Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 02:00 PM JST

PDB ID	:	7CAK
EMDB ID	:	EMD-30333
Title	:	SARS-CoV-2 S trimer with three RBD in the open state and complexed with three H014 Fab
Authors	:	Zhe, L.; Cao, L.; Deng, Y.; Sun, Y.; Wang, N.; Xie, L.; Wang, Y.; Rao, Z.; Qin, C.; Wang, X.
Deposited on	:	2020-06-08
Resolution	:	3.58 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

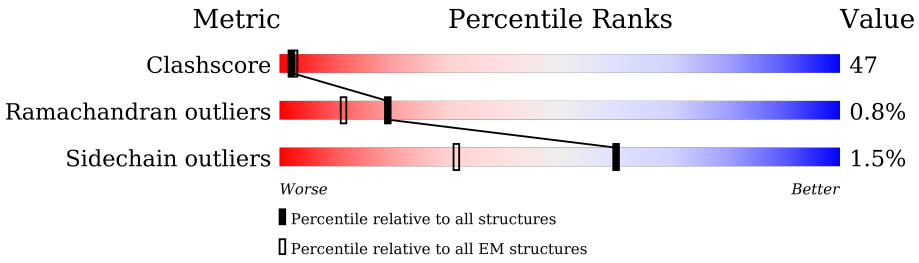
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1208	30% 49% 6% 15%
1	B	1208	30% 49% 6% 15%
1	C	1208	29% 49% 6% 15%
2	D	210	8% 22% 29% 49%
2	F	210	10% 21% 30% 49%
2	H	210	10% 21% 30% 49%
3	E	223	16% 38% 45%
3	G	223	22% 30% 45%

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Mol	Chain	Length	Quality of chain
3	I	223	17% 37% 45%
4	J	2	50% 50% 50%
4	K	2	100%
4	L	2	50% 50%
4	M	2	50% 50%
4	N	2	50% 50%
4	O	2	50% 50% 50%
4	P	2	100%
4	Q	2	50% 50%
4	R	2	50% 50%
4	S	2	50% 50%
4	T	2	50% 50% 50%
4	U	2	100%
4	V	2	50% 50%
4	W	2	50% 50%
4	X	2	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30263 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1028	Total	C	N	O	S	0	0
			8029	5128	1336	1528	37		
1	B	1028	Total	C	N	O	S	0	0
			8033	5130	1337	1529	37		
1	C	1028	Total	C	N	O	S	0	0
			8033	5130	1337	1529	37		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	835	MET	LYS	engineered mutation	UNP P0DTC2
A	844	MET	ILE	engineered mutation	UNP P0DTC2
A	846	TYR	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	835	MET	LYS	engineered mutation	UNP P0DTC2
B	844	MET	ILE	engineered mutation	UNP P0DTC2
B	846	TYR	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	835	MET	LYS	engineered mutation	UNP P0DTC2
C	844	MET	ILE	engineered mutation	UNP P0DTC2
C	846	TYR	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Light chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	107	Total	C	N	O	S	0	0
			837	534	140	161	2		
2	F	107	Total	C	N	O	S	0	0
			837	534	140	161	2		
2	H	107	Total	C	N	O	S	0	0
			837	534	140	161	2		

- Molecule 3 is a protein called Heavy chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	122	Total	C	N	O	S	0	0
			939	598	148	189	4		
3	G	122	Total	C	N	O	S	0	0
			939	598	148	189	4		
3	I	122	Total	C	N	O	S	0	0
			939	598	148	189	4		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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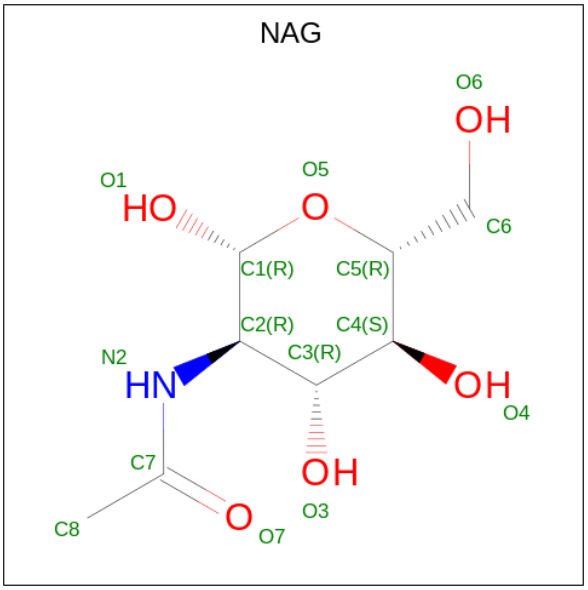
Mol	Chain	Residues	Atoms	AltConf	Trace
4	R	2	Total C N O 28 16 2 10	0	0
4	S	2	Total C N O 28 16 2 10	0	0
4	T	2	Total C N O 28 16 2 10	0	0
4	U	2	Total C N O 28 16 2 10	0	0
4	V	2	Total C N O 28 16 2 10	0	0
4	W	2	Total C N O 28 16 2 10	0	0
4	X	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0

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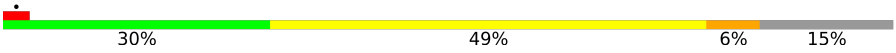
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

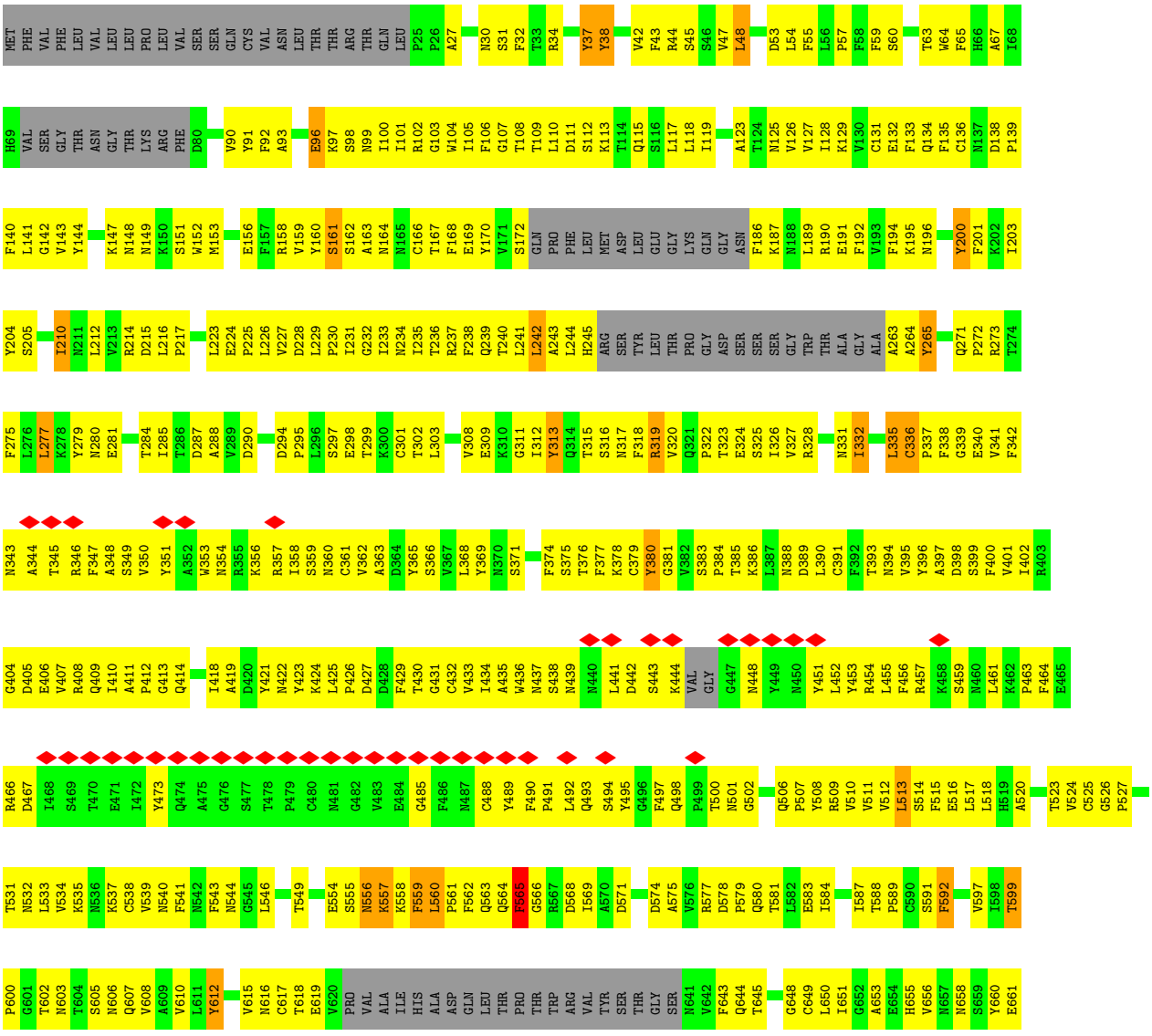
3 Residue-property plots (i)

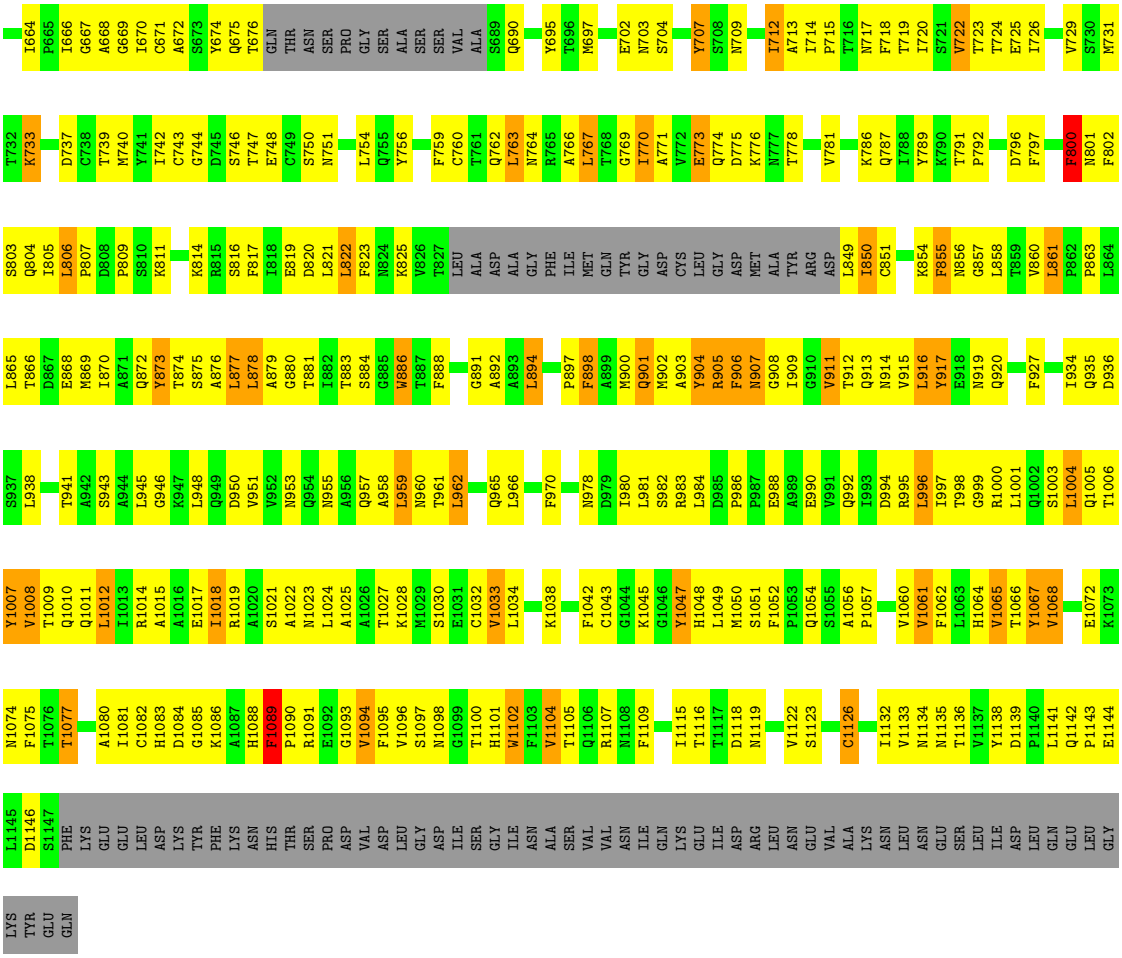
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein

Chain A:

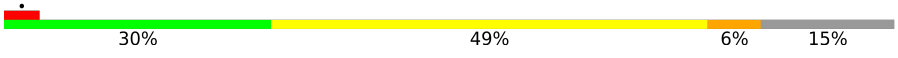


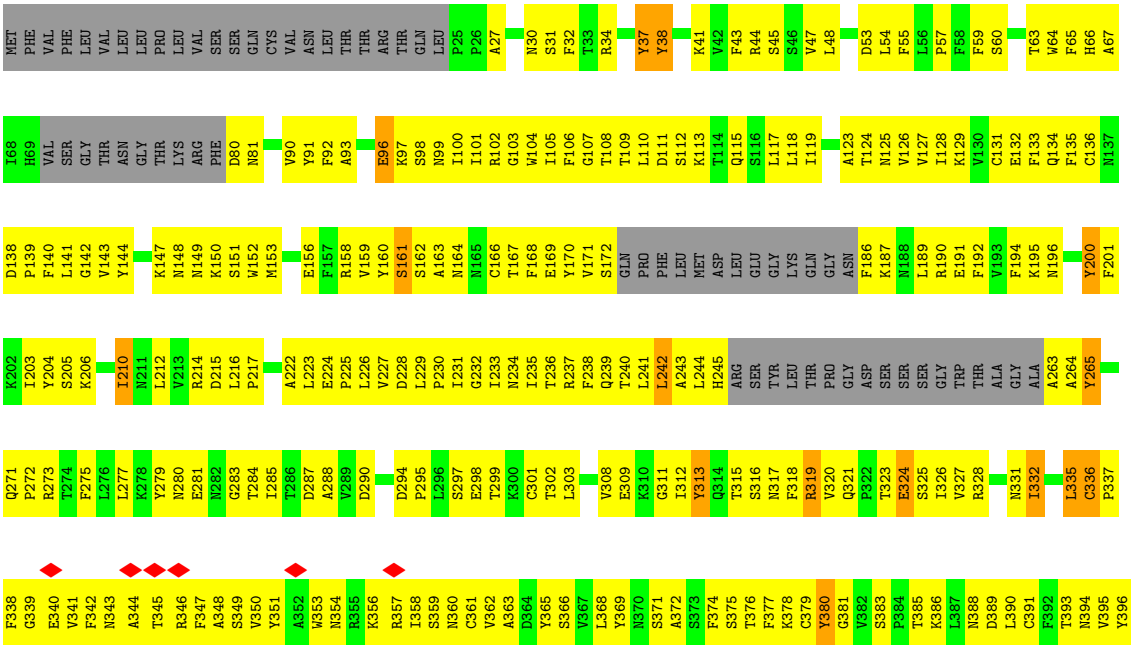


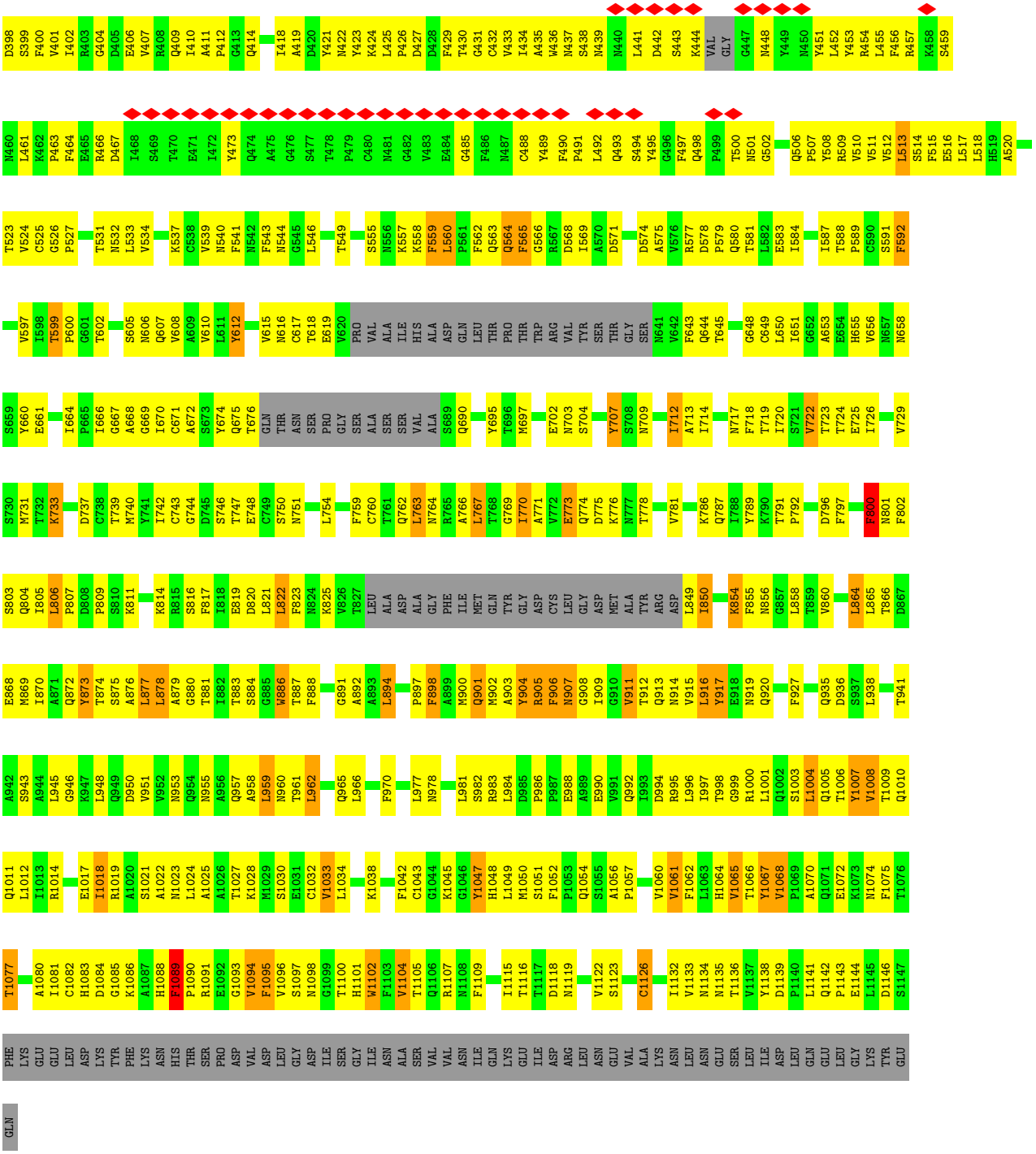


• Molecule 1: Spike glycoprotein

Chain B:

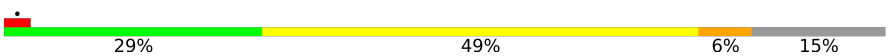


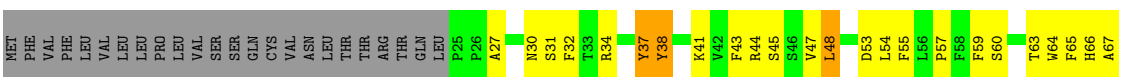


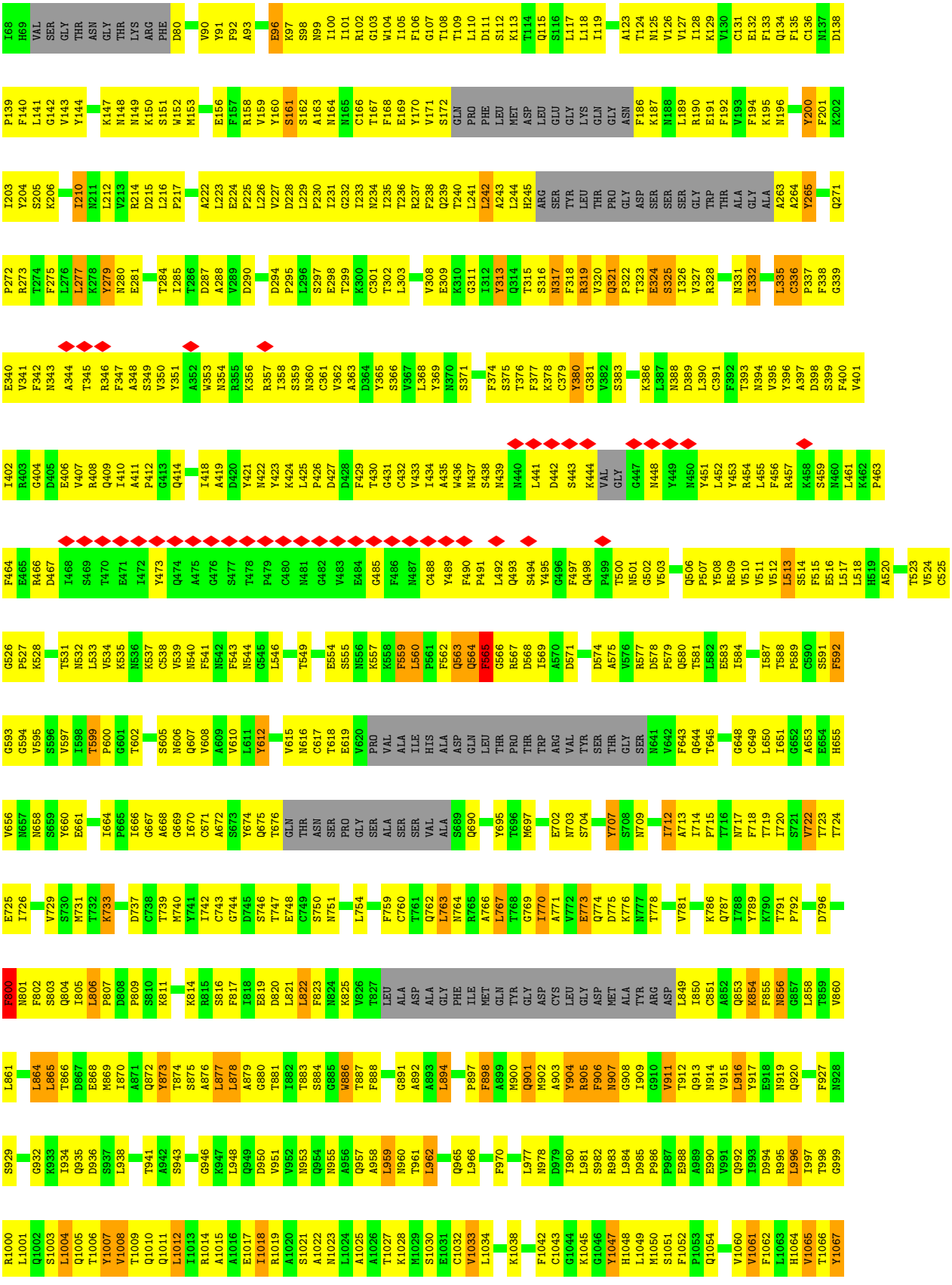


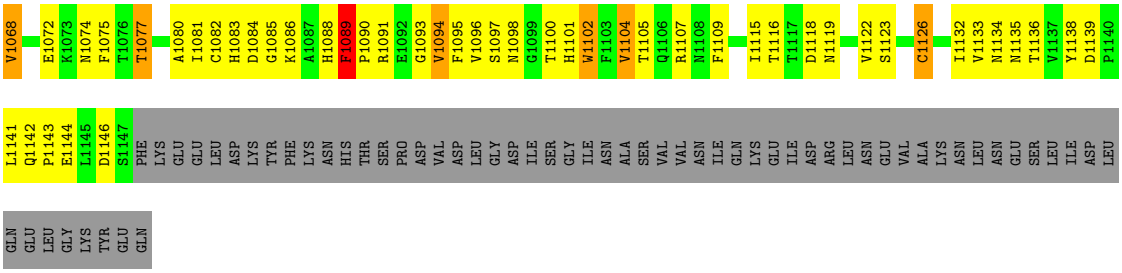
• Molecule 1: Spike glycoprotein

Chain C:

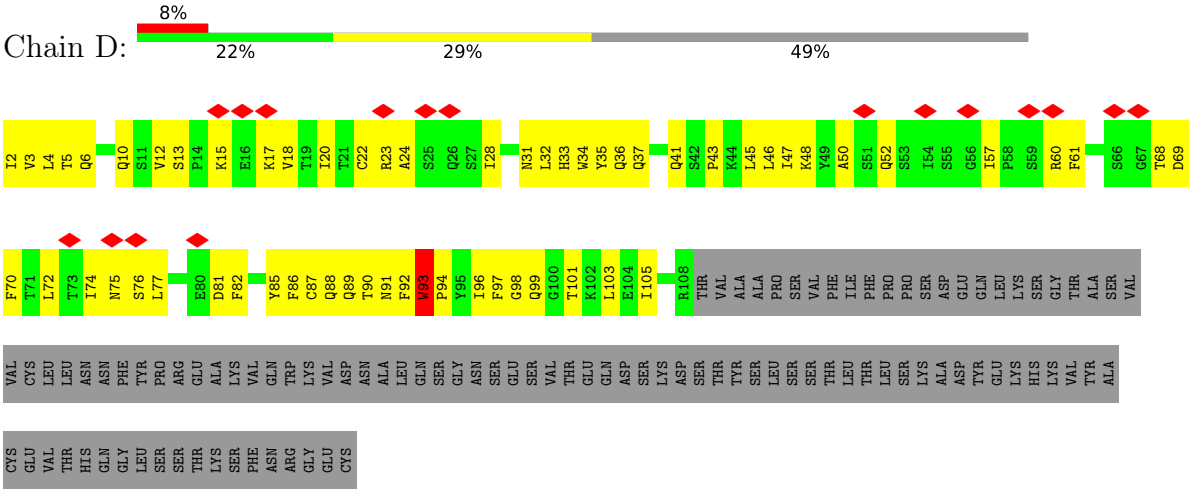




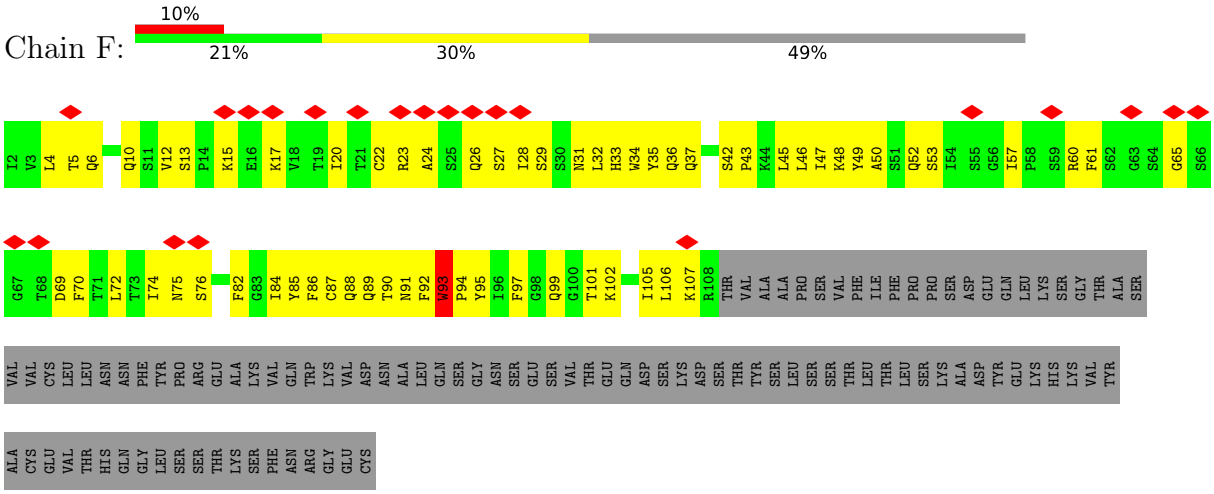




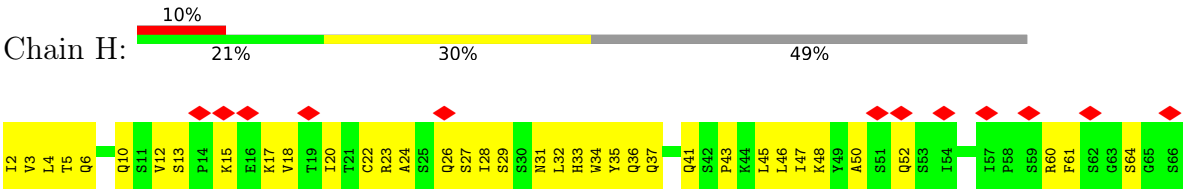
• Molecule 2: Light chain of H014 Fab

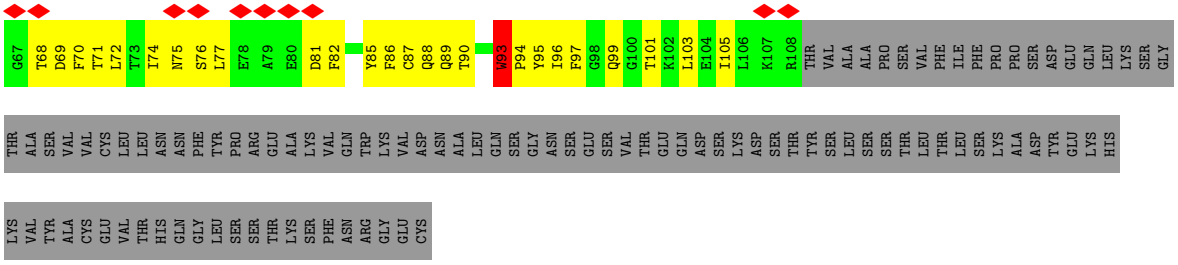


• Molecule 2: Light chain of H014 Fab



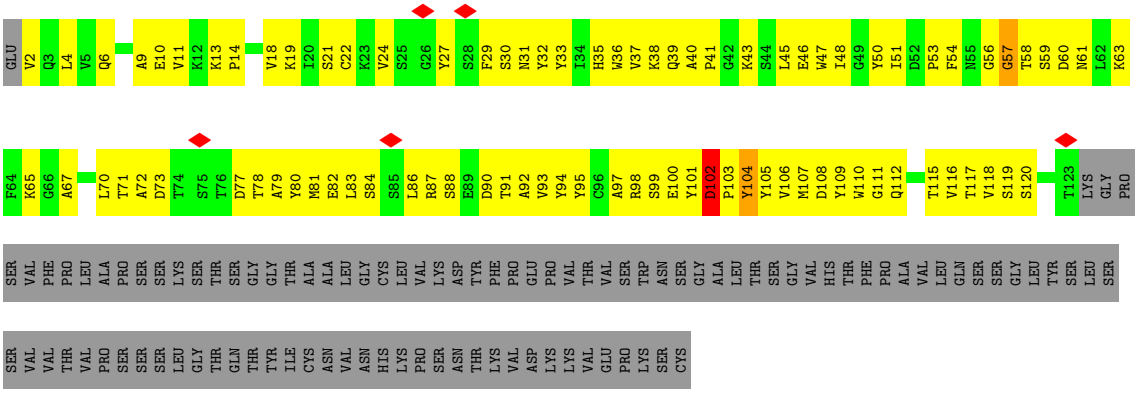
• Molecule 2: Light chain of H014 Fab





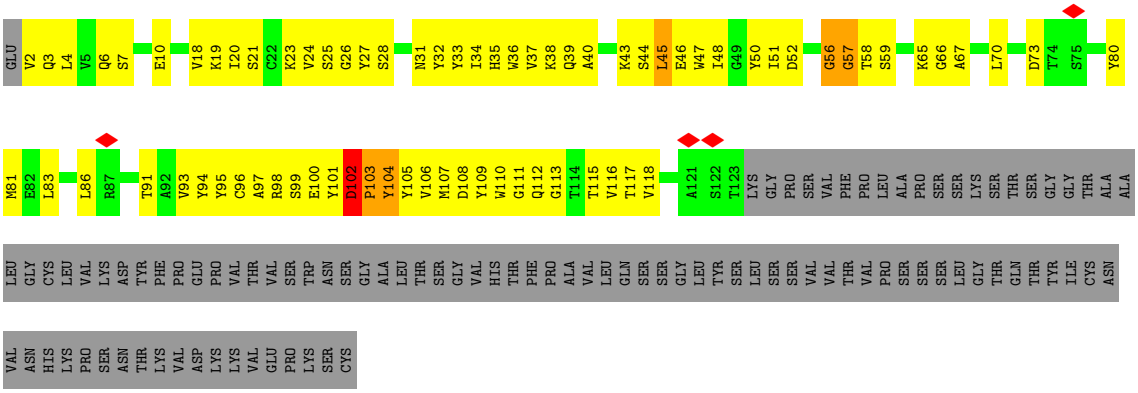
• Molecule 3: Heavy chain of H014 Fab

Chain E:



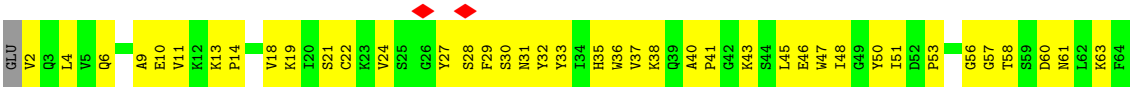
• Molecule 3: Heavy chain of H014 Fab

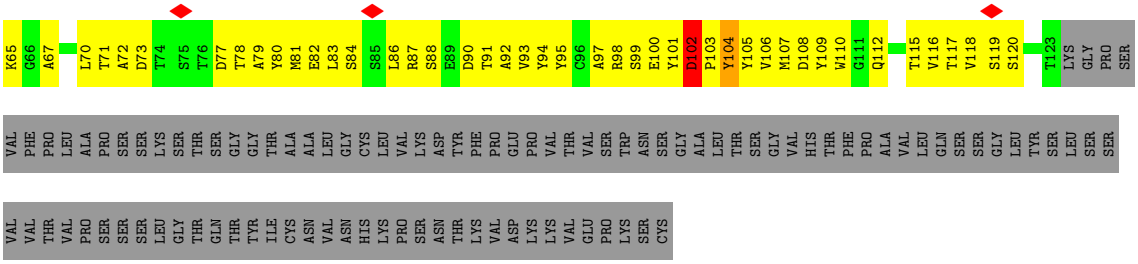
Chain G:



• Molecule 3: Heavy chain of H014 Fab

Chain I:



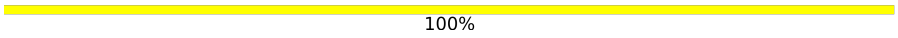


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

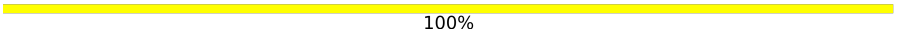
Chain N:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

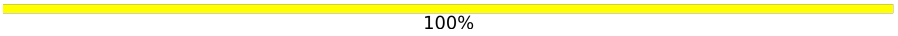
Chain S:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110970	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.41	101/8214 (1.2%)	0.92	22/11179 (0.2%)
1	B	1.41	99/8218 (1.2%)	0.91	22/11184 (0.2%)
1	C	1.41	101/8218 (1.2%)	0.91	22/11184 (0.2%)
2	D	0.41	0/857	0.66	0/1160
2	F	0.42	0/857	0.71	0/1160
2	H	0.41	0/857	0.66	0/1160
3	E	0.41	0/963	0.59	0/1311
3	G	0.44	0/963	0.65	1/1311 (0.1%)
3	I	0.41	0/963	0.59	0/1311
All	All	1.29	301/30110 (1.0%)	0.87	67/40960 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
1	C	0	7
2	D	0	1
2	F	0	1
2	H	0	1
3	G	0	2
3	I	0	1
All	All	0	26

All (301) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1060	VAL	CB-CG1	-9.27	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1060	VAL	CB-CG1	-9.24	1.33	1.52
1	B	1060	VAL	CB-CG1	-9.21	1.33	1.52
1	B	1102	TRP	CB-CG	-8.84	1.34	1.50
1	A	1102	TRP	CB-CG	-8.81	1.34	1.50
1	C	1102	TRP	CB-CG	-8.78	1.34	1.50
1	C	336	CYS	C-N	8.68	1.50	1.34
1	A	336	CYS	C-N	8.65	1.50	1.34
1	B	336	CYS	C-N	8.65	1.50	1.34
1	C	729	VAL	CB-CG1	-8.62	1.34	1.52
1	A	729	VAL	CB-CG1	-8.58	1.34	1.52
1	B	729	VAL	CB-CG1	-8.56	1.34	1.52
1	C	1067	TYR	CE2-CZ	-8.42	1.27	1.38
1	A	1067	TYR	CE2-CZ	-8.40	1.27	1.38
1	B	1067	TYR	CE2-CZ	-8.38	1.27	1.38
1	A	1047	TYR	CD2-CE2	-7.75	1.27	1.39
1	C	1047	TYR	CD2-CE2	-7.74	1.27	1.39
1	B	1047	TYR	CD2-CE2	-7.71	1.27	1.39
1	B	1067	TYR	CD2-CE2	-7.55	1.28	1.39
1	C	898	PHE	CB-CG	-7.52	1.38	1.51
1	B	898	PHE	CB-CG	-7.51	1.38	1.51
1	A	1067	TYR	CD2-CE2	-7.50	1.28	1.39
1	A	898	PHE	CB-CG	-7.49	1.38	1.51
1	A	1094	VAL	CB-CG2	-7.49	1.37	1.52
1	C	1067	TYR	CD2-CE2	-7.49	1.28	1.39
1	C	1094	VAL	CB-CG2	-7.48	1.37	1.52
1	B	1094	VAL	CB-CG2	-7.45	1.37	1.52
1	B	904	TYR	CD1-CE1	-7.42	1.28	1.39
1	A	904	TYR	CD1-CE1	-7.41	1.28	1.39
1	C	904	TYR	CD1-CE1	-7.41	1.28	1.39
1	C	1067	TYR	CG-CD2	-7.31	1.29	1.39
1	A	1067	TYR	CG-CD2	-7.31	1.29	1.39
1	B	1067	TYR	CG-CD2	-7.28	1.29	1.39
1	C	781	VAL	CB-CG1	-7.22	1.37	1.52
1	B	781	VAL	CB-CG1	-7.21	1.37	1.52
1	A	781	VAL	CB-CG1	-7.19	1.37	1.52
1	C	917	TYR	CD1-CE1	-7.08	1.28	1.39
1	A	917	TYR	CD1-CE1	-7.07	1.28	1.39
1	B	917	TYR	CD1-CE1	-7.05	1.28	1.39
1	A	1067	TYR	CE1-CZ	-6.99	1.29	1.38
1	C	1067	TYR	CE1-CZ	-6.96	1.29	1.38
1	B	1067	TYR	CE1-CZ	-6.95	1.29	1.38
1	A	729	VAL	CB-CG2	-6.88	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	729	VAL	CB-CG2	-6.88	1.38	1.52
1	C	729	VAL	CB-CG2	-6.85	1.38	1.52
1	A	1067	TYR	CG-CD1	-6.85	1.30	1.39
1	C	1067	TYR	CG-CD1	-6.81	1.30	1.39
1	B	901	GLN	CB-CG	-6.80	1.34	1.52
1	A	901	GLN	CB-CG	-6.77	1.34	1.52
1	B	1067	TYR	CG-CD1	-6.77	1.30	1.39
1	C	901	GLN	CB-CG	-6.76	1.34	1.52
1	B	1033	VAL	CB-CG2	-6.66	1.38	1.52
1	C	1094	VAL	CB-CG1	-6.65	1.38	1.52
1	A	1094	VAL	CB-CG1	-6.63	1.39	1.52
1	B	1065	VAL	CB-CG2	-6.63	1.39	1.52
1	B	1094	VAL	CB-CG1	-6.62	1.39	1.52
1	C	1033	VAL	CB-CG2	-6.62	1.39	1.52
1	A	1065	VAL	CB-CG2	-6.62	1.39	1.52
1	C	1065	VAL	CB-CG2	-6.61	1.39	1.52
1	A	1033	VAL	CB-CG2	-6.60	1.39	1.52
1	B	1060	VAL	CB-CG2	-6.58	1.39	1.52
1	B	1047	TYR	CD1-CE1	-6.57	1.29	1.39
1	C	873	TYR	CD1-CE1	-6.57	1.29	1.39
1	A	904	TYR	CB-CG	-6.57	1.41	1.51
1	C	1047	TYR	CD1-CE1	-6.56	1.29	1.39
1	B	873	TYR	CD1-CE1	-6.56	1.29	1.39
1	C	1060	VAL	CB-CG2	-6.55	1.39	1.52
1	A	873	TYR	CD1-CE1	-6.54	1.29	1.39
1	B	904	TYR	CB-CG	-6.53	1.41	1.51
1	B	707	TYR	CD1-CE1	-6.53	1.29	1.39
1	A	1068	VAL	CB-CG1	-6.53	1.39	1.52
1	A	1060	VAL	CB-CG2	-6.53	1.39	1.52
1	C	904	TYR	CB-CG	-6.51	1.41	1.51
1	C	1068	VAL	CB-CG1	-6.50	1.39	1.52
1	B	1068	VAL	CB-CG1	-6.50	1.39	1.52
1	A	707	TYR	CD1-CE1	-6.49	1.29	1.39
1	A	1047	TYR	CD1-CE1	-6.48	1.29	1.39
1	C	707	TYR	CD1-CE1	-6.47	1.29	1.39
1	B	789	TYR	CD2-CE2	-6.43	1.29	1.39
1	A	313	TYR	CD1-CE1	-6.40	1.29	1.39
1	A	789	TYR	CD2-CE2	-6.39	1.29	1.39
1	C	789	TYR	CD2-CE2	-6.38	1.29	1.39
1	B	1033	VAL	CB-CG1	-6.36	1.39	1.52
1	B	1032	CYS	CB-SG	-6.35	1.71	1.82
1	C	898	PHE	CG-CD2	-6.35	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1033	VAL	CB-CG1	-6.34	1.39	1.52
1	B	313	TYR	CD1-CE1	-6.34	1.29	1.39
1	A	898	PHE	CG-CD2	-6.33	1.29	1.38
1	A	1032	CYS	CB-SG	-6.33	1.71	1.82
1	B	898	PHE	CG-CD2	-6.32	1.29	1.38
1	C	313	TYR	CD1-CE1	-6.32	1.29	1.39
1	C	1033	VAL	CB-CG1	-6.31	1.39	1.52
1	C	1032	CYS	CB-SG	-6.29	1.71	1.82
1	A	886	TRP	CB-CG	-6.28	1.39	1.50
1	C	886	TRP	CB-CG	-6.27	1.39	1.50
1	B	886	TRP	CB-CG	-6.25	1.39	1.50
1	B	1062	PHE	CD2-CE2	-6.21	1.26	1.39
1	C	1062	PHE	CD2-CE2	-6.21	1.26	1.39
1	A	1062	PHE	CD2-CE2	-6.21	1.26	1.39
1	C	789	TYR	CD1-CE1	-6.18	1.30	1.39
1	A	789	TYR	CD1-CE1	-6.14	1.30	1.39
1	B	789	TYR	CD1-CE1	-6.11	1.30	1.39
1	A	1047	TYR	CE2-CZ	-6.06	1.30	1.38
1	C	1047	TYR	CE2-CZ	-6.04	1.30	1.38
1	B	1047	TYR	CE2-CZ	-6.04	1.30	1.38
1	A	1062	PHE	CE1-CZ	-6.03	1.25	1.37
1	C	1062	PHE	CE1-CZ	-6.02	1.25	1.37
1	B	1062	PHE	CE1-CZ	-6.01	1.25	1.37
1	A	917	TYR	CE1-CZ	-5.97	1.30	1.38
1	A	781	VAL	CB-CG2	-5.95	1.40	1.52
1	C	917	TYR	CE1-CZ	-5.94	1.30	1.38
1	C	781	VAL	CB-CG2	-5.93	1.40	1.52
1	B	781	VAL	CB-CG2	-5.93	1.40	1.52
1	B	917	TYR	CE1-CZ	-5.92	1.30	1.38
1	B	898	PHE	CG-CD1	-5.86	1.29	1.38
1	A	898	PHE	CG-CD1	-5.84	1.29	1.38
1	A	1052	PHE	CB-CG	-5.83	1.41	1.51
1	B	1062	PHE	CD1-CE1	-5.81	1.27	1.39
1	B	1007	TYR	CE1-CZ	-5.81	1.31	1.38
1	C	898	PHE	CG-CD1	-5.80	1.30	1.38
1	A	1062	PHE	CD1-CE1	-5.80	1.27	1.39
1	C	1007	TYR	CE1-CZ	-5.79	1.31	1.38
1	C	1062	PHE	CD1-CE1	-5.79	1.27	1.39
1	C	873	TYR	CD2-CE2	-5.79	1.30	1.39
1	B	1052	PHE	CB-CG	-5.78	1.41	1.51
1	C	898	PHE	CE1-CZ	-5.78	1.26	1.37
1	C	1052	PHE	CB-CG	-5.78	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	898	PHE	CE1-CZ	-5.76	1.26	1.37
1	B	911	VAL	CB-CG2	-5.76	1.40	1.52
1	C	911	VAL	CB-CG2	-5.76	1.40	1.52
1	B	873	TYR	CD2-CE2	-5.76	1.30	1.39
1	A	873	TYR	CD2-CE2	-5.75	1.30	1.39
1	B	898	PHE	CE1-CZ	-5.75	1.26	1.37
1	A	911	VAL	CB-CG2	-5.74	1.40	1.52
1	A	1007	TYR	CE1-CZ	-5.73	1.31	1.38
1	A	898	PHE	CD1-CE1	-5.72	1.27	1.39
1	C	898	PHE	CD1-CE1	-5.72	1.27	1.39
1	C	1068	VAL	CB-CG2	-5.71	1.40	1.52
1	B	898	PHE	CD1-CE1	-5.71	1.27	1.39
1	B	1068	VAL	CB-CG2	-5.70	1.40	1.52
1	A	1068	VAL	CB-CG2	-5.69	1.40	1.52
1	A	773	GLU	CB-CG	-5.64	1.41	1.52
1	B	773	GLU	CB-CG	-5.62	1.41	1.52
1	B	904	TYR	CD2-CE2	-5.62	1.30	1.39
1	C	773	GLU	CB-CG	-5.61	1.41	1.52
1	B	911	VAL	CB-CG1	-5.59	1.41	1.52
1	A	904	TYR	CD2-CE2	-5.59	1.30	1.39
1	A	911	VAL	CB-CG1	-5.59	1.41	1.52
1	C	904	TYR	CD2-CE2	-5.58	1.30	1.39
1	A	1061	VAL	CB-CG2	-5.56	1.41	1.52
1	B	279	TYR	CD1-CE1	-5.55	1.31	1.39
1	B	612	TYR	CD2-CE2	-5.54	1.31	1.39
1	C	612	TYR	CD2-CE2	-5.54	1.31	1.39
1	C	1061	VAL	CB-CG2	-5.54	1.41	1.52
1	C	911	VAL	CB-CG1	-5.53	1.41	1.52
1	C	279	TYR	CD1-CE1	-5.53	1.31	1.39
1	A	612	TYR	CD2-CE2	-5.53	1.31	1.39
1	B	610	VAL	CB-CG2	-5.53	1.41	1.52
1	B	1061	VAL	CB-CG2	-5.53	1.41	1.52
1	A	279	TYR	CD1-CE1	-5.52	1.31	1.39
1	C	610	VAL	CB-CG2	-5.52	1.41	1.52
1	A	1007	TYR	CE2-CZ	-5.51	1.31	1.38
1	B	707	TYR	CD2-CE2	-5.50	1.31	1.39
1	A	610	VAL	CB-CG2	-5.50	1.41	1.52
1	B	1007	TYR	CE2-CZ	-5.50	1.31	1.38
1	A	707	TYR	CD2-CE2	-5.49	1.31	1.39
1	C	707	TYR	CD2-CE2	-5.48	1.31	1.39
1	C	1007	TYR	CE2-CZ	-5.47	1.31	1.38
1	A	37	TYR	CD1-CE1	-5.46	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1096	VAL	CB-CG2	-5.45	1.41	1.52
1	C	1095	PHE	CE1-CZ	-5.44	1.27	1.37
1	A	906	PHE	CE1-CZ	-5.44	1.27	1.37
1	A	1095	PHE	CE1-CZ	-5.43	1.27	1.37
1	C	906	PHE	CE1-CZ	-5.42	1.27	1.37
1	B	906	PHE	CE1-CZ	-5.42	1.27	1.37
1	C	1096	VAL	CB-CG2	-5.41	1.41	1.52
1	A	1096	VAL	CB-CG2	-5.41	1.41	1.52
1	B	265	TYR	CD2-CE2	-5.41	1.31	1.39
1	B	1095	PHE	CE1-CZ	-5.41	1.27	1.37
1	C	37	TYR	CD1-CE1	-5.41	1.31	1.39
1	B	37	TYR	CD1-CE1	-5.40	1.31	1.39
1	B	1042	PHE	CD2-CE2	-5.40	1.28	1.39
1	A	1042	PHE	CD2-CE2	-5.40	1.28	1.39
1	A	265	TYR	CD2-CE2	-5.40	1.31	1.39
1	C	592	PHE	CB-CG	-5.40	1.42	1.51
1	A	789	TYR	CG-CD2	-5.38	1.32	1.39
1	C	265	TYR	CD2-CE2	-5.38	1.31	1.39
1	C	1042	PHE	CD2-CE2	-5.37	1.28	1.39
1	C	649	CYS	CB-SG	-5.37	1.73	1.81
1	B	789	TYR	CG-CD2	-5.37	1.32	1.39
1	C	789	TYR	CG-CD2	-5.36	1.32	1.39
1	A	313	TYR	CD2-CE2	-5.36	1.31	1.39
1	C	313	TYR	CD2-CE2	-5.36	1.31	1.39
1	B	649	CYS	CB-SG	-5.35	1.73	1.81
1	B	907	ASN	CB-CG	-5.34	1.38	1.51
1	A	592	PHE	CB-CG	-5.34	1.42	1.51
1	A	907	ASN	CB-CG	-5.34	1.38	1.51
1	B	592	PHE	CB-CG	-5.34	1.42	1.51
1	B	1067	TYR	CB-CG	-5.33	1.43	1.51
1	B	313	TYR	CD2-CE2	-5.33	1.31	1.39
1	A	898	PHE	CE2-CZ	-5.32	1.27	1.37
1	C	898	PHE	CE2-CZ	-5.32	1.27	1.37
1	A	1067	TYR	CB-CG	-5.32	1.43	1.51
1	C	907	ASN	CB-CG	-5.32	1.38	1.51
1	C	565	PHE	CB-CG	-5.32	1.42	1.51
1	C	1067	TYR	CB-CG	-5.32	1.43	1.51
1	A	565	PHE	CB-CG	-5.31	1.42	1.51
1	B	898	PHE	CE2-CZ	-5.31	1.27	1.37
1	C	1052	PHE	CD1-CE1	-5.30	1.28	1.39
1	A	1052	PHE	CD1-CE1	-5.30	1.28	1.39
1	B	917	TYR	CD2-CE2	-5.29	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1061	VAL	CB-CG1	-5.29	1.41	1.52
1	C	1061	VAL	CB-CG1	-5.29	1.41	1.52
1	C	722	VAL	CB-CG2	-5.28	1.41	1.52
1	A	1061	VAL	CB-CG1	-5.28	1.41	1.52
1	A	649	CYS	CB-SG	-5.27	1.73	1.81
1	B	1047	TYR	CB-CG	-5.26	1.43	1.51
1	C	1047	TYR	CB-CG	-5.26	1.43	1.51
1	A	1047	TYR	CB-CG	-5.26	1.43	1.51
1	B	1052	PHE	CD1-CE1	-5.26	1.28	1.39
1	A	722	VAL	CB-CG2	-5.25	1.41	1.52
1	C	917	TYR	CB-CG	-5.25	1.43	1.51
1	A	1062	PHE	CG-CD2	-5.25	1.30	1.38
1	A	1089	PHE	CD1-CE1	-5.25	1.28	1.39
1	B	722	VAL	CB-CG2	-5.25	1.41	1.52
1	A	1109	PHE	CB-CG	-5.24	1.42	1.51
1	C	1089	PHE	CD1-CE1	-5.24	1.28	1.39
1	C	1062	PHE	CG-CD2	-5.24	1.30	1.38
1	B	1089	PHE	CD1-CE1	-5.24	1.28	1.39
1	A	917	TYR	CB-CG	-5.24	1.43	1.51
1	C	873	TYR	CB-CG	-5.23	1.43	1.51
1	C	1065	VAL	CB-CG1	-5.23	1.41	1.52
1	C	1109	PHE	CB-CG	-5.22	1.42	1.51
1	A	335	LEU	C-N	5.22	1.46	1.34
1	B	800	PHE	CE1-CZ	-5.22	1.27	1.37
1	B	873	TYR	CB-CG	-5.21	1.43	1.51
1	C	38	TYR	CD2-CE2	-5.21	1.31	1.39
1	A	917	TYR	CD2-CE2	-5.21	1.31	1.39
1	B	1109	PHE	CB-CG	-5.21	1.42	1.51
1	B	1047	TYR	CE1-CZ	-5.21	1.31	1.38
1	A	873	TYR	CB-CG	-5.21	1.43	1.51
1	B	917	TYR	CB-CG	-5.21	1.43	1.51
1	A	38	TYR	CD2-CE2	-5.20	1.31	1.39
1	C	1008	VAL	CB-CG2	-5.20	1.42	1.52
1	B	1062	PHE	CG-CD2	-5.20	1.30	1.38
1	A	1008	VAL	CB-CG2	-5.20	1.42	1.52
1	B	1065	VAL	CB-CG1	-5.20	1.42	1.52
1	B	1089	PHE	CD2-CE2	-5.20	1.28	1.39
1	A	800	PHE	CE1-CZ	-5.20	1.27	1.37
1	B	898	PHE	CD2-CE2	-5.19	1.28	1.39
1	B	1133	VAL	CB-CG2	-5.19	1.42	1.52
1	C	1089	PHE	CD2-CE2	-5.19	1.28	1.39
1	C	335	LEU	C-N	5.18	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	917	TYR	CD2-CE2	-5.18	1.31	1.39
1	C	1133	VAL	CB-CG2	-5.18	1.42	1.52
1	A	1018	ILE	CB-CG2	-5.18	1.36	1.52
1	C	1047	TYR	CE1-CZ	-5.18	1.31	1.38
1	A	1047	TYR	CE1-CZ	-5.18	1.31	1.38
1	A	1133	VAL	CB-CG2	-5.18	1.42	1.52
1	A	898	PHE	CD2-CE2	-5.17	1.28	1.39
1	B	1008	VAL	CB-CG2	-5.17	1.42	1.52
1	A	1065	VAL	CB-CG1	-5.17	1.42	1.52
1	C	800	PHE	CE1-CZ	-5.17	1.27	1.37
1	B	335	LEU	C-N	5.17	1.46	1.34
1	B	1018	ILE	CB-CG2	-5.16	1.36	1.52
1	A	1089	PHE	CD2-CE2	-5.16	1.28	1.39
1	B	38	TYR	CD2-CE2	-5.15	1.31	1.39
1	A	37	TYR	CD2-CE2	-5.15	1.31	1.39
1	B	37	TYR	CD2-CE2	-5.15	1.31	1.39
1	C	1018	ILE	CB-CG2	-5.14	1.36	1.52
1	C	1047	TYR	CG-CD1	-5.14	1.32	1.39
1	C	898	PHE	CD2-CE2	-5.14	1.28	1.39
1	C	789	TYR	CB-CG	-5.14	1.44	1.51
1	A	1047	TYR	CG-CD1	-5.13	1.32	1.39
1	C	597	VAL	CB-CG1	-5.13	1.42	1.52
1	A	1052	PHE	CD2-CE2	-5.12	1.29	1.39
1	A	789	TYR	CB-CG	-5.11	1.44	1.51
1	B	597	VAL	CB-CG1	-5.11	1.42	1.52
1	C	37	TYR	CD2-CE2	-5.11	1.31	1.39
1	A	597	VAL	CB-CG1	-5.10	1.42	1.52
1	B	789	TYR	CB-CG	-5.09	1.44	1.51
1	B	1104	VAL	CB-CG1	-5.09	1.42	1.52
1	C	1104	VAL	CB-CG1	-5.08	1.42	1.52
1	B	789	TYR	CE1-CZ	-5.08	1.31	1.38
1	C	789	TYR	CE1-CZ	-5.08	1.31	1.38
1	B	1047	TYR	CG-CD1	-5.08	1.32	1.39
1	B	1052	PHE	CD2-CE2	-5.08	1.29	1.39
1	C	707	TYR	CE1-CZ	-5.08	1.31	1.38
1	C	722	VAL	CB-CG1	-5.07	1.42	1.52
1	A	1104	VAL	CB-CG1	-5.07	1.42	1.52
1	C	1052	PHE	CD2-CE2	-5.07	1.29	1.39
1	A	707	TYR	CE1-CZ	-5.07	1.31	1.38
1	B	707	TYR	CE1-CZ	-5.05	1.31	1.38
1	A	722	VAL	CB-CG1	-5.05	1.42	1.52
1	B	722	VAL	CB-CG1	-5.05	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	597	VAL	CB-CG2	-5.04	1.42	1.52
1	A	612	TYR	CD1-CE1	-5.03	1.31	1.39
1	A	789	TYR	CE1-CZ	-5.02	1.32	1.38
1	A	597	VAL	CB-CG2	-5.01	1.42	1.52
1	B	597	VAL	CB-CG2	-5.01	1.42	1.52
1	C	1096	VAL	CB-CG1	-5.00	1.42	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	878	LEU	CB-CG-CD2	-9.03	95.66	111.00
1	C	878	LEU	CB-CG-CD2	-9.02	95.67	111.00
1	B	878	LEU	CB-CG-CD2	-9.02	95.67	111.00
1	C	277	LEU	CA-CB-CG	-7.17	98.80	115.30
1	A	277	LEU	CA-CB-CG	-7.17	98.81	115.30
1	B	277	LEU	CA-CB-CG	-7.16	98.83	115.30
1	B	959	LEU	CB-CG-CD2	-6.99	99.12	111.00
1	C	959	LEU	CB-CG-CD2	-6.98	99.13	111.00
1	A	959	LEU	CB-CG-CD2	-6.98	99.14	111.00
1	C	916	LEU	CA-CB-CG	-6.83	99.59	115.30
1	A	916	LEU	CA-CB-CG	-6.82	99.61	115.30
1	B	916	LEU	CA-CB-CG	-6.82	99.62	115.30
1	C	1004	LEU	CB-CG-CD2	-6.59	99.79	111.00
1	B	1004	LEU	CB-CG-CD2	-6.58	99.82	111.00
1	A	1004	LEU	CB-CG-CD2	-6.58	99.82	111.00
1	A	763	LEU	CA-CB-CG	-6.34	100.71	115.30
1	C	763	LEU	CA-CB-CG	-6.33	100.74	115.30
1	B	763	LEU	CA-CB-CG	-6.33	100.75	115.30
1	A	48	LEU	CA-CB-CG	-6.31	100.79	115.30
1	B	48	LEU	CA-CB-CG	-6.27	100.87	115.30
1	C	48	LEU	CA-CB-CG	-6.27	100.87	115.30
1	A	894	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	B	894	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	C	894	LEU	CB-CG-CD2	-6.24	100.39	111.00
1	B	242	LEU	CB-CG-CD2	-6.12	100.59	111.00
1	A	242	LEU	CB-CG-CD2	-6.12	100.60	111.00
1	C	242	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	A	916	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	B	916	LEU	CB-CG-CD1	-6.06	100.69	111.00
1	C	916	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	C	822	LEU	CA-CB-CG	-6.04	101.40	115.30
1	B	822	LEU	CA-CB-CG	-6.04	101.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	822	LEU	CA-CB-CG	-6.04	101.42	115.30
1	B	767	LEU	CB-CG-CD2	-5.76	101.20	111.00
1	C	767	LEU	CB-CG-CD2	-5.76	101.20	111.00
1	B	959	LEU	CA-CB-CG	-5.76	102.05	115.30
1	C	959	LEU	CA-CB-CG	-5.76	102.05	115.30
1	A	959	LEU	CA-CB-CG	-5.76	102.06	115.30
1	B	1012	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	A	767	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	A	1012	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	C	1012	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	B	513	LEU	CA-CB-CG	5.61	128.21	115.30
1	C	513	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	996	LEU	CA-CB-CG	-5.58	102.46	115.30
1	A	513	LEU	CA-CB-CG	5.58	128.13	115.30
1	C	996	LEU	CA-CB-CG	-5.58	102.47	115.30
1	A	996	LEU	CA-CB-CG	-5.57	102.49	115.30
3	G	45	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	712	ILE	CG1-CB-CG2	-5.48	99.34	111.40
1	C	712	ILE	CG1-CB-CG2	-5.48	99.35	111.40
1	B	712	ILE	CG1-CB-CG2	-5.47	99.36	111.40
1	A	877	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	C	877	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	C	905	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	877	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	A	905	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	806	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	B	905	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	806	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	C	806	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	733	LYS	C-N-CA	-5.18	108.74	121.70
1	C	733	LYS	C-N-CA	-5.16	108.79	121.70
1	B	733	LYS	C-N-CA	-5.16	108.80	121.70
1	A	962	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	C	962	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	B	962	LEU	CB-CG-CD2	-5.08	102.37	111.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1126	CYS	Peptide
1	A	200	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	210	ILE	Peptide
1	A	380	TYR	Peptide
1	A	516	GLU	Peptide
1	A	565	PHE	Peptide
1	A	96	GLU	Peptide
1	B	1126	CYS	Peptide
1	B	200	TYR	Peptide
1	B	210	ILE	Peptide
1	B	380	TYR	Peptide
1	B	516	GLU	Peptide
1	B	96	GLU	Peptide
1	C	1126	CYS	Peptide
1	C	200	TYR	Peptide
1	C	210	ILE	Peptide
1	C	380	TYR	Peptide
1	C	516	GLU	Peptide
1	C	565	PHE	Peptide
1	C	96	GLU	Peptide
2	D	93	TRP	Peptide
2	F	93	TRP	Peptide
3	G	102	ASP	Peptide
3	G	56	GLY	Peptide
2	H	93	TRP	Peptide
3	I	102	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8029	0	7803	822	0
1	B	8033	0	7807	775	0
1	C	8033	0	7806	767	0
2	D	837	0	820	92	0
2	F	837	0	820	81	0
2	H	837	0	820	85	0
3	E	939	0	891	113	0
3	G	939	0	891	104	0
3	I	939	0	891	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	2	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	2	0
4	R	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	2	0
4	W	28	0	25	0	0
4	X	28	0	25	1	0
5	A	140	0	130	14	0
5	B	140	0	130	13	0
5	C	140	0	130	13	0
All	All	30263	0	29314	2778	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (2778) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CD2	1:B:559:PHE:HE1	1.02	1.63
1:A:43:PHE:CD2	1:B:559:PHE:CE1	1.93	1.56
1:B:324:GLU:CD	1:B:325:SER:H	1.07	1.46
1:C:318:PHE:CZ	1:C:615:VAL:HG11	1.62	1.33
1:A:43:PHE:CG	1:B:559:PHE:CE1	2.18	1.31
1:A:323:THR:HG22	1:A:324:GLU:OE1	1.34	1.26
2:H:95:TYR:OH	3:I:105:TYR:CD2	1.86	1.26
2:H:95:TYR:OH	3:I:105:TYR:CE2	1.81	1.22
1:C:559:PHE:CZ	1:C:565:PHE:O	1.93	1.22
1:B:318:PHE:CZ	1:B:615:VAL:HG11	1.78	1.19
1:B:324:GLU:CD	1:B:325:SER:N	1.92	1.18
1:A:559:PHE:HE2	1:A:564:GLN:O	1.26	1.17
1:A:319:ARG:NH1	1:C:740:MET:SD	2.18	1.16
1:C:320:VAL:HG23	1:C:591:SER:HB2	1.30	1.13
1:A:318:PHE:CZ	1:A:615:VAL:HG11	1.84	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:SD	1:B:319:ARG:NH1	2.25	1.09
1:C:408:ARG:HD3	3:I:102:ASP:CG	1.74	1.07
3:G:102:ASP:HB3	3:G:103:PRO:CD	1.84	1.06
1:A:318:PHE:HZ	1:A:615:VAL:HG11	0.93	1.06
1:B:850:ILE:H	1:B:850:ILE:HD12	1.19	1.06
1:C:559:PHE:CE2	1:C:565:PHE:O	2.08	1.06
1:C:318:PHE:HZ	1:C:615:VAL:CG1	1.70	1.05
1:C:408:ARG:HD3	3:I:102:ASP:OD2	1.54	1.05
1:A:559:PHE:CE2	1:A:564:GLN:O	2.09	1.04
3:E:102:ASP:HB3	3:E:103:PRO:HD2	1.34	1.04
1:B:318:PHE:HZ	1:B:615:VAL:CG1	1.71	1.03
3:G:99:SER:OG	3:G:105:TYR:HD1	1.40	1.03
1:B:324:GLU:CG	1:B:325:SER:H	1.72	1.02
1:B:43:PHE:HB2	1:C:563:GLN:HG2	1.42	0.99
1:B:318:PHE:HZ	1:B:615:VAL:HG11	0.85	0.99
1:B:324:GLU:CG	1:B:325:SER:N	2.27	0.98
1:B:320:VAL:HG23	1:B:591:SER:HB2	1.46	0.98
1:A:323:THR:CG2	1:A:324:GLU:OE1	2.13	0.97
1:C:865:LEU:HD23	1:C:870:ILE:HD13	1.45	0.95
3:I:102:ASP:HB3	3:I:103:PRO:CD	1.97	0.95
1:A:43:PHE:HD2	1:B:559:PHE:HE1	1.11	0.94
2:F:35:TYR:HB2	2:F:86:PHE:HB2	1.49	0.94
1:A:375:SER:HA	2:D:92:PHE:H	1.30	0.94
3:E:102:ASP:HB3	3:E:103:PRO:CD	1.98	0.94
2:H:95:TYR:CZ	3:I:105:TYR:CD2	2.54	0.94
1:C:850:ILE:H	1:C:850:ILE:HD12	1.29	0.94
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.01	0.94
1:C:320:VAL:HG23	1:C:591:SER:CB	1.98	0.93
2:F:10:GLN:HG3	2:F:20:ILE:HG12	1.47	0.93
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.01	0.93
1:A:328:ARG:HH22	1:A:533:LEU:HB2	1.34	0.92
1:A:559:PHE:HB2	1:A:584:ILE:HD11	1.52	0.92
1:A:559:PHE:HE2	1:A:564:GLN:C	1.73	0.92
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.02	0.91
1:C:328:ARG:HH22	1:C:533:LEU:HB2	1.34	0.91
3:G:35:HIS:HB2	3:G:97:ALA:HB3	1.53	0.91
1:A:557:LYS:O	1:A:584:ILE:HG21	1.69	0.90
1:B:328:ARG:HH22	1:B:533:LEU:HB2	1.34	0.90
1:A:375:SER:HA	2:D:92:PHE:N	1.86	0.90
3:G:99:SER:HG	3:G:105:TYR:HD1	1.18	0.90
1:C:559:PHE:HZ	1:C:565:PHE:C	1.76	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:HG23	1:A:591:SER:HB2	1.53	0.89
3:G:102:ASP:HB3	3:G:103:PRO:HD2	1.52	0.89
1:A:43:PHE:HA	1:B:563:GLN:NE2	1.85	0.89
3:G:10:GLU:HB2	3:G:116:VAL:HG22	1.51	0.89
1:A:318:PHE:HZ	1:A:615:VAL:CG1	1.85	0.88
3:G:102:ASP:OD2	3:G:103:PRO:HD3	1.74	0.88
1:A:353:TRP:O	1:A:466:ARG:NH2	2.07	0.88
3:E:103:PRO:O	3:E:105:TYR:CD2	2.27	0.88
1:A:43:PHE:CB	1:B:559:PHE:CE1	2.56	0.88
1:C:359:SER:HA	1:C:523:THR:HB	1.56	0.88
1:B:1019:ARG:NH2	1:B:1023:ASN:OD1	2.07	0.88
1:B:133:PHE:HB3	1:B:163:ALA:HA	1.55	0.87
1:A:323:THR:HG21	1:A:537:LYS:NZ	1.89	0.87
1:C:353:TRP:O	1:C:466:ARG:NH2	2.07	0.87
1:B:353:TRP:O	1:B:466:ARG:NH2	2.07	0.87
1:C:318:PHE:HZ	1:C:615:VAL:HG11	0.77	0.87
1:C:1019:ARG:NH2	1:C:1023:ASN:OD1	2.07	0.87
1:C:559:PHE:CZ	1:C:565:PHE:C	2.47	0.87
1:B:359:SER:HA	1:B:523:THR:HB	1.56	0.87
1:C:133:PHE:HB3	1:C:163:ALA:HA	1.55	0.87
1:C:559:PHE:HZ	1:C:565:PHE:O	1.57	0.87
1:C:786:LYS:NZ	1:C:891:GLY:O	2.08	0.87
1:A:133:PHE:HB3	1:A:163:ALA:HA	1.55	0.87
1:A:1019:ARG:NH2	1:A:1023:ASN:OD1	2.07	0.86
1:B:786:LYS:NZ	1:B:891:GLY:O	2.08	0.86
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.09	0.86
1:A:786:LYS:NZ	1:A:891:GLY:O	2.08	0.86
1:A:898:PHE:O	1:A:901:GLN:N	2.08	0.85
1:B:898:PHE:O	1:B:901:GLN:N	2.09	0.85
1:C:101:ILE:HG12	1:C:242:LEU:HD21	1.57	0.85
1:C:309:GLU:OE1	1:C:309:GLU:N	2.09	0.85
1:A:309:GLU:OE1	1:A:309:GLU:N	2.09	0.85
3:G:93:VAL:HG22	3:G:115:THR:HG22	1.58	0.85
1:A:359:SER:HA	1:A:523:THR:HB	1.56	0.85
1:B:1043:CYS:HB3	1:B:1048:HIS:CD2	2.12	0.85
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.10	0.85
2:D:24:ALA:HB3	2:D:28:ILE:HG22	1.59	0.85
1:A:101:ILE:HG12	1:A:242:LEU:HD21	1.57	0.85
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.09	0.85
1:B:703:ASN:OD1	1:B:704:SER:N	2.10	0.84
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.12	0.84
1:B:309:GLU:N	1:B:309:GLU:OE1	2.09	0.84
1:C:898:PHE:O	1:C:901:GLN:N	2.08	0.84
1:A:703:ASN:OD1	1:A:704:SER:N	2.10	0.84
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.10	0.84
1:C:316:SER:O	1:C:595:VAL:N	2.11	0.84
1:C:1043:CYS:HB3	1:C:1048:HIS:CD2	2.12	0.84
3:I:35:HIS:HB2	3:I:97:ALA:HB3	1.60	0.84
1:A:405:ASP:HA	3:E:103:PRO:HG3	1.58	0.83
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.09	0.83
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.43	0.83
3:G:102:ASP:CB	3:G:103:PRO:CD	2.56	0.83
1:B:101:ILE:HG12	1:B:242:LEU:HD21	1.57	0.83
1:C:703:ASN:OD1	1:C:704:SER:N	2.10	0.83
1:A:850:ILE:HD12	1:A:850:ILE:H	1.42	0.83
1:B:864:LEU:HD12	1:B:864:LEU:O	1.78	0.83
1:C:287:ASP:OD1	1:C:288:ALA:N	2.12	0.83
1:C:318:PHE:CZ	1:C:615:VAL:CG1	2.52	0.83
1:A:559:PHE:HB2	1:A:584:ILE:CD1	2.09	0.82
1:A:112:SER:OG	1:A:164:ASN:ND2	2.12	0.82
1:A:773:GLU:O	1:A:776:LYS:N	2.13	0.82
3:E:35:HIS:HB2	3:E:97:ALA:HB3	1.60	0.82
1:C:112:SER:OG	1:C:164:ASN:ND2	2.12	0.82
2:H:24:ALA:HB3	2:H:28:ILE:HG22	1.59	0.82
1:B:287:ASP:OD1	1:B:288:ALA:N	2.12	0.82
1:B:773:GLU:O	1:B:776:LYS:N	2.13	0.82
1:C:544:ASN:HD21	1:C:579:PRO:HB3	1.43	0.82
1:B:379:CYS:HA	1:B:432:CYS:HA	1.62	0.82
1:A:43:PHE:CG	1:B:559:PHE:CD1	2.68	0.81
1:A:225:PRO:HD2	1:B:562:PHE:CD2	2.14	0.81
1:B:112:SER:OG	1:B:164:ASN:ND2	2.12	0.81
1:B:115:GLN:HA	1:B:132:GLU:HG2	1.61	0.81
1:B:544:ASN:HD21	1:B:579:PRO:HB3	1.43	0.81
1:C:773:GLU:O	1:C:776:LYS:N	2.13	0.81
1:C:317:ASN:HB3	1:C:593:GLY:O	1.81	0.81
1:B:858:LEU:H	1:B:858:LEU:HD12	1.44	0.81
1:A:287:ASP:OD1	1:A:288:ALA:N	2.12	0.81
3:I:102:ASP:OD2	3:I:103:PRO:HD3	1.81	0.81
1:A:115:GLN:HA	1:A:132:GLU:HG2	1.61	0.81
1:B:99:ASN:O	1:B:102:ARG:NE	2.15	0.80
1:C:115:GLN:HA	1:C:132:GLU:HG2	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:HZ	1:B:566:GLY:CA	1.95	0.80
1:A:280:ASN:OD1	1:A:284:THR:N	2.15	0.80
1:B:436:TRP:HE1	1:B:509:ARG:HD2	1.46	0.80
1:A:559:PHE:CE1	1:C:43:PHE:HB3	2.17	0.80
1:B:90:VAL:HG12	1:B:91:TYR:O	1.82	0.80
1:C:280:ASN:OD1	1:C:284:THR:N	2.15	0.80
1:A:379:CYS:HA	1:A:432:CYS:HA	1.62	0.80
1:A:299:THR:O	1:A:302:THR:N	2.14	0.80
1:A:436:TRP:HE1	1:A:509:ARG:HD2	1.46	0.79
1:A:99:ASN:O	1:A:102:ARG:NE	2.15	0.79
1:C:99:ASN:O	1:C:102:ARG:NE	2.15	0.79
1:A:375:SER:HB3	2:D:91:ASN:HB2	1.63	0.79
1:A:43:PHE:HD1	1:B:563:GLN:OE1	1.64	0.79
1:A:90:VAL:HG12	1:A:91:TYR:O	1.82	0.79
1:C:901:GLN:O	1:C:904:TYR:N	2.15	0.79
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.16	0.79
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.16	0.79
1:C:379:CYS:HA	1:C:432:CYS:HA	1.62	0.79
1:C:438:SER:HB3	1:C:509:ARG:HG3	1.64	0.79
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.16	0.79
1:B:280:ASN:OD1	1:B:284:THR:N	2.15	0.79
1:C:90:VAL:HG12	1:C:91:TYR:O	1.82	0.79
1:C:299:THR:O	1:C:302:THR:N	2.14	0.79
1:B:901:GLN:O	1:B:904:TYR:N	2.15	0.79
1:C:869:MET:O	1:C:872:GLN:N	2.16	0.78
1:B:320:VAL:HG23	1:B:591:SER:CB	2.14	0.78
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.64	0.78
1:B:869:MET:O	1:B:872:GLN:N	2.16	0.78
2:D:4:LEU:HA	2:D:24:ALA:HA	1.66	0.78
1:C:436:TRP:HE1	1:C:509:ARG:HD2	1.46	0.78
1:A:901:GLN:O	1:A:904:TYR:N	2.15	0.78
2:F:6:GLN:O	2:F:99:GLN:NE2	2.16	0.78
1:A:438:SER:HB3	1:A:509:ARG:HG3	1.64	0.78
3:I:93:VAL:HG22	3:I:115:THR:HG22	1.65	0.78
1:A:737:ASP:OD1	1:A:739:THR:N	2.17	0.78
1:A:557:LYS:O	1:A:584:ILE:HG13	1.85	0.77
1:B:299:THR:O	1:B:302:THR:N	2.15	0.77
1:B:737:ASP:OD1	1:B:739:THR:N	2.17	0.77
1:B:796:ASP:OD1	1:B:796:ASP:N	2.15	0.77
1:C:737:ASP:OD1	1:C:739:THR:N	2.17	0.77
1:B:461:LEU:HD21	1:B:467:ASP:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:ASP:OD1	1:C:796:ASP:N	2.15	0.77
1:B:134:GLN:O	1:B:161:SER:N	2.17	0.77
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.17	0.77
2:F:6:GLN:NE2	2:F:87:CYS:SG	2.58	0.77
1:C:461:LEU:HD21	1:C:467:ASP:HB2	1.67	0.77
2:F:22:CYS:N	2:F:70:PHE:O	2.18	0.77
2:D:93:TRP:CD2	2:D:94:PRO:HD3	2.19	0.77
3:E:93:VAL:HG22	3:E:115:THR:HG22	1.65	0.77
3:G:100:GLU:HB2	3:G:104:TYR:O	1.85	0.77
1:A:461:LEU:HD21	1:A:467:ASP:HB2	1.67	0.76
1:A:863:PRO:O	1:A:865:LEU:O	2.02	0.76
2:F:93:TRP:CD2	2:F:94:PRO:HD3	2.19	0.76
1:A:1072:GLU:N	1:A:1072:GLU:OE1	2.17	0.76
2:H:4:LEU:HA	2:H:24:ALA:HA	1.66	0.76
1:A:424:LYS:HB3	1:A:461:LEU:HB2	1.67	0.76
1:C:317:ASN:CB	1:C:593:GLY:O	2.34	0.76
1:C:320:VAL:HG21	1:C:591:SER:OG	1.84	0.76
2:F:48:LYS:N	2:F:52:GLN:O	2.14	0.76
1:B:454:ARG:HD3	1:B:457:ARG:HB2	1.68	0.76
2:F:97:PHE:HD2	3:G:45:LEU:HB3	1.50	0.76
2:H:93:TRP:CD2	2:H:94:PRO:HD3	2.19	0.76
1:A:375:SER:CB	2:D:91:ASN:HB2	2.15	0.76
1:C:559:PHE:HZ	1:C:566:GLY:N	1.83	0.76
3:E:102:ASP:CB	3:E:103:PRO:CD	2.63	0.76
1:A:869:MET:O	1:A:872:GLN:N	2.16	0.76
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.17	0.76
1:B:331:ASN:OD1	1:B:332:ILE:N	2.19	0.76
1:C:331:ASN:HB3	5:C:1304:NAG:C7	2.16	0.76
2:F:24:ALA:HB3	2:F:28:ILE:HG22	1.68	0.76
1:B:560:LEU:HB2	1:B:563:GLN:HB2	1.65	0.75
1:C:134:GLN:O	1:C:161:SER:N	2.17	0.75
1:C:850:ILE:HD12	1:C:850:ILE:N	2.02	0.75
1:A:796:ASP:OD1	1:A:796:ASP:N	2.15	0.75
1:A:320:VAL:HG23	1:A:591:SER:CB	2.15	0.75
1:A:331:ASN:OD1	1:A:332:ILE:N	2.19	0.75
1:A:454:ARG:HD3	1:A:457:ARG:HB2	1.68	0.75
1:B:43:PHE:HB2	1:C:563:GLN:CG	2.16	0.75
1:B:331:ASN:HB3	5:B:1304:NAG:C7	2.16	0.75
1:C:424:LYS:HB3	1:C:461:LEU:HB2	1.67	0.75
1:A:873:TYR:O	1:A:876:ALA:N	2.20	0.75
1:A:134:GLN:O	1:A:161:SER:N	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:TYR:O	1:C:876:ALA:N	2.20	0.75
3:I:102:ASP:CB	3:I:103:PRO:CD	2.65	0.75
1:A:281:GLU:HB2	5:A:1303:NAG:H82	1.69	0.75
1:A:331:ASN:HB3	5:A:1304:NAG:C7	2.16	0.75
1:A:405:ASP:OD2	3:E:104:TYR:OH	2.04	0.75
1:C:331:ASN:OD1	1:C:332:ILE:N	2.19	0.75
3:G:102:ASP:HB3	3:G:103:PRO:HD3	1.67	0.75
1:B:564:GLN:OE1	1:B:564:GLN:HA	1.87	0.74
2:D:12:VAL:HG21	2:D:18:VAL:HB	1.68	0.74
1:A:861:LEU:N	1:A:861:LEU:HD23	2.02	0.74
3:I:102:ASP:HB3	3:I:103:PRO:HD3	1.70	0.74
1:C:311:GLY:HA2	1:C:664:ILE:HG23	1.70	0.74
1:B:424:LYS:HB3	1:B:461:LEU:HB2	1.67	0.74
1:B:873:TYR:O	1:B:876:ALA:N	2.20	0.74
1:C:568:ASP:OD1	1:C:569:ILE:N	2.20	0.74
1:C:880:GLY:O	1:C:884:SER:OG	2.05	0.74
1:A:196:ASN:HD21	1:A:235:ILE:HD12	1.53	0.74
1:B:196:ASN:HD21	1:B:235:ILE:HD12	1.53	0.74
1:B:880:GLY:O	1:B:884:SER:OG	2.05	0.74
1:A:408:ARG:HD3	3:E:102:ASP:CG	2.07	0.74
1:A:540:ASN:OD1	1:A:541:PHE:N	2.21	0.74
1:C:196:ASN:HD21	1:C:235:ILE:HD12	1.53	0.74
1:C:454:ARG:HD3	1:C:457:ARG:HB2	1.68	0.73
2:H:12:VAL:HG21	2:H:18:VAL:HB	1.68	0.73
1:B:123:ALA:HB3	5:B:1302:NAG:H83	1.71	0.73
1:B:540:ASN:OD1	1:B:541:PHE:N	2.21	0.73
1:B:568:ASP:OD1	1:B:569:ILE:N	2.20	0.73
1:A:311:GLY:HA2	1:A:664:ILE:HG23	1.70	0.73
1:A:850:ILE:HD12	1:A:850:ILE:N	2.03	0.73
1:B:850:ILE:HD12	1:B:850:ILE:N	2.01	0.73
1:C:123:ALA:HB3	5:C:1302:NAG:H83	1.71	0.73
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.22	0.73
1:B:323:THR:HG21	1:B:537:LYS:NZ	2.04	0.73
1:C:375:SER:N	1:C:435:ALA:O	2.22	0.73
1:B:281:GLU:HB2	5:B:1303:NAG:H82	1.69	0.73
1:B:375:SER:N	1:B:435:ALA:O	2.22	0.73
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.22	0.73
1:C:540:ASN:OD1	1:C:541:PHE:N	2.21	0.73
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.71	0.73
1:B:311:GLY:HA2	1:B:664:ILE:HG23	1.70	0.73
1:B:876:ALA:O	1:B:879:ALA:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:PHE:O	1:A:909:ILE:N	2.21	0.73
1:B:747:THR:O	1:B:751:ASN:N	2.19	0.73
1:C:865:LEU:HD23	1:C:870:ILE:CD1	2.19	0.73
1:C:906:PHE:O	1:C:909:ILE:N	2.21	0.73
1:A:123:ALA:HB3	5:A:1302:NAG:H83	1.71	0.72
1:A:880:GLY:O	1:A:884:SER:OG	2.05	0.72
1:A:357:ARG:HH12	1:C:167:THR:HA	1.53	0.72
1:A:375:SER:N	1:A:435:ALA:O	2.22	0.72
1:A:717:ASN:OD1	1:A:718:PHE:N	2.23	0.72
1:A:876:ALA:O	1:A:879:ALA:N	2.22	0.72
1:C:281:GLU:HB2	5:C:1303:NAG:H82	1.69	0.72
1:A:568:ASP:OD1	1:A:569:ILE:N	2.21	0.72
1:C:560:LEU:HB2	1:C:563:GLN:HB2	1.70	0.72
1:C:1100:THR:HG1	1:C:1101:HIS:HD1	1.37	0.72
1:B:108:THR:O	1:B:237:ARG:NH2	2.23	0.72
1:B:717:ASN:OD1	1:B:718:PHE:N	2.23	0.72
1:A:339:GLY:O	1:A:343:ASN:N	2.23	0.72
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.22	0.72
1:C:402:ILE:O	1:C:508:TYR:N	2.23	0.72
1:C:350:VAL:HG21	1:C:418:ILE:HD12	1.72	0.72
1:C:876:ALA:O	1:C:879:ALA:N	2.22	0.72
1:C:717:ASN:OD1	1:C:718:PHE:N	2.23	0.72
3:I:102:ASP:CB	3:I:103:PRO:HD3	2.20	0.72
1:B:339:GLY:O	1:B:343:ASN:N	2.23	0.71
2:D:5:THR:HB	2:D:23:ARG:HB3	1.72	0.71
3:G:99:SER:OG	3:G:105:TYR:CD1	2.30	0.71
1:A:1139:ASP:OD1	1:A:1141:LEU:N	2.23	0.71
1:B:190:ARG:HB3	1:B:192:PHE:CZ	2.25	0.71
1:A:108:THR:O	1:A:237:ARG:NH2	2.23	0.71
1:C:108:THR:O	1:C:237:ARG:NH2	2.23	0.71
1:C:190:ARG:HB3	1:C:192:PHE:CZ	2.25	0.71
1:A:562:PHE:CE2	1:C:225:PRO:HD2	2.26	0.71
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.71	0.71
3:G:65:LYS:HE3	3:G:67:ALA:HA	1.72	0.71
1:A:856:ASN:O	1:A:858:LEU:N	2.24	0.71
1:B:1139:ASP:OD1	1:B:1141:LEU:N	2.23	0.71
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.71	0.71
1:A:350:VAL:HG21	1:A:418:ILE:HD12	1.72	0.70
1:A:402:ILE:O	1:A:508:TYR:N	2.23	0.70
1:B:316:SER:OG	1:B:317:ASN:N	2.24	0.70
1:A:380:TYR:N	1:A:431:GLY:O	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:THR:OG1	1:A:600:PRO:O	2.09	0.70
1:B:906:PHE:O	1:B:909:ILE:N	2.21	0.70
1:C:320:VAL:CG2	1:C:591:SER:CB	2.70	0.70
1:C:1139:ASP:OD1	1:C:1141:LEU:N	2.23	0.70
1:A:190:ARG:HB3	1:A:192:PHE:CZ	2.25	0.70
1:C:599:THR:OG1	1:C:600:PRO:O	2.09	0.70
3:E:29:PHE:HZ	3:E:72:ALA:HB1	1.57	0.70
1:A:414:GLN:NE2	3:E:101:TYR:OH	2.22	0.70
1:B:339:GLY:HA2	5:B:1305:NAG:H81	1.74	0.70
1:B:599:THR:OG1	1:B:600:PRO:O	2.09	0.70
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.26	0.70
2:H:5:THR:HB	2:H:23:ARG:HB3	1.72	0.70
1:A:281:GLU:OE1	1:A:281:GLU:N	2.20	0.70
1:B:380:TYR:N	1:B:431:GLY:O	2.18	0.70
1:C:351:TYR:HA	1:C:422:ASN:HB2	1.73	0.70
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.26	0.70
1:A:1100:THR:HG1	1:A:1101:HIS:HD1	1.38	0.70
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.26	0.70
1:B:350:VAL:HG21	1:B:418:ILE:HD12	1.72	0.70
1:C:850:ILE:H	1:C:850:ILE:CD1	2.03	0.70
1:C:851:CYS:HA	1:C:854:LYS:HE2	1.72	0.70
3:I:29:PHE:HZ	3:I:72:ALA:HB1	1.57	0.70
1:A:361:CYS:N	1:A:523:THR:O	2.17	0.69
1:B:351:TYR:HA	1:B:422:ASN:HB2	1.73	0.69
1:A:316:SER:OG	1:A:317:ASN:N	2.24	0.69
1:B:709:ASN:ND2	5:B:1309:NAG:O7	2.25	0.69
1:B:1100:THR:HG1	1:B:1101:HIS:HD1	1.38	0.69
2:D:6:GLN:NE2	2:D:87:CYS:SG	2.66	0.69
1:A:357:ARG:NH1	1:C:167:THR:HA	2.08	0.69
1:C:339:GLY:O	1:C:343:ASN:N	2.23	0.69
1:A:532:ASN:OD1	1:A:533:LEU:N	2.23	0.69
1:A:854:LYS:HZ3	1:A:854:LYS:HB3	1.56	0.69
1:C:339:GLY:HA2	5:C:1305:NAG:H81	1.74	0.69
1:C:747:THR:O	1:C:751:ASN:N	2.19	0.69
1:A:709:ASN:ND2	5:A:1309:NAG:O7	2.25	0.69
1:A:858:LEU:N	1:A:858:LEU:HD12	2.07	0.69
1:C:709:ASN:ND2	5:C:1309:NAG:O7	2.25	0.69
1:B:676:THR:H	1:B:690:GLN:HG2	1.58	0.69
1:C:126:VAL:HB	1:C:172:SER:HB2	1.75	0.69
1:C:422:ASN:HB3	1:C:454:ARG:H	1.57	0.69
1:A:128:ILE:HD12	1:A:170:TYR:HD2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:O	1:A:210:ILE:N	2.21	0.69
1:A:422:ASN:HB3	1:A:454:ARG:H	1.57	0.69
1:A:763:LEU:O	1:A:766:ALA:N	2.25	0.69
1:B:763:LEU:O	1:B:766:ALA:N	2.25	0.69
1:B:850:ILE:H	1:B:850:ILE:CD1	1.98	0.69
1:C:532:ASN:OD1	1:C:533:LEU:N	2.23	0.69
3:G:102:ASP:CB	3:G:103:PRO:HD3	2.22	0.69
2:H:6:GLN:NE2	2:H:87:CYS:SG	2.65	0.69
1:C:763:LEU:O	1:C:766:ALA:N	2.25	0.69
2:F:22:CYS:HB3	2:F:70:PHE:HB2	1.74	0.69
1:A:339:GLY:HA2	5:A:1305:NAG:H81	1.74	0.69
1:B:128:ILE:HD12	1:B:170:TYR:HD2	1.58	0.69
3:E:65:LYS:HE3	3:E:67:ALA:HA	1.75	0.69
1:B:402:ILE:O	1:B:508:TYR:N	2.23	0.68
1:B:532:ASN:OD1	1:B:533:LEU:N	2.23	0.68
3:G:38:LYS:O	3:G:46:GLU:N	2.26	0.68
1:B:422:ASN:HB3	1:B:454:ARG:H	1.57	0.68
1:B:858:LEU:HD12	1:B:858:LEU:N	2.08	0.68
1:C:143:VAL:N	1:C:244:LEU:O	2.27	0.68
1:A:143:VAL:N	1:A:244:LEU:O	2.27	0.68
1:A:351:TYR:HA	1:A:422:ASN:HB2	1.73	0.68
1:A:866:THR:O	1:A:869:MET:N	2.26	0.68
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.75	0.68
1:A:143:VAL:HB	1:A:245:HIS:HA	1.76	0.68
1:B:134:GLN:HE21	1:B:135:PHE:H	1.41	0.68
1:B:866:THR:O	1:B:869:MET:N	2.26	0.68
1:B:1093:GLY:HA2	1:B:1107:ARG:HH11	1.57	0.68
1:C:1093:GLY:HA2	1:C:1107:ARG:HH11	1.57	0.68
1:A:43:PHE:CE2	1:B:559:PHE:CE1	2.75	0.68
1:A:676:THR:H	1:A:690:GLN:HG2	1.58	0.68
1:B:143:VAL:HB	1:B:245:HIS:HA	1.76	0.68
1:B:348:ALA:O	1:B:400:PHE:HA	1.94	0.68
1:C:406:GLU:HB3	1:C:418:ILE:HG13	1.76	0.68
3:G:35:HIS:O	3:G:97:ALA:N	2.25	0.68
1:A:126:VAL:HB	1:A:172:SER:HB2	1.75	0.68
1:C:320:VAL:CG2	1:C:591:SER:OG	2.41	0.68
1:C:676:THR:H	1:C:690:GLN:HG2	1.58	0.68
1:B:143:VAL:N	1:B:244:LEU:O	2.27	0.68
1:B:406:GLU:HB3	1:B:418:ILE:HG13	1.76	0.68
1:C:380:TYR:N	1:C:431:GLY:O	2.18	0.68
1:B:864:LEU:HD12	1:B:864:LEU:C	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:VAL:HG21	1:C:397:ALA:HB3	1.75	0.68
1:A:1093:GLY:HA2	1:A:1107:ARG:HH11	1.57	0.68
1:B:281:GLU:OE1	1:B:281:GLU:N	2.20	0.68
1:C:348:ALA:O	1:C:400:PHE:HA	1.94	0.68
2:D:6:GLN:O	2:D:99:GLN:NE2	2.27	0.68
3:E:40:ALA:HB3	3:E:43:LYS:HB2	1.75	0.68
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.75	0.68
2:H:5:THR:N	2:H:23:ARG:O	2.26	0.68
1:C:864:LEU:O	1:C:864:LEU:HD12	1.94	0.67
1:A:348:ALA:O	1:A:400:PHE:HA	1.94	0.67
1:B:126:VAL:HB	1:B:172:SER:HB2	1.75	0.67
1:A:43:PHE:HB3	1:B:559:PHE:CE1	2.28	0.67
1:A:323:THR:HG21	1:A:537:LYS:HZ2	1.59	0.67
1:B:200:TYR:HE1	1:B:230:PRO:HB3	1.60	0.67
1:C:128:ILE:HD12	1:C:170:TYR:HD2	1.58	0.67
1:C:866:THR:O	1:C:869:MET:N	2.26	0.67
2:D:5:THR:N	2:D:23:ARG:O	2.26	0.67
1:A:200:TYR:HE1	1:A:230:PRO:HB3	1.60	0.67
1:A:452:LEU:HD21	1:A:492:LEU:HB3	1.77	0.67
1:C:200:TYR:HE1	1:C:230:PRO:HB3	1.60	0.67
1:C:361:CYS:N	1:C:523:THR:O	2.17	0.67
1:A:747:THR:O	1:A:751:ASN:N	2.19	0.67
1:A:324:GLU:HG2	1:A:325:SER:H	1.60	0.67
2:H:6:GLN:O	2:H:99:GLN:NE2	2.27	0.67
3:I:65:LYS:HE3	3:I:67:ALA:HA	1.75	0.67
1:A:341:VAL:HG21	1:A:397:ALA:HB3	1.75	0.67
1:A:560:LEU:HD13	1:A:561:PRO:HD2	1.76	0.67
1:B:324:GLU:HG2	1:B:325:SER:N	2.08	0.67
1:B:341:VAL:HG21	1:B:397:ALA:HB3	1.75	0.67
1:A:406:GLU:HB3	1:A:418:ILE:HG13	1.76	0.67
1:C:143:VAL:HB	1:C:245:HIS:HA	1.76	0.66
1:A:323:THR:CB	1:A:537:LYS:HE3	2.25	0.66
3:I:40:ALA:HB3	3:I:43:LYS:HB2	1.75	0.66
1:B:1022:ALA:O	1:B:1025:ALA:N	2.28	0.66
1:A:378:LYS:HE2	3:E:57:GLY:HA2	1.76	0.66
1:A:1022:ALA:O	1:A:1025:ALA:N	2.28	0.66
1:B:361:CYS:N	1:B:523:THR:O	2.17	0.66
1:B:452:LEU:HD21	1:B:492:LEU:HB3	1.77	0.66
1:B:560:LEU:HD12	1:B:562:PHE:HE1	1.60	0.66
3:I:102:ASP:HB3	3:I:103:PRO:HD2	1.75	0.66
1:A:323:THR:HB	1:A:539:VAL:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CD1	1:B:563:GLN:OE1	2.48	0.66
1:A:134:GLN:HE21	1:A:135:PHE:H	1.41	0.66
1:A:323:THR:OG1	1:A:537:LYS:HE3	1.96	0.66
1:B:800:PHE:CD1	1:B:800:PHE:N	2.63	0.66
1:C:134:GLN:HE21	1:C:135:PHE:H	1.41	0.66
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.75	0.66
1:C:187:LYS:O	1:C:210:ILE:N	2.21	0.66
1:C:800:PHE:HD1	1:C:800:PHE:H	1.43	0.66
3:G:6:GLN:NE2	3:G:96:CYS:H	1.94	0.66
1:C:281:GLU:OE1	1:C:281:GLU:N	2.20	0.66
1:B:856:ASN:C	1:B:858:LEU:HD12	2.16	0.65
1:C:452:LEU:HD21	1:C:492:LEU:HB3	1.77	0.65
2:D:93:TRP:CE3	2:D:94:PRO:HD3	2.31	0.65
3:I:102:ASP:CG	3:I:103:PRO:HD3	2.17	0.65
2:H:93:TRP:CE3	2:H:94:PRO:HD3	2.31	0.65
1:B:800:PHE:H	1:B:800:PHE:HD1	1.44	0.65
1:C:103:GLY:HA3	1:C:241:LEU:HB2	1.79	0.65
3:G:97:ALA:HB1	3:G:107:MET:HB3	1.78	0.65
2:F:37:GLN:HB2	2:F:43:PRO:HG3	1.77	0.65
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.45	0.65
1:C:800:PHE:HD2	1:C:927:PHE:HD2	1.45	0.65
1:C:1022:ALA:O	1:C:1025:ALA:N	2.28	0.65
2:F:32:LEU:HD21	2:F:87:CYS:HB2	1.77	0.65
1:A:800:PHE:HD1	1:A:800:PHE:H	1.44	0.65
2:H:95:TYR:CE2	3:I:105:TYR:CG	2.85	0.65
1:A:43:PHE:HD2	1:B:559:PHE:CE1	1.92	0.65
1:A:418:ILE:HA	1:A:422:ASN:OD1	1.97	0.65
1:C:578:ASP:HB3	1:C:581:THR:O	1.97	0.65
1:A:901:GLN:O	1:A:903:ALA:N	2.30	0.65
1:C:978:ASN:HA	1:C:981:LEU:HD12	1.79	0.65
2:H:33:HIS:CE1	3:I:106:VAL:HG12	2.32	0.65
1:A:43:PHE:CD2	1:B:559:PHE:CD1	2.80	0.64
1:A:318:PHE:CZ	1:A:615:VAL:CG1	2.70	0.64
1:B:143:VAL:HG22	1:B:151:SER:HB2	1.79	0.64
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.61	0.64
1:C:800:PHE:HD1	1:C:800:PHE:N	1.95	0.64
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.61	0.64
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.28	0.64
2:F:48:LYS:HG3	3:G:106:VAL:HG11	1.79	0.64
1:A:578:ASP:HB3	1:A:581:THR:O	1.97	0.64
1:B:800:PHE:N	1:B:800:PHE:HD1	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:ASN:HA	1:B:981:LEU:HD12	1.79	0.64
1:C:351:TYR:CE2	1:C:452:LEU:HB3	2.33	0.64
2:D:22:CYS:N	2:D:70:PHE:O	2.31	0.64
2:D:33:HIS:CE1	3:E:106:VAL:HG12	2.32	0.64
3:G:2:VAL:HB	3:G:26:GLY:HA3	1.79	0.64
1:B:103:GLY:HA3	1:B:241:LEU:HB2	1.79	0.64
1:C:452:LEU:HA	1:C:494:SER:HA	1.80	0.64
1:A:43:PHE:HB2	1:B:563:GLN:HG2	1.79	0.64
1:A:143:VAL:HG22	1:A:151:SER:HB2	1.80	0.64
1:A:605:SER:OG	1:A:606:ASN:N	2.31	0.64
1:A:800:PHE:HD2	1:A:927:PHE:HD2	1.45	0.64
1:A:1100:THR:OG1	1:A:1101:HIS:ND1	2.30	0.64
1:B:376:THR:OG1	3:G:50:TYR:OH	2.14	0.64
1:C:418:ILE:HA	1:C:422:ASN:OD1	1.97	0.64
1:B:418:ILE:HA	1:B:422:ASN:OD1	1.97	0.64
2:H:64:SER:HG	2:H:71:THR:HG1	1.37	0.64
1:A:159:VAL:HB	1:A:160:TYR:HD1	1.62	0.64
1:A:374:PHE:O	2:D:93:TRP:N	2.30	0.64
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.28	0.64
1:B:144:TYR:N	1:B:151:SER:O	2.30	0.64
1:B:901:GLN:O	1:B:903:ALA:N	2.30	0.64
3:E:24:VAL:HG21	3:E:29:PHE:HD1	1.63	0.64
1:A:103:GLY:HA3	1:A:241:LEU:HB2	1.79	0.64
1:B:578:ASP:HB3	1:B:581:THR:O	1.97	0.64
1:C:159:VAL:HB	1:C:160:TYR:HD1	1.62	0.64
1:A:401:VAL:HA	1:A:509:ARG:HA	1.80	0.64
1:A:978:ASN:HA	1:A:981:LEU:HD12	1.79	0.64
1:B:605:SER:OG	1:B:606:ASN:N	2.31	0.64
1:C:901:GLN:O	1:C:903:ALA:N	2.30	0.64
1:A:589:PRO:HD3	1:C:855:PHE:CE1	2.32	0.63
1:B:105:ILE:C	1:B:106:PHE:HD1	2.01	0.63
1:B:328:ARG:HG3	1:B:579:PRO:HG2	1.80	0.63
1:B:351:TYR:CE2	1:B:452:LEU:HB3	2.33	0.63
1:B:381:GLY:HA3	1:B:430:THR:HG23	1.80	0.63
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.21	0.63
1:C:143:VAL:HG22	1:C:151:SER:HB2	1.79	0.63
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.62	0.63
1:B:855:PHE:CE1	1:C:589:PRO:HD3	2.32	0.63
1:C:361:CYS:O	1:C:525:CYS:N	2.29	0.63
1:B:904:TYR:OH	1:C:1094:VAL:HG12	1.98	0.63
1:C:1100:THR:OG1	1:C:1101:HIS:ND1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:OE1	1:A:324:GLU:N	2.32	0.63
1:A:328:ARG:HG3	1:A:579:PRO:HG2	1.80	0.63
1:A:351:TYR:CE2	1:A:452:LEU:HB3	2.33	0.63
1:B:452:LEU:HA	1:B:494:SER:HA	1.80	0.63
1:C:328:ARG:HG3	1:C:579:PRO:HG2	1.80	0.63
1:A:144:TYR:N	1:A:151:SER:O	2.30	0.63
2:F:69:ASP:OD1	2:F:70:PHE:N	2.32	0.63
1:A:324:GLU:HG2	1:A:325:SER:N	2.14	0.63
1:A:719:THR:HG22	1:A:1068:VAL:O	1.99	0.63
1:A:800:PHE:HD1	1:A:800:PHE:N	1.95	0.63
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.64	0.63
1:B:377:PHE:O	3:G:59:SER:HB3	1.99	0.63
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.30	0.63
3:I:72:ALA:HA	3:I:79:ALA:HA	1.81	0.63
1:A:452:LEU:HA	1:A:494:SER:HA	1.80	0.63
1:B:426:PRO:HD2	1:B:429:PHE:HB2	1.81	0.63
1:C:105:ILE:C	1:C:106:PHE:HD1	2.01	0.63
1:C:317:ASN:HB3	1:C:594:GLY:HA2	1.81	0.63
1:A:43:PHE:HB3	1:B:559:PHE:CZ	2.34	0.63
1:A:378:LYS:NZ	3:E:58:THR:O	2.20	0.63
1:C:401:VAL:HA	1:C:509:ARG:HA	1.80	0.63
1:B:224:GLU:H	1:B:224:GLU:CD	2.02	0.62
1:C:139:PRO:HB3	1:C:159:VAL:O	1.99	0.62
1:C:719:THR:HG22	1:C:1068:VAL:O	1.99	0.62
3:E:97:ALA:HB1	3:E:107:MET:HB2	1.80	0.62
3:E:102:ASP:CB	3:E:103:PRO:HD2	2.21	0.62
2:F:4:LEU:HA	2:F:24:ALA:HA	1.81	0.62
1:B:159:VAL:HB	1:B:160:TYR:HD1	1.62	0.62
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.28	0.62
1:C:224:GLU:H	1:C:224:GLU:CD	2.02	0.62
1:C:800:PHE:N	1:C:800:PHE:CD1	2.63	0.62
1:C:801:ASN:ND2	4:V:1:NAG:O7	2.32	0.62
1:A:167:THR:HA	1:B:357:ARG:HH12	1.64	0.62
1:A:224:GLU:CD	1:A:224:GLU:H	2.02	0.62
1:B:187:LYS:O	1:B:210:ILE:N	2.21	0.62
1:C:408:ARG:HD3	3:I:102:ASP:OD1	1.98	0.62
3:E:72:ALA:HA	3:E:79:ALA:HA	1.81	0.62
1:A:141:LEU:O	1:A:244:LEU:N	2.30	0.62
1:A:324:GLU:CG	1:A:325:SER:H	2.12	0.62
1:B:801:ASN:ND2	4:Q:1:NAG:O7	2.33	0.62
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:C	1:A:106:PHE:HD1	2.01	0.62
1:A:361:CYS:O	1:A:525:CYS:N	2.29	0.62
3:I:35:HIS:N	3:I:97:ALA:O	2.32	0.62
1:B:318:PHE:CZ	1:B:615:VAL:CG1	2.61	0.62
1:C:224:GLU:OE1	1:C:224:GLU:N	2.27	0.62
1:C:1018:ILE:O	1:C:1021:SER:N	2.33	0.62
3:I:24:VAL:HG21	3:I:29:PHE:HD1	1.63	0.62
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.82	0.62
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.47	0.62
1:B:401:VAL:HA	1:B:509:ARG:HA	1.80	0.62
1:A:139:PRO:HB3	1:A:159:VAL:O	1.99	0.62
1:A:800:PHE:N	1:A:800:PHE:CD1	2.63	0.62
1:B:906:PHE:O	1:B:907:ASN:C	2.38	0.62
1:B:1100:THR:OG1	1:B:1101:HIS:ND1	2.30	0.62
1:C:577:ARG:HA	1:C:583:GLU:O	2.00	0.62
1:C:865:LEU:HB3	1:C:870:ILE:HD11	1.82	0.62
2:F:88:GLN:HG2	2:F:97:PHE:CD1	2.34	0.62
1:B:719:THR:HG22	1:B:1068:VAL:O	1.98	0.62
3:G:6:GLN:NE2	3:G:96:CYS:SG	2.59	0.62
3:I:13:LYS:NZ	3:I:120:SER:O	2.33	0.62
1:A:577:ARG:HA	1:A:583:GLU:O	2.00	0.61
1:A:605:SER:OG	1:A:607:GLN:N	2.27	0.61
1:B:93:ALA:O	1:B:265:TYR:HB2	2.00	0.61
1:B:139:PRO:HB3	1:B:159:VAL:O	1.99	0.61
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.81	0.61
1:C:557:LYS:CB	1:C:584:ILE:HG21	2.29	0.61
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.21	0.61
1:C:992:GLN:O	1:C:995:ARG:N	2.33	0.61
3:I:97:ALA:HB1	3:I:107:MET:HB2	1.80	0.61
1:A:992:GLN:O	1:A:995:ARG:N	2.33	0.61
1:A:1018:ILE:O	1:A:1021:SER:N	2.33	0.61
1:B:577:ARG:HA	1:B:583:GLU:O	2.00	0.61
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.81	0.61
1:C:605:SER:OG	1:C:606:ASN:N	2.31	0.61
1:C:1102:TRP:HB2	1:C:1135:ASN:HD22	1.64	0.61
1:A:559:PHE:CE1	1:C:43:PHE:CB	2.83	0.61
1:A:801:ASN:ND2	4:L:1:NAG:O7	2.33	0.61
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.64	0.61
2:H:22:CYS:N	2:H:70:PHE:O	2.31	0.61
1:A:381:GLY:HA3	1:A:430:THR:HG23	1.81	0.61
1:A:559:PHE:CE2	1:A:564:GLN:C	2.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.47	0.61
1:B:992:GLN:O	1:B:995:ARG:N	2.33	0.61
1:C:323:THR:HG22	1:C:324:GLU:HG3	1.81	0.61
2:F:20:ILE:HD12	2:F:85:TYR:HD2	1.65	0.61
1:A:224:GLU:OE1	1:A:224:GLU:N	2.27	0.61
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.82	0.61
1:B:34:ARG:NH1	1:B:217:PRO:O	2.34	0.61
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.47	0.61
1:B:303:LEU:HD12	1:B:308:VAL:HG22	1.82	0.61
3:E:35:HIS:N	3:E:97:ALA:O	2.32	0.61
3:I:29:PHE:CZ	3:I:72:ALA:HB1	2.35	0.61
1:A:619:GLU:OE1	1:A:619:GLU:N	2.26	0.61
1:A:1094:VAL:HG12	1:C:904:TYR:OH	2.00	0.61
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.16	0.61
1:B:605:SER:OG	1:B:607:GLN:N	2.27	0.61
1:B:1018:ILE:O	1:B:1021:SER:N	2.33	0.61
1:C:93:ALA:O	1:C:265:TYR:HB2	2.00	0.61
1:C:906:PHE:O	1:C:907:ASN:C	2.38	0.61
1:A:34:ARG:NH1	1:A:217:PRO:O	2.34	0.61
1:A:1072:GLU:HG2	1:C:894:LEU:HD21	1.82	0.61
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.81	0.61
1:C:316:SER:O	1:C:595:VAL:HB	2.00	0.61
1:C:326:ILE:O	1:C:326:ILE:HG22	2.01	0.61
1:C:426:PRO:HD2	1:C:429:PHE:HB2	1.81	0.61
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.81	0.61
1:B:900:MET:SD	1:C:1077:THR:OG1	2.55	0.61
1:C:605:SER:OG	1:C:607:GLN:N	2.27	0.61
2:F:35:TYR:CZ	2:F:45:LEU:HD13	2.36	0.61
1:B:1089:PHE:N	1:B:1089:PHE:HD1	1.98	0.60
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.82	0.60
1:C:321:GLN:OE1	1:C:321:GLN:HA	1.99	0.60
2:F:34:TRP:HD1	2:F:47:ILE:HB	1.65	0.60
1:A:356:LYS:O	1:A:396:TYR:HA	2.01	0.60
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.30	0.60
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.16	0.60
1:C:34:ARG:NH1	1:C:217:PRO:O	2.34	0.60
1:A:1089:PHE:N	1:A:1089:PHE:HD1	1.98	0.60
1:B:323:THR:HG21	1:B:537:LYS:CE	2.32	0.60
1:C:748:GLU:CD	1:C:748:GLU:H	2.04	0.60
3:E:29:PHE:CZ	3:E:72:ALA:HB1	2.35	0.60
1:A:42:VAL:HG22	1:B:565:PHE:HE2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:THR:CG2	3:E:65:LYS:HE2	2.32	0.60
1:B:894:LEU:HD21	1:C:1072:GLU:HG2	1.82	0.60
1:C:515:PHE:HD2	1:C:517:LEU:H	1.49	0.60
2:H:37:GLN:HB2	2:H:43:PRO:HG3	1.82	0.60
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.84	0.60
3:G:91:THR:HG23	3:G:117:THR:HA	1.83	0.60
3:G:102:ASP:CG	3:G:103:PRO:HD3	2.21	0.60
1:A:93:ALA:O	1:A:265:TYR:HB2	2.00	0.60
1:A:904:TYR:OH	1:B:1094:VAL:HG12	2.01	0.60
1:B:444:LYS:HD2	1:B:448:ASN:HB2	1.83	0.60
1:C:970:PHE:CD2	1:C:999:GLY:HA3	2.36	0.60
1:C:1080:ALA:O	1:C:1081:ILE:HG13	2.02	0.60
1:A:970:PHE:CD2	1:A:999:GLY:HA3	2.36	0.60
1:B:1088:HIS:ND1	1:B:1122:VAL:HG22	2.17	0.60
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.37	0.60
1:B:970:PHE:CD2	1:B:999:GLY:HA3	2.36	0.60
1:C:860:VAL:O	1:C:860:VAL:HG12	2.01	0.60
1:A:57:PRO:HG2	1:A:271:GLN:OE1	2.02	0.60
1:A:515:PHE:HD2	1:A:517:LEU:H	1.49	0.60
1:B:190:ARG:HB3	1:B:192:PHE:CE1	2.37	0.60
1:B:356:LYS:O	1:B:396:TYR:HA	2.01	0.60
1:C:356:LYS:O	1:C:396:TYR:HA	2.01	0.60
1:C:430:THR:HG21	1:C:517:LEU:HG	1.84	0.60
2:D:37:GLN:HB2	2:D:43:PRO:HG3	1.82	0.60
3:E:18:VAL:HG12	3:E:86:LEU:HD21	1.84	0.60
1:A:748:GLU:CD	1:A:748:GLU:H	2.04	0.60
1:B:361:CYS:O	1:B:525:CYS:N	2.29	0.60
1:B:854:LYS:HA	1:B:858:LEU:O	2.02	0.60
1:B:1080:ALA:O	1:B:1081:ILE:HG13	2.02	0.60
1:C:444:LYS:HD2	1:C:448:ASN:HB2	1.83	0.60
1:C:600:PRO:HB3	1:C:674:TYR:HB2	1.84	0.60
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.16	0.60
2:H:32:LEU:HD21	2:H:87:CYS:HB2	1.84	0.60
1:A:134:GLN:NE2	1:A:135:PHE:H	2.00	0.59
1:B:134:GLN:NE2	1:B:135:PHE:H	2.00	0.59
1:C:1089:PHE:N	1:C:1089:PHE:CD1	2.70	0.59
2:D:33:HIS:NE2	3:E:105:TYR:O	2.35	0.59
3:E:13:LYS:NZ	3:E:120:SER:O	2.33	0.59
1:A:906:PHE:O	1:A:907:ASN:C	2.38	0.59
1:A:1080:ALA:O	1:A:1081:ILE:HG13	2.02	0.59
1:B:434:ILE:O	1:B:510:VAL:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TYR:HB2	2:D:86:PHE:HB2	1.84	0.59
1:A:434:ILE:O	1:A:510:VAL:HA	2.03	0.59
1:A:860:VAL:O	1:A:860:VAL:HG12	2.01	0.59
1:C:434:ILE:O	1:C:510:VAL:HA	2.03	0.59
1:C:559:PHE:HB2	1:C:584:ILE:HD11	1.83	0.59
1:A:430:THR:HG21	1:A:517:LEU:HG	1.84	0.59
1:B:385:THR:HG21	3:G:65:LYS:HE2	1.83	0.59
1:B:430:THR:HG21	1:B:517:LEU:HG	1.84	0.59
1:C:1088:HIS:ND1	1:C:1122:VAL:HG22	2.17	0.59
1:C:1089:PHE:N	1:C:1089:PHE:HD1	1.98	0.59
1:A:327:VAL:O	1:A:531:THR:N	2.35	0.59
1:A:363:ALA:N	1:A:525:CYS:O	2.34	0.59
1:A:1089:PHE:N	1:A:1089:PHE:CD1	2.70	0.59
1:B:860:VAL:O	1:B:860:VAL:HG12	2.01	0.59
1:C:57:PRO:HG2	1:C:271:GLN:OE1	2.02	0.59
2:D:88:GLN:HG2	2:D:97:PHE:CD1	2.37	0.59
1:A:854:LYS:O	1:A:854:LYS:HG2	2.02	0.59
1:B:309:GLU:H	1:B:309:GLU:CD	2.05	0.59
1:B:525:CYS:SG	1:B:526:GLY:N	2.76	0.59
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.37	0.59
1:C:525:CYS:SG	1:C:526:GLY:N	2.76	0.59
2:D:32:LEU:HD21	2:D:87:CYS:HB2	1.84	0.59
1:A:398:ASP:O	1:A:511:VAL:HA	2.02	0.59
1:C:323:THR:OG1	1:C:537:LYS:HE3	2.03	0.59
1:B:141:LEU:O	1:B:244:LEU:N	2.30	0.59
1:B:363:ALA:N	1:B:525:CYS:O	2.34	0.59
1:C:107:GLY:H	1:C:235:ILE:HG23	1.68	0.59
1:C:239:GLN:HG2	1:C:240:THR:O	2.03	0.59
2:F:95:TYR:HB2	2:F:97:PHE:HE1	1.68	0.59
2:H:88:GLN:HG2	2:H:97:PHE:CD1	2.37	0.59
1:A:107:GLY:H	1:A:235:ILE:HG23	1.68	0.59
1:A:650:LEU:HD21	1:A:653:ALA:HB3	1.85	0.59
1:A:1088:HIS:ND1	1:A:1122:VAL:HG22	2.17	0.59
1:B:515:PHE:HD2	1:B:517:LEU:H	1.49	0.59
1:B:132:GLU:O	1:B:164:ASN:N	2.36	0.58
1:C:864:LEU:HD12	1:C:864:LEU:C	2.24	0.58
1:A:132:GLU:O	1:A:164:ASN:N	2.36	0.58
1:A:395:VAL:HA	1:A:514:SER:O	2.03	0.58
1:A:444:LYS:HD2	1:A:448:ASN:HB2	1.83	0.58
1:A:849:LEU:HD23	1:A:849:LEU:O	2.03	0.58
1:A:855:PHE:CE1	1:B:589:PRO:HD3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:TYR:HB2	1:B:514:SER:HB2	1.85	0.58
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.38	0.58
1:B:498:GLN:O	1:B:501:ASN:N	2.36	0.58
1:C:134:GLN:NE2	1:C:135:PHE:H	2.00	0.58
1:C:395:VAL:HA	1:C:514:SER:O	2.03	0.58
1:C:587:ILE:HG22	1:C:588:THR:H	1.68	0.58
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.84	0.58
1:A:97:LYS:HE2	1:A:186:PHE:HE1	1.68	0.58
1:A:309:GLU:H	1:A:309:GLU:CD	2.06	0.58
1:A:365:TYR:HD1	1:A:368:LEU:HD12	1.69	0.58
1:A:377:PHE:HB3	2:D:93:TRP:CD1	2.39	0.58
1:A:587:ILE:HG22	1:A:588:THR:H	1.68	0.58
1:B:587:ILE:HG22	1:B:588:THR:H	1.68	0.58
1:B:856:ASN:O	1:B:858:LEU:HD12	2.03	0.58
1:C:97:LYS:HE2	1:C:186:PHE:HE1	1.68	0.58
1:C:309:GLU:H	1:C:309:GLU:CD	2.05	0.58
1:A:239:GLN:HG2	1:A:240:THR:O	2.03	0.58
1:A:986:PRO:O	1:A:990:GLU:HG2	2.03	0.58
1:B:107:GLY:H	1:B:235:ILE:HG23	1.68	0.58
1:C:365:TYR:HD1	1:C:368:LEU:HD12	1.69	0.58
1:C:396:TYR:HB2	1:C:514:SER:HB2	1.85	0.58
3:E:58:THR:HG22	3:E:70:LEU:HB2	1.85	0.58
1:A:676:THR:HG23	1:A:690:GLN:HA	1.86	0.58
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.84	0.58
1:B:398:ASP:O	1:B:511:VAL:HA	2.02	0.58
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.30	0.58
1:C:398:ASP:O	1:C:511:VAL:HA	2.02	0.58
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.85	0.58
1:A:856:ASN:C	1:A:858:LEU:H	2.07	0.58
1:A:1077:THR:OG1	1:C:900:MET:SD	2.58	0.58
1:B:57:PRO:HG2	1:B:271:GLN:OE1	2.02	0.58
1:B:97:LYS:HE2	1:B:186:PHE:HE1	1.68	0.58
3:E:100:GLU:HG2	3:E:106:VAL:HG22	1.85	0.58
3:I:35:HIS:CD2	3:I:99:SER:HB2	2.39	0.58
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.85	0.58
1:A:408:ARG:CD	3:E:102:ASP:CG	2.71	0.58
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.84	0.58
1:B:1089:PHE:N	1:B:1089:PHE:CD1	2.70	0.58
1:C:170:TYR:OH	1:C:172:SER:OG	2.20	0.58
2:H:35:TYR:HB2	2:H:86:PHE:HB2	1.84	0.58
3:I:18:VAL:HG12	3:I:86:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:CYS:SG	1:A:526:GLY:N	2.76	0.58
1:A:894:LEU:HD21	1:B:1072:GLU:HG2	1.85	0.58
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.21	0.58
1:C:363:ALA:N	1:C:525:CYS:O	2.34	0.58
1:C:800:PHE:HD2	1:C:927:PHE:CD2	2.21	0.58
3:I:47:TRP:HZ2	3:I:50:TYR:HB3	1.69	0.58
3:I:100:GLU:HG2	3:I:106:VAL:HG22	1.85	0.58
1:A:393:THR:HB	1:A:520:ALA:HB3	1.86	0.58
1:B:986:PRO:O	1:B:990:GLU:HG2	2.03	0.58
2:D:35:TYR:CZ	2:D:45:LEU:HD13	2.38	0.58
3:E:47:TRP:HZ2	3:E:50:TYR:HB3	1.69	0.58
2:F:5:THR:N	2:F:23:ARG:O	2.36	0.58
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.38	0.58
1:A:616:ASN:ND2	5:A:1307:NAG:O7	2.37	0.58
1:A:955:ASN:O	1:A:958:ALA:N	2.37	0.58
1:A:1088:HIS:HD1	1:A:1122:VAL:HG22	1.69	0.58
1:A:1089:PHE:HB3	1:A:1090:PRO:HD2	1.86	0.58
1:B:616:ASN:ND2	5:B:1307:NAG:O7	2.37	0.58
1:B:650:LEU:HD21	1:B:653:ALA:HB3	1.85	0.58
1:C:132:GLU:O	1:C:164:ASN:N	2.36	0.58
1:C:676:THR:HG23	1:C:690:GLN:HA	1.86	0.58
1:C:807:PRO:HA	1:C:816:SER:HB3	1.86	0.58
1:A:957:GLN:O	1:A:957:GLN:NE2	2.37	0.57
1:B:239:GLN:HG2	1:B:240:THR:O	2.03	0.57
1:B:320:VAL:HG21	1:B:591:SER:OG	2.03	0.57
1:C:616:ASN:ND2	5:C:1307:NAG:O7	2.37	0.57
2:H:35:TYR:CZ	2:H:45:LEU:HD13	2.38	0.57
1:A:807:PRO:HA	1:A:816:SER:HB3	1.86	0.57
1:B:27:ALA:O	1:B:64:TRP:HB3	2.05	0.57
1:B:125:ASN:HB2	5:B:1302:NAG:H81	1.86	0.57
1:B:395:VAL:HA	1:B:514:SER:O	2.03	0.57
3:G:73:ASP:HB2	3:G:80:TYR:HE2	1.70	0.57
1:B:327:VAL:O	1:B:531:THR:N	2.35	0.57
1:B:600:PRO:HB3	1:B:674:TYR:HB2	1.85	0.57
1:B:748:GLU:H	1:B:748:GLU:CD	2.04	0.57
1:B:800:PHE:CD2	1:B:927:PHE:HD2	2.22	0.57
1:C:393:THR:HB	1:C:520:ALA:HB3	1.86	0.57
3:E:38:LYS:NZ	3:E:46:GLU:OE1	2.24	0.57
1:A:856:ASN:C	1:A:858:LEU:N	2.57	0.57
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.38	0.57
1:C:574:ASP:OD2	1:C:575:ALA:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:THR:OG1	1:C:648:GLY:N	2.29	0.57
2:F:34:TRP:O	2:F:46:LEU:N	2.36	0.57
1:A:404:GLY:HA2	1:A:508:TYR:CD2	2.40	0.57
1:A:786:LYS:HG3	1:A:787:GLN:H	1.70	0.57
1:A:800:PHE:HD2	1:A:927:PHE:CD2	2.22	0.57
1:C:1089:PHE:HB3	1:C:1090:PRO:HD2	1.86	0.57
1:A:485:GLY:H	1:A:488:CYS:HB2	1.69	0.57
1:B:343:ASN:ND2	5:B:1305:NAG:O7	2.38	0.57
1:B:955:ASN:O	1:B:958:ALA:N	2.37	0.57
1:B:1089:PHE:HB3	1:B:1090:PRO:HD2	1.86	0.57
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.40	0.57
1:C:986:PRO:O	1:C:990:GLU:HG2	2.03	0.57
2:F:12:VAL:O	2:F:105:ILE:HA	2.03	0.57
1:A:125:ASN:HB2	5:A:1302:NAG:H81	1.86	0.57
1:A:1043:CYS:HB3	1:A:1048:HIS:HD2	1.68	0.57
1:B:224:GLU:OE1	1:B:224:GLU:N	2.27	0.57
1:B:393:THR:HB	1:B:520:ALA:HB3	1.86	0.57
1:B:574:ASP:OD2	1:B:575:ALA:N	2.38	0.57
1:B:807:PRO:HA	1:B:816:SER:HB3	1.86	0.57
1:C:141:LEU:O	1:C:244:LEU:N	2.30	0.57
2:F:22:CYS:SG	2:F:32:LEU:HD11	2.45	0.57
2:F:43:PRO:HD2	3:G:110:TRP:HZ3	1.68	0.57
2:F:93:TRP:CE3	2:F:94:PRO:HD3	2.39	0.57
1:A:800:PHE:CD2	1:A:927:PHE:HD2	2.22	0.57
1:B:365:TYR:HD1	1:B:368:LEU:HD12	1.68	0.57
1:B:438:SER:O	1:B:442:ASP:N	2.38	0.57
1:C:619:GLU:OE1	1:C:619:GLU:N	2.26	0.57
3:E:35:HIS:CD2	3:E:99:SER:HB2	2.39	0.57
3:G:4:LEU:HD23	3:G:24:VAL:HG22	1.86	0.57
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.87	0.57
1:B:676:THR:HG23	1:B:690:GLN:HA	1.86	0.57
1:B:786:LYS:HG3	1:B:787:GLN:H	1.70	0.57
3:E:73:ASP:O	3:E:77:ASP:N	2.38	0.57
3:G:6:GLN:OE1	3:G:113:GLY:N	2.31	0.57
3:I:58:THR:HG22	3:I:70:LEU:HB2	1.85	0.57
3:I:73:ASP:O	3:I:77:ASP:N	2.38	0.57
1:A:390:LEU:HD11	1:A:518:LEU:HD11	1.87	0.57
1:A:574:ASP:OD2	1:A:575:ALA:N	2.38	0.57
1:B:390:LEU:HD11	1:B:518:LEU:HD11	1.87	0.57
1:B:559:PHE:CZ	1:B:566:GLY:CA	2.83	0.57
1:C:485:GLY:H	1:C:488:CYS:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:ALA:O	1:C:769:GLY:N	2.38	0.57
1:B:1088:HIS:HD1	1:B:1122:VAL:HG22	1.69	0.56
1:C:144:TYR:N	1:C:151:SER:O	2.30	0.56
1:C:502:GLY:O	1:C:506:GLN:HG3	2.05	0.56
1:C:858:LEU:HD12	1:C:858:LEU:N	2.20	0.56
3:G:33:TYR:CE1	3:G:101:TYR:CD1	2.92	0.56
1:B:485:GLY:H	1:B:488:CYS:HB2	1.69	0.56
1:C:27:ALA:O	1:C:64:TRP:HB3	2.05	0.56
2:F:34:TRP:CD1	2:F:47:ILE:HB	2.39	0.56
1:A:498:GLN:O	1:A:501:ASN:N	2.36	0.56
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.21	0.56
1:A:766:ALA:O	1:A:769:GLY:N	2.38	0.56
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.40	0.56
1:B:957:GLN:NE2	1:B:957:GLN:O	2.37	0.56
1:C:327:VAL:O	1:C:531:THR:N	2.37	0.56
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.87	0.56
1:C:800:PHE:CD2	1:C:927:PHE:HD2	2.22	0.56
1:A:27:ALA:O	1:A:64:TRP:HB3	2.04	0.56
1:A:343:ASN:ND2	5:A:1305:NAG:O7	2.38	0.56
1:A:347:PHE:CE2	1:A:509:ARG:HB3	2.40	0.56
1:B:766:ALA:O	1:B:769:GLY:N	2.38	0.56
1:C:125:ASN:HB2	5:C:1302:NAG:H81	1.86	0.56
1:B:502:GLY:O	1:B:506:GLN:HG3	2.05	0.56
1:B:645:THR:OG1	1:B:648:GLY:N	2.29	0.56
1:B:914:ASN:HD22	1:C:1123:SER:HB2	1.69	0.56
1:C:347:PHE:CE2	1:C:509:ARG:HB3	2.40	0.56
1:C:557:LYS:O	1:C:584:ILE:HG13	2.05	0.56
1:C:955:ASN:O	1:C:958:ALA:N	2.37	0.56
3:I:37:VAL:O	3:I:95:TYR:N	2.36	0.56
1:A:336:CYS:SG	1:A:524:VAL:HG22	2.46	0.56
1:C:655:HIS:CD2	1:C:656:VAL:H	2.24	0.56
1:A:655:HIS:CD2	1:A:656:VAL:H	2.24	0.56
1:B:404:GLY:HA2	1:B:508:TYR:CD2	2.40	0.56
1:C:336:CYS:SG	1:C:524:VAL:HG22	2.46	0.56
1:C:901:GLN:HE21	1:C:905:ARG:NE	2.04	0.56
2:D:36:GLN:NE2	2:D:81:ASP:O	2.38	0.56
2:F:33:HIS:HA	2:F:47:ILE:O	2.05	0.56
1:B:37:TYR:HA	1:B:223:LEU:H	1.71	0.56
1:C:438:SER:O	1:C:442:ASP:N	2.38	0.56
1:C:786:LYS:HG3	1:C:787:GLN:H	1.70	0.56
1:C:957:GLN:O	1:C:957:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:LYS:HG2	2:F:75:ASN:HA	1.88	0.56
1:A:228:ASP:OD1	1:A:229:LEU:N	2.39	0.56
1:C:343:ASN:ND2	5:C:1305:NAG:O7	2.38	0.56
1:C:390:LEU:HD11	1:C:518:LEU:HD11	1.87	0.56
1:A:37:TYR:HA	1:A:223:LEU:H	1.71	0.56
1:A:438:SER:O	1:A:442:ASP:N	2.38	0.56
1:A:901:GLN:HE21	1:A:905:ARG:NE	2.04	0.56
1:B:323:THR:HG21	1:B:537:LYS:HE3	1.87	0.56
1:B:336:CYS:SG	1:B:524:VAL:HG22	2.46	0.56
1:B:655:HIS:CD2	1:B:656:VAL:H	2.24	0.56
1:B:655:HIS:CD2	1:B:656:VAL:N	2.74	0.56
1:C:498:GLN:O	1:C:501:ASN:N	2.36	0.56
3:E:56:GLY:O	3:E:58:THR:N	2.38	0.56
1:A:354:ASN:HD22	1:A:399:SER:HB3	1.71	0.55
1:A:365:TYR:CD1	1:A:368:LEU:HD12	2.41	0.55
1:A:560:LEU:HD12	1:A:562:PHE:HE1	1.70	0.55
1:B:147:LYS:CB	1:B:152:TRP:HE1	2.19	0.55
1:B:324:GLU:OE1	1:B:325:SER:N	2.35	0.55
1:B:1050:MET:O	1:B:1051:SER:OG	2.21	0.55
1:B:1067:TYR:CD2	1:B:1067:TYR:O	2.60	0.55
1:C:37:TYR:HA	1:C:223:LEU:H	1.71	0.55
1:C:1050:MET:O	1:C:1051:SER:OG	2.21	0.55
3:E:35:HIS:O	3:E:97:ALA:N	2.30	0.55
2:H:36:GLN:NE2	2:H:81:ASP:O	2.38	0.55
3:I:90:ASP:O	3:I:94:TYR:OH	2.19	0.55
1:A:655:HIS:CD2	1:A:656:VAL:N	2.74	0.55
1:A:900:MET:SD	1:B:1077:THR:OG1	2.61	0.55
1:B:645:THR:OG1	1:B:648:GLY:O	2.15	0.55
1:C:1088:HIS:HD1	1:C:1122:VAL:HG22	1.69	0.55
2:F:34:TRP:O	2:F:45:LEU:HD12	2.06	0.55
2:H:15:LYS:HA	2:H:76:SER:HA	1.88	0.55
3:I:56:GLY:O	3:I:58:THR:N	2.38	0.55
1:A:557:LYS:O	1:A:584:ILE:CG2	2.49	0.55
1:A:731:MET:HG2	1:A:774:GLN:OE1	2.07	0.55
1:A:854:LYS:HZ3	1:A:854:LYS:CB	2.19	0.55
1:B:365:TYR:CD1	1:B:368:LEU:HD12	2.41	0.55
1:B:375:SER:CB	1:B:436:TRP:HA	2.36	0.55
1:B:914:ASN:HD22	1:C:1123:SER:CB	2.19	0.55
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.41	0.55
3:G:40:ALA:HB3	3:G:43:LYS:HB2	1.88	0.55
1:B:409:GLN:HB3	1:B:418:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:LYS:HA	2:D:76:SER:HA	1.89	0.55
1:A:502:GLY:O	1:A:506:GLN:HG3	2.05	0.55
1:B:1141:LEU:O	1:B:1144:GLU:N	2.39	0.55
3:G:58:THR:HG22	3:G:70:LEU:HB2	1.89	0.55
1:A:1067:TYR:CD2	1:A:1067:TYR:O	2.60	0.55
1:B:148:ASN:OD1	1:B:149:ASN:N	2.40	0.55
1:B:378:LYS:O	1:B:433:VAL:N	2.34	0.55
1:B:1027:THR:O	1:B:1030:SER:N	2.40	0.55
1:C:375:SER:CB	1:C:436:TRP:HA	2.37	0.55
1:C:409:GLN:HB3	1:C:418:ILE:HB	1.89	0.55
1:C:1067:TYR:CD2	1:C:1067:TYR:O	2.60	0.55
1:B:320:VAL:CG2	1:B:591:SER:OG	2.54	0.55
1:B:901:GLN:HE21	1:B:905:ARG:NE	2.04	0.55
1:C:147:LYS:CB	1:C:152:TRP:HE1	2.19	0.55
1:C:861:LEU:N	1:C:861:LEU:HD23	2.21	0.55
1:A:295:PRO:O	1:A:298:GLU:N	2.39	0.55
1:A:544:ASN:ND2	1:A:579:PRO:HB3	2.19	0.55
1:B:167:THR:HA	1:C:357:ARG:HH12	1.72	0.55
1:C:1116:THR:H	1:C:1119:ASN:ND2	2.05	0.55
3:I:6:GLN:HA	3:I:21:SER:O	2.07	0.55
1:A:147:LYS:CB	1:A:152:TRP:HE1	2.19	0.55
1:A:375:SER:CB	1:A:436:TRP:HA	2.36	0.55
1:A:409:GLN:HB3	1:A:418:ILE:HB	1.89	0.55
1:B:354:ASN:HD22	1:B:399:SER:HB3	1.71	0.55
1:C:228:ASP:OD1	1:C:229:LEU:N	2.39	0.55
1:C:1043:CYS:HB3	1:C:1048:HIS:HD2	1.68	0.55
3:E:38:LYS:O	3:E:46:GLU:N	2.40	0.55
3:G:112:GLN:OE1	3:G:112:GLN:N	2.36	0.55
1:A:201:PHE:CE2	1:A:203:ILE:HG13	2.42	0.55
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.41	0.55
1:C:655:HIS:CD2	1:C:656:VAL:N	2.74	0.55
1:C:1000:ARG:O	1:C:1003:SER:N	2.40	0.55
3:E:6:GLN:HA	3:E:21:SER:O	2.07	0.55
1:A:136:CYS:H	1:A:139:PRO:HG3	1.72	0.54
1:A:1027:THR:O	1:A:1030:SER:N	2.40	0.54
1:B:201:PHE:CE2	1:B:203:ILE:HG13	2.42	0.54
1:B:228:ASP:OD1	1:B:229:LEU:N	2.39	0.54
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.87	0.54
1:B:731:MET:HG2	1:B:774:GLN:OE1	2.07	0.54
1:A:1000:ARG:O	1:A:1003:SER:N	2.40	0.54
1:C:365:TYR:CD1	1:C:368:LEU:HD12	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:ASN:ND2	1:C:579:PRO:HB3	2.19	0.54
1:C:1004:LEU:O	1:C:1007:TYR:N	2.41	0.54
3:G:4:LEU:N	3:G:109:TYR:HE2	2.05	0.54
1:A:1084:ASP:HB2	1:A:1086:LYS:NZ	2.22	0.54
1:B:118:LEU:HD23	1:B:129:LYS:HE2	1.89	0.54
1:B:1000:ARG:O	1:B:1003:SER:N	2.40	0.54
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.42	0.54
1:A:144:TYR:HD2	1:A:152:TRP:CD1	2.25	0.54
1:B:1084:ASP:HB2	1:B:1086:LYS:NZ	2.22	0.54
1:B:1143:PRO:HA	1:B:1146:ASP:HB2	1.90	0.54
1:A:43:PHE:HD1	1:B:563:GLN:CD	2.10	0.54
1:A:412:PRO:HB3	1:A:426:PRO:O	2.08	0.54
1:A:1116:THR:H	1:A:1119:ASN:ND2	2.05	0.54
1:B:100:ILE:HG22	1:B:242:LEU:HD22	1.89	0.54
1:B:1085:GLY:HA2	1:B:1126:CYS:SG	2.48	0.54
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.42	0.54
1:C:201:PHE:CE2	1:C:203:ILE:HG13	2.42	0.54
1:C:214:ARG:HB3	1:C:214:ARG:CZ	2.38	0.54
1:C:365:TYR:CE2	1:C:369:TYR:CE1	2.96	0.54
1:A:118:LEU:HD23	1:A:129:LYS:HE2	1.89	0.54
1:A:557:LYS:HB2	1:A:584:ILE:CG2	2.38	0.54
1:B:214:ARG:HB3	1:B:214:ARG:CZ	2.38	0.54
1:C:1027:THR:O	1:C:1030:SER:N	2.40	0.54
1:C:1085:GLY:HA2	1:C:1126:CYS:SG	2.48	0.54
2:D:28:ILE:HG21	2:D:68:THR:HA	1.90	0.54
3:G:6:GLN:HE22	3:G:96:CYS:H	1.55	0.54
3:G:33:TYR:CZ	3:G:101:TYR:CD1	2.95	0.54
1:B:90:VAL:HG21	1:B:238:PHE:CE1	2.42	0.54
1:B:144:TYR:HD2	1:B:152:TRP:CD1	2.25	0.54
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.90	0.54
1:C:731:MET:HG2	1:C:774:GLN:OE1	2.06	0.54
3:G:28:SER:OG	3:G:31:ASN:ND2	2.41	0.54
1:A:42:VAL:HG22	1:B:565:PHE:CE2	2.43	0.54
1:A:320:VAL:CG2	1:A:591:SER:OG	2.56	0.54
1:A:557:LYS:CB	1:A:584:ILE:HG21	2.38	0.54
1:A:1008:VAL:O	1:A:1011:GLN:N	2.41	0.54
1:B:136:CYS:H	1:B:139:PRO:HG3	1.72	0.54
1:C:354:ASN:HD22	1:C:399:SER:HB3	1.71	0.54
1:C:897:PRO:HD2	1:C:900:MET:HB2	1.90	0.54
2:F:34:TRP:CE3	2:F:72:LEU:HB2	2.43	0.54
1:B:110:LEU:HD13	1:B:237:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:GLU:OE1	1:B:619:GLU:N	2.26	0.54
1:C:148:ASN:OD1	1:C:149:ASN:N	2.40	0.54
1:C:350:VAL:HB	1:C:402:ILE:HG22	1.90	0.54
1:C:1141:LEU:O	1:C:1144:GLU:N	2.39	0.54
2:D:33:HIS:HA	2:D:47:ILE:O	2.08	0.54
3:I:91:THR:HA	3:I:116:VAL:O	2.08	0.54
1:A:214:ARG:HB3	1:A:214:ARG:CZ	2.38	0.54
1:A:562:PHE:CD2	1:C:225:PRO:HD2	2.43	0.54
1:C:53:ASP:OD1	1:C:54:LEU:N	2.41	0.54
1:C:100:ILE:HG22	1:C:242:LEU:HD22	1.89	0.54
1:C:959:LEU:O	1:C:962:LEU:N	2.41	0.54
3:E:37:VAL:O	3:E:95:TYR:N	2.36	0.54
3:I:18:VAL:O	3:I:83:LEU:N	2.34	0.54
1:A:53:ASP:OD1	1:A:54:LEU:N	2.41	0.53
1:A:148:ASN:OD1	1:A:149:ASN:N	2.40	0.53
1:A:376:THR:HG22	1:A:435:ALA:H	1.73	0.53
1:A:1004:LEU:O	1:A:1007:TYR:N	2.41	0.53
1:B:318:PHE:CE1	1:B:592:PHE:O	2.61	0.53
1:B:365:TYR:CE2	1:B:369:TYR:CE1	2.96	0.53
1:B:378:LYS:NZ	3:G:56:GLY:O	2.25	0.53
1:C:136:CYS:H	1:C:139:PRO:HG3	1.72	0.53
1:C:406:GLU:OE2	1:C:495:TYR:OH	2.19	0.53
1:A:110:LEU:HD13	1:A:237:ARG:NH2	2.23	0.53
1:A:320:VAL:HG21	1:A:591:SER:OG	2.08	0.53
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.41	0.53
1:A:1085:GLY:HA2	1:A:1126:CYS:SG	2.48	0.53
1:B:65:PHE:HD2	1:B:265:TYR:HH	1.53	0.53
1:B:559:PHE:HZ	1:B:566:GLY:HA3	1.72	0.53
1:C:360:ASN:H	1:C:523:THR:HA	1.74	0.53
1:C:1084:ASP:HB2	1:C:1086:LYS:NZ	2.22	0.53
2:H:33:HIS:HA	2:H:47:ILE:O	2.08	0.53
3:I:51:ILE:HD12	3:I:70:LEU:HB3	1.90	0.53
1:A:187:LYS:HD2	1:A:210:ILE:O	2.08	0.53
1:A:360:ASN:H	1:A:523:THR:HA	1.74	0.53
1:A:437:ASN:HA	1:A:508:TYR:HD1	1.74	0.53
1:B:140:PHE:HD2	1:B:141:LEU:O	1.91	0.53
1:C:187:LYS:HD2	1:C:210:ILE:O	2.09	0.53
1:C:412:PRO:HB3	1:C:426:PRO:O	2.08	0.53
3:G:27:TYR:CE2	3:G:98:ARG:HD3	2.43	0.53
1:A:91:TYR:CG	1:A:92:PHE:N	2.76	0.53
1:A:108:THR:OG1	1:A:109:THR:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:LEU:O	1:A:962:LEU:N	2.41	0.53
1:B:1004:LEU:O	1:B:1007:TYR:N	2.41	0.53
1:C:110:LEU:HD13	1:C:237:ARG:NH2	2.23	0.53
1:C:144:TYR:HD2	1:C:152:TRP:CD1	2.25	0.53
1:C:1008:VAL:O	1:C:1011:GLN:N	2.41	0.53
1:A:350:VAL:HB	1:A:402:ILE:HG22	1.90	0.53
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.90	0.53
1:B:959:LEU:O	1:B:962:LEU:N	2.41	0.53
1:B:1116:THR:H	1:B:1119:ASN:ND2	2.05	0.53
1:C:376:THR:HG22	1:C:435:ALA:H	1.73	0.53
2:D:93:TRP:CG	2:D:94:PRO:HD3	2.43	0.53
3:E:60:ASP:OD2	3:E:65:LYS:NZ	2.42	0.53
1:A:93:ALA:HB1	1:A:189:LEU:HD11	1.91	0.53
1:A:100:ILE:HG22	1:A:242:LEU:HD22	1.89	0.53
1:A:365:TYR:CE2	1:A:369:TYR:CE1	2.96	0.53
1:A:568:ASP:O	1:A:571:ASP:N	2.34	0.53
1:B:360:ASN:H	1:B:523:THR:HA	1.74	0.53
1:B:412:PRO:HB3	1:B:426:PRO:O	2.08	0.53
1:B:453:TYR:N	1:B:493:GLN:O	2.39	0.53
1:C:140:PHE:HD2	1:C:141:LEU:O	1.91	0.53
3:E:51:ILE:HD12	3:E:70:LEU:HB3	1.90	0.53
2:F:91:ASN:N	2:F:95:TYR:HE1	2.07	0.53
3:G:4:LEU:HD12	3:G:110:TRP:HA	1.91	0.53
1:A:323:THR:HG21	1:A:537:LYS:HZ1	1.71	0.53
1:B:53:ASP:OD1	1:B:54:LEU:N	2.41	0.53
1:B:93:ALA:HB1	1:B:189:LEU:HD11	1.91	0.53
1:B:375:SER:OG	1:B:436:TRP:HA	2.09	0.53
1:C:91:TYR:CG	1:C:92:PHE:N	2.76	0.53
1:C:378:LYS:O	1:C:433:VAL:N	2.34	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.91	0.53
2:H:31:ASN:CG	2:H:90:THR:HG21	2.29	0.53
2:H:34:TRP:CZ3	2:H:87:CYS:HB3	2.44	0.53
1:A:105:ILE:HG13	1:A:241:LEU:HD11	1.91	0.53
1:A:914:ASN:HD22	1:B:1123:SER:CB	2.22	0.53
1:B:320:VAL:CG2	1:B:591:SER:CB	2.86	0.53
1:C:128:ILE:HD12	1:C:170:TYR:CD2	2.43	0.53
1:C:555:SER:OG	1:C:584:ILE:O	2.22	0.53
1:C:1143:PRO:HA	1:C:1146:ASP:HB2	1.90	0.53
2:D:23:ARG:HE	2:D:69:ASP:HB2	1.74	0.53
2:D:34:TRP:CZ3	2:D:87:CYS:HB3	2.44	0.53
3:E:4:LEU:HD21	3:E:27:TYR:OH	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:91:THR:HA	3:E:116:VAL:O	2.08	0.53
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.90	0.53
1:B:897:PRO:HD2	1:B:900:MET:HB2	1.90	0.53
1:C:240:THR:OG1	1:C:241:LEU:N	2.42	0.53
1:C:375:SER:OG	1:C:436:TRP:HA	2.09	0.53
1:C:437:ASN:HA	1:C:508:TYR:HD1	1.74	0.53
1:C:886:TRP:O	1:C:888:PHE:N	2.42	0.53
2:D:31:ASN:CG	2:D:90:THR:HG21	2.29	0.53
2:D:43:PRO:HD2	3:E:110:TRP:HZ3	1.74	0.53
3:E:19:LYS:HA	3:E:82:GLU:HA	1.91	0.53
3:E:30:SER:HA	3:E:53:PRO:HB2	1.91	0.53
2:H:28:ILE:HG21	2:H:68:THR:HA	1.90	0.53
2:H:36:GLN:HB2	2:H:46:LEU:HD11	1.91	0.53
3:I:4:LEU:HD21	3:I:27:TYR:OH	2.09	0.53
1:B:1100:THR:OG1	1:B:1101:HIS:N	2.42	0.53
1:C:295:PRO:O	1:C:298:GLU:N	2.39	0.53
2:F:97:PHE:CZ	3:G:47:TRP:HB2	2.44	0.53
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.44	0.52
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.44	0.52
1:B:376:THR:HG22	1:B:435:ALA:H	1.73	0.52
1:B:1043:CYS:HB3	1:B:1048:HIS:HD2	1.68	0.52
1:C:108:THR:HG21	4:T:1:NAG:O5	2.10	0.52
2:F:22:CYS:O	2:F:70:PHE:N	2.41	0.52
3:G:37:VAL:O	3:G:95:TYR:N	2.38	0.52
3:I:35:HIS:O	3:I:97:ALA:N	2.30	0.52
1:A:886:TRP:O	1:A:888:PHE:N	2.42	0.52
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ3	1.74	0.52
1:B:340:GLU:O	1:B:344:ALA:HB2	2.09	0.52
1:B:437:ASN:HA	1:B:508:TYR:HD1	1.74	0.52
1:B:886:TRP:O	1:B:888:PHE:N	2.42	0.52
1:B:1084:ASP:HB2	1:B:1086:LYS:HZ3	1.74	0.52
1:C:93:ALA:HB1	1:C:189:LEU:HD11	1.91	0.52
1:C:118:LEU:HD23	1:C:129:LYS:HE2	1.89	0.52
1:C:559:PHE:CE2	1:C:565:PHE:C	2.80	0.52
1:C:877:LEU:O	1:C:881:THR:OG1	2.22	0.52
3:I:19:LYS:HA	3:I:82:GLU:HA	1.91	0.52
1:A:108:THR:HG21	4:J:1:NAG:O5	2.10	0.52
1:B:91:TYR:CG	1:B:92:PHE:N	2.76	0.52
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.91	0.52
1:B:534:VAL:HG11	1:B:537:LYS:HE2	1.92	0.52
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1100:THR:OG1	1:C:1101:HIS:N	2.42	0.52
2:F:97:PHE:HD2	3:G:45:LEU:CB	2.21	0.52
3:G:33:TYR:CE1	3:G:101:TYR:HD1	2.27	0.52
1:A:140:PHE:HD2	1:A:141:LEU:O	1.91	0.52
1:A:290:ASP:O	1:A:297:SER:HB3	2.10	0.52
1:A:294:ASP:OD1	1:A:294:ASP:N	2.42	0.52
1:A:340:GLU:O	1:A:344:ALA:HB2	2.09	0.52
1:A:603:ASN:OD1	5:A:1306:NAG:O5	2.23	0.52
1:A:914:ASN:HD22	1:B:1123:SER:HB2	1.74	0.52
1:A:1143:PRO:HA	1:A:1146:ASP:HB2	1.90	0.52
1:B:295:PRO:O	1:B:298:GLU:N	2.39	0.52
1:B:748:GLU:OE1	1:B:748:GLU:N	2.39	0.52
1:C:105:ILE:HG13	1:C:241:LEU:HD11	1.91	0.52
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.90	0.52
1:C:1091:ARG:N	1:C:1119:ASN:O	2.31	0.52
3:E:10:GLU:HG3	3:E:18:VAL:HG23	1.91	0.52
3:I:21:SER:HA	3:I:80:TYR:HD1	1.74	0.52
3:I:30:SER:HA	3:I:53:PRO:HB2	1.91	0.52
1:A:534:VAL:HG11	1:A:537:LYS:HE2	1.92	0.52
1:A:897:PRO:HD2	1:A:900:MET:HB2	1.90	0.52
1:B:191:GLU:O	1:B:205:SER:HA	2.10	0.52
1:C:340:GLU:O	1:C:344:ALA:HB2	2.09	0.52
1:C:866:THR:O	1:C:868:GLU:N	2.43	0.52
2:D:34:TRP:O	2:D:46:LEU:N	2.38	0.52
3:G:50:TYR:O	3:G:58:THR:HA	2.09	0.52
2:H:77:LEU:HD22	2:H:105:ILE:HD11	1.91	0.52
1:A:65:PHE:HD2	1:A:265:TYR:HH	1.56	0.52
1:A:748:GLU:OE1	1:A:748:GLU:N	2.39	0.52
1:B:105:ILE:HG13	1:B:241:LEU:HD11	1.91	0.52
1:B:127:VAL:HG11	5:B:1302:NAG:H5	1.91	0.52
1:B:187:LYS:HD2	1:B:210:ILE:O	2.08	0.52
1:C:645:THR:OG1	1:C:648:GLY:O	2.15	0.52
3:G:3:GLN:HA	3:G:109:TYR:OH	2.09	0.52
3:G:38:LYS:N	3:G:46:GLU:O	2.31	0.52
1:A:191:GLU:O	1:A:205:SER:HA	2.10	0.52
1:A:377:PHE:HA	1:A:434:ILE:HG12	1.92	0.52
1:A:866:THR:O	1:A:868:GLU:N	2.43	0.52
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.75	0.52
2:D:97:PHE:HD2	3:E:45:LEU:HB3	1.75	0.52
3:E:27:TYR:CD1	3:E:32:TYR:HD2	2.27	0.52
2:F:93:TRP:CG	2:F:94:PRO:HD3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:CYS:N	1:A:1132:ILE:HD11	2.25	0.52
1:A:1100:THR:OG1	1:A:1101:HIS:N	2.42	0.52
1:A:1123:SER:HB2	1:C:914:ASN:HD22	1.75	0.52
1:B:103:GLY:HA2	1:B:119:ILE:O	2.10	0.52
1:B:290:ASP:O	1:B:297:SER:HB3	2.10	0.52
1:B:406:GLU:OE2	1:B:495:TYR:OH	2.19	0.52
1:B:866:THR:O	1:B:868:GLU:N	2.43	0.52
1:C:1082:CYS:N	1:C:1132:ILE:HD11	2.25	0.52
2:D:34:TRP:O	2:D:45:LEU:HD12	2.10	0.52
3:E:38:LYS:N	3:E:46:GLU:O	2.23	0.52
2:H:93:TRP:CG	2:H:94:PRO:HD3	2.43	0.52
1:A:127:VAL:HG11	5:A:1302:NAG:H5	1.91	0.52
1:A:240:THR:OG1	1:A:241:LEU:N	2.42	0.52
1:A:347:PHE:HB2	1:A:401:VAL:HG23	1.91	0.52
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.75	0.52
1:C:378:LYS:HE3	1:C:380:TYR:HA	1.92	0.52
1:C:994:ASP:O	1:C:998:THR:N	2.42	0.52
1:A:587:ILE:HG22	1:A:588:THR:N	2.25	0.52
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.91	0.52
1:B:225:PRO:HD2	1:C:562:PHE:CD2	2.45	0.52
1:C:150:LYS:O	1:C:151:SER:OG	2.23	0.52
1:C:294:ASP:N	1:C:294:ASP:OD1	2.42	0.52
1:C:323:THR:HG21	1:C:537:LYS:NZ	2.25	0.52
3:I:60:ASP:OD2	3:I:65:LYS:NZ	2.42	0.52
1:A:103:GLY:HA2	1:A:119:ILE:O	2.10	0.51
1:B:995:ARG:O	1:B:999:GLY:N	2.36	0.51
1:C:365:TYR:HE2	1:C:369:TYR:CE1	2.28	0.51
1:C:560:LEU:HD12	1:C:562:PHE:HE1	1.74	0.51
2:F:6:GLN:HE22	2:F:87:CYS:N	2.08	0.51
2:H:23:ARG:HE	2:H:69:ASP:HB2	1.74	0.51
1:A:375:SER:OG	1:A:436:TRP:HA	2.09	0.51
1:A:861:LEU:HD23	1:A:861:LEU:H	1.72	0.51
1:A:1141:LEU:O	1:A:1144:GLU:N	2.39	0.51
1:B:128:ILE:HD12	1:B:170:TYR:CD2	2.42	0.51
1:B:1083:HIS:HB2	1:B:1088:HIS:CD2	2.45	0.51
1:C:453:TYR:N	1:C:493:GLN:O	2.39	0.51
1:C:559:PHE:HZ	1:C:566:GLY:CA	2.24	0.51
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.43	0.51
1:C:748:GLU:N	1:C:748:GLU:OE1	2.39	0.51
2:D:22:CYS:HB3	2:D:70:PHE:HB2	1.92	0.51
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:O	1:B:243:ALA:HA	2.10	0.51
1:B:376:THR:HG1	3:G:50:TYR:HH	1.45	0.51
1:B:435:ALA:HA	1:B:510:VAL:HG22	1.93	0.51
1:C:127:VAL:HG11	5:C:1302:NAG:H5	1.91	0.51
1:C:290:ASP:O	1:C:297:SER:HB3	2.10	0.51
1:C:421:TYR:HD1	1:C:457:ARG:HB3	1.75	0.51
1:C:435:ALA:HA	1:C:510:VAL:HG22	1.93	0.51
1:C:534:VAL:HG11	1:C:537:LYS:HE2	1.92	0.51
1:C:901:GLN:C	1:C:903:ALA:N	2.63	0.51
2:D:3:VAL:HG22	2:D:96:ILE:HD13	1.92	0.51
3:G:35:HIS:CD2	3:G:99:SER:HB2	2.45	0.51
2:H:95:TYR:CE2	3:I:105:TYR:CD2	2.97	0.51
1:A:54:LEU:HD23	1:A:272:PRO:HA	1.93	0.51
1:A:141:LEU:O	1:A:243:ALA:HA	2.10	0.51
1:A:302:THR:HG22	1:A:303:LEU:HD23	1.93	0.51
1:A:365:TYR:HE2	1:A:369:TYR:CE1	2.28	0.51
1:A:429:PHE:HE1	1:A:514:SER:HA	1.76	0.51
1:B:1082:CYS:N	1:B:1132:ILE:HD11	2.25	0.51
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.44	0.51
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.92	0.51
1:C:429:PHE:HE1	1:C:514:SER:HA	1.76	0.51
1:C:540:ASN:HA	1:C:549:THR:HG23	1.93	0.51
1:C:723:THR:OG1	1:C:724:THR:N	2.41	0.51
2:D:77:LEU:HD22	2:D:105:ILE:HD11	1.91	0.51
2:H:97:PHE:HD2	3:I:45:LEU:HB3	1.75	0.51
1:A:135:PHE:HA	1:A:160:TYR:HA	1.93	0.51
1:A:559:PHE:CZ	1:A:566:GLY:CA	2.90	0.51
1:B:108:THR:HG21	4:O:1:NAG:O5	2.10	0.51
1:B:302:THR:HG22	1:B:303:LEU:HD23	1.93	0.51
1:B:323:THR:HB	1:B:539:VAL:HG12	1.93	0.51
1:C:103:GLY:HA2	1:C:119:ILE:O	2.10	0.51
1:C:191:GLU:O	1:C:205:SER:HA	2.10	0.51
3:E:24:VAL:HB	3:E:77:ASP:HB3	1.93	0.51
3:E:103:PRO:O	3:E:105:TYR:CE2	2.62	0.51
2:H:34:TRP:O	2:H:45:LEU:HD12	2.10	0.51
3:I:61:ASN:OD1	3:I:63:LYS:HD3	2.10	0.51
1:A:419:ALA:O	1:A:424:LYS:HD3	2.11	0.51
1:B:419:ALA:O	1:B:424:LYS:HD3	2.11	0.51
1:B:453:TYR:CE2	1:B:455:LEU:HB2	2.46	0.51
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.11	0.51
1:C:347:PHE:HB2	1:C:401:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1083:HIS:HB2	1:C:1088:HIS:CD2	2.45	0.51
3:E:21:SER:HA	3:E:80:TYR:HD1	1.74	0.51
3:I:38:LYS:O	3:I:46:GLU:N	2.40	0.51
1:A:342:PHE:HE1	1:A:511:VAL:HG11	1.75	0.51
1:A:563:GLN:HG2	1:C:41:LYS:O	2.11	0.51
1:A:858:LEU:N	1:A:858:LEU:CD1	2.73	0.51
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.11	0.51
1:A:1123:SER:CB	1:C:914:ASN:HD22	2.24	0.51
1:B:240:THR:OG1	1:B:241:LEU:N	2.42	0.51
1:B:901:GLN:C	1:B:903:ALA:N	2.63	0.51
1:C:65:PHE:HD2	1:C:265:TYR:CZ	2.29	0.51
1:C:141:LEU:O	1:C:243:ALA:HA	2.10	0.51
1:C:302:THR:HG22	1:C:303:LEU:HD23	1.93	0.51
3:I:24:VAL:HB	3:I:77:ASP:HB3	1.93	0.51
3:I:27:TYR:CD1	3:I:32:TYR:HD2	2.27	0.51
1:A:65:PHE:HD2	1:A:265:TYR:CZ	2.29	0.51
1:A:886:TRP:HB2	1:A:1034:LEU:O	2.11	0.51
1:B:135:PHE:HA	1:B:160:TYR:HA	1.93	0.51
1:B:294:ASP:OD1	1:B:294:ASP:N	2.42	0.51
1:B:429:PHE:HE1	1:B:514:SER:HA	1.76	0.51
1:B:994:ASP:O	1:B:998:THR:N	2.42	0.51
1:B:1043:CYS:CB	1:B:1048:HIS:CD2	2.92	0.51
1:C:453:TYR:CE2	1:C:455:LEU:HB2	2.46	0.51
1:C:656:VAL:HG12	1:C:658:ASN:H	1.76	0.51
2:D:36:GLN:HB2	2:D:46:LEU:HD11	1.91	0.51
3:I:10:GLU:HG3	3:I:18:VAL:HG23	1.91	0.51
1:A:324:GLU:CG	1:A:325:SER:N	2.73	0.51
1:A:435:ALA:HA	1:A:510:VAL:HG22	1.93	0.51
1:A:901:GLN:C	1:A:903:ALA:N	2.63	0.51
1:B:618:THR:OG1	1:B:619:GLU:N	2.43	0.51
1:B:1008:VAL:O	1:B:1011:GLN:N	2.41	0.51
1:C:675:GLN:HG3	1:C:676:THR:O	2.11	0.51
1:C:904:TYR:O	1:C:906:PHE:N	2.44	0.51
1:C:1084:ASP:HB2	1:C:1086:LYS:HZ3	1.75	0.51
3:E:61:ASN:OD1	3:E:63:LYS:HD3	2.10	0.51
1:A:43:PHE:CD1	1:B:559:PHE:CD1	2.99	0.51
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.44	0.51
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.44	0.51
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.92	0.51
1:B:587:ILE:HG22	1:B:588:THR:N	2.25	0.51
1:B:886:TRP:HB2	1:B:1034:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:SER:O	1:C:132:GLU:HB3	2.11	0.51
1:C:316:SER:O	1:C:595:VAL:CB	2.58	0.51
2:F:48:LYS:O	2:F:52:GLN:HB2	2.11	0.51
3:G:35:HIS:N	3:G:97:ALA:O	2.34	0.51
1:A:112:SER:O	1:A:132:GLU:HB3	2.11	0.50
1:A:453:TYR:N	1:A:493:GLN:O	2.39	0.50
1:A:540:ASN:HA	1:A:549:THR:HG23	1.93	0.50
1:A:854:LYS:CB	1:A:854:LYS:NZ	2.73	0.50
1:B:112:SER:O	1:B:132:GLU:HB3	2.11	0.50
1:B:544:ASN:ND2	1:B:579:PRO:HB3	2.19	0.50
1:B:740:MET:HA	1:B:743:CYS:O	2.11	0.50
1:C:719:THR:HG23	1:C:720:ILE:N	2.26	0.50
2:H:22:CYS:HB3	2:H:70:PHE:HB2	1.92	0.50
3:I:4:LEU:N	3:I:109:TYR:HE2	2.09	0.50
1:A:91:TYR:O	1:A:92:PHE:HB2	2.11	0.50
1:A:315:THR:OG1	1:A:316:SER:N	2.44	0.50
1:A:378:LYS:HE3	1:A:380:TYR:HA	1.92	0.50
1:A:398:ASP:HB2	1:A:512:VAL:HB	1.92	0.50
1:A:402:ILE:HG12	1:A:508:TYR:O	2.12	0.50
1:A:645:THR:OG1	1:A:648:GLY:N	2.29	0.50
1:A:1083:HIS:HB2	1:A:1088:HIS:CD2	2.45	0.50
1:B:402:ILE:HG12	1:B:508:TYR:O	2.12	0.50
1:B:421:TYR:HD1	1:B:457:ARG:HB3	1.75	0.50
1:C:97:LYS:HE2	1:C:186:PHE:CE1	2.46	0.50
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.94	0.50
1:A:453:TYR:CE2	1:A:455:LEU:HB2	2.46	0.50
1:A:719:THR:HG23	1:A:720:ILE:N	2.26	0.50
1:A:851:CYS:HA	1:A:854:LYS:HZ3	1.77	0.50
1:B:65:PHE:HD2	1:B:265:TYR:CZ	2.29	0.50
1:B:192:PHE:HB3	1:B:194:PHE:CE1	2.47	0.50
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.94	0.50
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.93	0.50
1:B:904:TYR:O	1:B:906:PHE:N	2.44	0.50
1:C:91:TYR:O	1:C:92:PHE:HB2	2.11	0.50
1:C:135:PHE:HA	1:C:160:TYR:HA	1.93	0.50
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.11	0.50
3:G:51:ILE:HG12	3:G:52:ASP:N	2.26	0.50
3:I:38:LYS:N	3:I:46:GLU:O	2.23	0.50
1:A:421:TYR:HD1	1:A:457:ARG:HB3	1.75	0.50
1:A:618:THR:OG1	1:A:619:GLU:N	2.43	0.50
1:A:656:VAL:HG12	1:A:658:ASN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:TYR:O	1:A:906:PHE:N	2.44	0.50
1:B:376:THR:O	1:B:434:ILE:HG23	2.12	0.50
1:C:315:THR:OG1	1:C:316:SER:N	2.44	0.50
2:D:47:ILE:HA	2:D:52:GLN:O	2.12	0.50
2:F:26:GLN:HG3	2:F:27:SER:H	1.76	0.50
2:F:42:SER:HB2	3:G:110:TRP:CE3	2.46	0.50
3:G:20:ILE:HD12	3:G:94:TYR:HD2	1.76	0.50
2:H:17:LYS:HG2	2:H:75:ASN:HA	1.93	0.50
1:A:64:TRP:CD1	1:A:65:PHE:N	2.80	0.50
1:B:117:LEU:HD21	1:B:119:ILE:HD11	1.93	0.50
1:B:656:VAL:HG12	1:B:658:ASN:H	1.76	0.50
1:C:377:PHE:HA	1:C:434:ILE:HG12	1.92	0.50
1:C:564:GLN:OE1	1:C:564:GLN:HA	2.06	0.50
1:C:587:ILE:HG22	1:C:588:THR:N	2.25	0.50
1:C:656:VAL:HG12	1:C:658:ASN:N	2.27	0.50
2:D:17:LYS:HG2	2:D:75:ASN:HA	1.94	0.50
2:H:3:VAL:HG22	2:H:96:ILE:HD13	1.92	0.50
1:A:877:LEU:O	1:A:881:THR:OG1	2.22	0.50
1:B:97:LYS:HE2	1:B:186:PHE:CE1	2.46	0.50
1:B:378:LYS:HE3	1:B:380:TYR:HA	1.92	0.50
1:C:64:TRP:CD1	1:C:65:PHE:N	2.80	0.50
1:C:192:PHE:HB3	1:C:194:PHE:CE1	2.47	0.50
2:D:12:VAL:HG12	2:D:13:SER:N	2.27	0.50
2:F:84:ILE:HG12	2:F:102:LYS:HA	1.93	0.50
3:G:33:TYR:HD2	3:G:105:TYR:HE1	1.60	0.50
1:A:388:ASN:HA	1:A:527:PRO:HD2	1.94	0.50
1:A:560:LEU:HB2	1:A:563:GLN:HB2	1.94	0.50
1:B:64:TRP:CD1	1:B:65:PHE:N	2.80	0.50
1:B:407:VAL:HG21	1:B:435:ALA:HB2	1.94	0.50
1:B:733:LYS:HE3	1:B:771:ALA:O	2.12	0.50
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.44	0.50
1:C:376:THR:O	1:C:434:ILE:HG23	2.12	0.50
3:E:11:VAL:HG22	3:E:117:THR:HB	1.94	0.50
2:H:12:VAL:HG12	2:H:13:SER:N	2.27	0.50
3:I:11:VAL:HG22	3:I:117:THR:HB	1.94	0.50
1:A:430:THR:HG22	1:A:515:PHE:CE2	2.47	0.50
1:A:560:LEU:HD12	1:A:562:PHE:CE1	2.47	0.50
1:B:377:PHE:HA	1:B:434:ILE:HG12	1.92	0.50
1:C:108:THR:HG23	1:C:234:ASN:O	2.12	0.50
1:C:441:LEU:HD22	1:C:509:ARG:HH21	1.77	0.50
1:C:618:THR:OG1	1:C:619:GLU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:GLN:H	3:G:112:GLN:HE22	1.59	0.50
2:H:5:THR:O	2:H:23:ARG:N	2.35	0.50
1:A:115:GLN:OE1	1:A:115:GLN:N	2.45	0.50
1:A:740:MET:HA	1:A:743:CYS:O	2.11	0.50
1:B:143:VAL:HG13	1:B:151:SER:HA	1.94	0.50
1:B:540:ASN:HA	1:B:549:THR:HG23	1.93	0.50
1:B:936:ASP:N	1:B:936:ASP:OD1	2.44	0.50
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.94	0.50
1:C:1142:GLN:O	1:C:1146:ASP:N	2.45	0.50
2:D:34:TRP:CE3	2:D:72:LEU:HB2	2.47	0.50
2:D:82:PHE:HD2	2:D:105:ILE:HD12	1.77	0.50
3:E:4:LEU:N	3:E:109:TYR:HE2	2.09	0.50
2:H:43:PRO:HD2	3:I:110:TRP:HZ3	1.75	0.50
1:A:143:VAL:HG13	1:A:151:SER:HA	1.94	0.49
1:A:656:VAL:HG12	1:A:658:ASN:H	1.76	0.49
1:A:709:ASN:OD1	1:A:709:ASN:N	2.43	0.49
1:B:656:VAL:HG12	1:B:658:ASN:N	2.27	0.49
1:C:54:LEU:HD23	1:C:272:PRO:HA	1.93	0.49
1:C:233:ILE:HG22	1:C:234:ASN:O	2.12	0.49
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.93	0.49
1:C:419:ALA:O	1:C:424:LYS:HD3	2.11	0.49
1:C:733:LYS:HE3	1:C:771:ALA:O	2.12	0.49
1:C:886:TRP:HB2	1:C:1034:LEU:O	2.11	0.49
1:A:225:PRO:HD2	1:B:562:PHE:CE2	2.47	0.49
1:A:233:ILE:HG22	1:A:234:ASN:O	2.12	0.49
1:A:349:SER:HB2	1:A:351:TYR:CE2	2.47	0.49
1:B:54:LEU:HD23	1:B:272:PRO:HA	1.93	0.49
1:B:115:GLN:OE1	1:B:115:GLN:N	2.45	0.49
1:B:233:ILE:HG22	1:B:234:ASN:O	2.12	0.49
1:B:891:GLY:HA2	1:C:1045:LYS:HZ1	1.76	0.49
1:A:170:TYR:OH	1:A:172:SER:OG	2.20	0.49
1:A:441:LEU:HD22	1:A:509:ARG:HH21	1.77	0.49
1:A:1088:HIS:CE1	1:A:1122:VAL:HG22	2.48	0.49
1:C:407:VAL:HG21	1:C:435:ALA:HB2	1.94	0.49
3:G:35:HIS:ND1	3:G:50:TYR:HB3	2.27	0.49
1:A:107:GLY:N	1:A:235:ILE:HG23	2.27	0.49
1:A:192:PHE:HB3	1:A:194:PHE:CE1	2.47	0.49
1:A:436:TRP:NE1	1:A:509:ARG:HB2	2.27	0.49
1:B:91:TYR:O	1:B:92:PHE:HB2	2.11	0.49
1:B:365:TYR:HE2	1:B:369:TYR:CE1	2.28	0.49
1:B:650:LEU:HD23	1:B:650:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:ASN:N	1:B:709:ASN:OD1	2.43	0.49
1:C:1021:SER:O	1:C:1021:SER:OG	2.30	0.49
2:H:34:TRP:CE3	2:H:72:LEU:HB2	2.47	0.49
3:I:71:THR:O	3:I:80:TYR:N	2.28	0.49
1:A:376:THR:O	1:A:434:ILE:HG23	2.12	0.49
1:B:107:GLY:N	1:B:235:ILE:HG23	2.27	0.49
1:B:349:SER:HB2	1:B:351:TYR:CE2	2.47	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.13	0.49
1:B:568:ASP:O	1:B:571:ASP:N	2.34	0.49
1:B:858:LEU:H	1:B:858:LEU:CD1	2.18	0.49
1:C:402:ILE:HG12	1:C:508:TYR:O	2.12	0.49
1:C:740:MET:HA	1:C:743:CYS:O	2.11	0.49
1:C:883:THR:OG1	1:C:884:SER:N	2.45	0.49
3:G:10:GLU:HG3	3:G:18:VAL:HG23	1.95	0.49
3:G:91:THR:HA	3:G:116:VAL:O	2.12	0.49
2:H:47:ILE:HA	2:H:52:GLN:O	2.12	0.49
1:A:97:LYS:HE2	1:A:186:PHE:CE1	2.46	0.49
1:A:562:PHE:CE2	1:C:225:PRO:CD	2.95	0.49
1:A:675:GLN:HG3	1:A:676:THR:O	2.11	0.49
1:A:733:LYS:HE3	1:A:771:ALA:O	2.12	0.49
1:A:759:PHE:CD2	1:A:1001:LEU:HD21	2.48	0.49
1:B:441:LEU:HD22	1:B:509:ARG:HH21	1.77	0.49
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.54	0.49
1:C:65:PHE:HD2	1:C:265:TYR:HH	1.58	0.49
1:C:324:GLU:O	1:C:540:ASN:HB3	2.12	0.49
1:C:430:THR:HG22	1:C:515:PHE:CE2	2.47	0.49
1:C:709:ASN:N	1:C:709:ASN:OD1	2.43	0.49
2:F:82:PHE:HB3	2:F:105:ILE:HD12	1.93	0.49
3:G:47:TRP:HZ2	3:G:50:TYR:CD2	2.29	0.49
3:G:73:ASP:HB2	3:G:80:TYR:CE2	2.46	0.49
1:A:128:ILE:HD12	1:A:170:TYR:CD2	2.43	0.49
1:A:407:VAL:HG21	1:A:435:ALA:HB2	1.94	0.49
1:A:883:THR:OG1	1:A:884:SER:N	2.45	0.49
1:A:1091:ARG:N	1:A:1119:ASN:O	2.31	0.49
1:A:1142:GLN:O	1:A:1146:ASP:N	2.45	0.49
1:B:127:VAL:HG21	5:B:1302:NAG:H5	1.95	0.49
1:B:159:VAL:HB	1:B:160:TYR:CD1	2.46	0.49
1:B:906:PHE:O	1:B:908:GLY:N	2.46	0.49
1:C:349:SER:HB2	1:C:351:TYR:CE2	2.47	0.49
1:C:759:PHE:CD2	1:C:1001:LEU:HD21	2.48	0.49
3:E:6:GLN:H	3:E:112:GLN:HE22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:67:ALA:HB3	3:I:84:SER:OG	2.13	0.49
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.93	0.49
1:B:315:THR:OG1	1:B:316:SER:N	2.44	0.49
1:C:107:GLY:N	1:C:235:ILE:HG23	2.27	0.49
1:C:419:ALA:O	1:C:424:LYS:HB2	2.13	0.49
1:C:436:TRP:NE1	1:C:509:ARG:HB2	2.27	0.49
1:C:995:ARG:O	1:C:999:GLY:N	2.36	0.49
1:A:108:THR:HG23	1:A:234:ASN:O	2.12	0.49
1:A:167:THR:HA	1:B:357:ARG:NH1	2.28	0.49
1:A:650:LEU:C	1:A:650:LEU:HD23	2.33	0.49
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.46	0.49
1:B:378:LYS:HD3	3:G:57:GLY:HA2	1.94	0.49
1:B:658:ASN:ND2	1:B:660:TYR:OH	2.43	0.49
1:B:1088:HIS:CE1	1:B:1122:VAL:HG22	2.47	0.49
3:G:19:LYS:HA	3:G:81:MET:O	2.12	0.49
2:H:82:PHE:HD2	2:H:105:ILE:HD12	1.77	0.49
1:B:92:PHE:CD1	1:B:93:ALA:N	2.81	0.49
1:B:759:PHE:CD2	1:B:1001:LEU:HD21	2.48	0.49
1:B:821:LEU:O	1:B:825:LYS:HG2	2.13	0.49
1:B:1142:GLN:O	1:B:1146:ASP:N	2.45	0.49
1:C:115:GLN:N	1:C:115:GLN:OE1	2.45	0.49
1:C:117:LEU:HD21	1:C:119:ILE:HD11	1.93	0.49
1:C:503:VAL:HG21	2:H:29:SER:HA	1.94	0.49
1:C:906:PHE:O	1:C:908:GLY:N	2.46	0.49
1:A:227:VAL:HG12	1:A:228:ASP:N	2.28	0.48
1:A:375:SER:O	2:D:91:ASN:HA	2.13	0.48
1:A:821:LEU:O	1:A:825:LYS:HG2	2.13	0.48
1:B:430:THR:HG22	1:B:515:PHE:CE2	2.47	0.48
1:B:675:GLN:HG3	1:B:676:THR:O	2.11	0.48
1:C:105:ILE:HD12	1:C:241:LEU:HD21	1.95	0.48
1:C:402:ILE:HD13	1:C:410:ILE:HD12	1.95	0.48
3:E:87:ARG:HG3	3:E:90:ASP:H	1.78	0.48
2:H:43:PRO:HB2	3:I:110:TRP:CH2	2.48	0.48
1:A:127:VAL:HG21	5:A:1302:NAG:H5	1.94	0.48
1:A:402:ILE:HD13	1:A:410:ILE:HD12	1.95	0.48
1:A:984:LEU:HB3	1:A:988:GLU:OE1	2.13	0.48
1:B:746:SER:OG	1:B:748:GLU:OE1	2.15	0.48
1:B:1091:ARG:N	1:B:1119:ASN:O	2.31	0.48
1:C:388:ASN:HA	1:C:527:PRO:HD2	1.94	0.48
1:C:431:GLY:HA3	1:C:513:LEU:O	2.13	0.48
1:C:856:ASN:HB2	1:C:858:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:ASP:OD1	1:C:936:ASP:N	2.44	0.48
2:F:65:GLY:HA2	2:F:70:PHE:HA	1.95	0.48
2:H:34:TRP:HD1	2:H:47:ILE:HB	1.79	0.48
2:H:37:GLN:HG3	2:H:41:GLN:O	2.13	0.48
3:I:13:LYS:HD2	3:I:120:SER:HA	1.96	0.48
1:A:419:ALA:O	1:A:424:LYS:HB2	2.13	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.13	0.48
1:B:436:TRP:NE1	1:B:509:ARG:HB2	2.27	0.48
1:B:984:LEU:HB3	1:B:988:GLU:OE1	2.13	0.48
1:C:92:PHE:CD1	1:C:93:ALA:N	2.81	0.48
1:C:341:VAL:HG11	1:C:397:ALA:HB1	1.96	0.48
1:C:878:LEU:HD12	1:C:878:LEU:O	2.13	0.48
1:C:916:LEU:O	1:C:919:ASN:N	2.45	0.48
1:C:996:LEU:HA	1:C:996:LEU:HD23	1.46	0.48
2:D:34:TRP:HD1	2:D:47:ILE:HB	1.79	0.48
3:E:67:ALA:HB3	3:E:84:SER:OG	2.13	0.48
2:F:32:LEU:HD13	2:F:70:PHE:CG	2.48	0.48
3:G:4:LEU:CD2	3:G:24:VAL:HG22	2.43	0.48
1:A:328:ARG:HB3	1:A:543:PHE:CD1	2.48	0.48
1:A:349:SER:HG	1:A:451:TYR:HD1	1.62	0.48
1:B:106:PHE:CD1	1:B:106:PHE:N	2.81	0.48
1:B:108:THR:HG22	1:B:236:THR:H	1.79	0.48
1:B:436:TRP:O	1:B:508:TYR:HA	2.13	0.48
1:B:612:TYR:CE1	1:B:651:ILE:HD12	2.49	0.48
1:C:187:LYS:HA	1:C:210:ILE:O	2.14	0.48
1:C:323:THR:HG21	1:C:537:LYS:HZ2	1.78	0.48
1:C:821:LEU:O	1:C:825:LYS:HG2	2.13	0.48
1:C:914:ASN:OD1	1:C:915:VAL:N	2.47	0.48
1:C:1018:ILE:O	1:C:1022:ALA:N	2.43	0.48
1:A:555:SER:OG	1:A:584:ILE:O	2.22	0.48
1:B:419:ALA:O	1:B:424:LYS:HB2	2.13	0.48
1:C:143:VAL:HG13	1:C:151:SER:HA	1.94	0.48
1:C:328:ARG:HB3	1:C:543:PHE:CD1	2.48	0.48
1:C:984:LEU:HB3	1:C:988:GLU:OE1	2.13	0.48
2:D:43:PRO:HB2	3:E:110:TRP:CH2	2.48	0.48
3:E:65:LYS:HE3	3:E:67:ALA:CA	2.43	0.48
3:G:109:TYR:C	3:G:110:TRP:HD1	2.16	0.48
1:A:108:THR:HG22	1:A:236:THR:H	1.79	0.48
1:A:378:LYS:NZ	3:E:56:GLY:O	2.37	0.48
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.96	0.48
1:A:773:GLU:O	1:A:775:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:HG23	1:B:234:ASN:O	2.12	0.48
1:B:328:ARG:HB3	1:B:543:PHE:CD1	2.48	0.48
1:B:349:SER:HG	1:B:451:TYR:HD1	1.62	0.48
1:B:878:LEU:HD12	1:B:878:LEU:O	2.13	0.48
1:B:883:THR:OG1	1:B:884:SER:N	2.45	0.48
1:B:1021:SER:O	1:B:1021:SER:OG	2.30	0.48
1:B:1115:ILE:HA	1:B:1119:ASN:HD22	1.78	0.48
1:C:349:SER:HG	1:C:451:TYR:HD1	1.62	0.48
1:C:422:ASN:HB3	1:C:454:ARG:HB3	1.96	0.48
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.46	0.48
3:E:13:LYS:HD2	3:E:120:SER:HA	1.96	0.48
2:H:34:TRP:O	2:H:46:LEU:N	2.38	0.48
1:B:150:LYS:O	1:B:151:SER:OG	2.22	0.48
1:B:555:SER:OG	1:B:584:ILE:O	2.22	0.48
1:B:726:ILE:HG22	1:B:948:LEU:HD13	1.95	0.48
1:B:773:GLU:O	1:B:775:ASP:N	2.47	0.48
1:C:159:VAL:HB	1:C:160:TYR:CD1	2.46	0.48
1:C:280:ASN:HD21	1:C:284:THR:HB	1.78	0.48
1:C:391:CYS:CB	1:C:525:CYS:HA	2.44	0.48
2:F:15:LYS:HA	2:F:76:SER:HA	1.95	0.48
1:A:280:ASN:HD21	1:A:284:THR:HB	1.78	0.48
1:A:436:TRP:O	1:A:508:TYR:HA	2.13	0.48
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.49	0.48
1:A:906:PHE:O	1:A:908:GLY:N	2.46	0.48
1:A:1050:MET:O	1:A:1051:SER:OG	2.21	0.48
1:B:105:ILE:HD12	1:B:241:LEU:HD21	1.95	0.48
1:B:661:GLU:O	1:B:695:TYR:OH	2.30	0.48
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.46	0.48
1:C:106:PHE:CD1	1:C:106:PHE:N	2.81	0.48
1:C:436:TRP:O	1:C:508:TYR:HA	2.13	0.48
1:C:497:PHE:CE1	1:C:507:PRO:HB3	2.49	0.48
1:C:767:LEU:HD23	1:C:770:ILE:HD12	1.95	0.48
1:C:773:GLU:O	1:C:775:ASP:N	2.47	0.48
3:I:6:GLN:H	3:I:112:GLN:HE22	1.61	0.48
3:I:87:ARG:HG3	3:I:90:ASP:H	1.78	0.48
1:A:92:PHE:CD1	1:A:93:ALA:N	2.81	0.48
1:A:117:LEU:HD21	1:A:119:ILE:HD11	1.93	0.48
1:A:341:VAL:HG11	1:A:397:ALA:HB1	1.96	0.48
1:A:936:ASP:N	1:A:936:ASP:OD1	2.44	0.48
1:B:719:THR:HG23	1:B:720:ILE:N	2.26	0.48
1:C:108:THR:HG22	1:C:236:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:PHE:HE2	1:C:509:ARG:HB3	1.79	0.48
1:C:650:LEU:HD23	1:C:650:LEU:C	2.33	0.48
1:C:726:ILE:HG22	1:C:948:LEU:HD13	1.95	0.48
1:C:959:LEU:O	1:C:960:ASN:C	2.52	0.48
1:C:1139:ASP:CG	1:C:1142:GLN:H	2.17	0.48
2:F:20:ILE:HD12	2:F:85:TYR:CD2	2.47	0.48
1:A:105:ILE:HD12	1:A:241:LEU:HD21	1.95	0.48
1:A:497:PHE:CE1	1:A:507:PRO:HB3	2.49	0.48
1:A:559:PHE:CZ	1:C:43:PHE:HB3	2.48	0.48
1:A:1139:ASP:CG	1:A:1142:GLN:H	2.17	0.48
1:B:227:VAL:HG12	1:B:228:ASP:N	2.28	0.48
1:B:347:PHE:HE2	1:B:509:ARG:HB3	1.79	0.48
1:B:901:GLN:NE2	1:B:905:ARG:HE	2.11	0.48
3:G:109:TYR:O	3:G:110:TRP:HD1	1.97	0.48
3:I:38:LYS:NZ	3:I:46:GLU:OE1	2.24	0.48
1:A:347:PHE:HE2	1:A:509:ARG:HB3	1.79	0.47
1:A:914:ASN:OD1	1:A:915:VAL:N	2.47	0.47
1:A:1049:LEU:HA	1:A:1049:LEU:HD23	1.39	0.47
1:A:1115:ILE:HA	1:A:1119:ASN:HD22	1.78	0.47
1:B:331:ASN:H	1:B:580:GLN:HA	1.79	0.47
1:B:388:ASN:HA	1:B:527:PRO:HD2	1.94	0.47
1:B:391:CYS:CB	1:B:525:CYS:HA	2.44	0.47
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.95	0.47
1:B:914:ASN:OD1	1:B:915:VAL:N	2.47	0.47
1:B:959:LEU:O	1:B:960:ASN:C	2.52	0.47
1:B:966:LEU:HA	1:B:966:LEU:HD23	1.58	0.47
1:C:227:VAL:HG12	1:C:228:ASP:N	2.28	0.47
1:C:1088:HIS:CE1	1:C:1122:VAL:HG22	2.48	0.47
1:C:1100:THR:HG1	1:C:1101:HIS:CE1	2.29	0.47
1:C:1115:ILE:HA	1:C:1119:ASN:HD22	1.78	0.47
1:A:43:PHE:HB2	1:B:563:GLN:CG	2.44	0.47
1:A:129:LYS:HG2	1:A:169:GLU:OE1	2.14	0.47
1:A:187:LYS:HA	1:A:210:ILE:O	2.14	0.47
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.48	0.47
1:A:878:LEU:HD12	1:A:878:LEU:O	2.13	0.47
1:A:894:LEU:HA	1:A:894:LEU:HD23	1.52	0.47
1:B:31:SER:HG	1:B:60:SER:N	2.12	0.47
1:B:723:THR:OG1	1:B:724:THR:N	2.41	0.47
1:B:791:THR:HB	1:B:792:PRO:HD2	1.96	0.47
2:D:60:ARG:HB2	2:D:75:ASN:O	2.14	0.47
3:G:47:TRP:CZ2	3:G:50:TYR:HD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:CG2	1:A:591:SER:CB	2.91	0.47
1:A:560:LEU:CB	1:A:563:GLN:HB2	2.44	0.47
1:A:946:GLY:O	1:A:950:ASP:N	2.47	0.47
1:A:1018:ILE:O	1:A:1022:ALA:N	2.43	0.47
1:B:240:THR:O	1:B:241:LEU:HD23	2.15	0.47
1:C:66:HIS:N	1:C:80:ASP:OD2	2.43	0.47
1:C:108:THR:OG1	1:C:109:THR:N	2.42	0.47
1:C:331:ASN:H	1:C:580:GLN:HA	1.79	0.47
1:C:946:GLY:O	1:C:950:ASP:N	2.47	0.47
3:G:3:GLN:HB2	3:G:25:SER:OG	2.14	0.47
3:G:47:TRP:HZ2	3:G:50:TYR:HD2	1.61	0.47
1:A:107:GLY:HA2	1:A:235:ILE:HG12	1.96	0.47
1:A:117:LEU:HD12	1:A:118:LEU:H	1.80	0.47
1:A:159:VAL:HB	1:A:160:TYR:CD1	2.46	0.47
1:A:901:GLN:NE2	1:A:905:ARG:HE	2.11	0.47
1:B:66:HIS:N	1:B:80:ASP:OD2	2.43	0.47
1:B:117:LEU:HD12	1:B:118:LEU:H	1.80	0.47
1:B:129:LYS:HG2	1:B:169:GLU:OE1	2.14	0.47
1:B:167:THR:HA	1:C:357:ARG:NH1	2.30	0.47
1:B:341:VAL:HG11	1:B:397:ALA:HB1	1.96	0.47
1:B:402:ILE:HD13	1:B:410:ILE:HD12	1.94	0.47
1:B:422:ASN:HB3	1:B:454:ARG:HB3	1.96	0.47
1:B:426:PRO:HG3	1:B:463:PRO:HB3	1.96	0.47
1:C:568:ASP:O	1:C:571:ASP:N	2.34	0.47
1:C:853:GLN:O	1:C:858:LEU:HB2	2.15	0.47
1:A:429:PHE:CZ	1:A:512:VAL:HG13	2.50	0.47
1:A:994:ASP:O	1:A:998:THR:N	2.42	0.47
1:B:187:LYS:HA	1:B:210:ILE:O	2.14	0.47
1:B:497:PHE:CE1	1:B:507:PRO:HB3	2.49	0.47
1:C:117:LEU:HD12	1:C:118:LEU:H	1.80	0.47
1:C:473:TYR:N	1:C:489:TYR:O	2.46	0.47
1:C:612:TYR:CE1	1:C:651:ILE:HD12	2.49	0.47
3:E:10:GLU:O	3:E:116:VAL:HG13	2.15	0.47
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.54	0.47
2:H:89:GLN:HB3	2:H:96:ILE:H	1.80	0.47
1:A:391:CYS:CB	1:A:525:CYS:HA	2.44	0.47
1:A:439:ASN:HB2	1:A:507:PRO:HD2	1.97	0.47
1:A:873:TYR:O	1:A:875:SER:N	2.48	0.47
1:B:338:PHE:HB3	1:B:342:PHE:CE2	2.50	0.47
1:C:127:VAL:HG21	5:C:1302:NAG:H5	1.94	0.47
1:C:149:ASN:CG	1:C:152:TRP:HA	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:901:GLN:NE2	1:C:905:ARG:HE	2.11	0.47
2:D:37:GLN:HG3	2:D:41:GLN:O	2.13	0.47
3:E:48:ILE:HG21	3:E:81:MET:SD	2.55	0.47
2:F:32:LEU:HD21	2:F:87:CYS:CB	2.43	0.47
3:I:48:ILE:HG21	3:I:81:MET:SD	2.55	0.47
1:A:59:PHE:N	1:A:59:PHE:CD1	2.82	0.47
1:A:328:ARG:HG3	1:A:579:PRO:CG	2.45	0.47
1:A:375:SER:OG	2:D:91:ASN:ND2	2.48	0.47
1:A:425:LEU:HD11	1:A:512:VAL:HG21	1.97	0.47
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.97	0.47
1:A:767:LEU:HD23	1:A:770:ILE:HD12	1.95	0.47
1:B:191:GLU:C	1:B:192:PHE:CD1	2.88	0.47
1:B:600:PRO:HG3	1:B:674:TYR:CD1	2.50	0.47
1:B:914:ASN:HA	1:C:1089:PHE:CE2	2.50	0.47
1:B:1018:ILE:O	1:B:1022:ALA:N	2.43	0.47
1:C:107:GLY:HA2	1:C:235:ILE:HG12	1.96	0.47
1:C:196:ASN:ND2	1:C:235:ILE:HD12	2.27	0.47
1:C:350:VAL:HA	1:C:400:PHE:HB2	1.97	0.47
1:C:429:PHE:HD1	1:C:464:PHE:HZ	1.61	0.47
1:C:429:PHE:CZ	1:C:512:VAL:HG13	2.50	0.47
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.95	0.47
1:C:617:CYS:N	1:C:644:GLN:OE1	2.48	0.47
1:C:712:ILE:HB	1:C:1077:THR:HG21	1.97	0.47
1:C:791:THR:HB	1:C:792:PRO:HD2	1.97	0.47
1:C:873:TYR:O	1:C:875:SER:N	2.48	0.47
1:C:1083:HIS:CD2	1:C:1084:ASP:OD1	2.68	0.47
3:E:18:VAL:O	3:E:83:LEU:N	2.34	0.47
2:F:48:LYS:HG3	3:G:106:VAL:CG1	2.43	0.47
2:F:94:PRO:HB3	3:G:47:TRP:CZ3	2.50	0.47
1:A:63:THR:HG22	1:A:65:PHE:CE1	2.50	0.47
1:A:378:LYS:O	1:A:433:VAL:N	2.34	0.47
1:A:429:PHE:HD1	1:A:464:PHE:HZ	1.61	0.47
1:A:726:ILE:HG22	1:A:948:LEU:HD13	1.95	0.47
1:B:425:LEU:HD11	1:B:512:VAL:HG21	1.97	0.47
1:B:455:LEU:HG	1:B:456:PHE:CE2	2.50	0.47
1:C:59:PHE:N	1:C:59:PHE:CD1	2.82	0.47
1:C:959:LEU:HA	1:C:959:LEU:HD23	1.58	0.47
3:E:107:MET:HB2	3:E:110:TRP:HE1	1.80	0.47
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.96	0.47
1:B:231:ILE:HG13	1:B:232:GLY:N	2.30	0.47
1:B:393:THR:OG1	1:B:394:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ASN:HB2	1:C:507:PRO:HD2	1.97	0.47
2:D:22:CYS:HB2	2:D:34:TRP:CH2	2.50	0.47
2:D:61:PHE:HZ	2:D:81:ASP:OD1	1.98	0.47
2:H:22:CYS:HB2	2:H:34:TRP:CH2	2.50	0.47
1:A:43:PHE:HA	1:B:563:GLN:HE21	1.73	0.47
1:A:140:PHE:CZ	1:A:158:ARG:HD2	2.50	0.47
1:A:617:CYS:N	1:A:644:GLN:OE1	2.48	0.47
1:A:904:TYR:C	1:A:906:PHE:N	2.68	0.47
1:A:1045:LYS:HZ1	1:C:891:GLY:HA2	1.79	0.47
1:A:1083:HIS:CD2	1:A:1084:ASP:OD1	2.68	0.47
1:B:133:PHE:CD2	1:B:135:PHE:HE1	2.33	0.47
1:B:429:PHE:HD1	1:B:464:PHE:HZ	1.62	0.47
1:C:240:THR:O	1:C:241:LEU:HD23	2.15	0.47
1:C:426:PRO:HG3	1:C:463:PRO:HB3	1.96	0.47
1:C:600:PRO:HG3	1:C:674:TYR:CD1	2.50	0.47
1:C:822:LEU:HA	1:C:822:LEU:HD23	1.68	0.47
1:C:1012:LEU:HD23	1:C:1012:LEU:HA	1.60	0.47
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.54	0.47
1:A:231:ILE:HG13	1:A:232:GLY:N	2.30	0.46
1:A:323:THR:HG21	1:A:537:LYS:CE	2.44	0.46
1:A:455:LEU:HG	1:A:456:PHE:CE2	2.50	0.46
1:A:566:GLY:HA2	1:C:43:PHE:HB3	1.97	0.46
1:A:661:GLU:O	1:A:695:TYR:OH	2.30	0.46
1:A:676:THR:HG23	1:A:690:GLN:HG2	1.97	0.46
1:A:723:THR:OG1	1:A:724:THR:N	2.41	0.46
1:A:855:PHE:CD1	1:B:589:PRO:HG3	2.50	0.46
1:B:280:ASN:HD21	1:B:284:THR:HB	1.78	0.46
1:C:191:GLU:C	1:C:192:PHE:CD1	2.88	0.46
1:C:338:PHE:HB3	1:C:342:PHE:CE2	2.50	0.46
2:D:48:LYS:N	2:D:52:GLN:O	2.40	0.46
1:A:191:GLU:C	1:A:192:PHE:CD1	2.88	0.46
1:A:240:THR:O	1:A:241:LEU:HD23	2.15	0.46
1:A:331:ASN:H	1:A:580:GLN:HA	1.79	0.46
1:A:453:TYR:HB3	1:A:495:TYR:CE2	2.51	0.46
1:B:328:ARG:HG3	1:B:579:PRO:CG	2.45	0.46
1:B:429:PHE:CZ	1:B:512:VAL:HG13	2.50	0.46
1:B:1027:THR:O	1:B:1028:LYS:C	2.53	0.46
1:B:1083:HIS:CD2	1:B:1084:ASP:OD1	2.68	0.46
1:C:425:LEU:HD11	1:C:512:VAL:HG21	1.97	0.46
1:C:451:TYR:O	1:C:494:SER:OG	2.33	0.46
1:C:661:GLU:O	1:C:695:TYR:OH	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:CG	1:A:152:TRP:HA	2.35	0.46
1:A:422:ASN:HB3	1:A:454:ARG:HB3	1.96	0.46
1:A:556:ASN:OD1	1:A:556:ASN:N	2.38	0.46
1:B:63:THR:HG22	1:B:65:PHE:CE1	2.50	0.46
1:B:366:SER:HA	1:B:369:TYR:CD2	2.51	0.46
1:B:873:TYR:O	1:B:875:SER:N	2.48	0.46
1:C:366:SER:HA	1:C:369:TYR:CD2	2.51	0.46
1:C:455:LEU:HG	1:C:456:PHE:CE2	2.50	0.46
2:D:5:THR:O	2:D:23:ARG:N	2.35	0.46
2:H:2:ILE:O	2:H:96:ILE:HD12	2.15	0.46
2:H:61:PHE:HZ	2:H:81:ASP:OD1	1.98	0.46
1:A:106:PHE:CD1	1:A:106:PHE:N	2.81	0.46
1:A:133:PHE:CD2	1:A:135:PHE:HE1	2.33	0.46
1:A:225:PRO:CD	1:B:562:PHE:CD2	2.95	0.46
1:A:802:PHE:O	1:A:805:ILE:N	2.49	0.46
1:A:961:THR:O	1:A:965:GLN:HG2	2.16	0.46
1:B:1139:ASP:CG	1:B:1142:GLN:H	2.17	0.46
1:C:327:VAL:HB	1:C:531:THR:HG23	1.95	0.46
2:D:46:LEU:HD22	2:D:61:PHE:CD2	2.50	0.46
3:G:86:LEU:HB3	3:G:118:VAL:HG21	1.97	0.46
2:H:10:GLN:O	2:H:103:LEU:HD12	2.15	0.46
3:I:107:MET:HB2	3:I:110:TRP:HE1	1.80	0.46
1:A:111:ASP:C	1:A:113:LYS:H	2.18	0.46
1:A:299:THR:O	1:A:301:CYS:N	2.49	0.46
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.97	0.46
1:A:377:PHE:CB	2:D:93:TRP:CD1	2.98	0.46
1:A:385:THR:HG21	3:E:65:LYS:HE2	1.95	0.46
1:A:600:PRO:HG3	1:A:674:TYR:CD1	2.50	0.46
1:A:891:GLY:HA2	1:B:1045:LYS:HZ1	1.81	0.46
1:A:913:GLN:O	1:A:916:LEU:N	2.49	0.46
1:A:1043:CYS:CB	1:A:1048:HIS:CD2	2.92	0.46
1:B:43:PHE:CD2	1:C:559:PHE:CE1	3.03	0.46
1:B:215:ASP:OD1	1:B:216:LEU:N	2.42	0.46
1:B:299:THR:O	1:B:301:CYS:N	2.49	0.46
1:B:439:ASN:HB2	1:B:507:PRO:HD2	1.97	0.46
1:B:451:TYR:O	1:B:494:SER:OG	2.33	0.46
1:B:911:VAL:HG12	1:B:912:THR:O	2.16	0.46
1:B:916:LEU:O	1:B:919:ASN:N	2.45	0.46
1:B:946:GLY:O	1:B:950:ASP:N	2.47	0.46
1:B:961:THR:O	1:B:965:GLN:HG2	2.16	0.46
1:C:129:LYS:HG2	1:C:169:GLU:OE1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:GLU:O	1:C:192:PHE:HD1	1.98	0.46
1:C:371:SER:HB3	5:C:1305:NAG:H3	1.97	0.46
2:F:28:ILE:HD13	2:F:70:PHE:CZ	2.50	0.46
1:A:806:LEU:HA	1:A:806:LEU:HD23	1.54	0.46
1:A:911:VAL:HG12	1:A:912:THR:O	2.16	0.46
1:B:111:ASP:C	1:B:113:LYS:H	2.18	0.46
1:B:676:THR:HG23	1:B:690:GLN:HG2	1.97	0.46
1:C:63:THR:HG22	1:C:65:PHE:CE1	2.50	0.46
1:C:231:ILE:HG13	1:C:232:GLY:N	2.30	0.46
1:C:328:ARG:HG3	1:C:579:PRO:CG	2.45	0.46
1:C:363:ALA:HB3	1:C:388:ASN:HA	1.98	0.46
1:C:559:PHE:HE2	1:C:565:PHE:O	1.87	0.46
3:E:41:PRO:HD3	3:E:92:ALA:HA	1.97	0.46
2:F:12:VAL:HG12	2:F:13:SER:H	1.81	0.46
2:F:35:TYR:CE1	2:F:88:GLN:HG3	2.50	0.46
1:A:115:GLN:HB2	1:A:233:ILE:HG12	1.98	0.46
1:A:363:ALA:HB3	1:A:388:ASN:HA	1.98	0.46
1:A:366:SER:HA	1:A:369:TYR:CD2	2.51	0.46
1:A:453:TYR:HE2	1:A:455:LEU:HD13	1.81	0.46
1:A:791:THR:HB	1:A:792:PRO:HD2	1.96	0.46
1:B:44:ARG:HB3	1:B:47:VAL:CG1	2.46	0.46
1:B:161:SER:OG	1:B:162:SER:N	2.48	0.46
1:B:913:GLN:O	1:B:916:LEU:N	2.49	0.46
1:C:136:CYS:N	1:C:139:PRO:HG3	2.31	0.46
1:C:161:SER:OG	1:C:162:SER:N	2.48	0.46
1:C:299:THR:O	1:C:301:CYS:N	2.49	0.46
1:C:374:PHE:O	2:H:93:TRP:HB2	2.15	0.46
3:E:10:GLU:HB2	3:E:116:VAL:HG22	1.98	0.46
3:E:33:TYR:CE1	3:E:101:TYR:CD1	3.02	0.46
2:F:13:SER:OG	2:F:106:LEU:HB2	2.16	0.46
2:F:31:ASN:OD1	2:F:32:LEU:N	2.49	0.46
2:H:46:LEU:HD22	2:H:61:PHE:CD2	2.50	0.46
2:H:60:ARG:HB2	2:H:75:ASN:O	2.14	0.46
1:A:136:CYS:O	1:A:139:PRO:HD3	2.16	0.46
1:A:215:ASP:OD1	1:A:216:LEU:N	2.42	0.46
1:A:429:PHE:HD1	1:A:464:PHE:CZ	2.33	0.46
1:B:41:LYS:HD3	1:C:562:PHE:O	2.16	0.46
1:B:371:SER:HB3	5:B:1305:NAG:H3	1.97	0.46
1:B:453:TYR:HB3	1:B:495:TYR:CE2	2.50	0.46
1:B:1049:LEU:HA	1:B:1049:LEU:HD23	1.39	0.46
1:C:38:TYR:CE2	1:C:285:ILE:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PHE:CZ	1:C:158:ARG:HD2	2.51	0.46
1:C:215:ASP:OD1	1:C:216:LEU:N	2.42	0.46
1:C:453:TYR:HE2	1:C:455:LEU:HD13	1.81	0.46
1:C:759:PHE:O	1:C:760:CYS:C	2.54	0.46
3:G:20:ILE:HD11	3:G:116:VAL:CG2	2.46	0.46
3:I:10:GLU:O	3:I:116:VAL:HG13	2.15	0.46
1:A:338:PHE:HB3	1:A:342:PHE:CE2	2.50	0.46
1:A:371:SER:HB3	5:A:1305:NAG:H3	1.97	0.46
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.51	0.46
1:B:140:PHE:CZ	1:B:158:ARG:HD2	2.51	0.46
1:B:149:ASN:CG	1:B:152:TRP:HA	2.35	0.46
1:B:432:CYS:HB2	1:B:513:LEU:H	1.81	0.46
1:B:671:CYS:O	1:B:695:TYR:CE1	2.69	0.46
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.81	0.46
1:C:335:LEU:C	1:C:361:CYS:HB2	2.37	0.46
1:C:336:CYS:SG	1:C:362:VAL:N	2.89	0.46
1:C:671:CYS:O	1:C:695:TYR:CE1	2.69	0.46
1:C:911:VAL:HG12	1:C:912:THR:O	2.16	0.46
1:C:961:THR:O	1:C:965:GLN:HG2	2.16	0.46
1:A:192:PHE:HB3	1:A:194:PHE:HE1	1.81	0.46
1:A:323:THR:OG1	1:A:537:LYS:CE	2.64	0.46
1:B:136:CYS:O	1:B:139:PRO:HD3	2.16	0.46
1:B:191:GLU:O	1:B:192:PHE:HD1	1.98	0.46
1:B:429:PHE:HD1	1:B:464:PHE:CZ	2.34	0.46
1:B:555:SER:OG	1:B:584:ILE:HG22	2.16	0.46
1:B:712:ILE:HB	1:B:1077:THR:HG21	1.97	0.46
1:C:111:ASP:C	1:C:113:LYS:H	2.18	0.46
1:C:115:GLN:HB2	1:C:233:ILE:HG12	1.98	0.46
1:C:136:CYS:O	1:C:139:PRO:HD3	2.16	0.46
1:C:802:PHE:O	1:C:805:ILE:N	2.49	0.46
1:C:913:GLN:O	1:C:916:LEU:N	2.49	0.46
2:F:45:LEU:HD23	3:G:108:ASP:OD1	2.15	0.46
2:F:91:ASN:N	2:F:95:TYR:CE1	2.84	0.46
3:I:37:VAL:HB	3:I:95:TYR:HB2	1.98	0.46
1:A:196:ASN:ND2	1:A:235:ILE:HD12	2.27	0.45
1:A:645:THR:OG1	1:A:648:GLY:O	2.15	0.45
1:A:856:ASN:CB	1:A:858:LEU:HD13	2.46	0.45
1:B:136:CYS:N	1:B:139:PRO:HG3	2.31	0.45
1:B:398:ASP:N	1:B:512:VAL:O	2.49	0.45
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.81	0.45
1:B:557:LYS:O	1:B:584:ILE:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:HD22	1:B:560:LEU:HA	1.82	0.45
1:B:770:ILE:O	1:B:773:GLU:N	2.49	0.45
1:C:707:TYR:C	1:C:707:TYR:CD1	2.90	0.45
2:D:89:GLN:HB3	2:D:96:ILE:H	1.80	0.45
2:F:33:HIS:ND1	3:G:106:VAL:HG12	2.31	0.45
3:G:4:LEU:O	3:G:111:GLY:HA2	2.16	0.45
3:G:27:TYR:CD1	3:G:32:TYR:HD2	2.34	0.45
3:G:97:ALA:HB1	3:G:107:MET:CB	2.44	0.45
1:B:242:LEU:HA	1:B:242:LEU:HD23	1.73	0.45
1:B:336:CYS:SG	1:B:362:VAL:N	2.89	0.45
1:B:617:CYS:N	1:B:644:GLN:OE1	2.48	0.45
1:B:1064:HIS:O	1:B:1066:THR:HG23	2.17	0.45
1:C:152:TRP:HB3	1:C:153:MET:H	1.57	0.45
1:C:313:TYR:CD1	1:C:313:TYR:N	2.85	0.45
1:C:408:ARG:CD	3:I:102:ASP:OD2	2.45	0.45
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.60	0.45
1:C:1043:CYS:CB	1:C:1048:HIS:CD2	2.92	0.45
2:D:69:ASP:OD1	2:D:70:PHE:N	2.50	0.45
2:F:12:VAL:HG12	2:F:13:SER:N	2.32	0.45
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.81	0.45
1:A:191:GLU:O	1:A:192:PHE:HD1	1.98	0.45
1:A:313:TYR:N	1:A:313:TYR:CD1	2.85	0.45
1:A:555:SER:OG	1:A:584:ILE:HG22	2.16	0.45
1:A:877:LEU:HA	1:A:877:LEU:HD23	1.79	0.45
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.58	0.45
1:A:1027:THR:O	1:A:1028:LYS:C	2.53	0.45
1:B:350:VAL:HA	1:B:400:PHE:HB2	1.97	0.45
1:B:363:ALA:HB3	1:B:388:ASN:HA	1.98	0.45
1:B:557:LYS:O	1:B:584:ILE:HG13	2.16	0.45
1:B:802:PHE:O	1:B:805:ILE:N	2.49	0.45
1:B:904:TYR:C	1:B:906:PHE:N	2.68	0.45
1:C:44:ARG:HB3	1:C:47:VAL:CG1	2.46	0.45
1:C:133:PHE:CD2	1:C:135:PHE:HE1	2.33	0.45
1:C:429:PHE:HD1	1:C:464:PHE:CZ	2.33	0.45
1:C:676:THR:HG23	1:C:690:GLN:HG2	1.97	0.45
2:D:48:LYS:HD2	3:E:106:VAL:HG11	1.97	0.45
3:G:4:LEU:N	3:G:109:TYR:CE2	2.84	0.45
3:G:86:LEU:HB3	3:G:118:VAL:CG2	2.46	0.45
3:I:4:LEU:HD21	3:I:24:VAL:HG22	1.98	0.45
3:I:41:PRO:HD3	3:I:92:ALA:HA	1.97	0.45
3:I:65:LYS:HE3	3:I:67:ALA:CA	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:HG11	1:A:524:VAL:HG21	1.98	0.45
1:A:418:ILE:HG23	1:A:423:TYR:HB3	1.98	0.45
1:A:770:ILE:O	1:A:773:GLU:N	2.49	0.45
1:A:959:LEU:O	1:A:960:ASN:C	2.52	0.45
1:B:805:ILE:HB	1:B:1054:GLN:HE22	1.82	0.45
1:C:904:TYR:C	1:C:906:PHE:N	2.68	0.45
1:C:1064:HIS:O	1:C:1066:THR:HG23	2.17	0.45
3:E:50:TYR:O	3:E:58:THR:HA	2.17	0.45
2:F:32:LEU:HB3	2:F:50:ALA:HB2	1.99	0.45
1:A:38:TYR:CE2	1:A:285:ILE:HG13	2.51	0.45
1:A:38:TYR:CG	1:B:562:PHE:HZ	2.35	0.45
1:A:136:CYS:N	1:A:139:PRO:HG3	2.31	0.45
1:A:378:LYS:HE2	3:E:57:GLY:CA	2.45	0.45
1:A:485:GLY:N	1:A:488:CYS:HB2	2.32	0.45
1:B:485:GLY:N	1:B:488:CYS:HB2	2.32	0.45
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.60	0.45
1:C:143:VAL:HG13	1:C:151:SER:CB	2.47	0.45
1:C:432:CYS:HB2	1:C:513:LEU:H	1.81	0.45
1:C:457:ARG:NH2	1:C:461:LEU:HD23	2.32	0.45
1:C:555:SER:OG	1:C:584:ILE:HG22	2.16	0.45
1:C:587:ILE:CG2	1:C:588:THR:H	2.29	0.45
1:C:1097:SER:OG	1:C:1098:ASN:N	2.50	0.45
3:E:37:VAL:HB	3:E:95:TYR:HB2	1.98	0.45
2:H:48:LYS:HD2	3:I:106:VAL:HG11	1.97	0.45
2:H:69:ASP:OD1	2:H:70:PHE:N	2.50	0.45
1:A:322:PRO:HA	1:A:538:CYS:SG	2.56	0.45
1:A:473:TYR:HB2	1:A:491:PRO:HB3	1.98	0.45
1:A:671:CYS:O	1:A:695:TYR:CE1	2.69	0.45
1:A:1021:SER:O	1:A:1021:SER:OG	2.30	0.45
1:B:335:LEU:C	1:B:361:CYS:HB2	2.37	0.45
1:B:353:TRP:H	1:B:466:ARG:HE	1.65	0.45
1:B:707:TYR:CD1	1:B:707:TYR:C	2.90	0.45
1:B:739:THR:O	1:B:742:ILE:N	2.49	0.45
1:B:894:LEU:HD13	1:C:715:PRO:HD3	1.99	0.45
1:C:453:TYR:HB3	1:C:495:TYR:CE2	2.51	0.45
1:C:739:THR:O	1:C:742:ILE:N	2.49	0.45
2:D:10:GLN:O	2:D:103:LEU:HD12	2.15	0.45
3:G:100:GLU:CB	3:G:104:TYR:O	2.60	0.45
2:H:12:VAL:HG12	2:H:13:SER:H	1.81	0.45
1:A:44:ARG:HB3	1:A:47:VAL:CG1	2.46	0.45
1:A:55:PHE:CD2	1:A:275:PHE:CD2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:HB3	1:A:152:TRP:HB2	1.99	0.45
1:A:323:THR:HG22	1:A:324:GLU:N	2.32	0.45
1:A:384:PRO:HG3	3:E:60:ASP:HB3	1.99	0.45
1:A:436:TRP:CE2	1:A:509:ARG:HB2	2.52	0.45
1:A:1064:HIS:O	1:A:1066:THR:HG23	2.17	0.45
1:B:59:PHE:N	1:B:59:PHE:CD1	2.82	0.45
1:B:877:LEU:O	1:B:881:THR:OG1	2.22	0.45
1:B:1088:HIS:C	1:B:1089:PHE:HD1	2.20	0.45
1:C:398:ASP:N	1:C:512:VAL:O	2.49	0.45
3:G:33:TYR:CE1	3:G:101:TYR:CE1	3.05	0.45
2:H:32:LEU:HD13	2:H:70:PHE:CB	2.47	0.45
3:I:50:TYR:O	3:I:58:THR:HA	2.17	0.45
1:A:133:PHE:CE2	1:A:135:PHE:HE1	2.35	0.45
1:A:336:CYS:SG	1:A:362:VAL:N	2.89	0.45
1:A:473:TYR:N	1:A:489:TYR:O	2.46	0.45
1:A:587:ILE:CG2	1:A:588:THR:H	2.29	0.45
1:A:715:PRO:HD3	1:C:894:LEU:HD13	1.99	0.45
1:A:739:THR:O	1:A:742:ILE:N	2.49	0.45
1:A:746:SER:OG	1:A:748:GLU:OE1	2.15	0.45
1:B:418:ILE:HG23	1:B:423:TYR:HB3	1.98	0.45
1:B:894:LEU:HA	1:B:894:LEU:HD23	1.52	0.45
1:C:322:PRO:HA	1:C:538:CYS:SG	2.56	0.45
1:C:353:TRP:H	1:C:466:ARG:HE	1.65	0.45
1:C:560:LEU:HD12	1:C:562:PHE:CE1	2.51	0.45
1:C:916:LEU:HA	1:C:916:LEU:HD12	1.54	0.45
3:E:2:VAL:N	3:E:27:TYR:HD2	2.15	0.45
3:I:2:VAL:N	3:I:27:TYR:HD2	2.15	0.45
3:I:10:GLU:HB2	3:I:116:VAL:HG22	1.98	0.45
1:A:916:LEU:O	1:A:919:ASN:N	2.45	0.45
1:B:200:TYR:CD1	1:B:230:PRO:HA	2.52	0.45
1:B:225:PRO:HD2	1:C:562:PHE:CE2	2.52	0.45
1:B:457:ARG:NH2	1:B:461:LEU:HD23	2.32	0.45
1:B:759:PHE:O	1:B:760:CYS:C	2.54	0.45
1:C:133:PHE:CE2	1:C:135:PHE:HE1	2.35	0.45
1:C:395:VAL:HG11	1:C:524:VAL:HG21	1.98	0.45
1:C:770:ILE:O	1:C:773:GLU:N	2.49	0.45
1:C:934:ILE:HD12	1:C:934:ILE:HG23	1.67	0.45
1:A:133:PHE:HD2	1:A:160:TYR:HB2	1.82	0.45
1:A:335:LEU:C	1:A:361:CYS:HB2	2.37	0.45
1:A:759:PHE:O	1:A:760:CYS:C	2.54	0.45
1:A:966:LEU:HA	1:A:966:LEU:HD23	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:SER:O	1:A:1003:SER:OG	2.35	0.45
1:B:323:THR:HG21	1:B:537:LYS:HZ2	1.78	0.45
1:B:395:VAL:HG11	1:B:524:VAL:HG21	1.98	0.45
1:B:587:ILE:CG2	1:B:588:THR:H	2.29	0.45
1:C:354:ASN:HB2	1:C:399:SER:HB3	1.99	0.45
1:C:1003:SER:O	1:C:1003:SER:OG	2.35	0.45
2:D:2:ILE:O	2:D:96:ILE:HD12	2.15	0.45
2:D:32:LEU:HD13	2:D:70:PHE:CB	2.47	0.45
2:D:43:PRO:HG2	3:E:45:LEU:HD21	1.99	0.45
3:E:4:LEU:HD21	3:E:24:VAL:HG22	1.98	0.45
1:A:168:PHE:CG	1:A:169:GLU:N	2.86	0.44
1:A:200:TYR:CD1	1:A:230:PRO:HA	2.52	0.44
1:A:451:TYR:O	1:A:494:SER:OG	2.33	0.44
1:B:115:GLN:HB2	1:B:233:ILE:HG12	1.98	0.44
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.53	0.44
1:C:418:ILE:HG23	1:C:423:TYR:HB3	1.99	0.44
1:C:436:TRP:CE2	1:C:509:ARG:HB2	2.52	0.44
1:C:892:ALA:O	1:C:894:LEU:HG	2.18	0.44
1:C:1088:HIS:C	1:C:1089:PHE:HD1	2.20	0.44
1:A:318:PHE:O	1:A:318:PHE:CG	2.70	0.44
1:A:535:LYS:NZ	1:A:554:GLU:OE2	2.37	0.44
1:B:55:PHE:CD2	1:B:275:PHE:CD2	3.05	0.44
1:B:108:THR:OG1	1:B:109:THR:N	2.42	0.44
1:B:192:PHE:HB3	1:B:194:PHE:HE1	1.81	0.44
1:C:144:TYR:HB3	1:C:152:TRP:HB2	1.99	0.44
1:C:410:ILE:HG13	1:C:418:ILE:HG21	2.00	0.44
1:C:439:ASN:HA	1:C:443:SER:OG	2.18	0.44
1:C:809:PRO:O	1:C:814:LYS:HE2	2.18	0.44
1:C:877:LEU:HA	1:C:877:LEU:HD23	1.79	0.44
3:G:31:ASN:O	3:G:101:TYR:HB2	2.17	0.44
3:G:39:GLN:HG3	3:G:44:SER:O	2.18	0.44
1:A:353:TRP:H	1:A:466:ARG:HE	1.65	0.44
1:A:386:LYS:O	1:A:390:LEU:HB3	2.17	0.44
1:A:439:ASN:HA	1:A:443:SER:OG	2.18	0.44
1:A:581:THR:HG23	1:A:583:GLU:OE2	2.18	0.44
1:A:1088:HIS:C	1:A:1089:PHE:HD1	2.20	0.44
1:B:168:PHE:CG	1:B:169:GLU:N	2.86	0.44
1:B:473:TYR:N	1:B:489:TYR:O	2.46	0.44
1:C:141:LEU:HB3	1:C:243:ALA:HA	1.99	0.44
1:C:192:PHE:HB3	1:C:194:PHE:HE1	1.81	0.44
1:C:328:ARG:HH22	1:C:533:LEU:CB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:TYR:HB2	1:C:491:PRO:HB3	1.99	0.44
2:D:97:PHE:CZ	3:E:47:TRP:HB2	2.52	0.44
3:G:4:LEU:HG	3:G:109:TYR:CE2	2.52	0.44
1:A:386:LYS:HD3	1:A:389:ASP:HB3	2.00	0.44
1:A:869:MET:O	1:A:870:ILE:C	2.56	0.44
1:B:41:LYS:O	1:C:563:GLN:HA	2.16	0.44
1:B:152:TRP:HB3	1:B:153:MET:H	1.57	0.44
1:B:313:TYR:N	1:B:313:TYR:CD1	2.85	0.44
1:B:386:LYS:O	1:B:390:LEU:HB3	2.17	0.44
1:B:822:LEU:HA	1:B:822:LEU:HD23	1.68	0.44
1:B:873:TYR:C	1:B:875:SER:N	2.71	0.44
1:B:1097:SER:OG	1:B:1098:ASN:N	2.50	0.44
1:C:133:PHE:HD2	1:C:160:TYR:HB2	1.82	0.44
1:C:997:ILE:O	1:C:998:THR:C	2.56	0.44
2:D:31:ASN:OD1	2:D:32:LEU:N	2.51	0.44
1:A:559:PHE:CE1	1:C:43:PHE:CD2	3.05	0.44
1:A:707:TYR:CD1	1:A:707:TYR:C	2.90	0.44
1:A:805:ILE:HB	1:A:1054:GLN:HE22	1.82	0.44
1:A:809:PRO:O	1:A:814:LYS:HE2	2.18	0.44
1:A:892:ALA:O	1:A:894:LEU:HG	2.18	0.44
1:B:143:VAL:HG13	1:B:151:SER:CB	2.47	0.44
1:B:351:TYR:HB3	1:B:453:TYR:HA	2.00	0.44
1:B:436:TRP:NE1	1:B:509:ARG:HD2	2.24	0.44
1:B:912:THR:HG22	1:B:914:ASN:H	1.83	0.44
1:B:1038:LYS:HE3	1:B:1038:LYS:HB3	1.66	0.44
1:C:55:PHE:CD2	1:C:275:PHE:CD2	3.05	0.44
1:C:386:LYS:O	1:C:390:LEU:HB3	2.17	0.44
1:C:1081:ILE:HD13	1:C:1135:ASN:HB3	2.00	0.44
3:G:4:LEU:HA	3:G:23:LYS:O	2.18	0.44
1:A:54:LEU:O	1:A:55:PHE:HD1	2.00	0.44
1:A:161:SER:OG	1:A:162:SER:N	2.48	0.44
1:A:410:ILE:HG13	1:A:418:ILE:HG21	2.00	0.44
1:A:422:ASN:HB3	1:A:454:ARG:CB	2.48	0.44
1:A:802:PHE:O	1:A:804:GLN:N	2.50	0.44
1:A:1014:ARG:O	1:A:1017:GLU:N	2.47	0.44
1:A:1097:SER:OG	1:A:1098:ASN:N	2.50	0.44
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.33	0.44
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.81	0.44
1:B:144:TYR:HB3	1:B:152:TRP:HB2	1.99	0.44
1:B:191:GLU:C	1:B:192:PHE:HD1	2.21	0.44
1:B:326:ILE:HD12	1:B:532:ASN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ILE:HG13	1:B:418:ILE:HG21	2.00	0.44
1:B:802:PHE:O	1:B:804:GLN:N	2.50	0.44
1:C:200:TYR:CD1	1:C:230:PRO:HA	2.52	0.44
1:C:351:TYR:HB3	1:C:453:TYR:HA	2.00	0.44
1:C:386:LYS:HD3	1:C:389:ASP:HB3	2.00	0.44
1:C:805:ILE:HB	1:C:1054:GLN:HE22	1.82	0.44
1:C:869:MET:O	1:C:870:ILE:C	2.56	0.44
2:D:12:VAL:HG12	2:D:13:SER:H	1.81	0.44
2:H:32:LEU:HD13	2:H:70:PHE:CG	2.53	0.44
1:A:378:LYS:HZ3	3:E:58:THR:N	2.16	0.44
1:A:912:THR:HG22	1:A:914:ASN:H	1.83	0.44
1:B:809:PRO:O	1:B:814:LYS:HE2	2.18	0.44
1:B:892:ALA:O	1:B:894:LEU:HG	2.18	0.44
1:C:90:VAL:HG11	1:C:238:PHE:CZ	2.53	0.44
1:C:138:ASP:O	1:C:140:PHE:HD1	2.01	0.44
1:C:168:PHE:CG	1:C:169:GLU:N	2.86	0.44
1:C:191:GLU:C	1:C:192:PHE:HD1	2.21	0.44
1:C:802:PHE:O	1:C:804:GLN:N	2.50	0.44
2:F:34:TRP:CD2	2:F:72:LEU:HB2	2.52	0.44
3:G:10:GLU:HG3	3:G:18:VAL:CG2	2.48	0.44
2:H:60:ARG:O	2:H:74:ILE:HA	2.18	0.44
1:A:326:ILE:HD12	1:A:532:ASN:O	2.18	0.44
1:A:432:CYS:HB2	1:A:513:LEU:H	1.81	0.44
1:A:995:ARG:O	1:A:999:GLY:N	2.36	0.44
1:B:90:VAL:HG11	1:B:238:PHE:CZ	2.53	0.44
1:B:473:TYR:HB2	1:B:491:PRO:HB3	1.98	0.44
1:B:543:PHE:O	1:B:546:LEU:N	2.51	0.44
1:B:1134:ASN:O	1:B:1135:ASN:HB2	2.18	0.44
2:F:33:HIS:CE1	3:G:106:VAL:HG12	2.52	0.44
2:F:43:PRO:HD2	3:G:110:TRP:CZ3	2.51	0.44
3:G:7:SER:HB3	3:G:21:SER:OG	2.18	0.44
2:H:43:PRO:HG2	3:I:45:LEU:HD21	1.99	0.44
3:I:65:LYS:HA	3:I:65:LYS:HD2	1.71	0.44
1:A:141:LEU:HB3	1:A:243:ALA:HA	1.99	0.44
1:A:143:VAL:HG13	1:A:151:SER:CB	2.47	0.44
1:A:376:THR:HG22	1:A:435:ALA:N	2.33	0.44
1:A:457:ARG:NH2	1:A:461:LEU:HD23	2.32	0.44
1:B:141:LEU:HB3	1:B:243:ALA:HA	1.99	0.44
1:B:898:PHE:O	1:B:900:MET:N	2.50	0.44
1:B:1081:ILE:HD13	1:B:1135:ASN:HB3	2.00	0.44
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:TYR:C	1:C:875:SER:N	2.71	0.44
1:C:1038:LYS:HB3	1:C:1038:LYS:HE3	1.66	0.44
2:D:12:VAL:O	2:D:105:ILE:HA	2.18	0.44
2:D:74:ILE:HG21	2:D:77:LEU:HD23	2.00	0.44
3:E:41:PRO:HD3	3:E:91:THR:O	2.18	0.44
2:F:82:PHE:HB3	2:F:105:ILE:CD1	2.48	0.44
3:I:9:ALA:HA	3:I:115:THR:O	2.18	0.44
1:A:543:PHE:O	1:A:546:LEU:N	2.51	0.43
1:A:898:PHE:O	1:A:900:MET:N	2.50	0.43
1:B:436:TRP:CE2	1:B:509:ARG:HB2	2.52	0.43
1:C:318:PHE:CG	1:C:318:PHE:O	2.70	0.43
1:C:408:ARG:CD	3:I:102:ASP:OD1	2.65	0.43
1:C:897:PRO:O	1:C:900:MET:N	2.49	0.43
1:C:898:PHE:O	1:C:900:MET:N	2.51	0.43
1:C:919:ASN:O	1:C:920:GLN:C	2.57	0.43
2:F:31:ASN:OD1	2:F:49:TYR:HA	2.18	0.43
3:G:32:TYR:CD2	3:G:98:ARG:HD2	2.53	0.43
2:H:6:GLN:HE22	2:H:87:CYS:N	2.16	0.43
1:A:904:TYR:N	1:A:904:TYR:CD1	2.83	0.43
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.60	0.43
1:A:1134:ASN:O	1:A:1135:ASN:HB2	2.18	0.43
1:B:439:ASN:HA	1:B:443:SER:OG	2.18	0.43
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.33	0.43
2:H:12:VAL:O	2:H:105:ILE:HA	2.18	0.43
3:I:88:SER:HA	3:I:118:VAL:O	2.18	0.43
3:I:98:ARG:NH2	3:I:108:ASP:HB2	2.33	0.43
1:A:138:ASP:O	1:A:140:PHE:HD1	2.01	0.43
1:A:802:PHE:O	1:A:803:SER:C	2.56	0.43
1:A:916:LEU:HA	1:A:916:LEU:HD12	1.54	0.43
1:B:125:ASN:OD1	5:B:1302:NAG:H81	2.19	0.43
1:B:328:ARG:HH22	1:B:533:LEU:CB	2.17	0.43
1:B:342:PHE:CE1	1:B:511:VAL:HG11	2.53	0.43
1:B:869:MET:O	1:B:870:ILE:C	2.56	0.43
1:B:1003:SER:O	1:B:1003:SER:OG	2.35	0.43
1:B:1018:ILE:HD12	1:B:1018:ILE:HG23	1.56	0.43
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.33	0.43
1:C:54:LEU:O	1:C:55:PHE:HD1	2.00	0.43
1:C:759:PHE:HD1	1:C:762:GLN:HE21	1.66	0.43
1:C:825:LYS:HE2	1:C:938:LEU:O	2.19	0.43
1:C:966:LEU:HA	1:C:966:LEU:HD23	1.58	0.43
2:D:6:GLN:HE22	2:D:87:CYS:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:36:TRP:CD1	3:E:70:LEU:HD22	2.52	0.43
3:I:35:HIS:CG	3:I:47:TRP:HE1	2.36	0.43
1:A:354:ASN:HB2	1:A:399:SER:HB3	1.99	0.43
1:A:804:GLN:CD	1:A:935:GLN:NE2	2.72	0.43
1:A:825:LYS:HE2	1:A:938:LEU:O	2.19	0.43
1:B:123:ALA:O	1:B:124:THR:OG1	2.35	0.43
1:B:133:PHE:CE2	1:B:135:PHE:HE1	2.35	0.43
1:B:133:PHE:HD2	1:B:160:TYR:HB2	1.82	0.43
1:B:378:LYS:HA	1:B:378:LYS:HD2	1.74	0.43
1:B:619:GLU:H	1:B:619:GLU:CD	2.14	0.43
1:B:1139:ASP:OD2	1:B:1142:GLN:N	2.50	0.43
1:C:96:GLU:HB3	1:C:99:ASN:H	1.83	0.43
1:C:141:LEU:HD23	1:C:243:ALA:HB2	1.99	0.43
1:C:559:PHE:CD2	1:C:563:GLN:HB3	2.53	0.43
1:C:584:ILE:HA	1:C:584:ILE:HD13	1.77	0.43
3:E:33:TYR:HB2	3:E:99:SER:HB3	2.01	0.43
2:H:48:LYS:N	2:H:52:GLN:O	2.39	0.43
2:H:85:TYR:HE2	2:H:103:LEU:HD22	1.84	0.43
3:I:36:TRP:CD1	3:I:70:LEU:HD22	2.52	0.43
1:A:191:GLU:C	1:A:192:PHE:HD1	2.21	0.43
1:A:430:THR:HG21	1:A:517:LEU:CD2	2.49	0.43
1:A:884:SER:HA	1:A:894:LEU:O	2.19	0.43
1:A:919:ASN:O	1:A:920:GLN:C	2.57	0.43
1:A:997:ILE:O	1:A:998:THR:C	2.56	0.43
1:B:318:PHE:CG	1:B:318:PHE:O	2.70	0.43
1:B:437:ASN:HA	1:B:508:TYR:CD1	2.53	0.43
1:B:559:PHE:CZ	1:B:566:GLY:HA2	2.51	0.43
1:B:559:PHE:HD1	1:B:559:PHE:HA	1.72	0.43
1:B:1008:VAL:O	1:B:1009:THR:C	2.57	0.43
1:C:136:CYS:HB2	1:C:139:PRO:N	2.34	0.43
1:C:376:THR:HG22	1:C:435:ALA:N	2.33	0.43
1:C:402:ILE:HG21	1:C:410:ILE:HD11	2.01	0.43
1:C:1004:LEU:O	1:C:1005:GLN:C	2.56	0.43
2:D:85:TYR:HE2	2:D:103:LEU:HD22	1.84	0.43
2:F:20:ILE:CD1	2:F:85:TYR:HD2	2.31	0.43
3:G:109:TYR:C	3:G:110:TRP:CD1	2.92	0.43
2:H:97:PHE:CZ	3:I:47:TRP:HB2	2.52	0.43
1:A:136:CYS:HB2	1:A:139:PRO:N	2.34	0.43
1:A:351:TYR:HB3	1:A:453:TYR:HA	2.00	0.43
1:A:437:ASN:HA	1:A:508:TYR:CD1	2.53	0.43
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HD23	1:B:272:PRO:CA	2.49	0.43
1:B:141:LEU:HD23	1:B:243:ALA:HB2	1.99	0.43
1:B:422:ASN:HB3	1:B:454:ARG:CB	2.48	0.43
1:B:805:ILE:O	1:B:816:SER:OG	2.30	0.43
1:B:919:ASN:O	1:B:920:GLN:C	2.56	0.43
1:C:212:LEU:HD23	1:C:215:ASP:O	2.19	0.43
1:C:422:ASN:HB3	1:C:454:ARG:CB	2.48	0.43
1:C:619:GLU:H	1:C:619:GLU:CD	2.14	0.43
1:C:1027:THR:O	1:C:1028:LYS:C	2.53	0.43
3:E:33:TYR:CE1	3:E:101:TYR:HD1	2.37	0.43
3:E:71:THR:O	3:E:80:TYR:N	2.28	0.43
2:H:34:TRP:CD2	2:H:72:LEU:HB2	2.54	0.43
3:I:31:ASN:O	3:I:101:TYR:HB2	2.19	0.43
1:A:96:GLU:HB3	1:A:99:ASN:H	1.83	0.43
1:A:141:LEU:HD23	1:A:243:ALA:HB2	1.99	0.43
1:A:402:ILE:HG21	1:A:410:ILE:HD11	2.01	0.43
1:A:702:GLU:CD	1:A:703:ASN:N	2.72	0.43
1:A:778:THR:O	1:A:778:THR:HG22	2.19	0.43
1:A:1081:ILE:HD13	1:A:1135:ASN:HB3	2.00	0.43
1:B:402:ILE:HG21	1:B:410:ILE:HD11	2.01	0.43
1:B:825:LYS:HE2	1:B:938:LEU:O	2.19	0.43
1:B:884:SER:HA	1:B:894:LEU:O	2.19	0.43
1:B:1104:VAL:O	1:B:1104:VAL:HG13	2.19	0.43
1:C:737:ASP:OD1	1:C:737:ASP:C	2.57	0.43
1:C:884:SER:HA	1:C:894:LEU:O	2.19	0.43
2:D:23:ARG:HH11	2:D:69:ASP:HB2	1.83	0.43
3:E:9:ALA:HA	3:E:115:THR:O	2.18	0.43
2:F:36:GLN:OE1	2:F:46:LEU:HD21	2.18	0.43
2:H:23:ARG:HH11	2:H:69:ASP:HB2	1.83	0.43
1:A:90:VAL:HG11	1:A:238:PHE:CZ	2.53	0.43
1:A:342:PHE:CE1	1:A:511:VAL:HG11	2.53	0.43
1:B:386:LYS:HD3	1:B:389:ASP:HB3	2.00	0.43
1:B:581:THR:HG23	1:B:583:GLU:OE2	2.18	0.43
1:C:394:ASN:O	1:C:515:PHE:HA	2.19	0.43
1:C:581:THR:HG23	1:C:583:GLU:OE2	2.18	0.43
1:C:759:PHE:O	1:C:762:GLN:N	2.51	0.43
1:C:804:GLN:CD	1:C:935:GLN:NE2	2.72	0.43
2:D:85:TYR:N	2:D:101:THR:O	2.47	0.43
3:E:4:LEU:HD23	3:E:24:VAL:HA	2.00	0.43
3:E:35:HIS:CG	3:E:47:TRP:HE1	2.36	0.43
3:E:98:ARG:NH2	3:E:108:ASP:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:10:GLU:O	3:G:116:VAL:HA	2.18	0.43
1:A:308:VAL:HB	1:A:602:THR:HG23	2.00	0.43
1:A:359:SER:CA	1:A:523:THR:HB	2.40	0.43
1:A:393:THR:OG1	1:A:394:ASN:N	2.48	0.43
1:A:405:ASP:CG	3:E:104:TYR:OH	2.57	0.43
1:A:713:ALA:O	1:C:894:LEU:HD22	2.19	0.43
1:A:737:ASP:OD1	1:A:737:ASP:C	2.57	0.43
1:B:54:LEU:O	1:B:55:PHE:HD1	2.00	0.43
1:B:136:CYS:HB2	1:B:139:PRO:N	2.33	0.43
1:B:273:ARG:HA	1:B:273:ARG:HD3	1.68	0.43
1:B:308:VAL:HB	1:B:602:THR:HG23	2.00	0.43
1:B:737:ASP:OD1	1:B:737:ASP:C	2.57	0.43
1:B:876:ALA:O	1:B:877:LEU:C	2.57	0.43
1:C:54:LEU:HD23	1:C:272:PRO:CA	2.49	0.43
1:C:123:ALA:O	1:C:124:THR:OG1	2.35	0.43
1:C:318:PHE:CE1	1:C:592:PHE:O	2.72	0.43
1:C:341:VAL:CG2	1:C:356:LYS:HD3	2.49	0.43
1:C:412:PRO:HB3	1:C:427:ASP:HA	2.01	0.43
1:C:437:ASN:HA	1:C:508:TYR:CD1	2.53	0.43
1:C:805:ILE:HG21	1:C:805:ILE:HD13	1.73	0.43
1:C:950:ASP:O	1:C:951:VAL:C	2.56	0.43
3:E:88:SER:HA	3:E:118:VAL:O	2.18	0.43
2:H:31:ASN:OD1	2:H:32:LEU:N	2.51	0.43
3:I:41:PRO:HD3	3:I:91:THR:O	2.18	0.43
1:A:341:VAL:CG2	1:A:356:LYS:HD3	2.49	0.43
1:A:914:ASN:HA	1:B:1089:PHE:CE2	2.54	0.43
1:A:950:ASP:O	1:A:951:VAL:C	2.56	0.43
1:A:1136:THR:O	1:A:1136:THR:OG1	2.37	0.43
1:B:354:ASN:HB2	1:B:399:SER:HB3	1.99	0.43
1:B:430:THR:HG21	1:B:517:LEU:CD2	2.49	0.43
1:B:702:GLU:CD	1:B:703:ASN:N	2.72	0.43
1:B:1004:LEU:HA	1:B:1004:LEU:HD23	1.71	0.43
1:C:125:ASN:OD1	5:C:1302:NAG:H81	2.19	0.43
1:C:537:LYS:O	1:C:539:VAL:HG13	2.19	0.43
1:C:543:PHE:O	1:C:546:LEU:N	2.51	0.43
1:C:714:ILE:HD13	1:C:1105:THR:HG21	2.01	0.43
1:C:763:LEU:HA	1:C:763:LEU:HD23	1.62	0.43
1:C:1049:LEU:HA	1:C:1049:LEU:HD23	1.39	0.43
2:D:32:LEU:HD13	2:D:70:PHE:CG	2.53	0.43
2:D:60:ARG:O	2:D:74:ILE:HA	2.18	0.43
2:F:37:GLN:HB2	2:F:86:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD23	1:A:215:ASP:O	2.19	0.42
1:A:375:SER:HB2	1:A:436:TRP:HA	2.00	0.42
1:A:398:ASP:N	1:A:512:VAL:O	2.49	0.42
1:B:138:ASP:O	1:B:140:PHE:HD1	2.01	0.42
1:B:158:ARG:HG3	1:B:158:ARG:O	2.19	0.42
1:B:341:VAL:CG2	1:B:356:LYS:HD3	2.49	0.42
1:C:485:GLY:N	1:C:488:CYS:HB2	2.31	0.42
1:C:671:CYS:SG	1:C:697:MET:HB3	2.59	0.42
1:C:702:GLU:CD	1:C:703:ASN:N	2.72	0.42
1:C:912:THR:HG22	1:C:914:ASN:H	1.83	0.42
2:F:57:ILE:CG2	2:F:61:PHE:HD2	2.32	0.42
2:H:94:PRO:O	2:H:96:ILE:HG13	2.19	0.42
1:A:158:ARG:O	1:A:158:ARG:HG3	2.19	0.42
1:A:383:SER:HB2	1:A:386:LYS:HG2	2.01	0.42
1:A:412:PRO:CB	1:A:427:ASP:HA	2.49	0.42
1:A:671:CYS:SG	1:A:697:MET:HB3	2.59	0.42
1:B:381:GLY:CA	1:B:430:THR:HG23	2.49	0.42
1:B:950:ASP:O	1:B:951:VAL:C	2.56	0.42
1:C:92:PHE:CE1	1:C:93:ALA:O	2.72	0.42
1:C:381:GLY:CA	1:C:430:THR:HG23	2.49	0.42
1:C:778:THR:O	1:C:778:THR:HG22	2.19	0.42
1:C:858:LEU:HD12	1:C:858:LEU:H	1.84	0.42
1:C:1014:ARG:O	1:C:1017:GLU:N	2.47	0.42
2:D:4:LEU:HD23	2:D:89:GLN:HB2	2.01	0.42
2:D:94:PRO:O	2:D:96:ILE:HG13	2.19	0.42
2:H:74:ILE:HG21	2:H:77:LEU:HD23	2.00	0.42
3:I:4:LEU:HD23	3:I:24:VAL:HA	2.00	0.42
1:A:98:SER:OG	1:A:100:ILE:HG12	2.19	0.42
1:A:101:ILE:HA	1:A:242:LEU:CD2	2.49	0.42
1:A:108:THR:HG22	1:A:236:THR:N	2.35	0.42
1:A:897:PRO:O	1:A:900:MET:N	2.49	0.42
1:A:1004:LEU:HA	1:A:1004:LEU:HD23	1.71	0.42
1:B:96:GLU:HB3	1:B:99:ASN:H	1.83	0.42
1:B:388:ASN:CA	1:B:527:PRO:HD2	2.50	0.42
1:B:394:ASN:O	1:B:515:PHE:HA	2.19	0.42
1:B:671:CYS:SG	1:B:697:MET:HB3	2.59	0.42
1:B:804:GLN:CD	1:B:935:GLN:NE2	2.72	0.42
1:B:1143:PRO:O	1:B:1146:ASP:HB3	2.19	0.42
1:C:324:GLU:HB2	1:C:325:SER:H	1.56	0.42
1:C:773:GLU:O	1:C:774:GLN:C	2.57	0.42
1:C:1134:ASN:O	1:C:1135:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1138:TYR:OH	1:C:1143:PRO:HG3	2.20	0.42
3:I:18:VAL:HG13	3:I:83:LEU:HB3	2.02	0.42
1:A:48:LEU:H	1:A:48:LEU:HG	1.60	0.42
1:A:125:ASN:OD1	5:A:1302:NAG:H81	2.19	0.42
1:A:375:SER:CA	2:D:91:ASN:HB2	2.50	0.42
1:A:430:THR:HG21	1:A:517:LEU:CG	2.50	0.42
1:A:563:GLN:HA	1:C:41:LYS:O	2.19	0.42
1:A:876:ALA:O	1:A:877:LEU:C	2.57	0.42
1:A:1008:VAL:O	1:A:1009:THR:C	2.57	0.42
1:B:101:ILE:HA	1:B:242:LEU:CD2	2.49	0.42
1:B:108:THR:HG22	1:B:236:THR:N	2.35	0.42
1:B:431:GLY:HA2	1:B:515:PHE:CE1	2.55	0.42
1:B:816:SER:O	1:B:817:PHE:C	2.57	0.42
1:C:431:GLY:HA2	1:C:515:PHE:CE1	2.55	0.42
1:C:876:ALA:O	1:C:877:LEU:C	2.57	0.42
1:C:897:PRO:O	1:C:898:PHE:C	2.58	0.42
1:C:1104:VAL:HG13	1:C:1104:VAL:O	2.19	0.42
2:D:34:TRP:CD2	2:D:72:LEU:HB2	2.54	0.42
2:D:35:TYR:O	2:D:85:TYR:HA	2.20	0.42
2:H:35:TYR:O	2:H:85:TYR:HA	2.20	0.42
2:H:35:TYR:OH	3:I:107:MET:HG2	2.19	0.42
1:A:345:THR:HG22	1:A:346:ARG:NH1	2.35	0.42
1:A:412:PRO:HB3	1:A:427:ASP:HA	2.01	0.42
1:A:804:GLN:HE21	4:L:1:NAG:H62	1.85	0.42
1:A:1100:THR:HG1	1:A:1101:HIS:N	2.16	0.42
1:B:411:ALA:HB3	1:B:414:GLN:CG	2.50	0.42
1:B:498:GLN:O	1:B:500:THR:N	2.52	0.42
1:B:560:LEU:HD12	1:B:562:PHE:CE1	2.48	0.42
1:B:797:PHE:HD1	1:B:797:PHE:HA	1.65	0.42
1:C:44:ARG:HB3	1:C:47:VAL:HG11	2.02	0.42
1:C:319:ARG:H	1:C:319:ARG:HG2	1.66	0.42
1:C:375:SER:HB2	1:C:436:TRP:HA	2.00	0.42
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.37	0.42
1:C:712:ILE:HG21	1:C:712:ILE:HD13	1.82	0.42
1:A:44:ARG:HB3	1:A:47:VAL:HG11	2.02	0.42
1:A:378:LYS:NZ	3:E:58:THR:OG1	2.53	0.42
1:A:402:ILE:HD12	1:A:406:GLU:HB2	2.02	0.42
1:A:591:SER:O	1:A:592:PHE:HB2	2.19	0.42
1:A:819:GLU:O	1:A:823:PHE:HD2	2.03	0.42
1:A:894:LEU:HD22	1:B:713:ALA:O	2.19	0.42
1:B:229:LEU:HA	1:B:229:LEU:HD23	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:HG22	1:B:356:LYS:HD3	2.01	0.42
1:B:412:PRO:CB	1:B:427:ASP:HA	2.50	0.42
1:B:421:TYR:HB3	1:B:454:ARG:HG2	2.01	0.42
1:B:591:SER:O	1:B:592:PHE:HB2	2.19	0.42
1:B:712:ILE:HD13	1:B:712:ILE:HG21	1.82	0.42
1:B:759:PHE:HD1	1:B:762:GLN:HE21	1.66	0.42
1:B:950:ASP:O	1:B:953:ASN:N	2.53	0.42
1:B:1014:ARG:O	1:B:1017:GLU:N	2.47	0.42
1:C:98:SER:OG	1:C:100:ILE:HG12	2.19	0.42
1:C:383:SER:HB2	1:C:386:LYS:HG2	2.01	0.42
1:C:411:ALA:HB3	1:C:414:GLN:CG	2.50	0.42
1:C:498:GLN:O	1:C:500:THR:N	2.52	0.42
1:C:1011:GLN:O	1:C:1015:ALA:N	2.33	0.42
2:D:31:ASN:O	2:D:90:THR:OG1	2.32	0.42
3:I:27:TYR:CE2	3:I:98:ARG:HD3	2.55	0.42
1:A:54:LEU:HD23	1:A:272:PRO:CA	2.49	0.42
1:A:92:PHE:CE1	1:A:93:ALA:O	2.72	0.42
1:A:140:PHE:HB2	1:A:242:LEU:O	2.20	0.42
1:A:421:TYR:HB3	1:A:454:ARG:HG2	2.01	0.42
1:A:537:LYS:O	1:A:539:VAL:HG13	2.19	0.42
1:B:43:PHE:HB3	1:C:559:PHE:CZ	2.55	0.42
1:B:457:ARG:NH1	1:B:459:SER:O	2.51	0.42
1:B:759:PHE:O	1:B:762:GLN:N	2.51	0.42
1:B:763:LEU:HA	1:B:763:LEU:HD23	1.62	0.42
1:B:778:THR:O	1:B:778:THR:HG22	2.19	0.42
1:B:997:ILE:O	1:B:998:THR:C	2.56	0.42
1:C:31:SER:HG	1:C:60:SER:N	2.17	0.42
1:C:345:THR:HG22	1:C:346:ARG:NH1	2.35	0.42
1:C:421:TYR:HB3	1:C:454:ARG:HG2	2.01	0.42
1:C:763:LEU:O	1:C:764:ASN:C	2.58	0.42
2:F:10:GLN:HG2	2:F:101:THR:HG21	2.00	0.42
2:F:29:SER:HB2	2:F:90:THR:OG1	2.20	0.42
3:G:36:TRP:O	3:G:48:ILE:HG22	2.20	0.42
3:I:33:TYR:HB2	3:I:99:SER:HB3	2.01	0.42
3:I:116:VAL:HG12	3:I:118:VAL:HG23	2.01	0.42
1:A:31:SER:HG	1:A:60:SER:N	2.18	0.42
1:A:231:ILE:HG13	1:A:232:GLY:H	1.85	0.42
1:A:341:VAL:HG22	1:A:356:LYS:HD3	2.01	0.42
1:A:759:PHE:O	1:A:762:GLN:N	2.51	0.42
1:A:915:VAL:HG12	1:A:916:LEU:N	2.35	0.42
1:A:1104:VAL:HG13	1:A:1104:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:TYR:OH	1:A:1143:PRO:HG3	2.20	0.42
1:B:325:SER:O	1:B:326:ILE:HD13	2.20	0.42
1:B:709:ASN:ND2	5:B:1309:NAG:C7	2.83	0.42
1:B:804:GLN:HE21	4:Q:1:NAG:H62	1.85	0.42
1:C:108:THR:HG22	1:C:236:THR:N	2.35	0.42
1:C:341:VAL:HG22	1:C:356:LYS:HD3	2.01	0.42
1:C:430:THR:HG21	1:C:517:LEU:CD2	2.49	0.42
1:C:750:SER:O	1:C:754:LEU:HG	2.20	0.42
1:C:805:ILE:O	1:C:816:SER:OG	2.30	0.42
1:A:101:ILE:HA	1:A:242:LEU:HD23	2.02	0.42
1:A:325:SER:O	1:A:326:ILE:HD13	2.20	0.42
1:A:411:ALA:HB3	1:A:414:GLN:CG	2.50	0.42
1:A:431:GLY:HA2	1:A:515:PHE:CE1	2.55	0.42
1:A:773:GLU:C	1:A:775:ASP:N	2.72	0.42
1:A:805:ILE:HD13	1:A:805:ILE:HG21	1.73	0.42
1:B:30:ASN:HD22	1:B:32:PHE:HE1	1.67	0.42
1:B:98:SER:OG	1:B:100:ILE:HG12	2.19	0.42
1:B:212:LEU:HD23	1:B:215:ASP:O	2.19	0.42
1:B:719:THR:CG2	1:B:1068:VAL:HB	2.50	0.42
1:B:737:ASP:OD2	1:B:740:MET:N	2.48	0.42
1:B:747:THR:HG22	1:B:751:ASN:ND2	2.35	0.42
1:B:750:SER:O	1:B:754:LEU:HG	2.20	0.42
1:B:904:TYR:O	1:B:905:ARG:C	2.57	0.42
1:C:30:ASN:HD22	1:C:32:PHE:HE1	1.67	0.42
1:C:93:ALA:HA	1:C:190:ARG:O	2.20	0.42
1:C:308:VAL:HB	1:C:602:THR:HG23	2.00	0.42
1:C:402:ILE:HD12	1:C:406:GLU:HB2	2.02	0.42
1:C:412:PRO:CB	1:C:427:ASP:HA	2.50	0.42
1:C:567:ARG:HB3	1:C:568:ASP:H	1.71	0.42
1:C:588:THR:HG23	1:C:589:PRO:HD2	2.01	0.42
1:C:591:SER:O	1:C:592:PHE:HB2	2.19	0.42
1:C:737:ASP:OD2	1:C:740:MET:N	2.48	0.42
1:C:804:GLN:HE21	4:V:1:NAG:H62	1.85	0.42
3:E:18:VAL:HG13	3:E:83:LEU:HB3	2.02	0.42
2:H:4:LEU:HD23	2:H:89:GLN:HB2	2.01	0.42
3:I:14:PRO:HD3	3:I:119:SER:C	2.40	0.42
1:A:108:THR:HG22	1:A:236:THR:HG23	2.02	0.42
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.73	0.42
1:A:559:PHE:CE1	1:A:566:GLY:CA	3.03	0.42
1:A:560:LEU:HD22	1:A:560:LEU:HA	1.73	0.42
1:A:759:PHE:HD1	1:A:762:GLN:HE21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ILE:N	1:A:850:ILE:CD1	2.73	0.42
1:A:1089:PHE:CE2	1:C:914:ASN:HA	2.54	0.42
1:B:894:LEU:HD22	1:C:713:ALA:O	2.20	0.42
1:C:99:ASN:O	1:C:102:ARG:NH2	2.53	0.42
1:C:233:ILE:HD13	1:C:233:ILE:HG21	1.87	0.42
1:C:819:GLU:O	1:C:823:PHE:HD2	2.03	0.42
1:C:1018:ILE:HD12	1:C:1018:ILE:HG23	1.56	0.42
2:D:35:TYR:OH	3:E:107:MET:HG2	2.19	0.42
3:E:6:GLN:H	3:E:112:GLN:NE2	2.17	0.42
3:E:98:ARG:O	3:E:107:MET:HA	2.20	0.42
3:E:116:VAL:HG12	3:E:118:VAL:HG23	2.01	0.42
2:F:84:ILE:HA	2:F:102:LYS:HA	2.02	0.42
1:A:30:ASN:HD22	1:A:32:PHE:HE1	1.67	0.41
1:A:397:ALA:HB2	1:A:513:LEU:HD23	2.02	0.41
1:A:410:ILE:HG12	1:A:423:TYR:HD2	1.85	0.41
1:A:498:GLN:O	1:A:500:THR:N	2.52	0.41
1:A:816:SER:O	1:A:817:PHE:C	2.57	0.41
1:B:376:THR:HG22	1:B:435:ALA:N	2.33	0.41
1:B:584:ILE:HD13	1:B:584:ILE:HA	1.77	0.41
1:B:669:GLY:O	1:B:697:MET:HG2	2.20	0.41
1:B:897:PRO:O	1:B:898:PHE:C	2.58	0.41
1:C:816:SER:O	1:C:817:PHE:C	2.57	0.41
1:C:915:VAL:O	1:C:916:LEU:C	2.59	0.41
2:F:4:LEU:HD23	2:F:89:GLN:HB2	2.01	0.41
2:F:60:ARG:HG3	2:F:61:PHE:CD1	2.55	0.41
1:A:394:ASN:O	1:A:515:PHE:HA	2.19	0.41
1:A:588:THR:HG23	1:A:589:PRO:HD2	2.01	0.41
1:A:750:SER:O	1:A:754:LEU:HG	2.20	0.41
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.60	0.41
1:A:1116:THR:H	1:A:1119:ASN:HD22	1.68	0.41
1:A:1143:PRO:O	1:A:1146:ASP:HB3	2.19	0.41
1:B:92:PHE:CE1	1:B:93:ALA:O	2.72	0.41
1:B:375:SER:HB2	1:B:436:TRP:HA	2.00	0.41
1:B:397:ALA:HB2	1:B:513:LEU:HD23	2.02	0.41
1:B:402:ILE:HD12	1:B:406:GLU:HB2	2.02	0.41
1:B:588:THR:HG23	1:B:589:PRO:HD2	2.01	0.41
1:B:643:PHE:CD1	1:B:655:HIS:HB2	2.55	0.41
1:B:714:ILE:HD13	1:B:1105:THR:HG21	2.01	0.41
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	2.02	0.41
1:B:1138:TYR:OH	1:B:1143:PRO:HG3	2.20	0.41
1:C:140:PHE:HB2	1:C:242:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ASN:HB2	1:C:399:SER:H	1.85	0.41
1:C:709:ASN:ND2	5:C:1309:NAG:C7	2.83	0.41
1:C:759:PHE:HD1	1:C:762:GLN:NE2	2.18	0.41
1:C:802:PHE:O	1:C:803:SER:C	2.56	0.41
3:E:38:LYS:HG3	3:E:94:TYR:CE1	2.56	0.41
1:A:43:PHE:HB3	1:B:566:GLY:HA2	2.03	0.41
1:A:152:TRP:HB3	1:A:153:MET:H	1.57	0.41
1:A:357:ARG:NH1	1:C:166:CYS:O	2.53	0.41
1:A:457:ARG:NH1	1:A:459:SER:O	2.51	0.41
1:A:669:GLY:O	1:A:697:MET:HG2	2.20	0.41
1:A:744:GLY:O	1:A:746:SER:N	2.53	0.41
1:A:759:PHE:HD1	1:A:762:GLN:NE2	2.18	0.41
1:B:537:LYS:O	1:B:539:VAL:HG13	2.19	0.41
1:B:695:TYR:CD1	1:B:695:TYR:N	2.88	0.41
1:B:953:ASN:O	1:B:957:GLN:N	2.39	0.41
1:B:1024:LEU:HD12	1:B:1024:LEU:HA	1.72	0.41
1:C:101:ILE:HA	1:C:242:LEU:CD2	2.50	0.41
1:C:108:THR:HG22	1:C:236:THR:HG23	2.02	0.41
1:C:158:ARG:HG3	1:C:158:ARG:O	2.19	0.41
1:C:915:VAL:HG12	1:C:916:LEU:N	2.35	0.41
1:C:950:ASP:O	1:C:953:ASN:N	2.53	0.41
1:C:977:LEU:HA	1:C:977:LEU:HD12	1.75	0.41
1:C:1094:VAL:H	1:C:1094:VAL:HG22	1.67	0.41
1:C:1143:PRO:O	1:C:1146:ASP:HB3	2.19	0.41
3:E:35:HIS:HB3	3:E:47:TRP:HE1	1.85	0.41
2:F:46:LEU:O	2:F:53:SER:HA	2.19	0.41
3:G:47:TRP:CZ2	3:G:50:TYR:CD2	3.07	0.41
3:G:100:GLU:CG	3:G:104:TYR:O	2.68	0.41
3:I:35:HIS:HE1	3:I:105:TYR:CD1	2.38	0.41
1:A:385:THR:OG1	3:E:65:LYS:HE2	2.20	0.41
1:A:719:THR:CG2	1:A:1068:VAL:HB	2.50	0.41
1:B:64:TRP:NE1	1:B:65:PHE:O	2.53	0.41
1:B:915:VAL:HG12	1:B:916:LEU:N	2.35	0.41
1:B:917:TYR:HD2	1:C:1089:PHE:CE2	2.38	0.41
1:B:982:SER:OG	1:B:983:ARG:N	2.54	0.41
1:C:64:TRP:NE1	1:C:65:PHE:O	2.53	0.41
1:C:397:ALA:HB2	1:C:513:LEU:HD23	2.02	0.41
1:C:528:LYS:HE2	1:C:528:LYS:HB2	1.85	0.41
1:C:543:PHE:O	1:C:546:LEU:HB3	2.20	0.41
2:H:10:GLN:HG3	2:H:20:ILE:HG12	2.02	0.41
3:I:38:LYS:HG3	3:I:94:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:O	1:A:102:ARG:NH2	2.53	0.41
1:A:106:PHE:HD1	1:A:106:PHE:N	2.18	0.41
1:A:386:LYS:HA	1:A:389:ASP:HB3	2.02	0.41
1:A:709:ASN:ND2	5:A:1309:NAG:C7	2.83	0.41
1:A:1047:TYR:O	1:A:1066:THR:HB	2.20	0.41
1:B:44:ARG:HB3	1:B:47:VAL:HG11	2.02	0.41
1:B:337:PRO:HD2	1:B:358:ILE:HG23	2.03	0.41
1:B:717:ASN:O	1:B:1070:ALA:N	2.51	0.41
1:B:897:PRO:O	1:B:900:MET:N	2.49	0.41
1:C:118:LEU:N	1:C:129:LYS:O	2.53	0.41
1:C:337:PRO:HD2	1:C:358:ILE:HG12	2.03	0.41
1:C:773:GLU:C	1:C:775:ASP:N	2.72	0.41
1:C:791:THR:HG21	1:C:806:LEU:HD13	2.02	0.41
2:D:23:ARG:NE	2:D:69:ASP:HB2	2.36	0.41
3:E:6:GLN:N	3:E:112:GLN:HE22	2.19	0.41
3:E:14:PRO:HD3	3:E:119:SER:C	2.40	0.41
3:E:27:TYR:CE2	3:E:98:ARG:HD3	2.55	0.41
2:F:106:LEU:O	2:F:107:LYS:HB3	2.21	0.41
3:G:27:TYR:CE1	3:G:32:TYR:HD2	2.38	0.41
3:G:66:GLY:HA3	3:G:83:LEU:HD12	2.02	0.41
3:I:6:GLN:H	3:I:112:GLN:NE2	2.17	0.41
1:A:560:LEU:HB2	1:A:563:GLN:NE2	2.36	0.41
1:A:850:ILE:H	1:A:850:ILE:CD1	2.23	0.41
1:A:1004:LEU:O	1:A:1005:GLN:C	2.56	0.41
1:A:1011:GLN:O	1:A:1015:ALA:N	2.33	0.41
1:B:65:PHE:HD2	1:B:265:TYR:OH	2.04	0.41
1:B:345:THR:HG22	1:B:346:ARG:NH1	2.35	0.41
1:B:383:SER:HB2	1:B:386:LYS:HG2	2.01	0.41
1:B:412:PRO:HB3	1:B:427:ASP:HA	2.01	0.41
1:B:819:GLU:O	1:B:823:PHE:HD2	2.03	0.41
1:B:1095:PHE:HD1	1:B:1095:PHE:HA	1.70	0.41
1:C:353:TRP:CG	1:C:423:TYR:CE1	3.09	0.41
1:C:786:LYS:H	1:C:786:LYS:HG2	1.54	0.41
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.41
1:C:887:THR:H	1:C:887:THR:HG23	1.64	0.41
3:E:4:LEU:CD2	3:E:24:VAL:HG22	2.50	0.41
2:F:33:HIS:O	2:F:88:GLN:N	2.52	0.41
2:F:60:ARG:O	2:F:74:ILE:HA	2.21	0.41
2:H:23:ARG:NE	2:H:69:ASP:HB2	2.36	0.41
1:A:229:LEU:HD23	1:A:229:LEU:HA	1.78	0.41
1:A:353:TRP:CG	1:A:423:TYR:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ASN:HB2	1:A:399:SER:H	1.85	0.41
1:A:643:PHE:CD1	1:A:655:HIS:HB2	2.56	0.41
1:A:797:PHE:HD1	1:A:797:PHE:HA	1.65	0.41
1:A:874:THR:H	1:A:874:THR:HG23	1.60	0.41
1:A:980:ILE:H	1:A:980:ILE:HG13	1.63	0.41
1:A:982:SER:OG	1:A:983:ARG:N	2.54	0.41
1:A:1038:LYS:HE3	1:A:1038:LYS:HB3	1.66	0.41
1:A:1056:ALA:HB1	1:A:1057:PRO:HD2	2.02	0.41
1:A:1139:ASP:OD2	1:A:1142:GLN:N	2.50	0.41
1:B:106:PHE:HD1	1:B:106:PHE:N	2.18	0.41
1:B:140:PHE:HB2	1:B:242:LEU:O	2.20	0.41
1:B:666:ILE:HB	1:B:670:ILE:O	2.21	0.41
1:B:726:ILE:CG2	1:B:948:LEU:HD13	2.51	0.41
1:B:773:GLU:C	1:B:775:ASP:N	2.72	0.41
1:B:791:THR:HG21	1:B:806:LEU:HD13	2.02	0.41
1:B:1074:ASN:O	1:B:1075:PHE:CG	2.74	0.41
1:C:101:ILE:HA	1:C:242:LEU:HD23	2.02	0.41
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.85	0.41
1:C:226:LEU:HB2	1:C:227:VAL:HG23	2.02	0.41
1:C:409:GLN:CB	1:C:418:ILE:HB	2.51	0.41
1:C:719:THR:CG2	1:C:1068:VAL:HB	2.50	0.41
1:C:805:ILE:H	1:C:805:ILE:HG12	1.68	0.41
1:C:941:THR:HG22	1:C:943:SER:H	1.86	0.41
1:C:1047:TYR:O	1:C:1066:THR:HB	2.20	0.41
2:F:31:ASN:CG	2:F:49:TYR:HA	2.41	0.41
3:G:56:GLY:O	3:G:58:THR:N	2.53	0.41
1:A:226:LEU:HB2	1:A:227:VAL:HG23	2.02	0.41
1:A:273:ARG:HA	1:A:273:ARG:HD3	1.68	0.41
1:A:377:PHE:O	3:E:59:SER:HB3	2.21	0.41
1:A:378:LYS:HA	1:A:378:LYS:HD2	1.74	0.41
1:A:866:THR:C	1:A:868:GLU:N	2.74	0.41
1:A:873:TYR:C	1:A:875:SER:N	2.71	0.41
1:B:226:LEU:CB	1:B:227:VAL:HG23	2.51	0.41
1:B:312:ILE:O	1:B:312:ILE:HG23	2.21	0.41
1:B:587:ILE:HG21	1:B:587:ILE:HD13	1.80	0.41
1:B:759:PHE:HD1	1:B:762:GLN:NE2	2.18	0.41
1:B:915:VAL:O	1:B:916:LEU:C	2.59	0.41
1:B:916:LEU:HD12	1:B:916:LEU:HA	1.53	0.41
1:B:1004:LEU:O	1:B:1005:GLN:C	2.56	0.41
1:C:317:ASN:OD1	1:C:317:ASN:N	2.53	0.41
1:C:386:LYS:HA	1:C:389:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:980:ILE:H	1:C:980:ILE:HG13	1.63	0.41
1:C:982:SER:OG	1:C:983:ARG:N	2.54	0.41
1:C:1074:ASN:O	1:C:1075:PHE:CG	2.74	0.41
2:F:43:PRO:HB2	3:G:110:TRP:CH2	2.56	0.41
1:A:93:ALA:HA	1:A:190:ARG:O	2.20	0.41
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.85	0.41
1:A:328:ARG:HH22	1:A:533:LEU:CB	2.17	0.41
1:A:354:ASN:O	1:A:398:ASP:HA	2.21	0.41
1:A:584:ILE:HA	1:A:584:ILE:HD13	1.77	0.41
1:A:726:ILE:CG2	1:A:948:LEU:HD13	2.51	0.41
1:A:807:PRO:O	1:A:809:PRO:HD3	2.21	0.41
1:A:883:THR:H	1:A:883:THR:HG23	1.72	0.41
1:A:897:PRO:O	1:A:898:PHE:C	2.58	0.41
1:A:950:ASP:O	1:A:953:ASN:N	2.53	0.41
1:A:1074:ASN:O	1:A:1075:PHE:CG	2.74	0.41
1:B:97:LYS:H	1:B:97:LYS:HG2	1.64	0.41
1:B:101:ILE:HA	1:B:242:LEU:HD23	2.02	0.41
1:B:111:ASP:O	1:B:112:SER:HB3	2.21	0.41
1:B:203:ILE:CG2	1:B:204:TYR:N	2.84	0.41
1:B:206:LYS:HA	1:B:206:LYS:HD2	1.92	0.41
1:B:216:LEU:HA	1:B:216:LEU:HD23	1.84	0.41
1:B:331:ASN:N	1:B:580:GLN:HG2	2.36	0.41
1:B:354:ASN:O	1:B:398:ASP:HA	2.21	0.41
1:B:560:LEU:CB	1:B:563:GLN:HB2	2.44	0.41
1:B:864:LEU:HG	1:B:865:LEU:HD12	2.02	0.41
1:B:870:ILE:HG23	1:B:870:ILE:HD12	1.85	0.41
1:B:887:THR:H	1:B:887:THR:HG23	1.64	0.41
1:B:1047:TYR:O	1:B:1066:THR:HB	2.20	0.41
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.92	0.41
1:C:214:ARG:HG2	1:C:215:ASP:HB2	2.03	0.41
1:C:229:LEU:HA	1:C:229:LEU:HD23	1.78	0.41
1:C:279:TYR:CD1	1:C:279:TYR:N	2.89	0.41
1:C:388:ASN:CA	1:C:527:PRO:HD2	2.50	0.41
1:C:457:ARG:NH1	1:C:459:SER:O	2.51	0.41
1:C:560:LEU:CB	1:C:563:GLN:HB2	2.45	0.41
1:C:744:GLY:O	1:C:746:SER:N	2.53	0.41
1:C:929:SER:O	1:C:932:GLY:N	2.54	0.41
2:D:37:GLN:NE2	3:E:39:GLN:OE1	2.52	0.41
3:G:86:LEU:HD23	3:G:86:LEU:HA	1.92	0.41
2:H:26:GLN:HG3	2:H:27:SER:H	1.86	0.41
2:H:45:LEU:HD23	3:I:108:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:85:TYR:N	2:H:101:THR:O	2.47	0.41
3:I:30:SER:HA	3:I:53:PRO:CB	2.51	0.41
1:A:203:ILE:CG2	1:A:204:TYR:N	2.84	0.41
1:A:226:LEU:CB	1:A:227:VAL:HG23	2.51	0.41
1:A:337:PRO:HD2	1:A:358:ILE:HG12	2.03	0.41
1:A:388:ASN:CA	1:A:527:PRO:HD2	2.50	0.41
1:A:543:PHE:O	1:A:546:LEU:HB3	2.20	0.41
1:A:619:GLU:H	1:A:619:GLU:CD	2.14	0.41
1:A:714:ILE:HD13	1:A:1105:THR:HG21	2.01	0.41
1:A:822:LEU:HA	1:A:822:LEU:HD23	1.68	0.41
1:A:904:TYR:O	1:A:905:ARG:C	2.57	0.41
1:A:1093:GLY:HA2	1:A:1107:ARG:NH1	2.31	0.41
1:B:372:ALA:O	2:F:92:PHE:HA	2.20	0.41
1:B:744:GLY:O	1:B:746:SER:N	2.53	0.41
1:C:669:GLY:O	1:C:697:MET:HG2	2.20	0.41
1:C:786:LYS:HG3	1:C:787:GLN:N	2.35	0.41
1:C:854:LYS:HA	1:C:858:LEU:O	2.21	0.41
1:C:1004:LEU:HA	1:C:1004:LEU:HD23	1.71	0.41
3:E:92:ALA:O	3:E:115:THR:HA	2.21	0.41
2:H:32:LEU:HB3	2:H:50:ALA:HB2	2.03	0.41
1:A:45:SER:O	1:A:47:VAL:HG12	2.21	0.40
1:A:64:TRP:NE1	1:A:65:PHE:O	2.53	0.40
1:A:65:PHE:HD2	1:A:265:TYR:OH	2.04	0.40
1:A:216:LEU:HA	1:A:216:LEU:HD23	1.83	0.40
1:A:546:LEU:HD22	1:A:565:PHE:CE1	2.56	0.40
1:A:666:ILE:HB	1:A:670:ILE:O	2.21	0.40
1:A:667:GLY:O	1:A:668:ALA:C	2.59	0.40
1:A:715:PRO:HD3	1:C:894:LEU:CD1	2.51	0.40
1:A:756:TYR:HD1	1:B:970:PHE:HD1	1.69	0.40
1:A:915:VAL:O	1:A:916:LEU:C	2.59	0.40
1:A:941:THR:HG22	1:A:943:SER:H	1.86	0.40
1:A:945:LEU:O	1:A:946:GLY:C	2.59	0.40
1:B:170:TYR:CG	1:B:171:VAL:N	2.90	0.40
1:B:280:ASN:O	1:B:283:GLY:N	2.49	0.40
1:B:337:PRO:HD2	1:B:358:ILE:HG12	2.03	0.40
1:B:667:GLY:O	1:B:668:ALA:C	2.59	0.40
1:B:773:GLU:O	1:B:774:GLN:C	2.57	0.40
1:B:870:ILE:O	1:B:874:THR:HG23	2.21	0.40
1:B:1100:THR:HG1	1:B:1101:HIS:N	2.19	0.40
1:C:48:LEU:HA	1:C:48:LEU:HD23	1.90	0.40
1:C:222:ALA:C	1:C:223:LEU:HD12	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ILE:HG12	1:C:423:TYR:HD2	1.85	0.40
1:C:1139:ASP:OD2	1:C:1142:GLN:N	2.50	0.40
2:D:22:CYS:SG	2:D:32:LEU:HD11	2.62	0.40
2:D:45:LEU:HD23	3:E:108:ASP:OD1	2.21	0.40
3:E:31:ASN:O	3:E:101:TYR:HB2	2.21	0.40
3:G:6:GLN:CD	3:G:111:GLY:HA3	2.41	0.40
2:H:82:PHE:CD2	2:H:105:ILE:HB	2.56	0.40
3:I:4:LEU:CD2	3:I:24:VAL:HG22	2.50	0.40
3:I:28:SER:OG	3:I:31:ASN:HB2	2.22	0.40
3:I:98:ARG:O	3:I:107:MET:HA	2.20	0.40
1:A:413:GLY:HA3	3:E:54:PHE:CE2	2.56	0.40
1:A:419:ALA:C	1:A:424:LYS:HD3	2.42	0.40
1:A:670:ILE:HA	1:A:670:ILE:HD13	1.83	0.40
1:B:99:ASN:O	1:B:102:ARG:NH2	2.53	0.40
1:B:222:ALA:C	1:B:223:LEU:HD12	2.42	0.40
1:B:353:TRP:CG	1:B:423:TYR:CE1	3.09	0.40
1:B:354:ASN:HB2	1:B:399:SER:H	1.85	0.40
1:B:726:ILE:HD13	1:B:945:LEU:CD2	2.51	0.40
1:B:763:LEU:O	1:B:764:ASN:C	2.58	0.40
1:B:894:LEU:CD1	1:C:715:PRO:HD3	2.51	0.40
1:B:941:THR:HG22	1:B:943:SER:H	1.86	0.40
1:B:1116:THR:H	1:B:1119:ASN:HD22	1.68	0.40
1:C:131:CYS:HA	1:C:166:CYS:HA	2.03	0.40
1:C:170:TYR:CG	1:C:171:VAL:N	2.90	0.40
1:C:277:LEU:HA	1:C:277:LEU:HD23	1.48	0.40
1:C:695:TYR:CD1	1:C:695:TYR:N	2.88	0.40
1:C:737:ASP:OD2	1:C:740:MET:HB3	2.22	0.40
1:C:1008:VAL:O	1:C:1009:THR:C	2.57	0.40
2:D:10:GLN:HG3	2:D:20:ILE:HG12	2.02	0.40
2:D:32:LEU:HB3	2:D:50:ALA:HB2	2.03	0.40
1:A:32:PHE:HA	1:A:59:PHE:CD1	2.56	0.40
1:A:131:CYS:HA	1:A:166:CYS:HA	2.03	0.40
1:A:142:GLY:H	1:A:156:GLU:CB	2.34	0.40
1:A:212:LEU:HD11	1:A:214:ARG:NH1	2.37	0.40
1:A:312:ILE:O	1:A:312:ILE:HG23	2.21	0.40
1:A:327:VAL:HB	1:A:531:THR:HG23	2.04	0.40
1:A:331:ASN:N	1:A:580:GLN:HG2	2.36	0.40
1:A:455:LEU:HG	1:A:456:PHE:CD2	2.57	0.40
1:B:108:THR:HG22	1:B:236:THR:HG23	2.02	0.40
1:B:142:GLY:H	1:B:156:GLU:CB	2.34	0.40
1:B:543:PHE:O	1:B:546:LEU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:LYS:HG3	1:B:787:GLN:N	2.35	0.40
1:C:37:TYR:HB2	1:C:223:LEU:O	2.22	0.40
1:C:203:ILE:CG2	1:C:204:TYR:N	2.84	0.40
1:C:224:GLU:CD	1:C:224:GLU:N	2.72	0.40
1:C:643:PHE:CD1	1:C:655:HIS:HB2	2.55	0.40
1:C:666:ILE:HB	1:C:670:ILE:O	2.21	0.40
1:C:667:GLY:O	1:C:668:ALA:C	2.59	0.40
2:D:34:TRP:CD1	2:D:47:ILE:HB	2.55	0.40
3:E:4:LEU:O	3:E:111:GLY:HA2	2.22	0.40
2:F:29:SER:OG	2:F:91:ASN:OD1	2.26	0.40
3:G:34:ILE:HB	3:G:51:ILE:HG22	2.03	0.40
2:H:34:TRP:CD1	2:H:47:ILE:HB	2.55	0.40
3:I:92:ALA:O	3:I:115:THR:HA	2.21	0.40
4:X:1:NAG:H62	4:X:2:NAG:H82	2.04	0.40
1:A:31:SER:OG	1:A:60:SER:N	2.55	0.40
1:A:37:TYR:HB2	1:A:223:LEU:O	2.21	0.40
1:A:907:ASN:N	1:A:907:ASN:OD1	2.52	0.40
1:A:917:TYR:HD2	1:B:1089:PHE:CE2	2.40	0.40
1:A:934:ILE:HD12	1:A:934:ILE:HG23	1.67	0.40
1:B:31:SER:OG	1:B:60:SER:N	2.55	0.40
1:B:45:SER:O	1:B:47:VAL:HG12	2.21	0.40
1:B:131:CYS:HA	1:B:166:CYS:HA	2.03	0.40
1:B:214:ARG:HG2	1:B:215:ASP:HB2	2.03	0.40
1:B:453:TYR:CD1	1:B:495:TYR:CE2	3.10	0.40
1:B:1100:THR:HG1	1:B:1101:HIS:CE1	2.33	0.40
1:C:31:SER:OG	1:C:60:SER:N	2.55	0.40
1:C:142:GLY:H	1:C:156:GLU:CB	2.34	0.40
1:C:212:LEU:HD11	1:C:214:ARG:NH1	2.37	0.40
1:C:226:LEU:CB	1:C:227:VAL:HG23	2.51	0.40
3:E:22:CYS:O	3:E:78:THR:HA	2.21	0.40
3:E:97:ALA:HB1	3:E:107:MET:CB	2.50	0.40
3:I:6:GLN:N	3:I:112:GLN:HE22	2.19	0.40
3:I:22:CYS:O	3:I:78:THR:HA	2.21	0.40
1:A:106:PHE:HB3	1:A:235:ILE:HD13	2.04	0.40
1:A:725:GLU:C	1:A:726:ILE:HG13	2.42	0.40
1:A:737:ASP:OD2	1:A:740:MET:HB3	2.22	0.40
1:A:763:LEU:O	1:A:764:ASN:C	2.58	0.40
1:A:786:LYS:HG3	1:A:787:GLN:N	2.35	0.40
1:A:870:ILE:O	1:A:874:THR:HG23	2.21	0.40
1:A:1024:LEU:HA	1:A:1024:LEU:HD12	1.72	0.40
1:B:32:PHE:HA	1:B:59:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:ND2	1:B:239:GLN:HE21	2.19	0.40
1:B:231:ILE:HG13	1:B:232:GLY:H	1.85	0.40
1:B:347:PHE:CE2	1:B:509:ARG:HD3	2.57	0.40
1:B:430:THR:HG21	1:B:517:LEU:CG	2.50	0.40
1:B:737:ASP:OD2	1:B:740:MET:HB3	2.22	0.40
1:B:802:PHE:O	1:B:803:SER:C	2.56	0.40
1:B:977:LEU:HA	1:B:977:LEU:HD12	1.75	0.40
1:B:1086:LYS:HE2	1:B:1086:LYS:HB2	1.89	0.40
1:C:45:SER:O	1:C:47:VAL:HG12	2.21	0.40
1:C:317:ASN:HB2	1:C:593:GLY:O	2.17	0.40
1:C:985:ASP:N	1:C:988:GLU:OE1	2.52	0.40
2:D:35:TYR:CE2	2:D:45:LEU:HB2	2.57	0.40
2:D:57:ILE:CG2	2:D:61:PHE:HD2	2.34	0.40
2:D:87:CYS:O	2:D:98:GLY:N	2.46	0.40
3:I:35:HIS:HB3	3:I:47:TRP:HE1	1.85	0.40
4:S:1:NAG:H62	4:S:2:NAG:H82	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1012/1208 (84%)	899 (89%)	106 (10%)	7 (1%)	19 53
1	B	1012/1208 (84%)	906 (90%)	101 (10%)	5 (0%)	25 59
1	C	1012/1208 (84%)	900 (89%)	106 (10%)	6 (1%)	22 55
2	D	105/210 (50%)	96 (91%)	8 (8%)	1 (1%)	13 46
2	F	105/210 (50%)	98 (93%)	6 (6%)	1 (1%)	13 46
2	H	105/210 (50%)	96 (91%)	8 (8%)	1 (1%)	13 46
3	E	120/223 (54%)	113 (94%)	4 (3%)	3 (2%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	120/223 (54%)	112 (93%)	5 (4%)	3 (2%)	4 29
3	I	120/223 (54%)	112 (93%)	5 (4%)	3 (2%)	4 29
All	All	3711/4923 (75%)	3332 (90%)	349 (9%)	30 (1%)	19 51

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	856	ASN
3	G	102	ASP
3	I	102	ASP
1	A	332	ILE
1	A	557	LYS
1	A	857	GLY
1	B	332	ILE
1	C	332	ILE
3	E	104	TYR
1	A	161	SER
1	B	161	SER
1	C	161	SER
1	A	902	MET
1	B	902	MET
1	C	902	MET
3	E	57	GLY
3	E	102	ASP
3	I	57	GLY
3	I	104	TYR
2	F	93	TRP
3	G	103	PRO
1	A	1033	VAL
1	B	1033	VAL
1	C	1033	VAL
2	D	93	TRP
2	H	93	TRP
3	G	57	GLY
1	A	770	ILE
1	B	770	ILE
1	C	770	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	896/1054 (85%)	884 (99%)	12 (1%)	65 82
1	B	897/1054 (85%)	881 (98%)	16 (2%)	54 74
1	C	897/1054 (85%)	880 (98%)	17 (2%)	52 73
2	D	95/189 (50%)	95 (100%)	0	100 100
2	F	95/189 (50%)	95 (100%)	0	100 100
2	H	95/189 (50%)	95 (100%)	0	100 100
3	E	101/190 (53%)	100 (99%)	1 (1%)	73 85
3	G	101/190 (53%)	100 (99%)	1 (1%)	73 85
3	I	101/190 (53%)	100 (99%)	1 (1%)	73 85
All	All	3278/4299 (76%)	3230 (98%)	48 (2%)	60 79

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ARG
1	A	556	ASN
1	A	558	LYS
1	A	559	PHE
1	A	560	LEU
1	A	599	THR
1	A	800	PHE
1	A	850	ILE
1	A	855	PHE
1	A	861	LEU
1	A	1077	THR
1	A	1089	PHE
1	B	319	ARG
1	B	321	GLN
1	B	324	GLU
1	B	558	LYS
1	B	559	PHE
1	B	560	LEU

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Mol	Chain	Res	Type
1	B	564	GLN
1	B	565	PHE
1	B	599	THR
1	B	800	PHE
1	B	849	LEU
1	B	850	ILE
1	B	854	LYS
1	B	864	LEU
1	B	1077	THR
1	B	1089	PHE
1	C	317	ASN
1	C	319	ARG
1	C	321	GLN
1	C	324	GLU
1	C	325	SER
1	C	559	PHE
1	C	560	LEU
1	C	563	GLN
1	C	564	GLN
1	C	599	THR
1	C	800	PHE
1	C	849	LEU
1	C	854	LYS
1	C	864	LEU
1	C	865	LEU
1	C	1077	THR
1	C	1089	PHE
3	E	102	ASP
3	G	104	TYR
3	I	104	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	69	HIS
1	A	164	ASN
1	A	196	ASN
1	A	207	HIS
1	A	239	GLN
1	A	317	ASN
1	A	354	ASN

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Mol	Chain	Res	Type
1	A	414	GLN
1	A	437	ASN
1	A	655	HIS
1	A	779	GLN
1	A	804	GLN
1	A	901	GLN
1	A	935	GLN
1	A	1119	ASN
1	B	66	HIS
1	B	69	HIS
1	B	164	ASN
1	B	196	ASN
1	B	207	HIS
1	B	239	GLN
1	B	317	ASN
1	B	354	ASN
1	B	437	ASN
1	B	655	HIS
1	B	779	GLN
1	B	901	GLN
1	B	1119	ASN
1	C	66	HIS
1	C	69	HIS
1	C	164	ASN
1	C	196	ASN
1	C	207	HIS
1	C	239	GLN
1	C	354	ASN
1	C	437	ASN
1	C	655	HIS
1	C	779	GLN
1	C	804	GLN
1	C	901	GLN
1	C	935	GLN
1	C	1119	ASN
2	D	10	GLN
2	D	99	GLN
2	F	6	GLN
2	F	10	GLN
2	F	99	GLN
3	G	31	ASN
2	H	99	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

30 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	J	1	1,4	14,14,15	1.45	2 (14%)	17,19,21	1.45	2 (11%)
4	NAG	J	2	4	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
4	NAG	K	1	1,4	14,14,15	1.20	2 (14%)	17,19,21	0.60	0
4	NAG	K	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.61	0
4	NAG	L	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	0.68	0
4	NAG	L	2	4	14,14,15	1.08	1 (7%)	17,19,21	0.73	0
4	NAG	M	1	1,4	14,14,15	1.10	2 (14%)	17,19,21	0.78	0
4	NAG	M	2	4	14,14,15	0.34	0	17,19,21	0.44	0
4	NAG	N	1	1,4	14,14,15	1.33	2 (14%)	17,19,21	0.50	0
4	NAG	N	2	4	14,14,15	0.61	0	17,19,21	0.58	0
4	NAG	O	1	1,4	14,14,15	1.44	2 (14%)	17,19,21	1.45	2 (11%)
4	NAG	O	2	4	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
4	NAG	P	1	1,4	14,14,15	1.21	2 (14%)	17,19,21	0.59	0
4	NAG	P	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.61	0
4	NAG	Q	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	0.67	0
4	NAG	Q	2	4	14,14,15	1.08	1 (7%)	17,19,21	0.73	0
4	NAG	R	1	1,4	14,14,15	1.09	2 (14%)	17,19,21	0.78	0
4	NAG	R	2	4	14,14,15	0.33	0	17,19,21	0.44	0
4	NAG	S	1	1,4	14,14,15	1.34	2 (14%)	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	S	2	4	14,14,15	0.61	0	17,19,21	0.58	0
4	NAG	T	1	1,4	14,14,15	1.45	2 (14%)	17,19,21	1.45	2 (11%)
4	NAG	T	2	4	14,14,15	0.35	0	17,19,21	0.80	1 (5%)
4	NAG	U	1	1,4	14,14,15	1.20	2 (14%)	17,19,21	0.60	0
4	NAG	U	2	4	14,14,15	0.69	1 (7%)	17,19,21	0.62	0
4	NAG	V	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	0.67	0
4	NAG	V	2	4	14,14,15	1.07	1 (7%)	17,19,21	0.73	0
4	NAG	W	1	1,4	14,14,15	1.09	2 (14%)	17,19,21	0.78	0
4	NAG	W	2	4	14,14,15	0.33	0	17,19,21	0.44	0
4	NAG	X	1	1,4	14,14,15	1.34	2 (14%)	17,19,21	0.51	0
4	NAG	X	2	4	14,14,15	0.61	0	17,19,21	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-4.80	1.36	1.43
4	T	1	NAG	O5-C1	-4.80	1.36	1.43
4	O	1	NAG	O5-C1	-4.79	1.36	1.43
4	S	1	NAG	O5-C1	-4.32	1.36	1.43
4	X	1	NAG	O5-C1	-4.32	1.36	1.43
4	N	1	NAG	O5-C1	-4.31	1.36	1.43
4	L	2	NAG	O5-C1	-3.92	1.37	1.43
4	Q	2	NAG	O5-C1	-3.91	1.37	1.43
4	V	2	NAG	O5-C1	-3.87	1.37	1.43
4	U	1	NAG	O5-C1	-3.54	1.38	1.43
4	K	1	NAG	O5-C1	-3.54	1.38	1.43
4	P	1	NAG	O5-C1	-3.53	1.38	1.43
4	M	1	NAG	O5-C1	-2.74	1.39	1.43
4	R	1	NAG	O5-C1	-2.74	1.39	1.43
4	W	1	NAG	O5-C1	-2.72	1.39	1.43
4	M	1	NAG	C1-C2	-2.60	1.48	1.52
4	R	1	NAG	C1-C2	-2.55	1.48	1.52
4	W	1	NAG	C1-C2	-2.54	1.48	1.52
4	K	2	NAG	O5-C1	-2.50	1.39	1.43
4	P	2	NAG	O5-C1	-2.49	1.39	1.43
4	U	2	NAG	O5-C1	-2.46	1.39	1.43
4	L	1	NAG	O5-C1	-2.38	1.39	1.43
4	Q	1	NAG	O5-C1	-2.34	1.40	1.43
4	V	1	NAG	O5-C1	-2.34	1.40	1.43
4	P	1	NAG	C1-C2	-2.31	1.48	1.52
4	U	1	NAG	C1-C2	-2.24	1.49	1.52
4	X	1	NAG	C1-C2	-2.23	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	C1-C2	-2.22	1.49	1.52
4	N	1	NAG	C1-C2	-2.21	1.49	1.52
4	S	1	NAG	C1-C2	-2.21	1.49	1.52
4	J	1	NAG	C1-C2	-2.20	1.49	1.52
4	K	1	NAG	C1-C2	-2.19	1.49	1.52
4	O	1	NAG	C1-C2	-2.14	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1	NAG	C3-C4-C5	4.52	118.30	110.24
4	O	1	NAG	C3-C4-C5	4.52	118.30	110.24
4	T	1	NAG	C3-C4-C5	4.51	118.29	110.24
4	T	2	NAG	C1-O5-C5	2.80	115.99	112.19
4	O	2	NAG	C1-O5-C5	2.78	115.96	112.19
4	J	2	NAG	C1-O5-C5	2.75	115.92	112.19
4	T	1	NAG	O4-C4-C5	-2.08	104.14	109.30
4	O	1	NAG	O4-C4-C5	-2.07	104.16	109.30
4	J	1	NAG	O4-C4-C5	-2.06	104.18	109.30

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6

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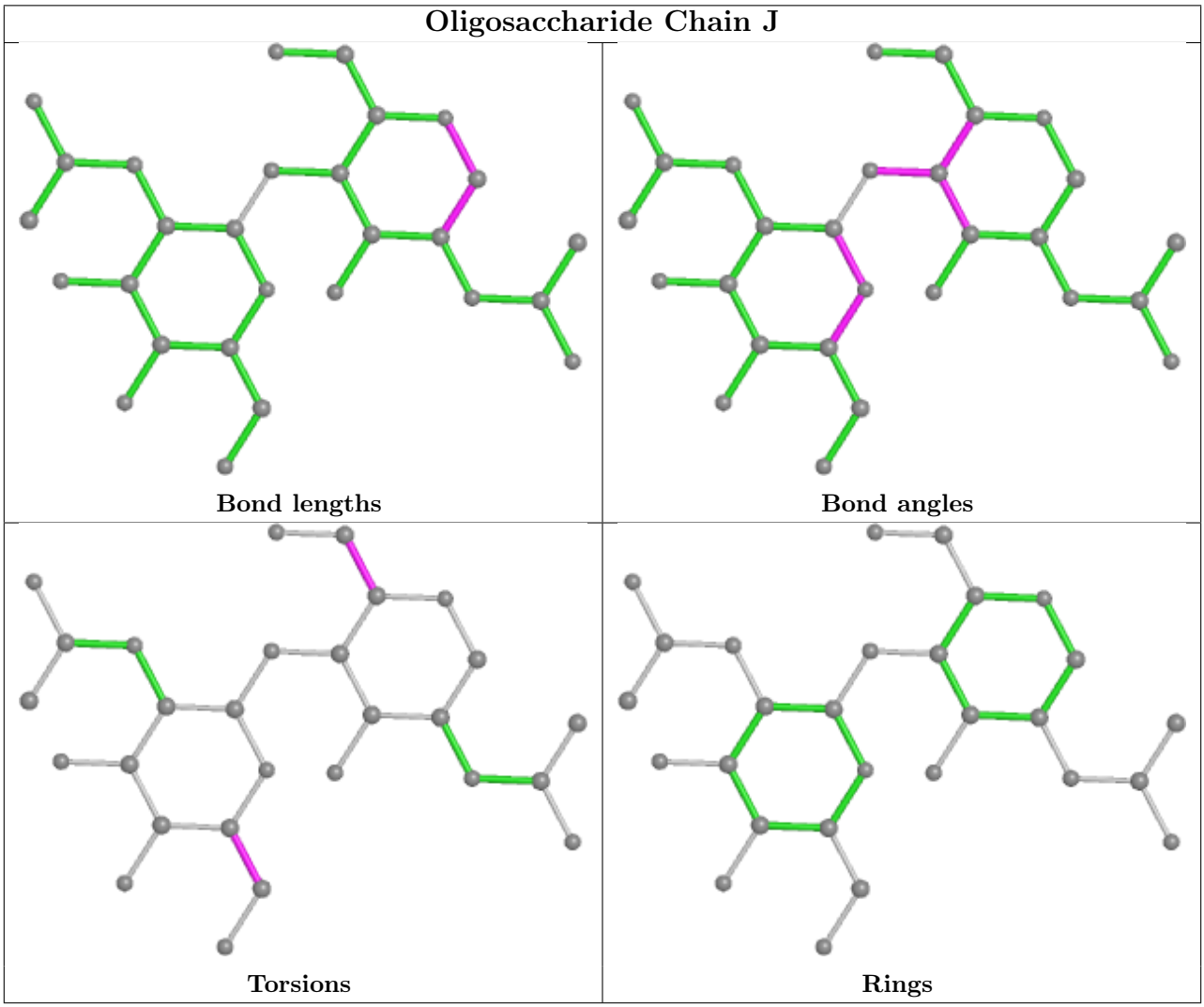
Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7

There are no ring outliers.

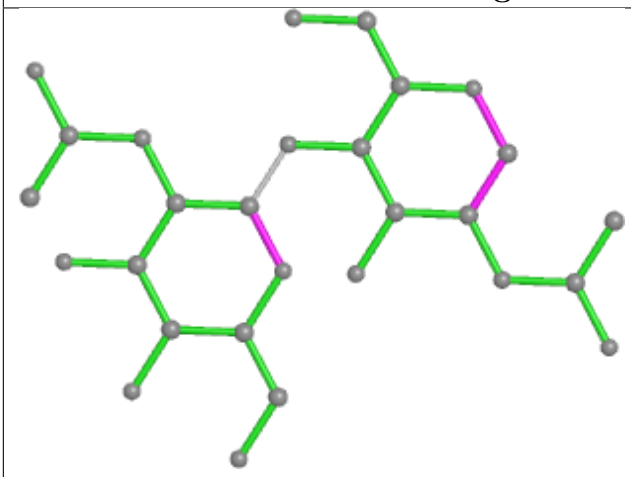
10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	1	0
4	O	1	NAG	1	0
4	L	1	NAG	2	0
4	J	1	NAG	1	0
4	X	1	NAG	1	0
4	T	1	NAG	1	0
4	S	2	NAG	1	0
4	X	2	NAG	1	0
4	V	1	NAG	2	0
4	Q	1	NAG	2	0

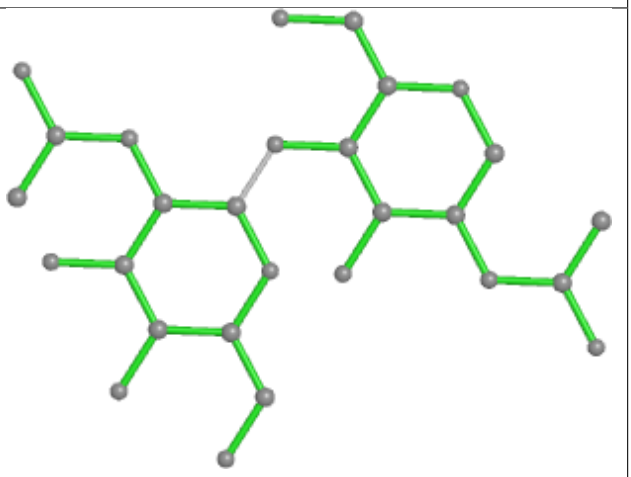
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



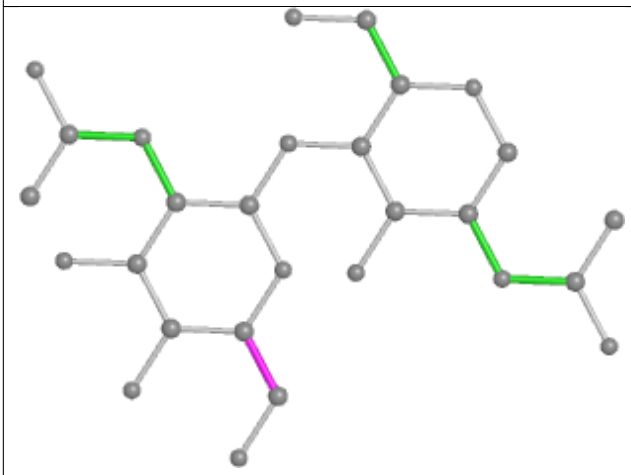
Oligosaccharide Chain K



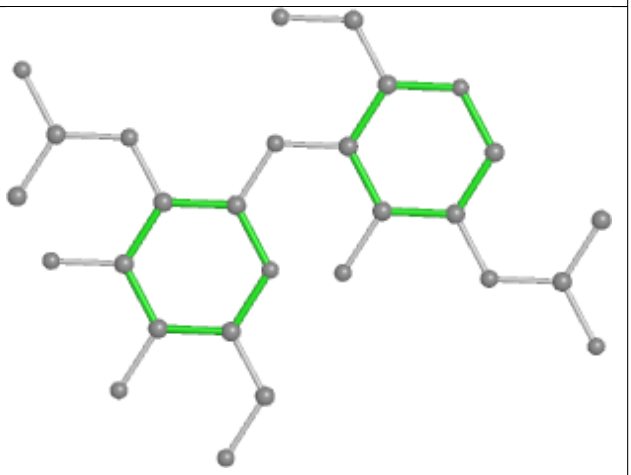
Bond lengths



Bond angles

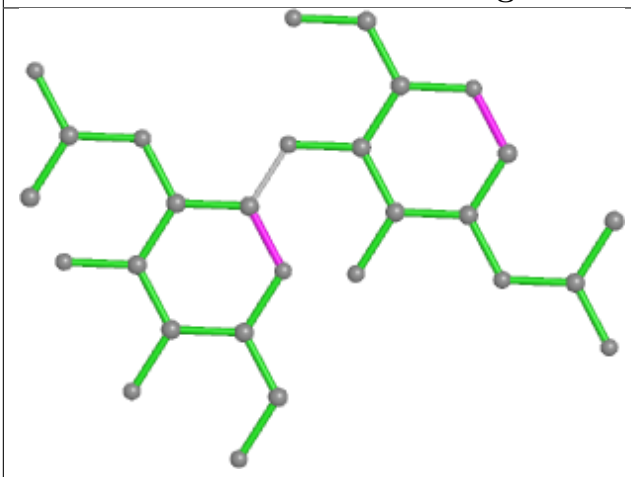


Torsions

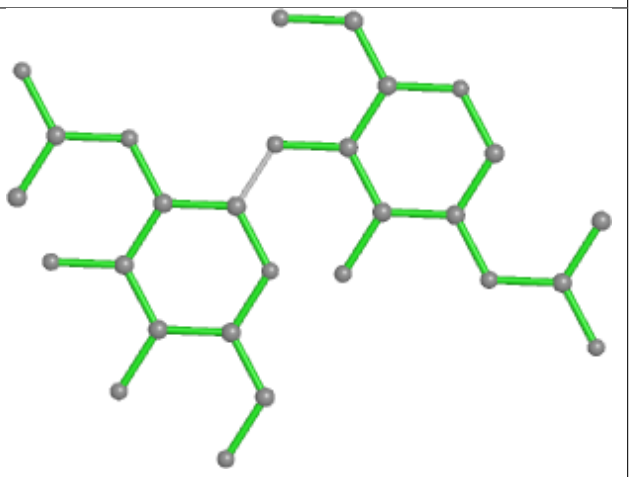


Rings

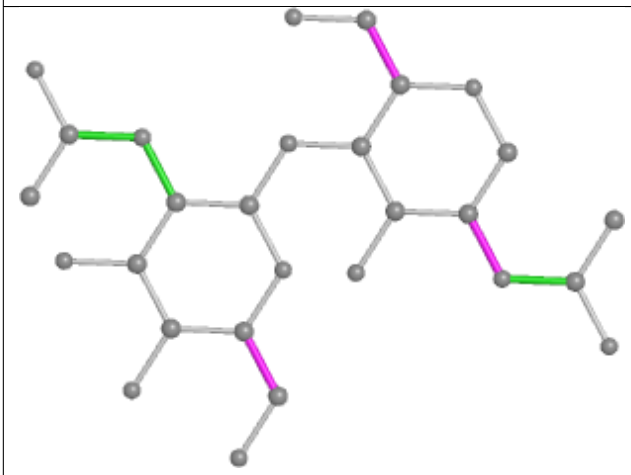
Oligosaccharide Chain L



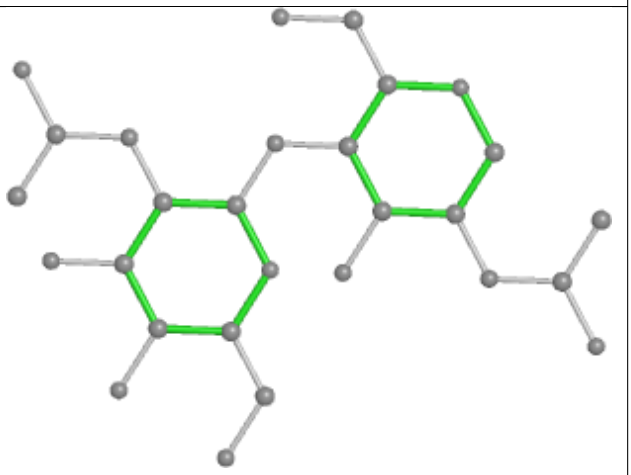
Bond lengths



Bond angles

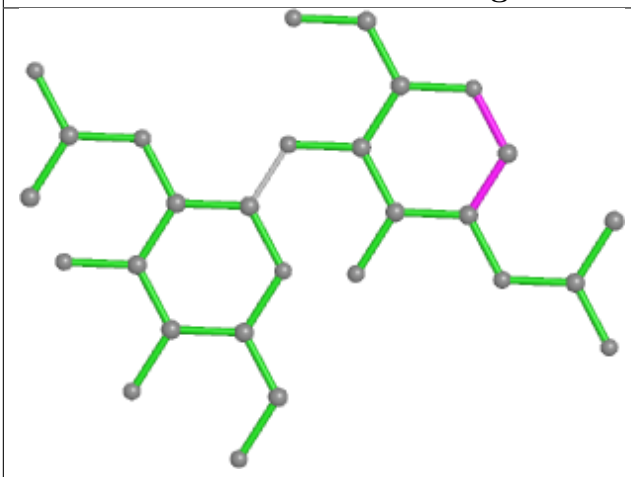


Torsions

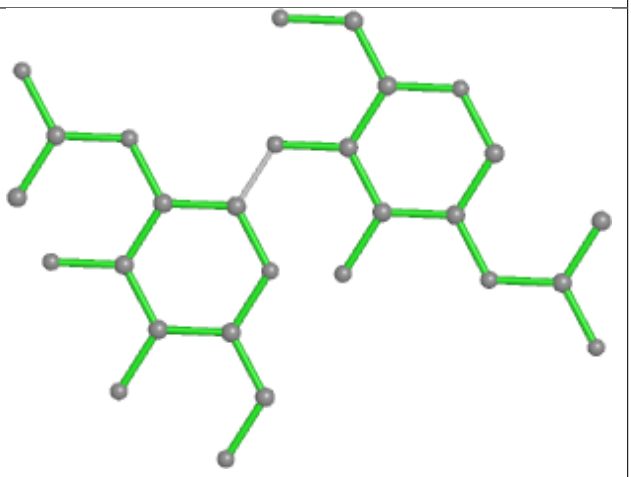


Rings

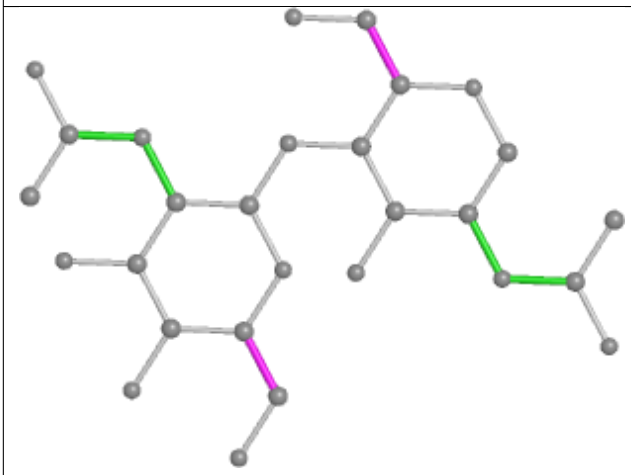
Oligosaccharide Chain M



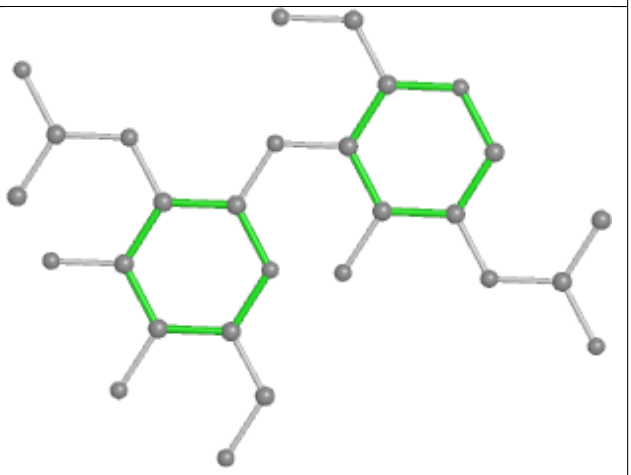
Bond lengths



Bond angles

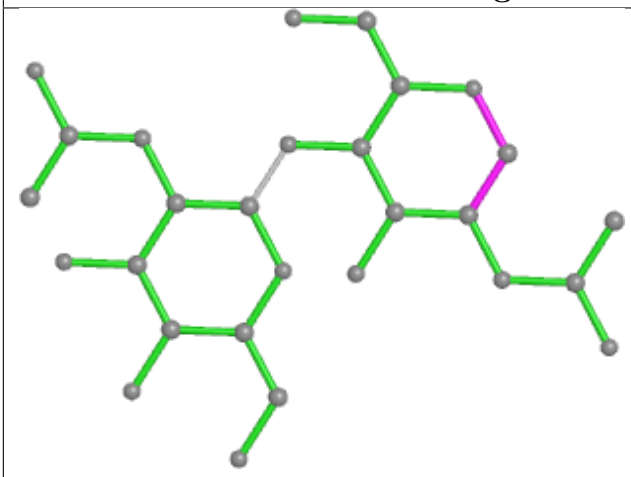


Torsions

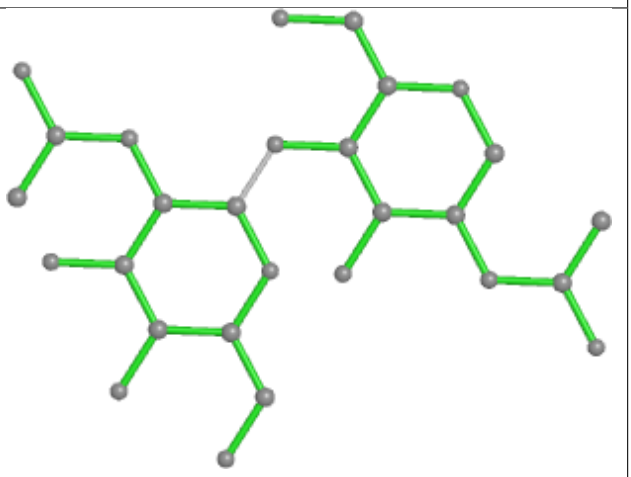


Rings

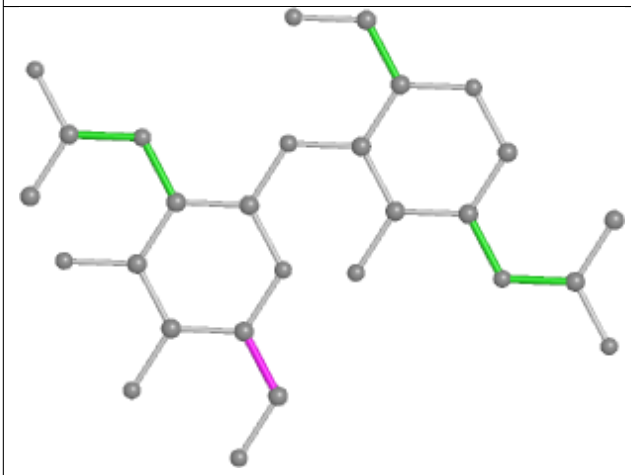
Oligosaccharide Chain N



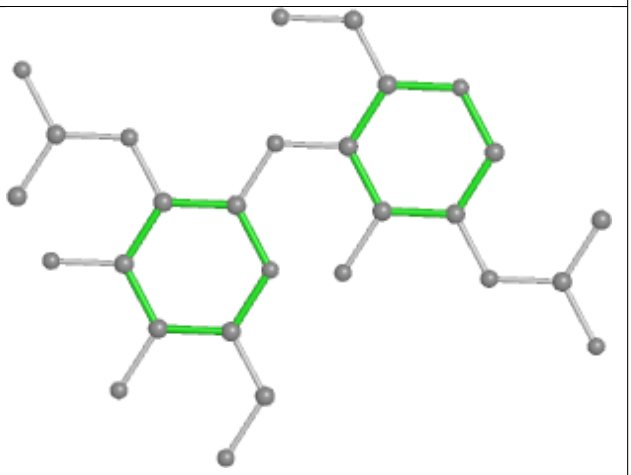
Bond lengths



Bond angles

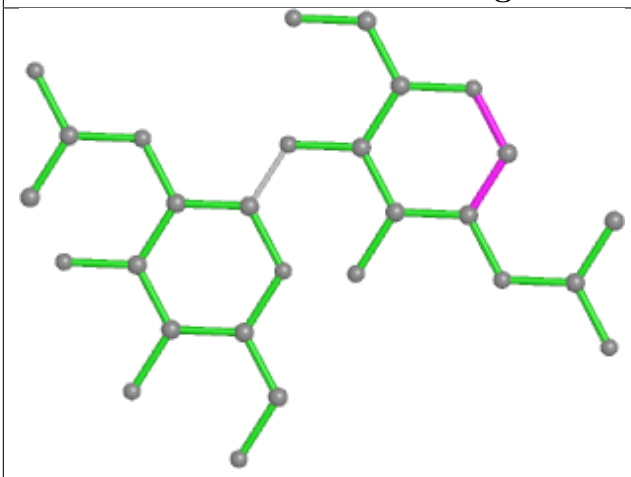


Torsions

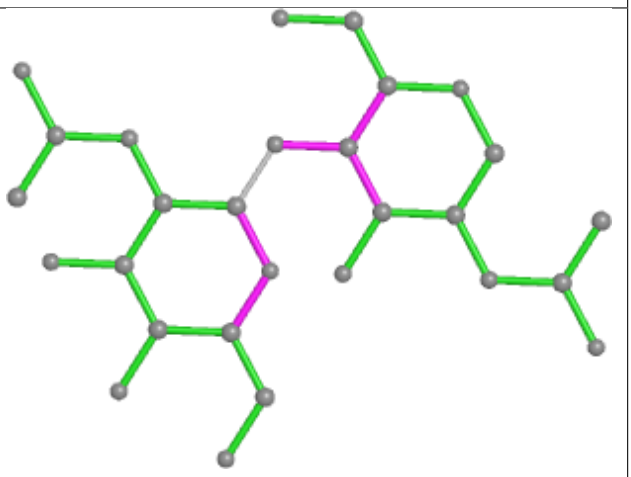


Rings

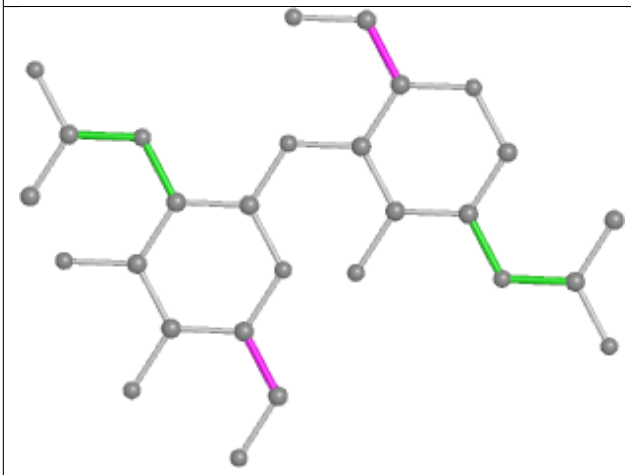
Oligosaccharide Chain O



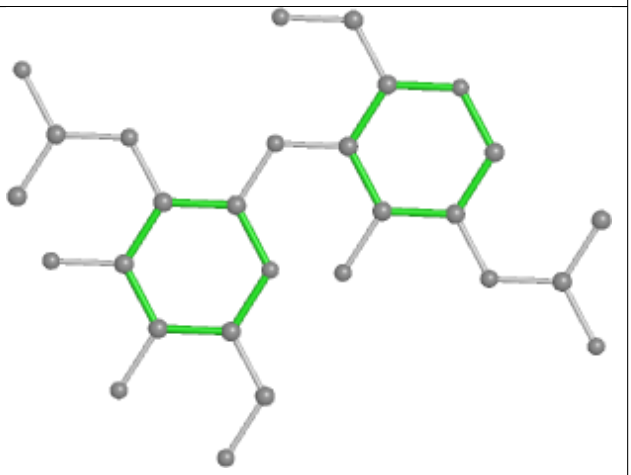
Bond lengths



Bond angles

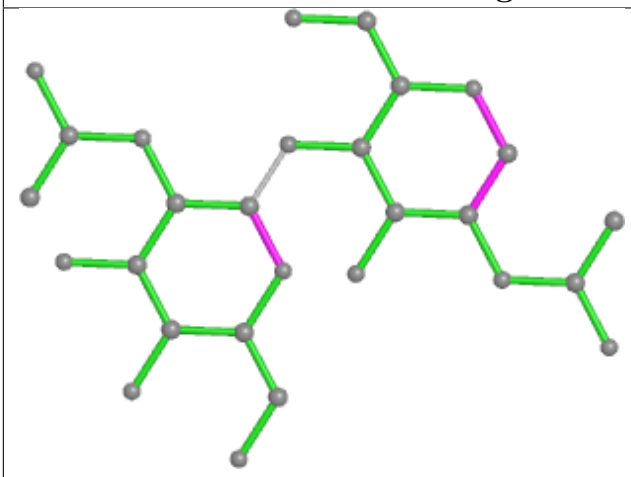


Torsions

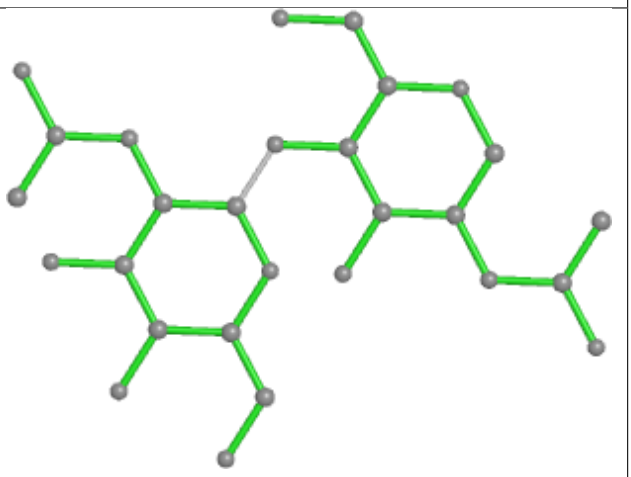


Rings

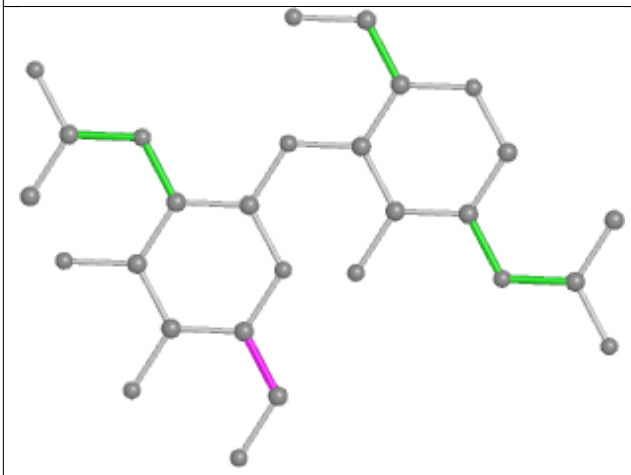
Oligosaccharide Chain P



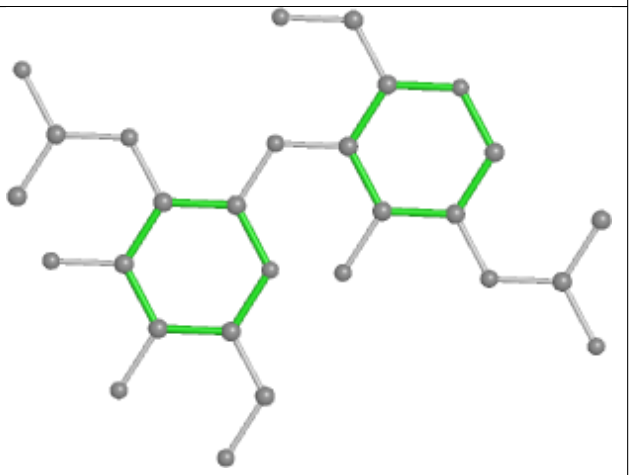
Bond lengths



Bond angles

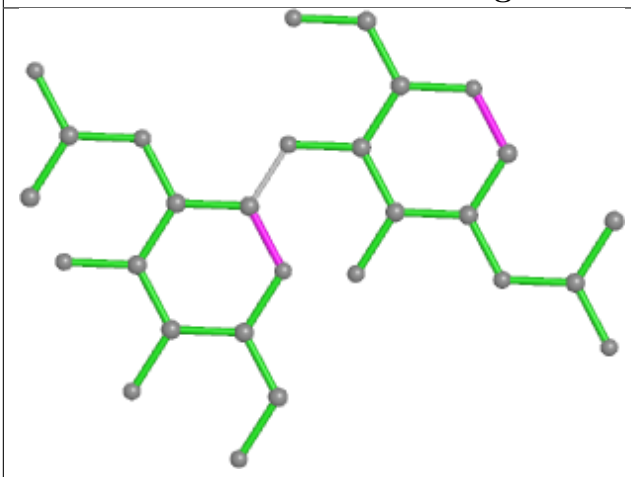


Torsions

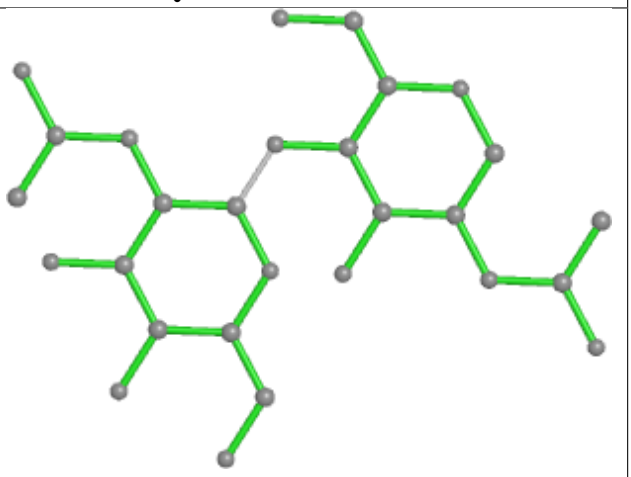


Rings

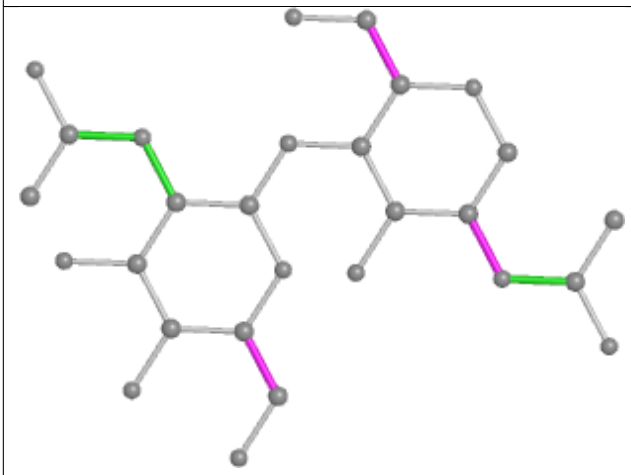
Oligosaccharide Chain Q



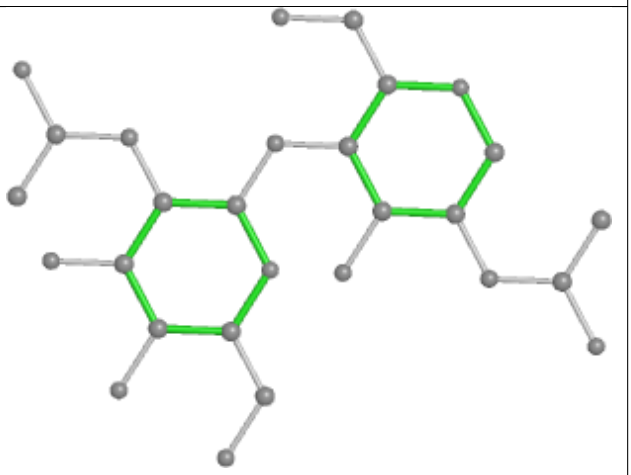
Bond lengths



Bond angles

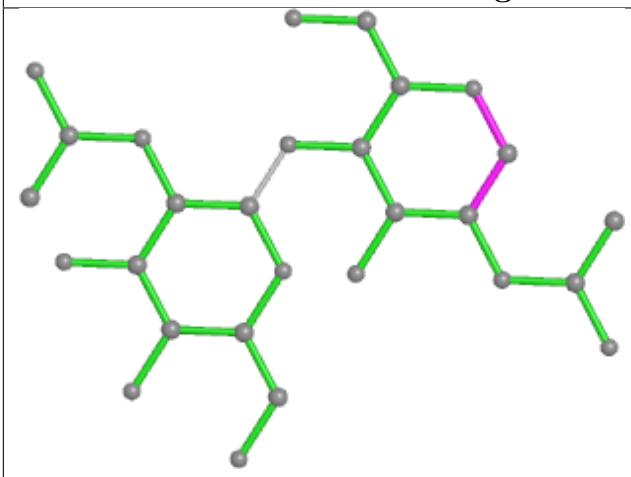


Torsions

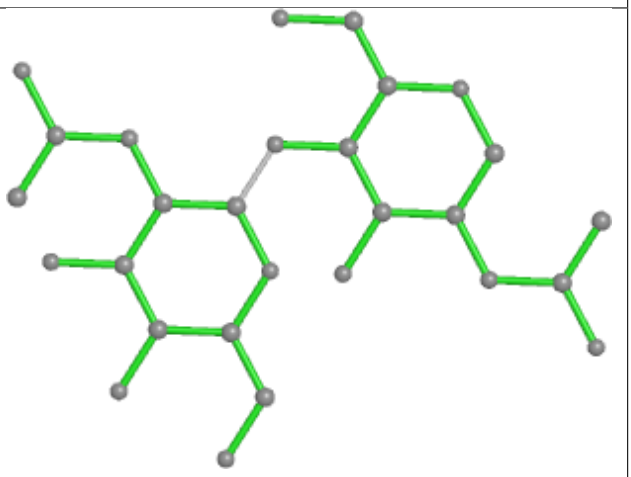


Rings

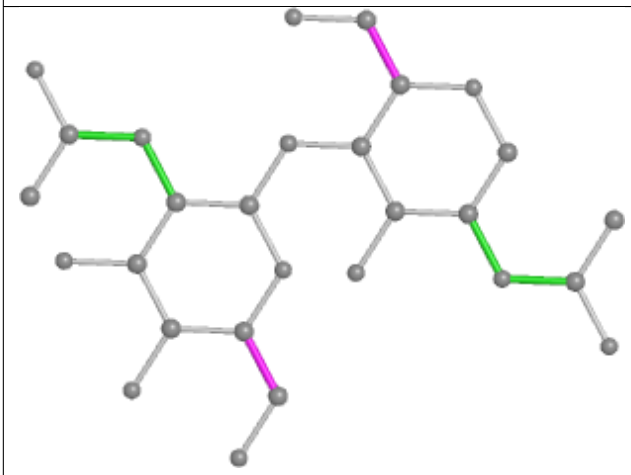
Oligosaccharide Chain R



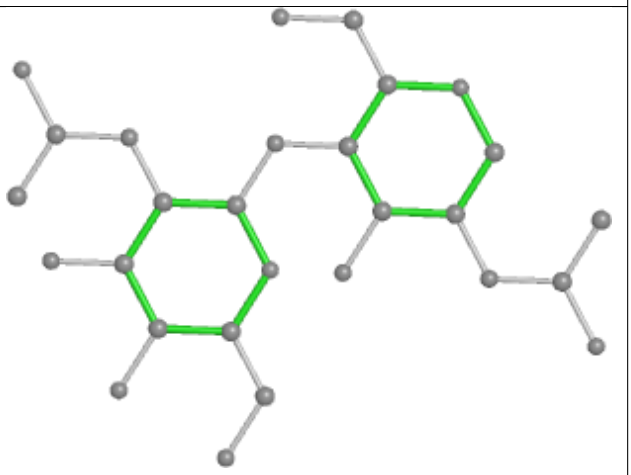
Bond lengths



Bond angles

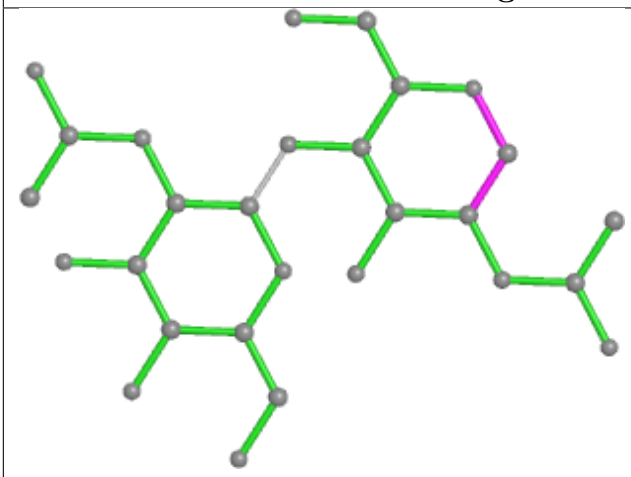


Torsions

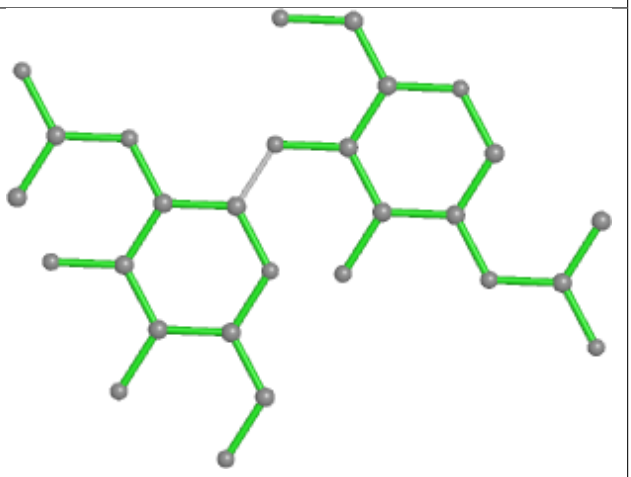


Rings

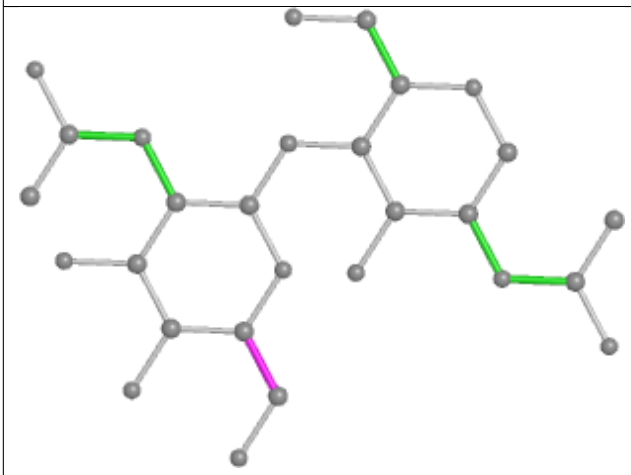
Oligosaccharide Chain S



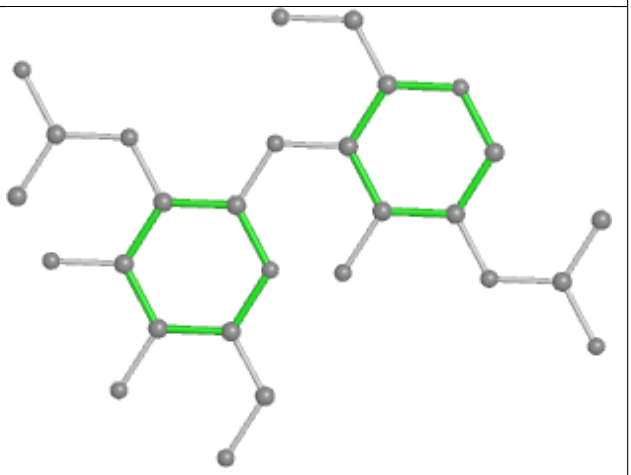
Bond lengths



Bond angles

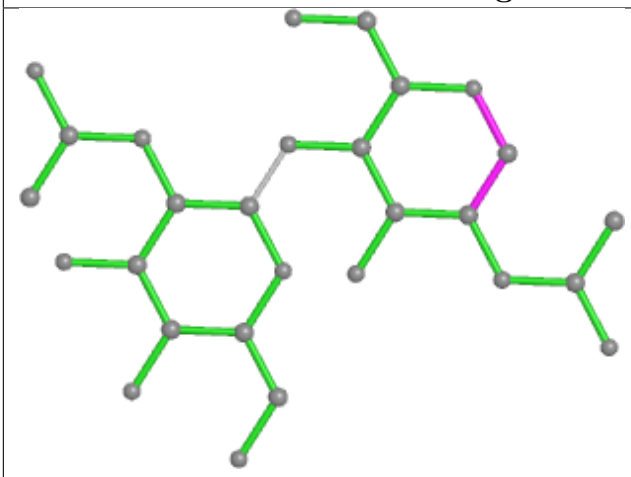


Torsions

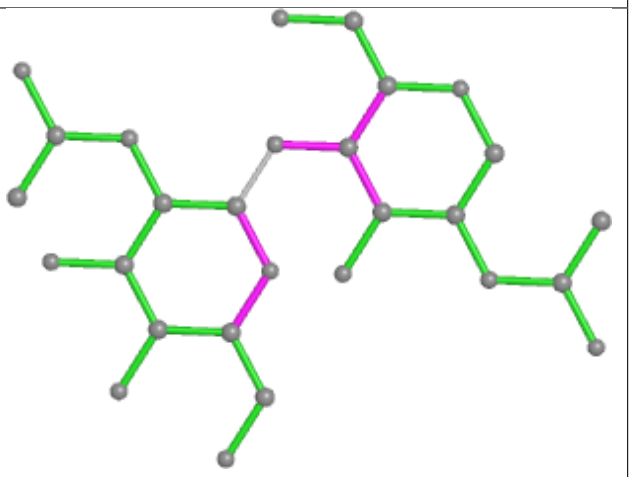


Rings

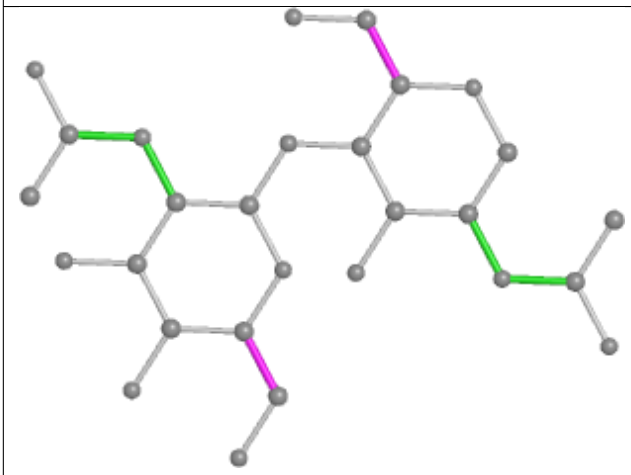
Oligosaccharide Chain T



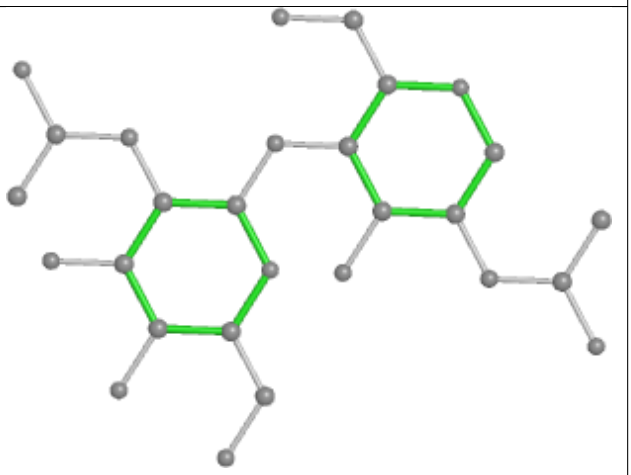
Bond lengths



Bond angles

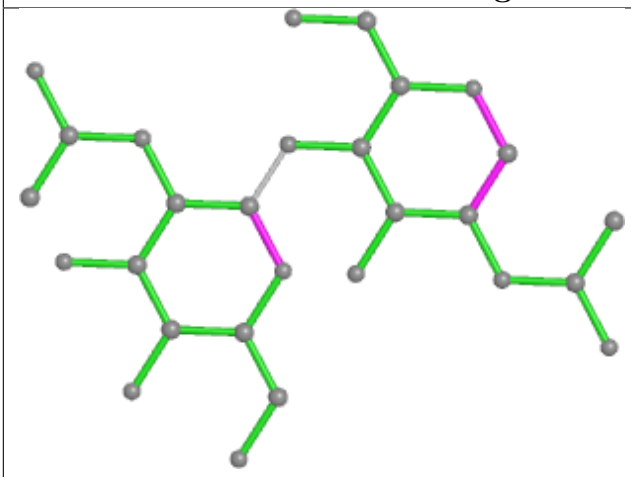


Torsions

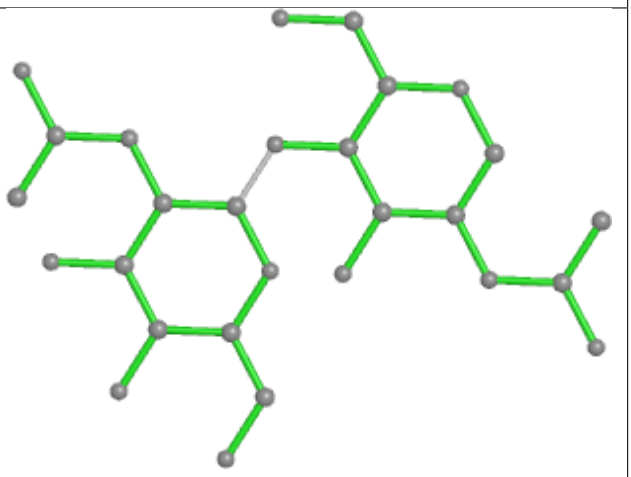


Rings

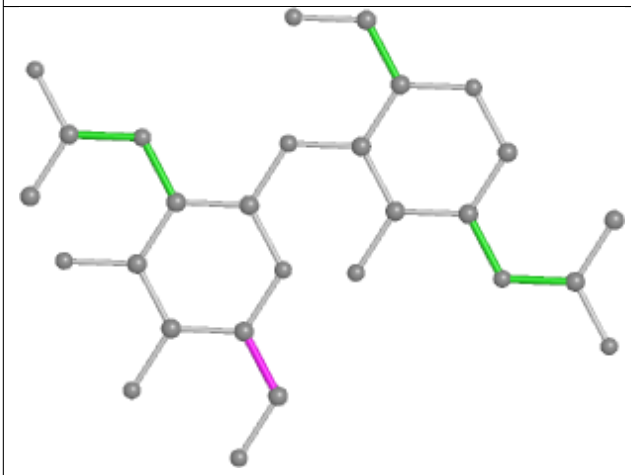
Oligosaccharide Chain U



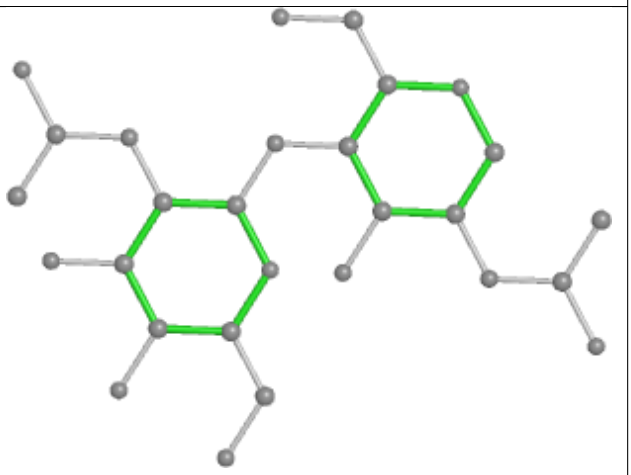
Bond lengths



Bond angles

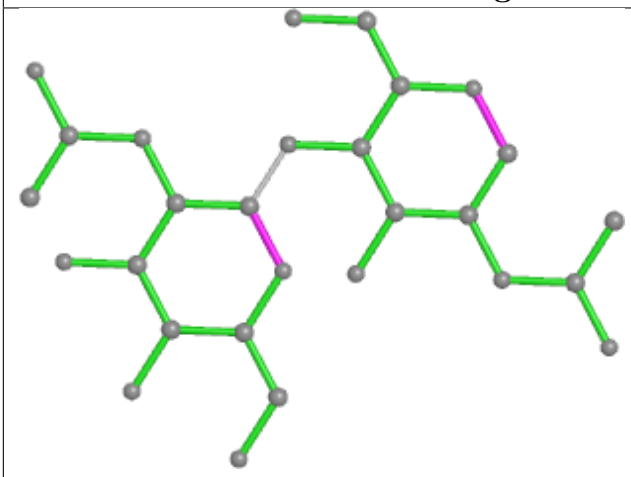


Torsions

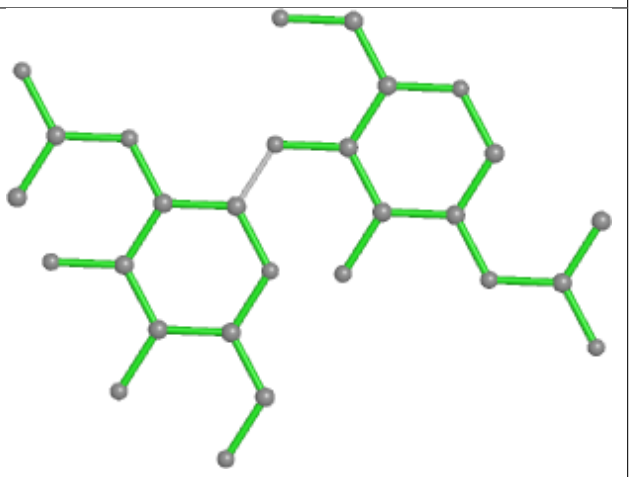


Rings

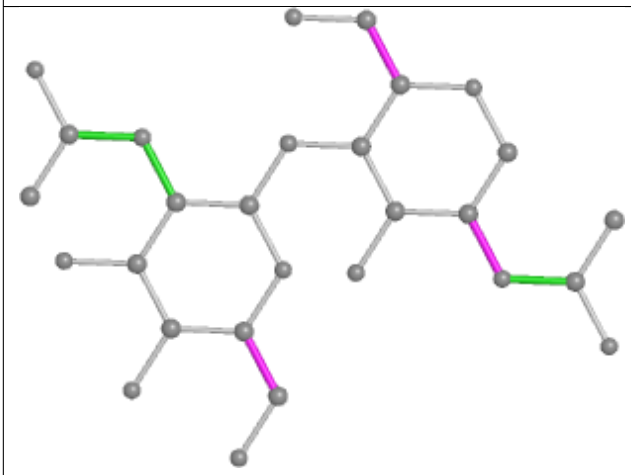
Oligosaccharide Chain V



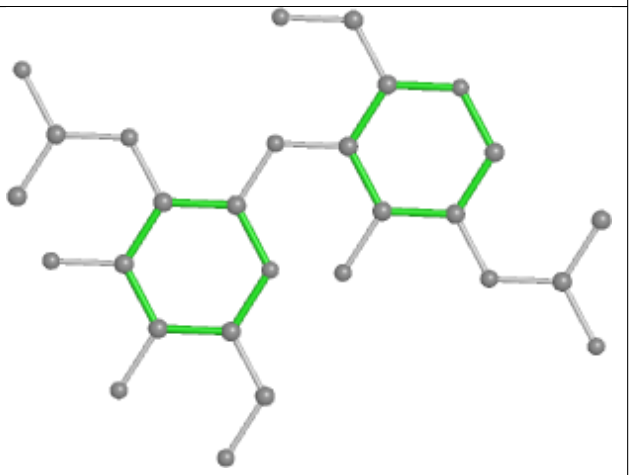
Bond lengths



Bond angles

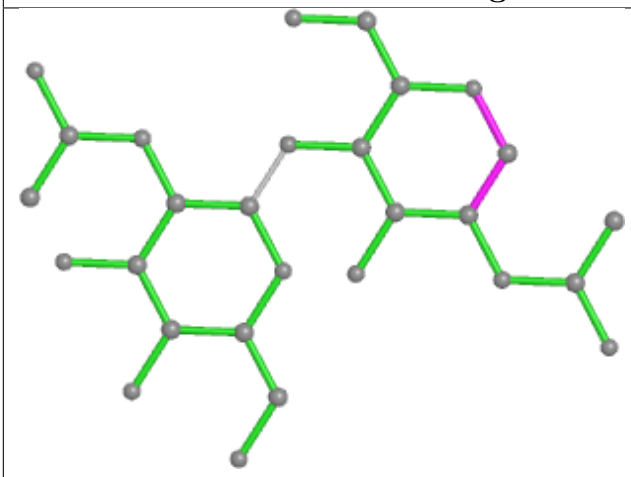


Torsions

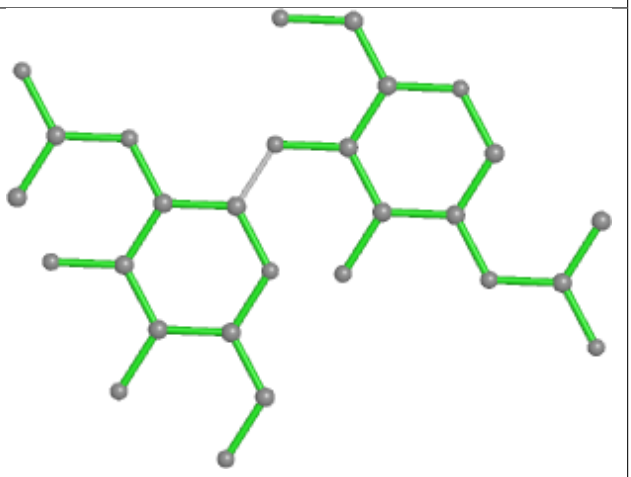


Rings

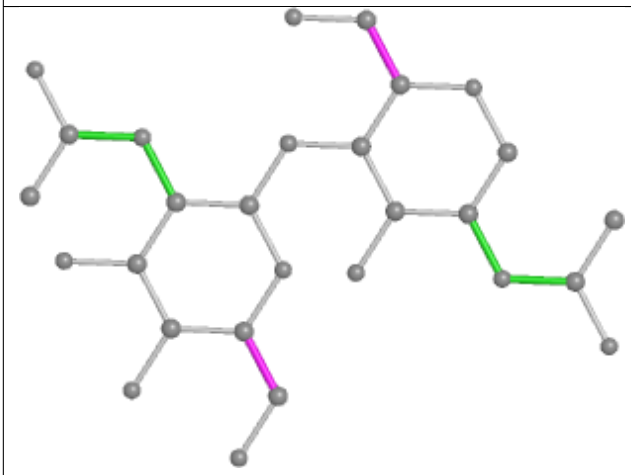
Oligosaccharide Chain W



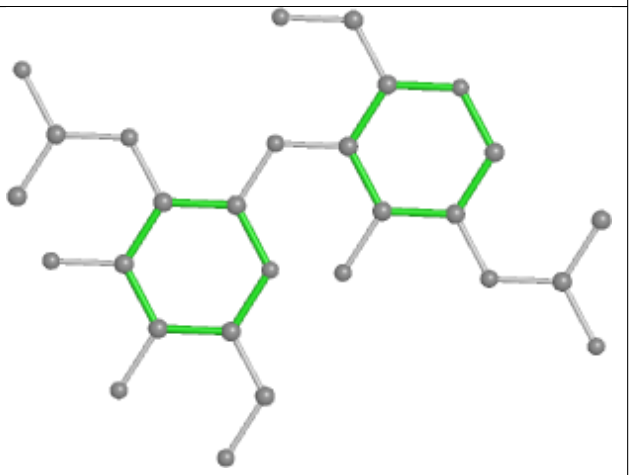
Bond lengths



Bond angles

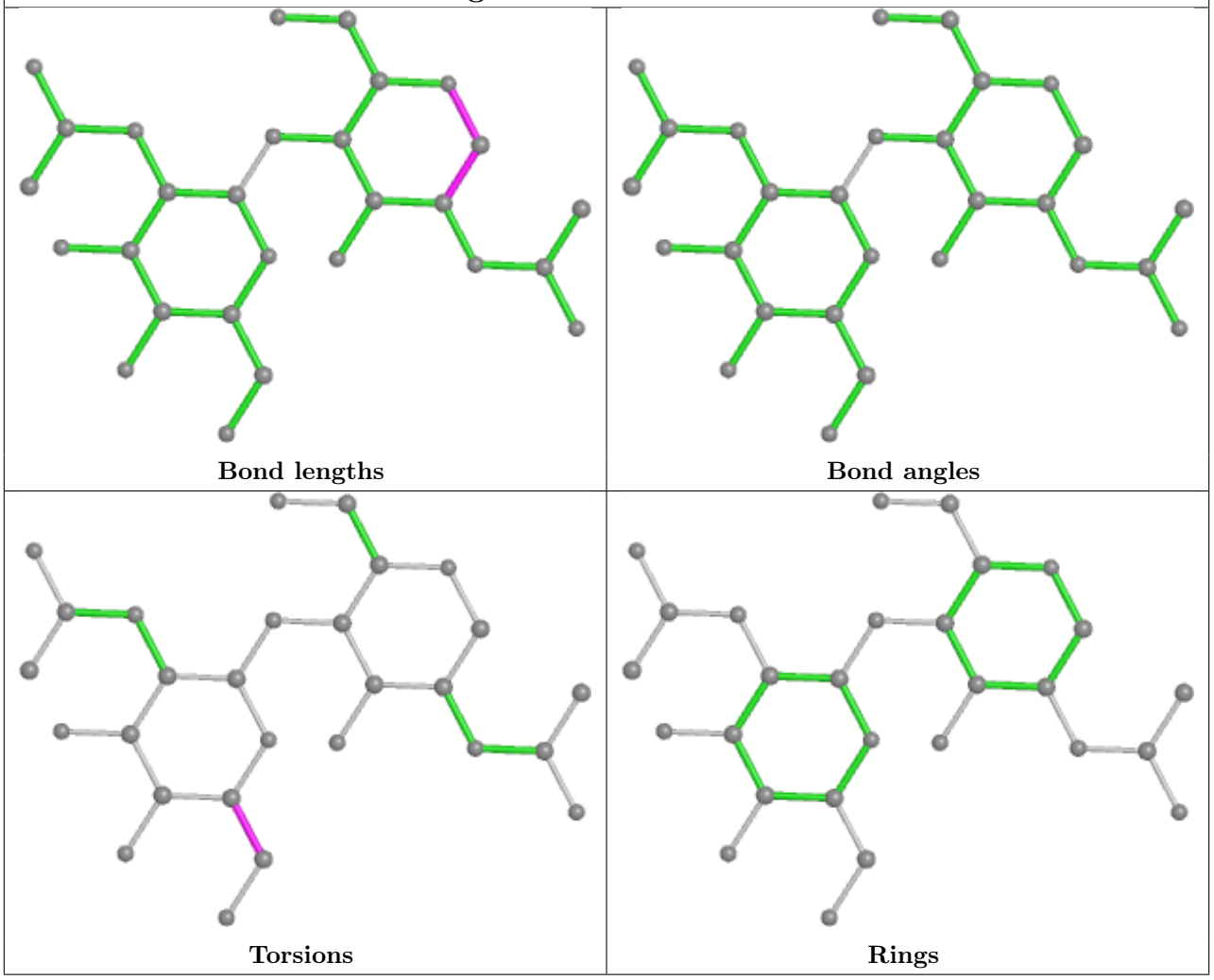


Torsions



Rings

Oligosaccharide Chain X



5.6 Ligand geometry (i)

30 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	1309	1	14,14,15	0.87	1 (7%)	17,19,21	0.49	0
5	NAG	A	1309	1	14,14,15	0.89	1 (7%)	17,19,21	0.49	0
5	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	C	1306	1	14,14,15	0.92	1 (7%)	17,19,21	2.13	1 (5%)
5	NAG	A	1301	1	14,14,15	0.77	1 (7%)	17,19,21	0.59	0
5	NAG	A	1305	1	14,14,15	0.40	0	17,19,21	0.32	0
5	NAG	C	1308	1	14,14,15	0.76	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	B	1309	1	14,14,15	0.89	1 (7%)	17,19,21	0.49	0
5	NAG	A	1306	1	14,14,15	1.64	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	B	1308	1	14,14,15	0.82	1 (7%)	17,19,21	1.12	1 (5%)
5	NAG	A	1303	1	14,14,15	0.40	0	17,19,21	0.61	0
5	NAG	C	1303	1	14,14,15	0.40	0	17,19,21	0.61	0
5	NAG	C	1307	1	14,14,15	0.45	0	17,19,21	0.62	0
5	NAG	B	1306	1	14,14,15	1.62	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	A	1304	1	14,14,15	0.32	0	17,19,21	1.05	1 (5%)
5	NAG	A	1307	1	14,14,15	0.45	0	17,19,21	0.63	0
5	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	B	1305	1	14,14,15	0.38	0	17,19,21	0.32	0
5	NAG	B	1310	1	14,14,15	0.47	0	17,19,21	0.63	0
5	NAG	B	1303	1	14,14,15	0.41	0	17,19,21	0.61	0
5	NAG	C	1301	1	14,14,15	0.76	1 (7%)	17,19,21	0.59	0
5	NAG	B	1301	1	14,14,15	0.76	1 (7%)	17,19,21	0.60	0
5	NAG	C	1305	1	14,14,15	0.39	0	17,19,21	0.33	0
5	NAG	B	1304	1	14,14,15	0.33	0	17,19,21	1.04	1 (5%)
5	NAG	B	1307	1	14,14,15	0.44	0	17,19,21	0.63	0
5	NAG	A	1308	1	14,14,15	0.72	1 (7%)	17,19,21	0.65	0
5	NAG	C	1310	1	14,14,15	0.48	0	17,19,21	0.63	0
5	NAG	A	1310	1	14,14,15	0.48	0	17,19,21	0.63	0
5	NAG	C	1304	1	14,14,15	0.32	0	17,19,21	1.05	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	1/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1306	NAG	O5-C1	-6.06	1.34	1.43
5	B	1306	NAG	O5-C1	-6.04	1.34	1.43
5	A	1309	NAG	O5-C1	-3.05	1.38	1.43
5	B	1309	NAG	O5-C1	-3.04	1.38	1.43
5	C	1309	NAG	O5-C1	-3.01	1.38	1.43
5	C	1306	NAG	O5-C1	2.92	1.48	1.43
5	B	1308	NAG	O5-C1	-2.85	1.39	1.43
5	A	1301	NAG	O5-C1	-2.69	1.39	1.43
5	C	1301	NAG	O5-C1	-2.66	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1301	NAG	O5-C1	-2.66	1.39	1.43
5	C	1308	NAG	O5-C1	-2.61	1.39	1.43
5	A	1308	NAG	O5-C1	-2.56	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1306	NAG	C1-O5-C5	8.49	123.69	112.19
5	B	1308	NAG	C1-O5-C5	4.18	117.86	112.19
5	A	1304	NAG	C1-O5-C5	3.60	117.06	112.19
5	C	1304	NAG	C1-O5-C5	3.58	117.05	112.19
5	B	1304	NAG	C1-O5-C5	3.56	117.02	112.19
5	C	1308	NAG	C1-O5-C5	3.21	116.54	112.19
5	B	1306	NAG	C1-O5-C5	-3.04	108.08	112.19
5	A	1306	NAG	C1-O5-C5	-2.58	108.70	112.19

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1308	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1305	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	C	1310	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	B	1308	NAG	C1-C2-N2-C7
5	A	1304	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	A	1302	NAG	C3-C2-N2-C7
5	A	1309	NAG	C3-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7
5	B	1309	NAG	C3-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7
5	C	1308	NAG	C3-C2-N2-C7
5	C	1309	NAG	C3-C2-N2-C7
5	A	1308	NAG	O5-C5-C6-O6
5	A	1305	NAG	C3-C2-N2-C7
5	B	1305	NAG	C3-C2-N2-C7
5	B	1308	NAG	C3-C2-N2-C7
5	C	1305	NAG	C3-C2-N2-C7

There are no ring outliers.

19 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1309	NAG	2	0
5	A	1309	NAG	2	0
5	A	1302	NAG	5	0

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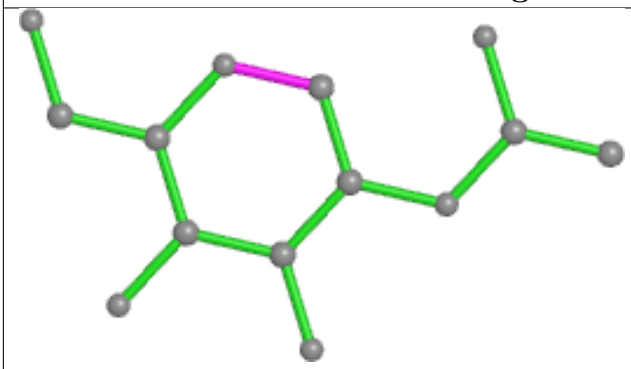
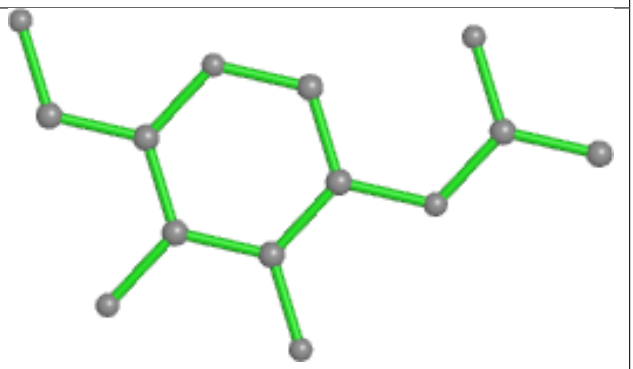
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1305	NAG	3	0
5	B	1309	NAG	2	0
5	A	1306	NAG	1	0
5	A	1303	NAG	1	0
5	C	1303	NAG	1	0
5	C	1307	NAG	1	0
5	B	1302	NAG	5	0
5	A	1304	NAG	1	0
5	A	1307	NAG	1	0
5	C	1302	NAG	5	0
5	B	1305	NAG	3	0
5	B	1303	NAG	1	0
5	C	1305	NAG	3	0
5	B	1304	NAG	1	0
5	B	1307	NAG	1	0
5	C	1304	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

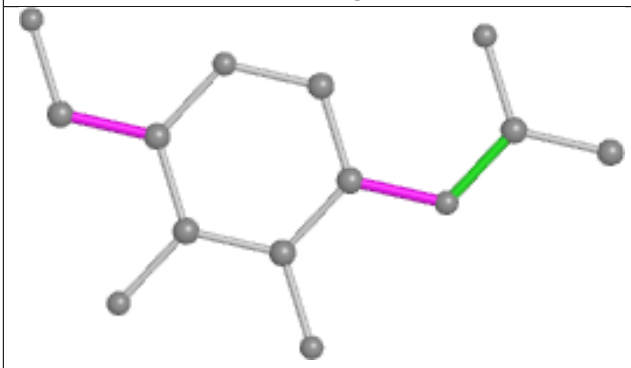
Ligand NAG C 1309



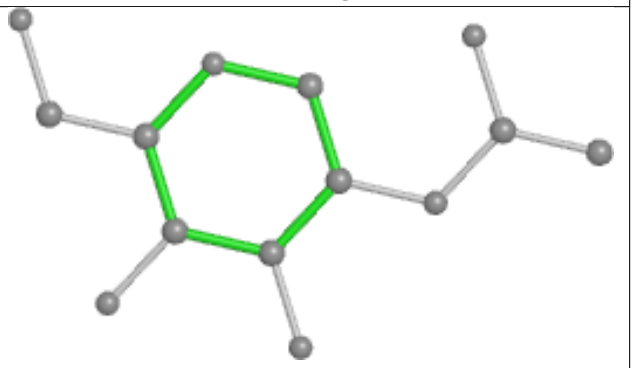
Bond lengths



Bond angles

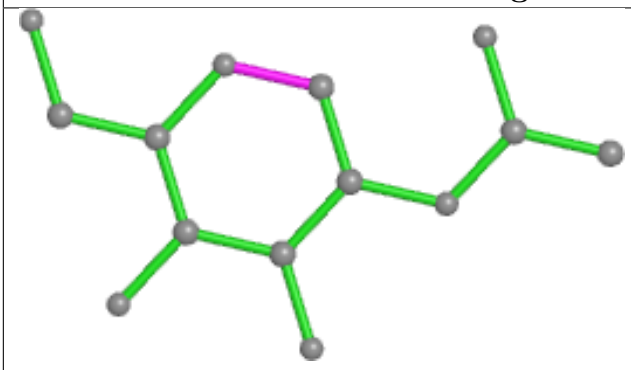


Torsions



Rings

Ligand NAG A 1309



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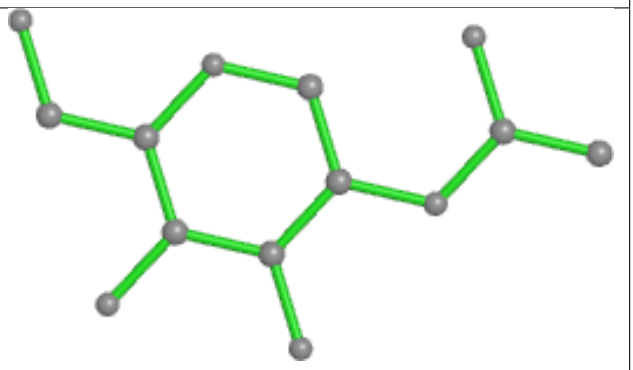
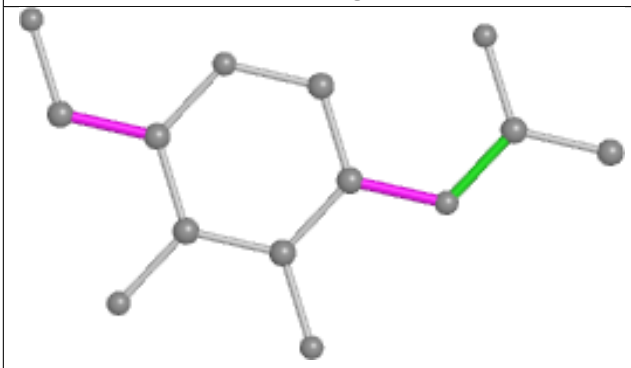


Bond angles



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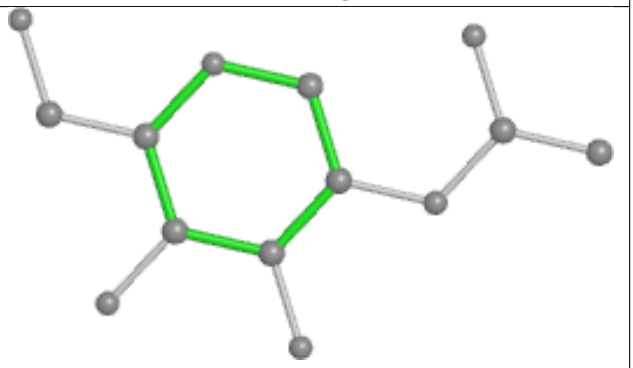
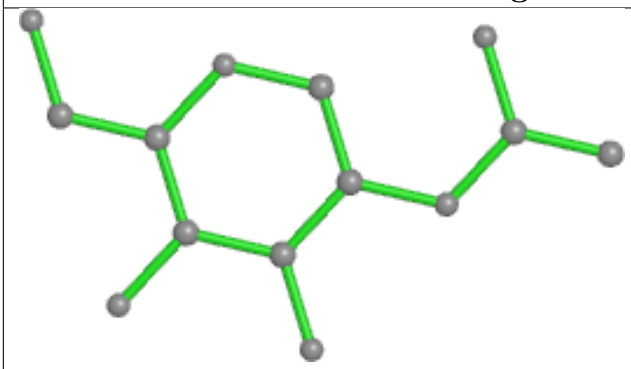
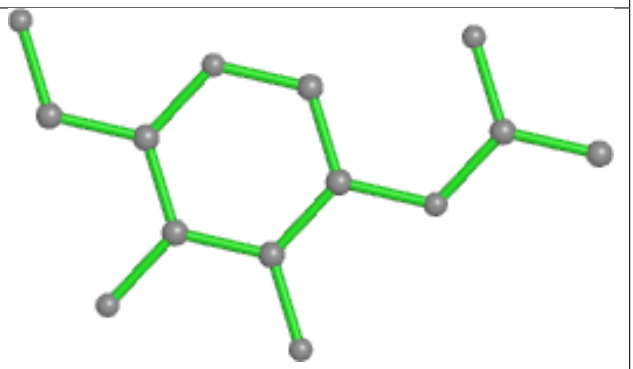


Rings

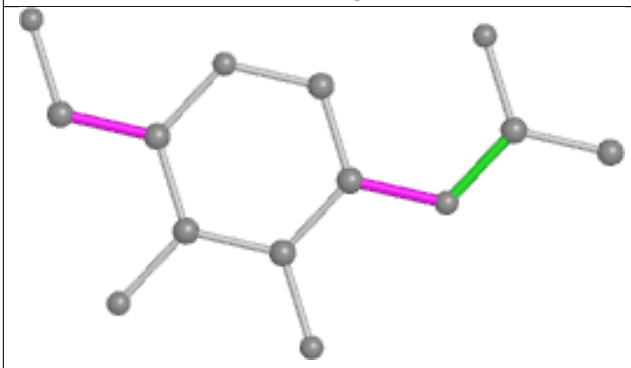
Ligand NAG A 1302



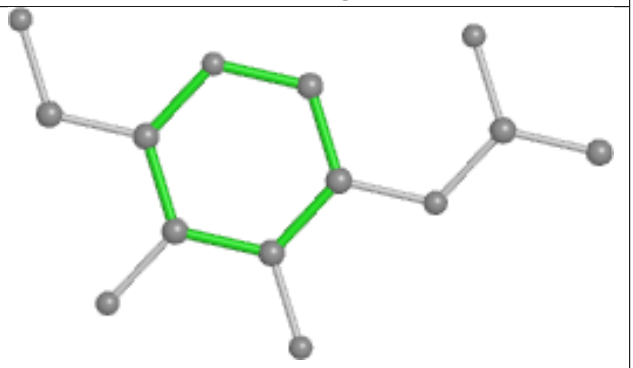
Bond lengths



Bond angles

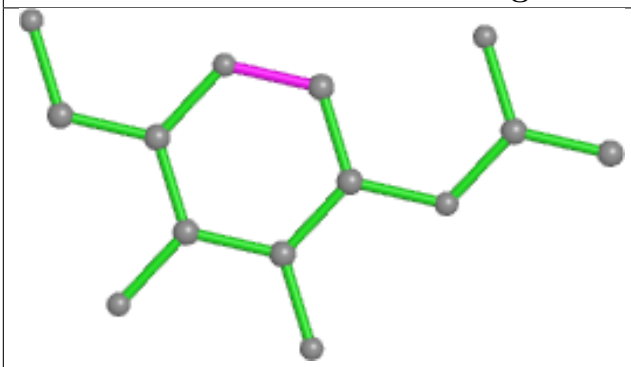


Torsions

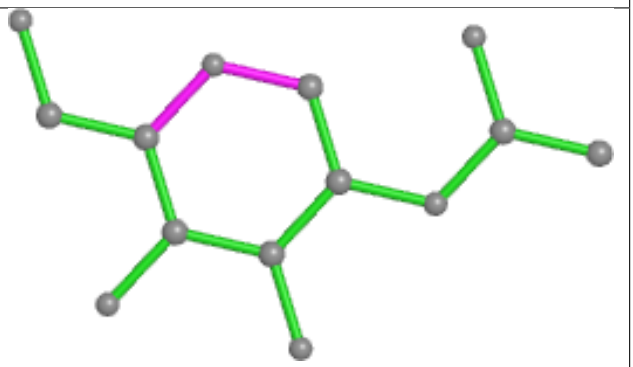


Rings

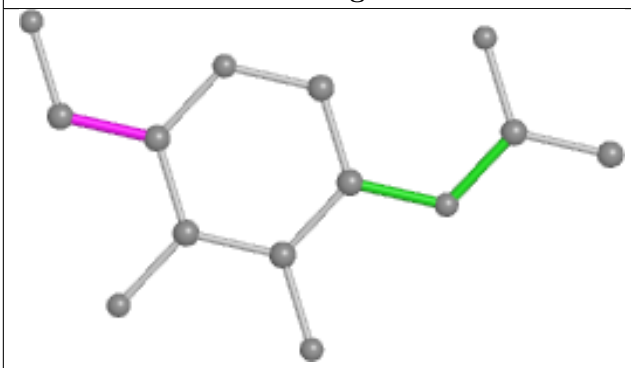
Ligand NAG C 1306



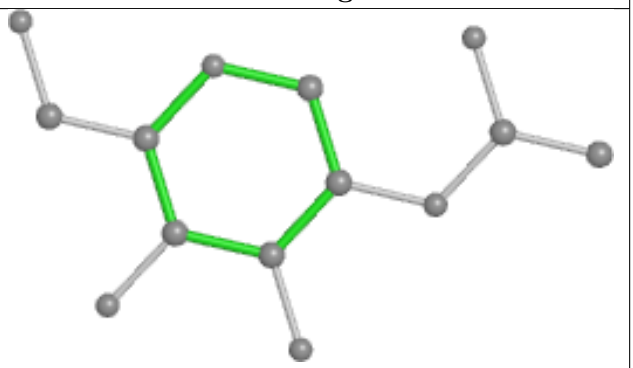
Bond lengths



Bond angles

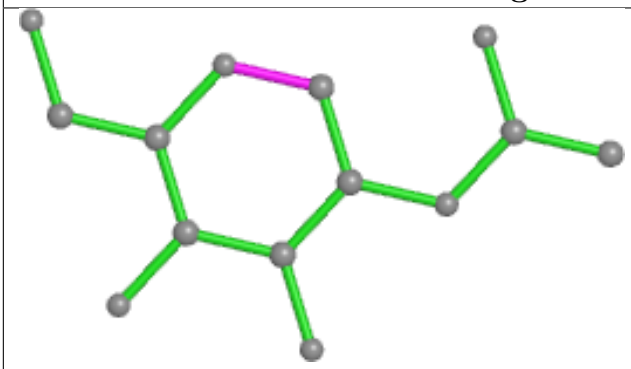


Torsions

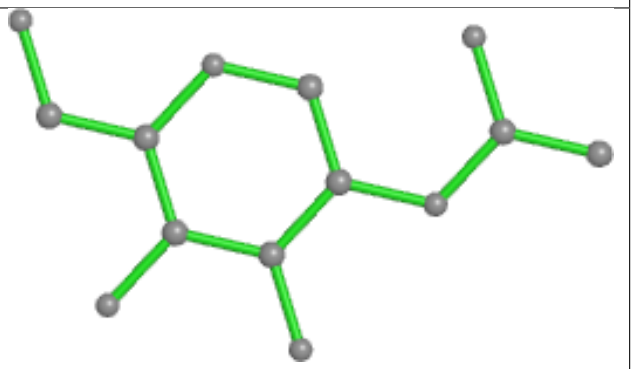


Rings

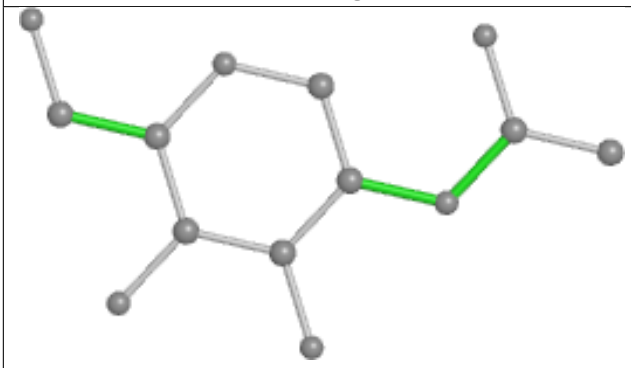
Ligand NAG A 1301



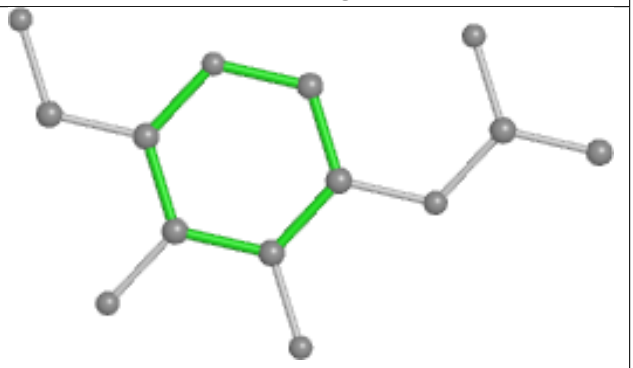
Bond lengths



Bond angles

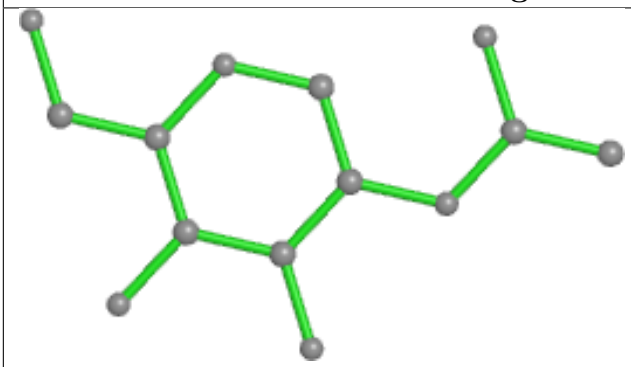


Torsions



Rings

Ligand NAG A 1305



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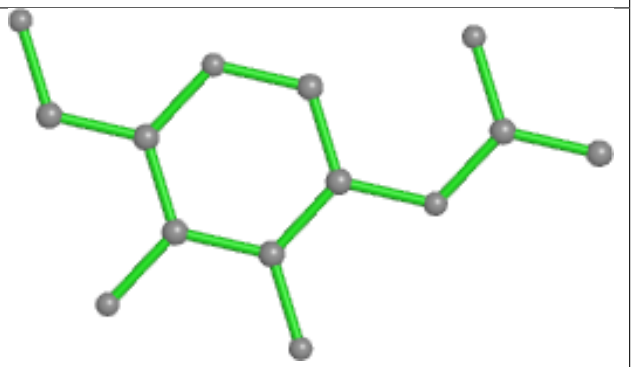
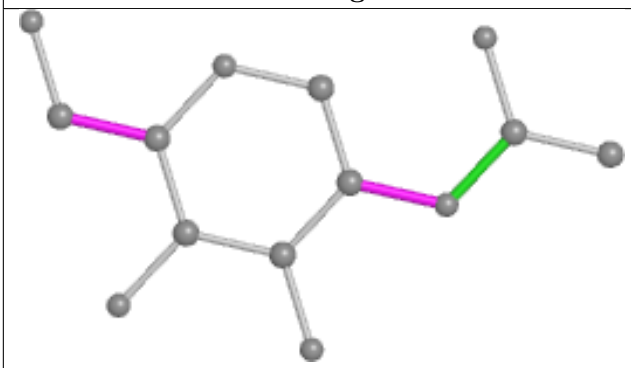


Bond angles



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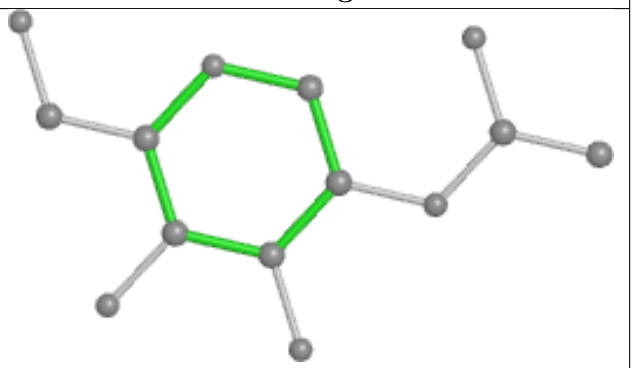
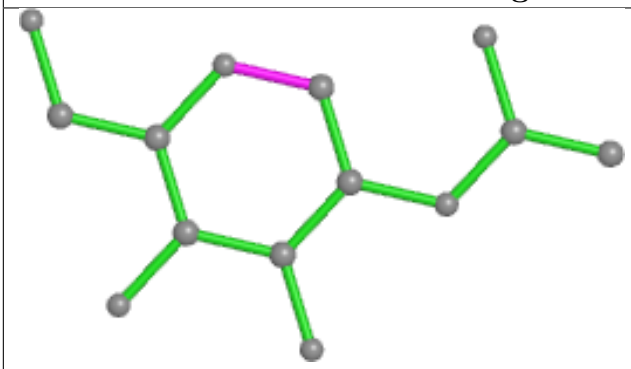
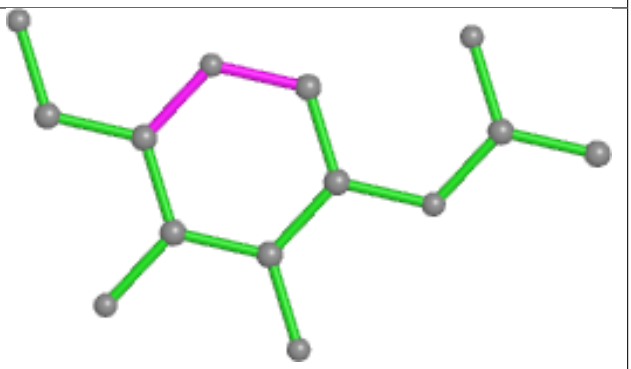
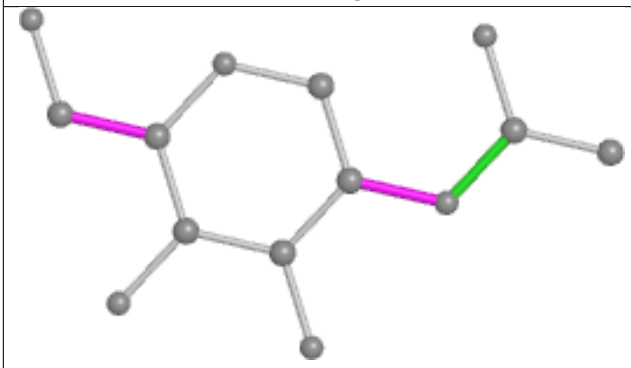
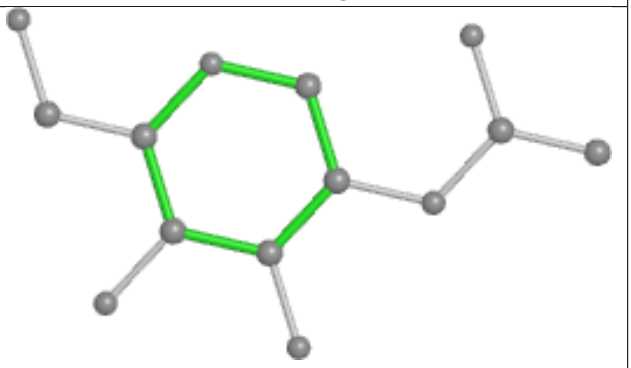
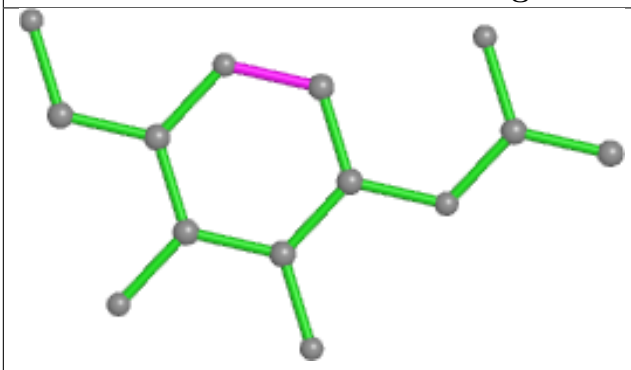
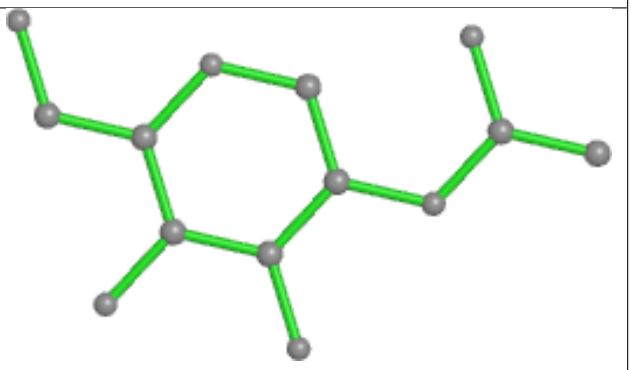
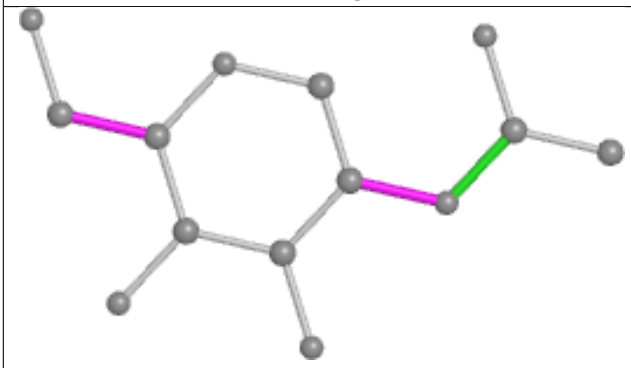
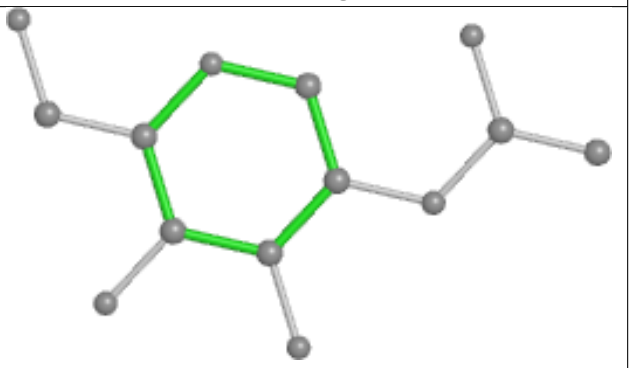
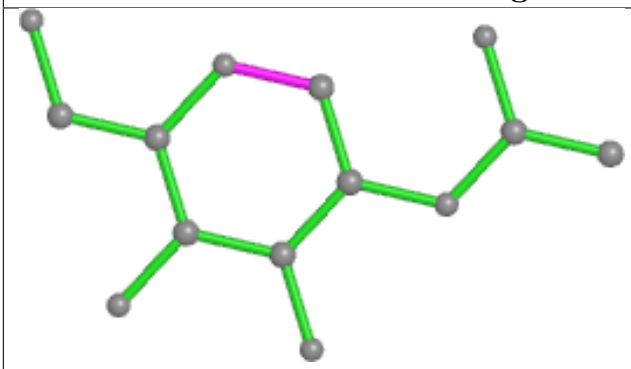
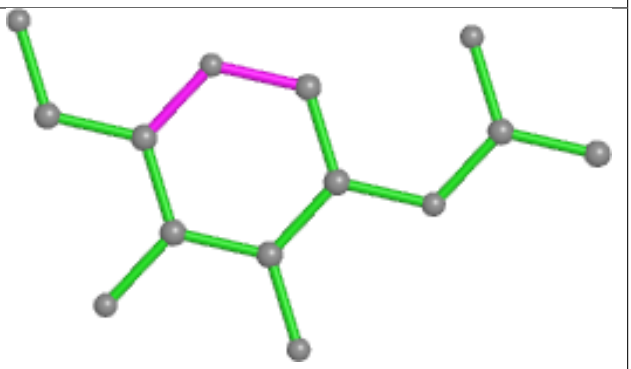
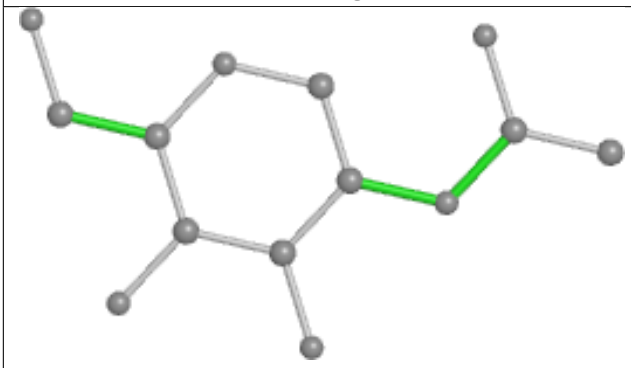
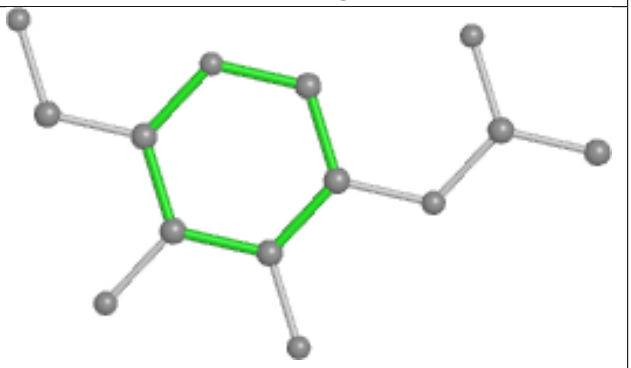
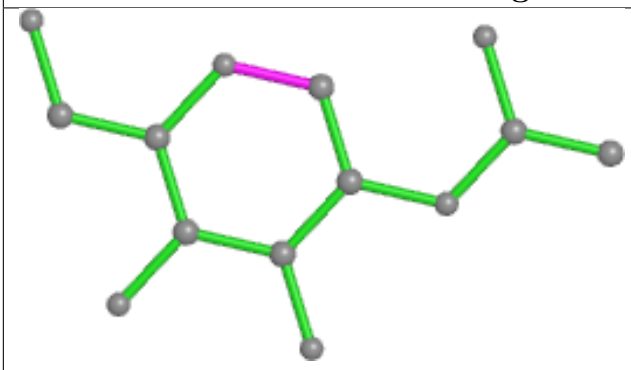
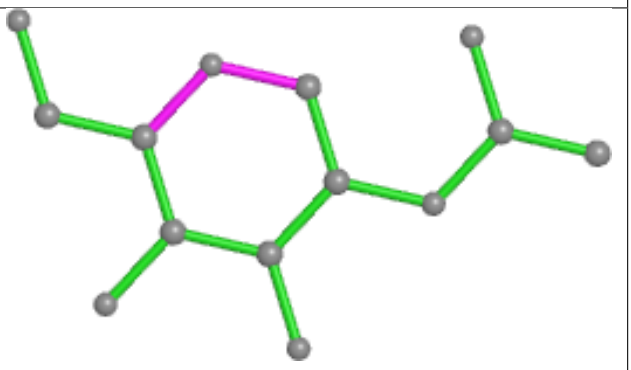
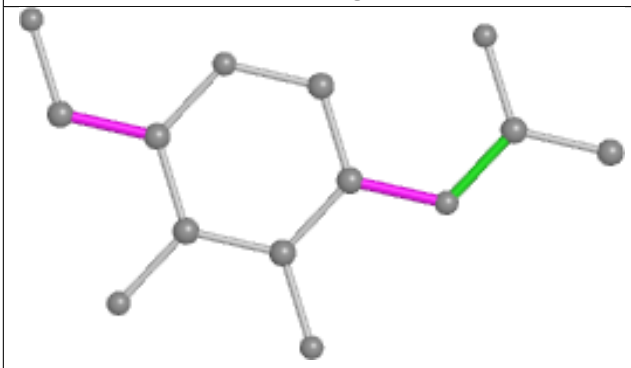
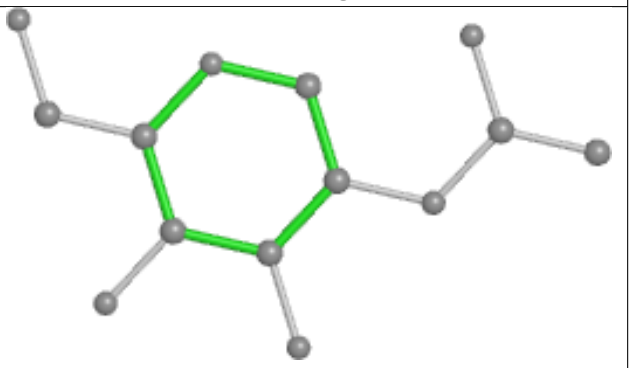


Rings

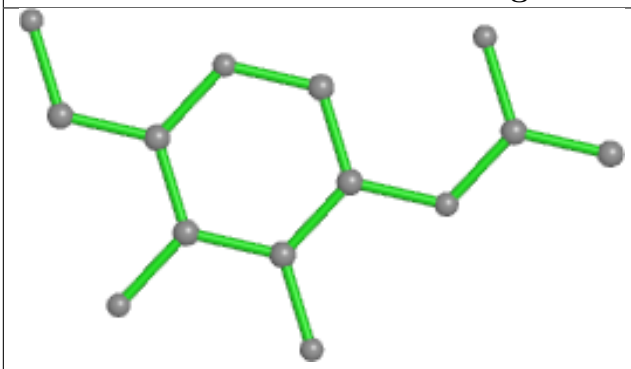
Ligand NAG C 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1309	
 Bond lengths	 Bond angles
 Torsions	 Rings

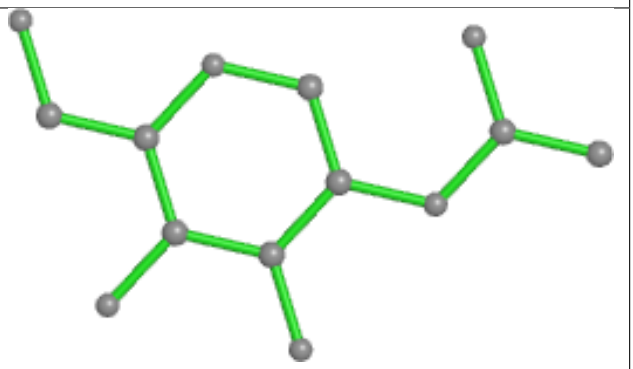
Ligand NAG A 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

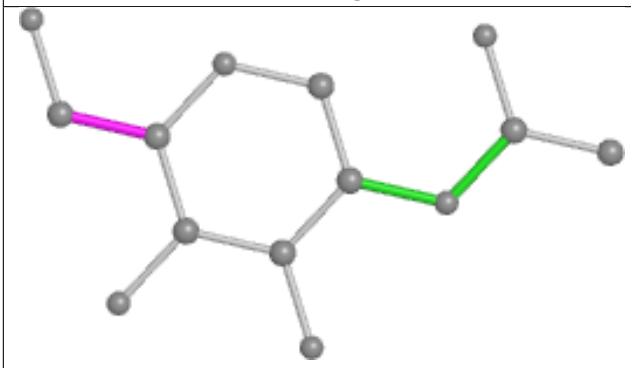
Ligand NAG A 1303



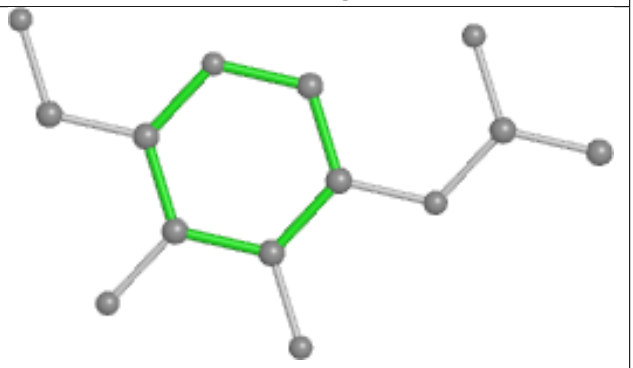
Bond lengths



Bond angles

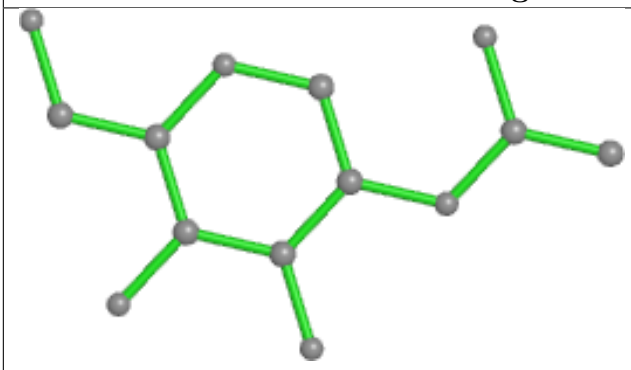


Torsions

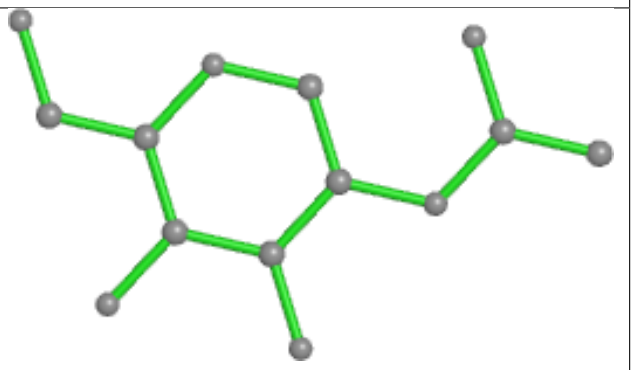


Rings

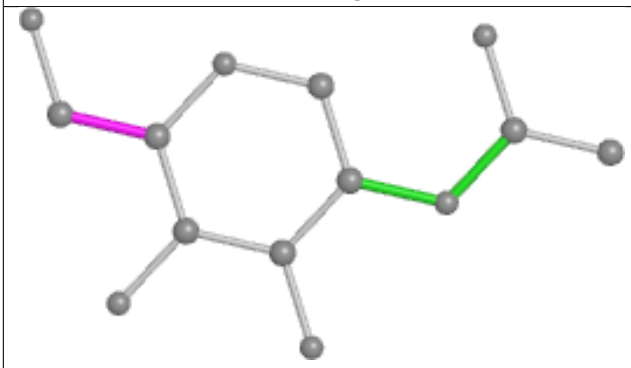
Ligand NAG C 1303



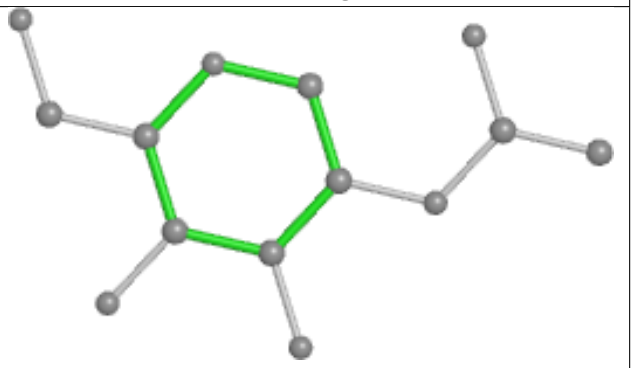
Bond lengths



Bond angles

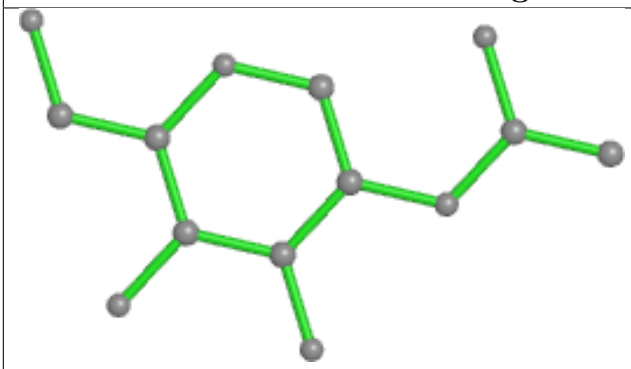


Torsions

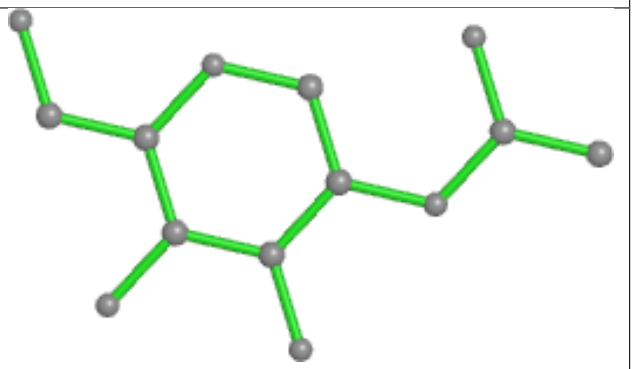


Rings

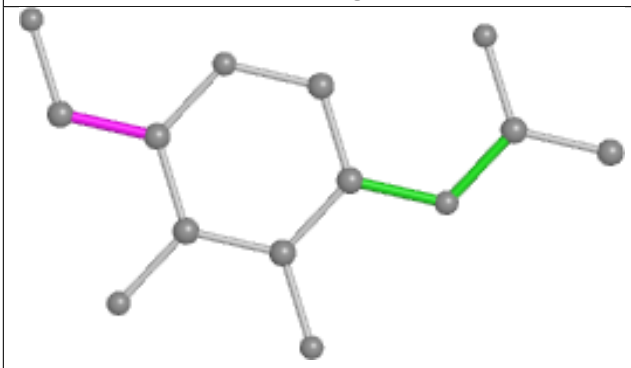
Ligand NAG C 1307



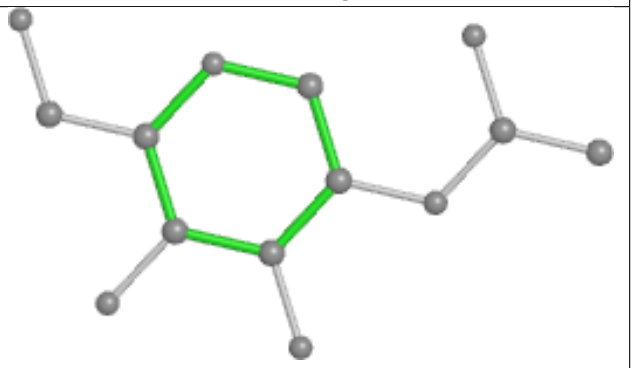
Bond lengths



Bond angles

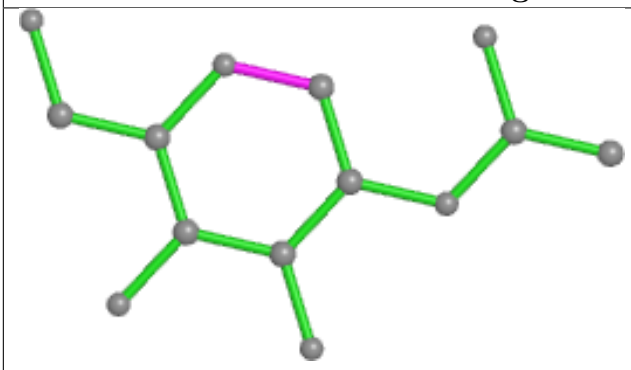


Torsions

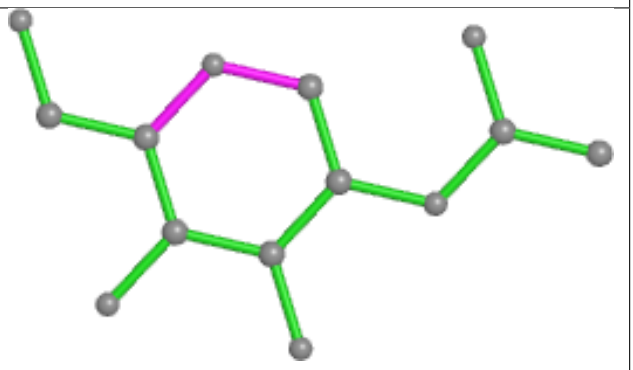


Rings

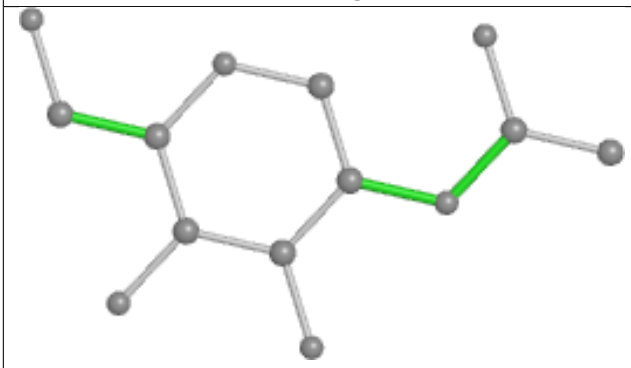
Ligand NAG B 1306



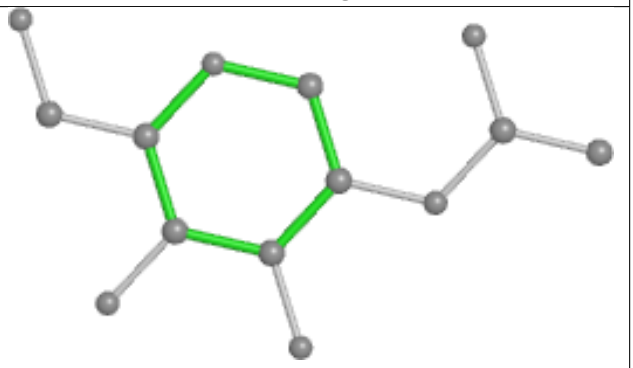
Bond lengths



Bond angles

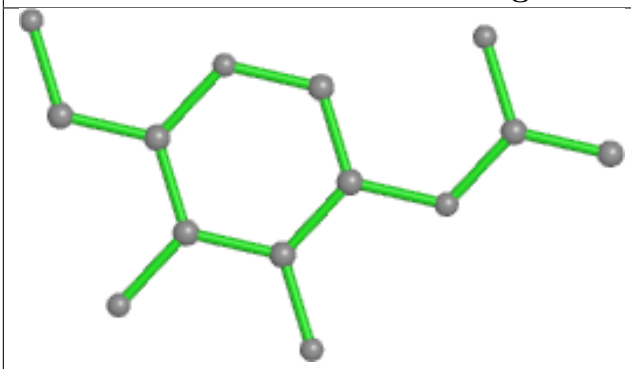


Torsions

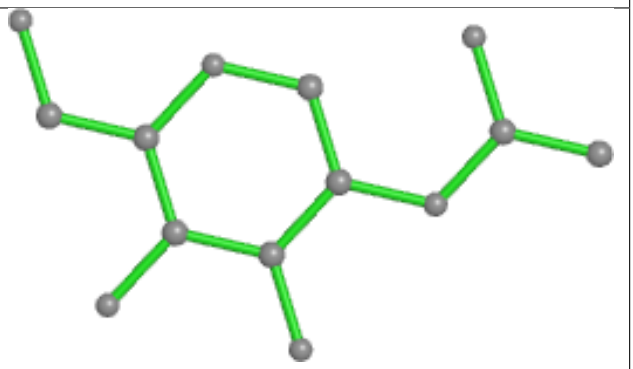


Rings

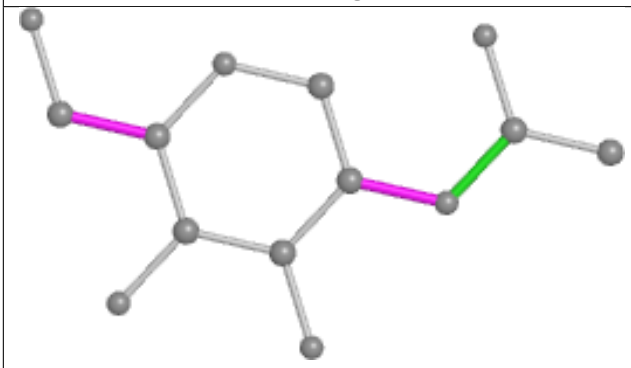
Ligand NAG B 1302



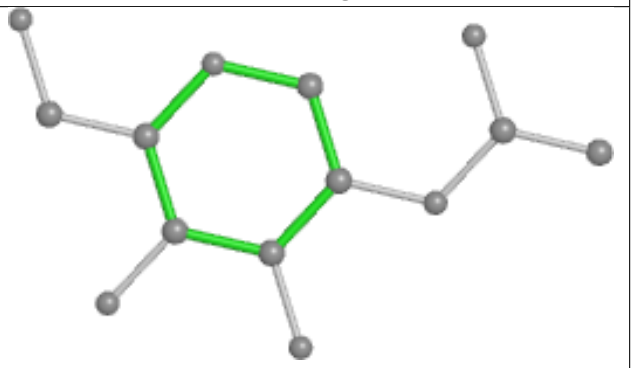
Bond lengths



Bond angles

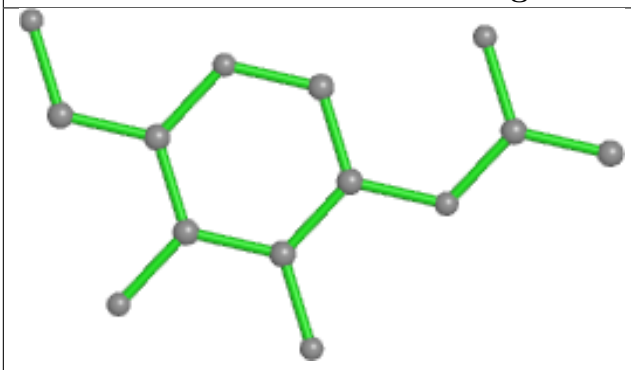


Torsions

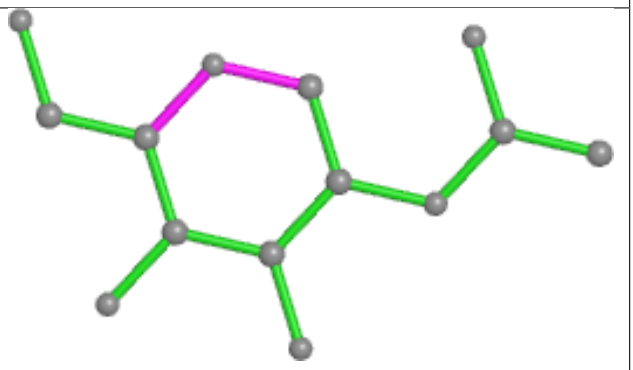


Rings

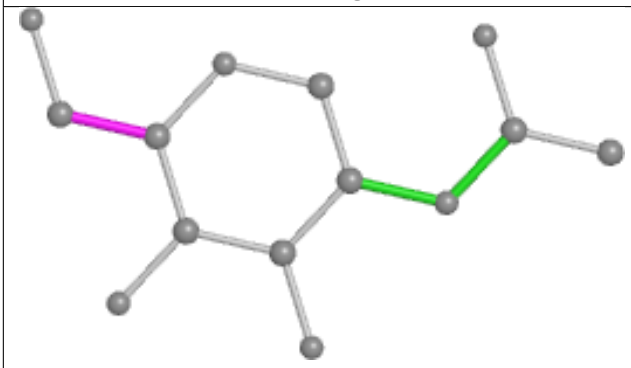
Ligand NAG A 1304



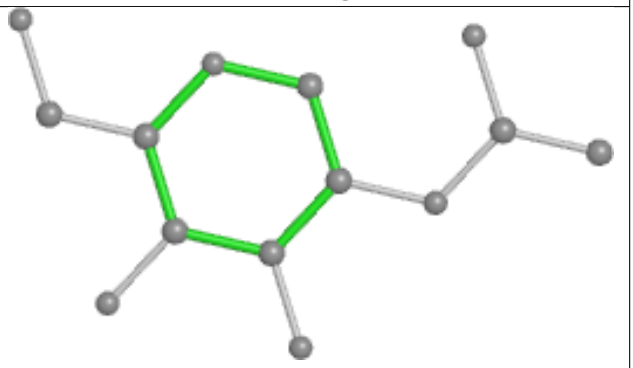
Bond lengths



Bond angles

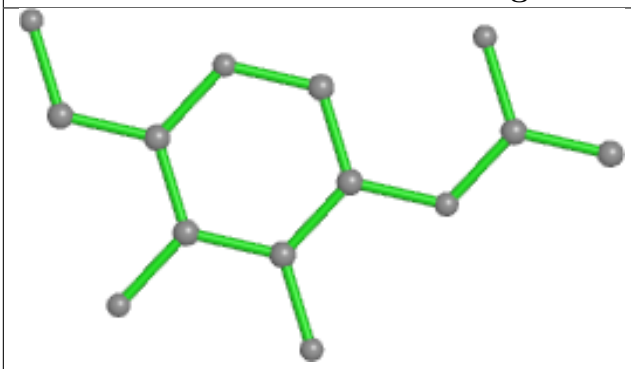


Torsions

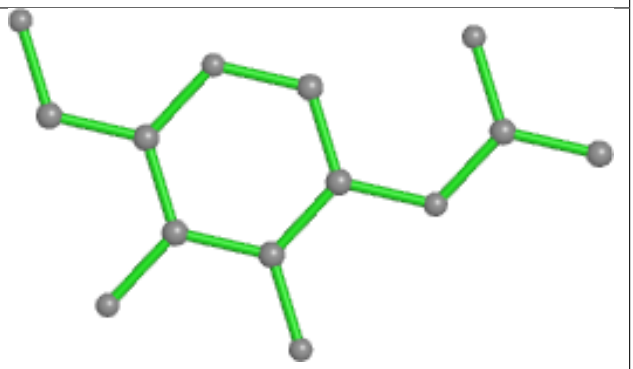


Rings

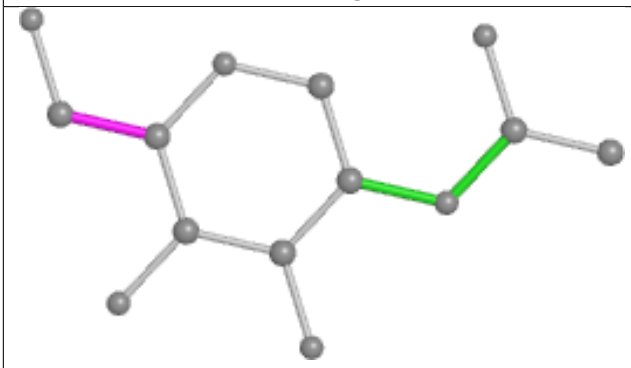
Ligand NAG A 1307



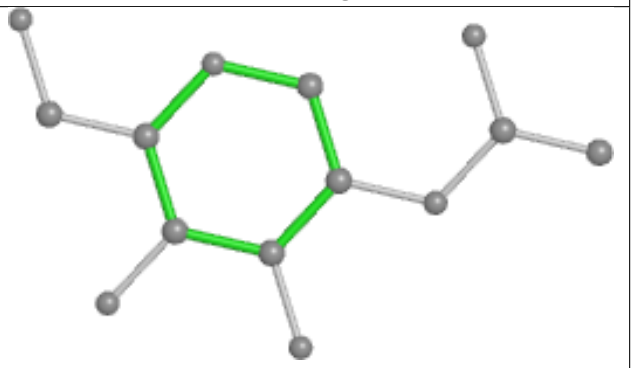
Bond lengths



Bond angles

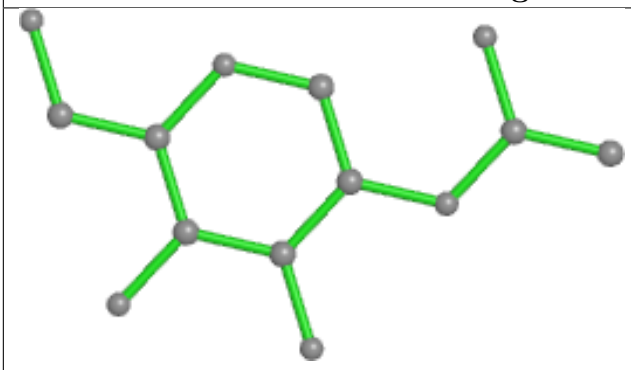


Torsions

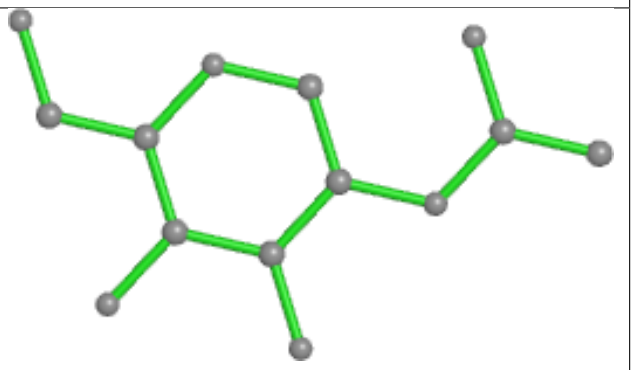


Rings

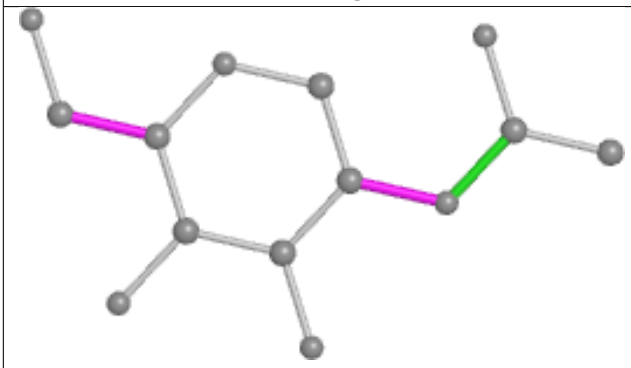
Ligand NAG C 1302



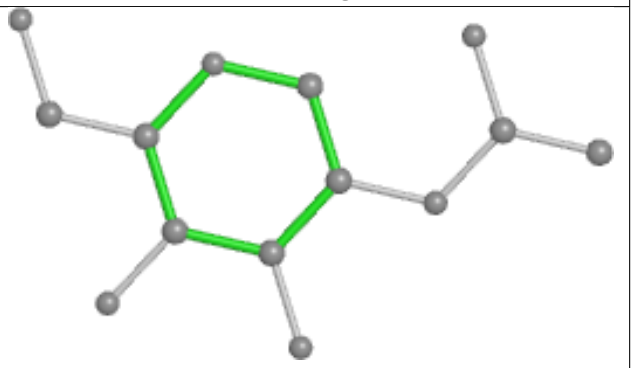
Bond lengths



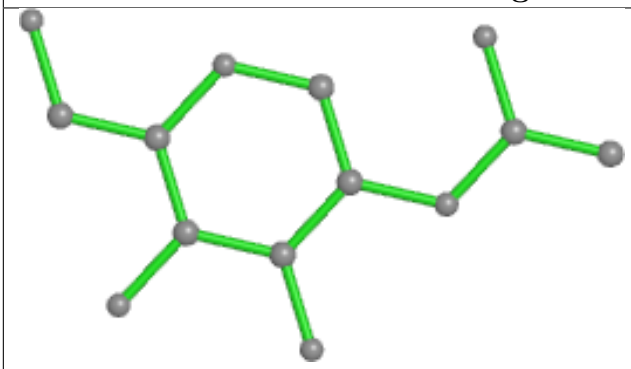
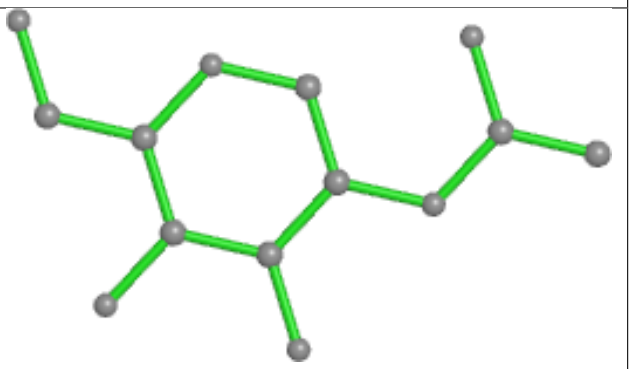
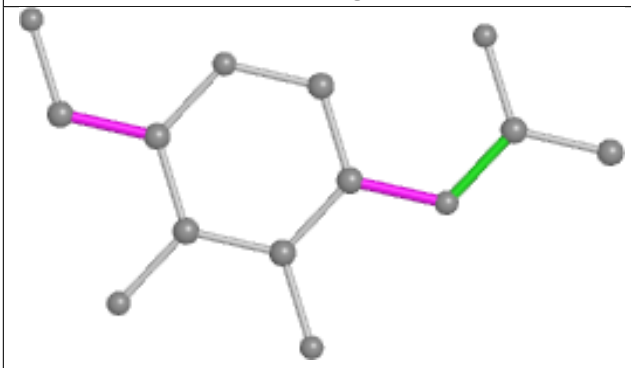
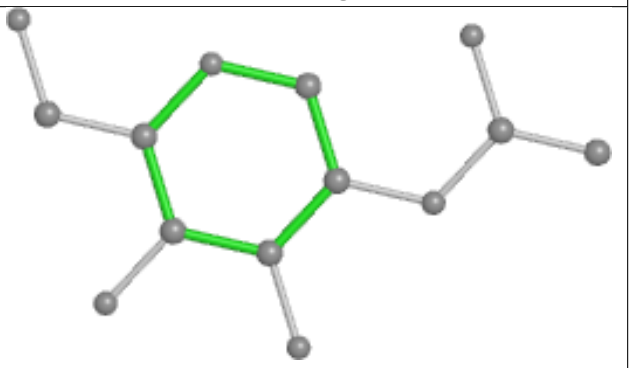
Bond angles

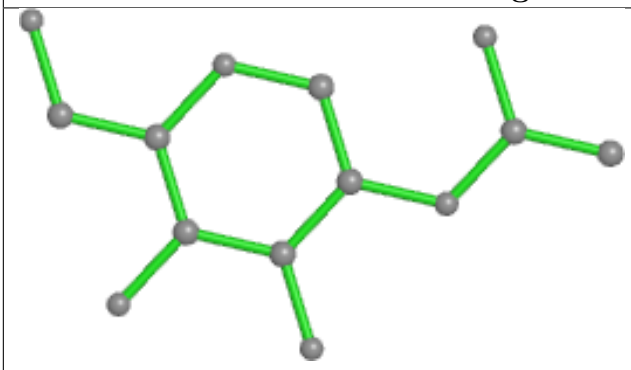
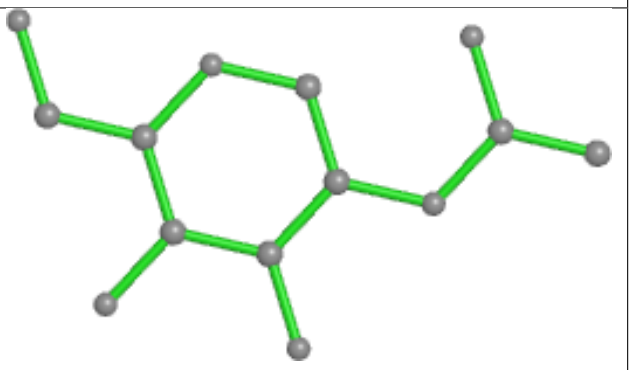
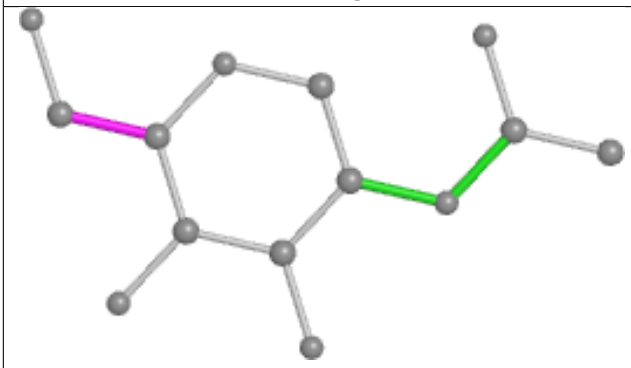
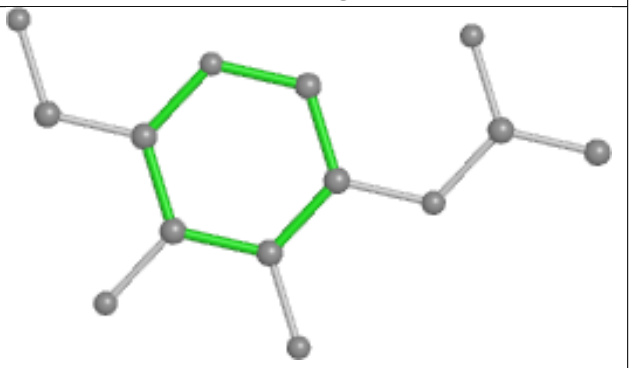


Torsions

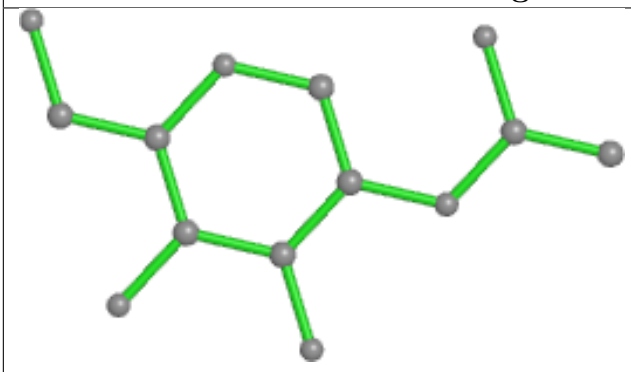


Rings

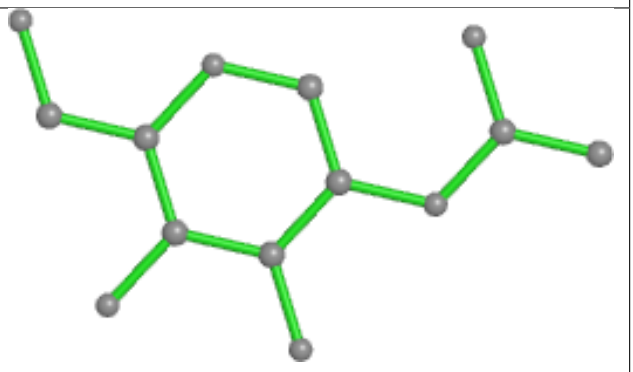
Ligand NAG B 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

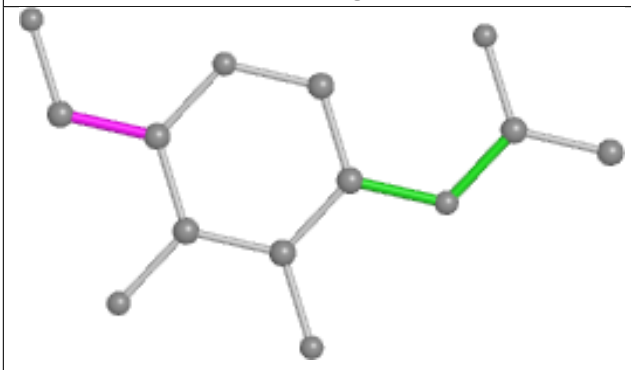
Ligand NAG B 1303



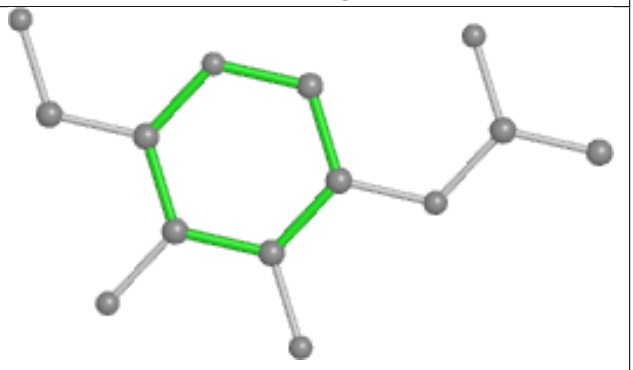
Bond lengths



Bond angles

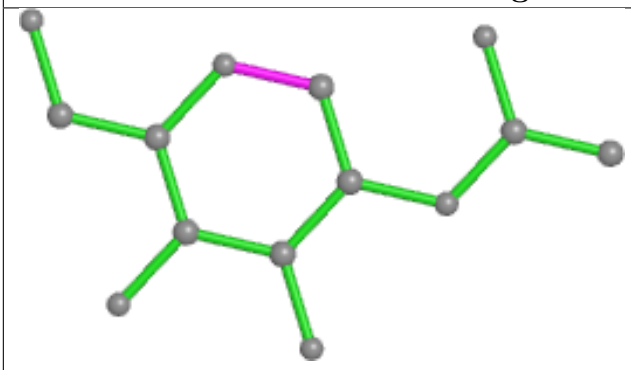


Torsions

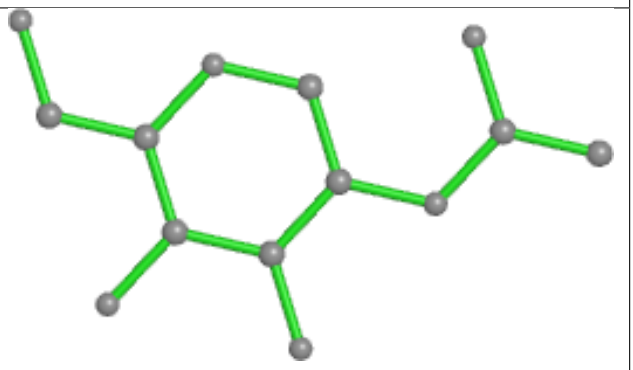


Rings

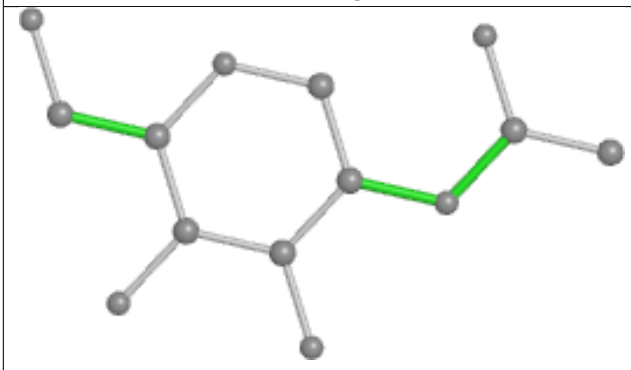
Ligand NAG C 1301



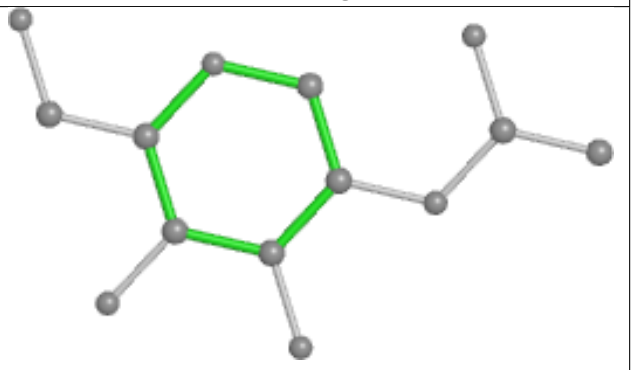
Bond lengths



Bond angles

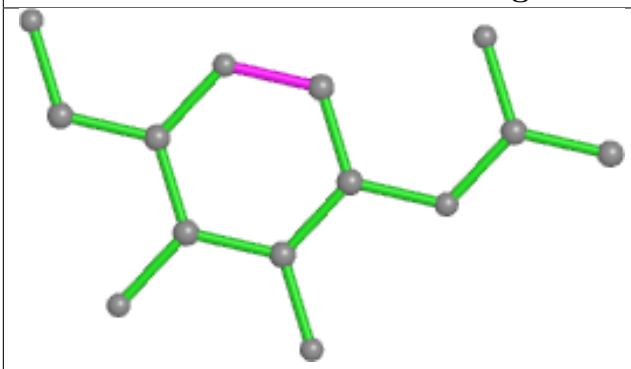


Torsions

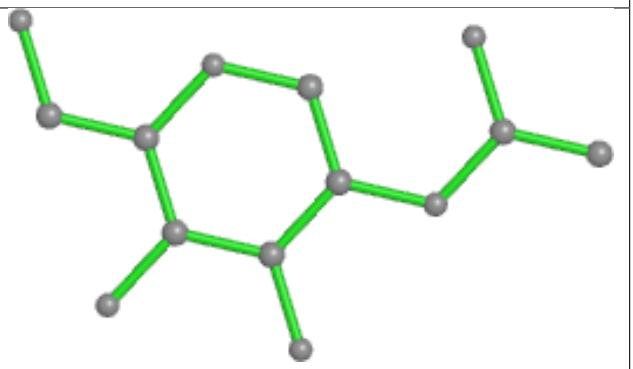


Rings

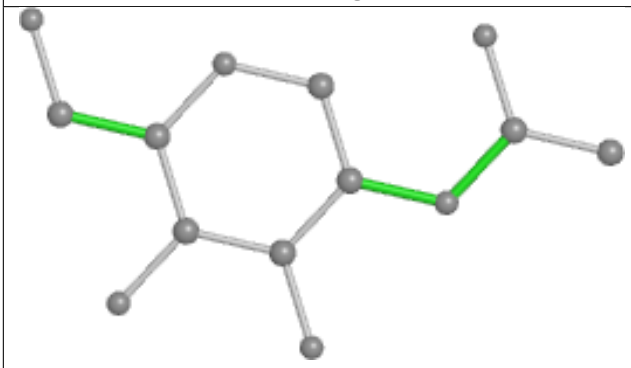
Ligand NAG B 1301



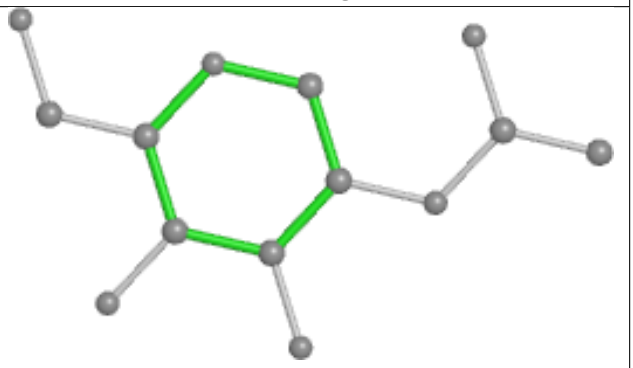
Bond lengths



Bond angles

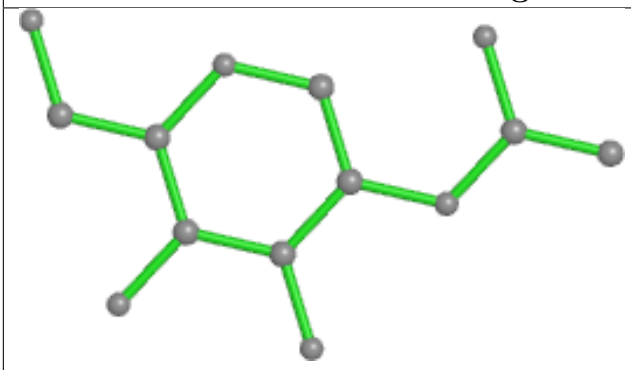


Torsions

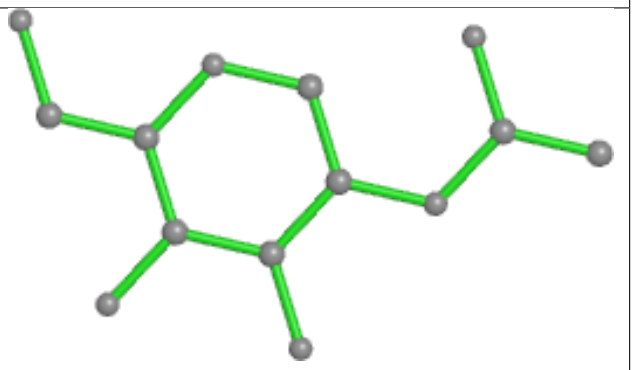


Rings

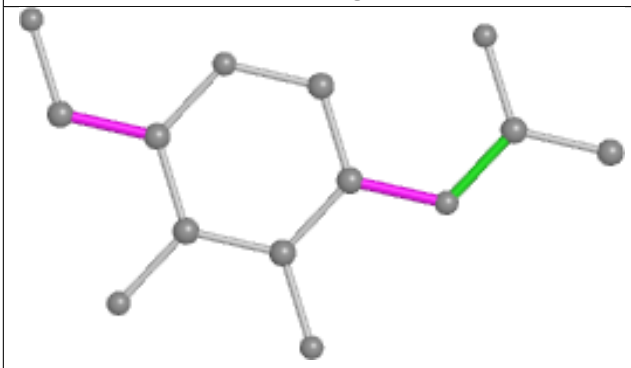
Ligand NAG C 1305



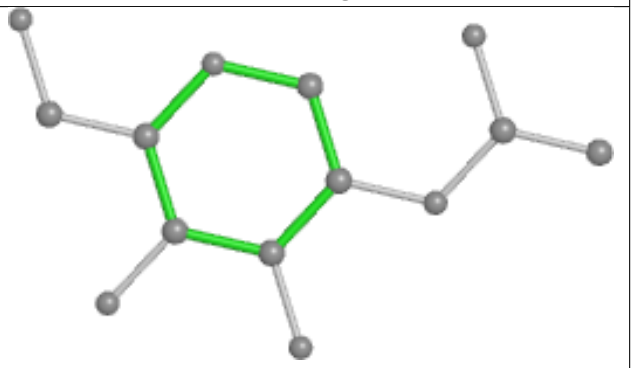
Bond lengths



Bond angles

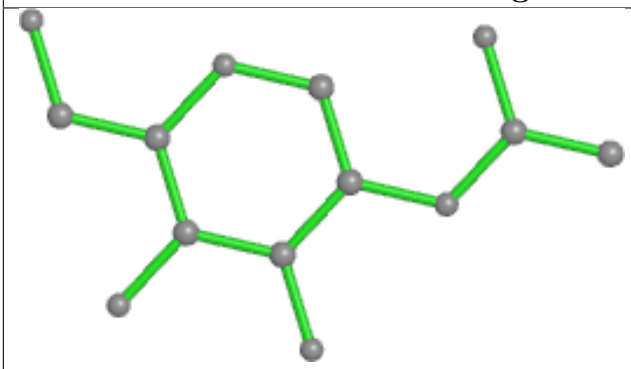


Torsions

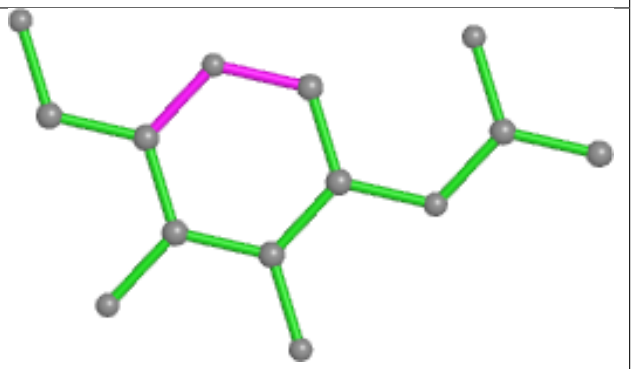


Rings

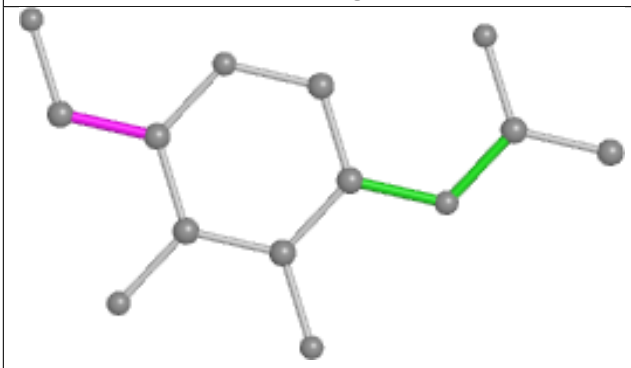
Ligand NAG B 1304



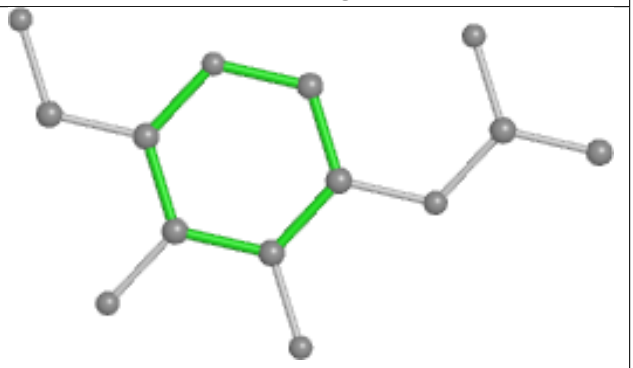
Bond lengths



Bond angles

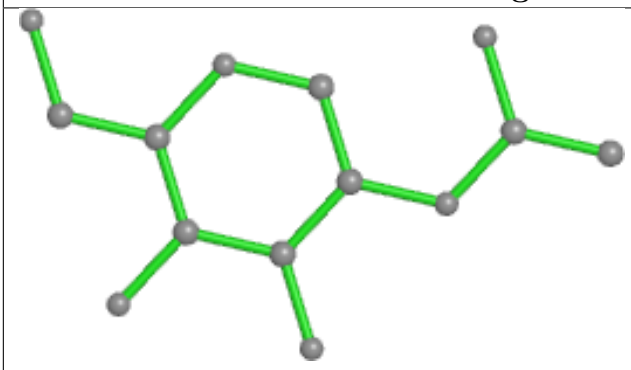


Torsions

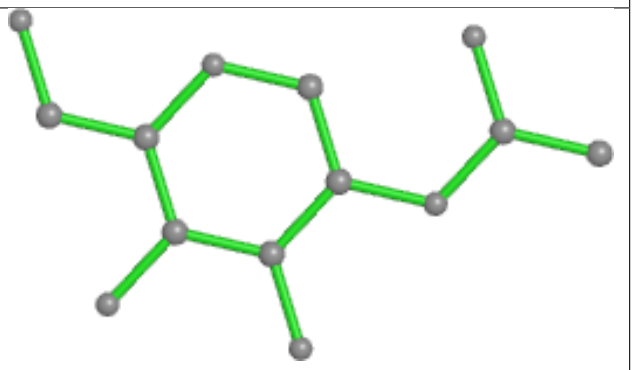


Rings

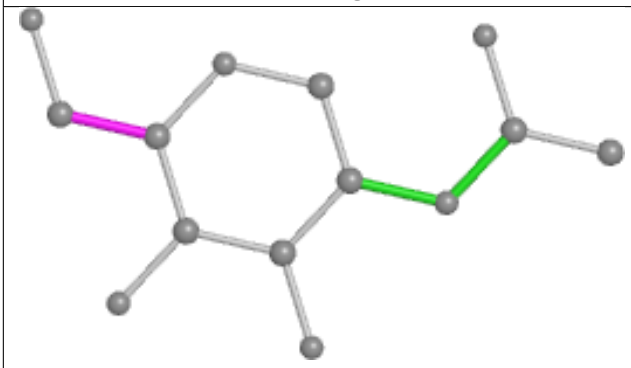
Ligand NAG B 1307



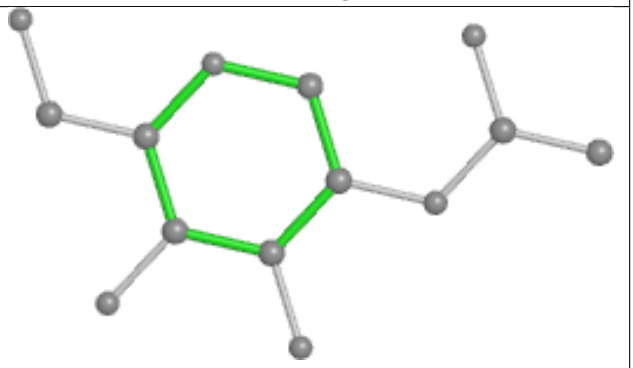
Bond lengths



Bond angles

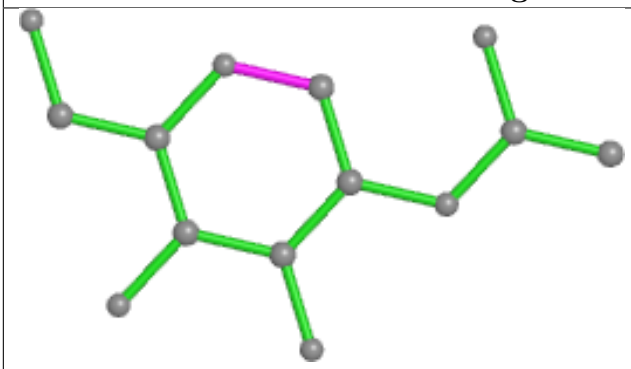


Torsions

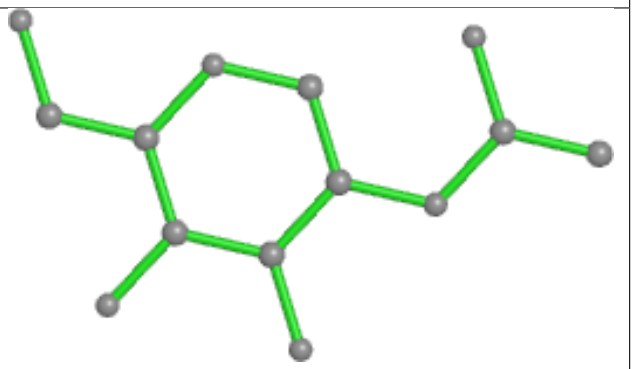


Rings

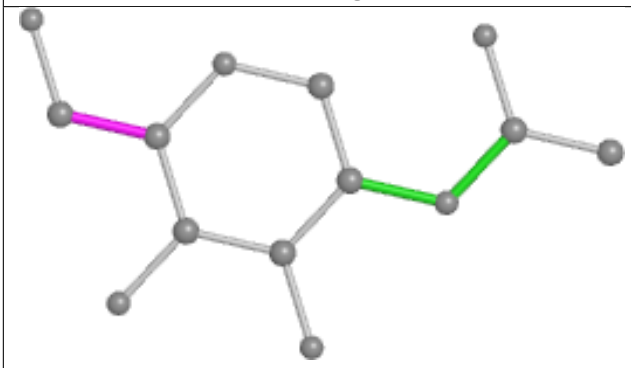
Ligand NAG A 1308



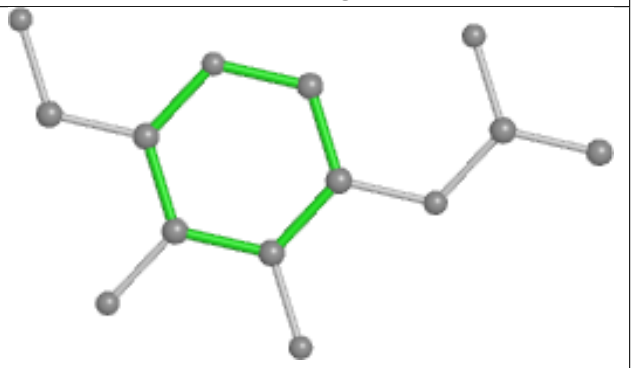
Bond lengths



Bond angles

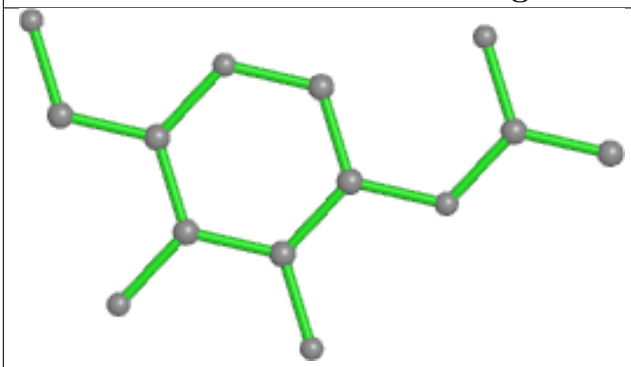


Torsions

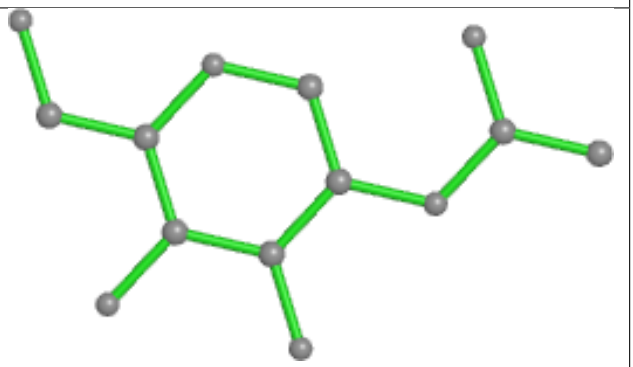


Rings

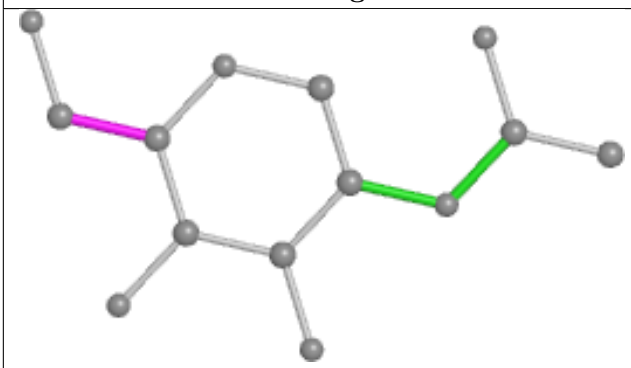
Ligand NAG C 1310



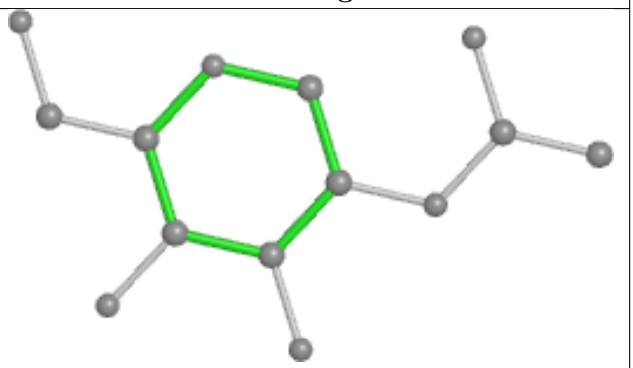
Bond lengths



Bond angles

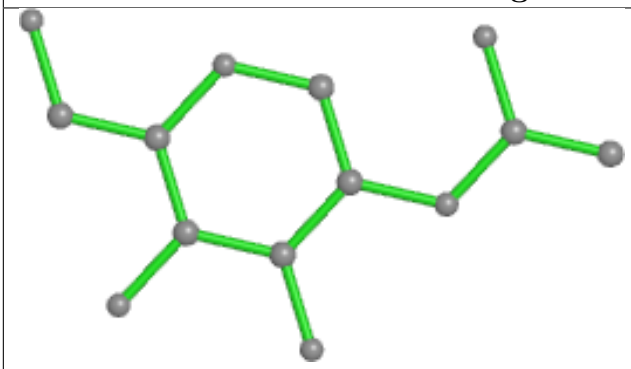


Torsions

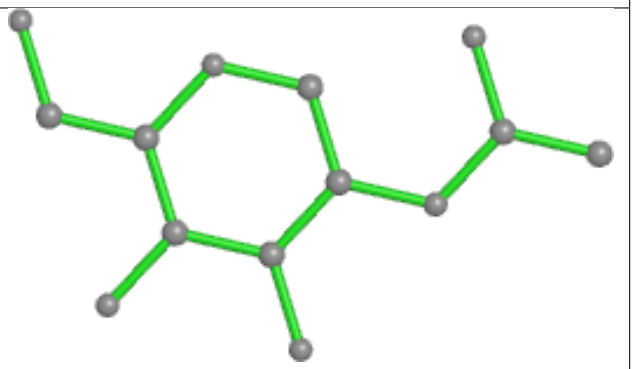


Rings

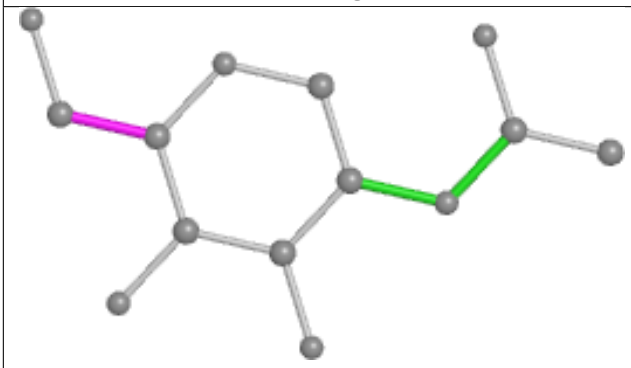
Ligand NAG A 1310



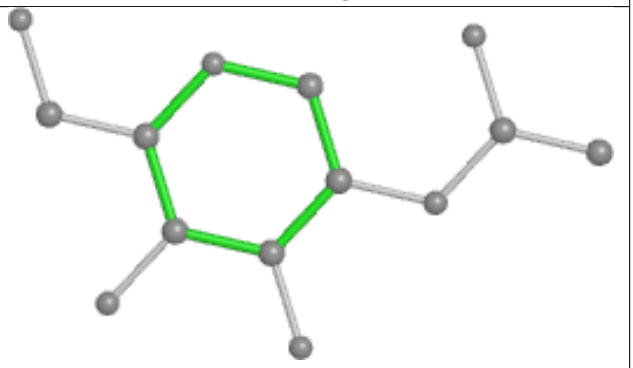
Bond lengths



Bond angles

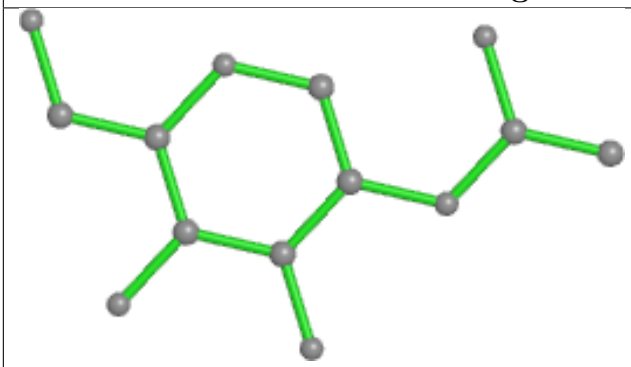


Torsions

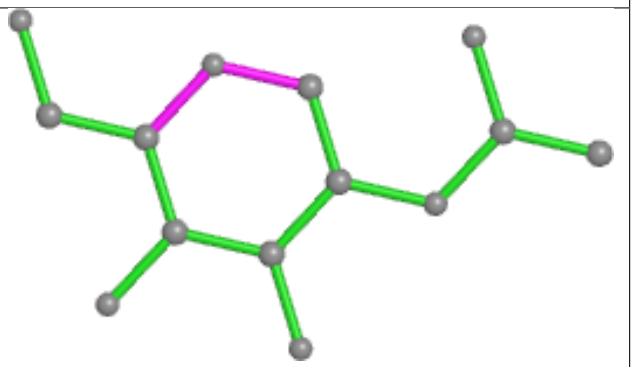


Rings

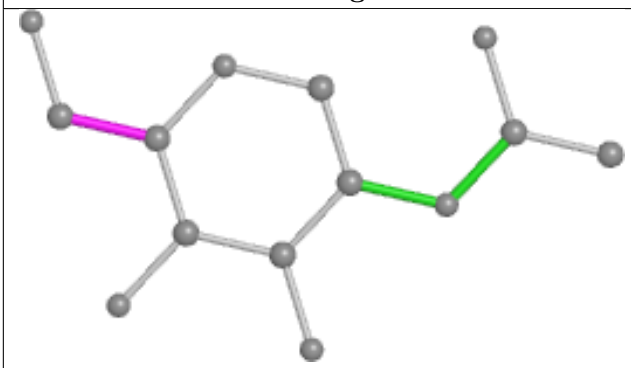
Ligand NAG C 1304



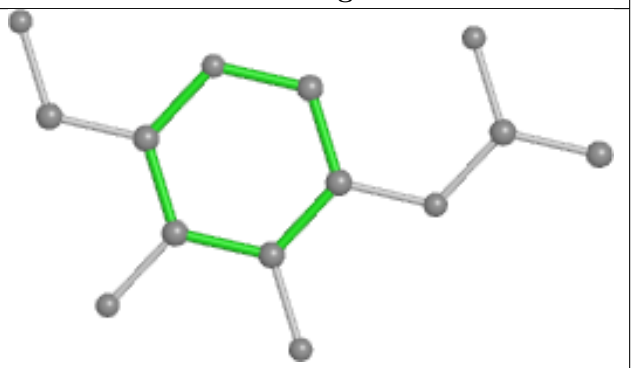
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

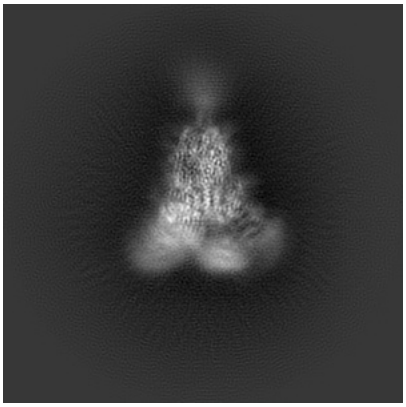
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30333. These allow visual inspection of the internal detail of the map and identification of artifacts.

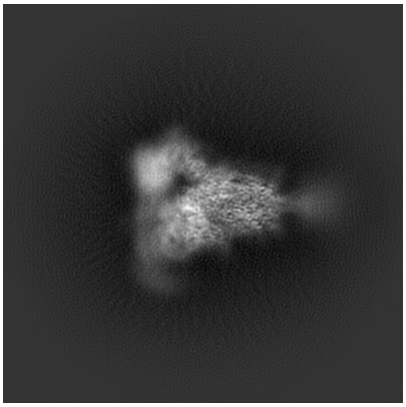
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

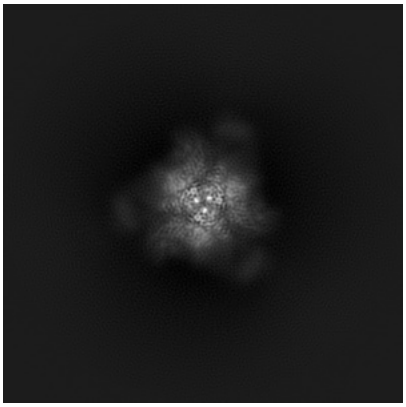
6.1.1 Primary map



X



Y

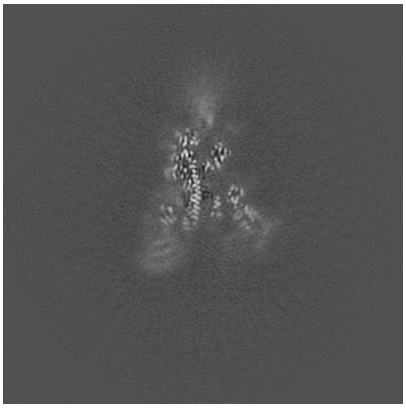


Z

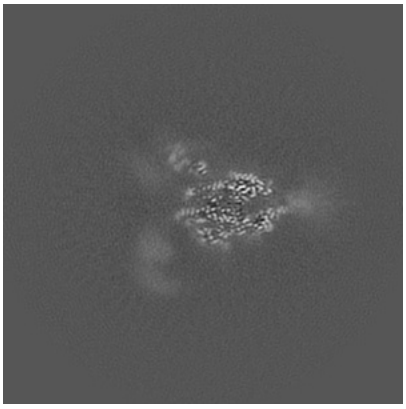
The images above show the map projected in three orthogonal directions.

6.2 Central slices

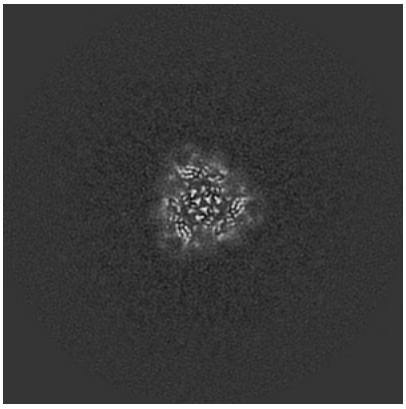
6.2.1 Primary map



X Index: 200



Y Index: 200

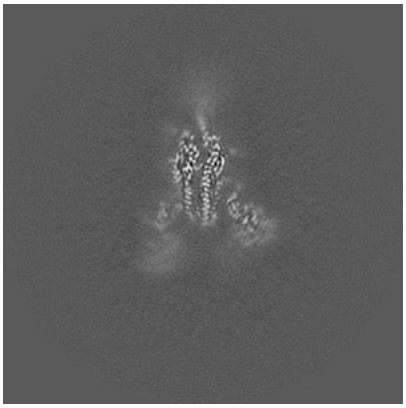


Z Index: 200

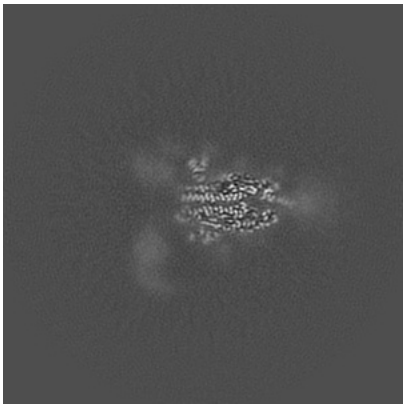
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

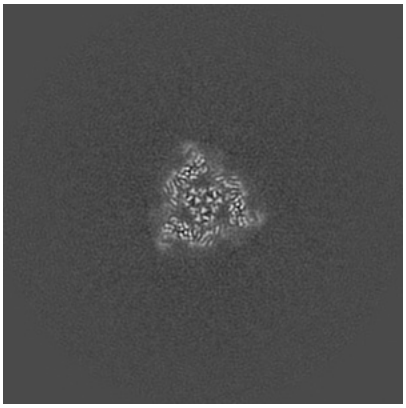
6.3.1 Primary map



X Index: 193



Y Index: 205

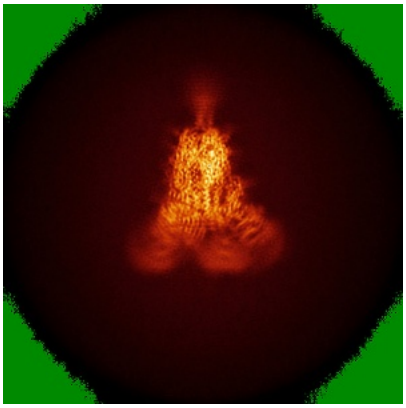


Z Index: 196

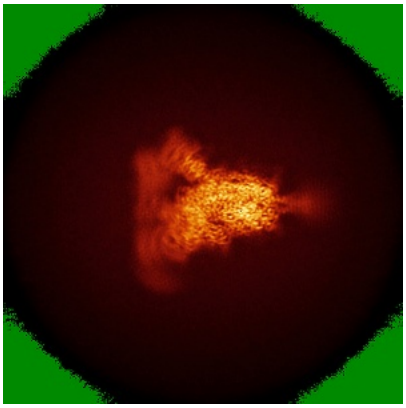
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

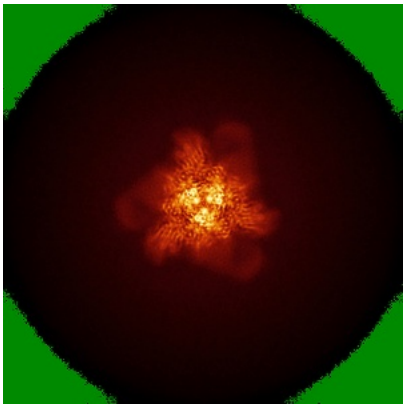
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

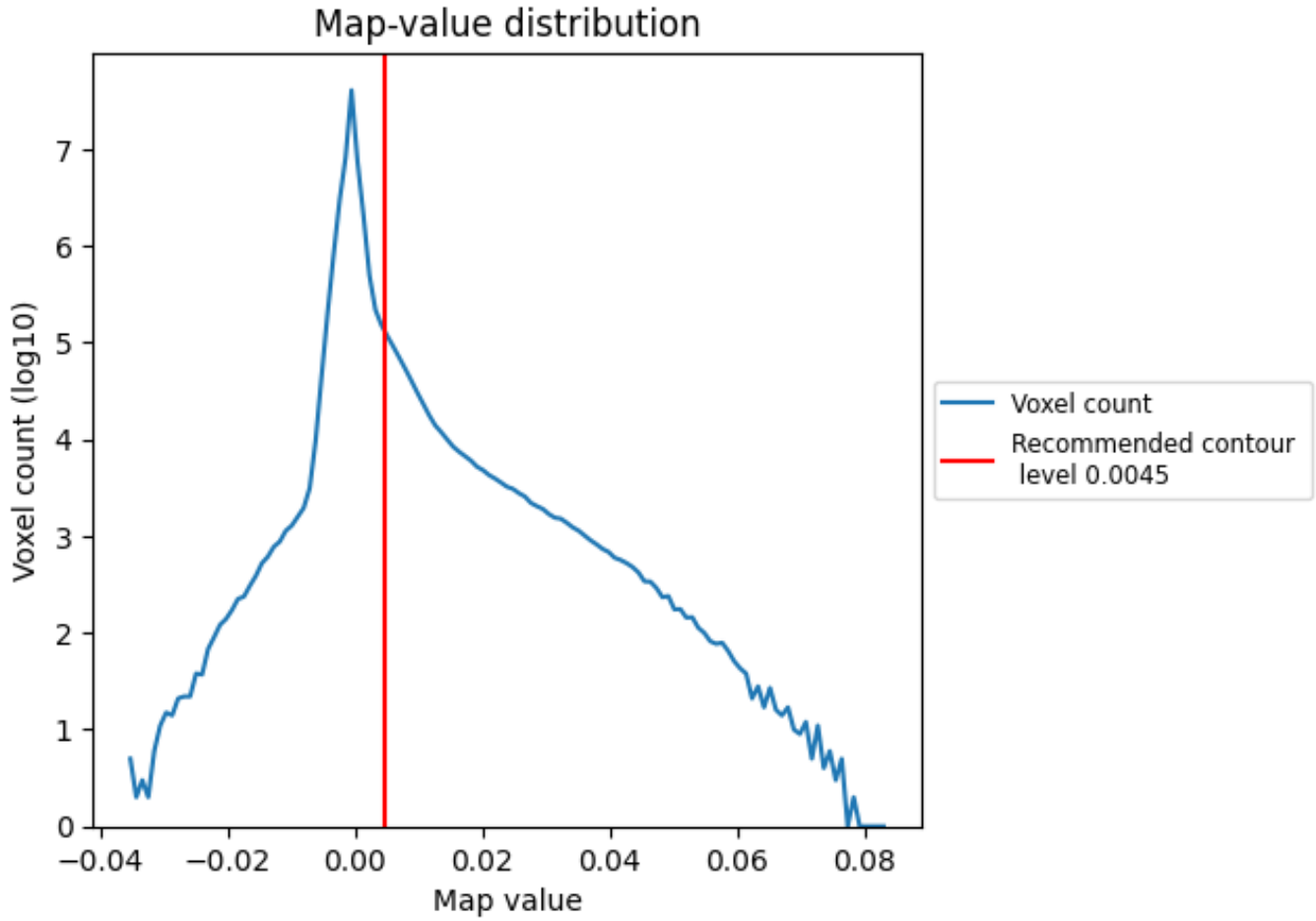
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

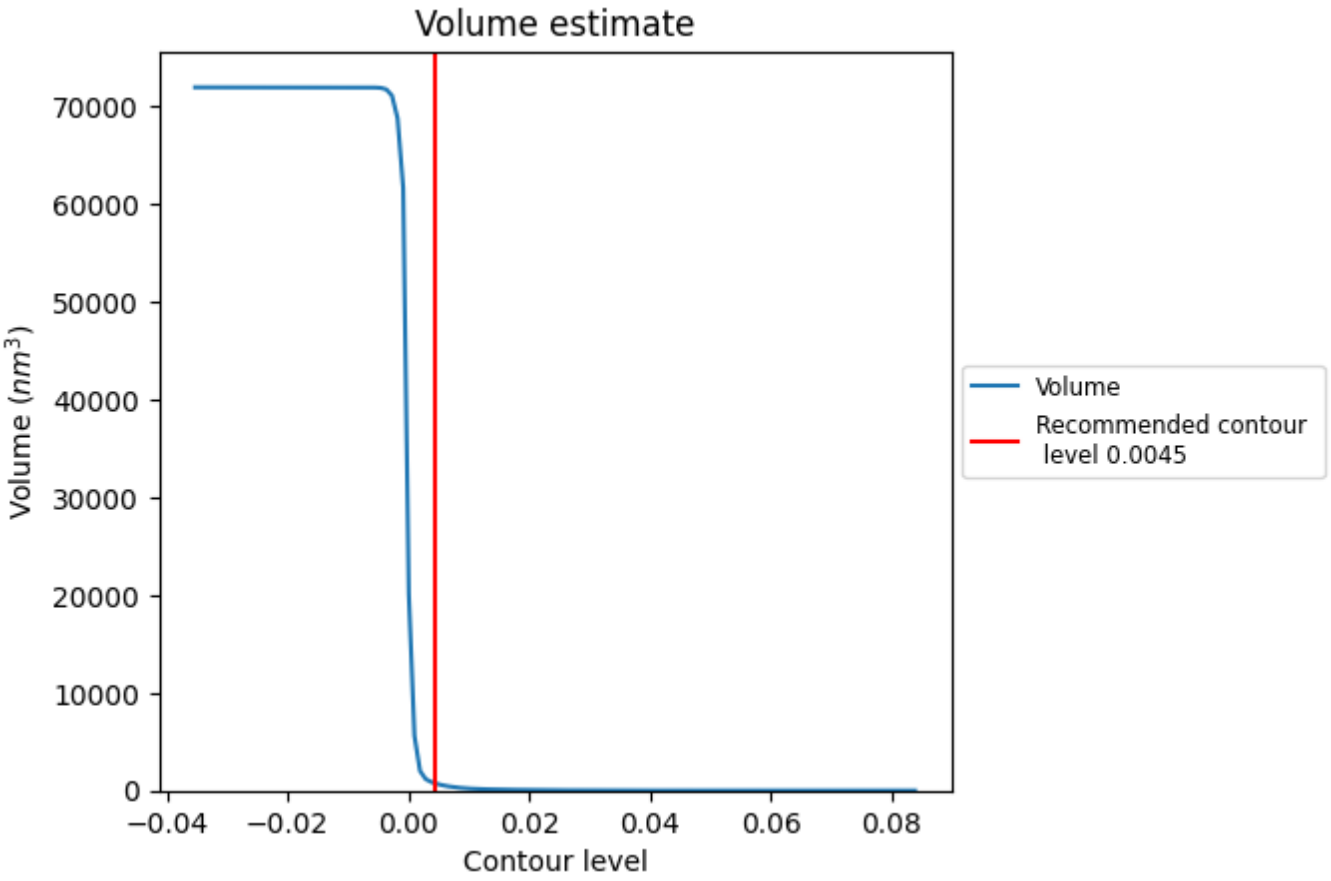
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

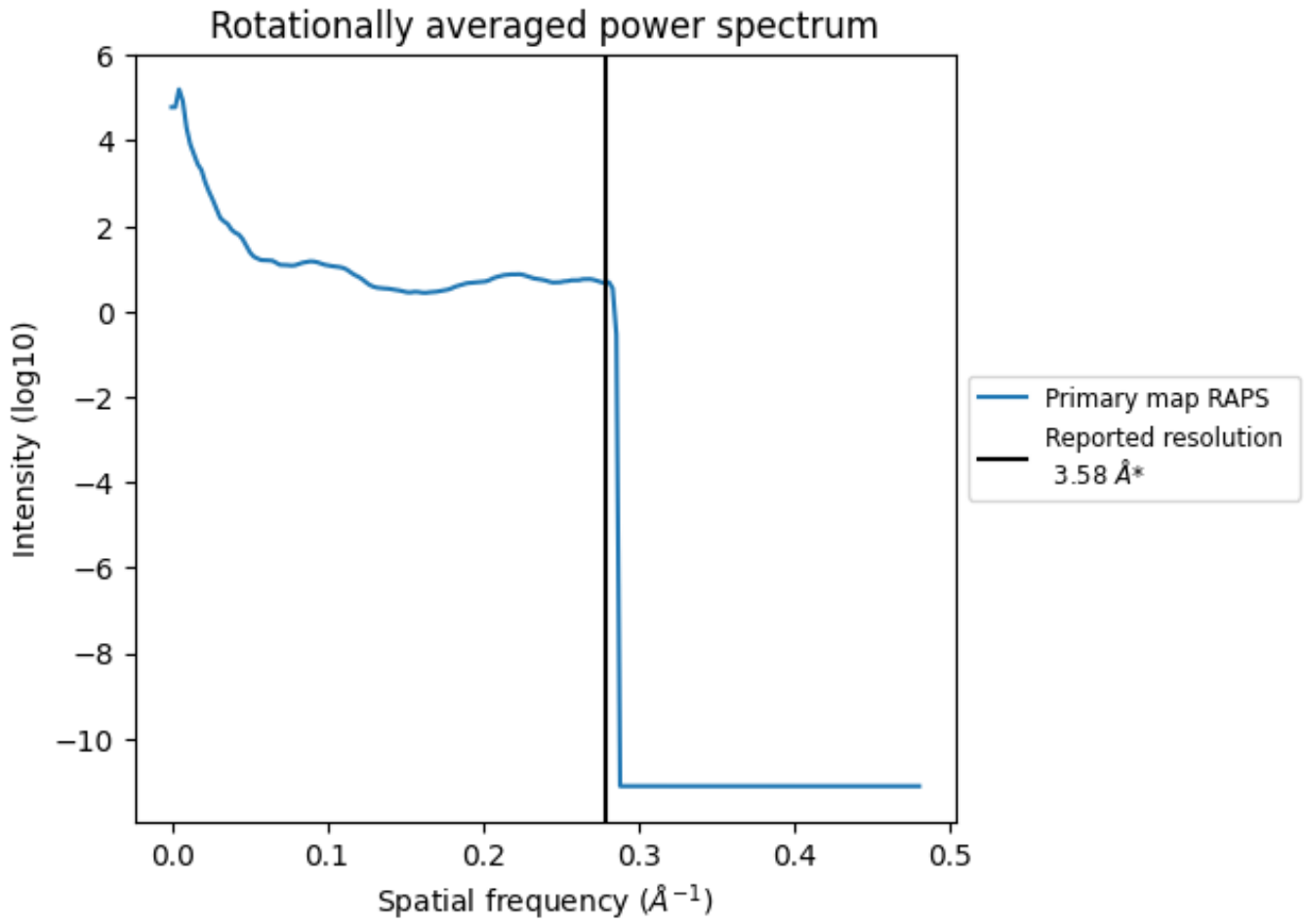
7.2 Volume estimate



The volume at the recommended contour level is 742 nm^3; this corresponds to an approximate mass of 670 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

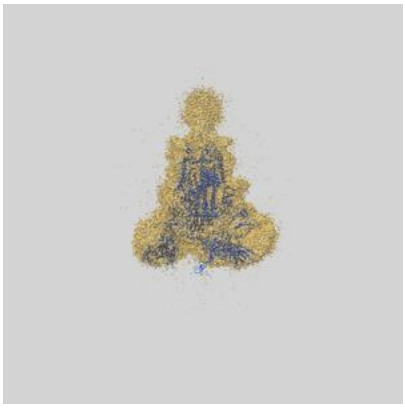
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

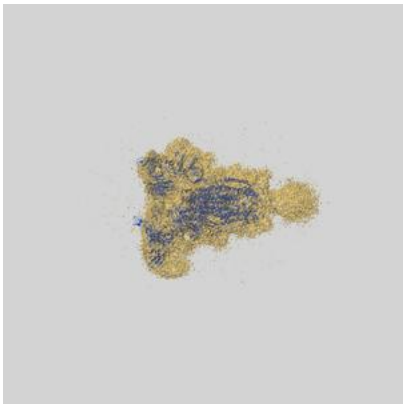
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30333 and PDB model 7CAK. Per-residue inclusion information can be found in section 3 on page 9.

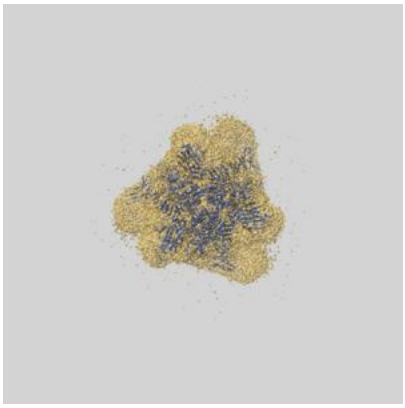
9.1 Map-model overlay



X



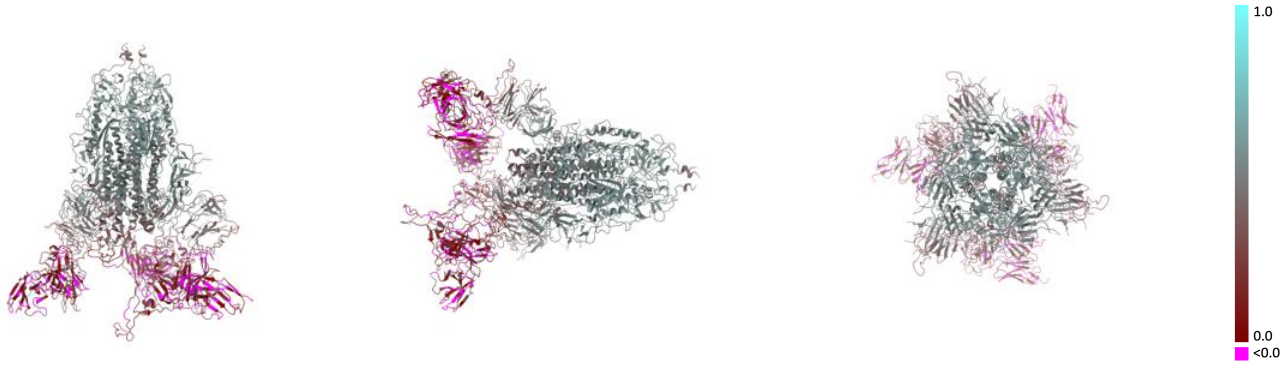
Y



Z

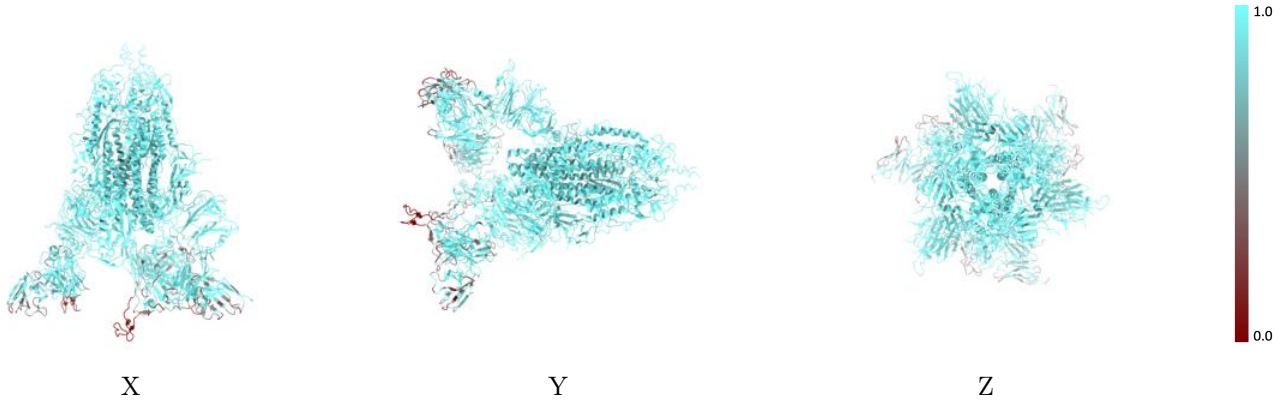
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



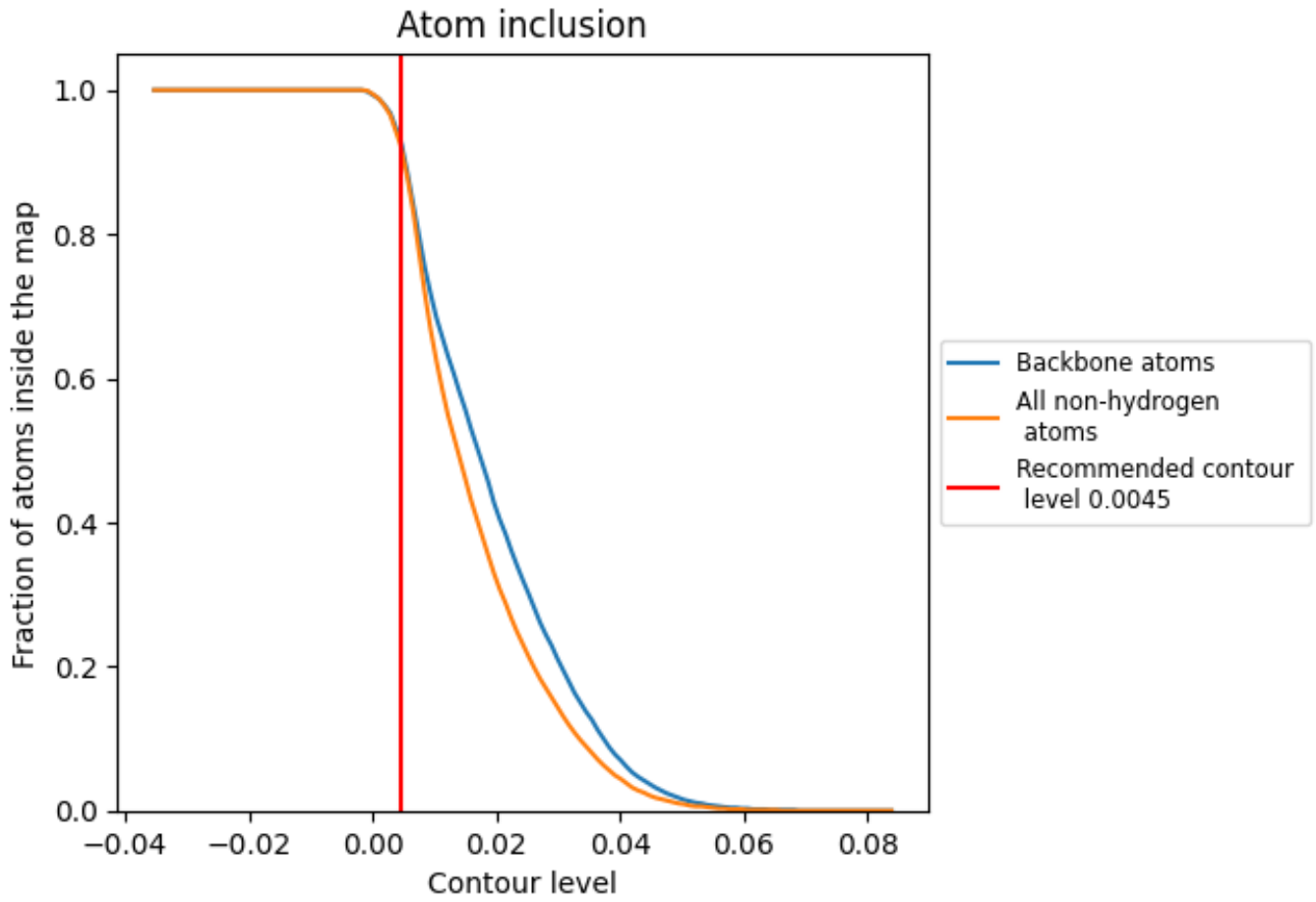
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0045).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9250	0.3620
A	0.9470	0.4240
B	0.9480	0.4230
C	0.9480	0.4230
D	0.7530	0.0360
E	0.8960	0.0620
F	0.7350	0.0980
G	0.8990	0.0700
H	0.7370	0.0670
I	0.8990	0.1020
J	0.5000	0.2390
K	1.0000	0.5040
L	1.0000	0.4490
M	1.0000	0.4810
N	1.0000	0.4540
O	0.5000	0.2330
P	1.0000	0.5150
Q	1.0000	0.4440
R	1.0000	0.4770
S	1.0000	0.4570
T	0.5000	0.2470
U	1.0000	0.4940
V	1.0000	0.4460
W	1.0000	0.4700
X	1.0000	0.4660