Full wwPDB EM Validation Report

Jun 29, 2025 – 07:15 am BST

PDB ID	:	7NVO / pdb_00007nvo
EMDB ID	:	EMD-12608
Title	:	Human TRiC complex in open state with nanobody bound
Authors	:	Kelly, J.J.; Chi, G.; Bulawa, C.; Paavilainen, V.O.; Bountra, C.; Huiskonen, J.T.; Yue, W.
Deposited on	:	2021-03-15
Resolution	:	3.50 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:

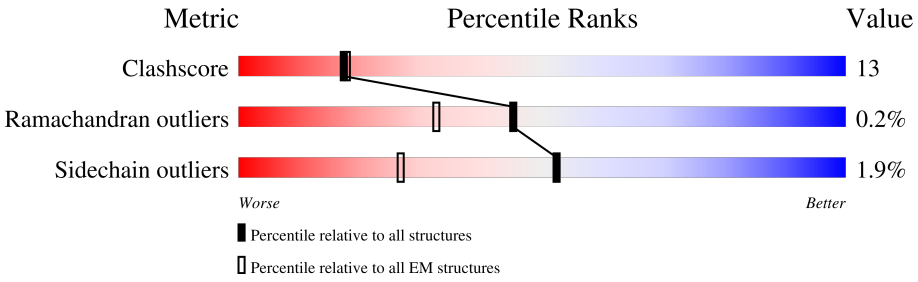
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 3.50 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	E	541	29% 17% 54%
1	e	541	29% 17% 54%
2	H	543	32% 14% 54%
2	h	543	32% 13% 54%
3	Q	548	47% 17% 36%
3	q	548	47% 17% 36%
4	Z	531	42% 19% 39%
4	z	531	42% 18% 39%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	G	545	32% 14% 54%
5	g	545	32% 13% 54%
6	A	556	33% 12% 55%
6	a	556	33% 12% 55%
7	D	539	29% 14% 54%
7	d	539	30% 14% 54%
8	B	535	39% 13% 47%
8	b	535	39% 13% 47%
9	N	129	8% 19% 9% 71%
9	n	129	15% 19% 9% 71%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ADP	Q	601	-	-	X	-
11	ADP	q	601	-	-	X	-
12	AF3	B	603	-	-	X	-
12	AF3	Z	603	-	-	X	-
12	AF3	b	603	-	-	X	-
12	AF3	z	603	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34246 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 T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	249	Total	C	N	O	S	0	0
			1873	1155	329	370	19		
1	e	249	Total	C	N	O	S	0	0
			1873	1155	329	370	19		

- Molecule 2 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	252	Total	C	N	O	S	0	0
			1900	1194	332	368	6		
2	h	252	Total	C	N	O	S	0	0
			1900	1194	332	368	6		

- Molecule 3 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	352	Total	C	N	O	S	0	0
			2685	1693	459	517	16		
3	q	352	Total	C	N	O	S	0	0
			2685	1693	459	517	16		

- Molecule 4 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	323	Total	C	N	O	S	0	0
			2417	1517	425	465	10		
4	z	323	Total	C	N	O	S	0	0
			2417	1517	425	465	10		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	249	Total	C	N	O	S	0	0
			1880	1179	328	358	15		
5	g	249	Total	C	N	O	S	0	0
			1880	1179	328	358	15		

- Molecule 6 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	249	Total	C	N	O	S	0	0
			1879	1187	322	365	5		
6	a	249	Total	C	N	O	S	0	0
			1879	1187	322	365	5		

- Molecule 7 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	247	Total	C	N	O	S	1	0
			1840	1150	318	363	9		
7	d	247	Total	C	N	O	S	1	0
			1840	1150	318	363	9		

- Molecule 8 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	282	Total	C	N	O	S	0	0
			2073	1282	364	415	12		
8	b	282	Total	C	N	O	S	0	0
			2073	1282	364	415	12		

- Molecule 9 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	37	Total	C	N	O	S	0	0
			323	208	56	57	2		
9	n	37	Total	C	N	O	S	0	0
			323	208	56	57	2		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

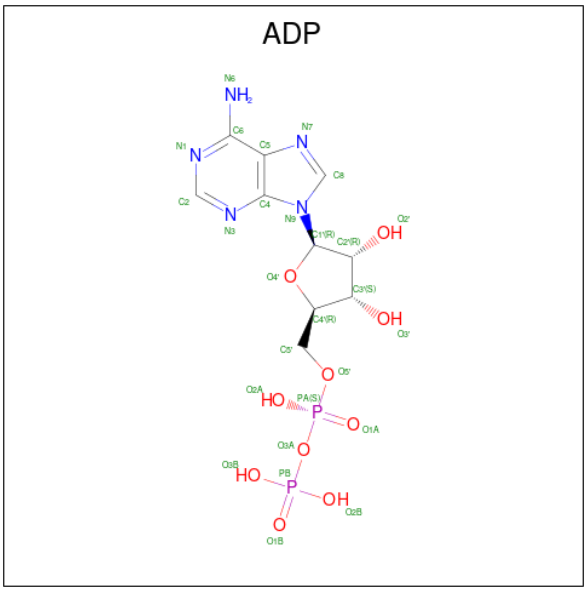
Mol	Chain	Residues	Atoms		AltConf
10	E	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
10	H	1	Total Mg 1 1	0
10	Q	1	Total Mg 1 1	0
10	Z	1	Total Mg 1 1	0
10	G	1	Total Mg 1 1	0
10	A	1	Total Mg 1 1	0
10	D	1	Total Mg 1 1	0
10	B	1	Total Mg 1 1	0
10	e	1	Total Mg 1 1	0
10	h	1	Total Mg 1 1	0
10	q	1	Total Mg 1 1	0
10	z	1	Total Mg 1 1	0
10	g	1	Total Mg 1 1	0
10	a	1	Total Mg 1 1	0
10	d	1	Total Mg 1 1	0
10	b	1	Total Mg 1 1	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



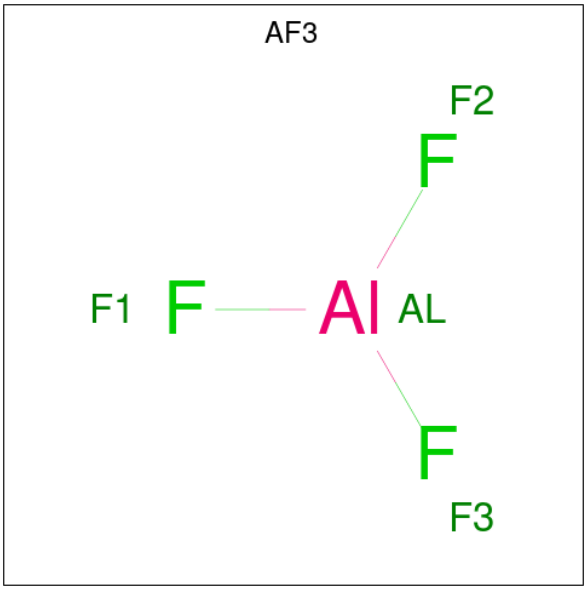
Mol	Chain	Residues	Atoms					AltConf
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	h	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	z	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	a	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
11	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	b	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			AltConf
12	H	1	Total	Al	F	0
			4	1	3	
12	Q	1	Total	Al	F	0
			4	1	3	
12	Z	1	Total	Al	F	0
			4	1	3	
12	G	1	Total	Al	F	0
			4	1	3	
12	A	1	Total	Al	F	0
			4	1	3	
12	B	1	Total	Al	F	0
			4	1	3	
12	h	1	Total	Al	F	0
			4	1	3	
12	q	1	Total	Al	F	0
			4	1	3	
12	z	1	Total	Al	F	0
			4	1	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
12	g	1	Total Al F 4 1 3	0
12	a	1	Total Al F 4 1 3	0
12	b	1	Total Al F 4 1 3	0

- Molecule 13 is water.

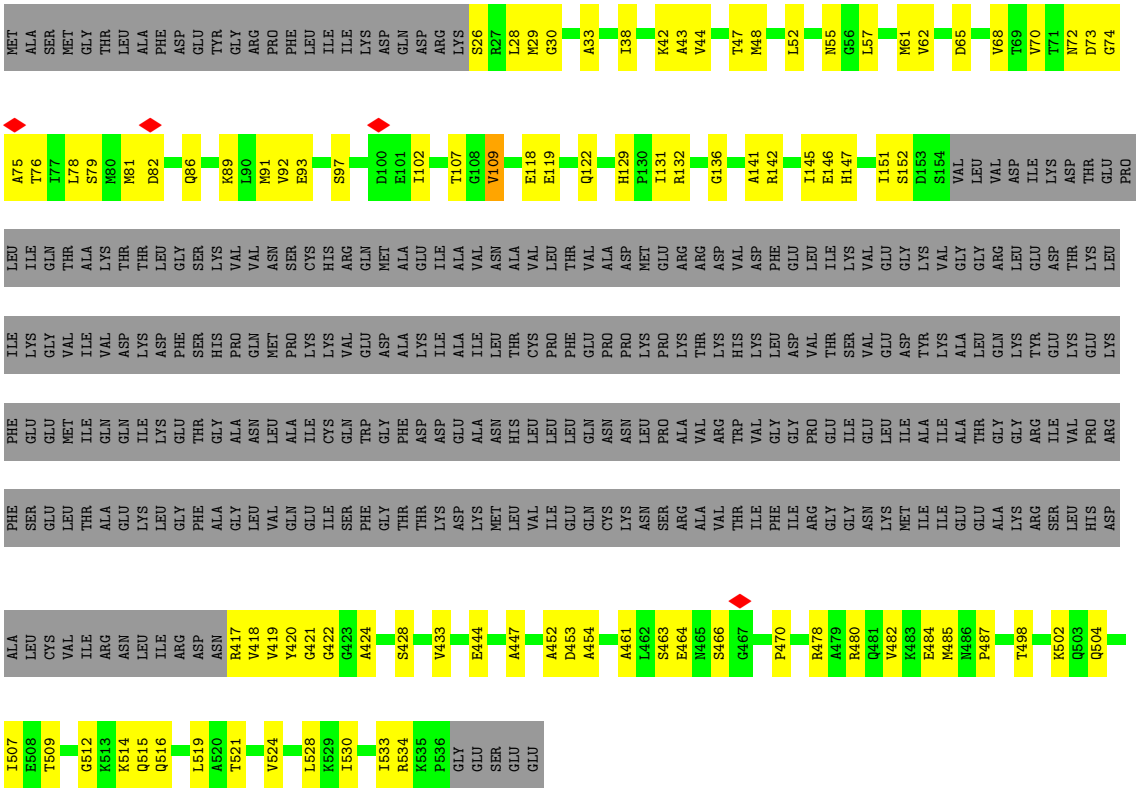
Mol	Chain	Residues	Atoms	AltConf
13	E	1	Total O 1 1	0
13	H	2	Total O 2 2	0
13	Q	1	Total O 1 1	0
13	D	1	Total O 1 1	0
13	e	1	Total O 1 1	0
13	h	2	Total O 2 2	0
13	q	1	Total O 1 1	0
13	d	1	Total O 1 1	0

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.

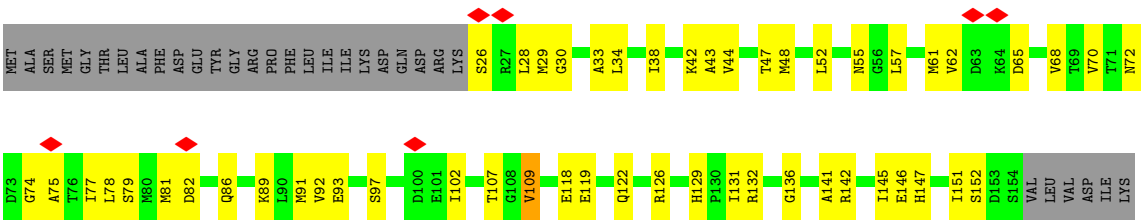
• Molecule 1: T-complex protein 1 subunit epsilon

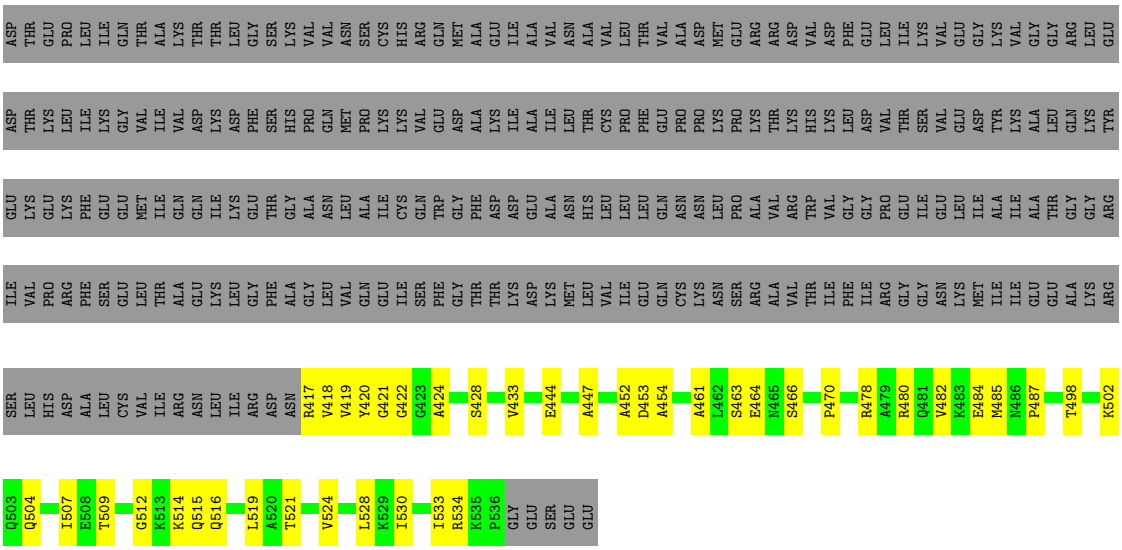
Chain E:



• Molecule 1: T-complex protein 1 subunit epsilon

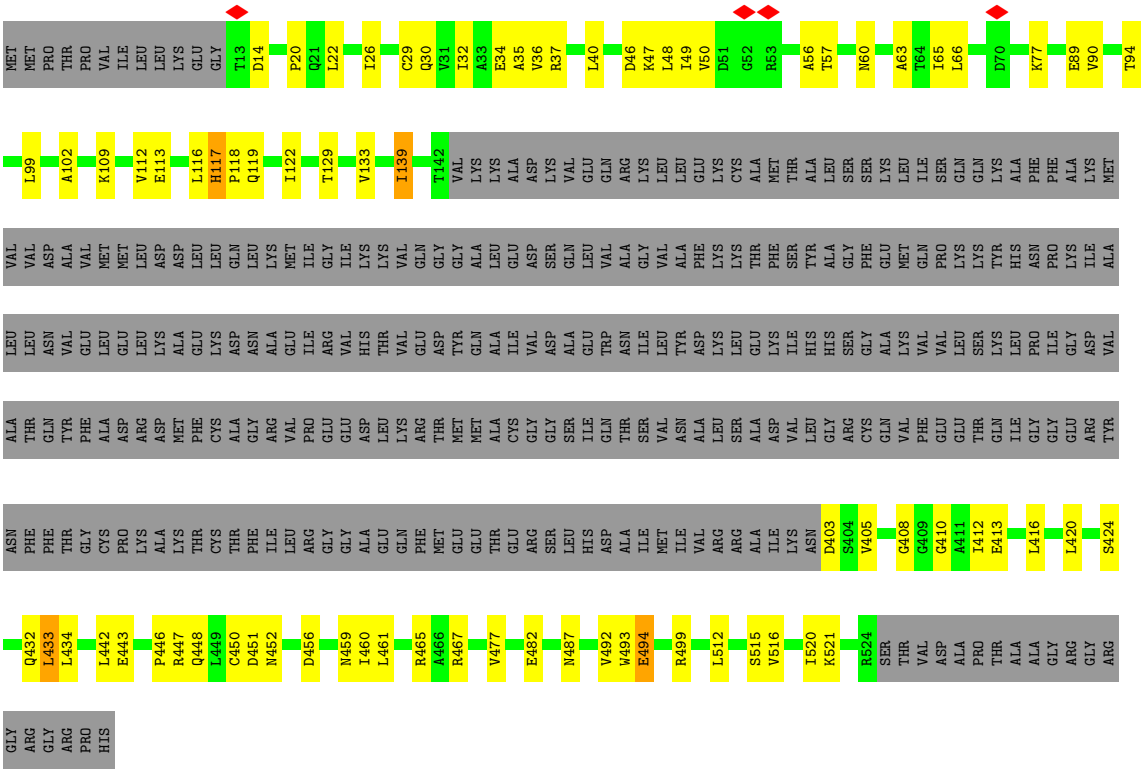
Chain e:





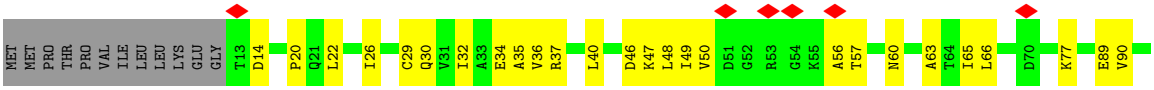
• Molecule 2: T-complex protein 1 subunit eta

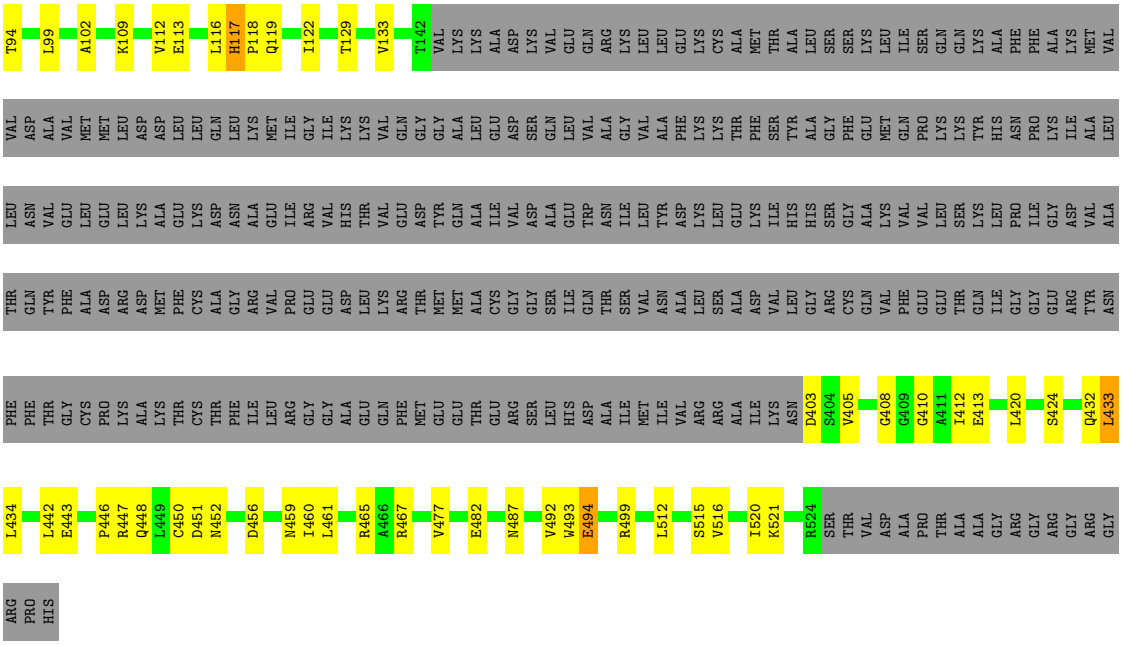
Chain H:



• Molecule 2: T-complex protein 1 subunit eta

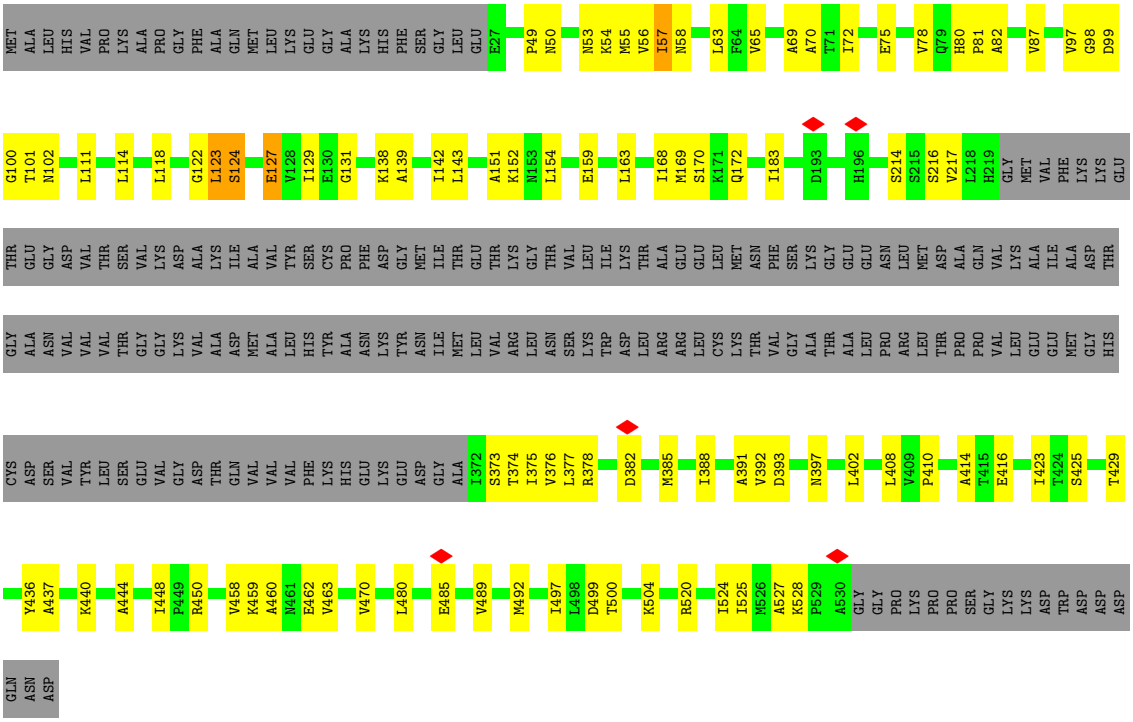
Chain h:





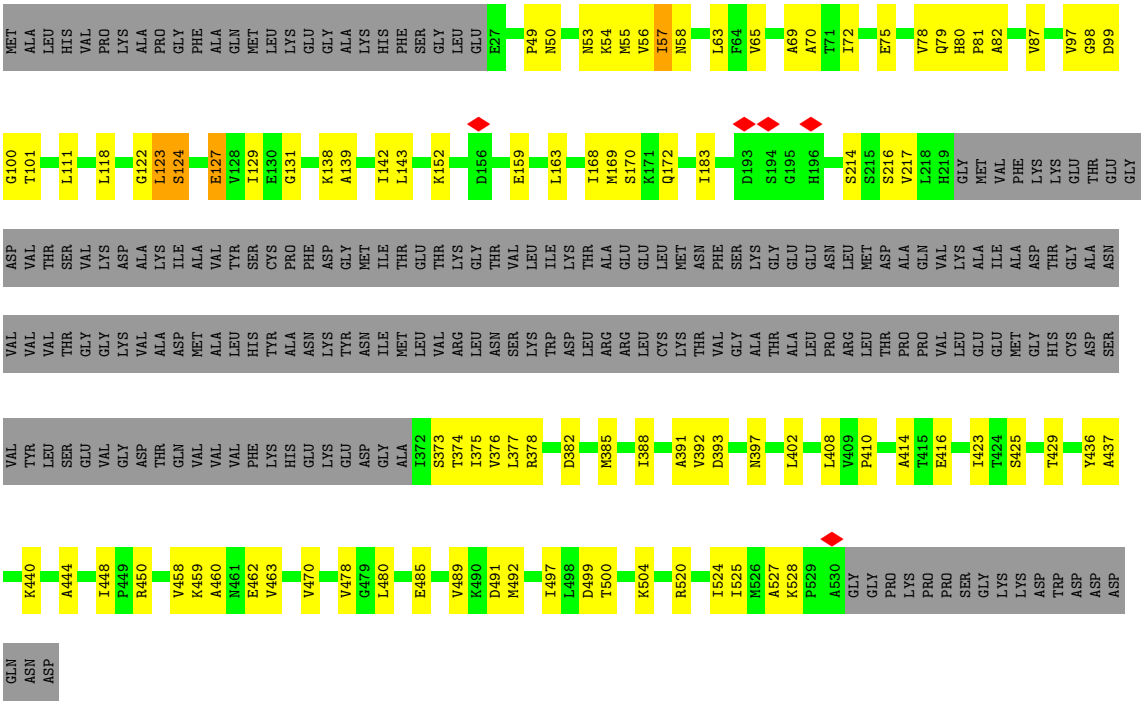
• Molecule 3: T-complex protein 1 subunit theta

Chain Q:



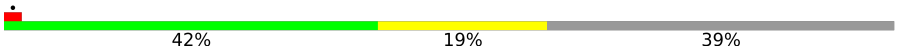
• Molecule 3: T-complex protein 1 subunit theta

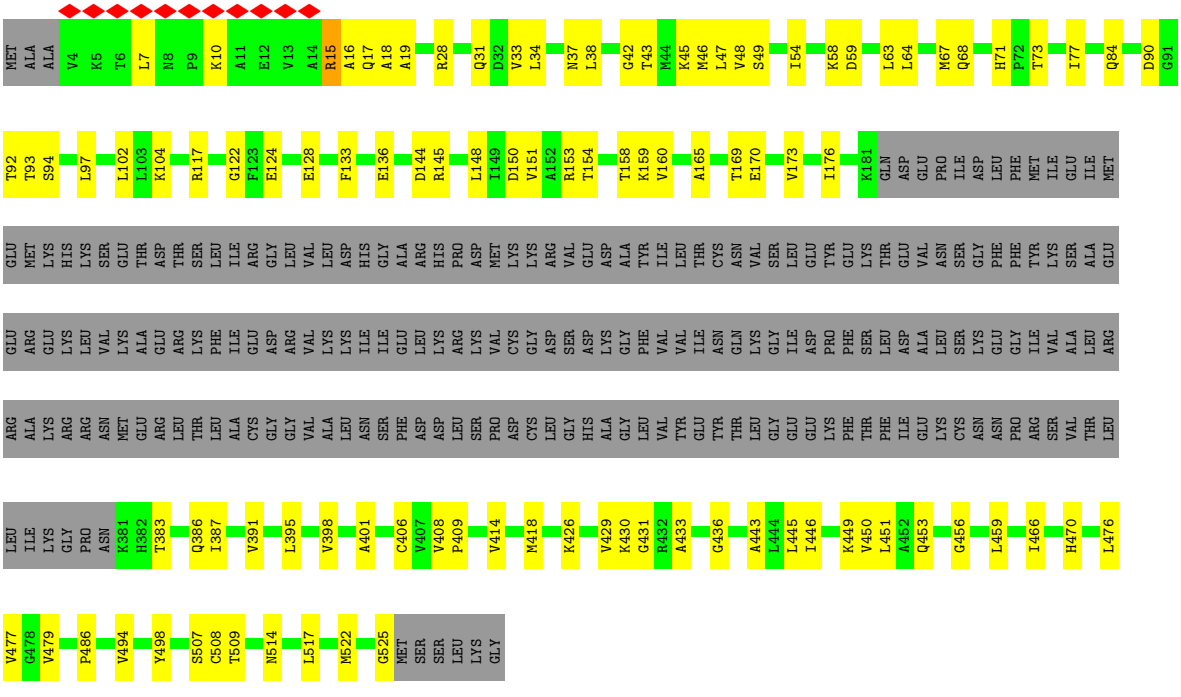
Chain q:



• Molecule 4: T-complex protein 1 subunit zeta

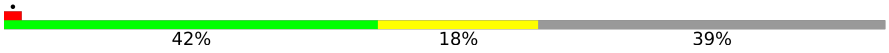
Chain Z:

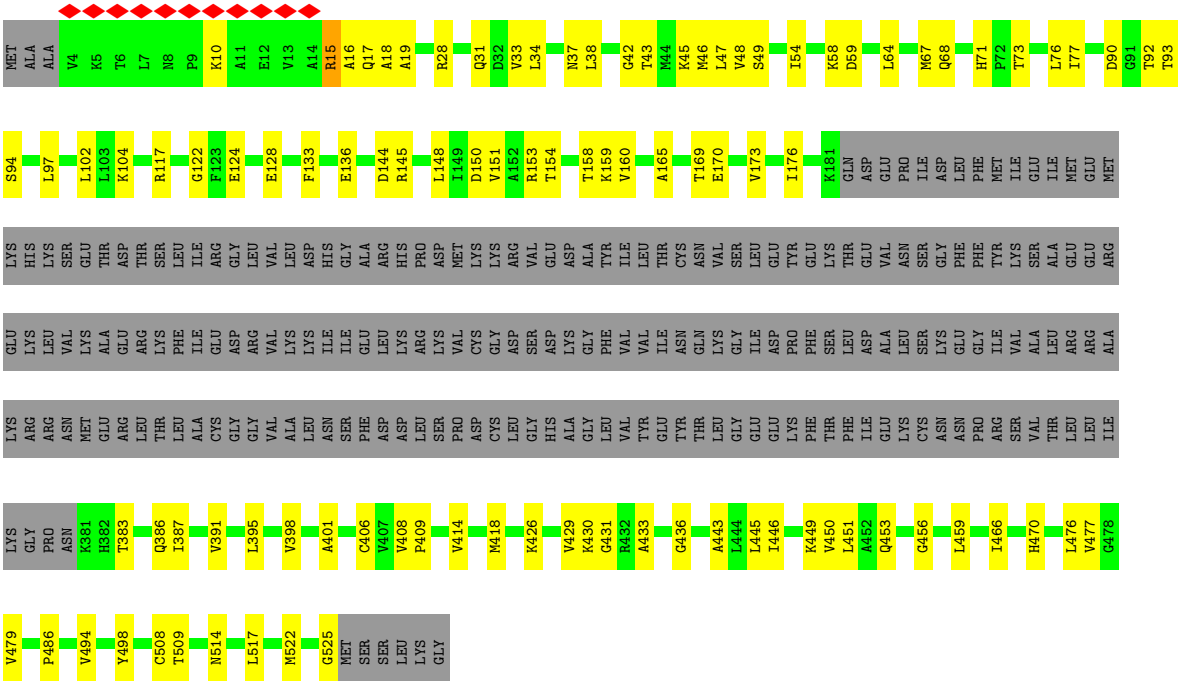




• Molecule 4: T-complex protein 1 subunit zeta

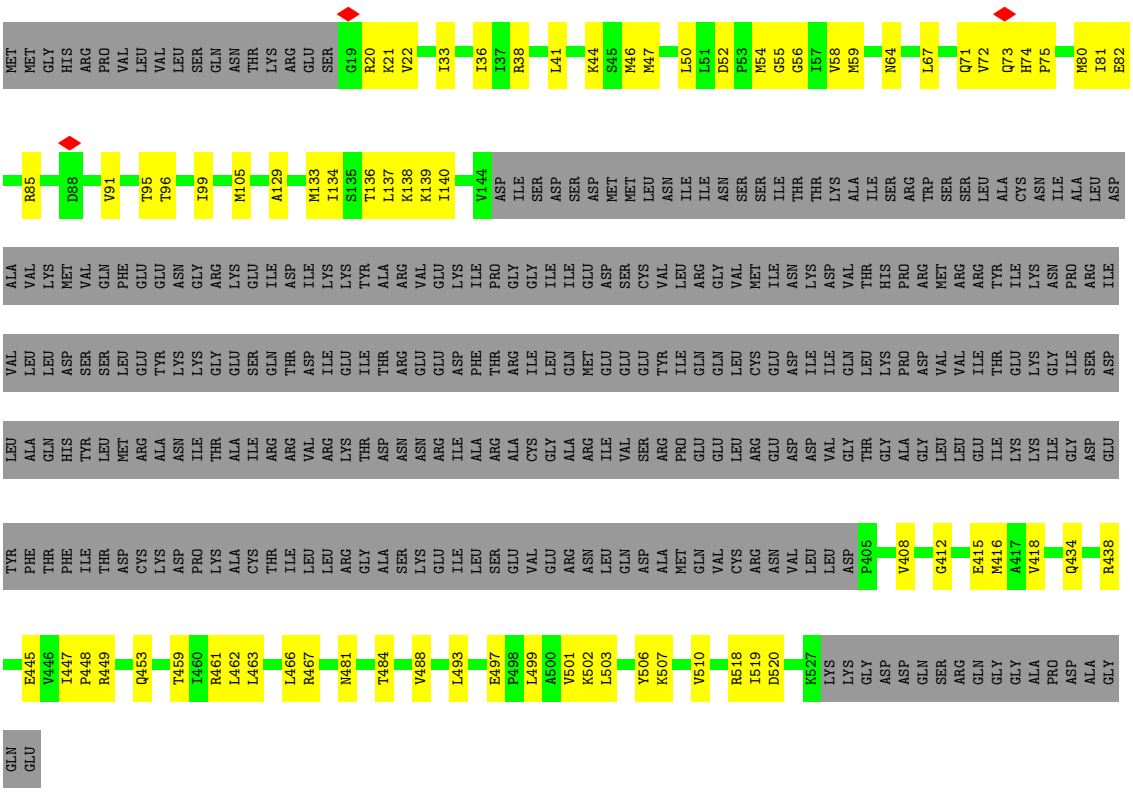
Chain z:





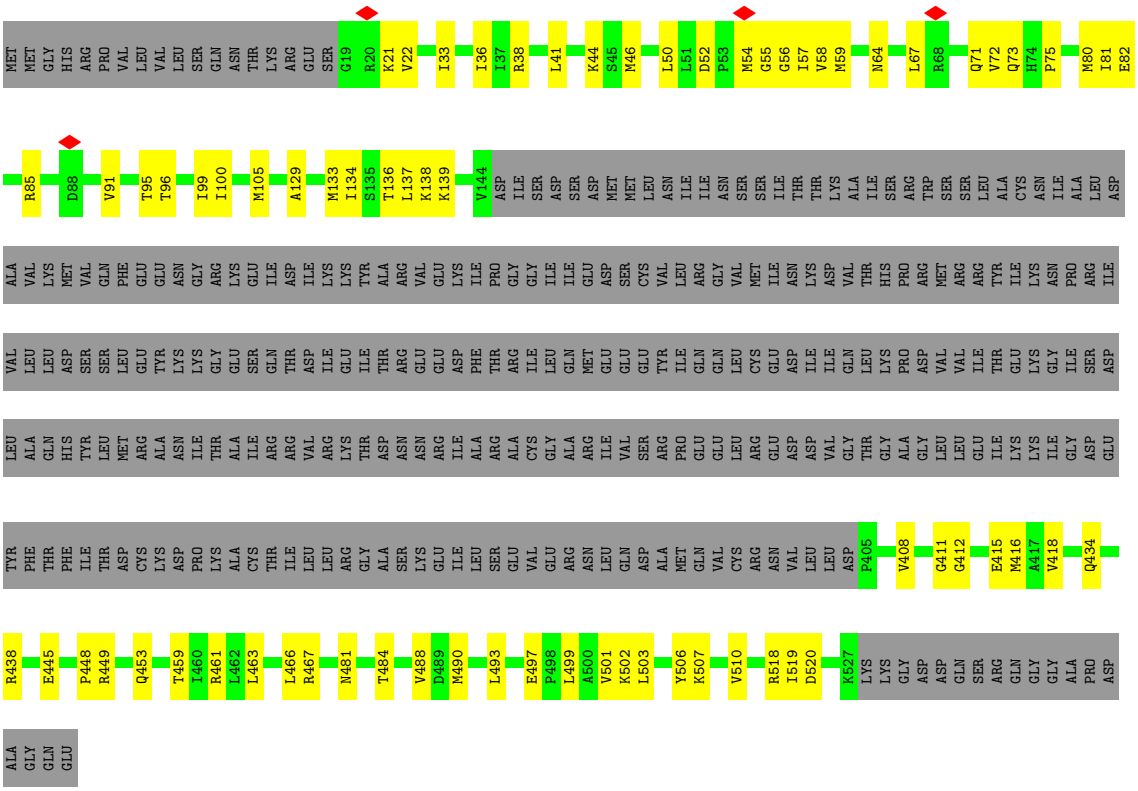
• Molecule 5: T-complex protein 1 subunit gamma

Chain G:



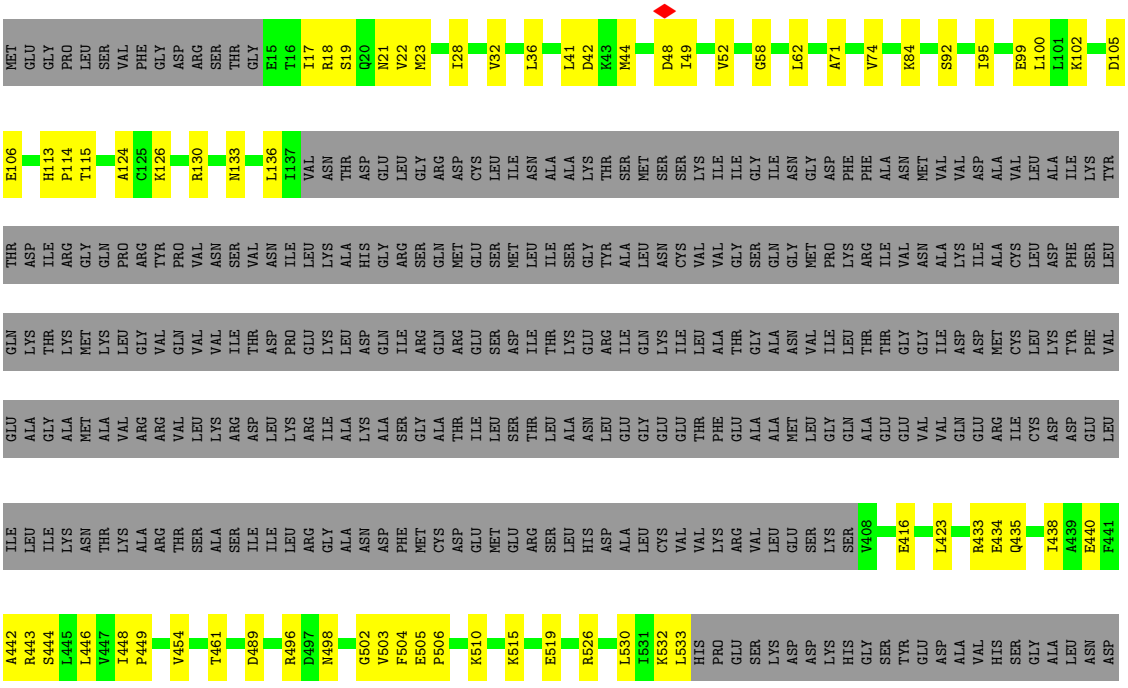
• Molecule 5: T-complex protein 1 subunit gamma

Chain g:



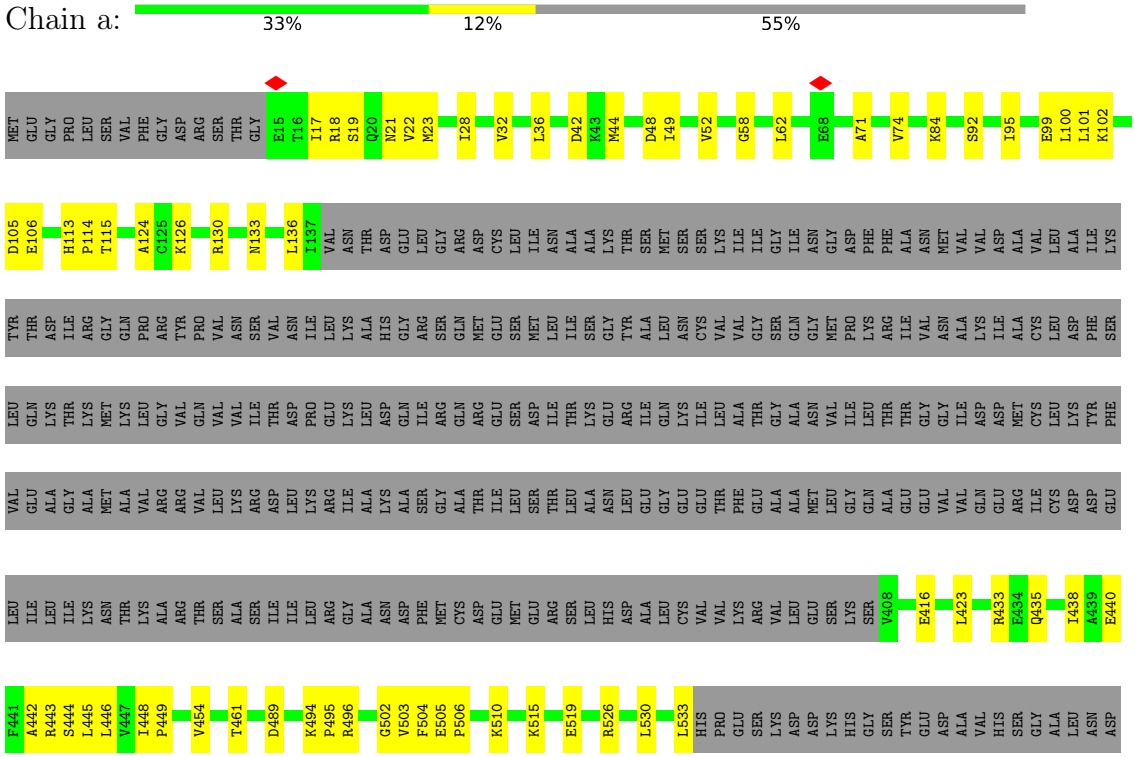
• Molecule 6: T-complex protein 1 subunit alpha

Chain A:



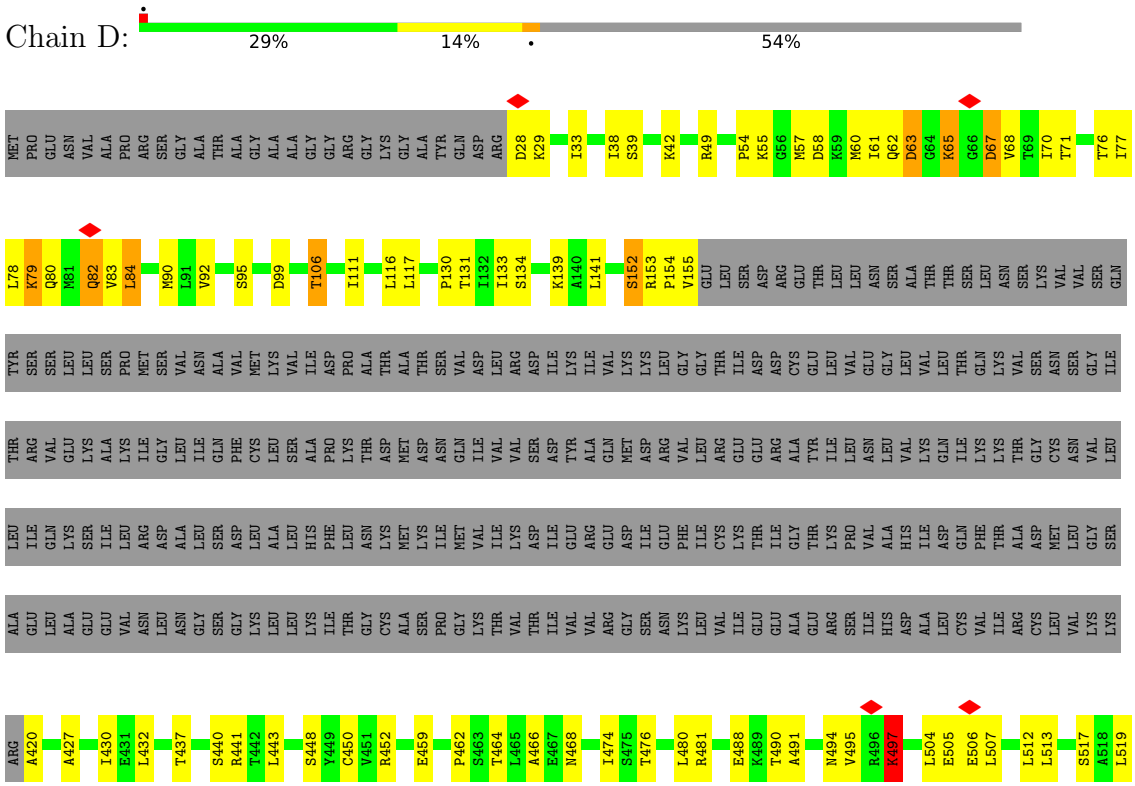
• Molecule 6: T-complex protein 1 subunit alpha

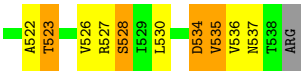
Chain a:



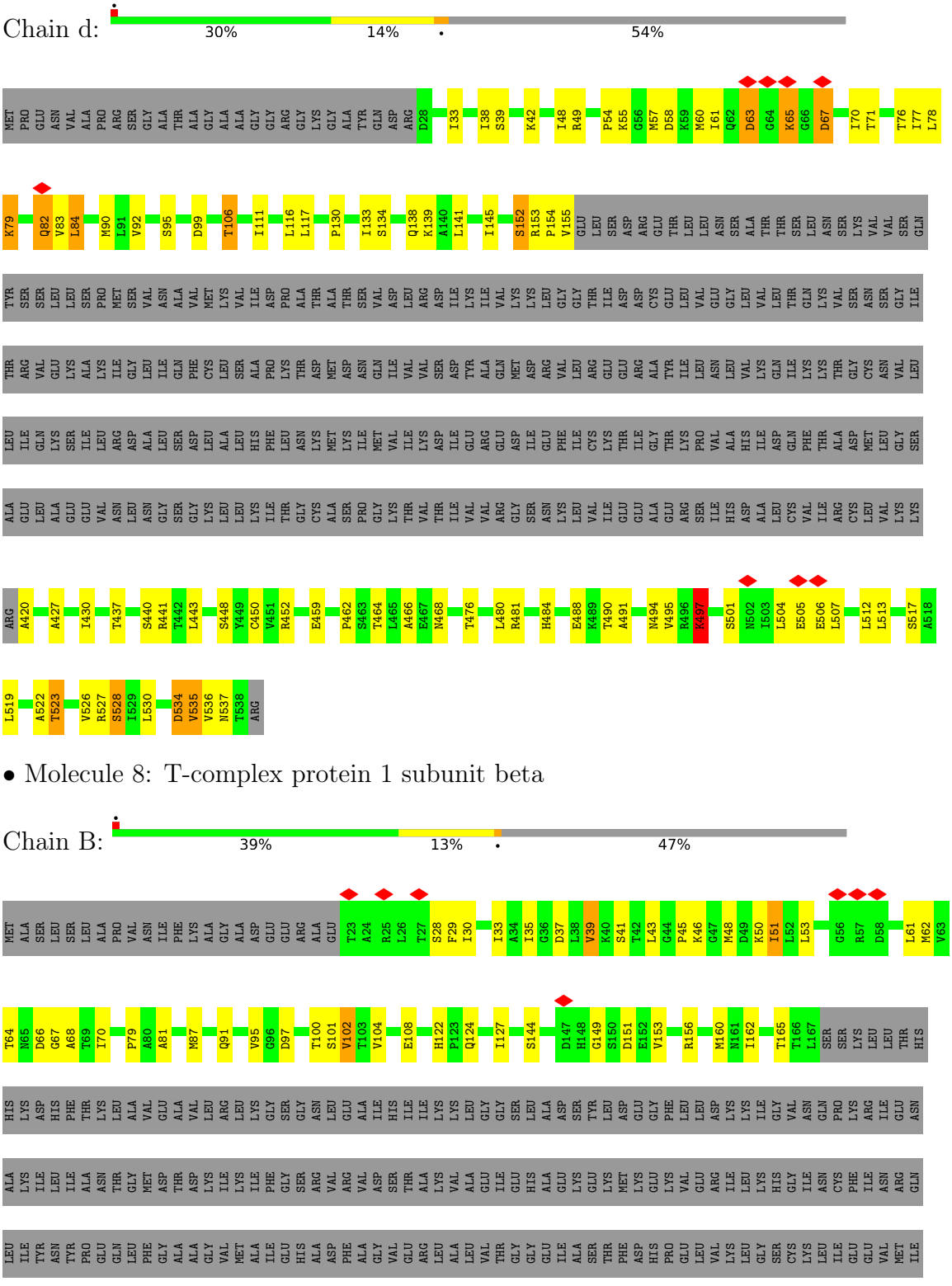
• Molecule 7: T-complex protein 1 subunit delta

Chain D:

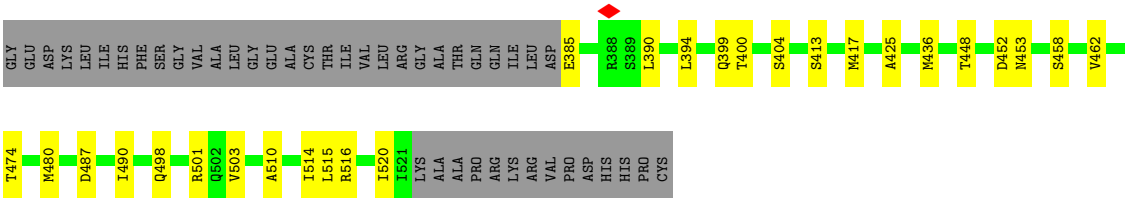


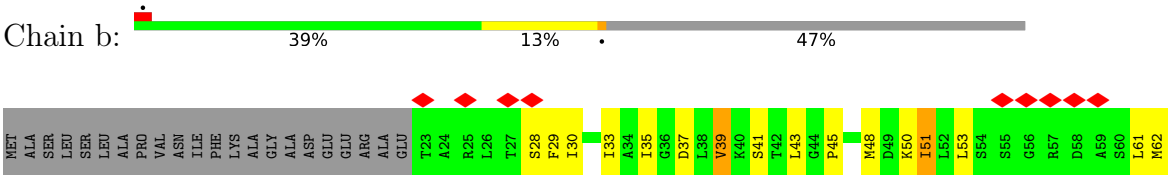


• Molecule 7: T-complex protein 1 subunit delta



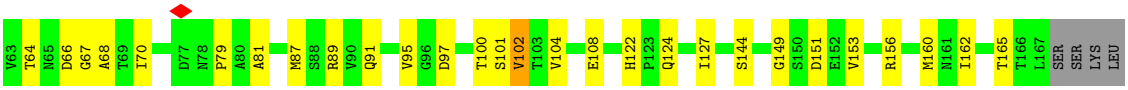
• Molecule 8: T-complex protein 1 subunit beta

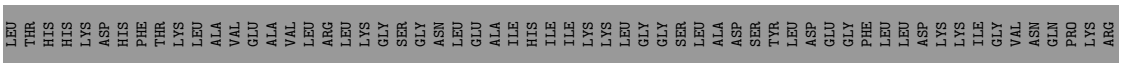


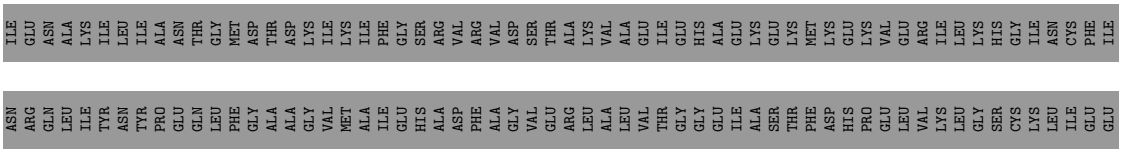


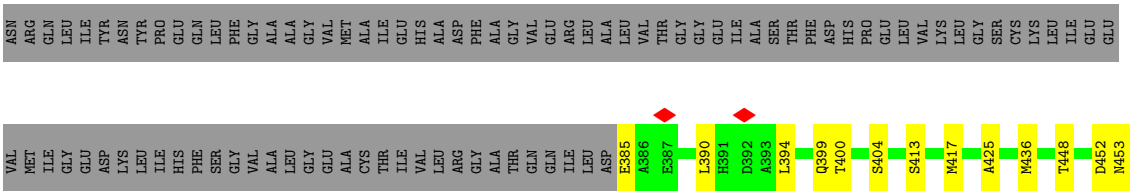
• Molecule 8: T-complex protein 1 subunit beta

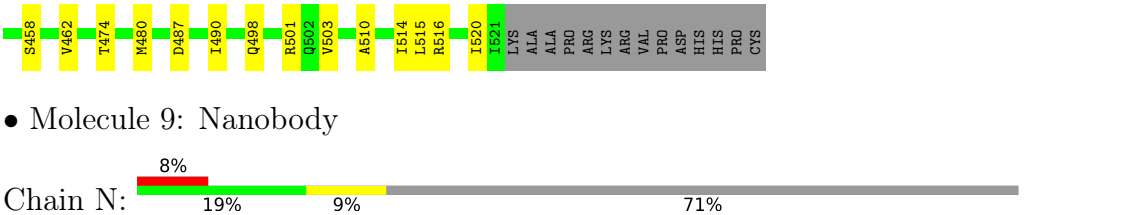
Chain b:

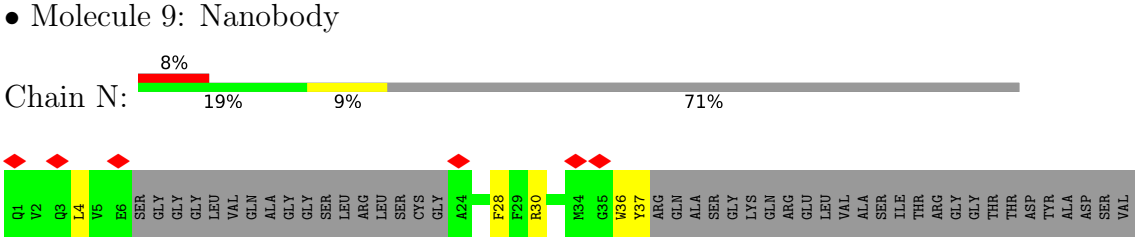






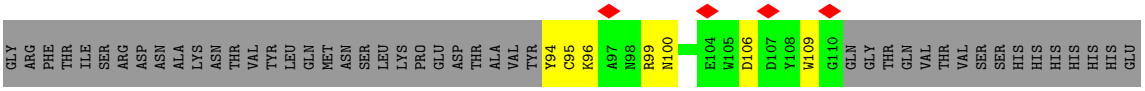






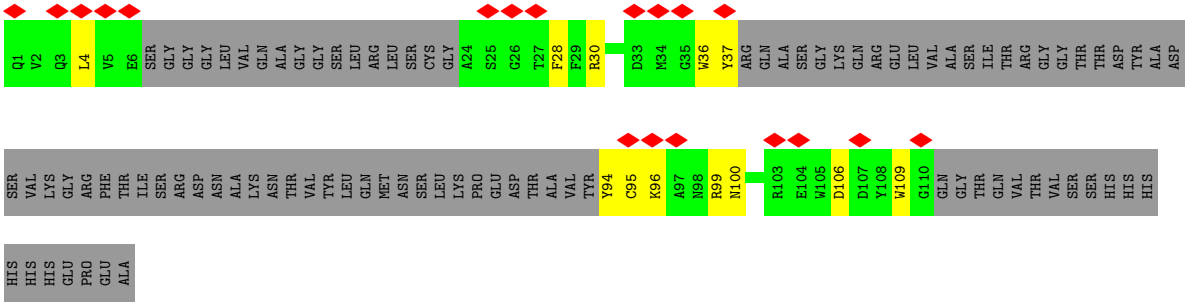
• Molecule 9: Nanobody

Chain N:



• Molecule 9: Nanobody

Chain n:


Q1 V2 Q3 L4 V5 E6 SER GLY GLY GLY LEU VAL GLN ALA GLY GLY SER LEU ARG LEU SER CYS GLY A24 S25 G26 T27 F28 F29 R30 D33 M34 G35 W36 Y37 ARG GLN ALA SER GLY LYS GLN ARG GLU LEU VAL ALA SER ILE THR ARG GLY GLY THR THR ASP TYR ALA ASP
SER VAL LYS GLY ARG PHE THR ILE SER ARG ASP ASN ALA LYS ASN THR VAL TYR LEU GLN MET ASN SER LEU LYS PRO GLU ASP THR ALA VAL TYR Y94 C95 K96 A97 N98 R99 N100 R103 E104 W105 D106 D107 Y108 W109 G110 GLN GLY THR GLN VAL THR VAL SER SER HIS HIS HIS
HIS HIS HIS GLU PRO GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	144903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, AF3

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	E	0.20	0/1888	0.43	0/2541
1	e	0.20	0/1888	0.43	0/2541
2	H	0.24	0/1924	0.39	0/2611
2	h	0.24	0/1924	0.39	0/2611
3	Q	0.22	0/2719	0.46	2/3677 (0.1%)
3	q	0.22	0/2719	0.46	2/3677 (0.1%)
4	Z	0.23	0/2439	0.47	0/3299
4	z	0.23	0/2439	0.47	0/3299
5	G	0.23	0/1904	0.41	0/2575
5	g	0.23	0/1904	0.41	0/2575
6	A	0.23	0/1898	0.43	0/2573
6	a	0.23	0/1898	0.43	0/2573
7	D	0.25	0/1856	0.51	1/2510 (0.0%)
7	d	0.25	0/1856	0.51	1/2510 (0.0%)
8	B	0.22	0/2089	0.39	0/2825
8	b	0.22	0/2089	0.39	0/2825
9	N	0.15	0/333	0.41	0/448
9	n	0.15	0/333	0.41	0/448
All	All	0.23	0/34100	0.44	6/46118 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	q	122	GLY	CA-C-N	-6.64	107.49	121.64
3	q	122	GLY	C-N-CA	-6.64	107.49	121.64
3	Q	122	GLY	CA-C-N	-6.62	107.55	121.64
3	Q	122	GLY	C-N-CA	-6.62	107.55	121.64
7	D	497	LYS	CA-CB-CG	5.25	124.59	114.10
7	d	497	LYS	CA-CB-CG	5.22	124.55	114.10

There are no chirality outliers.

There are no planarity outliers.

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	E	1873	0	1913	61	0
1	e	1873	0	1913	60	0
2	H	1900	0	1942	61	0
2	h	1900	0	1942	59	0
3	Q	2685	0	2737	82	0
3	q	2685	0	2737	78	0
4	Z	2417	0	2526	82	0
4	z	2417	0	2526	81	0
5	G	1880	0	1946	60	0
5	g	1880	0	1946	56	0
6	A	1879	0	1957	42	0
6	a	1879	0	1957	42	0
7	D	1840	0	1917	66	0
7	d	1840	0	1917	67	0
8	B	2073	0	2115	51	0
8	b	2073	0	2115	51	0
9	N	323	0	283	8	0
9	n	323	0	283	8	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	Q	1	0	0	0	0
10	Z	1	0	0	0	0
10	a	1	0	0	0	0
10	b	1	0	0	0	0
10	d	1	0	0	0	0
10	e	1	0	0	0	0
10	g	1	0	0	0	0
10	h	1	0	0	0	0
10	q	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	z	1	0	0	0	0
11	A	27	0	12	1	0
11	B	27	0	12	3	0
11	D	27	0	12	0	0
11	E	27	0	12	2	0
11	G	27	0	12	5	0
11	H	27	0	12	1	0
11	Q	27	0	12	13	0
11	Z	27	0	12	2	0
11	a	27	0	12	1	0
11	b	27	0	12	3	0
11	d	27	0	12	0	0
11	e	27	0	12	2	0
11	g	27	0	12	5	0
11	h	27	0	12	1	0
11	q	27	0	12	10	0
11	z	27	0	12	2	0
12	A	4	0	0	1	0
12	B	4	0	0	2	0
12	G	4	0	0	0	0
12	H	4	0	0	1	0
12	Q	4	0	0	1	0
12	Z	4	0	0	3	0
12	a	4	0	0	1	0
12	b	4	0	0	2	0
12	g	4	0	0	0	0
12	h	4	0	0	1	0
12	q	4	0	0	1	0
12	z	4	0	0	3	0
13	D	1	0	0	0	0
13	E	1	0	0	1	0
13	H	2	0	0	0	0
13	Q	1	0	0	0	0
13	d	1	0	0	0	0
13	e	1	0	0	1	0
13	h	2	0	0	0	0
13	q	1	0	0	0	0
All	All	34246	0	34864	925	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 13.

All (925) 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)
3:Q:170:SER:HB2	11:Q:601:ADP:H5'1	1.21	1.16
5:g:41:LEU:HD11	11:g:601:ADP:H5'1	1.21	1.12
5:G:41:LEU:HD11	11:G:601:ADP:H5'2	1.15	1.11
3:q:169:MET:SD	11:q:601:ADP:N6	2.23	1.10
5:G:41:LEU:HD11	11:G:601:ADP:C5'	1.82	1.09
5:g:41:LEU:CD1	11:g:601:ADP:H5'1	1.88	1.03
3:q:170:SER:HB2	11:q:601:ADP:H5'1	1.43	0.98
5:g:41:LEU:HD11	11:g:601:ADP:C5'	1.96	0.94
1:e:152:SER:HG	1:e:417:ARG:N	1.65	0.94
3:Q:170:SER:HB2	11:Q:601:ADP:C5'	1.98	0.92
1:E:152:SER:HG	1:E:417:ARG:N	1.69	0.91
3:Q:169:MET:SD	11:Q:601:ADP:N6	2.44	0.91
7:d:152:SER:HB3	7:d:512:LEU:HD11	1.55	0.89
7:D:152:SER:HB3	7:D:512:LEU:HD11	1.55	0.89
5:G:41:LEU:HD12	11:G:601:ADP:O1A	1.76	0.84
5:G:41:LEU:CD1	11:G:601:ADP:C5'	2.56	0.84
8:B:33:ILE:O	8:B:37:ASP:HB2	1.79	0.83
7:d:535:VAL:HG13	8:b:51:ILE:HG23	1.58	0.83
8:b:33:ILE:O	8:b:37:ASP:HB2	1.79	0.82
7:D:535:VAL:HG13	8:B:51:ILE:HG23	1.60	0.81
2:H:37:ARG:HG2	2:H:99:LEU:HD21	1.65	0.79
2:h:37:ARG:HG2	2:h:99:LEU:HD21	1.65	0.79
5:g:52:ASP:H	5:g:56:GLY:HA2	1.50	0.77
4:Z:46:MET:HE2	4:Z:54:ILE:HB	1.67	0.76
5:G:52:ASP:H	5:G:56:GLY:HA2	1.50	0.76
5:G:82:GLU:OE1	5:G:85:ARG:NH2	2.20	0.75
4:z:46:MET:HE2	4:z:54:ILE:HB	1.67	0.75
2:H:22:LEU:HD23	2:H:112:VAL:HG21	1.68	0.75
1:E:62:VAL:HG21	8:B:79:PRO:HB3	1.70	0.73
2:h:22:LEU:HD23	2:h:112:VAL:HG21	1.68	0.73
5:g:82:GLU:OE1	5:g:85:ARG:NH2	2.20	0.73
1:e:62:VAL:HG21	8:b:79:PRO:HB3	1.71	0.72
2:h:30:GLN:NE2	2:h:102:ALA:O	2.23	0.71
2:H:443:GLU:OE2	2:H:465:ARG:NH1	2.24	0.71
7:D:38:ILE:HG23	7:D:117:LEU:HB3	1.73	0.70
8:b:35:ILE:HG13	8:b:81:ALA:HB1	1.73	0.70
2:H:30:GLN:NE2	2:H:102:ALA:O	2.23	0.70
5:G:416:MET:HG3	5:G:466:LEU:HD13	1.73	0.70
5:G:38:ARG:NH1	5:G:453:GLN:OE1	2.25	0.70
7:d:38:ILE:HG23	7:d:117:LEU:HB3	1.73	0.70
5:g:416:MET:HG3	5:g:466:LEU:HD13	1.73	0.70
6:A:48:ASP:OD1	6:A:49:ILE:N	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:39:VAL:HG13	8:B:100:THR:HG23	1.74	0.70
5:g:38:ARG:NH1	5:g:453:GLN:OE1	2.25	0.70
5:g:137:LEU:HB3	5:g:499:LEU:HD11	1.74	0.70
6:a:48:ASP:OD1	6:a:49:ILE:N	2.24	0.69
5:g:519:ILE:HD13	6:a:44:MET:HE2	1.74	0.69
8:B:35:ILE:HG13	8:B:81:ALA:HB1	1.73	0.69
4:z:10:LYS:HZ1	5:g:73:GLN:HB2	1.57	0.69
2:h:443:GLU:OE2	2:h:465:ARG:NH1	2.24	0.69
8:b:39:VAL:HG13	8:b:100:THR:HG23	1.74	0.69
8:b:51:ILE:HD11	8:b:61:LEU:HD22	1.74	0.69
8:B:51:ILE:HD11	8:B:61:LEU:HD22	1.74	0.69
7:D:63:ASP:OD1	7:D:65:LYS:HG2	1.93	0.69
5:g:518:ARG:NE	6:a:42:ASP:OD1	2.24	0.69
7:d:63:ASP:OD1	7:d:65:LYS:HG2	1.93	0.68
5:G:137:LEU:HB3	5:G:499:LEU:HD11	1.73	0.68
5:G:38:ARG:HH22	5:G:449:ARG:HE	1.40	0.68
11:Z:601:ADP:O1B	12:Z:603:AF3:F1	2.01	0.68
4:z:514:ASN:HB3	5:g:59:MET:HE1	1.74	0.68
5:G:41:LEU:CD1	11:G:601:ADP:H5'1	2.24	0.68
2:H:433:LEU:HD21	6:a:461:THR:HB	1.75	0.68
7:D:459:GLU:OE2	7:D:481:ARG:NH1	2.23	0.68
11:z:601:ADP:O1B	12:z:603:AF3:F1	2.01	0.68
8:B:62:MET:HE2	8:B:64:THR:HG22	1.75	0.68
4:Z:28:ARG:HD3	4:Z:104:LYS:HB2	1.76	0.67
3:q:163:LEU:HD11	3:q:408:LEU:HD13	1.76	0.67
3:q:138:LYS:HE3	3:q:142:ILE:HD11	1.76	0.67
1:E:74:GLY:O	1:E:78:LEU:N	2.27	0.67
3:Q:100:GLY:N	11:Q:601:ADP:O3B	2.28	0.67
1:e:74:GLY:O	1:e:78:LEU:N	2.27	0.67
7:d:54:PRO:HG2	7:d:495:VAL:HG21	1.77	0.67
7:D:54:PRO:HG2	7:D:495:VAL:HG21	1.77	0.67
4:z:28:ARG:HD3	4:z:104:LYS:HB2	1.76	0.67
4:z:154:THR:HG21	4:z:494:VAL:HA	1.76	0.67
1:e:530:ILE:HG22	2:h:46:ASP:HB2	1.75	0.67
3:Q:163:LEU:HD11	3:Q:408:LEU:HD13	1.76	0.66
5:g:52:ASP:N	5:g:56:GLY:HA2	2.10	0.66
2:H:63:ALA:HB2	2:H:94:THR:HG21	1.77	0.66
1:E:52:LEU:HD12	1:E:461:ALA:HB3	1.78	0.66
3:Q:138:LYS:HE3	3:Q:142:ILE:HD11	1.76	0.66
5:g:38:ARG:HH22	5:g:449:ARG:HE	1.40	0.66
8:b:62:MET:HE2	8:b:64:THR:HG22	1.75	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:52:ASP:N	5:G:56:GLY:HA2	2.10	0.66
4:z:117:ARG:HD3	5:g:44:LYS:HB3	1.78	0.66
2:H:448:GLN:HA	2:H:451:ASP:HB2	1.78	0.66
1:E:498:THR:O	1:E:504:GLN:NE2	2.29	0.66
1:e:498:THR:O	1:e:504:GLN:NE2	2.29	0.65
3:q:98:GLY:HA3	3:q:397:ASN:HB3	1.78	0.65
11:E:602:ADP:O2A	13:E:701:HOH:O	2.14	0.65
4:Z:154:THR:HG21	4:Z:494:VAL:HA	1.76	0.65
2:h:63:ALA:HB2	2:h:94:THR:HG21	1.77	0.65
4:z:10:LYS:NZ	5:g:73:GLN:HB2	2.11	0.65
7:d:459:GLU:OE2	7:d:481:ARG:NH1	2.23	0.65
6:A:526:ARG:O	7:D:58:ASP:N	2.29	0.65
3:Q:102:ASN:HB2	11:Q:601:ADP:O1B	1.97	0.65
4:z:158:THR:HG22	4:z:159:LYS:HD3	1.79	0.65
8:B:45:PRO:HD2	8:B:480:MET:HE2	1.80	0.64
2:h:448:GLN:HA	2:h:451:ASP:HB2	1.78	0.64
1:e:52:LEU:HD12	1:e:461:ALA:HB3	1.77	0.64
3:Q:98:GLY:HA3	3:Q:397:ASN:HB3	1.78	0.64
4:Z:158:THR:HG22	4:Z:159:LYS:HD3	1.79	0.64
7:D:504:LEU:HA	7:D:507:LEU:HB2	1.79	0.64
8:b:45:PRO:HD2	8:b:480:MET:HE2	1.80	0.64
11:e:602:ADP:O2A	13:e:701:HOH:O	2.15	0.63
8:B:498:GLN:OE1	8:B:501:ARG:NH2	2.31	0.63
1:E:418:VAL:HG13	1:E:507:ILE:HG23	1.81	0.63
8:b:151:ASP:OD1	8:b:153:VAL:HG22	1.98	0.63
8:b:498:GLN:OE1	8:b:501:ARG:NH2	2.31	0.63
7:d:504:LEU:HA	7:d:507:LEU:HB2	1.79	0.63
8:b:95:VAL:HA	8:b:399:GLN:HE22	1.64	0.63
7:D:494:ASN:HD21	7:D:506:GLU:HG2	1.63	0.63
8:B:95:VAL:HA	8:B:399:GLN:HE22	1.64	0.63
1:E:530:ILE:HG22	2:H:46:ASP:HB2	1.80	0.63
8:B:91:GLN:HG3	8:B:102:VAL:HG11	1.81	0.63
1:e:418:VAL:HG13	1:e:507:ILE:HG23	1.81	0.63
1:e:89:LYS:O	1:e:93:GLU:HB2	1.99	0.63
8:B:151:ASP:OD1	8:B:153:VAL:HG22	1.98	0.62
3:q:100:GLY:N	11:q:601:ADP:O2B	2.30	0.62
7:d:494:ASN:HD21	7:d:506:GLU:HG2	1.63	0.62
3:Q:499:ASP:OD2	3:Q:504:LYS:NZ	2.32	0.62
1:e:48:MET:HE3	1:e:107:THR:HG23	1.81	0.62
3:q:499:ASP:OD2	3:q:504:LYS:NZ	2.32	0.62
4:Z:117:ARG:HD3	5:G:44:LYS:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:91:GLN:HG3	8:b:102:VAL:HG11	1.81	0.62
1:E:89:LYS:O	1:E:93:GLU:HB2	1.99	0.62
7:D:67:ASP:OD1	7:D:67:ASP:N	2.33	0.62
1:E:48:MET:HE3	1:E:107:THR:HG23	1.81	0.61
2:H:116:LEU:HD21	2:H:434:LEU:HD11	1.81	0.61
5:G:445:GLU:OE1	5:G:467:ARG:NH1	2.33	0.61
5:g:445:GLU:OE1	5:g:467:ARG:NH1	2.33	0.61
6:a:526:ARG:O	7:d:58:ASP:N	2.33	0.61
1:E:141:ALA:HB2	1:E:521:THR:HG21	1.82	0.61
2:H:89:GLU:HG3	2:H:90:VAL:HG23	1.82	0.61
7:d:139:LYS:HD3	7:d:443:LEU:HD21	1.81	0.61
1:e:141:ALA:HB2	1:e:521:THR:HG21	1.82	0.61
2:h:116:LEU:HD21	2:h:434:LEU:HD11	1.82	0.61
4:z:525:GLY:HA3	5:g:71:GLN:HE22	1.66	0.61
7:D:139:LYS:HD3	7:D:443:LEU:HD21	1.81	0.61
3:q:170:SER:HB2	11:q:601:ADP:C5'	2.23	0.61
4:z:38:LEU:HD22	4:z:450:VAL:HG13	1.83	0.61
3:Q:81:PRO:HG2	3:Q:524:ILE:HD13	1.83	0.60
7:D:141:LEU:HB2	7:D:523:THR:HG21	1.83	0.60
1:e:145:ILE:HG23	1:e:514:LYS:HG2	1.83	0.60
7:d:141:LEU:HB2	7:d:523:THR:HG21	1.83	0.60
1:E:145:ILE:HG23	1:E:514:LYS:HG2	1.84	0.60
6:A:446:LEU:HA	6:A:449:PRO:HD2	1.83	0.60
6:A:461:THR:HB	2:h:433:LEU:HD21	1.83	0.60
2:h:89:GLU:HG3	2:h:90:VAL:HG23	1.82	0.60
3:q:81:PRO:HG2	3:q:524:ILE:HD13	1.83	0.60
4:Z:38:LEU:HD22	4:Z:450:VAL:HG13	1.83	0.60
5:G:22:VAL:HG11	5:G:520:ASP:O	2.02	0.60
5:G:54:MET:HG3	5:G:55:GLY:H	1.65	0.60
5:g:54:MET:HG3	5:g:55:GLY:H	1.65	0.59
6:a:446:LEU:HA	6:a:449:PRO:HD2	1.83	0.59
5:g:22:VAL:HG11	5:g:520:ASP:O	2.02	0.59
2:H:49:ILE:O	2:H:57:THR:OG1	2.21	0.59
4:Z:145:ARG:NH2	4:Z:170:GLU:OE1	2.36	0.59
3:q:100:GLY:HA2	11:q:601:ADP:O2B	2.03	0.59
3:q:172:GLN:HE22	3:q:388:ILE:HG12	1.68	0.59
4:z:522:MET:HE1	5:g:36:ILE:HG23	1.84	0.59
4:Z:426:LYS:O	4:Z:429:VAL:HG12	2.03	0.59
4:z:145:ARG:NH2	4:z:170:GLU:OE1	2.36	0.59
4:z:426:LYS:O	4:z:429:VAL:HG12	2.03	0.59
4:Z:169:THR:O	4:Z:173:VAL:HG22	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:67:ASP:OD1	7:d:67:ASP:N	2.33	0.58
5:G:518:ARG:NE	6:A:42:ASP:OD1	2.35	0.58
8:b:487:ASP:HB3	8:b:490:ILE:HG12	1.84	0.58
8:B:487:ASP:HB3	8:B:490:ILE:HG12	1.84	0.58
2:h:49:ILE:O	2:h:57:THR:OG1	2.21	0.58
4:Z:10:LYS:HZ1	5:G:73:GLN:HB2	1.68	0.58
1:e:132:ARG:NH2	1:e:444:GLU:OE1	2.36	0.58
2:h:516:VAL:HG11	3:q:55:MET:HE2	1.84	0.58
7:d:82:GLN:HE21	7:d:84:LEU:HD12	1.69	0.58
1:E:485:MET:HB2	9:N:30:ARG:HG3	1.85	0.58
2:H:117:HIS:ND1	2:H:118:PRO:HD2	2.19	0.58
7:D:82:GLN:HE21	7:D:84:LEU:HD12	1.69	0.58
4:z:169:THR:O	4:z:173:VAL:HG22	2.03	0.58
1:E:132:ARG:NH2	1:E:444:GLU:OE1	2.36	0.57
3:Q:172:GLN:HE22	3:Q:388:ILE:HG12	1.68	0.57
4:Z:71:HIS:HD2	4:Z:73:THR:H	1.52	0.57
7:d:513:LEU:O	7:d:517:SER:HB3	2.05	0.57
1:e:65:ASP:N	1:e:65:ASP:OD1	2.36	0.57
3:q:528:LYS:HA	4:z:68:GLN:HE21	1.68	0.57
1:e:55:ASN:HB3	8:b:124:GLN:HG2	1.87	0.57
2:h:117:HIS:ND1	2:h:118:PRO:HD2	2.19	0.57
8:b:41:SER:HA	8:b:453:ASN:HD21	1.69	0.57
4:z:71:HIS:HD2	4:z:73:THR:H	1.52	0.57
7:D:513:LEU:O	7:D:517:SER:HB3	2.05	0.56
11:B:601:ADP:O3A	12:B:603:AF3:F1	2.13	0.56
2:H:117:HIS:CD2	2:H:119:GLN:HB2	2.40	0.56
7:D:443:LEU:HB3	7:D:448:SER:HB3	1.87	0.56
5:g:67:LEU:HD22	5:g:81:ILE:HG12	1.87	0.56
5:g:415:GLU:OE2	5:g:502:LYS:NZ	2.38	0.56
7:d:440:SER:O	7:d:448:SER:HB2	2.06	0.56
11:b:601:ADP:O3A	12:b:603:AF3:F1	2.13	0.56
4:Z:92:THR:O	12:Z:603:AF3:F3	2.14	0.56
5:G:67:LEU:HD22	5:G:81:ILE:HG12	1.87	0.56
2:h:117:HIS:CD2	2:h:119:GLN:HB2	2.40	0.56
4:Z:476:LEU:H	4:Z:476:LEU:HD23	1.71	0.56
4:Z:514:ASN:HB3	5:G:59:MET:HE1	1.86	0.56
4:z:92:THR:O	12:z:603:AF3:F3	2.14	0.56
5:g:133:MET:HG3	5:g:418:VAL:HG11	1.88	0.56
8:B:41:SER:HA	8:B:453:ASN:HD21	1.69	0.56
4:z:476:LEU:H	4:z:476:LEU:HD23	1.71	0.56
1:E:65:ASP:N	1:E:65:ASP:OD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:522:MET:HE1	5:G:36:ILE:HG23	1.88	0.56
7:d:443:LEU:HB3	7:d:448:SER:HB3	1.87	0.56
7:d:427:ALA:HB2	7:d:491:ALA:O	2.06	0.55
7:D:440:SER:O	7:D:448:SER:HB2	2.06	0.55
2:H:516:VAL:HG11	3:Q:55:MET:HE2	1.88	0.55
3:q:492:MET:HE3	3:q:497:ILE:HB	1.88	0.55
8:b:30:ILE:HA	8:b:33:ILE:HG12	1.88	0.55
4:Z:150:ASP:OD1	4:Z:153:ARG:NH2	2.40	0.55
4:Z:387:ILE:O	4:Z:391:VAL:HG23	2.06	0.55
2:h:34:GLU:OE2	2:h:37:ARG:HD2	2.07	0.55
3:q:152:LYS:HG2	3:q:159:GLU:OE2	2.07	0.55
3:Q:123:LEU:O	3:Q:124:SER:HB3	2.07	0.55
5:G:133:MET:HG3	5:G:418:VAL:HG11	1.88	0.55
3:q:123:LEU:O	3:q:124:SER:HB3	2.07	0.55
3:q:463:VAL:HG21	3:q:480:LEU:HD13	1.88	0.55
8:b:390:LEU:O	8:b:394:LEU:HD23	2.07	0.55
7:D:427:ALA:HB2	7:D:491:ALA:O	2.06	0.55
8:B:97:ASP:OD1	12:B:603:AF3:F1	2.15	0.55
1:e:534:ARG:HB2	2:h:49:ILE:HG22	1.89	0.55
4:z:150:ASP:OD1	4:z:153:ARG:NH2	2.40	0.55
1:e:29:MET:HE1	2:h:35:ALA:HA	1.89	0.55
4:z:387:ILE:O	4:z:391:VAL:HG23	2.06	0.55
5:G:434:GLN:OE1	5:G:438:ARG:NH2	2.33	0.55
8:B:30:ILE:HA	8:B:33:ILE:HG12	1.88	0.55
4:z:33:VAL:HG11	4:z:67:MET:HE1	1.89	0.55
2:H:40:LEU:O	2:H:452:ASN:ND2	2.39	0.54
3:Q:152:LYS:HG2	3:Q:159:GLU:OE2	2.07	0.54
3:Q:492:MET:HE3	3:Q:497:ILE:HB	1.88	0.54
3:Q:463:VAL:HG21	3:Q:480:LEU:HD13	1.88	0.54
5:G:64:ASN:HD21	5:G:95:THR:HG21	1.71	0.54
6:A:113:HIS:ND1	6:A:114:PRO:HD2	2.22	0.54
2:H:34:GLU:OE2	2:H:37:ARG:HD2	2.07	0.54
6:a:113:HIS:ND1	6:a:114:PRO:HD2	2.22	0.54
7:d:99:ASP:HB3	7:d:106:THR:CG2	2.37	0.54
1:E:55:ASN:HB3	8:B:124:GLN:HG2	1.90	0.54
7:D:99:ASP:HB3	7:D:106:THR:CG2	2.37	0.54
8:B:390:LEU:O	8:B:394:LEU:HD23	2.07	0.54
2:h:521:LYS:HA	3:q:57:ILE:HB	1.89	0.54
8:b:97:ASP:OD1	12:b:603:AF3:F1	2.15	0.54
4:Z:92:THR:C	4:Z:94:SER:H	2.15	0.54
4:Z:525:GLY:HA3	5:G:71:GLN:HE22	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:18:ARG:NH1	6:A:105:ASP:OD1	2.41	0.54
3:q:69:ALA:HA	3:q:72:ILE:HD12	1.89	0.54
6:a:18:ARG:NH1	6:a:105:ASP:OD1	2.41	0.54
9:N:4:LEU:HD21	9:N:95:CYS:HB3	1.89	0.54
5:g:64:ASN:HD21	5:g:95:THR:HG21	1.71	0.54
9:n:4:LEU:HD21	9:n:95:CYS:HB3	1.89	0.54
4:Z:33:VAL:HG11	4:Z:67:MET:HE1	1.89	0.54
4:z:446:ILE:HA	4:z:449:LYS:HB2	1.89	0.54
7:d:49:ARG:HA	7:d:111:ILE:HD11	1.90	0.54
3:Q:168:ILE:HG23	3:Q:391:ALA:HB1	1.90	0.53
4:Z:10:LYS:NZ	5:G:73:GLN:HB2	2.22	0.53
3:q:168:ILE:HG23	3:q:391:ALA:HB1	1.90	0.53
11:g:601:ADP:O2B	11:g:601:ADP:H5'2	2.08	0.53
5:G:136:THR:HA	5:G:139:LYS:HB3	1.90	0.53
7:D:49:ARG:HA	7:D:111:ILE:HD11	1.90	0.53
3:Q:58:ASN:HD22	3:Q:75:GLU:HG2	1.73	0.53
3:Q:69:ALA:HA	3:Q:72:ILE:HD12	1.89	0.53
1:e:102:ILE:HG12	1:e:515:GLN:HG3	1.91	0.53
4:Z:446:ILE:HA	4:Z:449:LYS:HB2	1.89	0.53
1:e:129:HIS:HD2	1:e:131:ILE:HB	1.74	0.53
5:g:488:VAL:HG21	5:g:493:LEU:HD22	1.90	0.53
7:d:153:ARG:HH11	7:d:154:PRO:HD2	1.74	0.53
1:E:42:LYS:HD2	1:E:118:GLU:HG3	1.91	0.53
1:E:102:ILE:HG12	1:E:515:GLN:HG3	1.91	0.53
1:E:129:HIS:HD2	1:E:131:ILE:HB	1.73	0.53
11:A:601:ADP:O3B	12:A:603:AF3:F3	2.17	0.53
3:q:58:ASN:HD22	3:q:75:GLU:HG2	1.73	0.53
4:z:92:THR:C	4:z:94:SER:H	2.15	0.53
8:B:452:ASP:OD1	8:B:458:SER:OG	2.23	0.53
8:b:45:PRO:HG3	11:b:601:ADP:C5	2.44	0.53
1:E:142:ARG:O	1:E:146:GLU:HB2	2.09	0.53
5:g:136:THR:HA	5:g:139:LYS:HB3	1.90	0.53
6:a:22:VAL:HG21	6:a:105:ASP:HB2	1.91	0.53
11:a:601:ADP:O3B	12:a:603:AF3:F3	2.17	0.53
7:d:155:VAL:H	7:d:420:ALA:HA	1.73	0.53
2:h:424:SER:O	2:h:432:GLN:HG3	2.09	0.52
3:q:100:GLY:CA	11:q:601:ADP:O2B	2.57	0.52
3:q:416:GLU:HG2	3:q:448:ILE:HB	1.92	0.52
5:G:488:VAL:HG21	5:G:493:LEU:HD22	1.90	0.52
5:g:91:VAL:CG1	5:g:501:VAL:HG12	2.39	0.52
7:d:133:ILE:HG13	7:d:530:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:528:LYS:HA	4:Z:68:GLN:HE21	1.74	0.52
4:Z:144:ASP:OD1	4:Z:144:ASP:N	2.41	0.52
4:z:59:ASP:HB3	4:z:159:LYS:HE2	1.91	0.52
3:q:497:ILE:HG21	11:q:601:ADP:C6	2.45	0.52
2:H:424:SER:O	2:H:432:GLN:HG3	2.09	0.52
6:A:22:VAL:HG21	6:A:105:ASP:HB2	1.91	0.52
6:a:99:GLU:HG3	6:a:444:SER:HB2	1.91	0.52
6:a:503:VAL:HG12	6:a:503:VAL:O	2.10	0.52
1:E:75:ALA:HA	1:E:79:SER:OG	2.09	0.52
1:e:75:ALA:HA	1:e:79:SER:OG	2.10	0.52
5:g:41:LEU:HD12	11:g:601:ADP:O1A	2.09	0.52
1:E:119:GLU:HG3	1:E:454:ALA:HB2	1.91	0.52
3:Q:416:GLU:HG2	3:Q:448:ILE:HB	1.92	0.52
6:A:21:ASN:HD22	6:A:71:ALA:HB2	1.75	0.52
6:A:99:GLU:HG3	6:A:444:SER:HB2	1.91	0.52
2:h:109:LYS:HA	2:h:112:VAL:HG12	1.92	0.52
4:z:453:GLN:HB2	4:z:459:LEU:HD23	1.91	0.52
2:H:29:CYS:HA	2:H:32:ILE:HG22	1.91	0.52
7:D:153:ARG:HH11	7:D:154:PRO:HD2	1.73	0.52
5:g:41:LEU:HD13	5:g:96:THR:HG23	1.91	0.52
5:g:434:GLN:OE1	5:g:438:ARG:NH2	2.33	0.52
8:b:413:SER:O	8:b:417:MET:HE2	2.10	0.52
4:Z:453:GLN:HB2	4:Z:459:LEU:HD23	1.91	0.52
5:G:519:ILE:HD13	6:A:44:MET:HE2	1.91	0.52
7:D:133:ILE:HG13	7:D:530:LEU:HD13	1.91	0.52
7:D:155:VAL:H	7:D:420:ALA:HA	1.73	0.52
8:B:45:PRO:HG3	11:B:601:ADP:C5	2.44	0.52
7:d:49:ARG:HH11	7:d:464:THR:HG22	1.75	0.52
5:G:415:GLU:OE2	5:G:502:LYS:NZ	2.38	0.52
7:D:153:ARG:HD3	7:D:154:PRO:HD2	1.92	0.52
1:e:42:LYS:HD2	1:e:118:GLU:HG3	1.91	0.52
1:e:142:ARG:O	1:e:146:GLU:HB2	2.09	0.52
4:z:48:VAL:HG12	4:z:54:ILE:HG22	1.92	0.52
2:H:109:LYS:HA	2:H:112:VAL:HG12	1.92	0.51
5:G:91:VAL:CG1	5:G:501:VAL:HG12	2.39	0.51
7:D:49:ARG:HH11	7:D:464:THR:HG22	1.75	0.51
1:e:26:SER:HB2	1:e:534:ARG:HH22	1.75	0.51
1:e:422:GLY:HA2	11:e:602:ADP:O2'	2.10	0.51
3:q:393:ASP:O	3:q:397:ASN:ND2	2.36	0.51
1:E:152:SER:OG	1:E:417:ARG:N	2.40	0.51
1:E:478:ARG:NH2	7:d:448:SER:OG	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:448:SER:OG	1:e:478:ARG:NH2	2.43	0.51
2:h:29:CYS:HA	2:h:32:ILE:HG22	1.91	0.51
3:Q:99:ASP:OD1	12:Q:603:AF3:F3	2.18	0.51
6:A:503:VAL:HG12	6:A:503:VAL:O	2.10	0.51
7:D:488:GLU:OE1	7:D:488:GLU:N	2.39	0.51
8:B:413:SER:O	8:B:417:MET:HE2	2.10	0.51
6:a:21:ASN:HD22	6:a:71:ALA:HB2	1.75	0.51
1:E:109:VAL:HG12	1:E:516:GLN:HG3	1.92	0.51
4:Z:133:PHE:HA	4:Z:136:GLU:HG2	1.92	0.51
5:G:41:LEU:HD13	5:G:96:THR:HG23	1.91	0.51
1:e:485:MET:HB2	9:n:30:ARG:HG3	1.93	0.51
2:h:37:ARG:HD3	2:h:448:GLN:NE2	2.25	0.51
4:Z:48:VAL:HG12	4:Z:54:ILE:HG22	1.92	0.51
4:Z:59:ASP:HB3	4:Z:159:LYS:HE2	1.91	0.51
1:e:119:GLU:HG3	1:e:454:ALA:HB2	1.91	0.51
1:E:482:VAL:HG21	7:d:441:ARG:O	2.11	0.51
1:E:422:GLY:HA2	11:E:602:ADP:O2'	2.10	0.51
4:Z:34:LEU:HD11	4:Z:64:LEU:HD21	1.93	0.51
1:e:109:VAL:HG12	1:e:516:GLN:HG3	1.92	0.51
4:z:34:LEU:HD11	4:z:64:LEU:HD21	1.93	0.51
6:a:515:LYS:O	6:a:519:GLU:HG2	2.11	0.51
9:N:96:LYS:HB2	9:N:109:TRP:CD1	2.46	0.51
3:Q:527:ALA:HB3	4:Z:49:SER:HA	1.93	0.51
2:H:456:ASP:OD2	2:H:459:ASN:ND2	2.39	0.51
5:g:67:LEU:HD11	5:g:99:ILE:HD13	1.92	0.51
1:E:26:SER:HB2	1:E:534:ARG:HH22	1.75	0.50
2:H:77:LYS:HD2	3:Q:63:LEU:HD12	1.93	0.50
3:q:99:ASP:OD1	12:q:603:AF3:F3	2.18	0.50
2:H:37:ARG:HD3	2:H:448:GLN:NE2	2.25	0.50
7:d:153:ARG:HD3	7:d:154:PRO:HD2	1.92	0.50
4:Z:414:VAL:O	4:Z:418:MET:HB2	2.11	0.50
8:B:50:LYS:HG3	8:B:70:ILE:HD13	1.93	0.50
4:Z:73:THR:O	4:Z:77:ILE:HG13	2.11	0.50
7:D:130:PRO:HB2	8:B:48:MET:HE1	1.92	0.50
2:H:408:GLY:O	2:H:487:ASN:ND2	2.37	0.50
6:A:515:LYS:O	6:A:519:GLU:HG2	2.11	0.50
8:b:50:LYS:HG3	8:b:70:ILE:HD13	1.93	0.50
2:H:521:LYS:HA	3:Q:57:ILE:HB	1.93	0.50
4:z:133:PHE:HA	4:z:136:GLU:HG2	1.92	0.50
9:n:28:PHE:HB2	9:n:99:ARG:HG3	1.94	0.50
7:D:497:LYS:HD3	7:D:497:LYS:C	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:66:ASP:OD2	8:B:68:ALA:N	2.44	0.50
4:z:73:THR:O	4:z:77:ILE:HG13	2.11	0.50
8:b:66:ASP:OD2	8:b:68:ALA:N	2.44	0.50
2:h:456:ASP:OD2	2:h:459:ASN:ND2	2.39	0.50
4:z:414:VAL:O	4:z:418:MET:HB2	2.11	0.50
7:d:497:LYS:HD3	7:d:497:LYS:C	2.36	0.50
9:N:28:PHE:HB2	9:N:99:ARG:HG3	1.94	0.49
2:h:40:LEU:O	2:h:452:ASN:ND2	2.39	0.49
4:Z:122:GLY:HA3	4:Z:436:GLY:HA3	1.94	0.49
4:Z:466:ILE:HG23	4:Z:477:VAL:HG13	1.94	0.49
6:A:102:LYS:O	6:A:106:GLU:HG2	2.12	0.49
7:D:60:MET:HG2	7:D:70:ILE:HG12	1.94	0.49
8:B:43:LEU:O	11:B:601:ADP:H5'1	2.12	0.49
1:e:152:SER:OG	1:e:417:ARG:N	2.40	0.49
3:q:139:ALA:HB2	3:q:423:ILE:HD11	1.94	0.49
7:d:497:LYS:HD3	7:d:497:LYS:O	2.11	0.49
9:n:96:LYS:HB2	9:n:109:TRP:CD1	2.46	0.49
3:Q:382:ASP:HA	3:Q:385:MET:HE2	1.94	0.49
7:D:437:THR:HG22	7:D:441:ARG:HH21	1.77	0.49
2:h:450:CYS:HB3	2:h:477:VAL:HG21	1.94	0.49
3:q:123:LEU:HD11	3:q:436:TYR:HD2	1.78	0.49
4:z:122:GLY:HA3	4:z:436:GLY:HA3	1.94	0.49
3:Q:525:ILE:HB	4:Z:47:LEU:HD23	1.94	0.49
6:a:102:LYS:O	6:a:106:GLU:HG2	2.12	0.49
1:E:421:GLY:HA3	1:E:424:ALA:HB3	1.94	0.49
3:Q:70:ALA:HB2	3:Q:101:THR:HG21	1.95	0.49
7:D:497:LYS:HD3	7:D:497:LYS:O	2.11	0.49
6:a:124:ALA:HB2	6:a:438:ILE:HG23	1.94	0.49
3:Q:123:LEU:HD11	3:Q:436:TYR:HD2	1.78	0.49
4:Z:429:VAL:HG13	4:Z:430:LYS:H	1.78	0.49
5:G:67:LEU:HD11	5:G:99:ILE:HD13	1.92	0.49
9:N:37:TYR:N	9:N:94:TYR:O	2.35	0.49
2:H:119:GLN:HG3	3:Q:50:ASN:HB3	1.95	0.49
3:Q:393:ASP:O	3:Q:397:ASN:ND2	2.36	0.49
5:g:519:ILE:HG21	6:a:44:MET:HE2	1.94	0.49
7:d:60:MET:HG2	7:d:70:ILE:HG12	1.94	0.49
6:A:124:ALA:HB2	6:A:438:ILE:HG23	1.94	0.49
8:B:101:SER:HA	8:B:104:VAL:HG12	1.93	0.49
8:b:101:SER:HA	8:b:104:VAL:HG12	1.93	0.49
1:E:57:LEU:HD11	8:B:122:HIS:CE1	2.48	0.49
4:Z:160:VAL:HG23	4:Z:165:ALA:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:36:LEU:HD13	6:A:95:ILE:HD12	1.95	0.49
7:d:448:SER:OG	7:d:448:SER:O	2.29	0.49
8:b:87:MET:HE3	8:b:87:MET:HB3	1.73	0.49
2:H:450:CYS:HB3	2:H:477:VAL:HG21	1.94	0.48
4:Z:10:LYS:NZ	5:G:72:VAL:O	2.46	0.48
5:G:105:MET:HE1	5:G:510:VAL:HG22	1.95	0.48
7:D:522:ALA:O	7:D:526:VAL:HG22	2.13	0.48
3:q:70:ALA:HB2	3:q:101:THR:HG21	1.95	0.48
3:q:214:SER:OG	3:q:378:ARG:NH1	2.41	0.48
4:z:160:VAL:HG23	4:z:165:ALA:HB2	1.93	0.48
4:z:429:VAL:HG13	4:z:430:LYS:N	2.28	0.48
4:z:466:ILE:HG23	4:z:477:VAL:HG13	1.94	0.48
1:E:38:ILE:O	1:E:42:LYS:HB2	2.13	0.48
2:H:516:VAL:HA	3:Q:53:ASN:O	2.13	0.48
3:Q:425:SER:O	3:Q:429:THR:HG23	2.14	0.48
6:a:36:LEU:HD13	6:a:95:ILE:HD12	1.95	0.48
4:Z:429:VAL:HG13	4:Z:430:LYS:N	2.28	0.48
8:B:104:VAL:O	8:B:108:GLU:HG2	2.14	0.48
2:h:467:ARG:HD2	2:h:467:ARG:HA	1.72	0.48
7:d:522:ALA:O	7:d:526:VAL:HG22	2.13	0.48
8:b:43:LEU:O	11:b:601:ADP:H5'1	2.12	0.48
1:E:509:THR:HG23	1:E:512:GLY:HA3	1.95	0.48
3:Q:139:ALA:HB2	3:Q:423:ILE:HD11	1.94	0.48
3:Q:497:ILE:HD13	11:Q:601:ADP:N6	2.28	0.48
4:z:144:ASP:OD1	4:z:144:ASP:N	2.41	0.48
1:e:421:GLY:HA3	1:e:424:ALA:HB3	1.94	0.48
7:d:437:THR:HG22	7:d:441:ARG:HH21	1.77	0.48
2:H:37:ARG:HB3	2:H:448:GLN:HE22	1.79	0.48
3:Q:373:SER:OG	3:Q:374:THR:N	2.46	0.48
4:Z:15:ARG:NH2	4:Z:17:GLN:OE1	2.47	0.48
1:e:38:ILE:O	1:e:42:LYS:HB2	2.13	0.48
1:e:86:GLN:HG3	2:h:50:VAL:HG11	1.96	0.48
3:q:382:ASP:HA	3:q:385:MET:HE2	1.94	0.48
6:a:17:ILE:HD13	6:a:530:LEU:HB2	1.96	0.48
3:q:97:VAL:HG22	3:q:98:GLY:H	1.78	0.48
3:q:377:LEU:HD11	3:q:388:ILE:HG22	1.96	0.48
2:h:37:ARG:HB3	2:h:448:GLN:HE22	1.79	0.48
4:z:429:VAL:HG13	4:z:430:LYS:H	1.78	0.48
3:Q:49:PRO:HG3	3:Q:170:SER:HA	1.95	0.48
2:h:22:LEU:HD12	2:h:22:LEU:HA	1.76	0.48
3:q:373:SER:OG	3:q:374:THR:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:497:ILE:HD13	11:q:601:ADP:C6	2.49	0.48
3:q:527:ALA:HB3	4:z:49:SER:HA	1.96	0.48
4:z:15:ARG:NH2	4:z:17:GLN:OE1	2.47	0.48
7:d:466:ALA:HB1	7:d:476:THR:HG21	1.96	0.48
1:E:428:SER:HB3	1:E:487:PRO:HB3	1.96	0.47
1:e:428:SER:HB3	1:e:487:PRO:HB3	1.96	0.47
2:H:447:ARG:HA	2:H:461:LEU:HD11	1.95	0.47
2:h:447:ARG:HA	2:h:461:LEU:HD11	1.95	0.47
3:q:425:SER:O	3:q:429:THR:HG23	2.14	0.47
5:g:105:MET:HE1	5:g:510:VAL:HG22	1.95	0.47
3:Q:97:VAL:HG22	3:Q:98:GLY:H	1.78	0.47
3:Q:377:LEU:HD11	3:Q:388:ILE:HG22	1.96	0.47
1:e:509:THR:HG23	1:e:512:GLY:HA3	1.95	0.47
3:q:163:LEU:HD11	3:q:408:LEU:CD1	2.44	0.47
4:z:42:GLY:HA3	4:z:58:LYS:HE2	1.96	0.47
7:d:116:LEU:HD23	7:d:526:VAL:HG21	1.96	0.47
8:b:104:VAL:O	8:b:108:GLU:HG2	2.14	0.47
2:H:109:LYS:O	2:H:113:GLU:HG2	2.15	0.47
3:q:49:PRO:HG3	3:q:170:SER:HA	1.95	0.47
5:g:75:PRO:HB3	6:a:52:VAL:HG11	1.96	0.47
2:H:459:ASN:HD21	6:a:433:ARG:HD2	1.79	0.47
3:Q:214:SER:OG	3:Q:378:ARG:NH1	2.41	0.47
3:Q:216:SER:OG	3:Q:217:VAL:N	2.48	0.47
4:Z:383:THR:O	4:Z:387:ILE:HG13	2.15	0.47
6:A:114:PRO:HB2	7:D:57:MET:HE1	1.95	0.47
7:D:65:LYS:HB3	7:D:65:LYS:HE2	1.64	0.47
1:e:147:HIS:CE1	1:e:151:ILE:HD11	2.49	0.47
8:b:79:PRO:HG2	8:b:520:ILE:HG21	1.97	0.47
1:E:147:HIS:CE1	1:E:151:ILE:HD11	2.49	0.47
8:B:79:PRO:HG2	8:B:520:ILE:HG21	1.97	0.47
8:B:124:GLN:HE22	8:B:516:ARG:HH12	1.63	0.47
4:z:408:VAL:HG22	4:z:414:VAL:HG21	1.97	0.47
6:a:19:SER:O	6:a:23:MET:HG2	2.15	0.47
8:b:124:GLN:HE22	8:b:516:ARG:HH12	1.63	0.47
4:Z:446:ILE:O	4:Z:450:VAL:N	2.33	0.47
4:Z:446:ILE:O	4:Z:450:VAL:HG12	2.15	0.47
4:Z:470:HIS:HD2	4:Z:476:LEU:HA	1.80	0.47
4:z:470:HIS:HD2	4:z:476:LEU:HA	1.80	0.47
1:E:433:VAL:HG23	1:E:452:ALA:HB2	1.97	0.47
1:E:482:VAL:C	1:E:484:GLU:H	2.23	0.47
4:Z:42:GLY:HA3	4:Z:58:LYS:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:73:GLN:HA	5:G:73:GLN:OE1	2.14	0.47
8:B:102:VAL:HG12	8:B:503:VAL:HG22	1.97	0.47
7:d:83:VAL:HG23	7:d:84:LEU:H	1.80	0.47
8:b:165:THR:HG22	8:b:165:THR:O	2.15	0.47
6:A:17:ILE:HD13	6:A:530:LEU:HB2	1.96	0.47
6:A:19:SER:O	6:A:23:MET:HG2	2.15	0.47
7:D:116:LEU:HD23	7:D:526:VAL:HG21	1.96	0.47
3:q:497:ILE:HD13	11:q:601:ADP:N6	2.29	0.47
4:z:383:THR:O	4:z:387:ILE:HG13	2.15	0.47
8:b:102:VAL:HG12	8:b:503:VAL:HG22	1.97	0.47
7:D:90:MET:HE1	7:D:528:SER:HB3	1.98	0.46
7:D:466:ALA:HB1	7:D:476:THR:HG21	1.96	0.46
8:B:127:ILE:HG13	8:B:515:LEU:HD23	1.97	0.46
2:h:109:LYS:O	2:h:113:GLU:HG2	2.15	0.46
5:g:73:GLN:OE1	5:g:73:GLN:HA	2.14	0.46
5:g:138:LYS:HE3	5:g:503:LEU:HD11	1.97	0.46
1:E:89:LYS:HA	1:E:92:VAL:HG22	1.96	0.46
3:Q:78:VAL:HG11	3:Q:87:VAL:HG21	1.97	0.46
4:Z:148:LEU:HD22	4:Z:398:VAL:HG23	1.97	0.46
2:h:516:VAL:HA	3:q:53:ASN:O	2.15	0.46
2:H:520:ILE:HB	3:Q:56:VAL:HG12	1.97	0.46
5:G:80:MET:HE3	5:G:80:MET:HB2	1.67	0.46
1:e:433:VAL:HG23	1:e:452:ALA:HB2	1.97	0.46
2:h:408:GLY:O	2:h:487:ASN:ND2	2.37	0.46
3:q:78:VAL:HG11	3:q:87:VAL:HG21	1.97	0.46
3:q:216:SER:OG	3:q:217:VAL:N	2.48	0.46
6:a:502:GLY:HA2	6:a:504:PHE:CE2	2.50	0.46
7:d:90:MET:HE1	7:d:528:SER:HB3	1.98	0.46
2:H:460:ILE:HD11	2:H:482:GLU:HG3	1.98	0.46
3:Q:524:ILE:HG23	4:Z:46:MET:HB3	1.97	0.46
5:G:134:ILE:HD13	5:G:507:LYS:HE2	1.98	0.46
8:B:28:SER:HB3	8:B:520:ILE:HD11	1.98	0.46
2:h:460:ILE:HD11	2:h:482:GLU:HG3	1.98	0.46
4:z:10:LYS:NZ	5:g:72:VAL:O	2.49	0.46
4:z:522:MET:HE2	4:z:522:MET:HB3	1.72	0.46
5:g:134:ILE:HD13	5:g:507:LYS:HE2	1.98	0.46
1:E:524:VAL:O	1:E:528:LEU:N	2.38	0.46
3:Q:402:LEU:HD21	3:Q:408:LEU:HD21	1.98	0.46
4:Z:15:ARG:NE	4:Z:15:ARG:O	2.49	0.46
4:Z:508:CYS:SG	4:Z:509:THR:N	2.88	0.46
7:D:430:ILE:CD1	7:D:480:LEU:HD13	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:87:MET:HE3	8:B:87:MET:HB3	1.73	0.46
4:z:446:ILE:O	4:z:450:VAL:HG12	2.15	0.46
2:H:14:ASP:HB3	2:H:20:PRO:HB3	1.98	0.46
3:Q:163:LEU:HD11	3:Q:408:LEU:CD1	2.44	0.46
4:Z:408:VAL:HG22	4:Z:414:VAL:HG21	1.97	0.46
6:A:502:GLY:HA2	6:A:504:PHE:CE2	2.50	0.46
7:D:83:VAL:HG23	7:D:84:LEU:H	1.80	0.46
7:D:452:ARG:NH2	1:e:453:ASP:OD2	2.49	0.46
1:e:34:LEU:HD23	1:e:34:LEU:HA	1.79	0.46
2:h:14:ASP:HB3	2:h:20:PRO:HB3	1.98	0.46
2:h:77:LYS:HD2	3:q:63:LEU:HD12	1.98	0.46
4:z:93:THR:O	4:z:97:LEU:HD13	2.15	0.46
7:d:65:LYS:HB3	7:d:65:LYS:HE2	1.64	0.46
3:q:56:VAL:O	3:q:56:VAL:HG23	2.16	0.46
4:z:15:ARG:O	4:z:15:ARG:NE	2.49	0.46
7:d:153:ARG:HA	7:d:153:ARG:NH1	2.31	0.46
1:E:480:ARG:O	1:E:484:GLU:HG3	2.16	0.46
3:Q:520:ARG:O	4:Z:43:THR:HG23	2.16	0.46
5:G:138:LYS:HE3	5:G:503:LEU:HD11	1.97	0.46
5:G:520:ASP:OD2	6:A:41:LEU:HD12	2.15	0.46
7:D:448:SER:OG	7:D:448:SER:O	2.29	0.46
3:q:402:LEU:HD21	3:q:408:LEU:HD21	1.98	0.46
8:b:29:PHE:O	8:b:33:ILE:HG23	2.16	0.46
8:b:510:ALA:O	8:b:514:ILE:HG13	2.16	0.46
2:H:467:ARG:HD2	2:H:467:ARG:HA	1.72	0.46
3:Q:170:SER:CB	11:Q:601:ADP:C5'	2.85	0.46
3:Q:393:ASP:OD1	3:Q:397:ASN:ND2	2.49	0.46
4:Z:470:HIS:HB2	4:Z:477:VAL:HG12	1.97	0.46
5:G:412:GLY:HA3	5:G:448:PRO:HG3	1.97	0.46
8:B:425:ALA:HB2	8:B:436:MET:HB2	1.97	0.46
3:q:54:LYS:HD2	3:q:72:ILE:HD13	1.98	0.46
4:z:148:LEU:HD22	4:z:398:VAL:HG23	1.97	0.46
8:b:425:ALA:HB2	8:b:436:MET:HB2	1.97	0.46
1:E:44:VAL:HG13	1:E:91:MET:HE2	1.98	0.46
3:Q:56:VAL:O	3:Q:56:VAL:HG23	2.16	0.46
7:D:83:VAL:HG11	7:D:92:VAL:HG21	1.97	0.46
1:e:44:VAL:HG13	1:e:91:MET:HE2	1.98	0.46
1:e:482:VAL:C	1:e:484:GLU:H	2.23	0.46
4:z:508:CYS:SG	4:z:509:THR:N	2.88	0.46
4:z:517:LEU:CD1	5:g:46:MET:HG2	2.46	0.46
6:a:92:SER:HB2	6:a:448:ILE:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:28:SER:HB3	8:b:520:ILE:HD11	1.98	0.46
8:b:127:ILE:HG13	8:b:515:LEU:HD23	1.97	0.46
5:G:461:ARG:NH2	4:z:456:GLY:O	2.50	0.45
8:B:165:THR:HG22	8:B:165:THR:O	2.15	0.45
1:e:89:LYS:HA	1:e:92:VAL:HG22	1.96	0.45
3:q:525:ILE:HB	4:z:47:LEU:HD23	1.98	0.45
7:d:83:VAL:HG11	7:d:92:VAL:HG21	1.97	0.45
7:d:430:ILE:CD1	7:d:480:LEU:HD13	2.46	0.45
4:Z:93:THR:O	4:Z:97:LEU:HD13	2.15	0.45
7:D:153:ARG:HA	7:D:153:ARG:NH1	2.31	0.45
1:E:70:VAL:HG22	1:E:72:ASN:H	1.80	0.45
2:H:413:GLU:HB3	2:H:442:LEU:O	2.16	0.45
3:Q:80:HIS:CD2	3:Q:82:ALA:HB3	2.52	0.45
8:B:29:PHE:O	8:B:33:ILE:HG23	2.16	0.45
1:E:464:GLU:C	1:E:466:SER:H	2.25	0.45
2:H:48:LEU:HD11	2:H:56:ALA:HB1	1.98	0.45
5:G:33:ILE:HD11	5:G:72:VAL:HG11	1.99	0.45
7:D:49:ARG:NH1	7:D:464:THR:HG22	2.32	0.45
3:q:216:SER:H	3:q:376:VAL:HG22	1.82	0.45
3:q:393:ASP:OD1	3:q:397:ASN:ND2	2.49	0.45
1:e:70:VAL:HG22	1:e:72:ASN:H	1.80	0.45
1:e:480:ARG:O	1:e:484:GLU:HG3	2.16	0.45
5:g:33:ILE:HD11	5:g:72:VAL:HG11	1.99	0.45
1:E:81:MET:HG3	1:E:82:ASP:OD2	2.17	0.45
1:E:420:TYR:CE2	1:E:502:LYS:HD2	2.52	0.45
3:Q:216:SER:H	3:Q:376:VAL:HG22	1.82	0.45
6:A:92:SER:HB2	6:A:448:ILE:HD11	1.98	0.45
4:z:470:HIS:HB2	4:z:477:VAL:HG12	1.97	0.45
5:g:412:GLY:HA3	5:g:448:PRO:HG3	1.97	0.45
1:E:29:MET:HG2	1:E:30:GLY:N	2.32	0.45
6:A:530:LEU:HD11	7:D:62:GLN:HB2	1.98	0.45
7:D:61:ILE:HD11	7:D:77:ILE:HG12	1.99	0.45
4:z:37:ASN:HD21	4:z:45:LYS:HG3	1.81	0.45
4:z:76:LEU:HD22	5:g:57:ILE:HG21	1.99	0.45
5:G:459:THR:O	5:G:463:LEU:HB2	2.17	0.45
7:D:76:THR:HA	7:D:79:LYS:HB2	1.99	0.45
7:D:474:ILE:HD11	1:e:126:ARG:O	2.17	0.45
8:B:510:ALA:O	8:B:514:ILE:HG13	2.16	0.45
1:e:29:MET:HG2	1:e:30:GLY:N	2.32	0.45
3:q:408:LEU:HD23	3:q:500:THR:HA	1.99	0.45
1:E:136:GLY:HA3	1:E:447:ALA:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:512:LEU:HD23	2:H:512:LEU:HA	1.79	0.45
3:Q:408:LEU:HD23	3:Q:500:THR:HA	1.99	0.45
4:Z:38:LEU:HG	11:Z:601:ADP:H5'1	1.99	0.45
4:Z:176:ILE:HD11	4:Z:395:LEU:HD22	1.98	0.45
7:D:537:ASN:HA	8:B:53:LEU:O	2.16	0.45
1:e:57:LEU:HD11	8:b:122:HIS:CE1	2.52	0.45
1:e:464:GLU:C	1:e:466:SER:H	2.25	0.45
4:z:90:ASP:OD2	12:z:603:AF3:F1	2.25	0.45
4:z:176:ILE:HD11	4:z:395:LEU:HD22	1.98	0.45
7:d:76:THR:HA	7:d:79:LYS:HB2	1.99	0.45
8:b:41:SER:HA	8:b:453:ASN:ND2	2.32	0.45
2:H:46:ASP:OD1	2:H:60:ASN:HB3	2.17	0.45
2:h:46:ASP:OD1	2:h:60:ASN:HB3	2.17	0.45
2:h:48:LEU:HD11	2:h:56:ALA:HB1	1.98	0.45
3:q:80:HIS:CD2	3:q:82:ALA:HB3	2.52	0.45
3:Q:54:LYS:HD2	3:Q:72:ILE:HD13	1.98	0.44
3:Q:143:LEU:HD23	3:Q:143:LEU:HA	1.82	0.44
4:Z:37:ASN:HD21	4:Z:45:LYS:HG3	1.81	0.44
2:h:413:GLU:HB3	2:h:442:LEU:O	2.16	0.44
7:d:488:GLU:OE1	7:d:488:GLU:N	2.39	0.44
9:n:99:ARG:HB3	9:n:106:ASP:OD2	2.17	0.44
4:Z:124:GLU:O	4:Z:128:GLU:HG2	2.17	0.44
3:q:217:VAL:HG12	3:q:375:ILE:HG12	2.00	0.44
4:z:38:LEU:HG	11:z:601:ADP:H5'1	1.99	0.44
6:a:126:LYS:O	6:a:130:ARG:HG2	2.18	0.44
3:Q:170:SER:CB	11:Q:601:ADP:H5'1	2.15	0.44
3:q:123:LEU:HD11	3:q:436:TYR:CD2	2.53	0.44
4:z:151:VAL:HG11	4:z:401:ALA:HB2	1.98	0.44
5:g:459:THR:O	5:g:463:LEU:HB2	2.17	0.44
7:d:61:ILE:HD11	7:d:77:ILE:HG12	1.99	0.44
2:H:515:SER:O	2:H:515:SER:OG	2.33	0.44
5:G:129:ALA:O	5:G:133:MET:N	2.49	0.44
6:A:489:ASP:HB2	6:A:496:ARG:HG2	1.98	0.44
6:a:440:GLU:HA	6:a:443:ARG:HG2	1.99	0.44
1:E:515:GLN:O	1:E:519:LEU:N	2.33	0.44
3:Q:123:LEU:HD11	3:Q:436:TYR:CD2	2.53	0.44
4:Z:90:ASP:OD2	12:Z:603:AF3:F1	2.25	0.44
4:Z:409:PRO:HG2	4:Z:476:LEU:HD11	2.00	0.44
6:A:505:GLU:HG3	6:A:506:PRO:HD2	1.99	0.44
2:h:410:GLY:C	2:h:412:ILE:H	2.25	0.44
11:h:601:ADP:O2A	12:h:603:AF3:F1	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:118:LEU:HD11	3:q:436:TYR:HB3	2.00	0.44
6:a:416:GLU:OE2	6:a:510:LYS:NZ	2.36	0.44
6:a:489:ASP:HB2	6:a:496:ARG:HG2	1.98	0.44
3:Q:217:VAL:HG12	3:Q:375:ILE:HG12	2.00	0.44
5:G:137:LEU:HD22	5:G:408:VAL:HG21	2.00	0.44
6:A:440:GLU:HA	6:A:443:ARG:HG2	1.99	0.44
1:e:420:TYR:CE2	1:e:502:LYS:HD2	2.52	0.44
3:q:127:GLU:HA	3:q:127:GLU:OE1	2.18	0.44
7:d:49:ARG:NH1	7:d:464:THR:HG22	2.32	0.44
7:d:535:VAL:HG13	8:b:51:ILE:CG2	2.37	0.44
4:Z:151:VAL:HG11	4:Z:401:ALA:HB2	1.98	0.44
8:B:162:ILE:HD12	8:B:400:THR:HG21	2.00	0.44
9:N:99:ARG:HB3	9:N:106:ASP:OD2	2.17	0.44
5:g:137:LEU:HD22	5:g:408:VAL:HG21	2.00	0.44
3:Q:497:ILE:HD13	11:Q:601:ADP:C6	2.53	0.44
5:G:136:THR:O	5:G:140:ILE:N	2.44	0.44
5:G:481:ASN:ND2	5:G:484:THR:OG1	2.51	0.44
7:D:28:ASP:HB3	7:D:29:LYS:H	1.57	0.44
8:B:41:SER:HA	8:B:453:ASN:ND2	2.32	0.44
2:h:494:GLU:HG2	2:h:499:ARG:HG2	1.99	0.44
6:a:533:LEU:HD12	7:d:63:ASP:HA	1.98	0.44
1:E:57:LEU:HD11	8:B:122:HIS:HE1	1.83	0.44
1:E:119:GLU:O	1:E:122:GLN:HG3	2.18	0.44
1:e:81:MET:HG3	1:e:82:ASP:OD2	2.17	0.44
4:z:124:GLU:O	4:z:128:GLU:HG2	2.18	0.44
5:g:481:ASN:ND2	5:g:484:THR:OG1	2.51	0.44
3:Q:127:GLU:HA	3:Q:127:GLU:OE1	2.18	0.43
2:h:119:GLN:HG3	3:q:50:ASN:HB3	1.99	0.43
8:b:452:ASP:OD1	8:b:458:SER:OG	2.23	0.43
1:E:453:ASP:OD2	7:d:452:ARG:NH2	2.48	0.43
2:H:410:GLY:C	2:H:412:ILE:H	2.25	0.43
4:Z:84:GLN:OE1	4:Z:507:SER:OG	2.28	0.43
3:q:450:ARG:HG3	3:q:460:ALA:HB1	2.00	0.43
6:a:505:GLU:HG3	6:a:506:PRO:HD2	1.99	0.43
11:H:601:ADP:O2A	12:H:603:AF3:F1	2.26	0.43
3:Q:118:LEU:HD11	3:Q:436:TYR:HB3	2.00	0.43
3:Q:450:ARG:HG3	3:Q:460:ALA:HB1	2.00	0.43
6:A:126:LYS:O	6:A:130:ARG:HG2	2.17	0.43
6:A:532:LYS:NZ	7:D:62:GLN:HG2	2.33	0.43
8:B:385:GLU:OE2	8:B:385:GLU:N	2.51	0.43
1:e:136:GLY:HA3	1:e:447:ALA:HB3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:385:GLU:OE2	8:b:385:GLU:N	2.51	0.43
5:G:75:PRO:HB3	6:A:52:VAL:HG11	2.00	0.43
3:q:143:LEU:HD23	3:q:143:LEU:HA	1.82	0.43
4:z:430:LYS:HG2	4:z:431:GLY:H	1.84	0.43
2:H:22:LEU:HA	2:H:22:LEU:HD12	1.76	0.43
3:Q:183:ILE:HD11	3:Q:392:VAL:HG22	2.00	0.43
7:D:78:LEU:HD22	7:D:92:VAL:HG22	2.01	0.43
4:z:409:PRO:HG2	4:z:476:LEU:HD11	2.00	0.43
7:d:134:SER:O	7:d:527:ARG:HD3	2.19	0.43
8:b:162:ILE:HD12	8:b:400:THR:HG21	2.00	0.43
4:Z:31:GLN:HG3	4:Z:97:LEU:HA	2.00	0.43
5:G:497:GLU:OE1	5:G:502:LYS:HE2	2.19	0.43
6:A:416:GLU:OE2	6:A:510:LYS:NZ	2.36	0.43
4:Z:15:ARG:N	4:Z:18:ALA:HB3	2.34	0.43
9:N:36:TRP:CZ3	9:N:95:CYS:HB2	2.54	0.43
1:e:43:ALA:O	1:e:47:THR:HG23	2.19	0.43
2:H:139:ILE:HD12	2:H:139:ILE:HA	1.85	0.43
4:Z:17:GLN:C	4:Z:19:ALA:N	2.76	0.43
4:Z:430:LYS:HG2	4:Z:431:GLY:H	1.84	0.43
7:D:134:SER:O	7:D:527:ARG:HD3	2.19	0.43
7:D:534:ASP:O	7:D:536:VAL:HG23	2.19	0.43
8:B:149:GLY:HA3	8:B:404:SER:HB2	2.00	0.43
8:B:474:THR:O	8:B:474:THR:OG1	2.33	0.43
4:z:406:CYS:HB2	4:z:498:TYR:HB3	2.00	0.43
5:g:129:ALA:O	5:g:133:MET:N	2.49	0.43
6:a:423:LEU:HB2	6:a:442:ALA:HB2	2.00	0.43
9:n:36:TRP:CZ3	9:n:95:CYS:HB2	2.54	0.43
1:e:61:MET:HB2	1:e:68:VAL:HB	2.01	0.43
1:e:533:ILE:HA	2:h:48:LEU:O	2.19	0.43
3:q:183:ILE:HD11	3:q:392:VAL:HG22	2.00	0.43
6:a:115:THR:HG21	7:d:468:ASN:O	2.19	0.43
3:Q:100:GLY:HA2	11:Q:601:ADP:O2B	2.19	0.42
4:Z:63:LEU:HD23	4:Z:63:LEU:HA	1.85	0.42
5:G:20:ARG:HD2	5:G:20:ARG:HA	1.87	0.42
5:G:47:MET:H	5:G:47:MET:HG2	1.65	0.42
1:e:119:GLU:O	1:e:122:GLN:HG3	2.18	0.42
2:h:515:SER:O	2:h:515:SER:OG	2.33	0.42
5:g:497:GLU:OE1	5:g:502:LYS:HE2	2.19	0.42
6:a:101:LEU:HD23	6:a:101:LEU:HA	1.86	0.42
7:d:78:LEU:HD22	7:d:92:VAL:HG22	2.01	0.42
1:E:29:MET:HE1	2:H:35:ALA:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:420:LEU:HD23	2:H:420:LEU:HA	1.79	0.42
3:Q:129:ILE:HD13	3:Q:520:ARG:HG3	2.01	0.42
11:Q:601:ADP:H3'	11:Q:601:ADP:H8	1.84	0.42
4:Z:430:LYS:HB3	4:Z:433:ALA:HB3	2.02	0.42
6:A:133:ASN:HA	6:A:136:LEU:HD22	2.00	0.42
6:A:423:LEU:HB2	6:A:442:ALA:HB2	2.00	0.42
2:h:512:LEU:HD23	2:h:512:LEU:HA	1.79	0.42
4:z:466:ILE:HD13	4:z:479:VAL:HG22	2.01	0.42
1:E:97:SER:HB2	1:E:519:LEU:HD11	2.02	0.42
2:H:412:ILE:O	2:H:416:LEU:N	2.41	0.42
4:Z:477:VAL:HG21	4:Z:486:PRO:HB2	2.01	0.42
4:Z:498:TYR:O	4:Z:498:TYR:CG	2.71	0.42
1:e:97:SER:HB2	1:e:519:LEU:HD11	2.02	0.42
1:e:524:VAL:O	1:e:528:LEU:N	2.38	0.42
1:E:43:ALA:O	1:E:47:THR:HG23	2.19	0.42
1:E:73:ASP:O	1:E:76:THR:OG1	2.23	0.42
6:A:44:MET:HG2	6:A:52:VAL:HB	2.01	0.42
2:h:26:ILE:O	2:h:30:GLN:HG2	2.20	0.42
2:h:520:ILE:HB	3:q:56:VAL:HG12	2.00	0.42
7:d:519:LEU:HD23	7:d:519:LEU:HA	1.84	0.42
8:B:67:GLY:HA3	8:B:100:THR:OG1	2.19	0.42
3:q:410:PRO:HB2	3:q:414:ALA:HB3	2.01	0.42
6:a:32:VAL:HG21	6:a:62:LEU:HD21	2.01	0.42
7:d:534:ASP:O	7:d:536:VAL:HG23	2.19	0.42
1:E:420:TYR:CD2	1:E:502:LYS:HA	2.54	0.42
2:H:26:ILE:O	2:H:30:GLN:HG2	2.20	0.42
2:H:494:GLU:HG2	2:H:499:ARG:HG2	2.00	0.42
3:q:79:GLN:H	3:q:79:GLN:HG2	1.74	0.42
1:E:533:ILE:HA	2:H:48:LEU:O	2.20	0.42
7:D:430:ILE:HG13	7:D:462:PRO:HG2	2.02	0.42
2:h:36:VAL:HG21	2:h:66:LEU:HD21	2.02	0.42
3:q:129:ILE:HD13	3:q:520:ARG:HG3	2.01	0.42
3:q:131:GLY:HA3	3:q:437:ALA:HB3	2.02	0.42
4:z:430:LYS:HB3	4:z:433:ALA:HB3	2.01	0.42
4:z:498:TYR:O	4:z:498:TYR:CG	2.71	0.42
6:a:133:ASN:HA	6:a:136:LEU:HD22	2.00	0.42
1:E:61:MET:HB2	1:E:68:VAL:HB	2.01	0.42
3:Q:154:LEU:HD23	3:Q:154:LEU:HA	1.90	0.42
4:Z:456:GLY:O	5:g:461:ARG:NH2	2.52	0.42
3:q:100:GLY:H	11:q:601:ADP:PB	2.43	0.42
4:z:150:ASP:O	4:z:154:THR:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:z:160:VAL:HG12	4:z:386:GLN:HE21	1.84	0.42
6:a:44:MET:HG2	6:a:52:VAL:HB	2.01	0.42
4:Z:160:VAL:HG12	4:Z:386:GLN:HE21	1.85	0.42
6:A:32:VAL:HG21	6:A:62:LEU:HD21	2.01	0.42
1:e:420:TYR:CD2	1:e:502:LYS:HA	2.54	0.42
6:a:84:LYS:HE2	6:a:84:LYS:HB3	1.74	0.42
3:Q:131:GLY:HA3	3:Q:437:ALA:HB3	2.02	0.42
3:Q:470:VAL:HG21	3:Q:489:VAL:HG11	2.02	0.42
4:Z:406:CYS:HB2	4:Z:498:TYR:HB3	2.00	0.42
6:A:71:ALA:HA	6:A:74:VAL:HG12	2.02	0.42
4:z:446:ILE:O	4:z:450:VAL:N	2.33	0.42
8:b:149:GLY:HA3	8:b:404:SER:HB2	2.00	0.42
1:E:534:ARG:HB2	2:H:49:ILE:HG22	2.02	0.41
3:Q:54:LYS:HE2	3:Q:54:LYS:HB3	1.80	0.41
3:Q:151:ALA:O	3:Q:152:LYS:C	2.63	0.41
5:G:50:LEU:HB2	5:G:58:VAL:HG13	2.02	0.41
5:G:54:MET:HG3	5:G:55:GLY:N	2.34	0.41
5:G:133:MET:HE3	5:G:133:MET:HB2	1.85	0.41
4:z:15:ARG:N	4:z:18:ALA:HB3	2.34	0.41
4:z:31:GLN:HG3	4:z:97:LEU:HA	2.00	0.41
7:d:537:ASN:HA	8:b:53:LEU:O	2.20	0.41
2:H:36:VAL:HG21	2:H:66:LEU:HD21	2.02	0.41
2:H:413:GLU:HB2	2:H:446:PRO:HD3	2.01	0.41
3:Q:111:LEU:HD12	3:Q:444:ALA:HB1	2.02	0.41
3:Q:410:PRO:HB2	3:Q:414:ALA:HB3	2.01	0.41
4:Z:150:ASP:O	4:Z:154:THR:HG23	2.20	0.41
2:h:413:GLU:HB2	2:h:446:PRO:HD3	2.01	0.41
3:q:118:LEU:HD22	3:q:440:LYS:HG3	2.03	0.41
5:g:50:LEU:HB2	5:g:58:VAL:HG13	2.02	0.41
8:b:156:ARG:O	8:b:160:MET:HG2	2.20	0.41
1:E:151:ILE:HB	1:E:419:VAL:HG23	2.02	0.41
3:Q:118:LEU:HD22	3:Q:440:LYS:HG3	2.02	0.41
4:Z:466:ILE:HD13	4:Z:479:VAL:HG22	2.01	0.41
4:Z:517:LEU:CD1	5:G:46:MET:HG2	2.51	0.41
8:B:156:ARG:O	8:B:160:MET:HG2	2.20	0.41
3:q:470:VAL:HG21	3:q:489:VAL:HG11	2.02	0.41
6:a:71:ALA:HA	6:a:74:VAL:HG12	2.02	0.41
7:d:130:PRO:HA	7:d:133:ILE:HG12	2.03	0.41
7:d:145:ILE:HD13	7:d:145:ILE:HA	1.89	0.41
8:b:160:MET:HE3	8:b:160:MET:HB3	1.98	0.41
1:E:28:LEU:O	1:E:33:ALA:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:SER:HB3	1:E:470:PRO:HA	2.01	0.41
6:A:115:THR:HG21	7:D:468:ASN:O	2.21	0.41
8:B:417:MET:HE3	8:B:417:MET:HB2	1.98	0.41
2:h:420:LEU:HD23	2:h:420:LEU:HA	1.79	0.41
4:z:414:VAL:HG12	4:z:418:MET:HE2	2.02	0.41
6:a:114:PRO:HB2	7:d:57:MET:HE1	2.01	0.41
4:Z:7:LEU:HA	5:G:74:HIS:CD2	2.56	0.41
6:A:433:ARG:HD2	2:h:459:ASN:HD21	1.86	0.41
1:e:151:ILE:HB	1:e:419:VAL:HG23	2.02	0.41
2:h:405:VAL:HG11	2:h:493:TRP:HB3	2.03	0.41
6:a:445:LEU:HD23	6:a:445:LEU:HA	1.82	0.41
7:d:459:GLU:OE2	7:d:481:ARG:HD2	2.20	0.41
8:b:474:THR:O	8:b:474:THR:OG1	2.33	0.41
7:D:55:LYS:O	7:D:468:ASN:HB3	2.21	0.41
8:B:448:THR:OG1	8:B:462:VAL:HG21	2.21	0.41
1:e:463:SER:HB3	1:e:470:PRO:HA	2.02	0.41
3:q:458:VAL:HG12	3:q:485:GLU:O	2.21	0.41
5:g:80:MET:HE3	5:g:80:MET:HB2	1.67	0.41
8:b:67:GLY:HA3	8:b:100:THR:OG1	2.19	0.41
2:H:47:LYS:HG3	2:H:65:ILE:HD13	2.03	0.41
2:H:405:VAL:HG11	2:H:493:TRP:HB3	2.03	0.41
2:H:492:VAL:O	2:H:492:VAL:HG13	2.21	0.41
2:H:515:SER:OG	3:Q:53:ASN:HB3	2.21	0.41
3:q:111:LEU:HD12	3:q:444:ALA:HB1	2.02	0.41
4:z:477:VAL:HG21	4:z:486:PRO:HB2	2.01	0.41
7:d:55:LYS:O	7:d:468:ASN:HB3	2.21	0.41
2:H:403:ASP:O	2:H:405:VAL:HG23	2.21	0.41
4:Z:414:VAL:HG12	4:Z:418:MET:HE2	2.02	0.41
7:D:42:LYS:HB3	7:D:42:LYS:HE2	1.76	0.41
7:D:62:GLN:HA	7:D:68:VAL:HG22	2.03	0.41
7:D:130:PRO:HA	7:D:133:ILE:HG12	2.03	0.41
3:q:520:ARG:O	4:z:43:THR:HG23	2.20	0.41
4:z:117:ARG:NE	4:z:517:LEU:HD11	2.36	0.41
7:d:33:ILE:HG22	7:d:33:ILE:O	2.20	0.41
2:H:129:THR:O	2:H:133:VAL:HG13	2.21	0.41
3:Q:55:MET:HG2	3:Q:65:VAL:HB	2.02	0.41
3:Q:99:ASP:OD1	11:Q:601:ADP:O3B	2.39	0.41
3:Q:497:ILE:HG21	11:Q:601:ADP:C6	2.56	0.41
5:G:447:ILE:HB	5:G:448:PRO:HD3	2.03	0.41
5:G:506:TYR:O	5:G:510:VAL:HG23	2.21	0.41
7:D:33:ILE:HG22	7:D:33:ILE:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:131:THR:HG21	8:B:46:LYS:HB3	2.02	0.41
1:e:28:LEU:O	1:e:33:ALA:HB2	2.20	0.41
2:h:122:ILE:HD11	2:h:515:SER:HB2	2.03	0.41
3:q:54:LYS:HB3	3:q:54:LYS:HE2	1.80	0.41
7:d:42:LYS:HE2	7:d:42:LYS:HB3	1.76	0.41
9:n:37:TYR:N	9:n:94:TYR:O	2.35	0.41
3:Q:524:ILE:HG12	4:Z:46:MET:HB2	2.03	0.41
4:Z:451:LEU:HD23	4:Z:451:LEU:HA	1.91	0.41
8:B:29:PHE:CZ	8:B:515:LEU:HD12	2.56	0.41
2:h:492:VAL:HG13	2:h:492:VAL:O	2.21	0.41
3:q:55:MET:HG2	3:q:65:VAL:HB	2.02	0.41
7:d:48:ILE:O	7:d:48:ILE:HG22	2.21	0.41
7:d:430:ILE:HG13	7:d:462:PRO:HG2	2.02	0.41
8:b:448:THR:OG1	8:b:462:VAL:HG21	2.21	0.41
2:H:122:ILE:HD11	2:H:515:SER:HB2	2.03	0.40
2:H:465:ARG:HE	6:a:435:GLN:HE22	1.69	0.40
3:Q:458:VAL:HG12	3:Q:485:GLU:O	2.21	0.40
3:Q:459:LYS:HB3	3:Q:462:GLU:HG2	2.03	0.40
4:Z:117:ARG:NE	4:Z:517:LEU:HD11	2.36	0.40
5:G:462:LEU:HD23	5:G:462:LEU:HA	1.83	0.40
6:A:435:GLN:HE22	2:h:465:ARG:HE	1.68	0.40
2:h:129:THR:O	2:h:133:VAL:HG13	2.21	0.40
2:h:403:ASP:O	2:h:405:VAL:HG23	2.21	0.40
2:h:515:SER:OG	3:q:53:ASN:HB3	2.21	0.40
7:d:484:HIS:HA	7:d:488:GLU:O	2.22	0.40
2:h:47:LYS:HG3	2:h:65:ILE:HD13	2.03	0.40
3:q:478:VAL:HA	3:q:491:ASP:HA	2.03	0.40
3:q:524:ILE:HG23	4:z:46:MET:HB3	2.04	0.40
5:g:411:GLY:HA3	5:g:490:MET:HE3	2.04	0.40
7:d:130:PRO:HB2	8:b:48:MET:HE1	2.03	0.40
1:E:86:GLN:HG3	2:H:50:VAL:HG11	2.02	0.40
6:A:84:LYS:HB3	6:A:84:LYS:HE2	1.74	0.40
6:A:100:LEU:HD23	6:A:444:SER:OG	2.22	0.40
6:A:533:LEU:HD12	7:D:63:ASP:HA	2.02	0.40
9:N:99:ARG:HG2	9:N:100:ASN:ND2	2.37	0.40
3:q:129:ILE:CD1	3:q:520:ARG:HG3	2.52	0.40
3:q:459:LYS:HB3	3:q:462:GLU:HG2	2.03	0.40
4:z:449:LYS:HD2	4:z:459:LEU:HD13	2.03	0.40
4:z:451:LEU:HD23	4:z:451:LEU:HA	1.91	0.40
5:g:506:TYR:O	5:g:510:VAL:HG23	2.21	0.40
6:a:100:LEU:HD23	6:a:444:SER:OG	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:29:PHE:CZ	8:b:515:LEU:HD12	2.56	0.40
6:A:496:ARG:NH1	6:A:498:ASN:OD1	2.55	0.40
7:D:432:LEU:HD11	7:D:519:LEU:HD11	2.04	0.40
1:e:77:ILE:HG22	1:e:81:MET:HE2	2.03	0.40
4:z:17:GLN:C	4:z:19:ALA:N	2.76	0.40
5:g:466:LEU:HD23	5:g:466:LEU:HA	1.90	0.40
7:d:138:GLN:OE1	7:d:527:ARG:NH1	2.55	0.40
9:n:99:ARG:HG2	9:n:100:ASN:ND2	2.37	0.40
3:Q:114:LEU:HB3	3:Q:440:LYS:HD2	2.04	0.40
3:Q:129:ILE:CD1	3:Q:520:ARG:HG3	2.51	0.40
4:Z:102:LEU:HD12	4:Z:443:ALA:CB	2.52	0.40
4:Z:443:ALA:C	4:Z:445:LEU:H	2.30	0.40
7:D:80:GLN:O	7:D:80:GLN:HG3	2.22	0.40
7:D:459:GLU:OE2	7:D:481:ARG:HD2	2.21	0.40
4:z:102:LEU:HD12	4:z:443:ALA:CB	2.52	0.40
4:z:443:ALA:C	4:z:445:LEU:H	2.30	0.40
5:g:38:ARG:HA	5:g:100:ILE:HD11	2.03	0.40
5:g:54:MET:HG3	5:g:55:GLY:N	2.34	0.40
6:a:494:LYS:HA	6:a:495:PRO:HD3	1.98	0.40
7:d:443:LEU:HB3	7:d:448:SER:CB	2.52	0.40
7:d:501:SER:O	7:d:507:LEU:HD11	2.22	0.40
8:b:89:ARG:H	8:b:89:ARG:HG2	1.72	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	E	245/541 (45%)	217 (89%)	28 (11%)	0	100	100
1	e	245/541 (45%)	217 (89%)	28 (11%)	0	100	100
2	H	248/543 (46%)	229 (92%)	18 (7%)	1 (0%)	30	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	248/543 (46%)	229 (92%)	18 (7%)	1 (0%)	30	64
3	Q	348/548 (64%)	327 (94%)	20 (6%)	1 (0%)	37	68
3	q	348/548 (64%)	327 (94%)	20 (6%)	1 (0%)	37	68
4	Z	319/531 (60%)	288 (90%)	30 (9%)	1 (0%)	37	68
4	z	319/531 (60%)	288 (90%)	30 (9%)	1 (0%)	37	68
5	G	245/545 (45%)	228 (93%)	17 (7%)	0	100	100
5	g	245/545 (45%)	229 (94%)	16 (6%)	0	100	100
6	A	245/556 (44%)	223 (91%)	21 (9%)	1 (0%)	30	64
6	a	245/556 (44%)	223 (91%)	21 (9%)	1 (0%)	30	64
7	D	244/539 (45%)	225 (92%)	19 (8%)	0	100	100
7	d	244/539 (45%)	224 (92%)	20 (8%)	0	100	100
8	B	278/535 (52%)	264 (95%)	14 (5%)	0	100	100
8	b	278/535 (52%)	264 (95%)	14 (5%)	0	100	100
9	N	31/129 (24%)	26 (84%)	5 (16%)	0	100	100
9	n	31/129 (24%)	26 (84%)	5 (16%)	0	100	100
All	All	4406/8934 (49%)	4054 (92%)	344 (8%)	8 (0%)	45	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	124	SER
3	q	124	SER
4	Z	16	ALA
4	z	16	ALA
2	H	117	HIS
2	h	117	HIS
6	A	58	GLY
6	a	58	GLY

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	E	204/456 (45%)	203 (100%)	1 (0%)	86 93
1	e	204/456 (45%)	203 (100%)	1 (0%)	86 93
2	H	202/443 (46%)	199 (98%)	3 (2%)	60 77
2	h	202/443 (46%)	200 (99%)	2 (1%)	73 84
3	Q	291/452 (64%)	288 (99%)	3 (1%)	73 84
3	q	291/452 (64%)	288 (99%)	3 (1%)	73 84
4	Z	260/442 (59%)	259 (100%)	1 (0%)	89 95
4	z	260/442 (59%)	259 (100%)	1 (0%)	89 95
5	G	206/469 (44%)	205 (100%)	1 (0%)	86 93
5	g	206/469 (44%)	205 (100%)	1 (0%)	86 93
6	A	205/463 (44%)	202 (98%)	3 (2%)	60 77
6	a	205/463 (44%)	203 (99%)	2 (1%)	73 84
7	D	203/452 (45%)	184 (91%)	19 (9%)	7 29
7	d	203/452 (45%)	184 (91%)	19 (9%)	7 29
8	B	219/427 (51%)	215 (98%)	4 (2%)	54 74
8	b	219/427 (51%)	215 (98%)	4 (2%)	54 74
9	N	31/105 (30%)	31 (100%)	0	100 100
9	n	31/105 (30%)	31 (100%)	0	100 100
All	All	3642/7418 (49%)	3574 (98%)	68 (2%)	52 73

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	109	VAL
2	H	139	ILE
2	H	433	LEU
2	H	494	GLU
3	Q	57	ILE
3	Q	123	LEU
3	Q	127	GLU
4	Z	15	ARG
5	G	21	LYS
6	A	28	ILE
6	A	434	GLU
6	A	454	VAL
7	D	39	SER
7	D	63	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	65	LYS
7	D	67	ASP
7	D	71	THR
7	D	79	LYS
7	D	82	GLN
7	D	84	LEU
7	D	95	SER
7	D	106	THR
7	D	152	SER
7	D	450	CYS
7	D	490	THR
7	D	497	LYS
7	D	505	GLU
7	D	523	THR
7	D	528	SER
7	D	534	ASP
7	D	535	VAL
8	B	39	VAL
8	B	51	ILE
8	B	102	VAL
8	B	144	SER
1	e	109	VAL
2	h	433	LEU
2	h	494	GLU
3	q	57	ILE
3	q	123	LEU
3	q	127	GLU
4	z	15	ARG
5	g	21	LYS
6	a	28	ILE
6	a	454	VAL
7	d	39	SER
7	d	63	ASP
7	d	65	LYS
7	d	67	ASP
7	d	71	THR
7	d	79	LYS
7	d	82	GLN
7	d	84	LEU
7	d	95	SER
7	d	106	THR
7	d	152	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	d	450	CYS
7	d	490	THR
7	d	497	LYS
7	d	505	GLU
7	d	523	THR
7	d	528	SER
7	d	534	ASP
7	d	535	VAL
8	b	39	VAL
8	b	51	ILE
8	b	102	VAL
8	b	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	55	ASN
1	E	98	GLN
1	E	129	HIS
1	E	147	HIS
1	E	435	GLN
1	E	469	ASN
1	E	499	ASN
1	E	522	GLN
2	H	21	GLN
2	H	25	ASN
2	H	459	ASN
2	H	480	ASN
2	H	481	ASN
3	Q	32	ASN
3	Q	50	ASN
3	Q	58	ASN
3	Q	140	HIS
3	Q	185	GLN
3	Q	196	HIS
3	Q	461	ASN
4	Z	68	GLN
4	Z	71	HIS
4	Z	105	GLN
4	Z	434	GLN
4	Z	470	HIS
5	G	64	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	G	442	GLN
5	G	454	ASN
5	G	472	GLN
5	G	481	ASN
6	A	21	ASN
6	A	435	GLN
6	A	455	ASN
6	A	472	ASN
6	A	475	GLN
6	A	492	ASN
7	D	82	GLN
7	D	98	GLN
7	D	125	GLN
7	D	482	ASN
7	D	494	ASN
8	B	161	ASN
8	B	391	HIS
8	B	399	GLN
8	B	419	HIS
8	B	453	ASN
8	B	464	GLN
9	N	32	ASN
9	N	98	ASN
9	N	100	ASN
1	e	55	ASN
1	e	98	GLN
1	e	129	HIS
1	e	147	HIS
1	e	435	GLN
1	e	499	ASN
1	e	522	GLN
2	h	21	GLN
2	h	25	ASN
2	h	480	ASN
2	h	481	ASN
3	q	32	ASN
3	q	50	ASN
3	q	58	ASN
3	q	140	HIS
3	q	196	HIS
3	q	435	GLN
3	q	461	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	z	68	GLN
4	z	71	HIS
4	z	105	GLN
4	z	434	GLN
4	z	470	HIS
4	z	503	GLN
5	g	64	ASN
5	g	118	HIS
5	g	442	GLN
5	g	454	ASN
5	g	472	GLN
5	g	481	ASN
6	a	21	ASN
6	a	82	GLN
6	a	435	GLN
6	a	455	ASN
6	a	472	ASN
6	a	475	GLN
6	a	492	ASN
7	d	82	GLN
7	d	98	GLN
7	d	125	GLN
7	d	129	HIS
7	d	494	ASN
8	b	161	ASN
8	b	399	GLN
8	b	419	HIS
8	b	453	ASN
8	b	464	GLN
9	n	32	ASN
9	n	98	ASN
9	n	100	ASN

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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 16 are monoatomic - leaving 28 for Mogul analysis.

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	$\#\|Z\| > 2$
11	ADP	e	602	10	24,29,29	0.90	1 (4%)	29,45,45	1.28	4 (13%)
11	ADP	d	602	10	24,29,29	0.97	1 (4%)	29,45,45	1.38	3 (10%)
11	ADP	h	601	10	24,29,29	0.91	1 (4%)	29,45,45	1.44	4 (13%)
11	ADP	g	601	10	24,29,29	0.68	0	29,45,45	0.79	1 (3%)
11	ADP	Z	601	10	24,29,29	0.92	1 (4%)	29,45,45	1.47	4 (13%)
12	AF3	h	603	-	0,3,3	-	-	-		
12	AF3	q	603	-	0,3,3	-	-	-		
11	ADP	Q	601	10	24,29,29	0.68	0	29,45,45	0.75	1 (3%)
12	AF3	z	603	-	0,3,3	-	-	-		
11	ADP	A	601	10	24,29,29	0.92	1 (4%)	29,45,45	1.42	4 (13%)
11	ADP	b	601	10	24,29,29	0.92	1 (4%)	29,45,45	1.45	4 (13%)
12	AF3	G	603	-	0,3,3	-	-	-		
12	AF3	H	603	-	0,3,3	-	-	-		
11	ADP	H	601	10	24,29,29	0.92	1 (4%)	29,45,45	1.44	4 (13%)
11	ADP	G	601	10	24,29,29	0.68	0	29,45,45	0.78	1 (3%)
12	AF3	A	603	-	0,3,3	-	-	-		
11	ADP	z	601	10	24,29,29	0.91	1 (4%)	29,45,45	1.47	4 (13%)
11	ADP	a	601	10	24,29,29	0.91	1 (4%)	29,45,45	1.43	4 (13%)
12	AF3	g	603	-	0,3,3	-	-	-		
12	AF3	Z	603	-	0,3,3	-	-	-		
12	AF3	a	603	-	0,3,3	-	-	-		
11	ADP	q	601	10	24,29,29	0.68	0	29,45,45	0.71	1 (3%)
12	AF3	b	603	-	0,3,3	-	-	-		
11	ADP	D	602	10	24,29,29	0.98	1 (4%)	29,45,45	1.37	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	AF3	Q	603	-	0,3,3	-	-	-		
12	AF3	B	603	-	0,3,3	-	-	-		
11	ADP	E	602	10	24,29,29	0.90	1 (4%)	29,45,45	1.28	4 (13%)
11	ADP	B	601	10	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)

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
11	ADP	H	601	10	-	4/12/32/32	0/3/3/3
11	ADP	Q	601	10	-	6/12/32/32	0/3/3/3
11	ADP	e	602	10	-	1/12/32/32	0/3/3/3
11	ADP	A	601	10	-	3/12/32/32	0/3/3/3
11	ADP	G	601	10	-	6/12/32/32	0/3/3/3
11	ADP	d	602	10	-	6/12/32/32	0/3/3/3
11	ADP	q	601	10	-	8/12/32/32	0/3/3/3
11	ADP	D	602	10	-	6/12/32/32	0/3/3/3
11	ADP	h	601	10	-	4/12/32/32	0/3/3/3
11	ADP	E	602	10	-	1/12/32/32	0/3/3/3
11	ADP	g	601	10	-	6/12/32/32	0/3/3/3
11	ADP	z	601	10	-	4/12/32/32	0/3/3/3
11	ADP	b	601	10	-	4/12/32/32	0/3/3/3
11	ADP	a	601	10	-	3/12/32/32	0/3/3/3
11	ADP	B	601	10	-	4/12/32/32	0/3/3/3
11	ADP	Z	601	10	-	4/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	d	602	ADP	C5-C4	2.35	1.47	1.40
11	A	601	ADP	C5-C4	2.34	1.47	1.40
11	a	601	ADP	C5-C4	2.32	1.47	1.40
11	D	602	ADP	C5-C4	2.30	1.47	1.40
11	b	601	ADP	C5-C4	2.30	1.47	1.40
11	B	601	ADP	C5-C4	2.30	1.47	1.40
11	h	601	ADP	C5-C4	2.29	1.47	1.40
11	H	601	ADP	C5-C4	2.28	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	z	601	ADP	C5-C4	2.24	1.46	1.40
11	Z	601	ADP	C5-C4	2.24	1.46	1.40
11	E	602	ADP	C5-C4	2.18	1.46	1.40
11	e	602	ADP	C5-C4	2.16	1.46	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	d	602	ADP	PA-O3A-PB	-3.92	119.36	132.83
11	D	602	ADP	PA-O3A-PB	-3.92	119.38	132.83
11	Z	601	ADP	PA-O3A-PB	-3.80	119.78	132.83
11	z	601	ADP	PA-O3A-PB	-3.80	119.80	132.83
11	B	601	ADP	PA-O3A-PB	-3.79	119.83	132.83
11	b	601	ADP	PA-O3A-PB	-3.78	119.86	132.83
11	h	601	ADP	PA-O3A-PB	-3.73	120.03	132.83
11	H	601	ADP	PA-O3A-PB	-3.72	120.06	132.83
11	a	601	ADP	PA-O3A-PB	-3.55	120.63	132.83
11	A	601	ADP	PA-O3A-PB	-3.55	120.64	132.83
11	Z	601	ADP	N3-C2-N1	-3.25	123.60	128.68
11	z	601	ADP	N3-C2-N1	-3.24	123.61	128.68
11	a	601	ADP	N3-C2-N1	-3.19	123.69	128.68
11	h	601	ADP	N3-C2-N1	-3.19	123.70	128.68
11	B	601	ADP	N3-C2-N1	-3.18	123.70	128.68
11	d	602	ADP	N3-C2-N1	-3.18	123.71	128.68
11	A	601	ADP	N3-C2-N1	-3.18	123.72	128.68
11	b	601	ADP	N3-C2-N1	-3.17	123.72	128.68
11	H	601	ADP	N3-C2-N1	-3.17	123.73	128.68
11	D	602	ADP	N3-C2-N1	-3.12	123.80	128.68
11	E	602	ADP	N3-C2-N1	-3.08	123.87	128.68
11	e	602	ADP	N3-C2-N1	-3.08	123.87	128.68
11	A	601	ADP	C3'-C2'-C1'	2.97	105.45	100.98
11	a	601	ADP	C3'-C2'-C1'	2.95	105.42	100.98
11	B	601	ADP	C3'-C2'-C1'	2.88	105.31	100.98
11	h	601	ADP	C3'-C2'-C1'	2.87	105.30	100.98
11	H	601	ADP	C3'-C2'-C1'	2.87	105.30	100.98
11	b	601	ADP	C3'-C2'-C1'	2.85	105.27	100.98
11	z	601	ADP	C3'-C2'-C1'	2.80	105.19	100.98
11	Z	601	ADP	C3'-C2'-C1'	2.79	105.18	100.98
11	d	602	ADP	C4-C5-N7	-2.76	106.52	109.40
11	D	602	ADP	C4-C5-N7	-2.76	106.53	109.40
11	Z	601	ADP	C4-C5-N7	-2.70	106.58	109.40
11	a	601	ADP	C4-C5-N7	-2.68	106.60	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	z	601	ADP	C4-C5-N7	-2.68	106.61	109.40
11	B	601	ADP	C4-C5-N7	-2.64	106.65	109.40
11	A	601	ADP	C4-C5-N7	-2.64	106.65	109.40
11	b	601	ADP	C4-C5-N7	-2.62	106.67	109.40
11	H	601	ADP	C4-C5-N7	-2.57	106.72	109.40
11	h	601	ADP	C4-C5-N7	-2.56	106.73	109.40
11	e	602	ADP	PA-O3A-PB	-2.51	124.22	132.83
11	E	602	ADP	PA-O3A-PB	-2.50	124.24	132.83
11	E	602	ADP	C4-C5-N7	-2.44	106.86	109.40
11	e	602	ADP	C4-C5-N7	-2.41	106.88	109.40
11	E	602	ADP	O4'-C1'-C2'	-2.36	103.48	106.93
11	e	602	ADP	O4'-C1'-C2'	-2.33	103.52	106.93
11	G	601	ADP	C5-C6-N6	2.26	123.78	120.35
11	g	601	ADP	C5-C6-N6	2.25	123.77	120.35
11	Q	601	ADP	C5-C6-N6	2.23	123.75	120.35
11	q	601	ADP	C5-C6-N6	2.22	123.73	120.35

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	601	ADP	PB-O3A-PA-O5'
11	H	601	ADP	C5'-O5'-PA-O1A
11	H	601	ADP	C5'-O5'-PA-O2A
11	Q	601	ADP	C5'-O5'-PA-O1A
11	Q	601	ADP	C5'-O5'-PA-O3A
11	Z	601	ADP	C5'-O5'-PA-O1A
11	Z	601	ADP	C5'-O5'-PA-O2A
11	G	601	ADP	PA-O3A-PB-O2B
11	A	601	ADP	C5'-O5'-PA-O2A
11	A	601	ADP	C5'-O5'-PA-O3A
11	D	602	ADP	C5'-O5'-PA-O1A
11	D	602	ADP	C5'-O5'-PA-O2A
11	B	601	ADP	PB-O3A-PA-O5'
11	B	601	ADP	C5'-O5'-PA-O1A
11	B	601	ADP	C5'-O5'-PA-O2A
11	h	601	ADP	PB-O3A-PA-O5'
11	h	601	ADP	C5'-O5'-PA-O1A
11	h	601	ADP	C5'-O5'-PA-O2A
11	q	601	ADP	PA-O3A-PB-O3B
11	q	601	ADP	C5'-O5'-PA-O1A
11	q	601	ADP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	z	601	ADP	C5'-O5'-PA-O1A
11	z	601	ADP	C5'-O5'-PA-O2A
11	g	601	ADP	PA-O3A-PB-O2B
11	a	601	ADP	C5'-O5'-PA-O2A
11	a	601	ADP	C5'-O5'-PA-O3A
11	d	602	ADP	C5'-O5'-PA-O1A
11	d	602	ADP	C5'-O5'-PA-O2A
11	b	601	ADP	PB-O3A-PA-O5'
11	b	601	ADP	C5'-O5'-PA-O1A
11	b	601	ADP	C5'-O5'-PA-O2A
11	D	602	ADP	C3'-C4'-C5'-O5'
11	d	602	ADP	C3'-C4'-C5'-O5'
11	D	602	ADP	O4'-C4'-C5'-O5'
11	d	602	ADP	O4'-C4'-C5'-O5'
11	Z	601	ADP	PB-O3A-PA-O5'
11	G	601	ADP	PB-O3A-PA-O5'
11	A	601	ADP	PB-O3A-PA-O5'
11	z	601	ADP	PB-O3A-PA-O5'
11	g	601	ADP	PB-O3A-PA-O5'
11	a	601	ADP	PB-O3A-PA-O5'
11	Z	601	ADP	C5'-O5'-PA-O3A
11	e	602	ADP	C5'-O5'-PA-O3A
11	z	601	ADP	C5'-O5'-PA-O3A
11	g	601	ADP	O4'-C4'-C5'-O5'
11	Q	601	ADP	PB-O3A-PA-O2A
11	g	601	ADP	PB-O3A-PA-O1A
11	G	601	ADP	C5'-O5'-PA-O1A
11	Q	601	ADP	C4'-C5'-O5'-PA
11	G	601	ADP	PB-O3A-PA-O1A
11	q	601	ADP	PB-O3A-PA-O1A
11	q	601	ADP	PB-O3A-PA-O2A
11	D	602	ADP	C4'-C5'-O5'-PA
11	d	602	ADP	C4'-C5'-O5'-PA
11	g	601	ADP	C3'-C4'-C5'-O5'
11	q	601	ADP	O4'-C4'-C5'-O5'
11	q	601	ADP	PA-O3A-PB-O1B
11	g	601	ADP	PA-O3A-PB-O1B
11	G	601	ADP	PA-O3A-PB-O3B
11	q	601	ADP	PA-O3A-PB-O2B
11	E	602	ADP	C5'-O5'-PA-O3A
11	H	601	ADP	C5'-O5'-PA-O3A
11	G	601	ADP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	D	602	ADP	C5'-O5'-PA-O3A
11	B	601	ADP	C5'-O5'-PA-O3A
11	h	601	ADP	C5'-O5'-PA-O3A
11	d	602	ADP	C5'-O5'-PA-O3A
11	b	601	ADP	C5'-O5'-PA-O3A
11	Q	601	ADP	O4'-C4'-C5'-O5'
11	Q	601	ADP	PB-O3A-PA-O1A

There are no ring outliers.

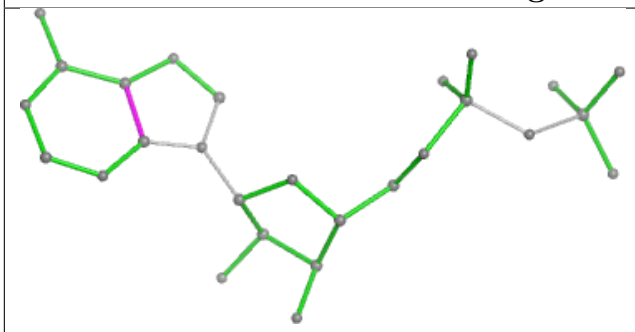
24 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	e	602	ADP	2	0
11	h	601	ADP	1	0
11	g	601	ADP	5	0
11	Z	601	ADP	2	0
12	h	603	AF3	1	0
12	q	603	AF3	1	0
11	Q	601	ADP	13	0
12	z	603	AF3	3	0
11	A	601	ADP	1	0
11	b	601	ADP	3	0
12	H	603	AF3	1	0
11	H	601	ADP	1	0
11	G	601	ADP	5	0
12	A	603	AF3	1	0
11	z	601	ADP	2	0
11	a	601	ADP	1	0
12	Z	603	AF3	3	0
12	a	603	AF3	1	0
11	q	601	ADP	10	0
12	b	603	AF3	2	0
12	Q	603	AF3	1	0
12	B	603	AF3	2	0
11	E	602	ADP	2	0
11	B	601	ADP	3	0

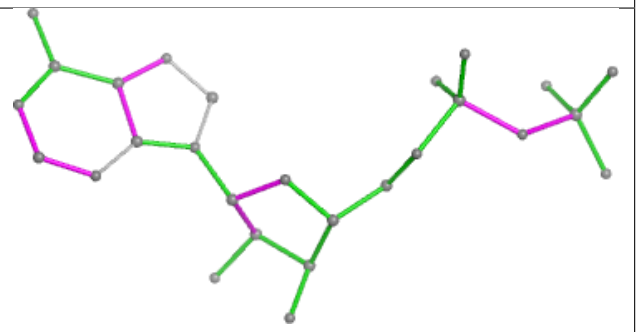
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

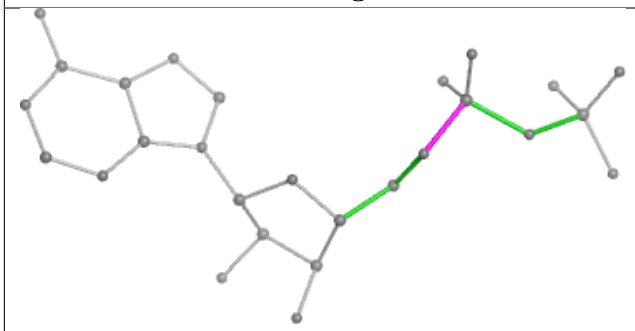
Ligand ADP e 602



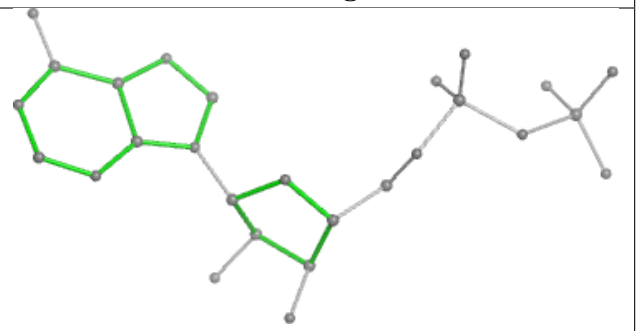
Bond lengths



Bond angles

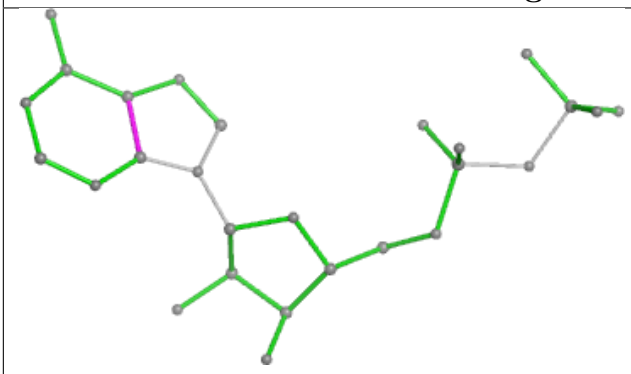


Torsions

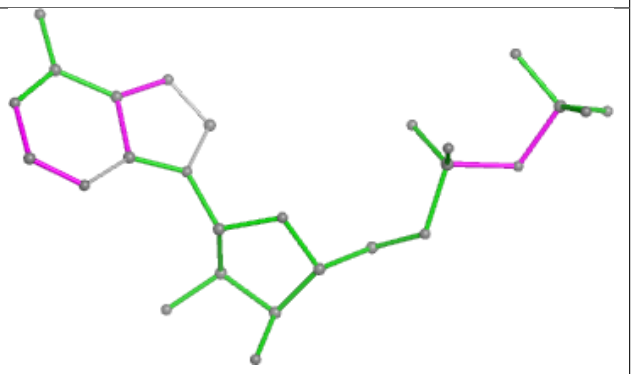


Rings

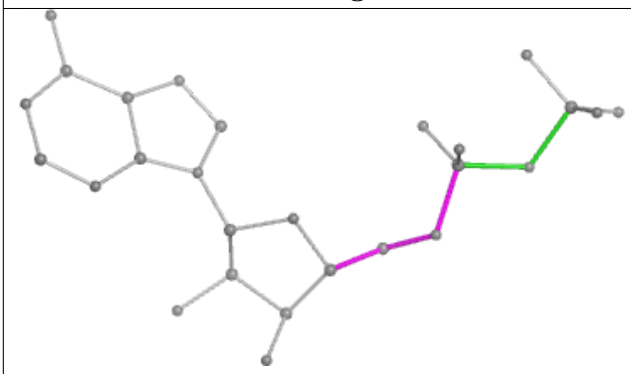
Ligand ADP d 602



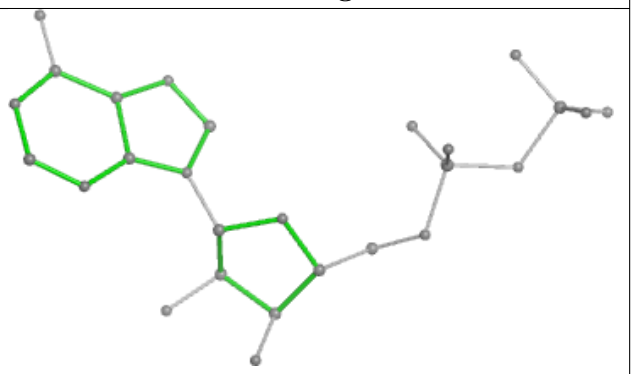
Bond lengths



Bond angles

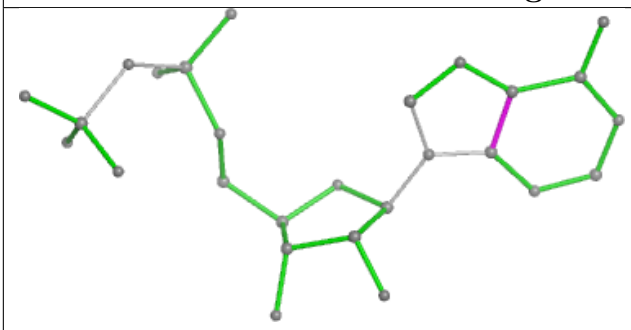


Torsions

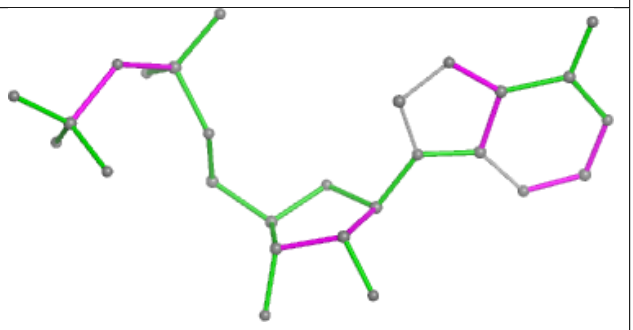


Rings

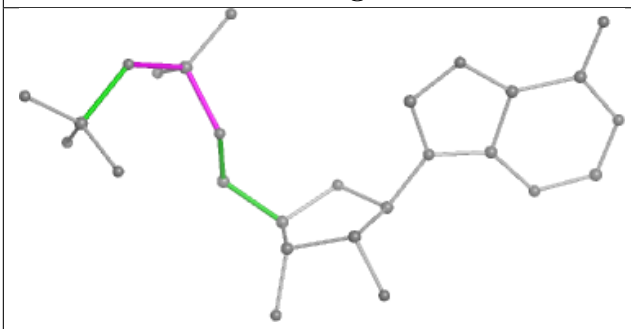
Ligand ADP h 601



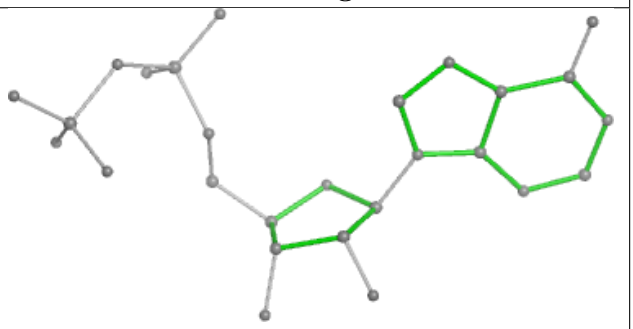
Bond lengths



Bond angles

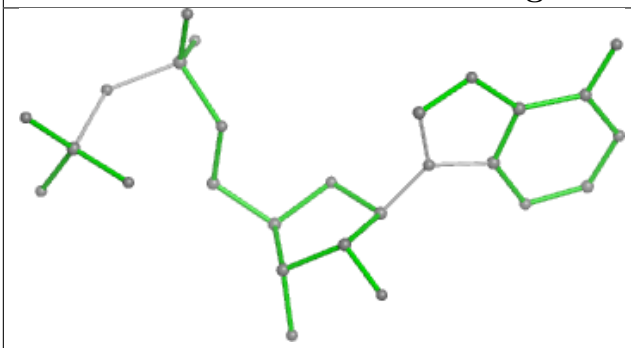


Torsions

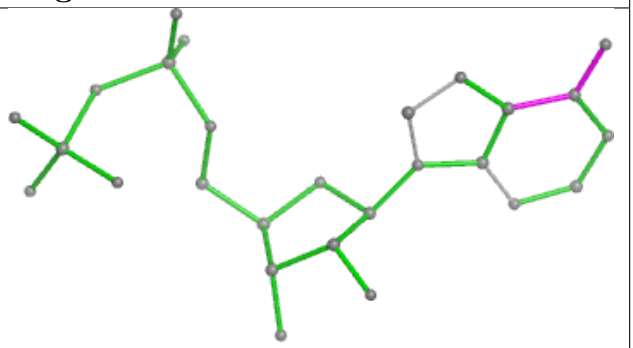


Rings

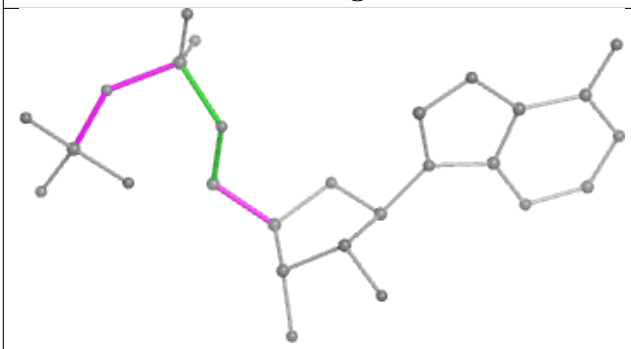
Ligand ADP g 601



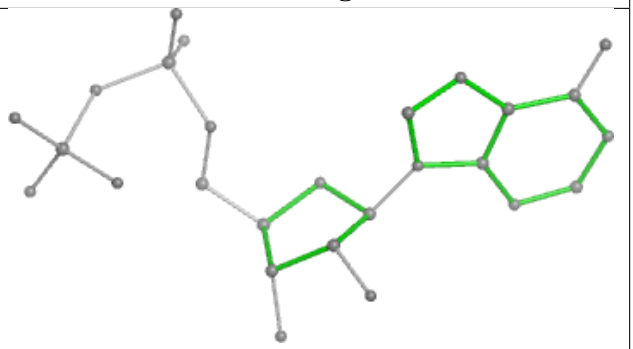
Bond lengths



Bond angles

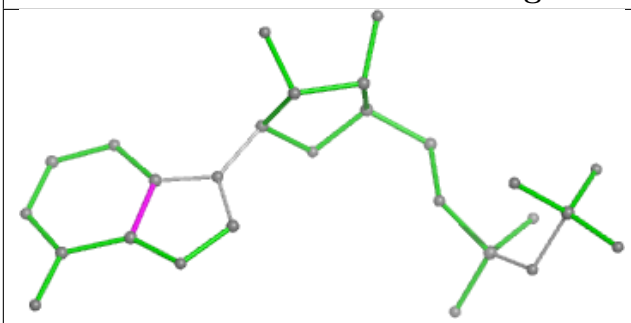


Torsions

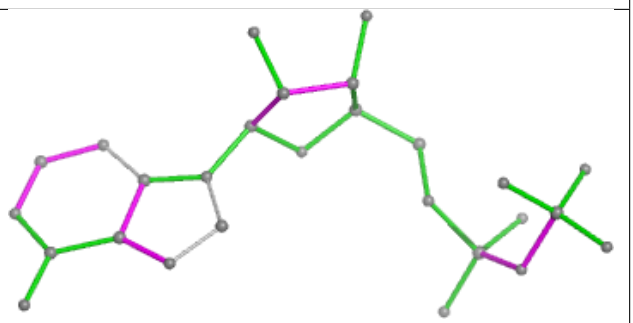


Rings

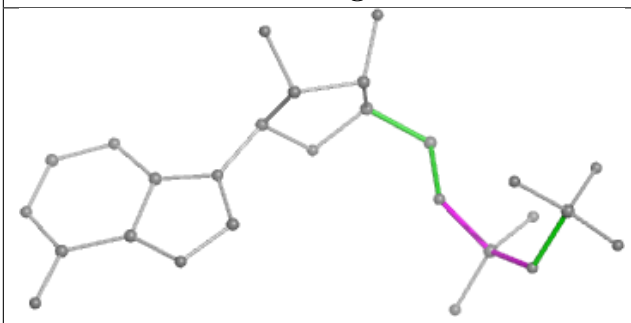
Ligand ADP Z 601



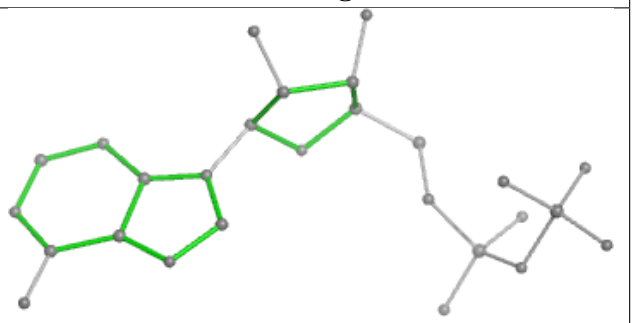
Bond lengths



Bond angles

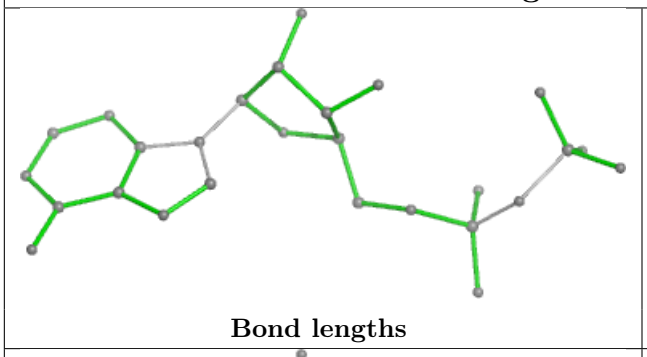


Torsions

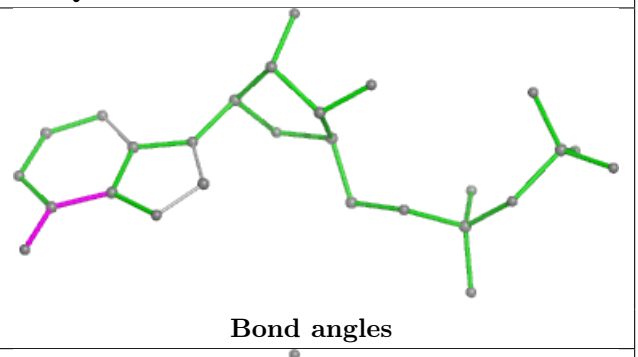


Rings

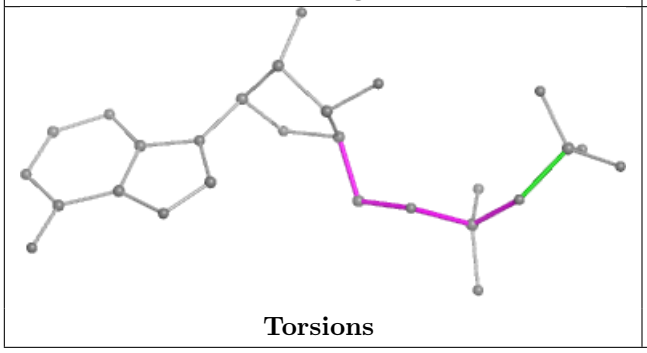
Ligand ADP Q 601



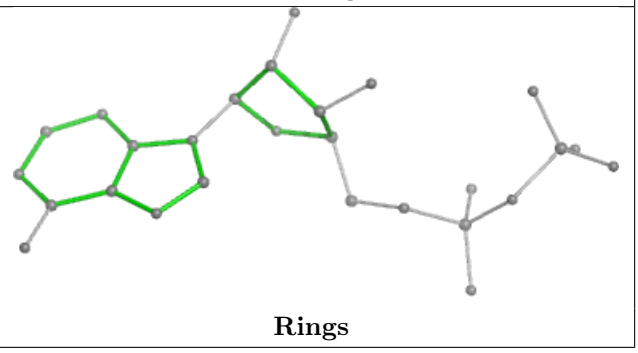
Bond lengths



Bond angles

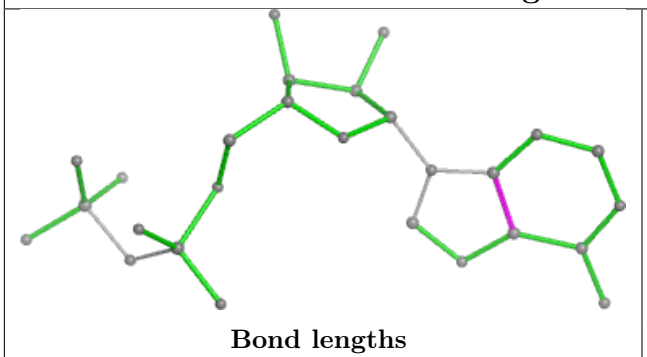


Torsions

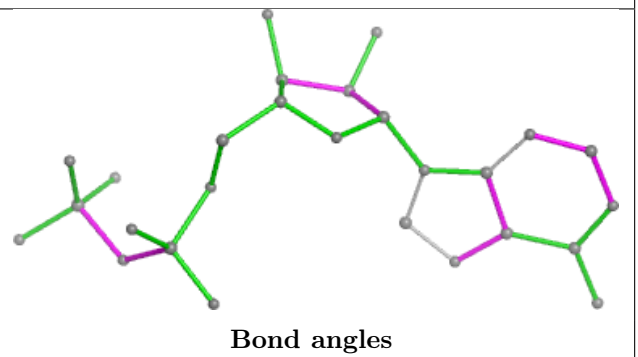


Rings

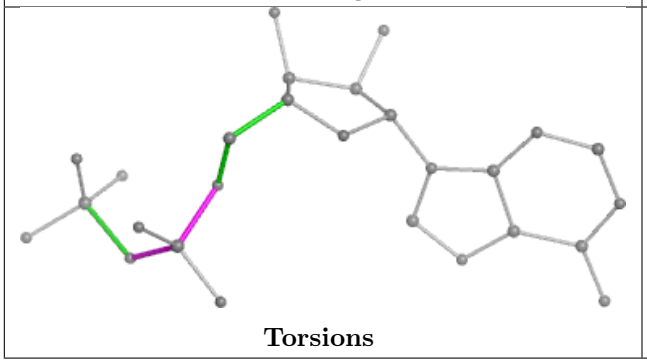
Ligand ADP A 601



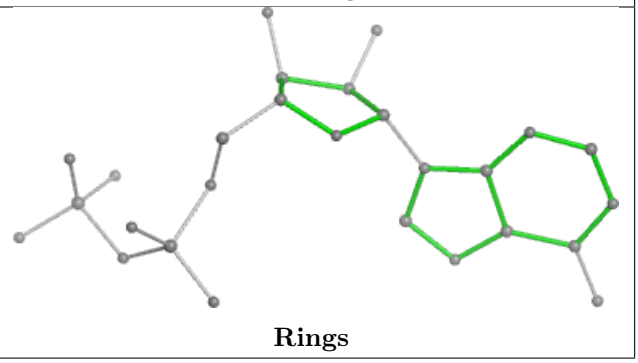
Bond lengths



Bond angles

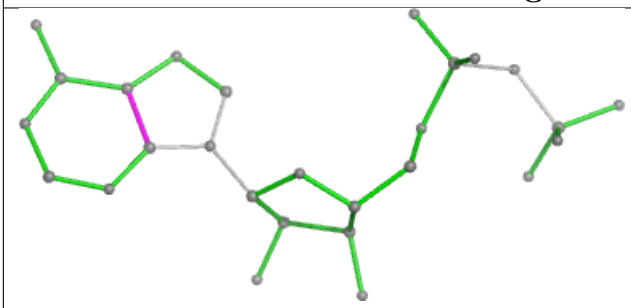


Torsions

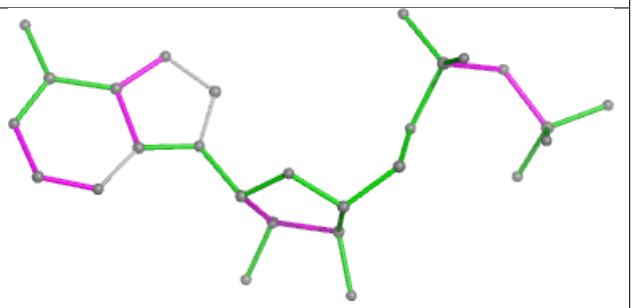


Rings

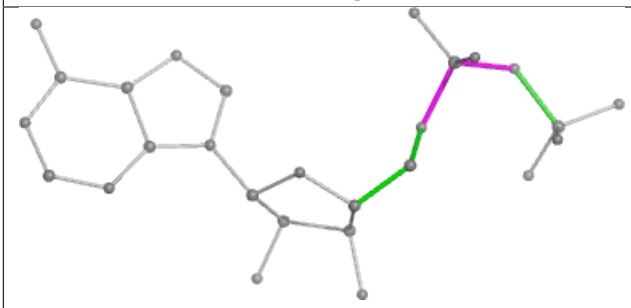
Ligand ADP b 601



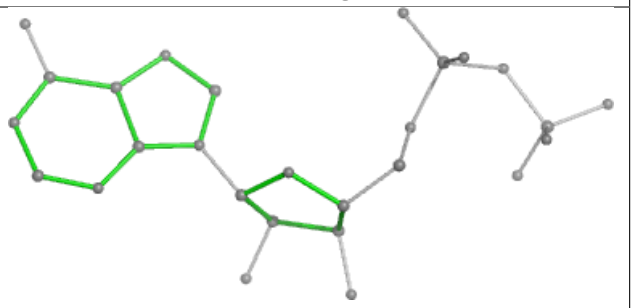
Bond lengths



Bond angles

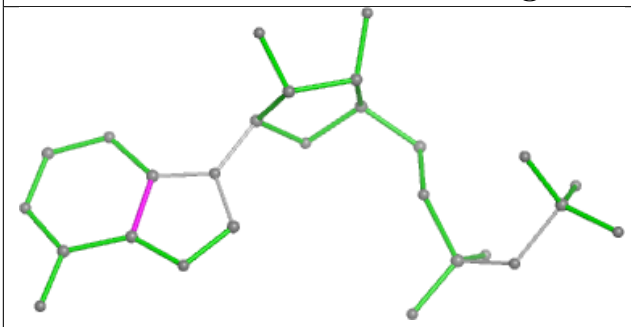


Torsions

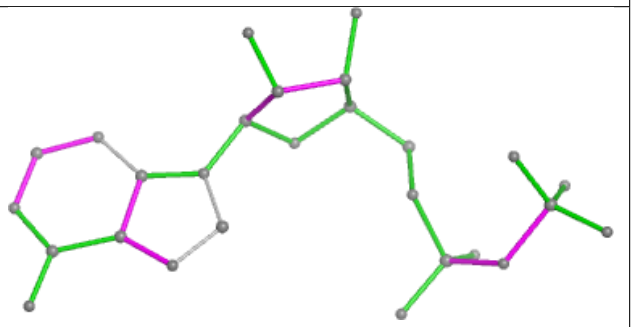


Rings

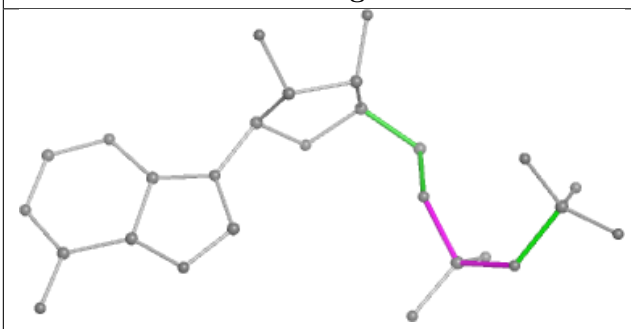
Ligand ADP H 601



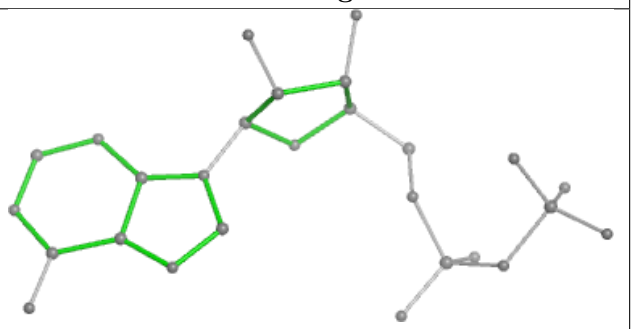
Bond lengths



Bond angles

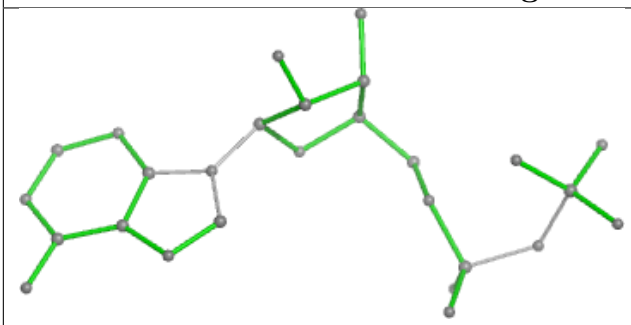


Torsions

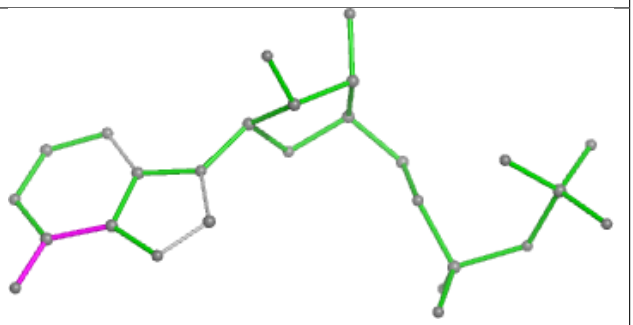


Rings

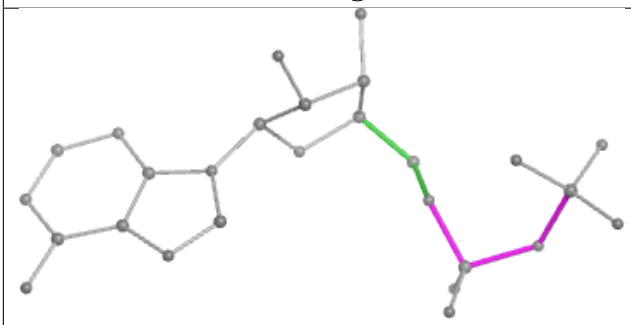
Ligand ADP G 601



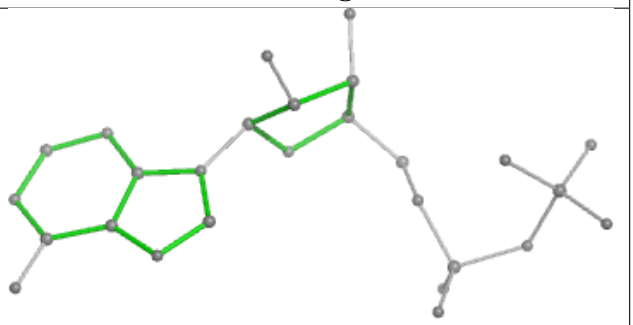
Bond lengths



Bond angles

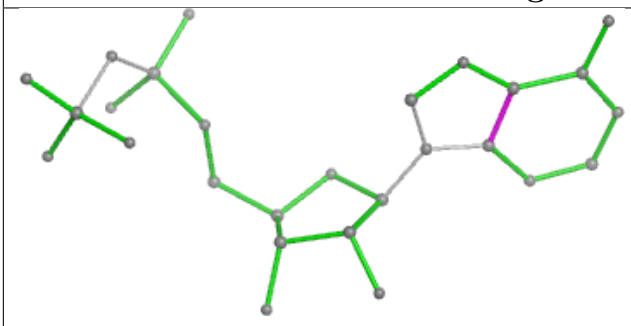


Torsions

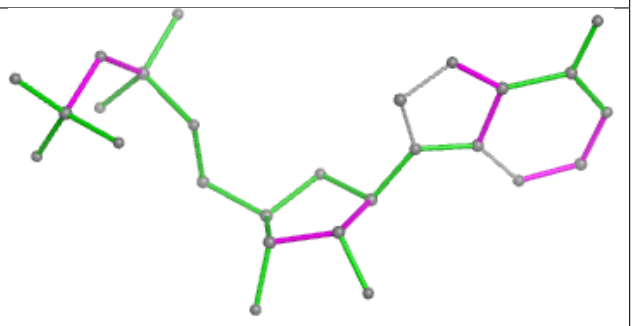


Rings

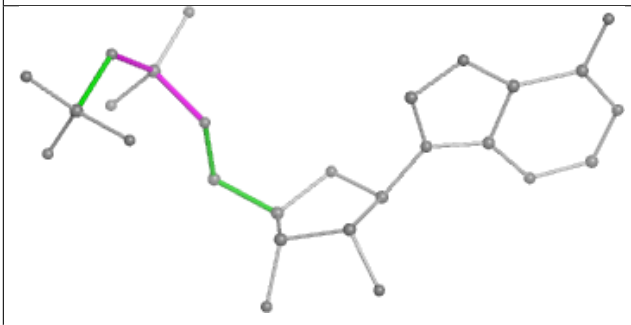
Ligand ADP z 601



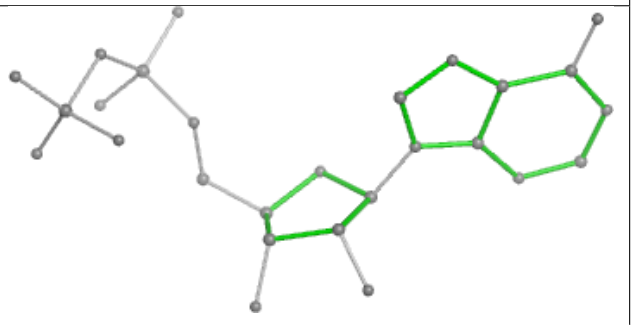
Bond lengths



Bond angles

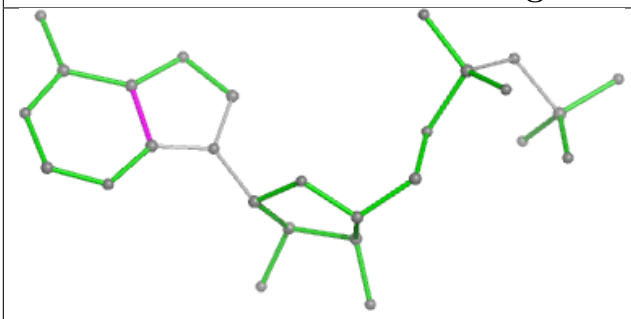


Torsions

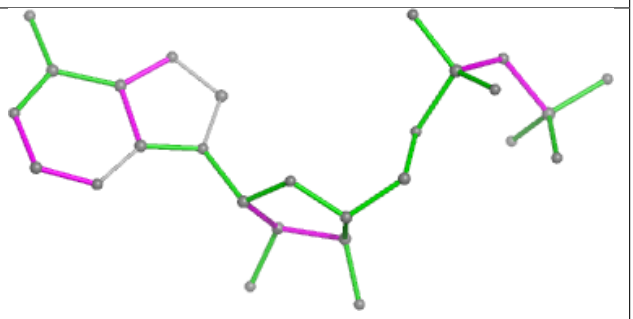


Rings

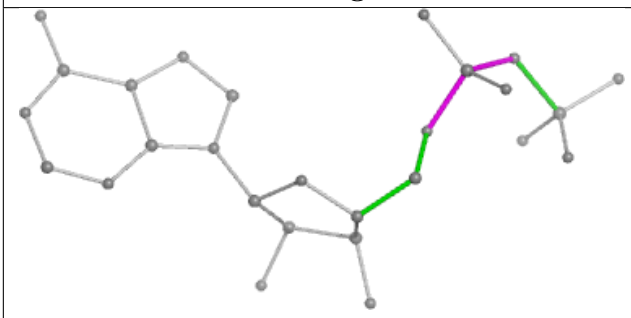
Ligand ADP a 601



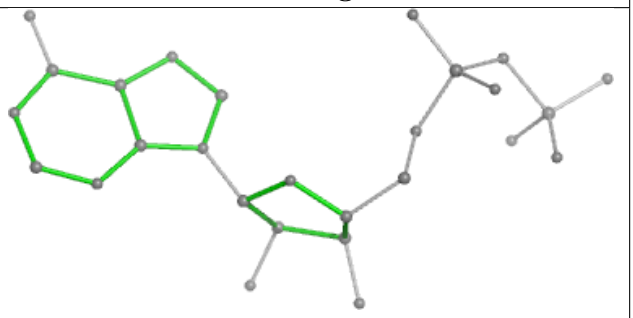
Bond lengths



Bond angles

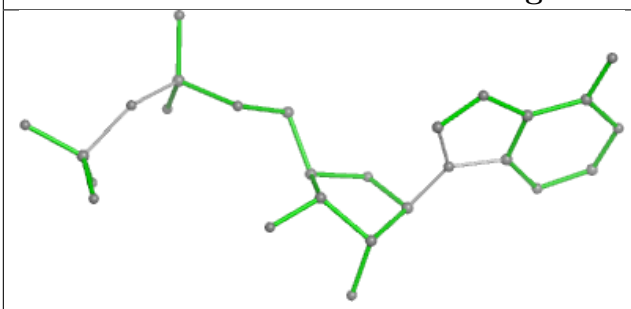


Torsions

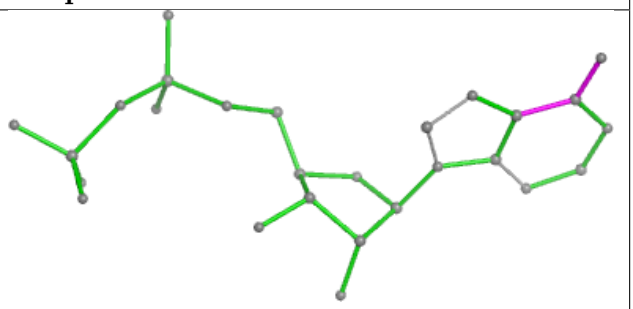


Rings

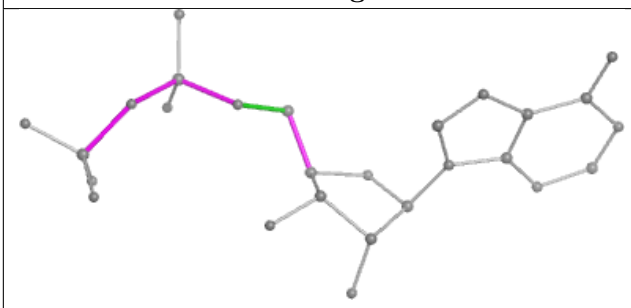
Ligand ADP q 601



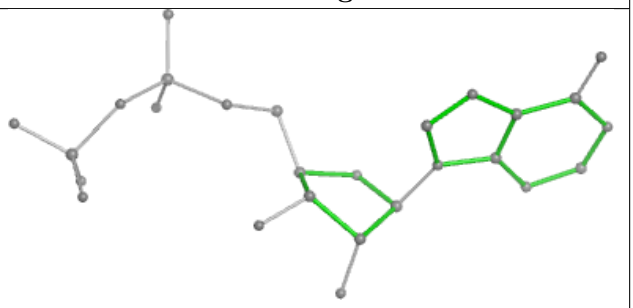
Bond lengths



Bond angles

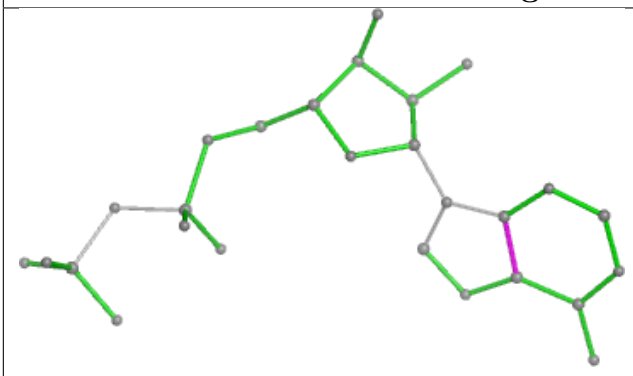


Torsions

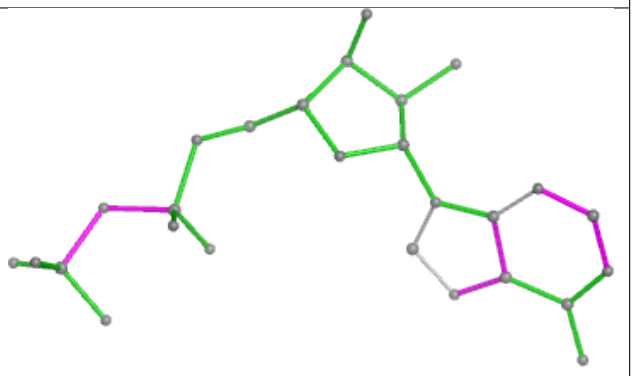


Rings

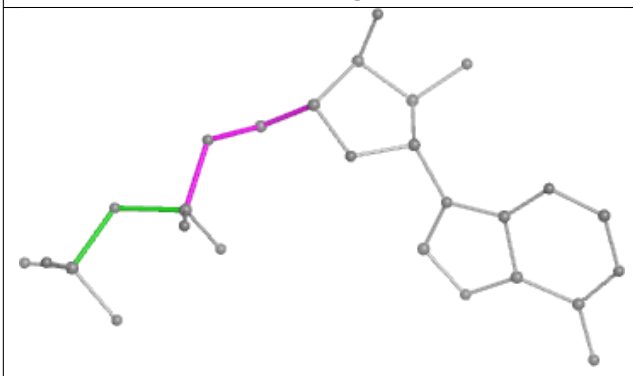
Ligand ADP D 602



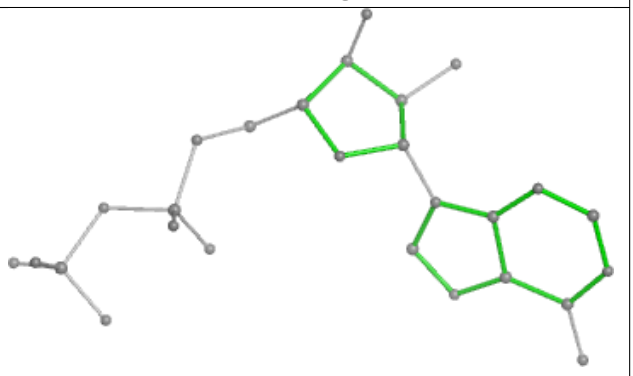
Bond lengths



Bond angles

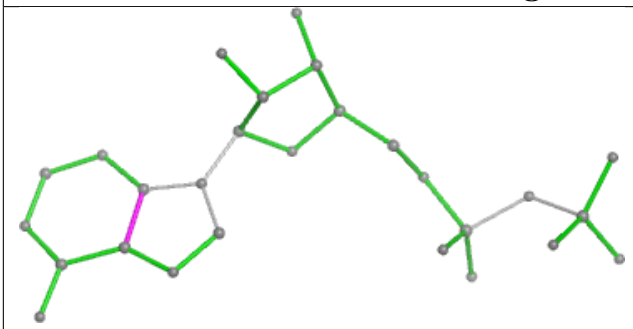


Torsions

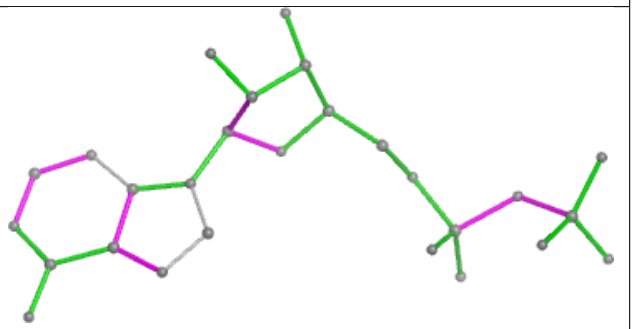


Rings

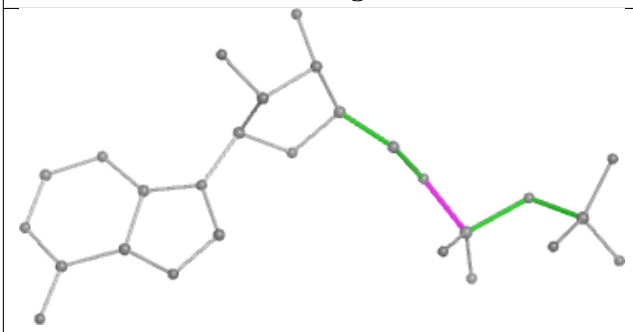
Ligand ADP E 602



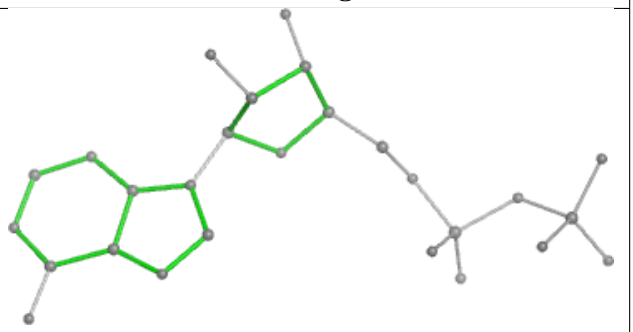
Bond lengths



Bond angles

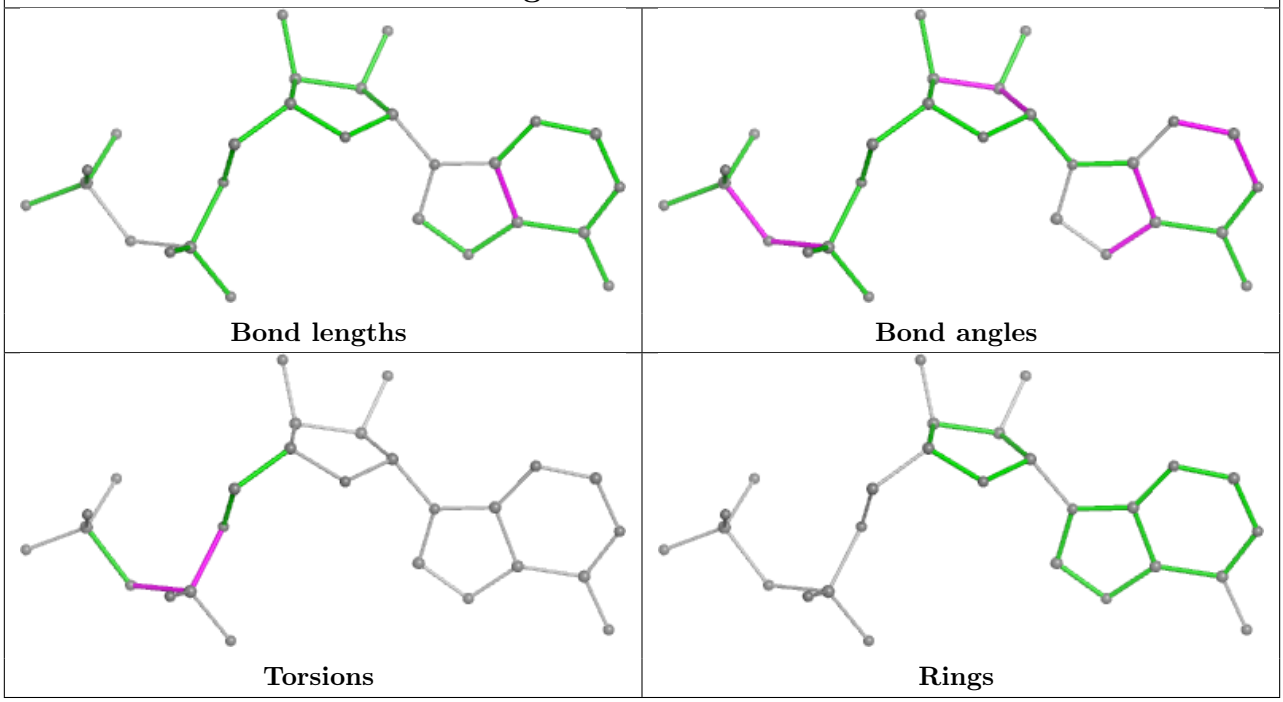


Torsions



Rings

Ligand ADP B 601



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.

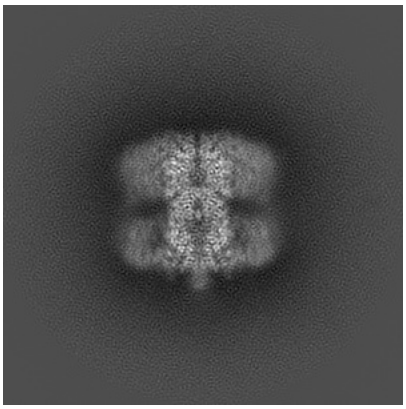
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12608. These allow visual inspection of the internal detail of the map and identification of artifacts.

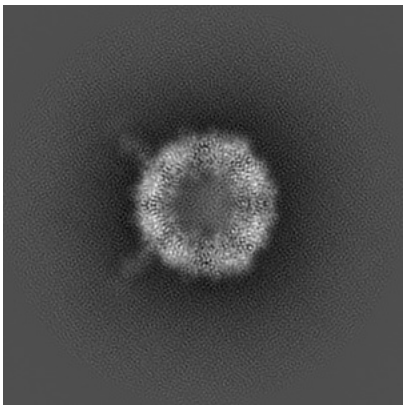
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

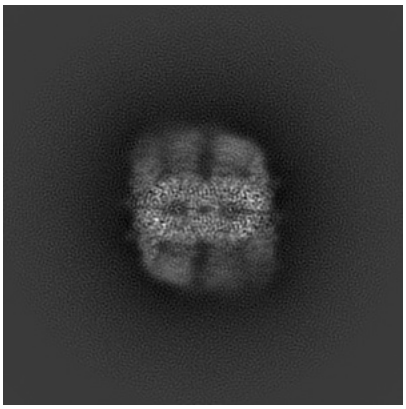
6.1.1 Primary map



X

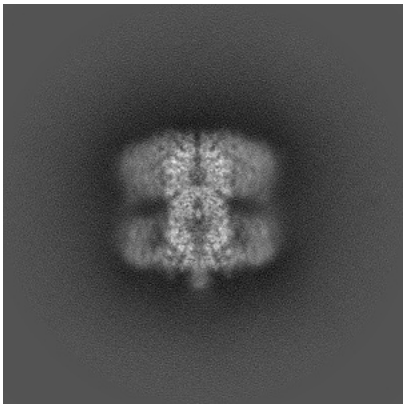


Y

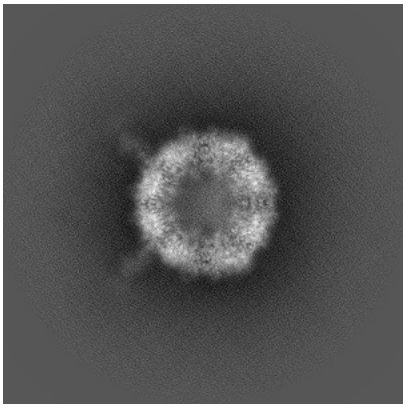


Z

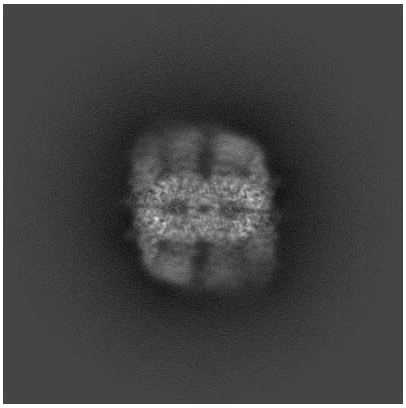
6.1.2 Raw map



X



Y

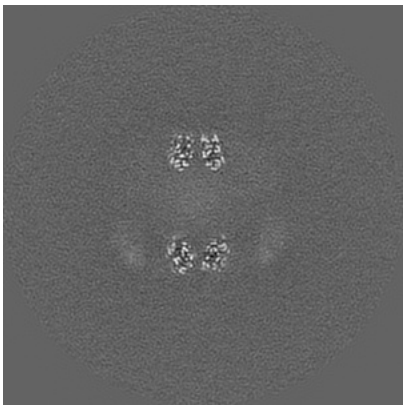


Z

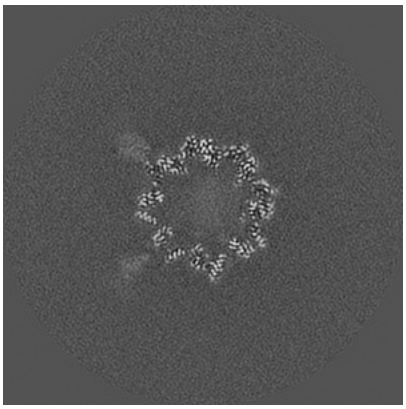
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

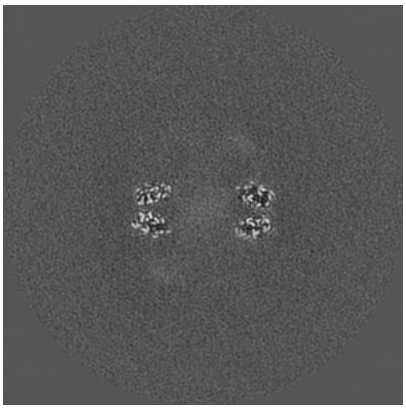
6.2.1 Primary map



X Index: 200

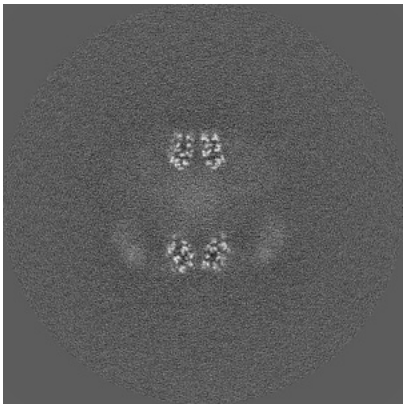


Y Index: 200

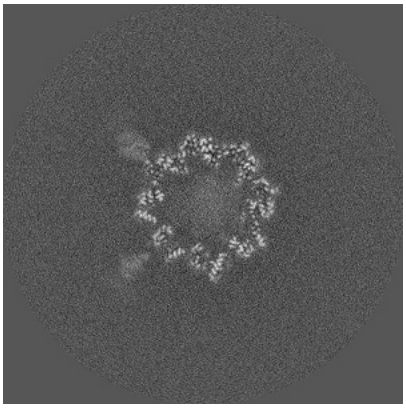


Z Index: 200

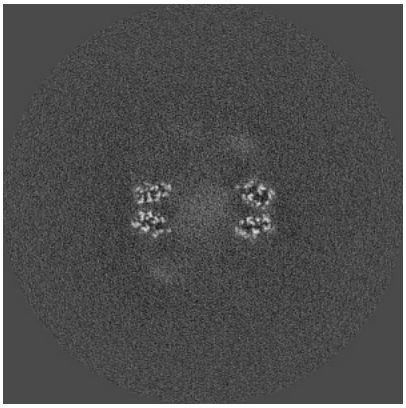
6.2.2 Raw map



X Index: 200



Y Index: 200

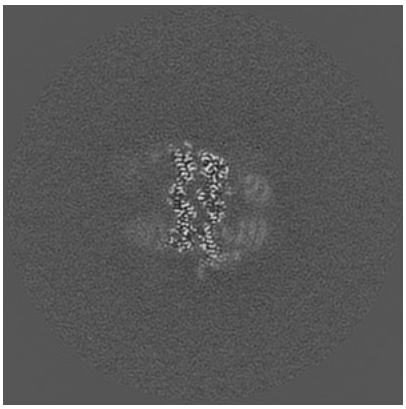


Z Index: 200

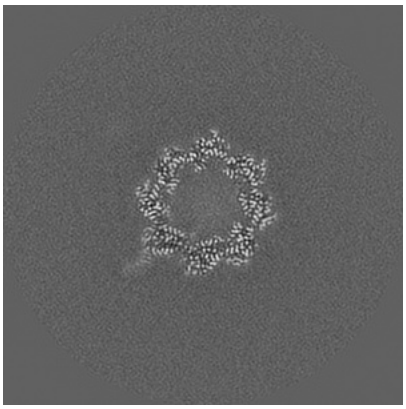
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

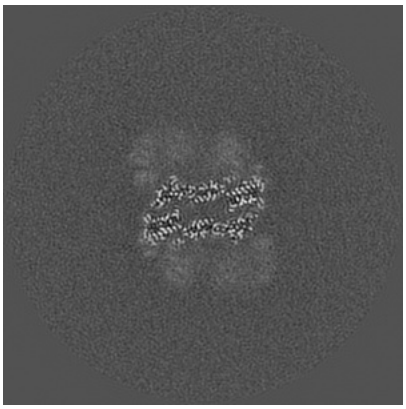
6.3.1 Primary map



X Index: 244

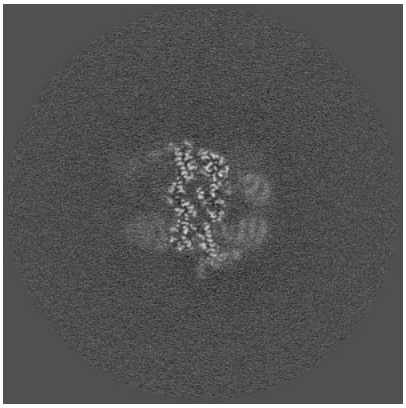


Y Index: 183

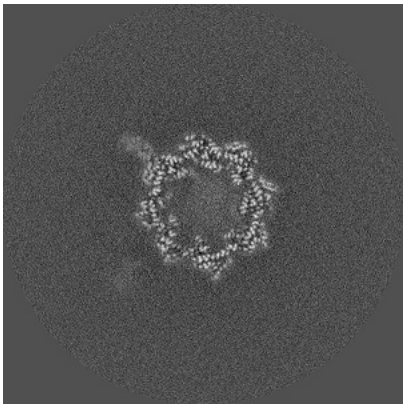


Z Index: 242

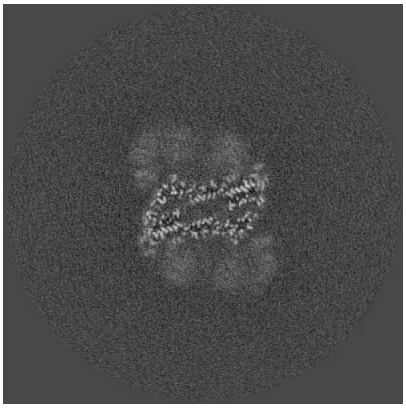
6.3.2 Raw map



X Index: 244



Y Index: 205

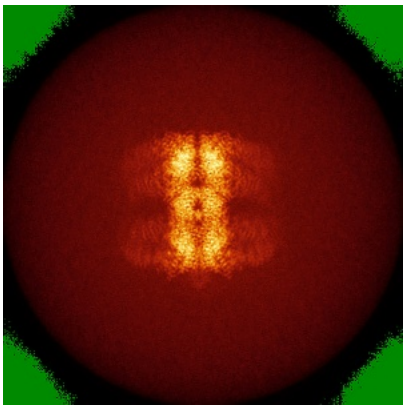


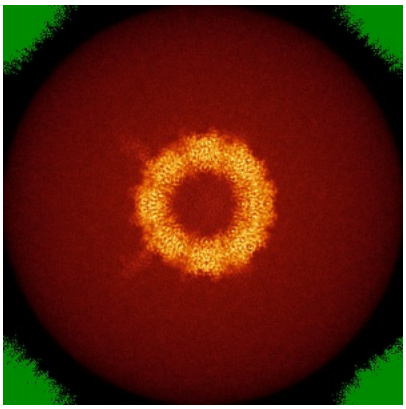
Z Index: 241

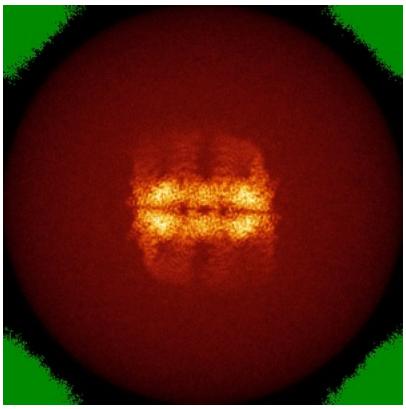
The images above show the largest variance slices of the map in three orthogonal directions.

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

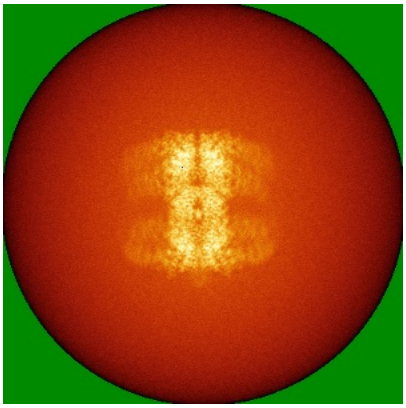
6.4.1 Primary map

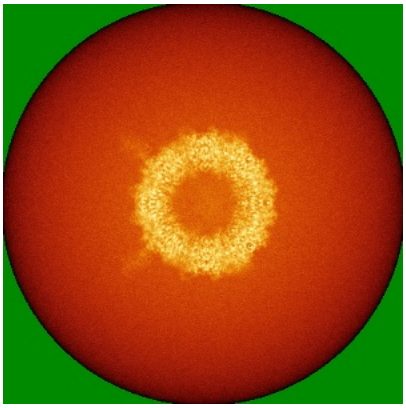

X

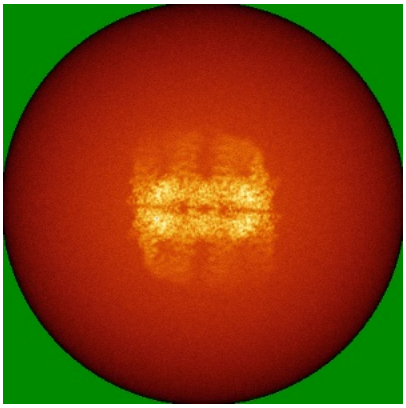

Y


Z

6.4.2 Raw map


X

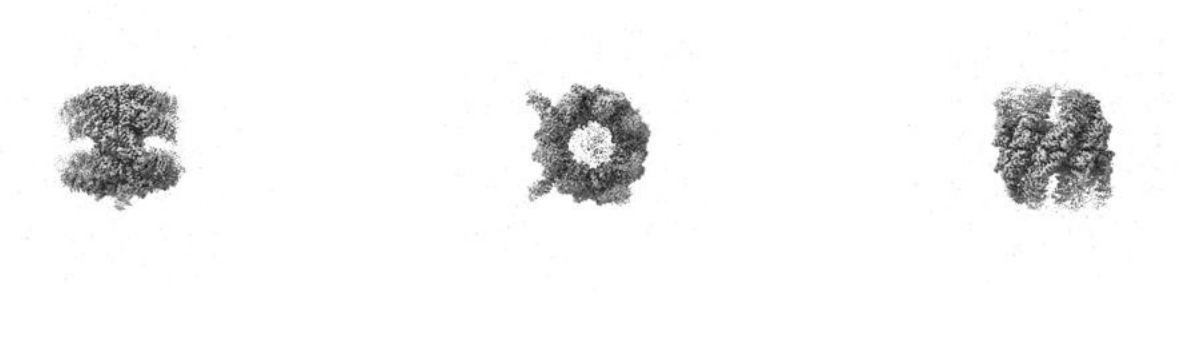

Y


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)

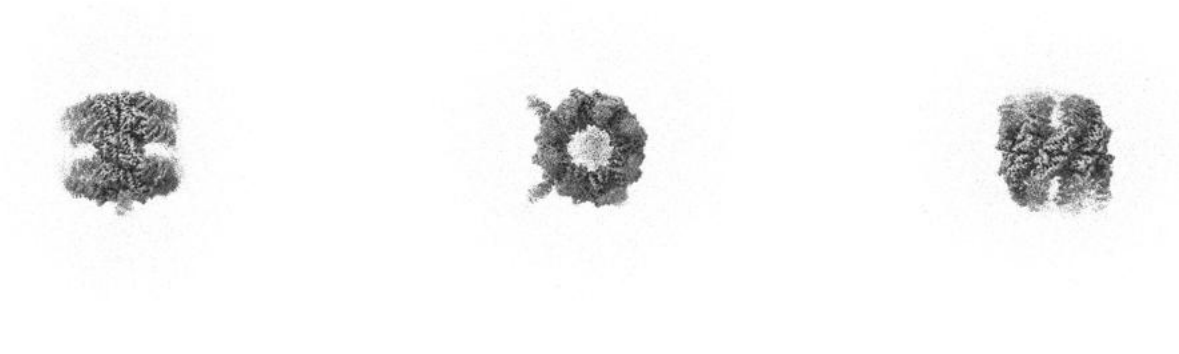
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

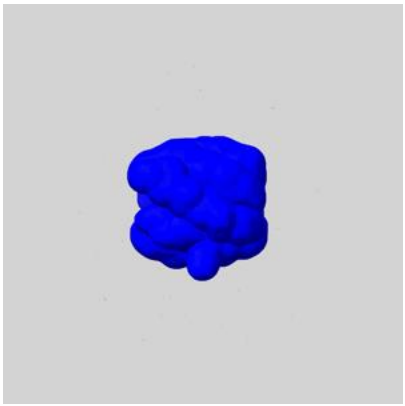
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

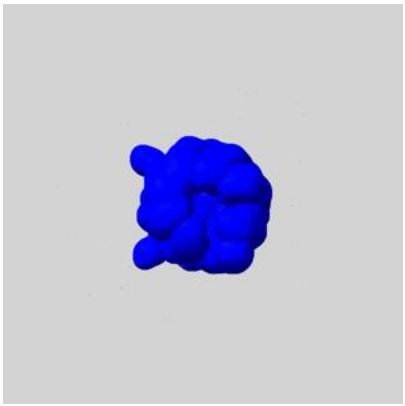
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

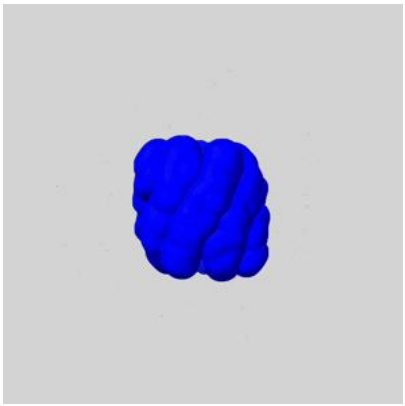
6.6.1 emd_12608_msk_1.map (i)



X



Y

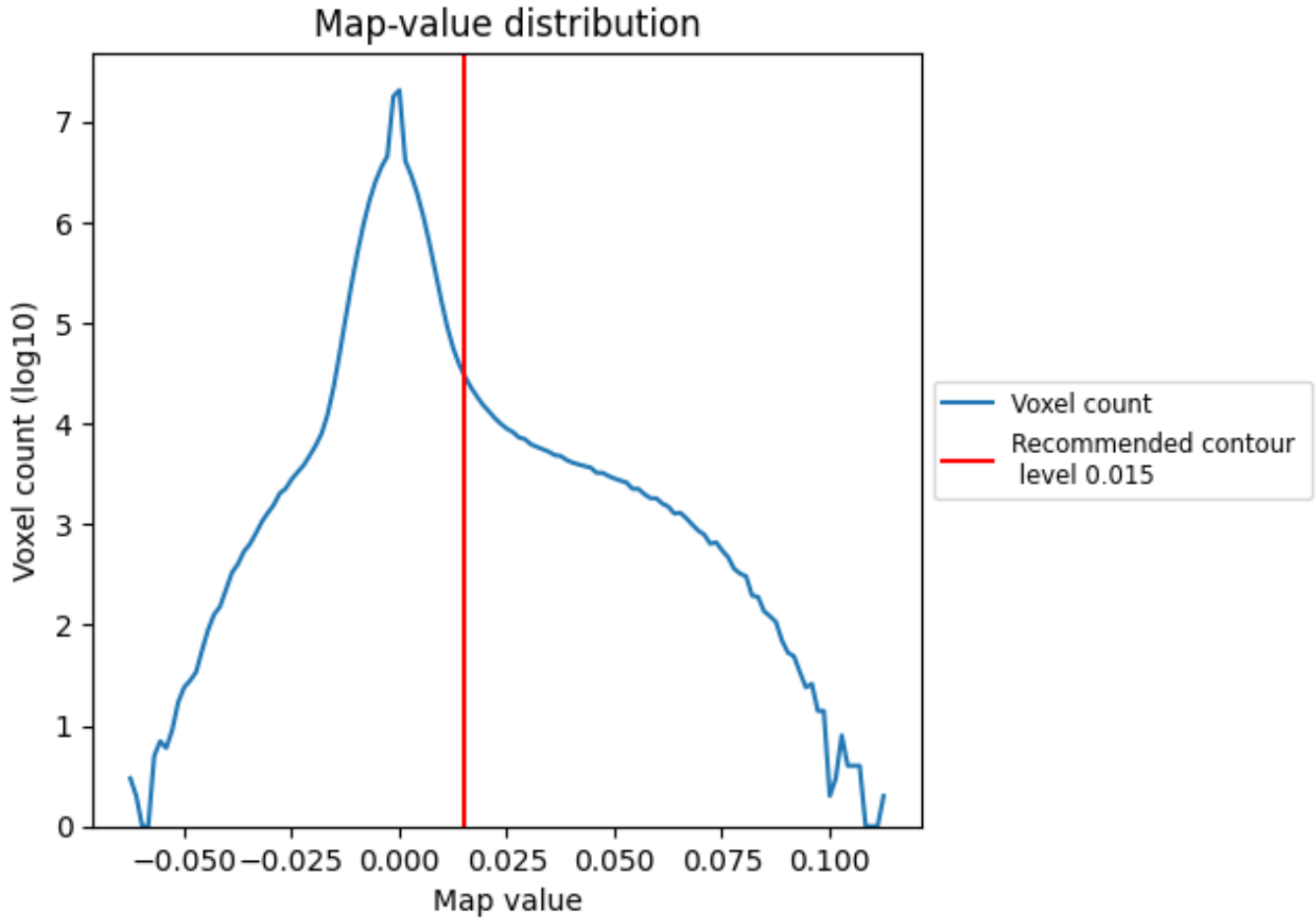


Z

7 Map analysis

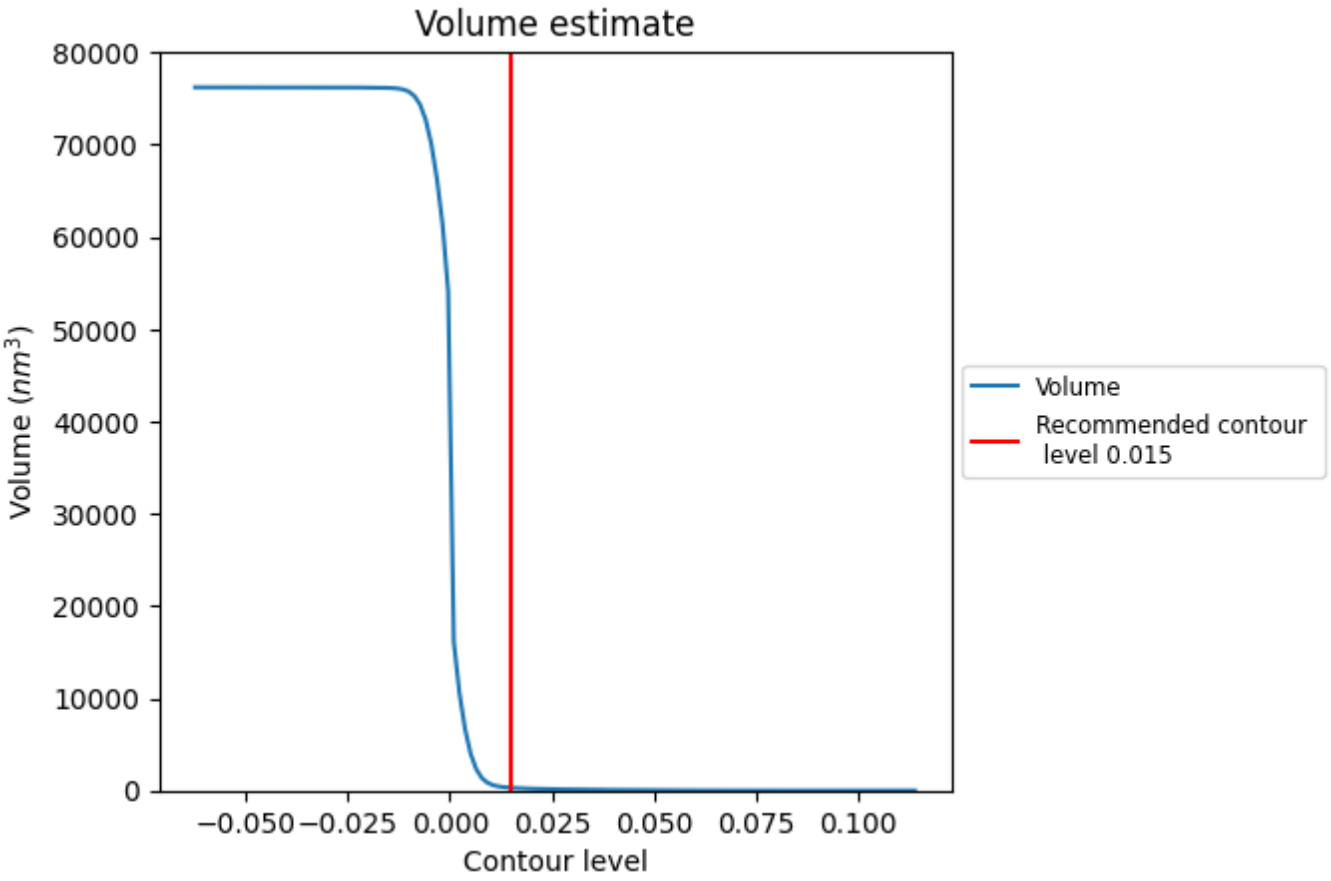
This section contains the results of statistical analysis of the map.

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.

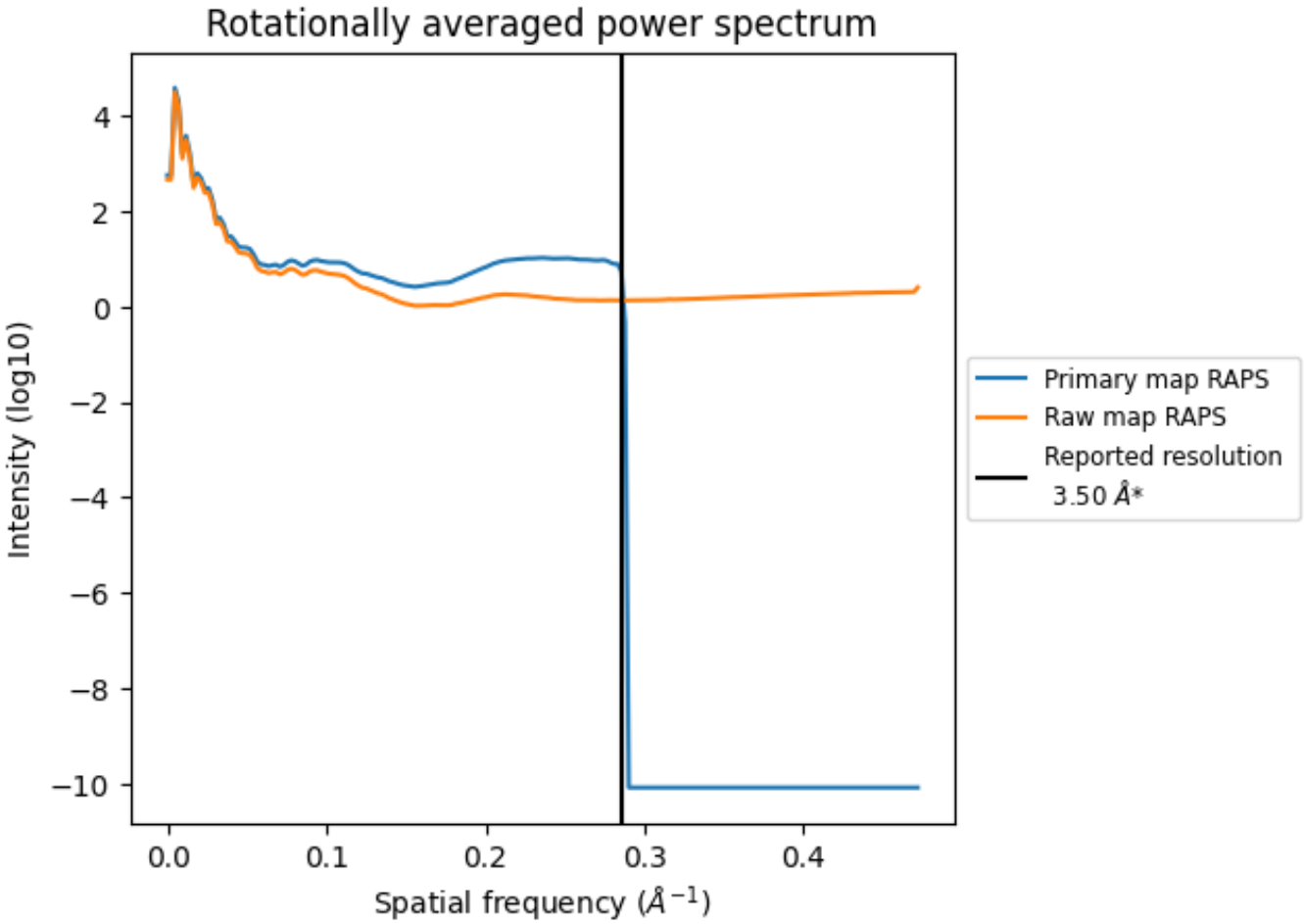
7.2 Volume estimate



The volume at the recommended contour level is 305 nm^3; this corresponds to an approximate mass of 275 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)

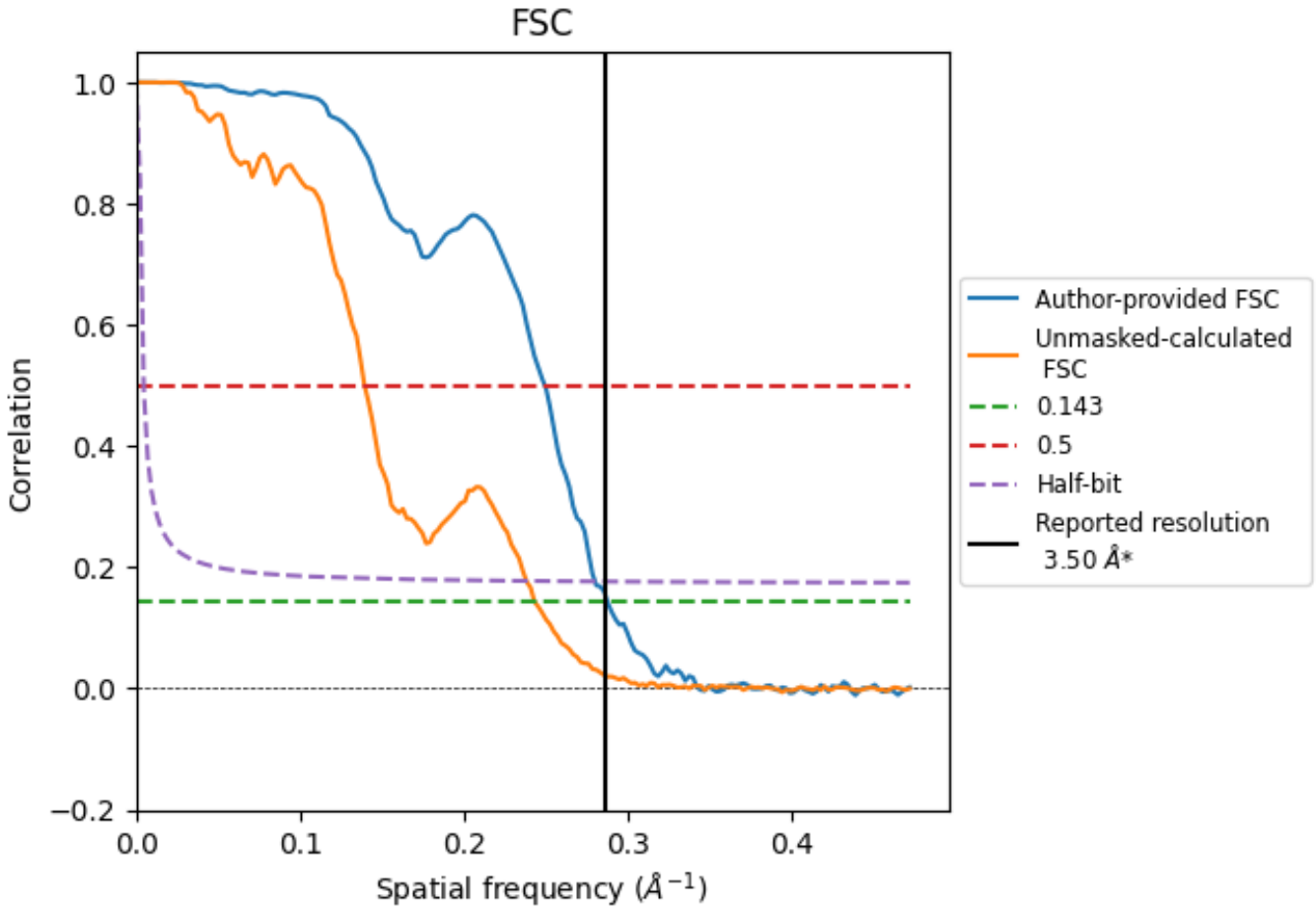


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

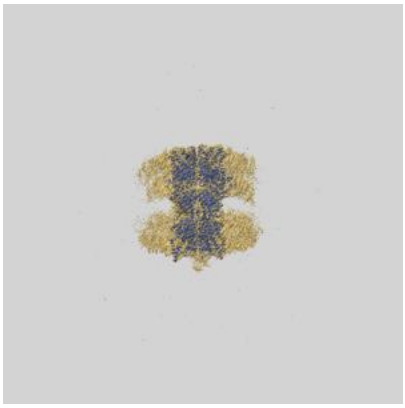
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.01	3.57
Unmasked-calculated*	4.12	7.18	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.5 by more than 10 %

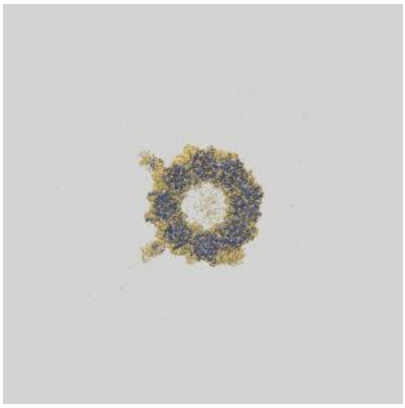
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12608 and PDB model 7NVO. Per-residue inclusion information can be found in section 3 on page 10.

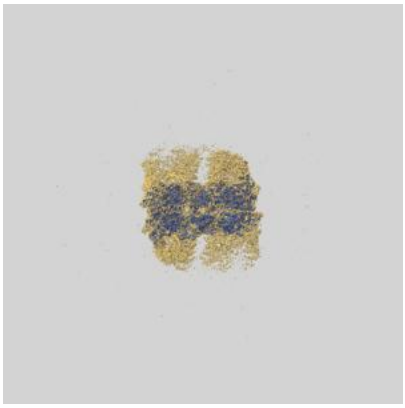
9.1 Map-model overlay



X



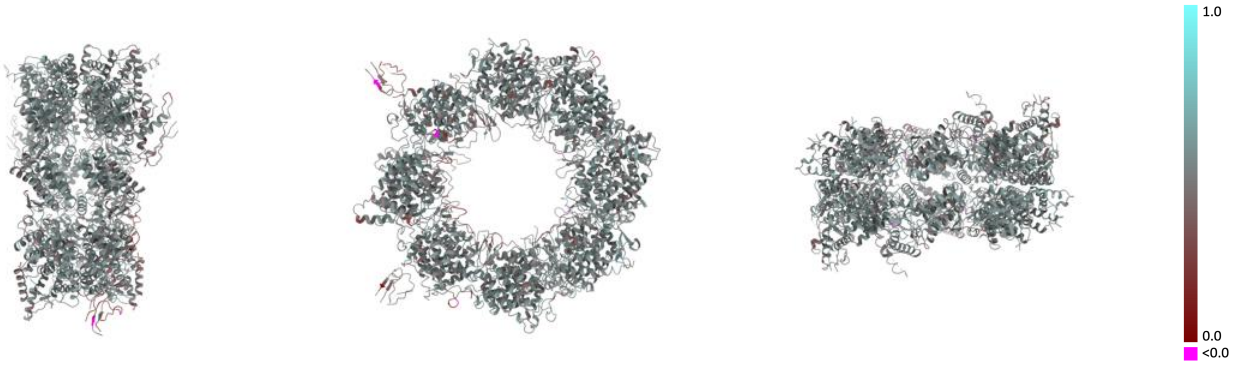
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

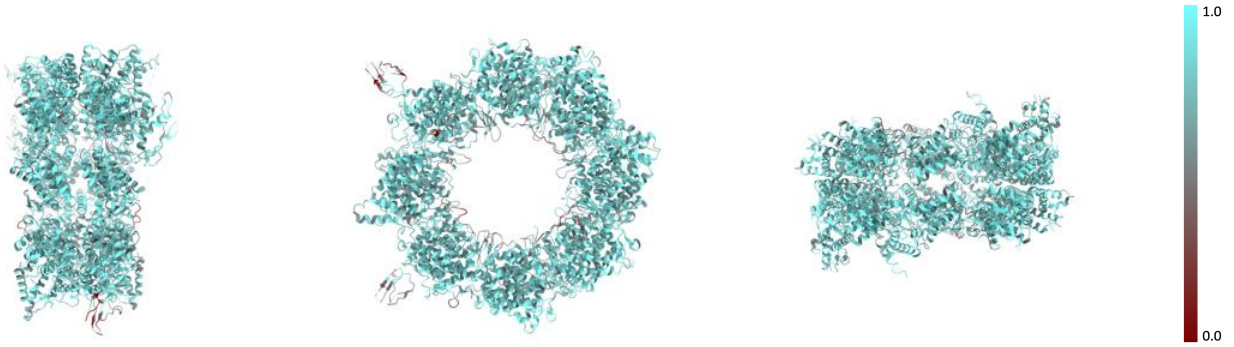
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

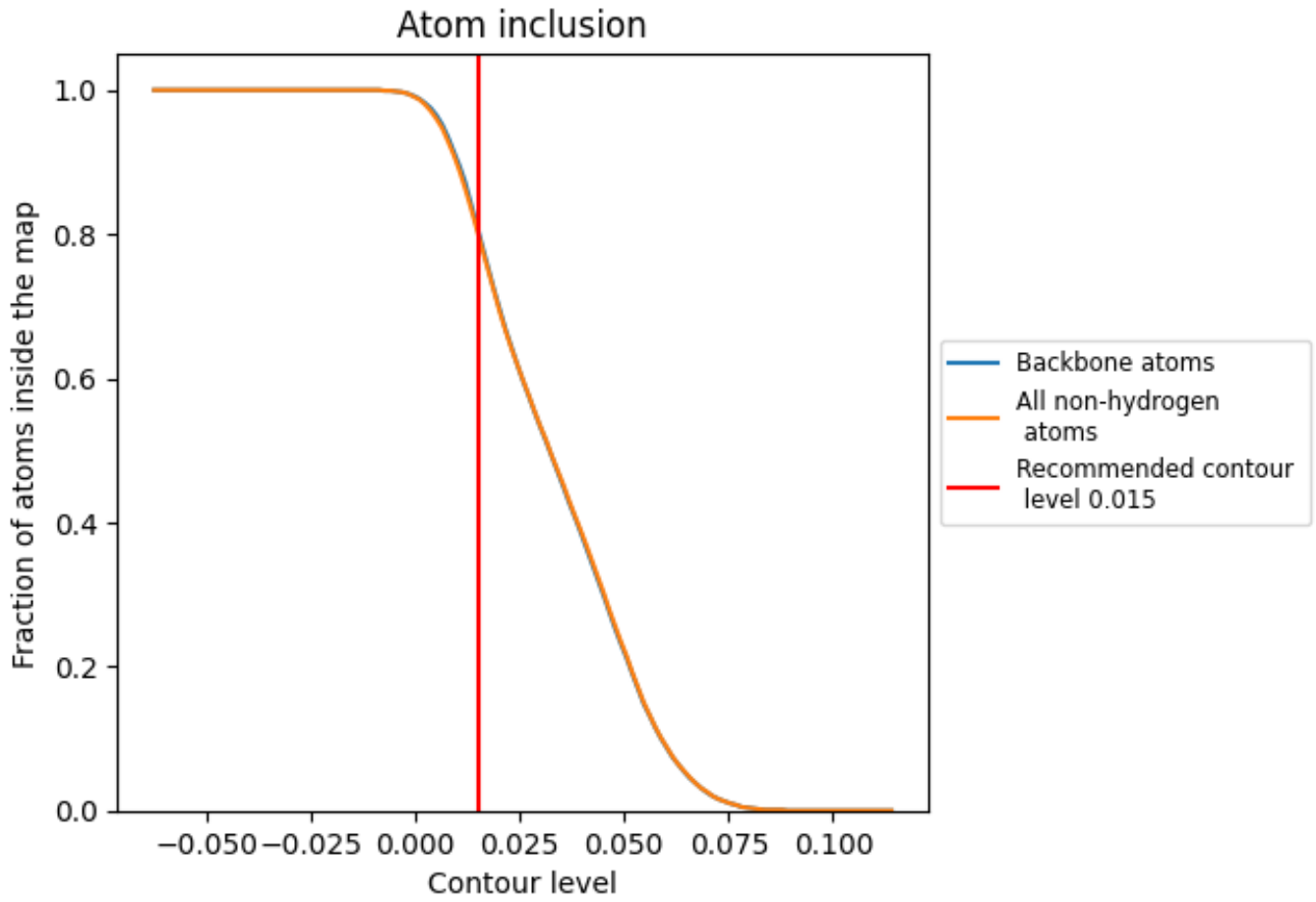
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.5020
A	0.8330	0.5190
B	0.7990	0.5090
D	0.8120	0.5100
E	0.7980	0.4960
G	0.8320	0.5230
H	0.8310	0.5140
N	0.5970	0.4150
Q	0.8380	0.5120
Z	0.8020	0.5120
a	0.8210	0.5070
b	0.7950	0.4980
d	0.7840	0.4810
e	0.7800	0.4750
g	0.8200	0.5140
h	0.8210	0.5050
n	0.4580	0.2920
q	0.8260	0.5010
z	0.7950	0.4950