Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 02:50 pm BST

PDB ID	:	8QKU / pdb_00008qku
EMDB ID	:	EMD-18471
Title	:	SWR1-nucleosome complex in configuration 1
Authors	:	Jalal, A.S.B.; Wigley, D.B.
Deposited on	:	2023-09-18
Resolution	:	3.80 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:

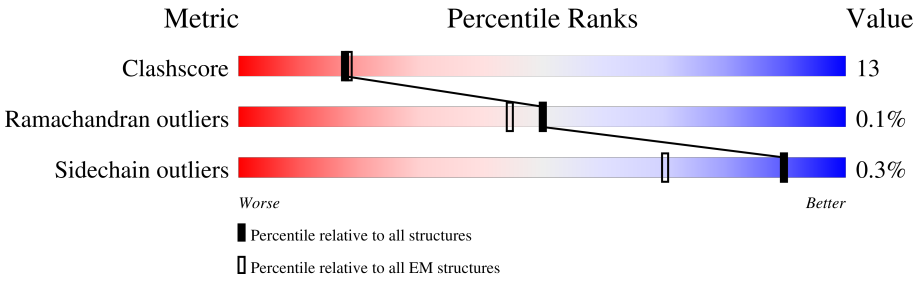
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	136	46% 25% 29%
1	B	136	46% 26% 29%
2	C	103	51% 28% 20%
2	D	103	44% 34% 22%
3	E	158	37% 28% 35%
3	F	158	38% 26% 36%
4	G	131	34% 39% 27%
4	H	131	33% 37% 31%

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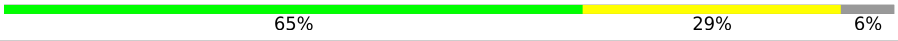
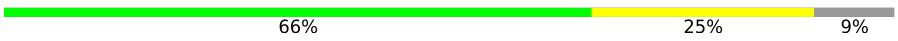
Mol	Chain	Length	Quality of chain
5	I	177	
6	J	177	
7	M	1514	
8	R	438	
9	S	280	
10	T	463	
10	V	463	
10	X	463	
11	U	471	
11	W	471	
11	Y	471	
12	Z	180	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 45395 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 Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	97	Total 796	C 506	N 152	O 138	0	0
1	B	97	Total 796	C 506	N 152	O 138	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLU	ASP	conflict	UNP P61830
B	123	GLU	ASP	conflict	UNP P61830

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	82	Total 651	C 410	N 126	O 115	0	0
2	D	80	Total 638	C 401	N 124	O 113	0	0

- Molecule 3 is a protein called Histone H2A.2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	103	Total 795	C 499	N 156	O 140	0	0
3	F	101	Total 779	C 489	N 153	O 137	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	127	GLU	-	expression tag	UNP P04912
E	128	VAL	-	expression tag	UNP P04912
E	129	CYS	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
E	130	GLN	-	expression tag	UNP P04912
E	131	ASP	-	expression tag	UNP P04912
E	132	CYS	-	expression tag	UNP P04912
E	133	GLN	-	expression tag	UNP P04912
E	134	SER	-	expression tag	UNP P04912
E	135	PHE	-	expression tag	UNP P04912
E	136	SER	-	expression tag	UNP P04912
E	137	ARG	-	expression tag	UNP P04912
E	138	THR	-	expression tag	UNP P04912
E	139	VAL	-	expression tag	UNP P04912
E	140	ARG	-	expression tag	UNP P04912
E	141	THR	-	expression tag	UNP P04912
E	142	GLU	-	expression tag	UNP P04912
E	143	LEU	-	expression tag	UNP P04912
E	144	LYS	-	expression tag	UNP P04912
E	145	ARG	-	expression tag	UNP P04912
E	146	ASN	-	expression tag	UNP P04912
E	147	LYS	-	expression tag	UNP P04912
E	148	ALA	-	expression tag	UNP P04912
E	149	ASN	-	expression tag	UNP P04912
E	150	GLN	-	expression tag	UNP P04912
E	151	THR	-	expression tag	UNP P04912
E	152	PHE	-	expression tag	UNP P04912
E	153	LEU	-	expression tag	UNP P04912
E	154	SER	-	expression tag	UNP P04912
E	155	PHE	-	expression tag	UNP P04912
E	156	GLY	-	expression tag	UNP P04912
E	157	VAL	-	expression tag	UNP P04912
F	127	GLU	-	expression tag	UNP P04912
F	128	VAL	-	expression tag	UNP P04912
F	129	CYS	-	expression tag	UNP P04912
F	130	GLN	-	expression tag	UNP P04912
F	131	ASP	-	expression tag	UNP P04912
F	132	CYS	-	expression tag	UNP P04912
F	133	GLN	-	expression tag	UNP P04912
F	134	SER	-	expression tag	UNP P04912
F	135	PHE	-	expression tag	UNP P04912
F	136	SER	-	expression tag	UNP P04912
F	137	ARG	-	expression tag	UNP P04912
F	138	THR	-	expression tag	UNP P04912
F	139	VAL	-	expression tag	UNP P04912
F	140	ARG	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
F	141	THR	-	expression tag	UNP P04912
F	142	GLU	-	expression tag	UNP P04912
F	143	LEU	-	expression tag	UNP P04912
F	144	LYS	-	expression tag	UNP P04912
F	145	ARG	-	expression tag	UNP P04912
F	146	ASN	-	expression tag	UNP P04912
F	147	LYS	-	expression tag	UNP P04912
F	148	ALA	-	expression tag	UNP P04912
F	149	ASN	-	expression tag	UNP P04912
F	150	GLN	-	expression tag	UNP P04912
F	151	THR	-	expression tag	UNP P04912
F	152	PHE	-	expression tag	UNP P04912
F	153	LEU	-	expression tag	UNP P04912
F	154	SER	-	expression tag	UNP P04912
F	155	PHE	-	expression tag	UNP P04912
F	156	GLY	-	expression tag	UNP P04912
F	157	VAL	-	expression tag	UNP P04912

- Molecule 4 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	96	Total	C	N	O	S	0	0
			741	465	129	146	1		
4	H	91	Total	C	N	O	S	0	0
			712	449	125	137	1		

- Molecule 5 is a DNA chain called DNA (177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	177	Total	C	N	O	P	0	0
			3608	1713	654	1064	177		

- Molecule 6 is a DNA chain called DNA (177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	177	Total	C	N	O	P	0	0
			3649	1726	686	1060	177		

- Molecule 7 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	688	Total	C	N	O	S	0	0
			5398	3438	960	974	26		

- Molecule 8 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	411	Total	C	N	O	S	0	0
			3335	2156	544	619	16		

- Molecule 9 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	208	Total	C	N	O	S	0	0
			1695	1071	302	312	10		

- Molecule 10 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	443	Total	C	N	O	S	0	0
			3391	2140	584	657	10		
10	V	434	Total	C	N	O	S	0	0
			3336	2107	574	645	10		
10	X	442	Total	C	N	O	S	0	0
			3397	2144	584	659	10		

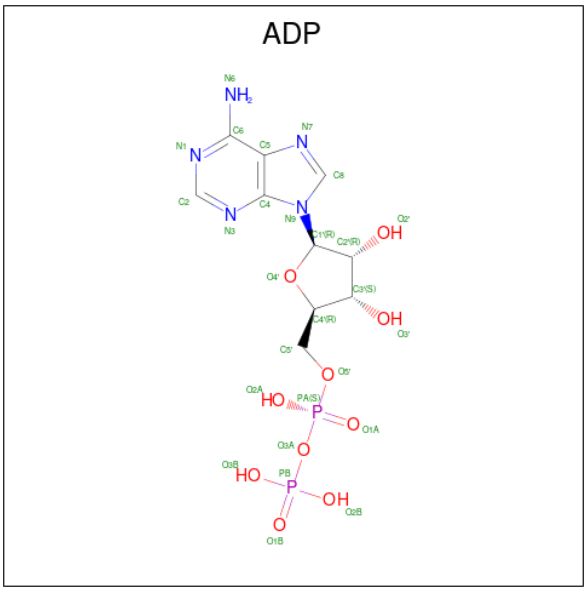
- Molecule 11 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	430	Total	C	N	O	S	0	0
			3299	2063	570	655	11		
11	W	433	Total	C	N	O	S	0	0
			3325	2085	572	657	11		
11	Y	447	Total	C	N	O	S	0	0
			3410	2133	590	675	12		

- Molecule 12 is a protein called Vacuolar protein sorting-associated protein 72.

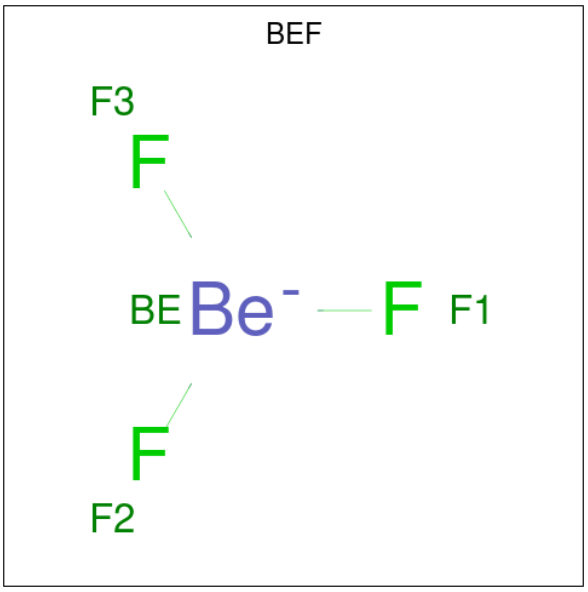
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	180	Total	C	N	O	S	0	0
			1410	885	255	266	4		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total Be F 4 1 3	0
14	R	1	Total Be F 4 1 3	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
15	M	1	Total Mg 1 1	0
15	R	1	Total Mg 1 1	0
15	U	2	Total Mg 2 2	0
15	V	1	Total Mg 1 1	0
15	W	1	Total Mg 1 1	0
15	X	1	Total Mg 1 1	0
15	Y	1	Total Mg 1 1	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

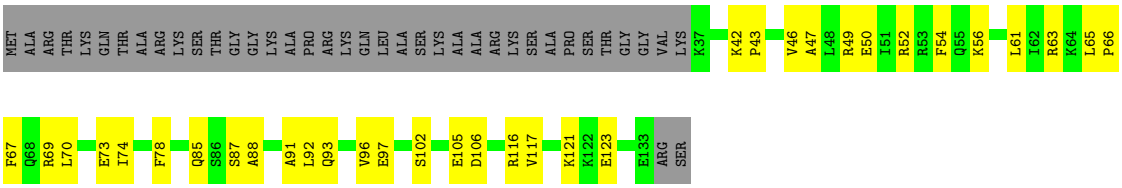
Mol	Chain	Residues	Atoms		AltConf
16	S	2	Total	Zn	0
			2	2	

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.

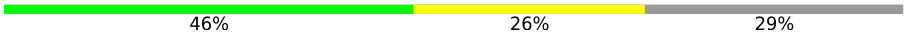
• Molecule 1: Histone H3

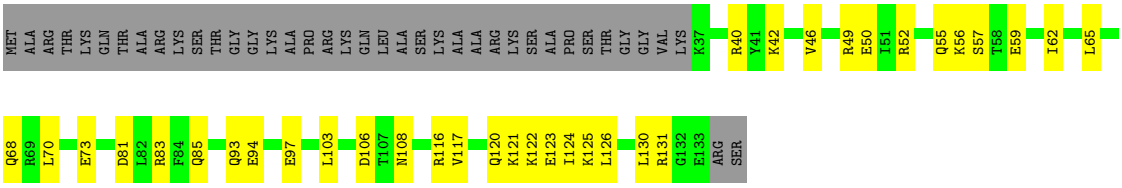
Chain A:



• Molecule 1: Histone H3

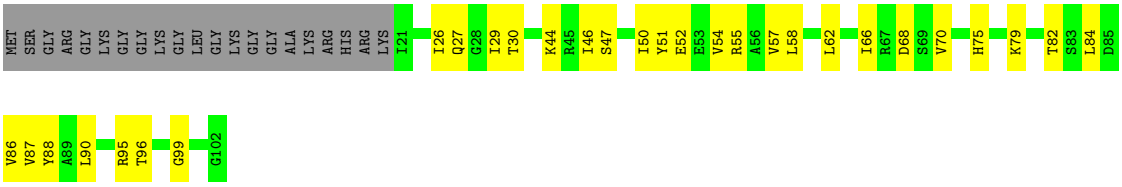
Chain B:





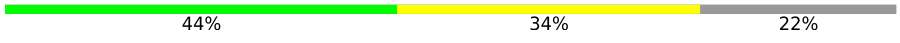
• Molecule 2: Histone H4

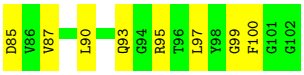
Chain C:



• Molecule 2: Histone H4

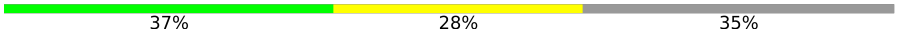
Chain D:

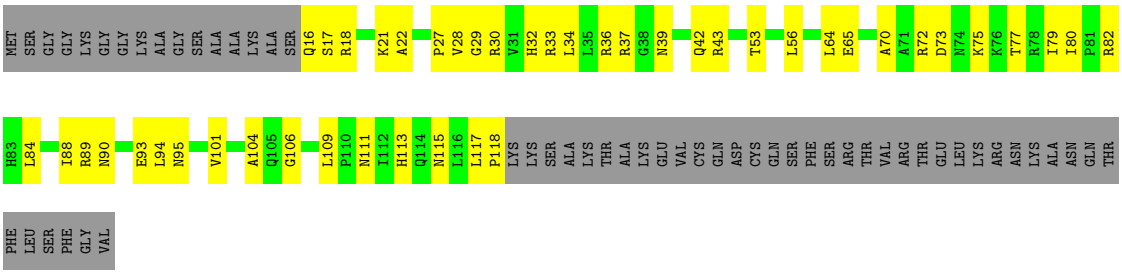




• Molecule 3: Histone H2A.2

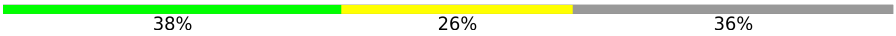
Chain E:

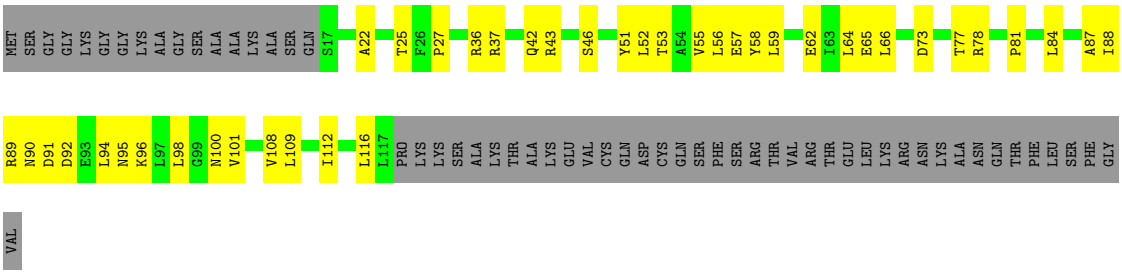




• Molecule 3: Histone H2A.2

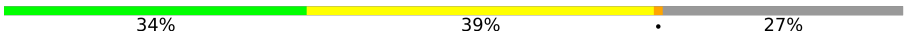
Chain F:

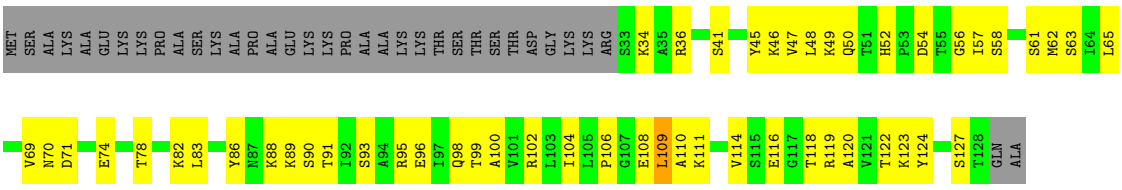




• Molecule 4: Histone H2B.1

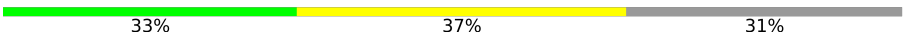
Chain G:

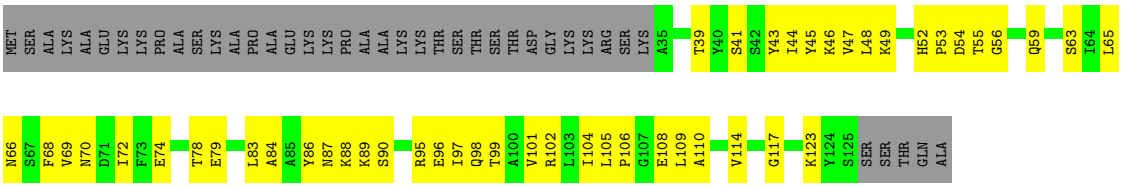




• Molecule 4: Histone H2B.1

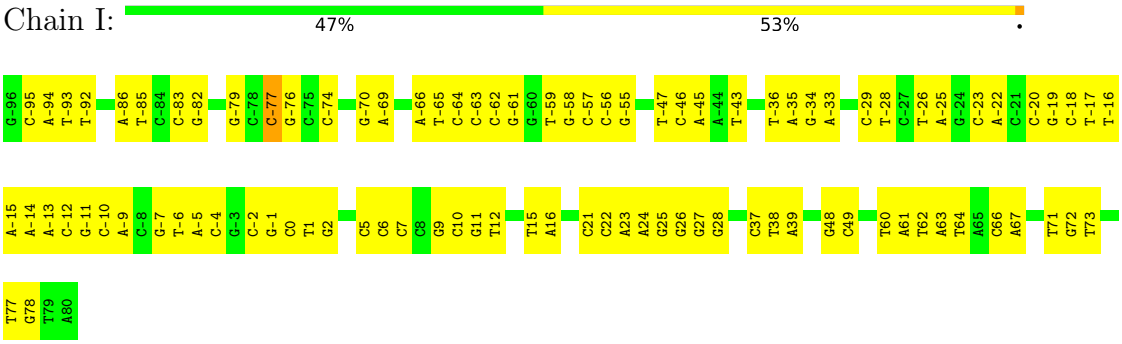
Chain H:





• Molecule 5: DNA (177-MER)

Chain I:

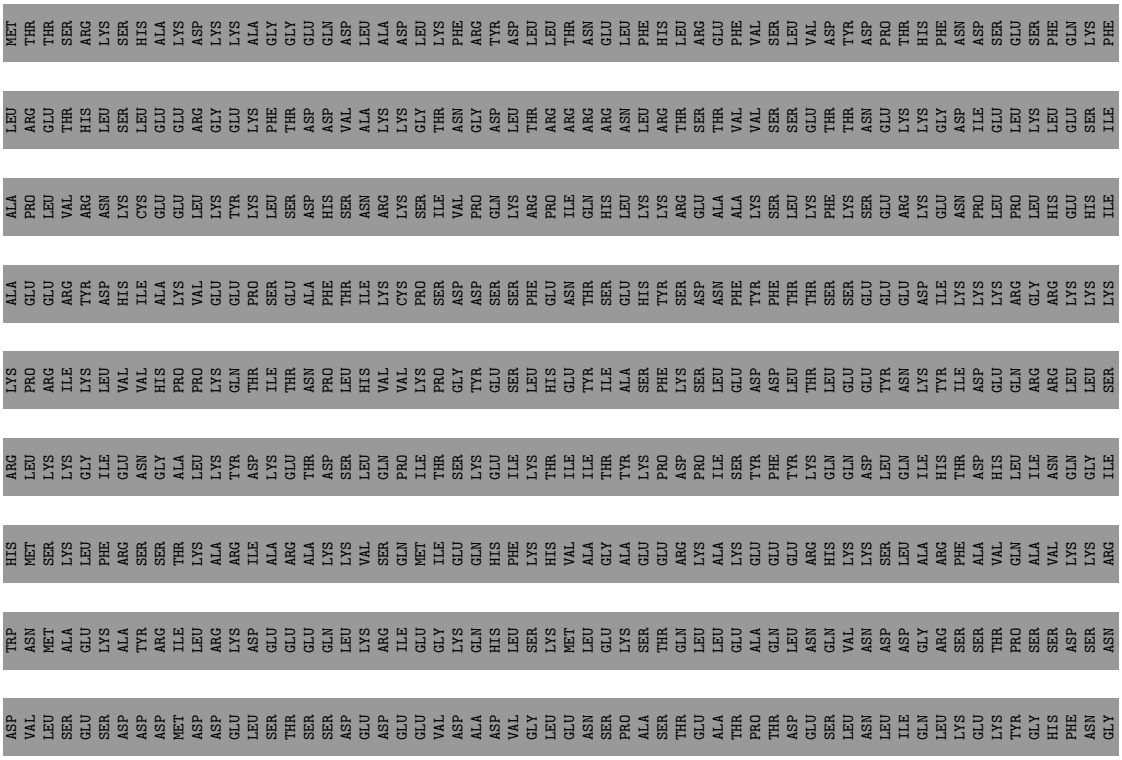


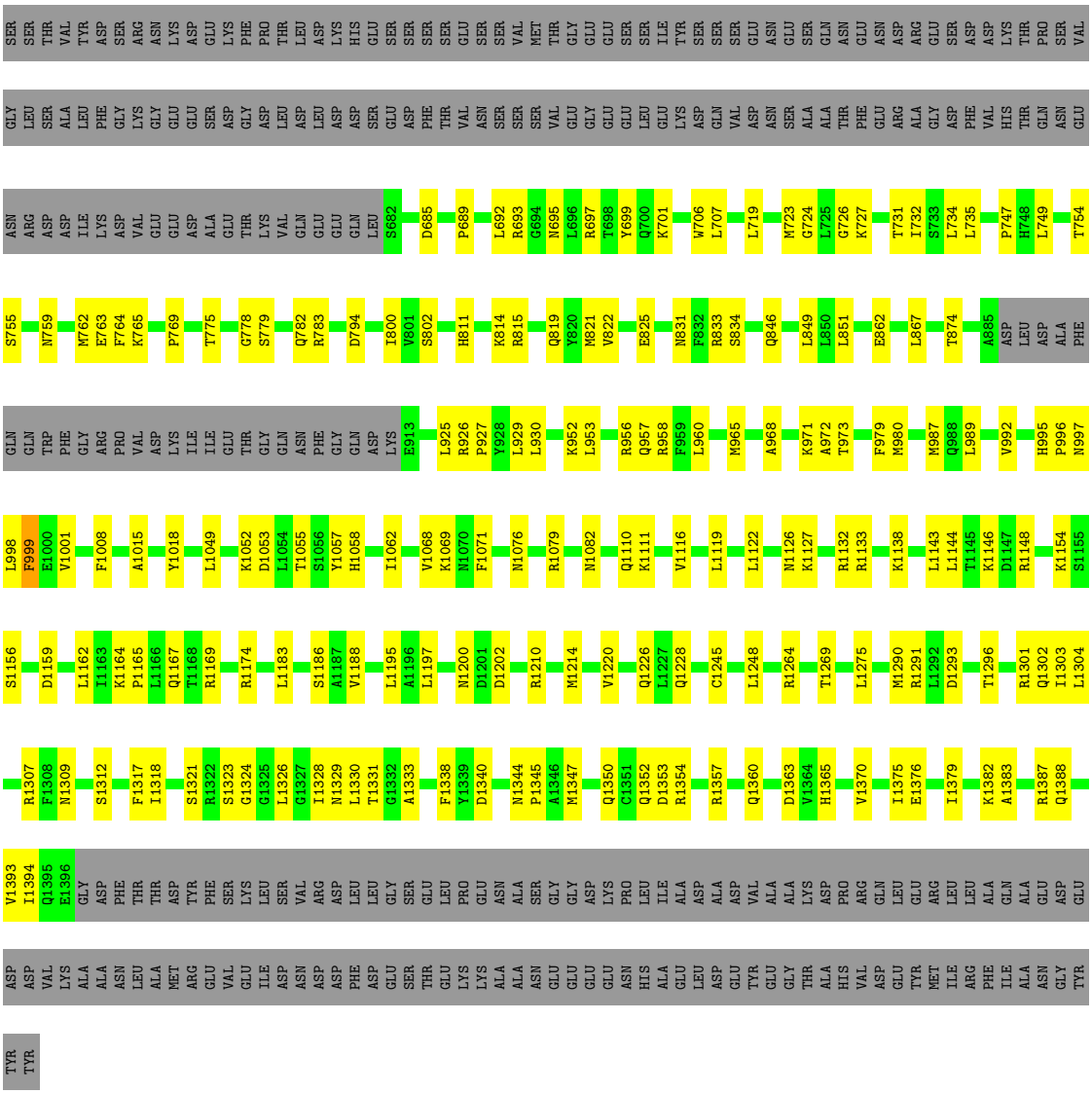
• Molecule 6: DNA (177-MER)

Chain J:

• Molecule 7: Helicase SWR1

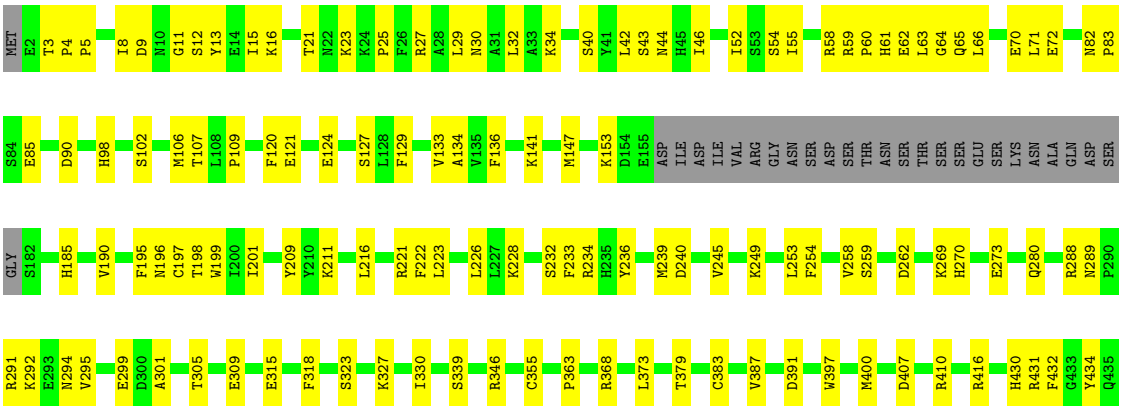
Chain M:





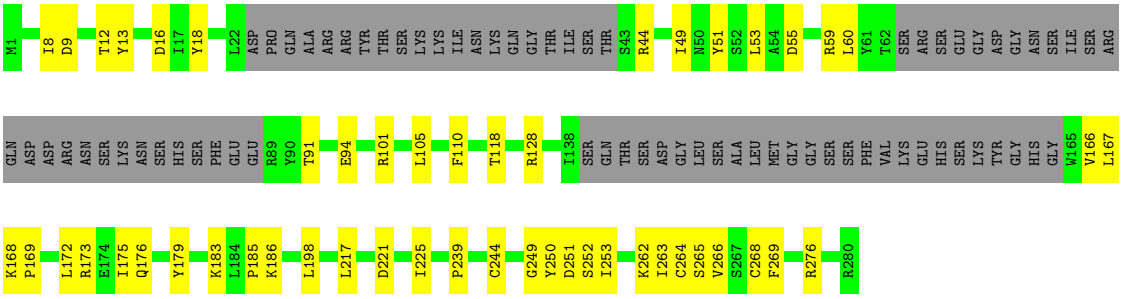
• Molecule 8: Actin-like protein ARP6

Chain R:



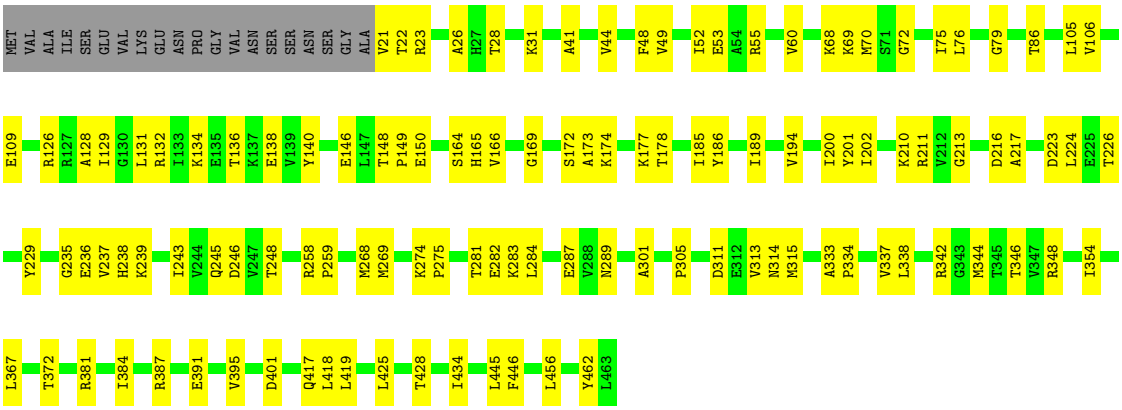
• Molecule 9: Vacuolar protein sorting-associated protein 71

Chain S:



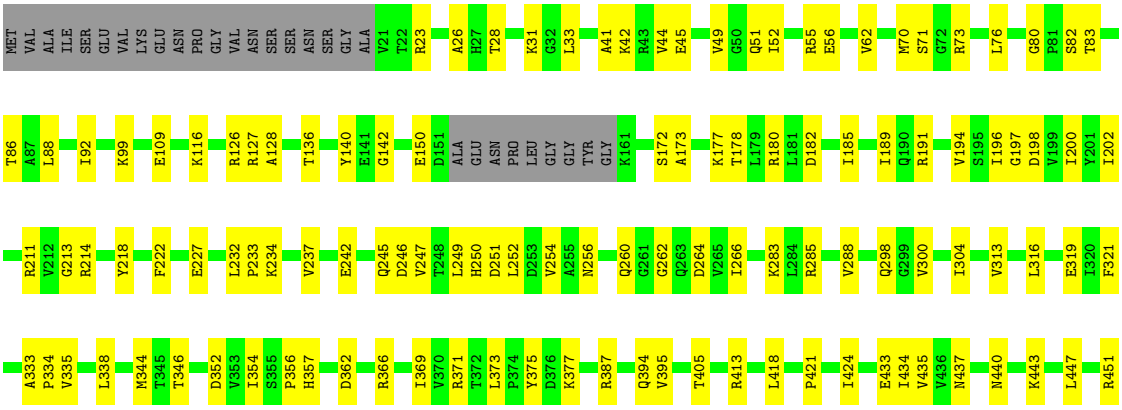
• Molecule 10: RuvB-like protein 1

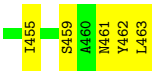
Chain T:



• Molecule 10: RuvB-like protein 1

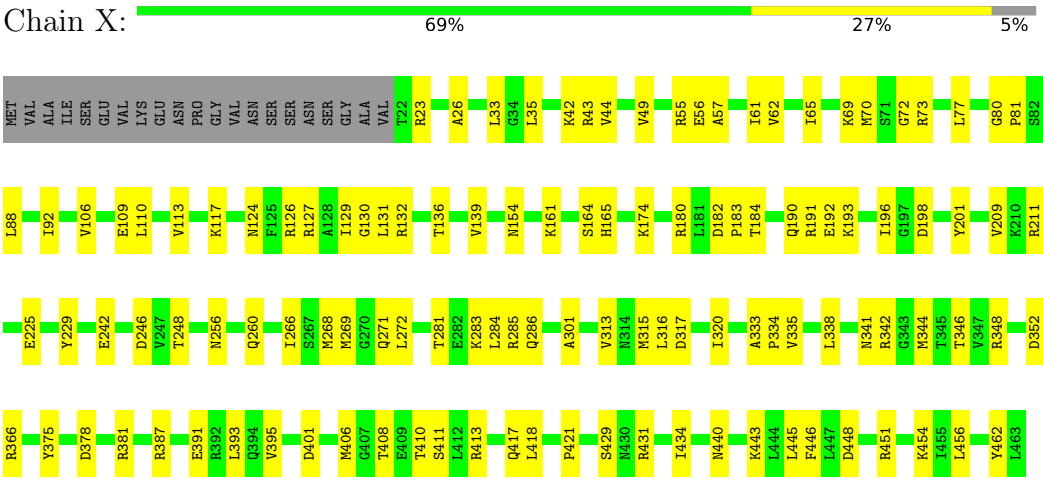
Chain V:





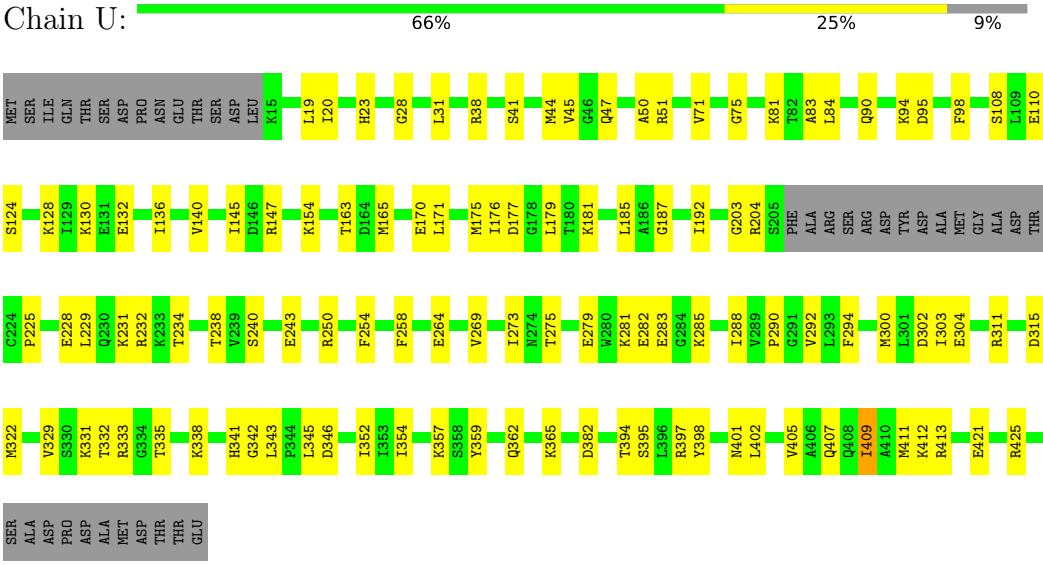
• Molecule 10: RuvB-like protein 1

Chain X:



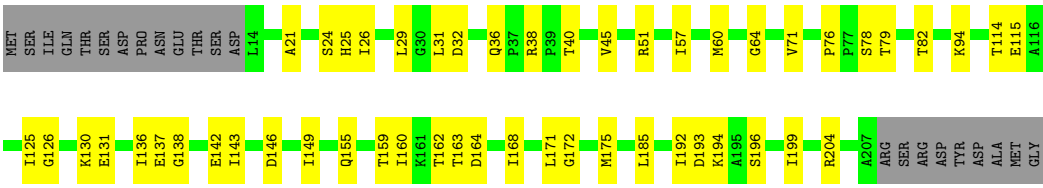
• Molecule 11: RuvB-like protein 2

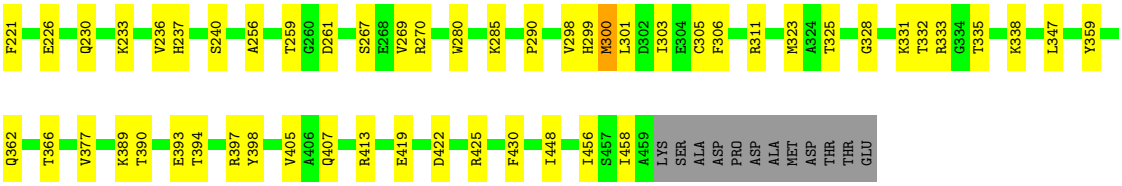
Chain U:



• Molecule 11: RuvB-like protein 2

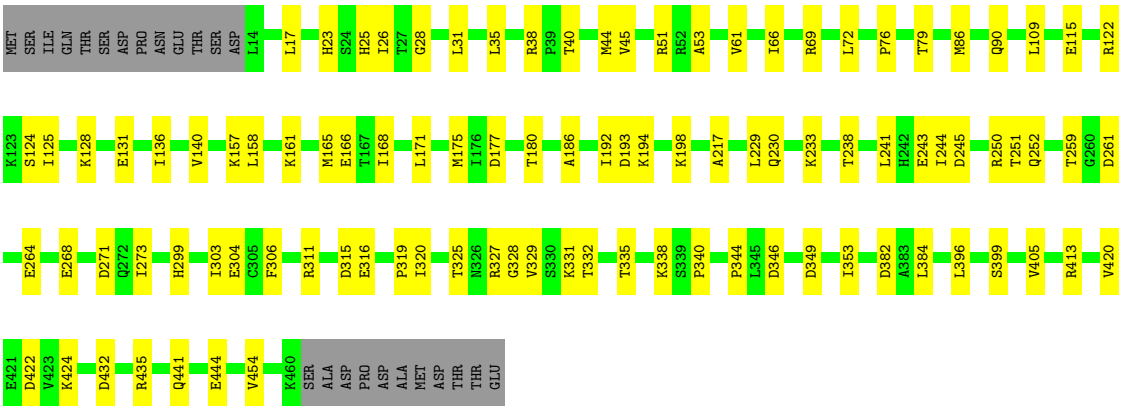
Chain W:





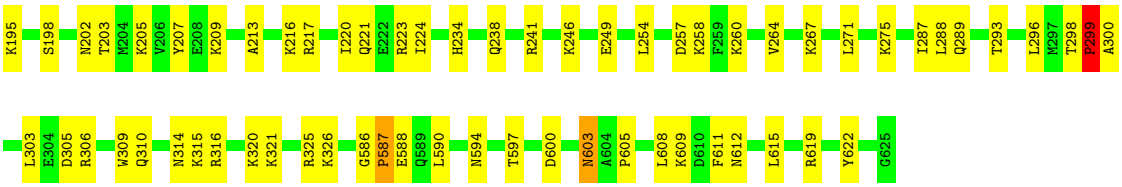
• Molecule 11: RuvB-like protein 2

Chain Y:



• Molecule 12: Vacuolar protein sorting-associated protein 72

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123591	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00197	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.16	0/807	0.44	0/1081
1	B	0.17	0/807	0.52	0/1081
2	C	0.14	0/658	0.43	0/880
2	D	0.16	0/645	0.44	0/862
3	E	0.13	0/806	0.33	0/1091
3	F	0.11	0/789	0.33	0/1067
4	G	0.18	0/750	0.51	0/1009
4	H	0.18	0/722	0.51	0/972
5	I	0.16	0/4042	0.39	2/6231 (0.0%)
6	J	0.17	0/4098	0.37	2/6328 (0.0%)
7	M	0.11	0/5495	0.30	0/7442
8	R	0.09	0/3429	0.23	0/4650
9	S	0.10	0/1722	0.28	0/2320
10	T	0.11	0/3433	0.26	0/4646
10	V	0.10	0/3375	0.25	0/4565
10	X	0.11	0/3439	0.28	0/4652
11	U	0.10	0/3333	0.26	0/4492
11	W	0.10	0/3361	0.24	0/4530
11	Y	0.10	0/3447	0.25	0/4649
12	Z	0.15	0/1431	0.52	4/1923 (0.2%)
All	All	0.12	0/46589	0.33	8/64471 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	-77	DC	OP1-P-O3'	-8.90	81.31	108.00
6	J	-77	DA	OP2-P-O3'	-8.39	82.84	108.00
6	J	-77	DA	OP1-P-O3'	-8.21	83.36	108.00
5	I	-77	DC	OP2-P-O3'	-7.75	84.75	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	587	PRO	CA-C-N	6.86	134.05	121.70
12	Z	587	PRO	C-N-CA	6.86	134.05	121.70
12	Z	299	PRO	CA-C-N	6.21	132.87	121.70
12	Z	299	PRO	C-N-CA	6.21	132.87	121.70

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	A	796	0	841	35	0
1	B	796	0	841	33	0
2	C	651	0	690	25	0
2	D	638	0	677	37	0
3	E	795	0	834	44	0
3	F	779	0	819	37	0
4	G	741	0	766	52	0
4	H	712	0	736	42	0
5	I	3608	0	1987	82	0
6	J	3649	0	1985	97	0
7	M	5398	0	5351	146	0
8	R	3335	0	3256	97	0
9	S	1695	0	1745	56	0
10	T	3391	0	3513	86	0
10	V	3336	0	3474	92	0
10	X	3397	0	3532	100	0
11	U	3299	0	3387	95	0
11	W	3325	0	3412	81	0
11	Y	3410	0	3465	67	0
12	Z	1410	0	1362	59	0
13	M	27	0	12	6	0
13	R	27	0	12	0	0
13	T	27	0	12	1	0
13	U	27	0	12	3	0
13	V	27	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	W	27	0	12	4	0
13	X	27	0	12	3	0
13	Y	27	0	12	1	0
14	M	4	0	0	1	0
14	R	4	0	0	0	0
15	M	1	0	0	0	0
15	R	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
16	S	2	0	0	0	0
All	All	45395	0	42769	1165	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 (1165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:O	1:A:78:PHE:HB2	1.62	0.98
11:Y:171:LEU:HD12	11:Y:175:MET:HG2	1.54	0.89
6:J:65:DA:H4'	12:Z:223:ARG:HH22	1.43	0.82
5:I:48:DG:N2	6:J:-48:DC:O2	2.12	0.82
5:I:48:DG:N1	6:J:-48:DC:N3	2.26	0.82
7:M:1345:PRO:HD2	7:M:1347:MET:HE1	1.62	0.81
5:I:-74:DC:O2	6:J:74:DG:N2	2.12	0.79
10:X:313:VAL:HG21	10:X:338:LEU:HB3	1.65	0.79
12:Z:603:ASN:O	12:Z:603:ASN:ND2	2.14	0.79
5:I:-74:DC:N3	6:J:74:DG:N1	2.28	0.79
5:I:-7:DG:N2	6:J:7:DC:O2	2.12	0.79
4:G:47:VAL:O	4:G:50:GLN:NE2	2.17	0.78
3:F:89:ARG:HA	3:F:95:ASN:HD21	1.48	0.78
1:B:122:LYS:HA	1:B:125:LYS:HG2	1.67	0.77
5:I:-46:DC:N3	6:J:46:DG:N1	2.29	0.75
10:V:313:VAL:HG21	10:V:338:LEU:HB3	1.67	0.75
10:X:183:PRO:HB2	12:Z:594:ASN:HD21	1.51	0.74
4:G:120:ALA:HA	4:G:123:LYS:HE3	1.70	0.73
10:T:68:LYS:HD2	10:T:305:PRO:HD2	1.70	0.73
5:I:-46:DC:O2	6:J:46:DG:N2	2.13	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:82:SER:HA	13:V:501:ADP:H5'1	1.70	0.73
1:B:117:VAL:HG21	2:C:44:LYS:HE2	1.69	0.73
5:I:-7:DG:N1	6:J:7:DC:N3	2.27	0.73
1:A:121:LYS:HZ3	2:D:50:ILE:HA	1.52	0.72
6:J:-46:DT:H2'	6:J:-45:DG:C8	2.25	0.72
2:D:33:ALA:HA	2:D:36:ARG:HE	1.54	0.72
10:T:76:LEU:HB3	10:T:367:LEU:HD13	1.71	0.72
7:M:1068:VAL:HG13	7:M:1069:LYS:HG3	1.70	0.71
7:M:1264:ARG:HB2	7:M:1333:ALA:HA	1.72	0.71
3:F:96:LYS:HD2	4:H:106:PRO:HG3	1.72	0.71
3:E:79:ILE:HD11	4:G:57:ILE:HG23	1.73	0.70
7:M:1144:LEU:O	7:M:1148:ARG:NH1	2.24	0.70
11:Y:28:GLY:H	11:Y:90:GLN:HB3	1.55	0.70
10:X:49:VAL:H	13:X:501:ADP:HN62	1.37	0.70
3:E:42:GLN:HE22	4:G:90:SER:HB3	1.55	0.70
10:V:42:LYS:O	10:V:55:ARG:NH2	2.25	0.70
12:Z:316:ARG:HH22	12:Z:320:LYS:HB3	1.56	0.70
10:T:44:VAL:HG22	10:T:49:VAL:HG12	1.74	0.69
3:E:64:LEU:HD22	4:G:48:LEU:HD21	1.74	0.69
2:C:29:ILE:H	2:C:29:ILE:HD12	1.57	0.69
4:G:34:LYS:NZ	6:J:50:DG:OP1	2.25	0.69
12:Z:605:PRO:HG2	12:Z:608:LEU:HB3	1.75	0.69
7:M:695:ASN:O	13:M:1601:ADP:N6	2.26	0.69
3:F:66:LEU:HB3	3:F:87:ALA:HB1	1.75	0.68
10:X:346:THR:HG22	10:X:354:ILE:HG12	1.74	0.68
2:C:84:LEU:HB2	2:C:88:TYR:HE2	1.59	0.68
11:Y:157:LYS:HB3	11:Y:168:ILE:HD11	1.75	0.67
10:X:42:LYS:O	10:X:55:ARG:NH2	2.27	0.67
4:G:118:THR:O	4:G:122:THR:HG23	1.94	0.67
5:I:-77:DC:N3	6:J:78:DG:N2	2.41	0.67
10:T:23:ARG:HH22	11:U:290:PRO:HB3	1.60	0.67
12:Z:303:LEU:HA	12:Z:306:ARG:HG2	1.76	0.67
1:A:92:LEU:O	1:A:96:VAL:HG23	1.94	0.67
7:M:995:HIS:ND1	7:M:1245:CYS:SG	2.67	0.67
5:I:-62:DC:H5'	12:Z:217:ARG:HB3	1.77	0.67
10:T:314:ASN:HD22	10:T:342:ARG:HG3	1.60	0.67
10:V:413:ARG:NH2	13:V:501:ADP:O1B	2.28	0.67
4:H:101:VAL:HG23	4:H:105:LEU:HD23	1.77	0.66
11:Y:432:ASP:H	11:Y:435:ARG:HD3	1.60	0.66
10:T:417:GLN:HB3	11:U:352:ILE:HD11	1.76	0.66
11:W:29:LEU:HB3	11:W:31:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:612:ASN:HA	12:Z:615:LEU:HG	1.77	0.66
2:D:33:ALA:O	2:D:37:LEU:HD12	1.96	0.66
3:E:43:ARG:HD2	6:J:38:DG:H4'	1.78	0.65
3:E:22:ALA:O	4:G:123:LYS:NZ	2.21	0.65
7:M:1154:LYS:HZ2	7:M:1156:SER:H	1.42	0.65
11:U:413:ARG:NH1	11:U:421:GLU:OE1	2.30	0.65
3:F:25:THR:HG21	4:H:47:VAL:HG23	1.78	0.65
8:R:397:TRP:HA	8:R:400:MET:HE2	1.79	0.65
2:D:70:VAL:O	2:D:74:GLU:HG2	1.97	0.65
10:V:44:VAL:HG22	10:V:49:VAL:HG12	1.79	0.65
10:X:44:VAL:HG22	10:X:49:VAL:HG12	1.78	0.65
2:C:96:THR:HG23	3:E:101:VAL:HG23	1.79	0.65
10:V:41:ALA:HB3	10:V:52:ILE:HG23	1.78	0.64
5:I:-20:DC:H2'	5:I:-19:DG:C8	2.32	0.64
5:I:-16:DT:H2"	5:I:-15:DA:H5'	1.78	0.64
11:Y:311:ARG:O	11:Y:311:ARG:NH1	2.31	0.64
7:M:965:MET:HA	7:M:965:MET:HE3	1.78	0.64
8:R:120:PHE:O	8:R:416:ARG:NH2	2.30	0.64
10:X:23:ARG:NH2	11:Y:316:GLU:O	2.30	0.64
4:H:39:THR:OG1	4:H:66:ASN:ND2	2.29	0.64
8:R:289:ASN:H	8:R:292:LYS:HE3	1.61	0.64
8:R:269:LYS:O	8:R:291:ARG:NH2	2.30	0.64
4:H:79:GLU:HG2	4:H:104:ILE:HD11	1.80	0.64
11:W:397:ARG:NH2	13:W:501:ADP:O1B	2.31	0.64
7:M:968:ALA:O	7:M:973:THR:N	2.31	0.64
1:B:46:VAL:O	1:B:50:GLU:HG3	1.97	0.64
6:J:52:DC:H2"	6:J:53:DC:C5	2.34	0.63
8:R:109:PRO:HD2	9:S:217:LEU:HD11	1.79	0.63
1:A:61:LEU:HD13	2:D:36:ARG:HB3	1.80	0.63
10:T:315:MET:HE3	10:T:315:MET:HA	1.80	0.63
10:V:126:ARG:HH12	10:V:285:ARG:HB3	1.62	0.63
10:V:377:LYS:HZ1	10:V:405:THR:HA	1.62	0.63
11:W:389:LYS:NZ	11:W:393:GLU:OE2	2.32	0.63
11:W:76:PRO:O	11:W:79:THR:OG1	2.15	0.63
10:T:174:LYS:HB2	10:T:236:GLU:HA	1.81	0.63
10:V:463:LEU:HG	11:W:76:PRO:HD3	1.81	0.63
4:G:116:GLU:HG2	4:G:119:ARG:HH21	1.64	0.63
1:B:65:LEU:HA	1:B:68:GLN:HG3	1.81	0.63
10:X:193:LYS:O	10:X:211:ARG:NH1	2.32	0.63
8:R:11:GLY:H	8:R:15:ILE:HD13	1.63	0.62
8:R:258:VAL:O	8:R:368:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:136:ILE:HB	11:Y:192:ILE:HG22	1.81	0.62
5:I:0:DC:H2'	5:I:1:DT:H71	1.81	0.62
2:D:99:GLY:O	4:H:63:SER:OG	2.16	0.62
7:M:1220:VAL:O	10:V:191:ARG:NH2	2.31	0.62
8:R:407:ASP:OD1	8:R:410:ARG:NH1	2.32	0.62
10:T:236:GLU:OE2	10:T:236:GLU:N	2.24	0.62
1:B:120:GLN:HG2	1:B:121:LYS:H	1.64	0.62
6:J:3:DC:H2"	6:J:4:DG:C8	2.35	0.62
8:R:315:GLU:OE2	8:R:368:ARG:NH2	2.33	0.62
9:S:16:ASP:HA	11:U:147:ARG:HE	1.63	0.62
11:U:175:MET:SD	11:U:175:MET:N	2.71	0.62
10:X:43:ARG:HG3	10:X:44:VAL:HG23	1.82	0.62
10:T:41:ALA:HB3	10:T:52:ILE:HG23	1.82	0.62
8:R:196:ASN:OD1	8:R:221:ARG:NH2	2.33	0.62
1:B:116:ARG:HH22	1:B:122:LYS:HZ1	1.46	0.62
10:X:406:MET:HE1	10:X:443:LYS:HB2	1.82	0.62
2:C:27:GLN:OE1	2:C:27:GLN:N	2.32	0.62
10:X:395:VAL:HG12	10:X:434:ILE:HD13	1.81	0.62
5:I:-79:DG:H22	6:J:79:DC:H2"	1.63	0.61
8:R:228:LYS:HD2	8:R:239:MET:HA	1.82	0.61
10:X:117:LYS:HD2	10:X:320:ILE:HD11	1.82	0.61
10:X:126:ARG:HD2	10:X:285:ARG:HD3	1.82	0.61
1:A:121:LYS:NZ	2:D:53:GLU:OE1	2.34	0.61
2:C:66:ILE:O	2:C:70:VAL:HG12	2.01	0.61
6:J:71:DC:H2'	6:J:72:DA:C8	2.35	0.61
11:Y:38:ARG:O	11:Y:51:ARG:NH2	2.30	0.61
1:A:88:ALA:H	2:D:100:PHE:HZ	1.46	0.61
8:R:289:ASN:OD1	8:R:291:ARG:NH1	2.33	0.61
6:J:-24:DT:H2"	6:J:-23:DT:H5'	1.82	0.61
10:V:28:THR:O	10:V:31:LYS:NZ	2.31	0.61
3:F:42:GLN:NE2	4:H:90:SER:O	2.32	0.61
10:T:236:GLU:HG2	10:T:237:VAL:H	1.66	0.61
11:U:154:LYS:NZ	11:U:177:ASP:OD1	2.33	0.61
11:W:40:THR:HG22	11:W:45:VAL:HG22	1.80	0.61
10:X:268:MET:HE3	10:X:268:MET:H	1.66	0.61
2:C:52:GLU:OE1	2:C:52:GLU:N	2.24	0.61
4:H:43:TYR:HA	4:H:46:LYS:NZ	2.15	0.61
2:C:47:SER:HB3	2:C:50:ILE:HG12	1.81	0.60
7:M:727:LYS:NZ	13:M:1601:ADP:O3B	2.34	0.60
7:M:1350:GLN:OE1	7:M:1354:ARG:NH1	2.33	0.60
10:T:26:ALA:H	10:T:387:ARG:HH22	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:75:GLY:O	11:U:81:LYS:NZ	2.34	0.60
7:M:1331:THR:O	7:M:1360:GLN:NE2	2.34	0.60
10:X:161:LYS:NZ	12:Z:600:ASP:O	2.34	0.60
5:I:-58:DG:O4'	7:M:815:ARG:NH1	2.34	0.60
7:M:1328:ILE:O	7:M:1354:ARG:NE	2.27	0.60
3:E:72:ARG:HH12	4:G:52:HIS:CE1	2.20	0.60
4:H:95:ARG:NH1	4:H:96:GLU:OE2	2.33	0.60
11:U:397:ARG:O	11:U:401:ASN:ND2	2.35	0.60
8:R:58:ARG:HB3	9:S:166:VAL:HG13	1.83	0.60
6:J:63:DG:H2"	6:J:64:DG:H5"	1.84	0.60
7:M:1303:ILE:HG23	12:Z:267:LYS:HD3	1.82	0.60
3:E:17:SER:HA	5:I:-43:DT:H5"	1.83	0.60
5:I:-59:DT:H1'	7:M:815:ARG:HH11	1.67	0.60
5:I:22:DC:H2'	7:M:833:ARG:HH22	1.65	0.60
7:M:1188:VAL:HG23	10:V:260:GLN:HB2	1.83	0.60
10:V:232:LEU:O	10:V:234:LYS:NZ	2.35	0.60
10:X:269:MET:HA	10:X:269:MET:HE3	1.84	0.60
3:F:89:ARG:HB3	3:F:109:LEU:HD21	1.84	0.60
4:H:41:SER:O	4:H:45:TYR:HB2	2.01	0.60
2:D:58:LEU:O	2:D:62:LEU:HG	2.02	0.59
10:V:23:ARG:NH1	11:W:64:GLY:O	2.35	0.59
10:V:194:VAL:HG12	10:V:211:ARG:HD2	1.83	0.59
3:F:51:TYR:HB3	4:H:97:ILE:HD11	1.83	0.59
7:M:747:PRO:HD2	7:M:819:GLN:HE22	1.67	0.59
9:S:251:ASP:OD1	9:S:252:SER:N	2.34	0.59
10:T:311:ASP:OD2	11:U:311:ARG:NH2	2.31	0.59
4:G:83:LEU:HD11	4:G:99:THR:HG23	1.84	0.59
7:M:1186:SER:OG	10:V:251:ASP:OD2	2.20	0.59
7:M:1326:LEU:O	7:M:1354:ARG:NH1	2.36	0.59
5:I:23:DA:H5"	7:M:833:ARG:HH12	1.68	0.59
7:M:755:SER:HA	7:M:1301:ARG:HD2	1.85	0.59
7:M:778:GLY:HA3	7:M:782:GLN:HB2	1.85	0.59
10:T:26:ALA:O	13:T:501:ADP:O3'	2.18	0.59
11:U:329:VAL:H	11:U:341:HIS:H	1.49	0.59
7:M:754:THR:HG22	7:M:802:SER:HB2	1.85	0.59
10:V:33:LEU:O	10:V:55:ARG:NH1	2.36	0.59
4:G:109:LEU:H	4:G:109:LEU:HD12	1.68	0.59
11:U:203:GLY:HA3	11:U:223:GLN:HE22	1.68	0.59
10:V:252:LEU:O	10:V:256:ASN:ND2	2.32	0.59
11:Y:332:THR:OG1	11:Y:335:THR:OG1	2.19	0.59
10:T:346:THR:HG22	10:T:354:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:84:GLY:N	13:X:501:ADP:O1A	2.36	0.59
12:Z:298:THR:C	12:Z:300:ALA:HA	2.28	0.59
3:E:73:ASP:O	3:E:75:LYS:NZ	2.36	0.58
7:M:1053:ASP:OD1	7:M:1053:ASP:N	2.36	0.58
7:M:1296:THR:O	7:M:1301:ARG:NH2	2.36	0.58
5:I:-59:DT:H2"	5:I:-58:DG:C8	2.39	0.58
7:M:1210:ARG:O	7:M:1214:MET:HG3	2.03	0.58
10:X:462:TYR:OH	11:Y:327:ARG:NH1	2.36	0.58
10:X:124:ASN:OD1	10:X:127:ARG:NH1	2.32	0.58
2:C:84:LEU:HB2	2:C:88:TYR:CE2	2.39	0.58
8:R:339:SER:O	8:R:346:ARG:NH2	2.36	0.58
7:M:1195:LEU:HD11	11:U:254:PHE:HZ	1.67	0.58
12:Z:238:GLN:OE1	12:Z:241:ARG:N	2.27	0.58
4:H:74:GLU:O	4:H:78:THR:HG22	2.04	0.58
9:S:239:PRO:HG3	10:T:217:ALA:HB1	1.85	0.58
10:T:132:ARG:HA	10:T:246:ASP:HA	1.86	0.58
10:V:362:ASP:O	10:V:366:ARG:NH1	2.37	0.58
10:V:455:ILE:O	10:V:459:SER:OG	2.22	0.58
11:U:19:LEU:HD12	10:V:71:SER:HB2	1.86	0.58
1:A:67:PHE:HZ	1:A:92:LEU:HB3	1.69	0.57
3:E:32:HIS:HB3	3:E:36:ARG:HH21	1.69	0.57
3:F:65:GLU:OE1	4:H:52:HIS:NE2	2.35	0.57
1:A:78:PHE:CE2	2:D:70:VAL:HG21	2.39	0.57
3:E:42:GLN:NE2	4:G:90:SER:HB3	2.18	0.57
8:R:197:CYS:SG	8:R:199:TRP:NE1	2.76	0.57
10:T:129:ILE:HG22	10:T:334:PRO:HB3	1.85	0.57
12:Z:289:GLN:HB3	12:Z:597:THR:HB	1.85	0.57
6:J:-17:DT:OP1	7:M:754:THR:OG1	2.21	0.57
8:R:12:SER:O	8:R:59:ARG:NH1	2.37	0.57
12:Z:257:ASP:OD1	12:Z:258:LYS:N	2.36	0.57
4:G:46:LYS:N	4:G:46:LYS:HD3	2.20	0.57
6:J:14:DT:H2"	6:J:15:DT:C5	2.39	0.57
7:M:1197:LEU:HD12	10:V:266:ILE:HG23	1.86	0.57
10:X:80:GLY:O	10:X:85:LYS:NZ	2.38	0.57
4:H:108:GLU:OE1	9:S:44:ARG:NH1	2.34	0.57
5:I:72:DG:H2"	5:I:73:DT:H5'	1.87	0.57
7:M:1132:ARG:NH1	11:Y:217:ALA:O	2.37	0.57
10:V:73:ARG:HB2	10:V:335:VAL:HG22	1.85	0.57
9:S:9:ASP:HB3	9:S:12:THR:HB	1.87	0.57
12:Z:217:ARG:HA	12:Z:220:ILE:HG22	1.87	0.57
5:I:-95:DC:H2"	5:I:-94:DA:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:244:CYS:HB2	9:S:264:CYS:HB3	1.86	0.57
7:M:1174:ARG:NH1	7:M:1226:GLN:OE1	2.38	0.57
7:M:1202:ASP:N	7:M:1202:ASP:OD1	2.38	0.57
11:Y:193:ASP:HB3	11:Y:198:LYS:H	1.70	0.57
7:M:953:LEU:HD23	7:M:958:ARG:HD2	1.86	0.56
7:M:1018:TYR:OH	11:U:243:GLU:OE1	2.21	0.56
7:M:1264:ARG:NH2	7:M:1312:SER:O	2.38	0.56
11:U:243:GLU:OE2	10:V:283:LYS:NZ	2.38	0.56
3:E:77:THR:O	4:G:56:GLY:N	2.32	0.56
10:V:264:ASP:OD1	10:V:264:ASP:N	2.34	0.56
12:Z:306:ARG:HA	12:Z:309:TRP:CD1	2.40	0.56
2:C:30:THR:OG1	6:J:-12:DA:OP2	2.23	0.56
5:I:-65:DT:H1'	5:I:-64:DC:H5'	1.88	0.56
5:I:-10:DC:H2"	5:I:-9:DA:H5'	1.87	0.56
7:M:1049:LEU:HD21	10:T:259:PRO:HG3	1.87	0.56
9:S:91:THR:OG1	9:S:94:GLU:OE1	2.22	0.56
10:T:236:GLU:H	10:T:236:GLU:CD	2.13	0.56
10:T:283:LYS:O	10:T:287:GLU:HG2	2.05	0.56
11:U:359:TYR:OH	13:U:502:ADP:N7	2.35	0.56
10:V:71:SER:OG	10:V:333:ALA:O	2.23	0.56
10:X:70:MET:HA	10:X:70:MET:HE2	1.87	0.56
3:F:64:LEU:HD13	4:H:48:LEU:HB2	1.87	0.56
4:H:65:LEU:O	4:H:69:VAL:HG13	2.06	0.56
8:R:120:PHE:HD1	8:R:416:ARG:HE	1.52	0.56
9:S:264:CYS:SG	9:S:265:SER:N	2.77	0.56
10:T:274:LYS:HA	11:U:250:ARG:HD3	1.86	0.56
4:G:47:VAL:HA	4:G:50:GLN:HE21	1.70	0.56
5:I:-36:DT:H2"	5:I:-35:DA:N7	2.21	0.56
7:M:689:PRO:HA	7:M:692:LEU:HD12	1.86	0.56
11:U:163:THR:H	11:U:225:PRO:HB2	1.71	0.56
10:V:196:ILE:O	10:V:214:ARG:NH2	2.39	0.56
3:E:80:ILE:HG22	3:E:82:ARG:H	1.70	0.56
3:E:64:LEU:HD13	4:G:48:LEU:HG	1.86	0.56
4:G:102:ARG:HA	4:G:110:ALA:HB1	1.86	0.56
6:J:55:DC:H2"	6:J:56:DG:C8	2.41	0.56
5:I:-35:DA:H2"	5:I:-34:DG:C8	2.41	0.56
6:J:-16:DT:H2"	6:J:-15:DA:C8	2.41	0.56
7:M:732:ILE:HG12	7:M:764:PHE:HE1	1.71	0.56
7:M:867:LEU:HD21	7:M:874:THR:HG21	1.88	0.56
4:G:58:SER:OG	4:G:61:SER:OG	2.18	0.56
4:H:97:ILE:O	4:H:101:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:953:LEU:HG	7:M:957:GLN:HB3	1.88	0.56
10:T:28:THR:O	10:T:31:LYS:NZ	2.34	0.56
10:V:344:MET:HE3	10:V:344:MET:HA	1.87	0.56
11:W:149:ILE:HD11	12:Z:288:LEU:HD22	1.88	0.56
11:W:306:PHE:HB3	11:W:347:LEU:HD11	1.88	0.56
8:R:190:VAL:HG23	8:R:201:ILE:HB	1.88	0.55
9:S:118:THR:HA	9:S:128:ARG:HG3	1.88	0.55
11:Y:40:THR:HG22	11:Y:45:VAL:HG22	1.87	0.55
5:I:-23:DC:H2"	5:I:-22:DA:C8	2.42	0.55
10:X:106:VAL:HG22	11:Y:311:ARG:HG2	1.87	0.55
12:Z:221:GLN:HA	12:Z:224:ILE:HB	1.87	0.55
12:Z:320:LYS:HG3	12:Z:321:LYS:HG3	1.88	0.55
1:A:78:PHE:HZ	2:D:67:ARG:HD2	1.71	0.55
7:M:1015:ALA:HA	11:U:258:PHE:HE2	1.70	0.55
8:R:30:ASN:ND2	8:R:72:GLU:OE2	2.34	0.55
8:R:228:LYS:HG2	8:R:245:VAL:HG21	1.87	0.55
10:T:235:GLY:HA3	10:T:239:LYS:HE3	1.88	0.55
11:U:115:GLU:HG3	11:U:264:GLU:HA	1.87	0.55
10:V:298:GLN:HB2	10:V:300:VAL:HG23	1.88	0.55
11:W:359:TYR:OH	13:W:501:ADP:N7	2.34	0.55
11:Y:128:LYS:HG2	11:Y:238:THR:HG22	1.89	0.55
3:E:42:GLN:OE1	3:E:42:GLN:N	2.38	0.55
11:W:413:ARG:NH1	11:W:422:ASP:OD1	2.38	0.55
7:M:685:ASP:OD2	7:M:701:LYS:NZ	2.39	0.55
7:M:1228:GLN:NE2	10:V:262:GLY:O	2.40	0.55
11:U:28:GLY:H	11:U:90:GLN:HB3	1.71	0.55
11:W:171:LEU:HD23	11:W:175:MET:HB3	1.88	0.55
2:C:90:LEU:HB3	2:C:95:ARG:HB2	1.88	0.55
10:T:70:MET:HE2	10:T:70:MET:HA	1.89	0.55
11:U:47:GLN:NE2	11:U:357:LYS:O	2.40	0.55
10:V:136:THR:HG22	10:V:242:GLU:HG2	1.88	0.55
10:V:126:ARG:HE	10:V:249:LEU:HD22	1.70	0.55
11:W:78:SER:HA	13:W:501:ADP:H5'1	1.89	0.55
4:G:83:LEU:HD22	4:G:96:GLU:HB3	1.88	0.54
8:R:29:LEU:HB2	8:R:43:SER:HB2	1.88	0.54
10:T:313:VAL:HG11	10:T:338:LEU:HB3	1.88	0.54
10:V:142:GLY:HA2	10:V:233:PRO:HG2	1.87	0.54
10:V:375:TYR:OH	13:V:501:ADP:N7	2.36	0.54
3:F:78:ARG:HH12	4:H:56:GLY:C	2.15	0.54
7:M:956:ARG:NH2	7:M:1001:VAL:O	2.40	0.54
8:R:83:PRO:HB3	8:R:90:ASP:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:190:GLN:HG2	10:X:191:ARG:HH22	1.71	0.54
11:Y:194:LYS:NZ	11:Y:230:GLN:OE1	2.39	0.54
12:Z:296:LEU:HD13	12:Z:588:GLU:HB3	1.90	0.54
4:H:102:ARG:HA	4:H:110:ALA:HB1	1.90	0.54
8:R:234:ARG:NH1	8:R:309:GLU:OE2	2.40	0.54
3:E:89:ARG:HB3	3:E:109:LEU:HD21	1.90	0.54
5:I:-18:DC:H2"	5:I:-17:DT:H5'	1.88	0.54
11:U:397:ARG:NH2	13:U:502:ADP:O3A	2.40	0.54
5:I:25:DG:H2"	5:I:26:DG:H5'	1.88	0.54
5:I:62:DT:H2"	5:I:63:DA:C8	2.42	0.54
11:W:204:ARG:O	11:W:221:PHE:N	2.40	0.54
3:E:18:ARG:HH21	3:E:29:GLY:HA2	1.73	0.54
5:I:-26:DT:H2"	5:I:-25:DA:N7	2.22	0.54
7:M:822:VAL:HG12	7:M:849:LEU:HB3	1.89	0.54
7:M:1127:LYS:NZ	10:T:136:THR:OG1	2.40	0.54
13:M:1601:ADP:O3B	14:M:1602:BEF:F1	2.16	0.54
8:R:299:GLU:HG3	8:R:301:ALA:H	1.72	0.54
11:U:425:ARG:NH1	10:V:56:GLU:OE2	2.39	0.54
10:X:62:VAL:HG22	10:X:92:ILE:HG13	1.90	0.54
10:X:440:ASN:HA	10:X:443:LYS:HD3	1.89	0.54
1:A:73:GLU:OE2	2:D:23:ARG:N	2.41	0.54
1:B:124:ILE:HD12	1:B:125:LYS:HD2	1.89	0.54
6:J:22:DT:H2"	6:J:23:DG:C8	2.43	0.54
8:R:434:TYR:OH	9:S:221:ASP:OD1	2.24	0.54
9:S:266:VAL:HA	11:U:165:MET:HE3	1.89	0.54
1:B:57:SER:HB2	1:B:59:GLU:OE1	2.08	0.54
11:W:163:THR:HG21	11:W:226:GLU:HG3	1.90	0.54
11:Y:26:ILE:HG22	11:Y:44:MET:HG2	1.90	0.54
10:T:344:MET:HE3	10:T:344:MET:HA	1.89	0.54
10:V:362:ASP:OD1	10:V:362:ASP:N	2.41	0.54
11:Y:396:LEU:O	11:Y:399:SER:OG	2.25	0.54
3:E:84:LEU:O	3:E:88:ILE:HG22	2.07	0.53
11:W:331:LYS:HA	11:W:338:LYS:HA	1.90	0.53
10:X:317:ASP:HB3	10:X:320:ILE:HG13	1.90	0.53
3:F:55:VAL:O	3:F:59:LEU:HD22	2.08	0.53
8:R:9:ASP:HB3	8:R:16:LYS:HB2	1.90	0.53
7:M:1183:LEU:HD12	11:W:269:VAL:HG13	1.90	0.53
10:T:149:PRO:HA	10:T:166:VAL:HG22	1.90	0.53
11:Y:122:ARG:NH1	11:Y:245:ASP:OD1	2.42	0.53
2:D:23:ARG:N	2:D:25:ASN:OD1	2.42	0.53
5:I:1:DT:H2'	5:I:2:DG:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:15:DT:H2"	5:I:16:DA:N7	2.23	0.53
7:M:759:ASN:O	7:M:763:GLU:HG2	2.08	0.53
11:U:124:SER:HB2	11:U:319:PRO:HG3	1.91	0.53
11:U:332:THR:OG1	11:U:335:THR:OG1	2.26	0.53
4:G:70:ASN:O	4:G:74:GLU:HG3	2.08	0.53
7:M:723:MET:SD	7:M:1354:ARG:NH2	2.81	0.53
10:T:224:LEU:HD21	11:U:171:LEU:HD23	1.90	0.53
10:X:129:ILE:HD11	10:X:334:PRO:HD3	1.90	0.53
8:R:141:LYS:HG3	8:R:185:HIS:CG	2.43	0.53
7:M:1138:LYS:HE2	7:M:1138:LYS:HA	1.90	0.53
8:R:13:TYR:HA	8:R:59:ARG:HH12	1.74	0.53
8:R:289:ASN:HB3	8:R:292:LYS:HE3	1.91	0.53
10:V:51:GLN:NE2	10:V:373:LEU:O	2.42	0.53
11:W:117:LEU:HD11	11:W:305:CYS:HB3	1.91	0.53
10:X:192:GLU:HG3	10:X:209:VAL:HG13	1.90	0.53
1:B:120:GLN:HG2	1:B:121:LYS:N	2.24	0.53
7:M:1383:ALA:O	7:M:1388:GLN:N	2.41	0.53
10:T:23:ARG:HD2	11:U:288:ILE:HD11	1.90	0.53
11:U:50:ALA:HB1	11:U:84:LEU:HD11	1.90	0.53
11:W:32:ASP:OD1	11:W:36:GLN:N	2.35	0.53
11:W:162:THR:HG23	11:W:164:ASP:H	1.74	0.53
7:M:1164:LYS:O	7:M:1169:ARG:NH2	2.42	0.52
10:X:73:ARG:HB2	10:X:335:VAL:HG22	1.89	0.52
10:X:281:THR:HG23	10:X:284:LEU:H	1.72	0.52
8:R:397:TRP:HA	8:R:400:MET:CE	2.39	0.52
8:R:430:HIS:O	8:R:436:ASN:ND2	2.42	0.52
10:V:252:LEU:HD11	10:V:288:VAL:HG13	1.91	0.52
10:V:395:VAL:HG22	10:V:434:ILE:HD12	1.91	0.52
10:X:216:ASP:HA	10:X:229:TYR:HB3	1.91	0.52
6:J:72:DA:H2"	6:J:73:DG:C8	2.44	0.52
7:M:1079:ARG:HA	7:M:1082:ASN:HB2	1.91	0.52
10:T:201:TYR:HB3	10:T:210:LYS:HG3	1.91	0.52
1:A:85:GLN:OE1	1:A:87:SER:OG	2.27	0.52
3:E:72:ARG:HD3	12:Z:207:TYR:CZ	2.44	0.52
4:G:78:THR:O	4:G:82:LYS:HG2	2.09	0.52
11:U:132:GLU:HG3	11:U:234:THR:HB	1.92	0.52
11:W:311:ARG:O	11:W:311:ARG:NH1	2.42	0.52
7:M:707:LEU:HD21	7:M:734:LEU:HD22	1.91	0.52
11:W:118:THR:O	11:W:122:ARG:HG2	2.10	0.52
3:F:100:ASN:OD1	3:F:100:ASN:N	2.42	0.52
6:J:64:DG:H2"	6:J:65:DA:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:992:VAL:HG23	7:M:998:LEU:HD13	1.90	0.52
10:T:456:LEU:HD13	11:U:329:VAL:HG23	1.92	0.52
11:U:38:ARG:HD2	11:U:41:SER:HB3	1.91	0.52
10:V:86:THR:N	13:V:501:ADP:O2A	2.43	0.52
11:W:115:GLU:OE2	11:W:270:ARG:NH2	2.43	0.52
11:W:299:HIS:HB3	11:W:325:THR:HG23	1.92	0.52
10:X:131:LEU:HD11	10:X:301:ALA:HB1	1.91	0.52
4:G:65:LEU:O	4:G:69:VAL:HG13	2.09	0.52
6:J:77:DG:C8	6:J:77:DG:H5"	2.44	0.52
10:V:211:ARG:NH2	10:V:227:GLU:OE2	2.43	0.52
5:I:-86:DA:H2"	5:I:-85:DT:C6	2.45	0.52
6:J:-28:DC:H4'	6:J:-27:DC:H5'	1.91	0.52
6:J:89:DA:H2'	6:J:90:DT:H71	1.92	0.52
7:M:1052:LYS:NZ	11:Y:252:GLN:OE1	2.42	0.52
10:T:172:SER:HB3	10:T:236:GLU:O	2.10	0.52
11:U:345:LEU:HD12	11:Y:454:VAL:HG12	1.91	0.52
11:Y:23:HIS:HB3	11:Y:26:ILE:HD11	1.92	0.52
1:A:91:ALA:HB2	2:D:100:PHE:HE2	1.75	0.52
6:J:-25:DC:H2"	6:J:-24:DT:H5"	1.92	0.52
8:R:273:GLU:HG2	8:R:305:THR:HG22	1.91	0.52
10:X:33:LEU:HB3	10:X:35:LEU:HD13	1.92	0.52
10:X:61:ILE:O	10:X:65:ILE:HG22	2.10	0.52
12:Z:271:LEU:O	12:Z:275:LYS:NZ	2.39	0.52
10:X:196:ILE:O	10:X:214:ARG:NH1	2.43	0.52
5:I:66:DC:H2"	5:I:67:DA:H5'	1.92	0.51
9:S:250:TYR:HA	9:S:253:ILE:HD11	1.92	0.51
10:T:200:ILE:HD12	10:T:202:ILE:HD11	1.92	0.51
10:T:281:THR:HG23	10:T:284:LEU:H	1.74	0.51
10:X:391:GLU:HB3	10:X:393:LEU:HD22	1.90	0.51
12:Z:305:ASP:HB3	12:Z:309:TRP:CZ2	2.45	0.51
3:F:91:ASP:OD1	9:S:44:ARG:NH2	2.43	0.51
4:G:88:LYS:HE2	4:G:88:LYS:HA	1.92	0.51
7:M:775:THR:HA	7:M:800:ILE:HG23	1.91	0.51
7:M:925:LEU:HD13	7:M:929:LEU:HD22	1.92	0.51
9:S:175:ILE:HG22	9:S:179:TYR:CE1	2.45	0.51
11:U:44:MET:HG2	11:U:51:ARG:HD3	1.93	0.51
10:V:394:GLN:HB2	10:V:433:GLU:HG2	1.92	0.51
11:W:331:LYS:HB2	11:W:338:LYS:HG2	1.91	0.51
11:W:332:THR:OG1	11:W:335:THR:OG1	2.23	0.51
11:W:362:GLN:O	11:W:366:THR:HG23	2.10	0.51
4:H:87:ASN:O	4:H:88:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:185:ILE:O	10:V:189:ILE:HG22	2.10	0.51
5:I:-34:DG:H2"	5:I:-33:DA:N7	2.25	0.51
7:M:723:MET:HE1	7:M:1353:ASP:HB3	1.91	0.51
8:R:65:GLN:HE21	8:R:107:THR:HA	1.75	0.51
10:T:129:ILE:O	10:T:248:THR:OG1	2.19	0.51
11:U:140:VAL:O	11:U:187:GLY:N	2.39	0.51
10:V:127:ARG:NH2	11:W:267:SER:OG	2.44	0.51
11:Y:86:MET:HE3	11:Y:86:MET:HA	1.93	0.51
11:Y:125:ILE:HG23	11:Y:241:LEU:HD13	1.92	0.51
6:J:-24:DT:H2'	6:J:-23:DT:H71	1.92	0.51
7:M:1307:ARG:HG2	12:Z:267:LYS:HD2	1.93	0.51
7:M:1363:ASP:OD2	7:M:1365:HIS:NE2	2.44	0.51
8:R:226:LEU:N	9:S:105:LEU:HD21	2.25	0.51
10:X:225:GLU:HG2	10:X:229:TYR:CE1	2.46	0.51
5:I:6:DC:H2"	5:I:7:DC:C5	2.45	0.51
8:R:134:ALA:HB1	8:R:190:VAL:HG21	1.92	0.51
11:W:425:ARG:NH2	10:X:56:GLU:OE2	2.44	0.51
10:X:378:ASP:N	10:X:378:ASP:OD1	2.42	0.51
11:U:154:LYS:HD3	11:U:176:ILE:HD12	1.93	0.51
11:U:398:TYR:OH	11:U:430:PHE:O	2.28	0.51
2:C:26:ILE:HD11	2:C:55:ARG:HG2	1.93	0.51
2:C:84:LEU:HA	2:C:87:VAL:HG12	1.93	0.51
4:G:45:TYR:O	4:G:49:LYS:HG2	2.10	0.51
5:I:-62:DC:H2"	5:I:-61:DG:C8	2.46	0.51
6:J:-35:DG:H2"	6:J:-34:DA:C8	2.46	0.51
8:R:61:HIS:CE1	8:R:66:LEU:HD23	2.46	0.51
5:I:5:DC:H2"	5:I:6:DC:C5	2.45	0.51
10:T:106:VAL:N	10:T:109:GLU:OE2	2.42	0.51
11:W:259:THR:HG23	11:W:261:ASP:H	1.76	0.51
3:F:42:GLN:HE22	4:H:90:SER:HB3	1.76	0.50
10:T:53:GLU:H	10:T:53:GLU:CD	2.17	0.50
11:Y:158:LEU:HG	11:Y:171:LEU:HD21	1.94	0.50
11:Y:346:ASP:OD1	11:Y:346:ASP:N	2.42	0.50
12:Z:310:GLN:NE2	12:Z:314:ASN:OD1	2.44	0.50
2:D:59:LYS:HA	2:D:59:LYS:HE2	1.92	0.50
9:S:244:CYS:HB3	9:S:249:GLY:N	2.26	0.50
10:T:48:PHE:HD2	10:T:55:ARG:HD3	1.75	0.50
10:T:53:GLU:OE1	10:T:53:GLU:N	2.25	0.50
10:X:352:ASP:OD1	10:X:352:ASP:N	2.43	0.50
3:F:77:THR:O	4:H:55:THR:OG1	2.28	0.50
6:J:62:DG:H2"	6:J:63:DG:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1382:LYS:NZ	7:M:1393:VAL:O	2.44	0.50
10:T:150:GLU:O	10:T:164:SER:N	2.44	0.50
11:U:108:SER:HA	10:V:116:LYS:HD3	1.92	0.50
3:E:65:GLU:HG2	4:G:52:HIS:HE1	1.77	0.50
4:G:54:ASP:OD1	4:G:54:ASP:N	2.44	0.50
11:U:402:LEU:HA	11:U:405:VAL:HG12	1.93	0.50
7:M:1110:GLN:NE2	7:M:1111:LYS:HG3	2.26	0.50
8:R:60:PRO:HD3	8:R:71:LEU:HD13	1.94	0.50
11:W:303:ILE:HD13	11:W:335:THR:HG23	1.92	0.50
12:Z:306:ARG:CZ	12:Z:309:TRP:HE1	2.24	0.50
1:A:70:LEU:O	1:A:74:ILE:HG13	2.11	0.50
5:I:-63:DC:H4'	12:Z:217:ARG:HD3	1.94	0.50
5:I:-46:DC:H2"	5:I:-45:DA:N7	2.27	0.50
7:M:765:LYS:HG2	12:Z:254:LEU:HD21	1.94	0.50
11:U:382:ASP:N	11:U:382:ASP:OD1	2.44	0.50
10:V:80:GLY:O	10:V:83:THR:OG1	2.22	0.50
2:C:82:THR:HG23	2:C:84:LEU:HG	1.93	0.50
4:H:54:ASP:OD1	4:H:54:ASP:N	2.44	0.50
10:T:60:VAL:HG11	11:Y:405:VAL:HG13	1.94	0.50
1:A:70:LEU:HD13	2:D:26:ILE:HA	1.94	0.50
1:A:93:GLN:O	1:A:97:GLU:HG3	2.12	0.50
4:G:71:ASP:HA	4:G:74:GLU:OE1	2.12	0.50
5:I:27:DG:H2"	5:I:28:DG:N7	2.27	0.50
6:J:-42:DG:H5'	6:J:-42:DG:H8	1.76	0.50
10:T:131:LEU:HD11	10:T:301:ALA:HB1	1.93	0.50
12:Z:619:ARG:HA	12:Z:622:TYR:HB2	1.93	0.50
4:H:106:PRO:HD2	4:H:109:LEU:HD12	1.94	0.50
5:I:-66:DA:H1'	5:I:-65:DT:H5'	1.94	0.50
7:M:1340:ASP:OD1	7:M:1340:ASP:N	2.44	0.50
10:T:381:ARG:NE	10:T:401:ASP:OD1	2.44	0.50
11:W:125:ILE:HD12	11:W:290:PRO:HA	1.93	0.50
3:F:53:THR:O	3:F:57:GLU:HG2	2.11	0.49
6:J:86:DT:H1'	6:J:87:DG:N7	2.27	0.49
7:M:1008:PHE:HD1	10:V:245:GLN:HE22	1.59	0.49
7:M:1293:ASP:O	7:M:1296:THR:OG1	2.30	0.49
11:W:146:ASP:HB2	11:W:155:GLN:HB2	1.94	0.49
11:Y:299:HIS:HB3	11:Y:325:THR:HG23	1.94	0.49
3:E:72:ARG:HD3	12:Z:207:TYR:CE1	2.47	0.49
7:M:724:GLY:H	13:M:1601:ADP:PB	2.35	0.49
10:T:268:MET:HE2	10:T:268:MET:N	2.27	0.49
11:U:333:ARG:NH2	10:V:319:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:106:VAL:HB	10:X:109:GLU:HG2	1.94	0.49
10:X:381:ARG:NE	10:X:401:ASP:OD1	2.43	0.49
6:J:-63:DT:H2"	6:J:-62:DA:C8	2.47	0.49
7:M:825:GLU:N	7:M:851:LEU:O	2.44	0.49
8:R:355:CYS:HB2	8:R:387:VAL:HG22	1.95	0.49
9:S:176:GLN:HA	9:S:179:TYR:CE2	2.47	0.49
11:W:142:GLU:OE2	12:Z:293:THR:OG1	2.26	0.49
7:M:1159:ASP:HA	7:M:1162:LEU:HB2	1.93	0.49
3:F:98:LEU:HB3	3:F:101:VAL:HB	1.95	0.49
7:M:979:PHE:HB3	7:M:980:MET:HE2	1.95	0.49
8:R:289:ASN:HD21	8:R:291:ARG:HB2	1.77	0.49
11:U:232:ARG:NH1	11:U:232:ARG:HA	2.28	0.49
11:W:300:MET:HB2	11:W:333:ARG:HD2	1.93	0.49
2:C:54:VAL:HA	2:C:57:VAL:HG12	1.94	0.49
8:R:136:PHE:CD2	8:R:400:MET:HG2	2.48	0.49
10:T:223:ASP:OD2	11:U:170:GLU:N	2.46	0.49
4:H:104:ILE:HG22	4:H:105:LEU:HD22	1.95	0.49
6:J:7:DC:H2"	6:J:8:DG:C8	2.47	0.49
7:M:1133:ARG:CZ	7:M:1133:ARG:HA	2.43	0.49
7:M:719:LEU:HG	7:M:930:LEU:HD23	1.94	0.49
7:M:731:THR:O	7:M:735:LEU:HG	2.13	0.49
8:R:136:PHE:CG	8:R:400:MET:HG2	2.48	0.49
9:S:244:CYS:HB3	9:S:249:GLY:H	1.78	0.49
11:W:175:MET:HA	11:W:175:MET:HE3	1.94	0.49
11:W:390:THR:O	11:W:394:THR:OG1	2.28	0.49
2:C:99:GLY:O	4:G:63:SER:OG	2.28	0.49
5:I:48:DG:O6	6:J:-48:DC:N4	2.34	0.49
6:J:-11:DC:H2"	6:J:-10:DG:H5'	1.95	0.49
7:M:987:MET:HA	7:M:987:MET:HE2	1.93	0.49
9:S:266:VAL:HA	11:U:165:MET:CE	2.42	0.49
10:T:172:SER:OG	10:T:173:ALA:N	2.46	0.49
11:U:275:THR:O	11:U:279:GLU:HG2	2.12	0.49
6:J:6:DA:H2"	6:J:7:DC:H5"	1.94	0.48
7:M:1290:MET:HE2	7:M:1317:PHE:CE1	2.48	0.48
9:S:172:LEU:O	9:S:176:GLN:HG2	2.13	0.48
11:U:331:LYS:HA	11:U:338:LYS:HA	1.94	0.48
1:B:124:ILE:CD1	1:B:125:LYS:HD2	2.43	0.48
5:I:-6:DT:H2"	5:I:-5:DA:N7	2.28	0.48
5:I:60:DT:H2"	5:I:61:DA:C8	2.47	0.48
7:M:732:ILE:HG12	7:M:764:PHE:CE1	2.47	0.48
8:R:21:THR:O	8:R:23:LYS:NZ	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:58:ARG:HH11	9:S:166:VAL:HG22	1.77	0.48
10:T:166:VAL:HG21	10:T:186:TYR:CG	2.48	0.48
11:W:430:PHE:HE1	10:X:57:ALA:HB1	1.77	0.48
12:Z:202:ASN:OD1	12:Z:203:THR:N	2.46	0.48
6:J:78:DG:H2"	6:J:79:DC:O5'	2.12	0.48
11:U:300:MET:O	11:U:333:ARG:NH1	2.44	0.48
11:U:346:ASP:OD1	11:U:346:ASP:N	2.42	0.48
10:V:461:ASN:N	10:V:461:ASN:OD1	2.46	0.48
3:F:84:LEU:O	3:F:88:ILE:HG12	2.14	0.48
8:R:430:HIS:HB3	8:R:431:ARG:HH21	1.79	0.48
10:T:177:LYS:HB3	10:T:237:VAL:HG21	1.94	0.48
11:W:280:TRP:CD1	11:W:285:LYS:HD3	2.48	0.48
11:W:448:ILE:HG21	10:X:342:ARG:HH11	1.79	0.48
3:E:88:ILE:HG13	3:E:94:LEU:HB3	1.96	0.48
6:J:5:DT:H2"	6:J:6:DA:N7	2.29	0.48
7:M:1071:PHE:CG	7:M:1126:ASN:HB2	2.49	0.48
11:U:128:LYS:HG2	11:U:238:THR:HG22	1.96	0.48
10:X:182:ASP:OD2	10:X:184:THR:OG1	2.31	0.48
4:G:95:ARG:O	4:G:99:THR:HG22	2.13	0.48
5:I:-85:DT:H3	6:J:85:DA:H61	1.61	0.48
6:J:19:DC:H2"	6:J:20:DG:H8	1.79	0.48
8:R:34:LYS:HA	8:R:40:SER:HA	1.96	0.48
8:R:63:LEU:HD12	8:R:64:GLY:H	1.78	0.48
1:A:117:VAL:HG13	3:F:116:LEU:HD11	1.96	0.48
4:G:47:VAL:CA	4:G:50:GLN:HE21	2.26	0.48
5:I:-57:DC:H2"	5:I:-56:DC:C6	2.48	0.48
7:M:778:GLY:O	7:M:783:ARG:N	2.47	0.48
10:T:138:GLU:OE1	10:T:238:HIS:NE2	2.37	0.48
10:T:140:TYR:CD1	10:T:238:HIS:HB2	2.49	0.48
10:T:226:THR:HG23	11:U:175:MET:HG3	1.96	0.48
10:V:177:LYS:HG2	10:V:237:VAL:HG21	1.95	0.48
11:Y:72:LEU:HD22	11:Y:353:ILE:HG23	1.96	0.48
11:Y:177:ASP:O	11:Y:180:THR:OG1	2.31	0.48
11:Y:331:LYS:HA	11:Y:338:LYS:HA	1.95	0.48
7:M:1269:THR:O	7:M:1321:SER:OG	2.31	0.48
10:X:190:GLN:HB3	10:X:191:ARG:NH1	2.29	0.48
11:Y:241:LEU:O	11:Y:244:ILE:N	2.46	0.48
1:B:123:GLU:O	1:B:126:LEU:HD23	2.13	0.48
3:E:16:GLN:HE21	3:E:21:LYS:HZ1	1.61	0.48
6:J:-45:DG:H2"	6:J:-44:DG:C8	2.48	0.48
6:J:44:DT:H2"	6:J:45:DT:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1165:PRO:HG3	10:X:260:GLN:HE21	1.78	0.48
10:T:246:ASP:OD1	10:T:246:ASP:N	2.43	0.48
11:U:110:GLU:N	11:U:110:GLU:OE1	2.47	0.48
10:V:211:ARG:HH21	10:V:213:GLY:HA2	1.79	0.48
1:B:94:GLU:HA	1:B:97:GLU:OE1	2.14	0.47
10:V:182:ASP:HB3	10:V:185:ILE:HG13	1.95	0.47
11:Y:115:GLU:HG3	11:Y:264:GLU:HG3	1.95	0.47
6:J:-44:DG:C8	6:J:-44:DG:H5'	2.49	0.47
7:M:1245:CYS:HB2	7:M:1248:LEU:HB2	1.97	0.47
8:R:9:ASP:OD1	8:R:102:SER:OG	2.30	0.47
10:V:189:ILE:HD11	10:V:194:VAL:HG21	1.96	0.47
7:M:980:MET:HE2	7:M:980:MET:N	2.29	0.47
7:M:1167:GLN:NE2	10:X:260:GLN:O	2.46	0.47
8:R:216:LEU:HG	8:R:327:LYS:HZ1	1.80	0.47
10:V:88:LEU:O	10:V:92:ILE:HG22	2.14	0.47
12:Z:306:ARG:NH1	12:Z:309:TRP:HE1	2.12	0.47
1:A:54:PHE:HB3	2:D:40:ARG:HD2	1.95	0.47
4:H:83:LEU:HD12	4:H:84:ALA:N	2.29	0.47
5:I:48:DG:H2"	5:I:49:DC:C4	2.49	0.47
6:J:92:DA:H2"	6:J:93:DA:N7	2.29	0.47
10:T:269:MET:N	10:T:269:MET:HE2	2.30	0.47
11:W:192:ILE:HG22	11:W:199:ILE:HA	1.96	0.47
12:Z:605:PRO:O	12:Z:609:LYS:N	2.41	0.47
6:J:-76:DT:H2"	6:J:-75:DG:C8	2.49	0.47
8:R:90:ASP:N	8:R:90:ASP:OD1	2.47	0.47
8:R:239:MET:HB2	9:S:110:PHE:HZ	1.79	0.47
10:T:395:VAL:HA	10:T:434:ILE:HB	1.94	0.47
11:W:159:THR:HG23	11:W:168:ILE:HG13	1.97	0.47
11:Y:420:VAL:HG12	11:Y:424:LYS:HZ2	1.79	0.47
3:E:18:ARG:HA	3:E:21:LYS:HZ3	1.79	0.47
3:F:89:ARG:HA	3:F:95:ASN:ND2	2.25	0.47
5:I:72:DG:H2'	5:I:73:DT:H71	1.96	0.47
7:M:1144:LEU:O	7:M:1148:ARG:HG2	2.15	0.47
11:W:456:ILE:HD12	10:X:81:PRO:HB2	1.96	0.47
4:G:61:SER:O	4:G:65:LEU:HD23	2.14	0.47
7:M:726:GLY:HA2	13:M:1601:ADP:H5'1	1.97	0.47
8:R:52:ILE:HA	8:R:55:ILE:HD11	1.97	0.47
11:W:131:GLU:OE2	11:W:237:HIS:NE2	2.38	0.47
10:X:33:LEU:O	10:X:55:ARG:NH1	2.48	0.47
11:Y:413:ARG:NH1	11:Y:422:ASP:OD1	2.48	0.47
1:B:46:VAL:O	1:B:49:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:68:PHE:O	4:H:72:ILE:HG13	2.15	0.47
7:M:1329:ASN:HB3	7:M:1357:ARG:HH21	1.80	0.47
4:H:86:TYR:HD1	4:H:86:TYR:O	1.97	0.47
6:J:-7:DG:H2"	6:J:-6:DG:C8	2.49	0.47
7:M:1387:ARG:HE	7:M:1387:ARG:HA	1.80	0.47
9:S:55:ASP:O	9:S:59:ARG:HG2	2.15	0.47
10:T:21:VAL:HG12	10:T:22:THR:HG23	1.97	0.47
11:W:397:ARG:NH1	10:X:365:ASP:OD1	2.47	0.47
1:A:67:PHE:CZ	1:A:92:LEU:HB3	2.48	0.47
9:S:186:LYS:HA	9:S:186:LYS:HD3	1.66	0.47
10:T:425:LEU:O	10:T:428:THR:OG1	2.32	0.47
11:U:294:PHE:HD1	11:U:322:MET:HG3	1.80	0.47
10:V:447:LEU:HD22	10:V:451:ARG:HD2	1.96	0.47
11:W:137:GLU:OE2	11:W:138:GLY:N	2.48	0.47
10:X:132:ARG:HG2	10:X:246:ASP:HB3	1.97	0.47
4:H:43:TYR:HA	4:H:46:LYS:HZ3	1.79	0.46
7:M:831:ASN:HD22	7:M:834:SER:HB3	1.80	0.46
11:U:98:PHE:HD1	11:U:292:VAL:HB	1.81	0.46
11:U:281:LYS:HZ1	11:U:288:ILE:HG12	1.80	0.46
11:Y:382:ASP:OD1	11:Y:382:ASP:N	2.44	0.46
4:G:100:ALA:O	4:G:104:ILE:HG22	2.14	0.46
6:J:58:DC:H2"	6:J:59:DA:C8	2.50	0.46
8:R:121:GLU:HB2	9:S:198:LEU:HD11	1.97	0.46
10:X:161:LYS:HE2	10:X:161:LYS:HB2	1.67	0.46
5:I:48:DG:H2"	5:I:49:DC:C5	2.50	0.46
9:S:8:ILE:O	10:V:178:THR:OG1	2.32	0.46
11:W:21:ALA:H	11:W:24:SER:HG	1.59	0.46
10:X:429:SER:OG	10:X:431:ARG:NH2	2.49	0.46
11:Y:441:GLN:HA	11:Y:444:GLU:HG3	1.97	0.46
1:A:42:LYS:HE3	1:A:43:PRO:HD2	1.98	0.46
4:G:46:LYS:HD3	4:G:46:LYS:H	1.80	0.46
7:M:1008:PHE:N	7:M:1186:SER:O	2.45	0.46
11:U:228:GLU:O	11:U:231:LYS:NZ	2.45	0.46
3:F:73:ASP:HB3	9:S:51:TYR:HB2	1.96	0.46
6:J:4:DG:H2"	6:J:5:DT:C5	2.50	0.46
12:Z:205:LYS:O	12:Z:209:LYS:HG2	2.15	0.46
1:B:55:GLN:NE2	3:E:111:ASN:O	2.42	0.46
5:I:71:DT:H2"	5:I:72:DG:H8	1.81	0.46
5:I:77:DT:H2"	5:I:78:DG:C8	2.51	0.46
6:J:13:DT:H2"	6:J:14:DT:C5	2.51	0.46
7:M:749:LEU:HD23	7:M:821:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:54:SER:OG	8:R:240:ASP:OD2	2.27	0.46
10:X:413:ARG:NE	11:Y:349:ASP:OD2	2.41	0.46
1:A:69:ARG:NH2	6:J:17:DA:OP1	2.49	0.46
5:I:-62:DC:H1'	12:Z:221:GLN:NE2	2.31	0.46
6:J:-35:DG:H2"	6:J:-34:DA:H8	1.80	0.46
7:M:1290:MET:HE1	7:M:1304:LEU:HB3	1.98	0.46
10:V:198:ASP:HA	10:V:214:ARG:HA	1.97	0.46
11:W:160:ILE:HD12	11:W:160:ILE:HA	1.85	0.46
10:X:271:GLN:O	10:X:272:LEU:HG	2.16	0.46
7:M:762:MET:HE3	7:M:762:MET:HA	1.98	0.46
8:R:9:ASP:N	8:R:16:LYS:O	2.43	0.46
11:U:23:HIS:HD2	11:U:83:ALA:HA	1.80	0.46
10:V:356:PRO:HB2	10:V:357:HIS:CE1	2.51	0.46
11:W:458:ILE:HD11	10:X:408:THR:HG22	1.98	0.46
11:Y:76:PRO:O	11:Y:79:THR:OG1	2.20	0.46
5:I:-5:DA:H2"	5:I:-4:DC:C5	2.51	0.46
7:M:952:LYS:HA	7:M:952:LYS:HD2	1.71	0.46
7:M:1338:PHE:CE2	7:M:1352:GLN:HB3	2.51	0.46
8:R:120:PHE:HE1	8:R:416:ARG:HA	1.81	0.46
10:T:128:ALA:HB3	10:T:334:PRO:HG3	1.97	0.46
10:X:375:TYR:OH	13:X:501:ADP:N7	2.41	0.46
10:X:456:LEU:HD13	11:Y:328:GLY:HA2	1.97	0.46
5:I:-47:DT:H2"	5:I:-46:DC:C5	2.51	0.46
5:I:-12:DC:H2"	5:I:-11:DG:C8	2.51	0.46
5:I:24:DA:H2'	5:I:25:DG:C8	2.51	0.46
7:M:1387:ARG:HA	7:M:1387:ARG:NE	2.31	0.46
8:R:147:MET:HA	8:R:147:MET:HE2	1.98	0.46
8:R:259:SER:OG	8:R:262:ASP:OD2	2.32	0.46
12:Z:246:LYS:O	12:Z:249:GLU:HG3	2.15	0.46
12:Z:316:ARG:NH2	12:Z:320:LYS:HD3	2.31	0.46
1:A:121:LYS:HD3	2:D:49:LEU:HB2	1.98	0.45
3:E:34:LEU:HD22	3:E:37:ARG:NH2	2.30	0.45
4:G:93:SER:H	4:G:96:GLU:HG2	1.81	0.45
7:M:1357:ARG:NH2	13:M:1601:ADP:O5'	2.49	0.45
10:T:126:ARG:NH2	10:T:289:ASN:OD1	2.49	0.45
1:B:116:ARG:HH22	1:B:122:LYS:NZ	2.12	0.45
3:E:93:GLU:OE1	4:G:106:PRO:HG2	2.15	0.45
5:I:-14:DA:H2"	5:I:-13:DA:C8	2.50	0.45
6:J:-38:DA:H2"	6:J:-37:DG:C8	2.52	0.45
7:M:1110:GLN:HE21	7:M:1111:LYS:HG3	1.81	0.45
7:M:1154:LYS:HD2	7:M:1156:SER:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:15:ILE:HD11	8:R:30:ASN:HD22	1.79	0.45
10:V:150:GLU:OE1	10:V:180:ARG:NH2	2.48	0.45
11:W:347:LEU:HD12	11:W:347:LEU:H	1.80	0.45
2:D:35:ARG:NH2	6:J:8:DG:OP2	2.49	0.45
5:I:-29:DC:C6	5:I:-28:DT:H72	2.52	0.45
7:M:1116:VAL:O	7:M:1119:LEU:HG	2.16	0.45
11:U:20:ILE:HB	10:V:70:MET:HA	1.97	0.45
12:Z:217:ARG:O	12:Z:220:ILE:HG22	2.15	0.45
2:D:40:ARG:HH22	3:F:108:VAL:HG22	1.82	0.45
3:F:27:PRO:HD3	4:H:43:TYR:CE1	2.51	0.45
4:G:41:SER:HA	4:G:62:MET:CE	2.47	0.45
6:J:-21:DG:H2"	6:J:-20:DC:O5'	2.16	0.45
7:M:1200:ASN:O	7:M:1210:ARG:NH1	2.50	0.45
9:S:53:LEU:HD12	9:S:53:LEU:H	1.81	0.45
10:V:200:ILE:HA	10:V:211:ARG:HA	1.99	0.45
12:Z:287:ILE:HG22	12:Z:288:LEU:H	1.82	0.45
2:C:75:HIS:CD2	4:H:99:THR:HG21	2.51	0.45
6:J:76:DC:H2"	6:J:77:DG:OP1	2.16	0.45
9:S:263:ILE:HD12	9:S:263:ILE:HA	1.76	0.45
1:B:83:ARG:HA	1:B:83:ARG:HD3	1.79	0.45
2:C:68:ASP:OD1	2:C:68:ASP:N	2.49	0.45
6:J:-1:DA:H2"	6:J:0:DG:H5"	1.97	0.45
7:M:1146:LYS:HE3	11:Y:131:GLU:HB2	1.99	0.45
8:R:82:ASN:OD1	9:S:183:LYS:NZ	2.41	0.45
9:S:244:CYS:N	9:S:249:GLY:O	2.47	0.45
10:T:216:ASP:HA	10:T:229:TYR:HB3	1.99	0.45
1:A:65:LEU:HD13	6:J:17:DA:H3'	1.99	0.45
2:D:76:ALA:O	2:D:77:LYS:HG2	2.16	0.45
3:E:18:ARG:HA	3:E:21:LYS:HG2	1.99	0.45
6:J:-20:DC:N4	6:J:-19:DG:O6	2.50	0.45
6:J:76:DC:C2	6:J:77:DG:N2	2.85	0.45
7:M:926:ARG:O	7:M:926:ARG:NE	2.50	0.45
8:R:239:MET:HB2	9:S:110:PHE:CZ	2.52	0.45
10:T:258:ARG:HH22	10:T:275:PRO:HA	1.81	0.45
10:V:128:ALA:HB3	10:V:334:PRO:HG3	1.97	0.45
10:X:154:ASN:N	10:X:154:ASN:OD1	2.49	0.45
11:Y:165:MET:SD	11:Y:229:LEU:HB2	2.56	0.45
1:A:78:PHE:HE2	2:D:70:VAL:HG21	1.78	0.45
2:C:84:LEU:O	2:C:88:TYR:CD2	2.70	0.45
3:E:117:LEU:HD12	3:E:118:PRO:HD2	1.99	0.45
4:H:49:LYS:HE3	4:H:53:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:45:DT:H2"	6:J:46:DG:C8	2.52	0.45
6:J:86:DT:H1'	6:J:87:DG:C8	2.52	0.45
10:X:88:LEU:O	10:X:92:ILE:HG22	2.16	0.45
11:Y:243:GLU:OE1	11:Y:243:GLU:N	2.37	0.45
11:Y:303:ILE:HD13	11:Y:335:THR:HG23	1.99	0.45
11:Y:329:VAL:HG22	11:Y:340:PRO:HA	1.97	0.45
3:F:112:ILE:HG22	9:S:60:LEU:HD13	1.98	0.45
10:T:150:GLU:HG3	10:T:165:HIS:CD2	2.52	0.45
11:W:398:TYR:OH	11:W:430:PHE:O	2.34	0.45
2:D:67:ARG:O	2:D:71:THR:OG1	2.27	0.45
4:G:102:ARG:HD3	4:G:114:VAL:HG11	1.98	0.45
4:H:79:GLU:HG2	4:H:104:ILE:CD1	2.47	0.45
7:M:971:LYS:HA	7:M:971:LYS:HD3	1.76	0.45
10:T:86:THR:OG1	11:U:311:ARG:NH2	2.50	0.45
11:W:25:HIS:CD2	11:W:26:ILE:HG13	2.52	0.45
11:W:185:LEU:HG	12:Z:590:LEU:HD12	1.99	0.45
12:Z:316:ARG:NE	12:Z:316:ARG:O	2.50	0.45
1:A:106:ASP:HB3	1:B:130:LEU:HD11	1.99	0.44
1:A:116:ARG:NH2	1:A:123:GLU:OE2	2.50	0.44
3:F:46:SER:OG	5:I:39:DA:OP1	2.31	0.44
6:J:19:DC:H2"	6:J:20:DG:C8	2.53	0.44
10:V:435:VAL:HG23	10:V:437:ASN:H	1.81	0.44
1:B:46:VAL:HG13	1:B:49:ARG:HD3	1.99	0.44
1:B:103:LEU:HD12	1:B:131:ARG:HH21	1.81	0.44
4:G:47:VAL:C	4:G:50:GLN:HE21	2.23	0.44
8:R:63:LEU:HD12	8:R:64:GLY:N	2.31	0.44
8:R:318:PHE:CE2	8:R:330:ILE:HD11	2.52	0.44
9:S:16:ASP:HA	11:U:147:ARG:NE	2.32	0.44
3:F:92:ASP:OD1	3:F:92:ASP:N	2.51	0.44
6:J:21:DG:H2"	6:J:22:DT:H71	2.00	0.44
7:M:706:TRP:CE3	7:M:930:LEU:HD22	2.53	0.44
9:S:185:PRO:O	9:S:186:LYS:NZ	2.37	0.44
10:T:384:ILE:HG23	10:T:419:LEU:HD11	1.99	0.44
11:U:94:LYS:HG2	11:U:95:ASP:H	1.81	0.44
10:V:109:GLU:HG2	11:W:114:THR:HG21	1.99	0.44
10:V:172:SER:OG	10:V:173:ALA:N	2.49	0.44
10:X:164:SER:O	10:X:165:HIS:ND1	2.50	0.44
10:X:283:LYS:O	10:X:286:GLN:HG3	2.16	0.44
12:Z:586:GLY:O	12:Z:588:GLU:HB2	2.17	0.44
3:E:93:GLU:CG	4:G:109:LEU:HD11	2.47	0.44
6:J:34:DC:H2"	6:J:35:DT:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:249:LYS:O	8:R:253:LEU:HB2	2.17	0.44
10:V:76:LEU:HD21	10:V:369:ILE:HG12	1.98	0.44
2:D:24:ASP:OD1	2:D:24:ASP:O	2.36	0.44
4:G:108:GLU:OE2	4:G:111:LYS:NZ	2.50	0.44
4:H:98:GLN:HG2	4:H:114:VAL:HG22	1.99	0.44
6:J:-42:DG:H5'	6:J:-42:DG:C8	2.52	0.44
6:J:-29:DT:H2"	6:J:-28:DC:C6	2.53	0.44
7:M:1076:ASN:HA	7:M:1079:ARG:HG2	2.00	0.44
8:R:124:GLU:HA	8:R:416:ARG:HH22	1.81	0.44
8:R:209:TYR:CE1	8:R:211:LYS:HB2	2.52	0.44
8:R:233:PHE:HD1	9:S:276:ARG:HH21	1.64	0.44
11:U:136:ILE:HA	11:U:229:LEU:O	2.18	0.44
10:X:344:MET:HA	10:X:344:MET:HE3	2.00	0.44
12:Z:220:ILE:CD1	12:Z:223:ARG:HE	2.30	0.44
2:D:84:LEU:HA	2:D:87:VAL:HG12	1.99	0.44
3:F:81:PRO:HA	3:F:84:LEU:HD12	1.99	0.44
7:M:727:LYS:HB3	7:M:851:LEU:HD11	1.99	0.44
9:S:265:SER:OG	9:S:266:VAL:N	2.51	0.44
11:Y:315:ASP:OD1	11:Y:316:GLU:N	2.50	0.44
3:F:22:ALA:HB1	4:H:123:LYS:HZ3	1.82	0.44
4:G:119:ARG:O	4:G:123:LYS:HG3	2.18	0.44
5:I:21:DC:OP2	7:M:831:ASN:ND2	2.49	0.44
9:S:168:LYS:HD3	9:S:168:LYS:HA	1.87	0.44
11:U:47:GLN:HG2	11:U:359:TYR:HE1	1.81	0.44
11:U:204:ARG:O	11:U:222:VAL:N	2.50	0.44
10:X:446:PHE:HE1	11:Y:53:ALA:HB1	1.82	0.44
11:Y:31:LEU:HD12	11:Y:35:LEU:C	2.42	0.44
6:J:-34:DA:H2"	6:J:-33:DG:H8	1.83	0.44
6:J:24:DC:H4'	6:J:25:DT:OP1	2.18	0.44
6:J:55:DC:H2"	6:J:56:DG:N7	2.33	0.44
7:M:995:HIS:O	7:M:997:ASN:N	2.47	0.44
7:M:1344:ASN:HA	7:M:1347:MET:SD	2.58	0.44
8:R:3:THR:OG1	8:R:4:PRO:HD3	2.17	0.44
8:R:323:SER:O	9:S:101:ARG:NH1	2.51	0.44
10:T:211:ARG:NH1	10:T:213:GLY:HA2	2.33	0.44
10:X:72:GLY:N	10:X:333:ALA:O	2.49	0.44
4:G:124:TYR:O	4:G:127:SER:OG	2.33	0.44
7:M:1122:LEU:HD23	7:M:1122:LEU:HA	1.85	0.44
7:M:1291:ARG:HG3	7:M:1318:ILE:HB	1.99	0.44
8:R:153:LYS:NZ	8:R:379:THR:O	2.35	0.44
10:V:387:ARG:HD2	10:V:387:ARG:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:85:LYS:HE3	10:X:341:ASN:HB3	1.99	0.44
12:Z:608:LEU:HA	12:Z:611:PHE:HB2	2.00	0.44
1:B:59:GLU:OE1	1:B:59:GLU:N	2.49	0.43
2:D:54:VAL:O	2:D:58:LEU:HD23	2.18	0.43
5:I:-77:DC:H2'	5:I:-76:DG:C8	2.53	0.43
5:I:11:DG:C8	5:I:12:DT:H72	2.53	0.43
6:J:85:DA:H2"	6:J:86:DT:O4'	2.18	0.43
10:V:346:THR:HG22	10:V:354:ILE:HG12	1.99	0.43
11:W:82:THR:HB	13:W:501:ADP:O1A	2.18	0.43
10:X:110:LEU:HD23	10:X:316:LEU:HD11	1.99	0.43
10:X:315:MET:HA	10:X:348:ARG:HD3	1.99	0.43
3:E:27:PRO:HB2	3:E:30:ARG:HB2	2.00	0.43
3:F:90:ASN:HB3	9:S:49:ILE:HG21	2.00	0.43
4:G:36:ARG:HD2	6:J:49:DC:H4'	1.99	0.43
5:I:63:DA:H2"	5:I:64:DT:H5'	1.99	0.43
10:T:109:GLU:HG2	11:U:114:THR:HG21	1.99	0.43
10:T:387:ARG:O	10:T:391:GLU:HG2	2.18	0.43
10:X:313:VAL:HA	10:X:316:LEU:HD23	2.00	0.43
11:Y:384:LEU:HD23	11:Y:384:LEU:HA	1.84	0.43
1:B:81:ASP:OD2	2:C:79:LYS:HD2	2.18	0.43
3:E:82:ARG:HA	3:E:106:GLY:HA2	1.99	0.43
8:R:25:PRO:HB3	8:R:397:TRP:CG	2.54	0.43
8:R:32:LEU:HD23	8:R:71:LEU:HD21	2.01	0.43
9:S:183:LYS:HD3	9:S:183:LYS:HA	1.70	0.43
10:X:418:LEU:C	10:X:421:PRO:HD2	2.43	0.43
1:B:40:ARG:HG2	5:I:10:DC:H5"	2.00	0.43
3:F:36:ARG:HD2	3:F:37:ARG:NH1	2.33	0.43
3:F:42:GLN:HE21	3:F:43:ARG:HB2	1.82	0.43
3:F:52:LEU:O	3:F:56:LEU:HD23	2.19	0.43
4:H:70:ASN:O	4:H:74:GLU:HG3	2.18	0.43
10:T:282:GLU:CD	10:T:282:GLU:H	2.25	0.43
11:Y:259:THR:OG1	11:Y:261:ASP:OD1	2.31	0.43
11:Y:344:PRO:HB2	11:Y:346:ASP:OD1	2.19	0.43
12:Z:195:LYS:O	12:Z:198:SER:OG	2.32	0.43
5:I:63:DA:H2'	5:I:64:DT:H71	2.00	0.43
9:S:262:LYS:HD3	9:S:262:LYS:N	2.33	0.43
1:A:52:ARG:O	1:A:56:LYS:HG2	2.19	0.43
1:B:70:LEU:HD12	1:B:73:GLU:OE2	2.19	0.43
3:E:43:ARG:HG3	4:G:91:THR:HG22	2.01	0.43
5:I:-6:DT:H2"	5:I:-5:DA:C8	2.53	0.43
6:J:68:DC:H2'	6:J:69:DT:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:5:PRO:HB3	8:R:98:HIS:HB2	1.99	0.43
8:R:198:THR:O	8:R:216:LEU:N	2.35	0.43
9:S:269:PHE:HB3	11:U:165:MET:HE1	2.00	0.43
10:T:72:GLY:N	10:T:333:ALA:O	2.51	0.43
11:U:431:LEU:HD11	10:V:371:ARG:HE	1.84	0.43
11:W:94:LYS:HA	11:W:94:LYS:HD3	1.60	0.43
2:C:58:LEU:HD12	2:C:62:LEU:HD23	2.00	0.43
2:D:90:LEU:HD22	2:D:97:LEU:HB2	2.00	0.43
6:J:-6:DG:H2"	6:J:-5:DG:N7	2.34	0.43
7:M:1323:SER:OG	7:M:1324:GLY:N	2.50	0.43
10:T:418:LEU:HD23	10:T:418:LEU:HA	1.86	0.43
11:W:143:ILE:O	12:Z:293:THR:HA	2.18	0.43
1:A:91:ALA:HB2	2:D:100:PHE:CE2	2.53	0.43
1:B:62:ILE:HG22	1:B:93:GLN:HE22	1.83	0.43
3:E:28:VAL:HA	3:E:53:THR:HG21	2.01	0.43
5:I:-83:DC:H2"	5:I:-82:DG:C8	2.54	0.43
5:I:-2:DC:H2"	5:I:-1:DG:C8	2.54	0.43
7:M:1055:THR:HG22	7:M:1058:HIS:HB2	2.01	0.43
8:R:27:ARG:NH2	8:R:391:ASP:OD2	2.52	0.43
8:R:98:HIS:ND1	8:R:127:SER:HB2	2.34	0.43
8:R:133:VAL:HA	8:R:136:PHE:HD2	1.84	0.43
8:R:254:PHE:HB2	8:R:363:PRO:HG2	1.99	0.43
9:S:91:THR:HG1	9:S:94:GLU:CD	2.27	0.43
11:U:81:LYS:HB2	11:U:81:LYS:HE3	1.80	0.43
10:V:99:LYS:HA	10:V:99:LYS:HD3	1.82	0.43
11:W:377:VAL:HG13	11:W:407:GLN:HG3	2.00	0.43
2:D:69:SER:O	2:D:73:THR:OG1	2.36	0.43
2:D:75:HIS:O	4:G:95:ARG:NH2	2.47	0.43
10:X:69:LYS:HE2	10:X:69:LYS:HB2	1.86	0.43
11:Y:66:ILE:HD11	11:Y:69:ARG:NH2	2.33	0.43
2:C:96:THR:HG23	2:C:96:THR:O	2.18	0.43
6:J:-7:DG:H2"	6:J:-6:DG:N7	2.34	0.43
7:M:851:LEU:HD12	7:M:851:LEU:HA	1.82	0.43
10:V:51:GLN:HE22	10:V:373:LEU:H	1.65	0.43
10:X:190:GLN:HB3	10:X:191:ARG:HH12	1.84	0.43
11:Y:303:ILE:HA	11:Y:306:PHE:HD2	1.83	0.43
1:B:93:GLN:O	1:B:97:GLU:HG3	2.19	0.42
4:G:98:GLN:O	4:G:102:ARG:HG2	2.19	0.42
7:M:1379:ILE:HG12	7:M:1394:ILE:HG13	2.00	0.42
11:W:136:ILE:HG12	11:W:230:GLN:HB2	2.01	0.42
11:W:298:VAL:HG11	11:W:323:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:440:ASN:O	10:X:443:LYS:HG2	2.19	0.42
12:Z:213:ALA:HA	12:Z:216:LYS:HG2	2.02	0.42
2:C:46:ILE:O	5:I:7:DC:H5”	2.18	0.42
2:D:95:ARG:HA	2:D:95:ARG:HD3	1.58	0.42
3:E:30:ARG:HA	3:E:33:ARG:HG2	2.00	0.42
6:J:-47:DC:H2’	6:J:-46:DT:H71	2.01	0.42
6:J:-37:DG:H2”	6:J:-36:DG:C8	2.54	0.42
11:U:232:ARG:HA	11:U:232:ARG:HH11	1.83	0.42
10:V:126:ARG:HH21	10:V:249:LEU:HD21	1.84	0.42
11:W:193:ASP:HB3	11:W:196:SER:HB2	2.01	0.42
10:X:418:LEU:O	10:X:421:PRO:HD2	2.18	0.42
1:A:121:LYS:NZ	2:D:50:ILE:HD13	2.35	0.42
1:B:49:ARG:HH12	5:I:-66:DA:H5”	1.83	0.42
1:B:106:ASP:OD1	1:B:106:ASP:N	2.51	0.42
6:J:61:DC:H2”	6:J:62:DG:C8	2.54	0.42
7:M:759:ASN:OD1	7:M:1302:GLN:NE2	2.32	0.42
8:R:44:ASN:ND2	8:R:85:GLU:OE2	2.53	0.42
11:U:283:GLU:OE1	11:U:285:LYS:NZ	2.52	0.42
10:V:140:TYR:HB2	10:V:202:ILE:HG23	2.01	0.42
10:X:113:VAL:HG11	11:Y:109:LEU:O	2.20	0.42
11:Y:45:VAL:H	13:Y:501:ADP:HN62	1.67	0.42
11:Y:268:GLU:HA	11:Y:271:ASP:OD2	2.19	0.42
3:E:34:LEU:HD22	3:E:37:ARG:HH22	1.85	0.42
6:J:-22:DG:N2	7:M:980:MET:SD	2.92	0.42
8:R:13:TYR:HB2	8:R:195:PHE:CG	2.54	0.42
11:U:181:LYS:HE3	11:U:181:LYS:HB3	1.87	0.42
10:V:26:ALA:H	10:V:387:ARG:HH22	1.65	0.42
2:D:33:ALA:HB2	2:D:36:ARG:HH21	1.84	0.42
9:S:167:LEU:HD11	9:S:172:LEU:HD21	2.01	0.42
9:S:173:ARG:HA	9:S:176:GLN:HG2	2.00	0.42
11:U:185:LEU:HD12	11:U:185:LEU:HA	1.90	0.42
11:W:331:LYS:HE2	11:W:331:LYS:HB3	1.87	0.42
4:H:59:GLN:N	4:H:59:GLN:CD	2.77	0.42
6:J:-15:DA:OP1	7:M:779:SER:OG	2.36	0.42
7:M:1055:THR:HG21	7:M:1057:TYR:CZ	2.54	0.42
8:R:25:PRO:HB3	8:R:397:TRP:CD1	2.54	0.42
8:R:407:ASP:HA	8:R:410:ARG:HD3	2.02	0.42
10:T:75:ILE:HG12	10:T:337:VAL:HG12	2.02	0.42
10:T:348:ARG:NH2	11:U:304:GLU:OE2	2.53	0.42
10:V:62:VAL:HG22	10:V:92:ILE:HG13	2.02	0.42
10:V:126:ARG:HA	10:V:126:ARG:HD2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:311:ARG:HA	11:W:311:ARG:HD2	1.90	0.42
11:Y:124:SER:HB2	11:Y:319:PRO:HG3	2.01	0.42
2:C:79:LYS:HD3	2:C:79:LYS:HA	1.75	0.42
4:H:123:LYS:HE3	4:H:123:LYS:HB3	1.75	0.42
5:I:-7:DG:O6	6:J:7:DC:N4	2.31	0.42
5:I:37:DC:H2"	5:I:38:DT:C5	2.55	0.42
9:S:18:TYR:HD2	11:U:145:ILE:HD12	1.85	0.42
10:T:26:ALA:N	10:T:387:ARG:HH22	2.17	0.42
10:T:169:GLY:HA2	10:T:178:THR:HA	2.01	0.42
11:U:147:ARG:HA	11:U:147:ARG:NH1	2.35	0.42
11:U:269:VAL:O	11:U:273:ILE:HG12	2.20	0.42
11:U:315:ASP:OD1	11:U:318:ALA:HB2	2.19	0.42
10:V:246:ASP:OD2	10:V:246:ASP:C	2.63	0.42
10:V:246:ASP:OD2	10:V:247:VAL:N	2.52	0.42
10:X:410:THR:OG1	10:X:411:SER:N	2.52	0.42
11:Y:140:VAL:HG13	11:Y:186:ALA:HA	2.00	0.42
1:A:47:ALA:O	1:A:50:GLU:HG2	2.19	0.42
4:G:111:LYS:HA	4:G:114:VAL:HG22	2.02	0.42
6:J:11:DC:H2"	6:J:12:DG:C8	2.55	0.42
7:M:1062:ILE:HG13	7:M:1133:ARG:HE	1.84	0.42
8:R:270:HIS:HA	8:R:291:ARG:NH2	2.35	0.42
10:T:146:GLU:OE1	10:T:148:THR:OG1	2.36	0.42
11:U:71:VAL:O	11:U:322:MET:HA	2.19	0.42
10:V:42:LYS:HD2	10:V:45:GLU:HB2	2.02	0.42
10:X:348:ARG:NH2	11:Y:304:GLU:OE2	2.52	0.42
3:E:113:HIS:ND1	3:E:115:ASN:HB3	2.35	0.42
5:I:9:DG:H2"	5:I:10:DC:C6	2.55	0.42
6:J:47:DA:H2"	6:J:48:DG:C8	2.55	0.42
7:M:1264:ARG:NH2	7:M:1312:SER:H	2.18	0.42
10:T:446:PHE:HE1	11:U:354:ILE:HD11	1.84	0.42
11:U:130:LYS:HE2	11:U:130:LYS:HB2	1.81	0.42
11:W:130:LYS:HA	11:W:236:VAL:HA	2.02	0.42
11:W:405:VAL:HG11	11:W:430:PHE:CE2	2.55	0.42
10:X:130:GLY:HA2	10:X:248:THR:HA	2.02	0.42
10:X:174:LYS:HE2	10:X:174:LYS:HB3	1.73	0.42
1:A:46:VAL:HA	1:A:49:ARG:HG2	2.02	0.41
3:E:39:ASN:O	3:E:39:ASN:ND2	2.53	0.41
7:M:1347:MET:H	7:M:1347:MET:HE3	1.84	0.41
8:R:280:GLN:OE1	8:R:280:GLN:N	2.47	0.41
10:T:243:ILE:HG22	10:T:245:GLN:H	1.85	0.41
10:X:61:ILE:HD13	10:X:61:ILE:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:190:GLN:CG	10:X:191:ARG:HH22	2.33	0.41
1:B:94:GLU:HG3	1:B:97:GLU:OE1	2.19	0.41
3:E:43:ARG:HA	3:E:43:ARG:HD3	1.75	0.41
3:E:65:GLU:HG2	4:G:52:HIS:CE1	2.55	0.41
4:H:89:LYS:NZ	6:J:-35:DG:H3'	2.35	0.41
5:I:-56:DC:H2"	5:I:-55:DG:N7	2.34	0.41
6:J:-80:DT:H2"	6:J:-79:DA:C5	2.55	0.41
8:R:42:LEU:O	8:R:46:ILE:HG13	2.19	0.41
8:R:63:LEU:O	8:R:196:ASN:ND2	2.48	0.41
10:T:189:ILE:HD11	10:T:194:VAL:HB	2.01	0.41
11:U:192:ILE:HD13	11:U:192:ILE:HA	1.91	0.41
12:Z:220:ILE:O	12:Z:223:ARG:HG3	2.20	0.41
12:Z:260:LYS:O	12:Z:264:VAL:HG22	2.20	0.41
5:I:22:DC:H2"	5:I:23:DA:O4'	2.19	0.41
7:M:811:HIS:HA	7:M:814:LYS:HE2	2.02	0.41
8:R:129:PHE:HA	8:R:432:PHE:CZ	2.55	0.41
10:T:185:ILE:O	10:T:189:ILE:HG22	2.20	0.41
10:V:197:GLY:HA3	10:V:218:TYR:HE2	1.84	0.41
10:V:462:TYR:HB2	11:W:328:GLY:HA3	2.02	0.41
10:X:191:ARG:HA	10:X:191:ARG:NE	2.35	0.41
10:X:448:ASP:OD1	10:X:451:ARG:NE	2.33	0.41
12:Z:234:HIS:HD2	12:Z:238:GLN:NE2	2.18	0.41
3:F:51:TYR:HB3	4:H:97:ILE:CD1	2.50	0.41
3:F:94:LEU:O	3:F:98:LEU:N	2.37	0.41
4:G:89:LYS:NZ	5:I:-33:DA:OP1	2.54	0.41
5:I:-93:DT:H2"	5:I:-92:DT:C5	2.54	0.41
9:S:16:ASP:HB3	11:U:147:ARG:HB2	2.02	0.41
10:T:105:LEU:HD12	10:T:105:LEU:HA	1.86	0.41
11:W:38:ARG:O	11:W:51:ARG:NH2	2.49	0.41
11:W:256:ALA:HA	11:W:259:THR:HG22	2.01	0.41
11:W:405:VAL:HG21	11:W:430:PHE:HE2	1.85	0.41
11:Y:250:ARG:HG3	11:Y:251:THR:N	2.35	0.41
12:Z:587:PRO:HA	12:Z:588:GLU:HB2	2.03	0.41
3:E:70:ALA:HA	3:E:73:ASP:OD2	2.21	0.41
3:F:64:LEU:HD12	4:H:47:VAL:HG12	2.02	0.41
8:R:373:LEU:HD23	8:R:383:CYS:SG	2.60	0.41
10:T:69:LYS:HD2	10:T:69:LYS:HA	1.67	0.41
11:U:342:GLY:O	11:U:343:LEU:HD23	2.20	0.41
10:V:440:ASN:HA	10:V:443:LYS:HD3	2.02	0.41
12:Z:603:ASN:C	12:Z:603:ASN:HD22	2.10	0.41
3:F:58:TYR:O	3:F:62:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:693:ARG:HD2	7:M:769:PRO:HD3	2.02	0.41
7:M:968:ALA:O	7:M:972:ALA:N	2.54	0.41
11:Y:17:LEU:HD13	11:Y:17:LEU:HA	1.95	0.41
2:D:75:HIS:CE1	4:G:83:LEU:HD21	2.56	0.41
7:M:1370:VAL:HG13	7:M:1376:GLU:HB2	2.03	0.41
8:R:62:GLU:N	8:R:65:GLN:O	2.48	0.41
9:S:169:PRO:O	9:S:173:ARG:HG2	2.20	0.41
10:T:79:GLY:HA3	10:T:372:THR:OG1	2.21	0.41
10:T:445:LEU:HD23	10:T:445:LEU:HA	1.92	0.41
10:X:393:LEU:HD12	10:X:434:ILE:HD11	2.01	0.41
10:X:445:LEU:HD23	10:X:445:LEU:HA	1.95	0.41
11:Y:25:HIS:CD2	11:Y:26:ILE:HG23	2.56	0.41
12:Z:223:ARG:HD2	12:Z:224:ILE:N	2.35	0.41
3:F:51:TYR:CE1	4:H:117:GLY:HA3	2.56	0.41
6:J:33:DT:H2"	6:J:34:DC:C6	2.56	0.41
7:M:706:TRP:CG	7:M:930:LEU:HD13	2.56	0.41
7:M:1143:LEU:O	7:M:1146:LYS:HG2	2.21	0.41
8:R:288:ARG:NH2	8:R:295:VAL:O	2.53	0.41
10:X:454:LYS:HB2	10:X:454:LYS:HE3	1.84	0.41
12:Z:605:PRO:HG2	12:Z:608:LEU:CB	2.47	0.41
1:A:42:LYS:HA	1:A:42:LYS:HD2	1.73	0.41
1:B:42:LYS:H	1:B:42:LYS:HG2	1.67	0.41
1:B:85:GLN:N	1:B:85:GLN:OE1	2.54	0.41
2:D:72:TYR:CE2	2:D:85:ASP:HA	2.55	0.41
4:G:83:LEU:HA	4:G:86:TYR:CZ	2.56	0.41
6:J:27:DG:H2"	6:J:28:DA:C8	2.56	0.41
7:M:723:MET:SD	7:M:1357:ARG:HD3	2.61	0.41
7:M:1375:ILE:H	7:M:1375:ILE:HD12	1.85	0.41
8:R:222:PHE:CD1	9:S:105:LEU:HD22	2.56	0.41
8:R:223:LEU:HB2	8:R:249:LYS:HZ2	1.86	0.41
11:U:31:LEU:HA	11:U:31:LEU:HD23	1.83	0.41
11:U:179:LEU:HD13	11:U:179:LEU:HA	1.96	0.41
11:W:397:ARG:HD2	10:X:366:ARG:HA	2.03	0.41
10:X:256:ASN:HB3	10:X:284:LEU:HD11	2.01	0.41
11:Y:233:LYS:HA	11:Y:233:LYS:HD2	1.76	0.41
1:B:94:GLU:OE1	3:E:104:ALA:HA	2.21	0.41
2:D:93:GLN:HE22	2:D:95:ARG:HG2	1.86	0.41
3:E:56:LEU:HD13	3:E:56:LEU:HA	1.88	0.41
5:I:-70:DG:H2"	5:I:-69:DA:C8	2.56	0.41
8:R:121:GLU:CB	9:S:198:LEU:HD11	2.50	0.41
11:U:302:ASP:OD1	11:U:303:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:409:ILE:H	11:U:409:ILE:HG13	1.60	0.41
11:W:45:VAL:HG11	11:W:366:THR:OG1	2.20	0.41
11:W:194:LYS:HA	11:W:194:LYS:HD2	1.61	0.41
11:W:233:LYS:HE2	11:W:233:LYS:HB2	1.87	0.41
11:W:430:PHE:CE1	10:X:57:ALA:HB1	2.56	0.41
10:X:77:LEU:HD12	10:X:85:LYS:HG2	2.02	0.41
10:X:136:THR:HG22	10:X:242:GLU:HG2	2.03	0.41
10:X:139:VAL:HG22	10:X:201:TYR:HE1	1.86	0.41
10:X:180:ARG:NH2	12:Z:315:LYS:HE2	2.35	0.41
10:X:266:ILE:HA	10:X:269:MET:HB2	2.03	0.41
12:Z:217:ARG:HA	12:Z:217:ARG:HD2	1.87	0.41
12:Z:296:LEU:HD23	12:Z:296:LEU:HA	1.82	0.41
1:A:63:ARG:HB2	1:A:66:PRO:HD2	2.03	0.40
1:B:52:ARG:O	1:B:56:LYS:HG3	2.21	0.40
6:J:50:DG:H2"	6:J:51:DG:H8	1.86	0.40
7:M:998:LEU:C	7:M:999:PHE:HD1	2.30	0.40
7:M:1275:LEU:HD13	7:M:1291:ARG:HD2	2.03	0.40
8:R:292:LYS:HD3	8:R:294:ASN:OD1	2.21	0.40
11:U:45:VAL:H	13:U:502:ADP:HN62	1.68	0.40
11:U:279:GLU:O	11:U:282:GLU:HG3	2.21	0.40
11:W:126:GLY:HA2	11:W:240:SER:HA	2.03	0.40
11:W:146:ASP:N	11:W:155:GLN:O	2.44	0.40
11:W:413:ARG:HH22	11:W:419:GLU:HG3	1.87	0.40
10:X:80:GLY:O	10:X:83:THR:OG1	2.32	0.40
1:A:43:PRO:HA	6:J:9:DT:H5'	2.02	0.40
1:A:87:SER:HB2	2:D:100:PHE:HE1	1.85	0.40
1:A:102:SER:HA	1:A:105:GLU:OE1	2.21	0.40
5:I:27:DG:H2"	5:I:28:DG:C8	2.56	0.40
6:J:-48:DC:H2"	6:J:-47:DC:C5	2.56	0.40
6:J:56:DG:H2"	6:J:57:DG:C8	2.56	0.40
7:M:727:LYS:O	7:M:731:THR:HG23	2.21	0.40
7:M:960:LEU:HD12	7:M:960:LEU:HA	1.92	0.40
7:M:989:LEU:HB3	7:M:1375:ILE:HD13	2.03	0.40
8:R:70:GLU:H	8:R:70:GLU:HG2	1.64	0.40
8:R:106:MET:HE3	9:S:225:ILE:HG12	2.04	0.40
8:R:232:SER:HA	8:R:236:TYR:O	2.21	0.40
10:T:456:LEU:HD23	10:T:456:LEU:HA	1.86	0.40
11:U:394:THR:OG1	11:U:395:SER:N	2.54	0.40
11:U:407:GLN:O	11:U:411:MET:SD	2.79	0.40
10:V:222:PHE:CD1	11:W:172:GLY:HA2	2.56	0.40
10:V:316:LEU:HB2	10:V:321:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:301:LEU:O	11:W:333:ARG:HB2	2.21	0.40
10:X:139:VAL:HG13	10:X:201:TYR:HD1	1.86	0.40
12:Z:299:PRO:N	12:Z:300:ALA:HA	2.36	0.40
5:I:-79:DG:H1	6:J:79:DC:H2"	1.87	0.40
7:M:794:ASP:OD1	7:M:794:ASP:N	2.52	0.40
7:M:1309:ASN:HD21	7:M:1330:LEU:HA	1.85	0.40
8:R:16:LYS:HB2	8:R:16:LYS:HE2	1.90	0.40
11:U:240:SER:HB3	11:U:243:GLU:HG3	2.04	0.40
11:U:362:GLN:HA	11:U:365:LYS:HE2	2.02	0.40
10:V:211:ARG:HE	10:V:211:ARG:HB2	1.76	0.40
10:V:250:HIS:O	10:V:254:VAL:HG13	2.21	0.40
10:V:418:LEU:C	10:V:421:PRO:HD2	2.46	0.40
10:V:424:ILE:HD11	11:W:60:MET:HB2	2.03	0.40
11:W:57:ILE:HD13	11:W:71:VAL:HG11	2.03	0.40
1:B:62:ILE:HD13	1:B:62:ILE:HA	1.89	0.40
3:E:89:ARG:HA	3:E:95:ASN:OD1	2.21	0.40
6:J:-38:DA:H2"	6:J:-37:DG:N7	2.36	0.40
7:M:926:ARG:N	7:M:927:PRO:HD2	2.35	0.40
7:M:996:PRO:HD2	7:M:1245:CYS:HG	1.85	0.40
9:S:263:ILE:HD11	9:S:268:CYS:HB3	2.04	0.40
11:U:409:ILE:HA	11:U:412:LYS:HB2	2.02	0.40
10:X:26:ALA:H	10:X:387:ARG:HH22	1.68	0.40
10:X:417:GLN:OE1	11:Y:69:ARG:HD2	2.22	0.40
11:Y:61:VAL:HG22	11:Y:320:ILE:HD13	2.03	0.40
11:Y:161:LYS:HA	11:Y:166:GLU:HB2	2.02	0.40
2:C:51:TYR:O	2:C:54:VAL:HG22	2.22	0.40
7:M:697:ARG:HD2	7:M:699:TYR:OH	2.21	0.40
7:M:819:GLN:HA	7:M:846:GLN:NE2	2.36	0.40
7:M:862:GLU:H	7:M:862:GLU:HG3	1.59	0.40
9:S:172:LEU:HD23	9:S:172:LEU:HA	1.94	0.40
10:T:134:LYS:HA	10:T:243:ILE:O	2.22	0.40
11:U:47:GLN:HE22	11:U:357:LYS:H	1.68	0.40
10:V:49:VAL:H	13:V:501:ADP:HN62	1.70	0.40
10:V:73:ARG:HD2	10:V:73:ARG:HA	1.89	0.40
10:V:234:LYS:HD3	10:V:234:LYS:HA	1.73	0.40
10:V:352:ASP:N	10:V:352:ASP:OD1	2.52	0.40
10:X:198:ASP:CG	10:X:211:ARG:HE	2.28	0.40
11:Y:273:ILE:HD13	11:Y:273:ILE:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/136 (70%)	89 (94%)	6 (6%)	0	100	100
1	B	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
2	C	80/103 (78%)	79 (99%)	1 (1%)	0	100	100
2	D	78/103 (76%)	73 (94%)	5 (6%)	0	100	100
3	E	101/158 (64%)	101 (100%)	0	0	100	100
3	F	99/158 (63%)	99 (100%)	0	0	100	100
4	G	94/131 (72%)	89 (95%)	5 (5%)	0	100	100
4	H	89/131 (68%)	86 (97%)	3 (3%)	0	100	100
7	M	684/1514 (45%)	628 (92%)	56 (8%)	0	100	100
8	R	407/438 (93%)	398 (98%)	9 (2%)	0	100	100
9	S	200/280 (71%)	196 (98%)	4 (2%)	0	100	100
10	T	441/463 (95%)	424 (96%)	17 (4%)	0	100	100
10	V	430/463 (93%)	418 (97%)	12 (3%)	0	100	100
10	X	440/463 (95%)	425 (97%)	15 (3%)	0	100	100
11	U	426/471 (90%)	408 (96%)	18 (4%)	0	100	100
11	W	429/471 (91%)	420 (98%)	9 (2%)	0	100	100
11	Y	445/471 (94%)	430 (97%)	15 (3%)	0	100	100
12	Z	176/180 (98%)	153 (87%)	20 (11%)	3 (2%)	7	34
All	All	4809/6270 (77%)	4608 (96%)	198 (4%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	Z	325	ARG
12	Z	299	PRO
12	Z	326	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	84/113 (74%)	84 (100%)	0	100 100
1	B	84/113 (74%)	83 (99%)	1 (1%)	67 77
2	C	68/81 (84%)	67 (98%)	1 (2%)	60 74
2	D	67/81 (83%)	67 (100%)	0	100 100
3	E	82/124 (66%)	81 (99%)	1 (1%)	67 77
3	F	80/124 (64%)	80 (100%)	0	100 100
4	G	82/109 (75%)	81 (99%)	1 (1%)	67 77
4	H	78/109 (72%)	77 (99%)	1 (1%)	65 76
7	M	574/1376 (42%)	573 (100%)	1 (0%)	92 94
8	R	372/396 (94%)	371 (100%)	1 (0%)	91 92
9	S	199/261 (76%)	198 (100%)	1 (0%)	86 90
10	T	371/391 (95%)	370 (100%)	1 (0%)	91 92
10	V	368/391 (94%)	367 (100%)	1 (0%)	91 92
10	X	374/391 (96%)	374 (100%)	0	100 100
11	U	367/403 (91%)	366 (100%)	1 (0%)	91 92
11	W	369/403 (92%)	368 (100%)	1 (0%)	91 92
11	Y	372/403 (92%)	372 (100%)	0	100 100
12	Z	143/171 (84%)	142 (99%)	1 (1%)	81 86
All	All	4134/5440 (76%)	4121 (100%)	13 (0%)	90 92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	108	ASN
2	C	86	VAL
3	E	90	ASN
4	G	109	LEU
4	H	44	ILE
7	M	999	PHE

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Mol	Chain	Res	Type
8	R	8	ILE
9	S	13	TYR
10	T	462	TYR
11	U	409	ILE
10	V	304	ILE
11	W	300	MET
12	Z	603	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	16	GLN
3	E	39	ASN
3	E	69	ASN
3	E	74	ASN
3	F	32	HIS
3	F	42	GLN
3	F	74	ASN
4	G	50	GLN
4	G	52	HIS
4	H	87	ASN
7	M	705	ASN
7	M	781	GLN
7	M	859	ASN
7	M	1110	GLN
7	M	1139	ASN
7	M	1228	GLN
7	M	1352	GLN
7	M	1356	HIS
8	R	22	ASN
8	R	319	HIS
9	S	176	GLN
10	T	250	HIS
10	T	461	ASN
11	U	23	HIS
11	U	119	GLN
11	U	223	GLN
11	U	401	ASN
11	U	446	GLN
10	V	51	GLN
10	V	205	ASN
11	W	47	GLN

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Mol	Chain	Res	Type
11	W	62	GLN
11	W	173	ASN
11	W	242	HIS
11	W	326	ASN
11	W	453	ASN
10	X	260	GLN
10	X	440	ASN
11	Y	47	GLN
11	Y	173	ASN
11	Y	242	HIS
12	Z	230	GLN
12	Z	234	HIS
12	Z	262	GLN
12	Z	310	GLN
12	Z	594	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\#\|Z\|>2$
13	ADP	X	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	T	501	15	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	M	1601	15	24,29,29	0.97	1 (4%)	29,45,45	1.44	4 (13%)
13	ADP	R	501	14,15	24,29,29	0.94	1 (4%)	29,45,45	1.48	4 (13%)
14	BEF	R	502	13	0,3,3	-	-	-		
14	BEF	M	1602	-	0,3,3	-	-	-		
13	ADP	U	502	15	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	W	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.40	4 (13%)
13	ADP	Y	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	V	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.41	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
13	ADP	X	501	15	-	3/12/32/32	0/3/3/3
13	ADP	T	501	15	-	5/12/32/32	0/3/3/3
13	ADP	M	1601	15	-	5/12/32/32	0/3/3/3
13	ADP	R	501	14,15	-	4/12/32/32	0/3/3/3
13	ADP	U	502	15	-	2/12/32/32	0/3/3/3
13	ADP	W	501	15	-	4/12/32/32	0/3/3/3
13	ADP	Y	501	15	-	2/12/32/32	0/3/3/3
13	ADP	V	501	15	-	5/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1601	ADP	C5-C4	2.49	1.47	1.40
13	W	501	ADP	C5-C4	2.48	1.47	1.40
13	Y	501	ADP	C5-C4	2.48	1.47	1.40
13	X	501	ADP	C5-C4	2.47	1.47	1.40
13	V	501	ADP	C5-C4	2.46	1.47	1.40
13	R	501	ADP	C5-C4	2.43	1.47	1.40
13	U	502	ADP	C5-C4	2.42	1.47	1.40
13	T	501	ADP	C5-C4	2.38	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	501	ADP	PA-O3A-PB	-4.14	118.62	132.83
13	Y	501	ADP	PA-O3A-PB	-3.97	119.22	132.83
13	R	501	ADP	PA-O3A-PB	-3.84	119.65	132.83
13	X	501	ADP	PA-O3A-PB	-3.80	119.77	132.83
13	U	502	ADP	PA-O3A-PB	-3.65	120.29	132.83
13	U	502	ADP	C3'-C2'-C1'	3.58	106.36	100.98
13	X	501	ADP	C3'-C2'-C1'	3.53	106.29	100.98
13	M	1601	ADP	C3'-C2'-C1'	3.44	106.16	100.98
13	V	501	ADP	C3'-C2'-C1'	3.19	105.78	100.98
13	M	1601	ADP	N3-C2-N1	-3.17	123.72	128.68
13	R	501	ADP	N3-C2-N1	-3.16	123.74	128.68
13	X	501	ADP	N3-C2-N1	-3.13	123.79	128.68
13	Y	501	ADP	N3-C2-N1	-3.12	123.80	128.68
13	T	501	ADP	N3-C2-N1	-3.11	123.81	128.68
13	Y	501	ADP	C3'-C2'-C1'	3.11	105.67	100.98
13	V	501	ADP	N3-C2-N1	-3.11	123.82	128.68
13	R	501	ADP	C3'-C2'-C1'	3.10	105.64	100.98
13	W	501	ADP	N3-C2-N1	-3.06	123.89	128.68
13	U	502	ADP	N3-C2-N1	-3.04	123.93	128.68
13	M	1601	ADP	PA-O3A-PB	-3.04	122.41	132.83
13	V	501	ADP	PA-O3A-PB	-3.03	122.42	132.83
13	W	501	ADP	PA-O3A-PB	-3.03	122.43	132.83
13	W	501	ADP	C3'-C2'-C1'	2.97	105.45	100.98
13	T	501	ADP	C3'-C2'-C1'	2.92	105.38	100.98
13	T	501	ADP	C4-C5-N7	-2.69	106.59	109.40
13	W	501	ADP	C4-C5-N7	-2.67	106.62	109.40
13	V	501	ADP	C4-C5-N7	-2.64	106.65	109.40
13	R	501	ADP	C4-C5-N7	-2.62	106.67	109.40
13	U	502	ADP	C4-C5-N7	-2.57	106.72	109.40
13	Y	501	ADP	C4-C5-N7	-2.57	106.72	109.40
13	X	501	ADP	C4-C5-N7	-2.56	106.73	109.40
13	M	1601	ADP	C4-C5-N7	-2.54	106.75	109.40

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PB-O3A-PA-O5'
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	C3'-C4'-C5'-O5'
13	T	501	ADP	C5'-O5'-PA-O2A
13	U	502	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
13	V	501	ADP	PA-O3A-PB-O2B
13	V	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	PA-O3A-PB-O2B
13	W	501	ADP	C5'-O5'-PA-O1A
13	W	501	ADP	C5'-O5'-PA-O3A
13	X	501	ADP	C5'-O5'-PA-O3A
13	Y	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	O4'-C4'-C5'-O5'
13	T	501	ADP	O4'-C4'-C5'-O5'
13	T	501	ADP	C3'-C4'-C5'-O5'
13	X	501	ADP	C3'-C4'-C5'-O5'
13	M	1601	ADP	C5'-O5'-PA-O3A
13	T	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	C5'-O5'-PA-O1A
13	T	501	ADP	C5'-O5'-PA-O1A
13	U	502	ADP	C5'-O5'-PA-O1A
13	X	501	ADP	C5'-O5'-PA-O1A
13	Y	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	PA-O3A-PB-O1B
13	W	501	ADP	PA-O3A-PB-O3B
13	M	1601	ADP	O4'-C4'-C5'-O5'
13	M	1601	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

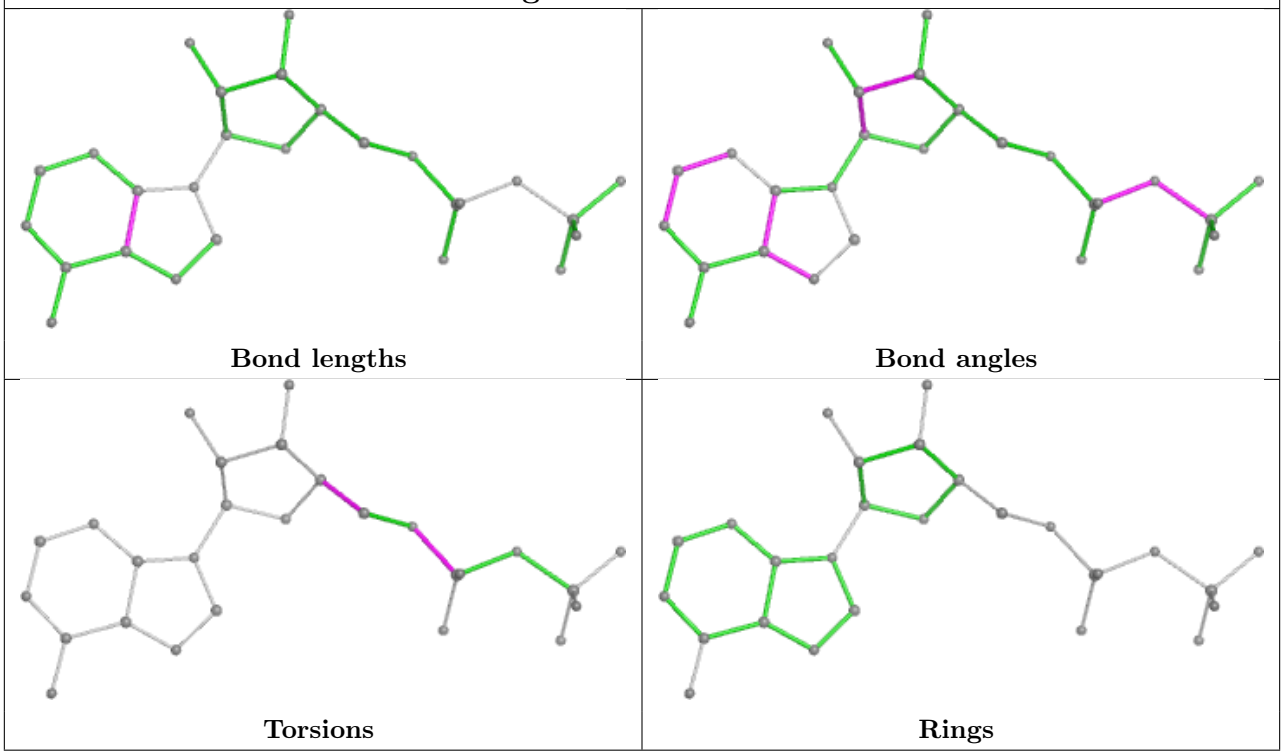
8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	X	501	ADP	3	0
13	T	501	ADP	1	0
13	M	1601	ADP	6	0
14	M	1602	BEF	1	0
13	U	502	ADP	3	0
13	W	501	ADP	4	0
13	Y	501	ADP	1	0
13	V	501	ADP	5	0

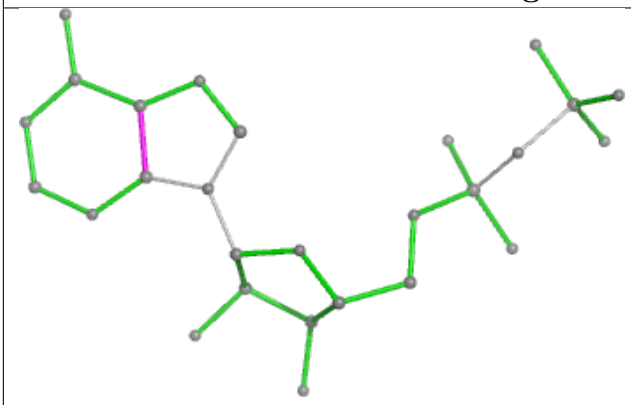
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

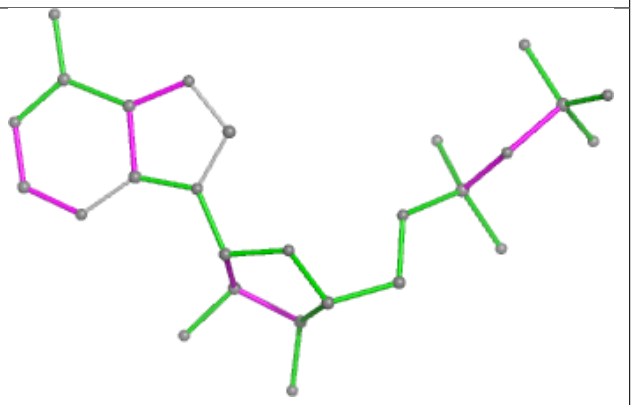
Ligand ADP X 501



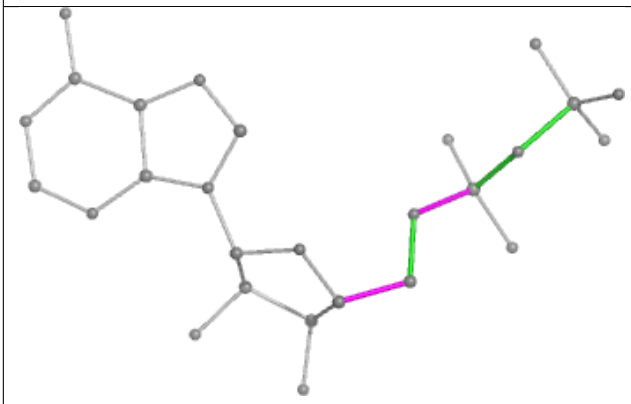
Ligand ADP T 501



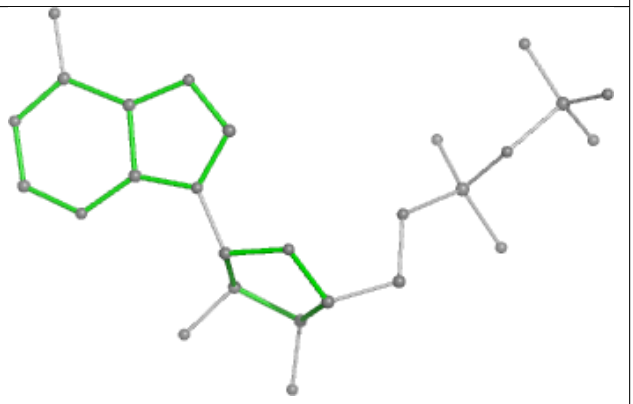
Bond lengths



Bond angles

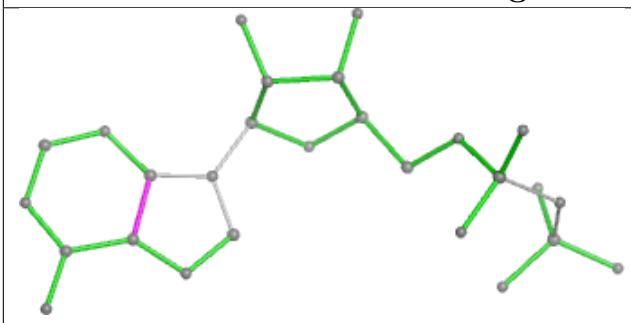


Torsions

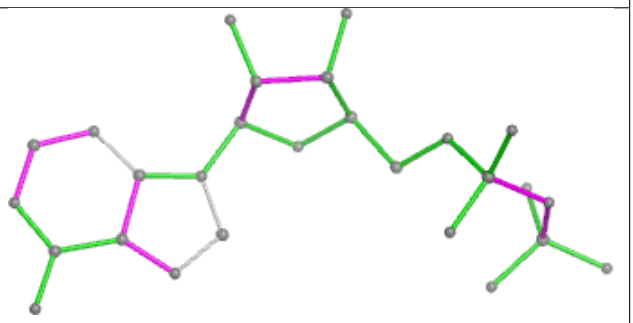


Rings

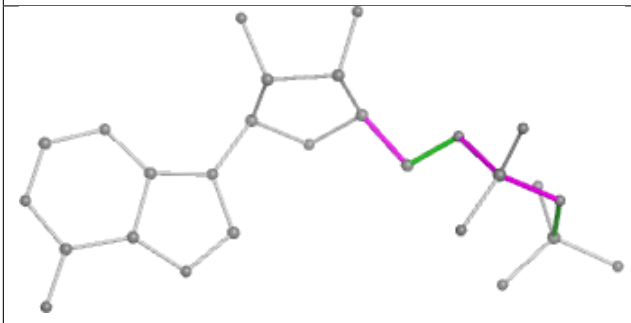
Ligand ADP M 1601



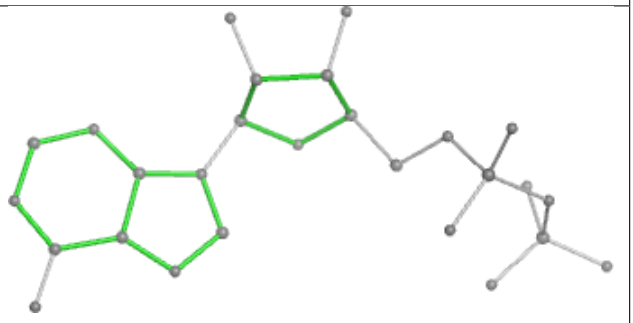
Bond lengths



Bond angles

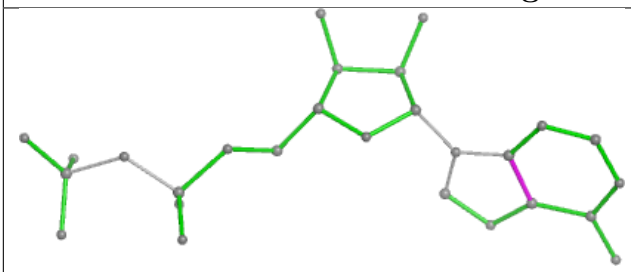


Torsions

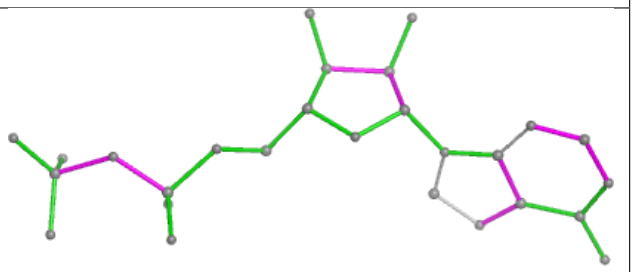


Rings

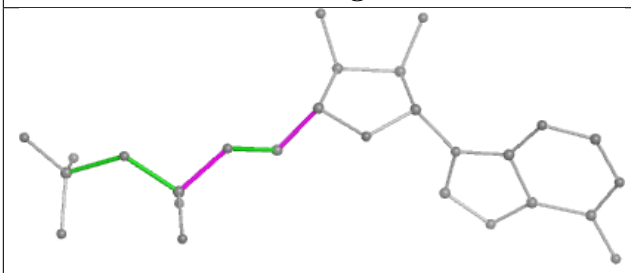
Ligand ADP R 501



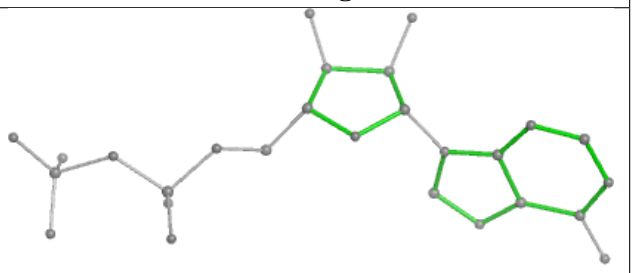
Bond lengths



Bond angles

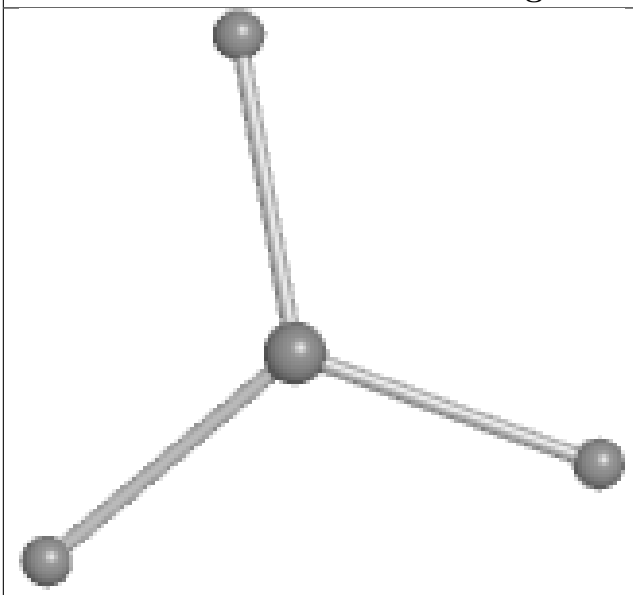


Torsions

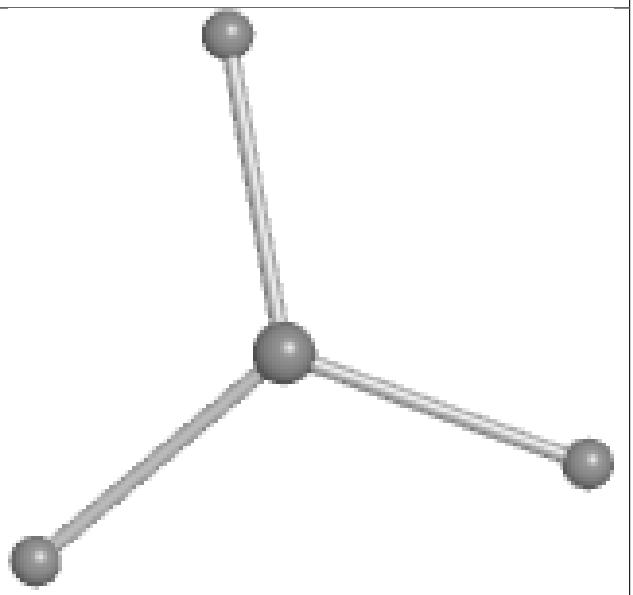


Rings

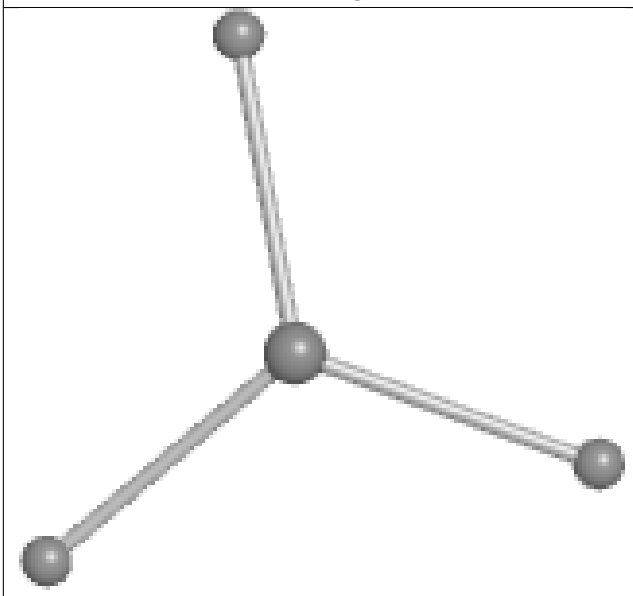
Ligand BEF R 502



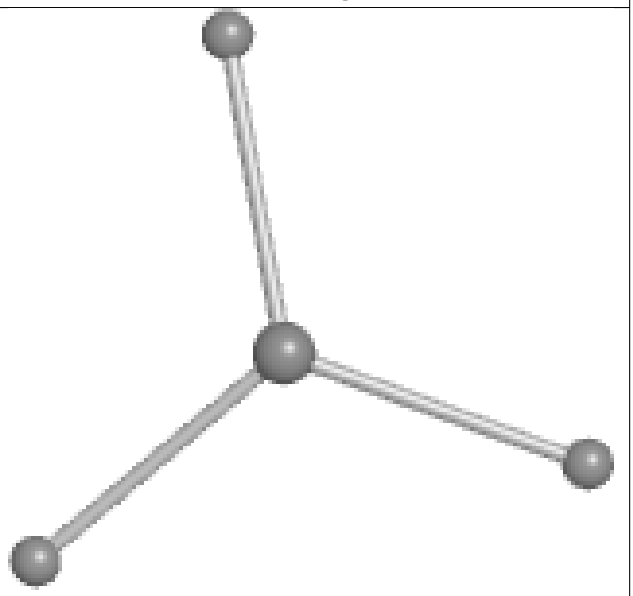
Bond lengths



Bond angles

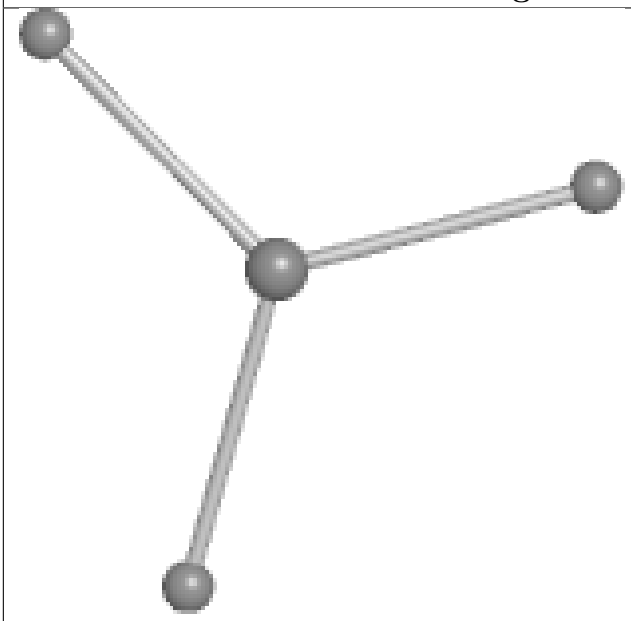


Torsions

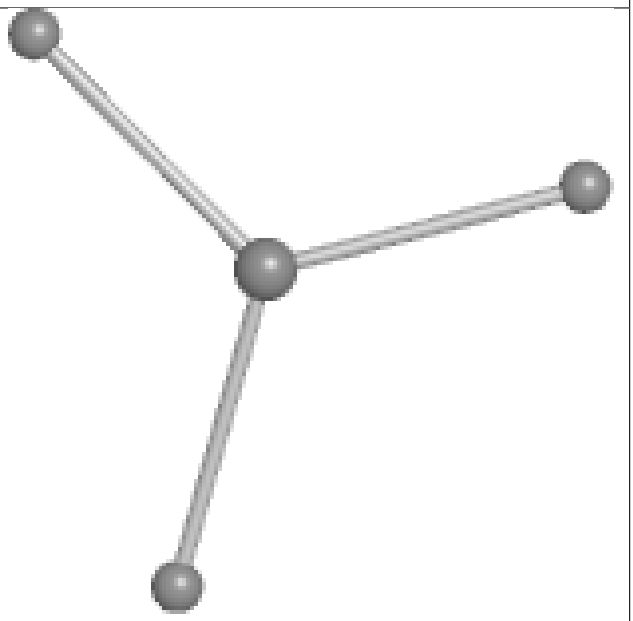


Rings

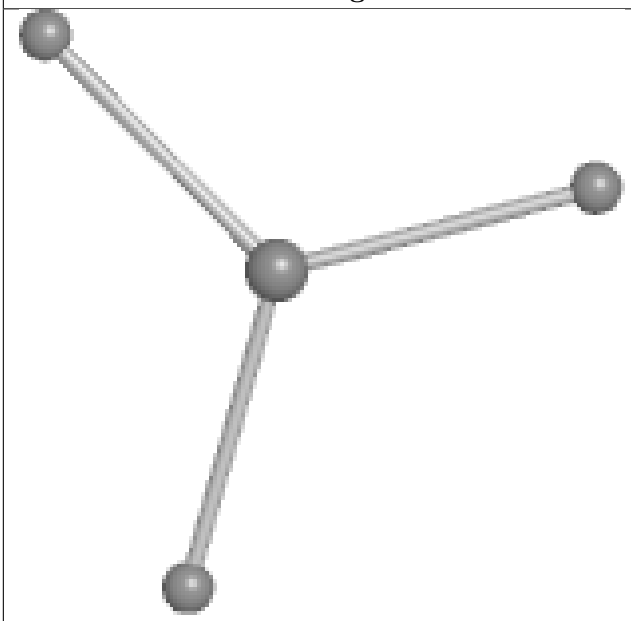
Ligand BEF M 1602



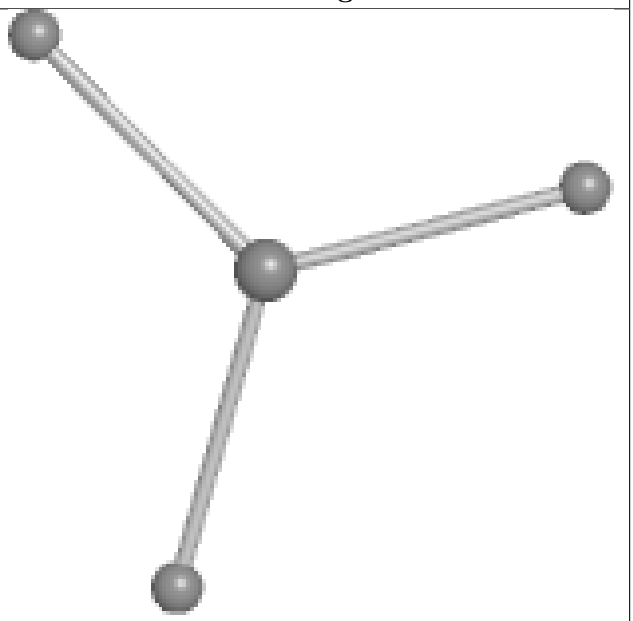
Bond lengths



Bond angles

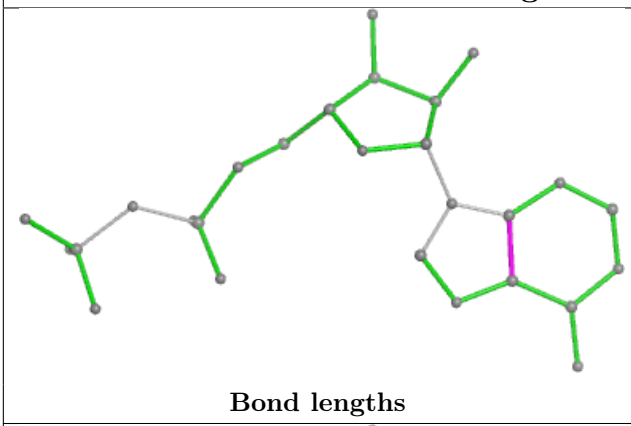


Torsions

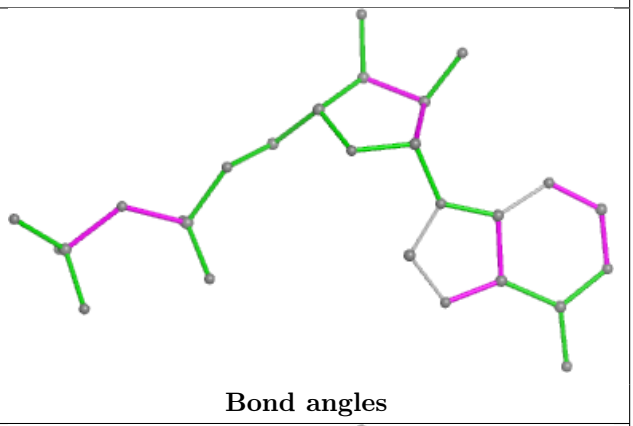


Rings

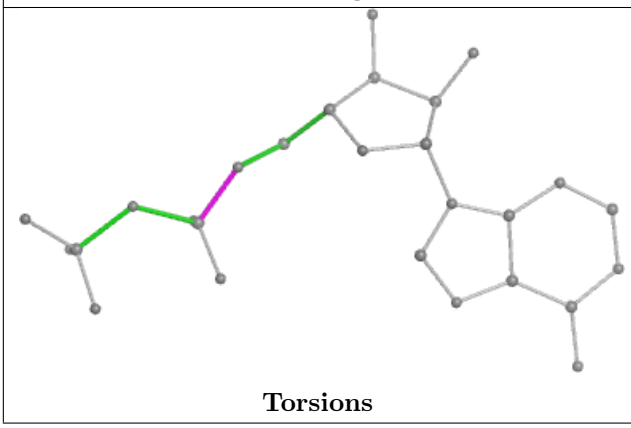
Ligand ADP U 502



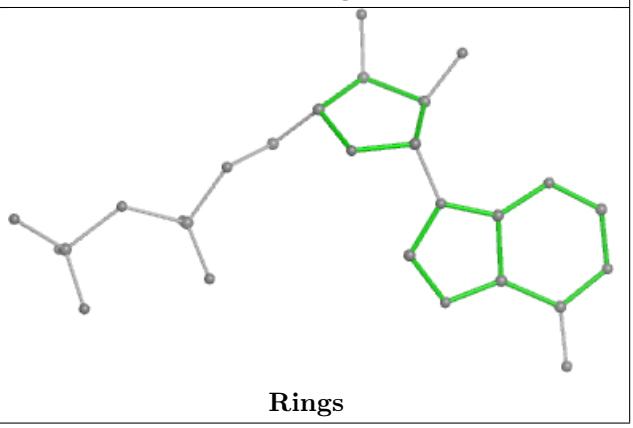
Bond lengths



Bond angles

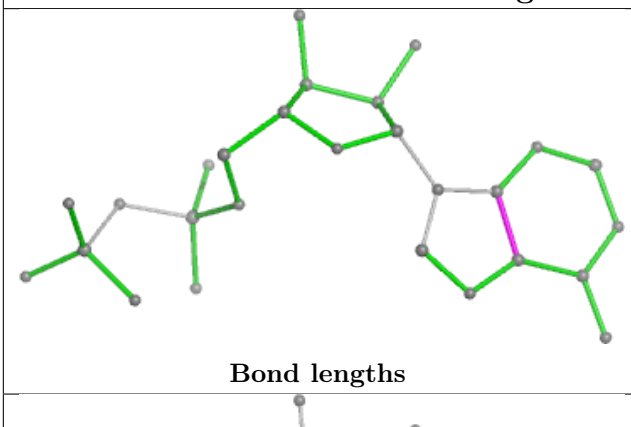


Torsions

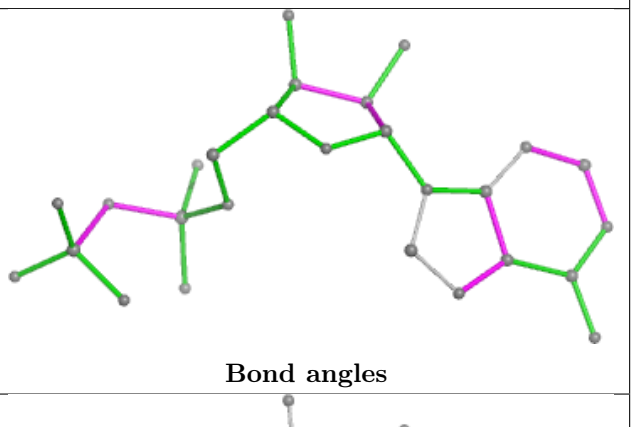


Rings

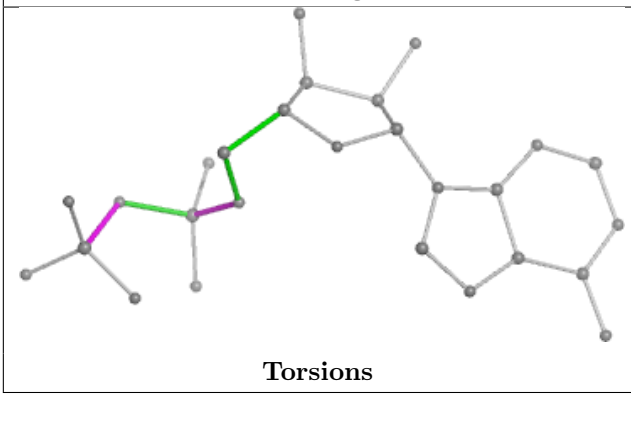
Ligand ADP W 501



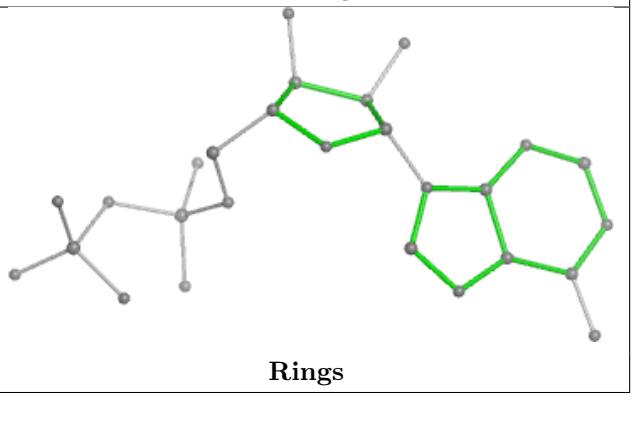
Bond lengths



Bond angles

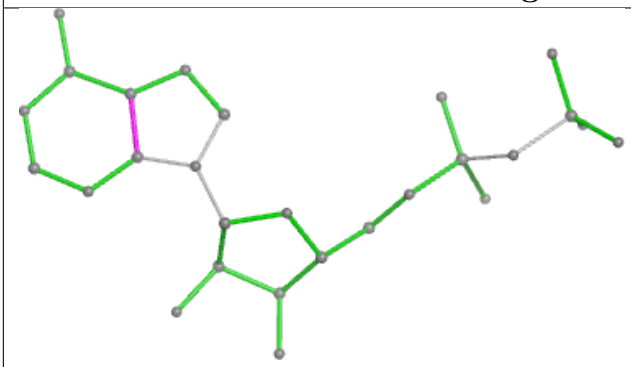


Torsions

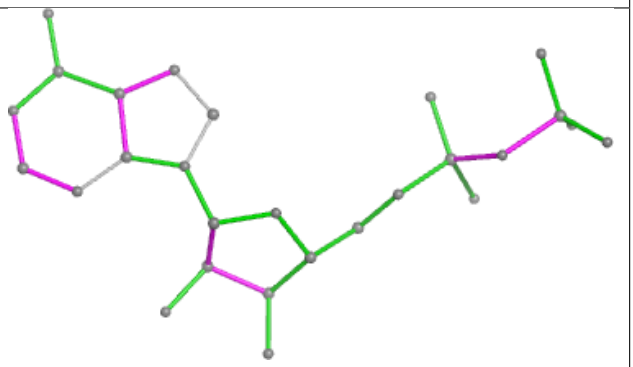


Rings

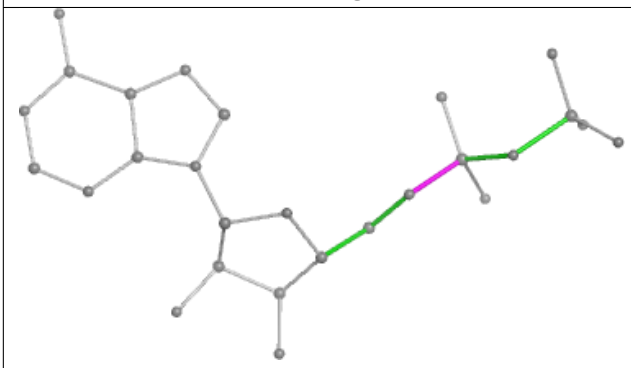
Ligand ADP Y 501



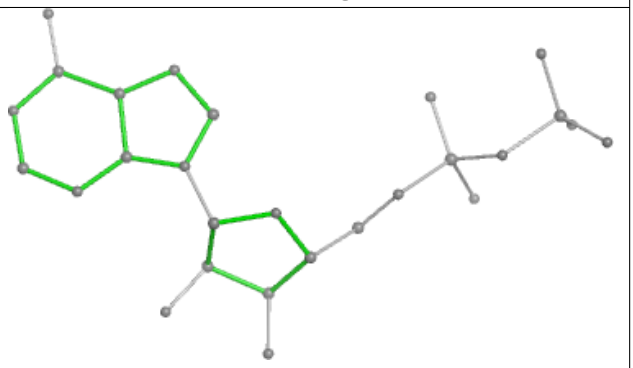
Bond lengths



Bond angles

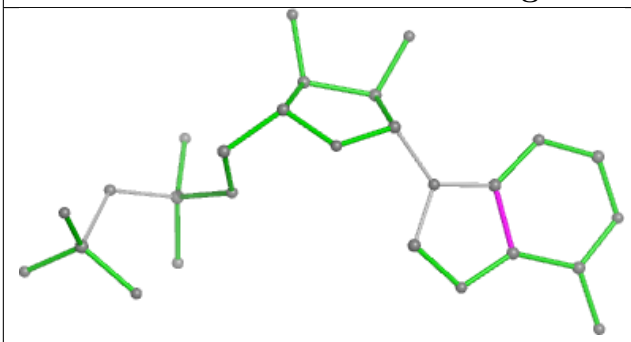


Torsions

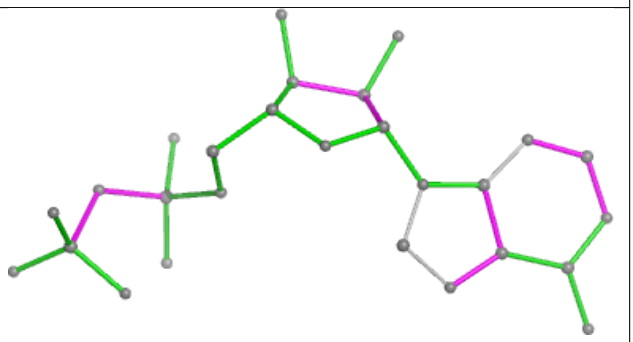


Rings

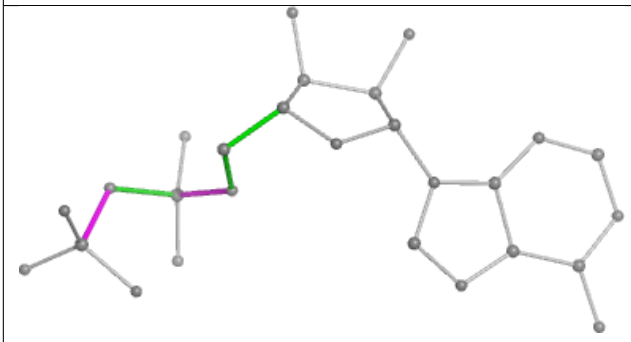
Ligand ADP V 501



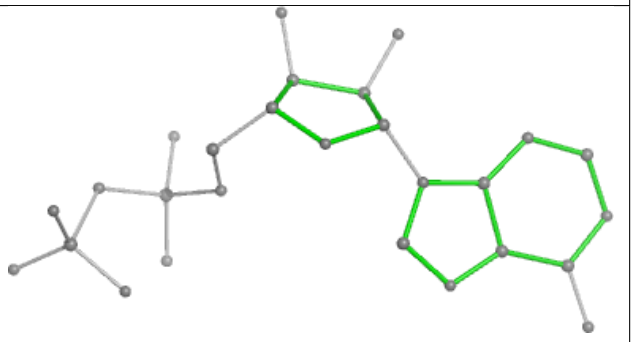
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	329:LYS	C	581:THR	N	65.95

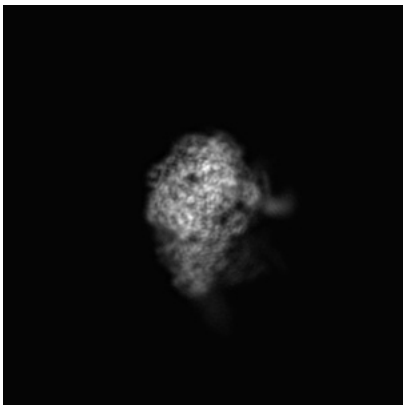
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18471. These allow visual inspection of the internal detail of the map and identification of artifacts.

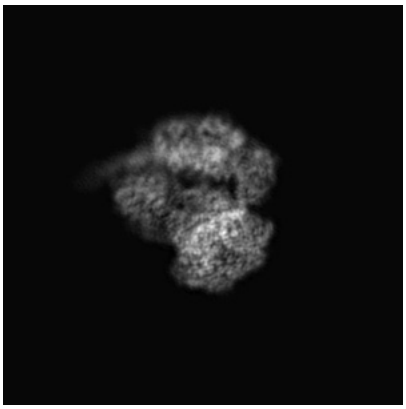
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

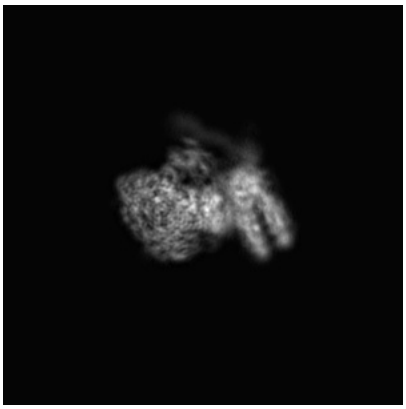
6.1.1 Primary map



X

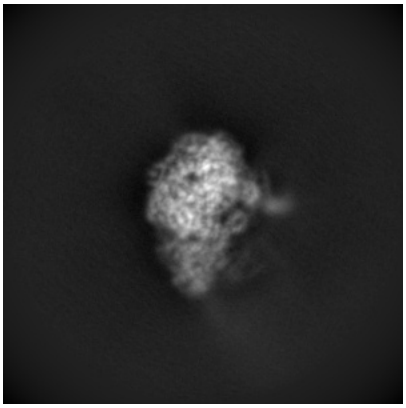


Y

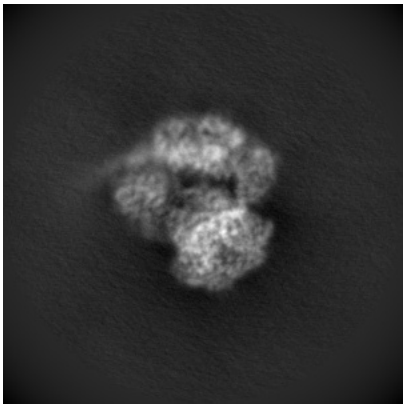


Z

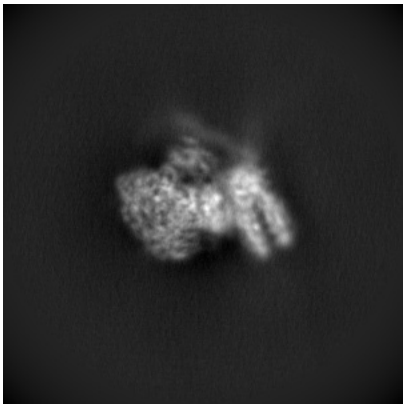
6.1.2 Raw map



X



Y

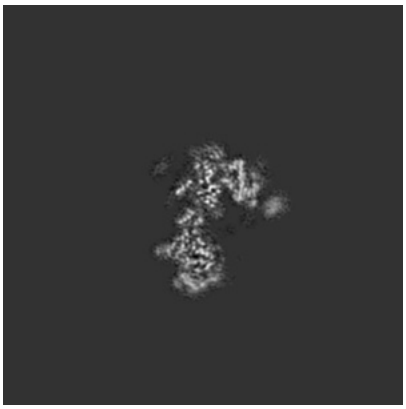


Z

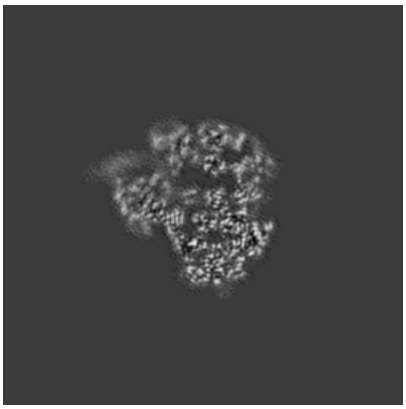
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

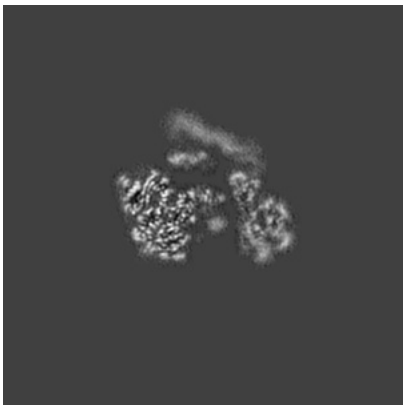
6.2.1 Primary map



X Index: 192

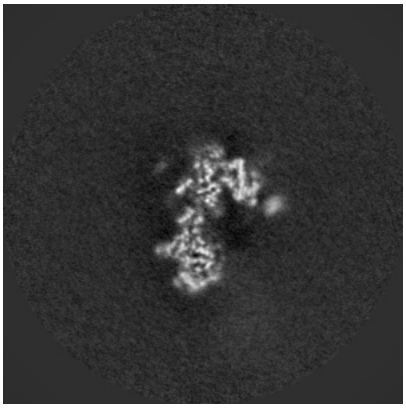


Y Index: 192

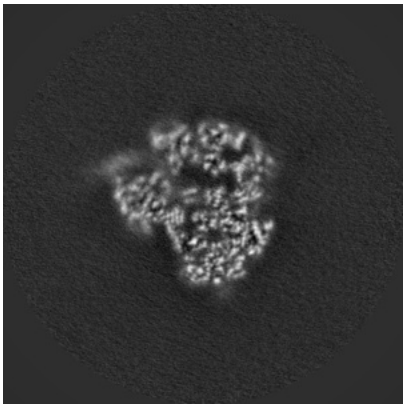


Z Index: 192

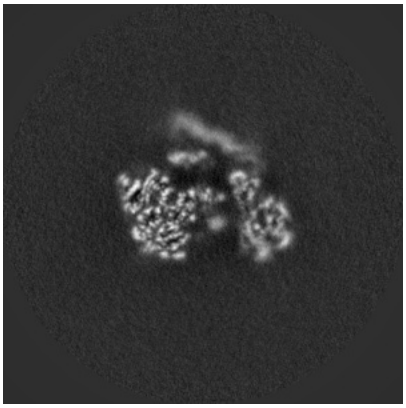
6.2.2 Raw map



X Index: 192



Y Index: 192

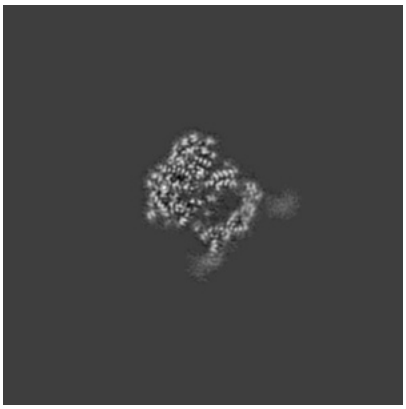


Z Index: 192

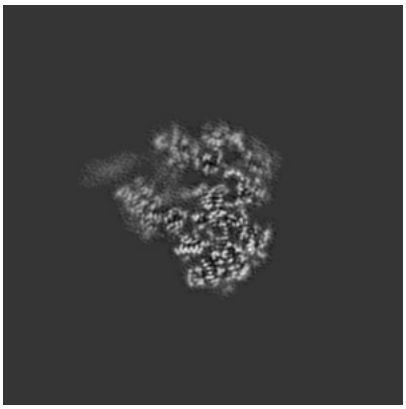
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

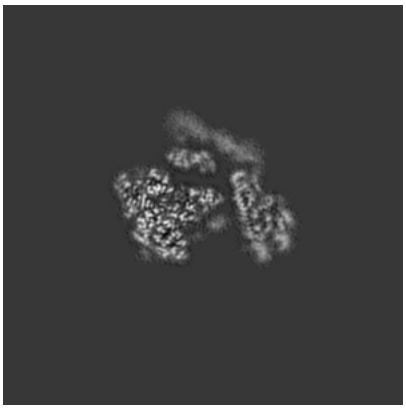
6.3.1 Primary map



X Index: 165

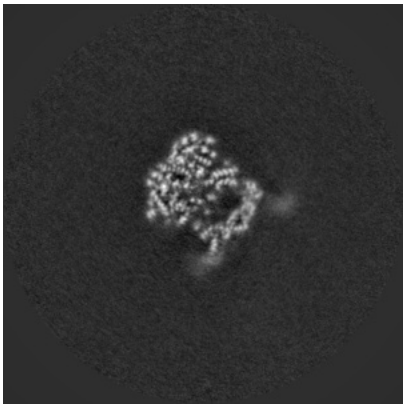


Y Index: 197

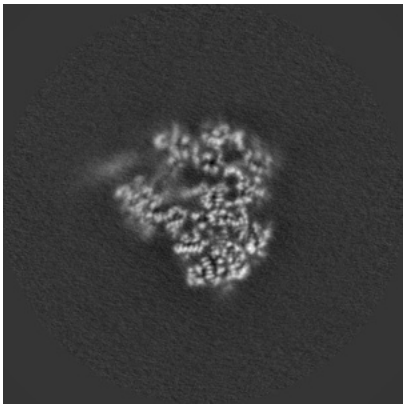


Z Index: 195

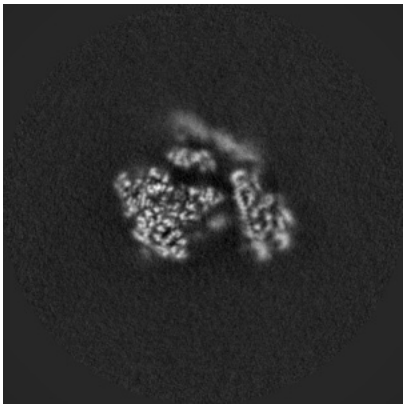
6.3.2 Raw map



X Index: 165



Y Index: 196

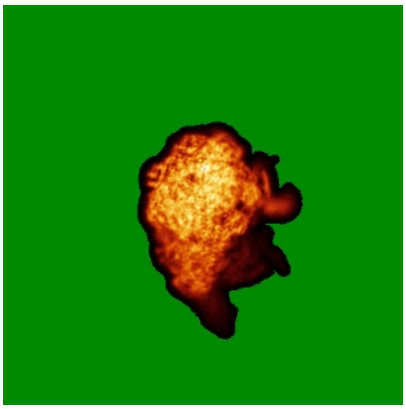


Z Index: 195

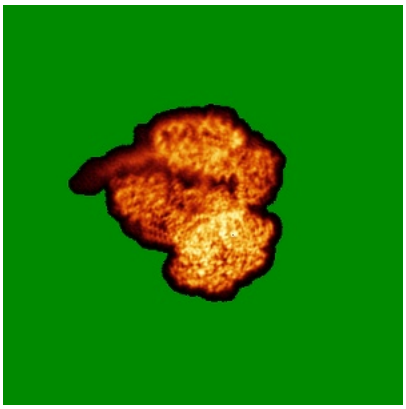
The images above show the largest variance slices of the map in three orthogonal directions.

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

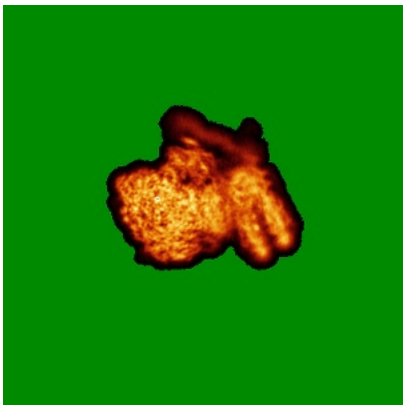
6.4.1 Primary map



X

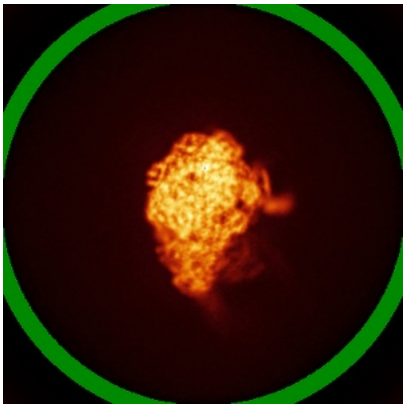


Y

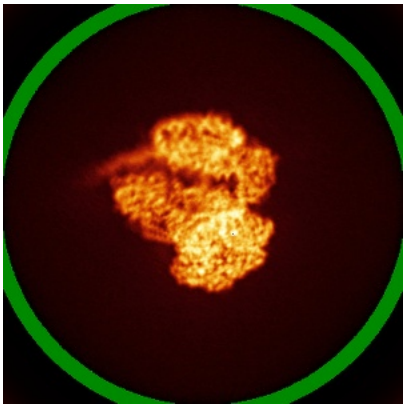


Z

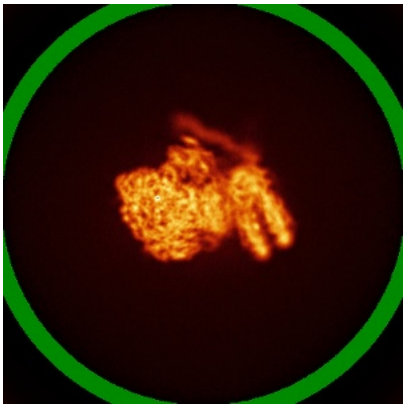
6.4.2 Raw map



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.

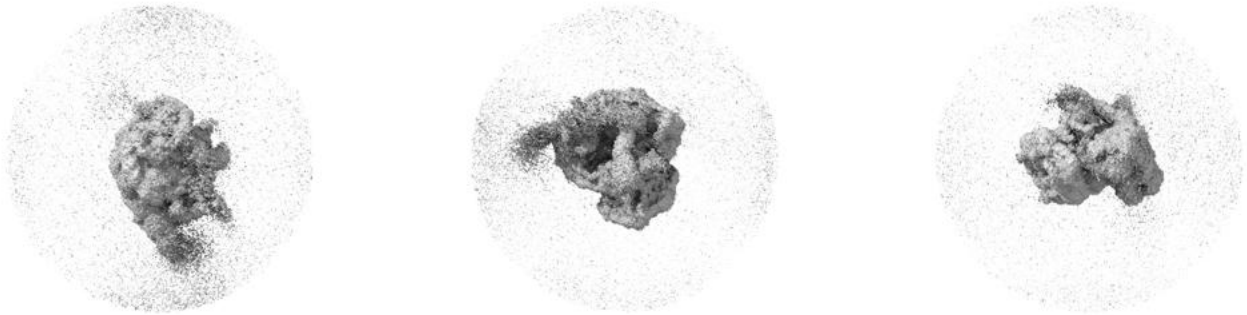
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00197. 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.

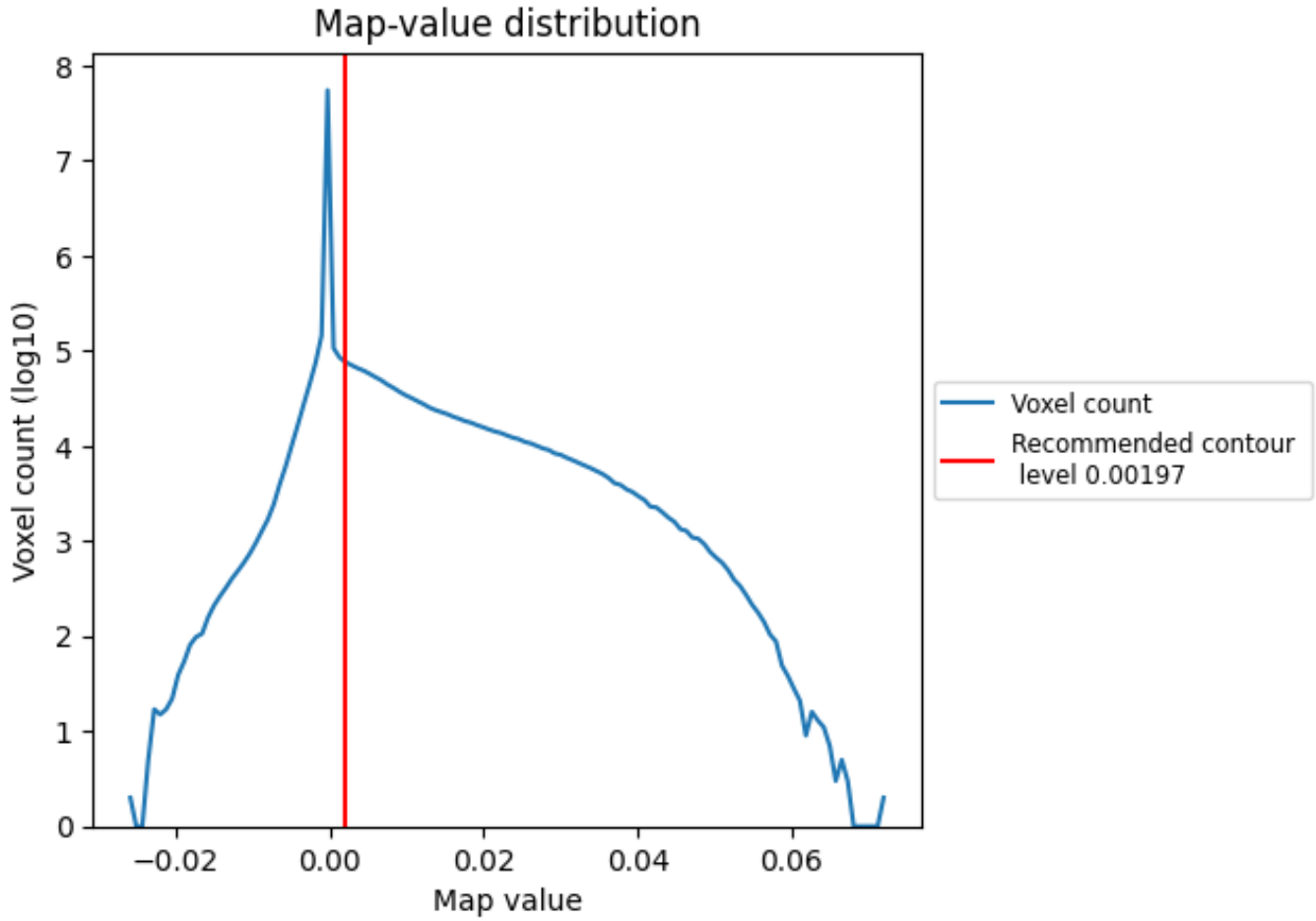
6.6 Mask visualisation (i)

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

7 Map analysis

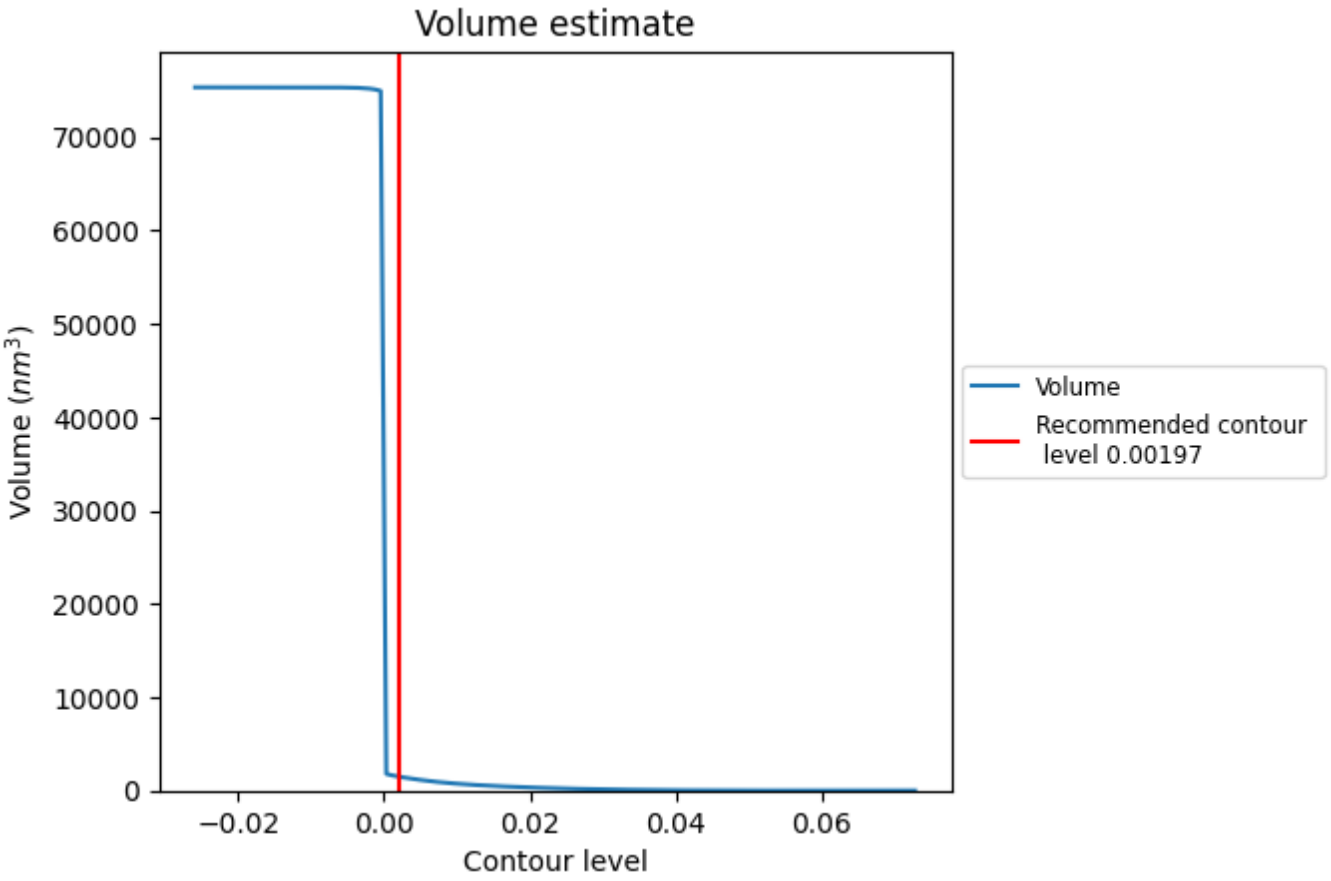
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

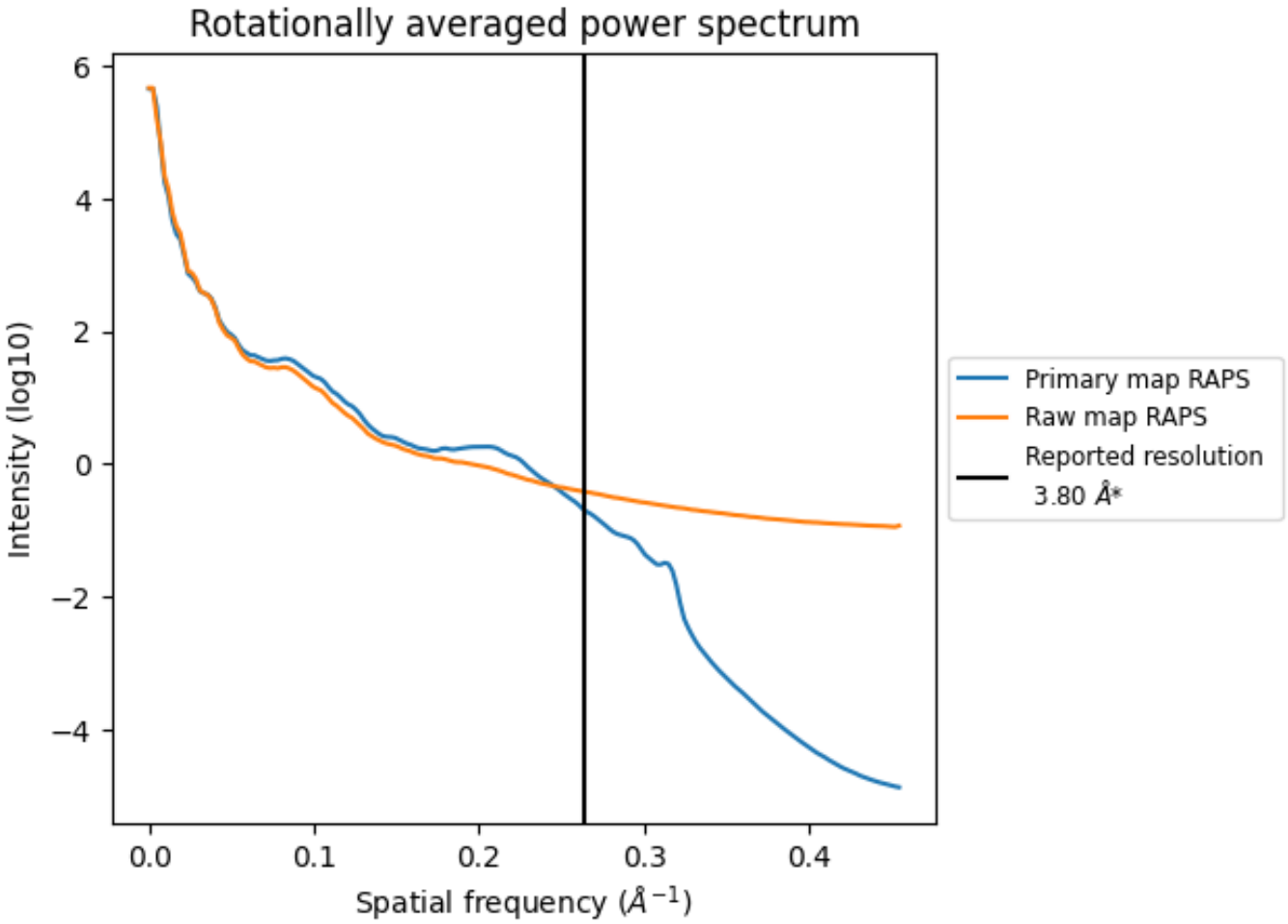
7.2 Volume estimate



The volume at the recommended contour level is 1501 nm^3; this corresponds to an approximate mass of 1356 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)

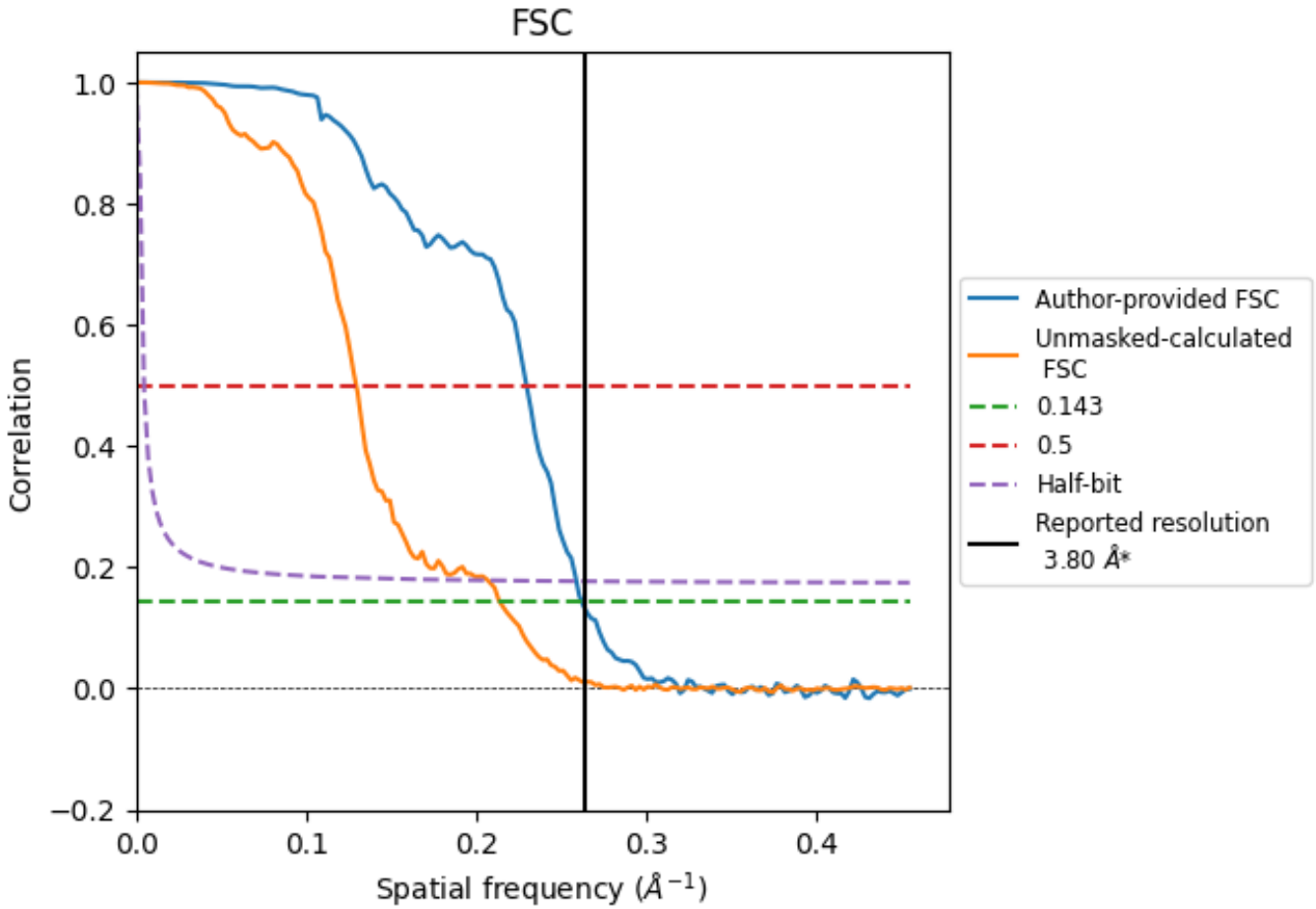


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

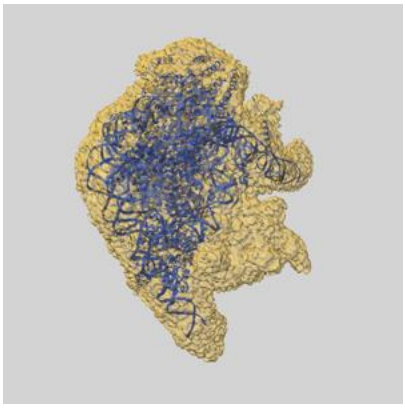
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.36	3.86
Unmasked-calculated*	4.68	7.73	4.84

*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 4.68 differs from the reported value 3.8 by more than 10 %

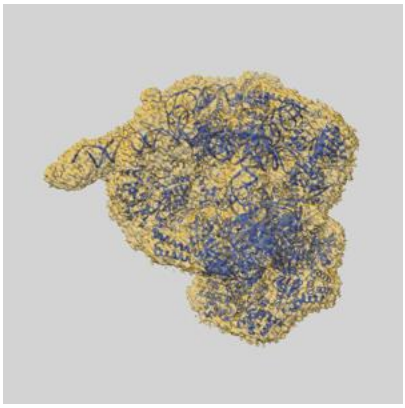
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18471 and PDB model 8QKU. Per-residue inclusion information can be found in section 3 on page 11.

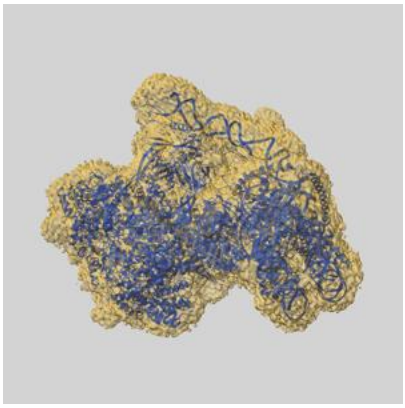
9.1 Map-model overlay



X



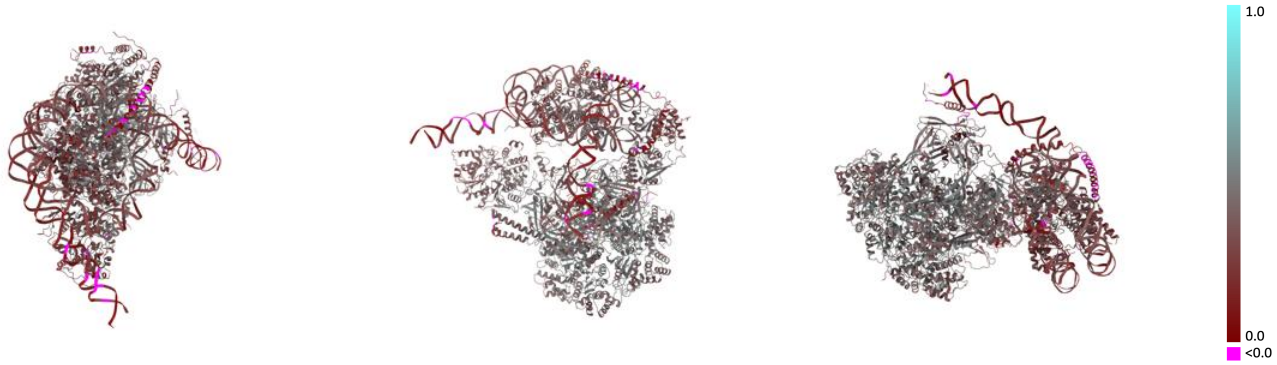
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00197 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.

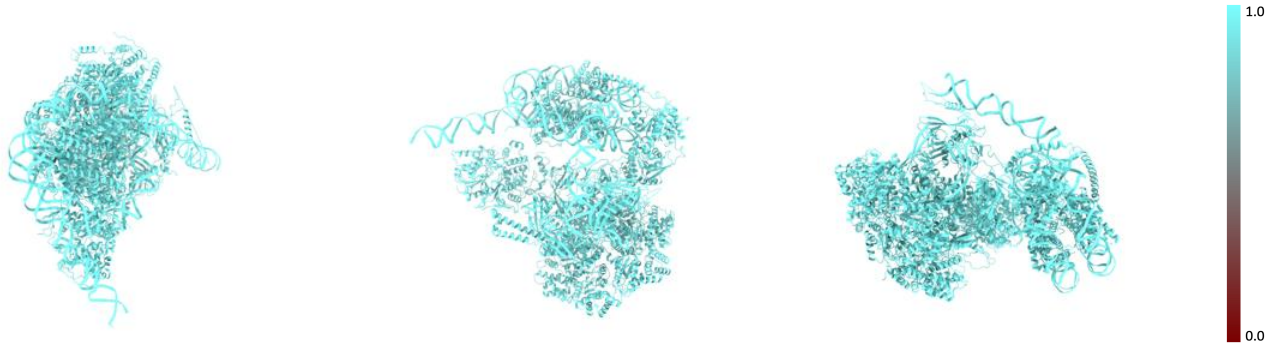
9.2 Q-score mapped to coordinate model (i)



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.

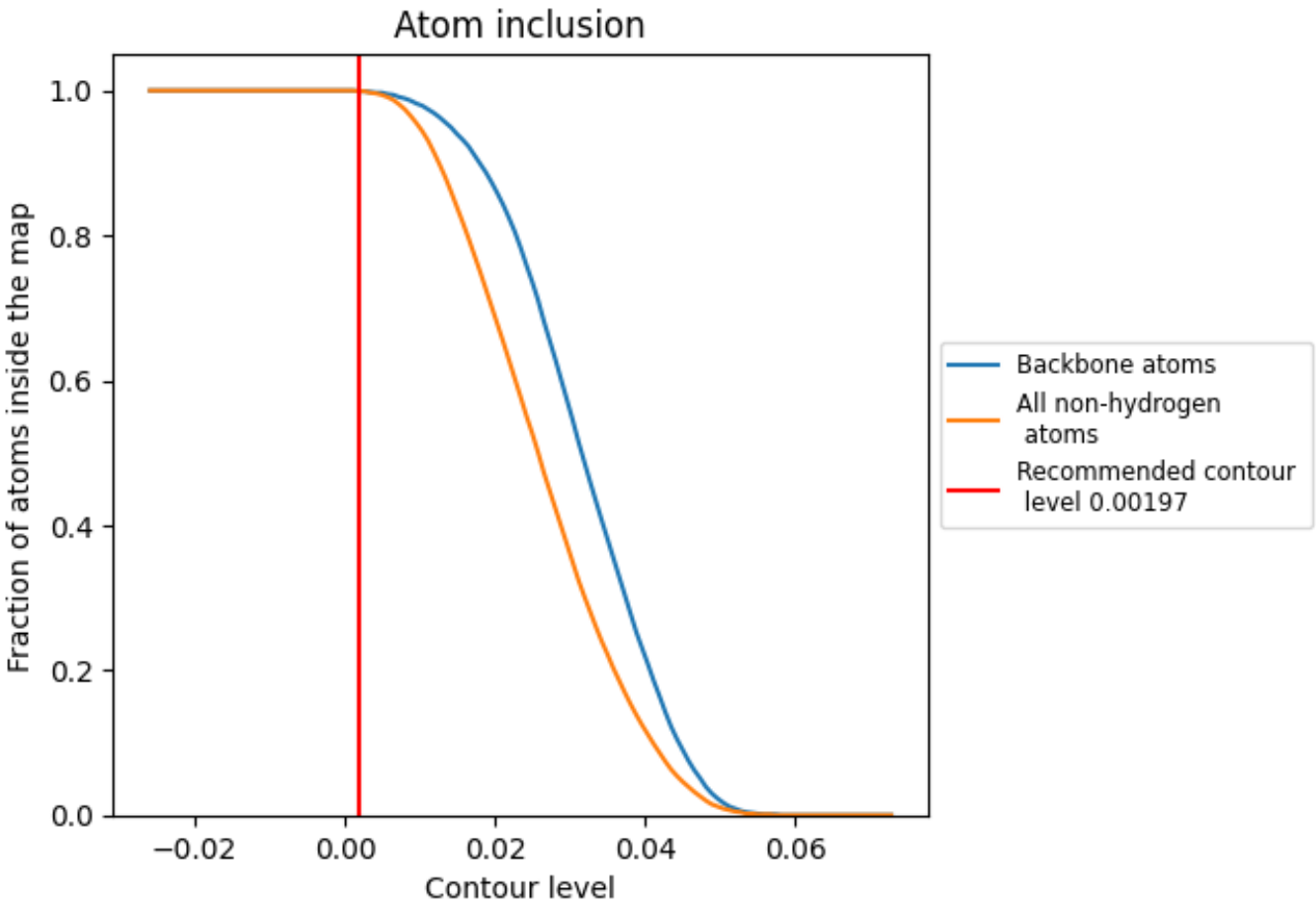
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00197).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.00197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9990	0.3630
A	1.0000	0.3070
B	0.9990	0.3810
C	0.9980	0.3840
D	0.9980	0.2990
E	1.0000	0.3460
F	1.0000	0.3070
G	1.0000	0.3020
H	1.0000	0.2980
I	0.9990	0.2310
J	1.0000	0.2340
M	0.9990	0.3800
R	0.9990	0.3510
S	1.0000	0.3260
T	1.0000	0.4390
U	1.0000	0.4230
V	1.0000	0.4400
W	1.0000	0.4380
X	1.0000	0.4250
Y	1.0000	0.4310
Z	0.9810	0.1900