Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 07:28 am BST

PDB ID	:	9FBW / pdb_00009fbw
EMDB ID	:	EMD-50297
Title	:	SWR1 lacking Swc5 subunit in complex with hexasome
Authors	:	Jalal, A.S.B.; Wigley, D.B.
Deposited on	:	2024-05-14
Resolution	:	4.40 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 (i) 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 (i)) were used in the production of this report:

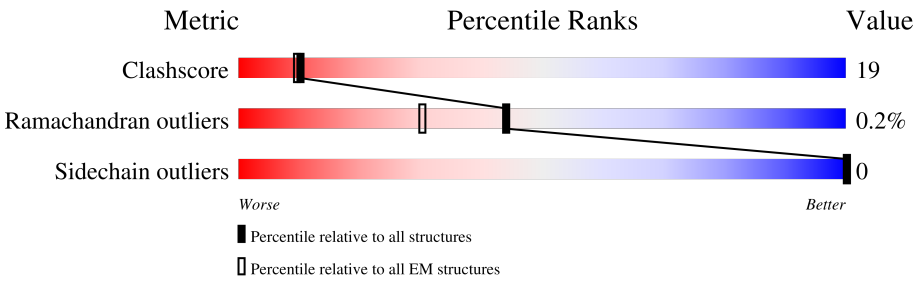
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

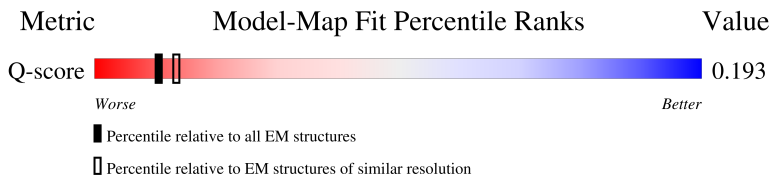
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	12% 42% 13% 45%
1	B	136	7% 40% 30% • 29%
2	C	103	13% 45% 31% • 23%
2	D	103	28% 44% 19% • 36%

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Mol	Chain	Length	Quality of chain
3	E	132	18% 61% 17% 23%
4	G	131	8% 34% 18% 49%
5	I	112	10% 28% 72%
6	J	112	12% 35% 65%
7	M	1514	27% 17% 56%
8	R	438	15% 45% 49% 6%
9	S	280	16% 39% 29% 32%
10	T	463	60% 35% 5%
10	V	463	53% 39% 8%
10	X	463	55% 40% 5%
11	U	471	60% 35% 5%
11	W	471	55% 37% 8%
11	Y	471	62% 32% 6%
12	Z	795	10% 6% 83%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	BEF	M	1602	-	-	X	-
14	BEF	R	502	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 39683 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
			Total	C	N	O		
1	A	75	612	390	113	109	0	0
1	B	97	762	485	147	130	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
			Total	C	N	O		
2	C	79	605	383	113	109	0	0
2	D	66	487	308	93	86	0	0

- Molecule 3 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	102	715	454	129	132	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	67	498	311	85	101	1	0	0

- Molecule 5 is a DNA chain called DNA (112-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	112	2281	1081	416	672	112	0	0

- Molecule 6 is a DNA chain called DNA (112-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	112	2311	1091	436	672	112	0	0

- Molecule 7 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	673	5248	3343	930	949	26	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	190	1536	971	271	285	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	T	439	3313	2090	573	640	10	0	0
			Total	C	N	O	S		
10	V	426	3245	2049	558	628	10	0	0
			Total	C	N	O	S		
10	X	441	3371	2128	581	653	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	U	446	3424	2140	592	680	12	0	0

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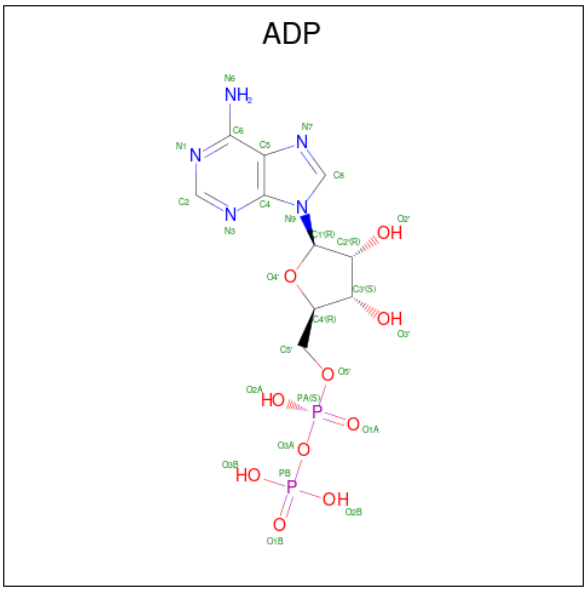
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	W	433	3303	2074	569	649	11	0	0
			Total	C	N	O	S		
11	Y	443	3342	2091	581	659	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Z	134	1061	663	191	203	4	0	0

- 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
			Total	C	N	O	P	
13	M	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	R	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	T	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	U	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	V	1	27	10	5	10	2	0
			Total	C	N	O	P	
13	W	1	27	10	5	10	2	0

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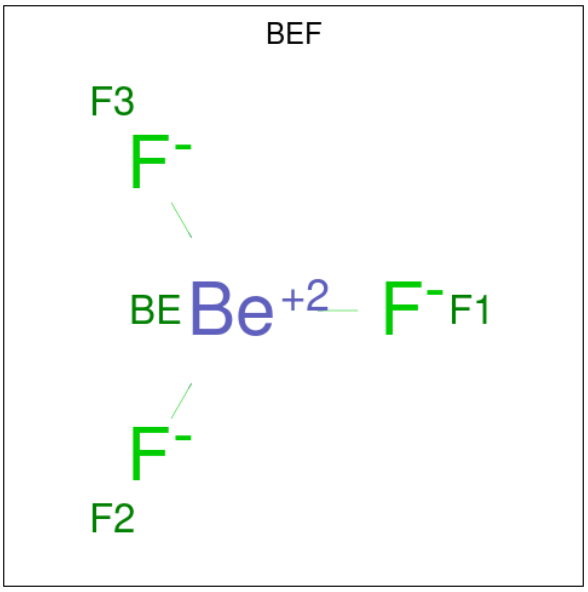
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	X	1	27	10	5	10	2	0
13	Y	1	27	10	5	10	2	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
14	M	1	4	1	3	0
14	R	1	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
			Total	Mg	
15	M	1	1	1	0
15	R	1	1	1	0
15	U	2	2	2	0
15	V	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	W	1	1	1	0
			Total	Mg	
15	X	1	1	1	0
			Total	Mg	
15	Y	1	1	1	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

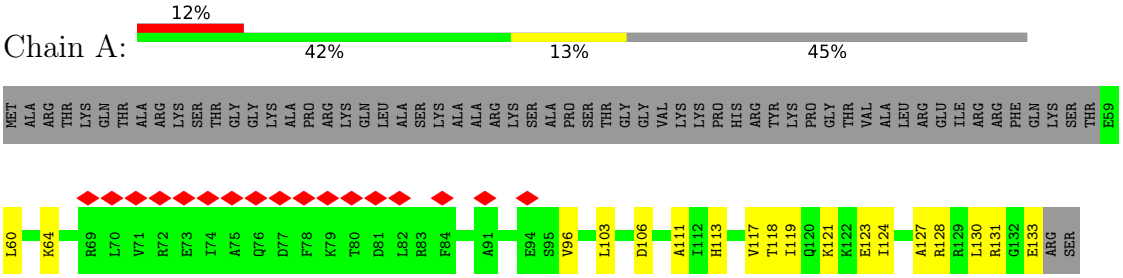
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	S	2	2	2	0

3 Residue-property plots (i)

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

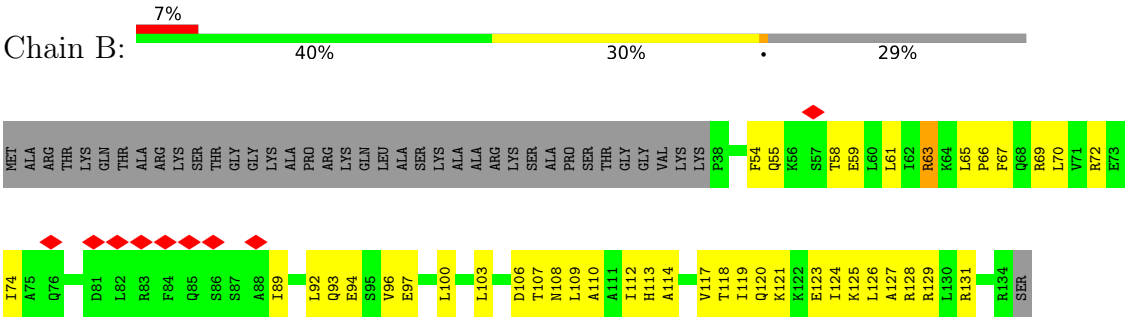
- Molecule 1: Histone H3

Chain A:



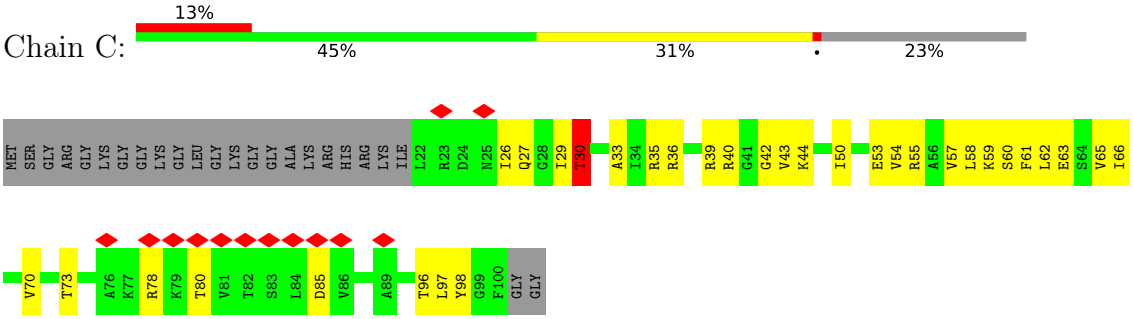
- Molecule 1: Histone H3

Chain B:



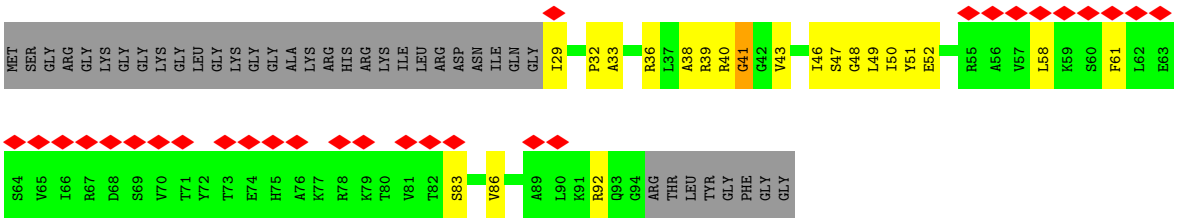
- Molecule 2: Histone H4

Chain C:



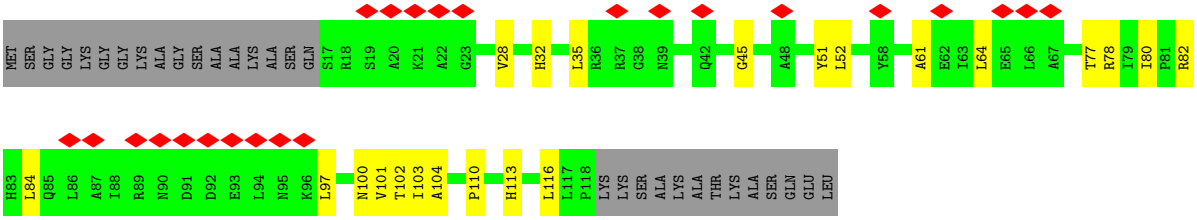
- Molecule 2: Histone H4

Chain D:



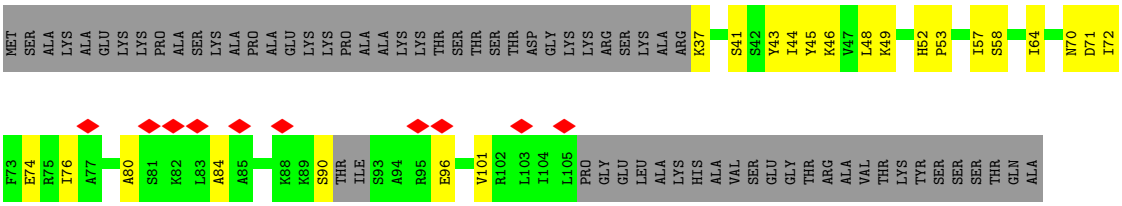
- Molecule 3: Histone H2A.1

Chain E:



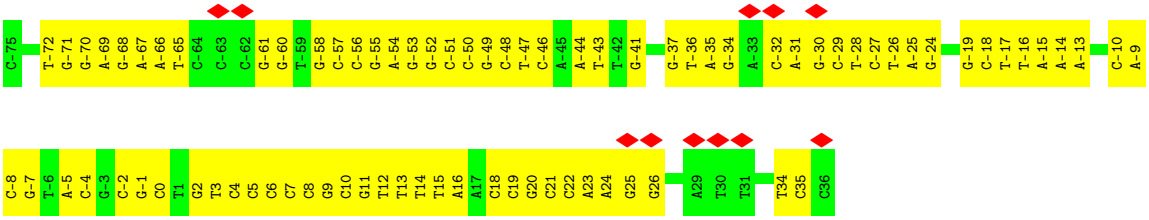
- Molecule 4: Histone H2B.1

Chain G:



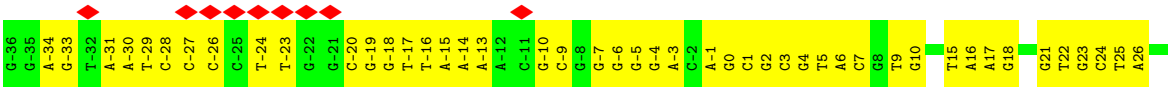
- Molecule 5: DNA (112-MER)

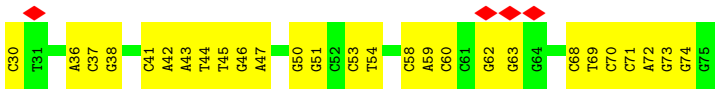
Chain I:



- Molecule 6: DNA (112-MER)

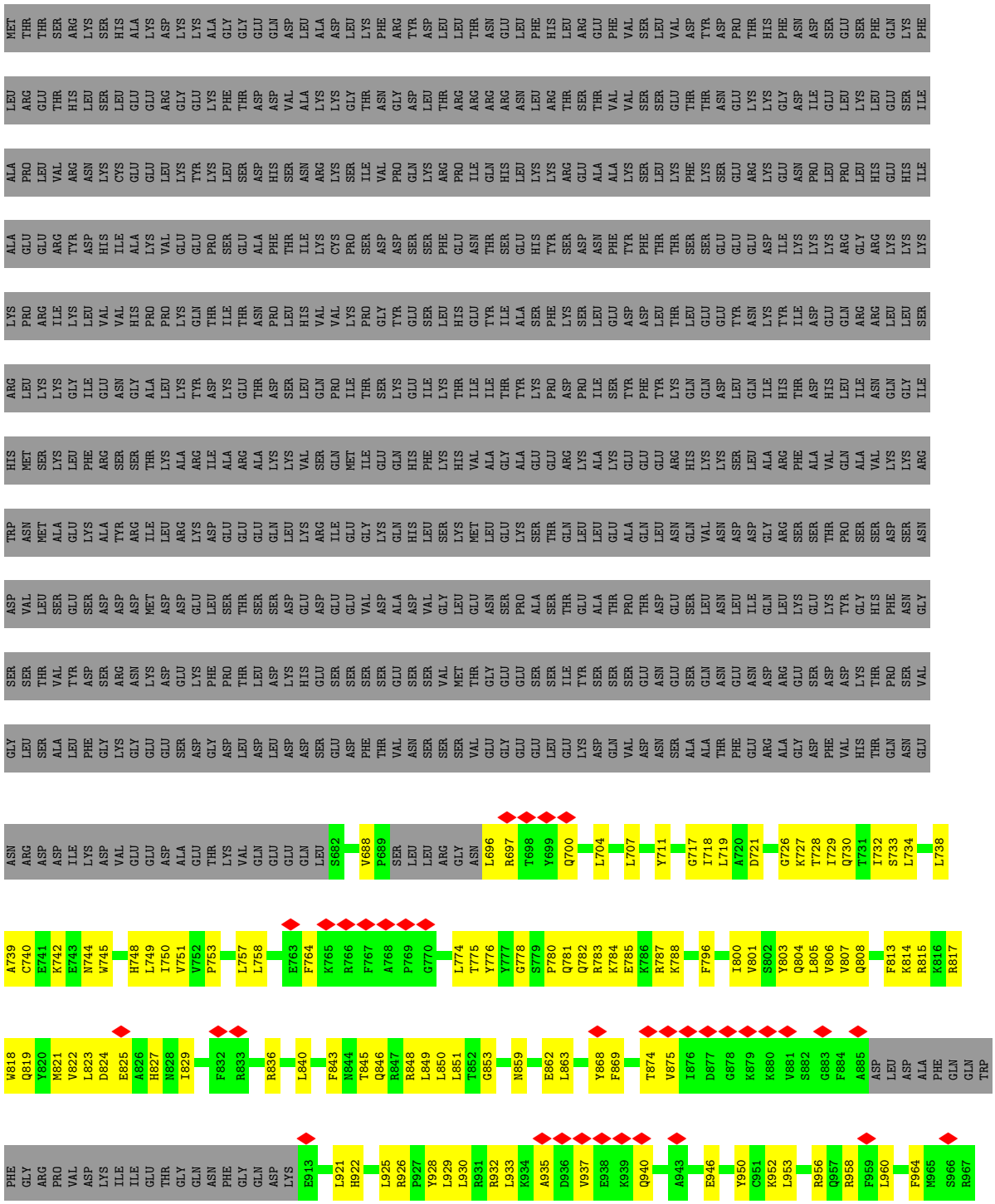
Chain J:

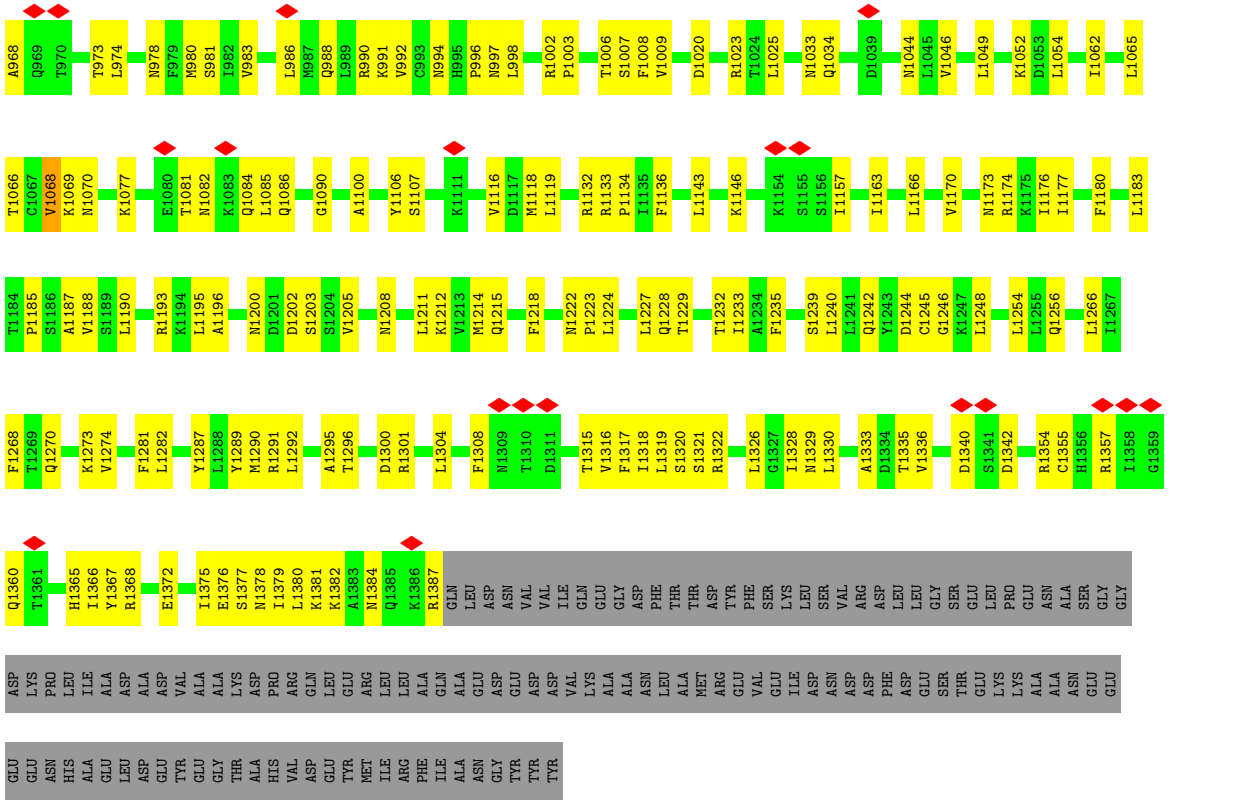




- Molecule 7: Helicase SWR1

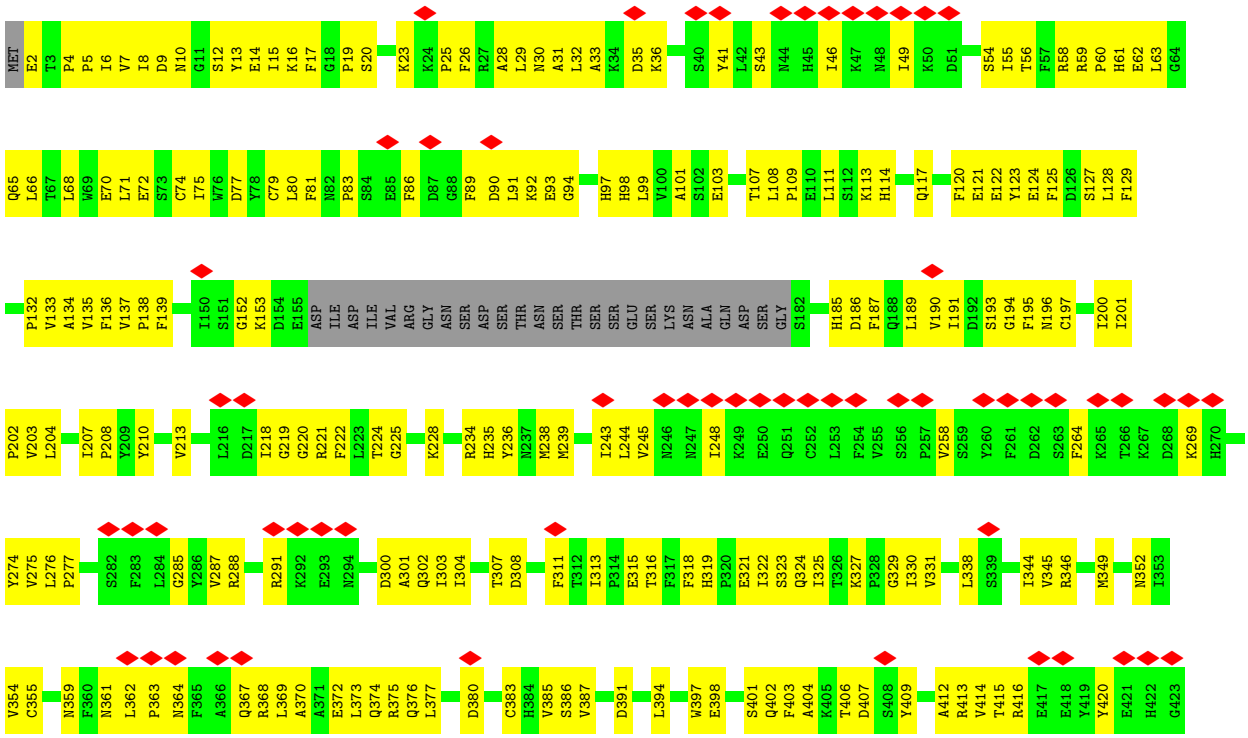
Chain M:

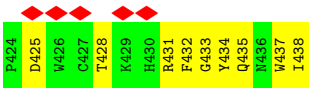




- Molecule 8: Actin-like protein ARP6

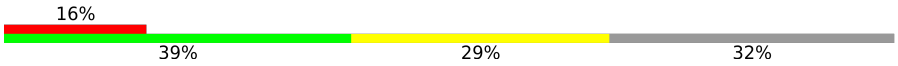
Chain R:

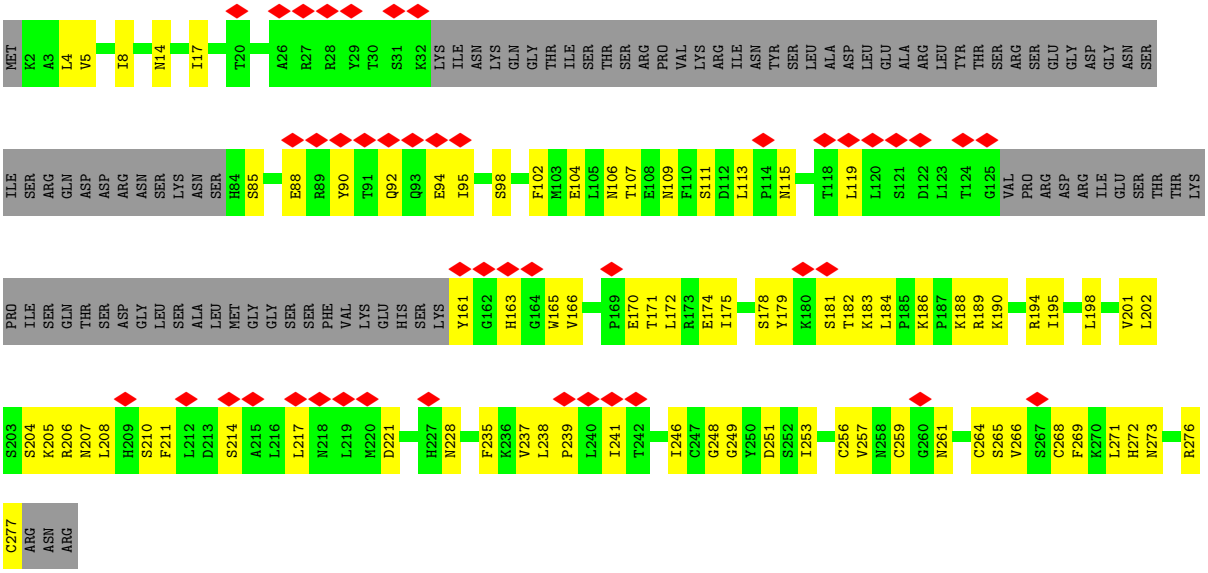




• Molecule 9: Vacuolar protein sorting-associated protein 71

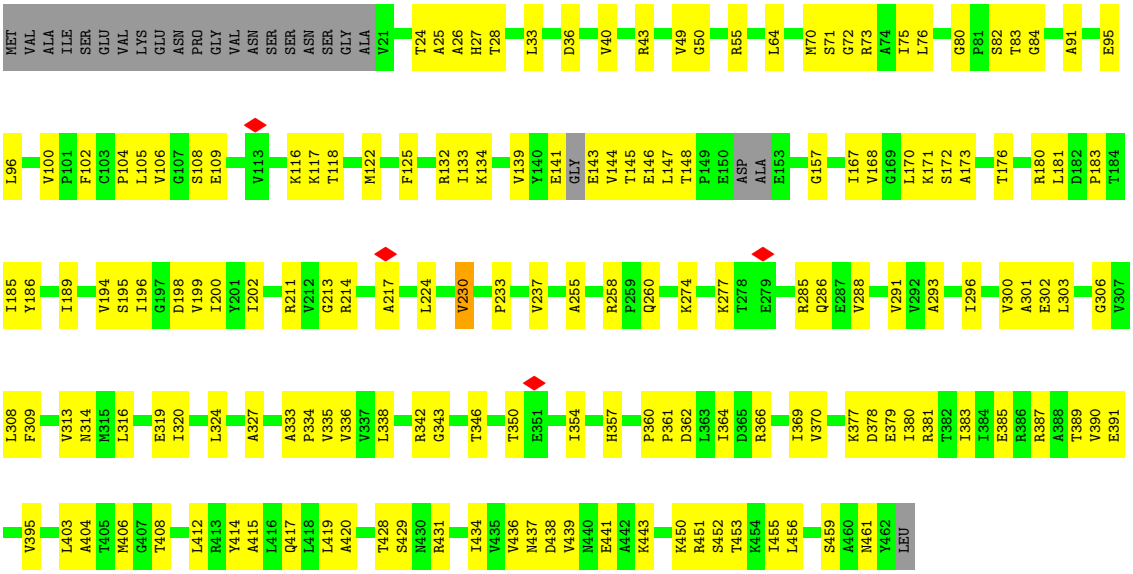
Chain S:





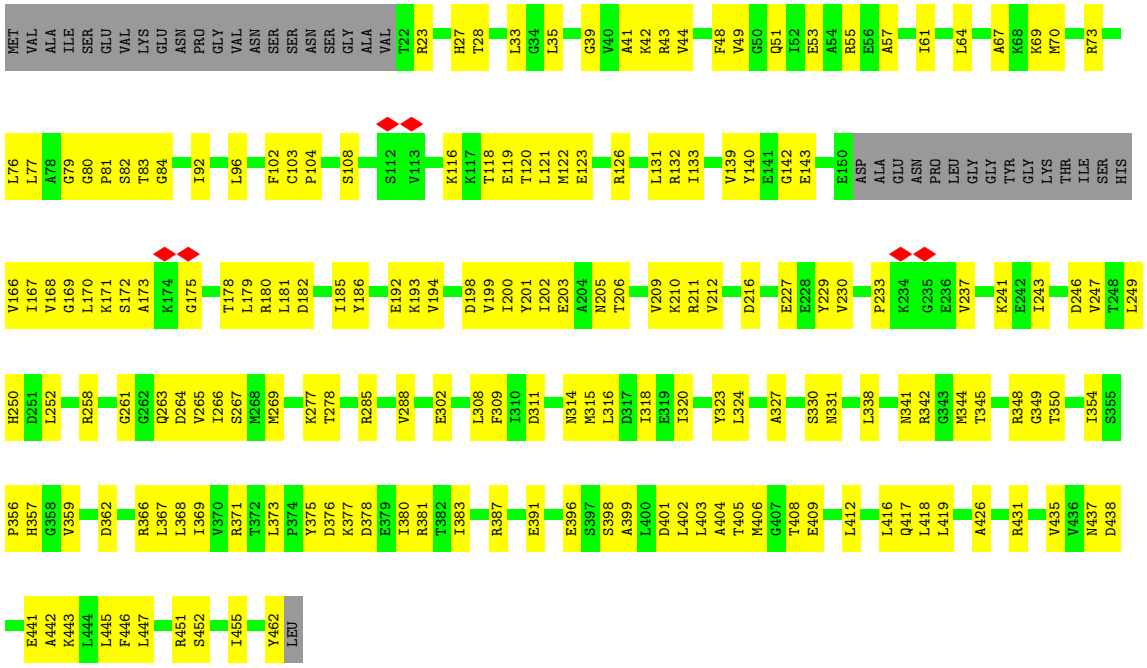
• Molecule 10: RuvB-like protein 1

Chain T:



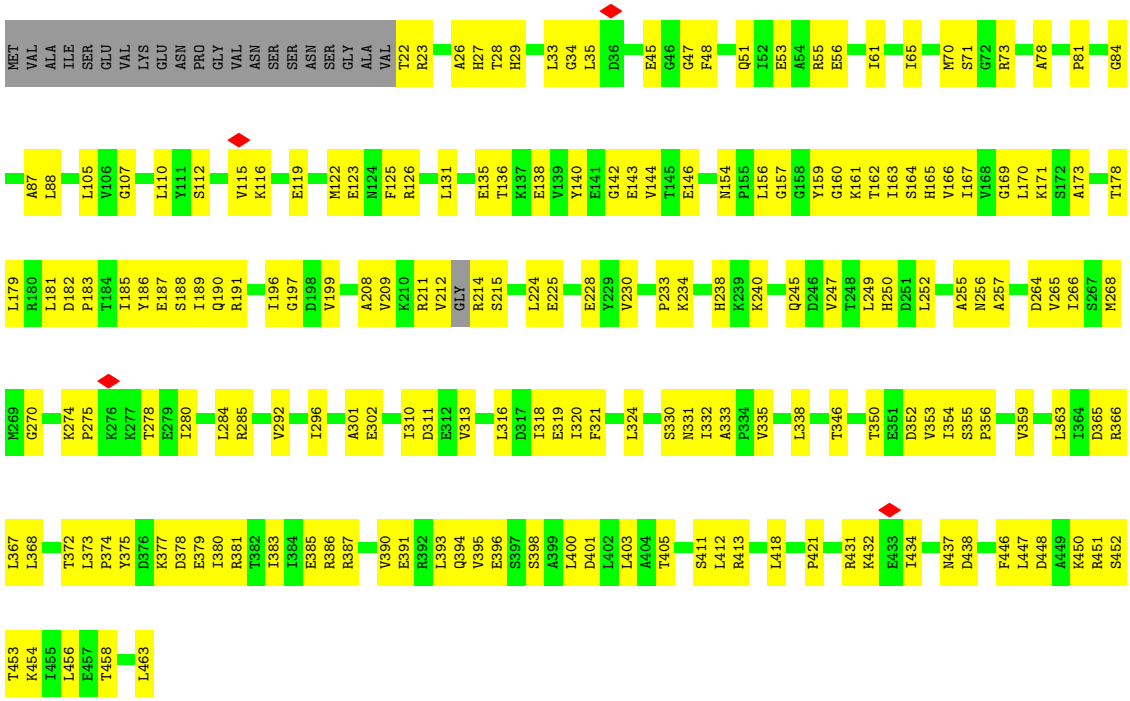
• Molecule 10: RuvB-like protein 1

Chain V:



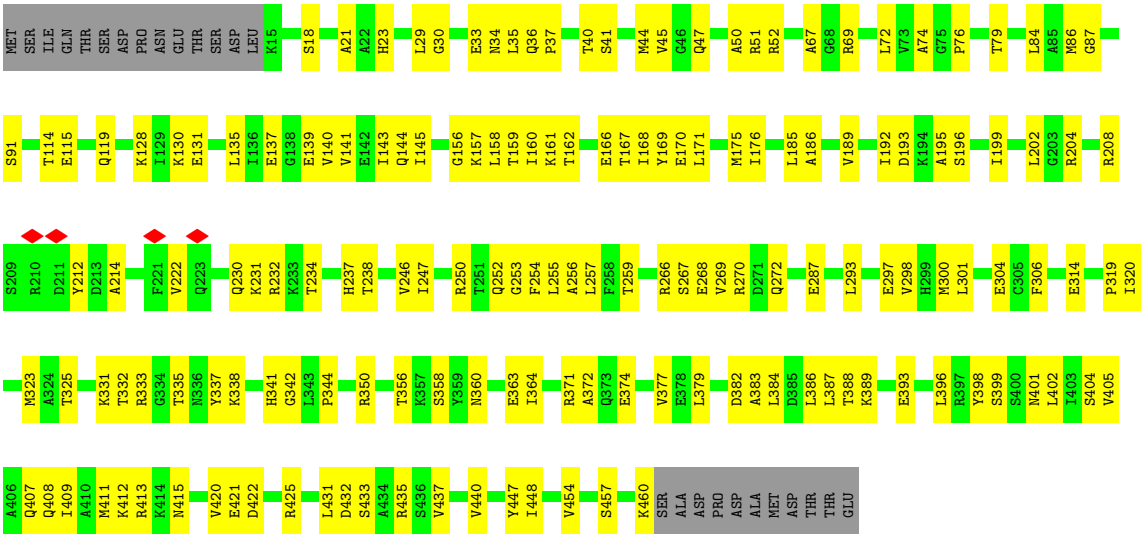
• Molecule 10: RuvB-like protein 1

Chain X:



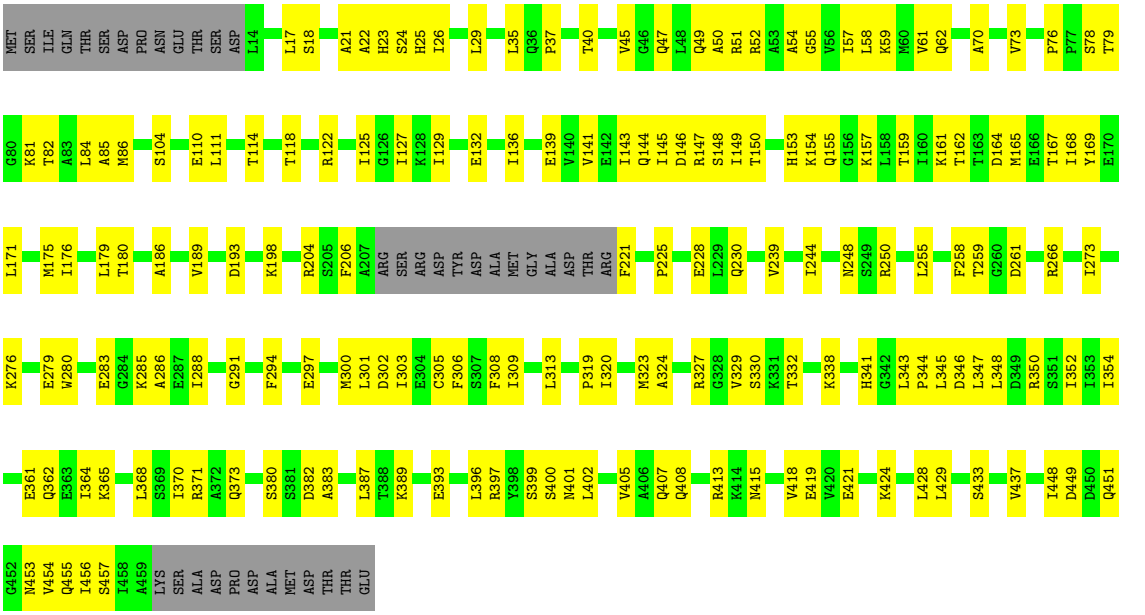
• Molecule 11: RuvB-like protein 2

Chain U:



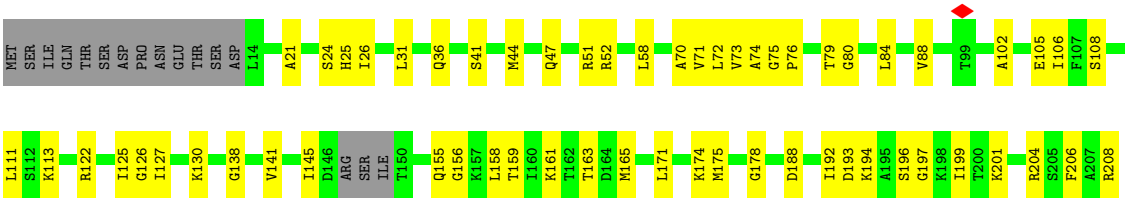
- Molecule 11: RuvB-like protein 2

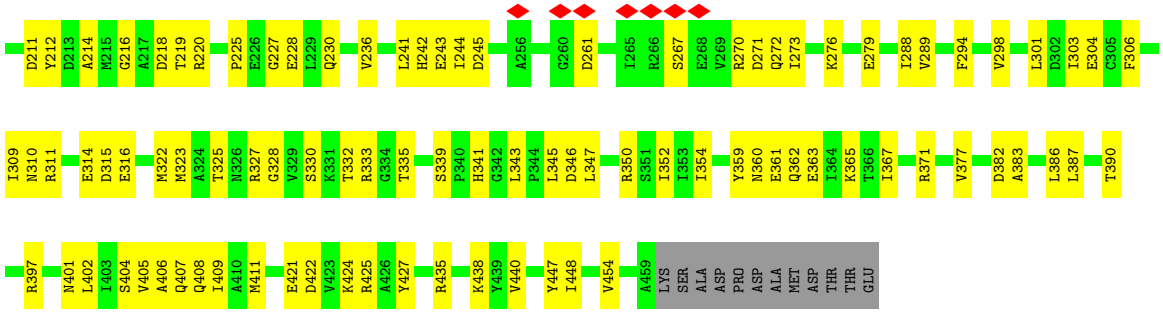
Chain W:



- Molecule 11: RuvB-like protein 2

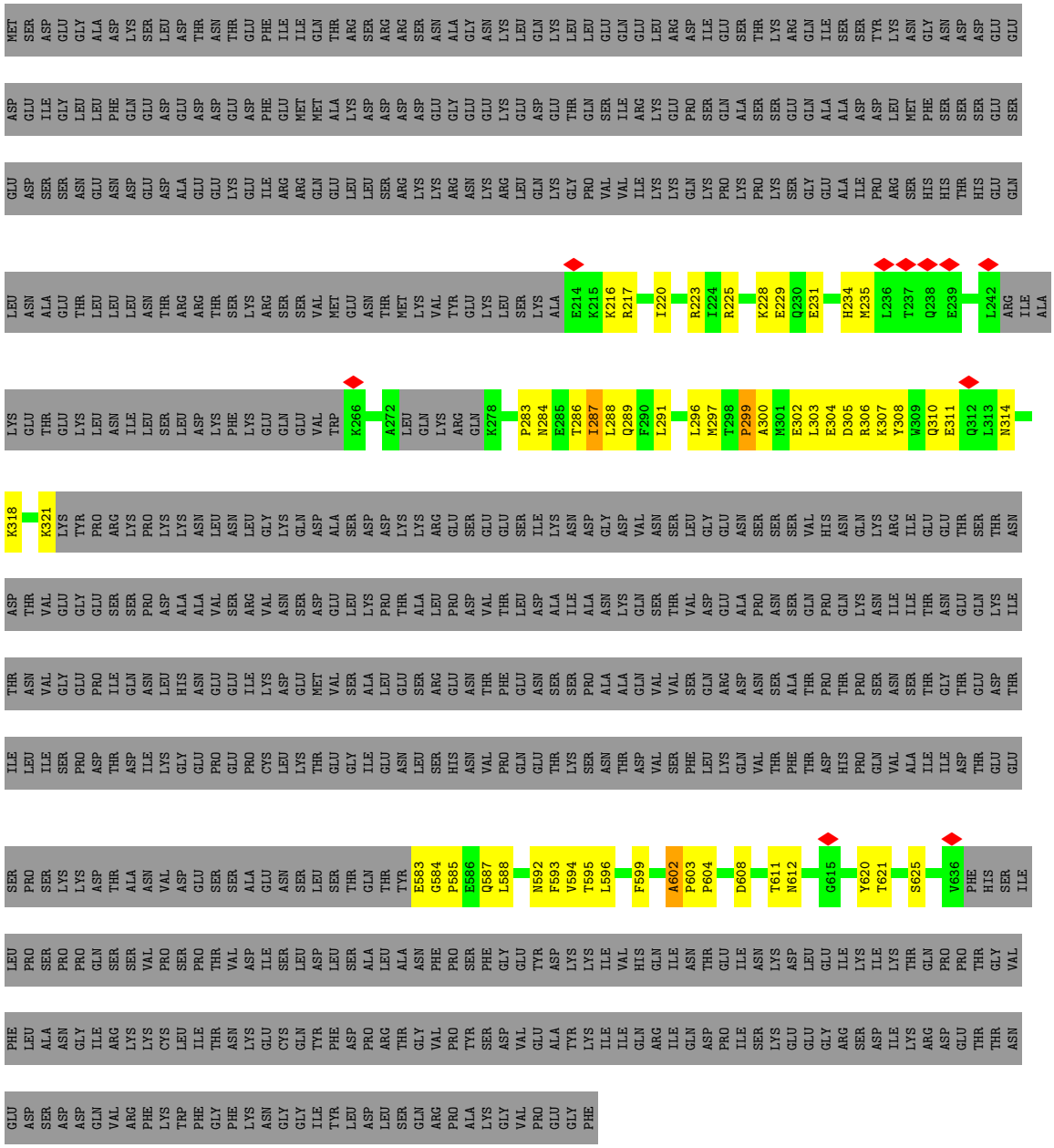
Chain Y:





- Molecule 12: Vacuolar protein sorting-associated protein 72

Chain Z: 10% 6% 83%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0011	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.11	0/618	0.29	0/827
1	B	0.13	0/772	0.37	0/1037
2	C	0.15	0/611	0.42	0/823
2	D	0.16	0/491	0.48	0/663
3	E	0.12	0/725	0.35	0/992
4	G	0.12	0/502	0.33	0/677
5	I	0.21	0/2555	0.45	0/3937
6	J	0.21	0/2595	0.39	0/4007
7	M	0.13	0/5342	0.38	0/7236
8	R	0.13	0/3429	0.35	0/4650
9	S	0.12	0/1564	0.40	2/2107 (0.1%)
10	T	0.13	0/3351	0.33	0/4537
10	V	0.13	0/3282	0.34	0/4443
10	X	0.11	0/3412	0.33	0/4618
11	U	0.12	0/3462	0.33	0/4667
11	W	0.12	0/3339	0.34	0/4503
11	Y	0.11	0/3378	0.31	0/4561
12	Z	0.15	0/1076	0.46	0/1446
All	All	0.14	0/40504	0.36	2/55731 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	S	115	ASN	CA-C-N	5.54	123.73	120.24
9	S	115	ASN	C-N-CA	5.54	123.73	120.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	63	ARG	Peptide
2	C	30	THR	Peptide
2	D	40	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	612	0	650	20	0
1	B	762	0	783	54	0
2	C	605	0	617	50	0
2	D	487	0	502	21	0
3	E	715	0	692	24	0
4	G	498	0	482	21	0
5	I	2281	0	1255	99	0
6	J	2311	0	1255	99	0
7	M	5248	0	5168	223	0
8	R	3335	0	3255	196	0
9	S	1536	0	1547	83	0
10	T	3313	0	3406	119	0
10	V	3245	0	3364	158	0
10	X	3371	0	3486	161	0
11	U	3424	0	3494	141	0
11	W	3303	0	3384	139	0
11	Y	3342	0	3369	118	0
12	Z	1061	0	1014	47	0
13	M	27	0	12	0	0
13	R	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	T	27	0	12	3	0
13	U	27	0	12	1	0
13	V	27	0	12	4	0
13	W	27	0	12	2	0
13	X	27	0	11	3	0
13	Y	27	0	12	4	0
14	M	4	0	0	2	0
14	R	4	0	0	2	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	39683	0	37818	1481	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 19.

All (1481) 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)
5:I:-30:DG:N2	6:J:30:DC:C2	2.37	0.92
5:I:-4:DC:O2	6:J:4:DG:N2	2.03	0.91
9:S:259:CYS:SG	9:S:272:HIS:CE1	2.66	0.88
7:M:778:GLY:HA3	7:M:782:GLN:HB3	1.56	0.87
10:X:131:LEU:HD11	10:X:301:ALA:HB1	1.56	0.86
10:X:163:ILE:HG12	12:Z:592:ASN:HD22	1.42	0.85
11:W:186:ALA:HB3	12:Z:296:LEU:H	1.41	0.84
5:I:6:DC:N3	6:J:-6:DG:N1	2.28	0.82
8:R:134:ALA:HB1	8:R:190:VAL:HG21	1.61	0.81
5:I:-69:DA:H2'	5:I:-68:DG:H8	1.45	0.80
7:M:825:GLU:HA	7:M:853:GLY:H	1.46	0.79
7:M:704:LEU:HD12	7:M:733:SER:HB2	1.62	0.79
11:W:343:LEU:HD12	11:W:344:PRO:HD2	1.63	0.79
7:M:727:LYS:HB2	7:M:851:LEU:HD12	1.65	0.78
10:X:330:SER:HB3	10:X:333:ALA:HB2	1.66	0.78
11:W:141:VAL:HB	11:W:161:LYS:HZ3	1.48	0.77
7:M:1379:ILE:HG22	7:M:1380:LEU:HG	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1009:VAL:HG11	10:V:205:ASN:HB3	1.66	0.77
9:S:261:ASN:HB2	9:S:272:HIS:HE1	1.48	0.77
10:X:196:ILE:O	10:X:214:ARG:NH1	2.16	0.76
8:R:9:ASP:HB3	8:R:16:LYS:HB2	1.68	0.76
7:M:1354:ARG:HH11	7:M:1357:ARG:HH22	1.34	0.75
6:J:-29:DT:OP2	7:M:981:SER:OG	2.04	0.75
10:X:394:GLN:HE22	10:X:432:LYS:HG3	1.52	0.75
11:U:41:SER:OG	11:U:44:MET:SD	2.45	0.74
5:I:-30:DG:N2	6:J:30:DC:O2	2.20	0.74
10:T:132:ARG:O	10:T:301:ALA:HA	1.87	0.74
11:Y:192:ILE:HD13	11:Y:199:ILE:HG13	1.69	0.74
5:I:6:DC:O2	6:J:-6:DG:N2	2.20	0.74
1:B:65:LEU:HD12	7:M:782:GLN:HB2	1.70	0.74
4:G:48:LEU:O	4:G:52:HIS:N	2.21	0.74
11:U:298:VAL:HG11	11:U:323:MET:HE2	1.69	0.74
10:T:167:ILE:HD13	10:T:180:ARG:HB3	1.69	0.74
11:U:135:LEU:HD13	11:U:137:GLU:HG2	1.69	0.74
1:B:117:VAL:HG22	6:J:-4:DG:H3'	1.70	0.73
10:T:76:LEU:HD13	10:T:338:LEU:HG	1.69	0.73
10:T:361:PRO:HA	10:T:364:ILE:HG12	1.69	0.73
5:I:23:DA:H2"	5:I:24:DA:H5"	1.68	0.73
1:B:74:ILE:HG23	2:C:66:ILE:HD13	1.69	0.73
7:M:776:TYR:OH	7:M:800:ILE:O	2.03	0.73
3:E:64:LEU:HD22	4:G:48:LEU:HB2	1.70	0.73
7:M:1378:ASN:HB3	7:M:1382:LYS:HE3	1.71	0.73
11:W:413:ARG:NH2	11:W:419:GLU:OE1	2.22	0.72
10:X:265:VAL:HA	10:X:268:MET:HE2	1.69	0.72
1:B:100:LEU:HD11	2:C:58:LEU:HB2	1.71	0.72
7:M:1002:ARG:NH1	11:W:279:GLU:OE1	2.21	0.72
5:I:22:DC:H2'	5:I:23:DA:C8	2.25	0.72
5:I:-69:DA:H2'	5:I:-68:DG:C8	2.25	0.72
7:M:707:LEU:HB3	7:M:734:LEU:HD22	1.72	0.72
10:T:213:GLY:HA3	10:T:230:VAL:HG21	1.70	0.72
7:M:1177:ILE:HD11	7:M:1227:LEU:HB2	1.73	0.71
9:S:253:ILE:HA	9:S:264:CYS:HA	1.72	0.71
9:S:257:VAL:HG21	11:U:166:GLU:HG2	1.71	0.71
11:Y:406:ALA:HA	11:Y:409:ILE:HD12	1.71	0.71
5:I:-24:DG:N2	6:J:25:DT:O2	2.23	0.71
12:Z:310:GLN:NE2	12:Z:311:GLU:OE2	2.24	0.71
8:R:81:PHE:HE1	8:R:91:LEU:HD22	1.56	0.70
10:V:210:LYS:HB2	10:V:263:GLN:HE22	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:342:ARG:HG3	11:Y:448:ILE:HB	1.73	0.70
2:C:97:LEU:HD21	3:E:104:ALA:HB2	1.74	0.69
8:R:12:SER:OG	8:R:65:GLN:OE1	2.10	0.69
11:U:407:GLN:HG3	11:U:411:MET:HE1	1.75	0.69
7:M:996:PRO:HD2	7:M:1246:GLY:H	1.57	0.69
7:M:807:VAL:HG22	7:M:836:ARG:HB3	1.72	0.69
7:M:1232:THR:HG22	7:M:1233:ILE:H	1.58	0.69
1:A:118:THR:HA	2:D:46:ILE:HG22	1.73	0.69
8:R:23:LYS:NZ	8:R:398:GLU:O	2.26	0.69
9:S:256:CYS:HB3	9:S:259:CYS:SG	2.32	0.69
10:V:133:ILE:HG22	10:V:246:ASP:HA	1.75	0.69
10:V:344:MET:HB3	10:V:354:ILE:HD11	1.74	0.69
6:J:23:DG:H2"	6:J:24:DC:H5"	1.75	0.69
11:U:29:LEU:HD13	11:U:87:GLY:HA3	1.75	0.69
10:V:42:LYS:O	10:V:55:ARG:NH1	2.27	0.69
10:V:200:ILE:HA	10:V:211:ARG:HA	1.73	0.69
8:R:71:LEU:HD23	9:S:166:VAL:HB	1.74	0.68
11:Y:407:GLN:HG3	11:Y:411:MET:HE2	1.75	0.68
11:W:147:ARG:HH22	11:W:153:HIS:H	1.41	0.68
7:M:933:LEU:HD12	7:M:935:ALA:H	1.58	0.68
10:T:181:LEU:HD22	11:Y:214:ALA:H	1.58	0.68
11:W:371:ARG:HH21	11:W:400:SER:HB2	1.59	0.68
10:T:255:ALA:O	10:T:260:GLN:NE2	2.25	0.68
10:X:144:VAL:HB	10:X:197:GLY:H	1.59	0.68
8:R:5:PRO:HA	8:R:98:HIS:HB2	1.76	0.68
8:R:153:LYS:HA	8:R:374:GLN:HG2	1.76	0.68
11:U:128:LYS:HG2	11:U:238:THR:HG22	1.75	0.68
10:X:313:VAL:HG21	10:X:338:LEU:HD12	1.74	0.68
1:B:55:GLN:HB3	3:E:110:PRO:HB3	1.76	0.68
1:B:108:ASN:ND2	2:C:42:GLY:O	2.27	0.68
10:T:443:LYS:HE3	10:T:451:ARG:HH21	1.59	0.68
10:T:461:ASN:HB2	11:U:76:PRO:HB3	1.76	0.68
1:B:61:LEU:HD12	2:C:40:ARG:HD3	1.76	0.67
11:U:298:VAL:HG21	11:U:323:MET:HB2	1.74	0.67
11:W:419:GLU:HG2	11:W:421:GLU:H	1.60	0.67
1:A:121:LYS:HZ2	2:D:52:GLU:HB2	1.59	0.67
1:B:103:LEU:HD23	2:C:54:VAL:HG13	1.76	0.67
10:X:47:GLY:O	10:X:386:ARG:NH1	2.28	0.67
11:W:70:ALA:HB1	11:W:323:MET:HE1	1.77	0.67
12:Z:304:GLU:O	12:Z:308:TYR:N	2.26	0.67
10:V:180:ARG:NH1	10:V:182:ASP:OD1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:275:VAL:HG22	8:R:303:ILE:HG12	1.76	0.67
10:T:366:ARG:NH2	13:Y:501:ADP:O3B	2.27	0.67
8:R:113:LYS:HE3	8:R:428:THR:HB	1.76	0.67
6:J:-15:DA:H5'	7:M:785:GLU:HB2	1.77	0.67
7:M:1384:ASN:O	7:M:1387:ARG:NH1	2.28	0.67
10:V:380:ILE:HG12	10:V:412:LEU:HD13	1.75	0.67
7:M:950:TYR:OH	7:M:1378:ASN:N	2.26	0.66
8:R:219:GLY:H	8:R:222:PHE:HB2	1.60	0.66
8:R:269:LYS:HE2	8:R:291:ARG:HH21	1.60	0.66
11:U:140:VAL:HB	11:U:160:ILE:HG13	1.75	0.66
10:X:167:ILE:HD13	12:Z:314:ASN:HD22	1.60	0.66
7:M:1049:LEU:O	7:M:1052:LYS:NZ	2.28	0.66
4:G:57:ILE:HG22	4:G:58:SER:H	1.60	0.66
6:J:4:DG:H2"	6:J:5:DT:C5	2.31	0.66
8:R:121:GLU:HB2	9:S:198:LEU:HD21	1.77	0.66
11:W:148:SER:HA	12:Z:289:GLN:HA	1.78	0.66
1:B:107:THR:HG23	1:B:123:GLU:HB2	1.77	0.66
7:M:1193:ARG:HH11	9:S:4:LEU:HD21	1.60	0.66
3:E:80:ILE:HG22	3:E:82:ARG:H	1.61	0.66
11:Y:80:GLY:O	11:Y:84:LEU:N	2.29	0.66
11:U:186:ALA:O	11:U:204:ARG:NH1	2.29	0.65
1:B:107:THR:HG21	1:B:119:ILE:HG23	1.78	0.65
5:I:21:DC:H2'	5:I:22:DC:H6	1.61	0.65
8:R:58:ARG:HD3	9:S:163:HIS:HA	1.77	0.65
7:M:1355:CYS:O	7:M:1360:GLN:NE2	2.30	0.65
10:V:76:LEU:HD21	10:V:369:ILE:HG13	1.77	0.65
11:Y:188:ASP:OD2	11:Y:201:LYS:NZ	2.29	0.65
11:U:50:ALA:HB1	11:U:84:LEU:HD12	1.76	0.65
7:M:814:LYS:O	7:M:815:ARG:NH1	2.29	0.65
11:U:332:THR:OG1	11:U:335:THR:OG1	2.14	0.65
10:X:123:GLU:OE2	10:X:285:ARG:NH2	2.29	0.65
5:I:19:DC:H1'	7:M:804:GLN:HG3	1.78	0.65
7:M:1033:ASN:OD1	7:M:1034:GLN:N	2.27	0.65
11:U:298:VAL:HG13	11:U:301:LEU:HD12	1.78	0.65
10:T:170:LEU:HB3	10:T:237:VAL:HG21	1.79	0.65
11:W:204:ARG:O	11:W:221:PHE:N	2.30	0.65
1:B:55:GLN:HE21	2:C:40:ARG:HA	1.60	0.65
5:I:-53:DG:H1'	5:I:-52:DG:N7	2.13	0.64
8:R:65:GLN:HG3	8:R:107:THR:HG22	1.79	0.64
10:T:25:ALA:HB2	11:U:67:ALA:HB3	1.79	0.64
11:U:250:ARG:HH22	11:U:256:ALA:HB2	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:142:GLY:HA3	10:X:170:LEU:HB3	1.79	0.64
11:W:23:HIS:HB3	11:W:86:MET:HE3	1.79	0.64
8:R:203:VAL:HA	8:R:208:PRO:HA	1.80	0.64
2:C:70:VAL:HA	2:C:73:THR:HG22	1.78	0.64
6:J:-18:DG:N7	7:M:1301:ARG:NH1	2.45	0.64
11:W:136:ILE:HG22	11:W:230:GLN:HG3	1.79	0.64
8:R:196:ASN:O	8:R:221:ARG:NH1	2.30	0.64
7:M:1065:LEU:O	7:M:1133:ARG:NH1	2.31	0.64
10:V:79:GLY:O	10:V:341:ASN:ND2	2.28	0.64
8:R:191:ILE:HG23	8:R:200:ILE:HG12	1.79	0.64
11:Y:36:GLN:OE1	11:Y:52:ARG:NH1	2.31	0.64
1:B:55:GLN:NE2	2:C:39:ARG:O	2.30	0.64
8:R:20:SER:O	8:R:401:SER:OG	2.16	0.64
8:R:258:VAL:O	8:R:368:ARG:NH1	2.31	0.64
10:X:437:ASN:OD1	10:X:438:ASP:N	2.31	0.64
11:Y:377:VAL:HG22	11:Y:407:GLN:HG2	1.79	0.64
1:B:117:VAL:HB	3:E:116:LEU:HD22	1.79	0.63
11:W:255:LEU:HD21	10:X:266:ILE:HD13	1.80	0.63
12:Z:592:ASN:OD1	12:Z:593:PHE:N	2.31	0.63
10:T:180:ARG:NH2	11:Y:211:ASP:O	2.31	0.63
11:U:23:HIS:HB3	11:U:86:MET:SD	2.38	0.63
10:X:453:THR:HA	10:X:456:LEU:HD12	1.80	0.63
10:V:447:LEU:HD22	10:V:451:ARG:HD2	1.79	0.63
12:Z:288:LEU:HD13	12:Z:604:PRO:HB2	1.81	0.63
1:A:130:LEU:HD13	1:B:127:ALA:HA	1.80	0.63
7:M:750:ILE:HD11	7:M:800:ILE:HG13	1.81	0.63
6:J:45:DT:H2"	6:J:46:DG:N7	2.13	0.63
10:V:132:ARG:HB3	10:V:302:GLU:HG2	1.81	0.63
7:M:1239:SER:O	7:M:1240:LEU:HG	1.99	0.63
10:T:285:ARG:NH1	10:T:286:GLN:OE1	2.31	0.63
10:T:431:ARG:NH2	10:T:438:ASP:OD2	2.31	0.63
10:V:82:SER:HA	13:V:501:ADP:H5'1	1.80	0.63
10:V:315:MET:HA	10:V:348:ARG:HD3	1.80	0.63
10:X:252:LEU:O	10:X:256:ASN:ND2	2.32	0.62
11:U:300:MET:O	11:U:333:ARG:NH1	2.32	0.62
10:V:377:LYS:HG3	10:V:408:THR:HG21	1.81	0.62
10:X:154:ASN:HB3	10:X:159:TYR:HA	1.81	0.62
10:V:203:GLU:OE1	10:V:206:THR:N	2.31	0.62
1:B:120:GLN:HB3	1:B:123:GLU:HG2	1.80	0.62
10:T:102:PHE:HD2	10:T:104:PRO:HD3	1.64	0.62
11:U:360:ASN:N	11:U:363:GLU:OE2	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:241:LYS:HG3	10:V:243:ILE:HD11	1.81	0.62
10:V:342:ARG:HE	10:V:345:THR:HG21	1.64	0.62
7:M:1333:ALA:O	7:M:1360:GLN:NE2	2.32	0.62
10:V:122:MET:HB3	10:V:285:ARG:HH21	1.65	0.62
11:W:413:ARG:HH22	11:W:415:ASN:HD21	1.48	0.62
8:R:14:GLU:HA	8:R:30:ASN:H	1.64	0.62
8:R:345:VAL:O	8:R:349:MET:N	2.33	0.62
11:W:368:LEU:HD22	11:W:387:LEU:HB3	1.81	0.62
11:U:29:LEU:HG	11:U:30:GLY:H	1.64	0.62
8:R:435:GLN:NE2	9:S:221:ASP:OD1	2.33	0.62
10:X:316:LEU:HD12	10:X:320:ILE:HG21	1.80	0.62
1:B:89:ILE:HD12	1:B:92:LEU:HD11	1.82	0.61
8:R:125:PHE:O	8:R:416:ARG:NH1	2.33	0.61
10:V:266:ILE:HA	10:V:269:MET:HE2	1.81	0.61
11:W:29:LEU:HD12	11:W:51:ARG:HG3	1.81	0.61
11:W:437:VAL:HG22	10:X:356:PRO:HG3	1.81	0.61
7:M:1315:THR:HG23	7:M:1316:VAL:HG23	1.81	0.61
10:T:73:ARG:HB2	10:T:335:VAL:HG22	1.82	0.61
1:B:103:LEU:HA	1:B:131:ARG:HH22	1.64	0.61
11:W:362:GLN:HA	11:W:365:LYS:HZ3	1.65	0.61
5:I:-30:DG:N1	6:J:30:DC:N3	2.49	0.61
8:R:373:LEU:O	8:R:377:LEU:N	2.21	0.61
10:X:107:GLY:HA2	10:X:110:LEU:HD23	1.82	0.61
11:W:258:PHE:HB3	10:X:284:LEU:HD22	1.82	0.61
10:T:108:SER:HB3	11:U:304:GLU:HB2	1.82	0.61
11:Y:310:ASN:ND2	11:Y:346:ASP:OD1	2.33	0.61
11:Y:397:ARG:NH2	13:Y:501:ADP:O3A	2.34	0.61
11:W:114:THR:HG23	11:W:308:PHE:HE2	1.66	0.61
10:X:122:MET:HB3	10:X:285:ARG:HH12	1.66	0.61
1:A:119:ILE:HD11	2:D:50:ILE:HG22	1.83	0.61
1:B:69:ARG:HE	2:C:26:ILE:HD12	1.65	0.61
6:J:2:DG:C8	6:J:2:DG:H5'	2.35	0.61
10:V:265:VAL:HG22	10:V:269:MET:HE1	1.82	0.61
11:Y:303:ILE:HG21	11:Y:335:THR:HG23	1.82	0.61
1:B:63:ARG:HH11	6:J:-15:DA:H2'	1.65	0.61
10:T:258:ARG:O	10:T:260:GLN:NE2	2.33	0.61
11:U:413:ARG:NE	11:U:422:ASP:OD1	2.33	0.61
7:M:1188:VAL:HG21	10:V:206:THR:HG22	1.83	0.61
11:U:189:VAL:HB	11:U:202:LEU:HB2	1.83	0.61
11:W:139:GLU:N	11:W:161:LYS:O	2.29	0.61
11:W:193:ASP:OD1	11:W:198:LYS:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:204:ARG:HH21	11:Y:208:ARG:HE	1.49	0.61
7:M:821:MET:HE1	7:M:840:LEU:HD22	1.81	0.60
8:R:113:LYS:HD2	8:R:425:ASP:HA	1.82	0.60
8:R:325:ILE:HG23	8:R:327:LYS:H	1.65	0.60
10:T:116:LYS:HD2	10:T:117:LYS:N	2.15	0.60
11:U:440:VAL:HG21	10:V:356:PRO:HB3	1.81	0.60
1:B:121:LYS:HA	1:B:124:ILE:HD12	1.82	0.60
7:M:1132:ARG:NH1	11:Y:216:GLY:O	2.34	0.60
3:E:113:HIS:HB2	3:E:116:LEU:HD23	1.83	0.60
5:I:-49:DG:H2"	5:I:-48:DC:C5	2.35	0.60
7:M:822:VAL:HG12	7:M:849:LEU:HB3	1.84	0.60
8:R:2:GLU:O	8:R:98:HIS:NE2	2.32	0.60
5:I:21:DC:H2'	5:I:22:DC:C6	2.37	0.60
8:R:193:SER:HB2	8:R:359:ASN:HB2	1.82	0.60
8:R:413:ARG:HH22	8:R:415:THR:HA	1.67	0.60
10:T:43:ARG:HH22	10:T:50:GLY:HA2	1.67	0.60
11:U:297:GLU:HB2	11:U:300:MET:HE3	1.84	0.60
10:X:156:LEU:HD23	12:Z:291:LEU:HD21	1.82	0.60
1:B:63:ARG:HE	2:C:36:ARG:HH22	1.47	0.60
7:M:774:LEU:H	7:M:796:PHE:HB3	1.66	0.60
11:U:156:GLY:N	11:U:170:GLU:OE2	2.34	0.60
11:W:297:GLU:H	11:W:324:ALA:HB3	1.67	0.60
11:W:17:LEU:HD11	10:X:296:ILE:HD12	1.83	0.60
10:V:49:VAL:HG21	10:V:383:ILE:HD11	1.84	0.60
6:J:-16:DT:H5"	7:M:775:THR:HB	1.82	0.59
7:M:764:PHE:HE2	7:M:800:ILE:HG12	1.65	0.59
11:U:413:ARG:NH1	11:U:421:GLU:OE2	2.34	0.59
10:V:132:ARG:HD3	10:V:246:ASP:OD1	2.02	0.59
11:Y:397:ARG:O	11:Y:401:ASN:ND2	2.35	0.59
1:A:111:ALA:HB2	1:A:119:ILE:HG22	1.83	0.59
4:G:84:ALA:HB1	4:G:90:SER:HA	1.84	0.59
7:M:1245:CYS:HB3	7:M:1248:LEU:HB2	1.83	0.59
10:V:376:ASP:OD1	10:V:377:LYS:N	2.31	0.59
11:W:380:SER:OG	11:W:418:VAL:O	2.20	0.59
7:M:1291:ARG:HE	7:M:1295:ALA:HB3	1.67	0.59
8:R:313:ILE:O	8:R:316:THR:HG22	2.03	0.59
10:X:161:LYS:NZ	12:Z:592:ASN:HD21	2.01	0.59
10:X:187:GLU:O	10:X:191:ARG:N	2.32	0.59
10:X:313:VAL:HA	10:X:316:LEU:HD23	1.85	0.59
10:T:71:SER:OG	10:T:333:ALA:O	2.18	0.59
10:V:43:ARG:HG2	10:V:44:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:141:VAL:O	11:Y:159:THR:OG1	2.17	0.59
11:Y:343:LEU:HD22	11:Y:347:LEU:HD23	1.85	0.59
5:I:5:DC:O2	6:J:-4:DG:N2	2.36	0.59
9:S:172:LEU:O	9:S:175:ILE:HG22	2.03	0.58
10:V:43:ARG:NH2	10:V:378:ASP:OD2	2.35	0.58
1:B:93:GLN:HG2	7:M:781:GLN:NE2	2.18	0.58
6:J:71:DC:H2"	6:J:72:DA:N7	2.18	0.58
9:S:186:LYS:HE3	9:S:188:LYS:HB2	1.85	0.58
10:T:157:GLY:HA2	11:Y:145:ILE:HG22	1.85	0.58
10:X:26:ALA:O	13:X:501:ADP:O3'	2.20	0.58
7:M:1185:PRO:HA	11:W:266:ARG:HH12	1.68	0.58
6:J:-29:DT:H2'	7:M:981:SER:HB3	1.85	0.58
10:T:296:ILE:HG22	10:T:301:ALA:HB3	1.86	0.58
10:V:103:CYS:HB2	10:V:308:LEU:HA	1.85	0.58
11:Y:171:LEU:HB3	11:Y:175:MET:HB2	1.85	0.58
7:M:848:ARG:NH1	7:M:869:PHE:O	2.33	0.58
7:M:1062:ILE:O	7:M:1066:THR:OG1	2.13	0.58
8:R:55:ILE:O	9:S:109:ASN:ND2	2.37	0.58
8:R:98:HIS:HA	8:R:127:SER:HB2	1.85	0.58
11:W:118:THR:HG22	11:W:122:ARG:HD2	1.85	0.58
1:B:121:LYS:HG3	2:C:53:GLU:HG3	1.84	0.58
5:I:-48:DC:H2"	5:I:-47:DT:C5	2.39	0.58
10:T:26:ALA:O	13:T:501:ADP:O3'	2.21	0.58
10:V:316:LEU:HD22	10:V:320:ILE:HG21	1.86	0.58
10:V:342:ARG:H	10:V:357:HIS:HA	1.67	0.58
10:V:443:LYS:O	10:V:451:ARG:NH1	2.37	0.58
10:X:156:LEU:HG	10:X:157:GLY:H	1.69	0.58
11:Y:21:ALA:O	11:Y:371:ARG:NH1	2.36	0.58
5:I:-30:DG:C2	6:J:30:DC:C2	2.92	0.58
11:W:146:ASP:OD2	11:W:157:LYS:NZ	2.37	0.58
10:X:162:THR:HA	12:Z:592:ASN:HB3	1.83	0.58
10:X:225:GLU:HG3	11:Y:174:LYS:HB2	1.86	0.58
8:R:234:ARG:NH1	8:R:307:THR:OG1	2.37	0.58
11:U:314:GLU:OE2	11:U:350:ARG:NH2	2.36	0.58
5:I:-37:DG:H2"	5:I:-36:DT:H71	1.85	0.57
8:R:74:CYS:HB3	9:S:175:ILE:HD13	1.86	0.57
8:R:221:ARG:NE	9:S:106:ASN:OD1	2.36	0.57
11:W:54:ALA:HB2	11:W:84:LEU:HD11	1.86	0.57
11:W:155:GLN:HB3	12:Z:283:PRO:HG2	1.86	0.57
11:W:347:LEU:HA	11:W:350:ARG:HG2	1.85	0.57
11:Y:72:LEU:O	11:Y:354:ILE:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:ARG:NH1	2:C:43:VAL:O	2.37	0.57
11:W:401:ASN:OD1	10:X:73:ARG:NH1	2.37	0.57
7:M:805:LEU:HB3	7:M:813:PHE:CE2	2.39	0.57
11:W:171:LEU:HB3	11:W:175:MET:HB3	1.85	0.57
1:B:65:LEU:HD21	7:M:780:PRO:HG2	1.85	0.57
10:T:24:THR:OG1	10:T:391:GLU:OE2	2.22	0.57
11:W:448:ILE:HG12	11:W:454:VAL:HB	1.86	0.57
10:X:165:HIS:CD2	10:X:182:ASP:HA	2.39	0.57
10:X:380:ILE:HD11	10:X:412:LEU:HD13	1.86	0.57
5:I:23:DA:H5"	7:M:1270:GLN:HG2	1.86	0.57
6:J:17:DA:H2"	6:J:18:DG:C8	2.38	0.57
7:M:1180:PHE:O	11:W:248:ASN:ND2	2.38	0.57
11:Y:241:LEU:HD13	11:Y:244:ILE:HD12	1.86	0.57
5:I:-72:DT:H2"	5:I:-71:DG:N7	2.20	0.57
6:J:3:DC:H4'	6:J:4:DG:H5'	1.87	0.57
8:R:354:VAL:HG22	8:R:386:SER:HB2	1.85	0.57
11:W:456:ILE:HD12	10:X:81:PRO:HB2	1.86	0.57
5:I:-57:DC:H4'	7:M:817:ARG:HA	1.86	0.57
7:M:1183:LEU:HB2	11:W:248:ASN:HB3	1.87	0.57
8:R:17:PHE:O	8:R:26:PHE:HB2	2.05	0.57
9:S:251:ASP:OD2	11:U:232:ARG:NH2	2.38	0.57
10:T:125:PHE:HD1	10:T:334:PRO:HD2	1.69	0.57
11:W:149:ILE:HG22	11:W:150:THR:HG23	1.86	0.57
7:M:753:PRO:HD2	7:M:824:ASP:HB3	1.85	0.57
11:U:162:THR:O	11:U:208:ARG:NH1	2.38	0.57
6:J:41:DC:H2"	6:J:42:DA:C8	2.39	0.57
10:T:456:LEU:HD11	11:U:341:HIS:CE1	2.40	0.57
11:U:37:PRO:HB3	11:U:51:ARG:HB3	1.86	0.57
10:V:53:GLU:OE2	10:V:371:ARG:NH2	2.37	0.57
10:V:108:SER:OG	11:W:114:THR:OG1	2.22	0.57
10:V:252:LEU:HD11	10:V:288:VAL:HG13	1.87	0.57
10:X:34:GLY:HA3	10:X:55:ARG:HH21	1.70	0.57
10:X:112:SER:OG	10:X:115:VAL:O	2.22	0.57
11:Y:211:ASP:OD1	11:Y:212:TYR:N	2.38	0.57
10:V:49:VAL:HG11	10:V:383:ILE:HG13	1.87	0.57
10:X:143:GLU:H	10:X:171:LYS:H	1.51	0.57
10:X:214:ARG:N	10:X:228:GLU:O	2.38	0.57
10:X:448:ASP:OD2	10:X:450:LYS:NZ	2.37	0.57
5:I:-41:DG:C6	6:J:42:DA:N1	2.73	0.56
8:R:81:PHE:CE1	8:R:91:LEU:HD22	2.39	0.56
10:T:343:GLY:O	10:T:357:HIS:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:69:ARG:HB2	11:U:320:ILE:HG23	1.87	0.56
10:V:143:GLU:O	10:V:171:LYS:N	2.38	0.56
11:W:162:THR:HG23	11:W:164:ASP:H	1.70	0.56
11:Y:74:ALA:N	11:Y:354:ILE:O	2.31	0.56
5:I:-49:DG:N1	6:J:50:DG:O6	2.38	0.56
7:M:1044:ASN:ND2	7:M:1134:PRO:O	2.38	0.56
9:S:198:LEU:O	9:S:202:LEU:HB2	2.05	0.56
10:X:105:LEU:O	10:X:310:ILE:HA	2.06	0.56
3:E:28:VAL:O	3:E:32:HIS:N	2.31	0.56
7:M:925:LEU:HB3	7:M:929:LEU:HD13	1.86	0.56
8:R:338:LEU:HD12	8:R:346:ARG:HG2	1.87	0.56
8:R:431:ARG:HG3	8:R:432:PHE:CD1	2.41	0.56
9:S:237:VAL:HG13	9:S:238:LEU:HD12	1.87	0.56
11:W:76:PRO:O	11:W:81:LYS:NZ	2.38	0.56
11:Y:106:ILE:HD11	11:Y:301:LEU:HD22	1.87	0.56
7:M:1222:ASN:ND2	7:M:1228:GLN:OE1	2.39	0.56
11:Y:448:ILE:HG12	11:Y:454:VAL:HB	1.86	0.56
5:I:-57:DC:H2"	5:I:-56:DC:H5	1.70	0.56
8:R:195:PHE:O	8:R:220:GLY:N	2.36	0.56
10:T:314:ASN:HD21	10:T:342:ARG:HD3	1.70	0.56
11:U:401:ASN:OD1	10:V:73:ARG:NH1	2.38	0.56
10:X:173:ALA:HB3	10:X:234:LYS:HA	1.87	0.56
5:I:-41:DG:C2	6:J:42:DA:C2	2.94	0.56
10:V:330:SER:OG	10:V:331:ASN:N	2.36	0.56
10:X:381:ARG:NH1	10:X:385:GLU:OE2	2.39	0.56
5:I:11:DG:H2'	5:I:12:DT:H71	1.87	0.56
8:R:373:LEU:HB3	8:R:377:LEU:HD23	1.87	0.56
11:U:115:GLU:OE2	11:U:119:GLN:NE2	2.33	0.56
11:U:139:GLU:N	11:U:161:LYS:O	2.38	0.56
7:M:1290:MET:O	7:M:1317:PHE:HA	2.06	0.56
8:R:79:CYS:SG	8:R:80:LEU:N	2.79	0.56
10:T:133:ILE:HG22	10:T:301:ALA:HB2	1.87	0.56
11:U:34:ASN:O	11:U:36:GLN:NE2	2.29	0.56
11:U:259:THR:HB	10:V:278:THR:HG21	1.87	0.56
5:I:13:DT:H2"	5:I:14:DT:C5	2.41	0.56
7:M:863:LEU:HD13	7:M:921:LEU:HD11	1.88	0.56
7:M:1208:ASN:O	7:M:1212:LYS:NZ	2.39	0.56
10:V:441:GLU:OE2	11:W:52:ARG:NH2	2.29	0.56
8:R:210:TYR:O	9:S:228:ASN:ND2	2.39	0.55
11:W:169:TYR:OH	11:W:230:GLN:NE2	2.39	0.55
11:W:361:GLU:HA	11:W:364:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:84:GLY:O	10:X:88:LEU:N	2.26	0.55
2:C:73:THR:OG1	2:C:78:ARG:O	2.24	0.55
3:E:45:GLY:HA2	6:J:38:DG:H5"	1.86	0.55
5:I:-1:DG:H2"	5:I:0:DC:H5	1.71	0.55
10:T:143:GLU:HA	10:T:199:VAL:HA	1.89	0.55
11:U:204:ARG:HB2	11:U:222:VAL:HG11	1.88	0.55
11:U:386:LEU:HD11	11:U:420:VAL:HG13	1.87	0.55
5:I:-70:DG:H2"	5:I:-69:DA:H8	1.70	0.55
7:M:751:VAL:HA	7:M:801:VAL:O	2.06	0.55
7:M:1196:ALA:HA	11:U:255:LEU:HD11	1.88	0.55
8:R:26:PHE:HE2	8:R:86:PHE:HB3	1.72	0.55
8:R:228:LYS:HE2	8:R:239:MET:HA	1.88	0.55
10:V:318:ILE:H	10:V:349:GLY:HA3	1.71	0.55
8:R:274:TYR:HB3	8:R:304:ILE:HG13	1.87	0.55
11:W:250:ARG:NH2	11:W:261:ASP:OD1	2.39	0.55
6:J:-17:DT:O4	7:M:1301:ARG:NH1	2.40	0.55
8:R:133:VAL:HA	8:R:136:PHE:HD2	1.71	0.55
11:U:331:LYS:NZ	11:U:332:THR:O	2.38	0.55
10:V:126:ARG:HG3	10:V:250:HIS:HB2	1.89	0.55
6:J:46:DG:H2"	6:J:47:DA:N7	2.21	0.55
8:R:92:LYS:HG3	8:R:93:GLU:H	1.71	0.55
10:T:437:ASN:OD1	10:T:438:ASP:N	2.39	0.55
11:U:409:ILE:O	11:U:412:LYS:HG2	2.06	0.55
11:W:47:GLN:HB3	11:W:50:ALA:HB3	1.88	0.55
11:W:365:LYS:HA	11:W:368:LEU:HD12	1.89	0.55
5:I:2:DG:H2'	5:I:3:DT:C6	2.42	0.55
9:S:246:ILE:HG13	9:S:271:LEU:HD11	1.88	0.55
12:Z:299:PRO:HD2	12:Z:303:LEU:HD13	1.88	0.55
10:T:96:LEU:HD13	10:T:100:VAL:HG11	1.89	0.55
10:V:383:ILE:HG22	10:V:416:LEU:HD21	1.88	0.55
7:M:1009:VAL:HG22	10:V:206:THR:HG23	1.88	0.55
10:T:64:LEU:HB2	11:Y:408:GLN:HG2	1.89	0.55
10:T:132:ARG:HB2	10:T:302:GLU:HG2	1.88	0.55
10:T:450:LYS:O	10:T:453:THR:OG1	2.25	0.55
5:I:3:DT:H2"	5:I:4:DC:H5'	1.88	0.55
8:R:234:ARG:HH22	8:R:308:ASP:HB3	1.71	0.55
10:T:104:PRO:HB3	10:T:309:PHE:HB3	1.88	0.55
11:U:160:ILE:HD13	11:U:169:TYR:HD2	1.71	0.55
10:V:167:ILE:HG23	10:V:178:THR:HB	1.88	0.55
10:V:172:SER:OG	10:V:233:PRO:O	2.23	0.55
11:W:402:LEU:HA	11:W:405:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:220:ILE:HD12	12:Z:223:ARG:CZ	2.37	0.55
2:C:35:ARG:NE	5:I:8:DC:H5"	2.21	0.54
3:E:84:LEU:HD22	4:G:64:ILE:HD13	1.88	0.54
4:G:45:TYR:CG	5:I:-53:DG:H5"	2.41	0.54
7:M:950:TYR:HE2	7:M:1376:GLU:HA	1.72	0.54
10:V:371:ARG:HH21	10:V:373:LEU:HD21	1.71	0.54
10:V:462:TYR:HB2	11:W:327:ARG:HA	1.89	0.54
10:X:413:ARG:NH2	13:X:501:ADP:O3A	2.40	0.54
11:Y:387:LEU:HD21	11:Y:402:LEU:HD22	1.90	0.54
12:Z:608:ASP:O	12:Z:611:THR:OG1	2.23	0.54
5:I:-30:DG:C2	6:J:30:DC:O2	2.60	0.54
7:M:1229:THR:HG22	10:V:263:GLN:HB3	1.89	0.54
10:T:91:ALA:O	10:T:95:GLU:HG2	2.07	0.54
11:W:26:ILE:HG21	13:W:501:ADP:H2	1.73	0.54
11:W:309:ILE:O	11:W:313:LEU:HG	2.08	0.54
7:M:1023:ARG:NH1	11:U:195:ALA:O	2.41	0.54
7:M:1354:ARG:NH1	7:M:1357:ARG:HH22	2.05	0.54
8:R:6:ILE:HG23	8:R:19:PRO:HA	1.89	0.54
11:U:40:THR:HA	11:U:45:VAL:HG12	1.88	0.54
11:U:158:LEU:HD22	11:U:171:LEU:HG	1.89	0.54
7:M:956:ARG:HD3	7:M:996:PRO:HB2	1.90	0.54
8:R:186:ASP:OD1	8:R:187:PHE:N	2.40	0.54
8:R:244:LEU:HD11	8:R:274:TYR:CE2	2.42	0.54
8:R:274:TYR:HA	8:R:287:VAL:HG22	1.90	0.54
11:U:300:MET:HG2	11:U:333:ARG:HD3	1.90	0.54
5:I:-66:DA:H2"	5:I:-65:DT:C5	2.42	0.54
7:M:1200:ASN:HD21	7:M:1203:SER:HB3	1.72	0.54
10:V:48:PHE:HA	13:V:501:ADP:HN62	1.72	0.54
10:X:126:ARG:HH21	10:X:249:LEU:HB3	1.73	0.54
7:M:946:GLU:HA	7:M:1366:ILE:HB	1.88	0.54
8:R:58:ARG:NH1	8:R:59:ARG:O	2.41	0.54
9:S:207:ASN:N	9:S:210:SER:OG	2.33	0.54
5:I:-16:DT:H2"	5:I:-15:DA:N7	2.23	0.54
7:M:925:LEU:O	7:M:929:LEU:HB2	2.08	0.54
8:R:92:LYS:HB2	9:S:184:LEU:HD13	1.89	0.54
10:V:387:ARG:HH11	10:V:419:LEU:HD12	1.73	0.54
11:W:141:VAL:HB	11:W:161:LYS:NZ	2.20	0.54
7:M:784:LYS:HA	7:M:787:ARG:HD3	1.90	0.54
7:M:946:GLU:OE1	7:M:1368:ARG:NH2	2.37	0.54
8:R:31:ALA:HA	8:R:60:PRO:HD2	1.89	0.54
8:R:152:GLY:N	8:R:383:CYS:SG	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:346:THR:OG1	10:T:350:THR:OG1	2.23	0.54
11:Y:71:VAL:HG23	11:Y:352:ILE:HG13	1.89	0.54
11:Y:188:ASP:HB2	11:Y:204:ARG:HA	1.89	0.54
11:Y:267:SER:HA	11:Y:270:ARG:HG3	1.90	0.54
9:S:181:SER:O	9:S:182:THR:OG1	2.27	0.53
10:T:224:LEU:HB3	11:U:175:MET:HE3	1.90	0.53
10:V:324:LEU:HD12	10:V:327:ALA:HB3	1.89	0.53
11:W:303:ILE:HD12	11:W:306:PHE:HB2	1.90	0.53
10:X:185:ILE:O	10:X:188:SER:OG	2.18	0.53
12:Z:307:LYS:O	12:Z:310:GLN:HG3	2.08	0.53
1:B:93:GLN:O	1:B:97:GLU:HG3	2.07	0.53
7:M:990:ARG:NH2	7:M:1342:ASP:OD1	2.41	0.53
8:R:108:LEU:HD13	9:S:217:LEU:HD13	1.91	0.53
10:T:172:SER:HA	10:T:233:PRO:HG2	1.90	0.53
10:V:80:GLY:O	10:V:83:THR:OG1	2.21	0.53
10:X:22:THR:OG1	10:X:23:ARG:NH1	2.41	0.53
2:C:98:TYR:HB2	3:E:103:ILE:HD13	1.91	0.53
11:U:293:LEU:HD23	11:U:319:PRO:HG2	1.90	0.53
10:X:463:LEU:HB2	11:Y:76:PRO:HD3	1.89	0.53
10:X:125:PHE:HE1	10:X:333:ALA:HA	1.74	0.53
6:J:-20:DC:H2"	6:J:-19:DG:C8	2.44	0.53
7:M:1070:ASN:HD21	11:Y:206:PHE:HB2	1.74	0.53
8:R:63:LEU:HD12	9:S:119:LEU:HD22	1.89	0.53
8:R:66:LEU:HD22	8:R:72:GLU:HG2	1.91	0.53
10:V:338:LEU:HD22	10:V:367:LEU:HD21	1.90	0.53
11:W:143:ILE:HD11	11:W:145:ILE:HD11	1.89	0.53
11:W:370:ILE:HA	11:W:373:GLN:HG2	1.91	0.53
10:X:363:LEU:HA	10:X:366:ARG:HG2	1.91	0.53
10:X:463:LEU:HD13	11:Y:75:GLY:HA2	1.91	0.53
5:I:22:DC:H5"	7:M:1322:ARG:HB2	1.90	0.53
11:U:144:GLN:HB3	11:U:157:LYS:HB2	1.89	0.53
11:U:364:ILE:HD12	11:U:396:LEU:HD12	1.91	0.53
10:X:107:GLY:HA3	10:X:316:LEU:HD21	1.90	0.53
1:B:66:PRO:HG2	6:J:-14:DA:O3'	2.09	0.53
7:M:964:PHE:CE1	7:M:988:GLN:HG2	2.43	0.53
7:M:1291:ARG:NH2	7:M:1295:ALA:O	2.39	0.53
8:R:319:HIS:CE1	8:R:321:GLU:HB2	2.43	0.53
10:T:346:THR:HA	10:T:354:ILE:HA	1.91	0.53
11:Y:402:LEU:HA	11:Y:405:VAL:HG12	1.89	0.53
1:A:128:ARG:NH1	1:A:133:GLU:O	2.41	0.53
5:I:-44:DA:H2'	5:I:-43:DT:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:406:THR:HG22	8:R:407:ASP:H	1.74	0.53
7:M:1025:LEU:HD11	11:U:247:ILE:HG13	1.90	0.53
8:R:129:PHE:HA	8:R:432:PHE:CZ	2.44	0.53
10:V:181:LEU:HD13	10:V:186:TYR:HA	1.90	0.53
6:J:-15:DA:H2"	6:J:-14:DA:C8	2.44	0.53
10:T:141:GLU:H	10:T:237:VAL:HG23	1.74	0.53
10:V:116:LYS:HG3	10:V:119:GLU:HG2	1.90	0.53
10:V:199:VAL:O	10:V:212:VAL:N	2.40	0.53
10:V:264:ASP:O	10:V:267:SER:OG	2.24	0.53
10:X:61:ILE:O	10:X:65:ILE:HG12	2.08	0.53
6:J:-24:DT:H2"	6:J:-23:DT:O2	2.09	0.52
10:X:454:LYS:O	10:X:458:THR:OG1	2.18	0.52
1:B:61:LEU:HB3	2:C:36:ARG:HB3	1.91	0.52
10:T:417:GLN:NE2	11:U:350:ARG:O	2.35	0.52
11:W:306:PHE:HE2	11:W:332:THR:HB	1.74	0.52
11:Y:130:LYS:HG2	11:Y:236:VAL:HG22	1.91	0.52
6:J:-7:DG:H2"	6:J:-6:DG:C8	2.45	0.52
7:M:1190:LEU:HA	7:M:1193:ARG:HH12	1.74	0.52
7:M:1233:ILE:HG12	7:M:1235:PHE:H	1.73	0.52
11:W:343:LEU:HD11	11:W:347:LEU:HD23	1.91	0.52
10:X:165:HIS:HD2	10:X:182:ASP:HA	1.75	0.52
11:Y:303:ILE:N	11:Y:333:ARG:O	2.40	0.52
1:B:65:LEU:HG	7:M:781:GLN:HB2	1.92	0.52
2:C:35:ARG:HH22	2:C:50:ILE:HD13	1.74	0.52
7:M:937:VAL:HG12	7:M:940:GLN:HB2	1.90	0.52
10:T:378:ASP:HA	10:T:381:ARG:HG2	1.92	0.52
7:M:1100:ALA:O	8:R:352:ASN:ND2	2.41	0.52
8:R:13:TYR:HB2	8:R:195:PHE:HB3	1.91	0.52
8:R:111:LEU:HD21	9:S:211:PHE:CE2	2.44	0.52
10:T:308:LEU:HB3	10:T:336:VAL:HG12	1.92	0.52
11:U:332:THR:OG1	11:U:337:TYR:O	2.28	0.52
10:V:445:LEU:HD21	11:W:49:GLN:HE21	1.75	0.52
10:V:446:PHE:HB3	11:W:352:ILE:HG23	1.91	0.52
5:I:-8:DC:H2"	5:I:-7:DG:H5'	1.90	0.52
5:I:24:DA:H2"	5:I:25:DG:C8	2.45	0.52
7:M:719:LEU:HD23	7:M:721:ASP:HB2	1.92	0.52
9:S:90:TYR:HB3	9:S:94:GLU:OE2	2.09	0.52
10:T:145:THR:HG22	10:T:171:LYS:HG2	1.90	0.52
10:V:122:MET:HE3	10:V:323:TYR:OH	2.09	0.52
11:W:35:LEU:HD21	11:W:59:LYS:HE3	1.91	0.52
10:X:165:HIS:HA	10:X:183:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-67:DA:N1	6:J:68:DC:N4	2.58	0.52
7:M:1003:PRO:O	11:W:276:LYS:NZ	2.43	0.52
7:M:1173:ASN:HB3	7:M:1176:ILE:HB	1.91	0.52
10:T:144:VAL:O	10:T:171:LYS:NZ	2.41	0.52
10:T:185:ILE:O	10:T:189:ILE:HG12	2.10	0.52
11:Y:113:LYS:HZ1	11:Y:304:GLU:C	2.17	0.52
5:I:-5:DA:H2"	5:I:-4:DC:C4	2.44	0.52
7:M:1132:ARG:NH1	11:Y:219:THR:O	2.42	0.52
8:R:288:ARG:HH12	8:R:303:ILE:HD13	1.74	0.52
10:T:319:GLU:OE2	10:T:320:ILE:HG12	2.09	0.52
10:V:309:PHE:CZ	10:V:311:ASP:HB2	2.45	0.52
5:I:6:DC:H4'	5:I:7:DC:H5'	1.92	0.52
6:J:-18:DG:H4'	7:M:757:LEU:HB3	1.92	0.52
6:J:71:DC:H2"	6:J:72:DA:C8	2.45	0.52
7:M:983:VAL:HA	7:M:986:LEU:HB2	1.91	0.52
10:V:140:TYR:HB3	10:V:170:LEU:HD12	1.92	0.52
11:W:154:LYS:HD2	11:W:176:ILE:HG21	1.90	0.52
10:X:160:GLY:HA3	12:Z:599:PHE:CZ	2.45	0.52
10:X:318:ILE:HG13	10:X:350:THR:HG22	1.91	0.52
5:I:-26:DT:H2"	5:I:-25:DA:C8	2.45	0.52
7:M:726:GLY:O	7:M:730:GLN:HG3	2.10	0.52
8:R:191:ILE:HG13	8:R:200:ILE:HG23	1.91	0.52
9:S:92:GLN:HA	9:S:95:ILE:HG12	1.90	0.52
11:U:402:LEU:HA	11:U:405:VAL:HG12	1.92	0.52
11:W:343:LEU:HD23	11:W:348:LEU:HD23	1.92	0.52
12:Z:225:ARG:NH1	12:Z:229:GLU:HB2	2.25	0.52
1:B:128:ARG:HH11	2:C:57:VAL:HG22	1.75	0.51
11:W:259:THR:OG1	11:W:261:ASP:OD2	2.28	0.51
10:X:71:SER:OG	10:X:333:ALA:O	2.27	0.51
10:X:380:ILE:HD11	10:X:412:LEU:HB2	1.93	0.51
1:B:70:LEU:HG	2:C:26:ILE:HD13	1.93	0.51
1:B:125:LYS:NZ	2:C:53:GLU:OE2	2.42	0.51
6:J:-19:DG:H2'	7:M:1301:ARG:HD3	1.92	0.51
7:M:805:LEU:HB3	7:M:813:PHE:HE2	1.74	0.51
8:R:15:ILE:HG12	8:R:28:ALA:HB3	1.93	0.51
11:W:380:SER:OG	11:W:382:ASP:OD1	2.26	0.51
11:Y:156:GLY:H	12:Z:621:THR:HG23	1.74	0.51
6:J:53:DC:H2"	6:J:54:DT:H72	1.90	0.51
6:J:73:DG:H2"	6:J:74:DG:C8	2.45	0.51
7:M:784:LYS:HA	7:M:787:ARG:HB2	1.91	0.51
11:W:125:ILE:HD13	11:W:291:GLY:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:147:ARG:HD2	11:W:154:LYS:HD3	1.92	0.51
11:Y:193:ASP:HB3	11:Y:197:GLY:HA3	1.91	0.51
11:Y:409:ILE:HD11	11:Y:425:ARG:HH11	1.76	0.51
2:C:96:THR:HG23	3:E:101:VAL:HG13	1.92	0.51
7:M:1046:VAL:HG22	7:M:1049:LEU:HB2	1.92	0.51
8:R:189:LEU:HD12	8:R:202:PRO:HB3	1.92	0.51
12:Z:297:MET:O	12:Z:297:MET:HG2	2.10	0.51
1:A:103:LEU:HD21	1:A:124:ILE:HG23	1.92	0.51
5:I:-47:DT:H2"	5:I:-46:DC:C5	2.45	0.51
7:M:778:GLY:O	7:M:783:ARG:N	2.41	0.51
8:R:32:LEU:HD21	9:S:171:THR:HG21	1.93	0.51
8:R:68:LEU:HB3	8:R:70:GLU:OE1	2.10	0.51
8:R:194:GLY:O	8:R:359:ASN:ND2	2.44	0.51
8:R:311:PHE:HZ	9:S:248:GLY:HA3	1.74	0.51
10:T:459:SER:OG	10:T:461:ASN:O	2.29	0.51
10:V:258:ARG:HH22	10:V:277:LYS:HD3	1.76	0.51
11:Y:271:ASP:OD1	11:Y:272:GLN:N	2.43	0.51
12:Z:302:GLU:O	12:Z:305:ASP:HB2	2.10	0.51
6:J:-27:DC:H5	7:M:980:MET:HE1	1.75	0.51
9:S:201:VAL:HA	9:S:204:SER:HB2	1.92	0.51
10:X:131:LEU:HD13	10:X:296:ILE:HD11	1.92	0.51
1:A:96:VAL:HG22	2:D:61:PHE:HD2	1.75	0.51
2:C:30:THR:HA	6:J:-13:DA:H2'	1.91	0.51
7:M:1232:THR:HG22	7:M:1233:ILE:N	2.25	0.51
8:R:20:SER:OG	8:R:401:SER:O	2.28	0.51
8:R:74:CYS:HB3	9:S:175:ILE:HG21	1.92	0.51
8:R:83:PRO:HD2	9:S:182:THR:HB	1.91	0.51
11:W:449:ASP:OD2	11:W:451:GLN:NE2	2.43	0.51
1:B:126:LEU:HD12	1:B:129:ARG:HH21	1.75	0.51
8:R:68:LEU:HD21	9:S:206:ARG:H	1.76	0.51
8:R:204:LEU:HD11	8:R:345:VAL:HG11	1.93	0.51
11:U:460:LYS:HD2	10:V:409:GLU:HG2	1.93	0.51
11:W:141:VAL:O	11:W:186:ALA:HB1	2.11	0.51
10:X:311:ASP:OD2	11:Y:311:ARG:NE	2.40	0.51
11:Y:367:ILE:HG12	13:Y:501:ADP:C2	2.45	0.51
8:R:361:ASN:ND2	8:R:391:ASP:OD1	2.40	0.51
10:V:362:ASP:HB2	10:V:366:ARG:HH12	1.75	0.51
10:X:224:LEU:HD13	11:Y:192:ILE:HG12	1.92	0.51
2:C:98:TYR:OH	4:G:71:ASP:OD2	2.19	0.50
10:T:148:THR:OG1	10:T:167:ILE:HB	2.11	0.50
7:M:1183:LEU:HD21	11:W:273:ILE:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:9:ASP:HB2	8:R:397:TRP:HD1	1.76	0.50
10:T:404:ALA:O	10:T:408:THR:HG23	2.10	0.50
4:G:43:TYR:HA	4:G:46:LYS:HD2	1.93	0.50
8:R:370:ALA:HB2	8:R:385:VAL:HG21	1.93	0.50
10:V:172:SER:N	10:V:175:GLY:O	2.40	0.50
10:X:144:VAL:N	10:X:197:GLY:HA2	2.27	0.50
1:A:117:VAL:HG21	2:D:43:VAL:HG22	1.93	0.50
6:J:-19:DG:H5"	7:M:1301:ARG:HD3	1.93	0.50
6:J:4:DG:H2"	6:J:5:DT:C6	2.46	0.50
8:R:239:MET:HE2	9:S:113:LEU:HD11	1.92	0.50
11:U:47:GLN:HB3	11:U:50:ALA:HB3	1.92	0.50
10:X:190:GLN:NE2	12:Z:608:ASP:OD1	2.38	0.50
1:B:66:PRO:O	1:B:69:ARG:HG2	2.11	0.50
2:C:30:THR:HG21	2:C:33:ALA:HB3	1.94	0.50
5:I:-1:DG:H2"	5:I:0:DC:C5	2.46	0.50
10:T:414:TYR:HE1	10:T:451:ARG:HH22	1.60	0.50
10:V:264:ASP:OD1	10:V:265:VAL:N	2.45	0.50
11:Y:360:ASN:N	11:Y:363:GLU:OE2	2.32	0.50
7:M:1200:ASN:ND2	7:M:1202:ASP:O	2.45	0.50
7:M:1300:ASP:HB3	7:M:1304:LEU:HD13	1.94	0.50
8:R:380:ASP:OD1	8:R:380:ASP:N	2.45	0.50
9:S:269:PHE:HA	9:S:272:HIS:HB3	1.92	0.50
11:U:382:ASP:OD1	11:U:383:ALA:N	2.43	0.50
11:Y:70:ALA:HB1	11:Y:323:MET:HE1	1.94	0.50
11:Y:315:ASP:OD1	11:Y:316:GLU:N	2.40	0.50
11:Y:382:ASP:OD1	11:Y:383:ALA:N	2.43	0.50
2:C:30:THR:HG22	6:J:-13:DA:H8	1.76	0.50
10:T:415:ALA:O	10:T:419:LEU:HG	2.11	0.50
11:U:267:SER:O	11:U:270:ARG:HG2	2.12	0.50
10:X:70:MET:HG2	10:X:73:ARG:CZ	2.41	0.50
10:X:225:GLU:O	11:Y:196:SER:HA	2.11	0.50
10:X:395:VAL:HG13	10:X:400:LEU:HB2	1.92	0.50
11:Y:421:GLU:HG2	11:Y:422:ASP:H	1.75	0.50
8:R:59:ARG:HE	8:R:61:HIS:HB2	1.77	0.50
10:T:316:LEU:HD13	10:T:320:ILE:HG21	1.93	0.50
11:W:345:LEU:HA	11:W:348:LEU:HD12	1.93	0.50
10:X:166:VAL:HG23	10:X:183:PRO:HA	1.94	0.50
10:X:188:SER:HB2	10:X:209:VAL:HG22	1.93	0.50
12:Z:302:GLU:OE1	12:Z:306:ARG:NH1	2.45	0.50
1:B:110:ALA:O	1:B:113:HIS:HB3	2.11	0.50
3:E:51:TYR:HE2	4:G:101:VAL:HG11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:803:TYR:CZ	7:M:829:ILE:HD12	2.46	0.50
10:T:134:LYS:NZ	10:T:300:VAL:O	2.42	0.50
10:X:446:PHE:CZ	11:Y:352:ILE:HD12	2.47	0.50
11:Y:41:SER:O	11:Y:44:MET:HG3	2.12	0.50
1:A:119:ILE:O	2:D:49:LEU:HG	2.12	0.49
7:M:1157:ILE:N	10:X:135:GLU:OE2	2.45	0.49
9:S:265:SER:OG	9:S:268:CYS:SG	2.70	0.49
10:V:426:ALA:HB1	10:V:431:ARG:HB3	1.94	0.49
10:X:310:ILE:HB	10:X:338:LEU:HD13	1.94	0.49
1:B:96:VAL:HG13	2:C:58:LEU:HD13	1.93	0.49
2:D:36:ARG:HA	2:D:39:ARG:HD2	1.93	0.49
6:J:-18:DG:H3'	7:M:758:LEU:HG	1.93	0.49
7:M:1242:GLN:HG3	7:M:1281:PHE:HD2	1.77	0.49
10:X:78:ALA:O	10:X:372:THR:N	2.41	0.49
10:X:396:GLU:OE2	10:X:398:SER:OG	2.30	0.49
8:R:7:VAL:HG23	8:R:20:SER:HB2	1.93	0.49
8:R:138:PRO:HB2	8:R:185:HIS:HB3	1.93	0.49
9:S:85:SER:HA	9:S:235:PHE:HB2	1.94	0.49
10:T:116:LYS:HD2	10:T:117:LYS:H	1.76	0.49
10:X:27:HIS:O	10:X:28:THR:OG1	2.30	0.49
10:X:65:ILE:HD12	10:X:335:VAL:HG11	1.93	0.49
5:I:-41:DG:N1	6:J:42:DA:C2	2.81	0.49
5:I:9:DG:H2"	5:I:10:DC:C6	2.48	0.49
10:T:452:SER:HA	10:T:455:ILE:HG22	1.93	0.49
10:X:29:HIS:CE1	10:X:387:ARG:HD3	2.47	0.49
11:Y:21:ALA:HB3	11:Y:24:SER:HB2	1.94	0.49
11:Y:163:THR:OG1	11:Y:227:GLY:O	2.31	0.49
5:I:14:DT:H2"	5:I:15:DT:C5	2.48	0.49
7:M:750:ILE:HG13	7:M:800:ILE:HA	1.94	0.49
7:M:1282:LEU:HD11	7:M:1316:VAL:HG21	1.95	0.49
11:W:300:MET:HE1	10:X:319:GLU:HA	1.95	0.49
8:R:362:LEU:HD12	8:R:363:PRO:HD2	1.93	0.49
11:W:127:ILE:HD12	11:W:288:ILE:HA	1.93	0.49
11:W:149:ILE:HB	12:Z:288:LEU:HG	1.95	0.49
10:X:447:LEU:HD22	10:X:451:ARG:HD2	1.94	0.49
11:Y:228:GLU:OE1	11:Y:230:GLN:N	2.45	0.49
5:I:-41:DG:N1	6:J:42:DA:N1	2.60	0.49
6:J:45:DT:H2"	6:J:46:DG:C5	2.48	0.49
7:M:1290:MET:HE3	7:M:1317:PHE:CE1	2.48	0.49
11:W:175:MET:HG2	11:W:179:LEU:HD23	1.94	0.49
7:M:922:HIS:O	7:M:926:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1223:PRO:HG3	10:X:264:ASP:HB2	1.95	0.49
8:R:364:ASN:ND2	8:R:367:GLN:OE1	2.39	0.49
10:T:429:SER:OG	10:T:431:ARG:NE	2.46	0.49
11:U:135:LEU:HB2	11:U:137:GLU:OE2	2.13	0.49
11:W:206:PHE:HB2	12:Z:584:GLY:HA2	1.95	0.49
10:X:144:VAL:H	10:X:197:GLY:HA2	1.78	0.49
11:Y:218:ASP:N	11:Y:218:ASP:OD1	2.46	0.49
1:B:70:LEU:HD22	2:C:59:LYS:HZ2	1.78	0.49
5:I:-19:DG:H2"	5:I:-18:DC:H5"	1.95	0.49
7:M:688:VAL:HG11	7:M:740:CYS:HB3	1.94	0.49
7:M:868:TYR:OH	7:M:875:VAL:O	2.28	0.49
8:R:94:GLY:HA2	8:R:97:HIS:HB2	1.95	0.49
8:R:416:ARG:NH2	8:R:420:TYR:OH	2.46	0.49
9:S:189:ARG:HB2	9:S:195:ILE:HD12	1.94	0.49
10:V:119:GLU:O	10:V:123:GLU:HG2	2.12	0.49
10:V:193:LYS:NZ	10:V:227:GLU:OE1	2.45	0.49
10:V:194:VAL:HG23	10:V:198:ASP:HB2	1.95	0.49
10:V:402:LEU:O	10:V:405:THR:OG1	2.22	0.49
10:X:122:MET:HB3	10:X:285:ARG:NH1	2.27	0.49
1:B:72:ARG:HH12	1:B:89:ILE:HD13	1.77	0.49
5:I:34:DT:H2"	5:I:35:DC:C5	2.48	0.49
6:J:-18:DG:H1'	6:J:-17:DT:H5'	1.94	0.49
8:R:91:LEU:HD21	8:R:125:PHE:HE1	1.78	0.49
8:R:108:LEU:HB2	8:R:111:LEU:HD23	1.94	0.49
10:T:33:LEU:O	10:T:55:ARG:NH2	2.44	0.49
11:U:408:GLN:HA	11:U:411:MET:HE2	1.95	0.49
11:W:302:ASP:OD1	11:W:303:ILE:N	2.45	0.49
2:D:92:ARG:NH2	3:E:97:LEU:O	2.33	0.48
3:E:84:LEU:HD21	4:G:64:ILE:HG21	1.95	0.48
7:M:1023:ARG:NH2	11:U:196:SER:OG	2.46	0.48
7:M:1266:LEU:HD22	7:M:1319:LEU:HD11	1.94	0.48
8:R:80:LEU:HD23	8:R:89:PHE:HZ	1.76	0.48
10:T:377:LYS:O	10:T:380:ILE:HG22	2.13	0.48
10:V:51:GLN:HG2	10:V:375:TYR:HE1	1.78	0.48
10:X:395:VAL:HG23	10:X:434:ILE:HB	1.95	0.48
11:Y:204:ARG:N	11:Y:220:ARG:O	2.37	0.48
2:C:63:GLU:HA	2:C:66:ILE:HG12	1.96	0.48
3:E:64:LEU:HD21	4:G:44:ILE:HG22	1.96	0.48
5:I:-55:DG:H2"	5:I:-54:DA:N7	2.29	0.48
7:M:785:GLU:HA	7:M:788:LYS:HE3	1.95	0.48
10:T:73:ARG:NH1	11:Y:401:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:441:GLU:OE2	11:U:52:ARG:NH1	2.46	0.48
10:V:452:SER:HA	10:V:455:ILE:HD12	1.94	0.48
10:V:452:SER:OG	11:W:341:HIS:NE2	2.46	0.48
1:A:106:ASP:HB2	1:A:127:ALA:HB1	1.95	0.48
6:J:-28:DC:H1'	6:J:-27:DC:H5'	1.94	0.48
8:R:122:GLU:HG2	9:S:198:LEU:HD13	1.96	0.48
8:R:355:CYS:HB2	8:R:387:VAL:HG22	1.94	0.48
11:U:161:LYS:HD3	11:U:166:GLU:HG3	1.95	0.48
11:U:171:LEU:HD22	11:U:175:MET:HB2	1.96	0.48
11:U:409:ILE:HD13	11:U:425:ARG:HB3	1.94	0.48
10:V:126:ARG:HB2	10:V:249:LEU:HD23	1.96	0.48
11:W:421:GLU:OE2	11:W:424:LYS:NZ	2.46	0.48
5:I:-32:DC:H2"	5:I:-31:DA:H8	1.78	0.48
8:R:9:ASP:HB2	8:R:397:TRP:CD1	2.49	0.48
8:R:17:PHE:CE1	8:R:28:ALA:HB2	2.48	0.48
8:R:308:ASP:OD2	9:S:248:GLY:N	2.41	0.48
10:T:84:GLY:N	13:T:501:ADP:O3B	2.41	0.48
10:T:122:MET:HA	10:T:122:MET:HE2	1.96	0.48
11:U:387:LEU:O	11:U:399:SER:OG	2.19	0.48
11:U:432:ASP:H	11:U:435:ARG:HB2	1.79	0.48
10:X:84:GLY:HA2	10:X:87:ALA:HB3	1.95	0.48
4:G:71:ASP:OD1	4:G:72:ILE:N	2.47	0.48
6:J:50:DG:H2"	6:J:51:DG:C8	2.49	0.48
8:R:56:THR:HG23	9:S:111:SER:HB3	1.94	0.48
8:R:99:LEU:HG	8:R:125:PHE:CZ	2.48	0.48
9:S:179:TYR:CG	9:S:183:LYS:HD2	2.49	0.48
10:V:401:ASP:O	10:V:405:THR:HG23	2.13	0.48
11:Y:245:ASP:OD1	11:Y:273:ILE:HG13	2.14	0.48
11:Y:386:LEU:O	11:Y:390:THR:HG23	2.14	0.48
12:Z:291:LEU:HB3	12:Z:593:PHE:CB	2.44	0.48
2:C:39:ARG:NH2	2:C:44:LYS:O	2.46	0.48
6:J:6:DA:H1'	6:J:7:DC:O4'	2.13	0.48
8:R:68:LEU:HD11	9:S:205:LYS:HA	1.95	0.48
8:R:319:HIS:HD1	8:R:322:ILE:HG13	1.79	0.48
10:V:76:LEU:HD22	10:V:367:LEU:HG	1.95	0.48
11:W:85:ALA:HB1	11:W:294:PHE:CE2	2.48	0.48
11:W:250:ARG:NH2	11:W:261:ASP:O	2.30	0.48
6:J:36:DA:H2"	6:J:37:DC:H5"	1.96	0.48
7:M:1086:GLN:HA	7:M:1090:GLY:HA3	1.94	0.48
8:R:420:TYR:HA	9:S:194:ARG:HH12	1.77	0.48
10:V:82:SER:N	13:V:501:ADP:O1B	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:126:ARG:HB3	10:V:285:ARG:HH12	1.78	0.48
10:X:169:GLY:HA2	10:X:178:THR:HA	1.95	0.48
5:I:19:DC:H2"	5:I:20:DG:C8	2.48	0.48
8:R:222:PHE:CE1	9:S:106:ASN:HB2	2.48	0.48
11:U:413:ARG:HH12	11:U:415:ASN:HD21	1.61	0.48
5:I:-44:DA:H2'	5:I:-43:DT:H6	1.78	0.48
7:M:801:VAL:HG12	7:M:806:VAL:HG23	1.95	0.48
10:T:180:ARG:H	10:T:180:ARG:HD3	1.79	0.48
2:C:58:LEU:HD12	2:C:62:LEU:HD23	1.96	0.48
6:J:62:DG:H2"	6:J:63:DG:C8	2.49	0.48
7:M:1023:ARG:CZ	11:U:196:SER:HA	2.44	0.48
8:R:6:ILE:HA	8:R:20:SER:H	1.78	0.48
8:R:60:PRO:HB3	9:S:166:VAL:HG21	1.95	0.48
11:U:169:TYR:OH	11:U:230:GLN:NE2	2.47	0.48
10:V:123:GLU:O	10:V:126:ARG:HG2	2.14	0.48
11:W:58:LEU:HA	11:W:61:VAL:HG22	1.96	0.48
11:U:413:ARG:NH1	11:U:415:ASN:HD21	2.11	0.47
11:Y:435:ARG:HA	11:Y:438:LYS:HE3	1.96	0.47
2:C:98:TYR:N	3:E:102:THR:O	2.36	0.47
4:G:70:ASN:O	4:G:74:GLU:HG2	2.14	0.47
6:J:15:DT:H2"	6:J:16:DA:C8	2.48	0.47
7:M:997:ASN:HA	7:M:1244:ASP:HB2	1.97	0.47
7:M:1242:GLN:HG3	7:M:1281:PHE:CD2	2.49	0.47
10:T:387:ARG:HA	10:T:390:VAL:HG12	1.96	0.47
10:V:324:LEU:HA	10:V:327:ALA:HB3	1.96	0.47
7:M:1195:LEU:HB3	11:U:254:PHE:HZ	1.80	0.47
8:R:26:PHE:CE2	8:R:86:PHE:HB3	2.49	0.47
9:S:207:ASN:OD1	9:S:208:LEU:N	2.40	0.47
10:V:35:LEU:HD23	10:V:41:ALA:HB2	1.96	0.47
11:Y:25:HIS:CD2	11:Y:26:ILE:HG12	2.49	0.47
1:B:106:ASP:OD2	1:B:131:ARG:NH2	2.28	0.47
7:M:859:ASN:O	7:M:862:GLU:HG2	2.15	0.47
9:S:246:ILE:HD11	9:S:276:ARG:HD2	1.94	0.47
11:U:360:ASN:O	11:U:364:ILE:HG12	2.14	0.47
10:V:102:PHE:CZ	10:V:309:PHE:HB2	2.50	0.47
11:W:147:ARG:HE	11:W:148:SER:N	2.12	0.47
3:E:52:LEU:HD13	4:G:76:ILE:HG21	1.95	0.47
8:R:19:PRO:HD3	8:R:89:PHE:HB2	1.96	0.47
10:T:106:VAL:HG23	10:T:109:GLU:HB2	1.96	0.47
11:U:131:GLU:OE2	11:U:237:HIS:ND1	2.33	0.47
10:X:51:GLN:HG2	10:X:375:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD13	2:C:59:LYS:HZ2	1.80	0.47
2:D:47:SER:OG	6:J:7:DC:H3'	2.15	0.47
5:I:-66:DA:H2"	5:I:-65:DT:C4	2.50	0.47
7:M:1377:SER:O	7:M:1381:LYS:HD2	2.14	0.47
9:S:266:VAL:HA	9:S:269:PHE:HD2	1.79	0.47
10:T:385:GLU:O	10:T:389:THR:HG23	2.14	0.47
11:U:44:MET:HA	13:U:502:ADP:N1	2.29	0.47
10:V:76:LEU:HD23	10:V:368:LEU:O	2.14	0.47
11:Y:194:LYS:NZ	11:Y:230:GLN:HE21	2.13	0.47
7:M:1242:GLN:HA	7:M:1245:CYS:SG	2.55	0.47
7:M:1292:LEU:N	7:M:1318:ILE:O	2.44	0.47
11:U:185:LEU:H	11:U:185:LEU:HD23	1.80	0.47
10:V:140:TYR:HB2	10:V:202:ILE:HG23	1.96	0.47
10:V:396:GLU:OE2	10:V:398:SER:OG	2.24	0.47
10:X:140:TYR:HB3	10:X:179:LEU:HD21	1.96	0.47
11:Y:141:VAL:O	11:Y:161:LYS:NZ	2.43	0.47
11:Y:314:GLU:HG3	11:Y:350:ARG:HH21	1.78	0.47
5:I:-26:DT:H73	6:J:26:DA:H61	1.80	0.47
7:M:1002:ARG:HH21	11:W:285:LYS:HB3	1.79	0.47
7:M:739:ALA:HA	7:M:745:TRP:CD1	2.50	0.47
8:R:132:PRO:HG2	8:R:135:VAL:HG23	1.97	0.47
10:T:383:ILE:HG21	10:T:412:LEU:HD21	1.96	0.47
10:V:435:VAL:HG13	10:V:437:ASN:H	1.79	0.47
11:W:176:ILE:O	11:W:180:THR:OG1	2.20	0.47
11:W:259:THR:O	10:X:278:THR:OG1	2.33	0.47
8:R:122:GLU:HG2	9:S:198:LEU:HD22	1.97	0.47
10:V:104:PRO:HA	10:V:309:PHE:HB3	1.96	0.47
12:Z:595:THR:HA	12:Z:596:LEU:HA	1.65	0.47
8:R:218:ILE:HG22	9:S:102:PHE:HZ	1.80	0.46
9:S:257:VAL:HG22	11:U:168:ILE:HG23	1.97	0.46
10:T:147:LEU:HD12	10:T:168:VAL:HA	1.98	0.46
12:Z:228:LYS:HA	12:Z:231:GLU:HG3	1.97	0.46
1:B:93:GLN:HG2	7:M:781:GLN:HE22	1.79	0.46
3:E:77:THR:N	6:J:58:DC:H5'	2.31	0.46
6:J:-27:DC:H2"	6:J:-26:DC:C5	2.50	0.46
7:M:1068:VAL:O	7:M:1069:LYS:HG2	2.15	0.46
7:M:1118:MET:HE2	7:M:1118:MET:HA	1.97	0.46
7:M:1317:PHE:CE2	7:M:1330:LEU:HD21	2.51	0.46
9:S:179:TYR:CD2	9:S:183:LYS:HD2	2.51	0.46
10:T:293:ALA:HA	10:T:296:ILE:HG12	1.96	0.46
11:U:135:LEU:HD21	11:U:231:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:247:ILE:HD13	11:U:253:GLY:HA3	1.97	0.46
12:Z:620:TYR:HD1	12:Z:625:SER:HA	1.81	0.46
7:M:776:TYR:O	7:M:776:TYR:CD2	2.68	0.46
7:M:1211:LEU:HD23	7:M:1214:MET:HE2	1.97	0.46
7:M:1256:GLN:OE1	7:M:1287:TYR:OH	2.33	0.46
7:M:1326:LEU:O	7:M:1354:ARG:NH2	2.38	0.46
8:R:8:ILE:HB	8:R:101:ALA:HA	1.96	0.46
11:W:153:HIS:ND1	12:Z:284:ASN:O	2.49	0.46
10:X:125:PHE:HZ	10:X:332:ILE:HB	1.80	0.46
5:I:26:DG:H5'	5:I:26:DG:C8	2.51	0.46
6:J:-19:DG:OP2	7:M:1296:THR:OG1	2.33	0.46
7:M:868:TYR:HE1	7:M:874:THR:HB	1.80	0.46
7:M:1224:LEU:HG	10:X:266:ILE:HD11	1.96	0.46
8:R:133:VAL:O	8:R:137:VAL:HG13	2.16	0.46
8:R:318:PHE:CD2	8:R:330:ILE:HD11	2.51	0.46
9:S:257:VAL:HA	11:U:168:ILE:HG12	1.97	0.46
10:T:303:LEU:HD23	10:T:303:LEU:H	1.79	0.46
10:T:324:LEU:HA	10:T:327:ALA:HB3	1.97	0.46
11:U:130:LYS:NZ	11:U:287:GLU:OE2	2.38	0.46
11:W:40:THR:HG23	11:W:45:VAL:HG22	1.97	0.46
4:G:57:ILE:HG22	4:G:58:SER:N	2.29	0.46
7:M:991:LYS:HE2	7:M:1273:LYS:HE3	1.98	0.46
8:R:319:HIS:ND1	8:R:322:ILE:HG13	2.31	0.46
11:U:331:LYS:HA	11:U:338:LYS:HB2	1.98	0.46
3:E:35:LEU:HD21	3:E:52:LEU:HD23	1.98	0.46
5:I:4:DC:H4'	5:I:5:DC:OP1	2.15	0.46
6:J:43:DA:H1'	6:J:44:DT:H5'	1.98	0.46
7:M:696:LEU:HB3	7:M:697:ARG:H	1.57	0.46
8:R:277:PRO:HB3	8:R:285:GLY:N	2.31	0.46
8:R:322:ILE:HD11	9:S:241:ILE:HD12	1.98	0.46
10:T:288:VAL:HA	10:T:291:VAL:HG22	1.98	0.46
10:V:212:VAL:HG12	10:V:230:VAL:HG21	1.97	0.46
11:W:144:GLN:HG2	11:W:157:LYS:HB2	1.97	0.46
7:M:718:ILE:HD12	7:M:850:LEU:HD23	1.97	0.46
7:M:1292:LEU:HB2	7:M:1317:PHE:CZ	2.50	0.46
8:R:319:HIS:ND1	8:R:319:HIS:O	2.49	0.46
10:T:27:HIS:O	10:T:28:THR:OG1	2.28	0.46
11:U:29:LEU:HB3	11:U:91:SER:HB3	1.98	0.46
11:U:34:ASN:HB3	11:U:36:GLN:HG2	1.98	0.46
10:V:140:TYR:HA	10:V:237:VAL:O	2.15	0.46
10:X:165:HIS:ND1	12:Z:311:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:OG1	6:J:-3:DA:OP1	2.34	0.46
5:I:-61:DG:H2"	5:I:-60:DG:N7	2.31	0.46
8:R:33:ALA:HA	8:R:58:ARG:H	1.81	0.46
9:S:14:ASN:HB2	9:S:17:ILE:HB	1.98	0.46
10:T:181:LEU:HB2	10:T:185:ILE:HD13	1.97	0.46
11:Y:242:HIS:ND1	11:Y:243:GLU:OE2	2.44	0.46
5:I:20:DG:OP1	7:M:807:VAL:HB	2.16	0.46
7:M:1174:ARG:HA	7:M:1177:ILE:HG22	1.98	0.46
10:T:117:LYS:HE2	10:T:319:GLU:OE2	2.16	0.46
11:U:18:SER:HB2	10:V:331:ASN:HB2	1.97	0.46
10:V:181:LEU:HB3	10:V:185:ILE:HG23	1.98	0.46
10:V:377:LYS:HB3	10:V:381:ARG:HH12	1.79	0.46
11:W:362:GLN:HA	11:W:365:LYS:NZ	2.30	0.46
7:M:688:VAL:HG22	12:Z:234:HIS:HD2	1.80	0.46
7:M:1077:LYS:HE3	7:M:1077:LYS:HB3	1.86	0.46
8:R:4:PRO:HA	8:R:5:PRO:HD3	1.83	0.46
8:R:23:LYS:HE3	8:R:398:GLU:HB2	1.98	0.46
8:R:81:PHE:HD2	9:S:183:LYS:NZ	2.14	0.46
8:R:90:ASP:N	8:R:90:ASP:OD1	2.49	0.46
8:R:133:VAL:HA	8:R:136:PHE:CD2	2.49	0.46
8:R:197:CYS:O	14:R:502:BEF:F3	2.24	0.46
8:R:276:LEU:HD13	8:R:302:GLN:O	2.16	0.46
8:R:331:VAL:HG21	8:R:376:GLN:HG3	1.98	0.46
10:X:452:SER:HB2	11:Y:341:HIS:CE1	2.50	0.46
11:Y:155:GLN:H	12:Z:621:THR:HA	1.81	0.46
2:D:83:SER:HA	2:D:86:VAL:HG22	1.98	0.45
3:E:78:ARG:NH2	5:I:-55:DG:OP2	2.45	0.45
10:T:49:VAL:HG23	10:T:379:GLU:HG3	1.98	0.45
10:T:75:ILE:HD11	10:T:370:VAL:HG23	1.97	0.45
10:T:143:GLU:N	10:T:171:LYS:HB2	2.31	0.45
10:T:377:LYS:HG3	10:T:378:ASP:H	1.80	0.45
11:W:382:ASP:OD1	11:W:383:ALA:N	2.49	0.45
10:X:138:GLU:HG3	10:X:240:LYS:HE2	1.97	0.45
11:Y:276:LYS:O	11:Y:279:GLU:HG3	2.17	0.45
6:J:-30:DA:H3'	7:M:974:LEU:C	2.41	0.45
6:J:70:DC:H6	6:J:70:DC:H5'	1.81	0.45
9:S:104:GLU:O	9:S:107:THR:OG1	2.25	0.45
11:U:159:THR:HG23	11:U:168:ILE:HG22	1.98	0.45
11:W:433:SER:OG	10:X:365:ASP:OD1	2.28	0.45
10:X:355:SER:OG	10:X:359:VAL:O	2.18	0.45
11:Y:362:GLN:O	11:Y:365:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:217:ARG:HA	12:Z:220:ILE:HG22	1.98	0.45
12:Z:299:PRO:HA	12:Z:300:ALA:HA	1.62	0.45
2:D:41:GLY:HA2	2:D:46:ILE:HD11	1.98	0.45
5:I:-58:DG:H5"	7:M:846:GLN:NE2	2.31	0.45
5:I:25:DG:H2"	5:I:26:DG:C8	2.51	0.45
8:R:83:PRO:HB3	8:R:90:ASP:HB3	1.98	0.45
8:R:220:GLY:O	8:R:224:THR:HG23	2.17	0.45
10:T:139:VAL:HG23	10:T:202:ILE:C	2.41	0.45
11:U:454:VAL:HG11	10:V:81:PRO:HD2	1.98	0.45
10:V:198:ASP:CG	10:V:211:ARG:HH22	2.25	0.45
10:X:215:SER:HA	10:X:230:VAL:H	1.81	0.45
10:X:367:LEU:HD23	10:X:368:LEU:N	2.31	0.45
11:Y:294:PHE:HB2	11:Y:322:MET:HB2	1.98	0.45
1:A:128:ARG:HH12	1:A:133:GLU:HB2	1.82	0.45
1:B:59:GLU:HA	7:M:788:LYS:HG2	1.99	0.45
2:C:26:ILE:HG13	2:C:27:GLN:H	1.82	0.45
7:M:717:GLY:HA2	7:M:928:TYR:CD2	2.52	0.45
7:M:742:LYS:HD3	7:M:744:ASN:H	1.80	0.45
11:U:140:VAL:HA	11:U:159:THR:O	2.15	0.45
11:U:399:SER:HA	11:U:402:LEU:HB2	1.99	0.45
11:U:432:ASP:OD1	11:U:433:SER:N	2.50	0.45
10:V:118:THR:HB	10:V:323:TYR:CE2	2.52	0.45
11:W:141:VAL:HA	11:W:186:ALA:C	2.42	0.45
10:X:245:GLN:HG3	10:X:247:VAL:HG13	1.98	0.45
5:I:-2:DC:H2"	5:I:-1:DG:C8	2.51	0.45
8:R:36:LYS:HD2	8:R:54:SER:HB3	1.97	0.45
8:R:201:ILE:HD13	8:R:213:VAL:HG12	1.98	0.45
9:S:264:CYS:SG	9:S:265:SER:N	2.90	0.45
10:T:76:LEU:HB3	10:T:369:ILE:HD13	1.99	0.45
10:T:171:LYS:HA	10:T:176:THR:HG22	1.99	0.45
11:U:33:GLU:CD	11:U:33:GLU:H	2.24	0.45
11:U:246:VAL:HG11	11:U:257:LEU:HG	1.99	0.45
11:U:304:GLU:OE1	11:U:304:GLU:N	2.49	0.45
11:W:147:ARG:HH11	11:W:154:LYS:HD3	1.81	0.45
11:W:407:GLN:NE2	11:W:408:GLN:OE1	2.48	0.45
10:X:45:GLU:OE2	10:X:55:ARG:NH2	2.50	0.45
11:Y:346:ASP:OD1	11:Y:347:LEU:N	2.49	0.45
5:I:6:DC:N4	6:J:-6:DG:O6	2.34	0.45
6:J:-20:DC:H2"	6:J:-19:DG:N7	2.32	0.45
6:J:-19:DG:H2"	6:J:-18:DG:H5'	1.97	0.45
8:R:315:GLU:O	8:R:319:HIS:N	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:194:VAL:HG11	10:T:200:ILE:HG22	1.98	0.45
10:T:314:ASN:ND2	10:T:342:ARG:HD3	2.32	0.45
11:U:143:ILE:HD13	11:U:158:LEU:HB2	1.98	0.45
11:U:409:ILE:HG23	11:U:412:LYS:HD3	1.99	0.45
10:X:33:LEU:HA	10:X:48:PHE:HD2	1.81	0.45
10:X:386:ARG:O	10:X:390:VAL:HG23	2.16	0.45
5:I:-53:DG:H4'	5:I:-52:DG:OP1	2.15	0.45
5:I:-28:DT:H2"	5:I:-27:DC:H6	1.81	0.45
7:M:1006:THR:HG22	7:M:1007:SER:H	1.81	0.45
7:M:1193:ARG:HE	10:V:261:GLY:H	1.63	0.45
10:T:105:LEU:HD12	10:T:109:GLU:OE1	2.17	0.45
11:Y:158:LEU:HD23	11:Y:171:LEU:HD11	1.98	0.45
11:Y:303:ILE:HA	11:Y:306:PHE:CD2	2.52	0.45
2:C:96:THR:HG22	3:E:100:ASN:O	2.16	0.45
7:M:994:ASN:HD21	7:M:1274:VAL:HG22	1.81	0.45
7:M:1195:LEU:HB3	11:U:254:PHE:CZ	2.52	0.45
8:R:14:GLU:HB3	8:R:29:LEU:HA	1.99	0.45
8:R:25:PRO:HB3	8:R:394:LEU:HD22	1.99	0.45
8:R:80:LEU:HD23	8:R:89:PHE:CZ	2.52	0.45
10:T:43:ARG:O	10:T:49:VAL:HA	2.17	0.45
11:W:25:HIS:CE1	11:W:26:ILE:HG12	2.52	0.45
2:C:60:SER:O	2:C:63:GLU:HG2	2.17	0.45
8:R:428:THR:O	8:R:433:GLY:HA3	2.17	0.45
9:S:8:ILE:HD13	10:V:180:ARG:HD3	1.99	0.45
9:S:261:ASN:HB2	9:S:272:HIS:CE1	2.39	0.45
10:T:360:PRO:HB2	10:T:362:ASP:OD1	2.16	0.45
11:U:192:ILE:HG13	11:U:199:ILE:HG12	1.97	0.45
10:V:169:GLY:HA2	10:V:178:THR:HG22	1.98	0.45
10:V:216:ASP:HA	10:V:229:TYR:HB3	1.97	0.45
10:V:258:ARG:NH2	10:V:277:LYS:HD3	2.31	0.45
10:X:173:ALA:N	10:X:233:PRO:O	2.38	0.45
10:X:270:GLY:O	10:X:275:PRO:HD3	2.17	0.45
2:C:29:ILE:HG21	2:C:55:ARG:HD2	1.99	0.44
2:C:30:THR:H	6:J:-13:DA:H3'	1.82	0.44
7:M:1002:ARG:NH2	11:W:283:GLU:HB3	2.33	0.44
8:R:20:SER:OG	8:R:404:ALA:HB3	2.17	0.44
8:R:43:SER:HB3	8:R:75:ILE:HD13	1.99	0.44
9:S:190:LYS:O	9:S:195:ILE:HG13	2.17	0.44
11:W:159:THR:HA	11:W:168:ILE:HA	1.99	0.44
2:C:62:LEU:HA	2:C:65:VAL:HG22	1.99	0.44
7:M:950:TYR:HB2	7:M:1372:GLU:CD	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:998:LEU:O	7:M:1240:LEU:HD22	2.18	0.44
8:R:9:ASP:HB3	8:R:16:LYS:HE2	1.99	0.44
8:R:70:GLU:HA	9:S:202:LEU:HG	1.99	0.44
10:X:225:GLU:HA	11:Y:175:MET:HG2	2.00	0.44
11:Y:79:THR:HG22	11:Y:359:TYR:HE1	1.81	0.44
12:Z:217:ARG:O	12:Z:220:ILE:HG22	2.17	0.44
1:A:119:ILE:H	2:D:46:ILE:HG22	1.82	0.44
2:C:33:ALA:HA	2:C:36:ARG:HE	1.82	0.44
7:M:825:GLU:HB2	7:M:827:HIS:NE2	2.32	0.44
9:S:161:TYR:OH	9:S:170:GLU:OE1	2.29	0.44
10:V:202:ILE:HD12	10:V:209:VAL:HB	1.99	0.44
10:V:431:ARG:NH1	10:V:438:ASP:OD1	2.51	0.44
11:W:428:LEU:HD12	11:W:429:LEU:HD22	1.99	0.44
10:X:379:GLU:O	10:X:383:ILE:HG13	2.17	0.44
11:Y:327:ARG:NH1	11:Y:328:GLY:H	2.16	0.44
7:M:953:LEU:HB3	7:M:958:ARG:HG2	2.00	0.44
7:M:1335:THR:HG23	7:M:1365:HIS:HB2	1.99	0.44
9:S:256:CYS:HB2	9:S:272:HIS:NE2	2.32	0.44
9:S:273:ASN:HA	9:S:277:CYS:HB3	1.98	0.44
11:U:405:VAL:O	11:U:409:ILE:HG13	2.18	0.44
11:W:228:GLU:OE1	11:W:230:GLN:N	2.50	0.44
10:X:146:GLU:OE2	12:Z:318:LYS:NZ	2.35	0.44
10:X:401:ASP:O	10:X:405:THR:HG23	2.18	0.44
11:Y:102:ALA:H	11:Y:105:GLU:CD	2.26	0.44
11:Y:303:ILE:HD12	11:Y:306:PHE:HD2	1.82	0.44
12:Z:620:TYR:CD1	12:Z:625:SER:HA	2.52	0.44
7:M:1166:LEU:O	7:M:1170:VAL:HG23	2.17	0.44
7:M:1268:PHE:CE2	7:M:1336:VAL:HG13	2.52	0.44
8:R:61:HIS:HB3	8:R:196:ASN:HD21	1.82	0.44
8:R:77:ASP:O	8:R:81:PHE:HB2	2.17	0.44
8:R:207:ILE:O	8:R:207:ILE:HG13	2.17	0.44
8:R:323:SER:C	8:R:324:GLN:HG3	2.43	0.44
10:T:314:ASN:HD22	10:T:342:ARG:HB2	1.82	0.44
11:U:457:SER:OG	10:V:409:GLU:O	2.28	0.44
10:V:168:VAL:HG23	10:V:181:LEU:HD11	1.99	0.44
10:X:143:GLU:O	10:X:170:LEU:HA	2.18	0.44
4:G:41:SER:HB2	5:I:-53:DG:OP2	2.18	0.44
4:G:80:ALA:HB1	4:G:96:GLU:HB3	1.99	0.44
5:I:6:DC:H1'	5:I:7:DC:C2	2.53	0.44
7:M:1106:TYR:OH	8:R:344:ILE:HA	2.17	0.44
8:R:331:VAL:HG23	8:R:373:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:109:GLU:HG3	11:U:114:THR:HG21	1.99	0.44
10:T:395:VAL:HA	10:T:434:ILE:HG22	1.99	0.44
10:V:342:ARG:N	10:V:357:HIS:HA	2.32	0.44
11:W:125:ILE:HG12	11:W:319:PRO:HG3	1.98	0.44
2:D:29:ILE:HG13	2:D:33:ALA:HB3	1.99	0.44
5:I:-72:DT:O2	6:J:73:DG:N2	2.51	0.44
5:I:-50:DC:H2'	5:I:-49:DG:O4'	2.18	0.44
6:J:-5:DG:H2"	6:J:-4:DG:C8	2.53	0.44
8:R:210:TYR:HB2	8:R:438:ILE:HA	1.99	0.44
11:Y:73:VAL:HA	11:Y:354:ILE:HB	2.00	0.44
11:Y:126:GLY:HA3	11:Y:289:VAL:HB	2.00	0.44
2:C:30:THR:HG23	6:J:-13:DA:OP2	2.18	0.44
5:I:-35:DA:H2"	5:I:-34:DG:C8	2.53	0.44
7:M:728:THR:O	7:M:732:ILE:HG13	2.17	0.44
7:M:776:TYR:HD2	7:M:805:LEU:HG	1.81	0.44
9:S:206:ARG:HG2	9:S:211:PHE:CE1	2.53	0.44
11:U:21:ALA:O	11:U:371:ARG:NH1	2.49	0.44
11:U:404:SER:HB3	10:V:70:MET:HE1	2.00	0.44
5:I:5:DC:H4'	5:I:6:DC:OP1	2.17	0.44
5:I:15:DT:O4	5:I:16:DA:N6	2.51	0.44
6:J:1:DC:H2"	6:J:2:DG:C8	2.53	0.44
7:M:727:LYS:NZ	14:M:1602:BEF:F3	2.33	0.44
7:M:748:HIS:ND1	7:M:819:GLN:HB2	2.33	0.44
7:M:1143:LEU:HD12	7:M:1146:LYS:HD3	2.00	0.44
8:R:114:HIS:O	8:R:117:GLN:HG2	2.17	0.44
8:R:368:ARG:HH21	8:R:372:GLU:HB3	1.83	0.44
9:S:5:VAL:HG12	9:S:5:VAL:O	2.18	0.44
9:S:85:SER:OG	9:S:88:GLU:OE1	2.26	0.44
9:S:272:HIS:O	9:S:277:CYS:N	2.51	0.44
10:T:116:LYS:HE3	10:T:118:THR:HB	2.00	0.44
10:V:166:VAL:HB	10:V:181:LEU:HB2	1.99	0.44
10:V:404:ALA:O	10:V:408:THR:HG23	2.17	0.44
11:W:162:THR:OG1	11:W:225:PRO:O	2.29	0.44
10:X:107:GLY:O	10:X:110:LEU:HB2	2.18	0.44
11:Y:298:VAL:HG12	11:Y:325:THR:HB	1.99	0.44
5:I:-51:DC:C2	5:I:-50:DC:C5	3.06	0.43
6:J:70:DC:H5'	6:J:70:DC:C6	2.53	0.43
7:M:968:ALA:HB1	7:M:973:THR:HG22	1.99	0.43
8:R:46:ILE:O	8:R:49:ILE:HG12	2.17	0.43
10:T:80:GLY:O	10:T:83:THR:OG1	2.24	0.43
10:V:167:ILE:HD12	10:V:178:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:173:ALA:N	10:V:233:PRO:O	2.48	0.43
10:V:362:ASP:HB2	10:V:366:ARG:NH1	2.33	0.43
11:W:189:VAL:HG22	11:W:225:PRO:HD3	1.99	0.43
11:W:330:SER:HA	11:W:338:LYS:NZ	2.33	0.43
10:X:378:ASP:OD1	10:X:379:GLU:N	2.48	0.43
5:I:23:DA:H5"	7:M:1270:GLN:HA	2.00	0.43
6:J:16:DA:H2"	6:J:17:DA:C8	2.53	0.43
7:M:719:LEU:HG	7:M:930:LEU:HB3	2.00	0.43
10:T:198:ASP:OD2	10:T:214:ARG:NH1	2.51	0.43
10:T:313:VAL:HG11	10:T:338:LEU:HD12	2.00	0.43
10:T:403:LEU:HD23	10:T:406:MET:HE2	2.00	0.43
11:U:371:ARG:NH2	11:U:374:GLU:HG2	2.33	0.43
11:U:398:TYR:CZ	11:U:402:LEU:HD11	2.52	0.43
10:V:67:ALA:HB1	10:V:69:LYS:HE2	1.99	0.43
10:V:92:ILE:O	10:V:96:LEU:HG	2.18	0.43
10:V:131:LEU:HB2	10:V:247:VAL:O	2.18	0.43
10:X:125:PHE:CE1	10:X:333:ALA:HA	2.53	0.43
10:X:136:THR:HB	10:X:240:LYS:HD2	2.00	0.43
10:X:161:LYS:HZ2	12:Z:592:ASN:HD21	1.65	0.43
10:X:431:ARG:NH1	10:X:437:ASN:OD1	2.49	0.43
7:M:1008:PHE:CZ	7:M:1187:ALA:HB2	2.53	0.43
7:M:1387:ARG:CZ	7:M:1387:ARG:HA	2.49	0.43
8:R:128:LEU:O	8:R:414:VAL:HG22	2.17	0.43
11:W:455:GLN:OE1	11:W:456:ILE:N	2.51	0.43
11:W:455:GLN:OE1	11:W:457:SER:N	2.42	0.43
10:X:84:GLY:N	13:X:501:ADP:N7	2.67	0.43
12:Z:286:THR:HG23	12:Z:287:ILE:HG12	1.99	0.43
6:J:37:DC:H2"	6:J:38:DG:C8	2.54	0.43
8:R:35:ASP:HB2	8:R:41:TYR:HE2	1.83	0.43
8:R:311:PHE:CZ	9:S:248:GLY:HA3	2.53	0.43
8:R:324:GLN:O	9:S:98:SER:HB2	2.18	0.43
9:S:170:GLU:O	9:S:174:GLU:HG2	2.19	0.43
11:U:269:VAL:O	11:U:272:GLN:HG3	2.18	0.43
11:U:437:VAL:HA	11:U:440:VAL:HG22	2.01	0.43
10:V:23:ARG:HH12	11:W:125:ILE:HD12	1.84	0.43
10:V:118:THR:O	10:V:122:MET:HG2	2.18	0.43
10:X:311:ASP:OD1	10:X:311:ASP:N	2.51	0.43
11:Y:80:GLY:N	13:Y:501:ADP:O1A	2.49	0.43
12:Z:602:ALA:HB1	12:Z:603:PRO:HD2	1.99	0.43
5:I:-17:DT:H6	5:I:-17:DT:H2'	1.64	0.43
7:M:1081:THR:HA	7:M:1084:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:145:ILE:HG23	11:U:176:ILE:HG12	2.00	0.43
11:W:59:LYS:HA	11:W:62:GLN:HG3	2.00	0.43
10:X:33:LEU:HB3	10:X:55:ARG:HG2	2.00	0.43
11:Y:31:LEU:HD11	11:Y:51:ARG:HG3	2.00	0.43
1:A:123:GLU:OE2	1:B:113:HIS:NE2	2.52	0.43
2:C:80:THR:OG1	2:C:85:ASP:OD2	2.36	0.43
7:M:960:LEU:HB3	7:M:992:VAL:HG23	2.01	0.43
7:M:1106:TYR:CG	7:M:1107:SER:N	2.87	0.43
11:W:55:GLY:O	11:W:58:LEU:HG	2.18	0.43
11:Y:204:ARG:HB3	11:Y:208:ARG:HG3	2.01	0.43
3:E:61:ALA:HA	3:E:64:LEU:HD12	1.99	0.43
8:R:434:TYR:O	8:R:438:ILE:HG13	2.18	0.43
10:T:194:VAL:HG12	10:T:211:ARG:CZ	2.49	0.43
10:V:441:GLU:O	10:V:445:LEU:HB2	2.19	0.43
10:X:186:TYR:CZ	10:X:187:GLU:HG2	2.53	0.43
11:Y:73:VAL:HG22	11:Y:354:ILE:HD12	2.01	0.43
11:Y:261:ASP:OD1	11:Y:261:ASP:N	2.50	0.43
11:U:161:LYS:HB3	11:U:167:THR:H	1.83	0.43
10:V:57:ALA:O	10:V:61:ILE:HG12	2.18	0.43
10:X:373:LEU:HG	10:X:374:PRO:HD2	2.01	0.43
6:J:9:DT:H2"	6:J:10:DG:N7	2.34	0.43
11:U:384:LEU:O	11:U:388:THR:HG23	2.19	0.43
11:W:389:LYS:NZ	11:W:393:GLU:OE2	2.37	0.43
10:X:164:SER:O	10:X:165:HIS:ND1	2.52	0.43
2:D:36:ARG:NH2	5:I:-14:DA:H5"	2.34	0.43
4:G:49:LYS:HD2	4:G:53:PRO:HA	2.01	0.43
5:I:-10:DC:H2"	5:I:-9:DA:C8	2.54	0.43
7:M:1002:ARG:CZ	11:W:280:TRP:HD1	2.32	0.43
11:U:431:LEU:HD11	10:V:371:ARG:HB2	2.01	0.43
11:Y:127:ILE:HD12	11:Y:288:ILE:HA	1.99	0.43
1:A:119:ILE:HD12	1:A:124:ILE:HG13	2.00	0.42
5:I:-57:DC:OP1	7:M:845:THR:HA	2.18	0.42
5:I:-52:DG:O5'	5:I:-52:DG:H8	2.01	0.42
7:M:1254:LEU:HD22	7:M:1367:TYR:CD2	2.54	0.42
8:R:113:LYS:HE2	8:R:113:LYS:HA	2.01	0.42
11:U:431:LEU:HB2	10:V:369:ILE:HB	2.00	0.42
10:V:166:VAL:HG21	10:V:186:TYR:CG	2.54	0.42
10:X:257:ALA:HB2	10:X:280:ILE:HD13	2.01	0.42
1:B:58:THR:HB	3:E:82:ARG:HG3	2.00	0.42
5:I:6:DC:H2"	5:I:7:DC:C5	2.54	0.42
6:J:-34:DA:H2"	6:J:-33:DG:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1212:LYS:HB3	7:M:1212:LYS:HE3	1.78	0.42
7:M:1340:ASP:OD1	7:M:1340:ASP:N	2.48	0.42
8:R:120:PHE:O	8:R:124:GLU:HA	2.19	0.42
8:R:139:PHE:HE2	8:R:402:GLN:HG3	1.84	0.42
10:T:380:ILE:HD11	10:T:412:LEU:HB2	2.01	0.42
10:V:35:LEU:HB3	10:V:39:GLY:HA2	2.01	0.42
10:X:391:GLU:HG3	10:X:393:LEU:HG	2.00	0.42
5:I:23:DA:H2"	5:I:24:DA:H8	1.84	0.42
6:J:21:DG:C4	6:J:22:DT:H72	2.54	0.42
6:J:59:DA:H2"	6:J:60:DC:C4	2.54	0.42
7:M:968:ALA:O	7:M:973:THR:N	2.53	0.42
10:X:199:VAL:HB	10:X:211:ARG:HG2	2.01	0.42
10:X:249:LEU:HD22	10:X:292:VAL:HG21	2.01	0.42
1:A:96:VAL:HG11	2:D:58:LEU:HD12	2.01	0.42
2:D:47:SER:OG	2:D:48:GLY:N	2.53	0.42
7:M:930:LEU:HD12	7:M:932:ARG:NH1	2.35	0.42
7:M:950:TYR:HB2	7:M:1372:GLU:OE1	2.20	0.42
7:M:1180:PHE:HB3	11:W:248:ASN:HD21	1.84	0.42
8:R:127:SER:CB	8:R:413:ARG:HE	2.32	0.42
10:T:420:ALA:HB3	11:U:69:ARG:HH12	1.84	0.42
11:U:408:GLN:HG3	10:V:64:LEU:HB2	2.01	0.42
10:X:452:SER:HB2	11:Y:341:HIS:HE1	1.84	0.42
11:Y:298:VAL:HG23	11:Y:301:LEU:HD12	2.01	0.42
5:I:-4:DC:C2	6:J:4:DG:N2	2.74	0.42
7:M:1054:LEU:HD11	7:M:1136:PHE:HA	2.00	0.42
7:M:1287:TYR:O	7:M:1289:TYR:HD1	2.02	0.42
8:R:239:MET:HE3	9:S:109:ASN:HA	2.01	0.42
9:S:210:SER:O	9:S:214:SER:N	2.53	0.42
10:T:36:ASP:OD1	10:T:40:VAL:N	2.34	0.42
11:W:141:VAL:HA	11:W:186:ALA:O	2.20	0.42
11:Y:47:GLN:O	11:Y:51:ARG:N	2.37	0.42
11:Y:306:PHE:O	11:Y:310:ASN:ND2	2.53	0.42
7:M:739:ALA:HA	7:M:745:TRP:HD1	1.84	0.42
7:M:1020:ASP:OD1	7:M:1020:ASP:N	2.53	0.42
8:R:10:ASN:HB2	8:R:103:GLU:HA	2.01	0.42
8:R:302:GLN:HE22	8:R:304:ILE:HG23	1.85	0.42
10:T:145:THR:OG1	10:T:146:GLU:N	2.53	0.42
10:T:183:PRO:O	10:T:186:TYR:N	2.52	0.42
11:U:159:THR:HA	11:U:168:ILE:HA	2.02	0.42
10:V:139:VAL:HG11	10:V:201:TYR:CE2	2.54	0.42
10:V:247:VAL:HG21	10:V:252:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:73:VAL:HG22	11:W:354:ILE:HB	2.01	0.42
10:X:53:GLU:O	10:X:56:GLU:HG3	2.18	0.42
11:Y:361:GLU:HG2	11:Y:362:GLN:N	2.34	0.42
6:J:-14:DA:C8	6:J:-14:DA:H5'	2.54	0.42
6:J:-1:DA:C2	6:J:0:DG:C6	3.07	0.42
6:J:42:DA:H2"	6:J:43:DA:C8	2.55	0.42
6:J:68:DC:H1'	6:J:69:DT:H5'	2.02	0.42
10:V:402:LEU:HD12	10:V:402:LEU:HA	1.85	0.42
10:X:296:ILE:HG23	10:X:302:GLU:HA	2.01	0.42
11:Y:138:GLY:HA2	11:Y:225:PRO:HD2	2.02	0.42
1:A:60:LEU:HD22	1:A:64:LYS:HA	2.02	0.42
1:B:69:ARG:NE	2:C:26:ILE:HA	2.35	0.42
1:B:109:LEU:HD12	1:B:112:ILE:HD11	2.01	0.42
2:C:97:LEU:HG	2:C:98:TYR:O	2.19	0.42
7:M:1328:ILE:HG13	7:M:1329:ASN:H	1.85	0.42
8:R:122:GLU:HA	9:S:189:ARG:HH21	1.83	0.42
8:R:134:ALA:O	8:R:137:VAL:HG22	2.20	0.42
10:V:142:GLY:HA2	10:V:233:PRO:HD2	2.00	0.42
11:W:37:PRO:HB3	11:W:51:ARG:HB3	2.01	0.42
11:Y:175:MET:C	11:Y:178:GLY:H	2.27	0.42
7:M:749:LEU:HB2	7:M:818:TRP:CE3	2.55	0.42
7:M:813:PHE:HB3	7:M:843:PHE:HZ	1.85	0.42
7:M:983:VAL:HA	7:M:986:LEU:HD12	2.02	0.42
7:M:1116:VAL:O	7:M:1119:LEU:HG	2.19	0.42
8:R:338:LEU:O	8:R:346:ARG:HG3	2.20	0.42
10:T:70:MET:HE1	11:Y:404:SER:HB2	2.02	0.42
11:U:140:VAL:HG13	11:U:140:VAL:O	2.20	0.42
11:U:332:THR:HG22	11:U:342:GLY:C	2.45	0.42
7:M:700:GLN:HA	7:M:730:GLN:HG2	2.02	0.42
7:M:823:LEU:HD13	7:M:829:ILE:HD13	2.01	0.42
7:M:1002:ARG:NH2	11:W:283:GLU:OE1	2.53	0.42
7:M:1006:THR:HG22	7:M:1007:SER:N	2.34	0.42
8:R:32:LEU:HG	8:R:33:ALA:H	1.85	0.42
10:V:116:LYS:O	10:V:120:THR:HG23	2.20	0.42
10:V:318:ILE:HB	10:V:350:THR:HG23	2.02	0.42
10:X:418:LEU:C	10:X:421:PRO:HD2	2.45	0.42
1:B:54:PHE:CD2	2:C:36:ARG:HG3	2.55	0.41
5:I:18:DC:H4'	7:M:780:PRO:HD2	2.02	0.41
7:M:1062:ILE:HG13	11:Y:220:ARG:HH21	1.85	0.41
9:S:239:PRO:HB3	10:T:217:ALA:HA	2.02	0.41
10:T:306:GLY:H	10:T:334:PRO:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:21:ALA:HB2	10:V:331:ASN:HA	2.01	0.41
10:V:140:TYR:CG	10:V:179:LEU:HD11	2.55	0.41
11:W:329:VAL:HG22	11:W:338:LYS:HB3	2.02	0.41
10:X:447:LEU:HA	10:X:451:ARG:CZ	2.49	0.41
7:M:1328:ILE:HG21	7:M:1330:LEU:HD13	2.02	0.41
8:R:208:PRO:O	8:R:437:TRP:HB3	2.20	0.41
8:R:244:LEU:HD11	8:R:274:TYR:HE2	1.85	0.41
11:U:300:MET:HG2	11:U:333:ARG:HH11	1.85	0.41
11:U:306:PHE:CE2	11:U:344:PRO:HD2	2.55	0.41
10:V:362:ASP:OD1	10:V:362:ASP:N	2.52	0.41
11:W:132:GLU:OE1	11:W:132:GLU:N	2.53	0.41
11:W:320:ILE:HD12	11:W:320:ILE:H	1.85	0.41
10:X:377:LYS:HA	10:X:380:ILE:HG22	2.02	0.41
12:Z:321:LYS:HA	12:Z:321:LYS:HD3	1.84	0.41
2:C:30:THR:N	6:J:-13:DA:H3'	2.35	0.41
8:R:139:PHE:CE2	8:R:402:GLN:HG3	2.55	0.41
9:S:8:ILE:HG21	10:V:180:ARG:HH11	1.84	0.41
11:U:141:VAL:HG12	11:U:159:THR:HB	2.01	0.41
11:W:110:GLU:HG3	11:W:111:LEU:HD13	2.01	0.41
10:X:199:VAL:HG11	10:X:212:VAL:H	1.85	0.41
10:X:214:ARG:HB3	10:X:215:SER:H	1.62	0.41
10:X:380:ILE:HD12	10:X:383:ILE:HD12	2.02	0.41
1:A:106:ASP:OD1	1:A:131:ARG:NH2	2.28	0.41
1:A:113:HIS:HE1	1:B:114:ALA:HB2	1.85	0.41
2:D:38:ALA:HB2	2:D:50:ILE:HD11	2.02	0.41
5:I:5:DC:C2	6:J:-4:DG:N2	2.88	0.41
8:R:62:GLU:HB2	8:R:65:GLN:O	2.20	0.41
11:U:372:ALA:HB1	11:U:379:LEU:HD13	2.02	0.41
11:U:447:TYR:CZ	10:V:79:GLY:HA2	2.56	0.41
10:V:314:ASN:OD1	10:V:314:ASN:N	2.54	0.41
11:W:22:ALA:O	11:W:25:HIS:ND1	2.54	0.41
11:W:79:THR:N	13:W:501:ADP:O2B	2.34	0.41
10:X:171:LYS:HE3	10:X:171:LYS:HB3	1.97	0.41
1:B:69:ARG:HH22	2:C:27:GLN:HB2	1.85	0.41
2:C:27:GLN:OE1	6:J:-13:DA:H4'	2.20	0.41
4:G:37:LYS:NZ	6:J:50:DG:H5"	2.36	0.41
8:R:61:HIS:NE2	8:R:66:LEU:HD23	2.35	0.41
8:R:409:TYR:HA	8:R:412:ALA:HB3	2.03	0.41
10:T:82:SER:N	13:T:501:ADP:O2B	2.51	0.41
10:V:121:LEU:HD21	10:V:324:LEU:HD13	2.01	0.41
10:V:202:ILE:HA	10:V:209:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:18:SER:OG	10:X:331:ASN:OD1	2.30	0.41
11:W:453:ASN:HA	11:Y:345:LEU:HD12	2.03	0.41
10:X:33:LEU:HD13	10:X:35:LEU:HD11	2.02	0.41
10:X:321:PHE:O	10:X:324:LEU:HG	2.21	0.41
11:Y:122:ARG:O	11:Y:125:ILE:HG12	2.20	0.41
11:Y:130:LYS:HE2	11:Y:130:LYS:HB2	1.91	0.41
1:B:67:PHE:CE1	2:C:29:ILE:HG23	2.55	0.41
2:D:32:PRO:HG3	5:I:-13:DA:H2'	2.02	0.41
2:D:41:GLY:O	2:D:46:ILE:HG12	2.21	0.41
5:I:-29:DC:H6	5:I:-29:DC:H2'	1.70	0.41
5:I:13:DT:H2"	5:I:14:DT:C6	2.55	0.41
6:J:-31:DA:H2"	6:J:-30:DA:N7	2.35	0.41
7:M:824:ASP:OD1	14:M:1602:BEF:F3	2.28	0.41
8:R:236:TYR:O	8:R:238:MET:HE2	2.21	0.41
8:R:300:ASP:OD1	8:R:301:ALA:N	2.53	0.41
8:R:327:LYS:NZ	8:R:329:GLY:H	2.19	0.41
11:U:212:TYR:HE2	11:U:214:ALA:HB3	1.85	0.41
11:U:332:THR:HG23	11:U:338:LYS:HA	2.03	0.41
11:W:129:ILE:HG12	11:W:286:ALA:HB2	2.02	0.41
11:W:346:ASP:OD2	11:W:350:ARG:NH2	2.48	0.41
10:X:181:LEU:HB2	10:X:185:ILE:HD13	2.03	0.41
11:Y:306:PHE:HA	11:Y:309:ILE:HG12	2.01	0.41
2:D:36:ARG:HH12	5:I:-14:DA:H3'	1.85	0.41
6:J:-10:DG:H2"	6:J:-9:DC:C5	2.55	0.41
7:M:1282:LEU:HD11	7:M:1316:VAL:HG11	2.03	0.41
8:R:109:PRO:HD3	8:R:434:TYR:HE1	1.86	0.41
8:R:225:GLY:O	8:R:228:LYS:HG2	2.21	0.41
8:R:264:PHE:CZ	9:S:249:GLY:HA2	2.56	0.41
13:R:501:ADP:O1B	14:R:502:BEF:F1	2.29	0.41
11:U:74:ALA:O	11:U:356:THR:OG1	2.35	0.41
11:U:266:ARG:HG3	11:U:268:GLU:CD	2.46	0.41
11:U:364:ILE:HG23	11:U:396:LEU:HD12	2.02	0.41
10:V:77:LEU:HD23	10:V:338:LEU:O	2.21	0.41
10:V:202:ILE:HB	10:V:209:VAL:HG23	2.03	0.41
10:V:418:LEU:HD22	10:V:442:ALA:HB1	2.02	0.41
10:X:274:LYS:O	10:X:274:LYS:HD2	2.20	0.41
10:X:352:ASP:OD1	10:X:353:VAL:HG23	2.20	0.41
1:A:119:ILE:HA	1:A:123:GLU:HG3	2.02	0.41
6:J:-16:DT:H5"	7:M:775:THR:CB	2.48	0.41
6:J:9:DT:H2"	6:J:10:DG:C8	2.55	0.41
8:R:123:TYR:HB3	8:R:125:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:210:TYR:CD2	8:R:437:TRP:HB2	2.56	0.41
9:S:175:ILE:HG13	9:S:178:SER:OG	2.20	0.41
11:U:37:PRO:HB2	11:U:51:ARG:HH11	1.86	0.41
11:U:448:ILE:O	10:V:342:ARG:HA	2.20	0.41
10:V:396:GLU:OE2	10:V:399:ALA:N	2.53	0.41
10:V:417:GLN:NE2	10:V:418:LEU:HG	2.36	0.41
11:W:258:PHE:O	10:X:280:ILE:HD12	2.21	0.41
11:W:301:LEU:HG	11:W:305:CYS:HB2	2.03	0.41
10:X:225:GLU:OE2	11:Y:175:MET:N	2.53	0.41
10:X:400:LEU:HA	10:X:403:LEU:HD12	2.02	0.41
10:X:448:ASP:O	10:X:452:SER:N	2.51	0.41
11:Y:298:VAL:HG22	11:Y:306:PHE:HE1	1.85	0.41
1:B:67:PHE:HB3	1:B:93:GLN:OE1	2.21	0.41
5:I:-15:DA:H5'	5:I:-15:DA:C8	2.56	0.41
6:J:5:DT:H1'	6:J:6:DA:C8	2.56	0.41
7:M:823:LEU:O	7:M:851:LEU:HB2	2.21	0.41
7:M:1163:ILE:HD12	10:X:255:ALA:HB3	2.03	0.41
7:M:1166:LEU:HD12	11:W:255:LEU:HD22	2.03	0.41
8:R:92:LYS:HG3	8:R:93:GLU:N	2.34	0.41
8:R:139:PHE:CD1	8:R:403:PHE:HD1	2.39	0.41
8:R:153:LYS:HG2	8:R:383:CYS:SG	2.61	0.41
8:R:213:VAL:HG23	8:R:213:VAL:O	2.21	0.41
11:U:389:LYS:O	11:U:393:GLU:HG2	2.21	0.41
10:V:192:GLU:C	10:V:193:LYS:HG3	2.46	0.41
10:V:341:ASN:OD1	10:V:341:ASN:O	2.39	0.41
10:V:357:HIS:HB2	10:V:359:VAL:HG23	2.02	0.41
10:V:387:ARG:HD3	10:V:419:LEU:HD12	2.02	0.41
11:W:23:HIS:HE1	11:W:82:THR:HG22	1.86	0.41
11:W:25:HIS:CD2	11:W:26:ILE:HG23	2.56	0.41
11:W:165:MET:HG2	11:W:167:THR:HG23	2.03	0.41
11:W:239:VAL:HG13	11:W:244:ILE:HD11	2.03	0.41
11:W:396:LEU:O	11:W:399:SER:OG	2.28	0.41
10:X:167:ILE:HA	10:X:179:LEU:O	2.21	0.41
10:X:352:ASP:OD1	10:X:353:VAL:N	2.54	0.41
10:X:411:SER:OG	10:X:412:LEU:N	2.53	0.41
11:Y:58:LEU:HD12	11:Y:88:VAL:HG13	2.02	0.41
11:Y:424:LYS:HD3	11:Y:427:TYR:HD2	1.86	0.41
12:Z:587:GLN:O	12:Z:588:LEU:HB2	2.19	0.41
6:J:-30:DA:H2'	7:M:974:LEU:HD23	2.02	0.41
8:R:245:VAL:HA	8:R:248:ILE:HG22	2.02	0.41
11:U:72:LEU:HA	11:U:323:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:79:THR:HG22	11:U:358:SER:HA	2.03	0.41
11:U:130:LYS:HB2	11:U:234:THR:HG22	2.03	0.41
11:U:193:ASP:HB3	11:U:196:SER:HB2	2.03	0.41
10:V:33:LEU:HD23	10:V:48:PHE:CZ	2.56	0.41
11:W:21:ALA:HB3	11:W:24:SER:HB3	2.02	0.41
10:X:123:GLU:OE1	10:X:250:HIS:ND1	2.53	0.41
10:X:310:ILE:HG22	10:X:313:VAL:HG22	2.03	0.41
11:Y:330:SER:O	11:Y:339:SER:N	2.46	0.41
4:G:45:TYR:CB	5:I:-53:DG:H5"	2.50	0.40
6:J:-1:DA:H2"	6:J:0:DG:N7	2.36	0.40
7:M:937:VAL:HG12	7:M:937:VAL:O	2.20	0.40
7:M:952:LYS:HB3	7:M:1375:ILE:O	2.21	0.40
10:V:387:ARG:NH1	10:V:391:GLU:OE1	2.55	0.40
10:X:48:PHE:CZ	10:X:88:LEU:HD22	2.56	0.40
10:X:138:GLU:HG2	10:X:238:HIS:HE1	1.87	0.40
11:Y:108:SER:OG	11:Y:111:LEU:HB2	2.20	0.40
11:Y:165:MET:HE1	11:Y:228:GLU:HB2	2.03	0.40
12:Z:583:GLU:C	12:Z:585:PRO:HD3	2.46	0.40
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.92	0.40
5:I:20:DG:OP2	7:M:808:GLN:NE2	2.53	0.40
7:M:1082:ASN:O	7:M:1085:LEU:HG	2.21	0.40
7:M:1205:VAL:HG13	11:U:252:GLN:HG3	2.03	0.40
7:M:1320:SER:OG	7:M:1321:SER:N	2.54	0.40
8:R:369:LEU:O	8:R:372:GLU:HG3	2.21	0.40
8:R:375:ARG:HG2	10:T:173:ALA:O	2.22	0.40
10:T:436:VAL:HA	10:T:439:VAL:HG12	2.04	0.40
10:X:116:LYS:HE2	10:X:119:GLU:HB2	2.03	0.40
10:X:189:ILE:O	12:Z:612:ASN:ND2	2.45	0.40
10:X:451:ARG:HA	10:X:454:LYS:HD2	2.04	0.40
11:Y:108:SER:OG	11:Y:111:LEU:O	2.33	0.40
11:Y:440:VAL:HG22	11:Y:447:TYR:HE2	1.86	0.40
1:B:94:GLU:HG3	3:E:104:ALA:HB1	2.04	0.40
7:M:1215:GLN:O	7:M:1218:PHE:HB2	2.21	0.40
8:R:55:ILE:HD13	8:R:243:ILE:H	1.86	0.40
8:R:235:HIS:CE1	8:R:304:ILE:HB	2.56	0.40
8:R:318:PHE:HA	8:R:330:ILE:HG12	2.03	0.40
10:T:195:SER:OG	10:T:196:ILE:N	2.54	0.40
10:T:274:LYS:HD2	11:U:250:ARG:NH1	2.36	0.40
10:V:27:HIS:O	10:V:28:THR:OG1	2.31	0.40
10:V:84:GLY:N	13:V:501:ADP:O2B	2.53	0.40
10:X:154:ASN:ND2	12:Z:594:VAL:H	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:346:THR:HA	10:X:354:ILE:HA	2.03	0.40
10:X:446:PHE:CE1	11:Y:352:ILE:HD12	2.56	0.40
11:Y:332:THR:O	11:Y:335:THR:OG1	2.35	0.40
2:D:47:SER:HB2	2:D:51:TYR:CZ	2.56	0.40
4:G:45:TYR:HB2	5:I:-53:DG:H5"	2.03	0.40
5:I:-68:DG:C6	5:I:-67:DA:C6	3.10	0.40
6:J:-29:DT:H4'	7:M:978:ASN:HB2	2.03	0.40
7:M:728:THR:HG23	7:M:729:ILE:HD12	2.04	0.40
7:M:1308:PHE:CE1	7:M:1330:LEU:HG	2.56	0.40
8:R:58:ARG:HH21	9:S:165:TRP:HA	1.86	0.40
10:T:277:LYS:HD2	10:T:277:LYS:HA	1.70	0.40
11:U:298:VAL:HB	11:U:325:THR:HG22	2.03	0.40
10:V:342:ARG:HA	10:V:342:ARG:HD2	1.95	0.40
10:V:403:LEU:HA	10:V:406:MET:HE2	2.03	0.40
11:W:57:ILE:O	11:W:61:VAL:HG13	2.21	0.40
11:W:104:SER:OG	10:X:319:GLU:OE2	2.38	0.40
12:Z:216:LYS:HG2	12:Z:217:ARG:HD3	2.02	0.40
1:B:65:LEU:HD23	7:M:781:GLN:OE1	2.22	0.40
2:C:61:PHE:O	2:C:65:VAL:HG13	2.21	0.40
7:M:711:TYR:CE2	7:M:738:LEU:HD13	2.56	0.40
8:R:81:PHE:HD2	9:S:183:LYS:HZ1	1.69	0.40
8:R:346:ARG:HH22	8:R:377:LEU:HD11	1.87	0.40
10:T:64:LEU:HD12	11:Y:408:GLN:HB2	2.03	0.40
10:T:72:GLY:N	10:T:333:ALA:O	2.55	0.40
10:T:428:THR:HG21	11:U:35:LEU:HD22	2.03	0.40
11:U:377:VAL:HG12	11:U:379:LEU:HD12	2.04	0.40
10:V:132:ARG:HB3	10:V:302:GLU:CG	2.50	0.40
11:W:78:SER:HB2	11:W:397:ARG:CZ	2.51	0.40
11:Y:421:GLU:HG2	11:Y:422:ASP:N	2.37	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	73/136 (54%)	71 (97%)	2 (3%)	0	100	100
1	B	95/136 (70%)	89 (94%)	6 (6%)	0	100	100
2	C	77/103 (75%)	66 (86%)	10 (13%)	1 (1%)	9	41
2	D	64/103 (62%)	54 (84%)	9 (14%)	1 (2%)	7	36
3	E	100/132 (76%)	95 (95%)	5 (5%)	0	100	100
4	G	63/131 (48%)	58 (92%)	5 (8%)	0	100	100
7	M	667/1514 (44%)	589 (88%)	77 (12%)	1 (0%)	48	83
8	R	407/438 (93%)	375 (92%)	32 (8%)	0	100	100
9	S	184/280 (66%)	163 (89%)	21 (11%)	0	100	100
10	T	433/463 (94%)	407 (94%)	25 (6%)	1 (0%)	43	77
10	V	422/463 (91%)	403 (96%)	19 (4%)	0	100	100
10	X	437/463 (94%)	415 (95%)	21 (5%)	1 (0%)	43	77
11	U	444/471 (94%)	412 (93%)	32 (7%)	0	100	100
11	W	429/471 (91%)	410 (96%)	19 (4%)	0	100	100
11	Y	439/471 (93%)	407 (93%)	32 (7%)	0	100	100
12	Z	126/795 (16%)	106 (84%)	16 (13%)	4 (3%)	3	21
All	All	4460/6570 (68%)	4120 (92%)	331 (7%)	9 (0%)	44	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	30	THR
7	M	1068	VAL
10	X	208	ALA
12	Z	602	ALA
12	Z	287	ILE
10	T	230	VAL
12	Z	235	MET
12	Z	299	PRO
2	D	41	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/113 (58%)	65 (100%)	0	100	100
1	B	75/113 (66%)	75 (100%)	0	100	100
2	C	60/81 (74%)	60 (100%)	0	100	100
2	D	48/81 (59%)	48 (100%)	0	100	100
3	E	65/99 (66%)	65 (100%)	0	100	100
4	G	52/109 (48%)	52 (100%)	0	100	100
7	M	553/1376 (40%)	553 (100%)	0	100	100
8	R	372/396 (94%)	372 (100%)	0	100	100
9	S	178/261 (68%)	178 (100%)	0	100	100
10	T	357/391 (91%)	357 (100%)	0	100	100
10	V	354/391 (90%)	354 (100%)	0	100	100
10	X	368/391 (94%)	368 (100%)	0	100	100
11	U	378/403 (94%)	378 (100%)	0	100	100
11	W	364/403 (90%)	364 (100%)	0	100	100
11	Y	359/403 (89%)	359 (100%)	0	100	100
12	Z	110/732 (15%)	110 (100%)	0	100	100
All	All	3758/5743 (65%)	3758 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
4	G	52	HIS
7	M	705	ASN
7	M	859	ASN
7	M	988	GLN
7	M	1036	ASN
7	M	1058	HIS
7	M	1167	GLN
7	M	1280	GLN
7	M	1283	ASN
7	M	1285	HIS
7	M	1378	ASN

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Mol	Chain	Res	Type
8	R	235	HIS
8	R	280	GLN
8	R	402	GLN
9	S	93	GLN
9	S	163	HIS
11	U	441	GLN
10	V	27	HIS
10	V	263	GLN
11	W	230	GLN
11	W	237	HIS
11	W	248	ASN
11	W	272	GLN
11	W	415	ASN
11	Y	47	GLN
11	Y	230	GLN
11	Y	237	HIS
11	Y	341	HIS
11	Y	441	GLN
12	Z	279	GLN
12	Z	314	ASN
12	Z	592	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	U	502	15	27,29,29	1.36	4 (14%)	42,45,45	1.99	10 (23%)
13	ADP	R	501	8	27,29,29	1.36	4 (14%)	42,45,45	1.94	11 (26%)
13	ADP	M	1601	7,15	27,29,29	1.36	4 (14%)	42,45,45	1.95	11 (26%)
13	ADP	Y	501	15	27,29,29	1.35	4 (14%)	42,45,45	2.02	9 (21%)
13	ADP	W	501	11,15	27,29,29	1.37	4 (14%)	42,45,45	1.98	9 (21%)
13	ADP	V	501	15	27,29,29	1.36	4 (14%)	42,45,45	1.97	10 (23%)
13	ADP	T	501	10	27,29,29	1.36	4 (14%)	42,45,45	2.04	11 (26%)
14	BEF	R	502	-	0,3,3	-	-	-		
13	ADP	X	501	10	27,29,29	1.36	4 (14%)	42,45,45	2.03	9 (21%)
14	BEF	M	1602	-	0,3,3	-	-	-		

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	U	502	15	-	4/16/32/32	0/3/3/3
13	ADP	R	501	8	-	5/16/32/32	0/3/3/3
13	ADP	M	1601	7,15	-	5/16/32/32	0/3/3/3
13	ADP	Y	501	15	-	3/16/32/32	0/3/3/3
13	ADP	W	501	11,15	-	5/16/32/32	0/3/3/3
13	ADP	V	501	15	-	4/16/32/32	0/3/3/3
13	ADP	T	501	10	-	2/16/32/32	0/3/3/3
13	ADP	X	501	10	-	4/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	501	ADP	C5-C4	4.67	1.47	1.39
13	W	501	ADP	C5-C4	4.65	1.47	1.39
13	Y	501	ADP	C5-C4	4.59	1.47	1.39
13	V	501	ADP	C5-C4	4.58	1.47	1.39
13	M	1601	ADP	C5-C4	4.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	U	502	ADP	C5-C4	4.57	1.47	1.39
13	R	501	ADP	C5-C4	4.51	1.47	1.39
13	T	501	ADP	C5-C4	4.45	1.47	1.39
13	R	501	ADP	C5-C6	2.73	1.48	1.41
13	M	1601	ADP	C5-C6	2.70	1.48	1.41
13	X	501	ADP	C5-C6	2.68	1.48	1.41
13	W	501	ADP	C5-C6	2.67	1.48	1.41
13	T	501	ADP	C5-C6	2.65	1.48	1.41
13	U	502	ADP	C5-C6	2.62	1.48	1.41
13	V	501	ADP	C5-C6	2.60	1.48	1.41
13	Y	501	ADP	C5-C6	2.60	1.48	1.41
13	R	501	ADP	C8-N7	2.48	1.36	1.31
13	M	1601	ADP	C8-N7	2.45	1.36	1.31
13	T	501	ADP	C8-N7	2.43	1.36	1.31
13	U	502	ADP	C8-N7	2.38	1.36	1.31
13	W	501	ADP	C8-N7	2.38	1.36	1.31
13	V	501	ADP	C8-N7	2.36	1.36	1.31
13	T	501	ADP	C5-N7	-2.34	1.34	1.39
13	X	501	ADP	C8-N7	2.27	1.35	1.31
13	Y	501	ADP	C8-N7	2.27	1.35	1.31
13	V	501	ADP	C5-N7	-2.26	1.34	1.39
13	U	502	ADP	C5-N7	-2.21	1.34	1.39
13	X	501	ADP	C5-N7	-2.20	1.34	1.39
13	Y	501	ADP	C5-N7	-2.20	1.34	1.39
13	W	501	ADP	C5-N7	-2.18	1.34	1.39
13	M	1601	ADP	C5-N7	-2.12	1.35	1.39
13	R	501	ADP	C5-N7	-2.05	1.35	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	X	501	ADP	C5-C4-N3	-6.44	118.34	126.75
13	Y	501	ADP	C5-C4-N3	-6.41	118.38	126.75
13	W	501	ADP	C5-C4-N3	-6.39	118.41	126.75
13	T	501	ADP	C5-C4-N3	-6.27	118.57	126.75
13	M	1601	ADP	C5-C4-N3	-6.26	118.59	126.75
13	V	501	ADP	C5-C4-N3	-6.23	118.63	126.75
13	U	502	ADP	C5-C4-N3	-6.11	118.78	126.75
13	R	501	ADP	C5-C4-N3	-6.04	118.87	126.75
13	Y	501	ADP	N3-C4-N9	5.21	135.66	127.08
13	X	501	ADP	N3-C4-N9	5.15	135.57	127.08
13	W	501	ADP	N3-C4-N9	5.12	135.51	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	501	ADP	N3-C4-N9	5.01	135.34	127.08
13	M	1601	ADP	N3-C4-N9	4.88	135.13	127.08
13	U	502	ADP	N3-C4-N9	4.83	135.03	127.08
13	T	501	ADP	N3-C4-N9	4.81	135.01	127.08
13	R	501	ADP	N3-C4-N9	4.65	134.75	127.08
13	T	501	ADP	C2-N3-C4	3.92	121.02	111.75
13	M	1601	ADP	C2-N3-C4	3.89	120.93	111.75
13	R	501	ADP	C2-N3-C4	3.85	120.84	111.75
13	W	501	ADP	C2-N3-C4	3.84	120.82	111.75
13	Y	501	ADP	C2-N3-C4	3.83	120.80	111.75
13	X	501	ADP	C2-N3-C4	3.81	120.75	111.75
13	U	502	ADP	PA-O3A-PB	-3.80	119.80	132.83
13	V	501	ADP	C2-N3-C4	3.78	120.68	111.75
13	U	502	ADP	C2-N3-C4	3.77	120.65	111.75
13	Y	501	ADP	PA-O3A-PB	-3.73	120.02	132.83
13	T	501	ADP	C4-C5-N7	-3.67	106.15	110.62
13	X	501	ADP	PA-O3A-PB	-3.63	120.38	132.83
13	T	501	ADP	PA-O3A-PB	-3.41	121.12	132.83
13	R	501	ADP	C4-C5-N7	-3.35	106.54	110.62
13	M	1601	ADP	C4-C5-N7	-3.30	106.61	110.62
13	T	501	ADP	C5-N7-C8	3.27	108.15	103.51
13	T	501	ADP	N3-C2-N1	-3.26	123.51	128.60
13	X	501	ADP	C4-C5-N7	-3.24	106.67	110.62
13	R	501	ADP	N3-C2-N1	-3.23	123.55	128.60
13	U	502	ADP	C4-C5-N7	-3.16	106.77	110.62
13	U	502	ADP	N3-C2-N1	-3.15	123.68	128.60
13	M	1601	ADP	N3-C2-N1	-3.15	123.68	128.60
13	V	501	ADP	C4-C5-N7	-3.14	106.80	110.62
13	V	501	ADP	PA-O3A-PB	-3.13	122.10	132.83
13	W	501	ADP	C4-C5-N7	-3.11	106.83	110.62
13	V	501	ADP	N3-C2-N1	-3.06	123.81	128.60
13	Y	501	ADP	C4-C5-N7	-3.05	106.91	110.62
13	Y	501	ADP	N3-C2-N1	-3.01	123.90	128.60
13	W	501	ADP	N3-C2-N1	-2.98	123.94	128.60
13	W	501	ADP	PA-O3A-PB	-2.94	122.74	132.83
13	X	501	ADP	N3-C2-N1	-2.88	124.09	128.60
13	M	1601	ADP	PA-O3A-PB	-2.84	123.07	132.83
13	R	501	ADP	PA-O3A-PB	-2.80	123.23	132.83
13	X	501	ADP	C5-N7-C8	2.79	107.47	103.51
13	M	1601	ADP	C5-N7-C8	2.79	107.47	103.51
13	R	501	ADP	C5-N7-C8	2.77	107.44	103.51
13	V	501	ADP	C5-N7-C8	2.73	107.39	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	X	501	ADP	C3'-C2'-C1'	2.70	106.56	101.43
13	T	501	ADP	C4-N9-C8	2.70	108.65	105.73
13	V	501	ADP	C4-N9-C8	2.69	108.64	105.73
13	R	501	ADP	C4-N9-C8	2.67	108.62	105.73
13	U	502	ADP	C5-N7-C8	2.65	107.27	103.51
13	Y	501	ADP	C3'-C2'-C1'	2.62	106.41	101.43
13	U	502	ADP	C3'-C2'-C1'	2.62	106.41	101.43
13	Y	501	ADP	C5-N7-C8	2.62	107.22	103.51
13	W	501	ADP	C5-N7-C8	2.61	107.22	103.51
13	Y	501	ADP	C4-N9-C8	2.61	108.55	105.73
13	W	501	ADP	C3'-C2'-C1'	2.60	106.37	101.43
13	M	1601	ADP	C4-N9-C8	2.56	108.50	105.73
13	U	502	ADP	C4-N9-C8	2.52	108.46	105.73
13	X	501	ADP	C4-N9-C8	2.52	108.46	105.73
13	W	501	ADP	C4-N9-C8	2.48	108.41	105.73
13	T	501	ADP	N9-C8-N7	-2.41	110.62	113.91
13	M	1601	ADP	C3'-C2'-C1'	2.41	106.00	101.43
13	T	501	ADP	C6-C5-N7	2.36	136.41	132.02
13	V	501	ADP	C3'-C2'-C1'	2.34	105.87	101.43
13	R	501	ADP	C6-C5-N7	2.32	136.34	132.02
13	T	501	ADP	C3'-C2'-C1'	2.19	105.59	101.43
13	R	501	ADP	C3'-C2'-C1'	2.17	105.55	101.43
13	M	1601	ADP	C6-C5-N7	2.17	136.06	132.02
13	R	501	ADP	N9-C8-N7	-2.12	111.02	113.91
13	U	502	ADP	C6-C5-N7	2.06	135.85	132.02
13	V	501	ADP	N9-C8-N7	-2.03	111.14	113.91
13	M	1601	ADP	N9-C8-N7	-2.03	111.14	113.91

There are no chirality outliers.

All (32) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
13	W	501	ADP	C5'-O5'-PA-O2A
13	X	501	ADP	C5'-O5'-PA-O1A
13	X	501	ADP	C5'-O5'-PA-O3A
13	Y	501	ADP	C5'-O5'-PA-O3A
13	M	1601	ADP	O4'-C4'-C5'-O5'
13	W	501	ADP	O4'-C4'-C5'-O5'
13	R	501	ADP	O4'-C4'-C5'-O5'
13	M	1601	ADP	C3'-C4'-C5'-O5'
13	X	501	ADP	C3'-C4'-C5'-O5'
13	W	501	ADP	C3'-C4'-C5'-O5'
13	X	501	ADP	O4'-C4'-C5'-O5'
13	M	1601	ADP	C5'-O5'-PA-O3A
13	U	502	ADP	C5'-O5'-PA-O3A
13	M	1601	ADP	C5'-O5'-PA-O1A
13	Y	501	ADP	C5'-O5'-PA-O2A
13	Y	501	ADP	O4'-C4'-C5'-O5'
13	V	501	ADP	PA-O3A-PB-O1B
13	V	501	ADP	PA-O3A-PB-O3B
13	R	501	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	C5'-O5'-PA-O3A
13	V	501	ADP	C5'-O5'-PA-O1A
13	U	502	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

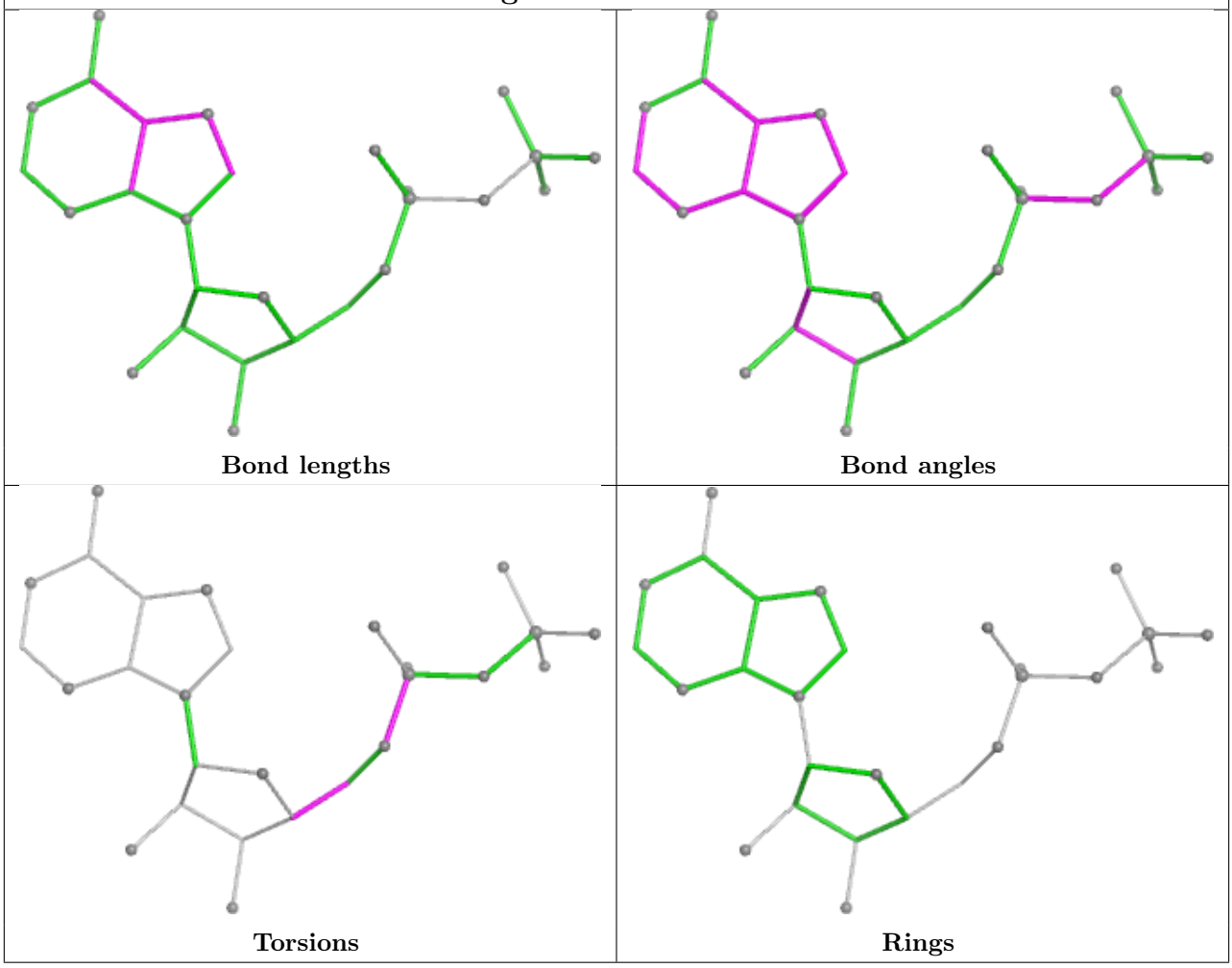
9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	502	ADP	1	0
13	R	501	ADP	1	0
13	Y	501	ADP	4	0
13	W	501	ADP	2	0
13	V	501	ADP	4	0
13	T	501	ADP	3	0
14	R	502	BEF	2	0
13	X	501	ADP	3	0
14	M	1602	BEF	2	0

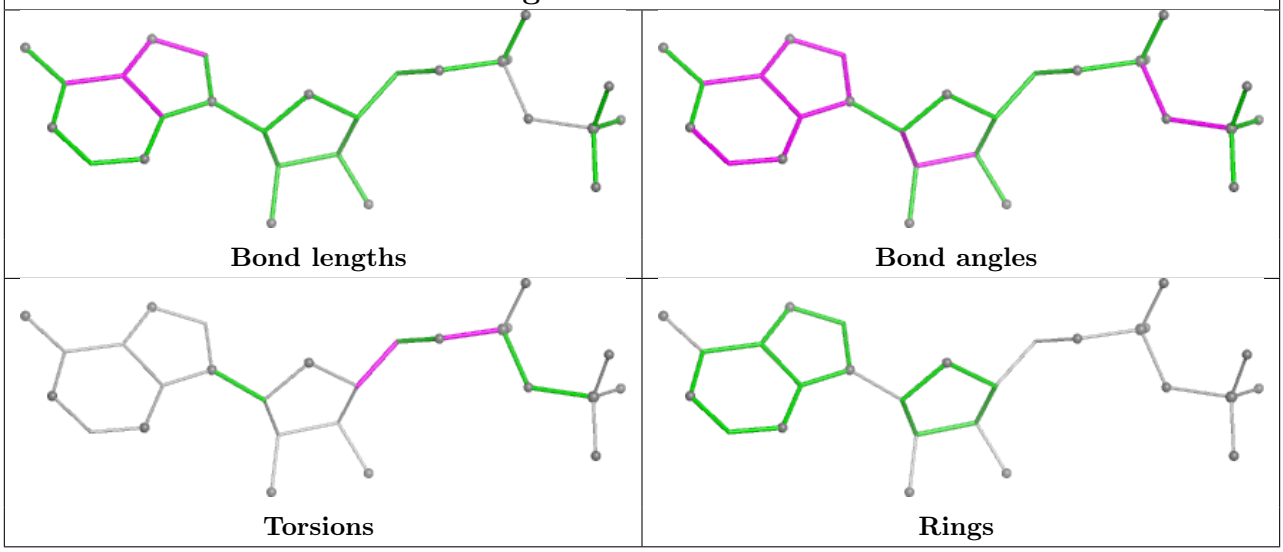
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

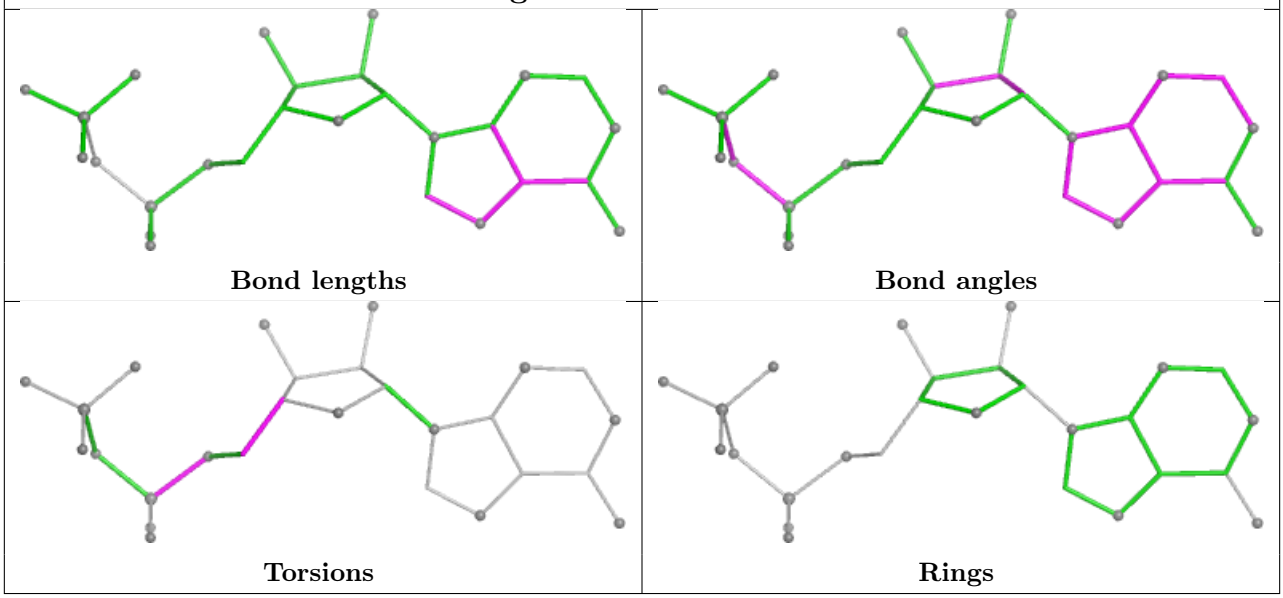
Ligand ADP U 502



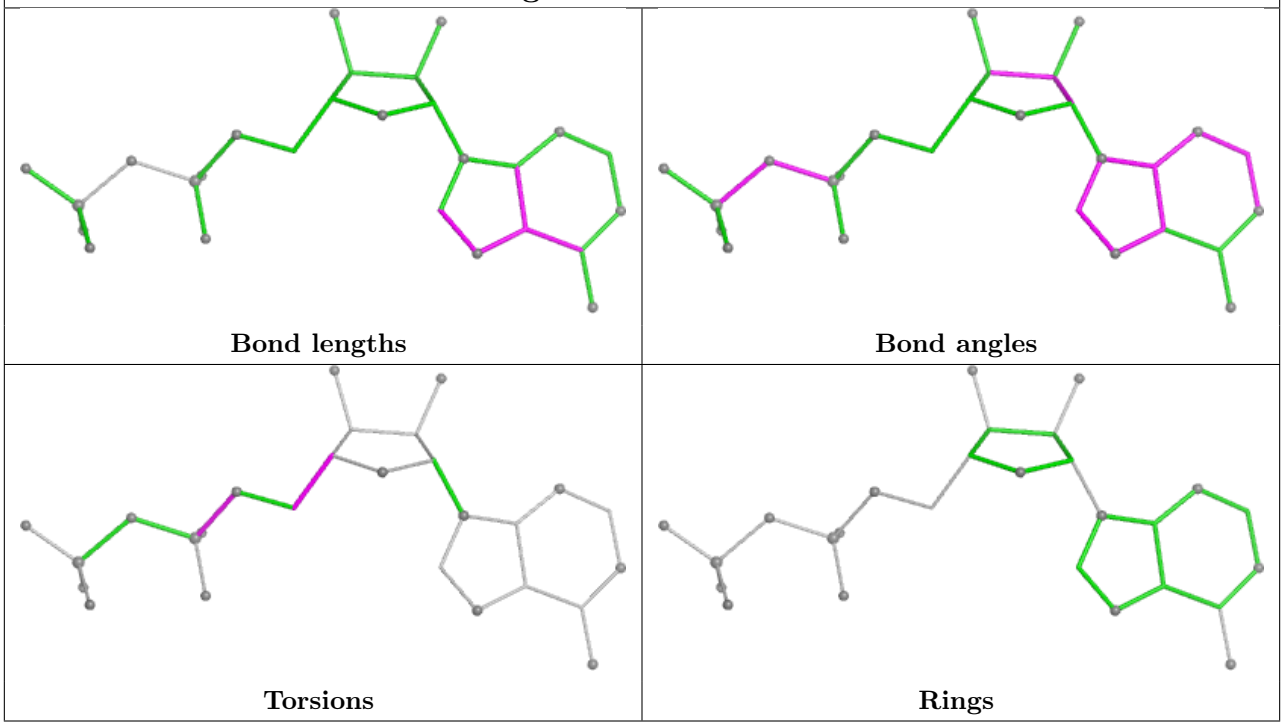
Ligand ADP R 501



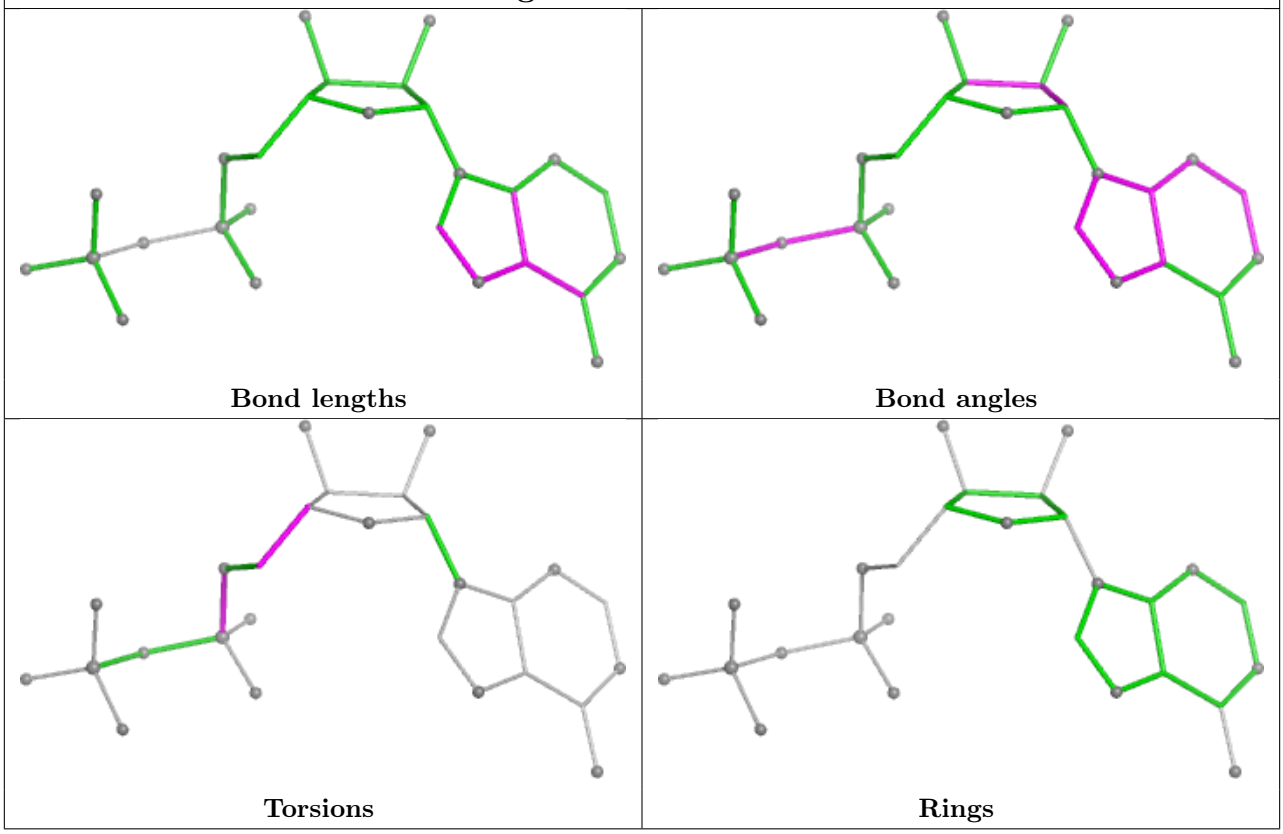
Ligand ADP M 1601

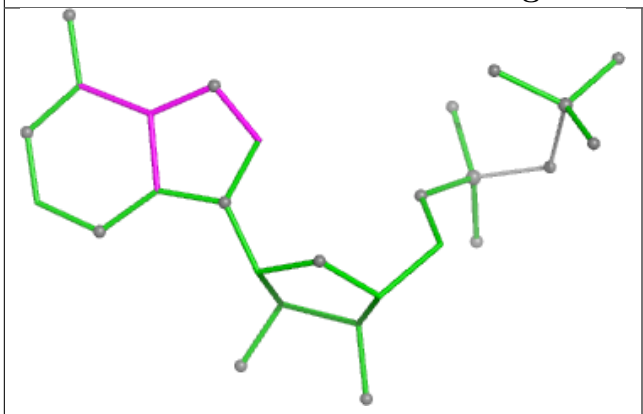
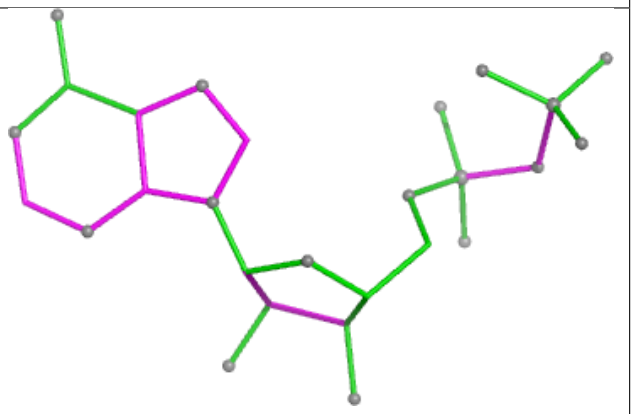
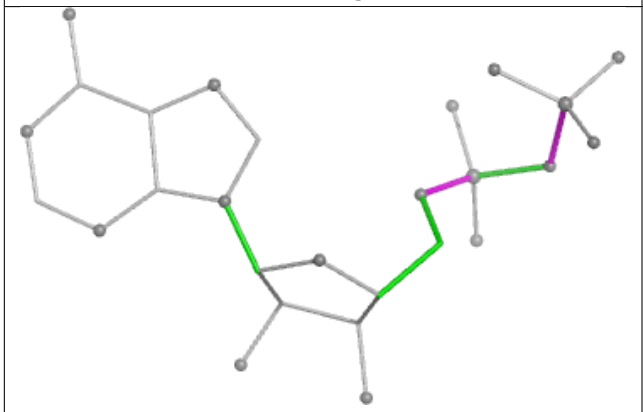
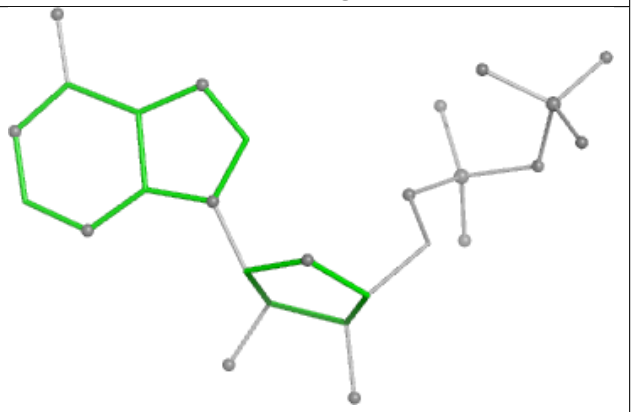


Ligand ADP Y 501

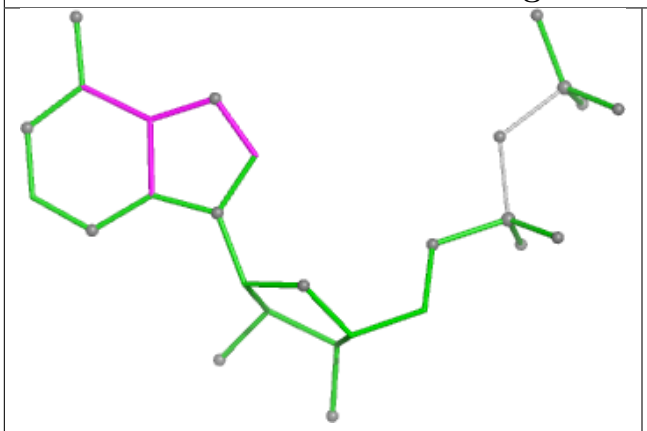


Ligand ADP W 501

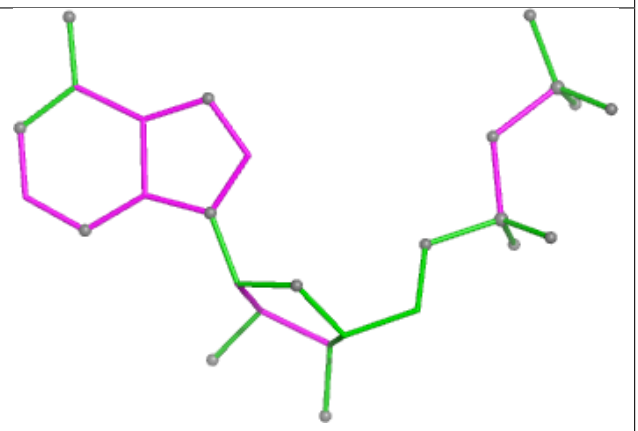


Ligand ADP V 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

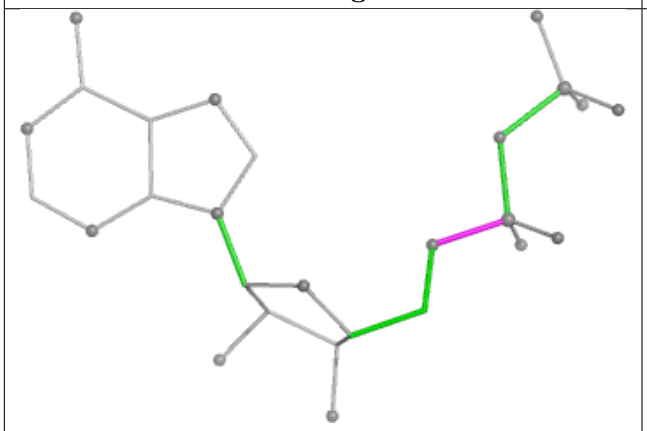
Ligand ADP T 501



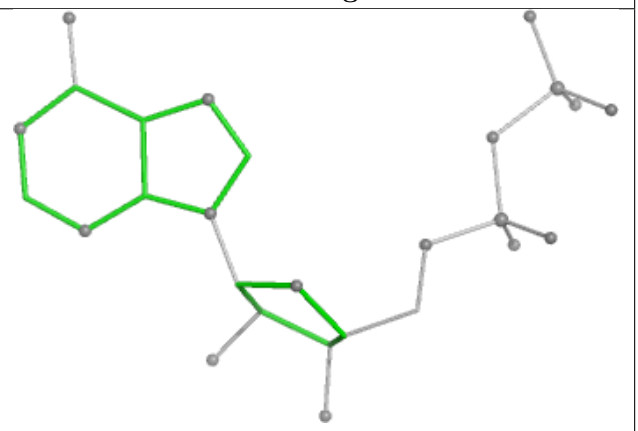
Bond lengths



Bond angles

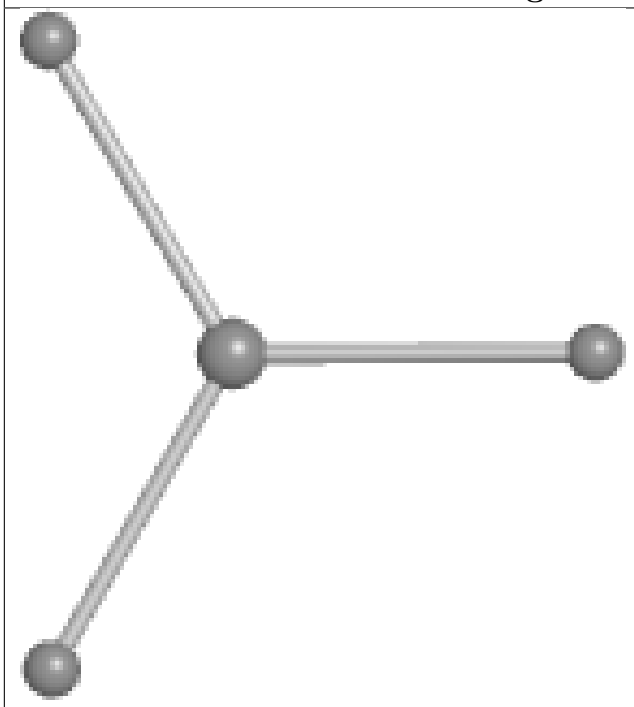


Torsions

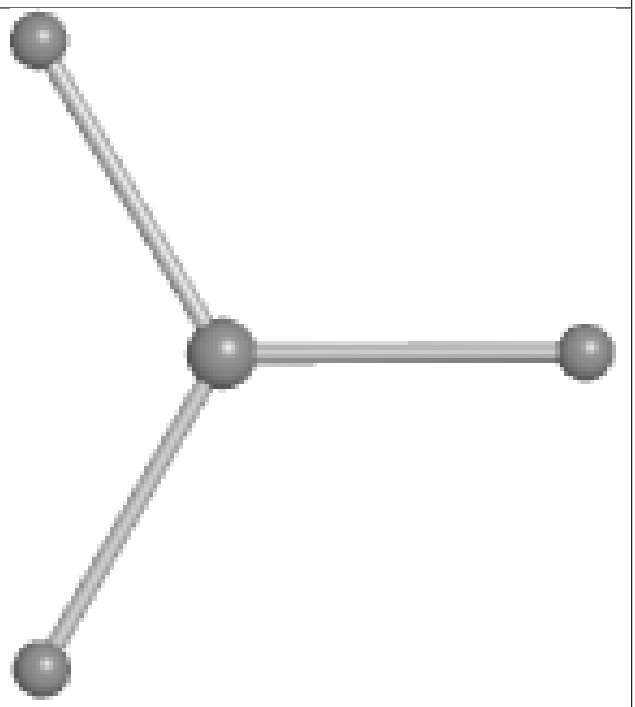


Rings

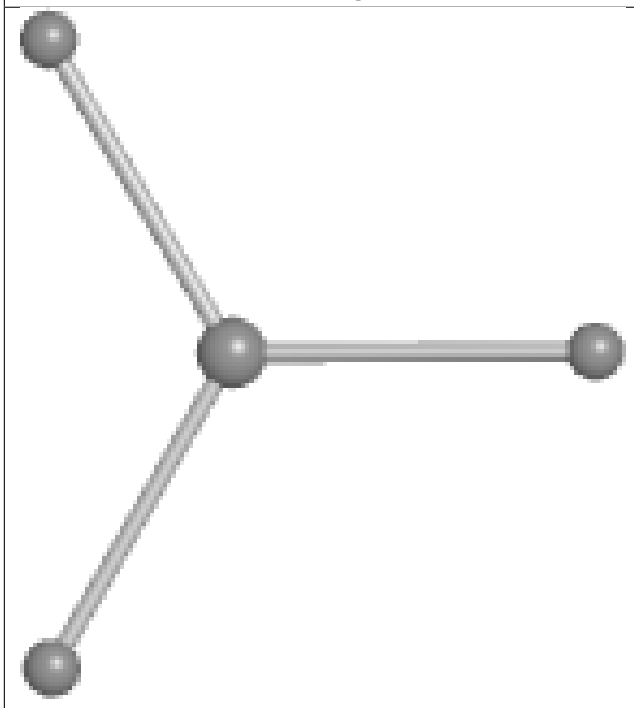
Ligand BEF R 502



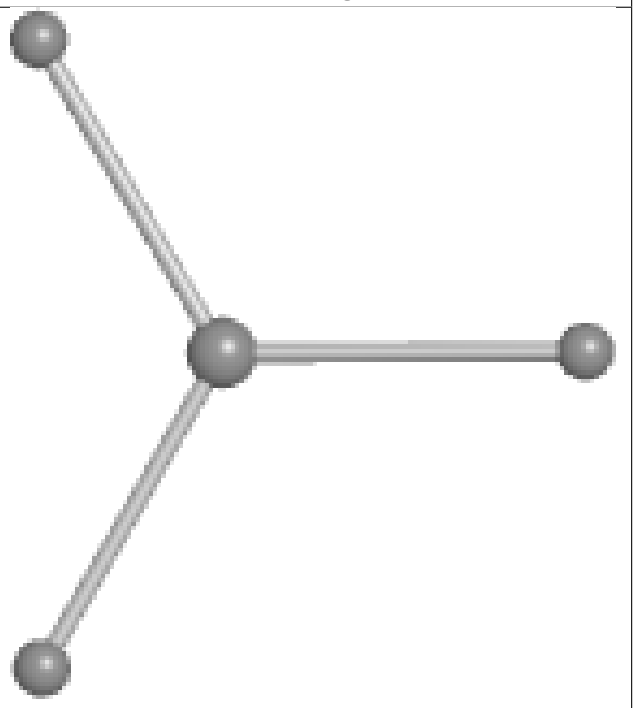
Bond lengths



Bond angles

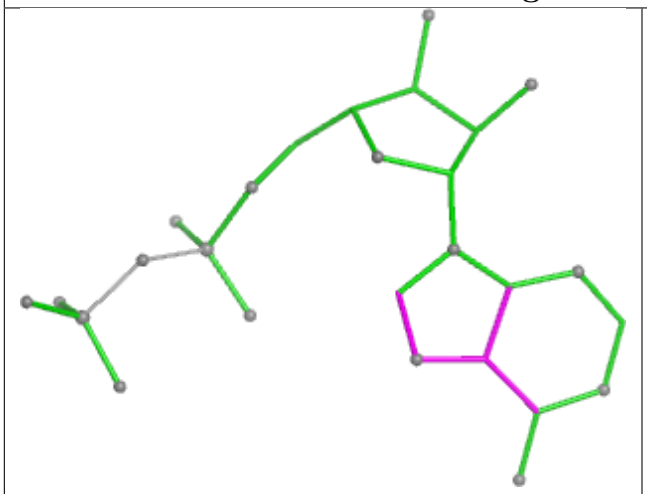


Torsions

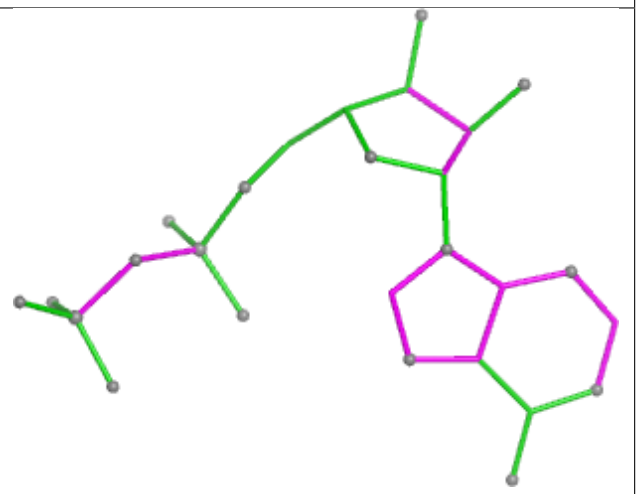


Rings

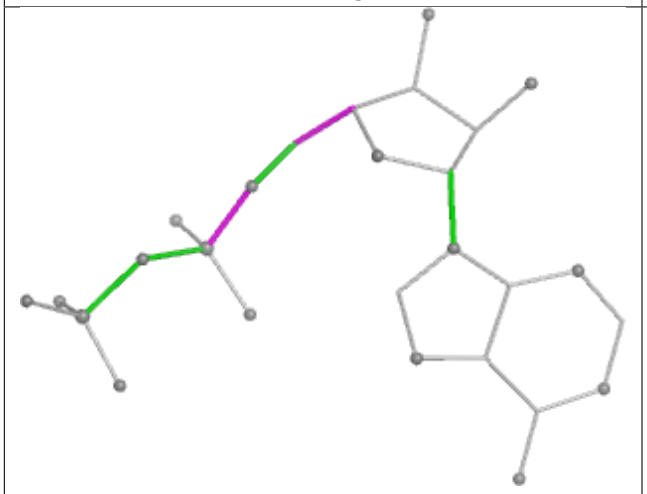
Ligand ADP X 501



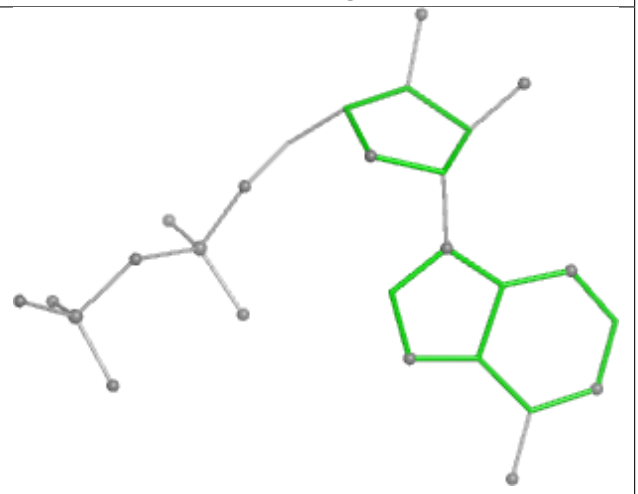
Bond lengths



Bond angles

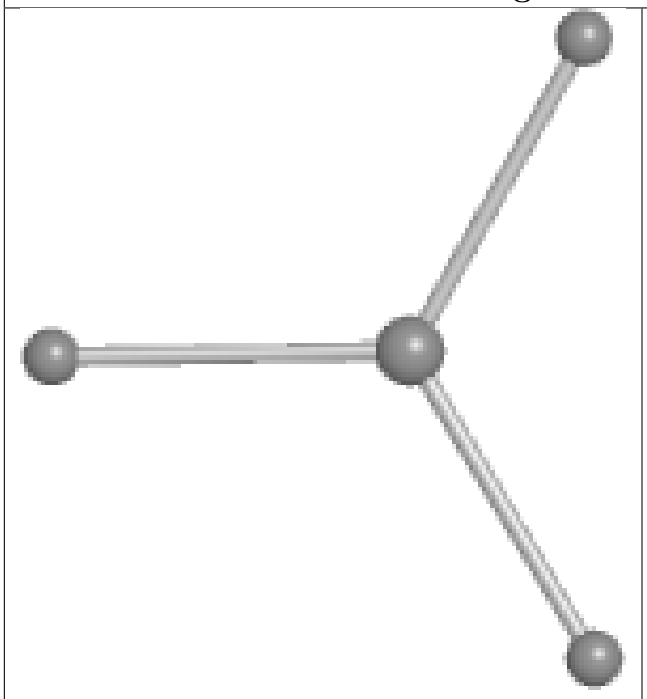


Torsions

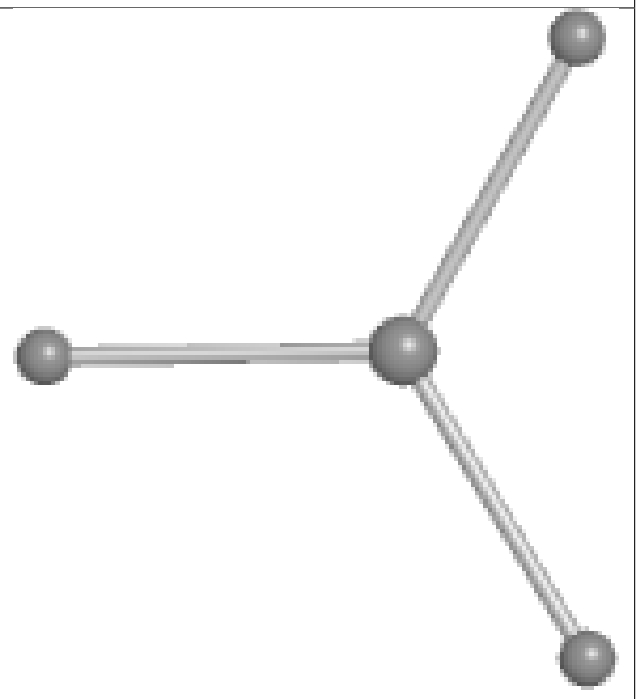


Rings

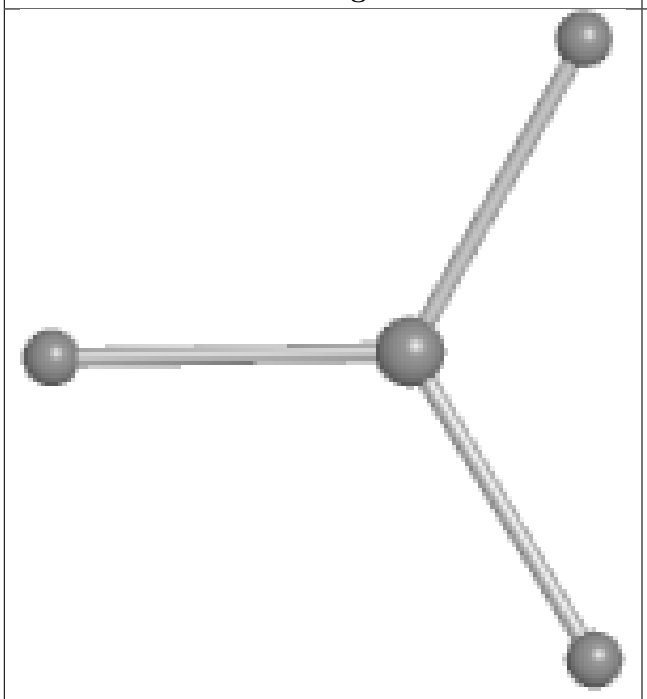
Ligand BEF M 1602



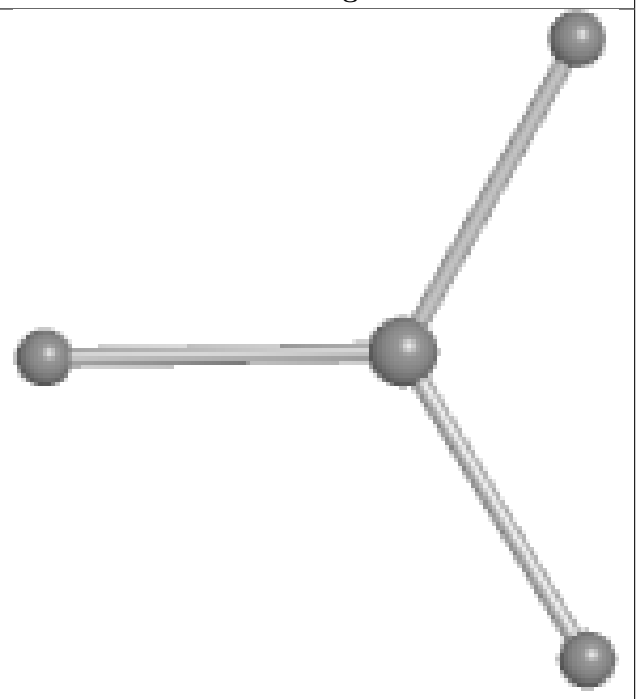
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

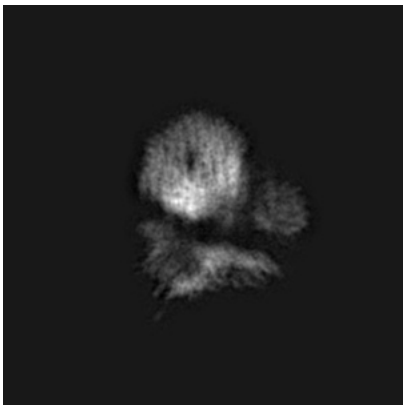
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-50297. These allow visual inspection of the internal detail of the map and identification of artifacts.

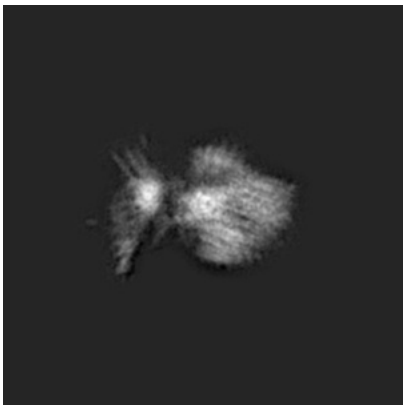
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

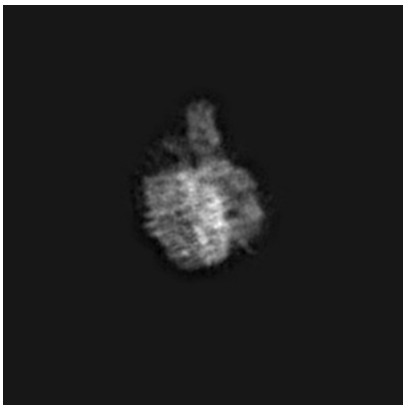
6.1.1 Primary map



X

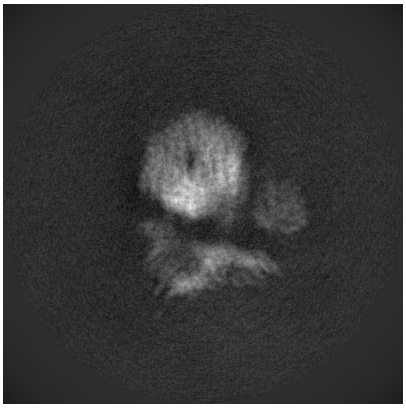


Y

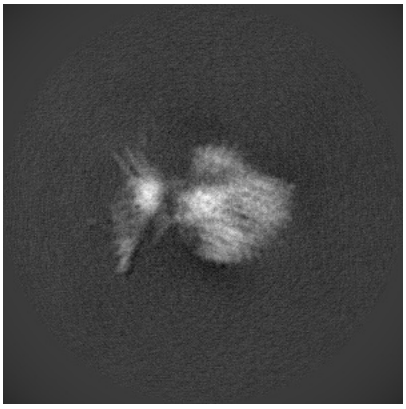


Z

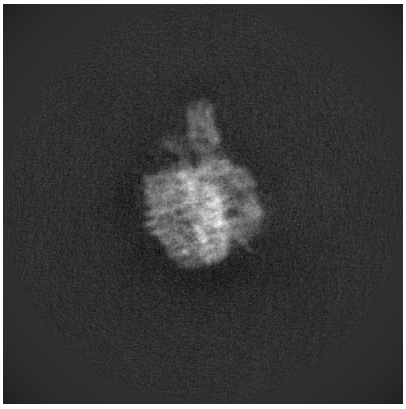
6.1.2 Raw map



X



Y

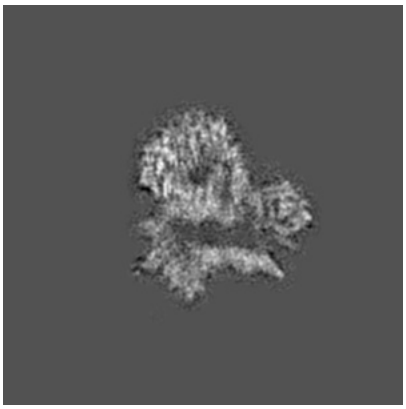


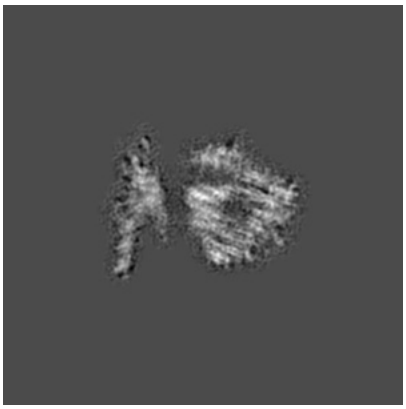
Z

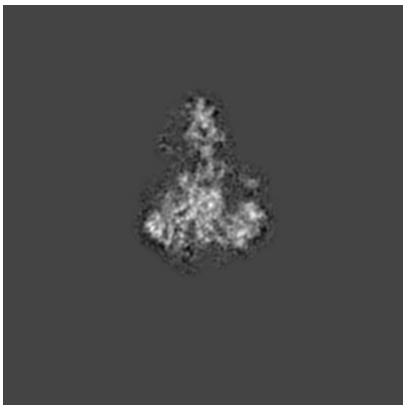
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

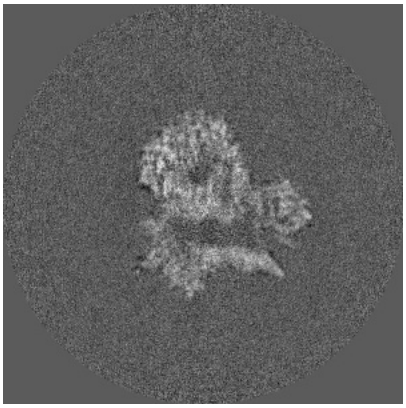
6.2.1 Primary map

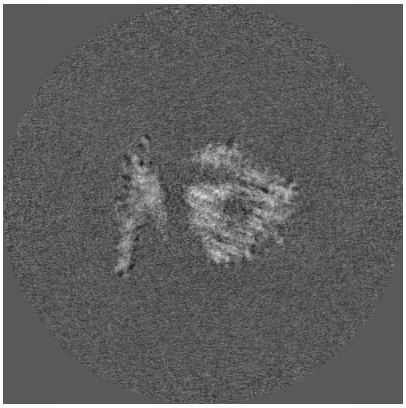

X Index: 240


Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240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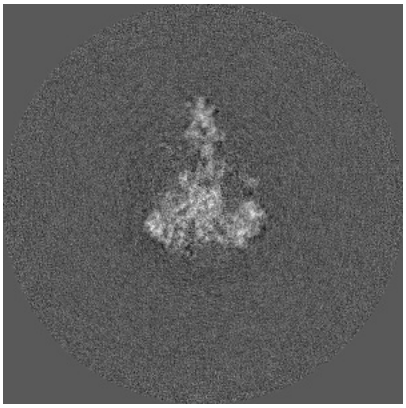
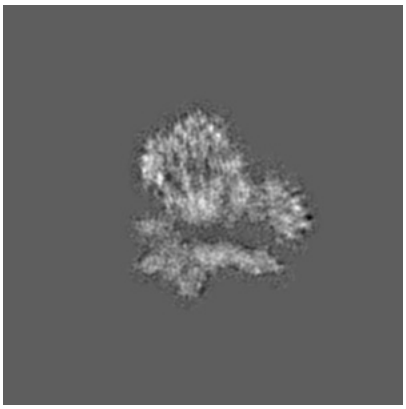
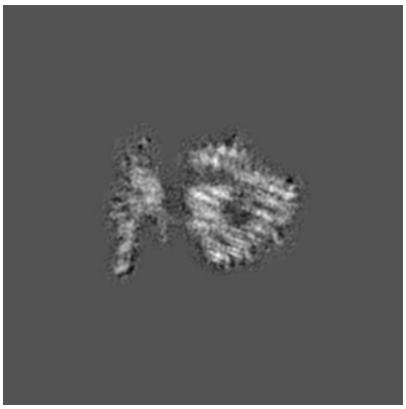

Z Index: 240

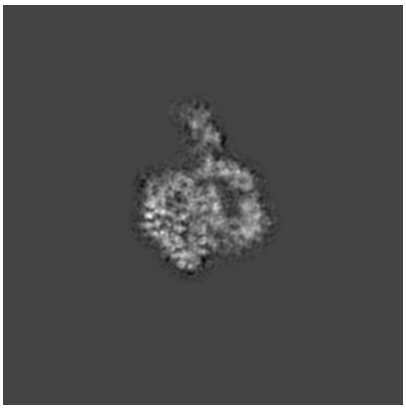
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

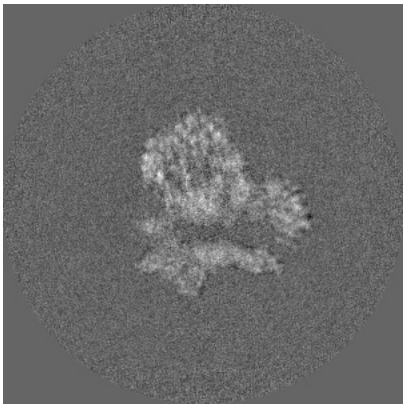
6.3.1 Primary map

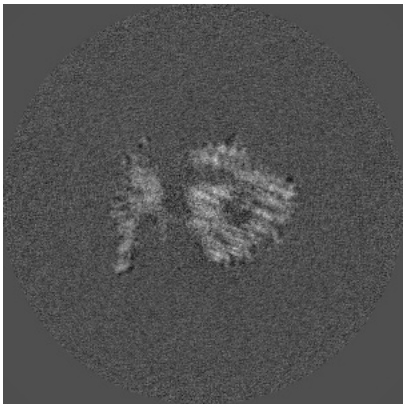

X Index: 247

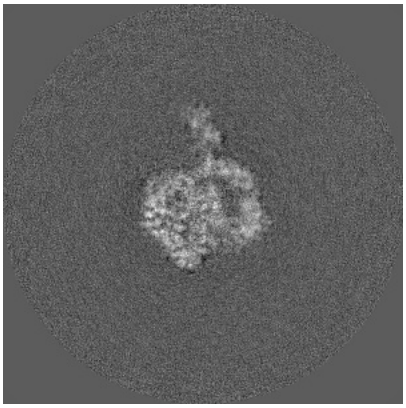

Y Index: 238


Z Index: 257

6.3.2 Raw map


X Index: 246

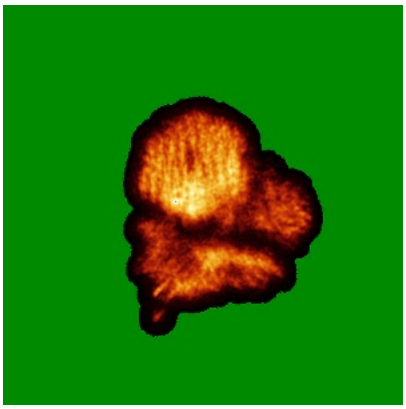

Y Index: 238


Z Index: 257

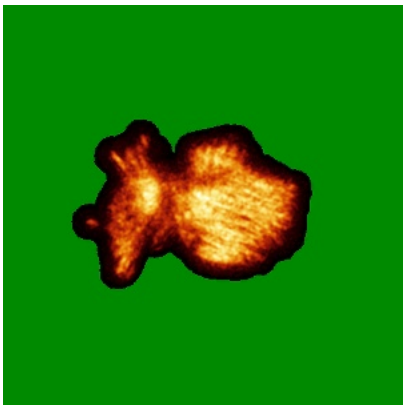
The images above show the largest variance slices of the map in three orthogonal directions.

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

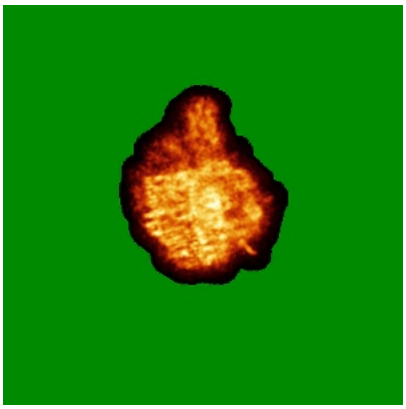
6.4.1 Primary map



X

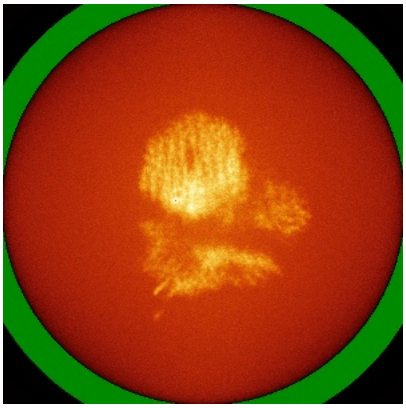


Y

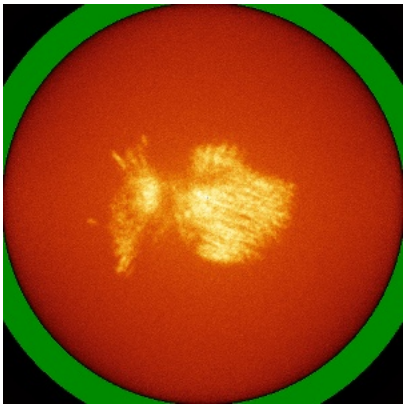


Z

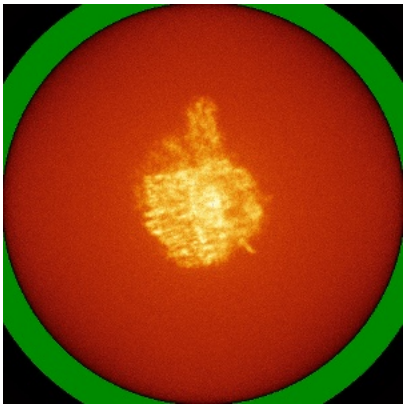
6.4.2 Raw map



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.

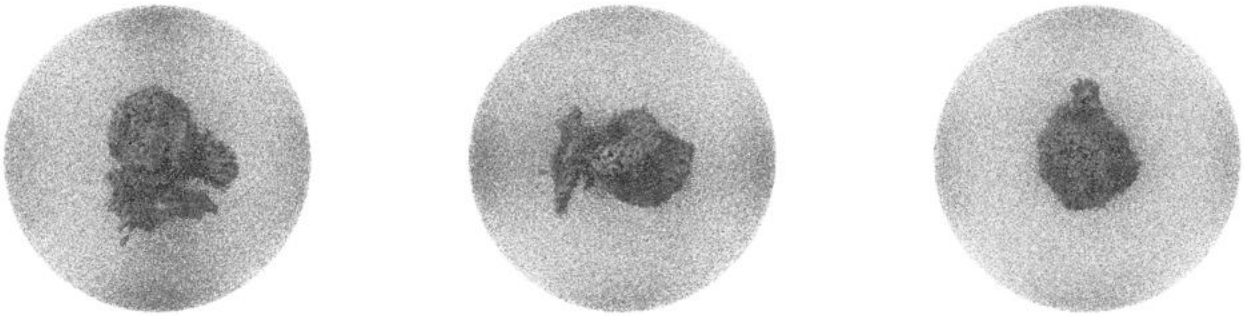
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0011. 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.

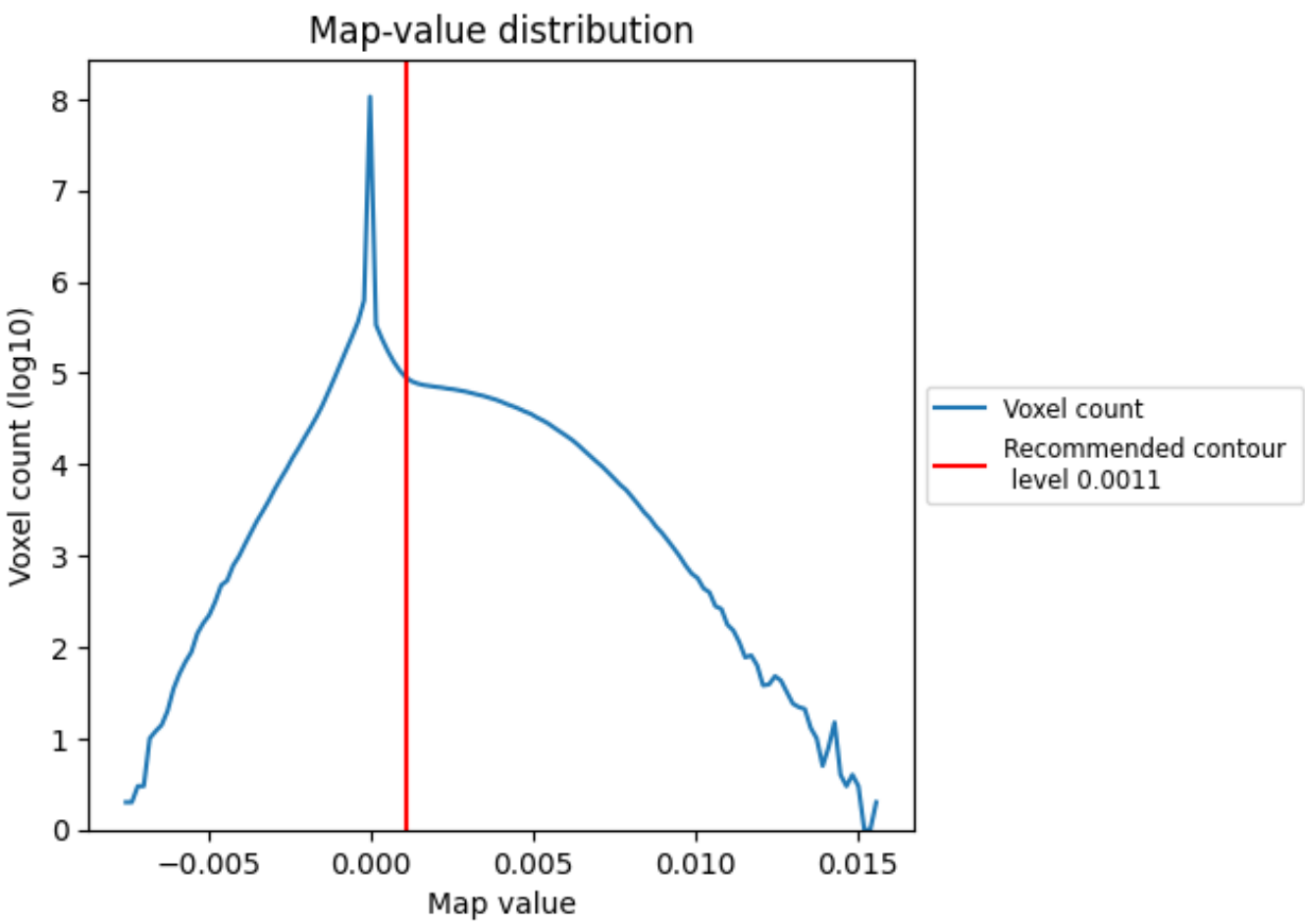
6.6 Mask visualisation (i)

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

7 Map analysis (i)

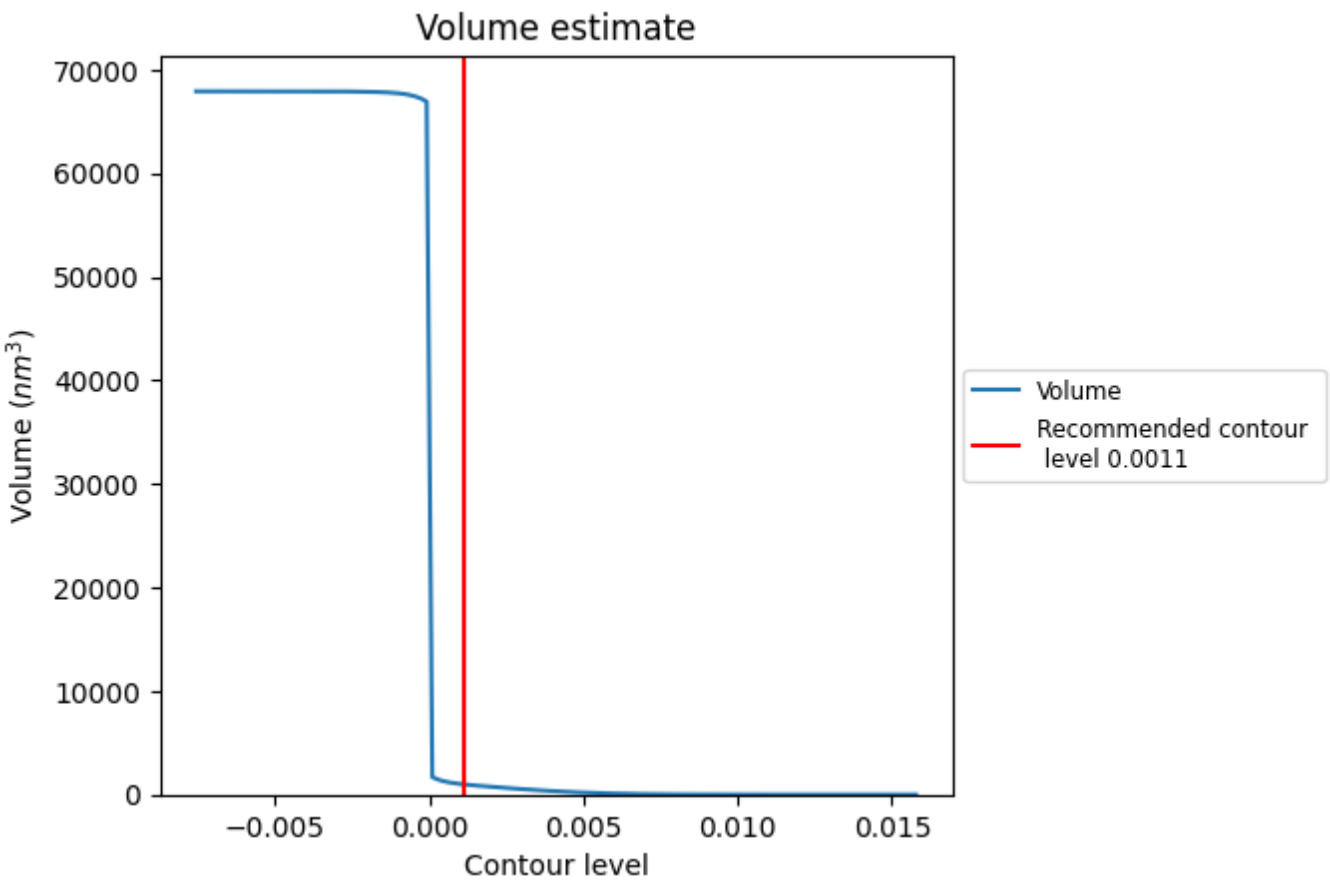
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

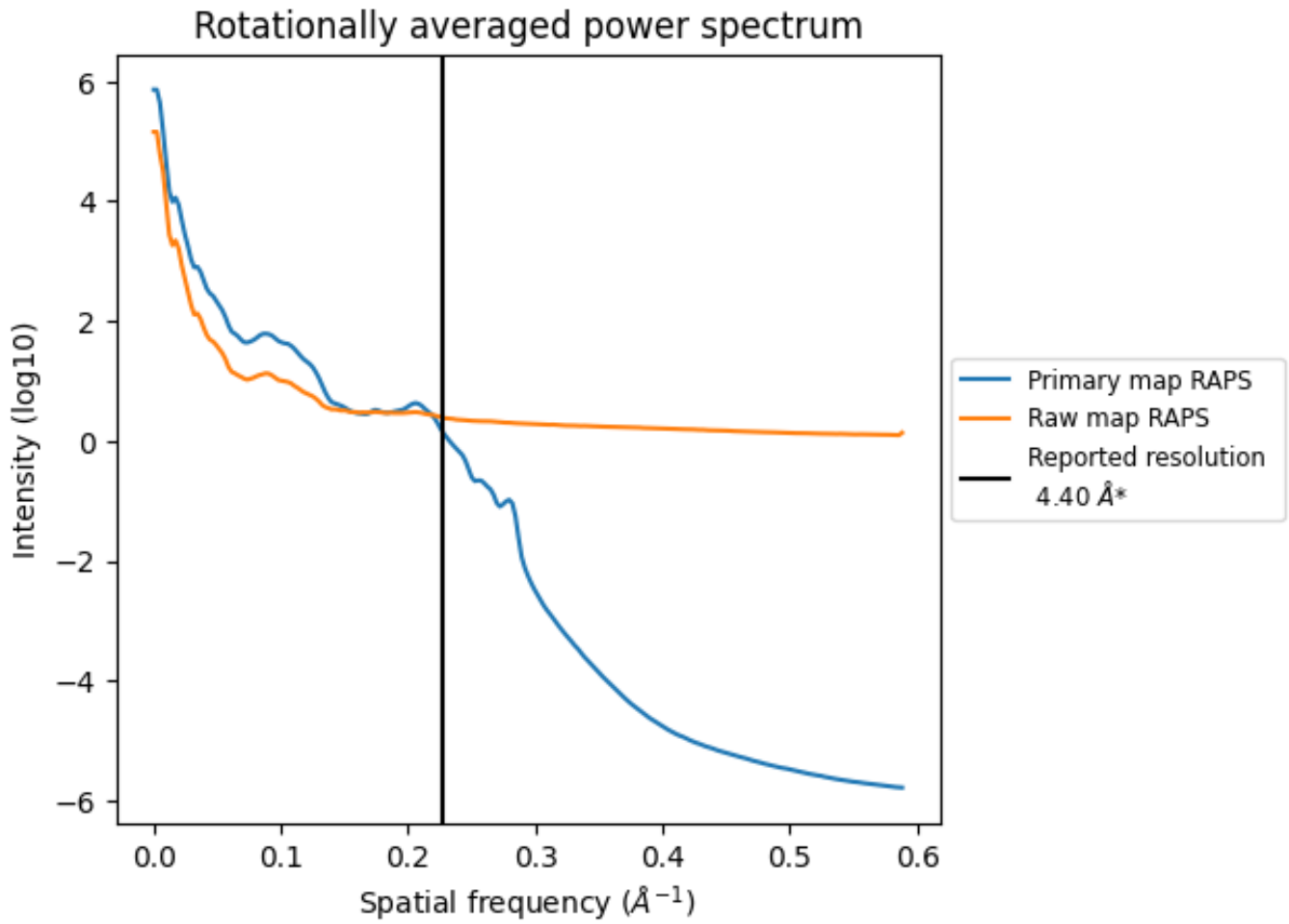
7.2 Volume estimate (i)



The volume at the recommended contour level is 986 nm^3; this corresponds to an approximate mass of 891 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)

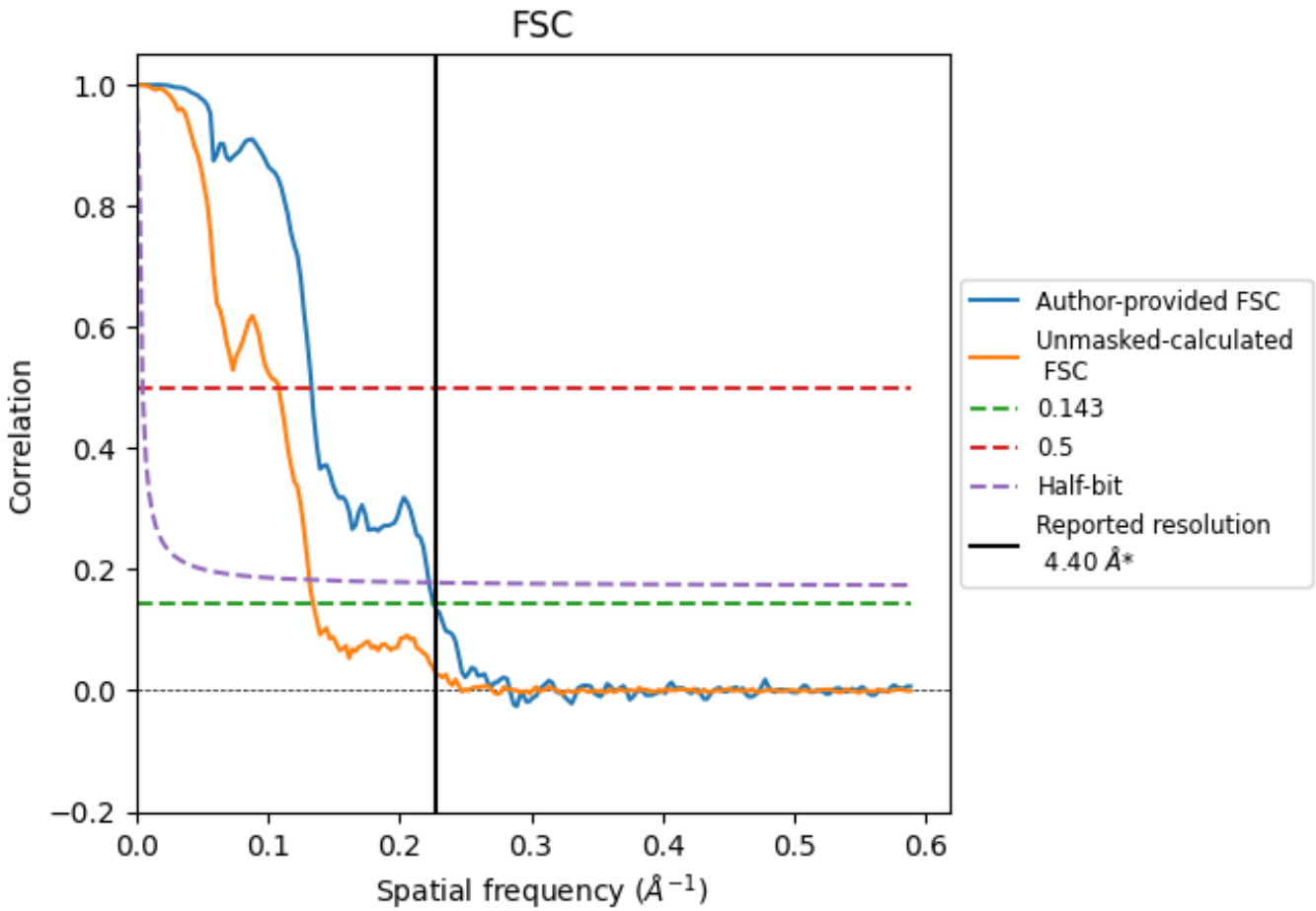


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

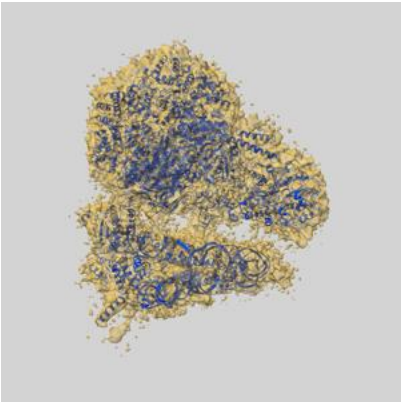
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	7.51	4.49
Unmasked-calculated*	7.43	9.24	7.60

*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 7.43 differs from the reported value 4.4 by more than 10 %

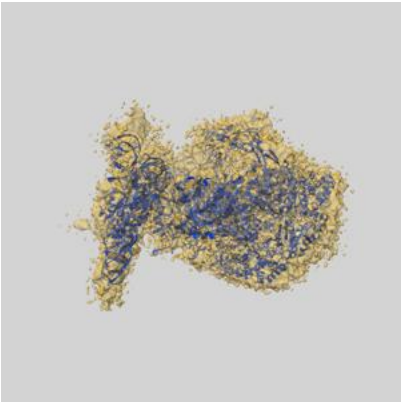
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-50297 and PDB model 9FBW. Per-residue inclusion information can be found in section 3 on page 9.

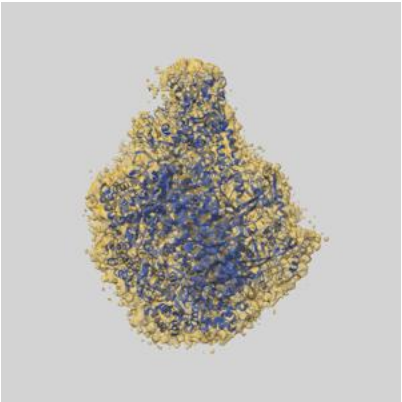
9.1 Map-model overlay (i)



X



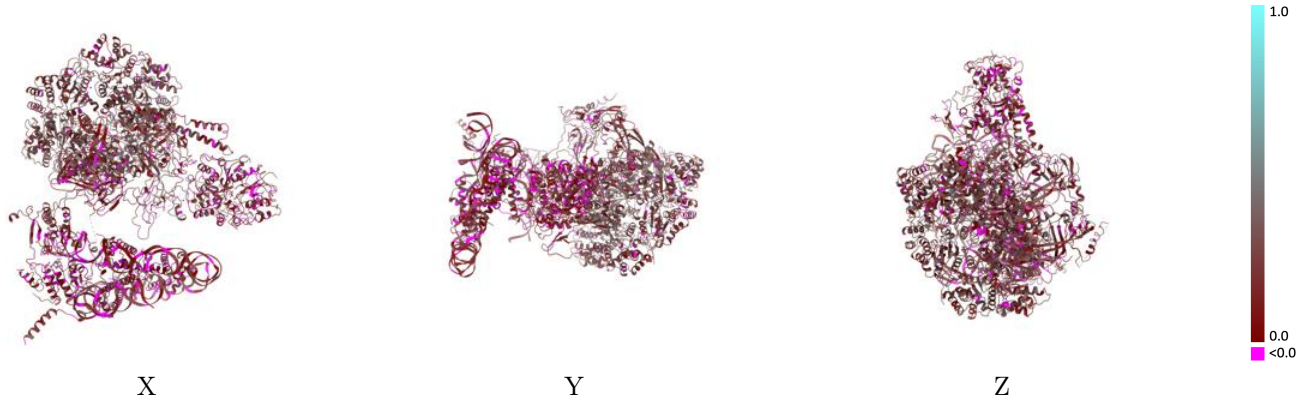
Y



Z

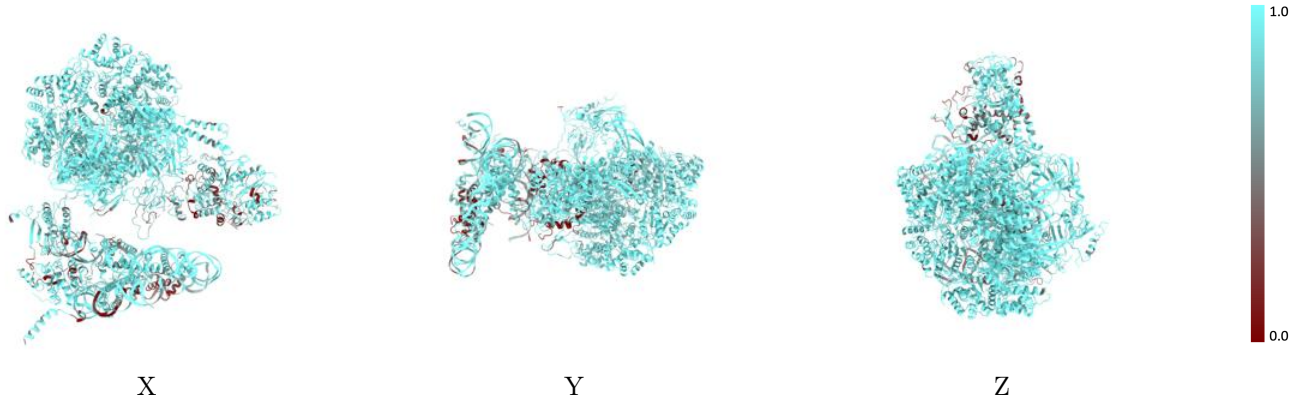
The images above show the 3D surface view of the map at the recommended contour level 0.0011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



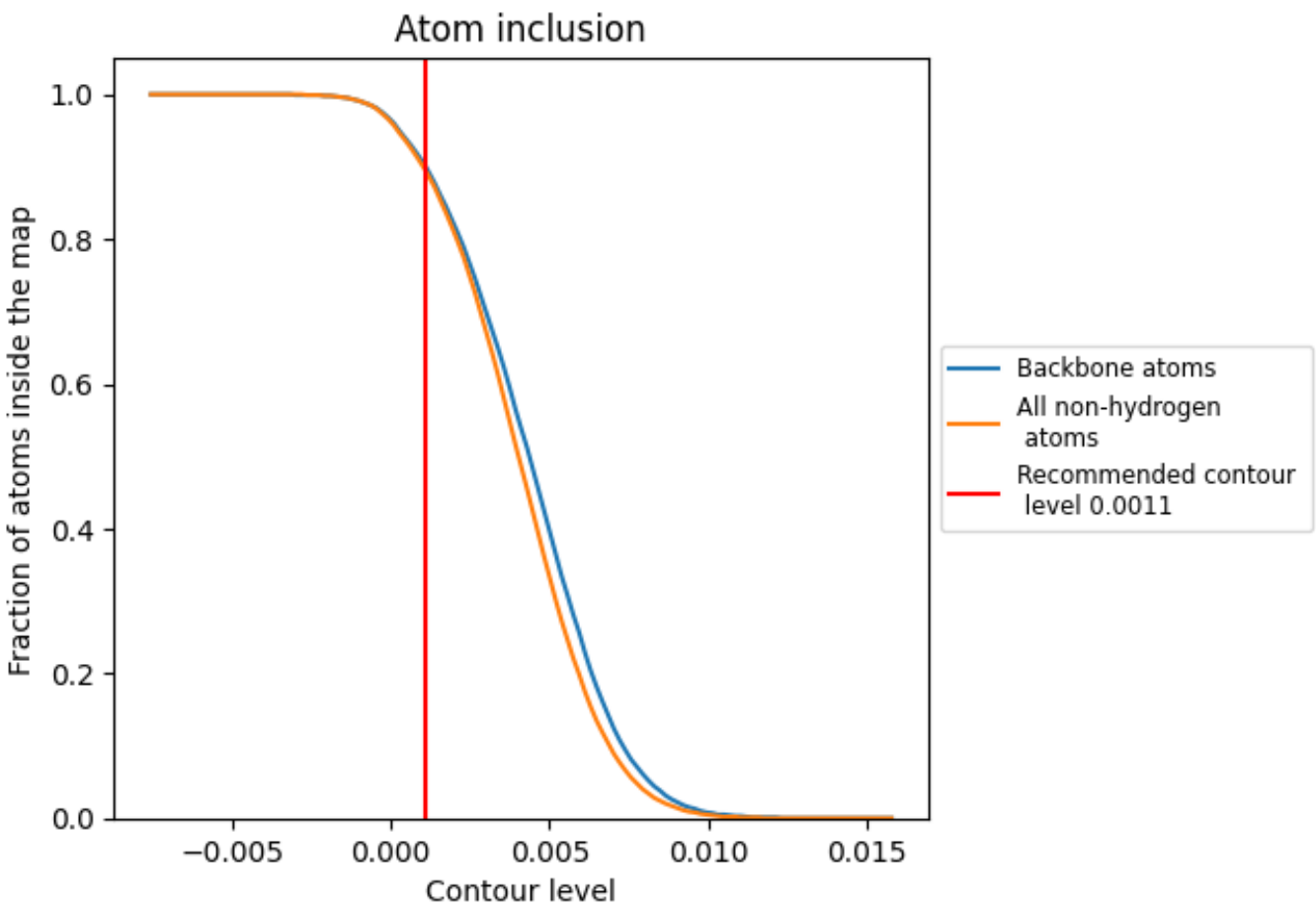
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0011).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.1930
A	0.6820	0.1120
B	0.8900	0.1410
C	0.7960	0.0930
D	0.5480	0.1270
E	0.7370	0.1230
G	0.7940	0.1430
I	0.8070	0.1120
J	0.8090	0.1170
M	0.8690	0.1760
R	0.7950	0.1430
S	0.7140	0.1470
T	0.9760	0.2490
U	0.9740	0.2450
V	0.9790	0.2280
W	0.9900	0.2500
X	0.9750	0.2290
Y	0.9680	0.2330
Z	0.8800	0.2110