



Full wwPDB EM Validation Report ⓘ

Sep 3, 2026 – 01:27 PM EDT

PDB ID : 36BL / pdb_000036bl
EMDB ID : EMD-77358
Title : yeast 26S proteasome base assembly intermediate, base-Rpn14-Hsm3-Nas6(2)
with Rpt4-EQ
Authors : Hsieh, H.H.; Martin, A.
Deposited on : 2026-05-28
Resolution : 3.91 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
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

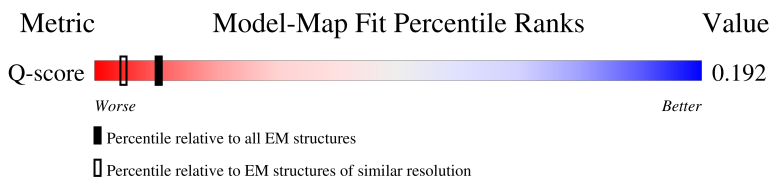
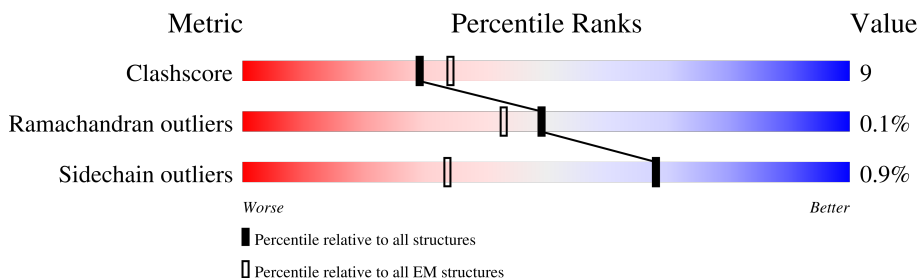
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 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.



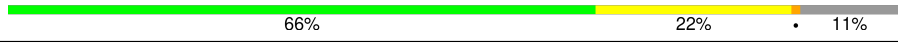
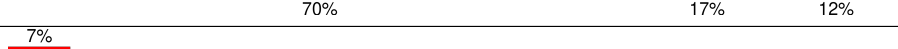
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7920 (3.41 - 4.41)

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 $\leq 5\%$. 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	467	8% 65% 16% 19%
2	B	437	69% 19% 12%
3	C	993	65% 20% 15%
4	D	480	20% 83% 14% .

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Mol	Chain	Length	Quality of chain
5	I	405	
6	J	428	
7	K	437	
8	L	156	
9	M	417	
10	N	228	
11	P	434	
12	Z	945	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 41522 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 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			2962	1860	529	557	16		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	384	Total	C	N	O	S	0	0
			3011	1894	507	593	17		

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	847	Total	C	N	O	S	0	0
			6573	4172	1076	1296	29		

- Molecule 4 is a protein called DNA mismatch repair protein HSM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	466	Total	C	N	O	S	0	0
			3804	2450	608	732	14		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	381	Total	C	N	O	S	0	0
			2994	1882	536	559	17		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	379	Total	C	N	O	S	0	0
			2989	1878	525	575	11		

- Molecule 7 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	383	Total	C	N	O	S	0	0
			3037	1914	542	569	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	282	GLN	GLU	engineered mutation	UNP P53549

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	131	Total	C	N	O	S	0	0
			1061	681	173	201	6		

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	417	Total	C	N	O	S	0	0
			3267	2049	557	650	11		

- Molecule 10 is a protein called Probable 26S proteasome regulatory subunit p28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	228	Total	C	N	O	S	0	0
			1808	1159	307	335	7		

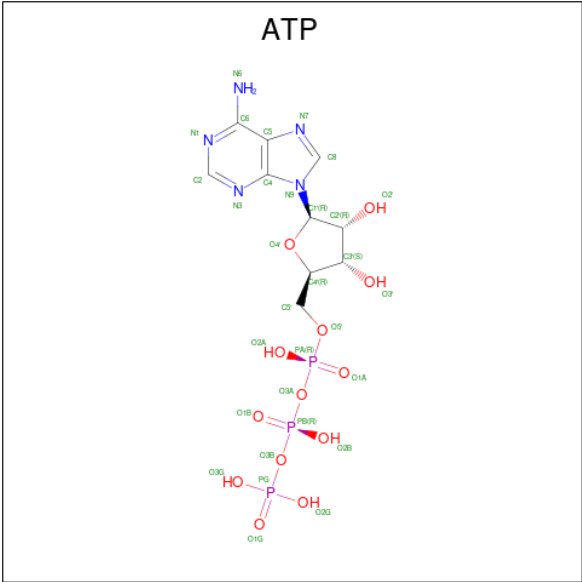
- Molecule 11 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	390	Total	C	N	O	S	0	0
			3054	1911	535	596	12		

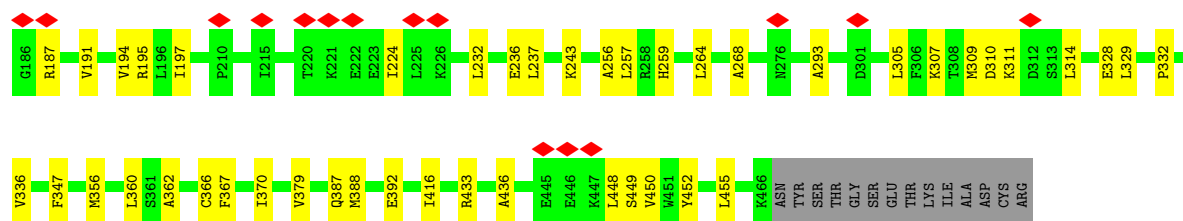
- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	880	Total	C	N	O	S	0	0
			6776	4305	1140	1303	28		

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

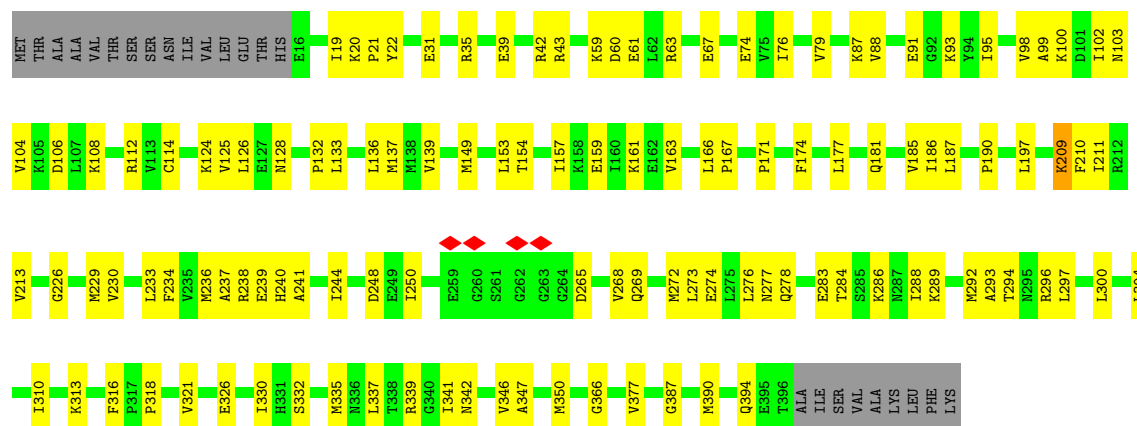


Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	P	1	Total	C	N	O	P	0
			31	10	5	13	3	



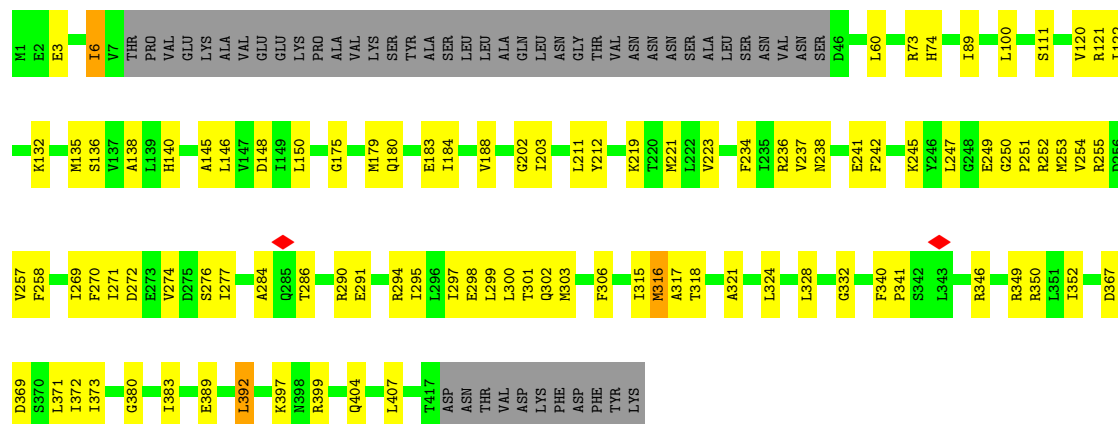
• Molecule 5: 26S proteasome regulatory subunit 8 homolog

Chain I: 65% 29% 6%



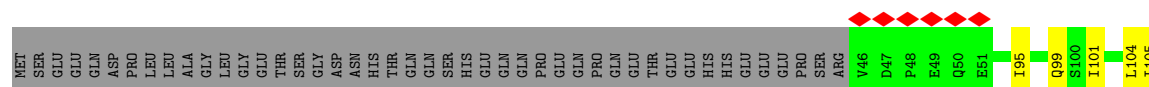
• Molecule 6: 26S proteasome regulatory subunit 6B homolog

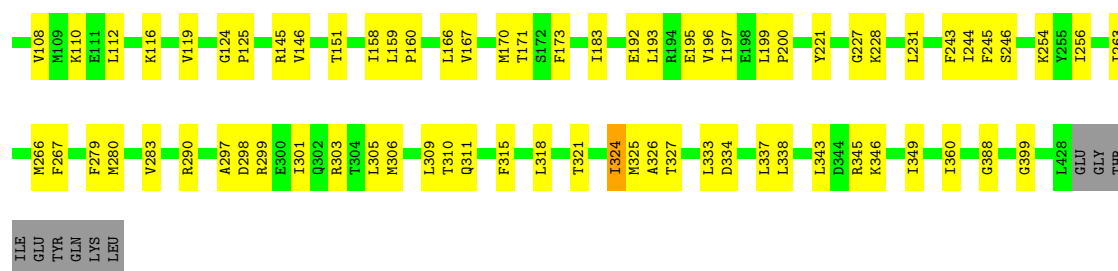
Chain J: 66% 22% 11%



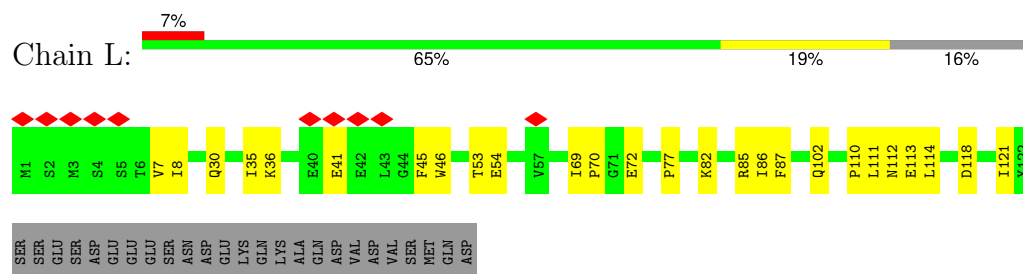
• Molecule 7: 26S proteasome subunit RPT4

Chain K: 70% 17% 12%

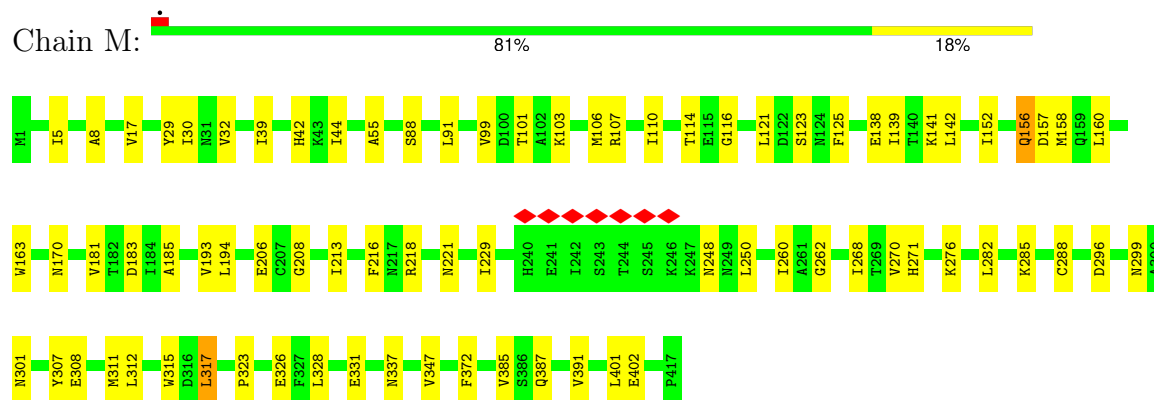




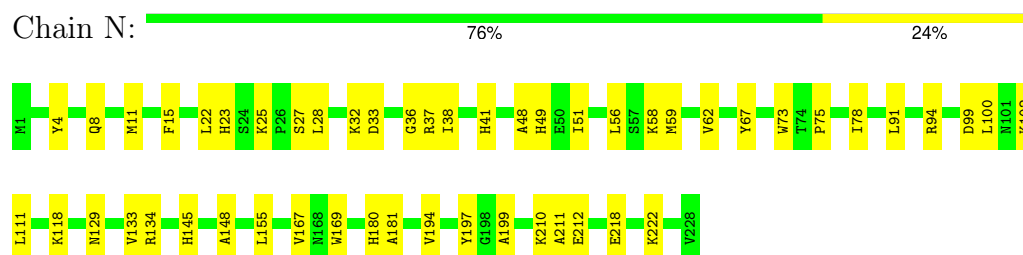
- Molecule 8: 26S proteasome regulatory subunit RPN13



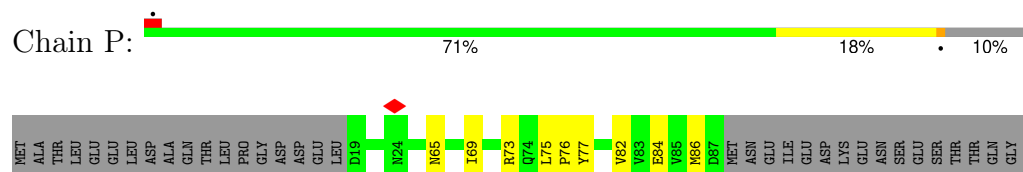
- Molecule 9: 26S proteasome regulatory subunit RPN14



- Molecule 10: Probable 26S proteasome regulatory subunit p28



- Molecule 11: 26S proteasome regulatory subunit 6A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208110	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.372	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	536.576, 536.576, 536.576	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.12	0/3008	0.37	0/4051
2	B	0.13	0/3052	0.39	0/4113
3	C	0.14	0/6690	0.36	0/9074
4	D	0.09	0/3871	0.28	1/5241 (0.0%)
5	I	0.15	0/3033	0.42	0/4074
6	J	0.13	0/3028	0.37	0/4086
7	K	0.12	0/3083	0.34	0/4146
8	L	0.15	0/1087	0.39	0/1470
9	M	0.11	0/3328	0.34	0/4505
10	N	0.13	0/1851	0.35	0/2506
11	P	0.12	0/3091	0.34	0/4162
12	Z	0.14	0/6884	0.38	0/9313
All	All	0.13	0/42006	0.36	1/56741 (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
2	B	0	1
4	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	449	SER	CB-CA-C	-5.01	110.42	117.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	292	TYR	Peptide
4	D	7	ASN	Peptide

5.2 Too-close contacts

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	2962	0	3029	65	0
2	B	3011	0	3085	62	0
3	C	6573	0	6526	133	0
4	D	3804	0	3840	43	0
5	I	2994	0	3120	92	0
6	J	2989	0	3069	81	0
7	K	3037	0	3116	58	0
8	L	1061	0	1050	19	0
9	M	3267	0	3175	48	0
10	N	1808	0	1792	40	0
11	P	3054	0	3120	58	0
12	Z	6776	0	6872	136	0
13	A	31	0	12	0	0
13	B	31	0	12	1	0
13	I	31	0	12	1	0
13	J	31	0	12	5	0
13	K	31	0	12	2	0
13	P	31	0	12	5	0
All	All	41522	0	41866	778	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 9.

All (778) 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)
4:D:388:MET:HE2	4:D:433:ARG:HA	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:76:PRO:HG2	11:P:150:LYS:HE2	1.61	0.82
12:Z:521:LEU:HA	12:Z:524:ILE:HD12	1.62	0.82
1:A:169:GLU:H	1:A:172:MET:HE1	1.41	0.80
1:A:278:GLU:HG2	1:A:282:LYS:HD3	1.61	0.80
6:J:397:LYS:HD2	6:J:399:ARG:HH21	1.44	0.80
3:C:253:VAL:HG11	3:C:265:LEU:HD21	1.64	0.79
6:J:271:ILE:HB	6:J:316:MET:HE1	1.64	0.78
7:K:101:ILE:HG13	11:P:152:SER:HA	1.66	0.78
7:K:195:GLU:HA	7:K:199:LEU:HD23	1.66	0.76
11:P:133:GLY:HA3	11:P:155:ILE:HG22	1.68	0.76
10:N:48:ALA:HB1	10:N:51:ILE:HD13	1.69	0.75
5:I:136:LEU:HD21	6:J:300:LEU:HD12	1.69	0.74
9:M:8:ALA:HB1	9:M:30:ILE:HD11	1.67	0.74
6:J:179:MET:HE3	6:J:179:MET:H	1.53	0.74
6:J:138:ALA:HB3	6:J:148:ASP:HB2	1.69	0.74
3:C:427:GLN:HE22	3:C:905:ASN:HB3	1.53	0.73
4:D:9:VAL:HG22	4:D:39:ASN:HB3	1.69	0.73
12:Z:520:GLY:HA2	12:Z:523:LEU:HD13	1.71	0.72
1:A:144:LYS:HG3	11:P:75:LEU:HD21	1.71	0.72
2:B:265:ARG:HA	2:B:312:GLN:HE21	1.54	0.72
12:Z:217:MET:HE3	12:Z:220:CYS:HA	1.69	0.72
2:B:65:ILE:HA	3:C:756:MET:HE1	1.72	0.71
2:B:160:LEU:HD22	5:I:95:ILE:HD11	1.72	0.71
3:C:827:LEU:HD23	3:C:855:LEU:HD11	1.71	0.71
5:I:99:ALA:HB3	5:I:102:ILE:HG12	1.72	0.71
3:C:278:LEU:HD22	3:C:297:VAL:HG13	1.71	0.71
7:K:283:VAL:HG22	7:K:327:THR:HB	1.72	0.71
2:B:106:ILE:HD11	5:I:95:ILE:HG13	1.73	0.70
5:I:181:GLN:HB2	5:I:284:THR:HB	1.74	0.70
5:I:347:ALA:HA	5:I:350:MET:HE3	1.72	0.70
1:A:306:ILE:HD12	1:A:351:VAL:HG22	1.74	0.70
7:K:280:MET:HG2	7:K:283:VAL:HG12	1.73	0.70
7:K:112:LEU:HB2	7:K:116:LYS:HG3	1.73	0.69
3:C:53:VAL:HG12	3:C:57:LYS:HZ2	1.58	0.69
9:M:288:CYS:HB2	9:M:308:GLU:HB3	1.73	0.69
12:Z:163:LEU:HD22	12:Z:205:SER:HB3	1.74	0.69
12:Z:657:MET:HB2	12:Z:682:PHE:HE1	1.58	0.69
10:N:59:MET:HE3	10:N:94:ARG:HH12	1.58	0.68
7:K:167:VAL:HA	7:K:170:MET:HE3	1.75	0.68
8:L:30:GLN:HA	8:L:102:GLN:HE22	1.58	0.67
1:A:102:CYS:HA	1:A:147:ILE:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:337:ASN:HD22	9:M:387:GLN:HA	1.60	0.67
5:I:226:GLY:HA2	5:I:229:MET:HE3	1.77	0.67
11:P:327:THR:HG21	11:P:333:LEU:HD11	1.77	0.67
5:I:76:ILE:HD11	5:I:87:LYS:HB2	1.76	0.66
12:Z:872:THR:HG22	12:Z:873:ARG:H	1.59	0.66
5:I:332:SER:HB2	5:I:337:LEU:HD11	1.78	0.66
3:C:460:SER:HA	3:C:496:ALA:HA	1.78	0.66
11:P:139:LYS:HD2	11:P:139:LYS:O	1.95	0.66
12:Z:339:MET:HG3	12:Z:707:ASN:HB2	1.77	0.66
2:B:284:ILE:HG21	2:B:326:MET:SD	2.36	0.66
3:C:291:GLU:HA	3:C:294:ILE:HD12	1.78	0.66
12:Z:236:GLY:HA2	12:Z:239:LEU:HD12	1.77	0.66
5:I:197:LEU:HD22	13:I:501:ATP:H2'	1.76	0.65
7:K:334:ASP:HB3	7:K:337:LEU:HD23	1.78	0.65
1:A:72:SER:HB3	5:I:79:VAL:HG13	1.78	0.65
7:K:171:THR:HG22	7:K:244:ILE:HG12	1.79	0.65
5:I:19:ILE:HD12	12:Z:144:CYS:HB2	1.78	0.65
11:P:220:MET:HE1	11:P:228:LYS:HD2	1.78	0.64
4:D:310:ASP:HA	4:D:314:LEU:HB2	1.77	0.64
8:L:8:ILE:HD12	8:L:35:ILE:HB	1.78	0.64
3:C:303:ASP:HB3	3:C:306:MET:HB2	1.79	0.64
4:D:293:ALA:HB2	4:D:329:LEU:HB3	1.80	0.64
6:J:255:ARG:HA	6:J:302:GLN:NE2	2.13	0.64
3:C:265:LEU:HB3	3:C:284:LEU:HD21	1.80	0.64
3:C:522:THR:HA	3:C:525:MET:HE1	1.79	0.64
5:I:19:ILE:HG12	12:Z:140:MET:HG2	1.79	0.64
12:Z:233:ASN:HA	12:Z:269:LEU:HD12	1.80	0.63
3:C:282:ILE:HB	3:C:297:VAL:HG11	1.80	0.63
11:P:146:VAL:HG12	11:P:158:THR:HG22	1.78	0.63
5:I:136:LEU:HD13	6:J:297:ILE:HG23	1.78	0.63
8:L:8:ILE:HG12	8:L:124:LYS:HD3	1.79	0.63
9:M:141:LYS:HG3	9:M:183:ASP:HA	1.79	0.63
9:M:160:LEU:HD11	9:M:181:VAL:HG11	1.80	0.63
12:Z:732:GLY:HA2	12:Z:748:PHE:HB3	1.80	0.63
7:K:228:LYS:HG2	7:K:349:ILE:HG21	1.80	0.63
10:N:38:ILE:HD13	10:N:67:TYR:HD1	1.63	0.63
12:Z:150:LEU:HD22	12:Z:173:LYS:HE2	1.81	0.63
2:B:75:PHE:HB2	3:C:621:LEU:HD12	1.81	0.62
5:I:273:LEU:HD23	5:I:276:LEU:HD12	1.80	0.62
12:Z:703:GLN:HA	12:Z:706:MET:HG2	1.82	0.62
3:C:826:ARG:HH21	3:C:830:LEU:HD11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:ARG:HD2	2:B:343:ARG:HH21	1.63	0.62
12:Z:215:MET:HE1	12:Z:241:LEU:HD13	1.81	0.62
10:N:25:LYS:HG3	10:N:28:LEU:HG	1.82	0.61
2:B:175:LYS:HA	2:B:243:THR:HG23	1.81	0.61
5:I:335:MET:HA	6:J:202:GLY:HA3	1.83	0.61
11:P:132:VAL:HG11	11:P:137:PRO:HB3	1.83	0.61
3:C:568:LEU:HD13	3:C:886:VAL:HG21	1.82	0.61
4:D:328:GLU:HG3	4:D:356:MET:HG2	1.82	0.61
3:C:575:MET:HB3	3:C:606:CYS:HB3	1.83	0.61
1:A:50:LYS:HD3	1:A:50:LYS:N	2.16	0.60
1:A:173:ARG:HB2	1:A:187:LEU:HB2	1.83	0.60
5:I:19:ILE:HA	5:I:22:TYR:HB3	1.82	0.60
3:C:934:GLU:HG2	3:C:936:VAL:HG22	1.82	0.60
5:I:366:GLY:HA3	6:J:203:ILE:HG21	1.83	0.60
3:C:776:VAL:HG23	3:C:777:PRO:HD3	1.83	0.60
10:N:51:ILE:HD12	10:N:51:ILE:H	1.66	0.60
3:C:207:ILE:HG22	3:C:211:PHE:HE2	1.66	0.60
3:C:613:ASP:HB3	3:C:616:LEU:HD13	1.84	0.60
1:A:222:ARG:HB2	4:D:38:LEU:HD21	1.84	0.60
3:C:827:LEU:HD12	3:C:830:LEU:HD12	1.84	0.59
5:I:61:GLU:HG3	6:J:121:ARG:HE	1.67	0.59
7:K:338:LEU:HD22	7:K:346:LYS:HE2	1.84	0.59
3:C:353:VAL:HG22	3:C:355:GLU:H	1.67	0.59
9:M:328:LEU:HD21	9:M:331:GLU:HB2	1.83	0.59
1:A:104:LYS:HE2	11:P:159:LEU:HD21	1.84	0.59
7:K:327:THR:HG21	7:K:333:LEU:HD11	1.84	0.59
10:N:32:LYS:HB3	10:N:36:GLY:HA2	1.84	0.59
5:I:167:PRO:HB2	5:I:289:LYS:HE3	1.84	0.59
6:J:350:ARG:HG2	6:J:372:ILE:HG21	1.84	0.59
1:A:444:LEU:HD21	4:D:232:LEU:HD12	1.85	0.59
2:B:148:LEU:HD21	2:B:160:LEU:HB2	1.85	0.59
3:C:224:LEU:HD23	3:C:227:ILE:HD11	1.85	0.58
3:C:495:ILE:HD11	3:C:903:MET:HA	1.86	0.58
1:A:75:GLY:HA2	2:B:140:LEU:HD13	1.85	0.58
12:Z:498:ILE:HG23	12:Z:521:LEU:HD11	1.86	0.58
10:N:73:TRP:CE3	10:N:104:THR:HG21	2.39	0.58
3:C:160:GLU:O	3:C:164:VAL:HG12	2.04	0.58
9:M:311:MET:HE1	9:M:326:GLU:HB3	1.85	0.58
11:P:69:ILE:HG22	11:P:73:ARG:HE	1.69	0.58
1:A:280:VAL:HG12	1:A:329:VAL:HG22	1.86	0.57
3:C:863:THR:HB	3:C:911:LYS:HD3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:N	1:A:172:MET:HE1	2.17	0.57
5:I:161:LYS:HB3	9:M:156:GLN:HE22	1.69	0.57
9:M:106:MET:HE1	9:M:123:SER:H	1.69	0.57
12:Z:809:ARG:NH2	12:Z:812:ALA:HB3	2.19	0.57
2:B:220:ILE:HG23	2:B:326:MET:HG3	1.86	0.57
3:C:615:LEU:HD11	12:Z:807:THR:HA	1.86	0.57
7:K:318:LEU:H	7:K:318:LEU:HD23	1.70	0.57
11:P:135:VAL:HB	11:P:140:LEU:HD21	1.86	0.57
12:Z:596:LEU:HD11	12:Z:717:LEU:HG	1.86	0.57
1:A:280:VAL:HG13	1:A:314:VAL:HG22	1.87	0.57
3:C:453:LEU:HB2	3:C:488:ALA:HB1	1.85	0.57
12:Z:606:VAL:HA	12:Z:609:LEU:HD12	1.87	0.57
3:C:279:THR:HG21	3:C:974:THR:HA	1.86	0.56
12:Z:104:LYS:O	12:Z:108:MET:HE2	2.04	0.56
6:J:100:LEU:HD11	6:J:111:SER:HB3	1.86	0.56
3:C:509:LEU:HB2	3:C:530:LEU:HD21	1.86	0.56
6:J:175:GLY:N	13:J:501:ATP:HN62	2.03	0.56
9:M:157:ASP:C	9:M:158:MET:HE2	2.31	0.56
10:N:100:LEU:HD11	10:N:129:ASN:HB2	1.88	0.56
12:Z:663:ILE:HG22	12:Z:664:LEU:HD23	1.86	0.56
12:Z:60:MET:HA	12:Z:60:MET:HE2	1.88	0.56
12:Z:533:ASP:HA	12:Z:536:ILE:HD12	1.87	0.56
3:C:568:LEU:HD11	3:C:882:LEU:HB3	1.87	0.56
9:M:183:ASP:HB3	9:M:229:ILE:HG12	1.88	0.56
3:C:905:ASN:HA	3:C:908:ILE:HD12	1.88	0.56
6:J:316:MET:HE3	6:J:316:MET:HA	1.87	0.56
5:I:241:ALA:HB2	5:I:288:ILE:HD11	1.88	0.55
9:M:114:THR:HA	9:M:138:GLU:HG3	1.88	0.55
5:I:100:LYS:HD3	5:I:100:LYS:N	2.21	0.55
4:D:336:VAL:HG11	4:D:366:CYS:HA	1.88	0.55
5:I:132:PRO:HG2	6:J:290:ARG:HH22	1.72	0.55
2:B:154:MET:N	2:B:154:MET:HE2	2.22	0.55
3:C:793:PHE:HA	3:C:796:LEU:HB2	1.89	0.55
3:C:928:ARG:HD2	3:C:948:TRP:CD1	2.42	0.55
8:L:118:ASP:HA	8:L:121:ILE:HD12	1.88	0.55
9:M:185:ALA:HB3	9:M:194:LEU:HB2	1.89	0.55
2:B:161:GLN:HG2	2:B:269:LYS:HZ1	1.72	0.55
5:I:283:GLU:HG2	5:I:286:LYS:HD2	1.88	0.55
7:K:145:ARG:HB2	7:K:159:LEU:HB2	1.89	0.55
3:C:71:LEU:O	3:C:75:ILE:HG13	2.05	0.55
9:M:44:ILE:HG23	9:M:55:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:56:LEU:HD11	10:N:91:LEU:HD23	1.88	0.55
12:Z:168:SER:HA	12:Z:171:LYS:HE3	1.87	0.55
1:A:200:VAL:HG13	1:A:272:ILE:HG12	1.88	0.54
6:J:175:GLY:H	13:J:501:ATP:HN62	1.55	0.54
12:Z:144:CYS:SG	12:Z:149:GLU:HB2	2.47	0.54
4:D:84:VAL:HG13	4:D:92:VAL:HG11	1.89	0.54
5:I:167:PRO:HG3	5:I:174:PHE:HE2	1.72	0.54
7:K:399:GLY:HA3	11:P:212:ILE:HD13	1.89	0.54
10:N:8:GLN:HA	10:N:11:MET:HE1	1.87	0.54
3:C:547:MET:HE1	3:C:591:ILE:HD11	1.90	0.54
9:M:103:LYS:HA	9:M:107:ARG:HA	1.89	0.54
11:P:159:LEU:HB3	11:P:160:PRO:HD3	1.90	0.54
4:D:34:ARG:HD3	4:D:75:TYR:CZ	2.42	0.54
11:P:130:PRO:HG2	11:P:131:MET:HE1	1.88	0.54
2:B:171:MET:HE3	2:B:267:ILE:HD12	1.88	0.54
6:J:188:VAL:HG21	6:J:315:ILE:HD11	1.90	0.54
7:K:283:VAL:HG11	7:K:325:MET:HB3	1.90	0.54
12:Z:211:PHE:HB2	12:Z:228:VAL:HG11	1.90	0.54
2:B:154:MET:HE2	2:B:154:MET:H	1.73	0.54
1:A:46:ALA:HA	1:A:50:LYS:NZ	2.23	0.53
3:C:427:GLN:HG2	3:C:428:TRP:CE3	2.43	0.53
6:J:179:MET:H	6:J:179:MET:CE	2.20	0.53
7:K:183:ILE:HD13	7:K:231:LEU:HD13	1.89	0.53
3:C:844:ALA:O	3:C:848:THR:HG23	2.08	0.53
5:I:346:VAL:HG12	5:I:350:MET:HE2	1.88	0.53
6:J:249:GLU:HA	6:J:252:ARG:HB3	1.90	0.53
10:N:59:MET:SD	10:N:62:VAL:HB	2.47	0.53
12:Z:270:LEU:O	12:Z:274:VAL:HG12	2.07	0.53
6:J:404:GLN:HG2	10:N:73:TRP:HE1	1.73	0.53
7:K:305:LEU:HD11	7:K:337:LEU:HD21	1.90	0.53
6:J:132:LYS:HB2	6:J:135:MET:HE3	1.91	0.53
6:J:295:ILE:O	6:J:299:LEU:HD13	2.09	0.53
10:N:22:LEU:HD22	10:N:58:LYS:NZ	2.24	0.53
12:Z:230:VAL:HG12	12:Z:724:THR:HG21	1.91	0.53
12:Z:518:ALA:HB1	12:Z:550:GLY:HA3	1.90	0.53
6:J:252:ARG:O	6:J:255:ARG:HG2	2.09	0.53
12:Z:436:ASP:HB3	12:Z:439:VAL:HB	1.91	0.53
3:C:92:LEU:HG	3:C:122:LEU:HD13	1.91	0.52
5:I:42:ARG:HA	5:I:42:ARG:CZ	2.38	0.52
12:Z:412:TYR:HB3	12:Z:416:GLY:HA3	1.91	0.52
11:P:228:LYS:HB2	13:P:501:ATP:O1B	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:209:LYS:NZ	5:I:210:PHE:H	2.07	0.52
7:K:166:LEU:HG	7:K:170:MET:HE2	1.92	0.52
9:M:110:ILE:HD12	9:M:142:LEU:HD22	1.91	0.52
12:Z:220:CYS:HB2	12:Z:222:TYR:CE1	2.45	0.52
12:Z:680:LYS:HA	12:Z:683:LEU:HD12	1.91	0.52
5:I:22:TYR:HD1	12:Z:103:SER:HB3	1.75	0.52
5:I:112:ARG:HB3	5:I:126:LEU:HB2	1.91	0.52
6:J:221:MET:SD	13:J:501:ATP:H2'	2.50	0.52
6:J:392:LEU:HD11	7:K:345:ARG:HE	1.75	0.52
7:K:388:GLY:HA3	13:K:501:ATP:C8	2.44	0.52
2:B:382:THR:HG23	2:B:384:LYS:H	1.75	0.52
3:C:748:LEU:HD21	3:C:866:VAL:HG11	1.89	0.52
6:J:272:ASP:HA	6:J:317:ALA:HB3	1.92	0.52
9:M:301:ASN:HA	9:M:317:LEU:HD21	1.91	0.52
12:Z:136:ILE:HG23	12:Z:139:ARG:HH21	1.73	0.52
6:J:238:ASN:HB3	6:J:241:GLU:HG3	1.92	0.52
6:J:291:GLU:O	6:J:295:ILE:HG13	2.10	0.52
7:K:279:PHE:HA	7:K:324:ILE:HG23	1.92	0.52
10:N:103:ILE:HD12	10:N:107:GLY:HA2	1.91	0.52
8:L:82:LYS:HA	8:L:112:ASN:HB3	1.90	0.52
9:M:88:SER:HA	9:M:91:LEU:HB2	1.91	0.52
3:C:244:ARG:NH1	3:C:939:ALA:HA	2.26	0.51
3:C:260:GLU:O	3:C:264:PHE:HB2	2.09	0.51
12:Z:303:LEU:HB3	12:Z:343:THR:HG22	1.91	0.51
3:C:862:MET:HE2	3:C:862:MET:HA	1.92	0.51
4:D:392:GLU:HA	4:D:436:ALA:HB2	1.91	0.51
5:I:88:VAL:HG13	5:I:91:GLU:OE2	2.10	0.51
7:K:306:MET:O	7:K:310:THR:HG23	2.10	0.51
11:P:84:GLU:HG3	11:P:254:MET:HE3	1.92	0.51
11:P:224:PRO:HA	11:P:228:LYS:NZ	2.26	0.51
12:Z:521:LEU:HD21	12:Z:535:LEU:HD21	1.92	0.51
2:B:257:LEU:HD11	2:B:302:ILE:HG13	1.91	0.51
3:C:581:VAL:HB	3:C:585:LEU:HD23	1.92	0.51
11:P:69:ILE:HG23	11:P:134:LEU:HD13	1.92	0.51
12:Z:329:HIS:CE1	12:Z:359:ALA:HB2	2.46	0.51
12:Z:627:ILE:HG23	12:Z:733:LEU:HD13	1.92	0.51
1:A:299:ARG:HA	1:A:349:ILE:HD11	1.92	0.51
11:P:230:LEU:HD22	13:P:501:ATP:H2'	1.93	0.51
1:A:245:GLY:HA2	1:A:351:VAL:O	2.11	0.51
4:D:256:ALA:HA	4:D:259:HIS:CE1	2.45	0.51
6:J:349:ARG:HG2	6:J:383:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:717:LEU:HD13	12:Z:729:SER:HB3	1.93	0.51
1:A:287:GLY:HA2	1:A:290:MET:SD	2.51	0.51
1:A:436:LYS:HA	2:B:211:MET:HE1	1.91	0.51
12:Z:448:LEU:O	12:Z:452:LEU:HD12	2.11	0.51
9:M:213:ILE:HG23	9:M:248:ASN:HD22	1.74	0.51
12:Z:202:PHE:CE2	12:Z:206:ILE:HD11	2.46	0.51
3:C:108:ASP:HB3	3:C:111:LEU:HB2	1.93	0.51
12:Z:406:TYR:OH	12:Z:747:HIS:HB2	2.09	0.51
3:C:165:TYR:CD2	3:C:227:ILE:HA	2.46	0.50
11:P:357:ARG:HG2	11:P:391:LEU:HD11	1.93	0.50
12:Z:606:VAL:HB	12:Z:621:THR:HG23	1.94	0.50
1:A:84:ILE:HG13	2:B:99:ILE:HG13	1.93	0.50
8:L:110:PRO:HG2	8:L:113:GLU:HB2	1.94	0.50
11:P:186:LEU:HD13	11:P:349:PHE:CE2	2.47	0.50
12:Z:313:LEU:HD11	12:Z:683:LEU:HD21	1.93	0.50
2:B:263:LEU:O	2:B:267:ILE:HG12	2.11	0.50
2:B:326:MET:HE1	2:B:338:LEU:HD13	1.92	0.50
3:C:779:ALA:HA	3:C:782:ILE:HD12	1.93	0.50
5:I:74:GLU:HB2	5:I:87:LYS:HB3	1.93	0.50
5:I:337:LEU:HB3	5:I:341:ILE:HD12	1.93	0.50
6:J:253:MET:O	6:J:257:VAL:HG23	2.12	0.50
9:M:99:VAL:HG21	9:M:401:LEU:HD23	1.93	0.50
12:Z:207:LEU:HD13	12:Z:231:ASN:HB3	1.92	0.50
3:C:208:VAL:HG13	3:C:209:PRO:HD3	1.93	0.50
3:C:261:ASP:O	3:C:265:LEU:HG	2.11	0.50
3:C:427:GLN:HA	3:C:458:SER:HA	1.92	0.50
3:C:812:ILE:HG21	3:C:848:THR:HG22	1.93	0.50
8:L:123:ASN:HA	8:L:126:ILE:HD12	1.94	0.50
9:M:30:ILE:HG23	9:M:42:HIS:HB2	1.93	0.50
12:Z:179:THR:HG23	12:Z:217:MET:SD	2.51	0.50
6:J:252:ARG:HA	6:J:255:ARG:HE	1.76	0.50
1:A:224:VAL:HG21	1:A:246:ILE:HB	1.92	0.50
2:B:142:GLU:HB3	2:B:145:CYS:HB3	1.92	0.50
3:C:105:LYS:HG3	9:M:285:LYS:HA	1.94	0.50
6:J:120:VAL:HB	6:J:145:ALA:HA	1.93	0.50
8:L:45:PHE:C	8:L:46:TRP:HD1	2.19	0.50
12:Z:889:ARG:HH22	12:Z:912:GLU:HB2	1.77	0.50
1:A:291:VAL:HG12	1:A:339:GLN:HG3	1.93	0.50
2:B:214:LYS:HD3	2:B:215:PRO:HD2	1.94	0.50
8:L:70:PRO:HA	8:L:129:LEU:HA	1.94	0.50
9:M:116:GLY:HA2	9:M:139:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:331:ALA:HB2	12:Z:697:PHE:CD2	2.47	0.50
1:A:197:MET:HE1	1:A:290:MET:HE2	1.94	0.50
1:A:275:ILE:HG13	1:A:278:GLU:HB2	1.93	0.50
6:J:297:ILE:O	6:J:301:THR:HG23	2.12	0.50
1:A:57:LYS:HE2	1:A:57:LYS:HA	1.94	0.49
1:A:200:VAL:HG22	1:A:272:ILE:HG23	1.94	0.49
2:B:142:GLU:CD	2:B:144:GLY:H	2.20	0.49
5:I:59:LYS:O	5:I:63:ARG:HG3	2.12	0.49
11:P:248:ALA:HB1	11:P:286:ILE:HG12	1.94	0.49
12:Z:360:GLN:H	12:Z:363:ALA:HB3	1.77	0.49
3:C:970:TYR:HB3	3:C:983:LEU:HB3	1.94	0.49
6:J:245:LYS:HD2	7:K:299:ARG:HB3	1.93	0.49
7:K:173:PHE:CE1	7:K:243:PHE:HB3	2.46	0.49
10:N:134:ARG:HD2	10:N:169:TRP:HZ3	1.77	0.49
12:Z:389:TYR:HA	12:Z:395:ALA:HB2	1.95	0.49
3:C:249:MET:HA	3:C:264:PHE:HE2	1.77	0.49
3:C:249:MET:O	3:C:253:VAL:HG23	2.12	0.49
5:I:42:ARG:HA	5:I:42:ARG:NH1	2.27	0.49
10:N:15:PHE:HD1	10:N:51:ILE:HG13	1.77	0.49
11:P:365:SER:HB3	11:P:370:THR:HG21	1.95	0.49
2:B:306:MET:HE3	2:B:306:MET:HA	1.93	0.49
7:K:110:LYS:HZ3	7:K:112:LEU:HA	1.78	0.49
2:B:375:VAL:HA	2:B:413:ALA:HB2	1.94	0.49
6:J:294:ARG:HA	6:J:297:ILE:HD12	1.95	0.49
3:C:765:MET:HE3	3:C:799:PHE:CD1	2.48	0.49
10:N:4:TYR:CZ	10:N:33:ASP:HA	2.47	0.49
12:Z:809:ARG:NH2	12:Z:813:ARG:HD2	2.28	0.49
5:I:190:PRO:HG3	5:I:318:PRO:HG3	1.95	0.49
6:J:242:PHE:CE2	6:J:254:VAL:HG22	2.47	0.49
3:C:935:THR:HB	3:C:942:PRO:HG2	1.95	0.49
9:M:260:ILE:HG22	9:M:270:VAL:HG22	1.94	0.49
10:N:38:ILE:HG12	10:N:41:HIS:ND1	2.27	0.49
3:C:472:LEU:HA	3:C:475:GLN:NE2	2.27	0.48
6:J:237:VAL:O	6:J:271:ILE:HA	2.13	0.48
1:A:75:GLY:HA3	2:B:159:VAL:HG23	1.95	0.48
1:A:227:LEU:HD13	4:D:38:LEU:HB3	1.95	0.48
3:C:324:GLU:CD	3:C:324:GLU:H	2.21	0.48
12:Z:378:ASN:HD21	12:Z:381:GLU:HB2	1.78	0.48
12:Z:872:THR:HG22	12:Z:873:ARG:N	2.28	0.48
1:A:406:LEU:HD21	4:D:191:VAL:HA	1.95	0.48
3:C:427:GLN:HG3	3:C:457:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:558:LEU:HA	3:C:563:VAL:HG21	1.95	0.48
1:A:406:LEU:HB3	4:D:232:LEU:HD21	1.96	0.48
4:D:367:PHE:HA	4:D:370:ILE:HG12	1.95	0.48
8:L:85:ARG:HD3	8:L:114:LEU:HA	1.96	0.48
1:A:257:THR:HG21	1:A:273:ARG:HH21	1.78	0.48
1:A:274:VAL:HG21	1:A:294:LEU:HD22	1.96	0.48
3:C:400:ILE:HG12	3:C:406:TRP:CD1	2.49	0.48
4:D:268:ALA:HB2	4:D:309:MET:HE3	1.96	0.48
5:I:149:MET:SD	5:I:197:LEU:HD11	2.53	0.48
7:K:197:ILE:C	7:K:200:PRO:HD2	2.38	0.48
7:K:227:GLY:O	7:K:231:LEU:HD22	2.14	0.48
12:Z:91:ILE:O	12:Z:102:VAL:HG21	2.13	0.48
2:B:109:LEU:HD23	2:B:143:PRO:HA	1.94	0.48
5:I:296:ARG:HA	5:I:296:ARG:NH1	2.29	0.48
10:N:111:LEU:HD21	10:N:133:VAL:HG12	1.95	0.48
11:P:219:LEU:HB2	11:P:343:LEU:HD13	1.95	0.48
1:A:218:ILE:O	1:A:222:ARG:HG3	2.14	0.48
1:A:149:LEU:HD11	1:A:155:PHE:HB2	1.96	0.48
3:C:241:THR:O	3:C:245:VAL:HG23	2.14	0.48
3:C:259:PRO:HD3	12:Z:813:ARG:HD3	1.96	0.48
5:I:137:MET:HB3	5:I:213:VAL:HG22	1.96	0.48
11:P:220:MET:HE3	11:P:220:MET:C	2.38	0.48
3:C:570:LEU:HD21	3:C:588:ILE:HD11	1.95	0.47
12:Z:270:LEU:HD12	12:Z:271:GLU:N	2.29	0.47
12:Z:532:ALA:O	12:Z:536:ILE:HG13	2.14	0.47
1:A:104:LYS:HB3	1:A:146:VAL:HB	1.96	0.47
3:C:778:LEU:HD23	3:C:810:ASN:HB3	1.95	0.47
5:I:87:LYS:HD3	5:I:93:LYS:HD3	1.97	0.47
11:P:388:GLY:HA3	13:P:501:ATP:C8	2.48	0.47
12:Z:625:LEU:HD23	12:Z:625:LEU:HA	1.72	0.47
1:A:291:VAL:HG11	1:A:336:LEU:HA	1.96	0.47
3:C:775:MET:HE3	3:C:775:MET:HA	1.96	0.47
7:K:306:MET:HA	7:K:309:LEU:HD12	1.96	0.47
8:L:69:ILE:HB	8:L:72:GLU:HB2	1.96	0.47
12:Z:372:GLY:HA2	12:Z:411:ILE:HD11	1.97	0.47
4:D:448:LEU:HD12	4:D:452:TYR:HD1	1.78	0.47
7:K:196:VAL:HG11	7:K:345:ARG:HD2	1.96	0.47
9:M:152:ILE:HD13	9:M:193:VAL:HG11	1.96	0.47
11:P:267:PHE:CD2	11:P:311:GLN:HB3	2.49	0.47
12:Z:112:GLU:HB3	12:Z:129:ILE:HG23	1.96	0.47
12:Z:871:MET:O	12:Z:871:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:HA	1:A:222:ARG:HE	1.79	0.47
2:B:186:GLY:HA3	2:B:357:THR:HG23	1.96	0.47
2:B:284:ILE:HG22	2:B:327:ALA:O	2.14	0.47
3:C:93:ARG:NE	3:C:125:THR:HB	2.29	0.47
1:A:283:TYR:HB3	1:A:290:MET:HE1	1.95	0.47
2:B:219:VAL:O	2:B:326:MET:HB3	2.14	0.47
3:C:883:THR:HB	3:C:903:MET:HG2	1.97	0.47
5:I:98:VAL:HG11	5:I:104:VAL:HG22	1.96	0.47
5:I:112:ARG:NH2	5:I:128:ASN:HA	2.29	0.47
5:I:234:PHE:CD2	5:I:278:GLN:HB3	2.50	0.47
5:I:239:GLU:HG2	5:I:240:HIS:CE1	2.49	0.47
7:K:243:PHE:HE2	7:K:245:PHE:HB2	1.80	0.47
11:P:137:PRO:HA	11:P:140:LEU:HG	1.96	0.47
12:Z:494:LYS:HA	12:Z:494:LYS:HD3	1.65	0.47
7:K:290:ARG:HH22	7:K:305:LEU:HD23	1.80	0.47
9:M:296:ASP:HB3	9:M:299:ASN:O	2.15	0.47
11:P:196:ALA:HB2	11:P:345:ARG:HD2	1.97	0.47
3:C:335:LEU:HD23	3:C:428:TRP:CD1	2.50	0.47
5:I:19:ILE:HD12	12:Z:144:CYS:CB	2.45	0.47
5:I:213:VAL:HG21	5:I:233:LEU:HD22	1.96	0.47
6:J:122:ILE:HG12	6:J:146:LEU:HD23	1.96	0.47
6:J:274:VAL:HB	6:J:316:MET:HE2	1.96	0.47
7:K:193:LEU:O	7:K:197:ILE:HG12	2.14	0.47
12:Z:481:ALA:O	12:Z:485:MET:HG3	2.15	0.47
12:Z:104:LYS:HB3	12:Z:108:MET:HE2	1.97	0.46
12:Z:770:LYS:HE2	12:Z:917:ILE:HD11	1.96	0.46
3:C:92:LEU:HD12	3:C:95:THR:OG1	2.15	0.46
4:D:347:PHE:HD1	4:D:356:MET:HE3	1.80	0.46
7:K:108:VAL:HA	7:K:119:VAL:HG12	1.97	0.46
7:K:170:MET:HG2	7:K:245:PHE:O	2.15	0.46
11:P:133:GLY:HA2	11:P:154:LEU:HD11	1.97	0.46
1:A:293:GLU:O	1:A:297:MET:HG2	2.16	0.46
2:B:380:LEU:HD21	2:B:416:PHE:HD2	1.80	0.46
3:C:351:PRO:HG2	3:C:398:LYS:HE3	1.97	0.46
5:I:186:ILE:HG13	5:I:292:MET:HB3	1.96	0.46
5:I:342:ASN:HB2	9:M:29:TYR:CD2	2.51	0.46
6:J:303:MET:HE2	6:J:332:GLY:O	2.15	0.46
10:N:148:ALA:HB1	10:N:181:ALA:HB2	1.96	0.46
12:Z:141:ILE:HD13	12:Z:165:ILE:HG21	1.97	0.46
1:A:283:TYR:CB	1:A:290:MET:HE1	2.46	0.46
2:B:194:ILE:HD13	2:B:232:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:857:LEU:O	3:C:862:MET:HB2	2.15	0.46
3:C:774:ARG:O	3:C:777:PRO:HD2	2.16	0.46
3:C:964:GLU:HA	3:C:977:ILE:HD12	1.96	0.46
7:K:95:ILE:O	7:K:99:GLN:HG3	2.15	0.46
7:K:315:PHE:CE2	7:K:321:THR:HB	2.50	0.46
9:M:121:LEU:HB3	9:M:125:PHE:HA	1.97	0.46
12:Z:298:TYR:OH	12:Z:766:GLN:HB3	2.15	0.46
12:Z:914:VAL:HB	12:Z:916:LEU:HG	1.98	0.46
2:B:361:ILE:HG12	13:B:501:ATP:N1	2.30	0.46
3:C:203:LEU:O	3:C:207:ILE:HG13	2.16	0.46
3:C:408:TYR:HA	3:C:415:MET:HE1	1.96	0.46
3:C:809:MET:HE1	3:C:844:ALA:N	2.31	0.46
6:J:346:ARG:HG2	6:J:349:ARG:NH2	2.31	0.46
7:K:360:ILE:HG12	13:K:501:ATP:N1	2.30	0.46
10:N:38:ILE:HG21	10:N:67:TYR:CD1	2.51	0.46
12:Z:452:LEU:HD12	12:Z:452:LEU:H	1.80	0.46
3:C:374:LEU:HD23	3:C:842:GLN:HG2	1.96	0.46
7:K:146:VAL:HG12	7:K:158:ILE:HG12	1.97	0.46
10:N:22:LEU:HD22	10:N:58:LYS:HZ2	1.80	0.46
10:N:210:LYS:HE3	10:N:212:GLU:HG2	1.96	0.46
11:P:130:PRO:HG2	11:P:131:MET:CE	2.46	0.46
2:B:362:LEU:HD21	2:B:380:LEU:HD23	1.97	0.46
5:I:60:ASP:HA	5:I:63:ARG:NE	2.31	0.46
5:I:163:VAL:HG11	5:I:185:VAL:HB	1.98	0.46
6:J:380:GLY:HA3	13:J:501:ATP:C8	2.51	0.46
12:Z:227:LYS:HA	12:Z:722:THR:HA	1.98	0.46
12:Z:521:LEU:HD21	12:Z:535:LEU:HD11	1.98	0.46
1:A:90:ARG:HH21	2:B:131:SER:HB2	1.81	0.46
3:C:357:ILE:HD12	3:C:856:HIS:CD2	2.51	0.46
4:D:264:LEU:HD13	4:D:305:LEU:HD21	1.98	0.46
7:K:256:ILE:HD11	7:K:303:ARG:NH2	2.31	0.46
12:Z:123:PHE:HB2	12:Z:128:ILE:HD12	1.96	0.46
12:Z:250:ASP:HB3	12:Z:253:LEU:HB3	1.98	0.46
1:A:44:PRO:HD2	3:C:159:LEU:HG	1.98	0.45
1:A:406:LEU:HD11	4:D:191:VAL:HG12	1.97	0.45
3:C:728:LYS:O	3:C:732:ILE:HG23	2.16	0.45
5:I:154:THR:HA	5:I:157:ILE:HD12	1.97	0.45
5:I:248:ASP:HA	5:I:293:ALA:HB3	1.98	0.45
5:I:326:GLU:O	5:I:330:ILE:HG12	2.16	0.45
8:L:30:GLN:HA	8:L:102:GLN:NE2	2.28	0.45
6:J:389:GLU:HA	6:J:392:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:210:LYS:HG2	10:N:211:ALA:N	2.31	0.45
10:N:218:GLU:O	10:N:222:LYS:HG2	2.16	0.45
12:Z:310:ASP:CG	12:Z:711:ARG:HH21	2.24	0.45
12:Z:666:GLN:HE21	12:Z:711:ARG:C	2.24	0.45
2:B:291:ARG:HD2	2:B:291:ARG:HA	1.71	0.45
3:C:433:LEU:HD22	3:C:455:ILE:HG23	1.98	0.45
5:I:390:MET:O	5:I:394:GLN:HG2	2.16	0.45
12:Z:339:MET:SD	12:Z:704:GLY:HA2	2.57	0.45
12:Z:502:PHE:HE1	12:Z:547:LEU:HD21	1.80	0.45
2:B:96:LEU:HD12	2:B:99:ILE:HB	1.99	0.45
4:D:224:ILE:HD13	4:D:237:LEU:HD13	1.98	0.45
6:J:255:ARG:HA	6:J:302:GLN:HE22	1.81	0.45
12:Z:575:ALA:HB2	12:Z:587:ALA:HB3	1.98	0.45
4:D:167:GLU:O	4:D:171:ARG:HG2	2.17	0.45
5:I:20:LYS:HB3	5:I:21:PRO:HD3	1.97	0.45
5:I:60:ASP:HA	5:I:63:ARG:HE	1.80	0.45
5:I:149:MET:HA	5:I:330:ILE:HG21	1.98	0.45
5:I:238:ARG:HE	5:I:286:LYS:HZ1	1.65	0.45
7:K:192:GLU:HG3	7:K:345:ARG:HH11	1.80	0.45
10:N:38:ILE:HG12	10:N:41:HIS:CE1	2.52	0.45
11:P:120:LYS:HD2	11:P:124:ARG:HA	1.98	0.45
3:C:863:THR:CG2	3:C:911:LYS:HB3	2.47	0.45
9:M:101:THR:HG21	9:M:391:VAL:HG22	1.98	0.45
10:N:91:LEU:HA	10:N:94:ARG:HD2	1.97	0.45
3:C:745:LEU:HD22	3:C:878:LEU:HD21	1.98	0.45
3:C:738:TYR:HE2	3:C:886:VAL:HG13	1.82	0.45
5:I:387:GLY:HA2	5:I:390:MET:HE1	1.97	0.45
7:K:95:ILE:HD11	11:P:65:ASN:OD1	2.16	0.45
2:B:285:ASP:O	2:B:289:THR:HG22	2.17	0.45
6:J:274:VAL:HG12	6:J:317:ALA:O	2.17	0.45
9:M:288:CYS:SG	9:M:307:TYR:HB3	2.57	0.45
11:P:244:LEU:HD21	11:P:269:LEU:HD23	1.99	0.45
12:Z:104:LYS:HB3	12:Z:108:MET:CE	2.47	0.45
3:C:124:MET:HG3	3:C:156:HIS:CG	2.52	0.45
3:C:809:MET:SD	3:C:847:ILE:HD12	2.57	0.45
6:J:250:GLY:O	6:J:254:VAL:HG23	2.17	0.45
11:P:190:ILE:HG12	11:P:231:LEU:HD11	1.99	0.45
3:C:913:ILE:HG12	3:C:978:GLU:HA	1.98	0.44
6:J:269:ILE:HG22	6:J:271:ILE:HD11	2.00	0.44
1:A:227:LEU:HD21	1:A:234:ARG:HH22	1.82	0.44
5:I:39:GLU:HB3	5:I:43:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:226:GLY:O	5:I:230:VAL:HG23	2.17	0.44
7:K:105:ILE:HD12	11:P:126:THR:HG22	2.00	0.44
7:K:192:GLU:HG3	7:K:345:ARG:NH1	2.32	0.44
7:K:246:SER:O	7:K:280:MET:HA	2.17	0.44
9:M:206:GLU:HB2	9:M:213:ILE:HD11	1.98	0.44
12:Z:674:GLN:O	12:Z:678:ILE:HG12	2.17	0.44
2:B:56:LYS:HE3	2:B:60:LEU:HD21	2.00	0.44
6:J:284:ALA:HB3	6:J:290:ARG:HD2	1.99	0.44
8:L:30:GLN:HB3	8:L:54:GLU:HG2	1.99	0.44
2:B:108:THR:O	2:B:121:THR:HG22	2.18	0.44
3:C:559:LYS:HE2	3:C:727:GLU:HG3	1.99	0.44
6:J:318:THR:HG21	6:J:324:LEU:HD21	1.99	0.44
9:M:315:TRP:CH2	9:M:323:PRO:HD3	2.53	0.44
10:N:194:VAL:HG22	10:N:199:ALA:HB3	1.99	0.44
12:Z:375:HIS:CD2	12:Z:385:VAL:HG11	2.53	0.44
2:B:150:HIS:HE1	2:B:152:LYS:HB2	1.82	0.44
2:B:248:VAL:HB	2:B:251:GLU:HB2	2.00	0.44
3:C:267:THR:O	3:C:271:ILE:HG12	2.17	0.44
6:J:371:LEU:HD11	6:J:407:LEU:HB3	1.99	0.44
7:K:283:VAL:HG13	7:K:326:ALA:O	2.17	0.44
9:M:5:ILE:HG12	9:M:372:PHE:HB2	2.00	0.44
12:Z:93:GLU:HB3	12:Z:98:VAL:HG21	1.98	0.44
12:Z:204:SER:HA	12:Z:207:LEU:HD12	2.00	0.44
12:Z:626:GLY:C	12:Z:662:MET:HE1	2.43	0.44
3:C:209:PRO:HG3	3:C:236:PHE:CD2	2.52	0.44
4:D:332:PRO:HG3	4:D:362:ALA:HB3	1.99	0.44
6:J:6:ILE:HG13	9:M:208:GLY:HA2	1.99	0.44
7:K:124:GLY:N	7:K:125:PRO:HD2	2.33	0.44
11:P:360:ILE:HG12	13:P:501:ATP:C6	2.53	0.44
2:B:291:ARG:CZ	2:B:303:GLN:HG2	2.48	0.44
3:C:933:VAL:HG21	3:C:946:THR:HG23	1.98	0.44
7:K:297:ALA:O	7:K:301:ILE:HG23	2.17	0.44
10:N:41:HIS:HD2	10:N:78:ILE:HD11	1.82	0.44
12:Z:76:GLU:HG2	12:Z:108:MET:HE1	1.99	0.44
12:Z:93:GLU:HB3	12:Z:98:VAL:HG11	1.98	0.44
12:Z:930:LEU:HD12	12:Z:931:PRO:HD2	2.00	0.44
3:C:224:LEU:HA	3:C:227:ILE:HG12	1.98	0.44
4:D:109:ILE:HG22	4:D:111:PRO:HD2	2.00	0.44
5:I:187:LEU:HB3	5:I:316:PHE:HE2	1.82	0.44
10:N:75:PRO:HA	10:N:78:ILE:HD12	1.99	0.44
10:N:145:HIS:HD2	10:N:180:HIS:CD2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:167:VAL:HG21	10:N:197:TYR:HB3	1.99	0.44
1:A:411:CYS:SG	1:A:451:ILE:HG13	2.58	0.44
2:B:300:ARG:HD3	2:B:300:ARG:HA	1.89	0.44
4:D:379:VAL:O	4:D:387:GLN:HG3	2.18	0.44
12:Z:729:SER:HA	12:Z:752:SER:HA	1.99	0.44
1:A:409:ARG:CZ	4:D:195:ARG:HG2	2.48	0.43
2:B:142:GLU:HG2	2:B:143:PRO:HD2	2.00	0.43
3:C:469:PRO:HA	3:C:472:LEU:HG	2.00	0.43
3:C:605:SER:OG	3:C:742:GLY:HA2	2.17	0.43
6:J:245:LYS:HD2	7:K:299:ARG:HD3	1.98	0.43
6:J:369:ASP:O	6:J:373:ILE:HG12	2.18	0.43
11:P:146:VAL:HG11	11:P:155:ILE:HD11	2.00	0.43
12:Z:106:ILE:HD13	12:Z:156:ILE:HD11	1.99	0.43
12:Z:731:VAL:O	12:Z:735:MET:HG2	2.18	0.43
12:Z:889:ARG:NH2	12:Z:912:GLU:HB2	2.32	0.43
3:C:750:GLU:HG3	3:C:753:GLY:H	1.82	0.43
8:L:41:GLU:HA	8:L:41:GLU:OE1	2.18	0.43
12:Z:479:GLU:HG3	12:Z:516:GLY:HA3	2.00	0.43
6:J:324:LEU:HD22	6:J:324:LEU:H	1.83	0.43
11:P:167:VAL:HG11	11:P:266:ALA:HA	1.99	0.43
11:P:362:GLN:HE21	11:P:376:TRP:CD1	2.36	0.43
12:Z:645:THR:O	12:Z:653:ARG:HD2	2.18	0.43
2:B:167:MET:HE3	2:B:267:ILE:HD13	1.99	0.43
3:C:44:LYS:O	3:C:44:LYS:HD3	2.18	0.43
4:D:197:ILE:HG21	4:D:236:GLU:HG3	1.99	0.43
5:I:153:LEU:HD13	5:I:316:PHE:HE1	1.83	0.43
6:J:3:GLU:CD	6:J:3:GLU:H	2.26	0.43
6:J:367:ASP:OD1	6:J:369:ASP:HB2	2.19	0.43
7:K:104:LEU:HD11	11:P:125:GLN:HB3	2.01	0.43
9:M:216:PHE:CE1	9:M:271:HIS:HB3	2.53	0.43
1:A:299:ARG:HA	1:A:299:ARG:HD3	1.88	0.43
2:B:142:GLU:OE1	2:B:262:ARG:HB2	2.19	0.43
2:B:285:ASP:CG	2:B:330:LYS:HB2	2.44	0.43
3:C:776:VAL:O	3:C:780:MET:HG2	2.18	0.43
4:D:142:LEU:HB2	4:D:156:ILE:HG21	2.00	0.43
5:I:108:LYS:N	5:I:108:LYS:HD2	2.33	0.43
5:I:114:CYS:HB2	5:I:124:LYS:HB3	2.00	0.43
9:M:206:GLU:HG3	9:M:250:LEU:HB3	1.99	0.43
10:N:118:LYS:HA	10:N:155:LEU:HD11	2.00	0.43
12:Z:564:ASN:O	12:Z:568:VAL:HG23	2.18	0.43
2:B:240:THR:O	2:B:241:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:31:GLU:HB3	5:I:35:ARG:NH2	2.34	0.43
6:J:223:VAL:HG11	6:J:270:PHE:CD2	2.53	0.43
7:K:290:ARG:HH22	7:K:305:LEU:HB3	1.82	0.43
11:P:159:LEU:HB3	11:P:160:PRO:CD	2.48	0.43
11:P:360:ILE:HG12	13:P:501:ATP:N1	2.33	0.43
12:Z:241:LEU:O	12:Z:245:LEU:HG	2.18	0.43
3:C:138:ARG:HG2	3:C:157:LEU:HD21	2.00	0.43
4:D:133:ASN:OD1	4:D:133:ASN:C	2.61	0.43
4:D:257:LEU:HD23	4:D:257:LEU:HA	1.83	0.43
6:J:303:MET:HE3	6:J:303:MET:O	2.17	0.43
8:L:30:GLN:HG3	8:L:53:THR:OG1	2.19	0.43
8:L:77:PRO:HB3	8:L:87:PHE:CZ	2.54	0.43
12:Z:297:ASP:CG	12:Z:921:ARG:HB2	2.44	0.43
2:B:148:LEU:HD12	2:B:158:GLY:HA3	2.00	0.43
2:B:167:MET:HE2	2:B:171:MET:SD	2.58	0.43
3:C:472:LEU:HD12	3:C:473:LEU:N	2.33	0.43
5:I:265:ASP:O	5:I:268:VAL:HG12	2.19	0.43
6:J:211:LEU:HB3	6:J:340:PHE:HE1	1.83	0.43
12:Z:370:SER:HA	12:Z:373:VAL:HG12	2.01	0.43
12:Z:890:PHE:HZ	12:Z:914:VAL:HG21	1.83	0.43
5:I:139:VAL:HG12	5:I:210:PHE:O	2.19	0.43
5:I:171:PRO:HB3	5:I:181:GLN:HE22	1.83	0.43
7:K:263:ILE:HA	7:K:266:MET:SD	2.59	0.43
12:Z:267:GLN:HA	12:Z:270:LEU:HG	2.00	0.43
12:Z:809:ARG:C	12:Z:809:ARG:HE	2.27	0.43
2:B:207:LEU:O	2:B:211:MET:HG2	2.19	0.43
3:C:253:VAL:HG21	3:C:265:LEU:HD23	2.01	0.43
5:I:91:GLU:CD	5:I:91:GLU:H	2.26	0.43
5:I:297:LEU:HD12	5:I:300:LEU:HD12	2.00	0.42
6:J:184:ILE:HD11	6:J:211:LEU:HD21	2.00	0.42
12:Z:106:ILE:HG12	12:Z:137:PHE:HD1	1.83	0.42
12:Z:455:MET:HA	12:Z:487:LEU:O	2.19	0.42
1:A:246:ILE:HG13	1:A:373:ARG:HB2	2.02	0.42
6:J:179:MET:O	6:J:183:GLU:HG2	2.19	0.42
7:K:159:LEU:HB3	7:K:160:PRO:HD2	2.00	0.42
7:K:290:ARG:NH2	7:K:305:LEU:HB3	2.34	0.42
8:L:111:LEU:HD12	8:L:111:LEU:O	2.19	0.42
12:Z:299:TYR:O	12:Z:303:LEU:HG	2.19	0.42
12:Z:466:LEU:HA	12:Z:469:VAL:HB	2.01	0.42
12:Z:604:ARG:H	12:Z:604:ARG:HG3	1.69	0.42
3:C:521:GLU:HG3	3:C:562:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:254:VAL:HG11	6:J:298:GLU:HG3	2.01	0.42
6:J:324:LEU:HB3	6:J:328:LEU:HD11	2.01	0.42
7:K:256:ILE:HD12	7:K:256:ILE:HA	1.80	0.42
12:Z:309:ILE:HB	12:Z:311:ILE:HG13	2.02	0.42
12:Z:334:VAL:HG22	12:Z:747:HIS:CE1	2.54	0.42
12:Z:768:ILE:HD11	12:Z:919:THR:HG22	2.00	0.42
1:A:74:THR:HB	2:B:100:ARG:HH22	1.83	0.42
3:C:204:CYS:O	3:C:208:VAL:HG12	2.20	0.42
3:C:857:LEU:HG	3:C:862:MET:HG3	2.00	0.42
3:C:864:MET:HE3	3:C:881:ILE:HG13	2.01	0.42
4:D:332:PRO:HB3	4:D:360:LEU:HA	2.01	0.42
11:P:84:GLU:HG2	11:P:86:MET:H	1.84	0.42
3:C:880:SER:HA	3:C:903:MET:SD	2.59	0.42
4:D:38:LEU:HD23	4:D:38:LEU:HA	1.91	0.42
6:J:89:ILE:HG23	6:J:140:HIS:ND1	2.34	0.42
9:M:337:ASN:ND2	9:M:387:GLN:HA	2.30	0.42
1:A:254:THR:HG21	1:A:377:PHE:HB3	2.01	0.42
2:B:177:PRO:HG2	2:B:237:ALA:HB3	2.00	0.42
3:C:776:VAL:CG2	3:C:777:PRO:HD3	2.49	0.42
5:I:236:MET:HE3	5:I:237:ALA:N	2.35	0.42
7:K:298:ASP:HA	7:K:301:ILE:HG12	2.01	0.42
10:N:58:LYS:O	10:N:58:LYS:HG2	2.20	0.42
11:P:309:LEU:HD22	11:P:342:ARG:HD3	2.01	0.42
12:Z:289:ILE:HA	12:Z:294:PRO:HG2	2.01	0.42
1:A:144:LYS:HB2	1:A:144:LYS:HE3	1.74	0.42
3:C:197:LYS:HB2	3:C:197:LYS:HE2	1.78	0.42
6:J:175:GLY:HA3	6:J:352:ILE:HA	2.02	0.42
6:J:251:PRO:HD3	6:J:295:ILE:HG12	2.02	0.42
7:K:343:LEU:HD23	7:K:343:LEU:HA	1.81	0.42
10:N:51:ILE:HD12	10:N:51:ILE:N	2.31	0.42
12:Z:544:GLU:HG3	12:Z:547:LEU:H	1.84	0.42
12:Z:651:PHE:HA	12:Z:654:GLN:HB3	2.02	0.42
1:A:223:GLU:HG2	1:A:227:LEU:HD22	2.02	0.42
2:B:291:ARG:HH11	2:B:306:MET:HG3	1.83	0.42
5:I:250:ILE:HG22	5:I:294:THR:HB	2.01	0.42
5:I:274:GLU:HA	5:I:277:ASN:HD21	1.83	0.42
9:M:282:LEU:HD23	9:M:282:LEU:HA	1.87	0.42
1:A:177:ASP:HB3	1:A:181:TYR:H	1.85	0.42
5:I:190:PRO:HD2	5:I:316:PHE:O	2.20	0.42
5:I:209:LYS:HZ1	5:I:210:PHE:H	1.66	0.42
6:J:258:PHE:HB2	6:J:302:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG23	1:A:281:GLN:H	1.85	0.42
1:A:412:PRO:HG3	4:D:243:LYS:NZ	2.35	0.42
3:C:550:PHE:CE2	3:C:595:MET:HE3	2.55	0.42
5:I:187:LEU:HB3	5:I:316:PHE:CE2	2.55	0.42
8:L:7:VAL:HG13	8:L:36:LYS:HA	2.01	0.42
9:M:163:TRP:CZ3	9:M:170:ASN:HB2	2.55	0.42
9:M:312:LEU:HD22	9:M:347:VAL:HG21	2.02	0.42
11:P:269:LEU:HA	11:P:272:GLU:OE2	2.20	0.42
5:I:136:LEU:HB2	6:J:297:ILE:HG12	2.02	0.41
5:I:210:PHE:O	5:I:211:ILE:HD13	2.19	0.41
10:N:194:VAL:HA	10:N:199:ALA:H	1.85	0.41
11:P:82:VAL:HA	11:P:119:VAL:HG12	2.00	0.41
11:P:84:GLU:OE2	11:P:86:MET:HB3	2.20	0.41
11:P:283:LEU:HD22	11:P:325:ALA:HB1	2.02	0.41
12:Z:540:LEU:HD12	12:Z:541:ALA:N	2.35	0.41
3:C:969:GLU:HA	3:C:989:TYR:CG	2.55	0.41
4:D:307:LYS:O	4:D:311:LYS:HG2	2.20	0.41
10:N:99:ASP:O	10:N:102:LYS:HG2	2.20	0.41
11:P:144:ASP:OD1	11:P:160:PRO:HD2	2.20	0.41
5:I:43:ARG:H	5:I:43:ARG:HG2	1.72	0.41
6:J:73:ARG:HE	6:J:74:HIS:N	2.18	0.41
6:J:404:GLN:HA	6:J:407:LEU:HD23	2.02	0.41
9:M:218:ARG:HB3	9:M:221:ASN:O	2.20	0.41
12:Z:603:PRO:HA	12:Z:625:LEU:HD21	2.03	0.41
3:C:206:ASP:O	3:C:209:PRO:HD2	2.21	0.41
3:C:904:LEU:O	3:C:908:ILE:HG13	2.20	0.41
4:D:416:ILE:HD11	4:D:455:LEU:HG	2.01	0.41
5:I:159:GLU:O	5:I:163:VAL:HG23	2.20	0.41
5:I:304:LEU:O	5:I:310:ILE:HG22	2.20	0.41
6:J:132:LYS:HB2	6:J:135:MET:CE	2.50	0.41
11:P:223:PRO:HD2	11:P:349:PHE:O	2.20	0.41
1:A:177:ASP:HB3	1:A:181:TYR:N	2.34	0.41
2:B:137:ASP:HB3	2:B:140:LEU:HD12	2.02	0.41
3:C:769:ASN:O	3:C:773:ARG:HG3	2.20	0.41
4:D:183:SER:O	4:D:187:ARG:HG3	2.21	0.41
5:I:166:LEU:HD21	9:M:158:MET:HE1	2.03	0.41
12:Z:298:TYR:HB3	12:Z:759:ILE:HD13	2.02	0.41
12:Z:650:ASP:HB3	12:Z:692:GLU:CD	2.46	0.41
12:Z:677:ASP:O	12:Z:680:LYS:HG2	2.21	0.41
5:I:63:ARG:O	5:I:67:GLU:HG3	2.21	0.41
6:J:219:LYS:HB2	13:J:501:ATP:O2B	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:213:ILE:HG23	9:M:248:ASN:ND2	2.36	0.41
10:N:25:LYS:HD2	10:N:27:SER:OG	2.21	0.41
3:C:578:GLY:O	3:C:581:VAL:HG22	2.21	0.41
6:J:136:SER:HB2	6:J:150:LEU:HD22	2.02	0.41
6:J:234:PHE:CZ	6:J:236:ARG:HB2	2.56	0.41
11:P:396:VAL:O	11:P:400:MET:HG3	2.21	0.41
12:Z:685:VAL:HA	12:Z:691:GLN:HG3	2.02	0.41
1:A:149:LEU:HD12	1:A:149:LEU:H	1.85	0.41
1:A:409:ARG:HD3	4:D:194:VAL:HG12	2.02	0.41
3:C:237:VAL:HG21	3:C:271:ILE:HG23	2.03	0.41
3:C:278:LEU:HD13	3:C:310:LEU:HD11	2.02	0.41
3:C:495:ILE:HD13	3:C:495:ILE:HA	1.88	0.41
4:D:163:LEU:HB3	4:D:169:ILE:HG13	2.02	0.41
5:I:321:VAL:HG11	9:M:39:ILE:HG13	2.02	0.41
6:J:286:THR:O	6:J:290:ARG:HG2	2.21	0.41
10:N:210:LYS:HE3	10:N:212:GLU:CG	2.50	0.41
11:P:284:ASP:O	11:P:288:THR:HG23	2.21	0.41
12:Z:109:TYR:OH	12:Z:162:ARG:HD3	2.20	0.41
12:Z:203:ARG:HA	12:Z:206:ILE:HD12	2.02	0.41
1:A:409:ARG:NH2	4:D:195:ARG:HG2	2.36	0.41
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.89	0.41
3:C:864:MET:HE3	3:C:881:ILE:CG1	2.50	0.41
4:D:49:MET:HE3	4:D:49:MET:O	2.21	0.41
5:I:103:ASN:HB3	5:I:106:ASP:OD2	2.20	0.41
5:I:297:LEU:HD21	5:I:313:LYS:HD2	2.03	0.41
6:J:180:GLN:NE2	6:J:341:PRO:HD3	2.36	0.41
6:J:276:SER:C	6:J:277:ILE:HD13	2.46	0.41
7:K:267:PHE:CD2	7:K:311:GLN:HB3	2.56	0.41
11:P:309:LEU:HD21	11:P:337:LEU:HG	2.03	0.41
11:P:312:LEU:HD13	11:P:342:ARG:HB3	2.02	0.41
12:Z:173:LYS:HG2	12:Z:185:ILE:HD13	2.03	0.41
12:Z:188:TYR:CZ	12:Z:192:LEU:HD11	2.55	0.41
12:Z:730:VAL:O	12:Z:734:VAL:HG23	2.20	0.41
2:B:256:TYR:HE1	2:B:263:LEU:HB2	1.86	0.41
3:C:258:PRO:HA	3:C:261:ASP:OD1	2.21	0.41
3:C:406:TRP:CE3	3:C:409:LYS:HD2	2.56	0.41
3:C:823:ASN:ND2	3:C:860:GLY:HA3	2.36	0.41
3:C:827:LEU:HD12	3:C:827:LEU:HA	1.96	0.41
5:I:133:LEU:HG	6:J:290:ARG:HH21	1.86	0.41
5:I:244:ILE:HD13	5:I:244:ILE:HA	1.91	0.41
5:I:339:ARG:HD3	9:M:17:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:303:MET:HA	6:J:306:PHE:CD2	2.55	0.41
8:L:86:ILE:HG13	12:Z:934:PHE:CE1	2.56	0.41
9:M:385:VAL:HG21	9:M:402:GLU:OE2	2.21	0.41
10:N:73:TRP:CZ3	10:N:104:THR:HG21	2.56	0.41
11:P:375:ASN:H	11:P:412:HIS:CE1	2.39	0.41
2:B:175:LYS:HE2	2:B:175:LYS:H	1.86	0.40
3:C:442:VAL:HG12	3:C:444:GLU:H	1.85	0.40
3:C:471:LEU:HB2	3:C:497:PHE:CZ	2.56	0.40
3:C:989:TYR:C	3:C:990:ARG:HD3	2.46	0.40
4:D:19:GLU:HA	4:D:22:GLU:HG3	2.03	0.40
12:Z:303:LEU:HD13	12:Z:341:ALA:O	2.21	0.40
12:Z:736:PHE:CD1	12:Z:736:PHE:C	2.99	0.40
12:Z:742:TRP:CE3	12:Z:742:TRP:HA	2.56	0.40
1:A:238:LEU:HD11	4:D:5:GLU:HA	2.03	0.40
1:A:425:GLU:HA	1:A:428:MET:HB3	2.03	0.40
2:B:150:HIS:CE1	2:B:152:LYS:HB2	2.56	0.40
5:I:269:GLN:HA	5:I:272:MET:SD	2.61	0.40
9:M:216:PHE:CZ	9:M:276:LYS:HA	2.56	0.40
11:P:197:ILE:C	11:P:200:PRO:HD2	2.46	0.40
12:Z:136:ILE:CG2	12:Z:139:ARG:HH21	2.34	0.40
12:Z:809:ARG:O	12:Z:809:ARG:NE	2.54	0.40
2:B:171:MET:HA	2:B:246:ARG:O	2.21	0.40
3:C:278:LEU:HD23	3:C:278:LEU:HA	1.88	0.40
3:C:624:LEU:HD13	3:C:764:LEU:HD11	2.03	0.40
3:C:865:ASP:OD2	3:C:865:ASP:N	2.53	0.40
3:C:988:ASP:OD1	3:C:988:ASP:O	2.38	0.40
7:K:221:TYR:HA	7:K:327:THR:O	2.22	0.40
12:Z:769:PRO:HB3	12:Z:914:VAL:HG11	2.02	0.40
1:A:293:GLU:O	1:A:296:GLU:HG3	2.22	0.40
6:J:212:TYR:HB2	6:J:321:ALA:HB2	2.04	0.40
12:Z:726:ASP:O	12:Z:730:VAL:HG23	2.22	0.40
12:Z:740:TRP:CD1	12:Z:740:TRP:C	2.99	0.40
1:A:168:ILE:HA	1:A:172:MET:HE1	2.02	0.40
3:C:159:LEU:HA	3:C:159:LEU:HD23	1.82	0.40
3:C:269:TYR:CE1	3:C:281:ALA:HB1	2.56	0.40
3:C:310:LEU:O	3:C:314:LEU:HG	2.22	0.40
6:J:60:LEU:HD22	12:Z:604:ARG:CZ	2.51	0.40
9:M:262:GLY:HA2	9:M:268:ILE:HD13	2.03	0.40
12:Z:207:LEU:HB2	12:Z:232:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	376/467 (80%)	365 (97%)	10 (3%)	1 (0%)	36	70
2	B	382/437 (87%)	375 (98%)	7 (2%)	0	100	100
3	C	841/993 (85%)	825 (98%)	16 (2%)	0	100	100
4	D	464/480 (97%)	458 (99%)	6 (1%)	0	100	100
5	I	379/405 (94%)	370 (98%)	9 (2%)	0	100	100
6	J	375/428 (88%)	366 (98%)	8 (2%)	1 (0%)	36	70
7	K	381/437 (87%)	374 (98%)	7 (2%)	0	100	100
8	L	129/156 (83%)	124 (96%)	5 (4%)	0	100	100
9	M	415/417 (100%)	403 (97%)	12 (3%)	0	100	100
10	N	226/228 (99%)	218 (96%)	8 (4%)	0	100	100
11	P	386/434 (89%)	377 (98%)	8 (2%)	1 (0%)	36	70
12	Z	874/945 (92%)	850 (97%)	24 (3%)	0	100	100
All	All	5228/5827 (90%)	5105 (98%)	120 (2%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	J	6	ILE
11	P	159	LEU
1	A	190	ARG

5.3.2 Protein sidechains ⓘ

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	320/399 (80%)	315 (98%)	5 (2%)	55	69
2	B	342/385 (89%)	338 (99%)	4 (1%)	63	73
3	C	723/850 (85%)	716 (99%)	7 (1%)	68	76
4	D	433/445 (97%)	430 (99%)	3 (1%)	76	79
5	I	332/352 (94%)	328 (99%)	4 (1%)	63	73
6	J	331/374 (88%)	328 (99%)	3 (1%)	70	76
7	K	328/377 (87%)	325 (99%)	3 (1%)	70	76
8	L	120/144 (83%)	120 (100%)	0	100	100
9	M	364/364 (100%)	361 (99%)	3 (1%)	73	77
10	N	198/198 (100%)	195 (98%)	3 (2%)	57	70
11	P	337/375 (90%)	334 (99%)	3 (1%)	70	76
12	Z	737/797 (92%)	732 (99%)	5 (1%)	76	79
All	All	4565/5060 (90%)	4522 (99%)	43 (1%)	68	76

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	58	ASP
1	A	63	ILE
1	A	162	ARG
1	A	294	LEU
2	B	129	TYR
2	B	159	VAL
2	B	189	SER
2	B	369	MET
3	C	115	LEU
3	C	146	PHE
3	C	161	ILE
3	C	208	VAL
3	C	276	ASN
3	C	541	ASP
3	C	790	MET
4	D	44	VAL
4	D	95	VAL
4	D	450	VAL
5	I	125	VAL
5	I	177	LEU
5	I	209	LYS

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Mol	Chain	Res	Type
5	I	377	VAL
6	J	247	LEU
6	J	316	MET
6	J	392	LEU
7	K	151	THR
7	K	254	LYS
7	K	324	ILE
9	M	32	VAL
9	M	156	GLN
9	M	317	LEU
10	N	23	HIS
10	N	37	ARG
10	N	49	HIS
11	P	77	TYR
11	P	150	LYS
11	P	254	MET
12	Z	241	LEU
12	Z	483	LEU
12	Z	606	VAL
12	Z	644	LEU
12	Z	743	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	339	GLN
2	B	161	GLN
2	B	312	GLN
2	B	352	ASN
3	C	379	GLN
3	C	771	HIS
4	D	7	ASN
4	D	251	GLN
4	D	269	GLN
4	D	359	ASN
4	D	387	GLN
6	J	72	GLN
6	J	302	GLN
6	J	375	ASN
7	K	282	GLN
8	L	131	ASN

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Mol	Chain	Res	Type
9	M	9	HIS
9	M	128	GLN
9	M	170	ASN
9	M	248	ASN
9	M	281	GLN
10	N	49	HIS
10	N	180	HIS
10	N	226	ASN
11	P	311	GLN
11	P	375	ASN
11	P	412	HIS
12	Z	226	ASN
12	Z	240	GLN
12	Z	510	HIS
12	Z	681	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	ATP	A	501	-	32,33,33	0.27	0	48,52,52	0.34	0
13	ATP	I	501	-	32,33,33	0.32	0	48,52,52	0.35	0
13	ATP	P	501	-	32,33,33	0.27	0	48,52,52	0.34	0
13	ATP	J	501	-	32,33,33	0.36	0	48,52,52	0.36	0
13	ATP	B	501	-	32,33,33	0.26	0	48,52,52	0.35	0
13	ATP	K	501	-	32,33,33	0.30	0	48,52,52	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ATP	A	501	-	-	3/22/38/38	0/3/3/3
13	ATP	I	501	-	-	4/22/38/38	0/3/3/3
13	ATP	P	501	-	-	6/22/38/38	0/3/3/3
13	ATP	J	501	-	-	2/22/38/38	0/3/3/3
13	ATP	B	501	-	-	5/22/38/38	0/3/3/3
13	ATP	K	501	-	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	501	ATP	PB-O3B-PG-O3G
13	B	501	ATP	C5'-O5'-PA-O2A
13	B	501	ATP	C5'-O5'-PA-O3A
13	K	501	ATP	C5'-O5'-PA-O1A
13	K	501	ATP	C5'-O5'-PA-O2A
13	K	501	ATP	C5'-O5'-PA-O3A
13	P	501	ATP	C5'-O5'-PA-O1A
13	P	501	ATP	C5'-O5'-PA-O2A
13	P	501	ATP	C5'-O5'-PA-O3A
13	I	501	ATP	O4'-C4'-C5'-O5'
13	B	501	ATP	PA-O3A-PB-O2B
13	J	501	ATP	PB-O3A-PA-O2A
13	B	501	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

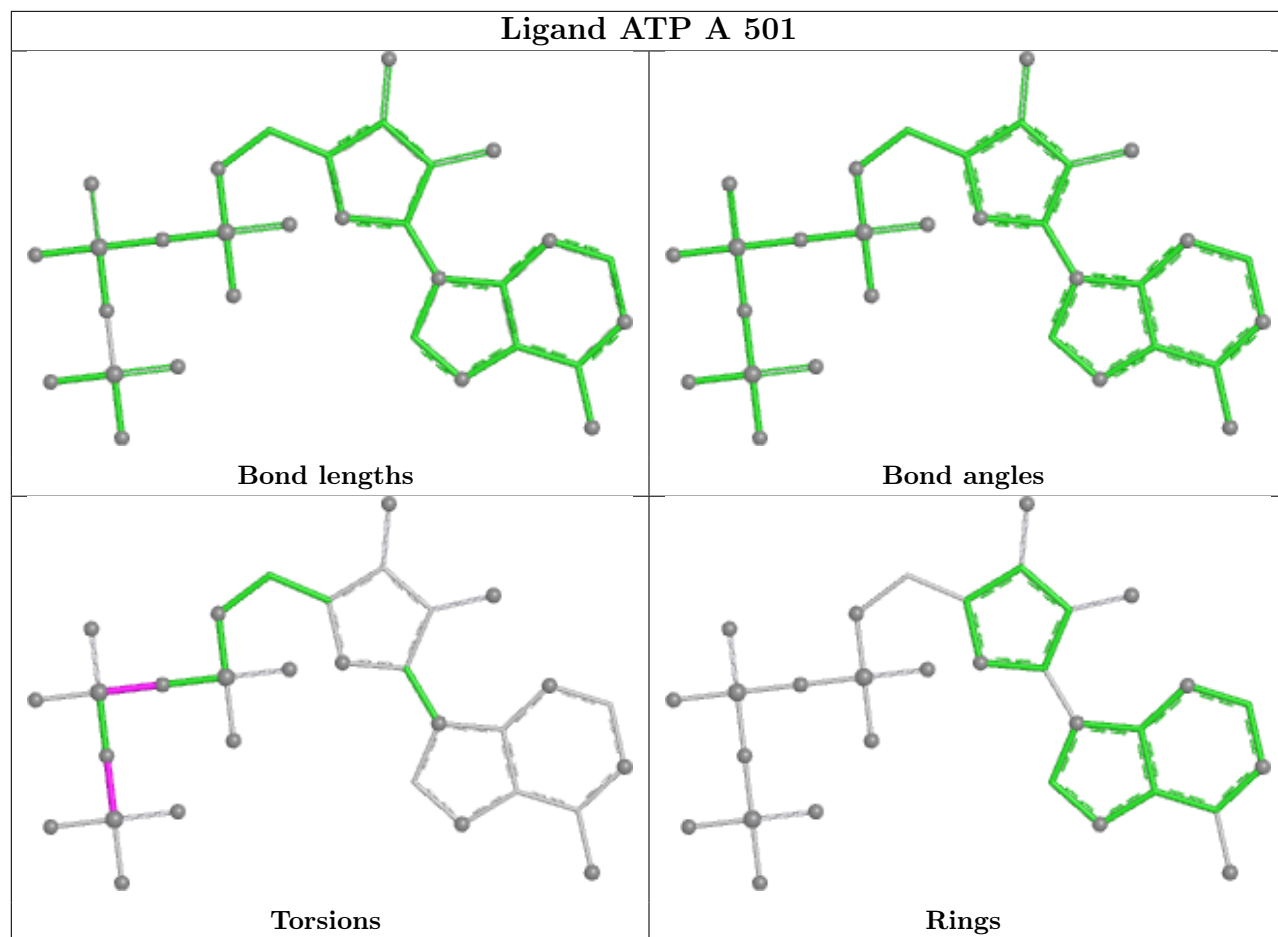
Mol	Chain	Res	Type	Atoms
13	I	501	ATP	PG-O3B-PB-O2B
13	P	501	ATP	C4'-C5'-O5'-PA
13	A	501	ATP	PA-O3A-PB-O3B
13	A	501	ATP	PA-O3A-PB-O1B
13	B	501	ATP	PA-O3A-PB-O1B
13	I	501	ATP	PG-O3B-PB-O1B
13	J	501	ATP	PB-O3A-PA-O1A
13	P	501	ATP	PG-O3B-PB-O2B
13	P	501	ATP	PB-O3A-PA-O1A
13	I	501	ATP	C3'-C4'-C5'-O5'

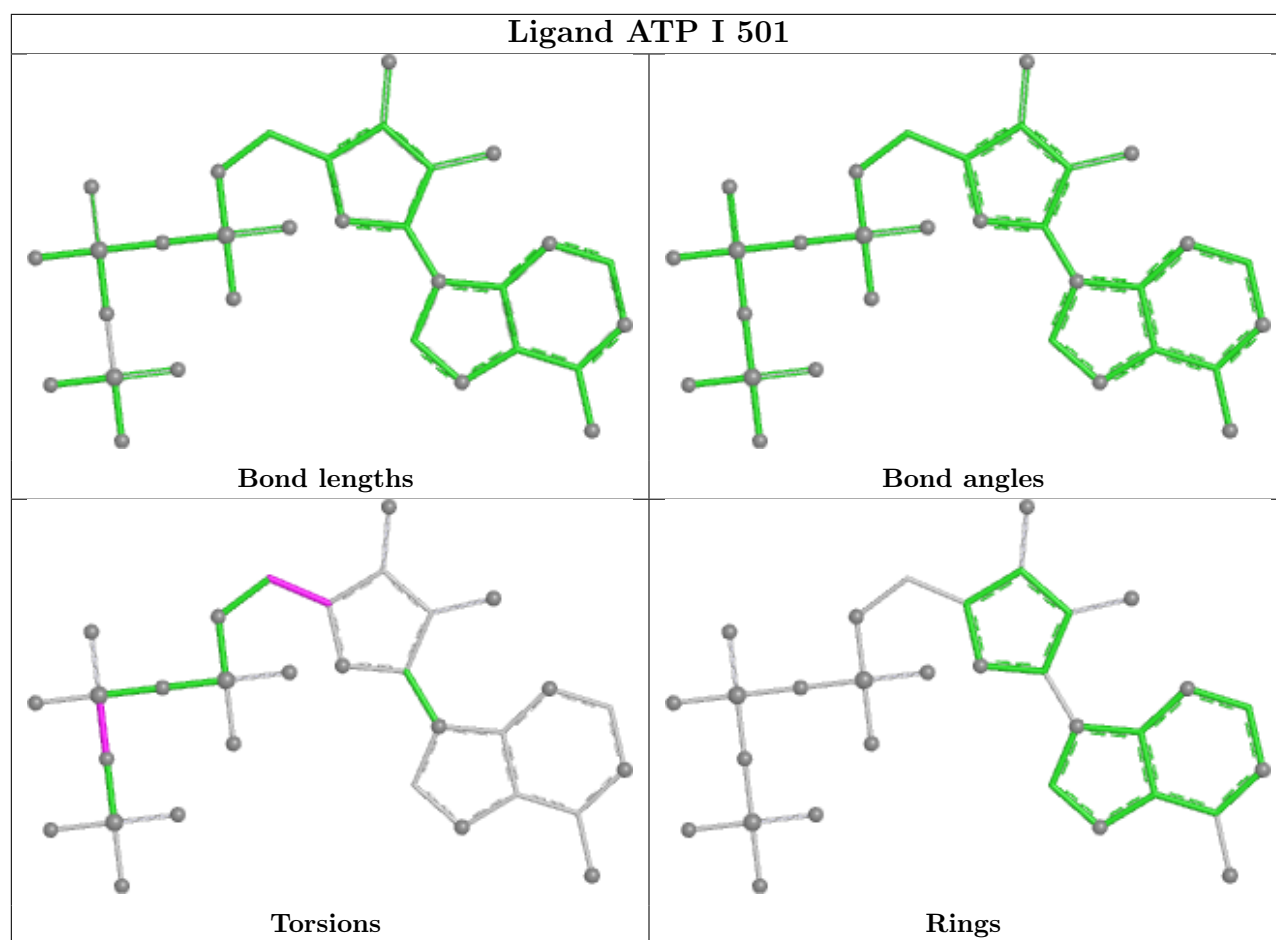
There are no ring outliers.

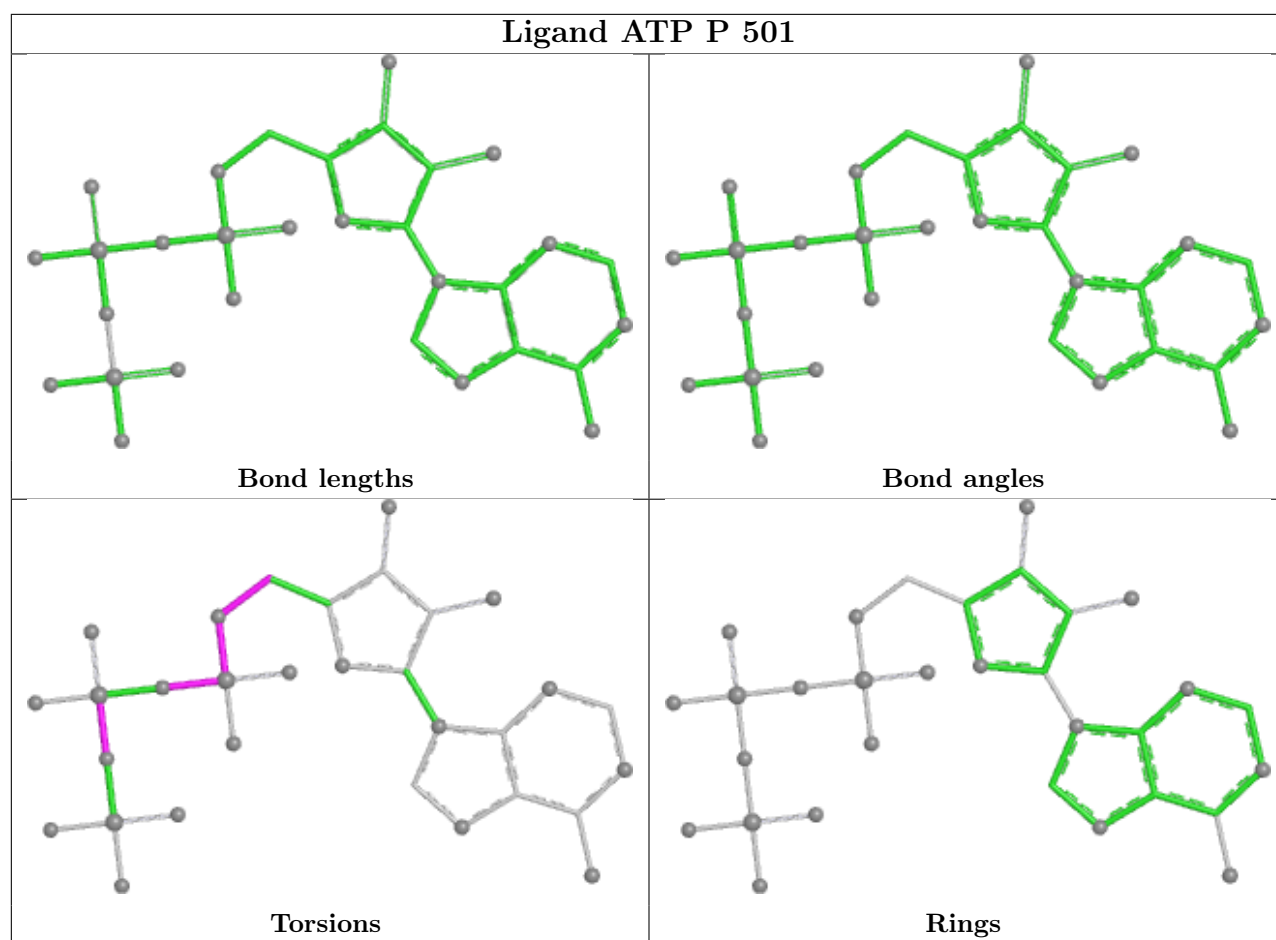
5 monomers are involved in 14 short contacts:

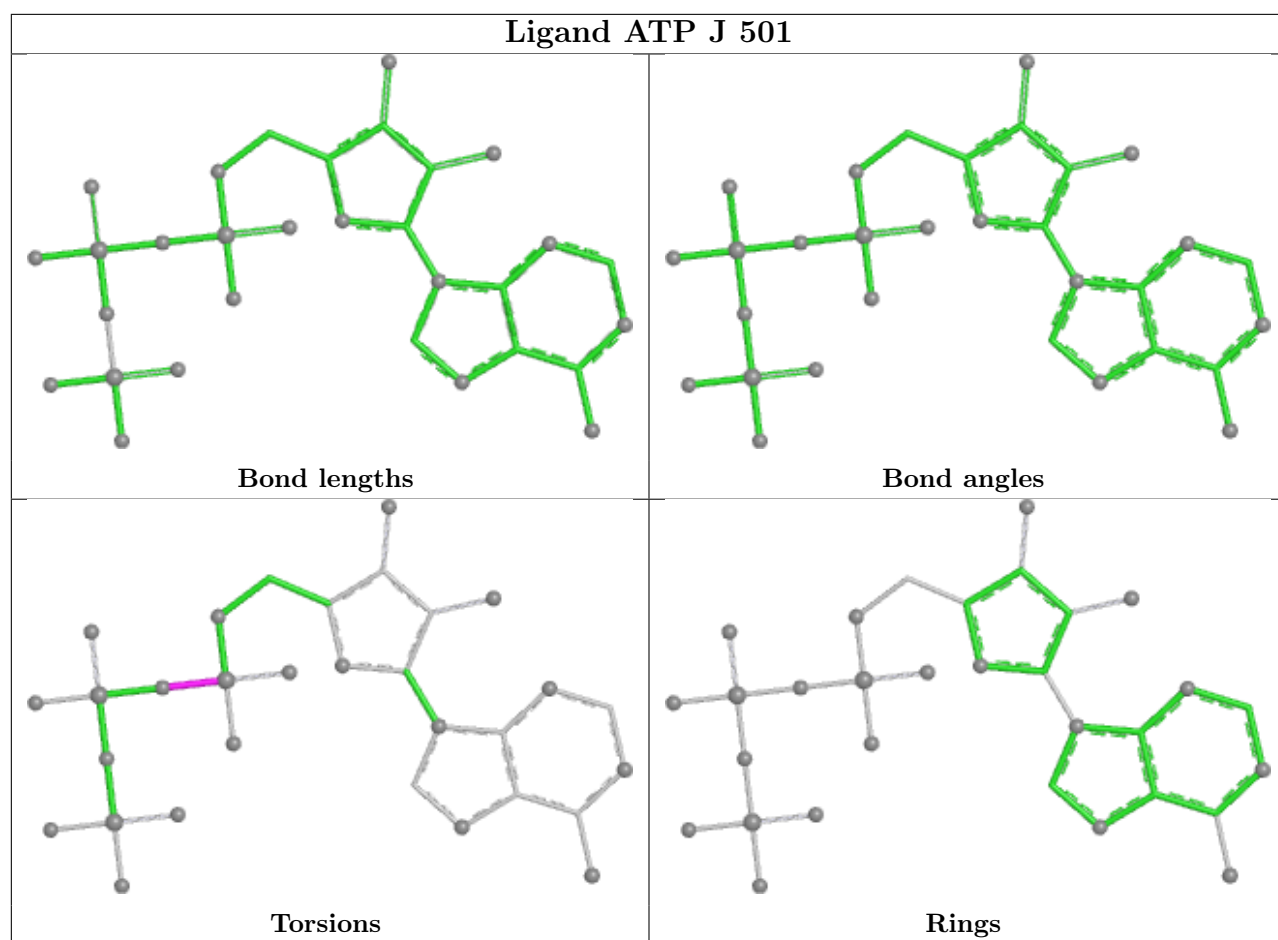
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	501	ATP	1	0
13	P	501	ATP	5	0
13	J	501	ATP	5	0
13	B	501	ATP	1	0
13	K	501	ATP	2	0

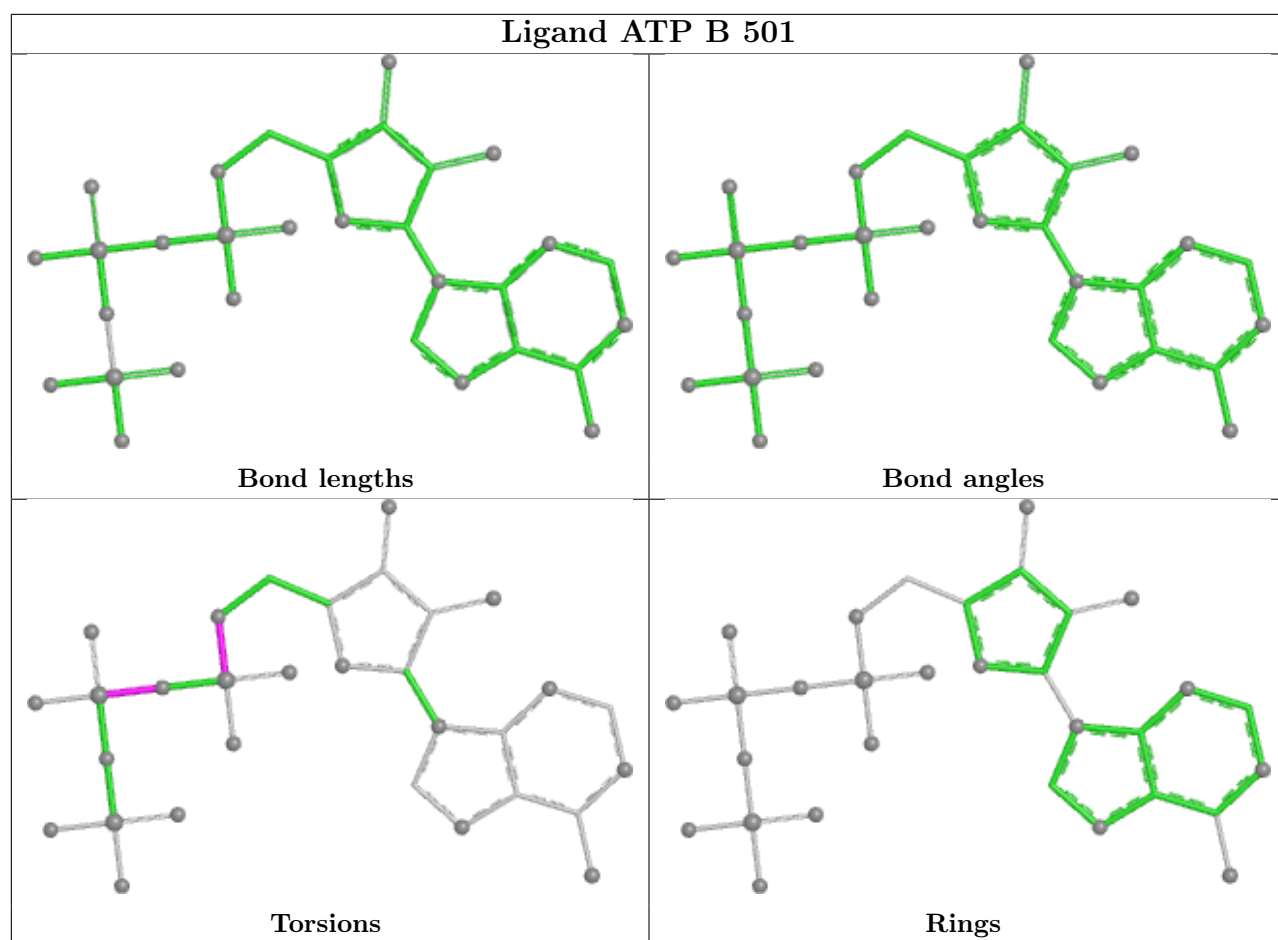
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

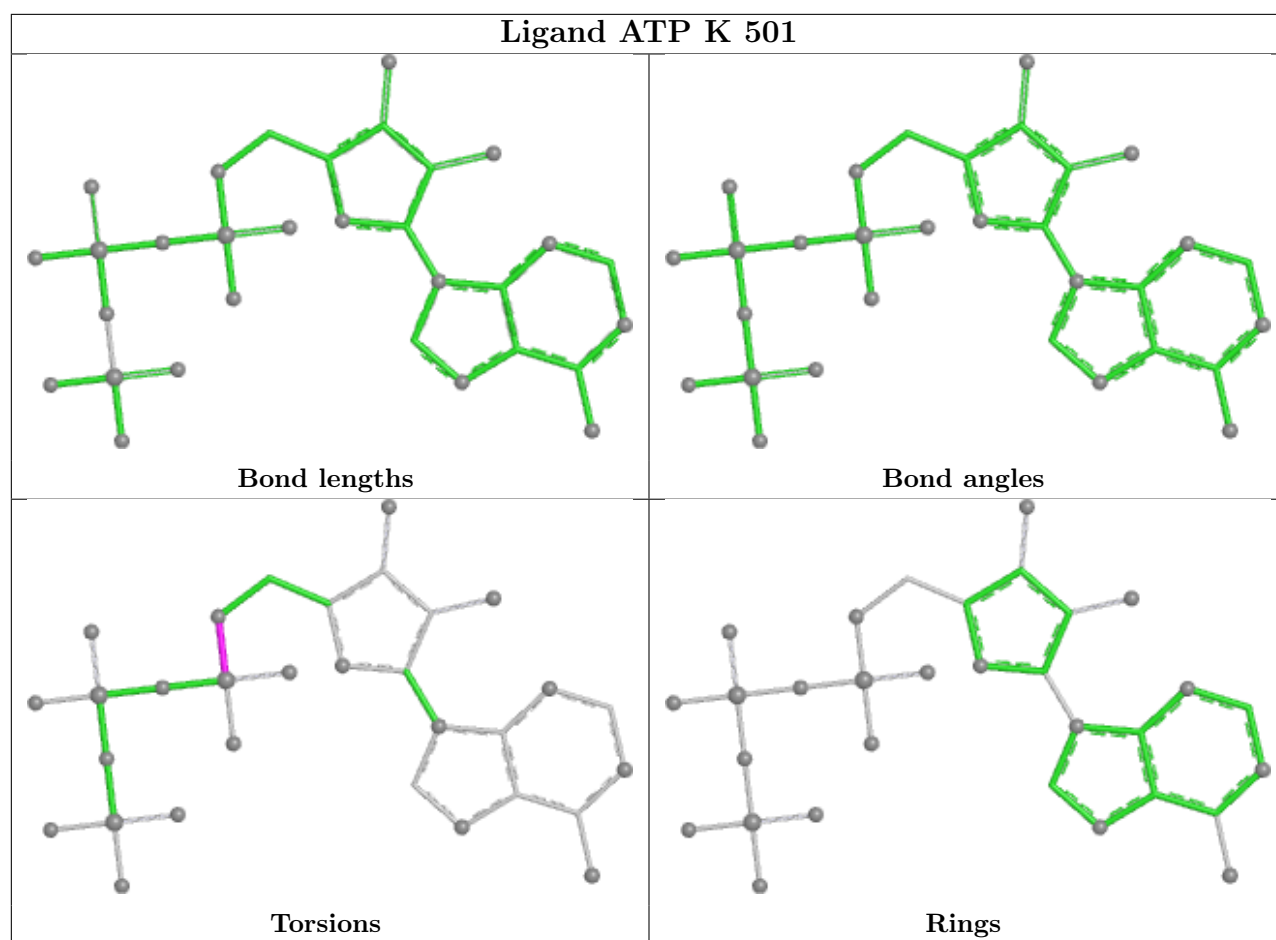












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

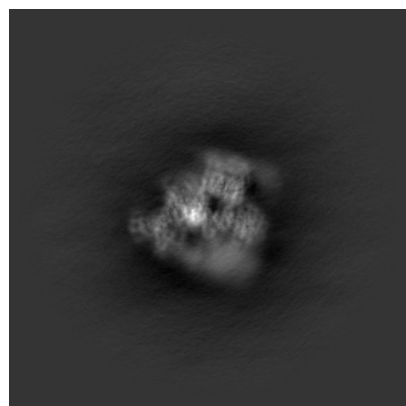
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77358. These allow visual inspection of the internal detail of the map and identification of artifacts.

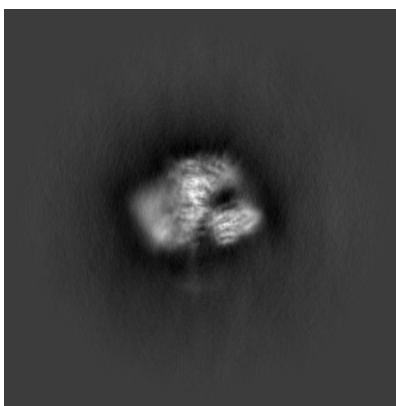
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

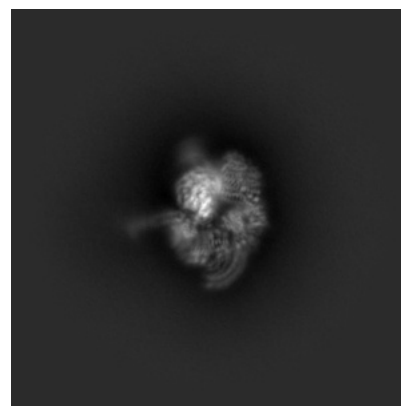
6.1.1 Primary map



X

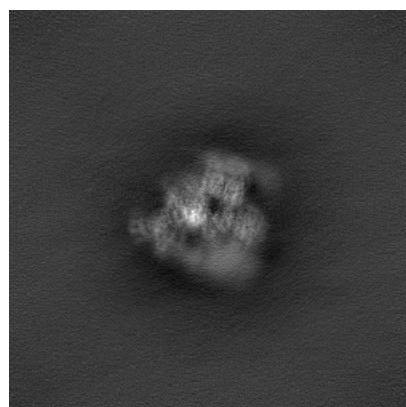


Y

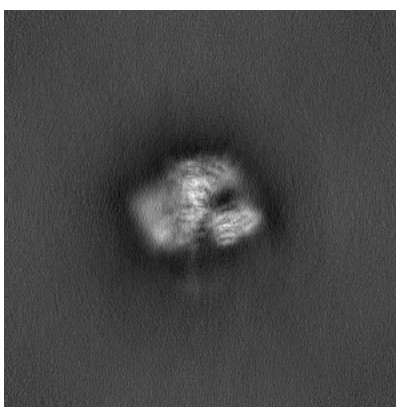


Z

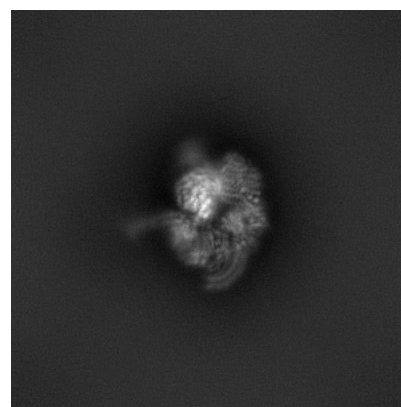
6.1.2 Raw map



X



Y

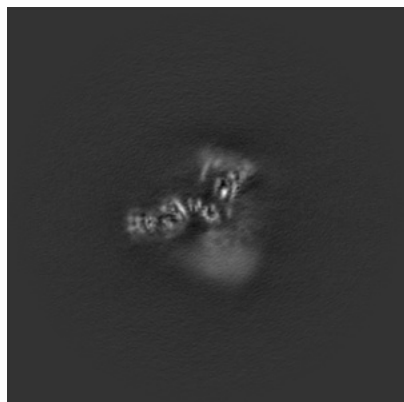


Z

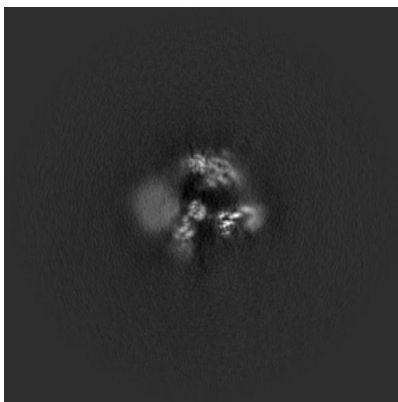
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

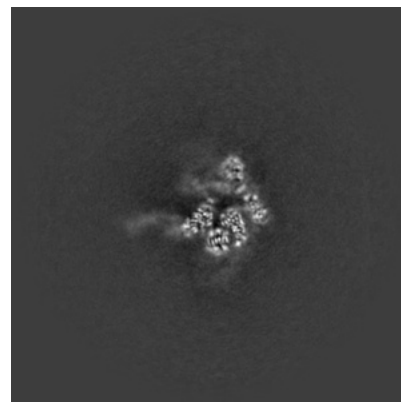
6.2.1 Primary map



X Index: 256

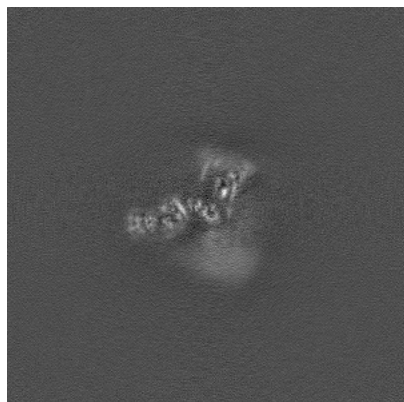


Y Index: 256

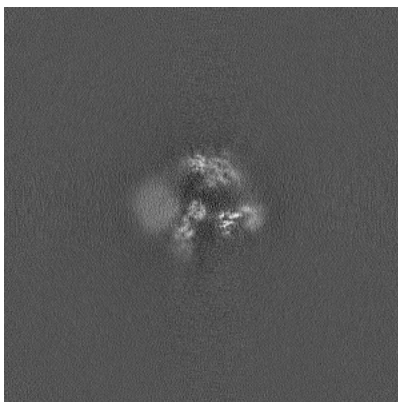


Z Index: 256

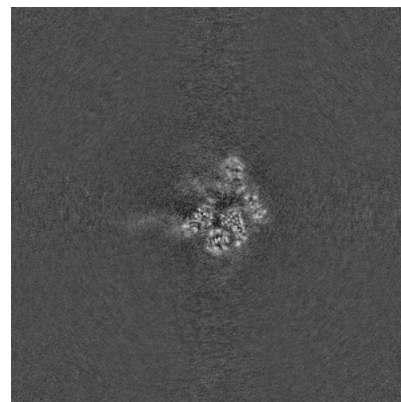
6.2.2 Raw map



X Index: 256



Y Index: 256

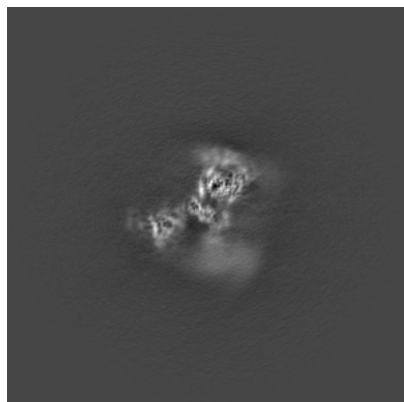


Z Index: 256

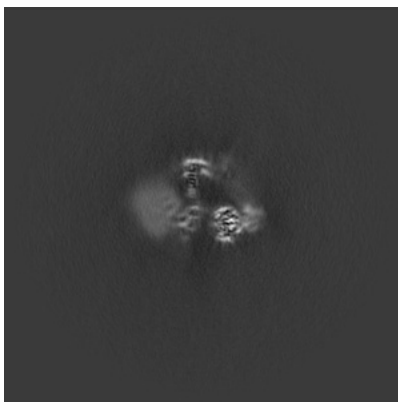
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

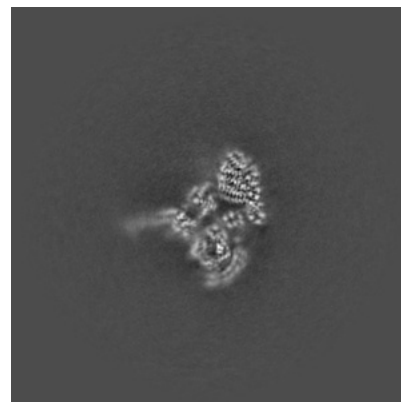
6.3.1 Primary map



X Index: 247

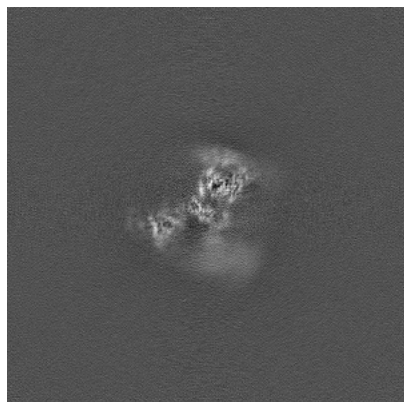


Y Index: 268



Z Index: 242

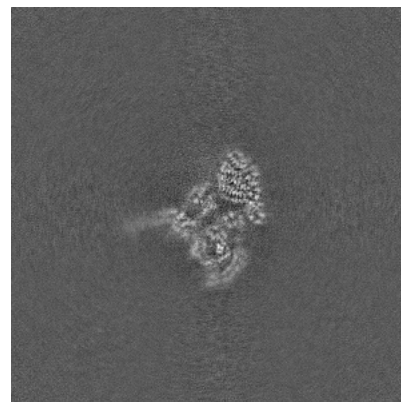
6.3.2 Raw map



X Index: 247



Y Index: 268

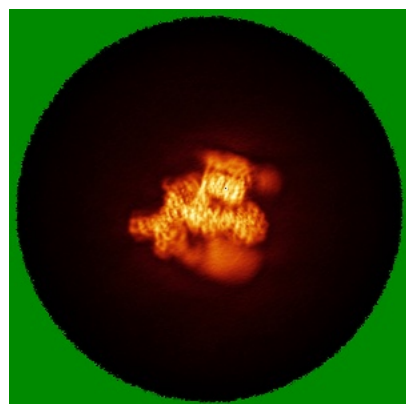


Z Index: 242

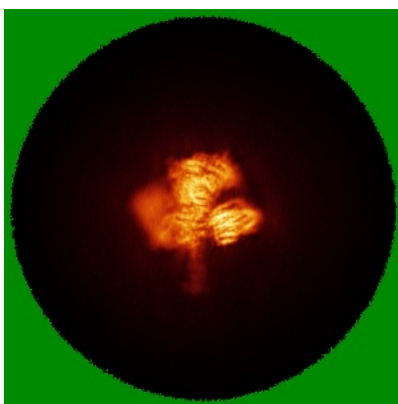
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

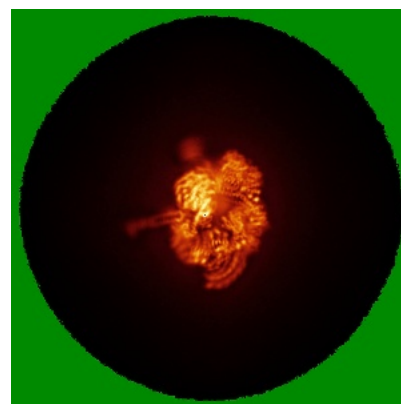
6.4.1 Primary map



X

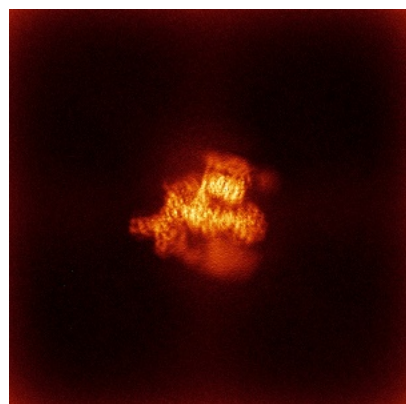


Y

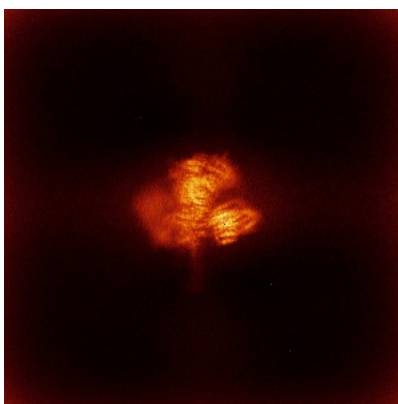


Z

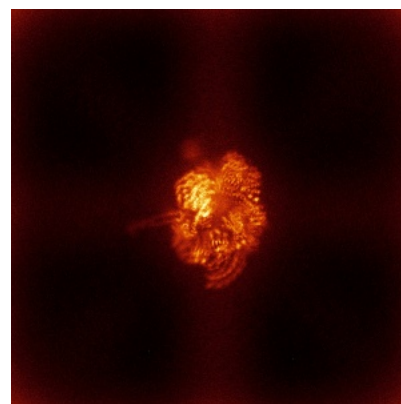
6.4.2 Raw map



X



Y

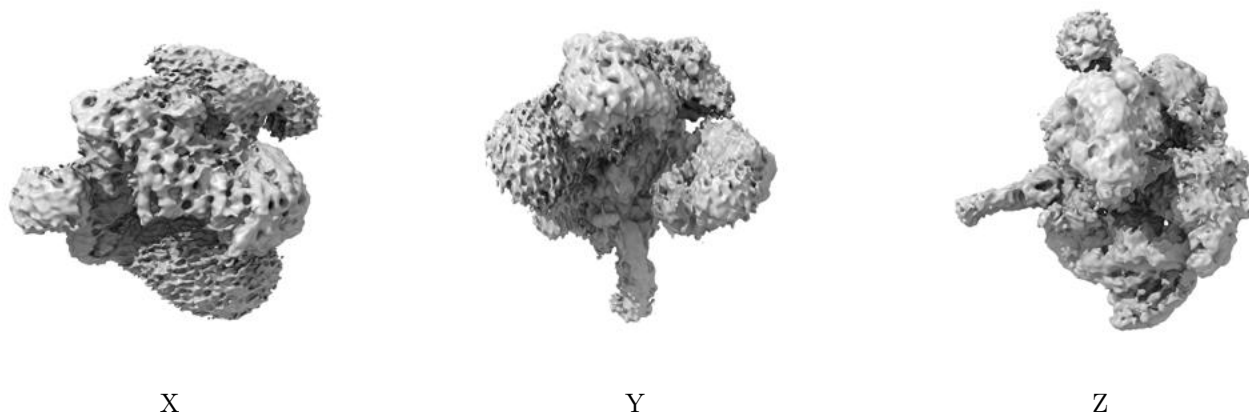


Z

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.

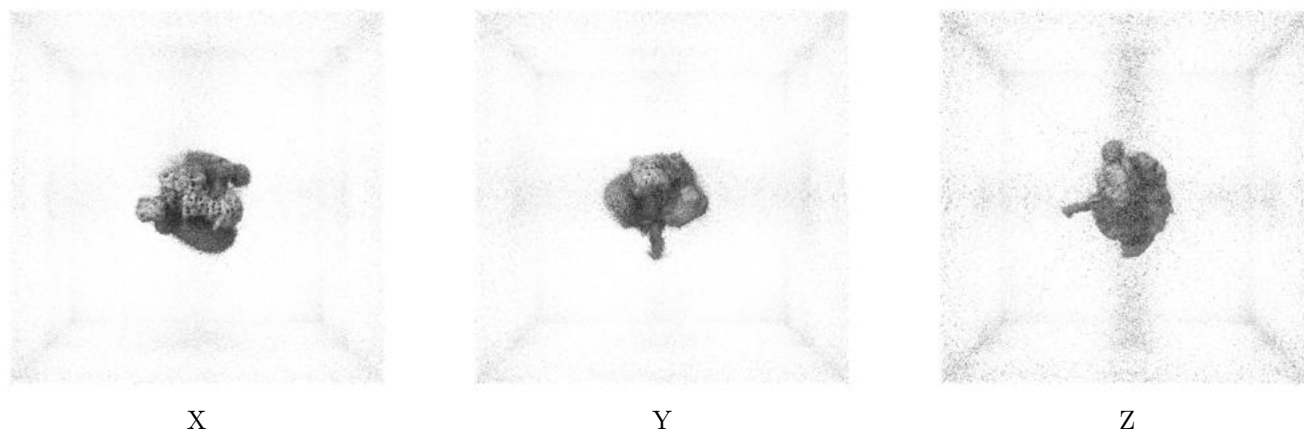
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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



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.

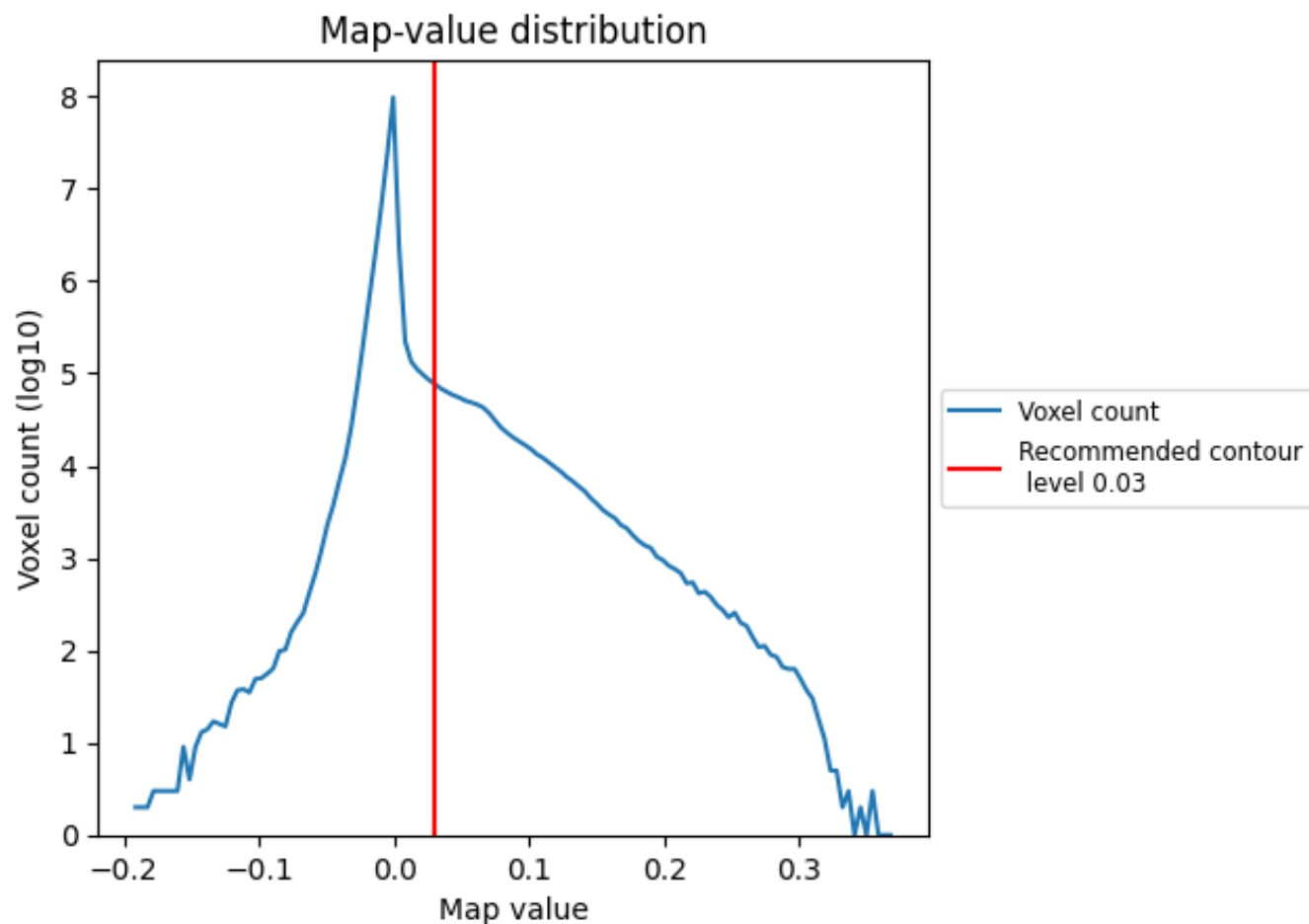
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

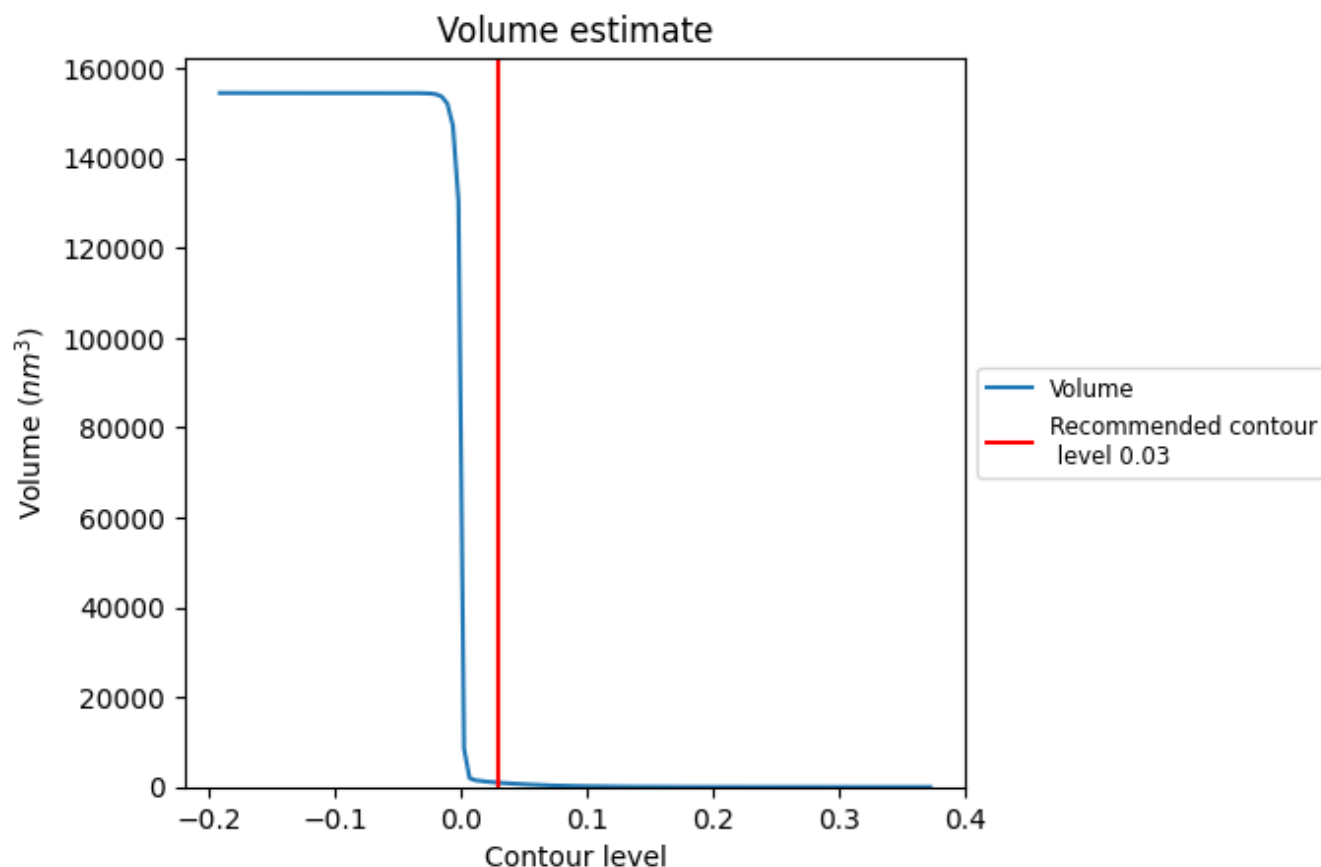
This section contains the results of statistical analysis of the map.

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.

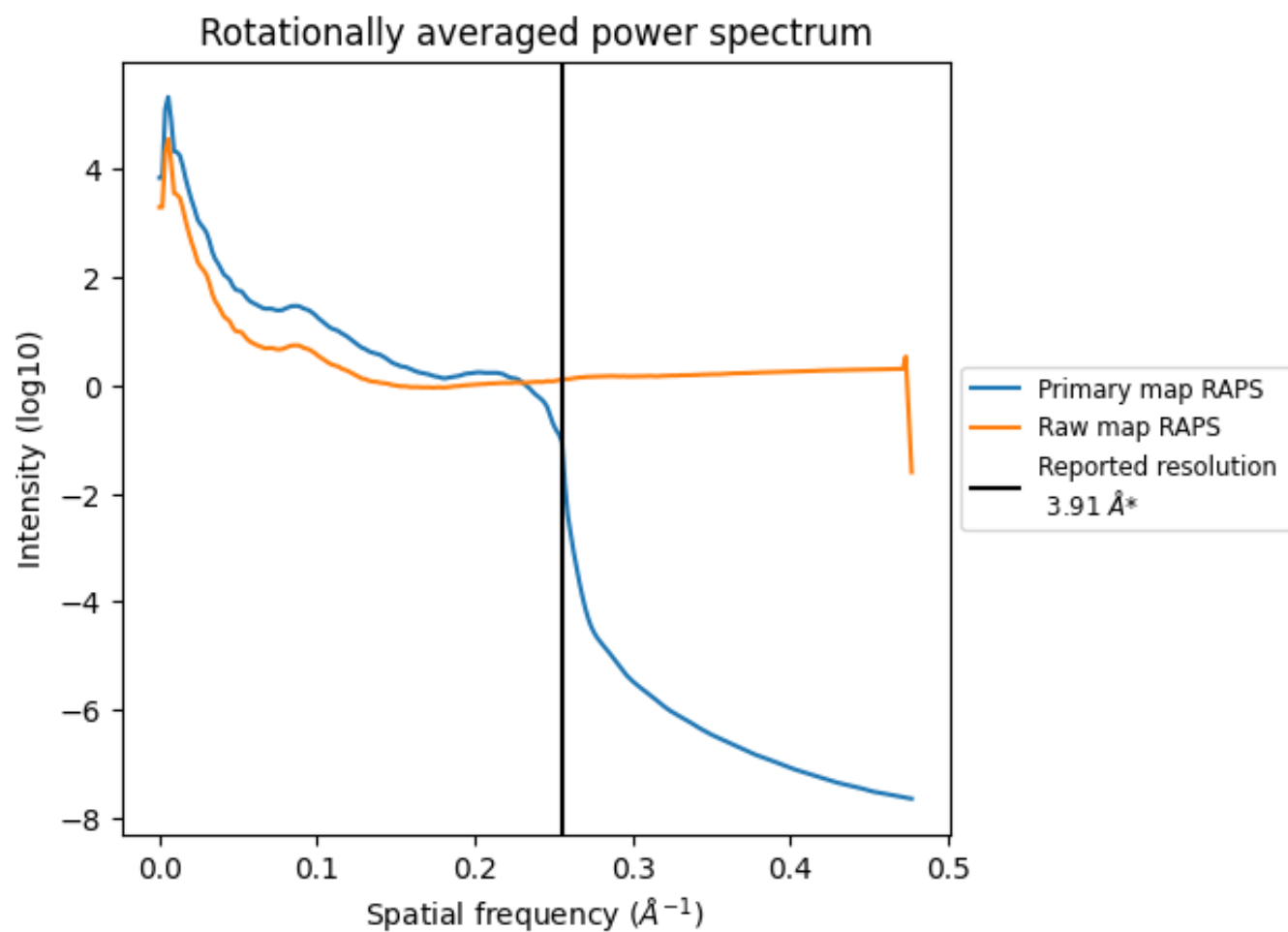
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 950 nm^3 ; this corresponds to an approximate mass of 858 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 ⓘ

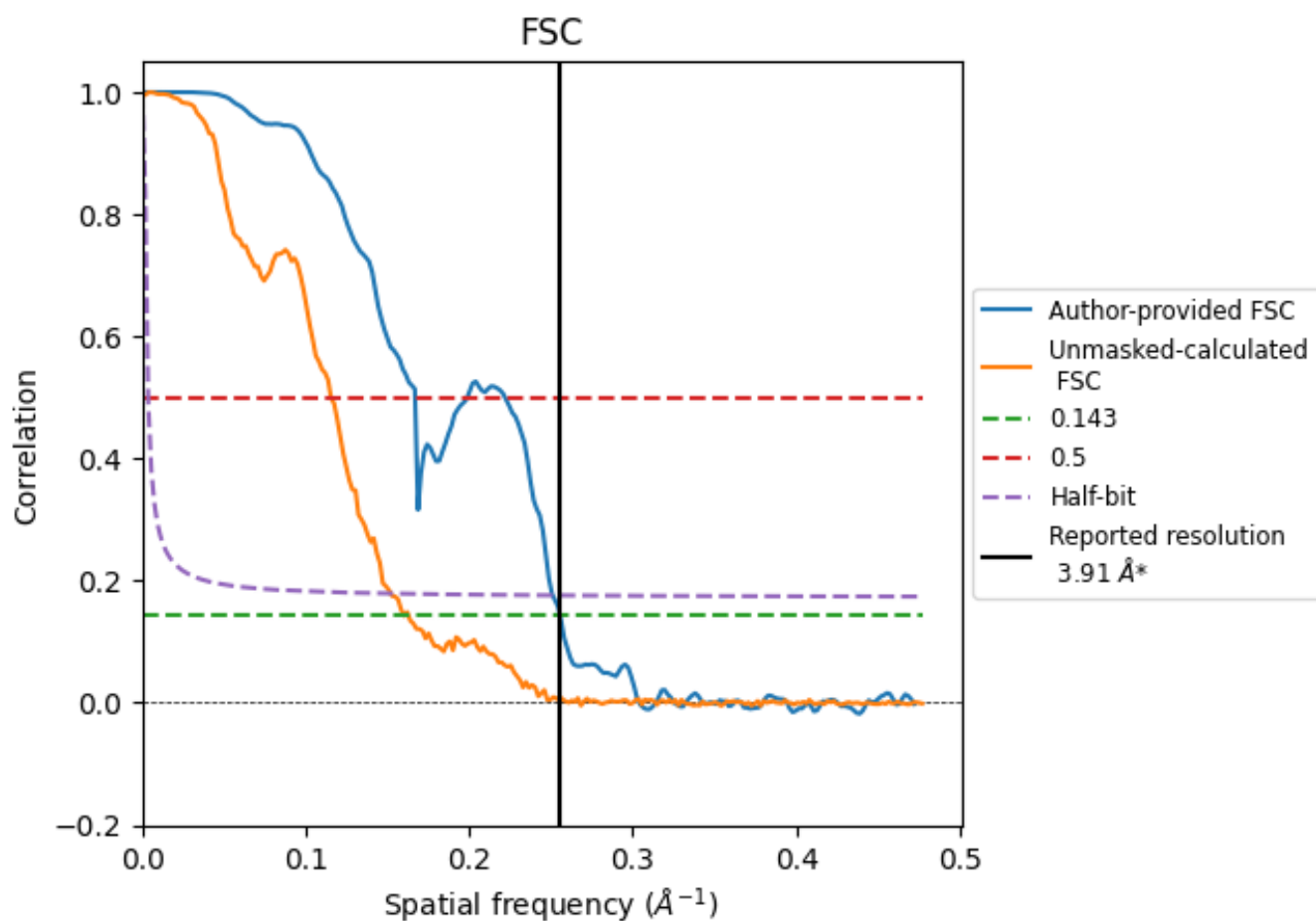


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

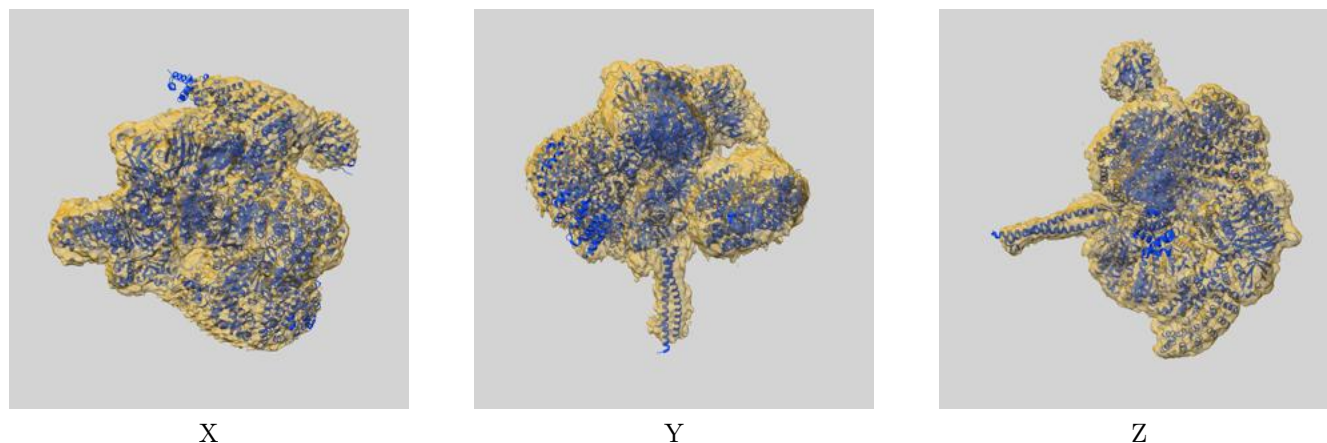
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.91	5.99	3.98
Unmasked-calculated*	6.24	8.66	6.58

*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 6.24 differs from the reported value 3.91 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77358 and PDB model 36BL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



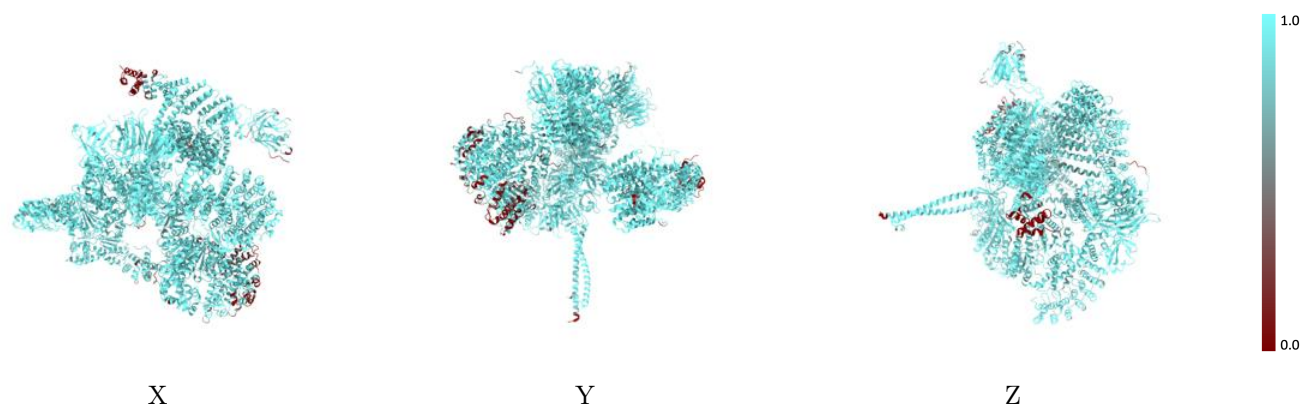
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



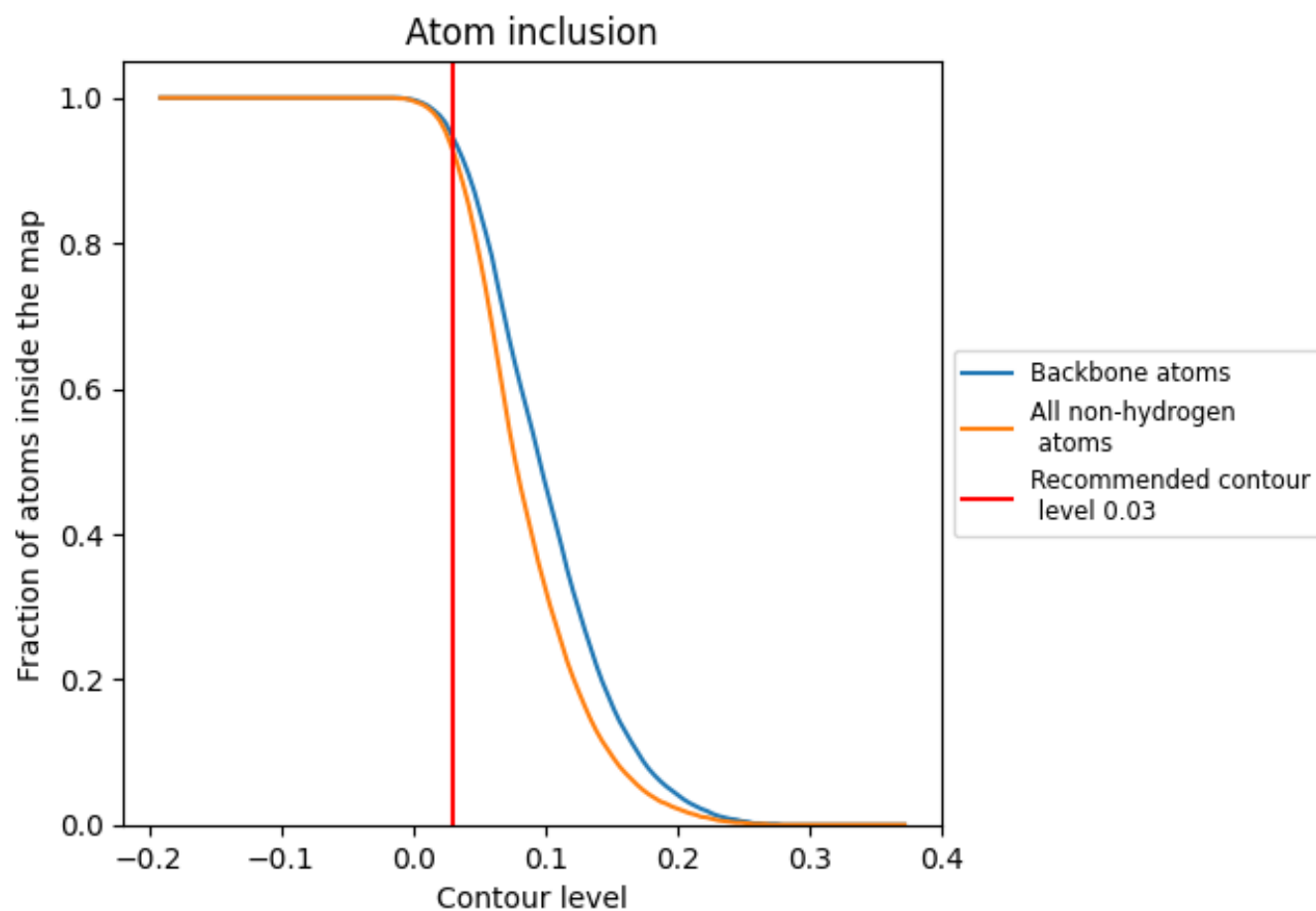
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.1920
A	0.8890	0.1130
B	0.9390	0.1230
C	0.9690	0.2580
D	0.7680	0.0510
I	0.9650	0.2700
J	0.9680	0.2630
K	0.9560	0.2070
L	0.8760	0.0980
M	0.9660	0.2350
N	0.9700	0.1810
P	0.9590	0.1350
Z	0.9080	0.2210

1.0

0.0

<0.0