



Full wwPDB EM Validation Report ⓘ

Sep 3, 2026 – 01:02 PM EDT

PDB ID : 36BM / pdb_000036bm
EMDB ID : EMD-77359
Title : yeast 26S proteasome base assembly intermediate, base-Hsm3-Nas6 with Rpt4-EQ
Authors : Hsieh, H.H.; Martin, A.
Deposited on : 2026-05-28
Resolution : 3.82 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:

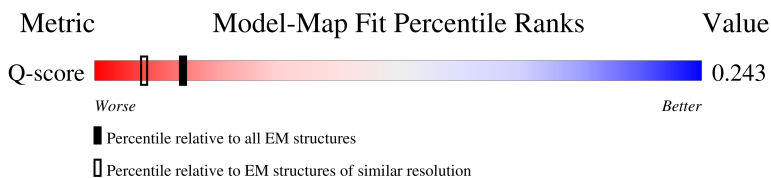
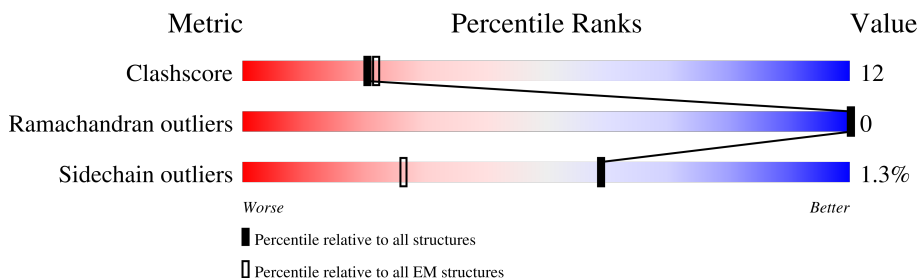
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.82 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	9152 (3.32 - 4.32)

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	
2	B	437	
3	C	993	
4	D	480	

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Mol	Chain	Length	Quality of chain
5	K	437	69%19%11%
6	P	434	66%23%11%
7	I	405	19%10%72%
8	J	428	57%29%13%
9	Z	945	8%70%25%5%
10	L	156	17%73%11%16%
11	N	228	64%36%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 36449 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	391	Total	C	N	O	S	0	0
			3042	1914	542	570	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	385	Total	C	N	O	S	0	0
			3020	1900	509	594	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	846	Total	C	N	O	S	0	0
			6569	4172	1074	1294	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	470	Total	C	N	O	S	0	0
			3832	2468	613	738	13		

- Molecule 5 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	391	Total	C	N	O	S	0	0
			3106	1957	552	585	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 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	387	Total	C	N	O	S	0	0
			3030	1892	531	595	12		

- Molecule 7 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	115	Total	C	N	O	S	0	0
			939	592	169	176	2		

- Molecule 8 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	372	Total	C	N	O	S	0	0
			2935	1843	518	564	10		

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	901	Total	C	N	O	S	0	0
			6952	4418	1166	1339	29		

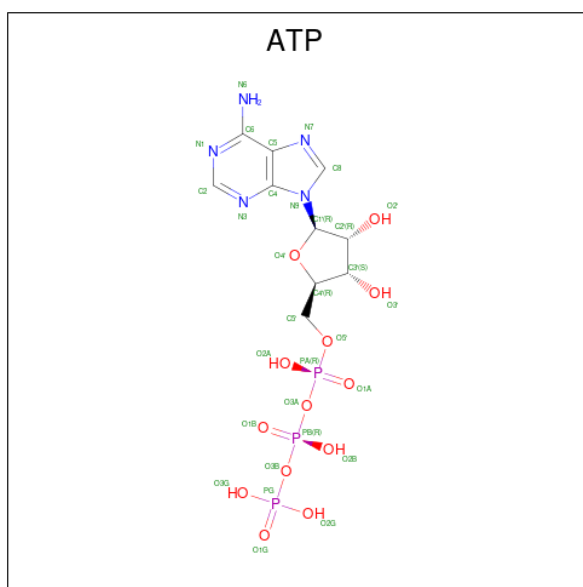
- Molecule 10 is a protein called 26S proteasome regulatory subunit RPN13.

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

- Molecule 11 is a protein called Probable 26S proteasome regulatory subunit p28.

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

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

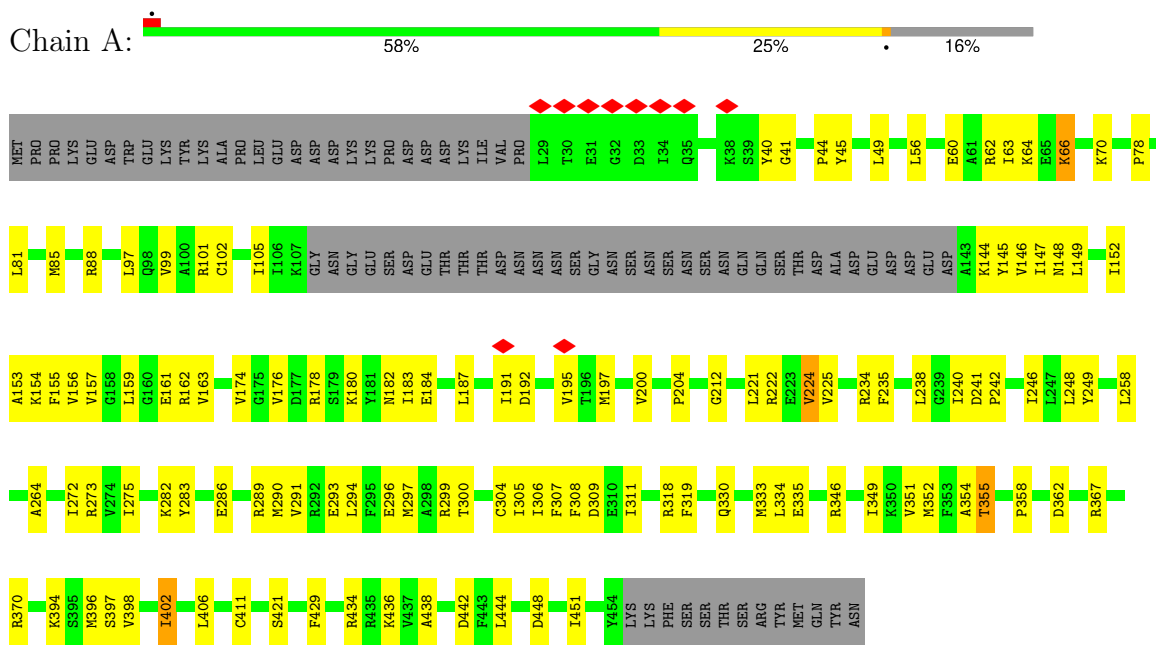


Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 31	C 10	N 5	O 13	P 3	0
12	B	1	Total 31	C 10	N 5	O 13	P 3	0
12	K	1	Total 31	C 10	N 5	O 13	P 3	0
12	P	1	Total 31	C 10	N 5	O 13	P 3	0
12	J	1	Total 31	C 10	N 5	O 13	P 3	0

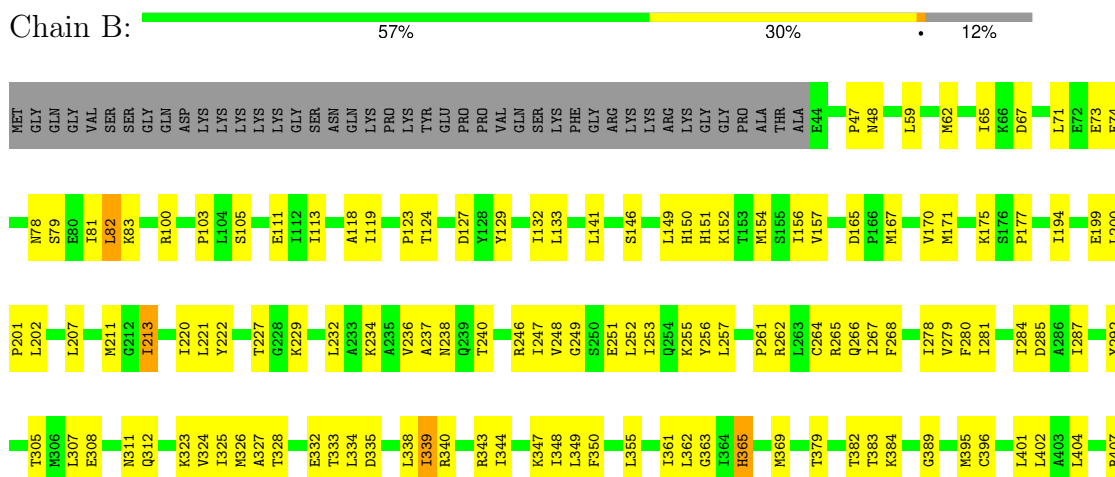
3 Residue-property plots

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: 26S proteasome regulatory subunit 7 homolog



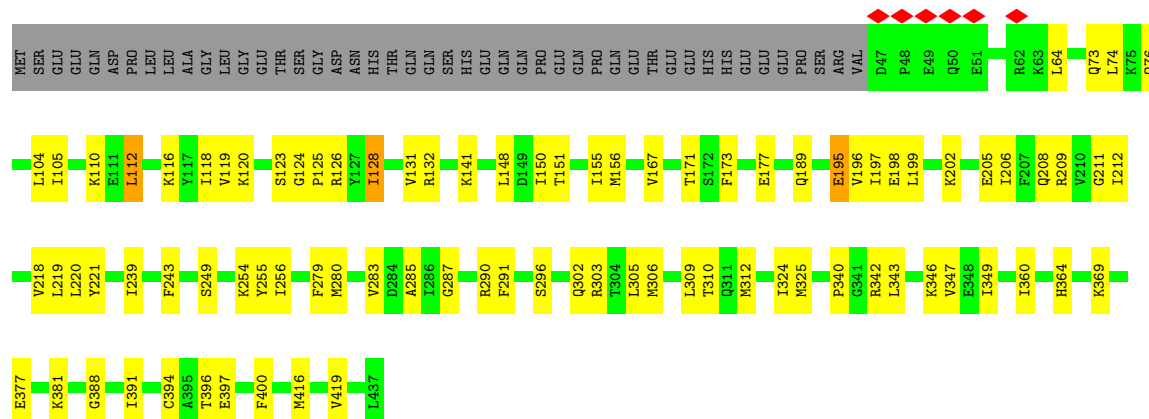
- Molecule 2: 26S proteasome regulatory subunit 4 homolog





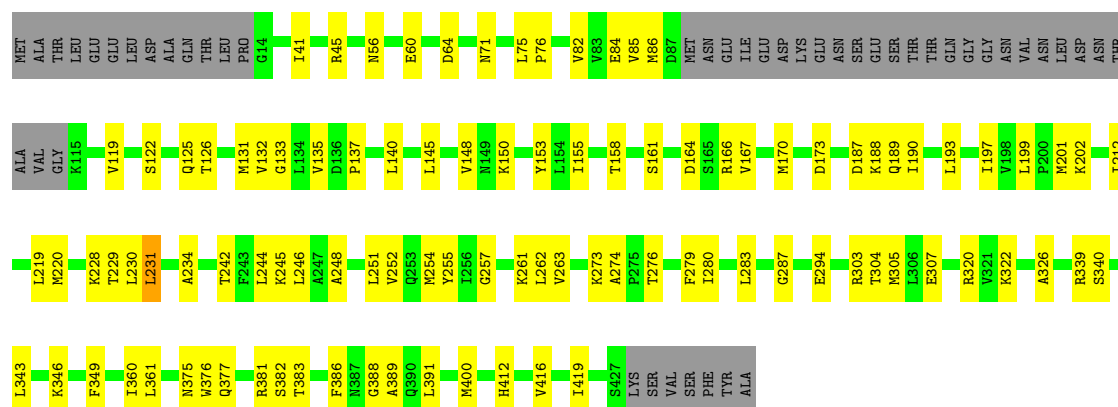
• Molecule 5: 26S proteasome subunit RPT4

Chain K: 69% 19% 11%



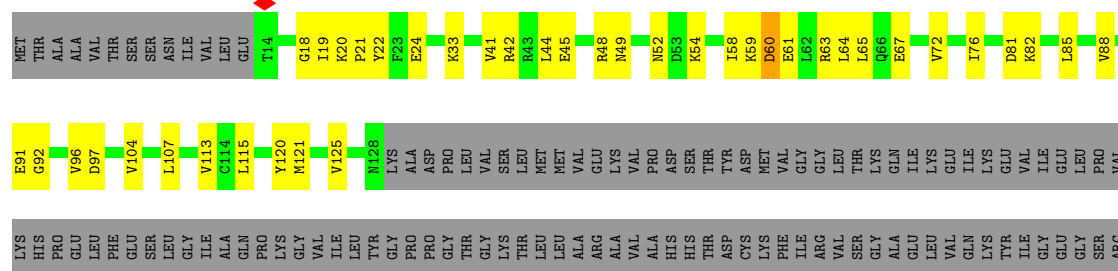
• Molecule 6: 26S proteasome regulatory subunit 6A

Chain P: 66% 23% 11%



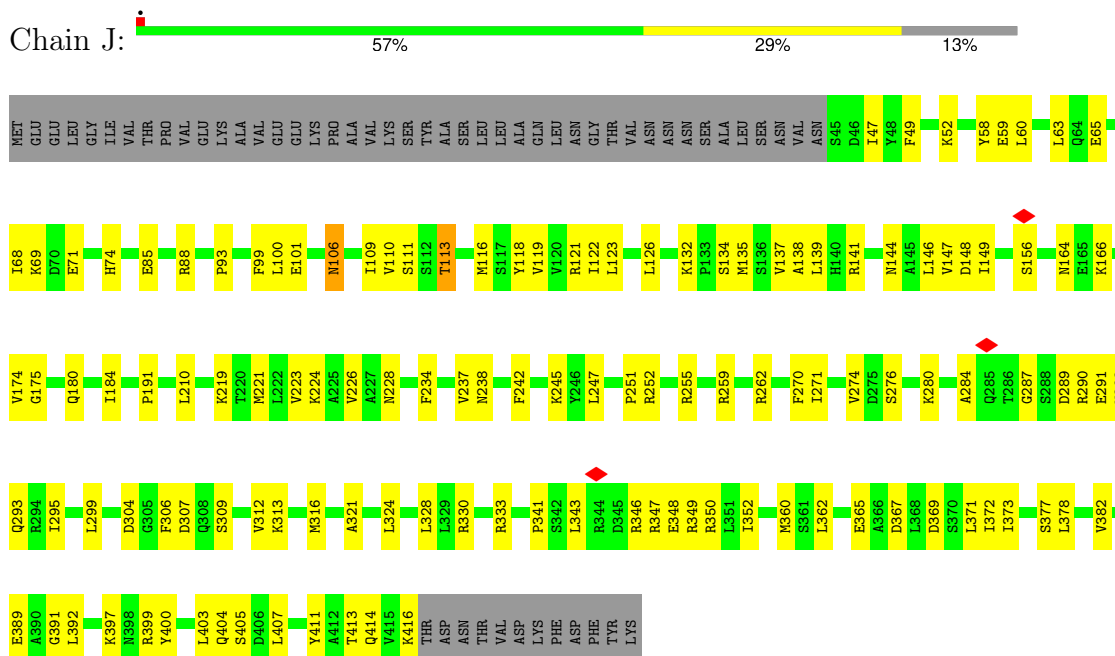
• Molecule 7: 26S proteasome regulatory subunit 8 homolog

Chain I: 19% 10% 72%

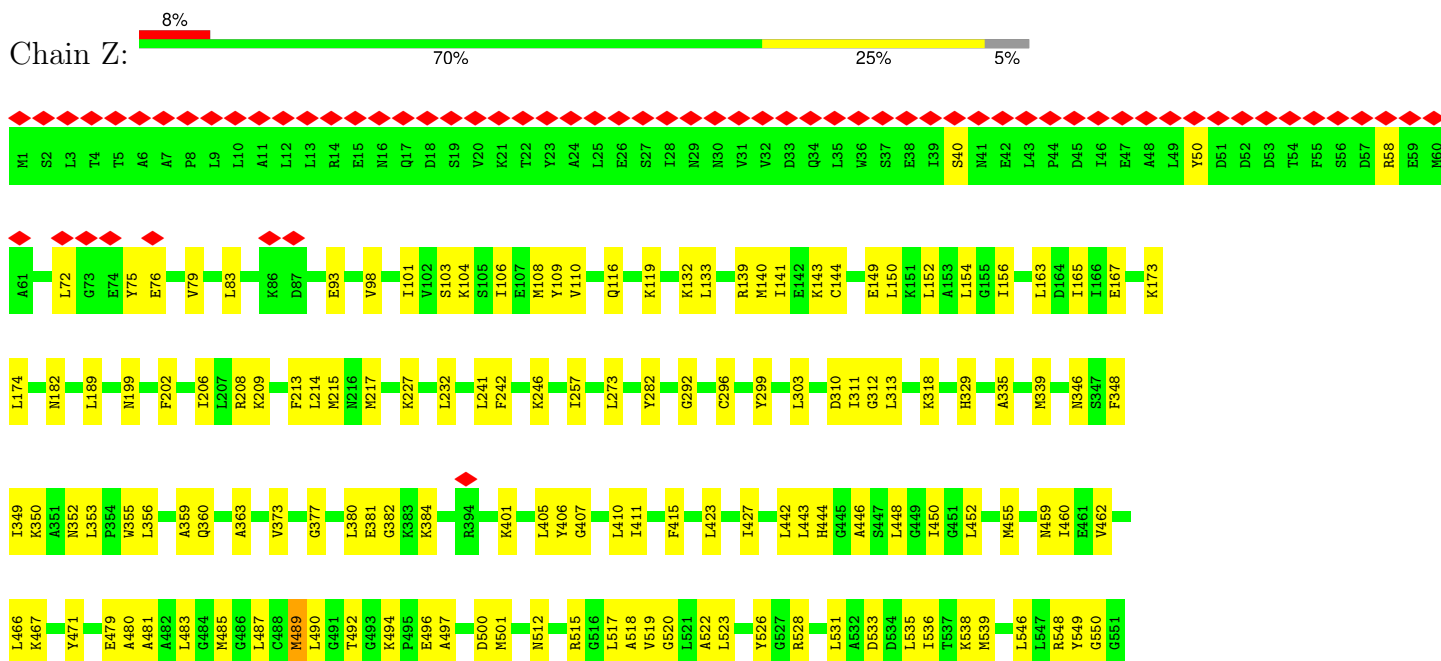


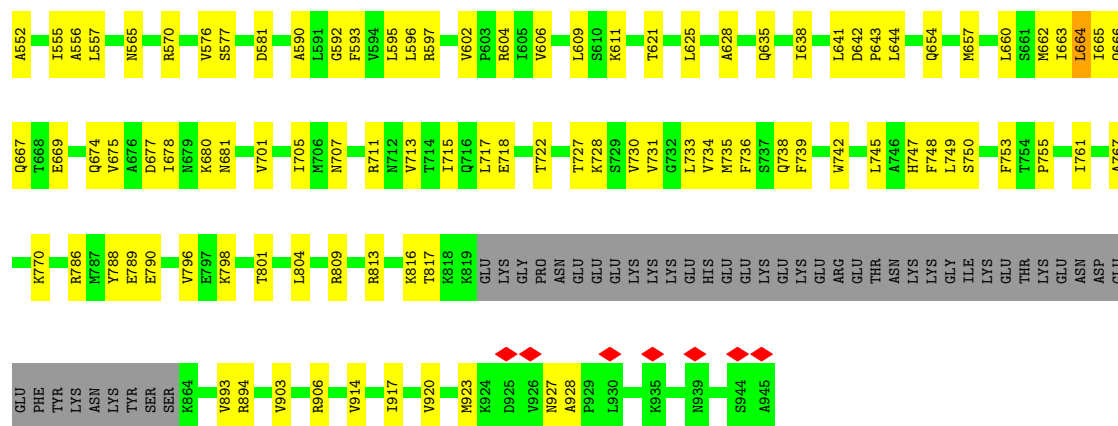
LYS MET ASN GLY CYS SER GLY ALA ASP VAL LYS VAL CYS THR TYR ALA LEU ARG GLU ARG ARG ILE HIS VAL THR THR GLN ASP PHE ASP GLU LEU LEU VAL VAL GLY LYS VAL MET MET ASN LYS ASN ASN GLN GLU THR THR ALA ALA LYS LYS PHE CYS

- Molecule 8: 26S proteasome regulatory subunit 6B homolog

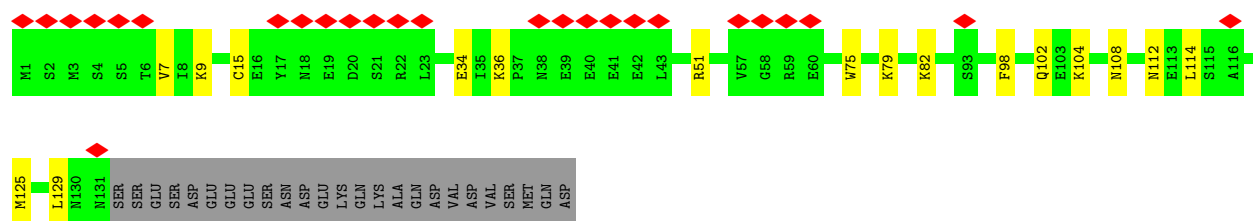
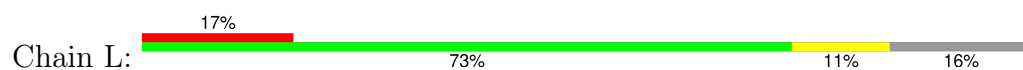


- Molecule 9: 26S proteasome regulatory subunit RPN2

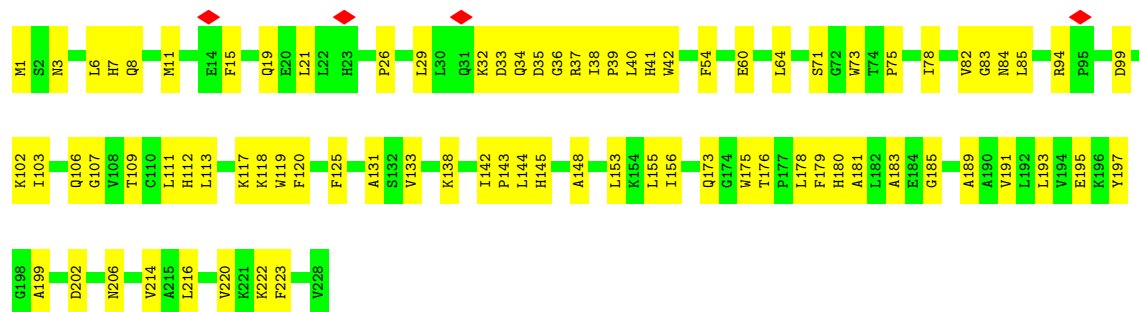




• Molecule 10: 26S proteasome regulatory subunit RPN13



• Molecule 11: Probable 26S proteasome regulatory subunit p28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241263	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	0.464	Depositor
Minimum map value	-0.192	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	536.576, 536.576, 536.576	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.20	0/3089	0.43	0/4162
2	B	0.15	0/3061	0.41	2/4124 (0.0%)
3	C	0.11	0/6687	0.30	0/9071
4	D	0.16	0/3900	0.35	0/5282
5	K	0.19	0/3153	0.36	0/4238
6	P	0.17	0/3065	0.35	0/4129
7	I	0.17	0/949	0.42	0/1271
8	J	0.16	0/2975	0.43	0/4016
9	Z	0.15	0/7067	0.36	0/9562
10	L	0.12	0/1087	0.34	0/1470
11	N	0.16	0/1851	0.44	0/2506
All	All	0.16	0/36884	0.37	2/49831 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	LEU	CA-C-N	-5.11	116.88	123.16
2	B	82	LEU	C-N-CA	-5.11	116.88	123.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	165	ASP	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	3042	0	3121	103	0
2	B	3020	0	3098	118	0
3	C	6569	0	6517	117	0
4	D	3832	0	3863	114	0
5	K	3106	0	3181	73	0
6	P	3030	0	3090	78	0
7	I	939	0	987	43	0
8	J	2935	0	3010	104	0
9	Z	6952	0	7033	171	0
10	L	1061	0	1050	12	0
11	N	1808	0	1792	63	0
12	A	31	0	12	2	0
12	B	31	0	12	2	0
12	J	31	0	12	1	0
12	K	31	0	12	3	0
12	P	31	0	12	6	0
All	All	36449	0	36802	887	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 12.

All (887) 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)
6:P:197:ILE:HD12	6:P:322:LYS:HB3	1.50	0.93
11:N:142:ILE:HD12	11:N:143:PRO:HD2	1.52	0.88
1:A:99:VAL:HG12	1:A:101:ARG:HH12	1.42	0.85
2:B:171:MET:HG3	2:B:247:ILE:HD11	1.63	0.81
6:P:219:LEU:HB2	6:P:343:LEU:HD13	1.60	0.81
4:D:324:THR:HG23	4:D:356:MET:HE2	1.66	0.78
6:P:220:MET:HG2	6:P:228:LYS:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:97:ASP:HB2	7:I:121:MET:HE1	1.67	0.76
8:J:403:LEU:HD23	8:J:405:SER:H	1.49	0.76
11:N:8:GLN:HA	11:N:11:MET:HE3	1.66	0.76
8:J:346:ARG:HH22	8:J:373:ILE:HA	1.49	0.76
5:K:219:LEU:HB2	5:K:343:LEU:HD13	1.68	0.76
1:A:49:LEU:HA	2:B:62:MET:HE1	1.67	0.75
7:I:44:LEU:HB3	8:J:68:ILE:HG21	1.66	0.75
7:I:64:LEU:HA	7:I:67:GLU:HG2	1.67	0.75
8:J:271:ILE:HB	8:J:316:MET:HE1	1.69	0.75
6:P:230:LEU:HD22	12:P:501:ATP:H2'	1.67	0.75
3:C:52:LEU:HD23	3:C:55:ARG:HH12	1.52	0.74
5:K:131:VAL:HG22	5:K:155:ILE:HD12	1.71	0.73
9:Z:717:LEU:HD21	9:Z:733:LEU:HD11	1.69	0.73
6:P:164:ASP:HB3	6:P:167:VAL:HG23	1.71	0.72
11:N:39:PRO:HA	11:N:42:TRP:HD1	1.54	0.72
2:B:113:ILE:HD11	2:B:119:ILE:HG13	1.72	0.72
2:B:249:GLY:HA2	2:B:252:LEU:HD12	1.72	0.71
4:D:310:ASP:HA	4:D:314:LEU:HB2	1.72	0.71
9:Z:606:VAL:HB	9:Z:621:THR:HG23	1.71	0.71
1:A:309:ASP:HA	1:A:354:ALA:HB3	1.72	0.70
5:K:112:LEU:HD11	5:K:118:ILE:HG13	1.72	0.70
6:P:76:PRO:HG2	6:P:150:LYS:HD3	1.73	0.70
9:Z:116:GLN:HA	9:Z:119:LYS:HZ3	1.57	0.69
2:B:220:ILE:HG22	2:B:347:LYS:HA	1.74	0.69
9:Z:150:LEU:HD22	9:Z:173:LYS:HD3	1.74	0.69
5:K:104:LEU:HD11	5:K:148:LEU:HD12	1.74	0.69
5:K:105:ILE:HD12	6:P:126:THR:HG22	1.75	0.69
8:J:316:MET:HE2	8:J:316:MET:HA	1.72	0.69
9:Z:489:MET:HE1	9:Z:497:ALA:HB3	1.73	0.69
4:D:336:VAL:HG21	4:D:366:CYS:HA	1.74	0.69
9:Z:786:ARG:HH12	9:Z:789:GLU:HB2	1.58	0.68
8:J:156:SER:HB3	8:J:259:ARG:HH12	1.56	0.68
8:J:347:ARG:HG2	8:J:350:ARG:HH22	1.58	0.68
8:J:397:LYS:HD2	8:J:399:ARG:HH21	1.57	0.68
6:P:248:ALA:HA	6:P:251:LEU:HD23	1.76	0.68
9:Z:535:LEU:HA	9:Z:538:LYS:HE2	1.75	0.68
4:D:109:ILE:HB	4:D:112:LEU:HD12	1.75	0.68
6:P:132:VAL:HG21	6:P:137:PRO:HB3	1.76	0.68
4:D:308:THR:HA	4:D:311:LYS:HE3	1.74	0.68
8:J:262:ARG:HH21	8:J:309:SER:HB3	1.59	0.68
3:C:460:SER:HA	3:C:496:ALA:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:293:ALA:HB2	4:D:329:LEU:HB3	1.76	0.68
8:J:99:PHE:HA	8:J:110:VAL:HG12	1.76	0.67
2:B:227:THR:HG21	2:B:350:PHE:HB3	1.74	0.67
3:C:827:LEU:HD22	3:C:855:LEU:HD13	1.75	0.67
3:C:285:ALA:HB1	3:C:294:ILE:HG12	1.76	0.67
1:A:308:PHE:HB3	1:A:311:ILE:HD13	1.76	0.67
3:C:750:GLU:HG3	3:C:753:GLY:H	1.59	0.67
9:Z:353:LEU:HA	9:Z:356:LEU:HD12	1.75	0.67
11:N:38:ILE:HD12	11:N:40:LEU:H	1.60	0.67
2:B:202:LEU:HB3	2:B:240:THR:HG21	1.76	0.66
11:N:71:SER:HG	11:N:73:TRP:CD1	2.13	0.66
1:A:45:TYR:HB3	2:B:59:LEU:HD22	1.78	0.66
5:K:126:ARG:HB3	8:J:113:THR:HG21	1.76	0.66
9:Z:500:ASP:HB2	9:Z:501:MET:HE2	1.77	0.66
2:B:132:ILE:HG12	2:B:156:ILE:HD12	1.77	0.66
4:D:261:LYS:HG2	4:D:305:LEU:HD22	1.77	0.66
6:P:131:MET:HE3	6:P:133:GLY:H	1.60	0.66
2:B:177:PRO:HB3	2:B:234:LYS:HG3	1.77	0.66
3:C:448:LYS:HE2	3:C:477:TYR:HE1	1.61	0.66
8:J:287:GLY:HA2	8:J:290:ARG:HD3	1.78	0.65
11:N:106:GLN:HA	11:N:138:LYS:HD2	1.78	0.65
1:A:290:MET:HE2	1:A:290:MET:H	1.60	0.65
4:D:166:ASP:HB3	4:D:169:ILE:HG22	1.77	0.65
2:B:83:LYS:HE2	3:C:626:PRO:HD2	1.78	0.65
9:Z:50:TYR:HA	9:Z:58:ARG:HB2	1.79	0.65
2:B:177:PRO:HB2	2:B:238:ASN:HB2	1.78	0.65
4:D:412:MET:HE3	4:D:412:MET:HA	1.79	0.65
9:Z:140:MET:HE3	9:Z:140:MET:HA	1.79	0.65
5:K:285:ALA:HB1	6:P:303:ARG:HG2	1.78	0.64
1:A:293:GLU:O	1:A:296:GLU:HG3	1.97	0.64
4:D:126:LYS:HB3	4:D:163:LEU:HD22	1.79	0.64
6:P:201:MET:HE2	6:P:322:LYS:HG2	1.80	0.64
9:Z:669:GLU:HG3	9:Z:675:VAL:HB	1.78	0.64
1:A:174:VAL:HB	1:A:183:ILE:HG23	1.80	0.64
8:J:330:ARG:HH11	8:J:333:ARG:HG3	1.62	0.64
9:Z:79:VAL:HG21	9:Z:104:LYS:HG3	1.80	0.64
1:A:148:ASN:HB2	1:A:154:LYS:HZ3	1.63	0.64
9:Z:75:TYR:HB3	9:Z:104:LYS:HG2	1.79	0.64
4:D:357:LEU:HG	4:D:393:THR:HG21	1.78	0.63
8:J:60:LEU:HB3	9:Z:604:ARG:HH22	1.62	0.63
2:B:265:ARG:HG2	2:B:312:GLN:HE21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:85:LEU:HD11	11:N:125:PHE:HD2	1.62	0.63
9:Z:641:LEU:HD23	9:Z:644:LEU:HD12	1.81	0.63
1:A:221:LEU:HD22	1:A:352:MET:HE2	1.81	0.63
3:C:813:PHE:HB2	3:C:847:ILE:HD11	1.80	0.62
10:L:15:CYS:HB2	10:L:98:PHE:HB3	1.81	0.62
1:A:146:VAL:HG22	1:A:156:VAL:HG22	1.80	0.62
3:C:824:ASN:H	3:C:855:LEU:HD11	1.64	0.62
7:I:49:ASN:HA	9:Z:611:LYS:HZ1	1.63	0.62
4:D:264:LEU:HD23	4:D:305:LEU:HD21	1.81	0.62
8:J:290:ARG:H	8:J:290:ARG:HD2	1.64	0.62
1:A:149:LEU:HD21	1:A:152:ILE:HD12	1.82	0.62
7:I:59:LYS:HG3	7:I:63:ARG:HH21	1.63	0.62
4:D:7:ASN:HD21	4:D:46:LEU:HD11	1.65	0.62
4:D:178:LEU:HA	4:D:181:LEU:HD12	1.81	0.62
5:K:340:PRO:HD2	8:J:382:VAL:HG22	1.81	0.62
8:J:139:LEU:HD13	8:J:144:ASN:HA	1.82	0.62
9:Z:93:GLU:HB3	9:Z:98:VAL:HG21	1.82	0.62
11:N:78:ILE:H	11:N:78:ILE:HD12	1.63	0.62
3:C:157:LEU:HD23	3:C:207:ILE:HD11	1.82	0.62
9:Z:539:MET:O	9:Z:548:ARG:HG2	2.00	0.62
7:I:72:VAL:HG22	8:J:119:VAL:HG23	1.81	0.62
9:Z:770:LYS:HD3	9:Z:917:ILE:HG13	1.81	0.61
1:A:56:LEU:HD11	2:B:62:MET:HG3	1.82	0.61
11:N:178:LEU:HD13	11:N:193:LEU:HD12	1.82	0.61
11:N:1:MET:HE3	11:N:3:ASN:H	1.65	0.61
6:P:219:LEU:HB3	6:P:346:LYS:HG2	1.83	0.61
3:C:756:MET:HE2	3:C:756:MET:N	2.15	0.61
2:B:167:MET:HE3	2:B:267:ILE:HG13	1.82	0.61
5:K:306:MET:HA	5:K:309:LEU:HD12	1.82	0.61
8:J:137:VAL:HG12	8:J:149:ILE:HA	1.83	0.60
9:Z:522:ALA:HB1	9:Z:557:LEU:HD13	1.83	0.60
1:A:183:ILE:H	1:A:183:ILE:HD12	1.66	0.60
6:P:360:ILE:HG22	6:P:391:LEU:HD22	1.83	0.60
4:D:109:ILE:HG22	4:D:111:PRO:HD2	1.83	0.60
4:D:55:LEU:HD11	4:D:83:LEU:HD12	1.83	0.60
9:Z:788:TYR:HE1	9:Z:790:GLU:HG3	1.67	0.60
2:B:324:VAL:HG22	2:B:326:MET:HE3	1.84	0.60
5:K:396:THR:HA	6:P:212:ILE:HG21	1.83	0.59
7:I:121:MET:HA	7:I:121:MET:HE2	1.83	0.59
1:A:162:ARG:HH22	1:A:184:GLU:CD	2.11	0.59
2:B:154:MET:HE2	2:B:154:MET:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:280:MET:HE3	5:K:283:VAL:HG23	1.84	0.59
9:Z:154:LEU:HD13	9:Z:189:LEU:HD21	1.85	0.59
9:Z:546:LEU:O	9:Z:549:TYR:HB3	2.01	0.59
2:B:422:ARG:HA	2:B:425:LYS:HE3	1.84	0.59
3:C:944:LYS:HB3	3:C:962:ARG:HH11	1.68	0.59
9:Z:654:GLN:HA	9:Z:657:MET:HE2	1.85	0.59
9:Z:104:LYS:HD2	9:Z:104:LYS:O	2.03	0.58
11:N:176:THR:HG23	11:N:178:LEU:H	1.68	0.58
4:D:339:HIS:HB3	4:D:342:VAL:HB	1.83	0.58
11:N:176:THR:HG22	11:N:179:PHE:CD1	2.38	0.58
1:A:187:LEU:HD22	2:B:119:ILE:HD11	1.86	0.58
2:B:281:ILE:HG22	2:B:326:MET:HA	1.85	0.58
2:B:335:ASP:HB3	2:B:338:LEU:HD13	1.83	0.58
3:C:279:THR:HG21	3:C:974:THR:HA	1.84	0.58
5:K:195:GLU:HA	5:K:199:LEU:HG	1.85	0.58
8:J:367:ASP:HB3	8:J:404:GLN:NE2	2.18	0.58
1:A:272:ILE:HB	1:A:306:ILE:HD13	1.85	0.58
9:Z:556:ALA:HB2	9:Z:590:ALA:HB1	1.86	0.58
3:C:282:ILE:HB	3:C:297:VAL:HG11	1.85	0.58
5:K:189:GLN:HG2	5:K:349:ILE:HD13	1.84	0.58
1:A:162:ARG:HE	1:A:162:ARG:H	1.50	0.58
8:J:191:PRO:HB2	8:J:313:LYS:HZ3	1.68	0.58
3:C:777:PRO:HA	3:C:780:MET:HG2	1.86	0.58
7:I:54:LYS:O	7:I:58:ILE:HG12	2.03	0.58
8:J:367:ASP:HB3	8:J:404:GLN:HE21	1.69	0.58
4:D:20:LEU:HD11	4:D:57:THR:HB	1.87	0.57
1:A:319:PHE:HB3	4:D:464:ASN:HD21	1.69	0.57
3:C:986:ASN:HB3	3:C:989:TYR:HB2	1.86	0.57
5:K:110:LYS:HB3	5:K:118:ILE:HD12	1.85	0.57
5:K:212:ILE:HG21	8:J:391:GLY:HA3	1.86	0.57
6:P:246:LEU:HD12	6:P:251:LEU:HD21	1.85	0.57
9:Z:609:LEU:HD12	9:Z:609:LEU:H	1.69	0.57
3:C:894:MET:O	3:C:894:MET:HE3	2.03	0.57
3:C:147:GLU:HA	3:C:154:ILE:HD11	1.87	0.57
1:A:161:GLU:HG2	1:A:162:ARG:HD3	1.86	0.57
5:K:177:GLU:CD	5:K:177:GLU:H	2.13	0.57
8:J:365:GLU:HB3	11:N:78:ILE:HG23	1.86	0.57
2:B:79:SER:HA	2:B:83:LYS:HE3	1.86	0.57
8:J:122:ILE:HG23	8:J:146:LEU:HD22	1.85	0.57
9:Z:460:ILE:HD12	9:Z:460:ILE:H	1.68	0.57
11:N:83:GLY:HA3	11:N:119:TRP:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:221:MET:HA	8:J:224:LYS:HD2	1.86	0.56
8:J:274:VAL:HB	8:J:316:MET:SD	2.45	0.56
2:B:103:PRO:HG3	7:I:120:TYR:CD1	2.40	0.56
2:B:253:ILE:HD13	2:B:287:ILE:HD12	1.85	0.56
3:C:894:MET:HE1	3:C:898:HIS:HA	1.88	0.56
9:Z:149:GLU:HB3	9:Z:152:LEU:HD12	1.87	0.56
1:A:144:LYS:HG2	6:P:75:LEU:HD11	1.87	0.56
2:B:395:MET:HE1	2:B:420:LYS:HB2	1.88	0.56
4:D:143:PHE:HA	4:D:195:ARG:HD2	1.87	0.56
5:K:209:ARG:HB3	8:J:400:TYR:HE1	1.69	0.56
9:Z:401:LYS:HB3	9:Z:442:LEU:HD11	1.86	0.56
9:Z:536:ILE:HA	9:Z:539:MET:HE1	1.88	0.56
6:P:231:LEU:HD23	6:P:349:PHE:HZ	1.70	0.56
11:N:82:VAL:HG12	11:N:84:ASN:H	1.70	0.56
4:D:307:LYS:HE3	4:D:338:TYR:CD2	2.40	0.56
3:C:894:MET:HE2	3:C:901:PHE:CZ	2.41	0.56
9:Z:665:ILE:HG23	9:Z:666:GLN:HG3	1.88	0.56
1:A:176:VAL:HG12	1:A:183:ILE:HA	1.88	0.56
3:C:224:LEU:HD23	3:C:227:ILE:HD11	1.87	0.56
2:B:154:MET:HE2	2:B:154:MET:N	2.21	0.56
5:K:131:VAL:HA	5:K:155:ILE:HB	1.88	0.56
1:A:178:ARG:HH22	2:B:154:MET:HE3	1.71	0.55
1:A:434:ARG:HH12	2:B:200:LEU:HD11	1.70	0.55
4:D:306:PHE:HA	4:D:309:MET:HB2	1.88	0.55
11:N:113:LEU:H	11:N:113:LEU:HD12	1.72	0.55
1:A:282:LYS:HA	2:B:292:TYR:HE1	1.70	0.55
4:D:319:GLU:HG3	4:D:322:LEU:HD12	1.89	0.55
6:P:375:ASN:HB3	6:P:412:HIS:HE1	1.69	0.55
2:B:292:TYR:CE2	4:D:425:ILE:HG12	2.41	0.55
7:I:88:VAL:HB	7:I:91:GLU:HG2	1.88	0.55
9:Z:713:VAL:HG12	9:Z:755:PRO:HA	1.89	0.55
2:B:78:ASN:HA	2:B:81:ILE:HD12	1.88	0.55
2:B:284:ILE:HG22	2:B:327:ALA:O	2.07	0.55
8:J:349:ARG:HD3	8:J:378:LEU:HD12	1.88	0.55
3:C:575:MET:HG3	3:C:875:LYS:HD3	1.87	0.55
11:N:41:HIS:CE1	11:N:75:PRO:HG3	2.42	0.55
11:N:173:GLN:HB2	11:N:175:TRP:CD1	2.42	0.55
4:D:353:SER:HA	4:D:356:MET:HE3	1.87	0.55
9:Z:318:LYS:HE3	9:Z:355:TRP:HB2	1.87	0.55
9:Z:736:PHE:CD2	9:Z:749:LEU:HB2	2.42	0.55
11:N:60:GLU:HA	11:N:94:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:824:ASN:N	3:C:855:LEU:HD11	2.22	0.55
4:D:231:ILE:HD13	4:D:279:ASP:HB3	1.88	0.55
1:A:294:LEU:HD21	1:A:306:ILE:HD12	1.89	0.55
3:C:173:ALA:HA	9:Z:816:LYS:HE3	1.89	0.55
4:D:117:CYS:HA	4:D:120:ILE:HD12	1.88	0.55
5:K:303:ARG:HG2	8:J:276:SER:HB2	1.89	0.55
1:A:70:LYS:HE2	7:I:81:ASP:H	1.71	0.54
4:D:317:GLY:HA2	4:D:323:ILE:HG12	1.89	0.54
4:D:367:PHE:HA	4:D:370:ILE:HG22	1.89	0.54
9:Z:593:PHE:HA	9:Z:596:LEU:HD23	1.89	0.54
11:N:142:ILE:HG13	11:N:144:LEU:H	1.72	0.54
1:A:224:VAL:HG21	1:A:246:ILE:HB	1.89	0.54
1:A:318:ARG:HH22	4:D:463:VAL:HG22	1.71	0.54
2:B:415:ASP:HA	2:B:418:GLN:NE2	2.22	0.54
3:C:285:ALA:HA	3:C:293:MET:HE1	1.88	0.54
1:A:238:LEU:HB3	1:A:240:ILE:HG22	1.89	0.54
9:Z:536:ILE:HA	9:Z:539:MET:CE	2.37	0.54
9:Z:701:VAL:O	9:Z:705:ILE:HG12	2.07	0.54
11:N:176:THR:HG22	11:N:179:PHE:HD1	1.72	0.54
2:B:167:MET:HE1	2:B:266:GLN:HB3	1.90	0.54
4:D:79:VAL:O	4:D:83:LEU:HG	2.08	0.54
1:A:299:ARG:HA	1:A:349:ILE:HD11	1.88	0.54
2:B:279:VAL:HG13	2:B:324:VAL:HG23	1.90	0.54
10:L:75:TRP:CG	10:L:125:MET:HG2	2.43	0.54
1:A:406:LEU:HD21	4:D:191:VAL:HG22	1.89	0.54
6:P:167:VAL:HA	6:P:170:MET:SD	2.48	0.54
7:I:107:LEU:HD12	7:I:107:LEU:H	1.72	0.54
8:J:175:GLY:HA3	8:J:352:ILE:HA	1.89	0.54
8:J:60:LEU:HB3	9:Z:604:ARG:HH12	1.73	0.54
2:B:281:ILE:HG21	2:B:284:ILE:HB	1.89	0.53
8:J:65:GLU:HA	8:J:68:ILE:HD12	1.90	0.53
9:Z:167:GLU:HG3	9:Z:213:PHE:CZ	2.43	0.53
9:Z:427:ILE:HD12	9:Z:443:LEU:HD22	1.89	0.53
4:D:448:LEU:HD12	4:D:452:TYR:HD1	1.74	0.53
1:A:290:MET:HE2	1:A:290:MET:N	2.23	0.53
4:D:67:SER:HA	4:D:73:TYR:HE2	1.73	0.53
5:K:156:MET:HE3	5:K:156:MET:HA	1.89	0.53
5:K:211:GLY:HA3	8:J:360:MET:HG2	1.90	0.53
5:K:388:GLY:HA2	5:K:391:ILE:HD12	1.90	0.53
1:A:221:LEU:HD21	1:A:248:LEU:HD21	1.90	0.53
4:D:476:ILE:HD12	8:J:247:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:100:LEU:HD11	8:J:111:SER:HB2	1.91	0.53
2:B:62:MET:HA	2:B:65:ILE:HD12	1.90	0.53
9:Z:215:MET:HE1	9:Z:241:LEU:HA	1.90	0.53
2:B:146:SER:N	2:B:262:ARG:HH12	2.05	0.53
4:D:445:GLU:HG2	4:D:452:TYR:CD2	2.44	0.53
6:P:242:THR:HB	6:P:276:THR:HG23	1.91	0.53
9:Z:106:ILE:HD11	9:Z:140:MET:HG3	1.90	0.53
11:N:133:VAL:O	11:N:142:ILE:HD11	2.09	0.53
2:B:105:SER:OG	2:B:149:LEU:HB2	2.09	0.53
3:C:894:MET:HE2	3:C:901:PHE:CE2	2.43	0.53
11:N:178:LEU:HD22	11:N:199:ALA:HB1	1.91	0.53
1:A:145:TYR:CE2	1:A:159:LEU:HG	2.44	0.53
7:I:48:ARG:HG3	8:J:71:GLU:OE2	2.08	0.53
8:J:166:LYS:HD3	8:J:228:ASN:HA	1.90	0.53
8:J:284:ALA:HB1	8:J:289:ASP:HB3	1.90	0.53
3:C:415:MET:SD	3:C:447:VAL:HG22	2.48	0.52
4:D:271:PHE:HB2	4:D:288:LEU:HD13	1.91	0.52
8:J:413:THR:HA	8:J:416:LYS:HE3	1.92	0.52
2:B:81:ILE:HG22	2:B:82:LEU:HG	1.91	0.52
2:B:133:LEU:HD12	2:B:157:VAL:HG12	1.92	0.52
4:D:401:SER:O	4:D:405:LEU:HD12	2.09	0.52
6:P:41:ILE:HG22	6:P:45:ARG:HE	1.74	0.52
6:P:187:ASP:HA	6:P:190:ILE:HD12	1.90	0.52
6:P:361:LEU:HA	6:P:391:LEU:HD21	1.92	0.52
6:P:377:GLN:O	6:P:381:ARG:HG3	2.08	0.52
8:J:93:PRO:HG2	8:J:141:ARG:HD2	1.91	0.52
11:N:7:HIS:CE1	11:N:33:ASP:HB3	2.44	0.52
5:K:388:GLY:HA3	12:K:501:ATP:C8	2.45	0.52
7:I:76:ILE:HB	7:I:85:LEU:HG	1.91	0.52
8:J:210:LEU:HA	8:J:316:MET:HB3	1.92	0.52
1:A:204:PRO:HG2	1:A:264:ALA:HB3	1.91	0.52
7:I:18:GLY:HA2	9:Z:140:MET:HE2	1.92	0.52
9:Z:329:HIS:CE1	9:Z:359:ALA:HB2	2.44	0.52
6:P:242:THR:HG21	6:P:273:LYS:HD3	1.91	0.52
9:Z:761:ILE:HG13	9:Z:767:ALA:O	2.09	0.52
1:A:318:ARG:CZ	1:A:318:ARG:HA	2.39	0.52
1:A:444:LEU:HD11	4:D:232:LEU:HB2	1.91	0.52
3:C:157:LEU:HD21	3:C:203:LEU:HD21	1.92	0.52
5:K:310:THR:HG21	8:J:238:ASN:ND2	2.24	0.52
6:P:84:GLU:HG3	6:P:86:MET:HE1	1.92	0.52
8:J:369:ASP:HA	8:J:372:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:HA	1:A:355:THR:O	2.10	0.52
4:D:120:ILE:HA	4:D:129:PHE:HE2	1.75	0.52
9:Z:174:LEU:HD23	9:Z:182:ASN:HB3	1.91	0.52
11:N:175:TRP:HZ3	11:N:214:VAL:HG21	1.74	0.52
4:D:394:LEU:HD13	4:D:404:LEU:HD13	1.92	0.51
7:I:19:ILE:HD12	9:Z:144:CYS:HB2	1.92	0.51
3:C:225:LEU:HB2	3:C:264:PHE:HZ	1.75	0.51
6:P:388:GLY:HA3	12:P:501:ATP:C8	2.45	0.51
8:J:65:GLU:HG2	8:J:69:LYS:NZ	2.25	0.51
8:J:251:PRO:HD3	8:J:295:ILE:HG12	1.92	0.51
9:Z:674:GLN:O	9:Z:678:ILE:HG12	2.10	0.51
1:A:258:LEU:HD22	12:A:501:ATP:H2'	1.92	0.51
2:B:326:MET:HA	2:B:326:MET:HE2	1.92	0.51
3:C:765:MET:HE2	3:C:799:PHE:CE2	2.45	0.51
7:I:20:LYS:NZ	9:Z:152:LEU:HD11	2.26	0.51
9:Z:552:ALA:O	9:Z:555:ILE:HG22	2.09	0.51
2:B:175:LYS:HE2	2:B:175:LYS:HA	1.93	0.51
3:C:990:ARG:H	3:C:990:ARG:HD3	1.75	0.51
2:B:332:GLU:HB2	4:D:429:THR:HG21	1.92	0.51
4:D:241:TYR:HA	4:D:244:PHE:HB3	1.92	0.51
11:N:120:PHE:HD2	11:N:155:LEU:HD22	1.74	0.51
1:A:225:VAL:HG21	1:A:305:ILE:HD11	1.92	0.51
3:C:290:GLU:O	3:C:294:ILE:HG13	2.11	0.51
5:K:254:LYS:O	5:K:254:LYS:HG2	2.10	0.51
9:Z:520:GLY:HA2	9:Z:523:LEU:HD12	1.92	0.51
10:L:125:MET:O	10:L:129:LEU:HD12	2.10	0.51
4:D:445:GLU:HG2	4:D:452:TYR:CG	2.46	0.51
7:I:19:ILE:HD13	9:Z:156:ILE:HG21	1.93	0.51
2:B:100:ARG:HG2	2:B:157:VAL:HB	1.93	0.51
9:Z:360:GLN:H	9:Z:363:ALA:HB3	1.74	0.51
2:B:365:HIS:HB3	2:B:396:CYS:SG	2.51	0.51
5:K:116:LYS:HB3	5:K:128:ILE:HD11	1.92	0.51
9:Z:660:LEU:HA	9:Z:663:ILE:HD12	1.91	0.51
11:N:1:MET:HE3	11:N:3:ASN:N	2.26	0.51
1:A:66:LYS:HZ1	2:B:73:GLU:HA	1.76	0.51
11:N:191:VAL:O	11:N:195:GLU:HG3	2.11	0.51
2:B:194:ILE:HD13	2:B:232:LEU:HG	1.93	0.50
4:D:328:GLU:HG2	4:D:356:MET:N	2.26	0.50
5:K:364:HIS:HE1	12:K:501:ATP:N3	2.09	0.50
1:A:99:VAL:HB	2:B:127:ASP:OD2	2.10	0.50
5:K:291:PHE:CZ	6:P:294:GLU:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:LEU:HD22	2:B:383:THR:HG23	1.92	0.50
4:D:125:PRO:HD2	4:D:128:LEU:HD21	1.93	0.50
4:D:367:PHE:CE2	4:D:400:THR:HA	2.46	0.50
8:J:106:ASN:HB3	8:J:121:ARG:HE	1.75	0.50
4:D:299:GLU:HG3	4:D:303:TYR:CE1	2.46	0.50
8:J:100:LEU:HB2	8:J:109:ILE:HG23	1.94	0.50
1:A:282:LYS:HD3	1:A:283:TYR:CZ	2.46	0.50
8:J:174:VAL:HG22	8:J:221:MET:HE2	1.94	0.50
9:Z:339:MET:HA	9:Z:707:ASN:O	2.12	0.50
7:I:41:VAL:O	7:I:45:GLU:HG3	2.11	0.50
7:I:63:ARG:HG3	7:I:64:LEU:HD22	1.94	0.50
8:J:292:VAL:HA	8:J:295:ILE:HD12	1.93	0.50
3:C:765:MET:HE1	3:C:773:ARG:HA	1.94	0.50
9:Z:479:GLU:O	9:Z:483:LEU:HD12	2.11	0.50
4:D:152:LEU:O	4:D:156:ILE:HG12	2.12	0.50
5:K:279:PHE:HD1	5:K:324:ILE:HB	1.77	0.50
5:K:312:MET:HE1	5:K:325:MET:HE1	1.93	0.50
4:D:126:LYS:HE2	4:D:166:ASP:HB2	1.93	0.50
5:K:123:SER:HB3	6:P:125:GLN:HG2	1.93	0.50
6:P:287:GLY:HA2	6:P:305:MET:HG3	1.93	0.50
9:Z:407:GLY:HA2	9:Z:410:LEU:HD12	1.94	0.50
11:N:193:LEU:HA	11:N:197:TYR:HD1	1.76	0.50
1:A:411:CYS:SG	1:A:451:ILE:HG13	2.52	0.49
4:D:468:TYR:HA	6:P:254:MET:HE1	1.93	0.49
8:J:123:LEU:HB3	8:J:126:LEU:CD1	2.42	0.49
1:A:396:MET:HE1	2:B:213:ILE:HG22	1.94	0.49
4:D:144:ASP:OD1	4:D:146:LYS:HG2	2.12	0.49
5:K:287:GLY:HA2	5:K:305:LEU:HD13	1.93	0.49
1:A:367:ARG:HB2	1:A:370:ARG:HD2	1.94	0.49
3:C:422:ILE:HB	3:C:436:LEU:HD21	1.93	0.49
6:P:199:LEU:HD13	6:P:202:LYS:HE2	1.94	0.49
8:J:71:GLU:HA	9:Z:576:VAL:HG11	1.95	0.49
2:B:150:HIS:CE1	2:B:152:LYS:HB2	2.48	0.49
3:C:617:ILE:HG23	3:C:743:ILE:HG12	1.95	0.49
4:D:139:LEU:HD12	4:D:143:PHE:CE2	2.47	0.49
5:K:123:SER:C	5:K:125:PRO:HD2	2.37	0.49
8:J:180:GLN:HE22	8:J:341:PRO:HD3	1.76	0.49
9:Z:678:ILE:HA	9:Z:681:ASN:ND2	2.27	0.49
11:N:222:LYS:HD2	11:N:223:PHE:N	2.28	0.49
1:A:97:LEU:HB2	2:B:129:TYR:HB3	1.94	0.49
2:B:246:ARG:HG3	2:B:280:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:26:PRO:O	11:N:29:LEU:HD22	2.13	0.49
2:B:280:PHE:HA	2:B:325:ILE:O	2.13	0.49
6:P:360:ILE:HG23	12:P:501:ATP:C2	2.47	0.49
9:Z:494:LYS:HD2	9:Z:497:ALA:H	1.78	0.49
11:N:37:ARG:HD3	11:N:41:HIS:HB2	1.94	0.49
3:C:374:LEU:HD23	3:C:842:GLN:HG2	1.93	0.49
4:D:474:THR:HA	6:P:255:TYR:CD2	2.48	0.49
6:P:228:LYS:HD2	6:P:326:ALA:HB1	1.93	0.49
8:J:63:LEU:HD21	9:Z:565:ASN:HB3	1.95	0.49
1:A:157:VAL:HG12	6:P:76:PRO:HB3	1.94	0.49
5:K:119:VAL:HG11	5:K:148:LEU:HD11	1.95	0.49
5:K:396:THR:HG22	5:K:400:PHE:CE2	2.48	0.49
9:Z:635:GLN:HA	9:Z:638:ILE:HD12	1.94	0.49
3:C:609:THR:HG21	3:C:878:LEU:HD21	1.94	0.49
8:J:328:LEU:HD12	8:J:328:LEU:H	1.78	0.49
1:A:195:VAL:HG21	2:B:311:ASN:HD22	1.78	0.49
8:J:289:ASP:O	8:J:293:GLN:HG3	2.13	0.49
1:A:44:PRO:HA	3:C:159:LEU:HD22	1.95	0.48
6:P:166:ARG:O	6:P:170:MET:HG3	2.13	0.48
8:J:65:GLU:HG2	8:J:69:LYS:HZ1	1.78	0.48
9:Z:382:GLY:HA3	9:Z:411:ILE:HG21	1.95	0.48
9:Z:606:VAL:HA	9:Z:609:LEU:HD13	1.95	0.48
11:N:185:GLY:HA3	11:N:216:LEU:HD13	1.94	0.48
3:C:790:MET:HA	3:C:793:PHE:CE2	2.48	0.48
4:D:135:ILE:HG21	4:D:172:ARG:HG2	1.94	0.48
8:J:262:ARG:HG2	8:J:312:VAL:HG21	1.94	0.48
9:Z:459:ASN:HB3	9:Z:462:VAL:HG22	1.94	0.48
3:C:970:TYR:HB3	3:C:983:LEU:HB3	1.94	0.48
4:D:328:GLU:HG2	4:D:355:GLY:C	2.39	0.48
5:K:205:GLU:HA	5:K:208:GLN:NE2	2.28	0.48
6:P:148:VAL:HG12	6:P:155:ILE:HD13	1.94	0.48
9:Z:662:MET:HE1	9:Z:715:ILE:HG21	1.96	0.48
2:B:111:GLU:OE1	2:B:119:ILE:HB	2.14	0.48
3:C:813:PHE:HE2	3:C:901:PHE:CE1	2.30	0.48
4:D:367:PHE:HE2	4:D:400:THR:HA	1.77	0.48
6:P:135:VAL:HG11	6:P:158:THR:HG23	1.94	0.48
7:I:61:GLU:O	7:I:65:LEU:HG	2.13	0.48
7:I:96:VAL:HG11	7:I:115:LEU:HD13	1.94	0.48
9:Z:167:GLU:HG3	9:Z:213:PHE:HZ	1.78	0.48
2:B:177:PRO:HG2	2:B:237:ALA:HB3	1.94	0.48
6:P:85:VAL:HG22	6:P:140:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:602:VAL:HG12	9:Z:625:LEU:HD23	1.96	0.48
3:C:781:GLY:HA3	3:C:817:LEU:HD12	1.96	0.48
6:P:82:VAL:HG21	6:P:140:LEU:HD11	1.96	0.48
3:C:570:LEU:HD23	3:C:603:VAL:HG21	1.96	0.48
9:Z:518:ALA:HB1	9:Z:550:GLY:HA3	1.95	0.48
1:A:66:LYS:NZ	2:B:73:GLU:HA	2.27	0.48
5:K:397:GLU:HA	5:K:400:PHE:HD2	1.77	0.48
1:A:147:ILE:HD11	1:A:155:PHE:HB2	1.96	0.48
1:A:197:MET:HE1	1:A:290:MET:HG2	1.96	0.48
6:P:375:ASN:HB3	6:P:412:HIS:CE1	2.48	0.47
8:J:223:VAL:HA	8:J:226:VAL:HB	1.96	0.47
9:Z:501:MET:HB3	9:Z:517:LEU:HD22	1.96	0.47
1:A:40:TYR:HA	3:C:124:MET:HE2	1.97	0.47
2:B:71:LEU:HD21	9:Z:804:LEU:HD11	1.95	0.47
4:D:347:PHE:CD1	4:D:370:ILE:HD11	2.49	0.47
7:I:20:LYS:HZ3	9:Z:152:LEU:HD11	1.77	0.47
9:Z:455:MET:HA	9:Z:487:LEU:O	2.14	0.47
4:D:204:PHE:HD1	4:D:207:ILE:HD11	1.79	0.47
5:K:206:ILE:H	5:K:206:ILE:HD12	1.79	0.47
6:P:246:LEU:HB2	6:P:280:ILE:HG12	1.95	0.47
9:Z:214:LEU:HA	9:Z:217:MET:HG2	1.95	0.47
9:Z:405:LEU:HD13	9:Z:446:ALA:HB2	1.95	0.47
9:Z:894:ARG:HH21	9:Z:903:VAL:HG22	1.79	0.47
1:A:41:GLY:HA2	3:C:152:GLU:HG2	1.97	0.47
3:C:530:LEU:HB3	3:C:542:ILE:HD13	1.96	0.47
5:K:150:ILE:HG23	5:K:151:THR:HG23	1.95	0.47
6:P:245:LYS:HB2	6:P:245:LYS:HZ3	1.79	0.47
2:B:151:HIS:CD2	2:B:152:LYS:HG3	2.49	0.47
2:B:285:ASP:HB2	2:B:333:THR:OG1	2.14	0.47
5:K:196:VAL:HG13	5:K:197:ILE:HG13	1.97	0.47
6:P:246:LEU:HB3	6:P:280:ILE:HG23	1.95	0.47
2:B:113:ILE:HG13	2:B:118:ALA:HA	1.97	0.47
2:B:123:PRO:HG2	7:I:91:GLU:O	2.14	0.47
3:C:864:MET:HE1	3:C:908:ILE:HG12	1.96	0.47
11:N:173:GLN:HB2	11:N:175:TRP:NE1	2.29	0.47
8:J:304:ASP:HB2	8:J:333:ARG:HE	1.78	0.47
9:Z:154:LEU:HD13	9:Z:189:LEU:HD11	1.97	0.47
9:Z:519:VAL:O	9:Z:523:LEU:HG	2.14	0.47
9:Z:528:ARG:HB3	9:Z:531:LEU:HB2	1.96	0.47
1:A:44:PRO:HB3	3:C:159:LEU:HB2	1.96	0.47
1:A:212:GLY:H	12:A:501:ATP:HN62	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:ILE:HG12	4:D:284:SER:HB3	1.97	0.47
5:K:221:TYR:CE1	5:K:346:LYS:HB3	2.50	0.47
6:P:382:SER:HB2	6:P:419:ILE:HD13	1.96	0.47
8:J:60:LEU:HA	8:J:63:LEU:HD12	1.97	0.47
8:J:156:SER:HB3	8:J:259:ARG:NH1	2.28	0.47
2:B:253:ILE:O	2:B:257:LEU:HB2	2.15	0.47
2:B:362:LEU:HD12	2:B:363:GLY:N	2.30	0.47
3:C:568:LEU:HD21	3:C:883:THR:HA	1.96	0.47
4:D:367:PHE:CD2	4:D:400:THR:HG22	2.50	0.47
9:Z:311:ILE:HD11	9:Z:348:PHE:HD2	1.78	0.47
9:Z:373:VAL:HG13	9:Z:750:SER:HB3	1.96	0.47
3:C:615:LEU:HD23	9:Z:804:LEU:HD12	1.97	0.47
3:C:823:ASN:ND2	3:C:860:GLY:HA3	2.30	0.47
5:K:255:TYR:HB3	8:J:245:LYS:HB3	1.96	0.47
9:Z:423:LEU:HB2	9:Z:450:ILE:HD13	1.96	0.47
9:Z:730:VAL:O	9:Z:734:VAL:HG23	2.15	0.47
9:Z:731:VAL:O	9:Z:735:MET:HG2	2.15	0.47
1:A:333:MET:HE1	1:A:362:ASP:HB3	1.97	0.46
2:B:247:ILE:HG22	2:B:281:ILE:HD12	1.97	0.46
2:B:395:MET:HE1	2:B:420:LYS:CB	2.45	0.46
4:D:7:ASN:ND2	4:D:46:LEU:HD11	2.30	0.46
4:D:57:THR:HG22	4:D:60:ARG:HH21	1.80	0.46
4:D:146:LYS:HD3	4:D:146:LYS:N	2.31	0.46
7:I:18:GLY:C	7:I:21:PRO:HD2	2.40	0.46
9:Z:79:VAL:HG22	9:Z:101:ILE:HG23	1.97	0.46
9:Z:750:SER:HA	9:Z:753:PHE:CD2	2.50	0.46
1:A:289:ARG:HG2	1:A:290:MET:CE	2.45	0.46
2:B:199:GLU:HB2	2:B:236:VAL:HG23	1.96	0.46
3:C:166:ASN:O	3:C:170:GLU:HG2	2.16	0.46
7:I:22:TYR:HD1	9:Z:103:SER:HB3	1.80	0.46
8:J:59:GLU:O	8:J:63:LEU:HG	2.16	0.46
8:J:389:GLU:HB2	8:J:414:GLN:HE21	1.79	0.46
9:Z:727:THR:O	9:Z:731:VAL:HG12	2.15	0.46
9:Z:742:TRP:HD1	9:Z:745:LEU:HG	1.79	0.46
11:N:103:ILE:HG22	11:N:109:THR:HG22	1.96	0.46
1:A:102:CYS:HA	1:A:147:ILE:HG22	1.96	0.46
2:B:47:PRO:HD3	3:C:756:MET:HE1	1.98	0.46
3:C:788:PRO:HA	3:C:818:CYS:SG	2.55	0.46
8:J:219:LYS:HZ3	12:J:501:ATP:PB	2.37	0.46
9:Z:299:TYR:O	9:Z:303:LEU:HG	2.15	0.46
1:A:293:GLU:O	1:A:297:MET:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:748:LEU:HD21	3:C:866:VAL:HG11	1.97	0.46
5:K:141:LYS:HD2	5:K:141:LYS:HA	1.68	0.46
5:K:290:ARG:HD2	5:K:302:GLN:OE1	2.15	0.46
6:P:283:LEU:O	6:P:283:LEU:HD12	2.15	0.46
7:I:59:LYS:CG	7:I:63:ARG:HH21	2.28	0.46
9:Z:745:LEU:O	9:Z:748:PHE:HD2	1.98	0.46
2:B:281:ILE:HG22	2:B:327:ALA:H	1.81	0.46
9:Z:664:LEU:HA	9:Z:667:GLN:HG2	1.98	0.46
3:C:427:GLN:HA	3:C:458:SER:HA	1.96	0.46
3:C:471:LEU:HD13	3:C:505:VAL:HG22	1.96	0.46
4:D:177:ASN:HA	4:D:180:TYR:CE1	2.51	0.46
5:K:148:LEU:HD23	5:K:155:ILE:HA	1.98	0.46
8:J:252:ARG:HA	8:J:255:ARG:HD2	1.96	0.46
8:J:262:ARG:NH2	8:J:307:ASP:HA	2.30	0.46
8:J:403:LEU:HD13	11:N:37:ARG:HH22	1.81	0.46
9:Z:40:SER:HB2	9:Z:72:LEU:HD11	1.98	0.46
9:Z:310:ASP:H	9:Z:707:ASN:HD21	1.64	0.46
9:Z:406:TYR:OH	9:Z:747:HIS:HB2	2.15	0.46
2:B:81:ILE:HG23	9:Z:796:VAL:HG22	1.97	0.46
2:B:334:LEU:HG	2:B:339:ILE:HD11	1.98	0.46
4:D:322:LEU:HB3	4:D:326:TRP:NE1	2.31	0.46
8:J:116:MET:HG3	8:J:118:TYR:CE2	2.51	0.46
9:Z:381:GLU:HB3	9:Z:384:LYS:HE3	1.97	0.46
9:Z:739:PHE:HA	9:Z:742:TRP:O	2.15	0.46
10:L:7:VAL:HG11	10:L:9:LYS:HE2	1.97	0.46
1:A:398:VAL:HG23	1:A:402:ILE:HD12	1.98	0.46
3:C:55:ARG:HD3	3:C:63:LEU:HB3	1.97	0.46
4:D:262:LYS:O	4:D:265:PRO:HD2	2.15	0.46
4:D:297:ARG:HA	4:D:331:ASN:ND2	2.31	0.46
9:Z:79:VAL:CG2	9:Z:104:LYS:HG3	2.45	0.46
4:D:347:PHE:CE2	4:D:356:MET:HB2	2.51	0.46
6:P:188:LYS:H	6:P:188:LYS:HD3	1.81	0.46
8:J:138:ALA:HB3	8:J:148:ASP:HB3	1.97	0.46
9:Z:928:ALA:HB2	10:L:104:LYS:HA	1.98	0.46
1:A:62:ARG:O	1:A:66:LYS:HG2	2.16	0.45
3:C:392:LEU:HD13	3:C:857:LEU:HD11	1.98	0.45
3:C:471:LEU:HB2	3:C:497:PHE:CZ	2.52	0.45
7:I:24:GLU:OE2	8:J:47:ILE:HG21	2.16	0.45
3:C:169:VAL:HG12	9:Z:809:ARG:NH1	2.31	0.45
4:D:38:LEU:HD23	4:D:38:LEU:HA	1.66	0.45
4:D:472:SER:O	4:D:473:GLU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:515:ARG:HH22	9:Z:738:GLN:HB3	1.80	0.45
1:A:282:LYS:HA	2:B:292:TYR:CE1	2.51	0.45
3:C:224:LEU:HA	3:C:227:ILE:HG12	1.98	0.45
5:K:196:VAL:HG11	5:K:218:VAL:HG21	1.98	0.45
8:J:321:ALA:HA	8:J:324:LEU:HG	1.99	0.45
4:D:123:SER:HB2	4:D:126:LYS:HA	1.97	0.45
6:P:56:ASN:O	6:P:60:GLU:HG2	2.16	0.45
6:P:119:VAL:HG11	6:P:155:ILE:HD11	1.99	0.45
7:I:42:ARG:HA	7:I:45:GLU:CD	2.41	0.45
8:J:343:LEU:HG	8:J:377:SER:HB2	1.99	0.45
3:C:813:PHE:CE1	3:C:817:LEU:HD21	2.50	0.45
5:K:397:GLU:HA	5:K:400:PHE:CD2	2.51	0.45
8:J:290:ARG:HD2	8:J:290:ARG:N	2.31	0.45
9:Z:108:MET:HE2	9:Z:108:MET:HA	1.99	0.45
11:N:99:ASP:HB3	11:N:102:LYS:HG2	1.98	0.45
1:A:145:TYR:HE2	1:A:159:LEU:N	2.14	0.45
4:D:188:MET:HE3	4:D:188:MET:HB2	1.89	0.45
6:P:188:LYS:HE2	6:P:188:LYS:HB2	1.68	0.45
6:P:219:LEU:HD23	6:P:346:LYS:HD3	1.98	0.45
8:J:74:HIS:CD2	9:Z:577:SER:HA	2.52	0.45
8:J:291:GLU:O	8:J:295:ILE:HG13	2.16	0.45
11:N:142:ILE:HG22	11:N:145:HIS:CE1	2.52	0.45
1:A:155:PHE:HE2	6:P:150:LYS:HG2	1.81	0.45
1:A:234:ARG:HB2	4:D:8:TYR:CD2	2.51	0.45
1:A:296:GLU:O	1:A:300:THR:HG23	2.16	0.45
1:A:319:PHE:HB3	4:D:464:ASN:ND2	2.32	0.45
3:C:448:LYS:HE2	3:C:477:TYR:CE1	2.45	0.45
4:D:137:ILE:O	4:D:141:ILE:HG22	2.16	0.45
6:P:361:LEU:HG	6:P:376:TRP:CE3	2.52	0.45
7:I:49:ASN:HA	9:Z:611:LYS:NZ	2.29	0.45
9:Z:227:LYS:HG3	9:Z:722:THR:HA	1.97	0.45
11:N:103:ILE:HD12	11:N:107:GLY:HA2	1.97	0.45
11:N:109:THR:HG23	11:N:112:HIS:CE1	2.52	0.45
2:B:349:LEU:HD12	2:B:350:PHE:H	1.82	0.45
3:C:49:LEU:HA	3:C:52:LEU:HD12	1.97	0.45
3:C:269:TYR:CZ	3:C:293:MET:HG2	2.51	0.45
9:Z:786:ARG:HH22	9:Z:789:GLU:H	1.64	0.45
11:N:37:ARG:CD	11:N:41:HIS:HB2	2.46	0.45
3:C:809:MET:HA	3:C:812:ILE:HD12	1.99	0.45
5:K:220:LEU:HD23	5:K:347:VAL:HB	1.98	0.45
5:K:249:SER:HB2	6:P:307:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:116:MET:HG3	8:J:118:TYR:CZ	2.51	0.45
1:A:436:LYS:NZ	2:B:207:LEU:HA	2.31	0.45
4:D:342:VAL:HG13	4:D:346:TYR:HE2	1.83	0.45
9:Z:736:PHE:CZ	9:Z:739:PHE:HE2	2.35	0.45
4:D:441:LEU:HA	4:D:448:LEU:HD11	1.99	0.44
7:I:81:ASP:O	7:I:104:VAL:HG21	2.17	0.44
8:J:270:PHE:HD1	8:J:271:ILE:N	2.15	0.44
9:Z:711:ARG:HH12	9:Z:786:ARG:HH21	1.66	0.44
1:A:153:ALA:HB1	6:P:122:SER:OG	2.17	0.44
2:B:268:PHE:N	2:B:268:PHE:CD1	2.84	0.44
3:C:335:LEU:HD11	3:C:910:PRO:HG3	1.99	0.44
5:K:309:LEU:HD22	5:K:342:ARG:HH11	1.81	0.44
7:I:41:VAL:HG12	7:I:45:GLU:OE1	2.17	0.44
9:Z:346:ASN:O	9:Z:350:LYS:HG2	2.18	0.44
9:Z:489:MET:HG3	9:Z:492:THR:OG1	2.16	0.44
1:A:436:LYS:HZ3	2:B:207:LEU:HA	1.81	0.44
3:C:242:PHE:CG	3:C:275:GLN:HG3	2.53	0.44
3:C:574:TYR:CZ	3:C:584:VAL:HG21	2.52	0.44
8:J:242:PHE:HE2	8:J:271:ILE:HG12	1.83	0.44
9:Z:141:ILE:HD13	9:Z:165:ILE:HG21	2.00	0.44
11:N:112:HIS:NE2	11:N:143:PRO:HD3	2.32	0.44
2:B:418:GLN:HA	2:B:421:GLU:HG2	2.00	0.44
4:D:46:LEU:HG	4:D:49:MET:SD	2.58	0.44
5:K:120:LYS:HE3	5:K:124:GLY:HA2	1.99	0.44
6:P:360:ILE:HG12	12:P:501:ATP:N1	2.32	0.44
6:P:375:ASN:H	6:P:412:HIS:CE1	2.35	0.44
7:I:33:LYS:HB3	8:J:58:TYR:CE1	2.52	0.44
9:Z:444:HIS:O	9:Z:448:LEU:HG	2.17	0.44
2:B:82:LEU:HD11	9:Z:798:LYS:HG2	2.00	0.44
2:B:255:LYS:HG3	2:B:256:TYR:CD2	2.52	0.44
2:B:264:CYS:SG	2:B:308:GLU:HG3	2.57	0.44
9:Z:526:TYR:CZ	9:Z:727:THR:HG23	2.53	0.44
10:L:75:TRP:CD1	10:L:125:MET:HG2	2.52	0.44
11:N:15:PHE:O	11:N:19:GLN:HG3	2.18	0.44
1:A:438:ALA:H	2:B:211:MET:HE1	1.83	0.44
2:B:292:TYR:CZ	4:D:425:ILE:HG12	2.53	0.44
3:C:412:GLY:O	3:C:415:MET:HB3	2.18	0.44
3:C:419:VAL:HB	3:C:450:GLY:HA3	2.00	0.44
3:C:559:LYS:HE2	3:C:727:GLU:HG3	2.00	0.44
3:C:830:LEU:O	3:C:834:LEU:HG	2.18	0.44
5:K:360:ILE:HG12	12:K:501:ATP:N1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:139:ARG:NH2	9:Z:143:LYS:HD2	2.32	0.44
9:Z:292:GLY:HA3	9:Z:415:PHE:CE1	2.53	0.44
2:B:221:LEU:HD12	2:B:229:LYS:HG2	1.99	0.44
4:D:301:ASP:HB3	4:D:304:SER:OG	2.18	0.44
5:K:198:GLU:O	5:K:202:LYS:HG2	2.17	0.44
2:B:420:LYS:O	2:B:424:MET:HG2	2.17	0.44
3:C:775:MET:HE3	3:C:889:VAL:HG13	2.00	0.44
9:Z:116:GLN:HA	9:Z:119:LYS:NZ	2.29	0.44
1:A:234:ARG:HG3	4:D:8:TYR:HB3	1.99	0.43
1:A:241:ASP:HA	1:A:346:ARG:HH12	1.83	0.43
3:C:52:LEU:HA	3:C:55:ARG:HH12	1.83	0.43
3:C:510:LEU:HA	3:C:530:LEU:HD11	2.00	0.43
9:Z:444:HIS:ND1	9:Z:480:ALA:HB2	2.33	0.43
9:Z:481:ALA:O	9:Z:485:MET:HG2	2.18	0.43
9:Z:597:ARG:HG2	9:Z:718:GLU:OE2	2.18	0.43
11:N:117:LYS:O	11:N:118:LYS:HG2	2.17	0.43
2:B:141:LEU:HD12	2:B:141:LEU:O	2.18	0.43
3:C:161:ILE:HG21	3:C:204:CYS:SG	2.58	0.43
3:C:515:SER:HB3	3:C:518:LEU:HD12	2.00	0.43
3:C:878:LEU:O	3:C:882:LEU:HG	2.18	0.43
4:D:49:MET:C	4:D:49:MET:HE2	2.43	0.43
8:J:371:LEU:HD23	8:J:411:TYR:HD2	1.84	0.43
8:J:371:LEU:HB3	8:J:411:TYR:CD2	2.52	0.43
9:Z:202:PHE:CE2	9:Z:206:ILE:HD11	2.53	0.43
2:B:382:THR:HG23	2:B:384:LYS:H	1.83	0.43
3:C:362:LEU:HD12	3:C:832:ARG:HH22	1.83	0.43
3:C:574:TYR:CD2	3:C:581:VAL:HG22	2.53	0.43
4:D:231:ILE:HG21	4:D:283:PHE:CD2	2.53	0.43
9:Z:335:ALA:O	9:Z:339:MET:HG2	2.18	0.43
11:N:7:HIS:CD2	11:N:39:PRO:HG3	2.54	0.43
5:K:239:ILE:HD12	5:K:239:ILE:HA	1.92	0.43
8:J:237:VAL:HG11	8:J:242:PHE:CE1	2.53	0.43
8:J:407:LEU:HD23	8:J:407:LEU:HA	1.77	0.43
9:Z:914:VAL:H	10:L:108:ASN:CG	2.26	0.43
1:A:282:LYS:HB3	1:A:283:TYR:CE2	2.53	0.43
5:K:112:LEU:HD12	5:K:112:LEU:H	1.83	0.43
3:C:763:HIS:HA	3:C:766:HIS:ND1	2.33	0.43
4:D:332:PRO:HB3	4:D:360:LEU:HA	2.01	0.43
4:D:475:LYS:HB3	6:P:255:TYR:CE2	2.53	0.43
9:Z:479:GLU:OE1	9:Z:512:ASN:HB3	2.18	0.43
11:N:64:LEU:HD22	11:N:75:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LYS:HD3	1:A:283:TYR:OH	2.18	0.43
1:A:286:GLU:HB3	1:A:289:ARG:HH11	1.83	0.43
3:C:389:PHE:HB3	3:C:857:LEU:HD13	2.00	0.43
4:D:264:LEU:HD21	4:D:295:VAL:HG22	2.01	0.43
4:D:326:TRP:CE3	4:D:330:ILE:HD11	2.53	0.43
1:A:85:MET:HE1	1:A:88:ARG:NH1	2.33	0.43
3:C:543:THR:O	3:C:547:MET:HE2	2.19	0.43
6:P:257:GLY:O	6:P:261:LYS:HB2	2.18	0.43
6:P:412:HIS:O	6:P:416:VAL:HG23	2.19	0.43
8:J:280:LYS:HD2	8:J:280:LYS:HA	1.83	0.43
9:Z:728:LYS:HE3	9:Z:728:LYS:HB2	1.85	0.43
11:N:148:ALA:HB1	11:N:181:ALA:HB2	2.01	0.43
1:A:159:LEU:HD22	1:A:163:VAL:HB	2.00	0.43
2:B:324:VAL:CG2	2:B:326:MET:HE3	2.47	0.43
3:C:357:ILE:HD11	3:C:390:LEU:HD13	2.01	0.43
3:C:564:ARG:HH12	3:C:890:SER:HB2	1.84	0.43
4:D:194:VAL:HG13	4:D:236:GLU:HG2	2.01	0.43
6:P:197:ILE:HD13	6:P:197:ILE:HA	1.89	0.43
9:Z:592:GLY:HA2	9:Z:628:ALA:HB2	2.00	0.43
3:C:407:VAL:HG12	3:C:415:MET:HE1	1.99	0.43
3:C:740:VAL:HG22	3:C:764:LEU:HD13	2.01	0.43
5:K:209:ARG:HB3	8:J:400:TYR:CE1	2.51	0.43
8:J:85:GLU:CD	8:J:88:ARG:HE	2.27	0.43
2:B:281:ILE:CG2	2:B:327:ALA:H	2.32	0.42
2:B:361:ILE:HG12	12:B:501:ATP:C6	2.54	0.42
3:C:588:ILE:HG22	3:C:596:THR:HG23	2.00	0.42
3:C:813:PHE:HE1	3:C:817:LEU:HD21	1.84	0.42
5:K:369:LYS:HA	5:K:369:LYS:HD3	1.84	0.42
9:Z:104:LYS:HD2	9:Z:104:LYS:C	2.43	0.42
9:Z:339:MET:HE3	9:Z:339:MET:HB3	1.90	0.42
9:Z:349:ILE:HG23	9:Z:356:LEU:HD11	2.00	0.42
1:A:429:PHE:HB3	1:A:442:ASP:OD1	2.18	0.42
9:Z:452:LEU:HD21	9:Z:748:PHE:HE1	1.84	0.42
10:L:34:GLU:HG2	10:L:36:LYS:NZ	2.35	0.42
4:D:266:VAL:HA	4:D:269:GLN:HG2	2.00	0.42
6:P:145:LEU:HB2	6:P:161:SER:HA	2.01	0.42
7:I:113:VAL:HG12	7:I:125:VAL:HG22	2.01	0.42
9:Z:625:LEU:HD23	9:Z:625:LEU:HA	1.81	0.42
11:N:145:HIS:HD2	11:N:180:HIS:CD2	2.38	0.42
1:A:330:GLN:O	1:A:334:LEU:HG	2.19	0.42
2:B:67:ASP:O	2:B:71:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:MET:HG3	3:C:264:PHE:CD2	2.53	0.42
4:D:342:VAL:HG13	4:D:346:TYR:CE2	2.54	0.42
1:A:191:ILE:HG22	1:A:192:ASP:H	1.85	0.42
2:B:278:ILE:HA	2:B:323:LYS:O	2.20	0.42
2:B:348:ILE:HD13	2:B:348:ILE:HA	1.84	0.42
3:C:158:ALA:HB1	3:C:223:LEU:HD13	2.02	0.42
3:C:362:LEU:HD12	3:C:832:ARG:NH2	2.35	0.42
3:C:765:MET:SD	3:C:776:VAL:HG11	2.59	0.42
4:D:66:VAL:HB	4:D:68:TYR:CE1	2.55	0.42
4:D:234:PHE:O	4:D:237:LEU:HB2	2.19	0.42
9:Z:927:ASN:HA	10:L:102:GLN:O	2.18	0.42
1:A:60:GLU:HG2	1:A:64:LYS:HE3	2.00	0.42
2:B:124:THR:HG21	7:I:91:GLU:HA	2.01	0.42
3:C:278:LEU:HB3	3:C:297:VAL:HG13	2.02	0.42
9:Z:246:LYS:HD2	9:Z:282:TYR:CE2	2.55	0.42
11:N:111:LEU:HD11	11:N:131:ALA:HB1	2.02	0.42
1:A:200:VAL:HG22	1:A:272:ILE:HG23	2.01	0.42
2:B:79:SER:HB3	3:C:767:TYR:CG	2.54	0.42
2:B:284:ILE:HD12	2:B:326:MET:SD	2.59	0.42
4:D:174:PHE:O	4:D:178:LEU:HB2	2.19	0.42
4:D:475:LYS:HB3	6:P:255:TYR:HE2	1.85	0.42
9:Z:208:ARG:HG3	9:Z:232:LEU:HD13	2.00	0.42
9:Z:462:VAL:O	9:Z:466:LEU:HG	2.19	0.42
5:K:173:PHE:CZ	5:K:243:PHE:HB3	2.55	0.42
9:Z:813:ARG:O	9:Z:817:THR:HG23	2.19	0.42
2:B:389:GLY:HA3	12:B:501:ATP:C8	2.54	0.42
8:J:101:GLU:H	8:J:109:ILE:HG22	1.84	0.42
8:J:164:ASN:OD1	8:J:164:ASN:C	2.63	0.42
9:Z:106:ILE:O	9:Z:110:VAL:HG23	2.20	0.42
11:N:189:ALA:O	11:N:193:LEU:HG	2.19	0.42
1:A:45:TYR:OH	3:C:222:ASP:HB3	2.20	0.41
2:B:248:VAL:HB	2:B:251:GLU:HB3	2.01	0.41
4:D:297:ARG:HA	4:D:331:ASN:HD22	1.84	0.41
4:D:473:GLU:HG3	5:K:296:SER:OG	2.20	0.41
5:K:394:CYS:SG	5:K:419:VAL:HG12	2.60	0.41
9:Z:241:LEU:HD21	9:Z:257:ILE:HG21	2.01	0.41
11:N:7:HIS:HD2	11:N:39:PRO:HG3	1.85	0.41
2:B:404:LEU:O	2:B:407:ARG:HD2	2.20	0.41
3:C:249:MET:SD	3:C:268:ALA:HB2	2.59	0.41
5:K:73:GLN:HA	5:K:76:GLN:HG3	2.01	0.41
7:I:96:VAL:HG21	7:I:115:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:132:LYS:HB2	8:J:135:MET:SD	2.60	0.41
8:J:242:PHE:CE2	8:J:271:ILE:HG12	2.56	0.41
9:Z:199:ASN:HB3	9:Z:202:PHE:HB3	2.02	0.41
9:Z:310:ASP:CG	9:Z:313:LEU:HG	2.44	0.41
9:Z:490:LEU:HD22	9:Z:490:LEU:H	1.85	0.41
11:N:153:LEU:HA	11:N:156:ILE:HD12	2.01	0.41
1:A:235:PHE:CE1	1:A:242:PRO:HA	2.55	0.41
1:A:434:ARG:NH1	2:B:200:LEU:HD11	2.34	0.41
3:C:258:PRO:HG2	9:Z:813:ARG:NH2	2.35	0.41
3:C:439:TYR:HB2	3:C:451:ALA:HB2	2.02	0.41
4:D:16:LEU:HA	4:D:32:LEU:HD21	2.01	0.41
4:D:265:PRO:HA	4:D:309:MET:SD	2.61	0.41
4:D:307:LYS:O	4:D:311:LYS:HG3	2.20	0.41
6:P:361:LEU:HG	6:P:376:TRP:CZ3	2.55	0.41
6:P:389:ALA:HB2	12:P:501:ATP:H5'1	2.02	0.41
8:J:68:ILE:HA	8:J:71:GLU:OE1	2.20	0.41
9:Z:349:ILE:HG22	9:Z:350:LYS:HD2	2.03	0.41
1:A:162:ARG:H	1:A:162:ARG:NE	2.17	0.41
1:A:222:ARG:HB3	4:D:38:LEU:HD11	2.01	0.41
1:A:249:TYR:CD2	1:A:358:PRO:HG3	2.55	0.41
1:A:448:ASP:OD1	1:A:448:ASP:C	2.63	0.41
2:B:246:ARG:HG3	2:B:280:PHE:CD2	2.55	0.41
3:C:53:VAL:HG12	3:C:57:LYS:HE3	2.01	0.41
3:C:138:ARG:HD2	3:C:153:TYR:OH	2.20	0.41
4:D:145:GLU:HG2	4:D:146:LYS:HD3	2.02	0.41
4:D:399:TYR:CE2	4:D:400:THR:HG23	2.55	0.41
6:P:361:LEU:CA	6:P:391:LEU:HD21	2.50	0.41
9:Z:920:VAL:HA	9:Z:923:MET:SD	2.60	0.41
11:N:33:ASP:HB2	11:N:34:GLN:OE1	2.20	0.41
1:A:99:VAL:HB	2:B:127:ASP:CG	2.46	0.41
2:B:343:ARG:O	2:B:344:ILE:HG13	2.20	0.41
3:C:49:LEU:HD23	3:C:52:LEU:HD12	2.02	0.41
4:D:474:THR:HG23	5:K:256:ILE:CD1	2.50	0.41
5:K:212:ILE:HD12	8:J:392:LEU:HD22	2.02	0.41
5:K:212:ILE:HG23	8:J:360:MET:SD	2.60	0.41
5:K:305:LEU:O	5:K:309:LEU:HG	2.21	0.41
7:I:60:ASP:HA	7:I:63:ARG:NE	2.35	0.41
9:Z:677:ASP:O	9:Z:680:LYS:HG2	2.20	0.41
11:N:6:LEU:HA	11:N:21:LEU:HD13	2.02	0.41
2:B:340:ARG:HB2	2:B:343:ARG:HE	1.85	0.41
3:C:161:ILE:HD11	3:C:203:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:297:ARG:HG3	4:D:331:ASN:HB2	2.03	0.41
5:K:416:MET:HA	5:K:419:VAL:HG22	2.02	0.41
6:P:274:ALA:HB1	6:P:320:ARG:HB3	2.03	0.41
7:I:91:GLU:HG3	7:I:92:GLY:N	2.35	0.41
8:J:365:GLU:CB	11:N:78:ILE:HG23	2.48	0.41
8:J:399:ARG:NH1	8:J:403:LEU:HB3	2.35	0.41
9:Z:109:TYR:HB2	9:Z:133:LEU:HD11	2.03	0.41
9:Z:296:CYS:HB3	9:Z:377:GLY:O	2.20	0.41
9:Z:536:ILE:HD11	9:Z:570:ARG:NH1	2.36	0.41
11:N:19:GLN:HG2	11:N:54:PHE:HE2	1.85	0.41
1:A:394:LYS:HE3	1:A:394:LYS:HB2	1.86	0.41
3:C:456:GLY:HA2	3:C:496:ALA:HB2	2.01	0.41
3:C:790:MET:HA	3:C:793:PHE:CZ	2.56	0.41
4:D:257:LEU:HG	4:D:261:LYS:HE3	2.02	0.41
4:D:268:ALA:HB2	4:D:309:MET:SD	2.60	0.41
4:D:385:LEU:O	4:D:389:GLN:HG3	2.20	0.41
5:K:309:LEU:HB3	5:K:342:ARG:NH1	2.36	0.41
6:P:339:ARG:HD2	6:P:340:SER:O	2.21	0.41
9:Z:76:GLU:HA	9:Z:104:LYS:HE3	2.02	0.41
9:Z:352:ASN:HB3	9:Z:355:TRP:HB3	2.03	0.41
9:Z:489:MET:HG3	9:Z:492:THR:HG1	1.85	0.41
9:Z:489:MET:CG	9:Z:489:MET:O	2.69	0.41
1:A:49:LEU:HG	2:B:59:LEU:HD13	2.03	0.41
1:A:291:VAL:HB	1:A:335:GLU:OE1	2.21	0.41
1:A:397:SER:HB3	2:B:211:MET:SD	2.60	0.41
2:B:402:LEU:HD13	2:B:418:GLN:HG2	2.02	0.41
3:C:804:ASP:HB3	3:C:807:VAL:HB	2.01	0.41
3:C:831:LEU:HD21	3:C:851:ALA:HB3	2.02	0.41
3:C:862:MET:HE2	3:C:862:MET:HA	2.03	0.41
8:J:346:ARG:HD3	11:N:183:ALA:HB1	2.02	0.41
9:Z:533:ASP:O	9:Z:536:ILE:HG13	2.21	0.41
11:N:173:GLN:HA	11:N:206:ASN:ND2	2.35	0.41
1:A:60:GLU:HA	1:A:63:ILE:HD12	2.03	0.41
1:A:78:PRO:HD2	1:A:81:LEU:HD12	2.02	0.41
2:B:200:LEU:HB3	2:B:201:PRO:HD3	2.03	0.41
2:B:332:GLU:HB3	4:D:384:TYR:HB3	2.03	0.41
3:C:108:ASP:HB3	3:C:111:LEU:HB2	2.02	0.41
3:C:782:ILE:O	3:C:785:VAL:HG23	2.21	0.41
5:K:283:VAL:HG21	5:K:325:MET:SD	2.61	0.41
6:P:343:LEU:HD23	6:P:343:LEU:HA	1.69	0.41
6:P:383:THR:O	6:P:386:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:52:LYS:HA	8:J:52:LYS:HD3	1.89	0.41
8:J:348:GLU:O	8:J:352:ILE:HG22	2.21	0.41
9:Z:312:GLY:HA3	9:Z:790:GLU:OE1	2.21	0.41
9:Z:494:LYS:HD3	9:Z:496:GLU:HB2	2.03	0.41
9:Z:711:ARG:HH12	9:Z:786:ARG:NH2	2.19	0.41
9:Z:788:TYR:CE1	9:Z:790:GLU:HG3	2.51	0.41
10:L:79:LYS:HD2	10:L:79:LYS:HA	1.80	0.41
10:L:82:LYS:HA	10:L:112:ASN:CG	2.45	0.41
11:N:32:LYS:HZ3	11:N:36:GLY:N	2.19	0.41
11:N:216:LEU:HB3	11:N:220:VAL:HG21	2.02	0.41
1:A:273:ARG:HG3	1:A:307:PHE:HB3	2.03	0.41
2:B:170:VAL:HG22	2:B:251:GLU:OE2	2.21	0.41
6:P:231:LEU:HD12	6:P:234:ALA:HB3	2.03	0.41
7:I:20:LYS:NZ	8:J:47:ILE:HD12	2.36	0.41
7:I:60:ASP:O	7:I:63:ARG:HG2	2.20	0.41
2:B:74:GLU:OE2	9:Z:801:THR:HA	2.22	0.40
2:B:200:LEU:HD12	2:B:200:LEU:HA	1.83	0.40
4:D:117:CYS:SG	4:D:156:ILE:HD13	2.61	0.40
4:D:347:PHE:HE2	4:D:356:MET:HB2	1.85	0.40
5:K:132:ARG:HD2	5:K:156:MET:HE3	2.03	0.40
5:K:167:VAL:O	5:K:171:THR:HG23	2.20	0.40
6:P:251:LEU:HD13	6:P:262:LEU:HD13	2.02	0.40
8:J:139:LEU:HA	8:J:147:VAL:HG22	2.02	0.40
9:Z:536:ILE:HD11	9:Z:570:ARG:HH11	1.86	0.40
1:A:148:ASN:HB2	1:A:154:LYS:NZ	2.33	0.40
3:C:225:LEU:HB2	3:C:264:PHE:CZ	2.56	0.40
4:D:231:ILE:HG12	4:D:283:PHE:HD2	1.85	0.40
5:K:377:GLU:O	5:K:381:LYS:HG3	2.21	0.40
7:I:76:ILE:HD12	7:I:85:LEU:HG	2.02	0.40
9:Z:163:LEU:HD22	9:Z:209:LYS:HD2	2.03	0.40
9:Z:642:ASP:HB3	9:Z:643:PRO:HD3	2.03	0.40
10:L:34:GLU:HB3	10:L:51:ARG:HH21	1.86	0.40
1:A:180:LYS:HG3	1:A:182:ASN:H	1.86	0.40
2:B:222:TYR:HA	2:B:328:THR:O	2.21	0.40
3:C:799:PHE:HB3	3:C:811:SER:OG	2.22	0.40
3:C:840:ARG:H	3:C:840:ARG:HG2	1.70	0.40
4:D:46:LEU:HD12	4:D:46:LEU:HA	1.86	0.40
5:K:150:ILE:HD12	6:P:153:TYR:HE2	1.86	0.40
6:P:228:LYS:HB2	12:P:501:ATP:O1B	2.21	0.40
6:P:229:THR:HG23	6:P:279:PHE:CE2	2.56	0.40
8:J:362:LEU:HD23	8:J:362:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:83:LEU:HD22	9:Z:132:LYS:HB3	2.03	0.40
9:Z:242:PHE:CE2	9:Z:273:LEU:HD21	2.56	0.40
9:Z:467:LYS:HE3	9:Z:471:TYR:OH	2.21	0.40
11:N:38:ILE:HG13	11:N:41:HIS:CE1	2.56	0.40
4:D:476:ILE:H	4:D:476:ILE:HG12	1.58	0.40
5:K:64:LEU:HD12	5:K:64:LEU:HA	1.86	0.40
11:N:202:ASP:OD1	11:N:202:ASP:N	2.52	0.40
2:B:247:ILE:HG22	2:B:281:ILE:CD1	2.52	0.40
2:B:261:PRO:HG3	2:B:305:THR:HA	2.03	0.40
2:B:307:LEU:HD12	2:B:307:LEU:HA	1.91	0.40
2:B:369:MET:HE1	2:B:396:CYS:HB3	2.04	0.40
3:C:165:TYR:CD1	3:C:227:ILE:HA	2.56	0.40
3:C:772:ILE:O	3:C:776:VAL:HG23	2.22	0.40
6:P:189:GLN:O	6:P:193:LEU:HG	2.21	0.40
7:I:52:ASN:HD22	9:Z:611:LYS:HE2	1.86	0.40
7:I:81:ASP:OD2	7:I:82:LYS:HG3	2.21	0.40
8:J:234:PHE:HZ	8:J:270:PHE:HD2	1.70	0.40
9:Z:893:VAL:HG13	9:Z:906:ARG:NH2	2.36	0.40
11:N:35:ASP:OD2	11:N:35:ASP:C	2.64	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	387/467 (83%)	374 (97%)	13 (3%)	0	100	100
2	B	383/437 (88%)	367 (96%)	16 (4%)	0	100	100
3	C	840/993 (85%)	829 (99%)	11 (1%)	0	100	100
4	D	468/480 (98%)	456 (97%)	12 (3%)	0	100	100
5	K	389/437 (89%)	379 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	P	383/434 (88%)	376 (98%)	7 (2%)	0	100	100
7	I	113/405 (28%)	113 (100%)	0	0	100	100
8	J	370/428 (86%)	360 (97%)	10 (3%)	0	100	100
9	Z	897/945 (95%)	880 (98%)	17 (2%)	0	100	100
10	L	129/156 (83%)	127 (98%)	2 (2%)	0	100	100
11	N	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
All	All	4585/5410 (85%)	4477 (98%)	108 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	328/399 (82%)	319 (97%)	9 (3%)	39	59
2	B	343/385 (89%)	337 (98%)	6 (2%)	53	67
3	C	722/850 (85%)	719 (100%)	3 (0%)	84	83
4	D	436/445 (98%)	429 (98%)	7 (2%)	55	68
5	K	335/377 (89%)	331 (99%)	4 (1%)	63	71
6	P	335/375 (89%)	326 (97%)	9 (3%)	39	59
7	I	107/352 (30%)	106 (99%)	1 (1%)	70	74
8	J	325/374 (87%)	318 (98%)	7 (2%)	45	63
9	Z	755/797 (95%)	750 (99%)	5 (1%)	76	77
10	L	120/144 (83%)	119 (99%)	1 (1%)	73	75
11	N	198/198 (100%)	198 (100%)	0	100	100
All	All	4004/4696 (85%)	3952 (99%)	52 (1%)	59	71

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	105	ILE
1	A	224	VAL
1	A	275	ILE
1	A	304	CYS
1	A	351	VAL
1	A	355	THR
1	A	402	ILE
1	A	421	SER
2	B	48	ASN
2	B	213	ILE
2	B	339	ILE
2	B	365	HIS
2	B	379	THR
2	B	401	LEU
3	C	405	ASN
3	C	581	VAL
3	C	799	PHE
4	D	37	SER
4	D	313	SER
4	D	405	LEU
4	D	408	MET
4	D	414	SER
4	D	450	VAL
4	D	476	ILE
5	K	74	LEU
5	K	112	LEU
5	K	128	ILE
5	K	195	GLU
6	P	64	ASP
6	P	71	ASN
6	P	173	ASP
6	P	231	LEU
6	P	244	LEU
6	P	252	VAL
6	P	263	VAL
6	P	304	THR
6	P	400	MET
7	I	60	ASP
8	J	49	PHE
8	J	106	ASN
8	J	113	THR
8	J	134	SER

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Mol	Chain	Res	Type
8	J	184	ILE
8	J	299	LEU
8	J	306	PHE
9	Z	380	LEU
9	Z	489	MET
9	Z	581	ASP
9	Z	595	LEU
9	Z	664	LEU
10	L	114	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
3	C	771	HIS
4	D	7	ASN
4	D	21	ASN
4	D	251	GLN
4	D	269	GLN
4	D	431	HIS
5	K	282	GLN
6	P	310	ASN
6	P	311	GLN
6	P	412	HIS
8	J	404	GLN
9	Z	499	HIS
9	Z	635	GLN
9	Z	672	ASN
9	Z	712	ASN
9	Z	927	ASN
10	L	112	ASN
11	N	7	HIS
11	N	180	HIS

5.3.3 RNA ⓘ

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](#)

5 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$
12	ATP	J	501	-	32,33,33	0.44	0	48,52,52	0.35	0
12	ATP	A	501	-	32,33,33	0.43	0	48,52,52	0.35	0
12	ATP	P	501	-	32,33,33	0.45	0	48,52,52	0.32	0
12	ATP	K	501	-	32,33,33	0.82	2 (6%)	48,52,52	0.36	0
12	ATP	B	501	-	32,33,33	0.38	0	48,52,52	0.34	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
12	ATP	J	501	-	-	2/22/38/38	0/3/3/3
12	ATP	A	501	-	-	6/22/38/38	0/3/3/3
12	ATP	P	501	-	-	6/22/38/38	0/3/3/3
12	ATP	K	501	-	-	1/22/38/38	0/3/3/3
12	ATP	B	501	-	-	3/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	501	ATP	PB-O3B	-3.75	1.55	1.59
12	K	501	ATP	PA-O3A	-2.09	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	501	ATP	PB-O3B-PG-O3G
12	B	501	ATP	PB-O3B-PG-O2G
12	J	501	ATP	PA-O3A-PB-O2B
12	A	501	ATP	C5'-O5'-PA-O1A
12	A	501	ATP	C5'-O5'-PA-O2A
12	A	501	ATP	C5'-O5'-PA-O3A
12	P	501	ATP	C5'-O5'-PA-O2A
12	A	501	ATP	O4'-C4'-C5'-O5'
12	P	501	ATP	C3'-C4'-C5'-O5'
12	P	501	ATP	O4'-C4'-C5'-O5'
12	P	501	ATP	C4'-C5'-O5'-PA
12	B	501	ATP	PB-O3B-PG-O1G
12	B	501	ATP	PB-O3B-PG-O3G
12	K	501	ATP	C4'-C5'-O5'-PA
12	P	501	ATP	PG-O3B-PB-O2B
12	P	501	ATP	PB-O3A-PA-O2A
12	J	501	ATP	PA-O3A-PB-O1B
12	A	501	ATP	PB-O3A-PA-O2A

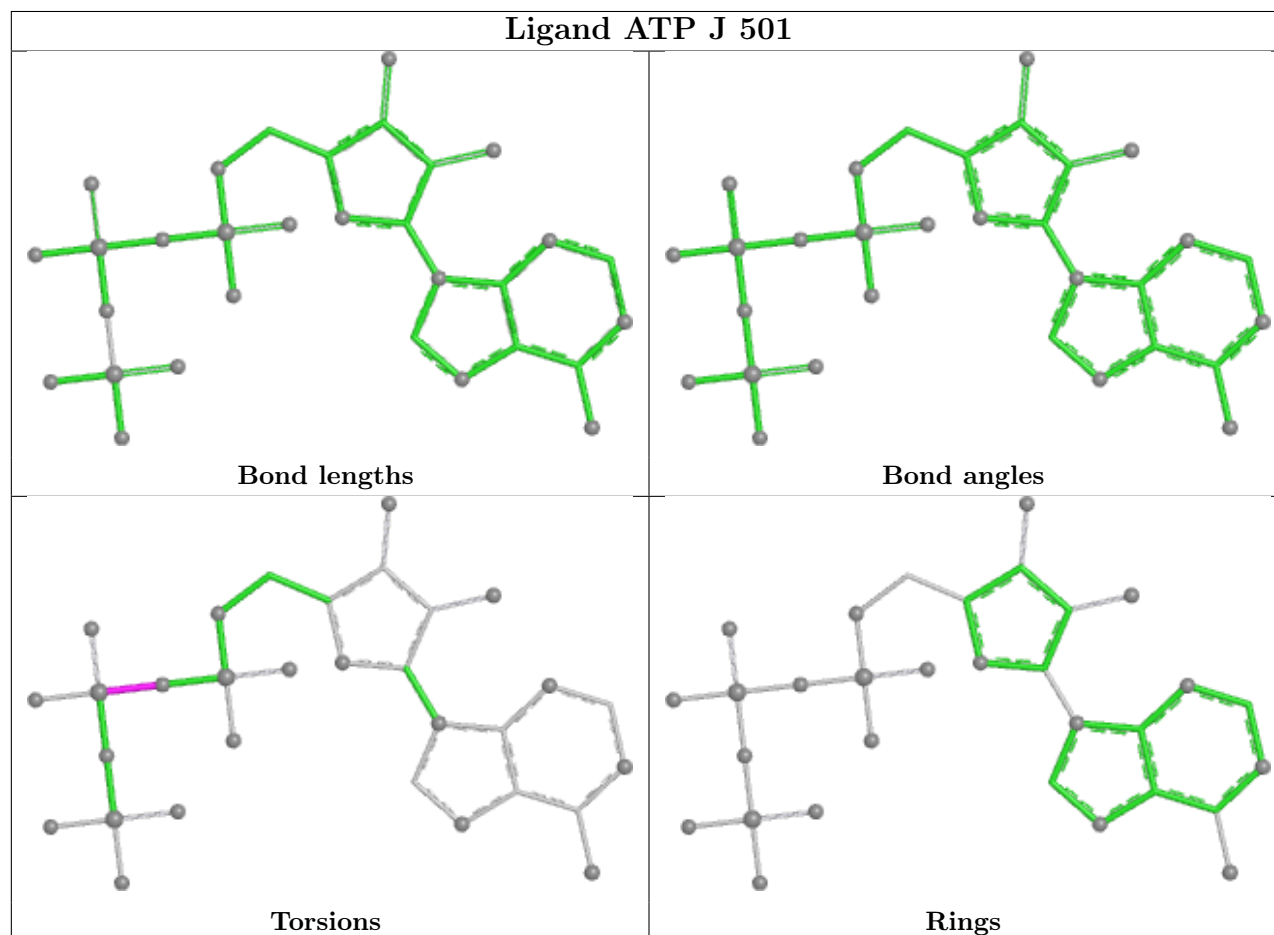
There are no ring outliers.

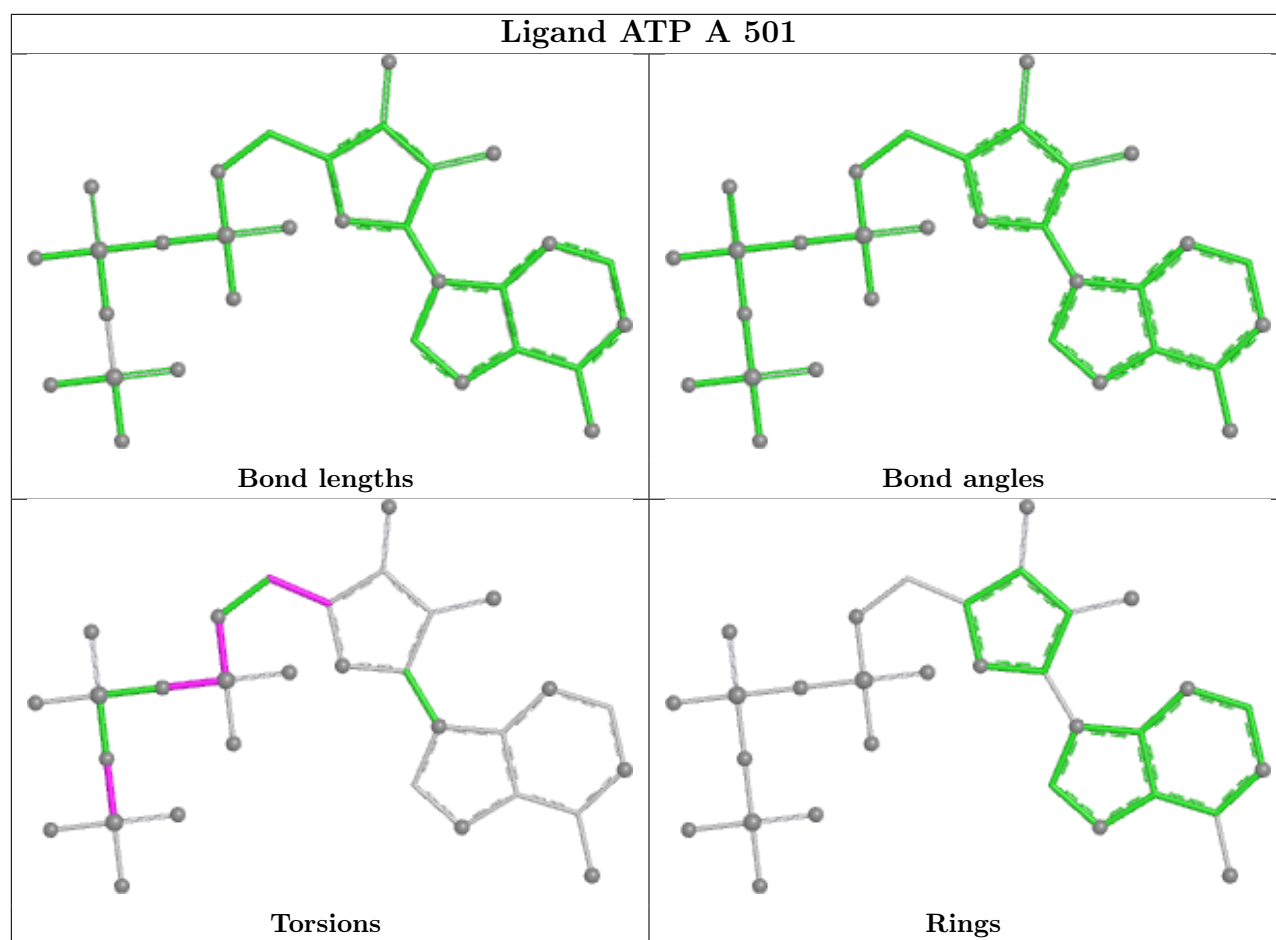
5 monomers are involved in 14 short contacts:

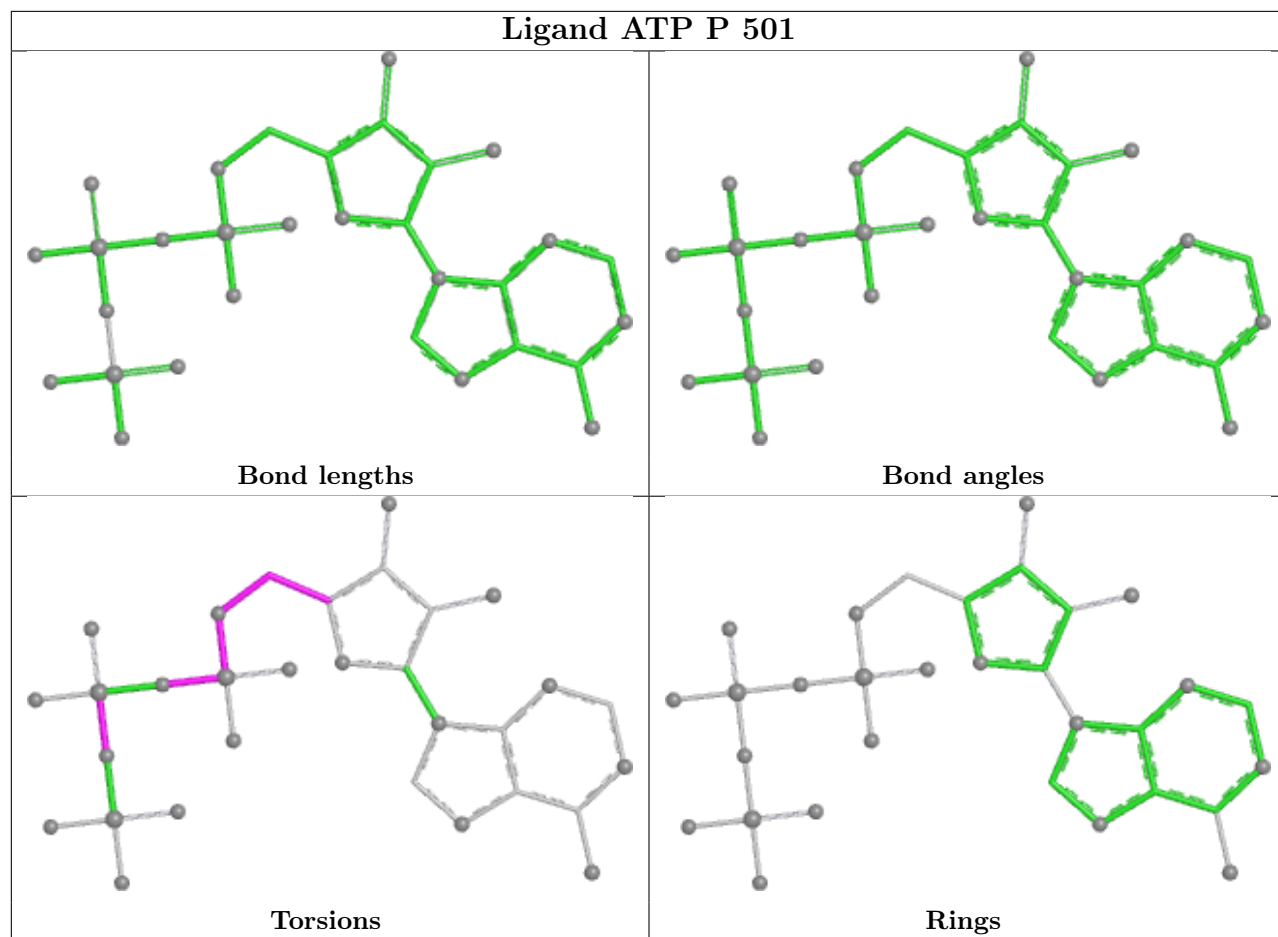
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	J	501	ATP	1	0
12	A	501	ATP	2	0
12	P	501	ATP	6	0
12	K	501	ATP	3	0
12	B	501	ATP	2	0

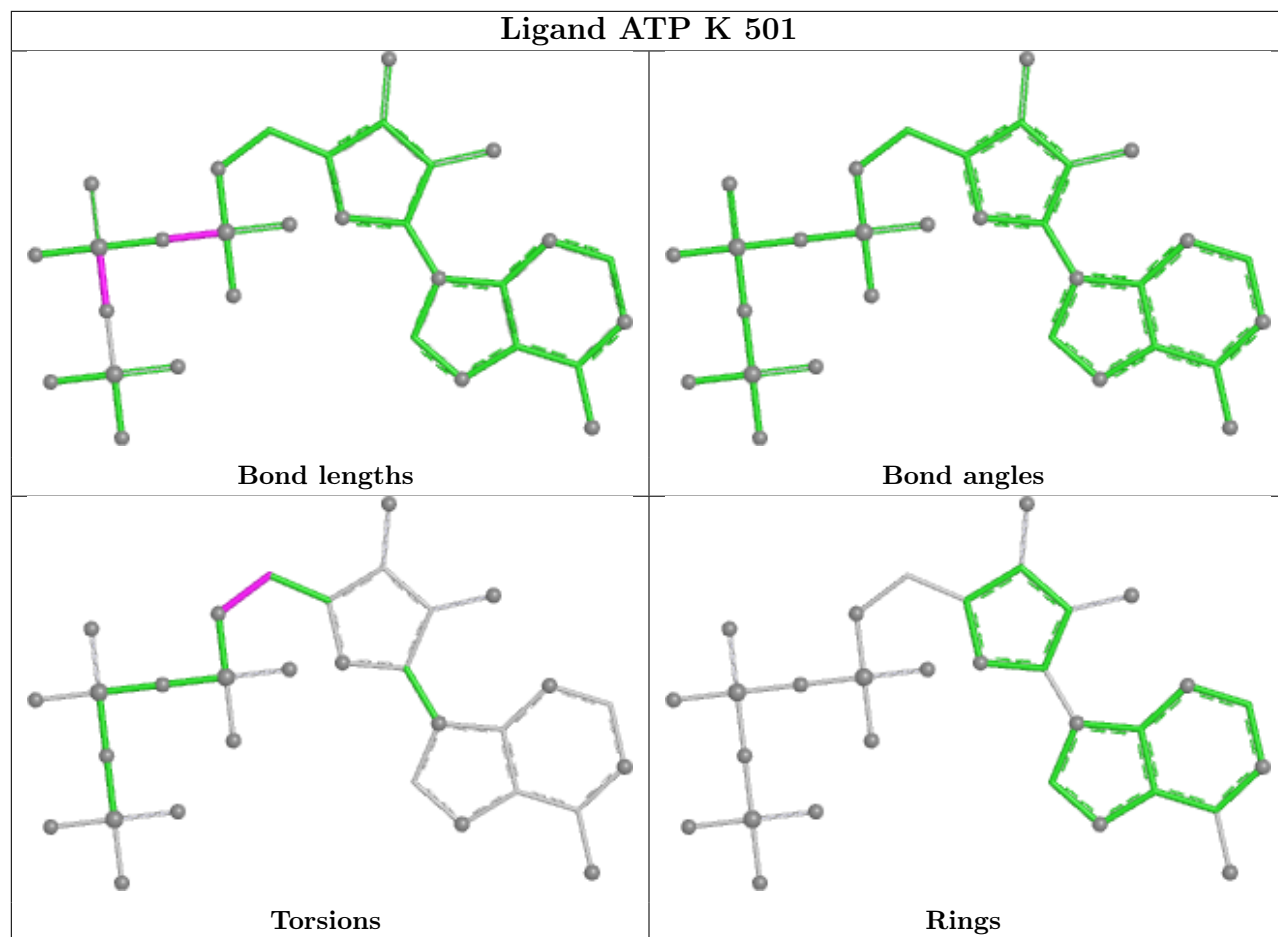
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

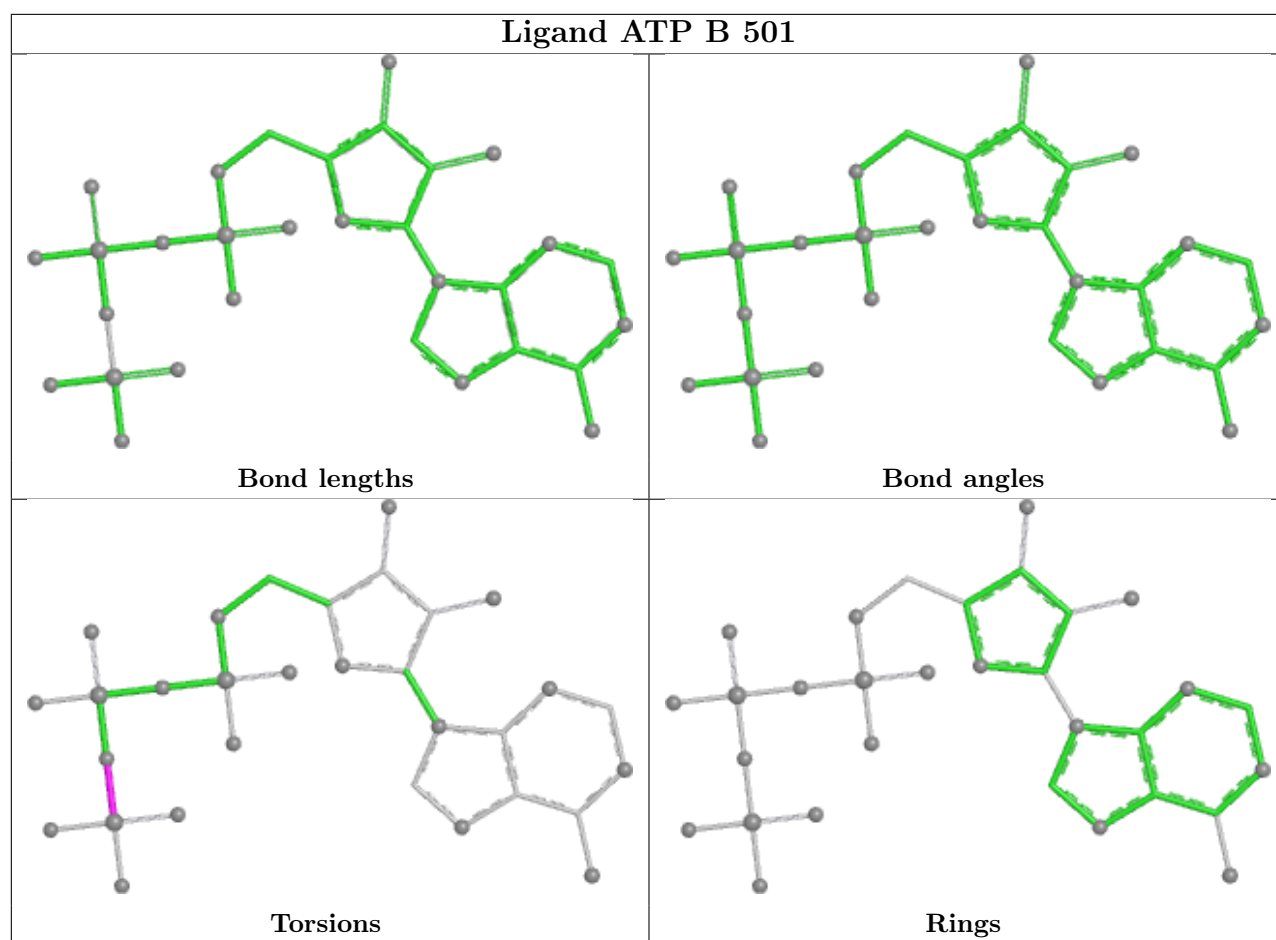
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

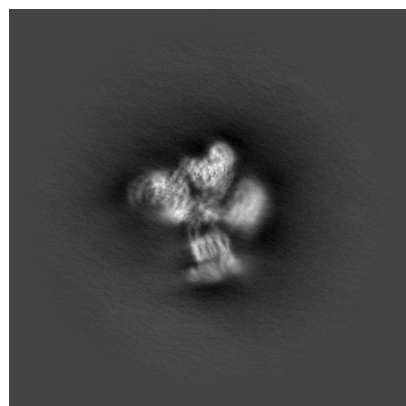
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77359. These allow visual inspection of the internal detail of the map and identification of artifacts.

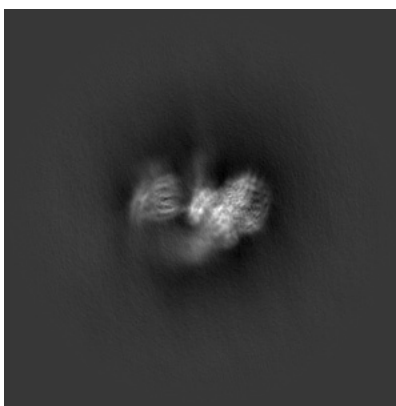
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

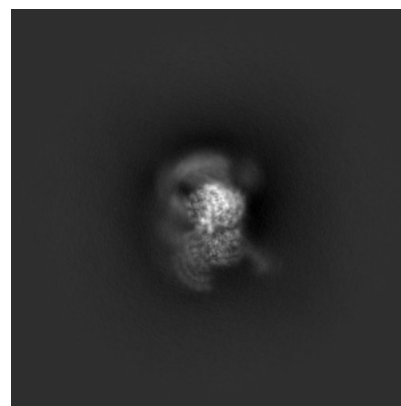
6.1.1 Primary map



X

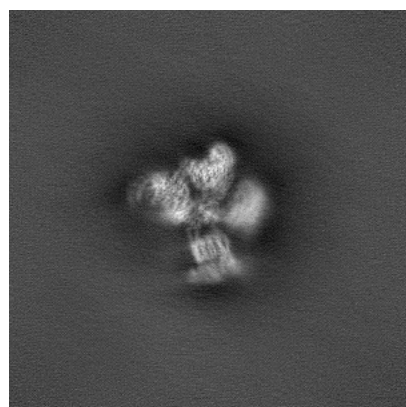


Y

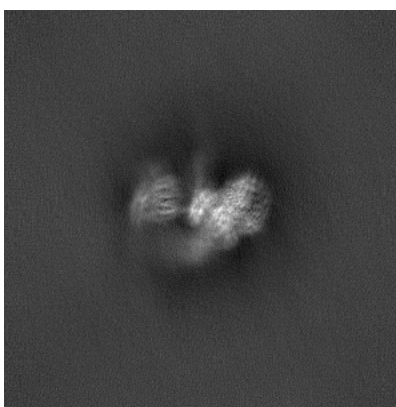


Z

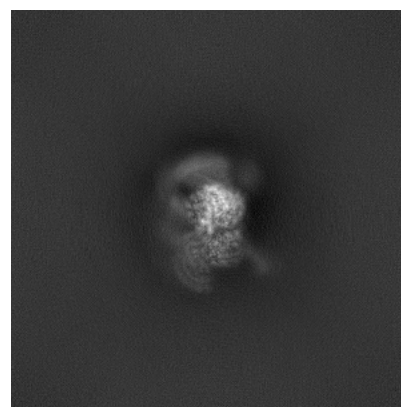
6.1.2 Raw map



X



Y

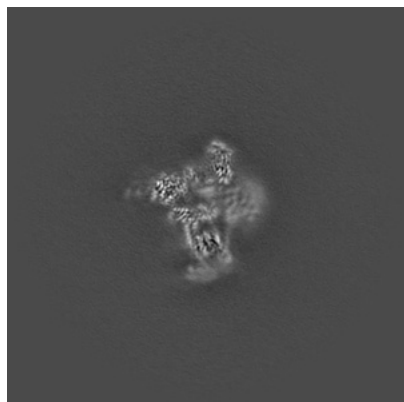


Z

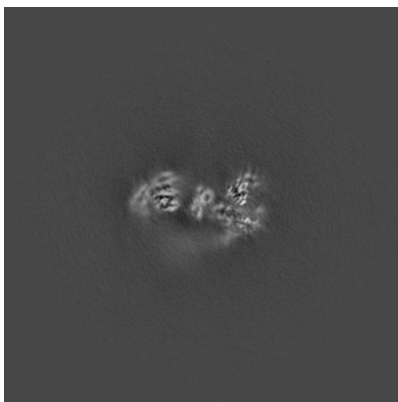
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

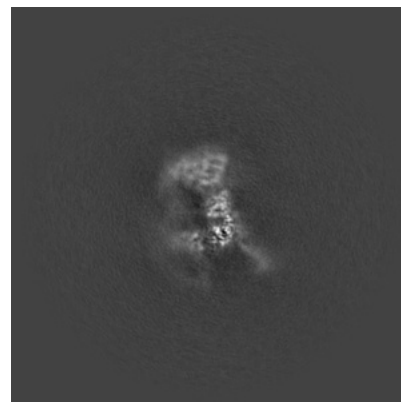
6.2.1 Primary map



X Index: 256

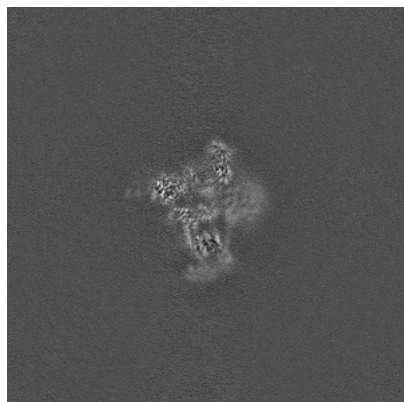


Y Index: 256



Z Index: 256

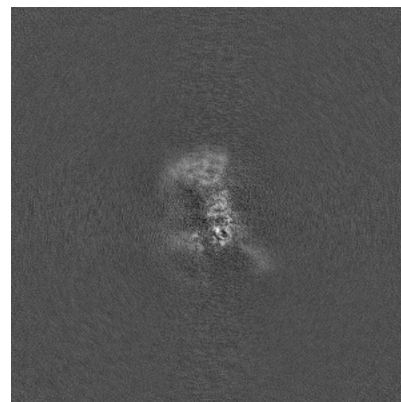
6.2.2 Raw map



X Index: 256



Y Index: 256

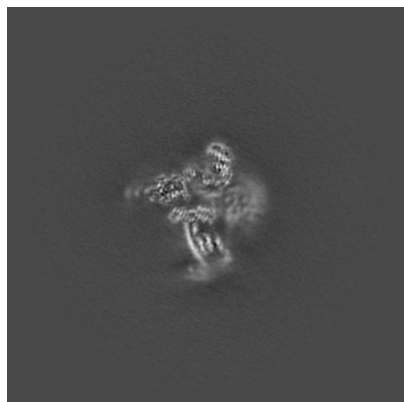


Z Index: 256

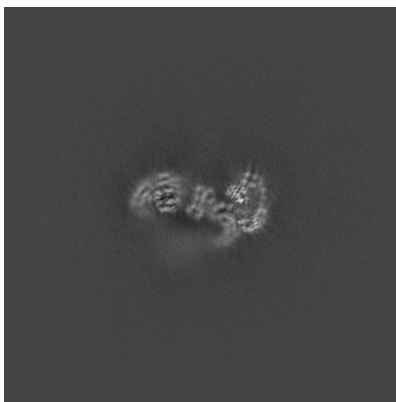
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

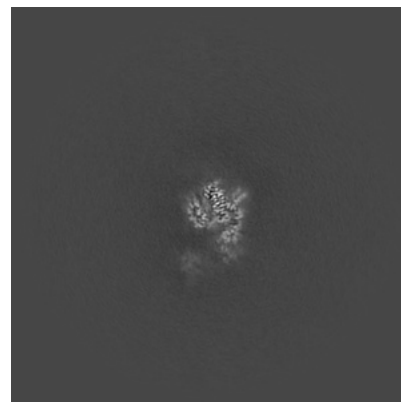
6.3.1 Primary map



X Index: 253



Y Index: 260



Z Index: 304

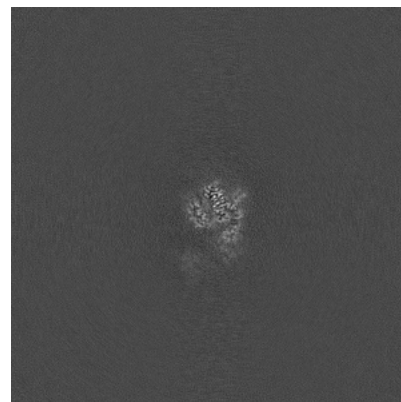
6.3.2 Raw map



X Index: 264



Y Index: 260



Z Index: 304

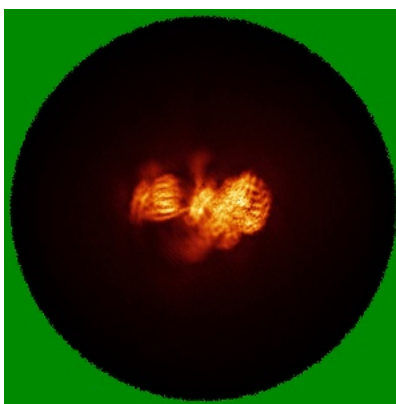
The images above show the largest variance slices of the map in three orthogonal directions.

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

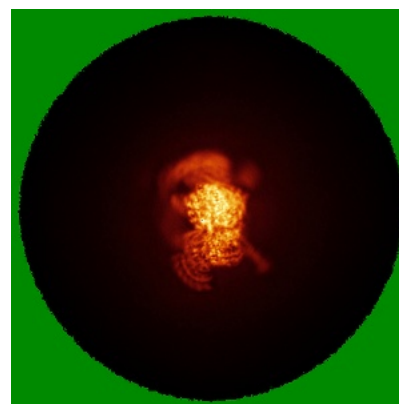
6.4.1 Primary map



X

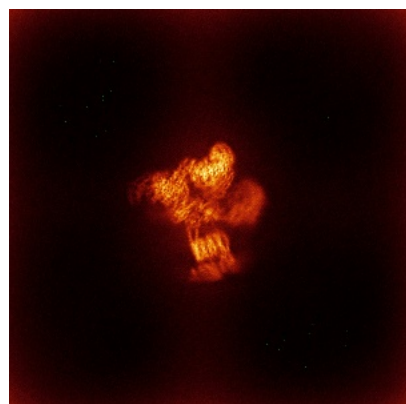


Y

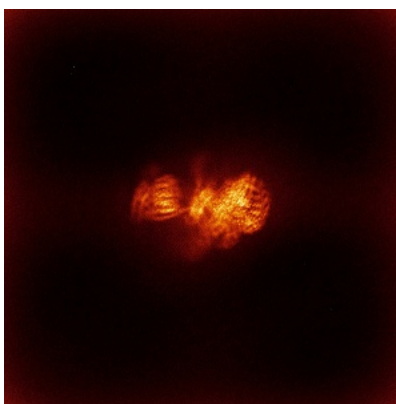


Z

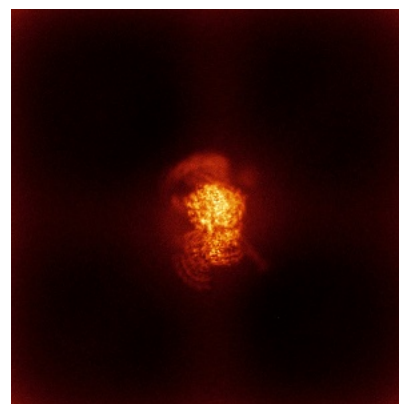
6.4.2 Raw map



X



Y

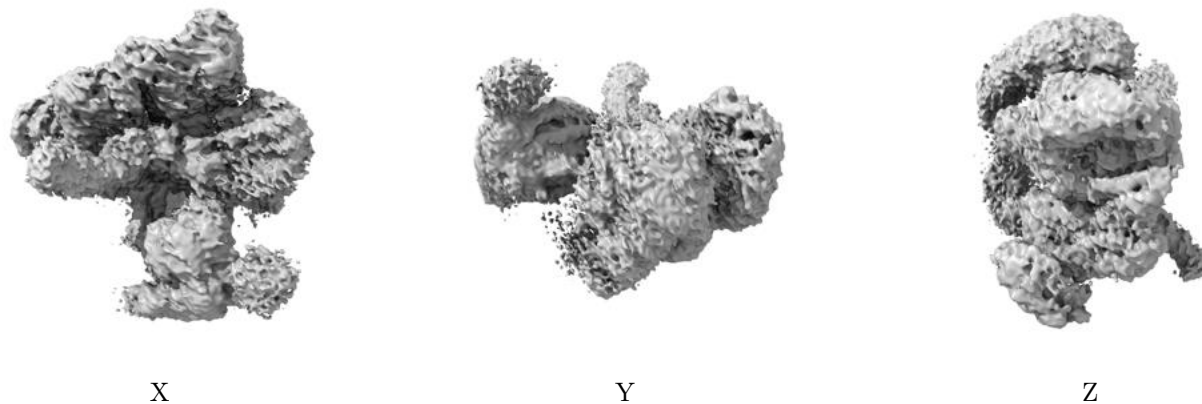


Z

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.

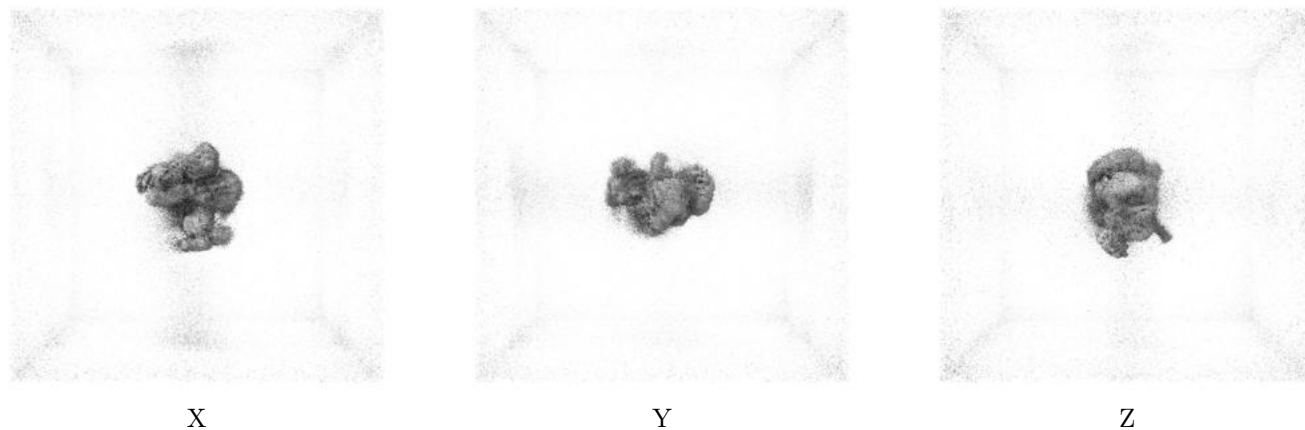
6.5 Orthogonal surface views [i](#)

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.

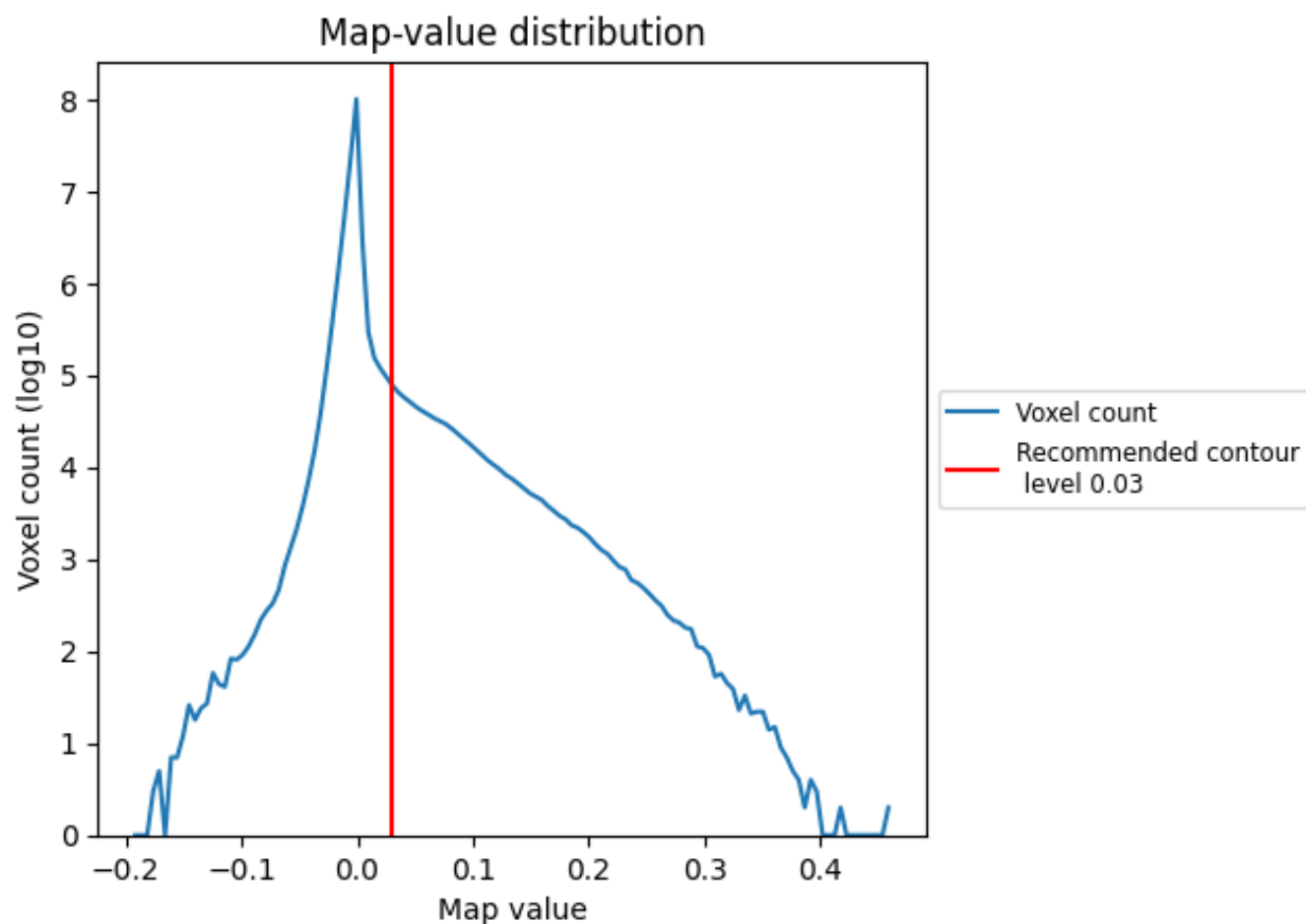
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

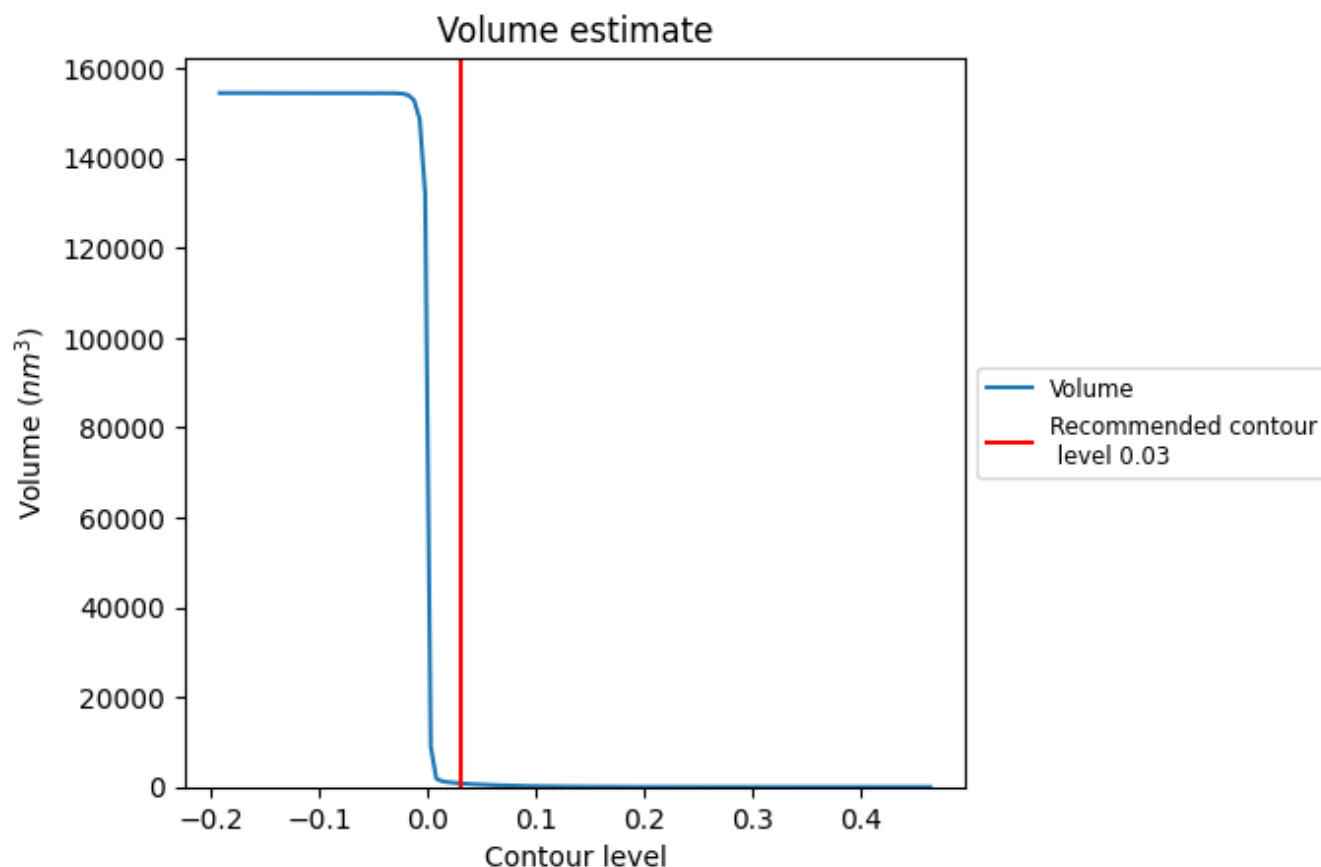
This section contains the results of statistical analysis of the map.

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.

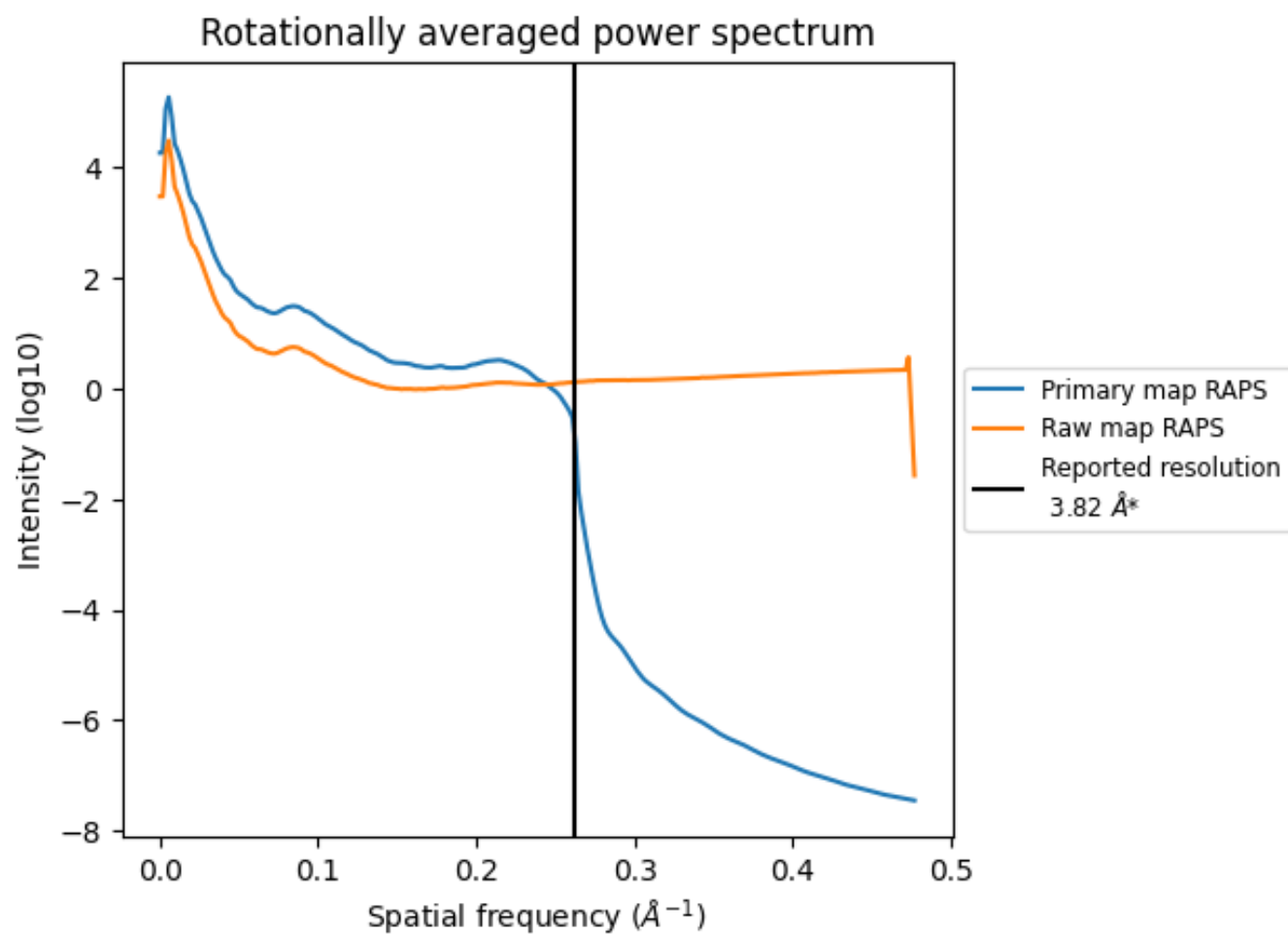
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 804 nm^3 ; this corresponds to an approximate mass of 726 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 ⓘ

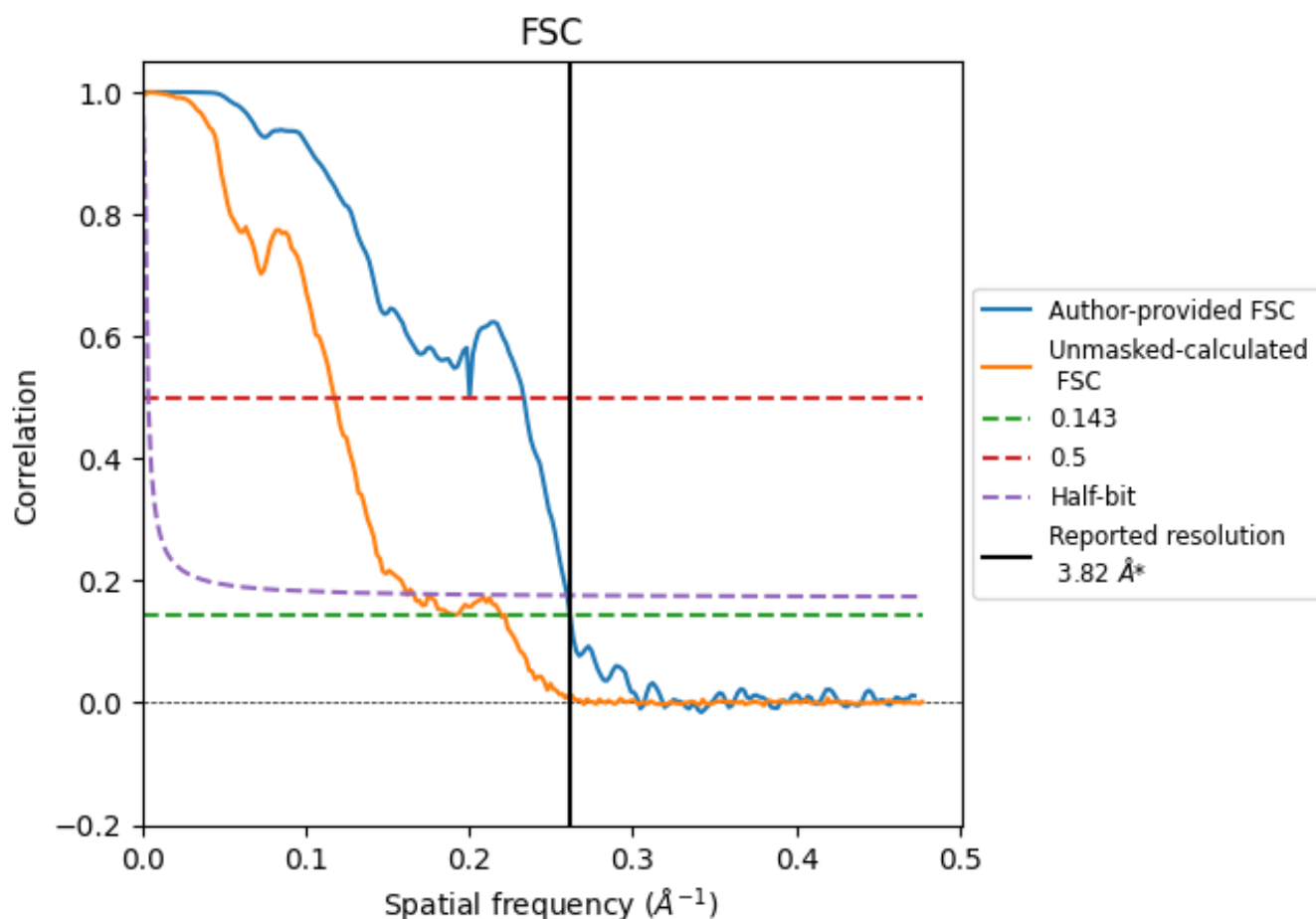


*Reported resolution corresponds to spatial frequency of 0.262 $\text{\AA}^{-1}$

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 0.262 $\text{\AA}^{-1}$

8.2 Resolution estimates

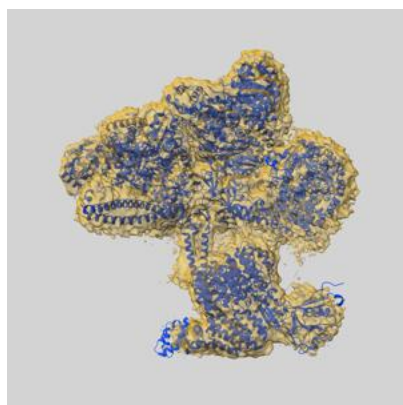
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.82	4.28	3.85
Unmasked-calculated*	4.56	8.50	6.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.56 differs from the reported value 3.82 by more than 10 %

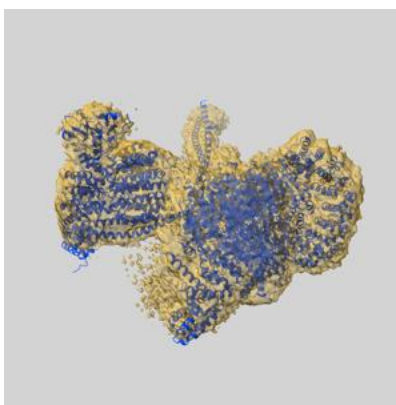
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77359 and PDB model 36BM. Per-residue inclusion information can be found in section 3 on page 7.

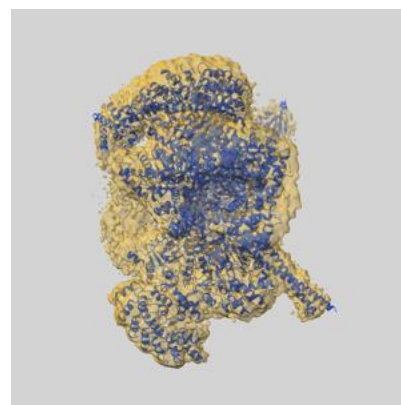
9.1 Map-model overlay [i](#)



X



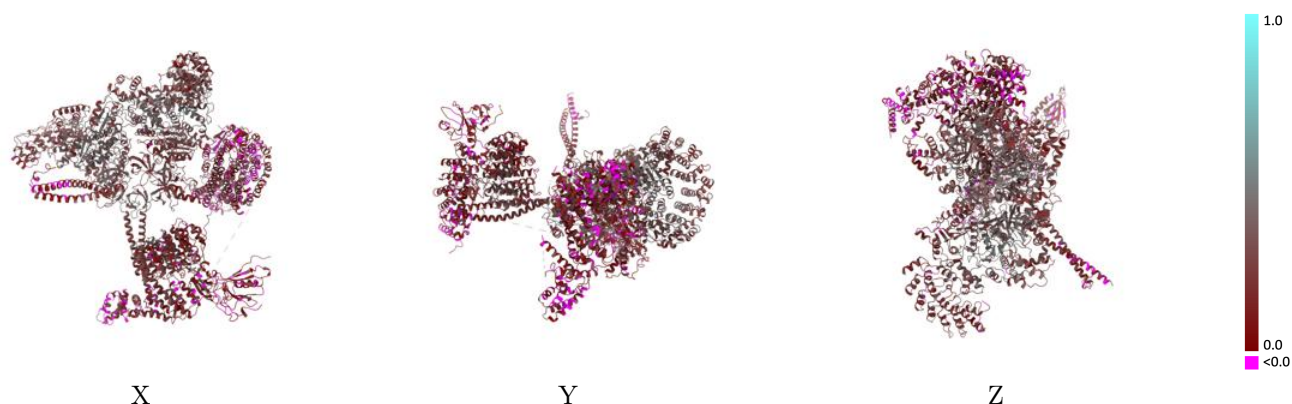
Y



Z

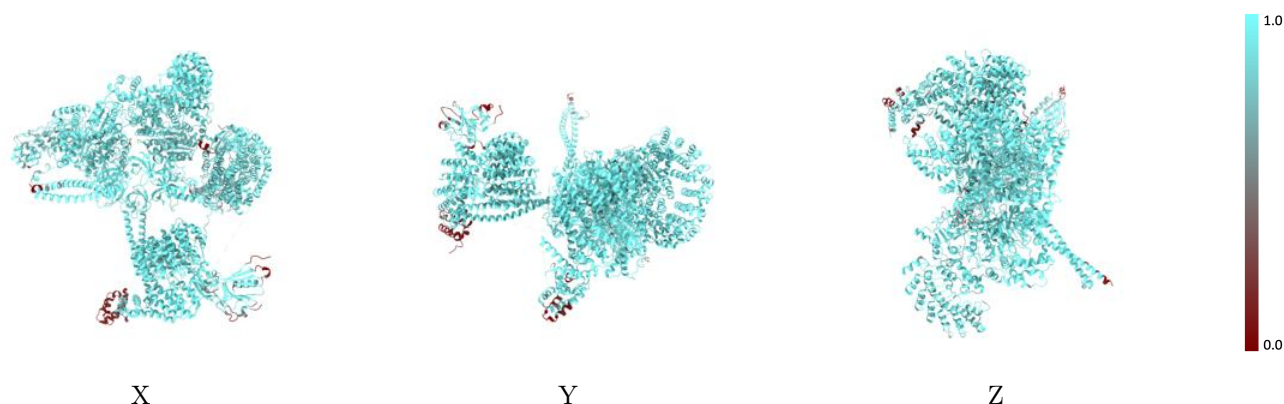
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



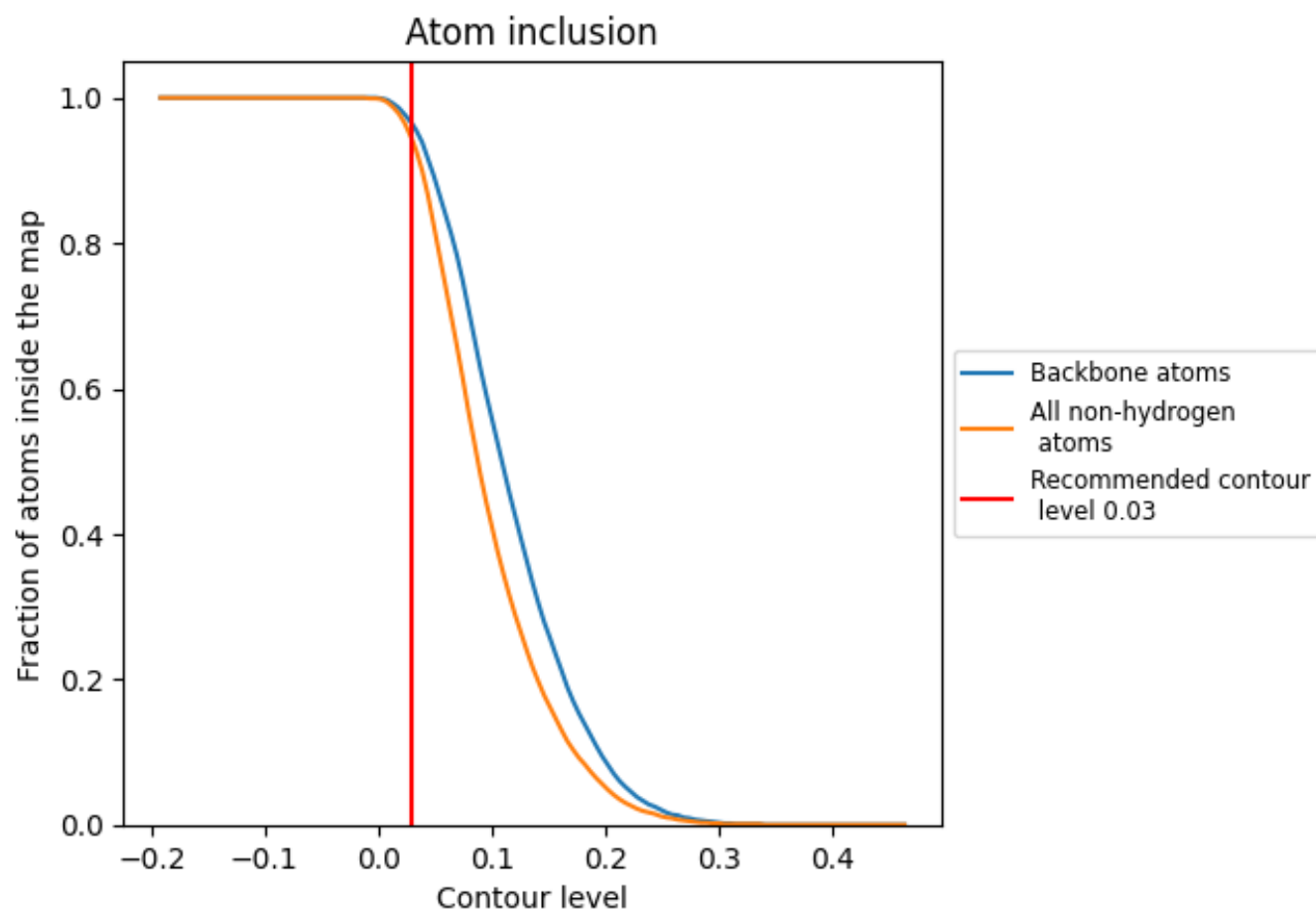
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 96% of all backbone atoms, 94% 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	 0.9420	 0.2430
A	 0.9630	 0.3380
B	 0.9740	 0.2420
C	 0.9420	 0.1200
D	 0.9900	 0.3170
I	 0.9730	 0.2580
J	 0.9640	 0.2820
K	 0.9700	 0.3300
L	 0.7610	 0.1290
N	 0.8850	 0.2240
P	 0.9790	 0.3270
Z	 0.8950	 0.2050

