



Full wwPDB EM Validation Report ⓘ

Sep 3, 2026 – 01:29 PM EDT

PDB ID : 36BD / pdb_000036bd
EMDB ID : EMD-77350
Title : yeast 26S proteasome base assembly intermediate, base-Rpn14-Hsm3-Nas6
with Rpt4-EQ
Authors : Hsieh, H.H.; Martin, A.
Deposited on : 2026-05-28
Resolution : 3.93 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:

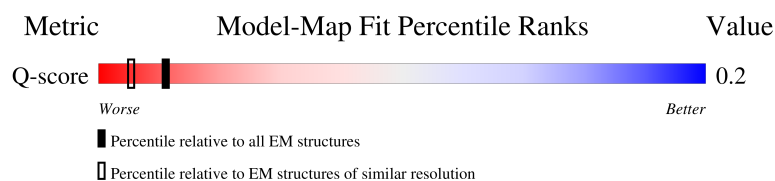
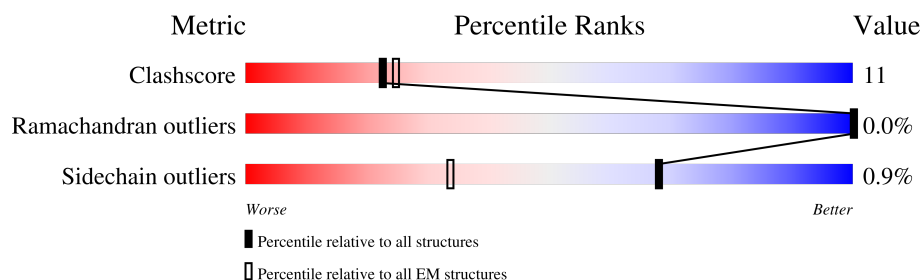
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.93 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	7811 (3.43 - 4.43)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	405	 64%31%5%
6	J	428	 61%27%11%
7	L	156	 58%26%16%
8	M	417	 7%83%17%
9	N	228	 67%32%.
10	Z	945	 5%72%21%7%
11	K	437	 66%20%.13%
12	P	434	 74%16%.10%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 41622 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	395	Total	C	N	O	S	0	0
			3071	1929	546	580	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	386	Total	C	N	O	S	0	0
			3028	1903	510	598	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	848	Total	C	N	O	S	0	0
			6584	4181	1077	1297	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	460	Total	C	N	O	S	0	0
			3756	2422	601	720	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	384	Total	C	N	O	S	0	0
			3013	1894	539	563	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 regulatory subunit RPN13.

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

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN14.

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

- Molecule 9 is a protein called Probable 26S proteasome regulatory subunit p28.

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

- Molecule 10 is a protein called 26S proteasome regulatory subunit RPN2.

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

- Molecule 11 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	382	Total	C	N	O	S	0	0
			3029	1908	541	568	12		

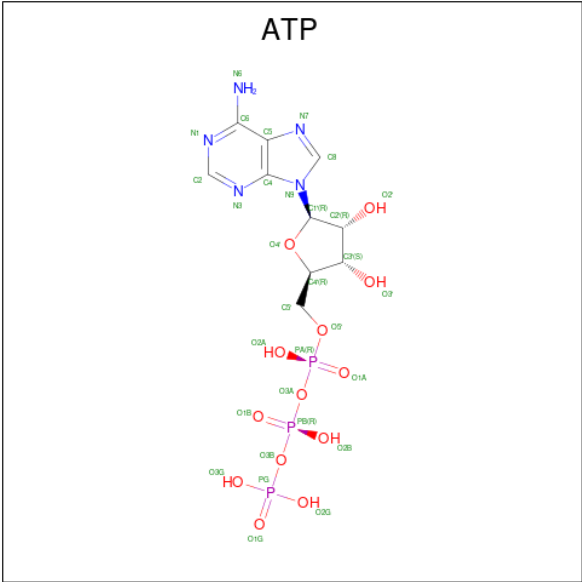
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called 26S proteasome regulatory subunit 6A.

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

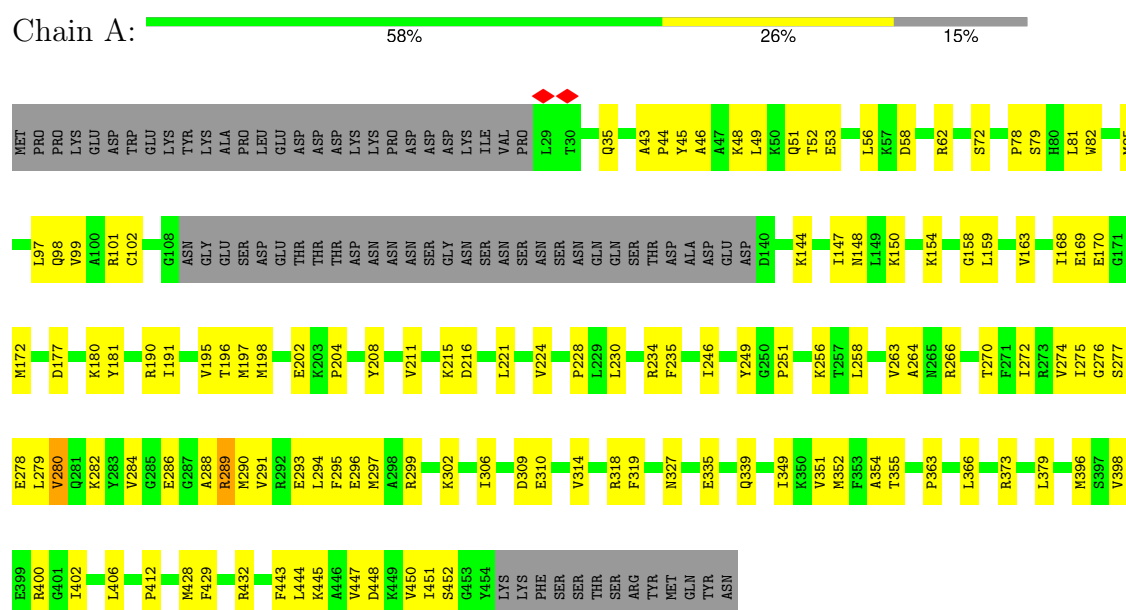
- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



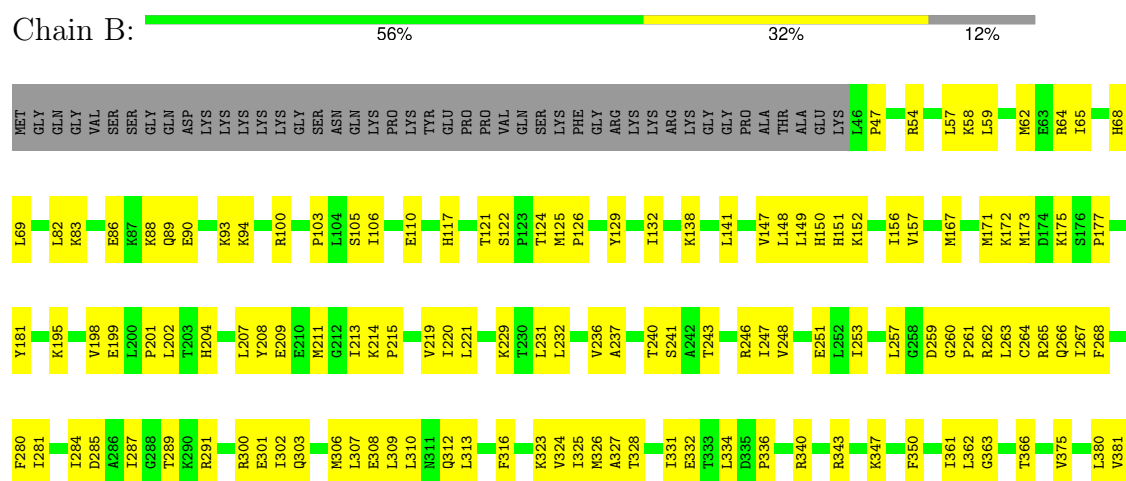
3 Residue-property plots

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.

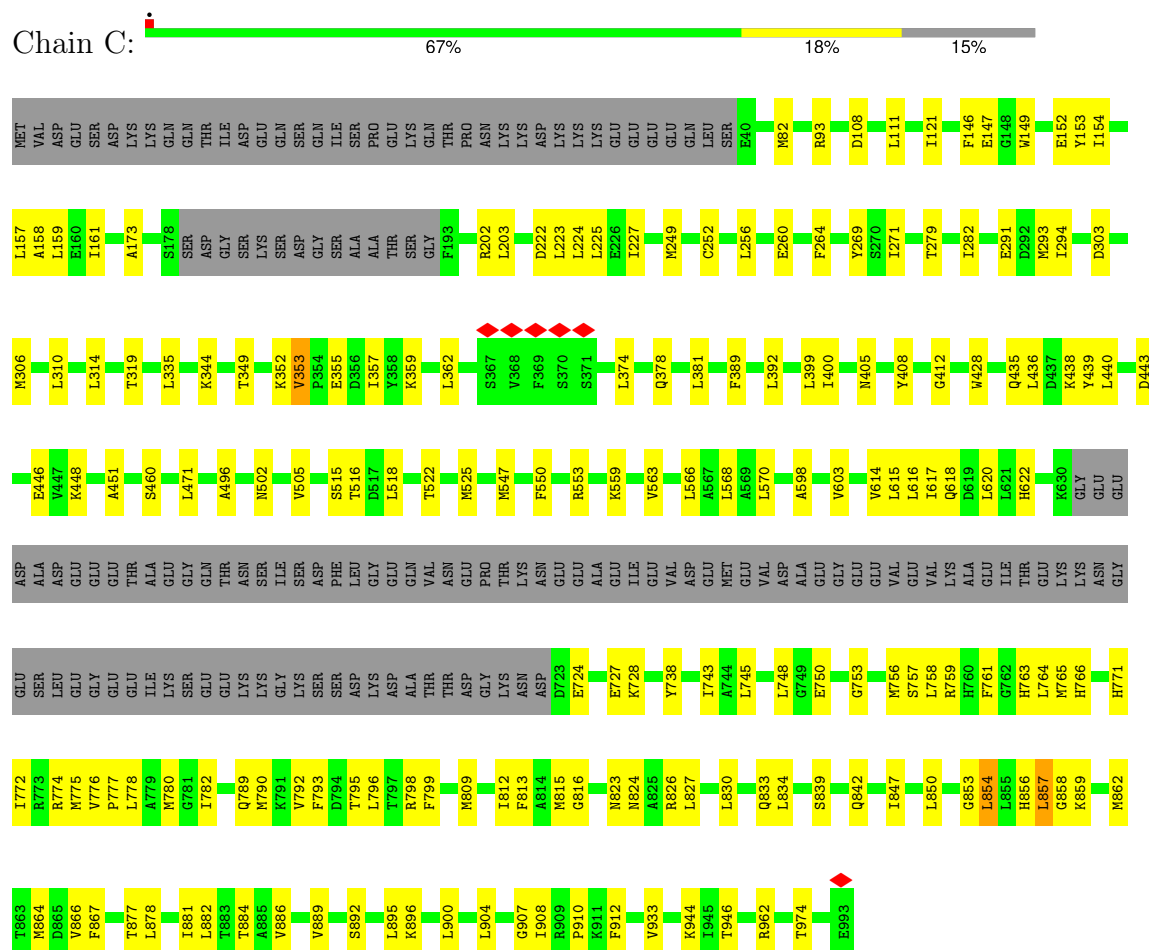
- Molecule 1: 26S proteasome regulatory subunit 7 homolog



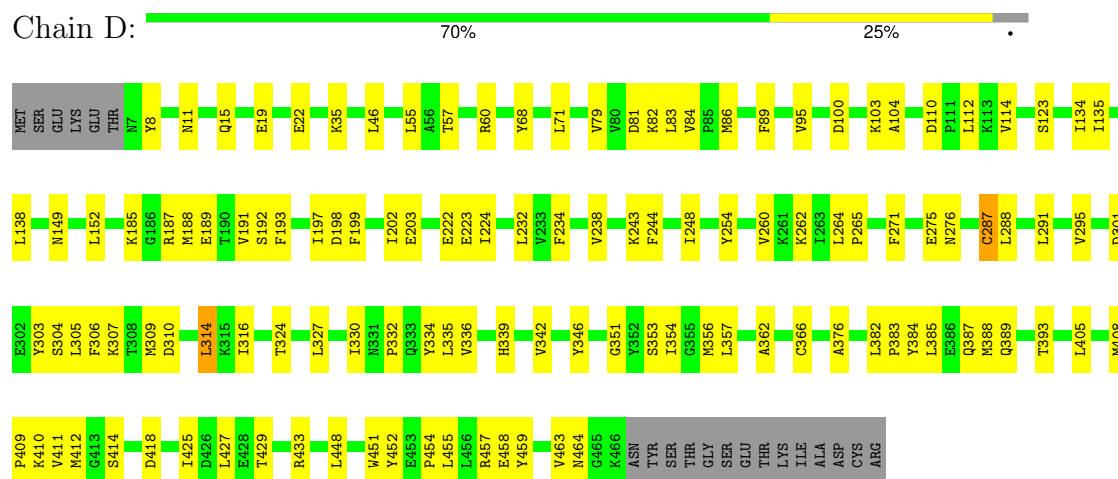
- Molecule 2: 26S proteasome regulatory subunit 4 homolog



- Molecule 3: 26S proteasome regulatory subunit RPN1

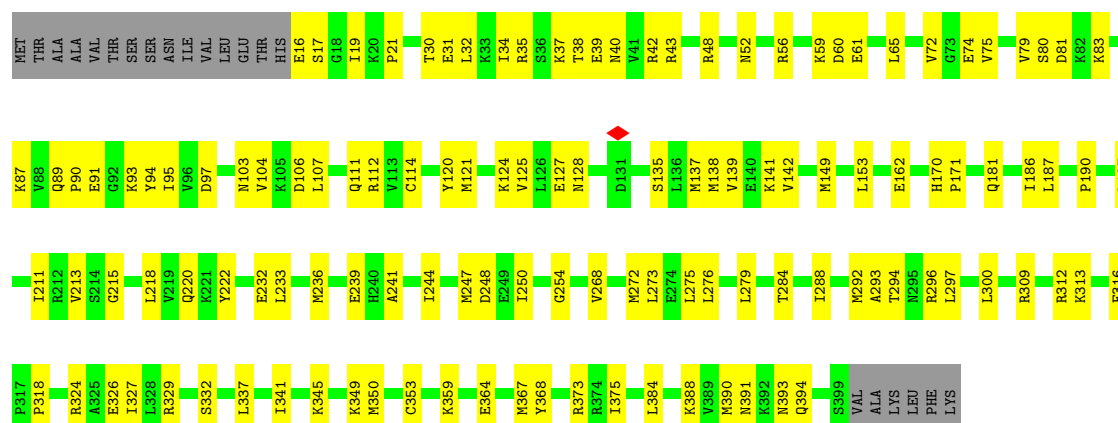


- Molecule 4: DNA mismatch repair protein HSM3



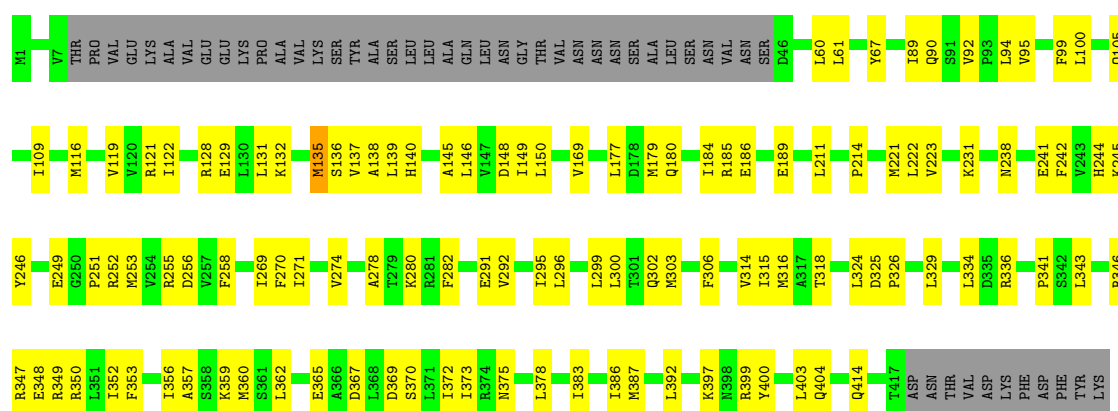
- Molecule 5: 26S proteasome regulatory subunit 8 homolog

Chain I:  64% 31% 5%



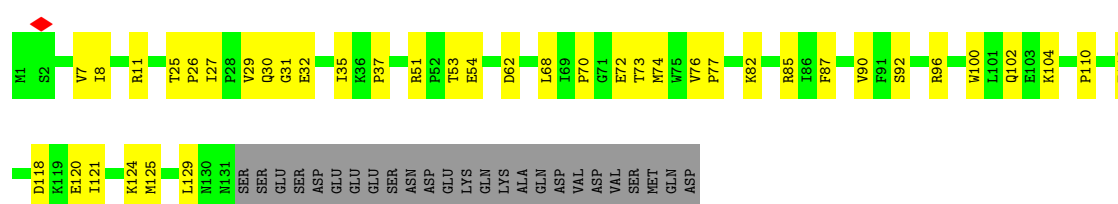
- Molecule 6: 26S proteasome regulatory subunit 6B homolog

Chain J:  61% 27% 11%



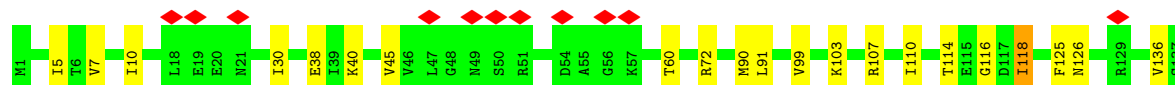
- Molecule 7: 26S proteasome regulatory subunit RPN13

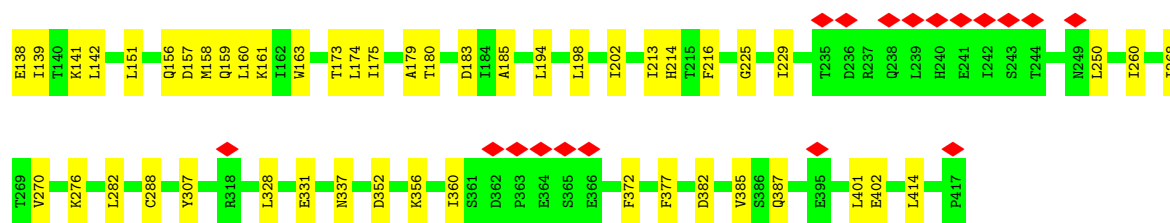
Chain L:  58% 26% 16%



- Molecule 8: 26S proteasome regulatory subunit RPN14

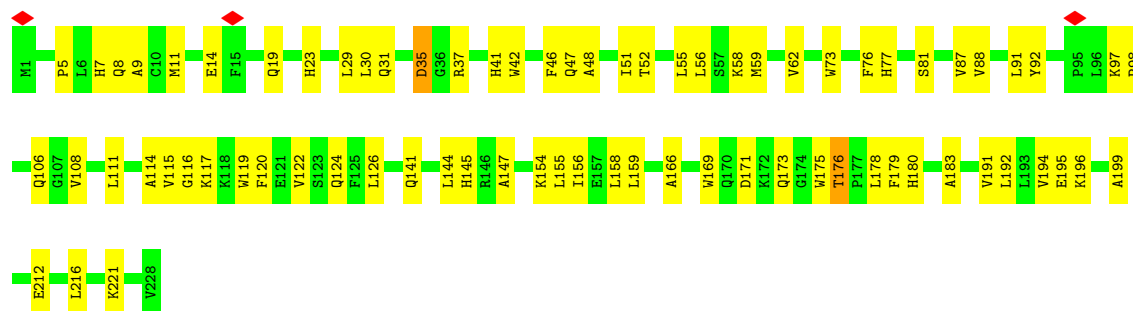
Chain M:  7% 83% 17%





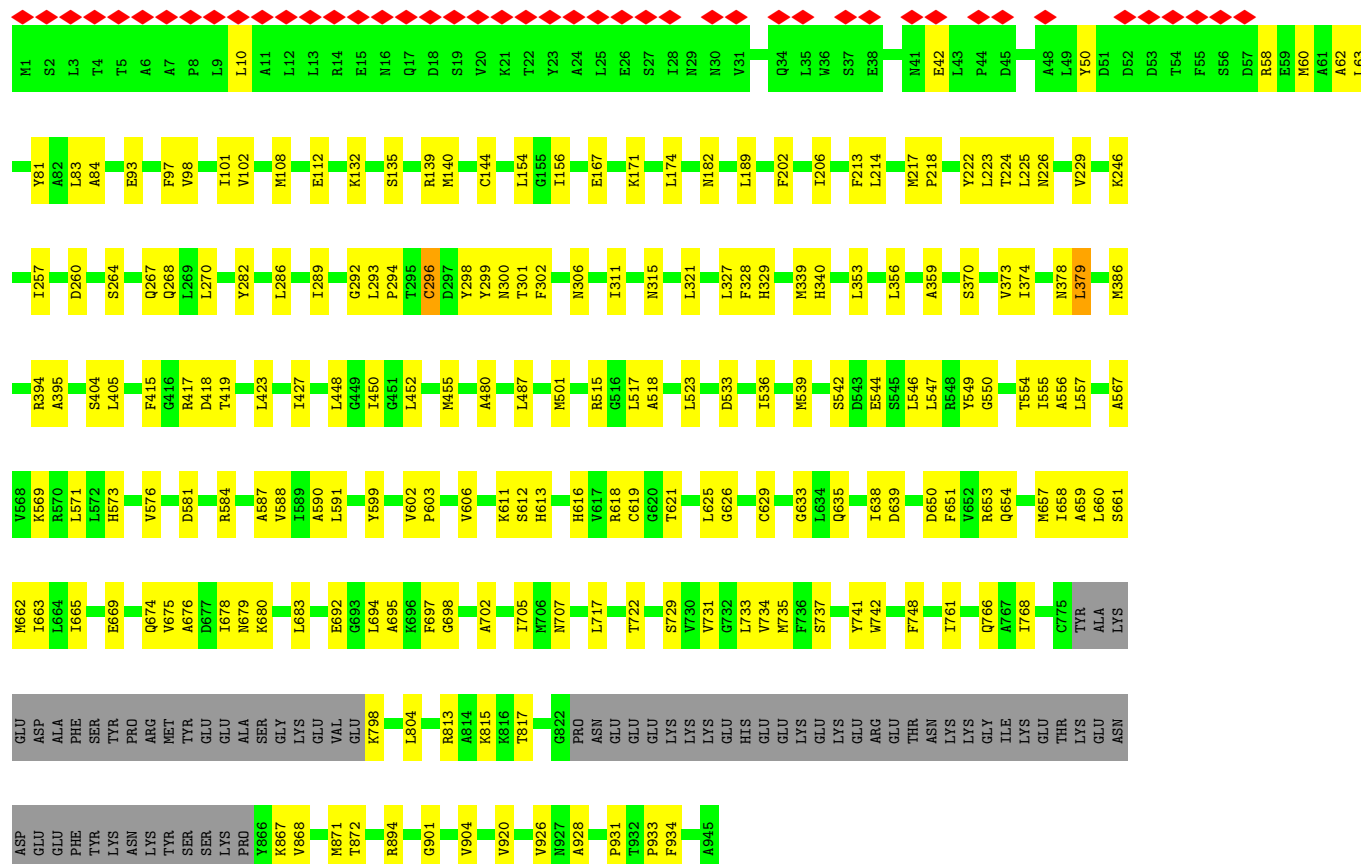
- Molecule 9: Probable 26S proteasome regulatory subunit p28

Chain N: 67% 32%



- Molecule 10: 26S proteasome regulatory subunit RPN2

Chain Z: 5% 72% 21% 7%



Chain K:

66% 20% 13%

MET SER GLU GLU GLN ASP PRO LEU LEU ALA P125 GLY LEU Y127 I128 GLY GLU THR SER GLY ASP ASN HIS THR GLN GLN SER SER HIS GLU GLN GLN PRO PRO GLU GLN GLN THR THR GLU GLU HIS HIS GLU PRO PRO SER ARG V46 D47 P48 E49 L64 E85 I95 L98 I105 M109 K110 E111 L112 I118 S123 G124 P125 R126 Y127 I128 R132 V135 K139 K142 L148 L149 L153 T154 E162 T163 M170 T171 T187 R191 E192 I193 R194 E195 V196 I197 E198 L199 I206 R209 V210 G211 I212 P215 V218 L219 L220 K228 T229 L230 V235 I239 G240 A241 I244 F245 S246 P247 K254 Y255 I256 G257 E258 I263 M266 F267 I277 I278 M280 F279 V283 G287 R290 E293 Q302 L305 M306 L309 M312 I323 I324 M325 A326 T327 D334 L337 R342 I343 D344

Chain P:

Amino Acid	Count	Percentage
ASP	1	
ASN	1	
THR	1	
ALA	1	
VAL	1	
G114	1	
K115	1	
A116	1	
A117	1	
V118	1	
S122	1	
S123	1	
R124	1	
Q125	1	
T126	1	
L129	1	
V132	1	
P137	1	
L140	1	
K141	1	
P142	1	
L145	1	
V146	1	
T155	1	
L159	1	
M170	1	
T190	1	
L193	1	
V194	1	
V198	1	
L199	1	
P200	1	
M201	1	
M210	1	
G211	1	
I212	1	
M220	1	
K228	1	
L231	1	
C235	1	
L246	1	
L247	1	
D19	1	
I22	1	
L30	1	
L37	1	
H53	1	
M58	1	
L75	1	
P76	1	
V79	1	
V83	1	
E84	1	
D87	1	
MET	1	
ASN	1	
GLU	1	
ILE	1	
GLU	1	
ASP	1	
LYS	1	
ASN	1	
SER	1	
GLU	1	
THR	1	
THR	1	
GLN	1	
GLY	1	
ASN	1	
VAL	1	
ASN	1	
THR	1	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	310130	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	0.447	Depositor
Minimum map value	-0.254	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	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	0.21	0/3118	0.38	0/4201
2	B	0.17	0/3069	0.38	0/4136
3	C	0.14	0/6702	0.31	0/9090
4	D	0.19	0/3823	0.37	0/5178
5	I	0.19	0/3052	0.40	0/4100
6	J	0.19	0/3028	0.44	0/4086
7	L	0.15	0/1087	0.42	0/1470
8	M	0.11	0/3328	0.32	0/4505
9	N	0.16	0/1851	0.42	0/2506
10	Z	0.24	0/6884	0.37	0/9313
11	K	0.16	0/3075	0.36	0/4135
12	P	0.13	0/3091	0.35	0/4162
All	All	0.18	0/42108	0.37	0/56882

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3071	0	3138	97	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3028	0	3097	121	0
3	C	6584	0	6535	115	0
4	D	3756	0	3791	91	0
5	I	3013	0	3141	101	0
6	J	2989	0	3069	96	0
7	L	1061	0	1050	31	0
8	M	3267	0	3175	43	0
9	N	1808	0	1792	53	0
10	Z	6776	0	6872	139	0
11	K	3029	0	3105	80	0
12	P	3054	0	3120	55	0
13	A	31	0	12	1	0
13	B	31	0	12	4	0
13	I	31	0	12	2	0
13	J	31	0	12	4	0
13	K	31	0	12	5	0
13	P	31	0	12	2	0
All	All	41622	0	41957	941	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 11.

All (941) 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)
10:Z:761:ILE:HD11	10:Z:904:VAL:HG22	1.54	0.89
2:B:284:ILE:HG21	2:B:326:MET:HB2	1.56	0.87
1:A:198:MET:HB3	1:A:272:ILE:HD11	1.62	0.82
7:L:31:GLY:HA2	7:L:53:THR:H	1.44	0.82
3:C:809:MET:HB3	3:C:847:ILE:HG21	1.62	0.81
7:L:35:ILE:HG21	7:L:125:MET:HE1	1.63	0.81
6:J:179:MET:HE3	6:J:179:MET:H	1.46	0.81
2:B:265:ARG:HA	2:B:312:GLN:HE21	1.45	0.80
6:J:249:GLU:HB3	6:J:252:ARG:HH21	1.44	0.80
3:C:864:MET:HE1	3:C:904:LEU:HB3	1.63	0.80
3:C:460:SER:HA	3:C:496:ALA:HA	1.62	0.79
3:C:790:MET:HE3	3:C:790:MET:H	1.47	0.79
5:I:324:ARG:HD2	5:I:350:MET:HE2	1.63	0.78
4:D:384:TYR:HA	4:D:387:GLN:HE21	1.48	0.78
5:I:139:VAL:HG23	5:I:211:ILE:HG12	1.66	0.78
10:Z:501:MET:HB3	10:Z:517:LEU:HD22	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:72:VAL:HG22	6:J:119:VAL:HG23	1.66	0.77
12:P:253:GLN:HG2	12:P:258:GLU:HB3	1.66	0.77
4:D:310:ASP:HA	4:D:314:LEU:HB2	1.66	0.77
5:I:75:VAL:HG11	5:I:107:LEU:HD13	1.66	0.76
11:K:105:ILE:HD12	12:P:126:THR:HG22	1.68	0.76
10:Z:289:ILE:HA	10:Z:294:PRO:HG2	1.66	0.76
5:I:48:ARG:HH22	10:Z:612:SER:HA	1.50	0.75
2:B:313:LEU:HB3	2:B:343:ARG:HH21	1.51	0.75
9:N:7:HIS:HE1	9:N:31:GLN:HG3	1.51	0.75
9:N:212:GLU:HB2	9:N:221:LYS:HE3	1.69	0.74
10:Z:518:ALA:HB1	10:Z:550:GLY:HA3	1.68	0.74
1:A:309:ASP:HA	1:A:354:ALA:HB3	1.69	0.73
5:I:181:GLN:HB2	5:I:284:THR:HB	1.69	0.73
2:B:395:MET:HE3	2:B:420:LYS:HB2	1.70	0.73
11:K:162:GLU:HG3	12:P:256:ILE:HG12	1.70	0.73
2:B:231:LEU:HD22	13:B:501:ATP:H2'	1.70	0.73
10:Z:680:LYS:HA	10:Z:683:LEU:HD12	1.70	0.72
3:C:399:LEU:HB3	3:C:400:ILE:HD12	1.70	0.72
9:N:59:MET:HB2	9:N:62:VAL:HB	1.72	0.71
1:A:197:MET:HE1	1:A:274:VAL:HG22	1.72	0.71
8:M:90:MET:HE1	8:M:126:ASN:HA	1.73	0.71
2:B:214:LYS:HD3	2:B:215:PRO:HD2	1.72	0.71
1:A:246:ILE:HG22	1:A:352:MET:HA	1.70	0.71
2:B:122:SER:HB3	2:B:125:MET:HB2	1.71	0.70
5:I:350:MET:HE3	5:I:353:CYS:HB2	1.73	0.70
11:K:254:LYS:HB2	12:P:299:ARG:HH21	1.56	0.69
3:C:750:GLU:HG3	3:C:753:GLY:H	1.56	0.69
8:M:141:LYS:HG3	8:M:183:ASP:HA	1.73	0.69
1:A:211:VAL:HG22	1:A:258:LEU:HD23	1.75	0.69
6:J:280:LYS:HG2	6:J:326:PRO:HD3	1.74	0.69
5:I:40:ASN:HA	5:I:43:ARG:HE	1.58	0.69
11:K:358:LEU:HD23	11:K:380:VAL:HG21	1.74	0.68
7:L:82:LYS:NZ	10:Z:934:PHE:HB2	2.08	0.68
1:A:78:PRO:HD2	1:A:81:LEU:HD12	1.76	0.68
1:A:198:MET:HG2	1:A:294:LEU:HD11	1.75	0.68
4:D:187:ARG:HG3	4:D:189:GLU:HG3	1.75	0.68
2:B:313:LEU:HD22	2:B:343:ARG:HE	1.59	0.68
7:L:82:LYS:HZ3	10:Z:934:PHE:HB2	1.59	0.68
1:A:279:LEU:HB2	1:A:314:VAL:HG11	1.75	0.67
6:J:100:LEU:HB2	6:J:109:ILE:HG23	1.77	0.67
7:L:32:GLU:HG2	7:L:51:ARG:HH22	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:138:ALA:HB3	6:J:148:ASP:HB2	1.75	0.67
12:P:200:PRO:HB2	12:P:201:MET:HE2	1.77	0.67
6:J:350:ARG:HG3	6:J:372:ILE:HG21	1.77	0.67
3:C:826:ARG:HH21	3:C:830:LEU:HD21	1.58	0.66
3:C:570:LEU:HD23	3:C:603:VAL:HG21	1.77	0.66
11:K:309:LEU:HD22	11:K:342:ARG:HD3	1.78	0.66
8:M:185:ALA:HB3	8:M:194:LEU:HB2	1.78	0.66
6:J:346:ARG:HE	6:J:350:ARG:HH21	1.45	0.65
11:K:254:LYS:H	11:K:254:LYS:HD2	1.60	0.65
2:B:306:MET:HA	2:B:309:LEU:HG	1.78	0.65
3:C:378:GLN:HA	3:C:381:LEU:HD12	1.79	0.65
4:D:327:LEU:HB2	4:D:356:MET:HE1	1.79	0.65
9:N:55:LEU:HD23	9:N:58:LYS:HZ2	1.62	0.65
12:P:305:MET:HE1	12:P:334:ASP:HB3	1.78	0.65
1:A:72:SER:HB3	5:I:79:VAL:HG13	1.79	0.65
1:A:195:VAL:HA	1:A:198:MET:HE1	1.76	0.65
12:P:193:LEU:HD21	12:P:235:CYS:HB2	1.78	0.65
6:J:350:ARG:HG3	6:J:372:ILE:HD13	1.79	0.65
9:N:176:THR:HG23	9:N:178:LEU:H	1.62	0.65
2:B:246:ARG:HG3	2:B:280:PHE:HD2	1.62	0.65
8:M:103:LYS:HA	8:M:107:ARG:HA	1.78	0.64
10:Z:222:TYR:HB3	10:Z:257:ILE:HD11	1.78	0.64
6:J:369:ASP:HA	6:J:372:ILE:HD12	1.78	0.64
4:D:408:MET:HA	4:D:408:MET:HE2	1.79	0.64
10:Z:154:LEU:HD22	10:Z:189:LEU:HD13	1.79	0.64
10:Z:659:ALA:O	10:Z:663:ILE:HG12	1.97	0.64
3:C:795:THR:HG23	3:C:798:ARG:HH22	1.62	0.64
3:C:374:LEU:HD23	3:C:842:GLN:HG2	1.80	0.64
3:C:547:MET:HA	3:C:550:PHE:HB2	1.80	0.64
10:Z:665:ILE:HD13	10:Z:705:ILE:O	1.98	0.63
3:C:303:ASP:HB3	3:C:306:MET:HB3	1.80	0.63
3:C:813:PHE:HB2	3:C:847:ILE:HD11	1.79	0.63
9:N:155:LEU:HA	9:N:158:LEU:HD23	1.80	0.63
2:B:211:MET:HA	2:B:211:MET:HE2	1.79	0.63
2:B:260:GLY:HA2	2:B:263:LEU:HD12	1.80	0.63
2:B:362:LEU:HD21	2:B:380:LEU:HD23	1.80	0.63
5:I:248:ASP:HA	5:I:293:ALA:HB3	1.81	0.63
3:C:353:VAL:HG22	3:C:355:GLU:H	1.65	0.62
6:J:375:ASN:HB3	9:N:173:GLN:HE22	1.63	0.62
2:B:117:HIS:HB3	2:B:129:TYR:HE1	1.64	0.62
6:J:353:PHE:CD1	6:J:372:ILE:HG12	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:300:LEU:HA	6:J:303:MET:HE3	1.82	0.62
8:M:10:ILE:HG13	8:M:30:ILE:HG12	1.79	0.62
11:K:255:TYR:HB2	11:K:258:GLU:HB2	1.82	0.62
11:K:283:VAL:HG12	11:K:327:THR:HB	1.81	0.62
2:B:375:VAL:HA	2:B:413:ALA:HB2	1.82	0.62
1:A:224:VAL:HG21	1:A:246:ILE:HD13	1.82	0.61
2:B:312:GLN:O	2:B:316:PHE:HB3	2.00	0.61
6:J:211:LEU:HG	6:J:315:ILE:HD11	1.81	0.61
9:N:8:GLN:HA	9:N:11:MET:HG3	1.83	0.61
11:K:305:LEU:HD11	11:K:337:LEU:HD11	1.81	0.61
11:K:148:LEU:HA	11:K:154:THR:O	2.00	0.61
9:N:92:TYR:CE1	9:N:98:PRO:HG2	2.35	0.61
12:P:145:LEU:HB3	12:P:159:LEU:HB2	1.83	0.61
10:Z:353:LEU:HA	10:Z:356:LEU:HD12	1.83	0.61
10:Z:417:ARG:C	10:Z:417:ARG:HE	2.09	0.61
10:Z:556:ALA:HB2	10:Z:590:ALA:HB1	1.83	0.61
12:P:22:ILE:HG23	12:P:30:LEU:HD21	1.82	0.61
3:C:777:PRO:HA	3:C:780:MET:HG2	1.83	0.61
3:C:816:GLY:HA3	3:C:854:LEU:HD12	1.82	0.60
8:M:110:ILE:HD12	8:M:142:LEU:HD22	1.82	0.60
7:L:118:ASP:HA	7:L:121:ILE:HD12	1.83	0.60
2:B:382:THR:HG23	2:B:384:LYS:H	1.66	0.60
10:Z:735:MET:HE3	10:Z:735:MET:HA	1.83	0.60
4:D:304:SER:HA	4:D:307:LYS:HE2	1.84	0.60
7:L:30:GLN:HE22	7:L:102:GLN:HB3	1.65	0.60
5:I:137:MET:SD	5:I:233:LEU:HB2	2.41	0.60
6:J:136:SER:HB3	6:J:150:LEU:HD12	1.83	0.60
4:D:357:LEU:HG	4:D:393:THR:HG21	1.83	0.60
10:Z:638:ILE:HG23	10:Z:660:LEU:HD21	1.82	0.60
8:M:260:ILE:HG22	8:M:270:VAL:HG22	1.84	0.59
1:A:196:THR:HG21	2:B:306:MET:HE1	1.84	0.59
10:Z:606:VAL:HG12	10:Z:621:THR:HG23	1.84	0.59
3:C:809:MET:HB3	3:C:847:ILE:HD13	1.84	0.59
3:C:146:PHE:HD1	3:C:153:TYR:HE2	1.50	0.59
5:I:31:GLU:HB3	5:I:35:ARG:HH21	1.67	0.59
12:P:312:LEU:HD13	12:P:342:ARG:HB3	1.85	0.59
4:D:264:LEU:HD12	4:D:305:LEU:HD21	1.85	0.59
10:Z:329:HIS:CE1	10:Z:359:ALA:HB2	2.38	0.59
6:J:303:MET:HA	6:J:306:PHE:CE1	2.38	0.59
6:J:373:ILE:HG21	9:N:141:GLN:HE22	1.68	0.58
7:L:8:ILE:HG12	7:L:124:LYS:HE2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:35:ASP:HB2	9:N:37:ARG:HG3	1.84	0.58
2:B:138:LYS:HA	2:B:141:LEU:HD23	1.85	0.58
11:K:112:LEU:HD21	11:K:118:ILE:HG12	1.84	0.58
9:N:29:LEU:HG	9:N:30:LEU:HG	1.85	0.58
10:Z:296:CYS:HB3	10:Z:379:LEU:HD11	1.84	0.58
5:I:65:LEU:HD12	6:J:145:ALA:HB1	1.85	0.58
7:L:25:THR:HG23	10:Z:933:PRO:HG3	1.84	0.58
1:A:177:ASP:HB3	1:A:181:TYR:N	2.18	0.58
3:C:795:THR:HG22	3:C:799:PHE:HE2	1.69	0.58
6:J:169:VAL:HG11	6:J:221:MET:HG2	1.85	0.58
4:D:306:PHE:HA	4:D:309:MET:HG2	1.85	0.58
5:I:38:THR:O	5:I:42:ARG:HG3	2.04	0.58
10:Z:761:ILE:HG13	10:Z:904:VAL:HA	1.86	0.58
1:A:102:CYS:HA	1:A:147:ILE:HG22	1.86	0.57
3:C:173:ALA:HA	10:Z:815:LYS:HZ1	1.69	0.57
11:K:388:GLY:HA3	13:K:501:ATP:C8	2.39	0.57
3:C:357:ILE:HD12	3:C:856:HIS:CD2	2.39	0.57
1:A:318:ARG:HH21	1:A:327:ASN:ND2	2.02	0.57
2:B:147:VAL:HB	2:B:156:ILE:HD13	1.86	0.57
7:L:72:GLU:HG2	7:L:92:SER:HB3	1.85	0.57
6:J:318:THR:HG21	6:J:324:LEU:HD11	1.87	0.57
5:I:186:ILE:HG13	5:I:292:MET:HG3	1.85	0.57
1:A:221:LEU:HD23	1:A:263:VAL:HG21	1.85	0.57
6:J:291:GLU:O	6:J:295:ILE:HG13	2.04	0.57
10:Z:223:LEU:HG	10:Z:894:ARG:CZ	2.34	0.57
10:Z:557:LEU:HD21	10:Z:734:VAL:HG21	1.86	0.57
4:D:68:TYR:HB2	4:D:71:LEU:HB2	1.87	0.57
7:L:68:LEU:HA	7:L:73:THR:HG21	1.87	0.57
10:Z:321:LEU:HB3	10:Z:328:PHE:HB3	1.86	0.57
11:K:163:THR:HG23	12:P:256:ILE:HD13	1.86	0.57
10:Z:286:LEU:HD12	10:Z:289:ILE:HD12	1.86	0.57
1:A:190:ARG:HH21	1:A:191:ILE:HG13	1.70	0.56
6:J:400:TYR:HB3	11:K:206:ILE:HD12	1.87	0.56
10:Z:557:LEU:HD11	10:Z:734:VAL:HG11	1.87	0.56
3:C:615:LEU:HD23	10:Z:804:LEU:HD13	1.87	0.56
4:D:336:VAL:HG11	4:D:366:CYS:HA	1.87	0.56
7:L:32:GLU:HG2	7:L:51:ARG:NH2	2.19	0.56
11:K:195:GLU:HA	11:K:199:LEU:HD12	1.87	0.56
2:B:106:ILE:HD12	5:I:93:LYS:HB3	1.88	0.56
3:C:359:LYS:HB2	3:C:362:LEU:HD13	1.87	0.56
5:I:87:LYS:HD3	5:I:93:LYS:NZ	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MET:HE3	1:A:198:MET:HG3	1.88	0.56
5:I:364:GLU:HA	5:I:367:MET:SD	2.46	0.56
6:J:255:ARG:HA	6:J:302:GLN:HE21	1.71	0.56
1:A:43:ALA:HB3	1:A:46:ALA:HB2	1.87	0.56
2:B:291:ARG:HD2	2:B:302:ILE:HG22	1.86	0.56
11:K:123:SER:HA	12:P:124:ARG:NH1	2.21	0.56
3:C:862:MET:HB3	3:C:908:ILE:HD11	1.87	0.56
5:I:16:GLU:O	5:I:21:PRO:HG3	2.06	0.56
3:C:522:THR:HA	3:C:525:MET:HE2	1.88	0.56
8:M:337:ASN:HD22	8:M:387:GLN:HA	1.70	0.56
2:B:248:VAL:HB	2:B:251:GLU:HB2	1.86	0.56
3:C:502:ASN:HB3	3:C:505:VAL:HG22	1.87	0.56
10:Z:635:GLN:HA	10:Z:638:ILE:HD12	1.87	0.56
10:Z:669:GLU:HG2	10:Z:676:ALA:HB2	1.87	0.56
11:K:382:MET:HE2	11:K:420:ARG:HA	1.88	0.56
4:D:193:PHE:O	4:D:197:ILE:HG12	2.06	0.55
4:D:339:HIS:HB3	4:D:342:VAL:HB	1.88	0.55
8:M:156:GLN:HA	8:M:180:THR:HG23	1.87	0.55
8:M:183:ASP:HB2	8:M:229:ILE:HG12	1.87	0.55
11:K:142:LYS:HE2	11:K:256:ILE:HB	1.87	0.55
9:N:175:TRP:HE3	9:N:180:HIS:HD2	1.53	0.55
10:Z:60:MET:HE1	10:Z:63:LEU:HD23	1.87	0.55
2:B:268:PHE:CE2	2:B:312:GLN:HB3	2.42	0.55
3:C:108:ASP:HB3	3:C:111:LEU:HB2	1.89	0.55
7:L:110:PRO:HG2	7:L:113:GLU:HB2	1.89	0.55
11:K:171:THR:HG22	11:K:244:ILE:HG12	1.89	0.55
3:C:121:ILE:HD12	3:C:149:TRP:HB3	1.89	0.55
4:D:448:LEU:HD12	4:D:452:TYR:HD1	1.71	0.55
7:L:90:VAL:HG13	7:L:96:ARG:HG2	1.88	0.55
8:M:213:ILE:HG12	8:M:250:LEU:HD23	1.88	0.55
5:I:39:GLU:HA	5:I:42:ARG:HE	1.72	0.55
10:Z:633:GLY:HA2	10:Z:663:ILE:HG22	1.88	0.55
11:K:85:GLU:HG3	12:P:58:MET:HE1	1.87	0.55
3:C:282:ILE:HD11	3:C:314:LEU:HD21	1.88	0.55
3:C:748:LEU:HG	3:C:867:PHE:HE2	1.72	0.55
3:C:877:THR:O	3:C:881:ILE:HG12	2.07	0.54
3:C:389:PHE:HD2	3:C:853:GLY:HA3	1.73	0.54
4:D:376:ALA:HB1	4:D:410:LYS:HD2	1.87	0.54
6:J:105:GLN:CD	6:J:105:GLN:H	2.15	0.54
11:K:228:LYS:HG2	11:K:349:ILE:HG21	1.90	0.54
2:B:150:HIS:CE1	2:B:152:LYS:HB2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:26:PRO:HG2	10:Z:931:PRO:HG2	1.88	0.54
12:P:296:SER:HA	12:P:299:ARG:HD2	1.89	0.54
3:C:812:ILE:HA	3:C:815:MET:HG3	1.88	0.54
5:I:272:MET:HE1	5:I:275:LEU:HD23	1.89	0.54
10:Z:167:GLU:HG3	10:Z:213:PHE:CZ	2.42	0.54
12:P:124:ARG:O	12:P:124:ARG:HG2	2.06	0.54
3:C:471:LEU:HD13	3:C:505:VAL:HG12	1.87	0.54
4:D:301:ASP:HB2	4:D:304:SER:HB3	1.89	0.54
8:M:38:GLU:HB3	8:M:40:LYS:NZ	2.22	0.54
1:A:246:ILE:CD1	1:A:373:ARG:HB2	2.37	0.54
2:B:105:SER:OG	2:B:149:LEU:HB2	2.08	0.54
2:B:336:PRO:HB3	4:D:427:LEU:HD23	1.89	0.54
9:N:7:HIS:CE1	9:N:31:GLN:HG3	2.39	0.54
9:N:117:LYS:HB2	9:N:119:TRP:NE1	2.23	0.54
10:Z:571:LEU:HD22	10:Z:587:ALA:O	2.07	0.54
3:C:763:HIS:HA	3:C:766:HIS:ND1	2.23	0.54
6:J:95:VAL:HG22	11:K:127:TYR:HE1	1.73	0.54
11:K:254:LYS:HD3	12:P:299:ARG:HE	1.73	0.54
2:B:219:VAL:O	2:B:326:MET:HE3	2.08	0.54
1:A:398:VAL:HG23	1:A:402:ILE:HD12	1.90	0.54
8:M:158:MET:HE2	8:M:179:ALA:HA	1.90	0.54
1:A:276:GLY:H	1:A:310:GLU:HG3	1.73	0.53
1:A:277:SER:O	1:A:280:VAL:HG22	2.08	0.53
2:B:331:ILE:HA	2:B:334:LEU:HD23	1.90	0.53
3:C:745:LEU:HD21	3:C:882:LEU:HD11	1.91	0.53
5:I:59:LYS:HG3	5:I:60:ASP:N	2.23	0.53
5:I:236:MET:HA	5:I:239:GLU:HG3	1.91	0.53
5:I:97:ASP:HB2	5:I:121:MET:HE1	1.89	0.53
11:K:344:ASP:C	11:K:345:ARG:HD3	2.34	0.53
1:A:46:ALA:HA	1:A:49:LEU:HD12	1.90	0.53
1:A:406:LEU:HD21	4:D:191:VAL:HA	1.89	0.53
1:A:412:PRO:HG3	4:D:243:LYS:NZ	2.22	0.53
3:C:761:PHE:HA	3:C:764:LEU:HD12	1.90	0.53
8:M:114:THR:HA	8:M:138:GLU:HG3	1.89	0.53
11:K:230:LEU:HD22	13:K:501:ATP:H2'	1.91	0.53
4:D:198:ASP:O	4:D:202:ILE:HG12	2.08	0.53
6:J:92:VAL:HG12	11:K:128:ILE:HG13	1.91	0.53
8:M:328:LEU:HD21	8:M:331:GLU:HB2	1.91	0.53
3:C:778:LEU:O	3:C:782:ILE:HG12	2.09	0.53
11:K:132:ARG:HB3	11:K:135:VAL:HG23	1.91	0.53
11:K:389:ALA:HB2	13:K:501:ATP:H5'1	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:LEU:HB3	2:B:343:ARG:NH2	2.21	0.52
3:C:291:GLU:HA	3:C:294:ILE:HD12	1.92	0.52
5:I:149:MET:HE3	5:I:149:MET:O	2.09	0.52
4:D:351:GLY:O	4:D:354:ILE:HG12	2.09	0.52
10:Z:327:LEU:HG	10:Z:697:PHE:HD1	1.74	0.52
11:K:360:ILE:HG12	13:K:501:ATP:N1	2.24	0.52
12:P:84:GLU:HB2	12:P:255:TYR:CZ	2.45	0.52
6:J:221:MET:HE1	13:J:501:ATP:C2	2.44	0.52
1:A:306:ILE:HG23	1:A:351:VAL:HA	1.92	0.52
10:Z:731:VAL:O	10:Z:735:MET:HG2	2.10	0.52
1:A:450:VAL:HG12	1:A:451:ILE:HD13	1.91	0.52
3:C:314:LEU:HB3	3:C:319:THR:OG1	2.10	0.52
7:L:74:MET:HE3	7:L:90:VAL:HB	1.90	0.52
2:B:65:ILE:O	2:B:69:LEU:HG	2.10	0.52
4:D:244:PHE:O	4:D:248:ILE:HG12	2.10	0.52
9:N:154:LYS:HD2	9:N:154:LYS:O	2.10	0.52
1:A:52:THR:HG21	2:B:62:MET:HG3	1.92	0.52
3:C:858:GLY:HA3	3:C:862:MET:HG2	1.91	0.52
10:Z:97:PHE:O	10:Z:101:ILE:HG12	2.10	0.52
12:P:327:THR:HG21	12:P:333:LEU:HD11	1.91	0.52
4:D:222:GLU:OE2	4:D:223:GLU:HG3	2.10	0.52
6:J:253:MET:HA	6:J:256:ASP:HB2	1.92	0.52
1:A:154:LYS:HB3	12:P:79:VAL:HB	1.92	0.52
8:M:352:ASP:HB2	8:M:382:ASP:HB2	1.92	0.52
1:A:202:GLU:HA	1:A:270:THR:HG23	1.92	0.51
3:C:335:LEU:HD23	3:C:428:TRP:CD1	2.44	0.51
4:D:134:ILE:O	4:D:138:LEU:HG	2.09	0.51
3:C:748:LEU:HD21	3:C:866:VAL:HG11	1.92	0.51
5:I:59:LYS:HE3	10:Z:613:HIS:HB2	1.91	0.51
6:J:280:LYS:HG2	6:J:325:ASP:HA	1.93	0.51
6:J:292:VAL:HA	6:J:295:ILE:HD12	1.92	0.51
8:M:90:MET:O	8:M:90:MET:HG2	2.09	0.51
5:I:37:LYS:HB3	6:J:61:LEU:HD13	1.92	0.51
5:I:141:LYS:HD2	5:I:142:VAL:H	1.76	0.51
10:Z:108:MET:O	10:Z:112:GLU:HG2	2.11	0.51
10:Z:339:MET:HE3	10:Z:707:ASN:HD22	1.76	0.51
3:C:884:THR:HA	3:C:900:LEU:HD21	1.91	0.51
4:D:307:LYS:HG2	4:D:334:TYR:HE2	1.75	0.51
5:I:35:ARG:O	5:I:39:GLU:HG2	2.11	0.51
6:J:221:MET:SD	13:J:501:ATP:H2'	2.51	0.51
11:K:196:VAL:HG13	11:K:215:PRO:HG2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:253:GLN:HG3	12:P:255:TYR:H	1.76	0.51
5:I:39:GLU:HA	5:I:42:ARG:NE	2.25	0.51
5:I:74:GLU:OE1	5:I:112:ARG:HG2	2.11	0.51
9:N:11:MET:HA	9:N:46:PHE:CE1	2.45	0.51
12:P:190:ILE:HG12	12:P:231:LEU:HD11	1.93	0.51
10:Z:301:THR:HG22	10:Z:920:VAL:H	1.76	0.51
10:Z:717:LEU:HD13	10:Z:729:SER:HB3	1.93	0.51
11:K:235:VAL:O	11:K:239:ILE:HG22	2.11	0.51
1:A:53:GLU:HA	1:A:56:LEU:HD12	1.93	0.51
2:B:62:MET:HA	2:B:65:ILE:HD12	1.91	0.51
3:C:933:VAL:HG21	3:C:946:THR:HG23	1.92	0.51
5:I:40:ASN:HA	5:I:43:ARG:NE	2.25	0.51
6:J:349:ARG:HD3	6:J:378:LEU:HB2	1.92	0.51
2:B:220:ILE:HB	2:B:347:LYS:HG2	1.91	0.51
6:J:186:GLU:HB2	6:J:336:ARG:HH12	1.76	0.51
3:C:765:MET:HG3	3:C:799:PHE:CE1	2.46	0.51
5:I:197:LEU:HD22	13:I:501:ATP:H2'	1.92	0.51
6:J:245:LYS:HB2	11:K:293:GLU:HA	1.93	0.51
4:D:79:VAL:O	4:D:83:LEU:HG	2.11	0.50
6:J:280:LYS:HB2	6:J:282:PHE:CE1	2.45	0.50
12:P:388:GLY:HA3	13:P:501:ATP:C8	2.46	0.50
2:B:105:SER:HA	5:I:94:TYR:CD1	2.47	0.50
2:B:284:ILE:HG13	2:B:334:LEU:HD11	1.92	0.50
4:D:135:ILE:HA	4:D:138:LEU:HD12	1.94	0.50
4:D:383:PRO:O	4:D:387:GLN:HG3	2.11	0.50
11:K:123:SER:HA	12:P:124:ARG:HH12	1.75	0.50
12:P:210:MET:HG3	12:P:212:ILE:HD12	1.92	0.50
3:C:224:LEU:HD23	3:C:227:ILE:HD11	1.93	0.50
8:M:38:GLU:HB3	8:M:40:LYS:HZ2	1.77	0.50
10:Z:658:ILE:O	10:Z:662:MET:HG3	2.11	0.50
10:Z:246:LYS:HD2	10:Z:282:TYR:CE2	2.47	0.50
10:Z:544:GLU:HG3	10:Z:547:LEU:H	1.76	0.50
2:B:287:ILE:H	2:B:287:ILE:HD12	1.76	0.50
4:D:303:TYR:O	4:D:307:LYS:HG3	2.11	0.50
9:N:37:ARG:HH21	9:N:41:HIS:HB3	1.75	0.50
11:K:123:SER:C	11:K:125:PRO:HD2	2.36	0.50
3:C:269:TYR:CZ	3:C:293:MET:HB3	2.47	0.50
6:J:357:ALA:HA	6:J:387:MET:HE1	1.93	0.50
9:N:46:PHE:O	9:N:47:GLN:HG2	2.12	0.50
1:A:97:LEU:HB2	2:B:129:TYR:HD2	1.76	0.50
3:C:161:ILE:HD11	3:C:203:LEU:HD23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:279:LEU:HB3	5:I:309:ARG:HG3	1.94	0.50
11:K:220:LEU:HG	11:K:324:ILE:HD11	1.93	0.50
11:K:290:ARG:O	11:K:290:ARG:HD3	2.11	0.50
12:P:132:VAL:O	12:P:155:ILE:HG22	2.12	0.50
1:A:58:ASP:HB3	1:A:62:ARG:HH21	1.75	0.50
4:D:11:ASN:O	4:D:15:GLN:HG3	2.11	0.50
10:Z:452:LEU:HD11	10:Z:748:PHE:CE2	2.46	0.50
10:Z:306:ASN:OD1	10:Z:872:THR:HA	2.12	0.50
12:P:283:LEU:HD22	12:P:325:ALA:HB1	1.94	0.50
5:I:187:LEU:HD22	5:I:316:PHE:HE2	1.77	0.49
6:J:242:PHE:CD1	6:J:253:MET:HE1	2.47	0.49
5:I:19:ILE:HD13	10:Z:156:ILE:HG21	1.93	0.49
5:I:52:ASN:HD21	5:I:56:ARG:HH22	1.59	0.49
5:I:276:LEU:HB3	5:I:309:ARG:NH2	2.27	0.49
3:C:279:THR:HG21	3:C:974:THR:HA	1.95	0.49
5:I:31:GLU:HB3	5:I:35:ARG:NH2	2.27	0.49
7:L:77:PRO:HA	7:L:87:PHE:HA	1.93	0.49
9:N:145:HIS:CE1	9:N:171:ASP:HB3	2.47	0.49
10:Z:174:LEU:HD22	10:Z:217:MET:HE3	1.94	0.49
10:Z:419:THR:O	10:Z:423:LEU:HG	2.11	0.49
2:B:171:MET:HG3	2:B:173:MET:SD	2.52	0.49
2:B:306:MET:HE2	2:B:306:MET:C	2.37	0.49
1:A:148:ASN:HB2	1:A:154:LYS:HZ3	1.78	0.49
2:B:90:GLU:O	2:B:93:LYS:HG3	2.13	0.49
5:I:337:LEU:HB3	5:I:341:ILE:HD12	1.94	0.49
6:J:356:ILE:HD11	13:J:501:ATP:C2	2.48	0.49
10:Z:533:ASP:O	10:Z:536:ILE:HG22	2.12	0.49
12:P:220:MET:HE3	12:P:228:LYS:HB3	1.94	0.49
2:B:64:ARG:HG3	2:B:68:HIS:NE2	2.28	0.49
3:C:344:LYS:HD3	3:C:349:THR:HG21	1.94	0.49
6:J:349:ARG:HG2	6:J:383:ILE:HD11	1.95	0.49
4:D:100:ASP:HA	4:D:103:LYS:HE3	1.95	0.49
8:M:198:LEU:HD12	8:M:225:GLY:HA3	1.95	0.49
10:Z:611:LYS:O	10:Z:611:LYS:HG2	2.11	0.49
1:A:251:PRO:HG2	1:A:379:LEU:HD21	1.95	0.49
1:A:428:MET:HE1	2:B:208:TYR:CE1	2.48	0.49
1:A:208:TYR:CE2	1:A:266:ARG:HG3	2.48	0.49
1:A:208:TYR:CZ	1:A:266:ARG:HG3	2.48	0.49
2:B:167:MET:HE1	2:B:267:ILE:HA	1.94	0.49
5:I:93:LYS:HA	5:I:93:LYS:HD3	1.61	0.49
10:Z:417:ARG:HG3	10:Z:418:ASP:OD2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:423:LEU:HD12	10:Z:450:ILE:HA	1.94	0.49
4:D:55:LEU:HD13	4:D:95:VAL:HG11	1.94	0.48
5:I:149:MET:HG3	5:I:197:LEU:HD11	1.94	0.48
10:Z:658:ILE:HD11	10:Z:698:GLY:HA2	1.95	0.48
4:D:408:MET:HG3	4:D:411:VAL:HB	1.95	0.48
4:D:451:TRP:C	4:D:454:PRO:HD2	2.37	0.48
6:J:122:ILE:HG12	6:J:146:LEU:HD21	1.95	0.48
9:N:122:VAL:O	9:N:126:LEU:HG	2.13	0.48
10:Z:167:GLU:HG3	10:Z:213:PHE:HZ	1.77	0.48
1:A:99:VAL:HG12	1:A:101:ARG:NH1	2.28	0.48
6:J:246:TYR:HB2	6:J:249:GLU:HG3	1.94	0.48
11:K:312:MET:HE2	11:K:323:ILE:HD12	1.96	0.48
3:C:439:TYR:HB2	3:C:451:ALA:HB2	1.95	0.48
9:N:48:ALA:HB1	9:N:51:ILE:HD12	1.95	0.48
10:Z:674:GLN:O	10:Z:678:ILE:HG12	2.13	0.48
11:K:95:ILE:HA	11:K:98:LEU:HD12	1.95	0.48
3:C:440:LEU:O	3:C:448:LYS:HE3	2.14	0.48
10:Z:717:LEU:HD21	10:Z:733:LEU:HD11	1.95	0.48
4:D:330:ILE:HB	4:D:335:LEU:HD21	1.96	0.48
4:D:408:MET:O	4:D:412:MET:HE2	2.13	0.48
5:I:94:TYR:HE2	5:I:120:TYR:CZ	2.31	0.48
2:B:198:VAL:HG21	2:B:325:ILE:HD11	1.95	0.48
4:D:271:PHE:HB2	4:D:288:LEU:HD13	1.96	0.48
7:L:100:TRP:CH2	7:L:102:GLN:HG2	2.48	0.48
10:Z:202:PHE:CE2	10:Z:206:ILE:HD11	2.48	0.48
10:Z:515:ARG:HD3	10:Z:546:LEU:HD22	1.95	0.48
1:A:204:PRO:HG2	1:A:264:ALA:HB3	1.96	0.48
3:C:82:MET:HE1	3:C:152:GLU:HG2	1.96	0.48
3:C:793:PHE:HA	3:C:796:LEU:HB3	1.95	0.48
4:D:324:THR:HA	4:D:356:MET:HE2	1.96	0.48
5:I:87:LYS:HE3	5:I:89:GLN:HA	1.95	0.48
2:B:124:THR:HG21	5:I:91:GLU:HA	1.95	0.48
4:D:382:LEU:HB2	4:D:387:GLN:HG2	1.96	0.48
10:Z:217:MET:SD	10:Z:218:PRO:HD2	2.53	0.48
11:K:170:MET:SD	11:K:247:PRO:HD2	2.54	0.48
11:K:254:LYS:HD2	11:K:254:LYS:N	2.28	0.48
4:D:332:PRO:HG3	4:D:362:ALA:HB3	1.96	0.48
7:L:11:ARG:HA	7:L:32:GLU:HA	1.96	0.48
10:Z:761:ILE:HG22	10:Z:768:ILE:CD1	2.43	0.48
5:I:390:MET:HA	5:I:393:ASN:HB2	1.95	0.47
6:J:357:ALA:HA	6:J:360:MET:SD	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:99:VAL:HG21	8:M:401:LEU:HD23	1.95	0.47
11:K:110:LYS:HD3	11:K:111:GLU:H	1.77	0.47
12:P:364:HIS:HB3	12:P:395:THR:HG21	1.96	0.47
1:A:169:GLU:H	1:A:172:MET:HE3	1.79	0.47
5:I:373:ARG:HH12	5:I:375:ILE:HG23	1.78	0.47
6:J:222:LEU:HD12	6:J:222:LEU:H	1.79	0.47
6:J:346:ARG:HH21	6:J:373:ILE:HG12	1.79	0.47
6:J:137:VAL:HG12	6:J:149:ILE:HG22	1.95	0.47
10:Z:174:LEU:HD23	10:Z:182:ASN:HB3	1.96	0.47
11:K:239:ILE:HG21	11:K:277:ILE:HD12	1.95	0.47
2:B:389:GLY:HA3	13:B:501:ATP:C8	2.49	0.47
6:J:180:GLN:O	6:J:184:ILE:HG12	2.15	0.47
9:N:192:LEU:HB3	9:N:196:LYS:HZ2	1.77	0.47
11:K:254:LYS:HG2	12:P:293:SER:C	2.39	0.47
1:A:299:ARG:HA	1:A:349:ILE:HD11	1.96	0.47
2:B:204:HIS:HB3	2:B:207:LEU:HG	1.95	0.47
2:B:309:LEU:HD12	2:B:310:LEU:N	2.29	0.47
3:C:944:LYS:HB3	3:C:962:ARG:HH11	1.79	0.47
5:I:171:PRO:HB3	5:I:181:GLN:HE22	1.79	0.47
5:I:297:LEU:HD12	5:I:300:LEU:HD12	1.95	0.47
10:Z:692:GLU:OE2	10:Z:694:LEU:HB2	2.15	0.47
3:C:563:VAL:HA	3:C:566:LEU:HD12	1.97	0.47
6:J:249:GLU:HA	6:J:252:ARG:HB3	1.96	0.47
10:Z:599:TYR:HB2	10:Z:629:CYS:SG	2.54	0.47
11:K:206:ILE:O	11:K:210:VAL:HG23	2.14	0.47
1:A:85:MET:HE2	1:A:85:MET:HA	1.96	0.47
1:A:256:LYS:HB2	13:A:501:ATP:O2G	2.14	0.47
3:C:833:GLN:NE2	3:C:834:LEU:HG	2.30	0.47
3:C:877:THR:HA	3:C:907:GLY:HA3	1.96	0.47
4:D:55:LEU:HB3	4:D:95:VAL:HG21	1.96	0.47
4:D:459:TYR:O	4:D:463:VAL:HG12	2.15	0.47
6:J:129:GLU:HA	6:J:132:LYS:NZ	2.30	0.47
6:J:231:LYS:HD2	6:J:231:LYS:N	2.29	0.47
8:M:161:LYS:HG2	8:M:173:THR:HG23	1.97	0.47
10:Z:654:GLN:O	10:Z:658:ILE:HG12	2.15	0.47
4:D:457:ARG:HE	4:D:458:GLU:HG2	1.79	0.47
5:I:327:ILE:HG23	13:I:501:ATP:C2	2.49	0.47
8:M:136:VAL:HB	8:M:157:ASP:HB3	1.96	0.47
9:N:87:VAL:O	9:N:91:LEU:HG	2.14	0.47
1:A:396:MET:HE1	2:B:213:ILE:HG13	1.97	0.47
3:C:753:GLY:O	3:C:757:SER:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:90:GLN:O	6:J:94:LEU:HD11	2.15	0.47
8:M:268:ILE:HB	8:M:282:LEU:HD12	1.96	0.47
8:M:356:LYS:HE3	8:M:414:LEU:HD22	1.97	0.47
10:Z:293:LEU:HD13	10:Z:379:LEU:HD13	1.97	0.47
10:Z:302:PHE:HB2	10:Z:871:MET:SD	2.55	0.47
10:Z:379:LEU:HD12	10:Z:379:LEU:H	1.80	0.47
10:Z:555:ILE:HD11	10:Z:567:ALA:HA	1.97	0.47
12:P:194:VAL:HG13	12:P:198:VAL:HB	1.96	0.47
1:A:154:LYS:HB2	1:A:154:LYS:HE2	1.66	0.47
2:B:177:PRO:HG2	2:B:237:ALA:HB3	1.97	0.47
2:B:261:PRO:O	2:B:265:ARG:HG3	2.15	0.47
3:C:405:ASN:HA	3:C:408:TYR:CE1	2.50	0.47
10:Z:340:HIS:HB2	10:Z:374:ILE:HG12	1.97	0.47
5:I:39:GLU:HB3	5:I:42:ARG:HH21	1.80	0.46
9:N:183:ALA:O	9:N:216:LEU:HD13	2.15	0.46
11:K:239:ILE:HG13	11:K:241:ALA:H	1.81	0.46
12:P:132:VAL:HG21	12:P:137:PRO:HB3	1.97	0.46
1:A:443:PHE:O	1:A:447:VAL:HG12	2.15	0.46
3:C:352:LYS:HG2	3:C:859:LYS:HE2	1.96	0.46
3:C:392:LEU:HD13	3:C:857:LEU:HD11	1.97	0.46
5:I:32:LEU:HD23	5:I:35:ARG:HD2	1.96	0.46
6:J:255:ARG:HA	6:J:302:GLN:NE2	2.30	0.46
10:Z:581:ASP:HB3	10:Z:616:HIS:CG	2.50	0.46
12:P:170:MET:SD	12:P:246:LEU:HA	2.56	0.46
2:B:381:VAL:HG13	2:B:387:LEU:HD12	1.97	0.46
5:I:127:GLU:CD	5:I:127:GLU:H	2.23	0.46
5:I:391:ASN:HA	5:I:394:GLN:NE2	2.31	0.46
10:Z:296:CYS:CB	10:Z:379:LEU:HD11	2.45	0.46
2:B:58:LYS:HG2	2:B:62:MET:CE	2.45	0.46
4:D:342:VAL:HG13	4:D:346:TYR:HE2	1.80	0.46
4:D:463:VAL:HG13	4:D:464:ASN:OD1	2.15	0.46
7:L:77:PRO:HB3	7:L:87:PHE:CE1	2.50	0.46
11:K:287:GLY:HA2	11:K:305:LEU:HD13	1.98	0.46
2:B:68:HIS:CD2	3:C:756:MET:HG3	2.51	0.46
2:B:375:VAL:HG22	2:B:413:ALA:N	2.31	0.46
3:C:559:LYS:HE2	3:C:727:GLU:HG3	1.97	0.46
4:D:385:LEU:HG	4:D:389:GLN:HE21	1.81	0.46
6:J:253:MET:HE2	6:J:253:MET:C	2.40	0.46
2:B:172:LYS:HB3	2:B:172:LYS:HE2	1.75	0.46
3:C:260:GLU:HB3	3:C:264:PHE:HE2	1.81	0.46
5:I:186:ILE:CG2	5:I:313:LYS:HG2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:190:PRO:HG3	5:I:318:PRO:HG3	1.97	0.46
6:J:251:PRO:HD3	6:J:295:ILE:HG12	1.98	0.46
8:M:5:ILE:HG12	8:M:372:PHE:HB2	1.98	0.46
2:B:361:ILE:HG12	13:B:501:ATP:C6	2.51	0.46
3:C:147:GLU:HA	3:C:154:ILE:HD11	1.98	0.46
3:C:157:LEU:HD21	3:C:203:LEU:HD21	1.98	0.46
4:D:19:GLU:HA	4:D:22:GLU:HG3	1.97	0.46
4:D:189:GLU:HB2	4:D:192:SER:OG	2.16	0.46
7:L:27:ILE:HG22	7:L:29:VAL:HG23	1.97	0.46
8:M:7:VAL:HA	8:M:377:PHE:CZ	2.51	0.46
10:Z:140:MET:HA	10:Z:140:MET:HE2	1.98	0.46
4:D:376:ALA:HB2	4:D:408:MET:HE1	1.98	0.46
5:I:61:GLU:O	5:I:65:LEU:HD22	2.15	0.46
5:I:345:LYS:O	5:I:349:LYS:HG3	2.16	0.46
6:J:347:ARG:NH2	6:J:348:GLU:HG2	2.30	0.46
6:J:392:LEU:HD23	11:K:212:ILE:HD12	1.98	0.46
11:K:254:LYS:HB2	12:P:299:ARG:NH2	2.29	0.46
3:C:412:GLY:O	3:C:446:GLU:HG2	2.16	0.46
6:J:105:GLN:HA	6:J:128:ARG:NH1	2.31	0.46
6:J:244:HIS:CE1	6:J:252:ARG:HH22	2.33	0.46
10:Z:871:MET:O	10:Z:871:MET:HG3	2.16	0.46
2:B:324:VAL:O	2:B:325:ILE:HD13	2.16	0.46
7:L:11:ARG:NH2	10:Z:926:VAL:HB	2.31	0.46
9:N:97:LYS:HD2	9:N:98:PRO:O	2.14	0.46
9:N:147:ALA:HB1	9:N:156:ILE:HD13	1.97	0.46
10:Z:626:GLY:HA2	10:Z:663:ILE:HD11	1.97	0.46
1:A:282:LYS:NZ	4:D:425:ILE:HA	2.31	0.45
4:D:314:LEU:HD13	4:D:314:LEU:HA	1.78	0.45
5:I:135:SER:HA	5:I:138:MET:HE2	1.98	0.45
6:J:177:LEU:HD13	6:J:180:GLN:CD	2.41	0.45
10:Z:536:ILE:CD1	10:Z:554:THR:HB	2.47	0.45
11:K:162:GLU:HA	12:P:256:ILE:HD11	1.98	0.45
4:D:185:LYS:O	4:D:188:MET:HE3	2.17	0.45
6:J:99:PHE:CD1	6:J:131:LEU:HD11	2.50	0.45
8:M:202:ILE:HB	8:M:216:PHE:HB2	1.98	0.45
2:B:106:ILE:HD11	5:I:95:ILE:HG13	1.98	0.45
10:Z:93:GLU:HB3	10:Z:98:VAL:HG21	1.99	0.45
1:A:56:LEU:HD11	2:B:62:MET:HB2	1.97	0.45
2:B:181:TYR:OH	2:B:236:VAL:HA	2.15	0.45
2:B:221:LEU:O	2:B:327:ALA:HA	2.15	0.45
2:B:232:LEU:O	2:B:236:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:30:THR:O	5:I:34:ILE:HG12	2.17	0.45
5:I:211:ILE:HD13	5:I:236:MET:HE1	1.99	0.45
8:M:116:GLY:HA2	8:M:139:ILE:HG13	1.97	0.45
10:Z:657:MET:HE3	10:Z:657:MET:HB2	1.79	0.45
11:K:263:ILE:O	11:K:267:PHE:HD1	1.99	0.45
11:K:280:MET:SD	11:K:325:MET:HA	2.56	0.45
3:C:618:GLN:HG2	3:C:622:HIS:CE1	2.52	0.45
3:C:765:MET:HG3	3:C:799:PHE:CZ	2.51	0.45
3:C:862:MET:HE2	3:C:862:MET:HA	1.98	0.45
4:D:388:MET:HE3	4:D:433:ARG:HA	1.99	0.45
5:I:48:ARG:NH2	10:Z:612:SER:HA	2.25	0.45
7:L:74:MET:HG3	7:L:76:VAL:HG23	1.98	0.45
10:Z:50:TYR:HA	10:Z:58:ARG:HB2	1.98	0.45
1:A:286:GLU:HB3	1:A:289:ARG:NH1	2.32	0.45
2:B:202:LEU:HD21	2:B:323:LYS:HG2	1.99	0.45
4:D:291:LEU:O	4:D:295:VAL:HG23	2.16	0.45
10:Z:301:THR:CG2	10:Z:920:VAL:H	2.29	0.45
12:P:132:VAL:HG11	12:P:140:LEU:HD11	1.99	0.45
1:A:35:GLN:HB3	3:C:93:ARG:NH1	2.32	0.45
4:D:275:GLU:HG2	4:D:276:ASN:N	2.31	0.45
4:D:385:LEU:O	4:D:389:GLN:HG3	2.17	0.45
5:I:332:SER:HB2	5:I:337:LEU:HD11	1.98	0.45
7:L:30:GLN:HB3	7:L:54:GLU:HG2	1.99	0.45
10:Z:135:SER:O	10:Z:139:ARG:HG2	2.17	0.45
5:I:61:GLU:HG3	6:J:121:ARG:HE	1.82	0.45
1:A:297:MET:HE2	1:A:297:MET:HA	1.98	0.45
2:B:105:SER:HG	2:B:149:LEU:HB2	1.82	0.45
2:B:380:LEU:HD21	2:B:416:PHE:CD2	2.52	0.45
4:D:262:LYS:O	4:D:265:PRO:HD2	2.16	0.45
5:I:124:LYS:HD2	5:I:125:VAL:N	2.32	0.45
5:I:137:MET:HE2	5:I:213:VAL:HG11	1.98	0.45
6:J:89:ILE:HG23	6:J:140:HIS:HD2	1.82	0.45
6:J:346:ARG:NH2	6:J:373:ILE:HG12	2.32	0.45
9:N:175:TRP:HE3	9:N:180:HIS:CD2	2.34	0.45
9:N:175:TRP:CE3	9:N:179:PHE:HB3	2.52	0.45
4:D:57:THR:HA	4:D:60:ARG:NH1	2.32	0.45
5:I:111:GLN:HA	5:I:128:ASN:HD21	1.81	0.45
6:J:403:LEU:HD12	6:J:404:GLN:H	1.81	0.45
7:L:120:GLU:O	7:L:124:LYS:HG3	2.15	0.45
8:M:159:GLN:HG3	8:M:175:ILE:HG12	1.99	0.45
9:N:192:LEU:HD12	9:N:196:LYS:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:219:LEU:HD12	11:K:325:MET:HB2	1.99	0.45
11:K:246:SER:O	11:K:280:MET:HB2	2.17	0.45
12:P:269:LEU:HD11	12:P:273:LYS:HE3	1.99	0.45
12:P:284:ASP:O	12:P:288:THR:HG23	2.17	0.45
1:A:45:TYR:OH	3:C:222:ASP:HB3	2.17	0.44
1:A:276:GLY:HA3	1:A:310:GLU:O	2.18	0.44
2:B:307:LEU:HA	2:B:310:LEU:HD12	1.99	0.44
4:D:238:VAL:HG11	4:D:287:CYS:HB3	1.98	0.44
4:D:451:TRP:O	4:D:455:LEU:HD12	2.17	0.44
6:J:352:ILE:HG12	13:J:501:ATP:N6	2.32	0.44
6:J:373:ILE:HG21	9:N:141:GLN:NE2	2.31	0.44
6:J:399:ARG:HD2	6:J:400:TYR:H	1.81	0.44
9:N:76:PHE:HE1	9:N:88:VAL:HG13	1.82	0.44
11:K:334:ASP:HB3	11:K:337:LEU:HD13	1.99	0.44
1:A:144:LYS:HG2	12:P:75:LEU:HD11	2.00	0.44
2:B:253:ILE:HG12	2:B:287:ILE:HG13	1.98	0.44
3:C:790:MET:HA	3:C:793:PHE:CE2	2.53	0.44
5:I:74:GLU:HG2	5:I:89:GLN:NE2	2.32	0.44
5:I:296:ARG:HA	5:I:296:ARG:NH1	2.31	0.44
10:Z:83:LEU:HD22	10:Z:132:LYS:HB3	1.98	0.44
11:K:412:PRO:O	11:K:416:MET:HE2	2.17	0.44
1:A:154:LYS:H	12:P:122:SER:HB2	1.82	0.44
1:A:163:VAL:HG11	1:A:168:ILE:HD11	1.98	0.44
2:B:175:LYS:HE2	2:B:175:LYS:H	1.82	0.44
3:C:758:LEU:HD12	3:C:759:ARG:N	2.31	0.44
4:D:57:THR:HG23	4:D:60:ARG:HH12	1.82	0.44
5:I:273:LEU:HD23	5:I:276:LEU:HD12	1.99	0.44
6:J:180:GLN:NE2	6:J:341:PRO:HD3	2.33	0.44
7:L:70:PRO:HA	7:L:129:LEU:HA	1.99	0.44
8:M:288:CYS:SG	8:M:307:TYR:HB3	2.58	0.44
12:P:220:MET:HE2	12:P:326:ALA:HB2	1.99	0.44
12:P:246:LEU:HD12	12:P:278:ILE:HG23	2.00	0.44
2:B:117:HIS:HB3	2:B:129:TYR:CE1	2.50	0.44
2:B:148:LEU:O	2:B:156:ILE:HD12	2.17	0.44
2:B:167:MET:HG3	2:B:266:GLN:HG2	2.00	0.44
4:D:301:ASP:HB2	4:D:304:SER:CB	2.47	0.44
5:I:80:SER:OG	5:I:83:LYS:HG2	2.16	0.44
6:J:397:LYS:HA	6:J:397:LYS:HD3	1.84	0.44
10:Z:267:GLN:O	10:Z:270:LEU:HG	2.18	0.44
3:C:761:PHE:HD2	3:C:780:MET:HE1	1.83	0.44
9:N:76:PHE:CE1	9:N:88:VAL:HG13	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:171:LYS:HE2	10:Z:213:PHE:HE1	1.83	0.44
10:Z:742:TRP:HA	10:Z:742:TRP:CE3	2.53	0.44
11:K:266:MET:HE2	11:K:278:ILE:HG23	2.00	0.44
12:P:142:PRO:HG2	12:P:253:GLN:HE22	1.82	0.44
2:B:88:LYS:HD3	2:B:89:GLN:N	2.32	0.44
2:B:340:ARG:HB2	2:B:343:ARG:HG3	2.00	0.44
3:C:910:PRO:HB2	3:C:912:PHE:HD1	1.82	0.44
5:I:32:LEU:O	5:I:35:ARG:HG2	2.18	0.44
6:J:278:ALA:HA	6:J:296:LEU:HD13	1.99	0.44
6:J:329:LEU:HD23	6:J:334:LEU:HD12	2.00	0.44
6:J:356:ILE:O	6:J:359:LYS:HG2	2.18	0.44
10:Z:602:VAL:O	10:Z:606:VAL:HG23	2.18	0.44
10:Z:650:ASP:HA	10:Z:653:ARG:CZ	2.48	0.44
3:C:892:SER:HA	3:C:895:LEU:HG	1.99	0.44
4:D:188:MET:HA	4:D:193:PHE:HB2	1.99	0.44
4:D:260:VAL:O	4:D:264:LEU:HG	2.18	0.44
5:I:103:ASN:HB3	5:I:106:ASP:OD2	2.18	0.44
5:I:364:GLU:OE1	5:I:388:LYS:HE3	2.16	0.44
6:J:223:VAL:HG11	6:J:270:PHE:CD1	2.53	0.44
6:J:271:ILE:HD13	6:J:316:MET:HE1	2.00	0.44
8:M:179:ALA:HB1	8:M:198:LEU:HB3	2.00	0.44
1:A:275:ILE:CG1	1:A:278:GLU:HB2	2.48	0.44
2:B:58:LYS:O	2:B:62:MET:HE3	2.18	0.44
2:B:195:LYS:HG2	2:B:199:GLU:OE1	2.17	0.44
3:C:614:VAL:HA	3:C:617:ILE:HD12	1.98	0.44
9:N:117:LYS:HD3	9:N:117:LYS:N	2.32	0.44
10:Z:501:MET:CB	10:Z:517:LEU:HD22	2.44	0.44
12:P:256:ILE:H	12:P:256:ILE:HG13	1.63	0.44
2:B:309:LEU:HD12	2:B:310:LEU:HG	1.99	0.44
2:B:332:GLU:HB2	4:D:429:THR:HG21	2.00	0.44
2:B:388:SER:H	2:B:391:ASP:HB2	1.83	0.44
4:D:310:ASP:CG	4:D:316:ILE:HG12	2.43	0.44
4:D:405:LEU:O	4:D:412:MET:HE1	2.17	0.44
6:J:274:VAL:HG11	6:J:316:MET:HG3	2.00	0.44
10:Z:569:LYS:NZ	10:Z:573:HIS:HB2	2.33	0.44
11:K:263:ILE:HG23	11:K:267:PHE:CE1	2.52	0.44
12:P:83:VAL:HB	12:P:118:VAL:HG12	1.98	0.44
1:A:49:LEU:HD13	2:B:54:ARG:HD2	2.01	0.43
3:C:568:LEU:HD22	3:C:886:VAL:HG21	2.00	0.43
5:I:90:PRO:HD2	6:J:116:MET:SD	2.58	0.43
10:Z:10:LEU:HD13	10:Z:42:GLU:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:84:GLU:HB2	12:P:255:TYR:OH	2.18	0.43
12:P:360:ILE:HG12	13:P:501:ATP:N1	2.33	0.43
1:A:318:ARG:HH11	1:A:319:PHE:N	2.15	0.43
3:C:775:MET:SD	3:C:889:VAL:HA	2.58	0.43
3:C:793:PHE:CG	3:C:827:LEU:HD21	2.53	0.43
4:D:193:PHE:CE2	4:D:197:ILE:HD11	2.54	0.43
5:I:17:SER:HB2	10:Z:102:VAL:HG11	2.00	0.43
7:L:100:TRP:CZ2	7:L:102:GLN:HG2	2.53	0.43
10:Z:394:ARG:HD2	10:Z:395:ALA:N	2.33	0.43
10:Z:405:LEU:HA	10:Z:405:LEU:HD23	1.72	0.43
11:K:149:ASP:O	11:K:153:LEU:HD23	2.17	0.43
4:D:8:TYR:HA	4:D:11:ASN:ND2	2.33	0.43
5:I:359:LYS:HE3	5:I:359:LYS:HB2	1.67	0.43
6:J:238:ASN:HB3	6:J:241:GLU:HG3	2.00	0.43
11:K:354:GLU:O	11:K:358:LEU:HG	2.18	0.43
1:A:299:ARG:HA	1:A:299:ARG:HD3	1.80	0.43
2:B:132:ILE:HA	2:B:156:ILE:HG23	1.99	0.43
2:B:167:MET:HE3	2:B:167:MET:HB3	1.93	0.43
2:B:285:ASP:O	2:B:289:THR:HG22	2.19	0.43
7:L:7:VAL:HG22	7:L:37:PRO:HD2	1.99	0.43
10:Z:311:ILE:HG22	10:Z:315:ASN:ND2	2.33	0.43
10:Z:761:ILE:HG22	10:Z:768:ILE:HD11	2.00	0.43
2:B:90:GLU:C	2:B:94:LYS:HE3	2.43	0.43
2:B:264:CYS:SG	2:B:308:GLU:HG3	2.59	0.43
3:C:824:ASN:HB3	3:C:827:LEU:HB2	1.99	0.43
4:D:149:ASN:HB3	4:D:152:LEU:HB3	2.00	0.43
11:K:218:VAL:O	11:K:325:MET:HG2	2.18	0.43
1:A:249:TYR:HA	1:A:355:THR:O	2.19	0.43
1:A:288:ALA:O	1:A:335:GLU:HG2	2.19	0.43
2:B:58:LYS:HG2	2:B:62:MET:HE1	2.01	0.43
3:C:516:THR:HA	3:C:553:ARG:NH2	2.34	0.43
5:I:56:ARG:HA	5:I:59:LYS:HG2	2.00	0.43
5:I:87:LYS:HD3	5:I:93:LYS:HZ1	1.84	0.43
6:J:255:ARG:H	6:J:255:ARG:HG3	1.68	0.43
8:M:160:LEU:HB2	8:M:174:LEU:HB2	1.99	0.43
10:Z:62:ALA:O	10:Z:81:TYR:HB3	2.19	0.43
10:Z:576:VAL:HA	10:Z:584:ARG:NH2	2.34	0.43
11:K:345:ARG:HD3	11:K:345:ARG:N	2.34	0.43
1:A:98:GLN:NE2	2:B:126:PRO:HB2	2.34	0.43
3:C:436:LEU:HD22	3:C:451:ALA:HA	2.00	0.43
4:D:248:ILE:HG22	4:D:254:TYR:CD1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:60:THR:HG23	8:M:72:ARG:HH21	1.83	0.43
10:Z:603:PRO:HG3	10:Z:625:LEU:HD11	2.00	0.43
10:Z:675:VAL:HG12	10:Z:679:ASN:ND2	2.34	0.43
10:Z:264:SER:HB2	10:Z:722:THR:HG21	2.00	0.43
10:Z:300:ASN:HD21	10:Z:378:ASN:HA	1.84	0.43
2:B:82:LEU:HD11	10:Z:798:LYS:HG2	2.01	0.43
2:B:300:ARG:HH11	2:B:303:GLN:HB2	1.84	0.43
3:C:823:ASN:OD1	3:C:856:HIS:HA	2.19	0.43
5:I:81:ASP:O	5:I:104:VAL:HG21	2.19	0.43
11:K:302:GLN:O	11:K:306:MET:HG3	2.18	0.43
11:K:370:LYS:HB2	11:K:374:PHE:CE1	2.53	0.43
2:B:83:LYS:HB3	2:B:86:GLU:OE1	2.19	0.43
2:B:198:VAL:C	2:B:201:PRO:HD2	2.44	0.43
5:I:326:GLU:HG3	5:I:329:ARG:NH1	2.34	0.43
6:J:132:LYS:O	6:J:135:MET:HB2	2.19	0.43
10:Z:292:GLY:HA3	10:Z:415:PHE:CE1	2.54	0.43
1:A:79:SER:HA	1:A:82:TRP:CE2	2.53	0.42
1:A:215:LYS:HG3	1:A:216:ASP:N	2.34	0.42
1:A:284:VAL:O	1:A:286:GLU:HG3	2.19	0.42
3:C:256:LEU:HD13	3:C:264:PHE:CE2	2.54	0.42
3:C:761:PHE:O	3:C:764:LEU:HB2	2.19	0.42
1:A:180:LYS:HD2	12:P:76:PRO:HD3	2.01	0.42
5:I:89:GLN:HA	5:I:90:PRO:HA	1.79	0.42
8:M:385:VAL:HG21	8:M:402:GLU:OE2	2.19	0.42
1:A:44:PRO:HB3	3:C:159:LEU:HB2	2.01	0.42
1:A:293:GLU:O	1:A:296:GLU:HG3	2.19	0.42
1:A:295:PHE:CE2	1:A:339:GLN:HB3	2.54	0.42
3:C:249:MET:HE1	3:C:271:ILE:HD12	2.01	0.42
4:D:83:LEU:HD12	4:D:84:VAL:N	2.34	0.42
4:D:327:LEU:HB2	4:D:356:MET:SD	2.59	0.42
5:I:19:ILE:HD12	10:Z:144:CYS:HB2	2.01	0.42
5:I:153:LEU:HD13	5:I:316:PHE:HE1	1.83	0.42
6:J:365:GLU:HB2	9:N:81:SER:OG	2.18	0.42
6:J:399:ARG:HD2	6:J:400:TYR:N	2.34	0.42
9:N:5:PRO:O	9:N:8:GLN:HG3	2.18	0.42
11:K:162:GLU:CD	12:P:303:ARG:HH22	2.27	0.42
1:A:318:ARG:HE	1:A:327:ASN:ND2	2.18	0.42
2:B:175:LYS:HA	2:B:243:THR:HG23	2.01	0.42
3:C:878:LEU:HA	3:C:881:ILE:HD11	2.01	0.42
4:D:414:SER:HA	4:D:418:ASP:CG	2.44	0.42
5:I:368:TYR:CZ	5:I:384:LEU:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:89:ILE:HG23	6:J:140:HIS:CD2	2.55	0.42
11:K:110:LYS:NZ	11:K:142:LYS:HD2	2.34	0.42
12:P:199:LEU:HB3	12:P:200:PRO:HD3	2.00	0.42
2:B:93:LYS:HZ3	2:B:94:LYS:HG3	1.84	0.42
2:B:103:PRO:HG3	5:I:120:TYR:CD1	2.54	0.42
2:B:316:PHE:O	2:B:316:PHE:CG	2.72	0.42
5:I:220:GLN:HG3	5:I:222:TYR:H	1.84	0.42
9:N:116:GLY:C	9:N:117:LYS:HD3	2.45	0.42
10:Z:386:MET:SD	10:Z:404:SER:HB2	2.60	0.42
10:Z:417:ARG:C	10:Z:417:ARG:NE	2.76	0.42
10:Z:804:LEU:HD12	10:Z:804:LEU:H	1.84	0.42
12:P:146:VAL:HB	12:P:155:ILE:HD12	2.02	0.42
2:B:100:ARG:HG2	2:B:157:VAL:HB	2.01	0.42
3:C:202:ARG:NH2	3:C:203:LEU:HB2	2.34	0.42
3:C:790:MET:HA	3:C:793:PHE:CZ	2.55	0.42
4:D:454:PRO:HA	4:D:457:ARG:NH2	2.35	0.42
6:J:180:GLN:HE22	6:J:341:PRO:HD3	1.83	0.42
9:N:111:LEU:O	9:N:115:VAL:HG13	2.20	0.42
10:Z:515:ARG:NH2	10:Z:741:TYR:HB3	2.34	0.42
10:Z:606:VAL:CG1	10:Z:621:THR:HG23	2.48	0.42
11:K:187:THR:O	11:K:191:ARG:HG2	2.20	0.42
1:A:234:ARG:HD2	4:D:8:TYR:HB3	2.01	0.42
5:I:213:VAL:HG12	5:I:247:MET:CE	2.50	0.42
10:Z:588:VAL:HG23	10:Z:591:LEU:HD12	2.02	0.42
1:A:275:ILE:HG12	1:A:278:GLU:HB2	2.01	0.42
1:A:319:PHE:HD2	4:D:464:ASN:HD21	1.68	0.42
1:A:429:PHE:CE2	1:A:445:LYS:HB3	2.55	0.42
2:B:259:ASP:HB3	2:B:262:ARG:HH21	1.85	0.42
6:J:362:LEU:H	6:J:362:LEU:HD23	1.84	0.42
8:M:214:HIS:CG	8:M:276:LYS:HD2	2.55	0.42
10:Z:202:PHE:CZ	10:Z:206:ILE:HD11	2.55	0.42
10:Z:569:LYS:HD2	10:Z:569:LYS:HA	1.76	0.42
2:B:110:GLU:OE1	2:B:121:THR:HB	2.20	0.42
2:B:246:ARG:HG3	2:B:280:PHE:CD2	2.49	0.42
2:B:268:PHE:CD2	2:B:312:GLN:HB3	2.55	0.42
3:C:435:GLN:CD	3:C:435:GLN:H	2.28	0.42
7:L:104:LYS:HA	10:Z:928:ALA:HB2	2.01	0.42
8:M:151:LEU:HD11	8:M:163:TRP:HD1	1.85	0.42
9:N:9:ALA:HA	9:N:14:GLU:OE2	2.20	0.42
11:K:64:LEU:HD13	12:P:37:LEU:HD11	2.01	0.42
1:A:234:ARG:HB2	4:D:8:TYR:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ARG:HE	1:A:327:ASN:HD21	1.68	0.41
2:B:57:LEU:HD13	3:C:252:CYS:SG	2.60	0.41
8:M:136:VAL:HB	8:M:157:ASP:CB	2.49	0.41
10:Z:657:MET:HE1	10:Z:695:ALA:O	2.20	0.41
1:A:102:CYS:SG	1:A:170:GLU:HA	2.60	0.41
2:B:363:GLY:HA2	2:B:366:THR:HG22	2.02	0.41
3:C:616:LEU:O	3:C:620:LEU:HG	2.21	0.41
10:Z:619:CYS:HB2	10:Z:651:PHE:CD1	2.55	0.41
10:Z:867:LYS:HA	10:Z:867:LYS:HD3	1.89	0.41
3:C:771:HIS:O	3:C:775:MET:HE2	2.20	0.41
9:N:11:MET:HE2	9:N:42:TRP:CD2	2.55	0.41
9:N:144:LEU:HA	9:N:159:LEU:HD13	2.02	0.41
1:A:289:ARG:HG2	1:A:290:MET:SD	2.60	0.41
2:B:150:HIS:HE1	2:B:152:LYS:HB2	1.83	0.41
3:C:515:SER:HB3	3:C:518:LEU:HD12	2.02	0.41
3:C:827:LEU:HA	3:C:830:LEU:HD12	2.02	0.41
5:I:215:GLY:HA2	5:I:218:LEU:HG	2.02	0.41
6:J:269:ILE:HG23	6:J:314:VAL:HA	2.02	0.41
6:J:386:ILE:HG12	6:J:414:GLN:HB2	2.03	0.41
10:Z:298:TYR:OH	10:Z:766:GLN:HB3	2.20	0.41
10:Z:813:ARG:O	10:Z:817:THR:HG23	2.20	0.41
11:K:228:LYS:HB2	13:K:501:ATP:O1B	2.20	0.41
11:K:305:LEU:HD21	11:K:337:LEU:HD11	2.03	0.41
3:C:756:MET:SD	3:C:756:MET:N	2.94	0.41
6:J:177:LEU:HD13	6:J:180:GLN:OE1	2.19	0.41
1:A:148:ASN:HD22	1:A:154:LYS:NZ	2.19	0.41
1:A:400:ARG:HD2	1:A:400:ARG:C	2.46	0.41
2:B:257:LEU:HG	2:B:301:GLU:HG2	2.03	0.41
3:C:598:ALA:HB1	3:C:738:TYR:CD2	2.55	0.41
3:C:850:LEU:O	3:C:854:LEU:HG	2.21	0.41
8:M:159:GLN:CG	8:M:175:ILE:HG12	2.51	0.41
11:K:109:MET:HE2	11:K:126:ARG:HH12	1.86	0.41
1:A:230:LEU:HD21	4:D:35:LYS:HA	2.03	0.41
1:A:363:PRO:HA	1:A:366:LEU:HG	2.01	0.41
2:B:268:PHE:HB2	2:B:312:GLN:NE2	2.36	0.41
3:C:374:LEU:HD21	3:C:839:SER:O	2.21	0.41
3:C:774:ARG:HB2	3:C:775:MET:HE2	2.02	0.41
4:D:199:PHE:O	4:D:203:GLU:HG2	2.20	0.41
6:J:329:LEU:HA	6:J:334:LEU:HD12	2.02	0.41
9:N:191:VAL:HG12	9:N:195:GLU:OE2	2.20	0.41
9:N:194:VAL:HG12	9:N:199:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Z:226:ASN:HD22	10:Z:260:ASP:CG	2.28	0.41
10:Z:546:LEU:O	10:Z:549:TYR:HB3	2.21	0.41
11:K:109:MET:HE2	11:K:126:ARG:NH1	2.36	0.41
11:K:192:GLU:O	11:K:196:VAL:HG23	2.20	0.41
11:K:194:ARG:O	11:K:198:GLU:HB3	2.21	0.41
1:A:98:GLN:HE22	2:B:126:PRO:HB2	1.86	0.41
4:D:89:PHE:CZ	4:D:123:SER:HA	2.55	0.41
4:D:104:ALA:HB1	4:D:112:LEU:HG	2.01	0.41
4:D:224:ILE:HD11	4:D:234:PHE:CD1	2.56	0.41
6:J:185:ARG:O	6:J:189:GLU:HG3	2.20	0.41
8:M:118:ILE:HD13	8:M:142:LEU:HD21	2.01	0.41
8:M:141:LYS:HE3	8:M:141:LYS:HB3	1.94	0.41
9:N:141:GLN:NE2	9:N:145:HIS:HB3	2.36	0.41
9:N:176:THR:HG23	9:N:178:LEU:N	2.32	0.41
10:Z:214:LEU:HD13	10:Z:225:LEU:HG	2.03	0.41
11:K:64:LEU:HD12	11:K:64:LEU:HA	1.93	0.41
11:K:244:ILE:HD12	11:K:266:MET:HE1	2.03	0.41
1:A:148:ASN:HB2	1:A:154:LYS:HD3	2.03	0.41
1:A:158:GLY:O	1:A:159:LEU:HD23	2.21	0.41
1:A:228:PRO:HA	1:A:235:PHE:HE2	1.85	0.41
2:B:47:PRO:HD3	3:C:756:MET:HE1	2.03	0.41
2:B:284:ILE:HG12	2:B:327:ALA:O	2.21	0.41
2:B:303:GLN:HA	2:B:306:MET:SD	2.61	0.41
2:B:409:MET:HE2	2:B:409:MET:C	2.46	0.41
3:C:772:ILE:O	3:C:776:VAL:HG23	2.20	0.41
4:D:82:LYS:O	4:D:86:MET:HE3	2.21	0.41
4:D:353:SER:HB2	4:D:356:MET:HB2	2.03	0.41
5:I:114:CYS:HB2	5:I:124:LYS:HB3	2.03	0.41
5:I:170:HIS:CE1	8:M:136:VAL:HG13	2.56	0.41
5:I:186:ILE:HG22	5:I:312:ARG:O	2.21	0.41
5:I:218:LEU:HD11	5:I:247:MET:HE3	2.02	0.41
6:J:95:VAL:HG22	11:K:127:TYR:CE1	2.53	0.41
6:J:214:PRO:HB2	6:J:343:LEU:HD21	2.03	0.41
6:J:367:ASP:OD2	6:J:370:SER:HB3	2.21	0.41
8:M:118:ILE:HD12	8:M:163:TRP:CD1	2.56	0.41
9:N:52:THR:O	9:N:56:LEU:HG	2.20	0.41
9:N:216:LEU:HD12	9:N:216:LEU:HA	1.86	0.41
12:P:248:ALA:HB1	12:P:286:ILE:HG12	2.03	0.41
1:A:49:LEU:HG	2:B:59:LEU:HD11	2.03	0.41
1:A:291:VAL:HB	1:A:335:GLU:HG3	2.03	0.41
2:B:240:THR:O	2:B:241:SER:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:282:ILE:HD12	3:C:310:LEU:HB3	2.02	0.41
5:I:232:GLU:O	5:I:236:MET:HG3	2.21	0.41
5:I:254:GLY:HA2	5:I:272:MET:SD	2.60	0.41
6:J:179:MET:H	6:J:179:MET:CE	2.24	0.41
10:Z:299:TYR:OH	10:Z:901:GLY:HA2	2.20	0.41
10:Z:455:MET:HG2	10:Z:487:LEU:HD12	2.03	0.41
10:Z:542:SER:OG	10:Z:547:LEU:HD13	2.21	0.41
2:B:229:LYS:HG2	2:B:350:PHE:CG	2.56	0.40
2:B:284:ILE:HG12	2:B:328:THR:HB	2.03	0.40
2:B:403:ALA:HB2	2:B:411:VAL:HG23	2.03	0.40
3:C:435:GLN:O	3:C:438:LYS:HG2	2.22	0.40
3:C:789:GLN:HB2	3:C:792:VAL:HG23	2.03	0.40
4:D:327:LEU:HB2	4:D:356:MET:CE	2.46	0.40
5:I:220:GLN:C	5:I:222:TYR:H	2.30	0.40
5:I:250:ILE:HG22	5:I:294:THR:HB	2.03	0.40
11:K:124:GLY:N	11:K:125:PRO:HD2	2.36	0.40
12:P:357:ARG:HG2	12:P:391:LEU:HD11	2.02	0.40
1:A:412:PRO:HG3	4:D:243:LYS:HZ3	1.85	0.40
2:B:361:ILE:HG12	13:B:501:ATP:N1	2.36	0.40
4:D:110:ASP:O	4:D:114:VAL:HG23	2.22	0.40
5:I:241:ALA:HB2	5:I:288:ILE:HD11	2.02	0.40
6:J:94:LEU:HB3	6:J:139:LEU:O	2.21	0.40
7:L:30:GLN:CB	7:L:54:GLU:HG2	2.51	0.40
9:N:73:TRP:HA	9:N:77:HIS:ND1	2.36	0.40
9:N:106:GLN:HB2	9:N:108:VAL:HG23	2.03	0.40
10:Z:370:SER:HA	10:Z:373:VAL:HG23	2.02	0.40
10:Z:539:MET:HE3	10:Z:539:MET:HB3	1.89	0.40
10:Z:661:SER:HB3	10:Z:702:ALA:HB1	2.04	0.40
11:K:170:MET:SD	11:K:246:SER:HA	2.61	0.40
12:P:116:ALA:HB1	12:P:129:LEU:O	2.22	0.40
12:P:399:GLY:O	12:P:403:LEU:HG	2.20	0.40
1:A:48:LYS:HA	1:A:51:GLN:OE1	2.22	0.40
1:A:197:MET:CE	1:A:198:MET:HG3	2.51	0.40
1:A:448:ASP:O	1:A:452:SER:HB2	2.22	0.40
2:B:90:GLU:O	2:B:94:LYS:HG3	2.21	0.40
2:B:171:MET:CE	2:B:247:ILE:HG13	2.51	0.40
3:C:724:GLU:O	3:C:728:LYS:HG2	2.22	0.40
3:C:824:ASN:CG	3:C:827:LEU:HD23	2.46	0.40
3:C:895:LEU:HD12	3:C:896:LYS:HG3	2.04	0.40
6:J:258:PHE:HB2	6:J:302:GLN:NE2	2.36	0.40
6:J:296:LEU:O	6:J:299:LEU:HB3	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:62:ASP:OD2	7:L:62:ASP:C	2.63	0.40
8:M:91:LEU:HD22	8:M:125:PHE:CE1	2.56	0.40
9:N:42:TRP:HB3	9:N:46:PHE:HE1	1.87	0.40
10:Z:226:ASN:HA	10:Z:229:VAL:HG12	2.03	0.40
10:Z:448:LEU:HG	10:Z:480:ALA:HB1	2.03	0.40
10:Z:639:ASP:OD2	10:Z:639:ASP:N	2.54	0.40
11:K:209:ARG:HA	11:K:209:ARG:HD2	1.82	0.40
1:A:444:LEU:HD21	4:D:232:LEU:HD12	2.02	0.40
2:B:106:ILE:HA	2:B:147:VAL:O	2.22	0.40
2:B:151:HIS:NE2	2:B:152:LYS:HE3	2.37	0.40
4:D:15:GLN:HG3	4:D:15:GLN:H	1.73	0.40
4:D:409:PRO:HA	4:D:412:MET:CE	2.52	0.40
5:I:244:ILE:HD13	5:I:244:ILE:HA	1.89	0.40
9:N:114:ALA:HA	9:N:119:TRP:HD1	1.85	0.40
9:N:166:ALA:HB3	9:N:169:TRP:HE3	1.87	0.40
11:K:139:LYS:HD2	11:K:139:LYS:HA	1.88	0.40
1:A:429:PHE:HA	1:A:432:ARG:HD2	2.03	0.40
3:C:158:ALA:HB1	3:C:223:LEU:HD13	2.03	0.40
9:N:19:GLN:O	9:N:23:HIS:HB2	2.20	0.40
10:Z:50:TYR:CZ	10:Z:84:ALA:HB1	2.56	0.40
10:Z:214:LEU:HD11	10:Z:224:THR:HG22	2.03	0.40
10:Z:419:THR:HG22	10:Z:423:LEU:HD21	2.03	0.40
10:Z:618:ARG:O	10:Z:621:THR:HB	2.22	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	391/467 (84%)	372 (95%)	18 (5%)	1 (0%)	36 70
2	B	384/437 (88%)	376 (98%)	8 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	842/993 (85%)	831 (99%)	11 (1%)	0	100	100
4	D	458/480 (95%)	448 (98%)	10 (2%)	0	100	100
5	I	382/405 (94%)	367 (96%)	15 (4%)	0	100	100
6	J	375/428 (88%)	363 (97%)	12 (3%)	0	100	100
7	L	129/156 (83%)	117 (91%)	12 (9%)	0	100	100
8	M	415/417 (100%)	397 (96%)	18 (4%)	0	100	100
9	N	226/228 (99%)	217 (96%)	9 (4%)	0	100	100
10	Z	874/945 (92%)	857 (98%)	17 (2%)	0	100	100
11	K	380/437 (87%)	375 (99%)	5 (1%)	0	100	100
12	P	386/434 (89%)	378 (98%)	8 (2%)	0	100	100
All	All	5242/5827 (90%)	5098 (97%)	143 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	LYS

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	331/399 (83%)	328 (99%)	3 (1%)	70	76
2	B	344/385 (89%)	342 (99%)	2 (1%)	78	81
3	C	724/850 (85%)	718 (99%)	6 (1%)	73	77
4	D	427/445 (96%)	423 (99%)	4 (1%)	70	76
5	I	334/352 (95%)	332 (99%)	2 (1%)	78	81
6	J	331/374 (88%)	328 (99%)	3 (1%)	70	76
7	L	120/144 (83%)	119 (99%)	1 (1%)	73	77
8	M	364/364 (100%)	361 (99%)	3 (1%)	73	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	N	198/198 (100%)	194 (98%)	4 (2%)	48	66
10	Z	737/797 (92%)	730 (99%)	7 (1%)	70	76
11	K	327/377 (87%)	323 (99%)	4 (1%)	63	73
12	P	337/375 (90%)	333 (99%)	4 (1%)	63	73
All	All	4574/5060 (90%)	4531 (99%)	43 (1%)	68	76

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

Mol	Chain	Res	Type
1	A	280	VAL
1	A	289	ARG
1	A	302	LYS
2	B	209	GLU
2	B	281	ILE
3	C	225	LEU
3	C	353	VAL
3	C	443	ASP
3	C	743	ILE
3	C	854	LEU
3	C	857	LEU
4	D	46	LEU
4	D	81	ASP
4	D	287	CYS
4	D	314	LEU
5	I	162	GLU
5	I	268	VAL
6	J	60	LEU
6	J	67	TYR
6	J	135	MET
7	L	85	ARG
8	M	45	VAL
8	M	118	ILE
8	M	360	ILE
9	N	35	ASP
9	N	120	PHE
9	N	124	GLN
9	N	176	THR
10	Z	268	GLN
10	Z	296	CYS
10	Z	379	LEU
10	Z	427	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	Z	523	LEU
10	Z	737	SER
10	Z	868	VAL
11	K	112	LEU
11	K	128	ILE
11	K	170	MET
11	K	325	MET
12	P	53	HIS
12	P	193	LEU
12	P	256	ILE
12	P	305	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	327	ASN
2	B	68	HIS
2	B	295	ASN
2	B	312	GLN
3	C	132	HIS
3	C	871	HIS
4	D	387	GLN
4	D	389	GLN
6	J	302	GLN
7	L	30	GLN
8	M	9	HIS
8	M	156	GLN
9	N	23	HIS
9	N	141	GLN
9	N	145	HIS
10	Z	616	HIS
10	Z	738	GLN
12	P	53	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](#)

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	P	501	-	32,33,33	0.27	0	48,52,52	0.34	0
13	ATP	B	501	-	32,33,33	0.44	0	48,52,52	0.36	0
13	ATP	K	501	-	32,33,33	0.33	0	48,52,52	0.33	0
13	ATP	I	501	-	32,33,33	0.31	0	48,52,52	0.34	0
13	ATP	J	501	-	32,33,33	0.42	0	48,52,52	0.38	0
13	ATP	A	501	-	32,33,33	0.68	2 (6%)	48,52,52	0.41	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	P	501	-	-	4/22/38/38	0/3/3/3
13	ATP	B	501	-	-	2/22/38/38	0/3/3/3
13	ATP	K	501	-	-	2/22/38/38	0/3/3/3
13	ATP	I	501	-	-	3/22/38/38	0/3/3/3
13	ATP	J	501	-	-	7/22/38/38	0/3/3/3
13	ATP	A	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)
13	A	501	ATP	PA-O3A	-2.48	1.56	1.59
13	A	501	ATP	PB-O3B	-2.08	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

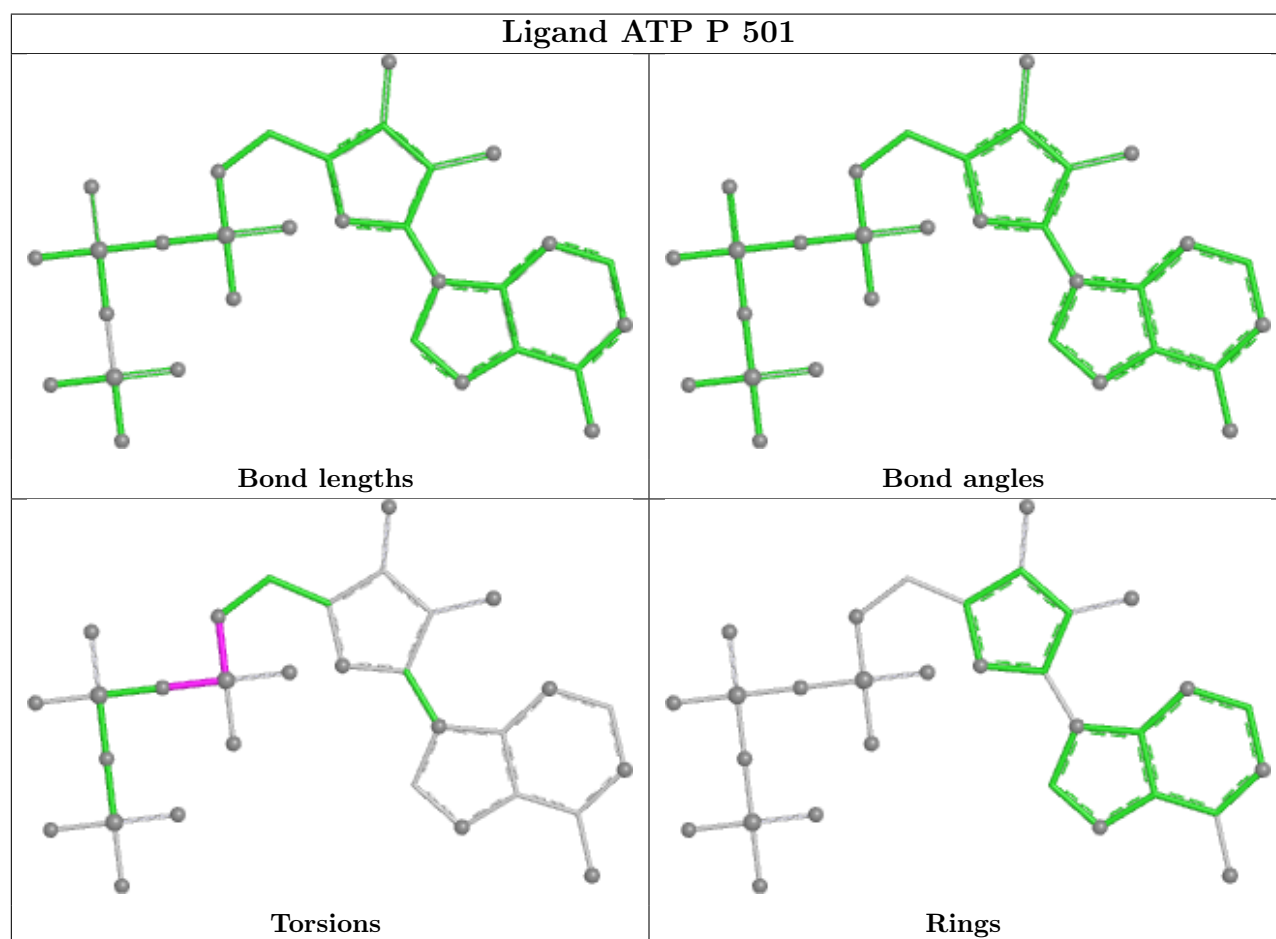
Mol	Chain	Res	Type	Atoms
13	A	501	ATP	C5'-O5'-PA-O1A
13	A	501	ATP	C5'-O5'-PA-O3A
13	B	501	ATP	C5'-O5'-PA-O3A
13	I	501	ATP	C5'-O5'-PA-O2A
13	J	501	ATP	C5'-O5'-PA-O1A
13	J	501	ATP	C5'-O5'-PA-O2A
13	J	501	ATP	C5'-O5'-PA-O3A
13	K	501	ATP	C5'-O5'-PA-O3A
13	P	501	ATP	C5'-O5'-PA-O2A
13	J	501	ATP	O4'-C4'-C5'-O5'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

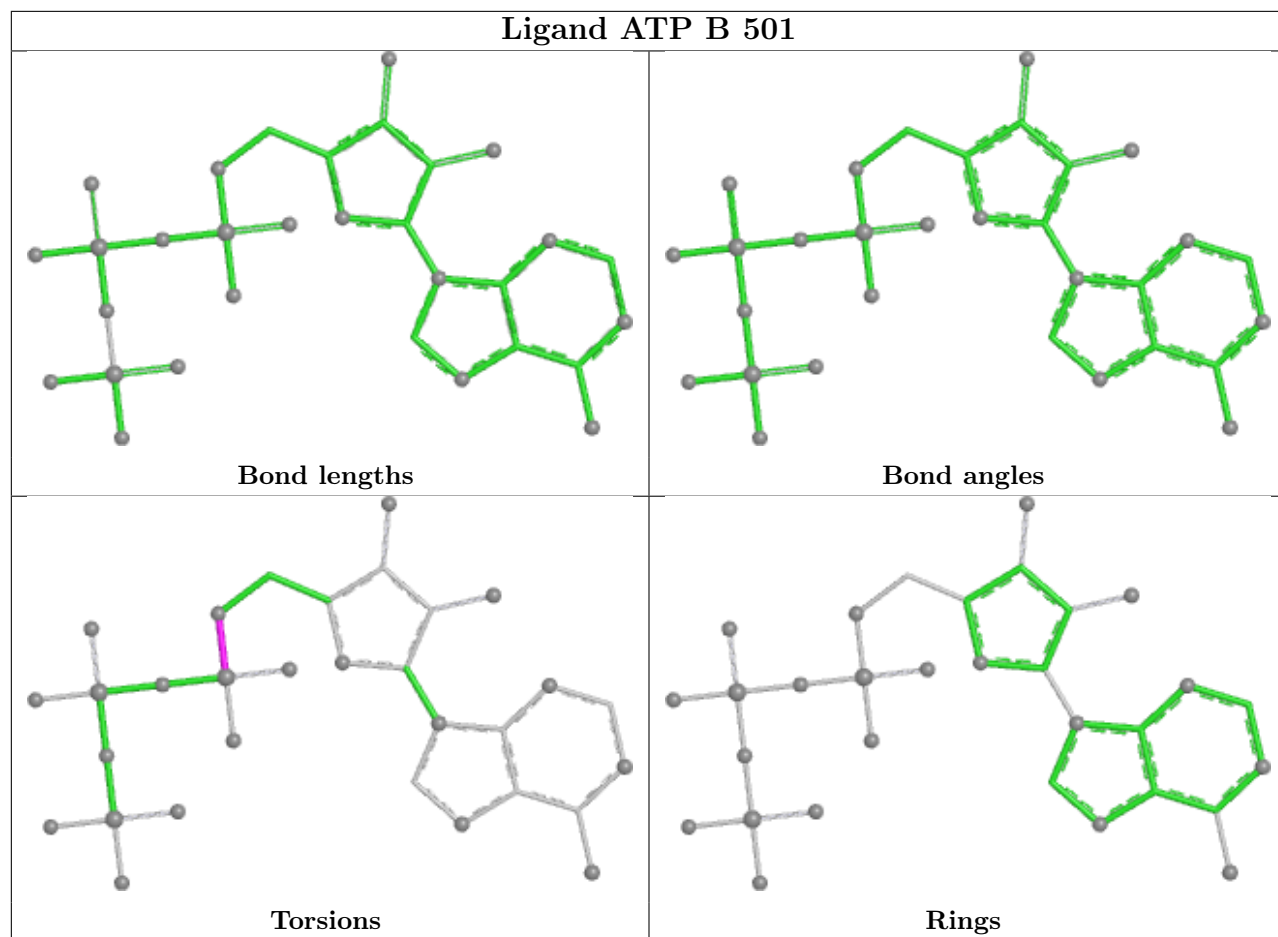
There are no ring outliers.

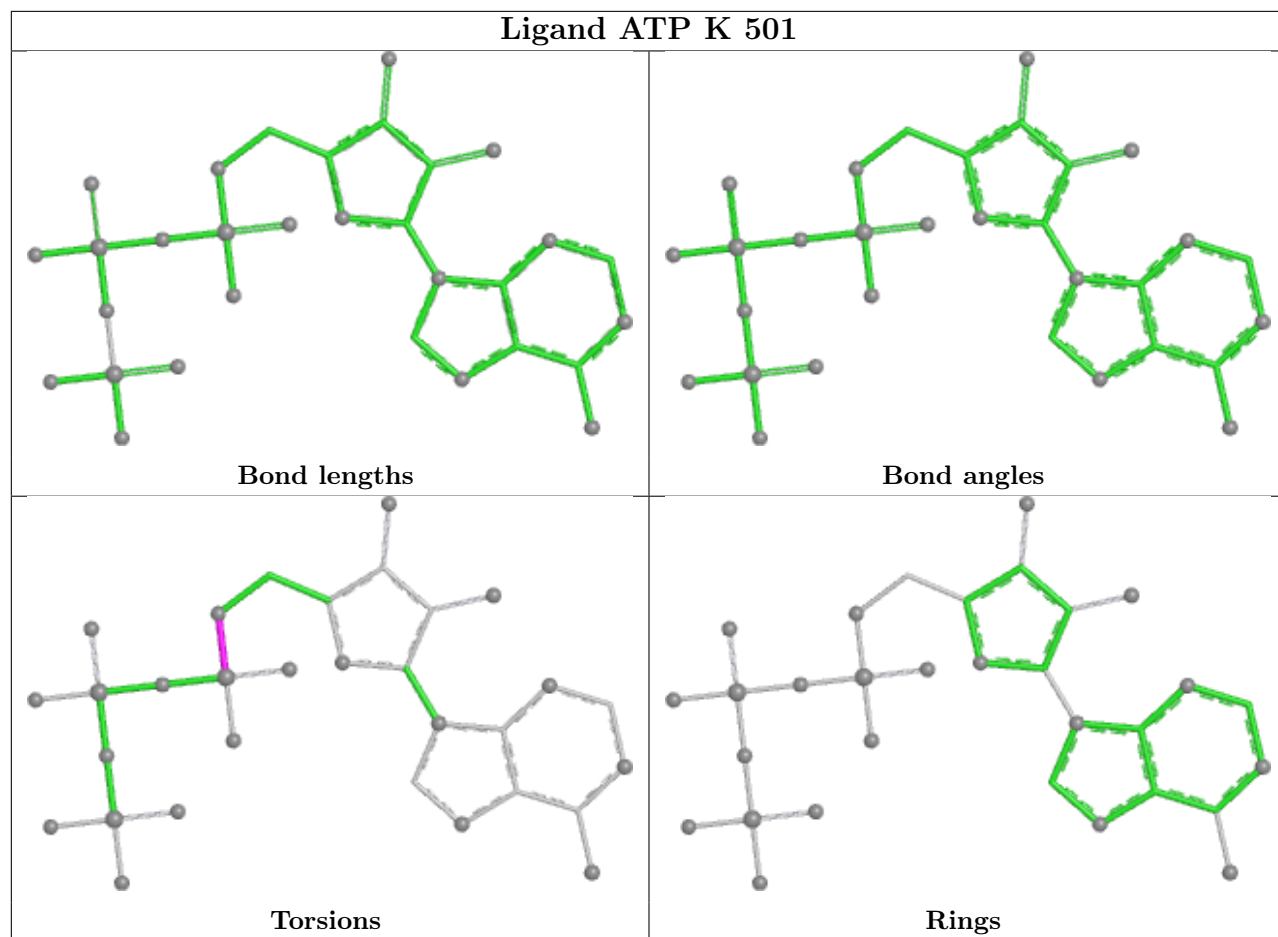
6 monomers are involved in 18 short contacts:

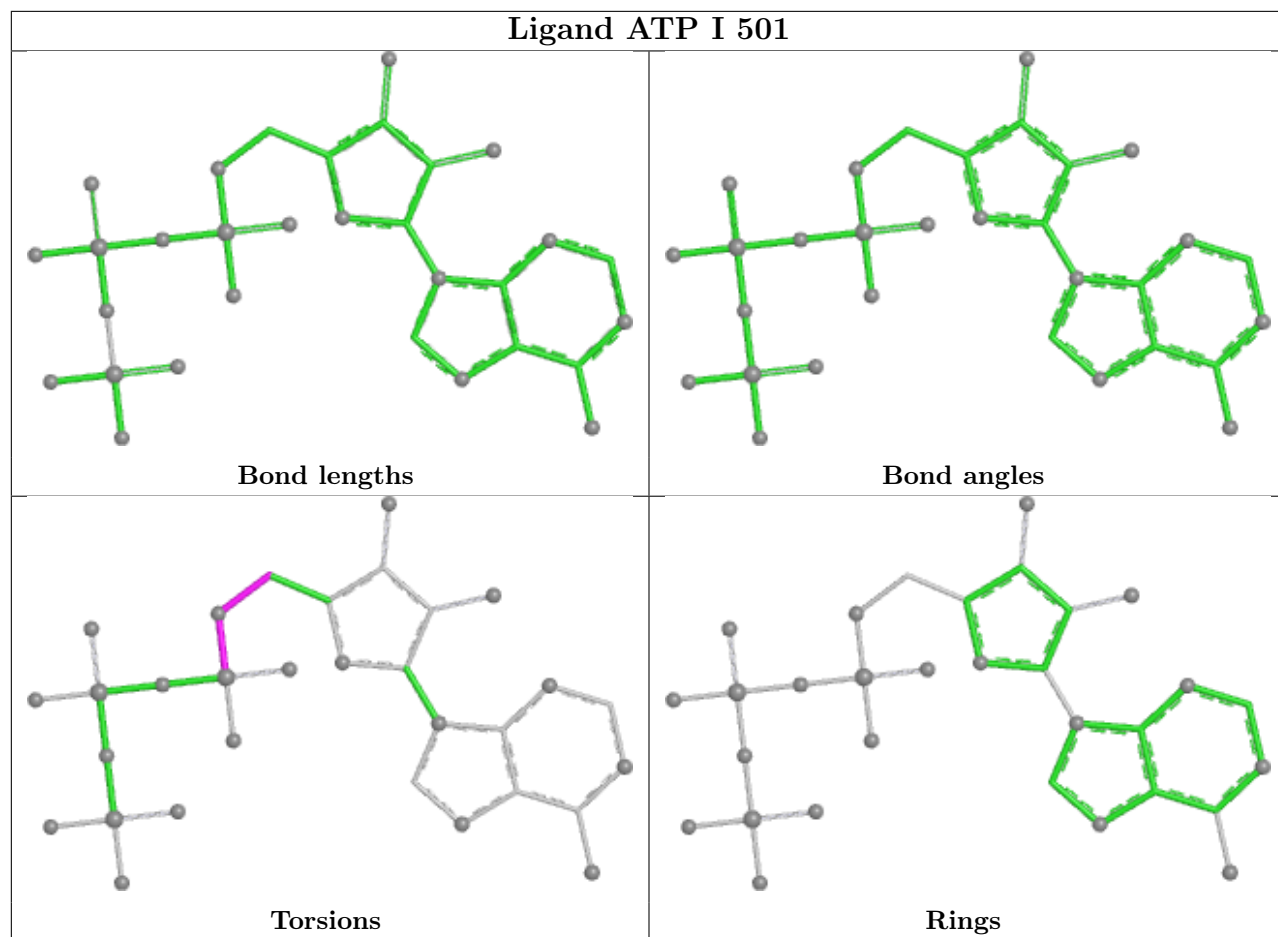
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	501	ATP	2	0
13	B	501	ATP	4	0
13	K	501	ATP	5	0
13	I	501	ATP	2	0
13	J	501	ATP	4	0
13	A	501	ATP	1	0

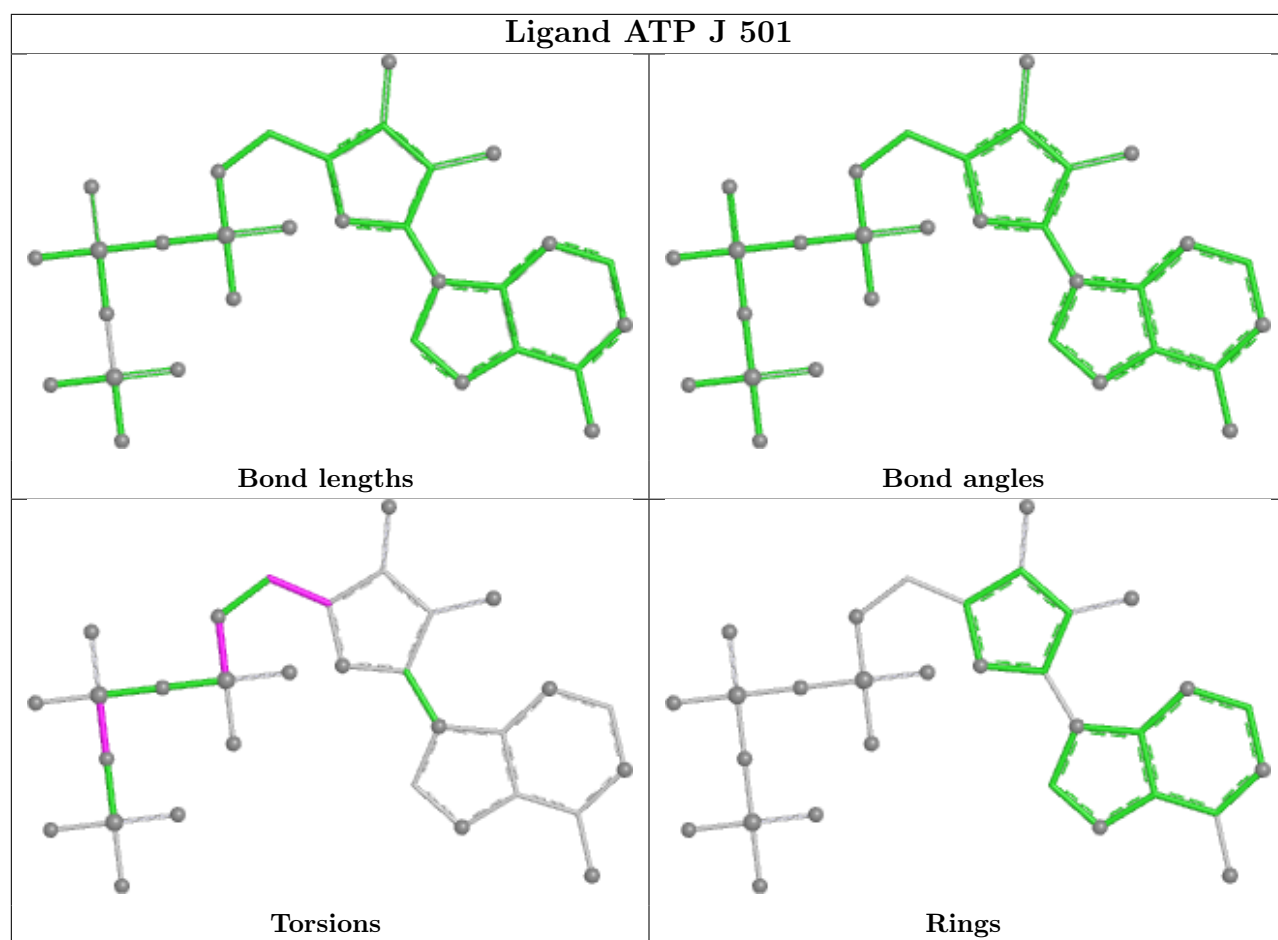
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

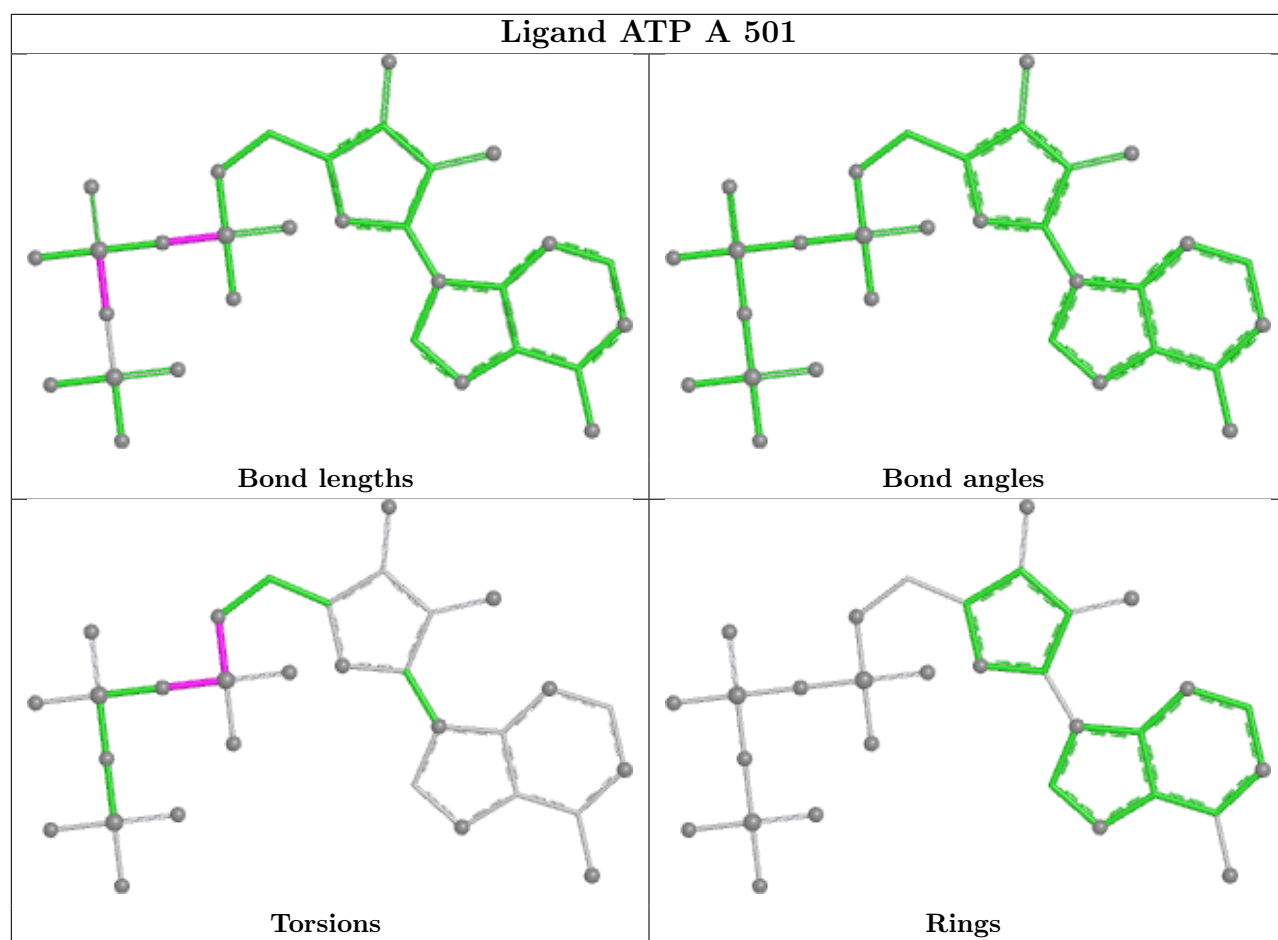












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

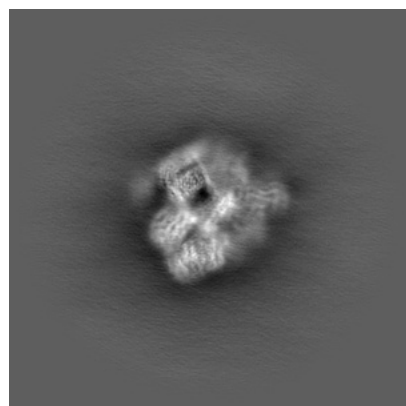
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77350. These allow visual inspection of the internal detail of the map and identification of artifacts.

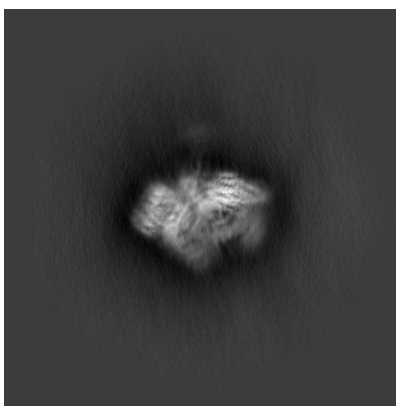
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

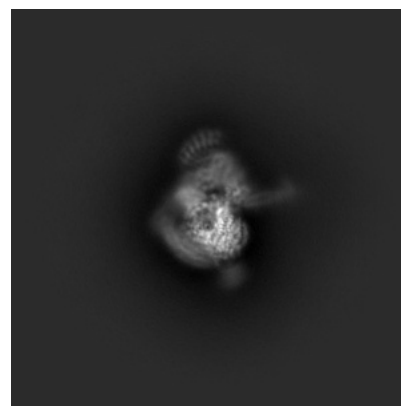
6.1.1 Primary map



X

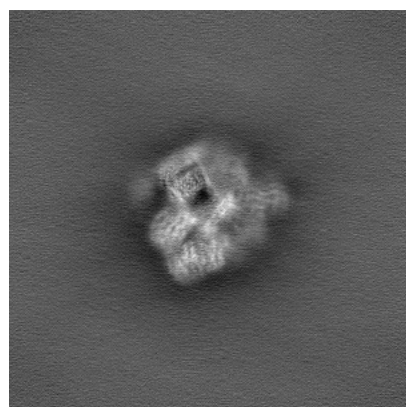


Y

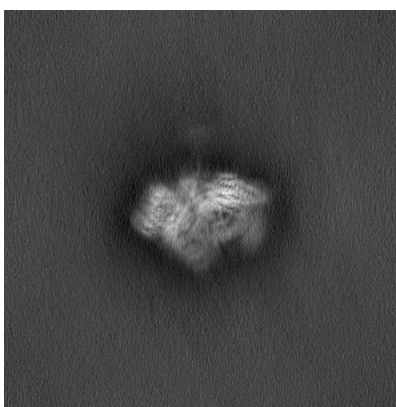


Z

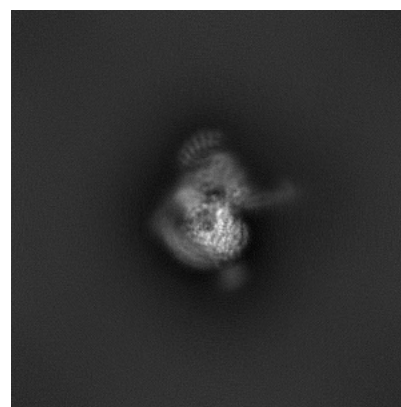
6.1.2 Raw map



X



Y

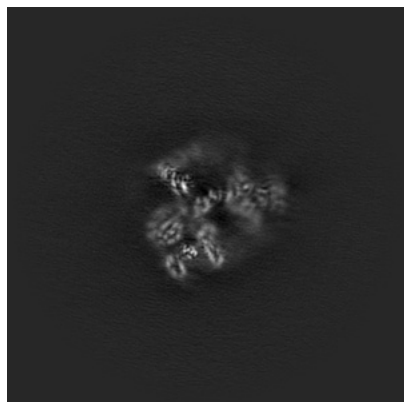


Z

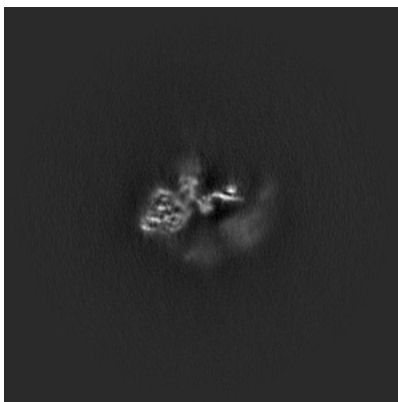
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

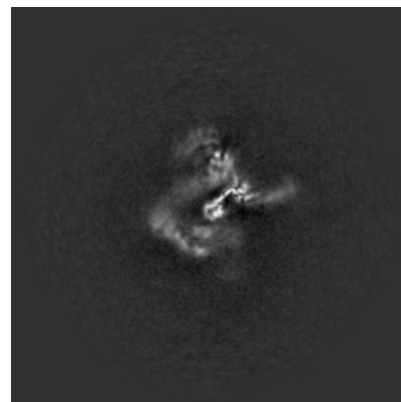
6.2.1 Primary map



X Index: 256

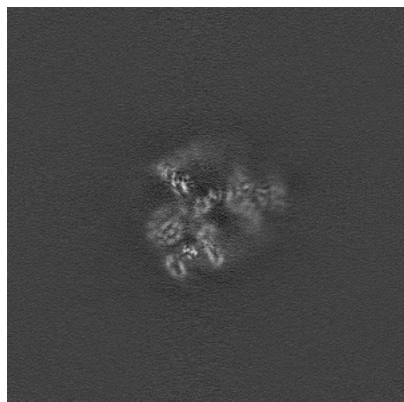


Y Index: 256



Z Index: 256

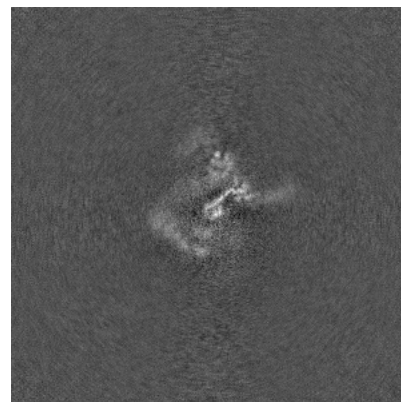
6.2.2 Raw map



X Index: 256



Y Index: 256

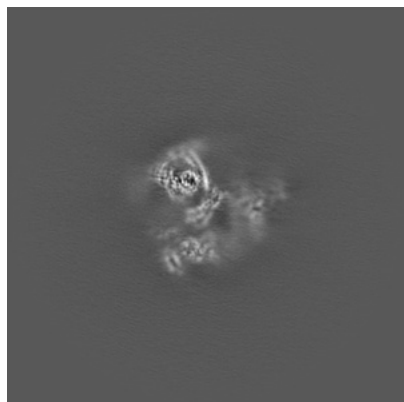


Z Index: 256

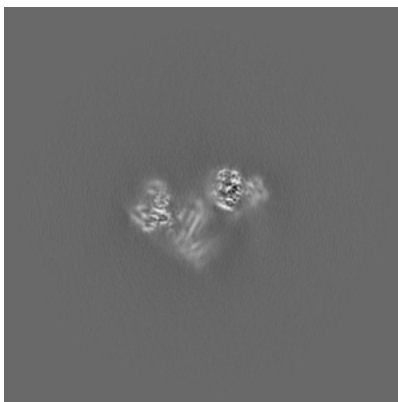
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

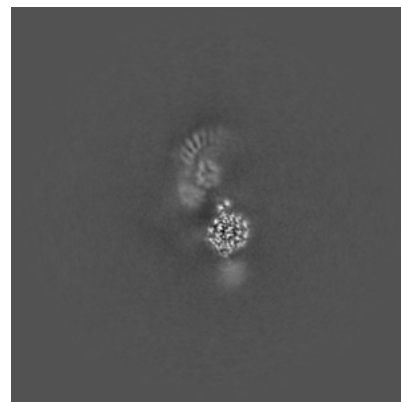
6.3.1 Primary map



X Index: 267

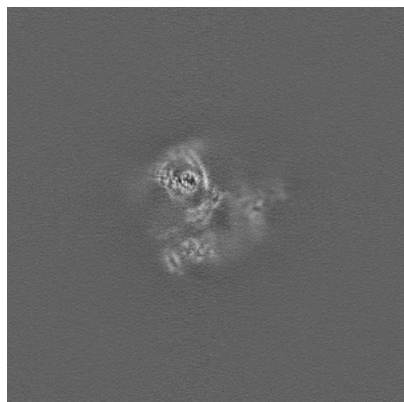


Y Index: 226



Z Index: 284

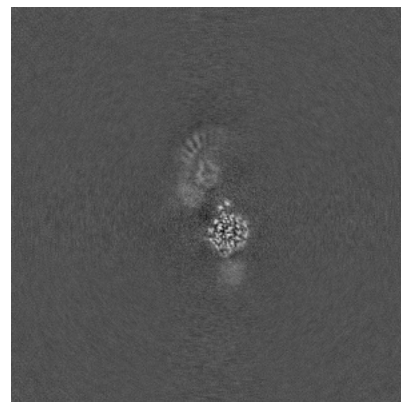
6.3.2 Raw map



X Index: 267



Y Index: 226

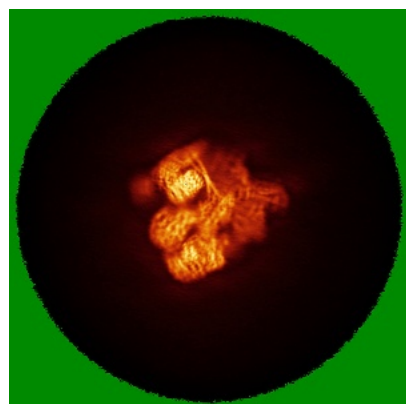


Z Index: 284

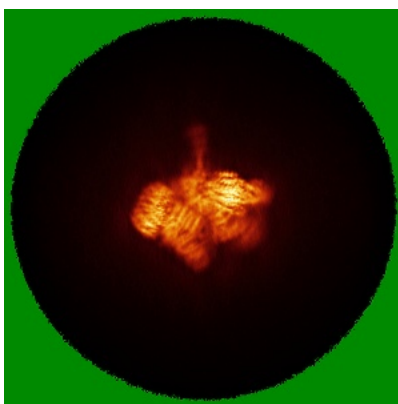
The images above show the largest variance slices of the map in three orthogonal directions.

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

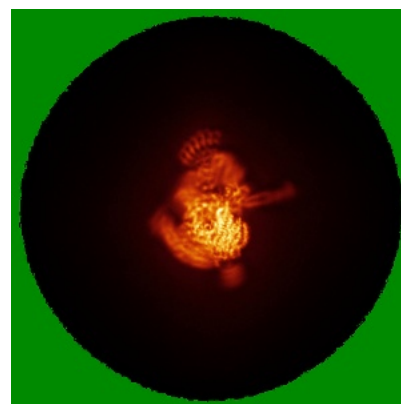
6.4.1 Primary map



X

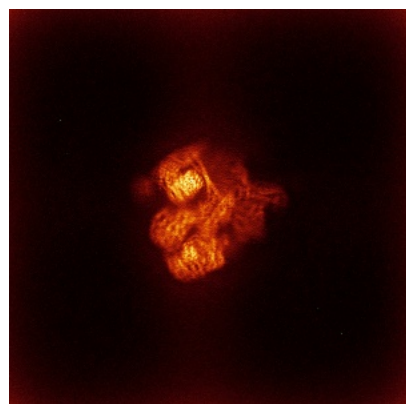


Y

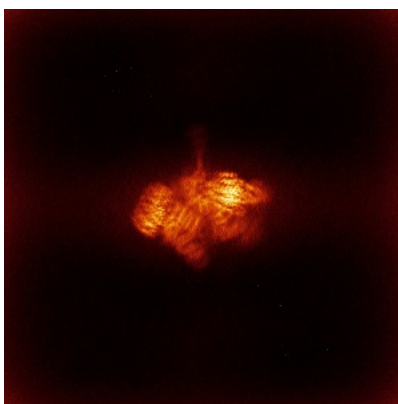


Z

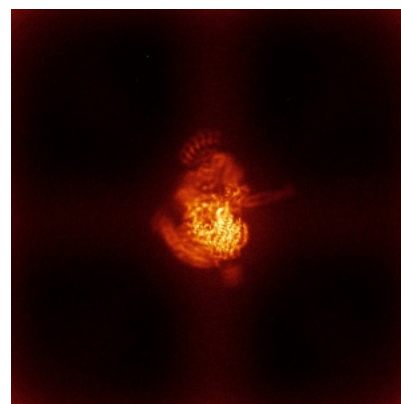
6.4.2 Raw map



X



Y

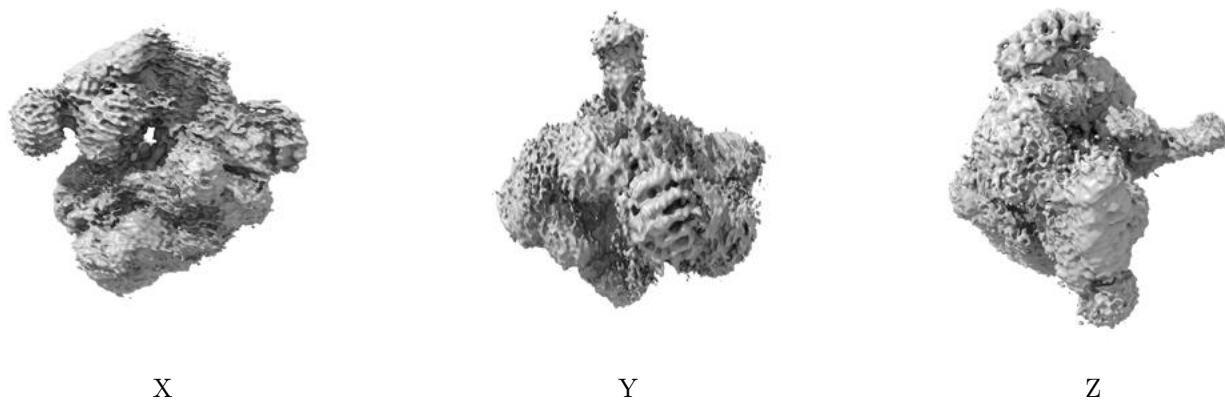


Z

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.

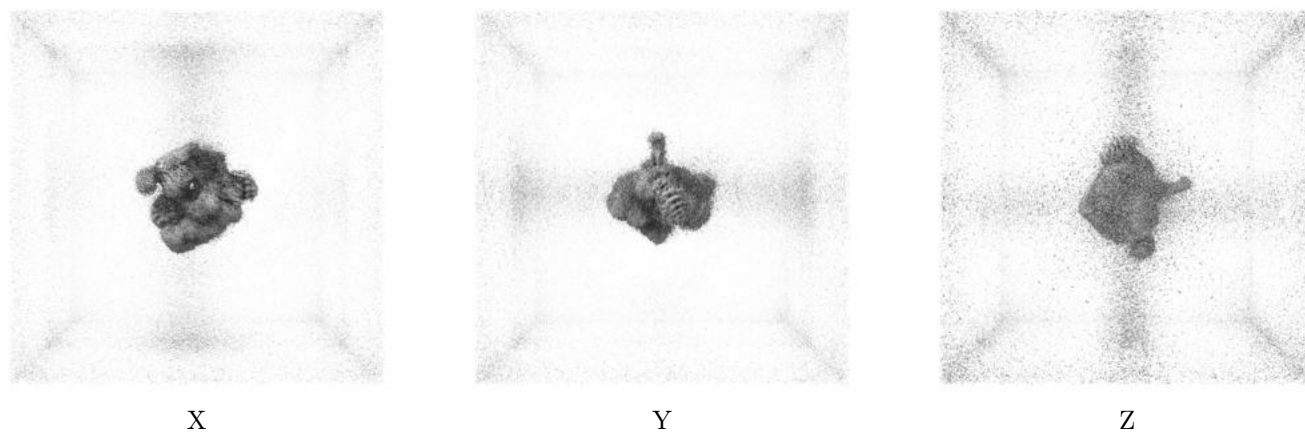
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

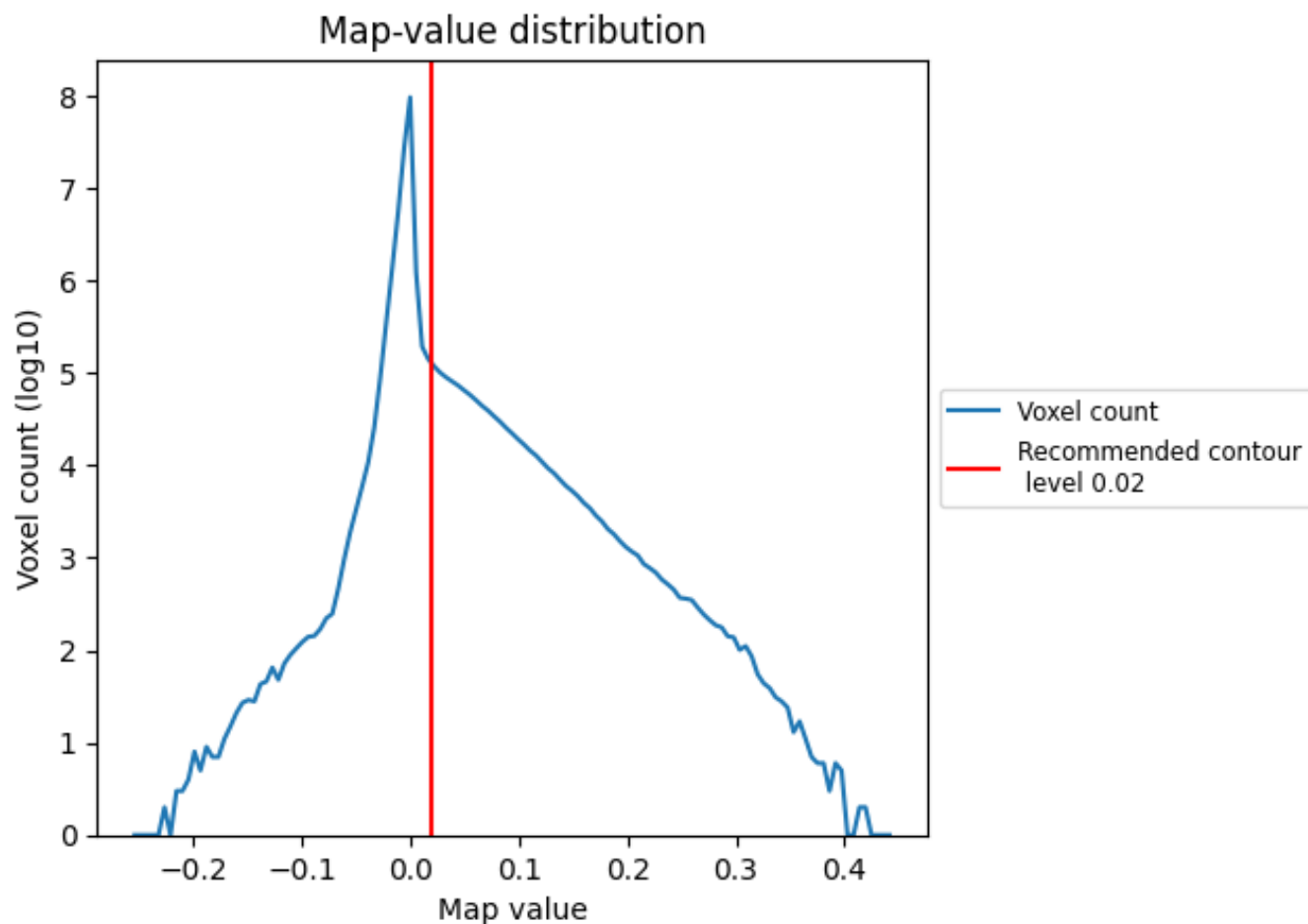
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

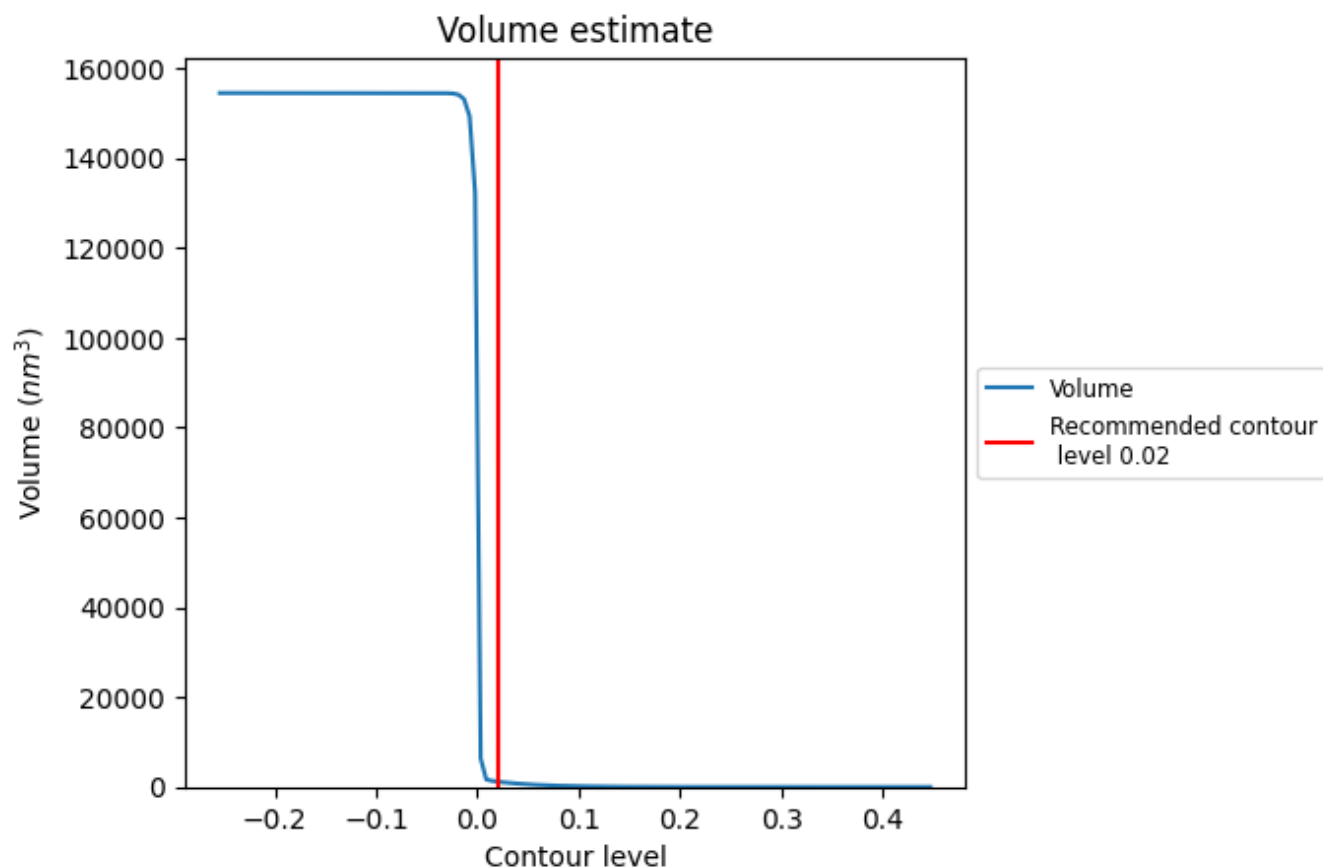
This section contains the results of statistical analysis of the map.

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.

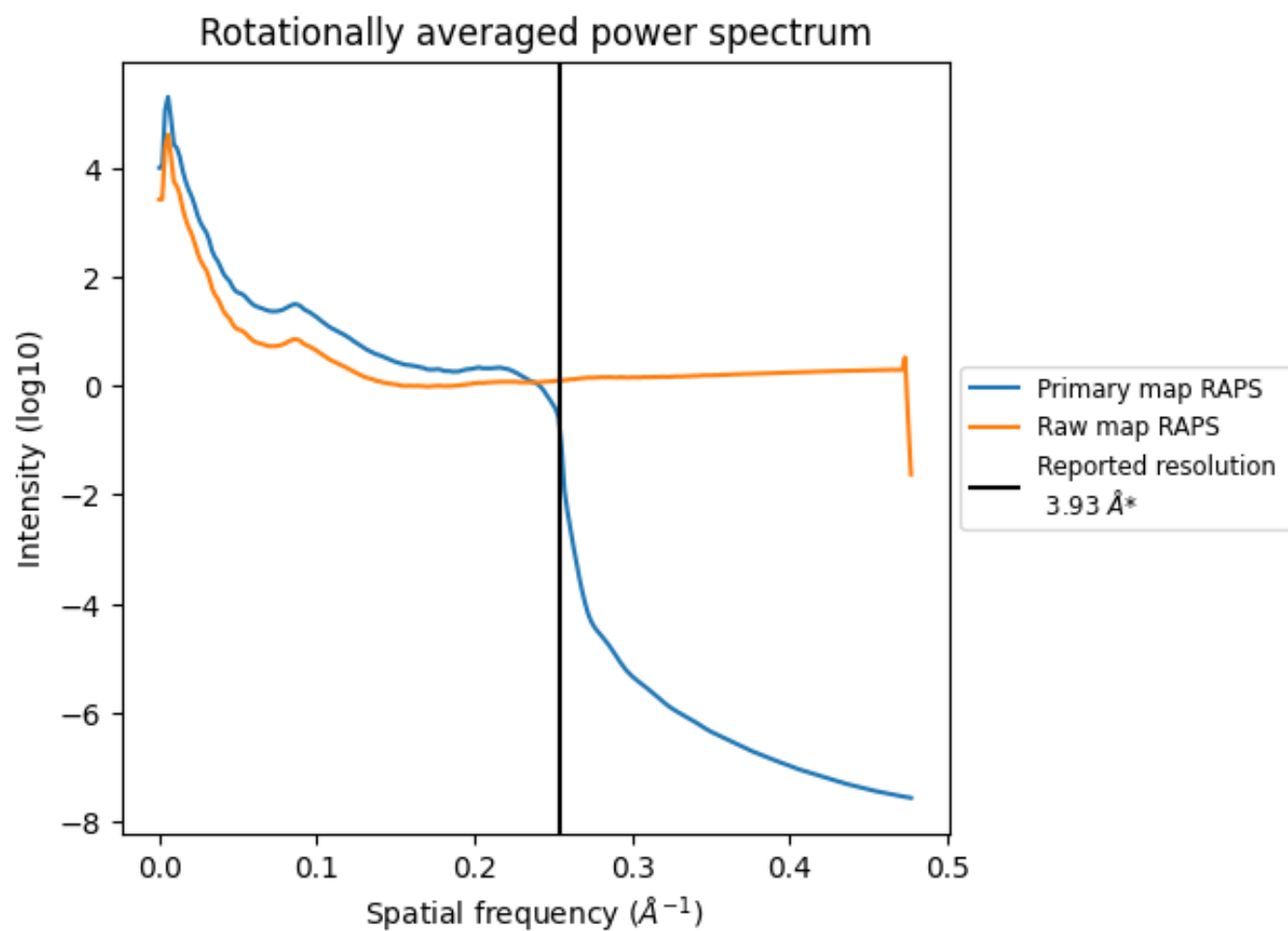
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1177 nm^3 ; this corresponds to an approximate mass of 1063 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 ⓘ

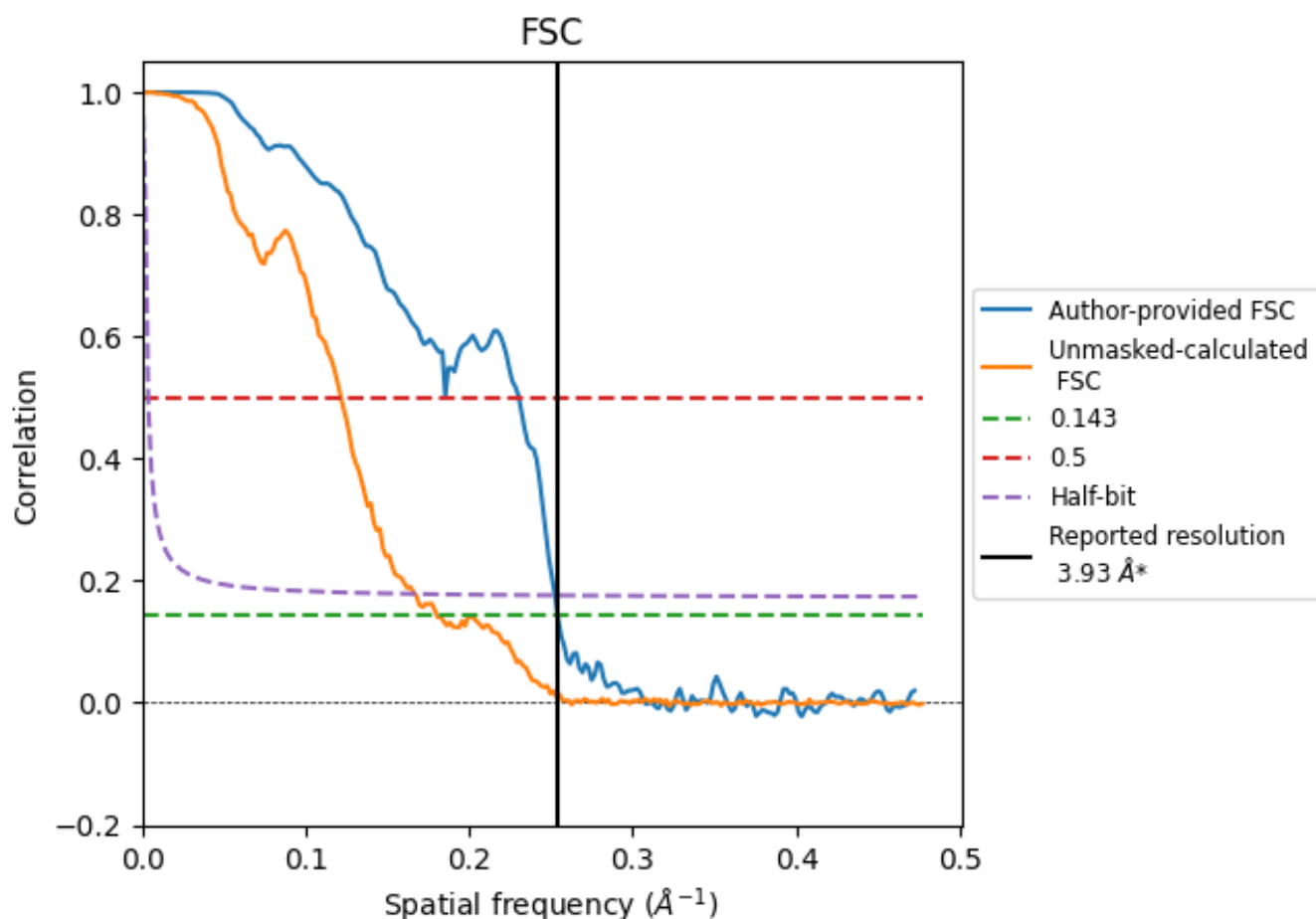


*Reported resolution corresponds to spatial frequency of 0.254 $\text{\AA}^{-1}$

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 0.254 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

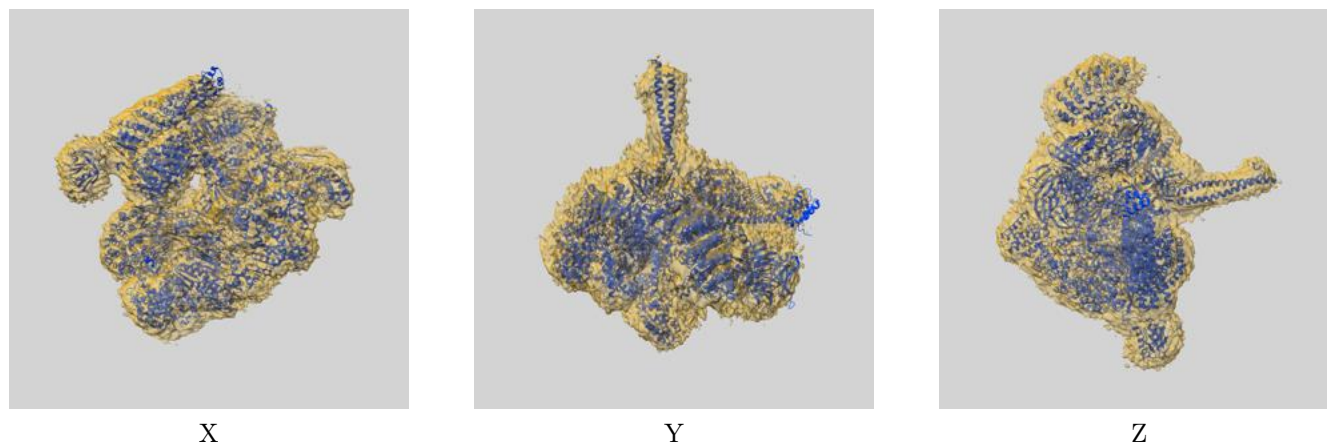
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.93	4.34	3.96
Unmasked-calculated*	5.55	8.22	6.00

*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 5.55 differs from the reported value 3.93 by more than 10 %

9 Map-model fit [i](#)

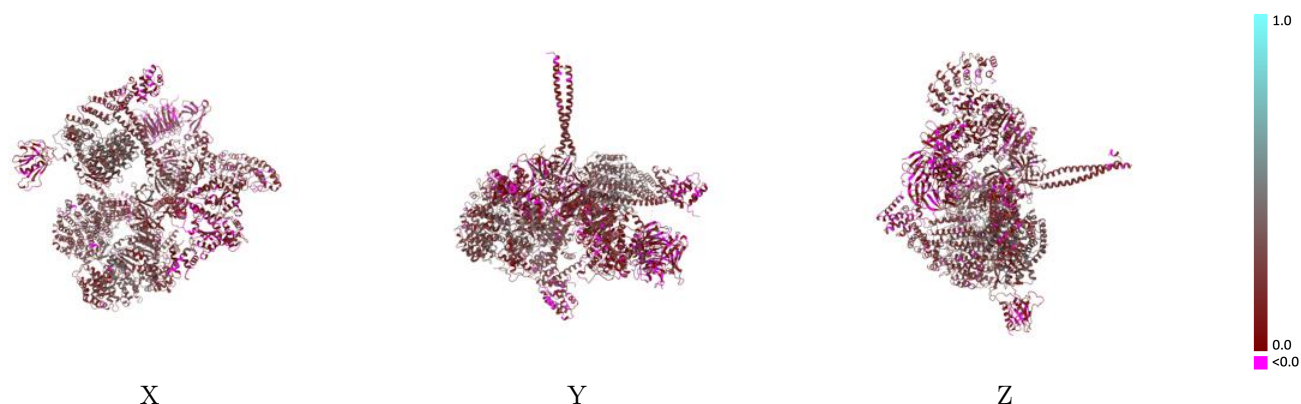
This section contains information regarding the fit between EMDB map EMD-77350 and PDB model 36BD. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



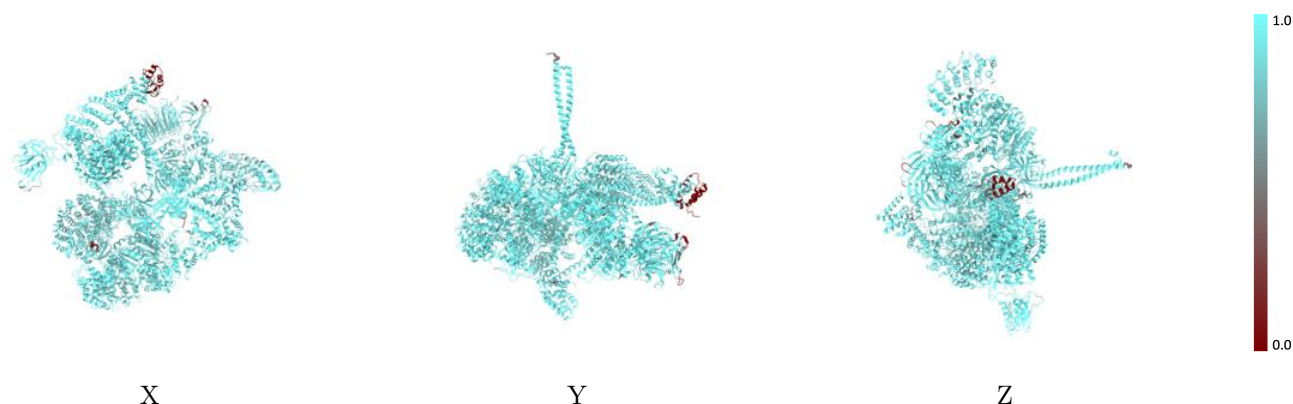
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



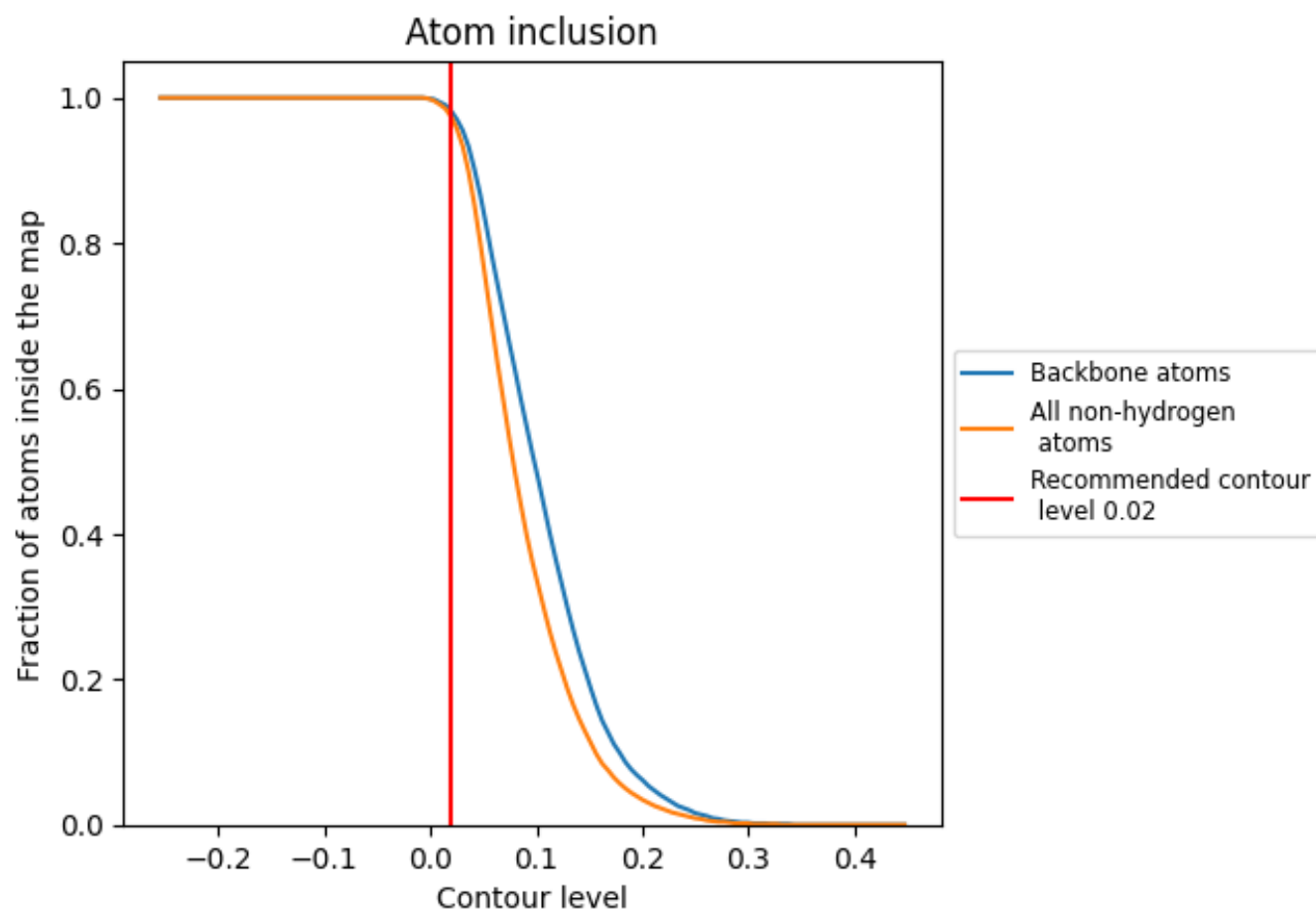
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9730	0.2000
A	0.9910	0.2690
B	0.9980	0.2300
C	0.9890	0.2000
D	0.9970	0.2420
I	0.9890	0.1660
J	0.9740	0.2100
K	0.9810	0.1610
L	0.9750	0.1140
M	0.9060	0.0770
N	0.9460	0.1610
P	0.9910	0.1220
Z	0.9450	0.2800

1.0

0.0

<0.0