



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 09:06 PM EDT

PDB ID : 9PRT / pdb_00009prt
EMDB ID : EMD-71813
Title : Human 19S proteasome bound to TXNL1 PITH domain but with low density for RPT1, RPT2, and RPN1
Authors : Chen, X.; Negi, H.; Walters, K.J.
Deposited on : 2025-07-24
Resolution : 3.02 Å (reported)
Based on initial models : 1WWY, 7WSI

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:

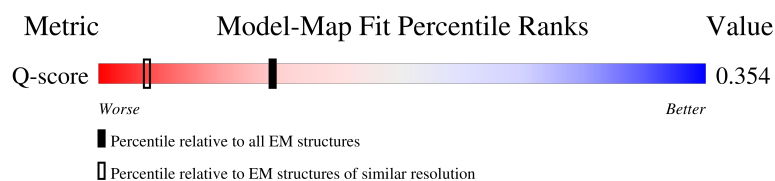
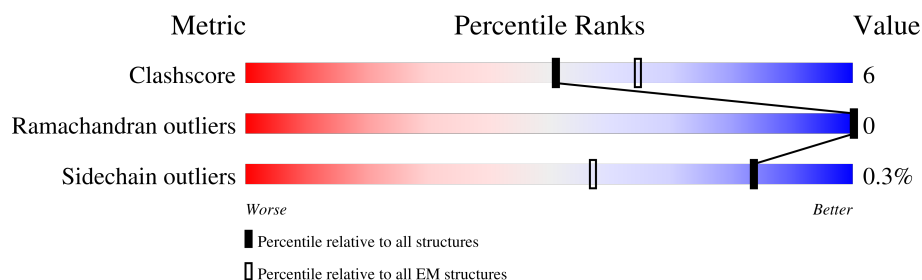
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.02 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.








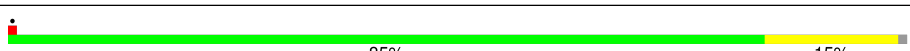
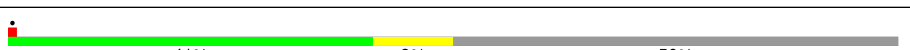
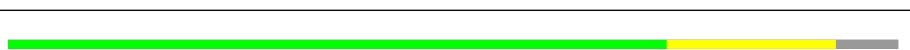


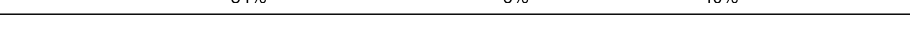
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	C	406	
2	D	418	
3	E	389	
4	F	439	

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Mol	Chain	Length	Quality of chain
5	U	953	
6	V	534	
7	W	456	
8	X	422	
9	Y	389	
10	Z	324	
11	a	376	
12	b	377	
13	c	310	
14	d	350	
15	e	70	
16	g	289	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 41604 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 RPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	370	Total	C	N	O	S	0	0
			2912	1831	523	541	17		

- Molecule 2 is a protein called RPT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	369	Total	C	N	O	S	0	0
			2935	1857	507	558	13		

- Molecule 3 is a protein called RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	380	Total	C	N	O	S	0	0
			3025	1900	542	567	16		

- Molecule 4 is a protein called RPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	376	Total	C	N	O	S	0	0
			2945	1854	508	565	18		

- Molecule 5 is a protein called RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	831	Total	C	N	O	S	0	0
			6472	4108	1099	1221	44		

- Molecule 6 is a protein called RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	464	Total	C	N	O	S	0	0
			3739	2374	666	686	13		

- Molecule 7 is a protein called RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	317	Total	C	N	O	S	0	0
			2605	1655	445	491	14		

- Molecule 8 is a protein called RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	104	Total	C	N	O	S	0	0
			836	536	139	159	2		

- Molecule 9 is a protein called RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 10 is a protein called RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

- Molecule 11 is a protein called RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

- Molecule 12 is a protein called RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	189	Total	C	N	O	S	0	0
			1449	905	259	277	8		

- Molecule 13 is a protein called RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	289	Total	C	N	O	S	0	0
			2272	1438	391	424	19		

- Molecule 14 is a protein called RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	265	Total	C	N	O	S	0	0
			2166	1402	355	400	9		

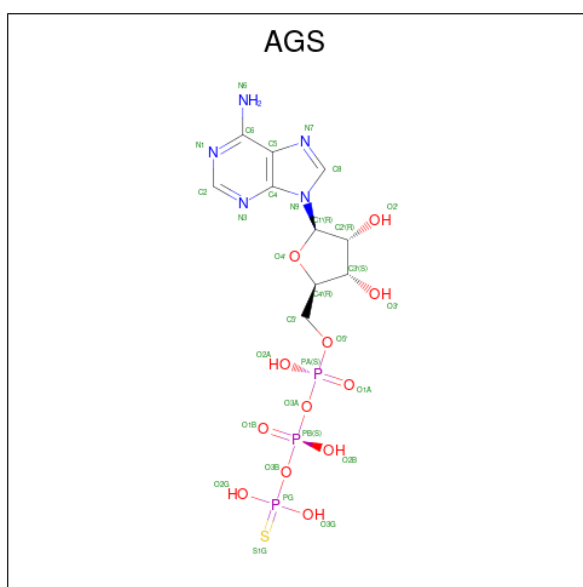
- Molecule 15 is a protein called DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 16 is a protein called TXNL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	173	Total	C	N	O	S	0	0
			1383	869	227	278	9		

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



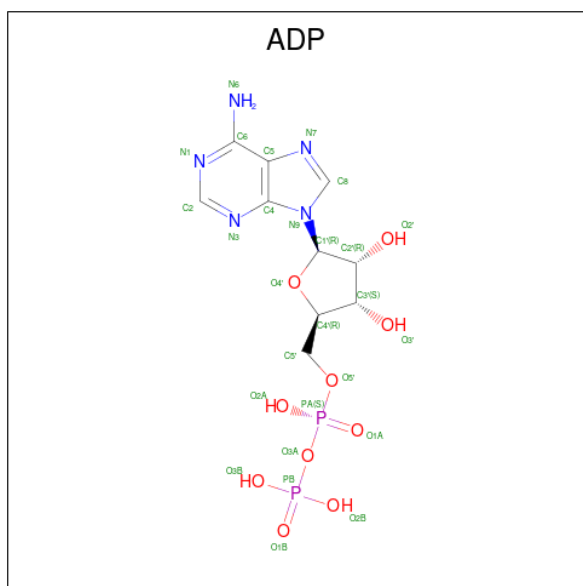
Mol	Chain	Residues	Atoms						AltConf
17	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	C	1	Total	Mg	0
			1	1	
18	D	1	Total	Mg	0
			1	1	

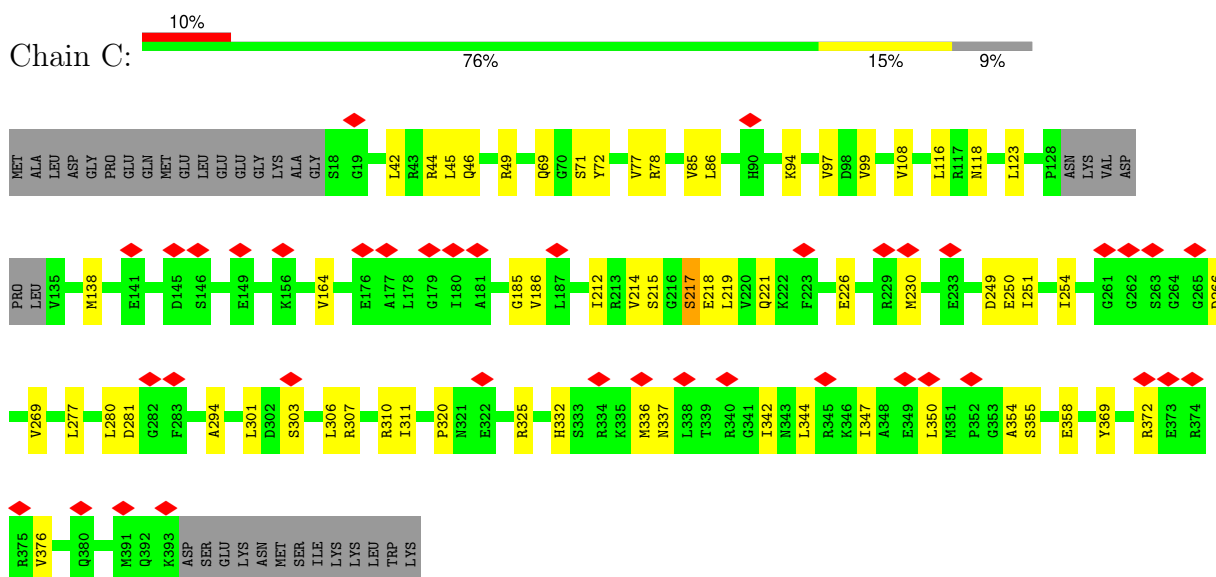
- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



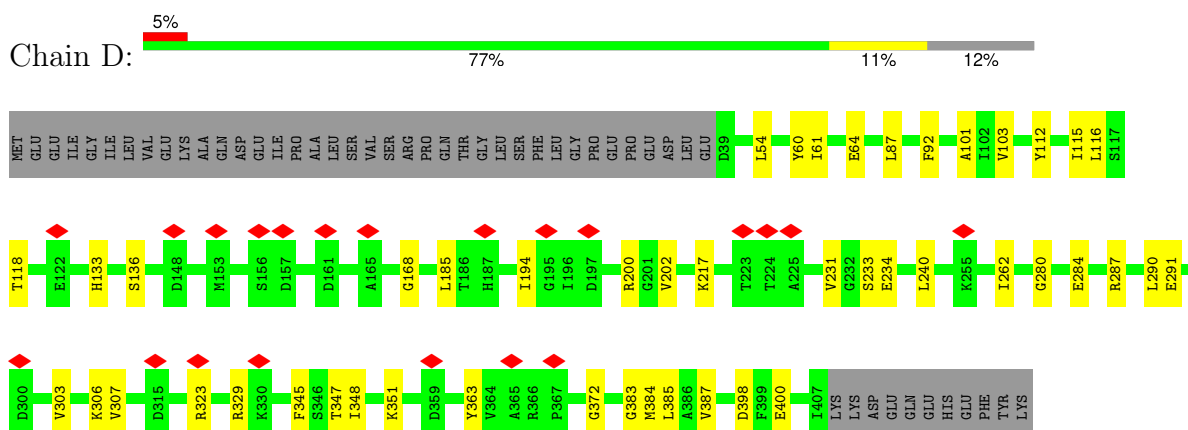
3 Residue-property plots

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.

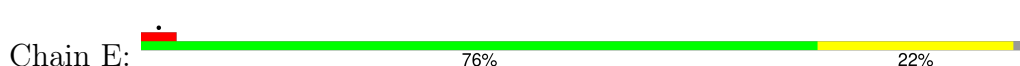
• Molecule 1: RPT6

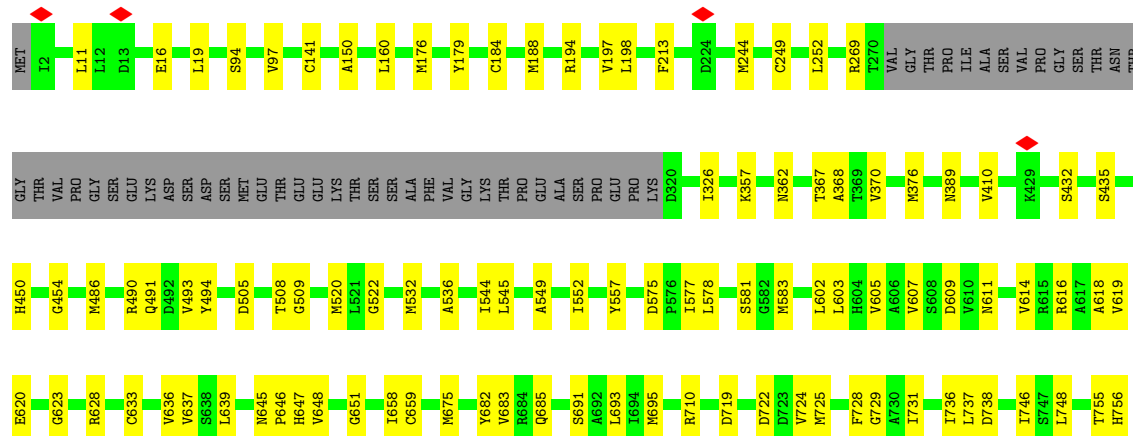


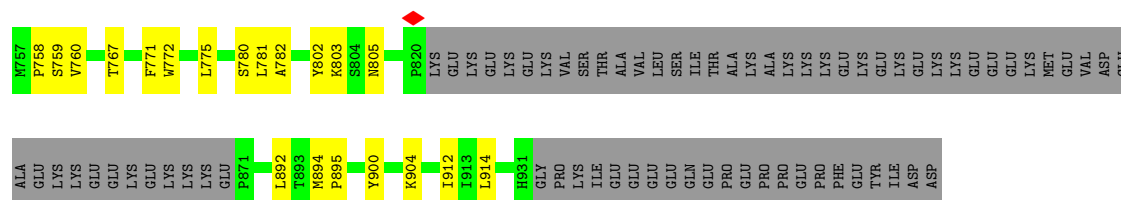
• Molecule 2: RPT3



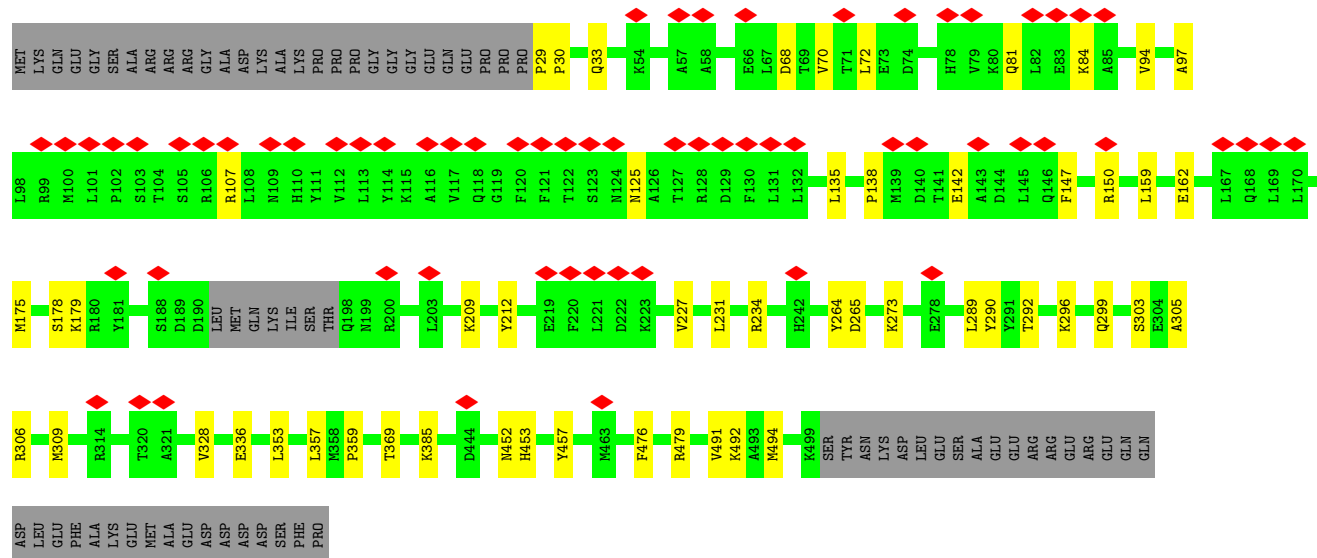
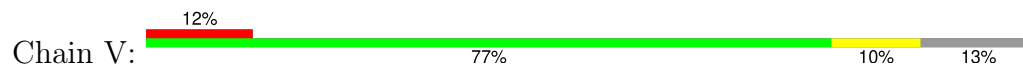
• Molecule 3: RPT4



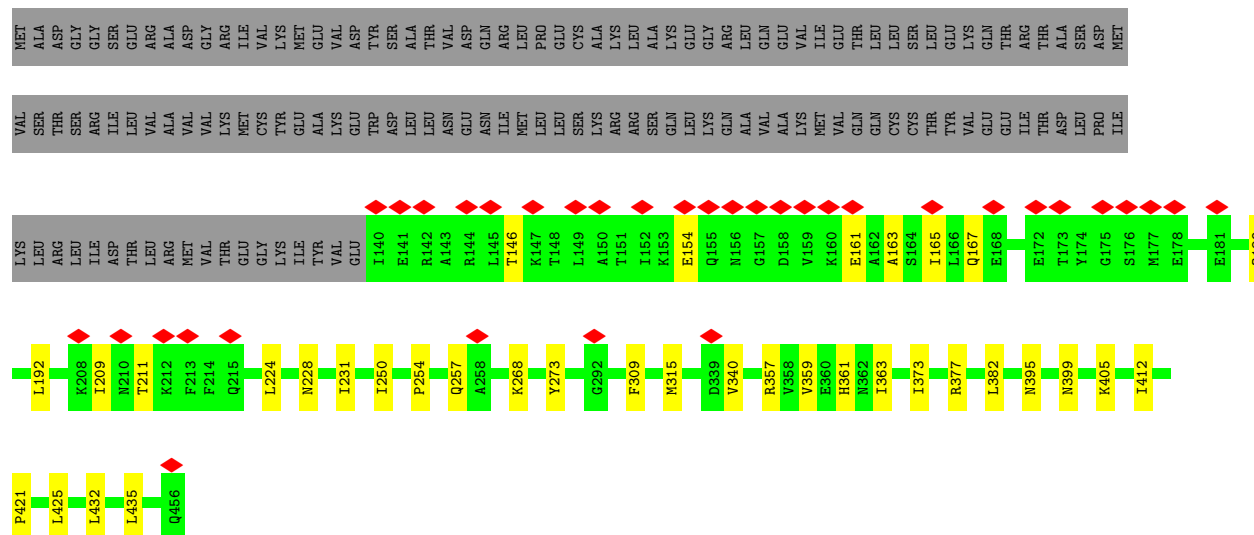




• Molecule 6: RPN3



• Molecule 7: RPN5

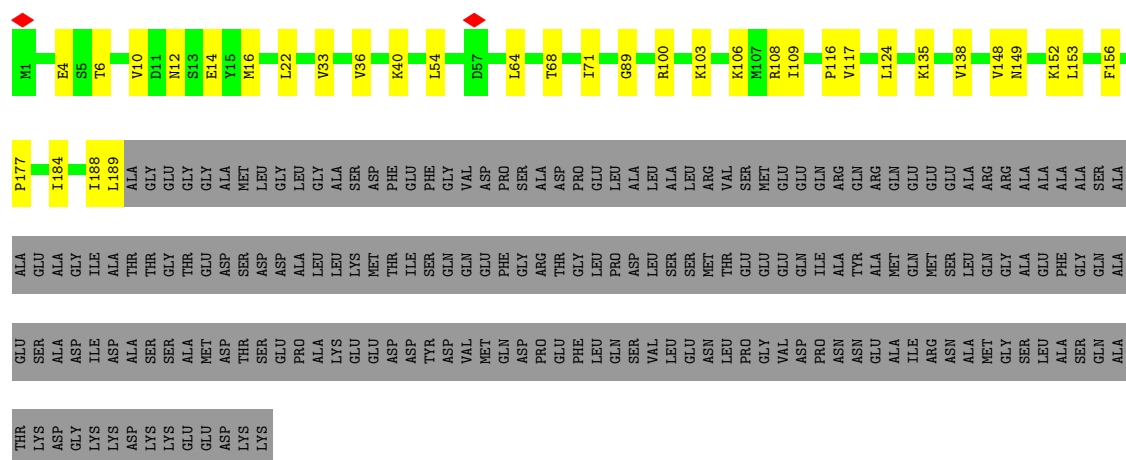


• Molecule 8: RPN6

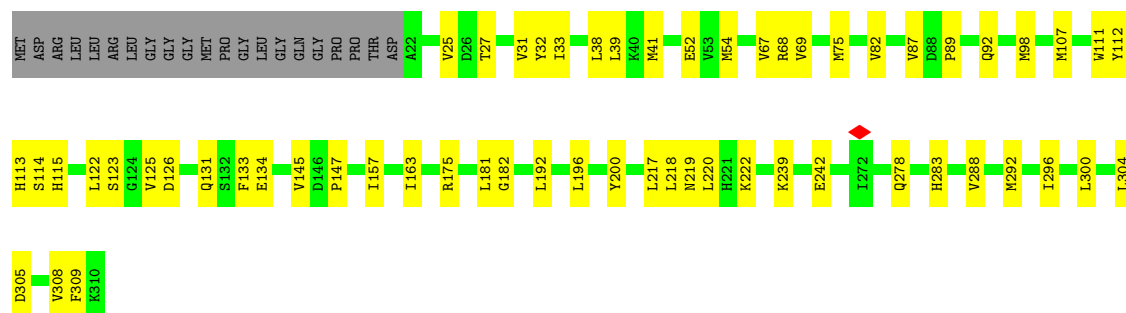




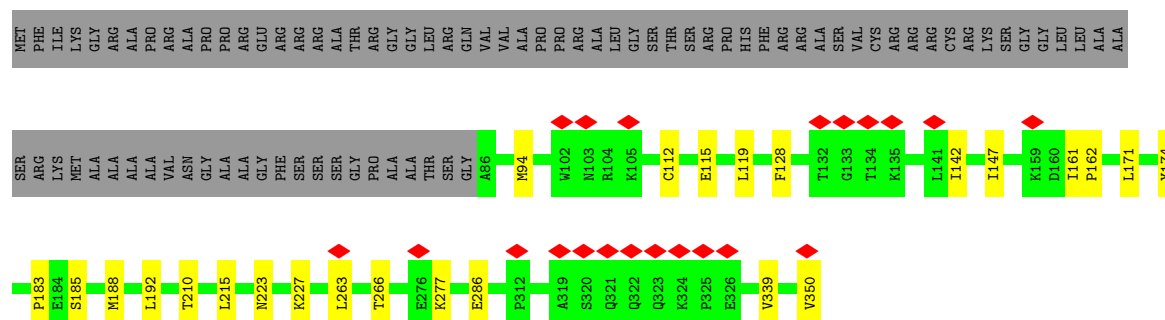
• Molecule 12: RPN10



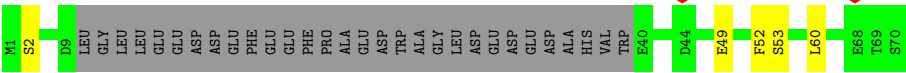
• Molecule 13: RPN11



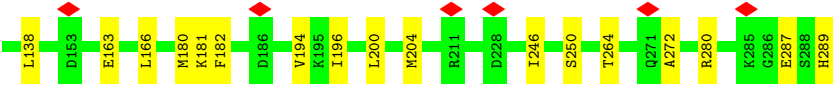
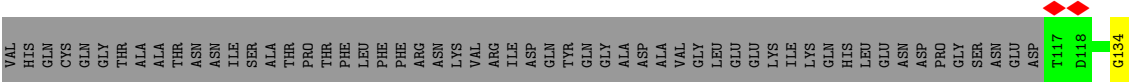
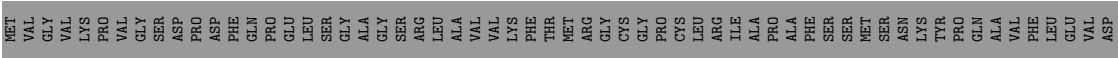
• Molecule 14: RPN12



• Molecule 15: DSS1



• Molecule 16: TXNL1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228010	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.348	Depositor
Minimum map value	-0.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	349.92, 349.92, 349.92	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.38	0/2949	0.71	0/3964
2	D	0.29	0/2982	0.61	0/4027
3	E	0.34	0/3071	0.73	0/4131
4	F	0.41	0/2982	0.77	0/4018
5	U	0.26	0/6589	0.57	0/8922
6	V	0.27	0/3811	0.61	0/5145
7	W	0.23	0/2645	0.58	0/3555
8	X	0.25	0/847	0.54	0/1139
9	Y	0.26	0/3173	0.59	0/4273
10	Z	0.27	0/2333	0.59	0/3162
11	a	0.32	0/3061	0.62	0/4144
12	b	0.32	0/1469	0.61	0/1989
13	c	0.25	0/2315	0.63	0/3129
14	d	0.31	0/2212	0.60	0/2988
15	e	0.27	0/338	0.64	0/450
16	g	0.24	0/1410	0.47	0/1902
All	All	0.30	0/42187	0.63	0/56938

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2912	0	3023	45	0
2	D	2935	0	2982	34	0
3	E	3025	0	3101	57	0
4	F	2945	0	3036	51	0
5	U	6472	0	6496	71	0
6	V	3739	0	3784	36	0
7	W	2605	0	2670	25	0
8	X	836	0	875	6	0
9	Y	3115	0	3120	39	0
10	Z	2290	0	2320	26	0
11	a	3003	0	3016	37	0
12	b	1449	0	1497	20	0
13	c	2272	0	2288	42	0
14	d	2166	0	2196	17	0
15	e	334	0	294	4	0
16	g	1383	0	1331	12	0
17	C	31	0	12	0	0
17	D	31	0	12	2	0
17	E	31	0	12	3	0
18	C	1	0	0	0	0
18	D	1	0	0	0	0
19	F	27	0	12	1	0
20	c	1	0	0	0	0
All	All	41604	0	42077	460	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 6.

All (460) 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)
13:c:113:HIS:HE2	13:c:115:HIS:CD2	1.97	0.82
5:U:583:MET:HE2	5:U:618:ALA:CB	2.13	0.79
3:E:206:LYS:HA	4:F:261:ILE:HG23	1.65	0.78
5:U:583:MET:HE1	5:U:602:LEU:HA	1.68	0.74
4:F:88:TYR:HE1	4:F:161:LEU:HD12	1.54	0.71
2:D:240:LEU:HD12	2:D:287:ARG:HH22	1.54	0.71
5:U:583:MET:HE2	5:U:618:ALA:HB1	1.71	0.69
10:Z:70:LEU:HD11	10:Z:108:ILE:HG23	1.76	0.68
3:E:335:SER:HB2	3:E:371:VAL:HG22	1.76	0.67
3:E:182:LEU:HA	3:E:185:ARG:HD2	1.76	0.66
1:C:71:SER:HB2	2:D:112:TYR:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:196:LEU:HD11	3:E:230:ILE:HG23	1.78	0.65
3:E:247:THR:H	3:E:250:ASP:HB2	1.62	0.65
5:U:619:VAL:HG21	5:U:648:VAL:HG13	1.80	0.64
11:a:56:LEU:HB2	11:a:86:GLN:HG3	1.80	0.63
5:U:616:ARG:HB2	5:U:647:HIS:HB3	1.80	0.63
3:E:210:GLU:O	3:E:214:LEU:HB2	1.99	0.62
6:V:162:GLU:HB3	6:V:175:MET:HB3	1.80	0.62
4:F:35:LYS:C	4:F:37:SER:H	2.07	0.62
12:b:36:VAL:HG12	12:b:189:LEU:HD11	1.82	0.61
1:C:249:ASP:HA	1:C:294:ALA:HB3	1.82	0.61
13:c:113:HIS:NE2	13:c:115:HIS:CD2	2.68	0.61
4:F:186:SER:HB2	4:F:364:ARG:NH2	2.16	0.61
9:Y:104:MET:HA	9:Y:107:LYS:HB2	1.83	0.60
11:a:74:LEU:HD13	11:a:109:GLU:HB3	1.82	0.60
3:E:322:LYS:HA	3:E:362:VAL:H	1.65	0.60
3:E:270:LEU:HD12	3:E:273:VAL:HG21	1.84	0.60
1:C:266:ASP:HB2	2:D:280:GLY:HA3	1.84	0.59
5:U:620:GLU:HG3	5:U:651:GLY:HA2	1.84	0.59
4:F:272:PHE:CD2	4:F:316:GLN:HB3	2.37	0.59
3:E:215:ILE:HA	3:E:218:MET:HG3	1.83	0.59
13:c:31:VAL:HG12	13:c:67:VAL:HB	1.84	0.59
11:a:360:VAL:HG22	13:c:308:VAL:HG13	1.84	0.59
1:C:69:GLN:HA	2:D:136:SER:HA	1.83	0.58
3:E:171:LEU:HB2	3:E:298:LYS:HA	1.84	0.58
2:D:231:VAL:HG12	2:D:233:SER:H	1.68	0.58
9:Y:237:ARG:O	9:Y:241:ILE:HB	2.03	0.58
1:C:355:SER:HB2	2:D:323:ARG:HH21	1.67	0.58
7:W:315:MET:HE1	7:W:361:HIS:HD2	1.69	0.58
4:F:73:ILE:HA	4:F:76:ASN:HB2	1.85	0.58
5:U:710:ARG:HG2	5:U:737:LEU:HD21	1.86	0.58
3:E:149:ILE:HD13	3:E:276:ILE:HD11	1.85	0.58
5:U:575:ASP:HB3	5:U:578:LEU:HB2	1.87	0.57
6:V:305:ALA:O	6:V:309:MET:HB2	2.05	0.56
11:a:18:GLN:HB2	11:a:19:PRO:HD3	1.86	0.56
6:V:296:LYS:HA	6:V:299:GLN:HG2	1.86	0.56
2:D:385:LEU:HD23	2:D:398:ASP:HA	1.87	0.56
1:C:221:GLN:HB2	1:C:226:GLU:HG3	1.88	0.56
1:C:72:TYR:HB2	1:C:116:LEU:HB2	1.88	0.56
11:a:267:GLN:O	11:a:271:LYS:HG2	2.05	0.56
10:Z:172:VAL:HG22	13:c:217:LEU:HD11	1.88	0.56
4:F:365:ILE:HA	4:F:368:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:LYS:HE2	3:E:267:PHE:HA	1.88	0.56
4:F:62:VAL:O	4:F:66:LEU:HB2	2.05	0.55
5:U:505:ASP:HB2	5:U:508:THR:HG22	1.88	0.55
5:U:486:MET:HE1	5:U:781:LEU:HD21	1.88	0.55
1:C:354:ALA:HB1	1:C:358:GLU:HB2	1.89	0.55
10:Z:40:LEU:HB3	10:Z:89:GLU:HB3	1.87	0.55
6:V:359:PRO:HG3	6:V:385:LYS:HD3	1.88	0.55
7:W:405:LYS:HD3	8:X:343:SER:HB3	1.89	0.55
6:V:70:VAL:HG21	15:e:2:SER:H	1.71	0.55
5:U:904:LYS:HE2	5:U:912:ILE:HG22	1.88	0.55
2:D:262:ILE:HB	2:D:307:VAL:HG23	1.88	0.55
7:W:209:ILE:HG22	7:W:211:THR:H	1.72	0.55
10:Z:9:VAL:HG12	10:Z:48:LEU:HB3	1.88	0.55
2:D:284:GLU:HA	2:D:287:ARG:HG2	1.88	0.54
5:U:376:MET:HE1	5:U:738:ASP:HB2	1.89	0.54
5:U:748:LEU:HD23	5:U:760:VAL:HG22	1.88	0.54
3:E:346:VAL:HG22	3:E:374:VAL:HG21	1.89	0.54
1:C:215:SER:HB2	1:C:218:GLU:HB2	1.90	0.54
13:c:25:VAL:HG23	13:c:175:ARG:HG2	1.89	0.54
9:Y:84:LEU:HB3	9:Y:107:LYS:HD3	1.89	0.54
5:U:719:ASP:HB3	5:U:722:ASP:HB2	1.88	0.54
13:c:131:GLN:HA	13:c:134:GLU:HG2	1.90	0.54
13:c:278:GLN:HB3	13:c:283:HIS:HE1	1.73	0.54
1:C:226:GLU:O	1:C:230:MET:HB2	2.08	0.54
12:b:103:LYS:HB2	16:g:134:GLY:HA2	1.90	0.54
3:E:372:ARG:HA	3:E:375:ALA:HB3	1.90	0.54
6:V:369:THR:HB	15:e:52:PHE:HZ	1.71	0.54
1:C:369:TYR:HA	1:C:372:ARG:HE	1.72	0.54
3:E:304:PRO:HD2	3:E:339:ASN:HA	1.88	0.54
4:F:186:SER:HB2	4:F:364:ARG:HH21	1.73	0.54
1:C:250:GLU:HB3	2:D:290:LEU:HD13	1.89	0.53
4:F:379:VAL:HG11	4:F:416:THR:HA	1.89	0.53
9:Y:221:THR:HG22	9:Y:256:VAL:HG21	1.90	0.53
3:E:355:ILE:HG21	4:F:204:LEU:HD21	1.91	0.53
7:W:167:GLN:HA	7:W:189:GLN:HE21	1.74	0.53
2:D:92:PHE:HA	2:D:103:VAL:HG12	1.90	0.53
4:F:260:PHE:HB2	4:F:263:ASP:HB2	1.89	0.53
5:U:756:HIS:HB3	5:U:759:SER:HB2	1.90	0.53
1:C:254:ILE:HG13	1:C:269:VAL:HB	1.90	0.53
3:E:230:ILE:HD13	3:E:273:VAL:HG13	1.89	0.53
3:E:233:ASP:HA	3:E:278:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HA	1:C:347:ILE:HD12	1.91	0.53
5:U:549:ALA:HA	5:U:581:SER:HB2	1.91	0.53
6:V:264:TYR:HB2	14:d:210:THR:HG23	1.91	0.53
6:V:452:ASN:HB3	6:V:457:TYR:HB2	1.90	0.53
14:d:142:ILE:HD11	14:d:183:PRO:HD2	1.91	0.53
3:E:142:ILE:HG12	3:E:183:LEU:HD11	1.91	0.53
3:E:359:HIS:HE1	3:E:363:VAL:HB	1.73	0.53
7:W:154:GLU:OE1	7:W:192:LEU:HD21	2.09	0.53
3:E:177:GLY:H	17:E:501:AGS:PB	2.32	0.52
13:c:54:MET:HB2	13:c:82:VAL:HG12	1.90	0.52
2:D:185:LEU:HB2	2:D:306:LYS:HE3	1.91	0.52
4:F:86:LEU:N	4:F:87:PRO:HD2	2.24	0.52
5:U:16:GLU:HG3	5:U:19:LEU:H	1.74	0.52
11:a:112:ILE:HG23	11:a:138:VAL:HG13	1.92	0.52
2:D:284:GLU:HG2	2:D:287:ARG:HE	1.74	0.52
6:V:227:VAL:HG22	6:V:231:LEU:HG	1.90	0.52
6:V:265:ASP:HB3	14:d:210:THR:HG21	1.91	0.52
2:D:202:VAL:HA	2:D:329:ARG:HB2	1.91	0.52
10:Z:77:ASN:ND2	13:c:98:MET:HE1	2.25	0.52
5:U:213:PHE:HB2	5:U:244:MET:HE2	1.91	0.52
9:Y:12:PRO:HD3	9:Y:176:ARG:HH21	1.74	0.52
12:b:22:LEU:HD23	12:b:177:PRO:HA	1.90	0.52
13:c:41:MET:HE3	13:c:112:TYR:HB2	1.90	0.52
4:F:381:TYR:HA	4:F:384:LEU:HB2	1.91	0.52
5:U:803:LYS:HE2	5:U:805:ASN:HB3	1.91	0.52
11:a:292:THR:HG22	11:a:330:ARG:HG2	1.92	0.52
5:U:160:LEU:HD21	5:U:197:VAL:HG22	1.91	0.52
11:a:225:LEU:HD11	11:a:230:ARG:HD2	1.92	0.52
11:a:324:ILE:HA	11:a:331:VAL:HG23	1.91	0.52
11:a:353:LEU:HD23	11:a:356:TRP:HE1	1.75	0.52
11:a:367:VAL:HG21	13:c:304:LEU:HD21	1.93	0.52
4:F:84:LYS:HG3	4:F:161:LEU:HD13	1.91	0.51
4:F:314:LEU:HD22	4:F:347:ARG:HD3	1.92	0.51
12:b:135:LYS:HG2	12:b:135:LYS:O	2.09	0.51
6:V:68:ASP:O	6:V:72:LEU:HB2	2.09	0.51
12:b:68:THR:HA	12:b:71:ILE:HD12	1.91	0.51
2:D:240:LEU:CD1	2:D:287:ARG:HH22	2.19	0.51
13:c:125:VAL:HB	16:g:289:HIS:CE1	2.46	0.51
1:C:86:LEU:HD11	1:C:94:LYS:HB3	1.92	0.51
1:C:277:LEU:HD12	1:C:310:ARG:HD3	1.93	0.51
2:D:87:LEU:HD22	2:D:133:HIS:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:84:ARG:HD3	3:E:108:MET:HG3	1.93	0.51
12:b:12:ASN:HA	12:b:16:MET:HG3	1.93	0.51
13:c:192:LEU:HD23	13:c:196:LEU:HB3	1.92	0.51
10:Z:65:ASP:HB3	10:Z:103:LYS:HB3	1.93	0.51
5:U:682:TYR:HA	5:U:685:GLN:HG2	1.93	0.51
13:c:145:VAL:HG23	13:c:157:ILE:HB	1.92	0.50
4:F:36:MET:HA	4:F:36:MET:HE2	1.92	0.50
1:C:332:HIS:O	1:C:336:MET:HB2	2.12	0.50
10:Z:94:TRP:CD1	10:Z:112:MET:HG3	2.46	0.50
11:a:201:GLY:HA3	11:a:233:LEU:HD21	1.92	0.50
3:E:320:ILE:HD12	4:F:217:ILE:HG22	1.93	0.50
13:c:54:MET:HE1	13:c:111:TRP:HB2	1.92	0.50
5:U:633:CYS:O	5:U:637:VAL:HB	2.11	0.50
11:a:217:LEU:HD21	11:a:237:LEU:HB3	1.92	0.50
17:D:501:AGS:S1G	3:E:294:ARG:NH2	2.85	0.50
3:E:322:LYS:HD2	3:E:326:ILE:HG13	1.94	0.50
3:E:328:TYR:HA	3:E:331:ILE:HD12	1.94	0.50
9:Y:297:ARG:HA	9:Y:300:ARG:HE	1.75	0.50
16:g:196:ILE:HG12	16:g:246:ILE:HG12	1.94	0.50
3:E:216:ARG:HA	3:E:263:GLN:HE22	1.77	0.49
10:Z:131:LEU:HD11	10:Z:200:GLY:HA2	1.94	0.49
9:Y:319:MET:HA	9:Y:322:ALA:HB3	1.93	0.49
10:Z:14:LEU:HD12	13:c:39:LEU:HB3	1.94	0.49
15:e:49:GLU:HG2	15:e:53:SER:HB2	1.94	0.49
4:F:93:VAL:HG21	4:F:145:LEU:HD11	1.94	0.49
4:F:232:GLY:HA2	19:F:501:ADP:H3'	1.94	0.49
5:U:410:VAL:HG13	5:U:780:SER:HB3	1.94	0.49
12:b:188:ILE:HG13	12:b:189:LEU:HD12	1.93	0.49
13:c:218:LEU:O	13:c:222:LYS:HB2	2.12	0.49
1:C:138:MET:HB3	1:C:212:ILE:HG23	1.95	0.49
4:F:175:MET:HE1	4:F:251:LEU:HB2	1.95	0.49
6:V:290:TYR:HD1	6:V:309:MET:HE1	1.77	0.49
10:Z:212:LEU:HD22	11:a:350:LYS:HB2	1.93	0.49
5:U:141:CYS:HB3	5:U:150:ALA:HB2	1.95	0.49
5:U:611:ASN:HB3	5:U:614:VAL:HG12	1.94	0.49
5:U:675:MET:HE3	5:U:683:VAL:HG13	1.95	0.49
10:Z:234:PHE:CE1	11:a:352:ARG:HB3	2.48	0.49
7:W:412:ILE:HG23	11:a:327:VAL:HG21	1.95	0.49
4:F:251:LEU:HD11	4:F:256:LEU:HD21	1.95	0.49
11:a:60:TYR:HA	11:a:64:ILE:HB	1.95	0.49
3:E:270:LEU:HB3	3:E:273:VAL:HB	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:450:HIS:HB3	5:U:454:GLY:HA2	1.94	0.48
4:F:314:LEU:HD21	4:F:342:LEU:HD23	1.95	0.48
5:U:623:GLY:HA2	5:U:659:CYS:HB2	1.95	0.48
7:W:405:LYS:HB3	8:X:343:SER:HB3	1.96	0.48
7:W:435:LEU:HD22	13:c:309:PHE:HE1	1.78	0.48
3:E:199:VAL:HG12	3:E:201:SER:H	1.77	0.48
7:W:254:PRO:HA	7:W:257:GLN:HB2	1.94	0.48
16:g:163:GLU:HG3	16:g:250:SER:HA	1.94	0.48
11:a:123:LEU:HD13	11:a:131:THR:HG21	1.96	0.48
3:E:132:TYR:HE1	3:E:142:ILE:HG21	1.79	0.48
8:X:368:MET:HG2	8:X:373:LYS:HG3	1.95	0.48
14:d:171:LEU:HA	14:d:174:TYR:HD2	1.79	0.48
11:a:109:GLU:HA	11:a:112:ILE:HD12	1.96	0.48
12:b:6:THR:HG22	12:b:108:ARG:HB3	1.94	0.48
3:E:198:VAL:HG13	3:E:232:MET:HG3	1.95	0.48
12:b:4:GLU:HA	12:b:106:LYS:H	1.78	0.48
2:D:345:PHE:HA	2:D:348:ILE:HG22	1.96	0.47
9:Y:51:ALA:HB3	9:Y:52:PRO:HD3	1.95	0.47
1:C:307:ARG:HB2	1:C:310:ARG:HD2	1.97	0.47
1:C:337:ASN:HB2	2:D:194:ILE:HA	1.96	0.47
4:F:35:LYS:C	4:F:37:SER:N	2.72	0.47
4:F:151:VAL:HG12	4:F:163:THR:HG23	1.95	0.47
5:U:802:TYR:HB3	5:U:892:LEU:HD11	1.95	0.47
2:D:168:GLY:HA2	2:D:347:THR:HG21	1.96	0.47
5:U:545:LEU:HB3	5:U:577:ILE:HG21	1.96	0.47
7:W:163:ALA:O	7:W:167:GLN:HB2	2.15	0.47
7:W:395:ASN:O	7:W:399:ASN:HB2	2.14	0.47
11:a:113:LEU:HD13	11:a:151:VAL:HG23	1.97	0.47
16:g:200:LEU:HD22	16:g:204:MET:HE3	1.95	0.47
3:E:181:THR:OG1	17:E:501:AGS:S1G	2.72	0.47
5:U:605:VAL:O	5:U:609:ASP:HB2	2.15	0.47
4:F:169:ASP:HB3	4:F:172:VAL:HG23	1.96	0.47
4:F:224:LEU:HB2	4:F:348:LEU:HG	1.96	0.47
5:U:900:TYR:HB3	5:U:914:LEU:HB3	1.96	0.47
11:a:8:LEU:HD13	11:a:26:GLU:HA	1.97	0.47
13:c:122:LEU:HD22	13:c:126:ASP:HB3	1.97	0.47
14:d:192:LEU:HD13	14:d:215:LEU:HD11	1.96	0.47
3:E:312:ILE:HD12	17:E:501:AGS:N1	2.29	0.47
4:F:310:MET:HG3	4:F:311:LEU:N	2.30	0.47
5:U:432:SER:HB3	5:U:435:SER:HB2	1.97	0.47
5:U:491:GLN:HA	5:U:494:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:421:PRO:HB2	10:Z:252:LYS:HE3	1.97	0.47
1:C:347:ILE:HA	1:C:350:LEU:HD12	1.97	0.47
2:D:372:GLY:C	17:D:501:AGS:H1'	2.39	0.47
5:U:249:CYS:HA	5:U:252:LEU:HD12	1.96	0.47
9:Y:16:ASP:HB2	9:Y:48:ASN:ND2	2.30	0.47
16:g:180:MET:HE2	16:g:182:PHE:HB2	1.96	0.46
2:D:116:LEU:HD23	2:D:118:THR:H	1.79	0.46
3:E:171:LEU:HB3	3:E:173:TYR:HD2	1.80	0.46
9:Y:247:LEU:HA	9:Y:250:LEU:HG	1.97	0.46
11:a:222:LEU:HD12	11:a:234:ILE:HG12	1.98	0.46
13:c:163:ILE:H	13:c:200:TYR:HA	1.79	0.46
3:E:81:VAL:HG12	3:E:105:LEU:HB3	1.98	0.46
12:b:116:PRO:HB3	12:b:148:VAL:HG11	1.97	0.46
6:V:94:VAL:HG13	6:V:142:GLU:HB2	1.97	0.46
1:C:49:ARG:HD2	5:U:639:LEU:HD13	1.98	0.46
4:F:180:ARG:HD2	4:F:242:ALA:HA	1.98	0.46
4:F:180:ARG:HE	4:F:245:LYS:HA	1.80	0.46
4:F:301:ALA:HA	4:F:304:ARG:HG2	1.97	0.46
8:X:377:ILE:HG12	9:Y:312:ARG:HB2	1.97	0.46
12:b:10:VAL:HG12	12:b:33:VAL:HG21	1.97	0.46
10:Z:15:VAL:HG13	10:Z:53:SER:HB2	1.98	0.46
1:C:44:ARG:CZ	6:V:492:LYS:HA	2.46	0.46
1:C:214:VAL:CG1	1:C:219:LEU:HD21	2.46	0.46
4:F:78:GLU:O	4:F:81:LYS:HG2	2.16	0.46
5:U:357:LYS:HD2	5:U:389:ASN:HD22	1.80	0.46
10:Z:209:ARG:HD2	11:a:354:GLU:HB3	1.98	0.46
12:b:54:LEU:HD12	12:b:89:GLY:HA3	1.97	0.46
14:d:119:LEU:HD21	14:d:147:ILE:HG12	1.98	0.46
10:Z:212:LEU:HD13	11:a:353:LEU:HD12	1.98	0.46
9:Y:131:THR:HG21	9:Y:137:ARG:HG2	1.98	0.46
2:D:231:VAL:HB	2:D:234:GLU:HB2	1.98	0.45
5:U:522:GLY:HA2	5:U:557:TYR:H	1.82	0.45
9:Y:53:TYR:C	9:Y:53:TYR:CD2	2.94	0.45
13:c:288:VAL:O	13:c:292:MET:HB2	2.17	0.45
13:c:304:LEU:O	13:c:308:VAL:HB	2.16	0.45
2:D:64:GLU:HA	5:U:607:VAL:HG11	1.98	0.45
4:F:259:MET:SD	4:F:259:MET:N	2.89	0.45
5:U:94:SER:HB3	5:U:97:VAL:HG12	1.98	0.45
6:V:135:LEU:HG	6:V:178:SER:HB2	1.99	0.45
6:V:147:PHE:HB2	6:V:150:ARG:HB3	1.97	0.45
6:V:289:LEU:HA	6:V:292:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:HD22	2:D:54:LEU:HG	1.98	0.45
5:U:725:MET:HA	5:U:728:PHE:HB3	1.98	0.45
6:V:33:GLN:CD	6:V:81:GLN:HA	2.42	0.45
9:Y:268:TYR:HA	9:Y:271:PHE:HB3	1.98	0.45
2:D:60:TYR:CD1	5:U:603:LEU:HB3	2.52	0.45
2:D:383:GLY:HA3	3:E:164:ILE:HD13	1.99	0.45
6:V:29:PRO:HB2	6:V:30:PRO:HD3	1.98	0.45
9:Y:101:ARG:HA	9:Y:101:ARG:HD2	1.77	0.45
5:U:636:VAL:HG13	5:U:637:VAL:HG23	1.99	0.45
1:C:69:GLN:H	1:C:118:ASN:HD22	1.63	0.45
1:C:85:VAL:HG11	1:C:108:VAL:HG11	1.97	0.45
1:C:99:VAL:HA	1:C:123:LEU:HB2	1.98	0.45
2:D:101:ALA:HB2	2:D:115:ILE:HD11	1.99	0.45
6:V:94:VAL:HG21	6:V:138:PRO:HG3	1.99	0.45
9:Y:16:ASP:HB2	9:Y:48:ASN:HD22	1.81	0.45
13:c:114:SER:HB2	13:c:147:PRO:HD3	1.97	0.45
6:V:159:LEU:HA	6:V:162:GLU:HB2	1.98	0.45
12:b:149:ASN:HB3	12:b:153:LEU:HD12	1.97	0.45
5:U:746:ILE:HG23	5:U:782:ALA:HB1	1.99	0.45
12:b:6:THR:HG21	12:b:40:LYS:HE3	1.98	0.45
16:g:138:LEU:HD12	16:g:166:LEU:HD23	1.98	0.45
2:D:387:VAL:HG21	3:E:158:LEU:HD21	1.99	0.45
1:C:221:GLN:HB2	1:C:226:GLU:CG	2.48	0.44
5:U:194:ARG:HG2	5:U:198:LEU:HD23	2.00	0.44
5:U:628:ARG:HH21	5:U:755:THR:HB	1.82	0.44
11:a:214:GLY:HA3	11:a:340:VAL:HB	2.00	0.44
4:F:35:LYS:O	4:F:37:SER:N	2.47	0.44
5:U:362:ASN:HD22	5:U:724:VAL:HG21	1.82	0.44
7:W:224:LEU:HD22	7:W:250:ILE:HG23	1.99	0.44
9:Y:314:LEU:HG	9:Y:319:MET:HE3	2.00	0.44
11:a:219:HIS:HD2	11:a:221:VAL:HG22	1.82	0.44
11:a:281:THR:HB	11:a:291:LEU:HD11	1.99	0.44
14:d:161:ILE:N	14:d:162:PRO:HD2	2.32	0.44
4:F:227:GLY:HA3	4:F:354:PHE:HB2	2.00	0.44
7:W:432:LEU:HD21	10:Z:238:PRO:HG3	1.99	0.44
16:g:194:VAL:HG13	16:g:246:ILE:HG23	1.99	0.44
1:C:277:LEU:CD1	1:C:310:ARG:HD3	2.46	0.44
6:V:97:ALA:H	6:V:107:ARG:HG3	1.82	0.44
6:V:303:SER:HA	6:V:306:ARG:HE	1.82	0.44
7:W:359:VAL:HB	7:W:382:LEU:HD22	1.99	0.44
10:Z:175:LEU:HD11	13:c:38:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:117:VAL:HB	12:b:152:LYS:HD2	1.99	0.44
13:c:219:ASN:HA	13:c:222:LYS:HB3	1.98	0.44
9:Y:35:ALA:HB1	9:Y:37:VAL:HG12	1.99	0.44
9:Y:149:LEU:HG	9:Y:286:TRP:HH2	1.83	0.44
10:Z:172:VAL:HG11	13:c:220:LEU:HD23	1.99	0.44
13:c:33:ILE:HA	13:c:69:VAL:HB	1.99	0.44
14:d:112:CYS:HA	14:d:115:GLU:HB2	1.99	0.44
5:U:691:SER:O	5:U:695:MET:HB2	2.18	0.44
6:V:84:LYS:HA	6:V:125:ASN:HB2	1.99	0.44
7:W:425:LEU:HD22	10:Z:252:LYS:HG3	2.00	0.44
9:Y:53:TYR:C	9:Y:53:TYR:HD2	2.25	0.44
1:C:45:LEU:HB3	2:D:61:ILE:HG21	1.99	0.44
3:E:201:SER:HB2	4:F:308:ARG:HB3	1.98	0.44
5:U:509:GLY:HA3	5:U:544:ILE:HG12	1.99	0.44
11:a:278:MET:HA	11:a:281:THR:HG22	1.98	0.44
14:d:94:MET:HG3	14:d:119:LEU:HD13	2.00	0.44
3:E:100:LEU:HG	3:E:107:ILE:HG13	2.00	0.44
5:U:367:THR:HA	5:U:370:VAL:HG22	2.00	0.44
5:U:772:TRP:HD1	5:U:775:LEU:HG	1.82	0.44
5:U:11:LEU:HD11	14:d:128:PHE:HE2	1.83	0.43
5:U:693:LEU:HD23	5:U:736:ILE:HG21	2.00	0.43
6:V:179:LYS:HE2	6:V:179:LYS:HB2	1.90	0.43
10:Z:40:LEU:HB2	10:Z:52:ASN:HB3	1.99	0.43
11:a:131:THR:O	11:a:135:ILE:HG12	2.18	0.43
5:U:685:GLN:HB2	5:U:729:GLY:HA3	1.99	0.43
7:W:309:PHE:HB3	7:W:357:ARG:HH12	1.83	0.43
9:Y:22:LEU:HB3	9:Y:37:VAL:HG21	1.98	0.43
9:Y:190:ALA:HB2	9:Y:287:LEU:HD22	2.00	0.43
9:Y:52:PRO:C	9:Y:54:TYR:N	2.77	0.43
1:C:303:SER:HA	1:C:306:LEU:HB2	2.01	0.43
5:U:269:ARG:HB3	5:U:326:ILE:HD11	2.00	0.43
5:U:614:VAL:O	5:U:618:ALA:HB2	2.18	0.43
5:U:894:MET:HE3	5:U:895:PRO:HD2	2.01	0.43
12:b:64:LEU:HD21	12:b:100:ARG:HG2	2.00	0.43
13:c:32:TYR:HB2	13:c:68:ARG:HA	2.00	0.43
3:E:152:PRO:HB3	3:E:166:PRO:HB3	2.00	0.43
9:Y:316:LEU:HD12	9:Y:352:GLU:HA	2.00	0.43
4:F:150:LEU:H	4:F:166:THR:HG22	1.83	0.43
4:F:260:PHE:HB2	4:F:263:ASP:CB	2.49	0.43
6:V:353:LEU:HB3	6:V:357:LEU:HD12	2.01	0.43
11:a:112:ILE:HG21	11:a:142:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:87:VAL:HG21	13:c:133:PHE:HZ	1.83	0.43
13:c:89:PRO:HA	13:c:92:GLN:HE21	1.83	0.43
14:d:223:ASN:O	14:d:227:LYS:HB2	2.18	0.43
1:C:164:VAL:HG21	1:C:186:VAL:HG21	2.01	0.43
9:Y:101:ARG:HH21	9:Y:131:THR:HG22	1.84	0.43
6:V:273:LYS:HA	6:V:273:LYS:HD3	1.85	0.43
6:V:309:MET:HE3	6:V:328:VAL:HG13	2.01	0.43
9:Y:45:VAL:HG22	9:Y:50:MET:HB2	2.01	0.43
9:Y:128:TYR:HA	9:Y:131:THR:HG23	2.01	0.43
13:c:305:ASP:O	13:c:309:PHE:HB2	2.19	0.43
2:D:384:MET:HA	2:D:387:VAL:HG22	2.00	0.43
5:U:494:TYR:HB2	5:U:520:MET:HE3	2.01	0.43
6:V:179:LYS:HE3	6:V:212:TYR:HA	2.00	0.43
13:c:27:THR:HB	13:c:182:GLY:HA3	2.01	0.43
13:c:239:LYS:HA	13:c:242:GLU:HG2	2.01	0.43
9:Y:52:PRO:HA	9:Y:54:TYR:CE1	2.53	0.43
4:F:219:PRO:HA	4:F:220:PRO:HD3	1.88	0.42
10:Z:48:LEU:HD11	10:Z:92:VAL:HG11	2.00	0.42
13:c:300:LEU:HB2	14:d:339:VAL:HG11	2.00	0.42
1:C:97:VAL:HG11	1:C:116:LEU:HD11	2.01	0.42
3:E:148:VAL:HG12	3:E:149:ILE:HG23	2.02	0.42
4:F:322:PRO:HB2	4:F:324:THR:HG23	2.02	0.42
5:U:490:ARG:HB3	5:U:493:VAL:HG12	2.01	0.42
9:Y:276:ALA:HB1	15:e:60:LEU:HD12	2.02	0.42
2:D:200:ARG:HD3	2:D:303:VAL:HA	2.00	0.42
5:U:536:ALA:HB1	5:U:578:LEU:HD21	2.01	0.42
11:a:35:HIS:CE1	12:b:14:GLU:HB3	2.54	0.42
11:a:131:THR:O	11:a:134:THR:HG22	2.18	0.42
13:c:292:MET:HE3	13:c:296:ILE:HD11	2.01	0.42
1:C:217:SER:OG	2:D:291:GLU:HB2	2.19	0.42
1:C:251:ILE:HG23	1:C:301:LEU:HD11	2.02	0.42
3:E:239:GLY:HA2	3:E:257:LEU:HD12	2.01	0.42
3:E:305:ASN:O	3:E:309:ARG:HG3	2.20	0.42
3:E:330:ALA:HA	3:E:333:LYS:HZ2	1.84	0.42
7:W:146:THR:HG23	7:W:165:ILE:HG22	2.00	0.42
4:F:365:ILE:HD13	4:F:393:GLY:HA2	2.01	0.42
5:U:645:ASN:HA	5:U:646:PRO:HD3	1.91	0.42
6:V:476:PHE:HA	6:V:479:ARG:HB2	2.01	0.42
7:W:373:ILE:HA	11:a:326:GLU:HB3	2.01	0.42
6:V:209:LYS:HZ3	6:V:234:ARG:HB3	1.85	0.42
7:W:161:GLU:O	7:W:165:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:228:ASN:HA	7:W:231:ILE:HD12	2.02	0.42
14:d:185:SER:HB3	14:d:188:MET:HB2	2.02	0.42
5:U:658:ILE:HD11	5:U:767:THR:HG21	2.01	0.42
9:Y:377:LEU:HD23	9:Y:377:LEU:HA	1.92	0.42
3:E:29:LEU:HB3	4:F:62:VAL:HG11	2.02	0.42
5:U:184:CYS:HA	5:U:188:MET:HE2	2.02	0.42
5:U:532:MET:HG2	5:U:552:ILE:HD11	2.02	0.42
12:b:124:LEU:HD21	12:b:156:PHE:HB2	2.02	0.42
3:E:316:HIS:HB3	3:E:347:CYS:SG	2.60	0.42
4:F:151:VAL:HA	4:F:164:LEU:H	1.85	0.42
9:Y:186:LEU:HD12	9:Y:286:TRP:HZ3	1.85	0.42
10:Z:144:VAL:HA	10:Z:151:THR:HG21	2.02	0.42
1:C:337:ASN:ND2	1:C:376:VAL:O	2.52	0.41
4:F:285:ILE:HG21	4:F:288:LEU:HD12	2.02	0.41
4:F:366:MET:HE3	4:F:381:TYR:HB3	2.02	0.41
9:Y:165:LYS:HA	9:Y:168:ILE:HG12	2.02	0.41
14:d:277:LYS:HD3	14:d:277:LYS:H	1.85	0.41
1:C:185:GLY:HA3	1:C:311:ILE:HA	2.03	0.41
1:C:320:PRO:HB2	1:C:325:ARG:HG3	2.02	0.41
11:a:353:LEU:O	11:a:356:TRP:HD1	2.03	0.41
13:c:52:GLU:HB3	13:c:82:VAL:HG13	2.02	0.41
14:d:263:LEU:HA	14:d:266:THR:HG22	2.03	0.41
4:F:190:GLY:HA3	4:F:361:ALA:HB2	2.01	0.41
4:F:426:GLU:HA	4:F:429:ALA:HA	2.02	0.41
8:X:421:LEU:HD21	9:Y:387:ILE:HD11	2.03	0.41
9:Y:261:PHE:O	9:Y:265:GLU:HB2	2.20	0.41
9:Y:282:MET:SD	9:Y:288:PHE:HB3	2.60	0.41
3:E:122:MET:HE1	3:E:196:LEU:HD13	2.03	0.41
10:Z:15:VAL:HG21	10:Z:50:VAL:HG12	2.02	0.41
1:C:221:GLN:HB2	1:C:226:GLU:CD	2.45	0.41
3:E:234:GLU:CD	4:F:311:LEU:HD13	2.45	0.41
6:V:491:VAL:HA	6:V:494:MET:HE3	2.02	0.41
11:a:245:VAL:HG21	11:a:300:ALA:HA	2.02	0.41
3:E:212:ALA:O	3:E:216:ARG:HB2	2.21	0.41
3:E:307:GLN:O	3:E:310:LEU:HB3	2.20	0.41
7:W:363:ILE:HD11	7:W:382:LEU:HD11	2.02	0.41
11:a:240:PHE:HZ	11:a:271:LYS:HB3	1.86	0.41
12:b:184:ILE:HA	12:b:189:LEU:HD22	2.03	0.41
1:C:277:LEU:HA	1:C:280:LEU:HG	2.03	0.41
3:E:135:ILE:HD13	3:E:183:LEU:HD22	2.01	0.41
3:E:148:VAL:HG11	3:E:170:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:392:ASN:HB2	4:F:395:GLN:H	1.86	0.41
5:U:771:PHE:HD1	13:c:181:LEU:HD11	1.84	0.41
7:W:273:TYR:CE2	7:W:340:VAL:HG22	2.56	0.41
9:Y:101:ARG:HE	9:Y:131:THR:HA	1.85	0.41
9:Y:275:LEU:HD11	9:Y:296:VAL:HG23	2.02	0.41
16:g:181:LYS:HB2	16:g:264:THR:HG22	2.03	0.41
1:C:281:ASP:OD2	1:C:310:ARG:HG2	2.21	0.41
3:E:20:LYS:HD3	3:E:20:LYS:HA	1.88	0.41
3:E:182:LEU:HD12	3:E:185:ARG:HD2	2.03	0.41
4:F:153:VAL:HG22	4:F:160:ILE:HA	2.03	0.41
5:U:633:CYS:HA	5:U:636:VAL:HG12	2.03	0.41
11:a:72:ASN:HA	11:a:73:PRO:HD3	1.95	0.41
13:c:123:SER:HB3	16:g:289:HIS:CE1	2.56	0.41
6:V:306:ARG:HD2	6:V:336:GLU:HG2	2.01	0.41
6:V:491:VAL:HB	14:d:350:VAL:HG11	2.03	0.41
10:Z:74:TYR:CE2	13:c:98:MET:HB3	2.56	0.41
10:Z:205:LEU:HD23	10:Z:205:LEU:HA	1.85	0.41
6:V:453:HIS:CE1	14:d:286:GLU:HG2	2.56	0.40
12:b:109:ILE:HB	12:b:138:VAL:HG22	2.03	0.40
13:c:75:MET:HE3	13:c:87:VAL:HG22	2.03	0.40
16:g:280:ARG:HH22	16:g:287:GLU:HB2	1.85	0.40
7:W:268:LYS:HB2	7:W:268:LYS:HE3	1.92	0.40
13:c:107:MET:HE3	16:g:272:ALA:HA	2.03	0.40
1:C:44:ARG:HG3	6:V:494:MET:HB2	2.02	0.40
2:D:363:TYR:HE1	2:D:400:GLU:HG2	1.87	0.40
3:E:171:LEU:HD11	3:E:290:LEU:HD22	2.04	0.40
3:E:175:PRO:HD2	3:E:301:ILE:O	2.22	0.40
4:F:401:VAL:HG13	4:F:405:MET:HE3	2.03	0.40
5:U:176:MET:HE1	5:U:179:TYR:HD2	1.86	0.40
7:W:377:ARG:HD2	7:W:377:ARG:HA	1.92	0.40
8:X:420:LYS:HE3	10:Z:280:ILE:HD12	2.03	0.40
9:Y:21:GLN:HB3	9:Y:286:TRP:HB2	2.03	0.40
1:C:46:GLN:HG2	5:U:639:LEU:HD11	2.03	0.40
1:C:77:VAL:O	1:C:78:ARG:HG3	2.22	0.40
3:E:184:ALA:HA	3:E:187:VAL:HG12	2.04	0.40
5:U:368:ALA:HB1	5:U:731:ILE:HB	2.04	0.40
5:U:756:HIS:CD2	5:U:758:PRO:HD2	2.57	0.40
5:U:772:TRP:CD1	5:U:775:LEU:HG	2.57	0.40
9:Y:50:MET:HB3	9:Y:53:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	366/406 (90%)	342 (93%)	24 (7%)	0	100	100
2	D	367/418 (88%)	343 (94%)	24 (6%)	0	100	100
3	E	378/389 (97%)	355 (94%)	23 (6%)	0	100	100
4	F	372/439 (85%)	347 (93%)	25 (7%)	0	100	100
5	U	825/953 (87%)	793 (96%)	32 (4%)	0	100	100
6	V	460/534 (86%)	429 (93%)	31 (7%)	0	100	100
7	W	315/456 (69%)	306 (97%)	9 (3%)	0	100	100
8	X	102/422 (24%)	102 (100%)	0	0	100	100
9	Y	376/389 (97%)	352 (94%)	24 (6%)	0	100	100
10	Z	285/324 (88%)	276 (97%)	9 (3%)	0	100	100
11	a	372/376 (99%)	358 (96%)	14 (4%)	0	100	100
12	b	187/377 (50%)	174 (93%)	13 (7%)	0	100	100
13	c	287/310 (93%)	275 (96%)	12 (4%)	0	100	100
14	d	263/350 (75%)	253 (96%)	10 (4%)	0	100	100
15	e	36/70 (51%)	33 (92%)	3 (8%)	0	100	100
16	g	171/289 (59%)	165 (96%)	6 (4%)	0	100	100
All	All	5162/6502 (79%)	4903 (95%)	259 (5%)	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	C	321/352 (91%)	319 (99%)	2 (1%)	78	87
2	D	322/366 (88%)	321 (100%)	1 (0%)	86	90
3	E	333/341 (98%)	332 (100%)	1 (0%)	86	90
4	F	325/379 (86%)	319 (98%)	6 (2%)	51	76
5	U	707/816 (87%)	707 (100%)	0	100	100
6	V	401/460 (87%)	401 (100%)	0	100	100
7	W	292/416 (70%)	292 (100%)	0	100	100
8	X	96/362 (26%)	96 (100%)	0	100	100
9	Y	334/344 (97%)	332 (99%)	2 (1%)	78	87
10	Z	258/295 (88%)	258 (100%)	0	100	100
11	a	334/336 (99%)	334 (100%)	0	100	100
12	b	167/312 (54%)	167 (100%)	0	100	100
13	c	253/268 (94%)	253 (100%)	0	100	100
14	d	235/294 (80%)	235 (100%)	0	100	100
15	e	38/63 (60%)	38 (100%)	0	100	100
16	g	157/253 (62%)	157 (100%)	0	100	100
All	All	4573/5657 (81%)	4561 (100%)	12 (0%)	84	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	217	SER
1	C	342	ILE
2	D	351	LYS
3	E	303	LEU
4	F	36	MET
4	F	86	LEU
4	F	257	VAL
4	F	261	ILE
4	F	313	LEU
4	F	315	ASN
9	Y	50	MET
9	Y	53	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	102	ASN
1	C	118	ASN
1	C	296	ASN
1	C	392	GLN
2	D	193	GLN
2	D	221	HIS
2	D	222	HIS
2	D	312	ASN
2	D	380	GLN
3	E	10	GLN
3	E	194	ASN
3	E	263	GLN
3	E	271	HIS
4	F	208	HIS
5	U	28	ASN
5	U	149	GLN
5	U	218	GLN
5	U	258	GLN
5	U	596	ASN
5	U	734	GLN
5	U	749	GLN
6	V	257	ASN
6	V	282	ASN
6	V	473	GLN
7	W	361	HIS
7	W	380	GLN
7	W	453	HIS
9	Y	77	ASN
9	Y	160	ASN
10	Z	77	ASN
10	Z	277	ASN
11	a	264	ASN
12	b	158	ASN
13	c	185	ASN
13	c	206	ASN
13	c	278	GLN
13	c	283	HIS
14	d	103	ASN
14	d	140	GLN
14	d	190	GLN
15	e	55	GLN
16	g	144	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
17	AGS	E	501	-	32,33,33	0.65	1 (3%)	45,52,52	0.56	0
17	AGS	C	501	18	32,33,33	0.67	1 (3%)	45,52,52	0.54	0
17	AGS	D	501	18	32,33,33	0.67	1 (3%)	45,52,52	0.60	0
19	ADP	F	501	-	28,29,29	1.37	3 (10%)	43,45,45	1.96	10 (23%)

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
17	AGS	E	501	-	-	4/21/38/38	0/3/3/3
17	AGS	C	501	18	-	0/21/38/38	0/3/3/3
17	AGS	D	501	18	-	1/21/38/38	0/3/3/3
19	ADP	F	501	-	-	4/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	501	ADP	C5-C4	4.58	1.47	1.39
19	F	501	ADP	C5-C6	2.57	1.48	1.41
19	F	501	ADP	C5-N7	-2.53	1.34	1.39
17	D	501	AGS	PG-S1G	2.22	1.95	1.90
17	C	501	AGS	PG-S1G	2.15	1.95	1.90
17	E	501	AGS	PG-S1G	2.01	1.95	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	501	ADP	C5-C4-N3	-6.10	118.31	126.72
19	F	501	ADP	N3-C4-N9	5.07	135.80	127.17
19	F	501	ADP	C2-N3-C4	3.87	121.28	111.83
19	F	501	ADP	N3-C2-N1	-3.34	123.52	128.58
19	F	501	ADP	C4-C5-N7	-3.25	106.86	110.58
19	F	501	ADP	C2'-C1'-N9	-2.97	105.93	113.30
19	F	501	ADP	C4-N9-C8	2.63	108.50	105.74
19	F	501	ADP	C3'-C2'-C1'	2.56	106.31	101.46
19	F	501	ADP	C5-N7-C8	2.45	107.30	103.45
19	F	501	ADP	O3A-PA-O1A	-2.12	104.33	110.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	F	501	ADP	O4'-C4'-C5'-O5'
17	E	501	AGS	PG-O3B-PB-O1B
19	F	501	ADP	PB-O3A-PA-O2A
19	F	501	ADP	C3'-C4'-C5'-O5'
17	E	501	AGS	PG-O3B-PB-O2B
17	E	501	AGS	PB-O3A-PA-O2A
19	F	501	ADP	PB-O3A-PA-O1A
17	E	501	AGS	C2'-C1'-N9-C8
17	D	501	AGS	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 6 short contacts:

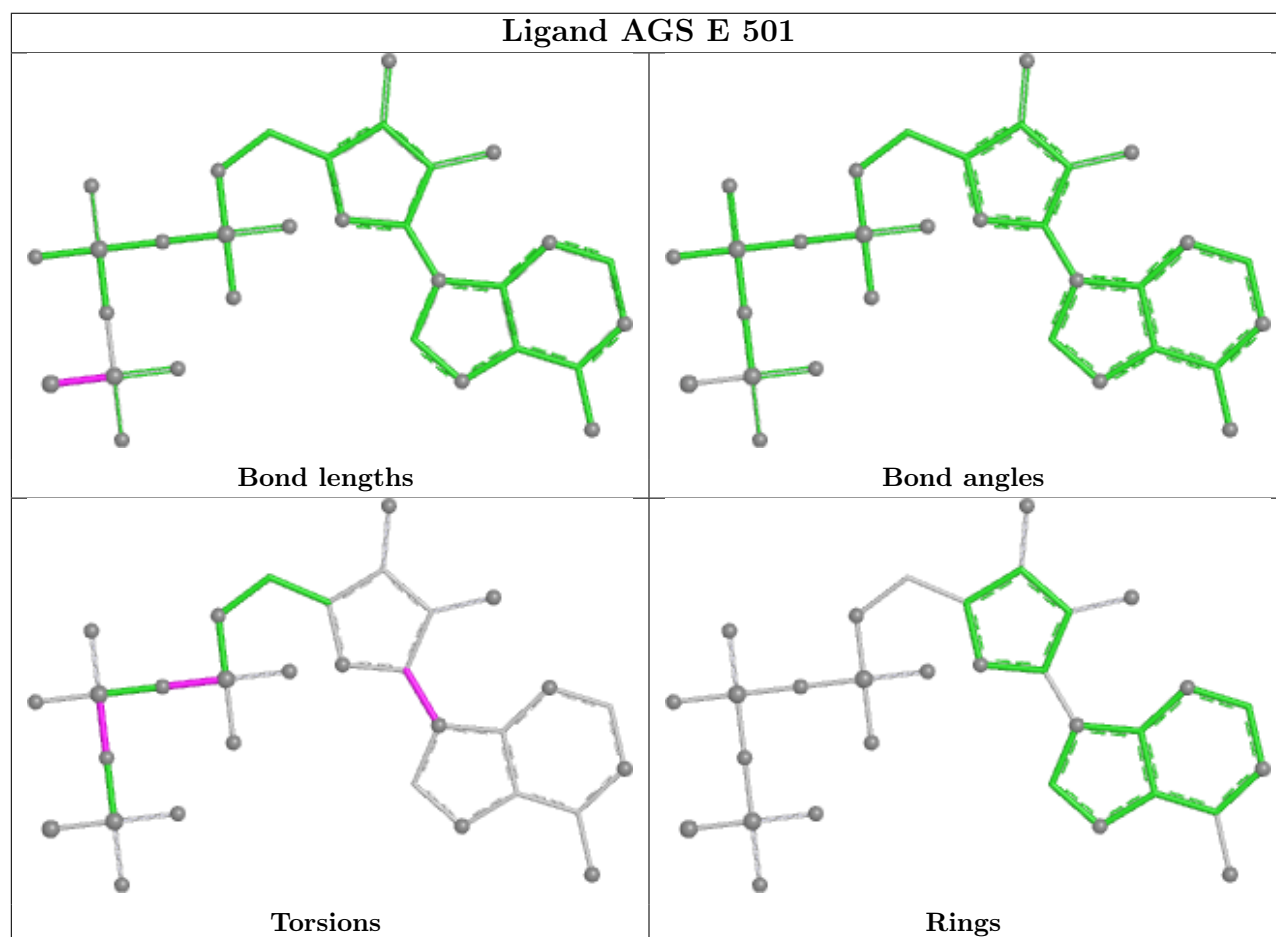
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	E	501	AGS	3	0

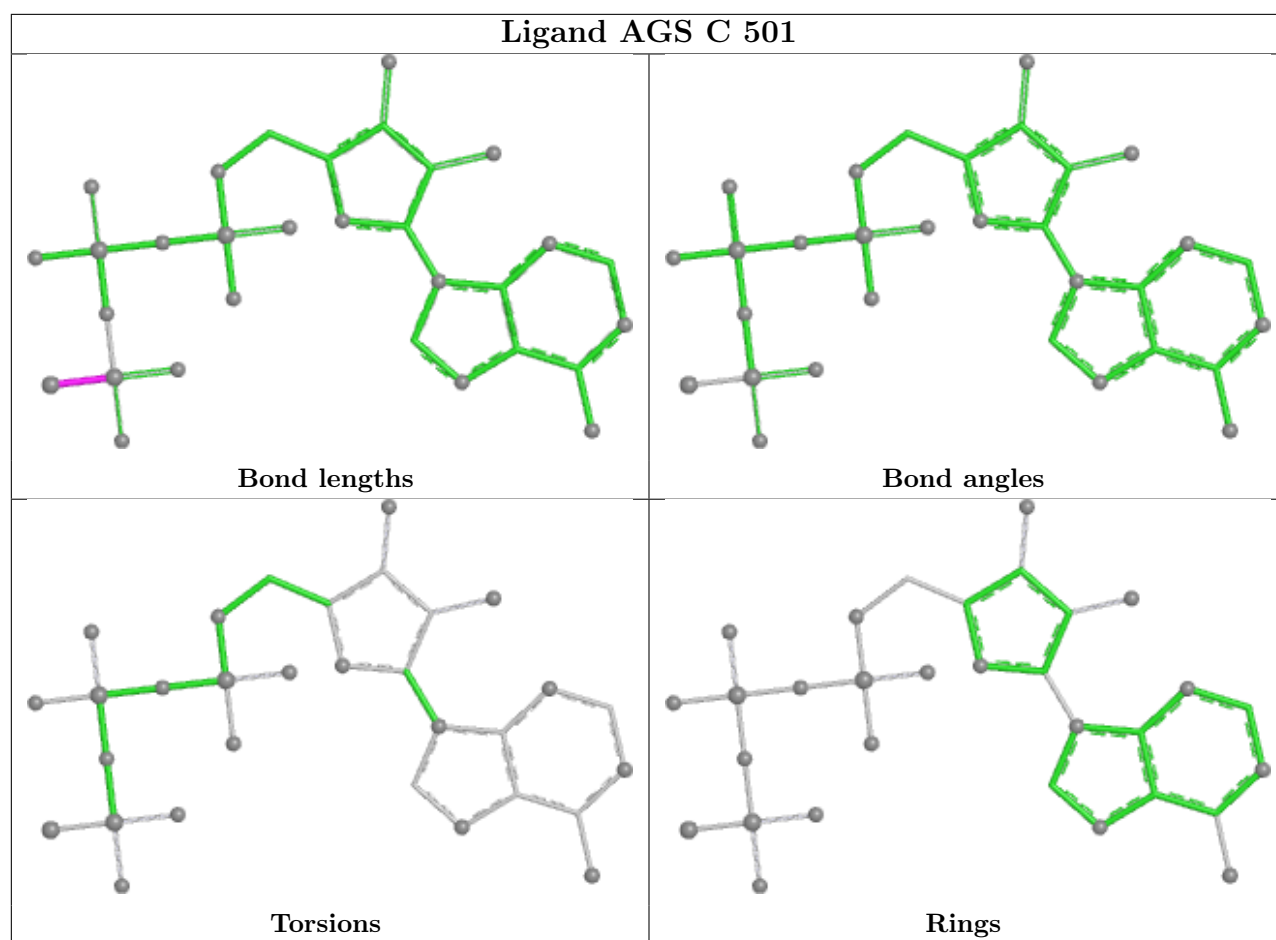
Continued on next page...

Continued from previous page...

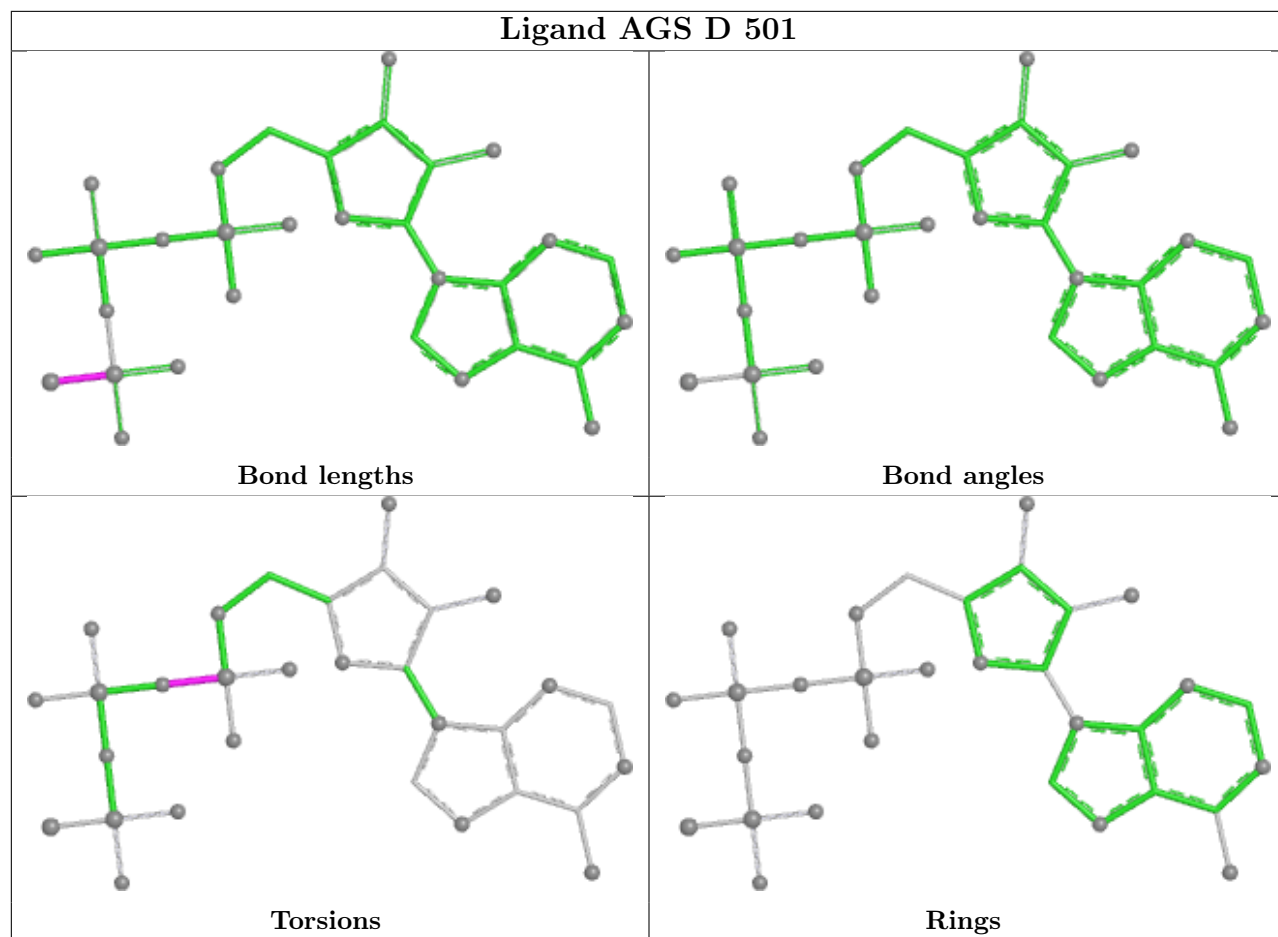
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	501	AGS	2	0
19	F	501	ADP	1	0

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.

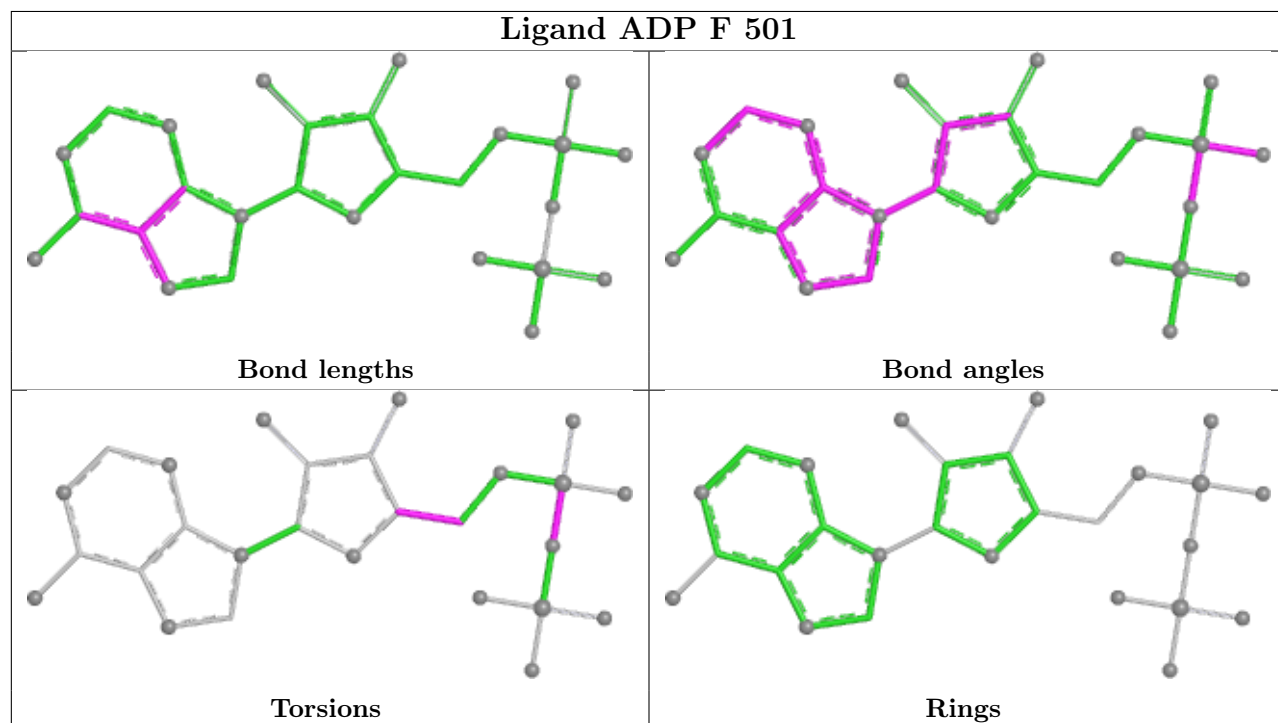




Ligand AGS D 501



Ligand ADP F 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

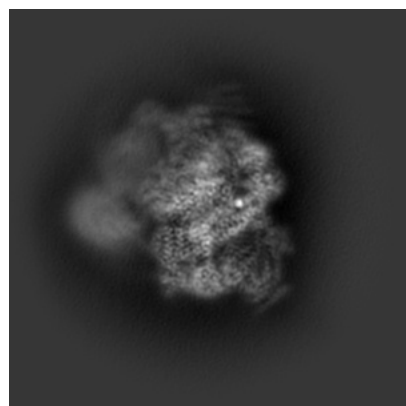
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71813. These allow visual inspection of the internal detail of the map and identification of artifacts.

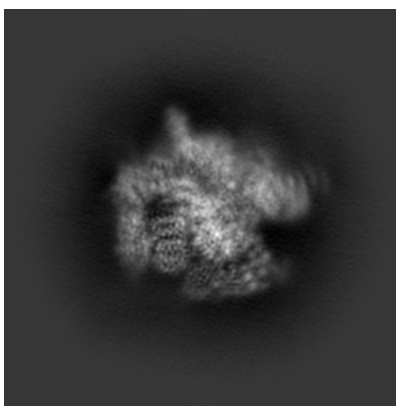
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

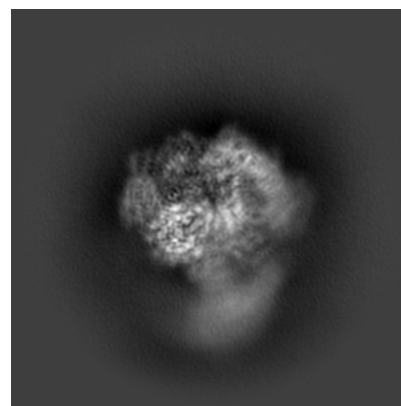
6.1.1 Primary map



X

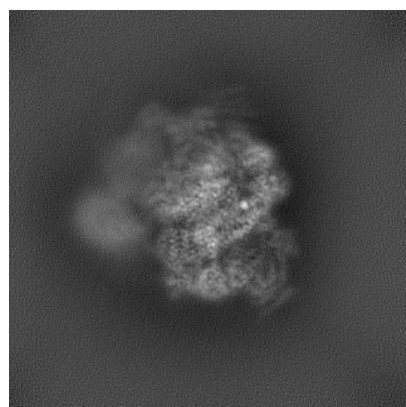


Y

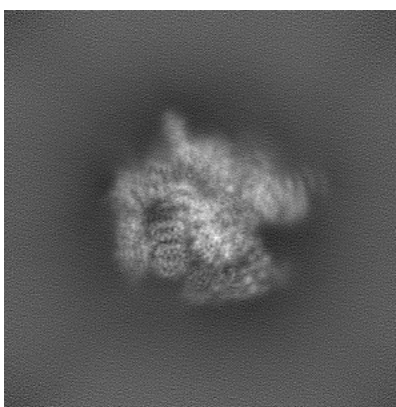


Z

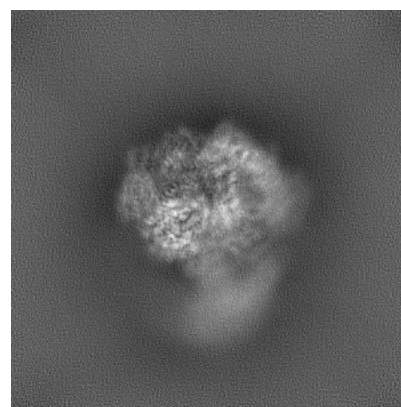
6.1.2 Raw map



X



Y

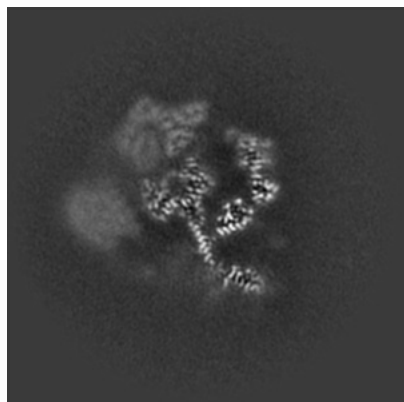


Z

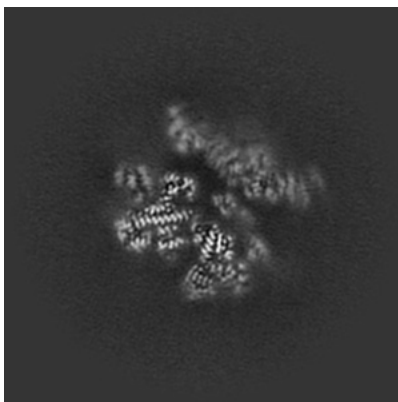
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

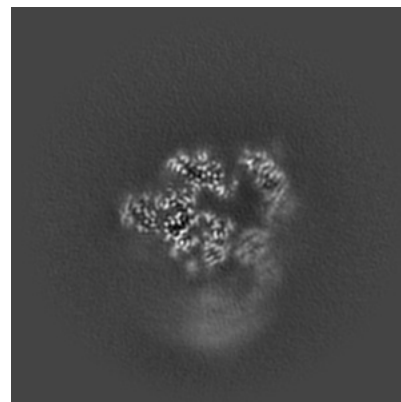
6.2.1 Primary map



X Index: 216

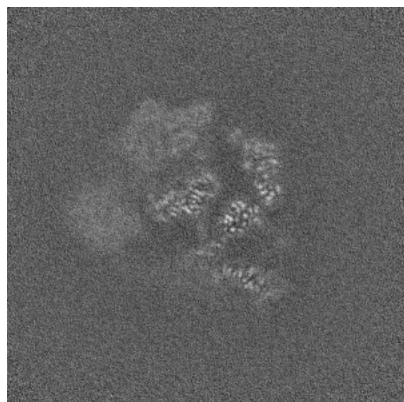


Y Index: 216

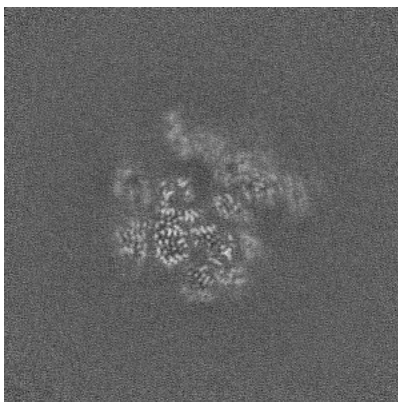


Z Index: 216

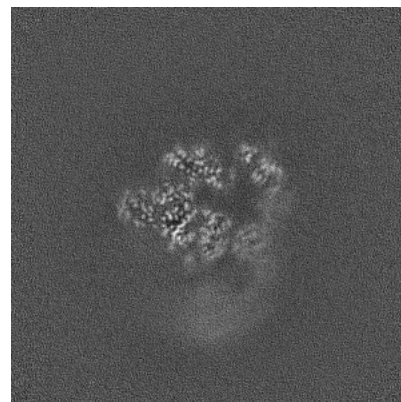
6.2.2 Raw map



X Index: 216



Y Index: 216

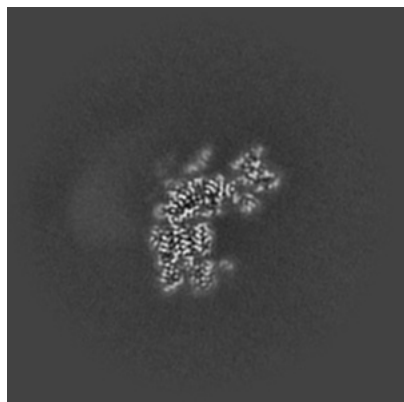


Z Index: 216

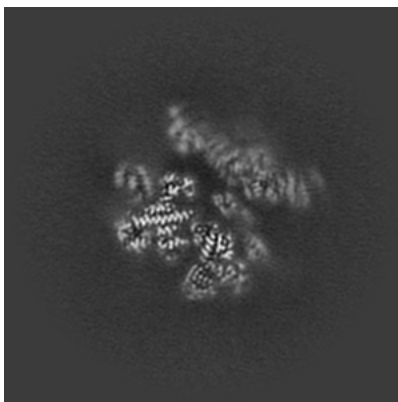
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

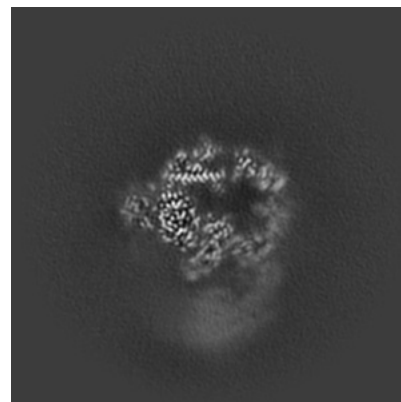
6.3.1 Primary map



X Index: 178

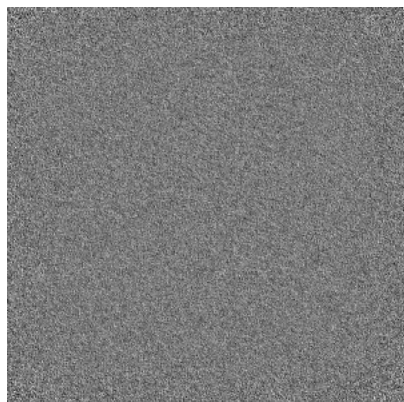


Y Index: 215

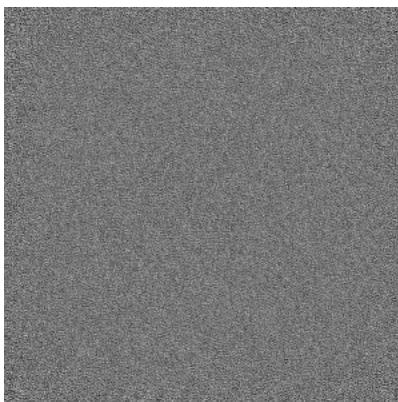


Z Index: 222

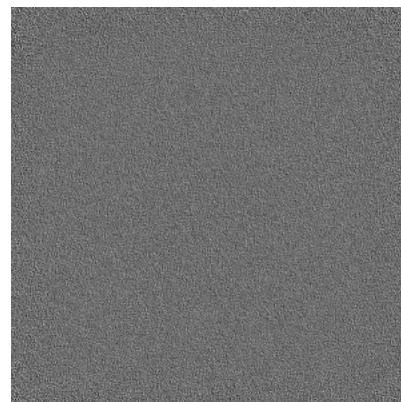
6.3.2 Raw map



X Index: 0



Y Index: 0

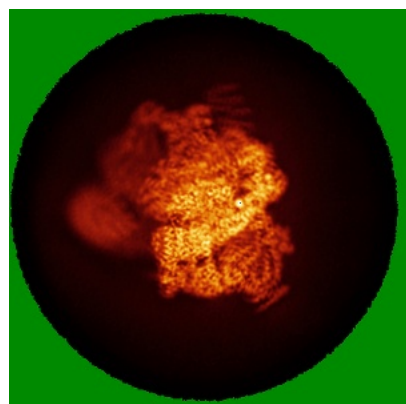


Z Index: 0

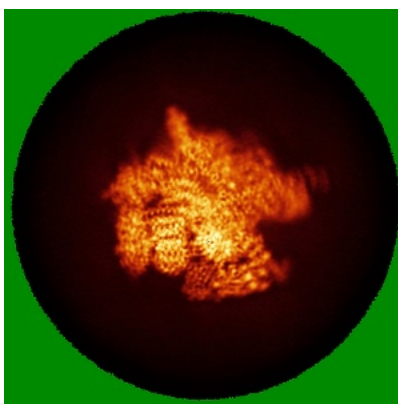
The images above show the largest variance slices of the map in three orthogonal directions.

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

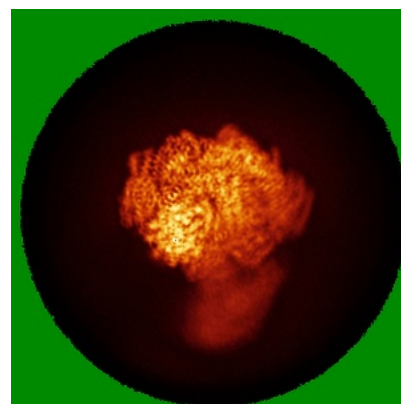
6.4.1 Primary map



X

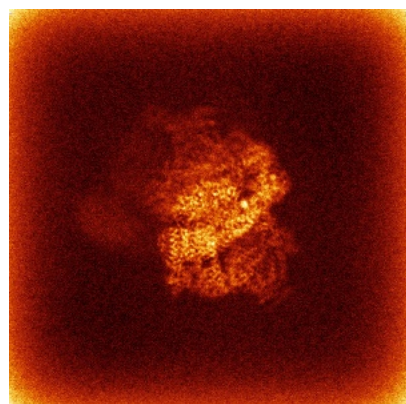


Y

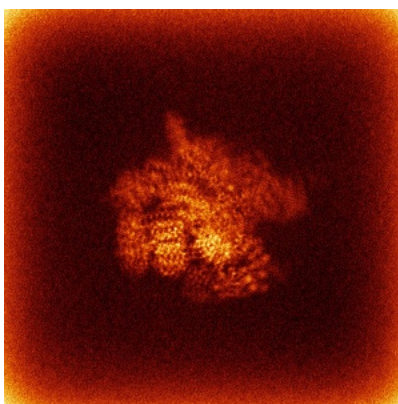


Z

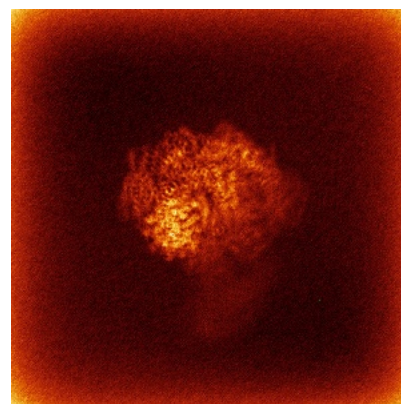
6.4.2 Raw map



X



Y

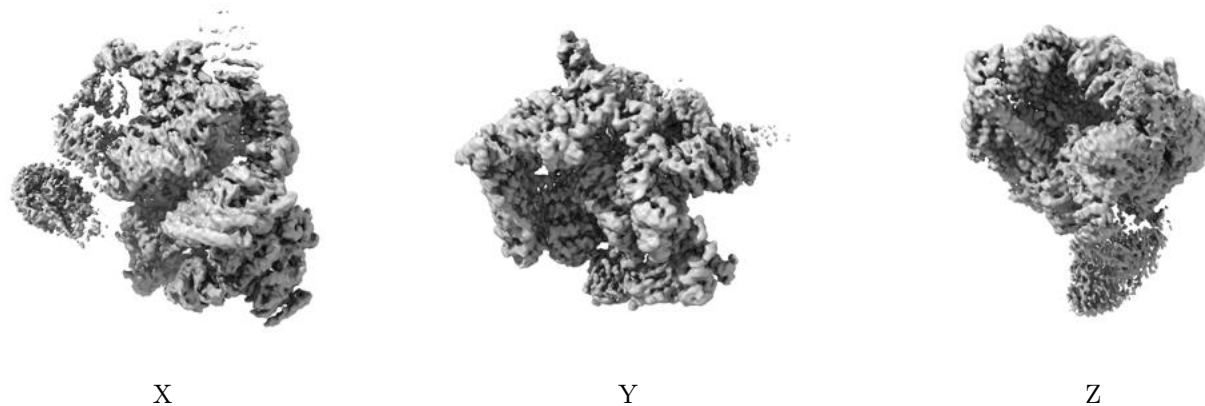


Z

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.

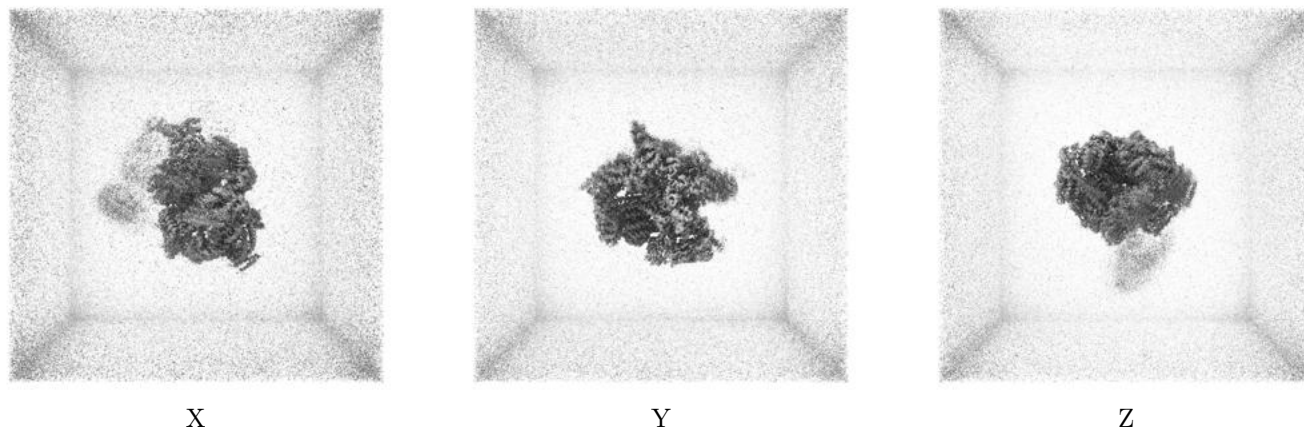
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

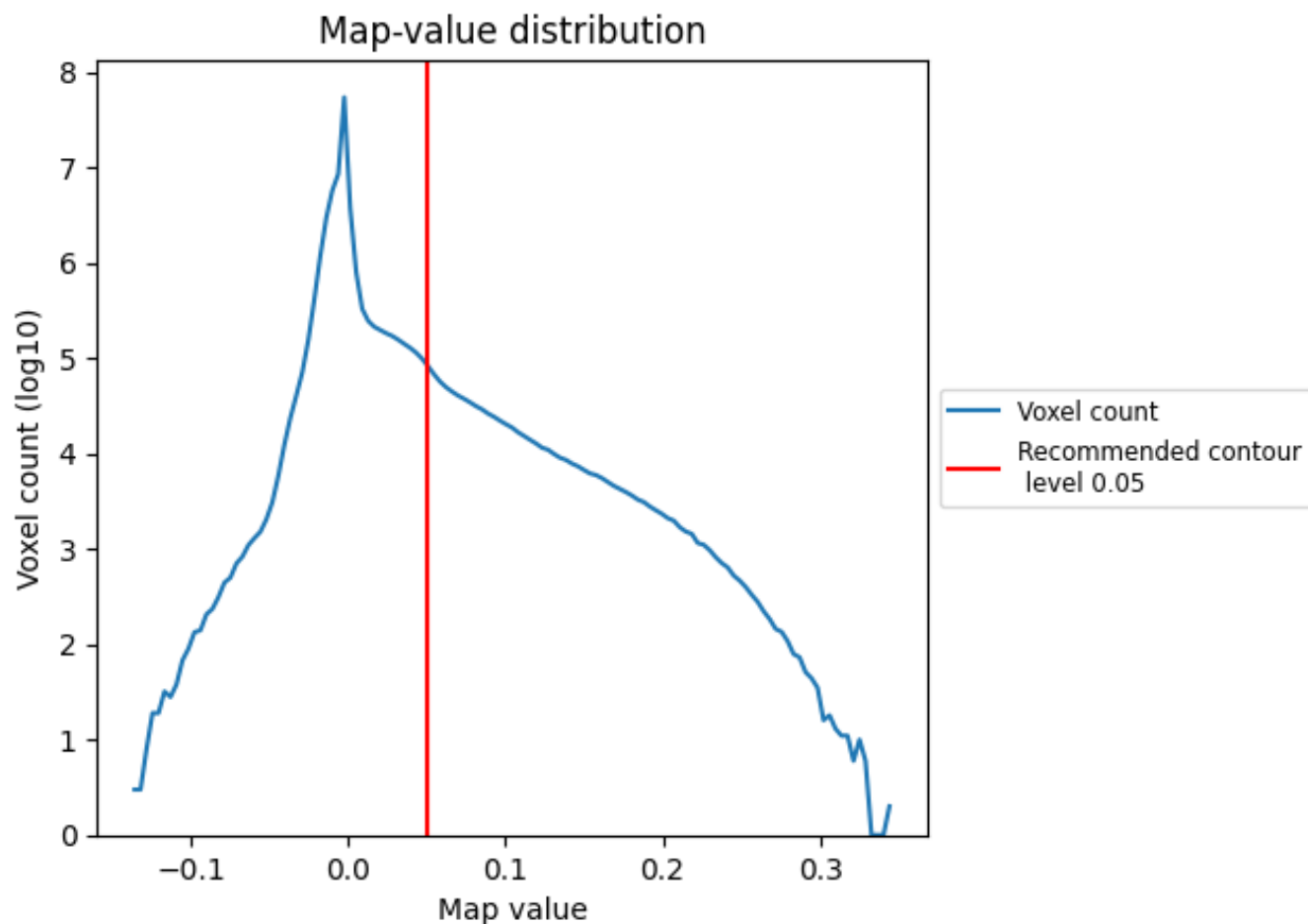
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

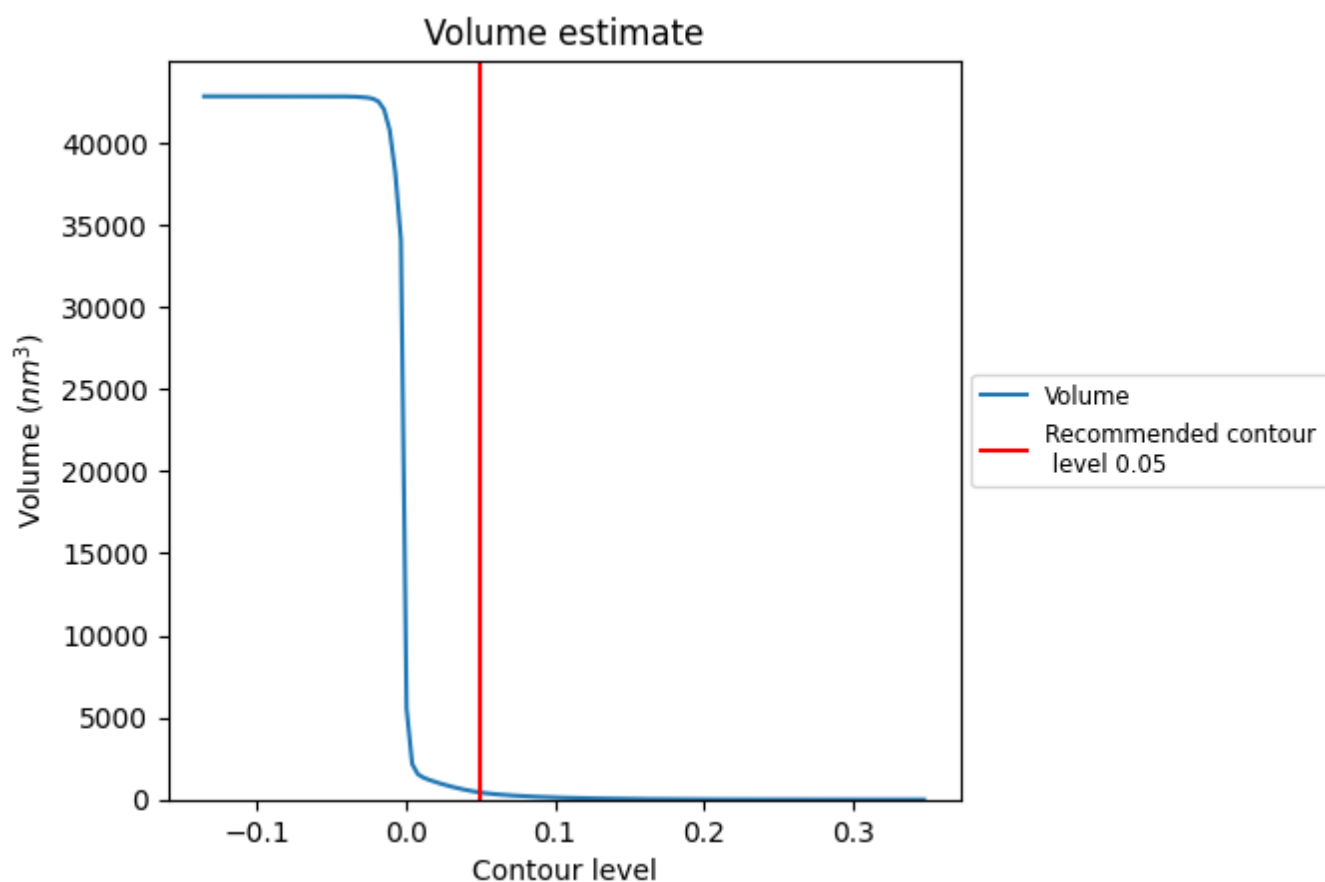
This section contains the results of statistical analysis of the map.

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.

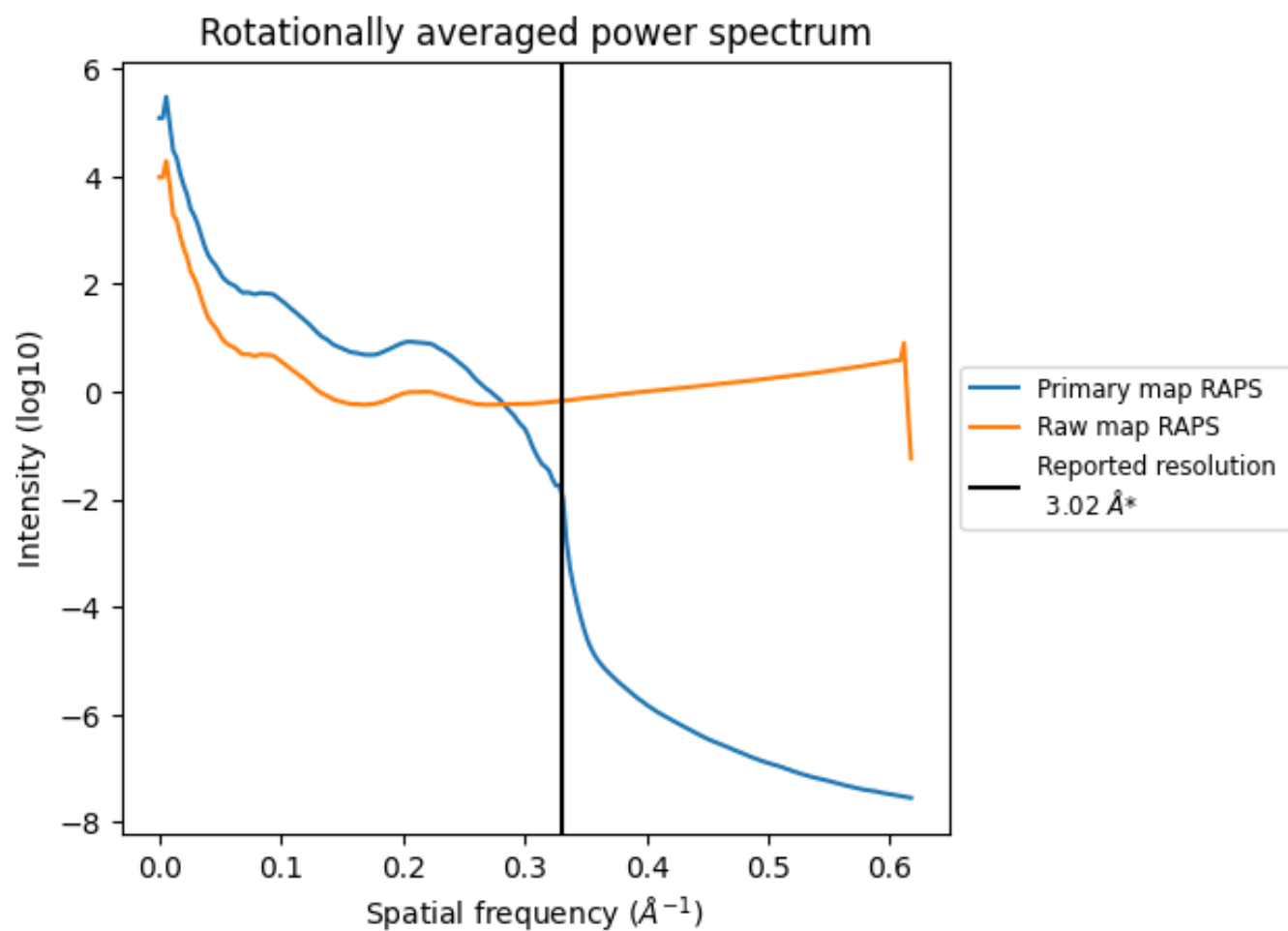
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 430 nm³; this corresponds to an approximate mass of 389 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 ⓘ

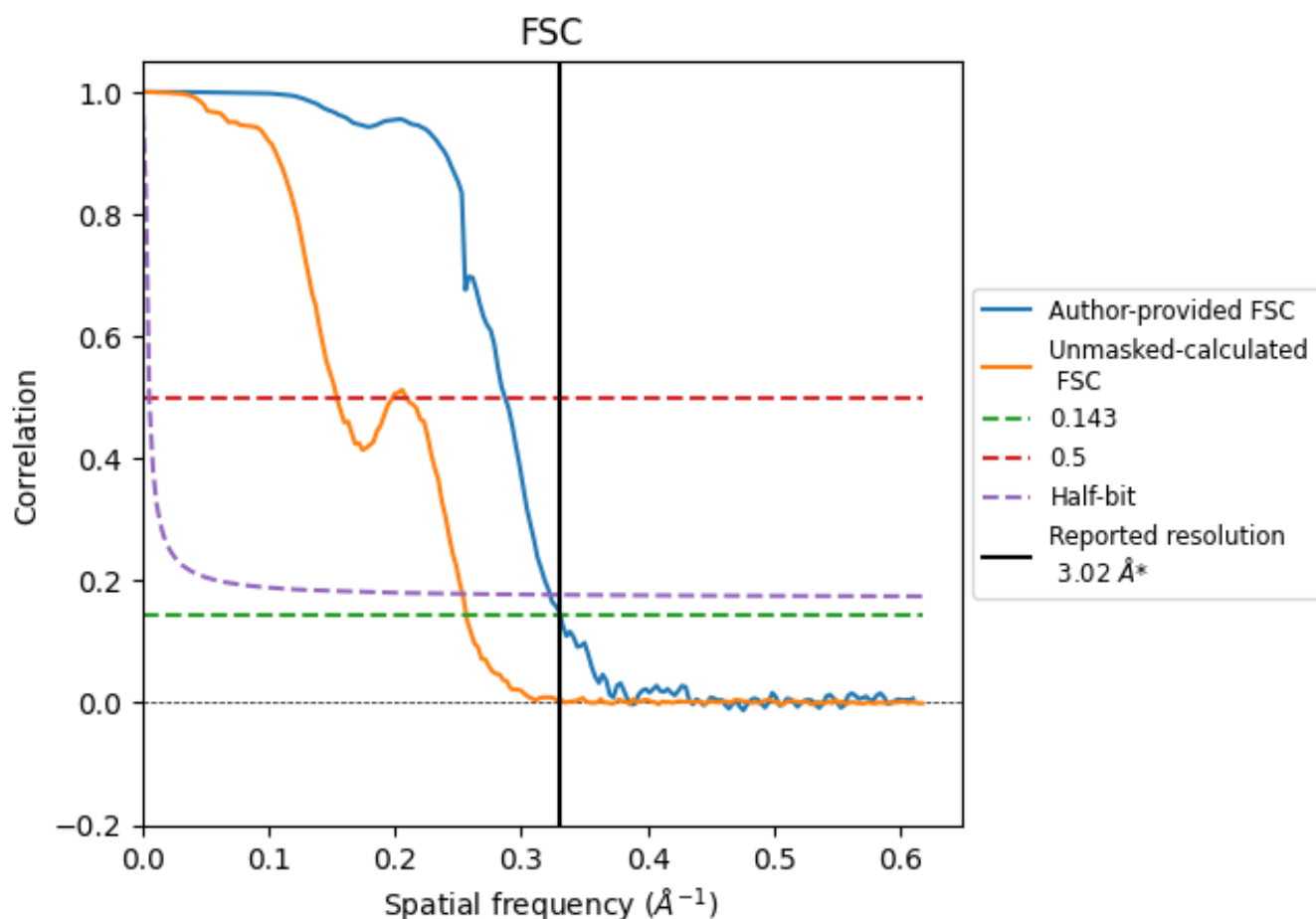


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.331 \AA^{-1}

8.2 Resolution estimates [i](#)

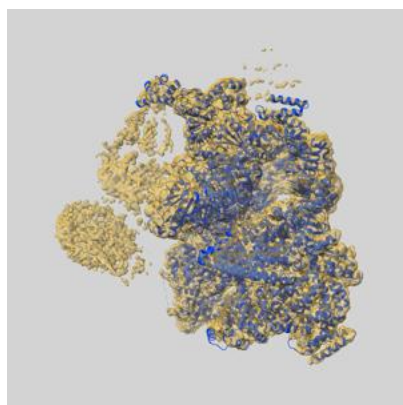
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.48	3.10
Unmasked-calculated*	3.90	6.50	3.94

*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 3.90 differs from the reported value 3.02 by more than 10 %

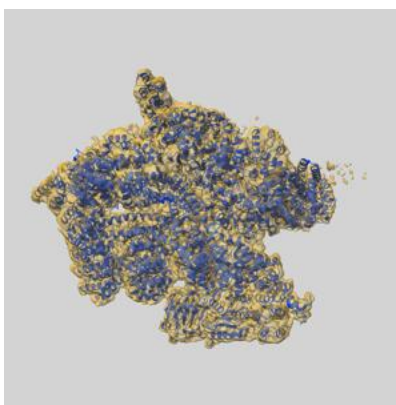
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71813 and PDB model 9PRT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

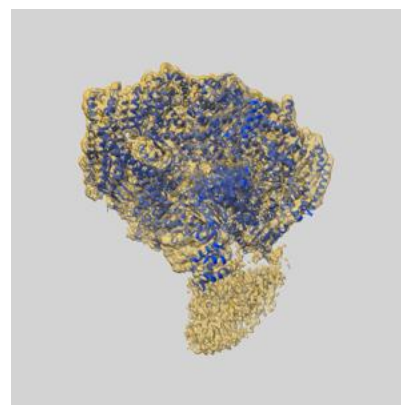
9.1 Map-model overlay [i](#)



X



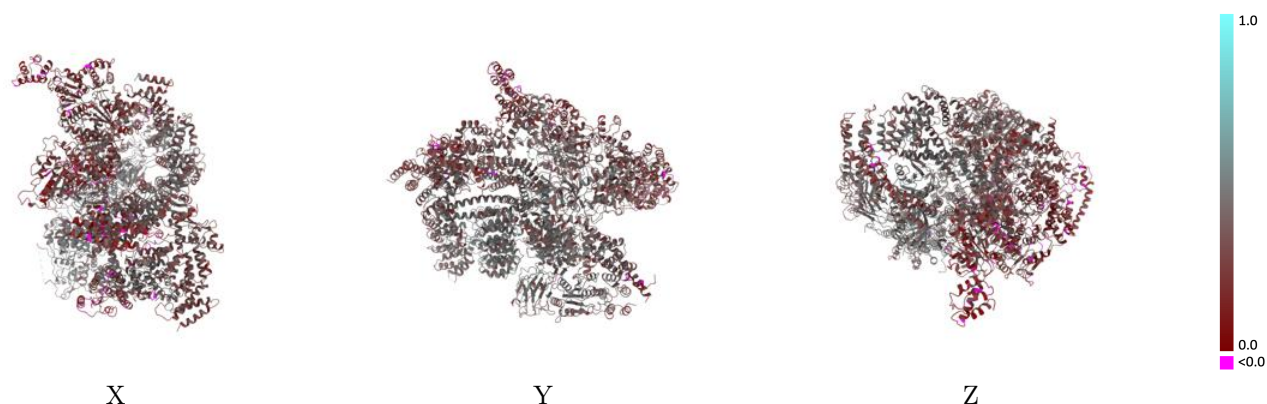
Y



Z

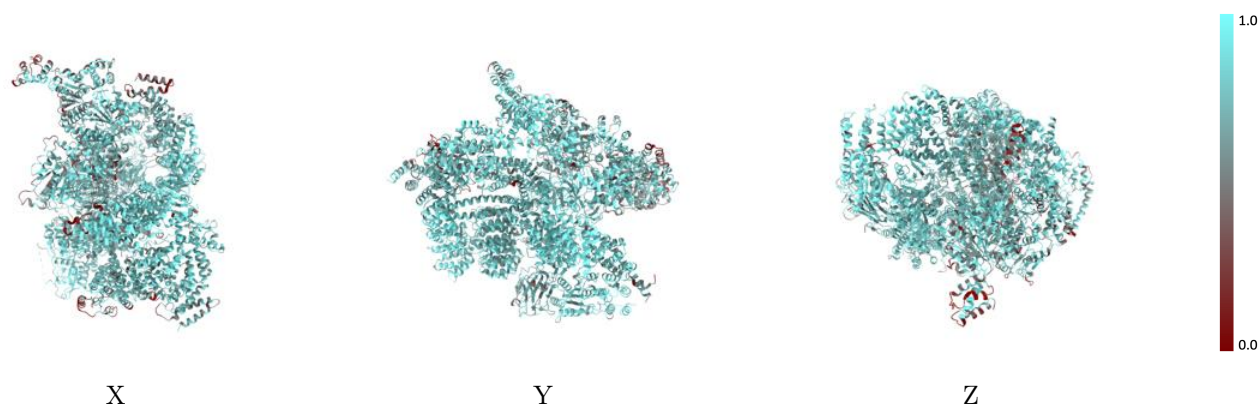
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



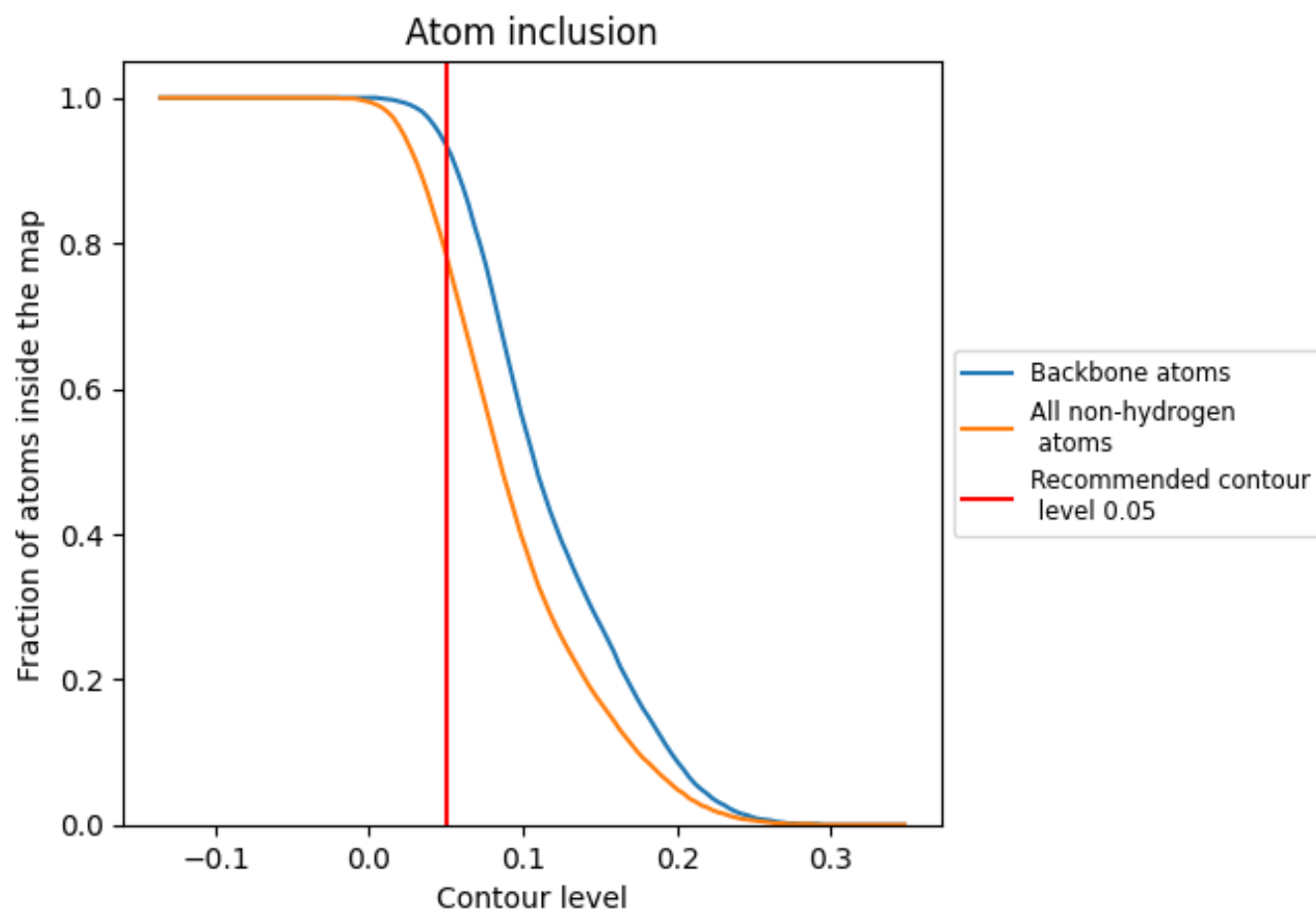
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7840	 0.3540
C	 0.7260	 0.2790
D	 0.7560	 0.3280
E	 0.7510	 0.3130
F	 0.6450	 0.2470
U	 0.8760	 0.4350
V	 0.7140	 0.3030
W	 0.7270	 0.3650
X	 0.8300	 0.3930
Y	 0.8130	 0.2800
Z	 0.8620	 0.4400
a	 0.8610	 0.3930
b	 0.8630	 0.3990
c	 0.8420	 0.4300
d	 0.7260	 0.3250
e	 0.7910	 0.2750
g	 0.7060	 0.4250

