Full wwPDB EM Validation Report

Jul 8, 2026 – 10:09 PM JST

PDB ID	:	22VL / pdb_000022vl
EMDB ID	:	EMD-68717
Title	:	Cryo-EM structure of Chlamydomonas reinhardtii chloroplast F1Fo-ATP synthase
Authors	:	Liu, J.; Li, D.Y.; Guan, Z.Y.; Yin, P.; Yan, J.J.
Deposited on	:	2026-01-25
Resolution	:	3.20 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:

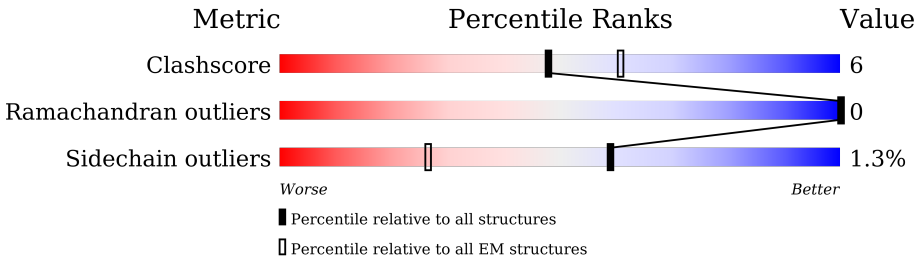
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

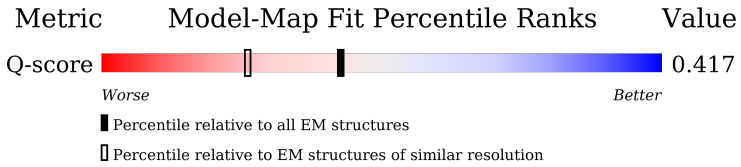
1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.





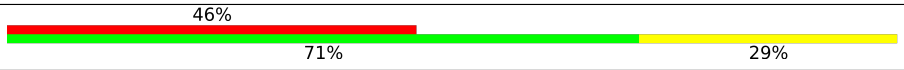
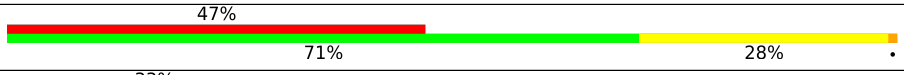
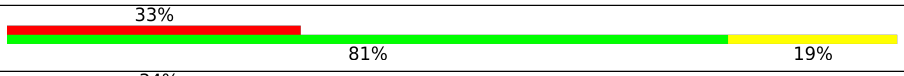
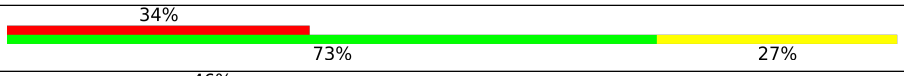
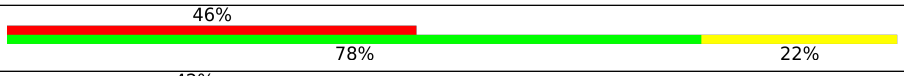
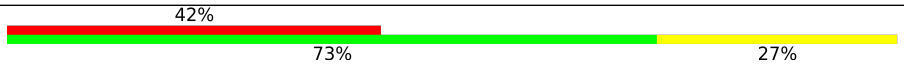
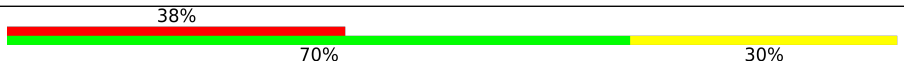
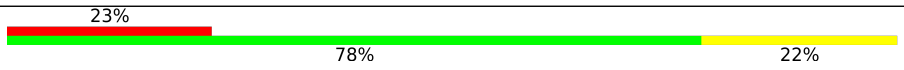
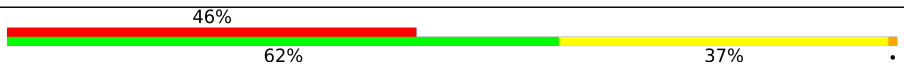
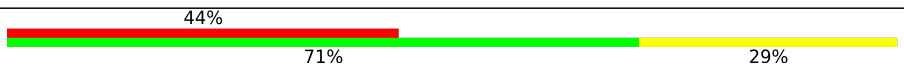
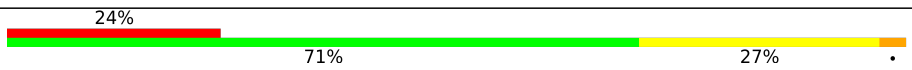
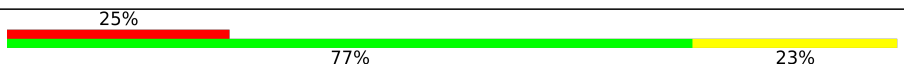
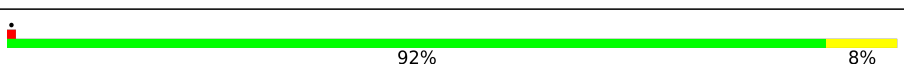
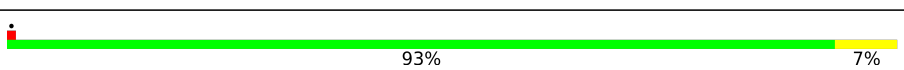
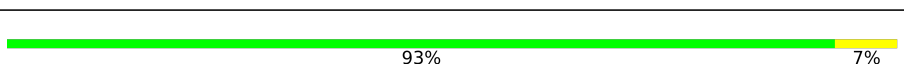
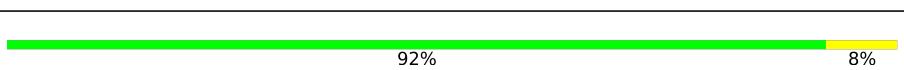
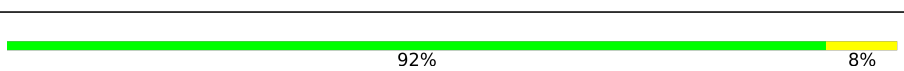
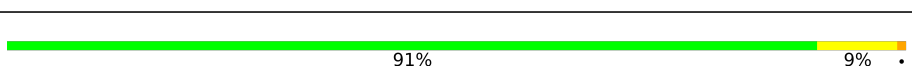
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	223	45% 88% 12%
2	p	129	82% 74% 26%
3	D	322	89% 11%
4	d	173	83% 82% 17%

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Mol	Chain	Length	Quality of chain
5	b	152	
6	e	136	
7	F	79	
7	G	79	
7	H	79	
7	I	79	
7	J	79	
7	K	79	
7	L	79	
7	M	79	
7	N	79	
7	O	79	
7	P	79	
7	Q	79	
7	R	79	
7	S	79	
8	A	484	
8	V	484	
9	B	482	
10	E	475	
10	T	475	
10	U	475	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 38386 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 ATP synthase subunit a, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	223	1742	1167	264	310	1	0	0

- Molecule 2 is a protein called ATP synthase subunit b', chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	p	129	989	623	164	198	4	0	0

- Molecule 3 is a protein called ATP synthase gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	322	2468	1549	432	474	13	0	0

- Molecule 4 is a protein called ATP synthase delta chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	173	1341	849	223	263	6	0	0

- Molecule 5 is a protein called ATP synthase subunit b, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	b	152	1238	781	225	231	1	0	0

- Molecule 6 is a protein called ATP synthase epsilon chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	e	130	1000	633	171	192	4	0	0

- Molecule 7 is a protein called ATP synthase subunit c, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	F	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	G	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	H	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	I	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	J	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	K	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	L	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	N	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	O	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	P	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	Q	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	R	79	Total	C	N	O	S	0	0
			548	358	89	99	2		
7	S	79	Total	C	N	O	S	0	0
			548	358	89	99	2		

- Molecule 8 is a protein called ATP synthase subunit alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	484	Total	C	N	O	S	0	0
			3655	2310	631	704	10		
8	V	484	Total	C	N	O	S	0	0
			3655	2310	631	704	10		

- Molecule 9 is a protein called ATP synthase subunit alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	482	Total	C	N	O	S	0	0
			3641	2301	628	702	10		

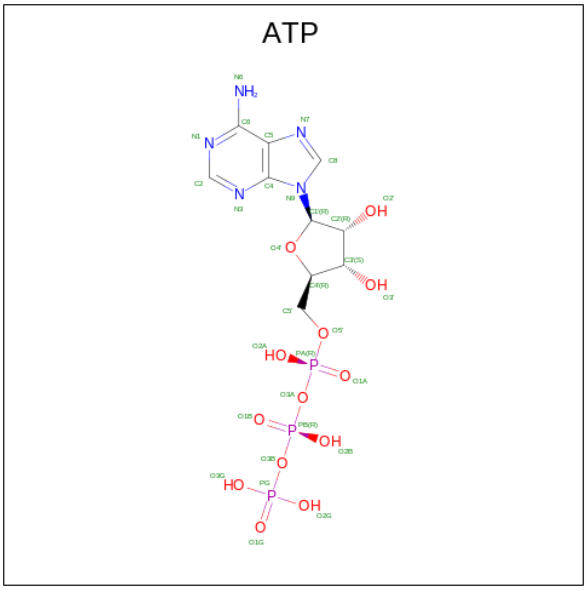
- Molecule 10 is a protein called ATP synthase subunit beta, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	475	Total	C	N	O	S	0	0
			3609	2292	612	689	16		
10	T	475	Total	C	N	O	S	0	0
			3609	2292	612	689	16		
10	U	475	Total	C	N	O	S	0	0
			3609	2292	612	689	16		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	V	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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Mol	Chain	Residues	Atoms					AltConf
12	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
12	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

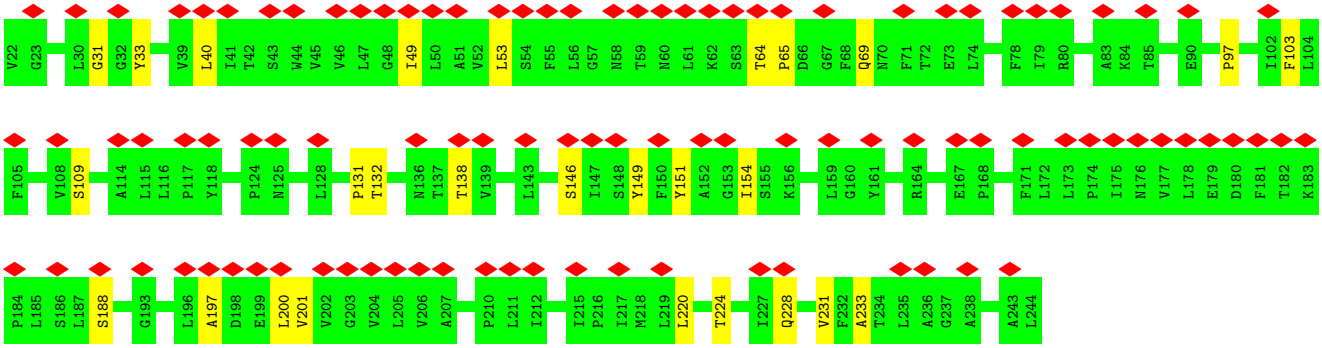
3 Residue-property plots (i)

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

• Molecule 1: ATP synthase subunit a, chloroplastic

Chain a:





• Molecule 2: ATP synthase subunit b', chloroplastic

Chain p:





• Molecule 3: ATP synthase gamma chain, chloroplastic

Chain D:



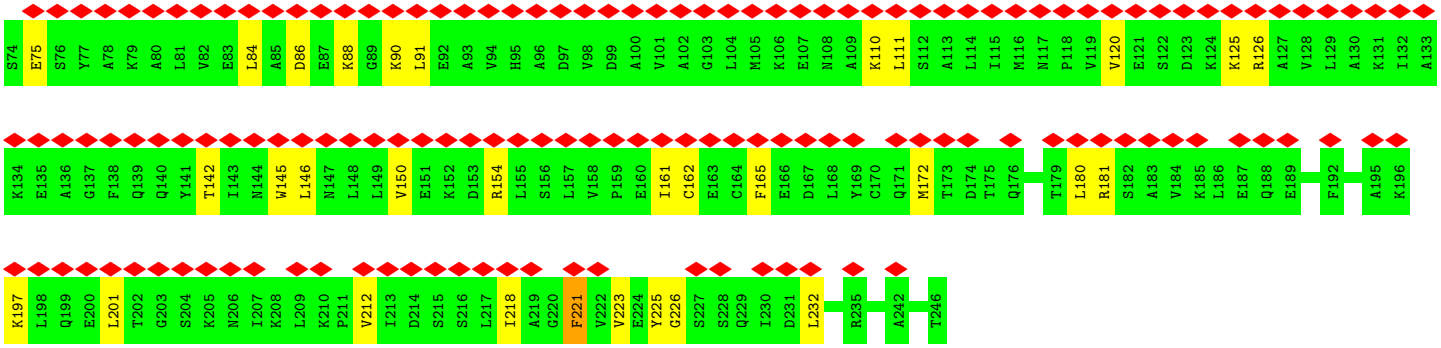




• Molecule 4: ATP synthase delta chain, chloroplastic

Chain d:

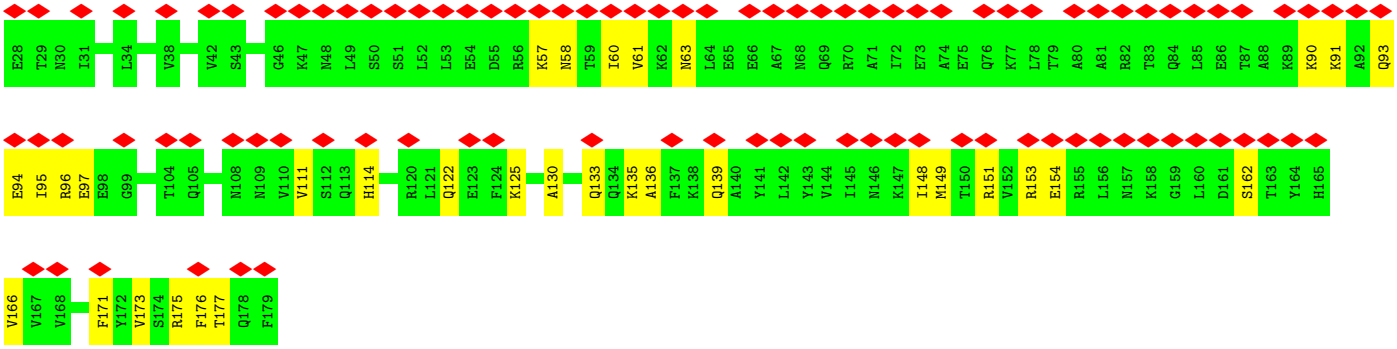




• Molecule 5: ATP synthase subunit b, chloroplastic

Chain b:

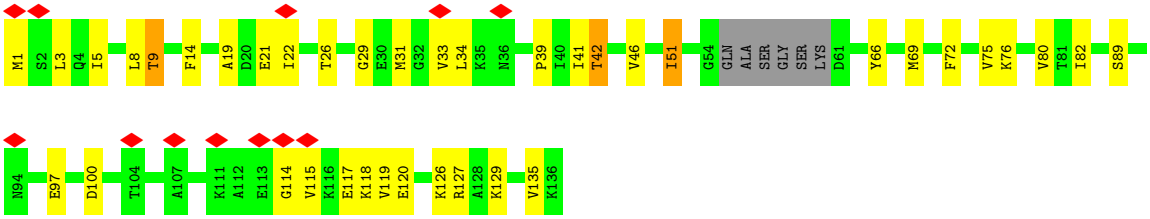




• Molecule 6: ATP synthase epsilon chain, chloroplastic

Chain e:

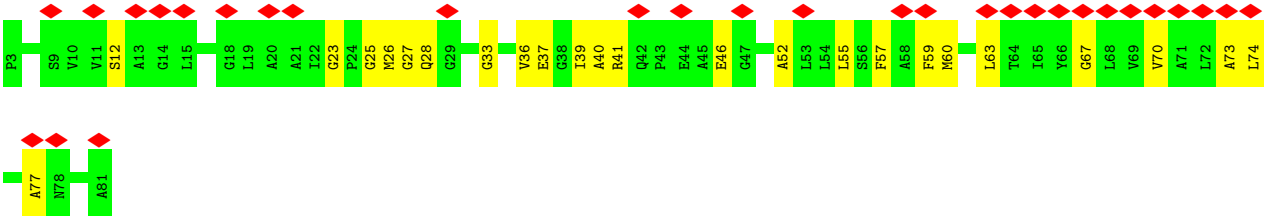




• Molecule 7: ATP synthase subunit c, chloroplastic

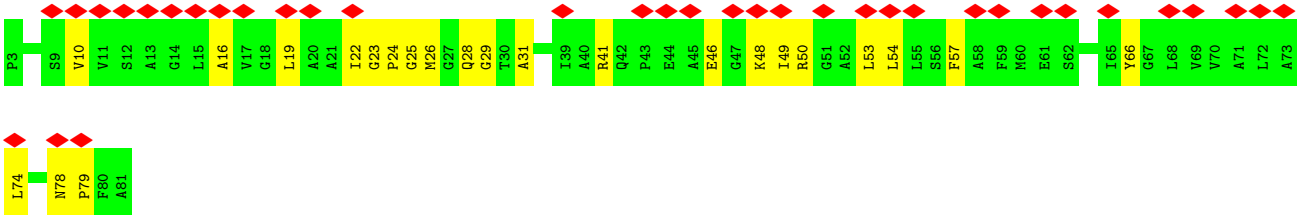
Chain M:



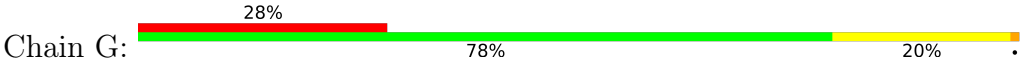


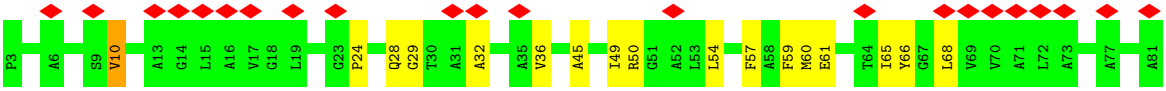
• Molecule 7: ATP synthase subunit c, chloroplastic





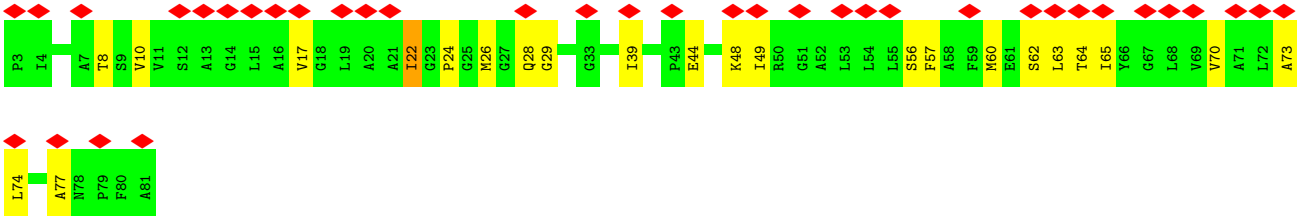
• Molecule 7: ATP synthase subunit c, chloroplastic



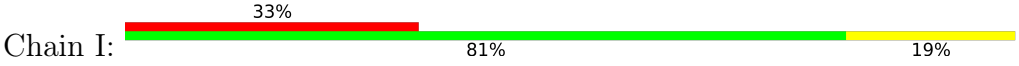


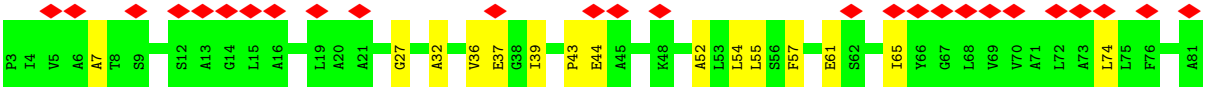
• Molecule 7: ATP synthase subunit c, chloroplastic





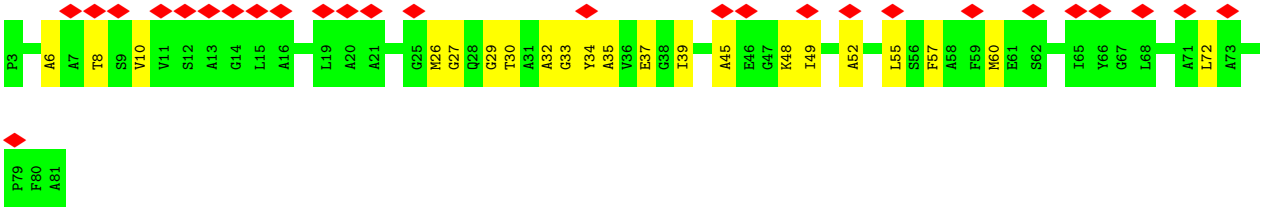
• Molecule 7: ATP synthase subunit c, chloroplastic





• Molecule 7: ATP synthase subunit c, chloroplastic

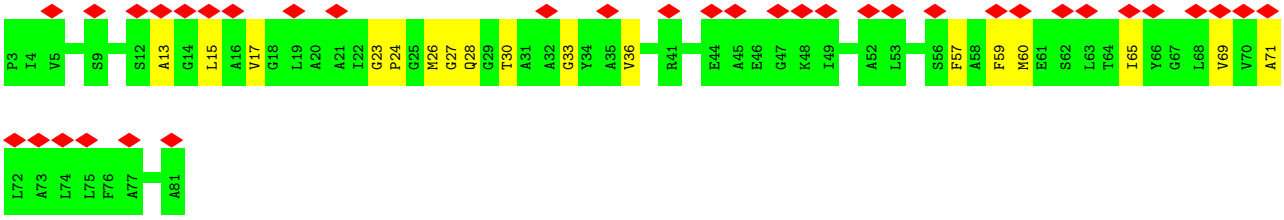




• Molecule 7: ATP synthase subunit c, chloroplastic

Chain K:

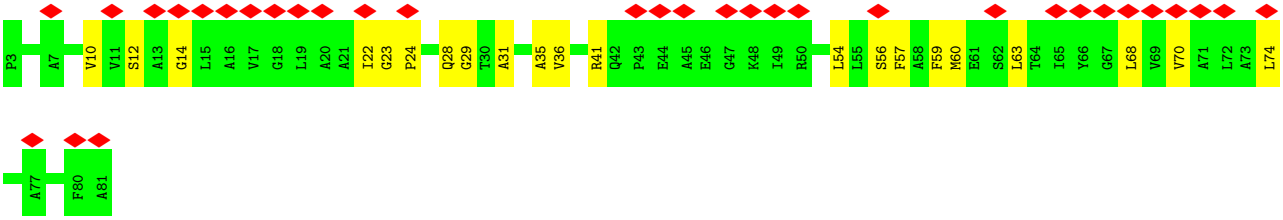




• Molecule 7: ATP synthase subunit c, chloroplastic

Chain L:

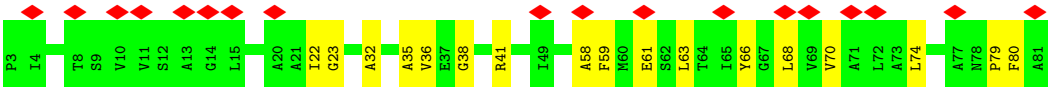




• Molecule 7: ATP synthase subunit c, chloroplastic

Chain N:

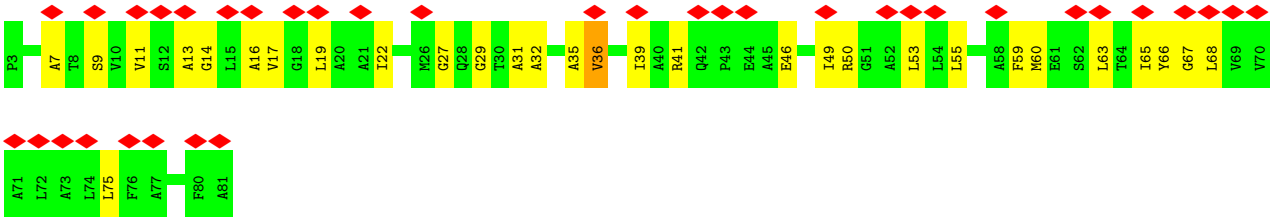




• Molecule 7: ATP synthase subunit c, chloroplastic

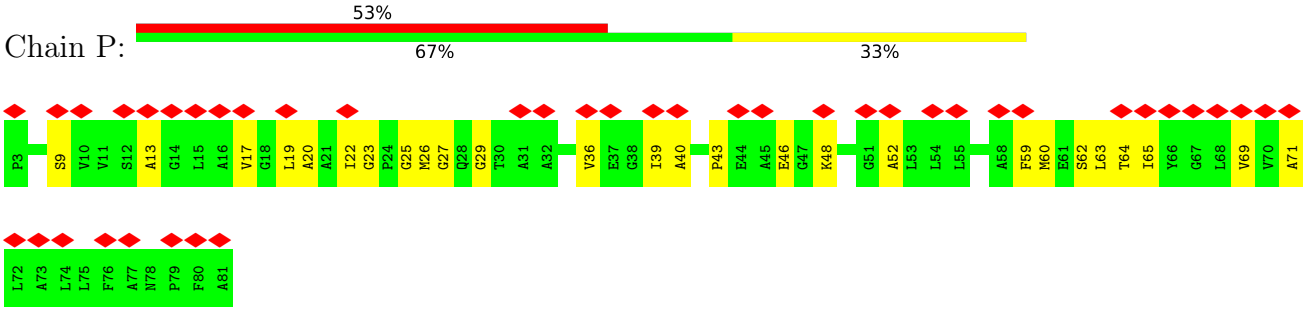
Chain O:





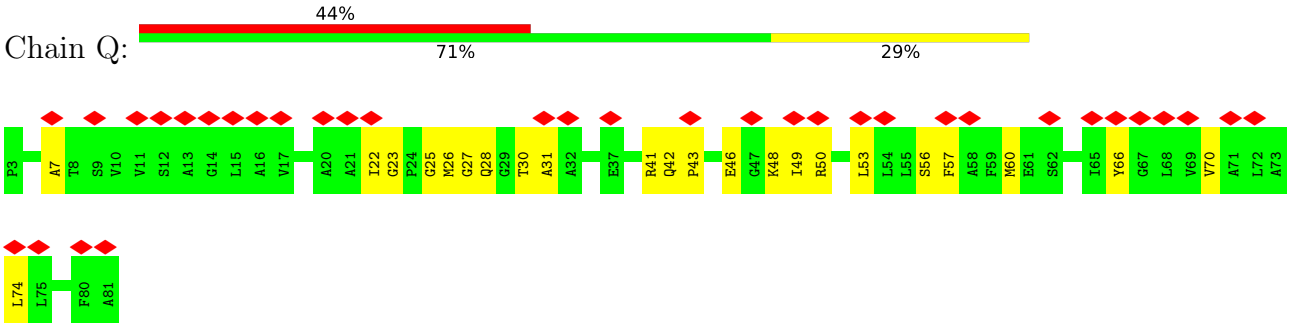
• Molecule 7: ATP synthase subunit c, chloroplastic

Chain P:



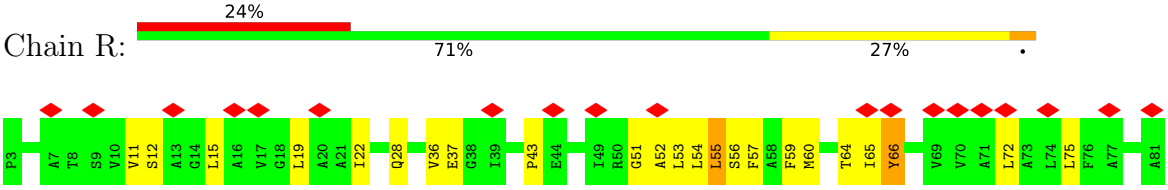
• Molecule 7: ATP synthase subunit c, chloroplastic

Chain Q:



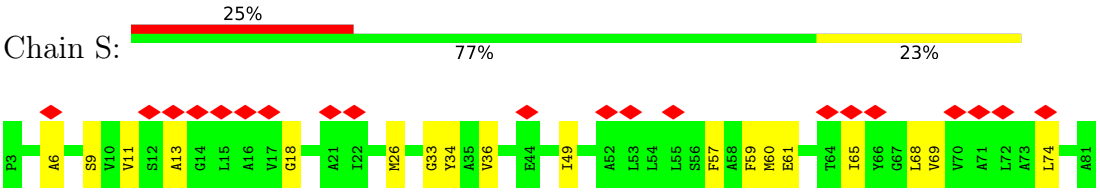
• Molecule 7: ATP synthase subunit c, chloroplastic

Chain R:



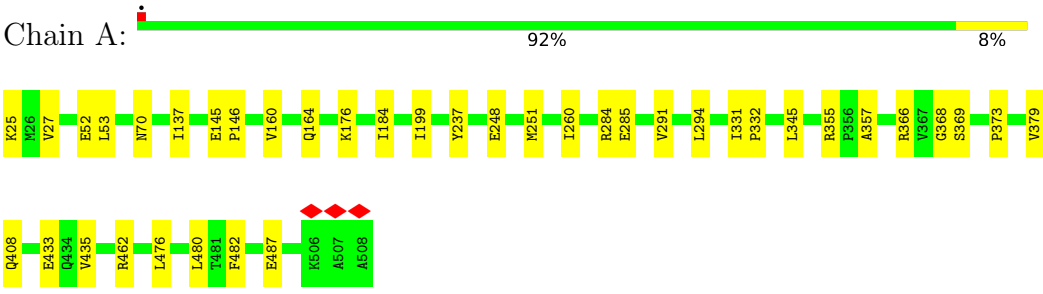
• Molecule 7: ATP synthase subunit c, chloroplastic

Chain S:



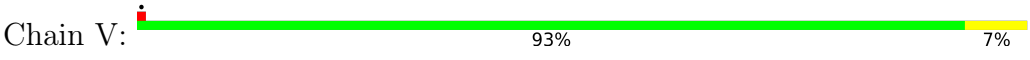
• Molecule 8: ATP synthase subunit alpha, chloroplastic

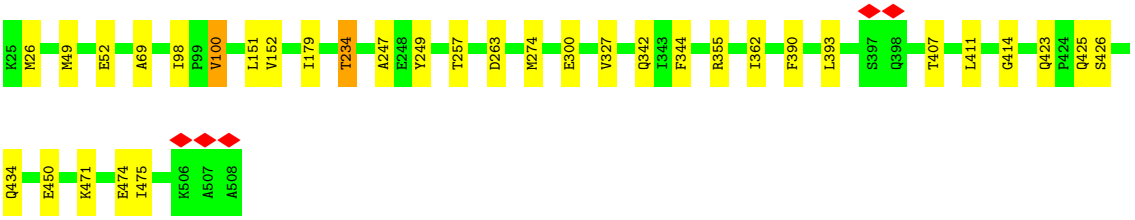
Chain A:



• Molecule 8: ATP synthase subunit alpha, chloroplastic

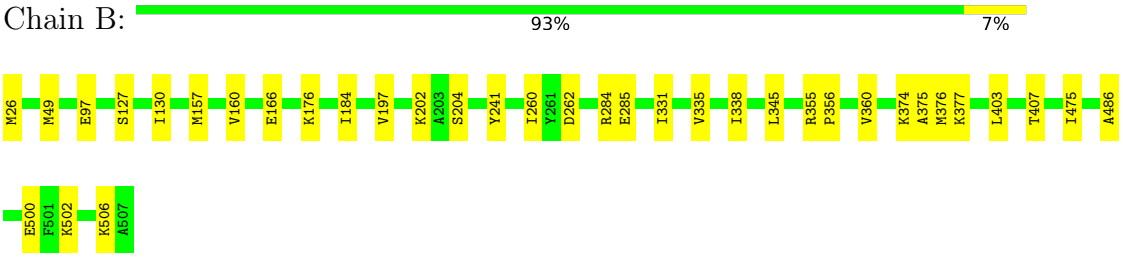
Chain V:





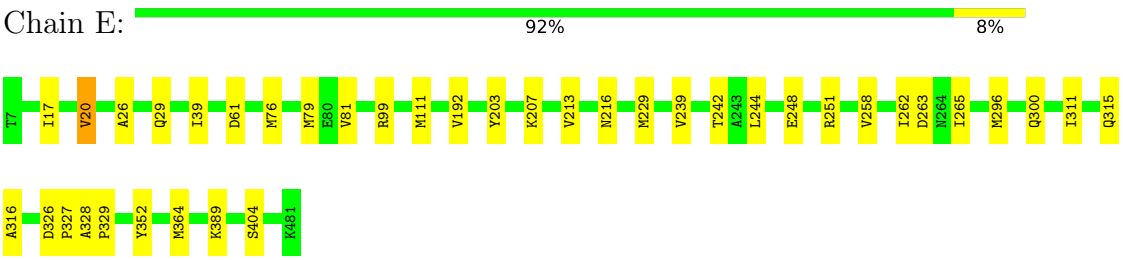
• Molecule 9: ATP synthase subunit alpha, chloroplastic

Chain B:



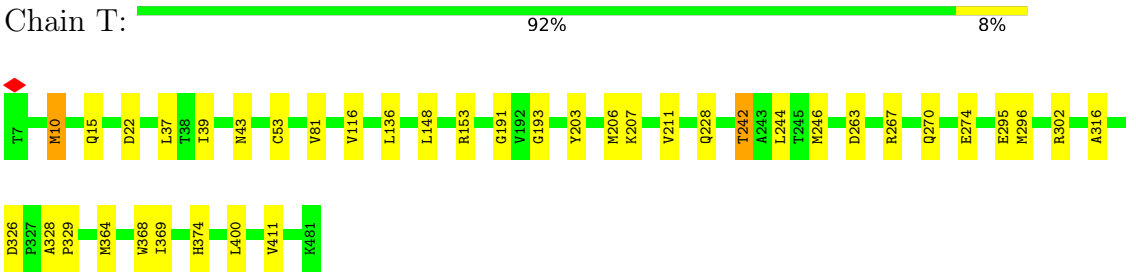
• Molecule 10: ATP synthase subunit beta, chloroplastic

Chain E:



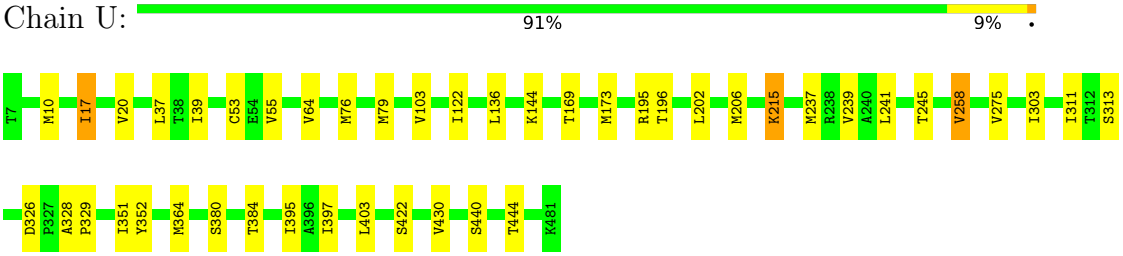
• Molecule 10: ATP synthase subunit beta, chloroplastic

Chain T:



• Molecule 10: ATP synthase subunit beta, chloroplastic

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64764	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.68	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.418	Depositor
Minimum map value	-0.683	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.15	0/1788	0.43	0/2447
2	p	0.16	0/996	0.37	0/1338
3	D	0.15	0/2495	0.34	0/3364
4	d	0.14	0/1354	0.42	0/1825
5	b	0.14	0/1251	0.37	0/1683
6	e	0.14	0/1015	0.41	0/1370
7	F	0.16	0/557	0.48	0/757
7	G	0.17	0/557	0.41	0/757
7	H	0.17	0/557	0.41	0/757
7	I	0.15	0/557	0.37	0/757
7	J	0.14	0/557	0.35	0/757
7	K	0.15	0/557	0.45	0/757
7	L	0.14	0/557	0.39	0/757
7	M	0.15	0/557	0.48	0/757
7	N	0.17	0/557	0.43	0/757
7	O	0.18	0/557	0.42	0/757
7	P	0.16	0/557	0.44	0/757
7	Q	0.15	0/557	0.42	0/757
7	R	0.16	0/557	0.39	0/757
7	S	0.14	0/557	0.42	0/757
8	A	0.16	0/3708	0.38	1/5021 (0.0%)
8	V	0.17	0/3708	0.39	0/5021
9	B	0.17	0/3694	0.37	0/5003
10	E	0.17	0/3667	0.37	0/4969
10	T	0.17	0/3667	0.37	0/4969
10	U	0.17	0/3667	0.39	0/4969
All	All	0.16	0/38808	0.39	1/52577 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	368	GLY	N-CA-C	5.54	120.56	114.40

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	a	1742	0	1779	16	0
2	p	989	0	1037	22	0
3	D	2468	0	2549	22	0
4	d	1341	0	1387	19	0
5	b	1238	0	1276	24	0
6	e	1000	0	1007	24	0
7	F	548	0	572	30	0
7	G	548	0	572	18	0
7	H	548	0	572	22	0
7	I	548	0	572	16	0
7	J	548	0	572	20	0
7	K	548	0	572	19	0
7	L	548	0	572	28	0
7	M	548	0	572	24	0
7	N	548	0	572	16	0
7	O	548	0	572	38	0
7	P	548	0	572	33	0
7	Q	548	0	572	24	0
7	R	548	0	572	20	0
7	S	548	0	572	13	0
8	A	3655	0	3730	22	0
8	V	3655	0	3729	23	0
9	B	3641	0	3711	23	0
10	E	3609	0	3683	22	0
10	T	3609	0	3683	23	0
10	U	3609	0	3683	27	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	31	0	12	1	0
12	B	31	0	12	0	0
12	T	31	0	12	0	0
12	U	31	0	12	0	0
12	V	31	0	12	1	0
All	All	38386	0	39322	458	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 (458) 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)
8:A:160:VAL:HA	8:A:164:GLN:HE21	1.39	0.88
2:p:181:ILE:HG12	5:b:125:LYS:HE2	1.60	0.82
7:M:57:PHE:HA	7:M:60:MET:HG2	1.61	0.82
6:e:46:VAL:HG21	6:e:127:ARG:HA	1.65	0.78
7:L:24:PRO:HB3	7:L:60:MET:HB3	1.67	0.76
3:D:346:LEU:HD21	9:B:284:ARG:H	1.51	0.76
7:M:26:MET:HB2	7:S:26:MET:HG3	1.68	0.75
10:T:43:ASN:HD21	8:V:49:MET:HE2	1.49	0.74
7:F:66:TYR:HB3	7:O:68:LEU:HD11	1.70	0.73
7:F:53:LEU:O	7:F:57:PHE:HB2	1.89	0.72
10:U:136:LEU:HD23	10:U:364:MET:HE1	1.74	0.70
7:G:50:ARG:HH22	7:I:55:LEU:HD13	1.54	0.70
7:L:68:LEU:HD11	7:O:66:TYR:HB3	1.72	0.70
7:K:17:VAL:HG11	7:L:70:VAL:HG21	1.74	0.70
1:a:64:THR:HB	5:b:57:LYS:HE2	1.73	0.70
4:d:142:THR:HA	4:d:145:TRP:CD1	2.27	0.70
7:M:27:GLY:HA2	7:H:29:GLY:HA3	1.74	0.69
7:M:28:GLN:HG2	7:M:60:MET:HG3	1.75	0.69
2:p:121:ASN:HA	2:p:124:ARG:HG2	1.76	0.68
7:J:57:PHE:HD2	7:K:59:PHE:HD2	1.42	0.67
7:F:26:MET:HE2	7:P:23:GLY:HA2	1.75	0.67
7:F:31:ALA:HB2	7:O:29:GLY:HA2	1.76	0.67
3:D:140:GLU:HG3	3:D:144:MET:HE2	1.75	0.67
7:P:62:SER:HA	7:P:65:ILE:HG12	1.75	0.67
6:e:22:ILE:HG13	6:e:33:VAL:HB	1.78	0.66
7:H:48:LYS:HB3	7:Q:46:GLU:HG3	1.78	0.65
10:U:122:ILE:HA	10:U:245:THR:HG21	1.78	0.65
7:P:43:PRO:HG3	7:Q:42:GLN:HE22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:471:LYS:O	8:V:475:ILE:HG12	1.97	0.64
10:E:39:ILE:HG12	10:E:81:VAL:HG22	1.80	0.64
7:K:24:PRO:HB3	7:K:60:MET:HB3	1.77	0.64
8:A:160:VAL:HA	8:A:164:GLN:NE2	2.13	0.64
10:U:144:LYS:HG2	10:U:444:THR:HG22	1.78	0.64
2:p:157:ALA:O	2:p:161:THR:HG23	1.98	0.63
3:D:50:THR:HG21	10:U:397:ILE:HD12	1.80	0.63
2:p:143:GLU:O	2:p:147:ILE:HG12	1.99	0.62
7:F:50:ARG:HD2	7:P:52:ALA:HB1	1.81	0.62
7:N:63:LEU:HD22	7:R:64:THR:HG21	1.81	0.62
1:a:146:SER:HA	1:a:149:TYR:CZ	2.34	0.61
7:M:39:ILE:HD11	7:M:46:GLU:HG3	1.80	0.61
2:p:97:PHE:O	2:p:101:MET:HG2	2.00	0.61
7:F:16:ALA:HB2	7:O:14:GLY:HA2	1.81	0.61
7:N:32:ALA:O	7:N:36:VAL:HG23	2.00	0.61
9:B:502:LYS:HA	9:B:506:LYS:HG3	1.82	0.61
7:M:40:ALA:HB1	7:M:41:ARG:HH21	1.65	0.61
7:G:24:PRO:HB3	7:G:60:MET:HG3	1.83	0.61
7:K:60:MET:HE2	7:K:60:MET:H	1.66	0.61
3:D:246:GLU:HB3	3:D:263:LYS:HD3	1.82	0.61
5:b:171:PHE:O	5:b:175:ARG:HG3	2.01	0.61
7:S:65:ILE:HA	7:S:68:LEU:HD12	1.81	0.60
8:A:176:LYS:HG2	8:A:345:LEU:HD12	1.83	0.60
2:p:95:GLY:HA2	2:p:98:LEU:HD12	1.83	0.60
7:O:32:ALA:O	7:O:36:VAL:HG12	2.01	0.60
2:p:148:LEU:HD21	9:B:500:GLU:HG3	1.82	0.60
3:D:111:VAL:HG11	3:D:141:LEU:HD13	1.83	0.60
7:F:53:LEU:HD23	7:F:54:LEU:HD23	1.83	0.60
7:F:74:LEU:HD23	7:O:75:LEU:HD11	1.83	0.60
7:N:74:LEU:HD21	7:R:75:LEU:HD21	1.84	0.60
7:P:40:ALA:HA	7:Q:42:GLN:HE21	1.67	0.60
8:A:403:LEU:H	8:A:403:LEU:HD23	1.67	0.60
7:J:32:ALA:HB2	7:J:57:PHE:HZ	1.67	0.59
6:e:126:LYS:HD2	6:e:129:LYS:HE3	1.84	0.59
7:L:28:GLN:HB3	7:O:60:MET:HE2	1.84	0.59
8:V:234:THR:HG23	8:V:274:MET:HE1	1.84	0.59
7:N:22:ILE:HG13	7:N:23:GLY:N	2.17	0.59
6:e:9:THR:HG22	6:e:14:PHE:HB2	1.84	0.58
7:G:66:TYR:CE1	7:N:68:LEU:HD22	2.38	0.58
8:V:393:LEU:HD23	8:V:407:THR:HG23	1.83	0.58
7:O:36:VAL:HA	7:O:39:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:106:ARG:HD2	3:D:107:PRO:HD2	1.85	0.58
3:D:141:LEU:HA	3:D:144:MET:HE3	1.85	0.57
7:H:60:MET:HB3	7:Q:28:GLN:OE1	2.04	0.57
7:K:26:MET:HE1	7:L:23:GLY:HA2	1.87	0.57
7:P:40:ALA:HB3	7:Q:41:ARG:HH21	1.68	0.57
7:G:65:ILE:O	7:G:68:LEU:HB3	2.04	0.57
8:V:342:GLN:HG3	8:V:344:PHE:CE2	2.39	0.57
3:D:81:ASN:HA	3:D:84:LYS:HG3	1.87	0.57
7:N:58:ALA:O	7:N:61:GLU:HG2	2.05	0.57
8:V:247:ALA:HB1	8:V:257:THR:HG21	1.85	0.57
2:p:136:ASP:O	2:p:139:LYS:HG2	2.04	0.57
7:M:37:GLU:OE1	7:S:34:TYR:HB3	2.04	0.57
7:F:31:ALA:HB1	7:O:32:ALA:HB3	1.87	0.57
7:I:43:PRO:HA	7:J:48:LYS:HE2	1.87	0.57
7:N:63:LEU:HD21	7:R:28:GLN:HE22	1.70	0.57
7:P:26:MET:HE2	7:P:26:MET:HA	1.85	0.56
7:M:33:GLY:O	7:M:37:GLU:HG2	2.04	0.56
7:P:20:ALA:HB1	7:P:64:THR:HA	1.87	0.56
7:F:29:GLY:HA3	7:P:27:GLY:HA2	1.85	0.56
9:B:338:ILE:HG23	10:E:229:MET:HE1	1.87	0.56
10:E:251:ARG:HD3	10:E:311:ILE:HG13	1.88	0.56
7:I:7:ALA:HB1	7:J:8:THR:HG21	1.86	0.56
7:J:39:ILE:HG12	7:J:49:ILE:HG21	1.88	0.56
6:e:26:THR:HB	6:e:31:MET:HE2	1.88	0.56
7:F:50:ARG:NE	7:F:50:ARG:HA	2.20	0.56
7:F:66:TYR:HB3	7:O:68:LEU:HD21	1.88	0.56
7:H:8:THR:HG21	7:Q:7:ALA:HB1	1.88	0.56
2:p:195:GLU:O	2:p:199:MET:HG2	2.06	0.56
7:F:48:LYS:HD3	7:O:46:GLU:HB2	1.88	0.56
7:I:61:GLU:O	7:I:65:ILE:HD12	2.05	0.56
7:O:39:ILE:HG12	7:O:49:ILE:HD13	1.88	0.56
10:E:326:ASP:HB3	10:E:329:PRO:HD2	1.86	0.56
7:G:10:VAL:HG13	7:I:74:LEU:HD22	1.87	0.55
7:J:35:ALA:O	7:J:39:ILE:HG13	2.07	0.55
10:E:76:MET:HG2	10:E:79:MET:HE3	1.88	0.55
4:d:142:THR:HA	4:d:145:TRP:HD1	1.71	0.55
8:A:184:ILE:HD11	8:A:260:ILE:HD13	1.88	0.55
3:D:203:VAL:HG22	3:D:224:LEU:HB2	1.88	0.55
4:d:232:LEU:HD13	5:b:176:PHE:HB2	1.88	0.55
3:D:77:PRO:HA	3:D:80:GLU:HB3	1.89	0.55
7:F:41:ARG:HH22	7:O:41:ARG:HH21	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:180:LEU:HB3	4:d:221:PHE:CZ	2.42	0.55
7:M:74:LEU:HD22	7:H:10:VAL:HG23	1.89	0.55
7:P:29:GLY:HA2	7:Q:31:ALA:HB2	1.88	0.55
7:F:22:ILE:HD11	7:P:19:LEU:HD22	1.89	0.55
8:A:373:PRO:HB3	8:A:480:LEU:HD12	1.89	0.55
6:e:75:VAL:HA	6:e:80:VAL:HG23	1.88	0.54
8:A:379:VAL:HG21	8:A:435:VAL:HG13	1.89	0.54
10:T:136:LEU:HD22	10:T:364:MET:HE1	1.88	0.54
4:d:84:LEU:O	4:d:88:LYS:HG3	2.08	0.54
8:A:369:SER:HB3	10:U:430:VAL:HB	1.90	0.54
7:G:29:GLY:HA3	7:I:27:GLY:HA2	1.90	0.54
9:B:97:GLU:OE2	9:B:127:SER:HB2	2.08	0.54
8:V:327:VAL:HG11	8:V:344:PHE:HE1	1.73	0.54
7:H:62:SER:HA	7:H:65:ILE:HD12	1.90	0.54
7:G:59:PHE:HZ	7:N:61:GLU:HB3	1.73	0.53
4:d:162:CYS:HA	4:d:165:PHE:HD2	1.72	0.53
7:F:50:ARG:HD3	7:F:54:LEU:HG	1.90	0.53
10:U:202:LEU:O	10:U:206:MET:HG2	2.07	0.53
6:e:46:VAL:HG23	6:e:69:MET:HA	1.91	0.53
7:F:23:GLY:HA3	7:O:22:ILE:HA	1.90	0.53
7:S:13:ALA:HB2	7:S:74:LEU:HD23	1.91	0.53
3:D:352:GLY:O	3:D:356:THR:HG23	2.09	0.53
10:T:270:GLN:O	10:T:274:GLU:HG3	2.09	0.53
1:a:49:ILE:O	1:a:53:LEU:HG	2.09	0.52
7:M:70:VAL:O	7:M:74:LEU:HG	2.09	0.52
7:O:60:MET:HA	7:O:63:LEU:HD12	1.91	0.52
4:d:197:LYS:HD3	5:b:176:PHE:CZ	2.45	0.52
7:L:54:LEU:HD11	7:O:55:LEU:HD23	1.91	0.52
7:F:49:ILE:HG12	7:O:36:VAL:HG23	1.92	0.52
10:E:296:MET:HE3	10:E:300:GLN:HE21	1.75	0.52
4:d:218:ILE:HG22	5:b:153:ARG:NH1	2.24	0.52
7:P:39:ILE:HG12	7:P:46:GLU:HA	1.92	0.52
8:A:291:VAL:O	8:A:294:LEU:HB3	2.09	0.52
7:H:73:ALA:HA	7:H:77:ALA:HB3	1.92	0.52
7:P:39:ILE:HG23	7:P:46:GLU:HB2	1.92	0.51
7:Q:23:GLY:O	7:Q:26:MET:HG2	2.10	0.51
3:D:137:ARG:HG3	3:D:220:ILE:HD13	1.91	0.51
7:F:25:GLY:HA3	7:P:23:GLY:HA3	1.91	0.51
7:G:59:PHE:CZ	7:N:61:GLU:HB3	2.45	0.51
7:H:56:SER:HB2	7:Q:57:PHE:CE2	2.45	0.51
7:M:37:GLU:O	7:M:41:ARG:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:137:ILE:HD13	10:U:196:THR:HG23	1.93	0.51
10:E:265:ILE:HG12	10:E:296:MET:HE1	1.91	0.51
7:K:36:VAL:HB	7:L:35:ALA:HA	1.93	0.51
6:e:22:ILE:HD11	6:e:80:VAL:HG11	1.93	0.51
7:K:26:MET:O	7:K:30:THR:HG22	2.11	0.51
7:K:28:GLN:HB3	7:L:60:MET:HE1	1.92	0.51
5:b:173:VAL:O	5:b:177:THR:HG23	2.11	0.51
7:I:39:ILE:HG22	7:J:48:LYS:NZ	2.25	0.51
7:L:68:LEU:HD21	7:O:66:TYR:HB3	1.93	0.50
10:T:37:LEU:HB2	10:T:53:CYS:SG	2.51	0.50
10:U:76:MET:O	10:U:79:MET:HG3	2.11	0.50
1:a:220:LEU:O	1:a:224:THR:HG23	2.11	0.50
7:I:32:ALA:O	7:I:36:VAL:HG23	2.11	0.50
10:T:193:GLY:HA3	10:T:267:ARG:HG3	1.93	0.50
6:e:5:ILE:O	6:e:5:ILE:HG13	2.11	0.50
7:N:38:GLY:HA2	7:N:41:ARG:HG2	1.93	0.50
7:P:17:VAL:HG21	7:Q:70:VAL:HG21	1.93	0.50
10:U:328:ALA:HB3	10:U:329:PRO:HD3	1.93	0.50
7:P:46:GLU:HG3	7:Q:48:LYS:HB3	1.92	0.50
10:T:153:ARG:HD2	10:T:364:MET:HE2	1.92	0.50
6:e:39:PRO:HB3	6:e:76:LYS:HA	1.94	0.50
6:e:115:VAL:O	6:e:119:VAL:HG12	2.12	0.49
7:L:28:GLN:HG3	7:L:60:MET:HG3	1.92	0.49
7:N:66:TYR:O	7:N:70:VAL:HG22	2.12	0.49
7:R:12:SER:HB3	7:S:11:VAL:HA	1.94	0.49
1:a:200:LEU:HD23	7:R:72:LEU:HD22	1.93	0.49
6:e:34:LEU:HD12	7:R:43:PRO:HD2	1.94	0.49
7:P:22:ILE:HD12	7:Q:22:ILE:HD11	1.94	0.49
7:O:50:ARG:CZ	7:O:50:ARG:HA	2.42	0.49
10:U:258:VAL:HG22	10:U:311:ILE:HG12	1.94	0.49
9:B:355:ARG:HB2	9:B:356:PRO:HD3	1.94	0.49
7:H:24:PRO:HD3	7:Q:22:ILE:HA	1.94	0.49
7:N:23:GLY:HA3	7:R:22:ILE:HA	1.95	0.49
5:b:90:LYS:O	5:b:94:GLU:HG2	2.12	0.49
6:e:21:GLU:HA	6:e:33:VAL:O	2.13	0.49
7:I:37:GLU:CG	7:J:34:TYR:HB3	2.42	0.49
7:J:6:ALA:O	7:J:10:VAL:HG13	2.13	0.49
7:R:52:ALA:HA	7:R:55:LEU:HD23	1.94	0.49
7:P:13:ALA:O	7:P:17:VAL:HG12	2.13	0.49
7:K:13:ALA:O	7:K:17:VAL:HG13	2.13	0.48
9:B:202:LYS:HE2	9:B:204:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:211:SER:O	2:p:215:LEU:HG	2.12	0.48
7:F:24:PRO:O	7:F:28:GLN:HG3	2.13	0.48
7:F:50:ARG:HD2	7:P:52:ALA:CB	2.41	0.48
7:O:65:ILE:HA	7:O:68:LEU:HD23	1.94	0.48
8:A:366:ARG:HH21	10:U:195:ARG:HH22	1.60	0.48
1:a:109:SER:OG	1:a:132:THR:HG23	2.14	0.48
1:a:138:THR:HB	1:a:188:SER:HB2	1.95	0.48
7:J:26:MET:O	7:J:30:THR:HG23	2.14	0.48
7:L:56:SER:O	7:L:60:MET:HE2	2.14	0.48
10:E:328:ALA:HB3	10:E:329:PRO:HD3	1.95	0.48
1:a:103:PHE:HB2	1:a:233:ALA:HB2	1.95	0.48
2:p:213:GLU:HG2	2:p:216:LYS:HE3	1.95	0.48
7:P:60:MET:HA	7:P:63:LEU:HD23	1.95	0.48
10:U:303:ILE:HD11	10:U:313:SER:HB2	1.95	0.48
2:p:142:LEU:O	2:p:146:THR:HG23	2.13	0.48
6:e:5:ILE:HD13	6:e:51:ILE:HD12	1.96	0.48
7:G:65:ILE:HG23	7:G:68:LEU:HD23	1.95	0.48
7:L:22:ILE:HD11	7:O:19:LEU:HG	1.96	0.48
10:E:192:VAL:HG22	10:E:239:VAL:HG13	1.95	0.48
10:U:241:LEU:O	10:U:245:THR:HG23	2.14	0.48
8:V:355:ARG:HA	8:V:355:ARG:HD3	1.70	0.48
5:b:149:MET:O	5:b:153:ARG:HG2	2.13	0.47
8:A:355:ARG:HB3	12:A:602:ATP:N6	2.29	0.47
10:E:26:ALA:HB3	10:E:29:GLN:HG2	1.96	0.47
2:p:185:VAL:O	2:p:189:ILE:HG12	2.14	0.47
5:b:136:ALA:O	5:b:139:GLN:HG3	2.14	0.47
10:T:191:GLY:HA2	10:T:263:ASP:HB3	1.96	0.47
5:b:151:ARG:HA	5:b:154:GLU:HG3	1.97	0.47
7:G:50:ARG:HH12	7:I:55:LEU:HD22	1.79	0.47
10:T:328:ALA:HB3	10:T:329:PRO:HD3	1.96	0.47
7:L:29:GLY:HA3	7:O:27:GLY:HA2	1.96	0.47
3:D:278:GLU:HB3	6:e:42:THR:HG22	1.97	0.47
4:d:197:LYS:O	4:d:201:LEU:HG	2.14	0.47
7:M:36:VAL:HG22	7:S:49:ILE:HG12	1.96	0.47
7:L:36:VAL:HB	7:O:35:ALA:HB2	1.95	0.47
7:L:68:LEU:HD21	7:O:66:TYR:CG	2.50	0.47
7:O:17:VAL:HA	7:O:67:GLY:HA3	1.96	0.47
7:R:59:PHE:CE1	7:S:57:PHE:HB3	2.49	0.47
10:T:15:GLN:HE21	8:V:69:ALA:HB2	1.80	0.47
10:U:351:ILE:HG23	10:U:422:SER:HB3	1.96	0.47
1:a:228:GLN:HA	1:a:231:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:ARG:HH11	7:I:52:ALA:HA	1.80	0.47
3:D:252:THR:O	10:E:404:SER:HB3	2.15	0.47
7:L:12:SER:HB3	7:L:74:LEU:HD13	1.97	0.47
7:L:14:GLY:HA2	7:O:16:ALA:HB2	1.97	0.47
4:d:146:LEU:O	4:d:150:VAL:HG23	2.15	0.47
7:G:28:GLN:HG3	7:G:60:MET:HG2	1.97	0.47
7:J:45:ALA:O	7:J:49:ILE:HG13	2.15	0.47
7:N:79:PRO:HG2	7:N:80:PHE:CE1	2.51	0.46
7:S:61:GLU:O	7:S:65:ILE:HG13	2.14	0.46
7:H:24:PRO:O	7:H:28:GLN:HG3	2.16	0.46
7:R:53:LEU:HG	7:R:57:PHE:CE2	2.50	0.46
6:e:21:GLU:HB2	6:e:34:LEU:HD23	1.97	0.46
7:M:36:VAL:O	7:M:39:ILE:HG22	2.16	0.46
2:p:119:ARG:HE	2:p:119:ARG:HA	1.81	0.46
2:p:174:TYR:OH	5:b:114:HIS:HB3	2.16	0.46
7:G:61:GLU:O	7:G:65:ILE:HG12	2.16	0.46
8:A:482:PHE:CE2	8:A:487:GLU:HG2	2.51	0.46
10:U:169:THR:O	10:U:173:MET:HG2	2.15	0.46
9:B:160:VAL:HG22	9:B:166:GLU:HG3	1.98	0.46
1:a:65:PRO:HA	1:a:69:GLN:HB3	1.96	0.46
3:D:46:SER:O	3:D:50:THR:HG23	2.14	0.46
7:F:41:ARG:HH22	7:O:41:ARG:NH2	2.13	0.46
3:D:126:TYR:HE1	3:D:208:THR:HG21	1.81	0.46
7:J:48:LYS:NZ	7:J:49:ILE:HG12	2.31	0.46
7:L:28:GLN:OE1	7:O:60:MET:HG3	2.16	0.46
7:P:17:VAL:HG11	7:Q:70:VAL:HG21	1.98	0.46
7:P:25:GLY:O	7:Q:27:GLY:HA3	2.16	0.46
7:Q:66:TYR:O	7:Q:70:VAL:HG22	2.15	0.46
8:A:248:GLU:HA	8:A:251:MET:HB3	1.97	0.46
1:a:31:GLY:C	1:a:33:TYR:H	2.24	0.46
7:R:56:SER:O	7:R:60:MET:HG2	2.15	0.46
10:T:43:ASN:HD21	8:V:49:MET:CE	2.23	0.46
7:M:26:MET:CE	7:H:26:MET:HB2	2.46	0.46
7:O:13:ALA:O	7:O:17:VAL:HG12	2.16	0.46
10:T:326:ASP:HB3	10:T:329:PRO:HD2	1.98	0.46
7:R:11:VAL:O	7:R:15:LEU:HG	2.16	0.45
9:B:49:MET:HE2	9:B:49:MET:HB3	1.84	0.45
10:T:39:ILE:HG12	10:T:81:VAL:HG22	1.98	0.45
7:F:23:GLY:N	7:F:24:PRO:HD2	2.31	0.45
7:H:24:PRO:HA	7:Q:25:GLY:HA3	1.98	0.45
8:A:25:LYS:HG2	8:A:27:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:91:LYS:O	5:b:95:ILE:HG22	2.16	0.45
10:T:242:THR:O	10:T:246:MET:HG3	2.16	0.45
1:a:97:PRO:HB3	2:p:101:MET:HE3	1.98	0.45
7:K:26:MET:CE	7:L:23:GLY:HA2	2.46	0.45
7:P:36:VAL:HG13	7:Q:49:ILE:HG12	1.98	0.45
10:E:203:TYR:CE2	10:E:207:LYS:HD2	2.52	0.45
8:A:433:GLU:HB3	8:A:462:ARG:HD3	1.98	0.45
2:p:131:LYS:HA	2:p:131:LYS:HD3	1.75	0.45
10:U:364:MET:HA	10:U:364:MET:HE2	1.98	0.45
5:b:94:GLU:O	5:b:97:GLU:HG2	2.16	0.45
7:K:33:GLY:CA	7:L:31:ALA:HA	2.46	0.45
9:B:374:LYS:HA	9:B:374:LYS:HE2	1.98	0.45
10:T:244:LEU:HD21	10:T:302:ARG:HB2	1.99	0.45
8:V:327:VAL:HG11	8:V:344:PHE:CE1	2.52	0.45
7:H:39:ILE:HG13	7:H:49:ILE:HG21	1.99	0.45
7:K:28:GLN:HG2	7:K:57:PHE:HD1	1.80	0.45
5:b:162:SER:HA	5:b:166:VAL:HG12	1.99	0.45
8:V:425:GLN:HA	12:V:602:ATP:C6	2.52	0.45
7:H:60:MET:HB2	7:H:63:LEU:HD11	1.99	0.44
7:L:28:GLN:HE22	7:O:59:PHE:HB3	1.82	0.44
7:L:54:LEU:HA	7:L:57:PHE:CD2	2.53	0.44
10:T:400:LEU:HD11	10:T:411:VAL:HG11	1.98	0.44
7:F:74:LEU:HA	7:O:75:LEU:HD11	1.99	0.44
7:I:44:GLU:H	7:I:44:GLU:CD	2.25	0.44
10:U:173:MET:HE1	10:U:202:LEU:HD13	2.00	0.44
7:M:25:GLY:O	7:S:60:MET:HE1	2.18	0.44
7:G:54:LEU:HA	7:G:57:PHE:HB2	2.00	0.44
7:P:17:VAL:HB	7:P:71:ALA:HB2	1.98	0.44
10:E:262:ILE:HD12	10:E:315:GLN:NE2	2.33	0.44
10:U:237:MET:HE1	10:U:275:VAL:HG21	2.00	0.44
8:A:52:GLU:HG2	8:A:53:LEU:H	1.82	0.44
3:D:78:PHE:C	3:D:78:PHE:CD2	2.95	0.44
5:b:93:GLN:HA	5:b:96:ARG:HG2	2.00	0.44
6:e:66:TYR:HB2	6:e:89:SER:HA	1.99	0.44
7:K:13:ALA:HB1	7:K:71:ALA:HB1	2.00	0.44
7:K:28:GLN:CB	7:L:60:MET:HE1	2.47	0.44
1:a:197:ALA:O	1:a:201:VAL:HG23	2.18	0.44
7:O:53:LEU:HD23	7:O:53:LEU:HA	1.85	0.44
7:S:6:ALA:HA	7:S:9:SER:HB2	2.00	0.44
6:e:114:GLY:O	6:e:118:LYS:HG2	2.18	0.44
4:d:126:ARG:HD3	4:d:150:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:181:ARG:HG3	4:d:212:VAL:HG23	1.99	0.43
7:H:28:GLN:HG2	7:H:60:MET:HE2	2.00	0.43
7:J:29:GLY:HA3	7:K:27:GLY:CA	2.48	0.43
7:R:51:GLY:O	7:R:54:LEU:HG	2.18	0.43
10:E:263:ASP:O	10:E:316:ALA:HB3	2.18	0.43
2:p:174:TYR:O	2:p:178:LYS:HG2	2.18	0.43
7:M:57:PHE:CE2	7:S:59:PHE:HB3	2.53	0.43
4:d:75:GLU:HB2	4:d:154:ARG:HH12	1.84	0.43
7:G:50:ARG:NH1	7:I:55:LEU:HD22	2.34	0.43
9:B:176:LYS:HG2	9:B:345:LEU:HD12	2.00	0.43
9:B:376:MET:O	9:B:376:MET:HG3	2.18	0.43
10:T:206:MET:SD	10:T:211:VAL:HG21	2.59	0.43
7:M:59:PHE:HB2	7:H:57:PHE:CZ	2.53	0.43
7:M:73:ALA:HA	7:M:77:ALA:HB3	1.99	0.43
7:I:54:LEU:O	7:I:57:PHE:HB2	2.19	0.43
8:V:152:VAL:HG22	8:V:434:GLN:HG2	2.00	0.43
7:F:79:PRO:HD2	7:O:75:LEU:HD22	1.98	0.43
1:a:40:LEU:HD23	2:p:93:MET:HE3	2.01	0.43
7:M:23:GLY:CA	7:H:22:ILE:HA	2.48	0.43
7:N:59:PHE:CE2	7:R:57:PHE:HB3	2.54	0.43
8:A:345:LEU:HA	8:A:357:ALA:O	2.19	0.43
10:T:148:LEU:HD12	10:T:374:HIS:CE1	2.53	0.43
5:b:135:LYS:HE3	5:b:135:LYS:HB3	1.83	0.43
7:J:33:GLY:O	7:J:37:GLU:HG2	2.19	0.43
7:J:52:ALA:O	7:J:55:LEU:HB3	2.19	0.43
8:V:49:MET:HG3	8:V:52:GLU:HB2	2.00	0.43
2:p:170:LEU:O	2:p:173:THR:HG22	2.18	0.43
4:d:225:TYR:CD2	4:d:226:GLY:N	2.87	0.43
7:L:29:GLY:HA3	7:O:27:GLY:CA	2.49	0.43
8:A:145:GLU:HA	8:A:146:PRO:HD3	1.89	0.43
2:p:170:LEU:HD21	5:b:111:VAL:HG13	2.01	0.43
7:K:65:ILE:O	7:K:69:VAL:HG23	2.18	0.43
7:L:10:VAL:HG21	7:O:9:SER:HA	1.99	0.43
7:P:59:PHE:O	7:P:63:LEU:HD23	2.19	0.43
7:Q:70:VAL:O	7:Q:74:LEU:HG	2.19	0.43
10:E:244:LEU:O	10:E:248:GLU:HG3	2.19	0.43
5:b:130:ALA:HA	5:b:133:GLN:HE21	1.84	0.42
5:b:151:ARG:O	5:b:154:GLU:HG3	2.19	0.42
10:E:99:ARG:NH2	10:E:111:MET:HB2	2.34	0.42
7:M:52:ALA:O	7:M:55:LEU:HB3	2.19	0.42
7:H:70:VAL:O	7:H:74:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:29:GLY:HA2	7:O:31:ALA:HB2	2.01	0.42
9:B:130:ILE:HG23	9:B:241:TYR:HB3	2.01	0.42
10:E:364:MET:HE2	10:E:364:MET:HB3	1.97	0.42
9:B:375:ALA:C	9:B:377:LYS:H	2.27	0.42
3:D:324:LYS:HB3	3:D:324:LYS:HE3	1.81	0.42
6:e:97:GLU:HA	6:e:100:ASP:OD1	2.18	0.42
7:H:44:GLU:OE1	7:Q:43:PRO:HG2	2.19	0.42
7:H:62:SER:HA	7:H:65:ILE:HB	2.01	0.42
9:B:375:ALA:O	9:B:376:MET:HB3	2.19	0.42
8:V:471:LYS:HA	8:V:474:GLU:HG2	2.01	0.42
6:e:117:GLU:HA	6:e:120:GLU:HG2	2.01	0.42
9:B:184:ILE:HD11	9:B:260:ILE:HD13	2.02	0.42
10:U:103:VAL:HG22	10:U:239:VAL:HB	2.01	0.42
5:b:58:ASN:O	5:b:61:VAL:HG12	2.18	0.42
10:E:389:LYS:HE2	10:E:389:LYS:HB3	1.84	0.42
8:V:26:MET:HE3	8:V:26:MET:HB3	1.90	0.42
5:b:60:ILE:HA	5:b:63:ASN:OD1	2.20	0.42
7:N:63:LEU:HD11	7:R:28:GLN:CD	2.45	0.42
7:P:46:GLU:CG	7:Q:48:LYS:HB3	2.50	0.42
7:R:37:GLU:OE2	7:R:37:GLU:HA	2.20	0.42
3:D:76:ARG:HH12	3:D:247:ILE:HG13	1.85	0.42
4:d:86:ASP:OD2	4:d:86:ASP:C	2.62	0.42
10:T:203:TYR:CZ	10:T:207:LYS:HD2	2.55	0.42
4:d:90:LYS:O	4:d:91:LEU:HD23	2.20	0.42
4:d:110:LYS:HG3	4:d:111:LEU:HG	2.01	0.42
7:F:10:VAL:HG11	7:P:9:SER:HA	2.01	0.42
7:J:45:ALA:HB1	7:J:48:LYS:HE3	2.02	0.42
7:P:65:ILE:O	7:P:69:VAL:HG23	2.20	0.42
8:V:425:GLN:HG2	8:V:426:SER:N	2.35	0.42
7:P:60:MET:O	7:P:63:LEU:HB2	2.20	0.42
8:A:404:ASP:O	8:A:408:GLN:HG3	2.20	0.42
10:U:326:ASP:HB3	10:U:329:PRO:HD2	2.01	0.42
10:U:440:SER:O	10:U:444:THR:HG23	2.20	0.42
8:V:344:PHE:CD2	8:V:362:ILE:HG12	2.55	0.42
7:F:29:GLY:CA	7:P:27:GLY:HA2	2.50	0.41
7:O:7:ALA:O	7:O:11:VAL:HB	2.20	0.41
10:E:17:ILE:O	10:E:20:VAL:HG22	2.20	0.41
7:L:41:ARG:HA	7:O:41:ARG:CD	2.50	0.41
7:S:33:GLY:O	7:S:36:VAL:HG12	2.20	0.41
8:V:390:PHE:HE1	8:V:411:LEU:HD13	1.84	0.41
3:D:226:MET:HG3	3:D:227:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:65:ILE:HD12	7:K:65:ILE:HA	1.94	0.41
10:U:17:ILE:O	10:U:20:VAL:HG22	2.20	0.41
1:a:151:TYR:HA	1:a:154:ILE:HG12	2.02	0.41
7:I:39:ILE:HG22	7:J:48:LYS:HZ3	1.85	0.41
9:B:403:LEU:HD13	9:B:407:THR:HG21	2.01	0.41
2:p:149:LYS:HD2	2:p:152:ARG:HH22	1.85	0.41
4:d:120:VAL:O	4:d:125:LYS:HE3	2.20	0.41
6:e:29:GLY:HA3	7:M:41:ARG:NH1	2.36	0.41
7:M:67:GLY:HA2	7:H:17:VAL:HG11	2.01	0.41
7:N:35:ALA:HA	7:R:36:VAL:HG11	2.03	0.41
7:R:19:LEU:O	7:R:22:ILE:HG22	2.21	0.41
9:B:197:VAL:O	9:B:262:ASP:HB2	2.19	0.41
10:U:380:SER:O	10:U:384:THR:HG23	2.20	0.41
7:F:28:GLN:OE1	7:P:60:MET:HB3	2.21	0.41
7:J:72:LEU:HD13	7:J:72:LEU:HA	1.95	0.41
6:e:41:ILE:HG13	6:e:72:PHE:HE2	1.86	0.41
7:Q:50:ARG:HA	7:Q:53:LEU:HB3	2.03	0.41
10:E:326:ASP:OD1	10:E:327:PRO:HD2	2.20	0.41
10:T:368:TRP:CE3	10:T:369:ILE:HG23	2.56	0.41
5:b:122:GLN:HA	5:b:125:LYS:HE3	2.01	0.41
7:F:74:LEU:O	7:F:78:ASN:HB2	2.21	0.41
10:T:10:MET:HB3	10:T:10:MET:HE3	1.74	0.41
10:U:55:VAL:HG13	10:U:64:VAL:HG13	2.03	0.41
10:U:395:ILE:HG12	10:U:403:LEU:HD11	2.02	0.41
1:a:109:SER:OG	1:a:131:PRO:HD2	2.21	0.41
4:d:225:TYR:HD2	9:B:26:MET:SD	2.43	0.41
7:M:63:LEU:HD22	7:H:64:THR:HB	2.02	0.41
7:J:26:MET:HB3	7:K:23:GLY:O	2.21	0.41
7:Q:56:SER:O	7:Q:60:MET:HG2	2.20	0.41
8:A:331:ILE:HB	8:A:332:PRO:HD3	2.02	0.41
9:B:284:ARG:O	9:B:285:GLU:HB2	2.20	0.41
10:U:37:LEU:HB2	10:U:53:CYS:SG	2.61	0.41
3:D:81:ASN:HD21	6:e:8:LEU:HD12	1.85	0.41
3:D:161:PHE:HD1	3:D:161:PHE:HA	1.74	0.41
7:M:33:GLY:O	7:M:36:VAL:HG12	2.21	0.41
7:G:32:ALA:O	7:G:36:VAL:HG12	2.22	0.41
7:G:45:ALA:O	7:G:49:ILE:HG22	2.21	0.40
7:G:50:ARG:NH1	7:I:52:ALA:HA	2.36	0.40
10:U:215:LYS:H	10:U:215:LYS:HG2	1.57	0.40
5:b:148:ILE:HD13	5:b:148:ILE:HA	1.96	0.40
7:F:46:GLU:HB2	7:P:48:LYS:NZ	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:213:VAL:HG12	10:E:216:ASN:H	1.85	0.40
7:J:27:GLY:C	7:J:60:MET:HE1	2.47	0.40
7:P:26:MET:HE1	7:Q:30:THR:OG1	2.21	0.40
7:R:19:LEU:HD11	7:S:18:GLY:HA2	2.03	0.40
9:B:157:MET:SD	9:B:360:VAL:HG21	2.61	0.40
9:B:475:ILE:HG21	9:B:486:ALA:HB2	2.03	0.40
10:T:296:MET:HE2	10:T:296:MET:HB2	1.93	0.40
6:e:3:LEU:HG	6:e:19:ALA:O	2.21	0.40
7:K:28:GLN:HG3	7:K:60:MET:HB2	2.03	0.40
7:L:59:PHE:O	7:L:63:LEU:HG	2.21	0.40
7:R:65:ILE:HG13	7:R:66:TYR:N	2.35	0.40
8:A:284:ARG:O	8:A:285:GLU:HB2	2.21	0.40
10:T:15:GLN:HB2	10:T:22:ASP:HB2	2.02	0.40
8:V:152:VAL:HG23	8:V:423:GLN:NE2	2.36	0.40
9:B:331:ILE:O	9:B:335:VAL:HG23	2.20	0.40
10:E:203:TYR:CZ	10:E:207:LYS:HD2	2.57	0.40
10:T:263:ASP:O	10:T:316:ALA:HB3	2.21	0.40
8:V:100:VAL:HG11	8:V:249:TYR:HB2	2.03	0.40
8:V:151:LEU:HD11	8:V:179:ILE:HG12	2.03	0.40
8:V:390:PHE:CG	8:V:414:GLY:HA3	2.56	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	221/223 (99%)	209 (95%)	12 (5%)	0	100	100
2	p	127/129 (98%)	127 (100%)	0	0	100	100
3	D	320/322 (99%)	313 (98%)	7 (2%)	0	100	100
4	d	171/173 (99%)	163 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	150/152 (99%)	150 (100%)	0	0	100	100
6	e	126/136 (93%)	121 (96%)	5 (4%)	0	100	100
7	F	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
7	G	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
7	H	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
7	I	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
7	J	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
7	K	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
7	L	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
7	M	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
7	N	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
7	O	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
7	P	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
7	Q	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
7	R	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
7	S	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
8	A	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
8	V	482/484 (100%)	459 (95%)	23 (5%)	0	100	100
9	B	480/482 (100%)	465 (97%)	15 (3%)	0	100	100
10	E	473/475 (100%)	454 (96%)	19 (4%)	0	100	100
10	T	473/475 (100%)	455 (96%)	18 (4%)	0	100	100
10	U	473/475 (100%)	456 (96%)	17 (4%)	0	100	100
All	All	5056/5116 (99%)	4881 (96%)	175 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	187/187 (100%)	187 (100%)	0	100 100
2	p	111/111 (100%)	111 (100%)	0	100 100
3	D	267/267 (100%)	261 (98%)	6 (2%)	45 71
4	d	148/148 (100%)	144 (97%)	4 (3%)	39 68
5	b	134/134 (100%)	134 (100%)	0	100 100
6	e	103/107 (96%)	97 (94%)	6 (6%)	18 51
7	F	51/51 (100%)	50 (98%)	1 (2%)	48 72
7	G	51/51 (100%)	50 (98%)	1 (2%)	48 72
7	H	51/51 (100%)	50 (98%)	1 (2%)	48 72
7	I	51/51 (100%)	51 (100%)	0	100 100
7	J	51/51 (100%)	51 (100%)	0	100 100
7	K	51/51 (100%)	50 (98%)	1 (2%)	48 72
7	L	51/51 (100%)	51 (100%)	0	100 100
7	M	51/51 (100%)	50 (98%)	1 (2%)	48 72
7	N	51/51 (100%)	51 (100%)	0	100 100
7	O	51/51 (100%)	50 (98%)	1 (2%)	48 72
7	P	51/51 (100%)	51 (100%)	0	100 100
7	Q	51/51 (100%)	51 (100%)	0	100 100
7	R	51/51 (100%)	49 (96%)	2 (4%)	28 62
7	S	51/51 (100%)	50 (98%)	1 (2%)	48 72
8	A	380/380 (100%)	376 (99%)	4 (1%)	65 79
8	V	380/380 (100%)	374 (98%)	6 (2%)	55 75
9	B	379/379 (100%)	379 (100%)	0	100 100
10	E	389/389 (100%)	384 (99%)	5 (1%)	61 78
10	T	389/389 (100%)	384 (99%)	5 (1%)	61 78
10	U	389/389 (100%)	383 (98%)	6 (2%)	57 76
All	All	3970/3974 (100%)	3919 (99%)	51 (1%)	59 78

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	123	CYS
3	D	167	TYR
3	D	203	VAL

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Mol	Chain	Res	Type
3	D	206	VAL
3	D	229	MET
3	D	247	ILE
4	d	161	ILE
4	d	172	MET
4	d	221	PHE
4	d	223	VAL
6	e	1	MET
6	e	9	THR
6	e	42	THR
6	e	51	ILE
6	e	82	ILE
6	e	135	VAL
7	M	12	SER
7	F	19	LEU
7	G	10	VAL
7	H	22	ILE
7	K	15	LEU
7	O	36	VAL
7	R	55	LEU
7	R	66	TYR
7	S	69	VAL
8	A	70	ASN
8	A	199	ILE
8	A	237	TYR
8	A	476	LEU
10	E	20	VAL
10	E	61	ASP
10	E	242	THR
10	E	258	VAL
10	E	352	TYR
10	T	10	MET
10	T	116	VAL
10	T	228	GLN
10	T	242	THR
10	T	295	GLU
10	U	10	MET
10	U	17	ILE
10	U	39	ILE
10	U	215	LYS
10	U	258	VAL
10	U	352	TYR

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Mol	Chain	Res	Type
8	V	98	ILE
8	V	100	VAL
8	V	234	THR
8	V	263	ASP
8	V	300	GLU
8	V	450	GLU

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

Mol	Chain	Res	Type
1	a	194	ASN
3	D	317	ASN
3	D	322	ASN
4	d	117	ASN
4	d	188	GLN
5	b	133	GLN
5	b	170	ASN
6	e	108	ASN
7	L	28	GLN
7	Q	42	GLN
7	R	28	GLN
8	A	295	HIS
8	A	389	GLN
10	E	70	ASN
10	E	256	GLN
10	E	366	GLN
10	E	462	GLN
10	T	9	ASN
10	T	15	GLN
10	T	43	ASN
10	T	56	GLN
10	T	62	ASN
10	T	264	ASN
10	T	366	GLN
10	T	374	HIS
10	U	70	ASN
10	U	254	ASN
10	U	386	GLN
8	V	295	HIS
8	V	372	GLN
8	V	398	GLN
8	V	443	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
12	ATP	V	602	11	29,33,33	0.33	0	44,52,52	0.50	1 (2%)
12	ATP	B	600	11	29,33,33	0.33	0	44,52,52	0.49	0
12	ATP	A	602	11	29,33,33	0.35	0	44,52,52	0.55	1 (2%)
12	ATP	T	501	-	29,33,33	0.31	0	44,52,52	0.49	1 (2%)
12	ATP	U	501	-	29,33,33	0.31	0	44,52,52	0.49	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ATP	V	602	11	-	0/22/38/38	0/3/3/3
12	ATP	B	600	11	-	0/22/38/38	0/3/3/3
12	ATP	A	602	11	-	2/22/38/38	0/3/3/3
12	ATP	T	501	-	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ATP	U	501	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	U	501	ATP	PB-O3B-PG	2.10	140.03	132.83
12	T	501	ATP	PB-O3B-PG	2.02	139.75	132.83
12	A	602	ATP	PB-O3B-PG	2.01	139.72	132.83
12	V	602	ATP	PB-O3B-PG	2.00	139.70	132.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	T	501	ATP	C5'-O5'-PA-O1A
12	T	501	ATP	C4'-C5'-O5'-PA
12	U	501	ATP	PB-O3B-PG-O2G
12	U	501	ATP	C3'-C4'-C5'-O5'
12	T	501	ATP	C3'-C4'-C5'-O5'
12	U	501	ATP	C4'-C5'-O5'-PA
12	U	501	ATP	O4'-C4'-C5'-O5'
12	T	501	ATP	O4'-C4'-C5'-O5'
12	A	602	ATP	O4'-C1'-N9-C4
12	A	602	ATP	O4'-C1'-N9-C8
12	T	501	ATP	C5'-O5'-PA-O3A
12	U	501	ATP	C5'-O5'-PA-O3A
12	T	501	ATP	PB-O3A-PA-O1A
12	T	501	ATP	PB-O3A-PA-O2A
12	U	501	ATP	C5'-O5'-PA-O2A
12	U	501	ATP	PB-O3B-PG-O1G

There are no ring outliers.

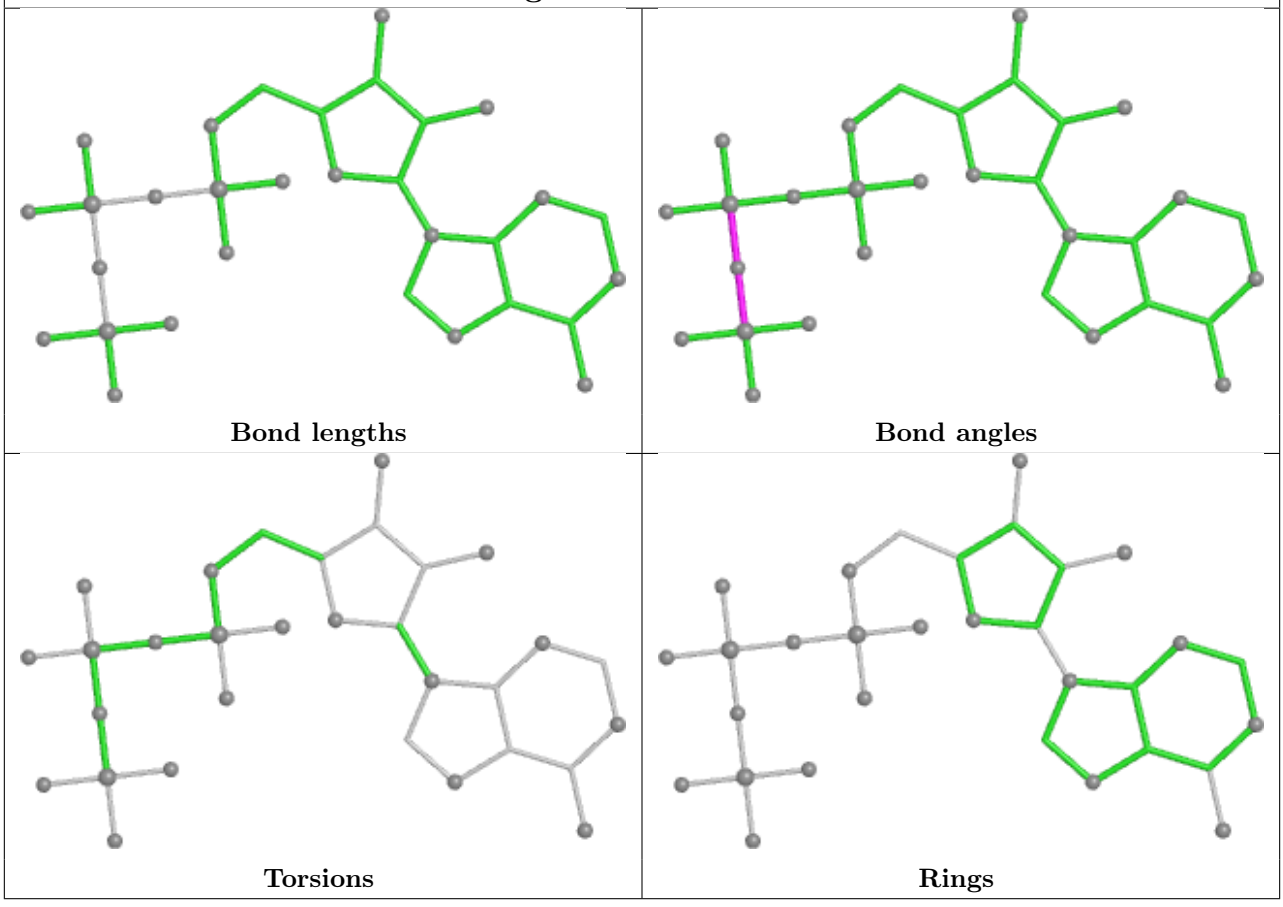
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	V	602	ATP	1	0
12	A	602	ATP	1	0

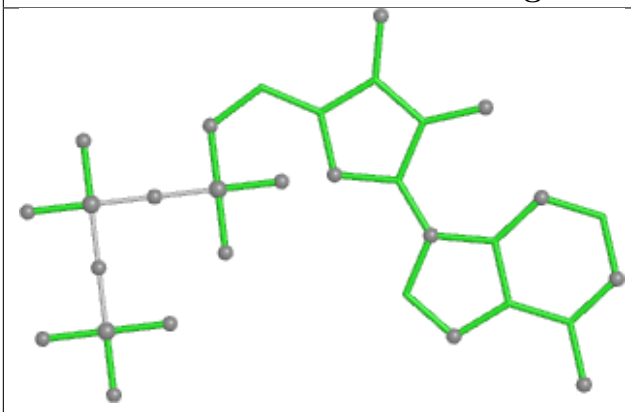
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

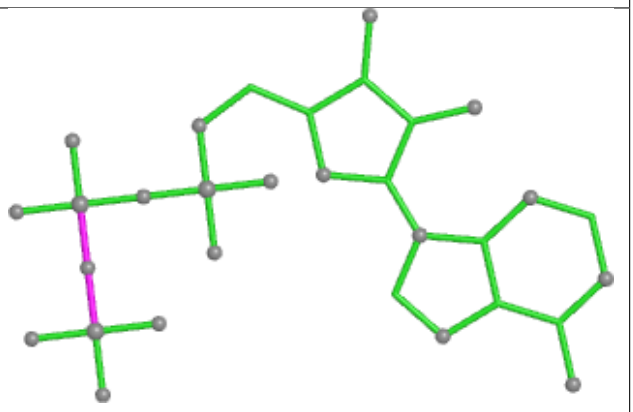
Ligand ATP V 602



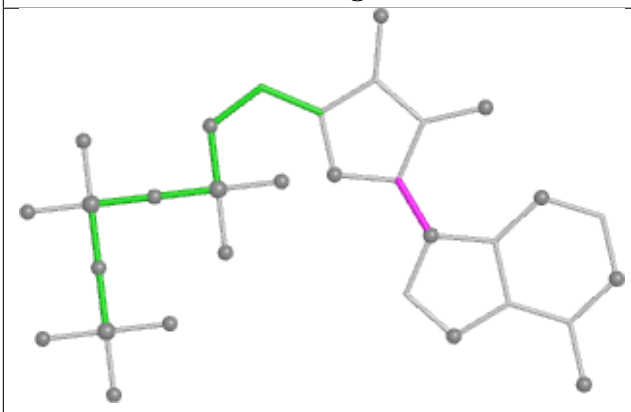
Ligand ATP A 602



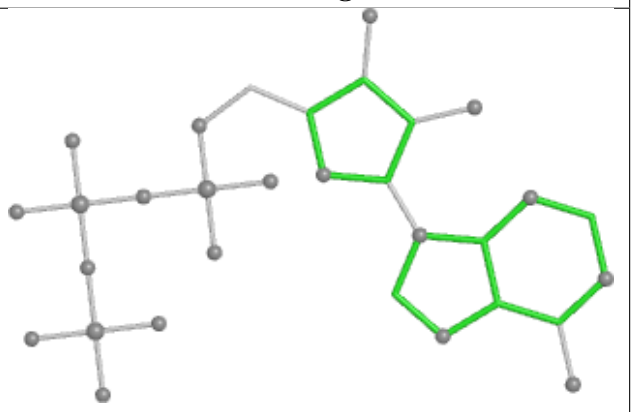
Bond lengths



Bond angles

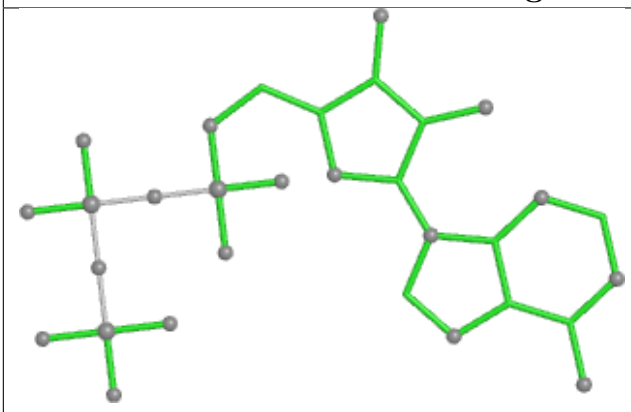


Torsions

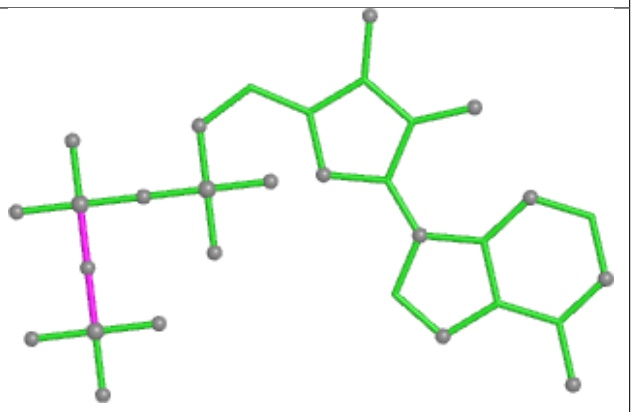


Rings

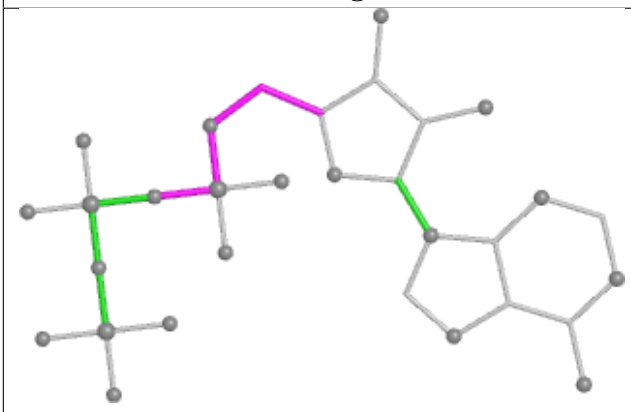
Ligand ATP T 501



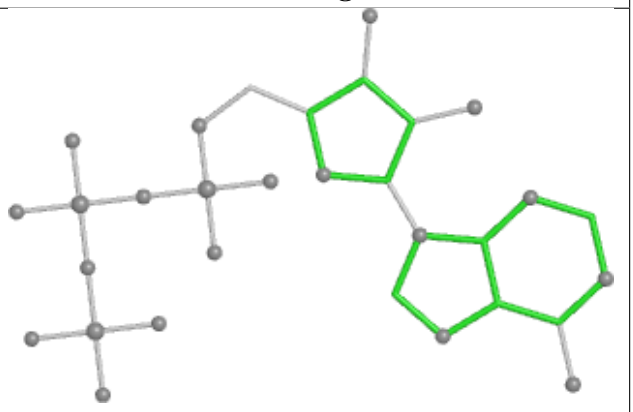
Bond lengths



Bond angles

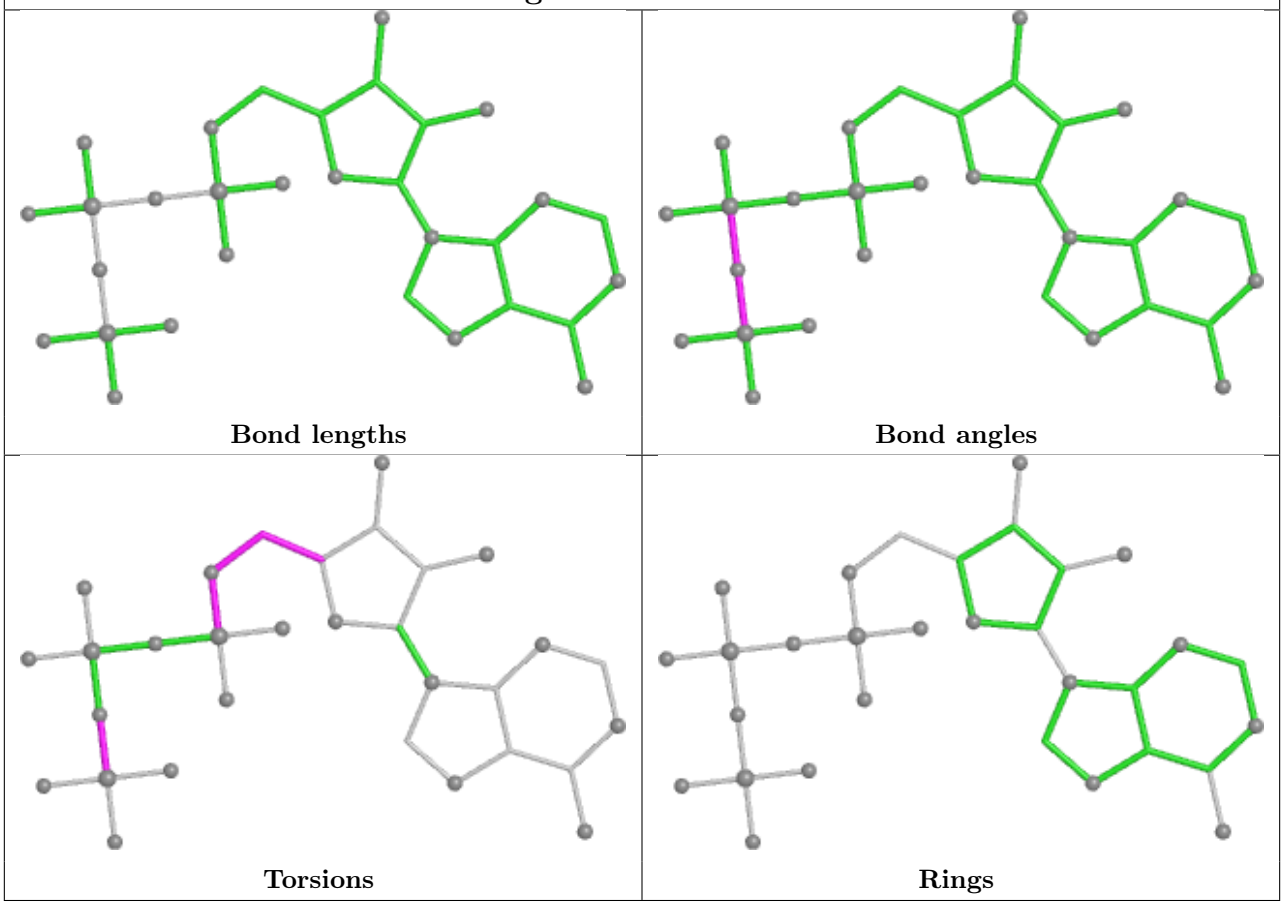


Torsions



Rings

Ligand ATP U 501



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.

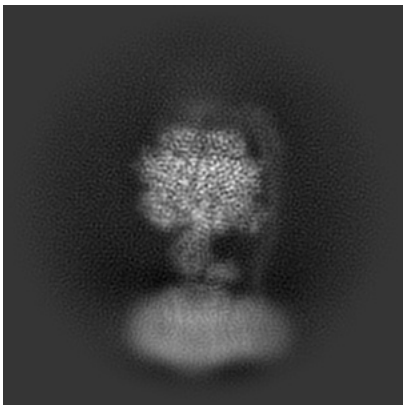
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-68717. These allow visual inspection of the internal detail of the map and identification of artifacts.

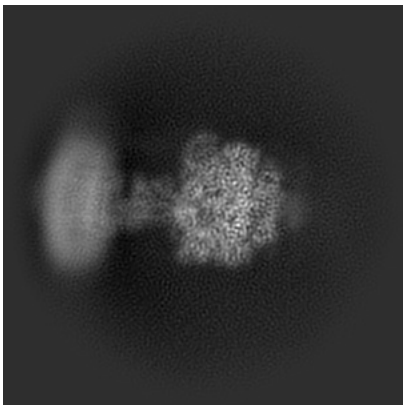
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

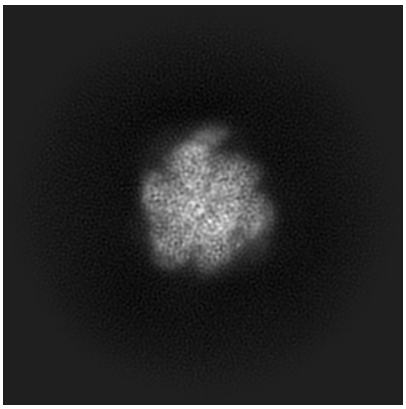
6.1.1 Primary map



X

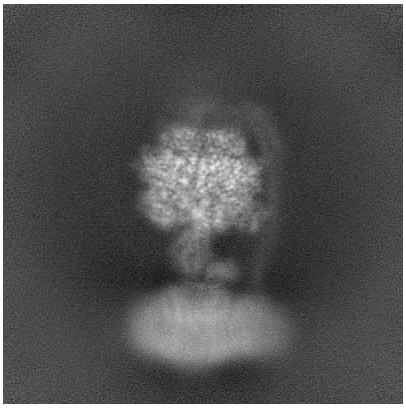


Y

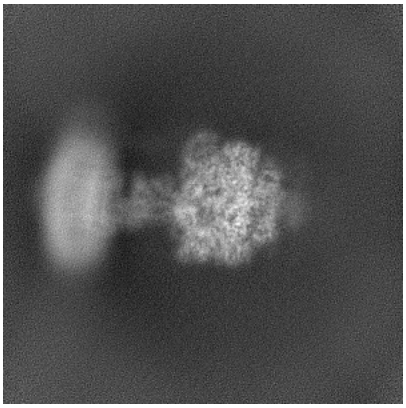


Z

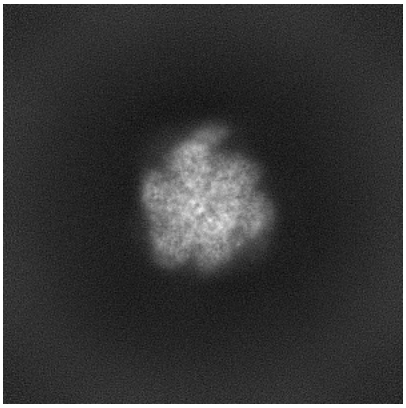
6.1.2 Raw map



X



Y

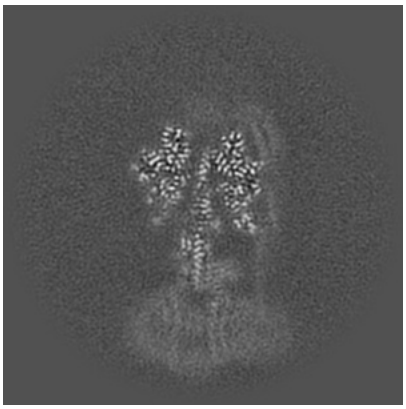


Z

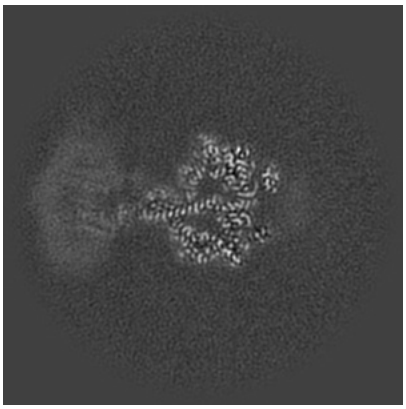
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

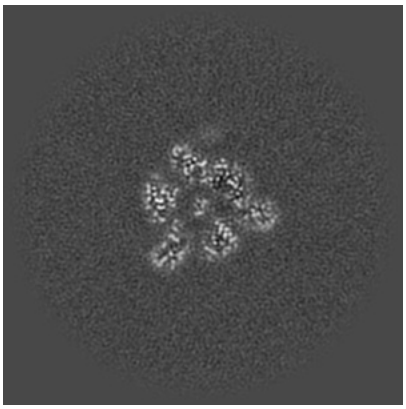
6.2.1 Primary map



X Index: 200

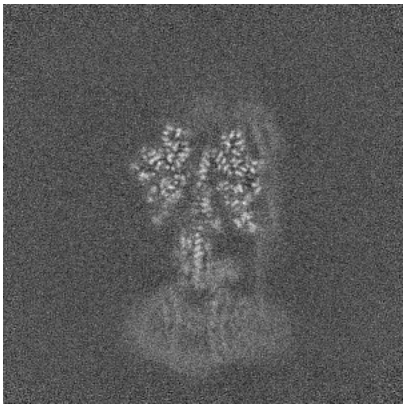


Y Index: 200

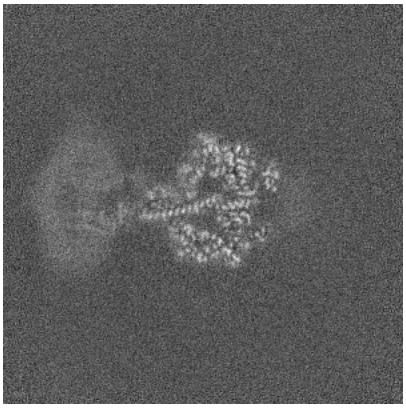


Z Index: 200

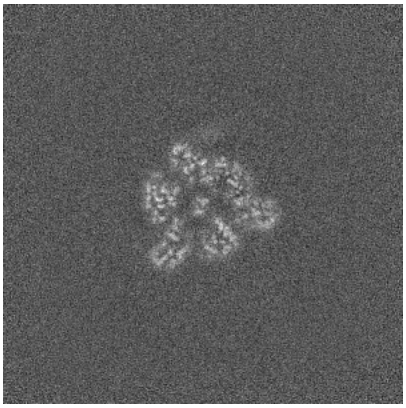
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

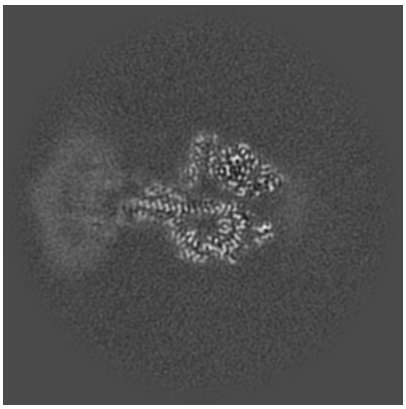
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

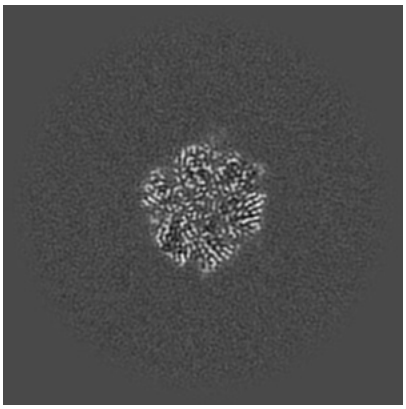
6.3.1 Primary map



X Index: 199

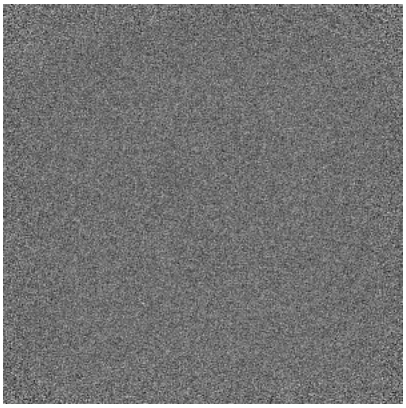


Y Index: 196

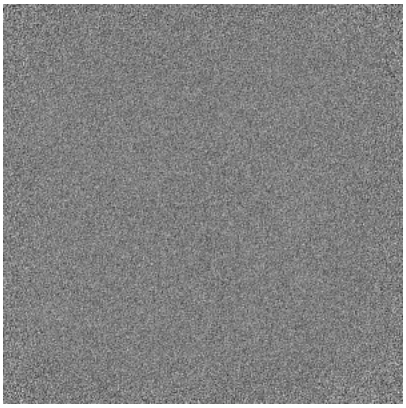


Z Index: 235

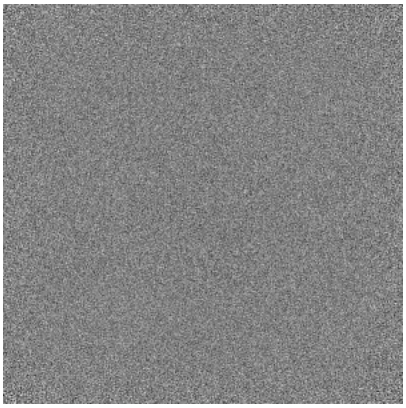
6.3.2 Raw map



X Index: 0



Y Index: 0

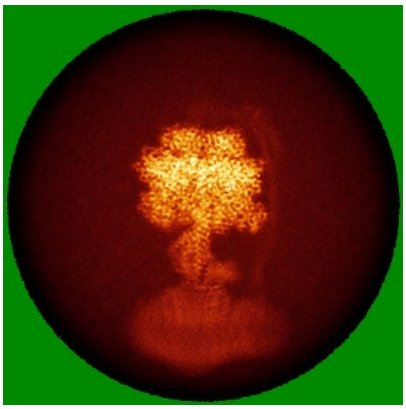


Z Index: 399

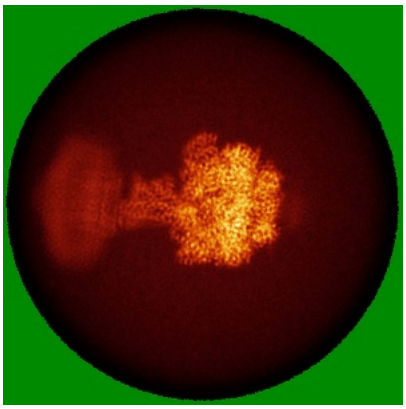
The images above show the largest variance slices of the map in three orthogonal directions.

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

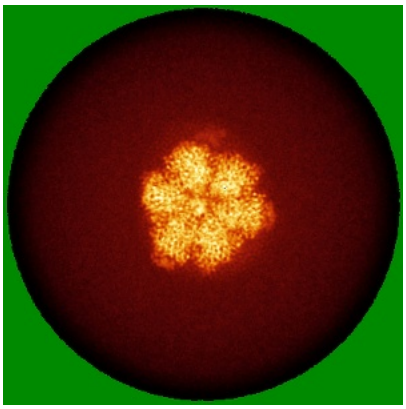
6.4.1 Primary map



X

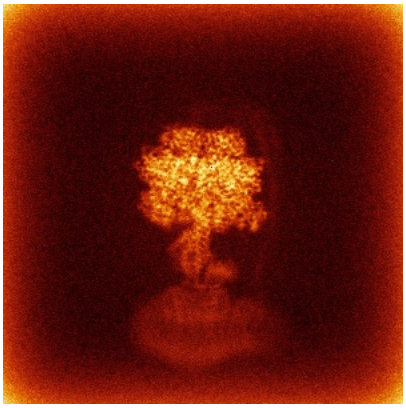


Y

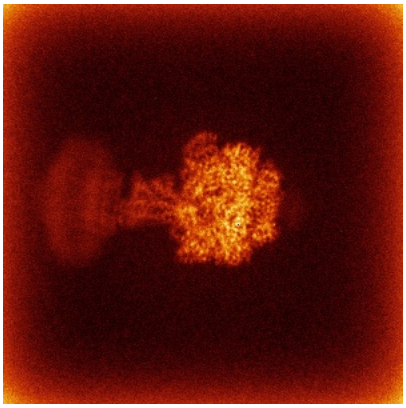


Z

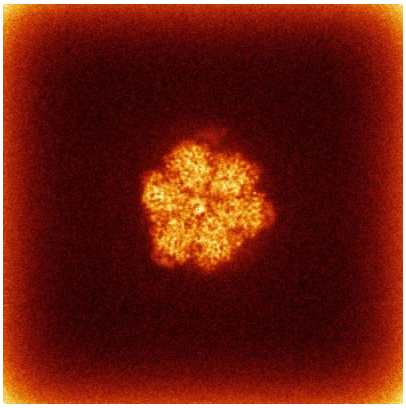
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

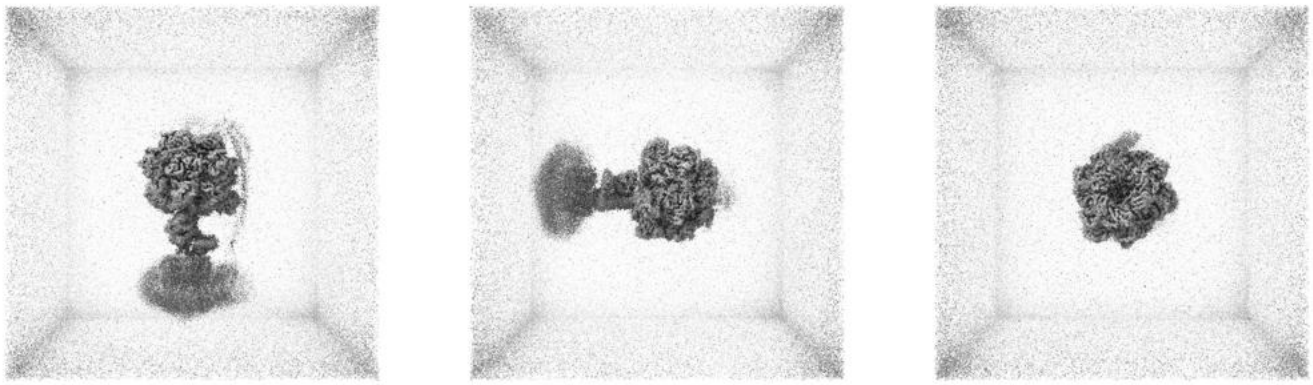
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

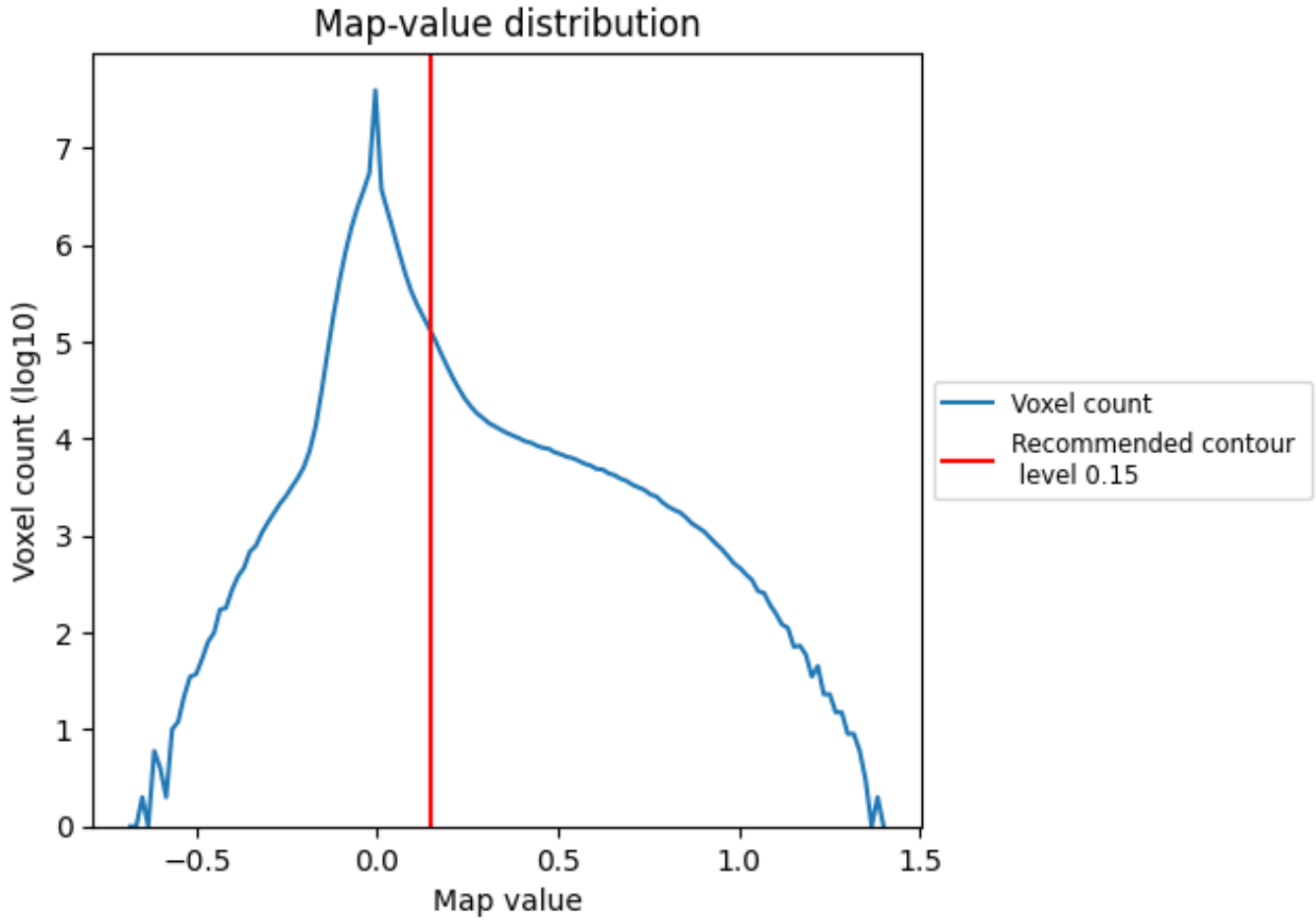
6.6 Mask visualisation (i)

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

7 Map analysis

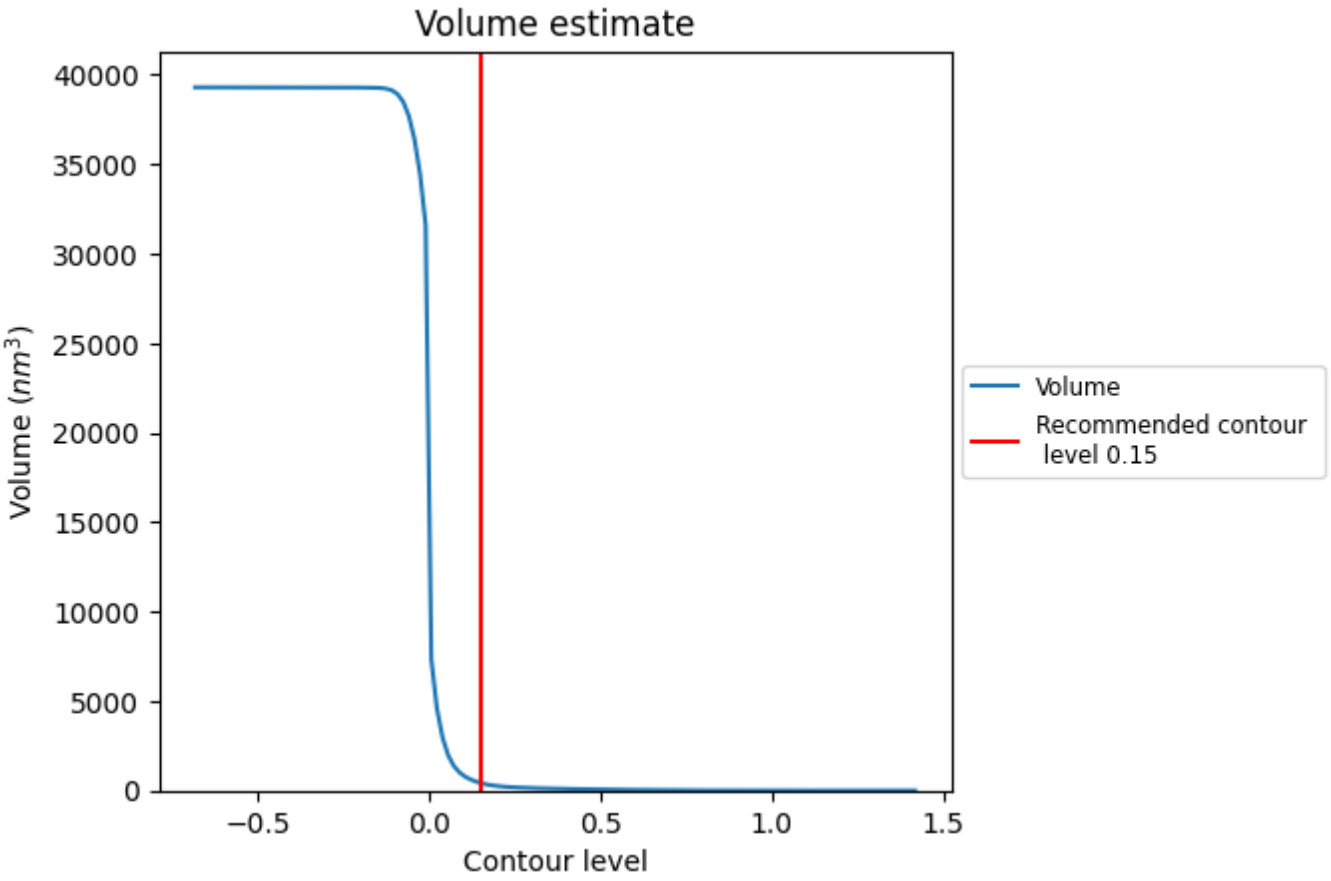
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

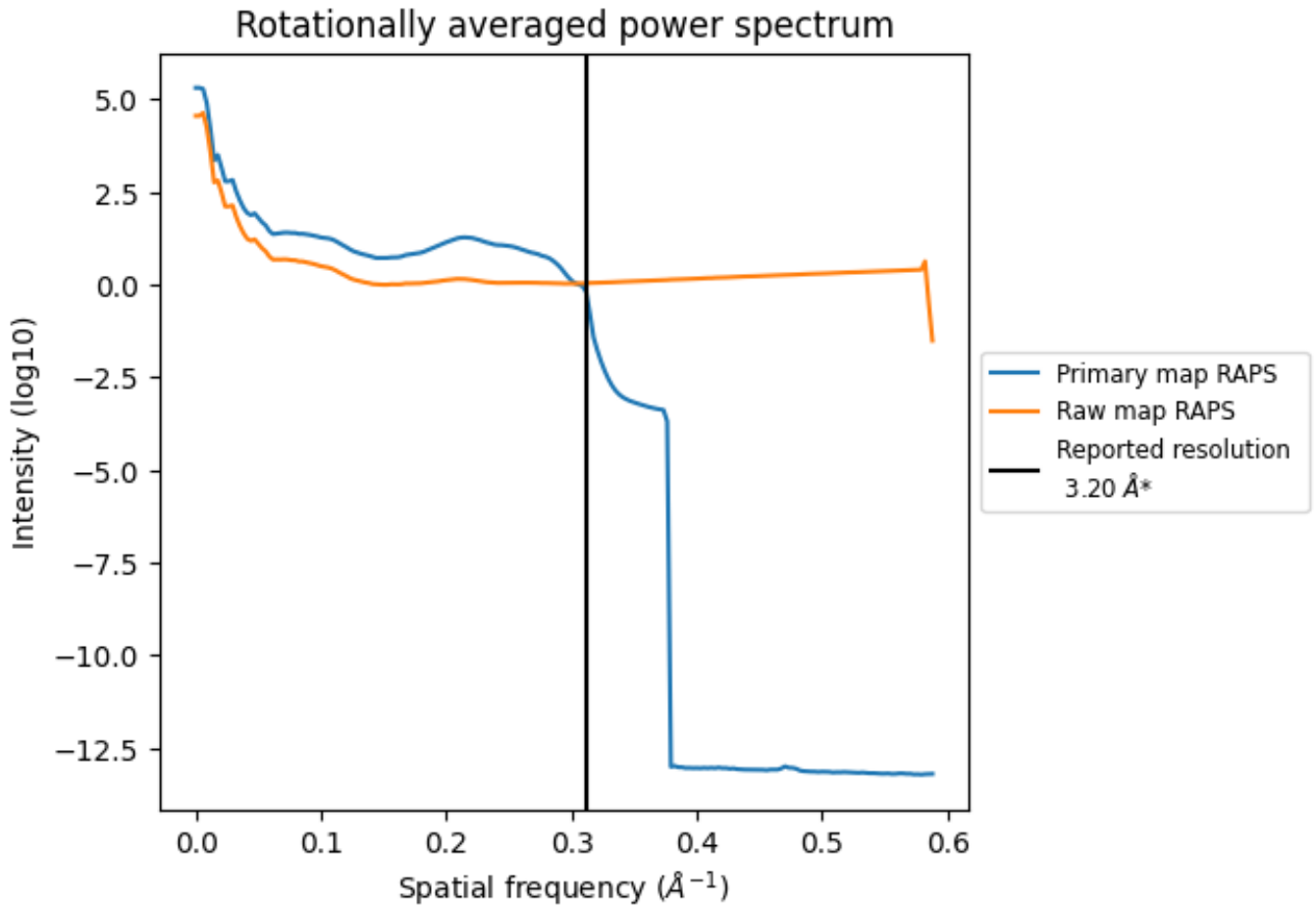
7.2 Volume estimate



The volume at the recommended contour level is 426 nm^3; this corresponds to an approximate mass of 385 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

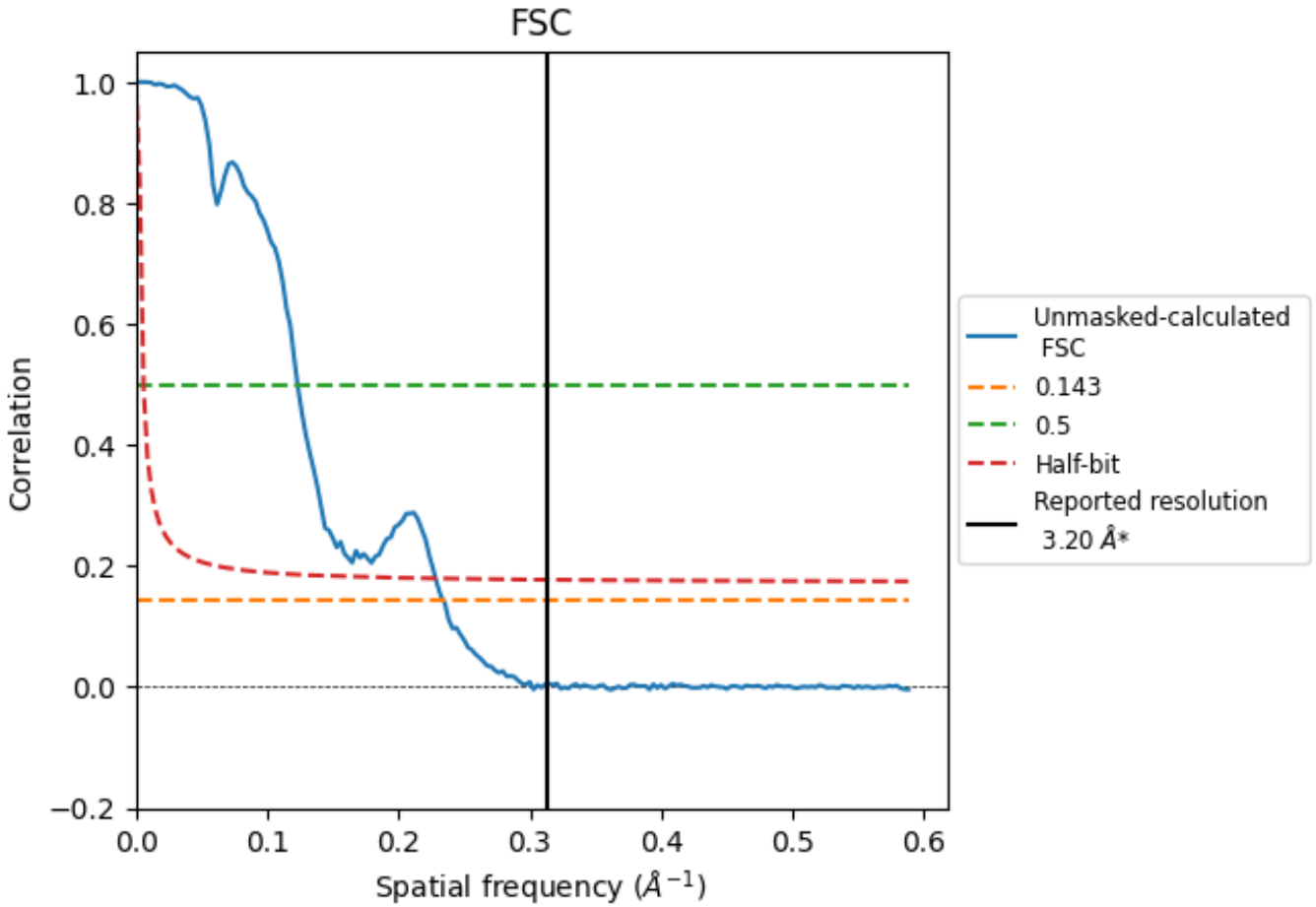


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

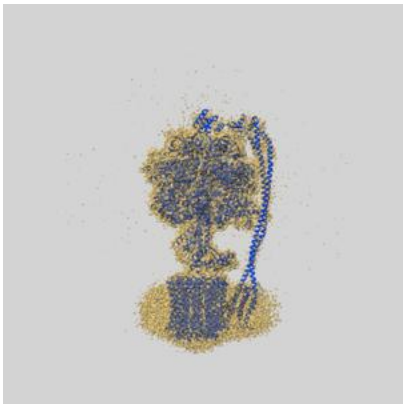
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.27	8.12	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.2 by more than 10 %

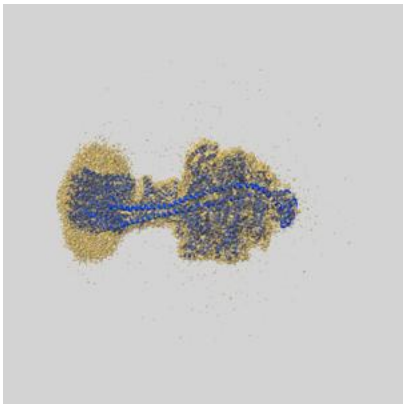
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-68717 and PDB model 22VL. Per-residue inclusion information can be found in section 3 on page 8.

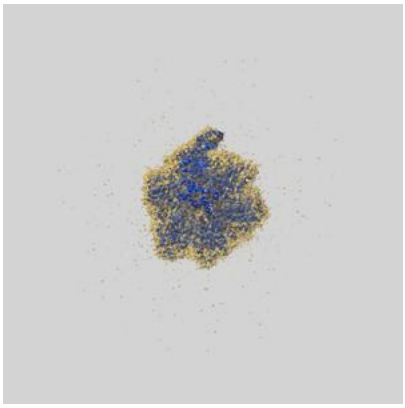
9.1 Map-model overlay



X



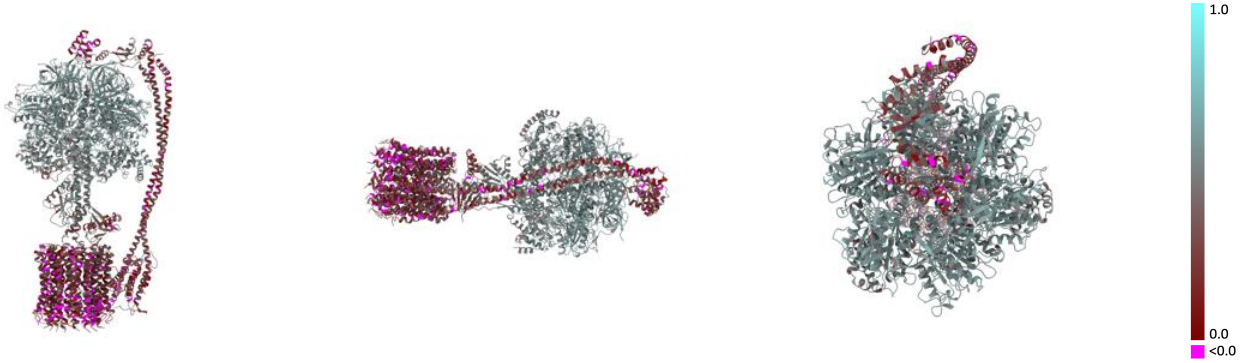
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

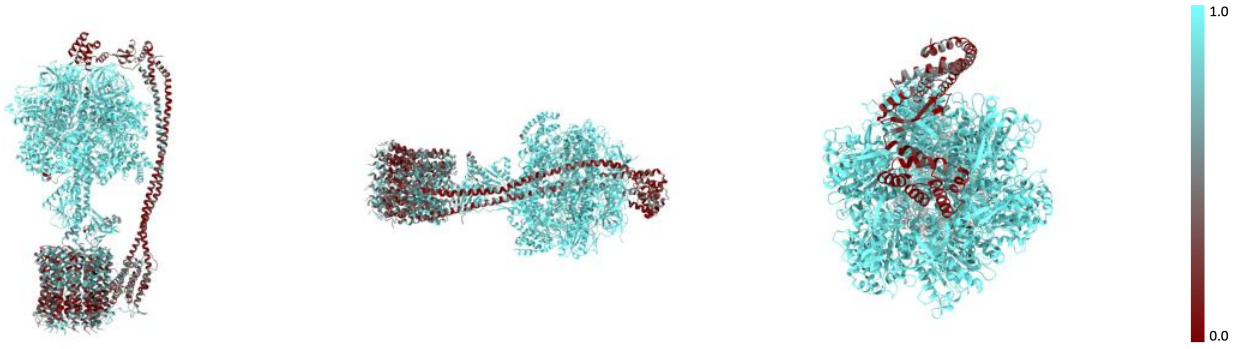
9.2 Q-score mapped to coordinate model



X Y Z

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

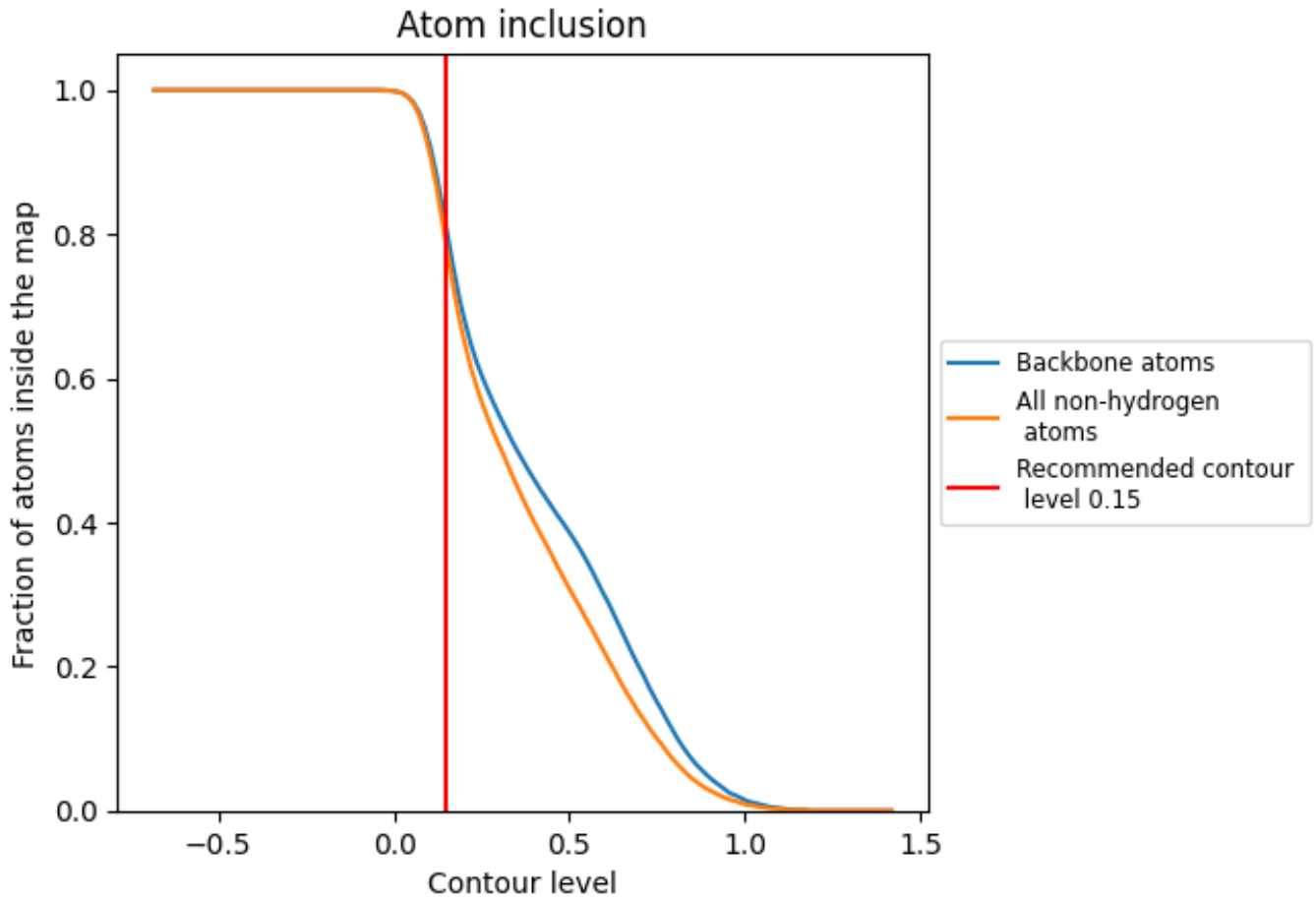
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 81% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.4170
A	0.9680	0.5370
B	0.9780	0.5520
D	0.9280	0.4640
E	0.9770	0.5470
F	0.4800	0.1600
G	0.6290	0.2350
H	0.4670	0.1550
I	0.5260	0.2110
J	0.5180	0.1870
K	0.4890	0.1560
L	0.4960	0.1590
M	0.4980	0.1920
N	0.6420	0.2140
O	0.4780	0.1730
P	0.4130	0.1550
Q	0.4540	0.1690
R	0.6720	0.2190
S	0.6160	0.2240
T	0.9750	0.5440
U	0.9700	0.5470
V	0.9670	0.5310
a	0.4410	0.2130
b	0.3280	0.2410
d	0.1780	0.2520
e	0.7960	0.2910
p	0.2100	0.2210

