



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:53 AM EST

PDB ID : 7MD3
EMDB ID : EMD-23764
Title : The F1 region of apoptolidin-bound *Saccharomyces cerevisiae* ATP synthase
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2021-04-03
Resolution : 3.30 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:

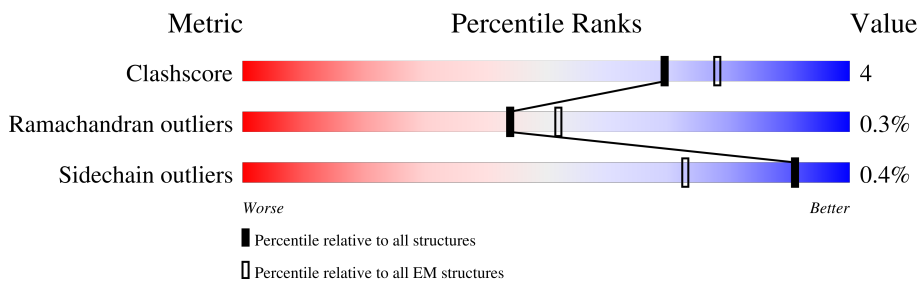
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	478	
2	E	478	
2	F	478	
3	G	278	
4	H	61	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 46124 atoms, of which 23093 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	483	Total	C	H	N	O	S	0	0
			7132	2261	3579	634	655	3		
1	B	479	Total	C	H	N	O	S	0	0
			6946	2220	3470	628	625	3		
1	C	485	Total	C	H	N	O	S	0	0
			7280	2293	3675	648	661	3		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	D	468	Total	C	H	N	O	S	0	0
			6747	2150	3380	590	621	6		
2	E	469	Total	C	H	N	O	S	0	0
			6897	2186	3469	599	638	5		
2	F	469	Total	C	H	N	O	S	0	0
			6893	2186	3471	597	633	6		

- Molecule 3 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	G	232	Total	C	H	N	O	S	0	0
			3309	1060	1641	292	307	9		

- Molecule 4 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	H	48	Total	C	H	N	O	0	0
			608	208	276	59	65		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

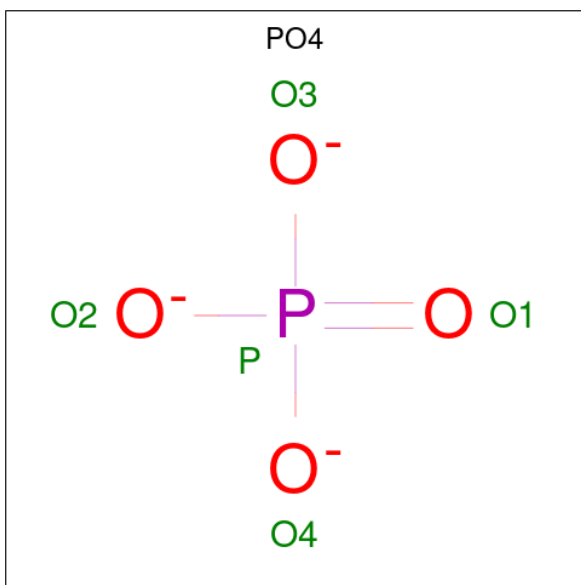


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
5	A	1	43	10	12	5	13	3	0
5	B	1	43	10	12	5	13	3	0
5	C	1	43	10	12	5	13	3	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

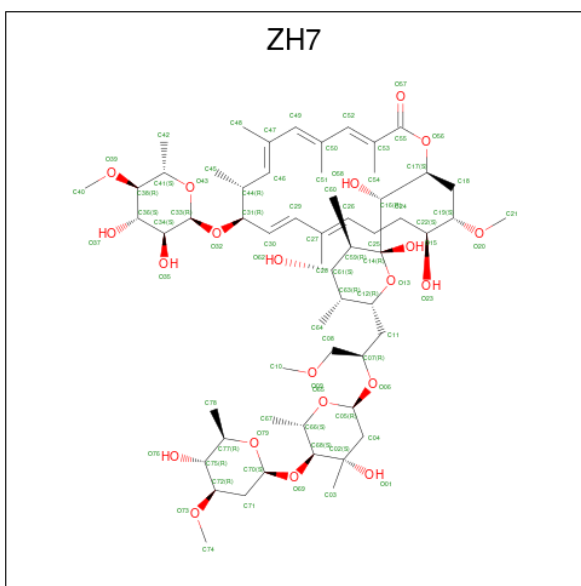
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0
6	B	1	1	1	0
6	C	1	1	1	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		AltConf
7	F	1	Total	O P	0
			5	4 1	

- Molecule 8 is (3 {E},5 {E},7 {E},9 {R},10 {R},11 {E},13 {E},17 {S},18 {S},20 {S})-18-methoxy-20-[({R})-(2 {R},3 {R},4 {S},5 {R},6 {R})-6-[(2 {R})-3-methoxy-2-[(2 {R},4 {S},5 {S},6 {S})-5-[(2 {S},4 {R},5 {R},6 {R})-4-methoxy-6-methyl-5-oxidanyl-oxan-2-yl]oxy-4,6-dimethyl-4-oxidanyl-oxan-2-yl]oxy-propyl]-3,5-dimethyl-2,4-bis(oxidanyl)oxan-2-yl]-oxidanyl-methyl]-10-[(2 {R},3 {S},4 {S},5 {R},6 {S})-5-methoxy-6-methyl-3,4-bis(oxidanyl)oxan-2-yl]oxy-3,5,7,9,13-pentamethyl-17-oxidanyl-1-oxacycloicosa-3,5,7,11,13-pentaen-2-one (three-letter code: ZH7) (formula: C₅₈H₉₆O₂₁) (labeled as "Ligand of Interest" by depositor).

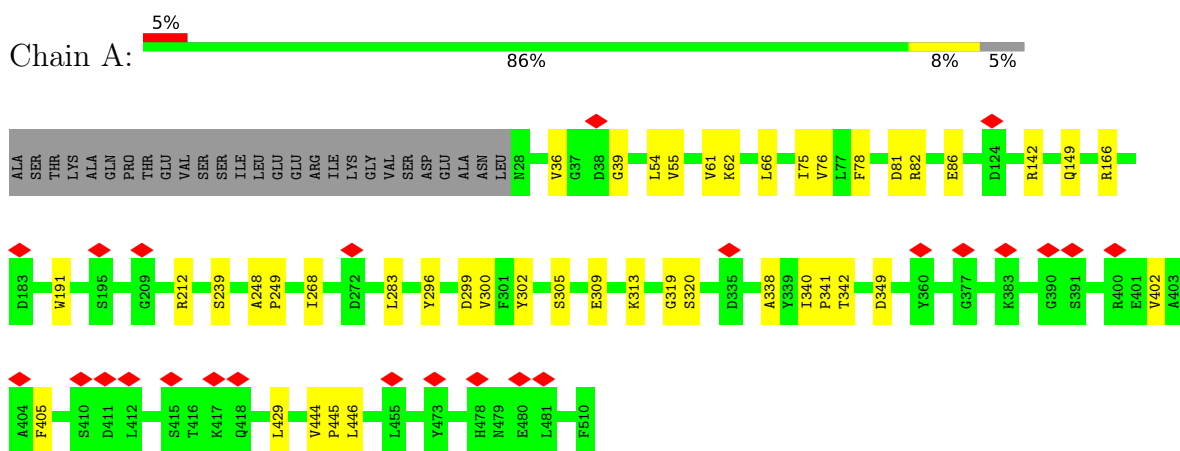


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
8	G	1	175	58	96	21	0

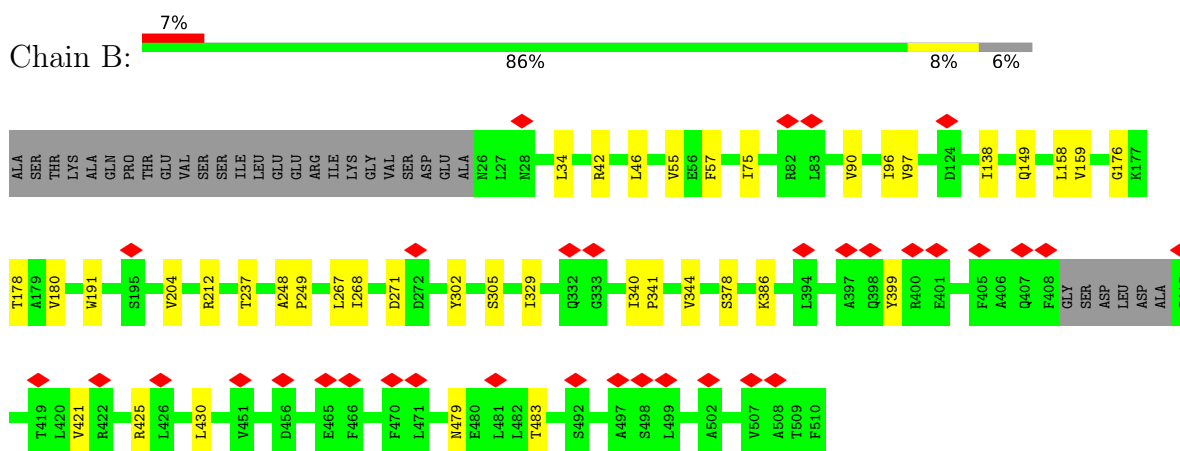
3 Residue-property plots

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

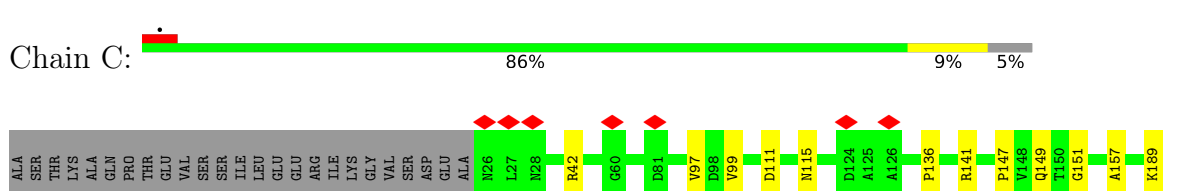
- Molecule 1: ATP synthase subunit alpha

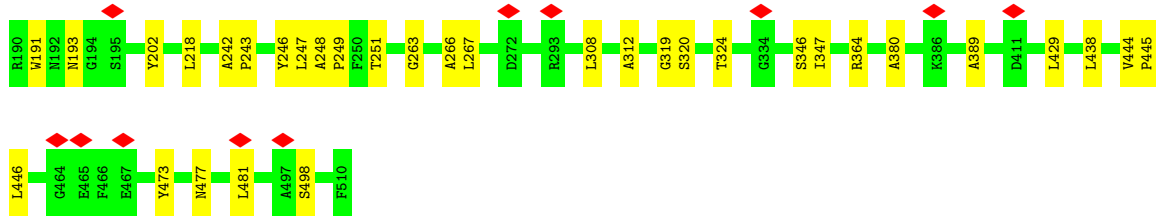


- Molecule 1: ATP synthase subunit alpha

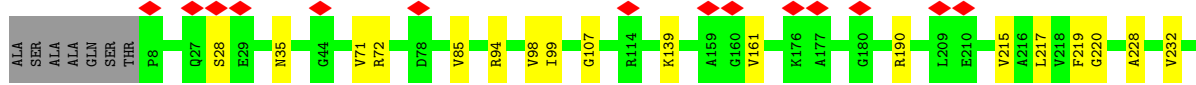
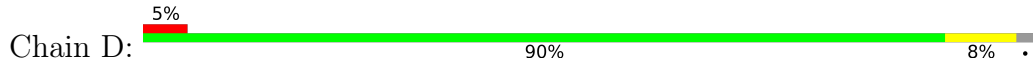


- Molecule 1: ATP synthase subunit alpha

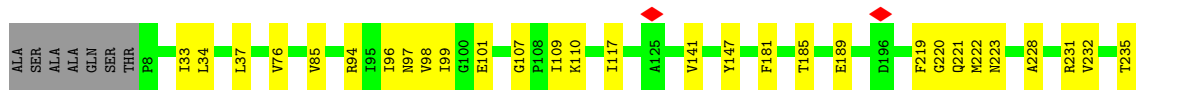
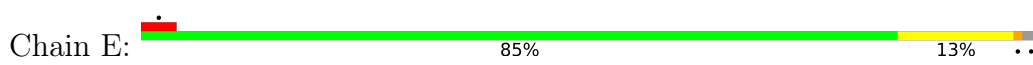




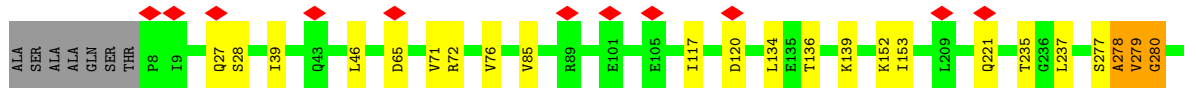
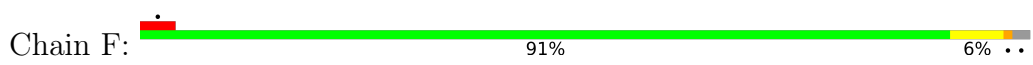
• Molecule 2: ATP synthase subunit beta



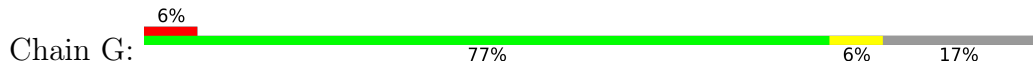
• Molecule 2: ATP synthase subunit beta

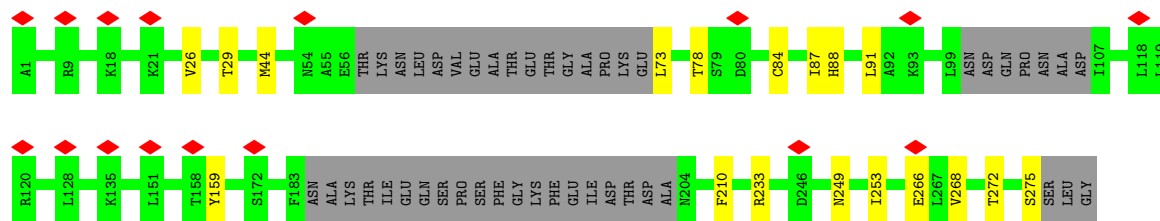


• Molecule 2: ATP synthase subunit beta

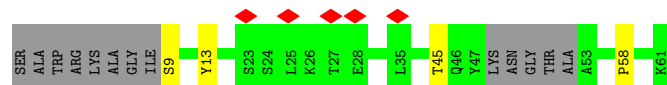
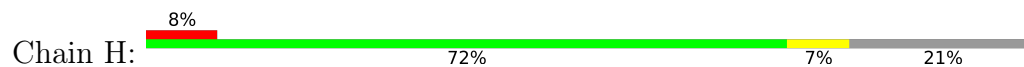


• Molecule 3: ATP synthase subunit gamma





• Molecule 4: ATP synthase subunit epsilon, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	477847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	135922	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.052	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	329.6, 329.6, 329.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2875, 1.2875, 1.2875	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZH7, ATP, 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	A	0.36	0/3610	0.46	0/4903
1	B	0.36	0/3531	0.46	0/4802
1	C	0.36	0/3662	0.47	0/4965
2	D	0.36	0/3421	0.47	0/4660
2	E	0.36	0/3484	0.47	0/4737
2	F	0.36	0/3478	0.47	0/4730
3	G	0.32	0/1687	0.43	0/2288
4	H	0.29	0/337	0.44	0/462
All	All	0.36	0/23210	0.47	0/31547

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	278	ALA	Peptide
2	E	278	ALA	Peptide

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	3553	3579	3579	27	0
1	B	3476	3470	3470	23	0
1	C	3605	3675	3675	24	0
2	D	3367	3380	3380	25	0
2	E	3428	3469	3469	41	0
2	F	3422	3471	3471	23	0
3	G	1668	1641	1641	10	0
4	H	332	276	276	2	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	F	5	0	0	0	0
8	G	79	96	0	1	0
All	All	23031	23093	22997	168	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 4.

All (168) 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)
2:E:278:ALA:O	2:E:280:GLY:N	1.99	0.95
2:F:278:ALA:O	2:F:280:GLY:N	2.08	0.86
2:D:278:ALA:O	2:D:280:GLY:N	2.10	0.83
2:D:228:ALA:O	2:D:232:VAL:HG23	1.81	0.80
3:G:84:CYS:SG	3:G:233:ARG:NH2	2.60	0.75
2:D:139:LYS:NZ	2:D:460:VAL:O	2.22	0.72
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.73	0.71
2:D:220:GLY:HA3	2:D:232:VAL:HG21	1.72	0.70
1:A:299:ASP:O	1:A:302:TYR:N	2.28	0.67
1:A:55:VAL:HG21	1:A:75:ILE:HD13	1.77	0.65
2:E:189:GLU:O	2:E:221:GLN:NE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.80	0.62
1:C:97:VAL:HG21	1:C:247:LEU:HD21	1.80	0.61
1:C:99:VAL:HG11	1:C:251:THR:HB	1.81	0.61
2:F:277:SER:O	2:F:278:ALA:O	2.19	0.61
2:F:152:LYS:HG2	2:F:329:LEU:HD23	1.83	0.60
2:F:27:GLN:O	2:F:28:SER:OG	2.18	0.59
2:D:400:ASP:OD2	8:G:301:ZH7:O76	2.21	0.59
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.86	0.57
2:E:277:SER:O	2:E:278:ALA:O	2.24	0.56
1:C:111:ASP:OD2	1:C:115:ASN:N	2.37	0.56
2:E:425:THR:HG22	2:E:425:THR:O	2.05	0.55
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.87	0.55
2:E:33:ILE:HG22	2:E:34:LEU:HG	1.86	0.55
1:A:212:ARG:NH2	1:A:239:SER:OG	2.40	0.55
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.88	0.55
1:C:189:LYS:O	1:C:193:ASN:ND2	2.40	0.54
2:D:161:VAL:HG22	2:D:161:VAL:O	2.08	0.54
4:H:45:THR:HG22	4:H:58:PRO:HA	1.88	0.54
1:B:158:LEU:HD11	1:B:430:LEU:HD13	1.89	0.54
2:D:217:LEU:HD22	2:D:219:PHE:CZ	2.43	0.54
1:A:338:ALA:O	1:A:342:THR:OG1	2.13	0.53
2:E:472:LYS:O	2:E:476:GLU:N	2.40	0.53
1:C:319:GLY:O	1:C:320:SER:OG	2.24	0.52
2:D:28:SER:O	2:D:28:SER:OG	2.27	0.52
1:B:138:ILE:H	1:B:138:ILE:HD12	1.75	0.52
1:C:346:SER:O	2:D:190:ARG:NH2	2.42	0.52
1:C:473:TYR:O	1:C:477:ASN:N	2.42	0.52
1:A:82:ARG:NH1	2:D:35:ASN:OD1	2.37	0.51
1:A:444:VAL:HG12	1:A:445:PRO:HD3	1.93	0.51
2:D:293:GLN:O	2:D:296:ILE:N	2.41	0.51
1:C:157:ALA:O	1:C:389:ALA:HB1	2.10	0.51
1:A:296:TYR:HB3	1:A:300:VAL:HG21	1.92	0.50
3:G:275:SER:O	3:G:275:SER:OG	2.28	0.50
2:E:94:ARG:NH2	2:E:107:GLY:O	2.40	0.50
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.94	0.50
2:F:139:LYS:NZ	2:F:413:PHE:O	2.35	0.50
2:E:243:PHE:CB	2:E:251:VAL:HG21	2.42	0.50
1:B:212:ARG:HG2	1:B:237:THR:HG21	1.93	0.49
2:E:452:ILE:CG2	2:E:456:ALA:HB3	2.43	0.49
3:G:73:LEU:HD12	3:G:159:TYR:HD2	1.78	0.49
2:D:94:ARG:NH2	2:D:107:GLY:O	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.94	0.49
2:F:120:ASP:OD1	2:F:120:ASP:N	2.46	0.49
1:B:204:VAL:N	1:B:267:LEU:O	2.45	0.49
1:A:340:ILE:HB	1:A:341:PRO:HD3	1.94	0.48
2:E:109:ILE:O	2:E:110:LYS:HG2	2.13	0.48
2:D:85:VAL:CG1	2:D:235:THR:HG23	2.41	0.48
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.95	0.48
2:F:237:LEU:HD22	2:F:292:LEU:HD12	1.95	0.48
1:B:340:ILE:HB	1:B:341:PRO:HD3	1.96	0.48
1:C:429:LEU:HG	1:C:446:LEU:HD21	1.96	0.48
3:G:268:VAL:O	3:G:272:THR:HG23	2.13	0.48
2:E:228:ALA:O	2:E:232:VAL:HG23	2.14	0.47
1:A:76:VAL:HG11	1:A:283:LEU:HD11	1.95	0.47
1:A:142:ARG:N	1:A:313:LYS:O	2.47	0.47
1:C:267:LEU:HD12	1:C:324:THR:HB	1.97	0.47
2:E:96:ILE:HG22	2:E:97:ASN:O	2.15	0.47
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.96	0.47
1:B:268:ILE:HG23	1:B:268:ILE:O	2.15	0.47
2:E:243:PHE:HB2	2:E:251:VAL:HG21	1.97	0.46
1:B:46:LEU:O	2:F:72:ARG:NH2	2.41	0.46
1:A:166:ARG:NH2	1:A:349:ASP:OD2	2.48	0.46
1:B:212:ARG:CG	1:B:237:THR:HG21	2.46	0.46
1:C:147:PRO:HB3	1:C:380:ALA:O	2.16	0.46
2:D:277:SER:C	2:D:278:ALA:O	2.53	0.46
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.46	0.46
1:A:54:LEU:HD13	1:A:78:PHE:CE2	2.51	0.46
2:E:37:LEU:HB3	2:E:76:VAL:HG12	1.97	0.46
3:G:26:VAL:O	3:G:29:THR:OG1	2.29	0.46
4:H:9:SER:O	4:H:13:TYR:N	2.39	0.45
2:E:436:ASP:N	2:E:436:ASP:OD1	2.49	0.45
2:E:456:ALA:O	2:E:460:VAL:HG11	2.16	0.45
2:E:460:VAL:HG12	2:E:469:LYS:HD2	1.99	0.45
1:B:159:VAL:O	1:B:159:VAL:HG13	2.16	0.45
3:G:249:ASN:O	3:G:253:ILE:HG13	2.16	0.45
1:B:138:ILE:HD11	2:F:221:GLN:OE1	2.17	0.45
2:E:241:GLU:OE1	2:E:295:ARG:NH2	2.44	0.45
3:G:78:THR:HG22	3:G:91:LEU:HD22	1.98	0.45
1:A:444:VAL:N	1:A:445:PRO:CD	2.80	0.45
2:D:296:ILE:HG23	2:D:304:VAL:O	2.17	0.45
2:F:359:ASP:O	2:F:363:VAL:HG22	2.16	0.45
1:A:268:ILE:HG23	1:A:268:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ALA:HB3	1:C:249:PRO:HD3	1.99	0.45
1:B:329:ILE:HD11	1:B:344:VAL:HG21	1.99	0.45
2:F:46:LEU:HD13	2:F:65:ASP:HB3	1.99	0.45
2:F:117:ILE:O	2:F:295:ARG:NH1	2.50	0.45
2:F:39:ILE:HD13	2:F:76:VAL:HG22	1.98	0.44
1:B:378:SER:HB3	1:B:386:LYS:HG3	1.99	0.44
1:C:141:ARG:NH2	1:C:312:ALA:HB2	2.33	0.44
1:C:151:GLY:HA2	1:C:438:LEU:O	2.18	0.44
1:C:263:GLY:HA2	1:C:319:GLY:O	2.17	0.44
2:D:279:VAL:HA	3:G:266:GLU:OE1	2.18	0.44
2:D:409:LYS:NZ	2:D:450:ASP:OD1	2.43	0.44
2:F:39:ILE:HD13	2:F:76:VAL:HG13	2.00	0.44
1:A:76:VAL:CB	1:A:283:LEU:HD11	2.48	0.44
2:D:253:LEU:N	2:D:305:THR:O	2.43	0.44
2:E:262:THR:HG23	2:E:285:LEU:HD13	1.98	0.44
2:E:452:ILE:HG23	2:E:470:ALA:HB2	2.00	0.44
1:B:421:VAL:HG13	1:B:425:ARG:CZ	2.48	0.43
3:G:78:THR:CG2	3:G:91:LEU:HD22	2.48	0.43
2:E:440:SER:HB3	2:E:463:ILE:HG23	1.99	0.43
2:F:134:LEU:O	2:F:136:THR:HG23	2.18	0.43
1:A:319:GLY:O	1:A:320:SER:OG	2.28	0.43
1:B:149:GLN:HB2	1:B:191:TRP:CH2	2.54	0.43
1:B:55:VAL:HG21	1:B:75:ILE:HD13	2.00	0.43
1:B:302:TYR:HA	1:B:305:SER:OG	2.19	0.43
2:E:384:LEU:O	2:E:387:ILE:HG22	2.19	0.43
1:A:429:LEU:CD2	1:A:446:LEU:HD12	2.49	0.43
1:C:202:TYR:O	1:C:266:ALA:HA	2.18	0.43
2:E:98:VAL:HG13	2:E:99:ILE:HG23	2.00	0.43
2:E:98:VAL:HG21	2:E:231:ARG:HB2	2.01	0.43
1:A:402:VAL:HG12	1:A:402:VAL:O	2.19	0.43
1:A:405:PHE:CD1	1:A:405:PHE:N	2.87	0.43
1:B:178:THR:OG1	1:B:271:ASP:OD2	2.36	0.42
1:A:66:LEU:HD12	1:A:76:VAL:HG11	2.00	0.42
1:A:248:ALA:HB3	1:A:249:PRO:HD3	2.01	0.42
1:B:57:PHE:CD2	1:B:90:VAL:HG22	2.54	0.42
1:B:34:LEU:N	1:B:42:ARG:O	2.51	0.42
1:C:429:LEU:HD11	1:C:446:LEU:HG	2.01	0.42
1:A:309:GLU:OE1	2:E:223:ASN:ND2	2.40	0.42
2:E:296:ILE:O	2:E:297:THR:HG23	2.19	0.42
1:B:176:GLY:O	1:B:180:VAL:HG23	2.20	0.42
2:E:277:SER:C	2:E:278:ALA:O	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ASN:O	1:B:483:THR:OG1	2.24	0.42
1:C:136:PRO:O	1:C:141:ARG:NH1	2.52	0.42
2:D:256:ASP:HA	2:D:257:ASN:HA	1.84	0.42
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.55	0.42
1:A:36:VAL:HG12	1:A:81:ASP:OD2	2.20	0.41
1:C:364:ARG:HD3	5:C:600:ATP:C2	2.55	0.41
2:D:98:VAL:HG13	2:D:99:ILE:HG23	2.00	0.41
1:B:248:ALA:HB3	1:B:249:PRO:HD3	2.02	0.41
2:E:279:VAL:O	2:E:279:VAL:HG22	2.19	0.41
2:E:117:ILE:HA	2:E:238:THR:OG1	2.20	0.41
1:A:61:VAL:HG22	1:A:62:LYS:N	2.35	0.41
1:C:149:GLN:HB2	1:C:191:TRP:CH2	2.56	0.41
2:D:71:VAL:HG12	2:D:72:ARG:O	2.21	0.41
2:E:185:THR:OG1	2:E:255:ILE:HD13	2.20	0.41
1:A:39:GLY:N	1:A:81:ASP:OD1	2.53	0.41
1:A:305:SER:HB2	2:E:222:MET:HB3	2.02	0.41
1:C:242:ALA:N	1:C:243:PRO:CD	2.84	0.41
2:D:215:VAL:O	2:D:215:VAL:HG13	2.20	0.41
2:E:141:VAL:HG13	2:E:147:TYR:CE1	2.56	0.41
2:E:181:PHE:O	2:E:251:VAL:HG13	2.21	0.41
3:G:87:ILE:HG22	3:G:88:HIS:N	2.35	0.41
1:A:149:GLN:HB2	1:A:191:TRP:CH2	2.56	0.41
2:E:97:ASN:OD1	2:E:101:GLU:N	2.40	0.41
1:B:96:ILE:HG22	1:B:97:VAL:N	2.36	0.40
2:F:279:VAL:HG22	2:F:279:VAL:O	2.21	0.40
1:C:308:LEU:HD12	1:C:347:ILE:HG21	2.03	0.40
2:D:346:PRO:HB3	2:D:418:PHE:CZ	2.56	0.40
2:F:237:LEU:HD23	2:F:295:ARG:HB2	2.03	0.40
1:C:444:VAL:HB	1:C:445:PRO:HD3	2.03	0.40
1:C:481:LEU:HD21	1:C:498:SER:HB3	2.03	0.40
2:F:71:VAL:HG12	2:F:72:ARG:O	2.21	0.40
2:F:153:ILE:C	2:F:329:LEU:HD22	2.42	0.40
2:F:278:ALA:C	2:F:280:GLY:H	2.24	0.40
2:E:298:THR:HG22	2:E:299:THR:N	2.36	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	481/510 (94%)	474 (98%)	7 (2%)	0	100	100
1	B	475/510 (93%)	459 (97%)	16 (3%)	0	100	100
1	C	483/510 (95%)	480 (99%)	3 (1%)	0	100	100
2	D	466/478 (98%)	453 (97%)	11 (2%)	2 (0%)	34	66
2	E	467/478 (98%)	449 (96%)	15 (3%)	3 (1%)	25	57
2	F	467/478 (98%)	454 (97%)	10 (2%)	3 (1%)	25	57
3	G	224/278 (81%)	222 (99%)	2 (1%)	0	100	100
4	H	44/61 (72%)	43 (98%)	1 (2%)	0	100	100
All	All	3107/3303 (94%)	3034 (98%)	65 (2%)	8 (0%)	44	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	278	ALA
2	D	279	VAL
2	E	278	ALA
2	E	279	VAL
2	F	278	ALA
2	F	279	VAL
2	E	280	GLY
2	F	280	GLY

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	356/412 (86%)	355 (100%)	1 (0%)	92	96
1	B	335/412 (81%)	334 (100%)	1 (0%)	92	96
1	C	367/412 (89%)	364 (99%)	3 (1%)	81	89
2	D	334/384 (87%)	334 (100%)	0	100	100
2	E	348/384 (91%)	345 (99%)	3 (1%)	78	87
2	F	347/384 (90%)	347 (100%)	0	100	100
3	G	162/236 (69%)	160 (99%)	2 (1%)	71	83
4	H	26/48 (54%)	26 (100%)	0	100	100
All	All	2275/2672 (85%)	2265 (100%)	10 (0%)	91	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLU
1	B	399	TYR
1	C	42	ARG
1	C	218	LEU
1	C	246	TYR
2	E	219	PHE
2	E	337	ARG
2	E	436	ASP
3	G	44	MET
3	G	210	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	220	GLN
1	A	224	GLN
1	A	282	GLN
1	A	304	HIS
2	D	118	HIS
2	D	178	HIS
2	D	328	HIS
2	D	375	GLN
2	E	35	ASN
2	F	328	HIS
2	F	367	HIS

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Mol	Chain	Res	Type
3	G	88	HIS

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 monosaccharides 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$
5	ATP	C	600	6	26,33,33	0.86	1 (3%)	31,52,52	1.66	5 (16%)
7	PO4	F	600	-	4,4,4	0.98	0	6,6,6	0.38	0
8	ZH7	G	301	-	82,83,83	2.24	24 (29%)	96,121,121	1.90	22 (22%)
5	ATP	B	600	6	26,33,33	0.90	1 (3%)	31,52,52	1.76	6 (19%)
5	ATP	A	600	6	26,33,33	0.85	1 (3%)	31,52,52	1.72	4 (12%)

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
5	ATP	B	600	6	-	2/18/38/38	0/3/3/3
8	ZH7	G	301	-	-	25/77/156/156	1/4/5/5
5	ATP	C	600	6	-	5/18/38/38	0/3/3/3
5	ATP	A	600	6	-	4/18/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	301	ZH7	C44-C31	10.44	1.66	1.54
8	G	301	ZH7	C22-C19	4.67	1.61	1.52
8	G	301	ZH7	C17-C16	4.31	1.61	1.53
8	G	301	ZH7	C49-C47	4.01	1.54	1.45
8	G	301	ZH7	C29-C27	3.83	1.54	1.45
8	G	301	ZH7	C52-C50	3.48	1.52	1.45
8	G	301	ZH7	C49-C50	3.47	1.40	1.35
8	G	301	ZH7	C18-C19	3.46	1.58	1.52
8	G	301	ZH7	C33-C34	3.44	1.62	1.52
8	G	301	ZH7	O56-C55	3.33	1.42	1.34
8	G	301	ZH7	C52-C53	3.13	1.41	1.33
8	G	301	ZH7	C38-C41	3.04	1.58	1.52
8	G	301	ZH7	O01-C02	-3.00	1.39	1.44
8	G	301	ZH7	C31-C30	2.73	1.59	1.50
8	G	301	ZH7	C75-C72	2.72	1.58	1.53
8	G	301	ZH7	C63-C12	2.54	1.57	1.53
8	G	301	ZH7	C55-C53	2.49	1.58	1.50
8	G	301	ZH7	C36-C34	2.44	1.58	1.52
8	G	301	ZH7	C75-C77	2.34	1.58	1.52
8	G	301	ZH7	C04-C02	2.34	1.58	1.53
8	G	301	ZH7	C71-C70	2.32	1.56	1.51
8	G	301	ZH7	C42-C41	2.24	1.56	1.51
5	B	600	ATP	C5-C4	2.14	1.46	1.40
5	C	600	ATP	C5-C4	2.11	1.46	1.40
8	G	301	ZH7	C08-C07	2.07	1.57	1.50
5	A	600	ATP	C5-C4	2.04	1.46	1.40
8	G	301	ZH7	C68-C66	2.00	1.58	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	301	ZH7	C48-C47-C49	-6.36	104.37	119.05
8	G	301	ZH7	C45-C44-C46	5.95	119.95	110.05
8	G	301	ZH7	C51-C50-C52	-5.76	105.75	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	301	ZH7	C31-C30-C29	5.61	136.76	124.94
5	C	600	ATP	PB-O3B-PG	-4.88	116.07	132.83
5	B	600	ATP	PB-O3B-PG	-4.87	116.10	132.83
5	A	600	ATP	PA-O3A-PB	-4.71	116.67	132.83
5	B	600	ATP	PA-O3A-PB	-4.40	117.73	132.83
5	A	600	ATP	PB-O3B-PG	-4.29	118.09	132.83
5	C	600	ATP	PA-O3A-PB	-4.06	118.90	132.83
8	G	301	ZH7	O69-C70-C71	4.01	116.15	108.41
5	A	600	ATP	N3-C2-N1	-4.00	122.43	128.68
5	B	600	ATP	N3-C2-N1	-3.71	122.88	128.68
8	G	301	ZH7	O13-C12-C11	3.38	110.27	105.95
8	G	301	ZH7	C51-C50-C49	-3.35	113.43	123.12
5	C	600	ATP	N3-C2-N1	-3.25	123.60	128.68
8	G	301	ZH7	O79-C70-C71	-3.08	106.22	110.87
8	G	301	ZH7	C36-C38-C41	-3.03	105.84	110.30
8	G	301	ZH7	C44-C46-C47	2.77	135.43	126.67
8	G	301	ZH7	O65-C66-C67	2.75	112.64	106.70
8	G	301	ZH7	O06-C05-C04	2.74	113.74	109.01
8	G	301	ZH7	C63-C61-C59	-2.69	108.05	111.47
5	B	600	ATP	C3'-C2'-C1'	2.60	104.89	100.98
8	G	301	ZH7	C54-C53-C52	-2.53	116.80	123.87
8	G	301	ZH7	O56-C55-O57	-2.49	118.58	123.32
8	G	301	ZH7	O65-C05-C04	-2.47	107.42	112.12
8	G	301	ZH7	O56-C55-C53	2.44	117.65	111.52
8	G	301	ZH7	C71-C72-C75	-2.38	106.30	110.77
8	G	301	ZH7	O79-C77-C78	2.32	111.70	106.70
5	B	600	ATP	C4-C5-N7	-2.30	107.01	109.40
8	G	301	ZH7	C42-C41-C38	-2.22	110.02	113.41
5	C	600	ATP	C4-C5-N7	-2.22	107.09	109.40
8	G	301	ZH7	C45-C44-C31	-2.19	107.95	111.28
8	G	301	ZH7	C05-O06-C07	2.17	119.54	115.20
5	A	600	ATP	C4-C5-N7	-2.14	107.16	109.40
5	C	600	ATP	N6-C6-N1	2.14	123.02	118.57
5	B	600	ATP	N6-C6-N1	2.03	122.79	118.57

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ATP	C5'-O5'-PA-O3A
5	C	600	ATP	C5'-O5'-PA-O3A
5	C	600	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	C	600	ATP	C3'-C4'-C5'-O5'
8	G	301	ZH7	C59-C14-C16-O58
8	G	301	ZH7	O13-C14-C16-C17
8	G	301	ZH7	O13-C14-C16-O58
8	G	301	ZH7	O15-C14-C16-C17
8	G	301	ZH7	C26-C27-C29-C30
8	G	301	ZH7	C44-C46-C47-C49
8	G	301	ZH7	C47-C49-C50-C52
8	G	301	ZH7	C51-C50-C52-C53
8	G	301	ZH7	C50-C52-C53-C54
8	G	301	ZH7	C50-C52-C53-C55
8	G	301	ZH7	C28-C27-C29-C30
8	G	301	ZH7	C30-C31-C44-C45
8	G	301	ZH7	C11-C07-C08-O09
8	G	301	ZH7	C44-C31-O32-C33
5	A	600	ATP	PB-O3B-PG-O3G
8	G	301	ZH7	O32-C31-C44-C46
8	G	301	ZH7	O06-C07-C08-O09
5	B	600	ATP	PG-O3B-PB-O2B
8	G	301	ZH7	C49-C50-C52-C53
5	A	600	ATP	C5'-O5'-PA-O1A
5	C	600	ATP	C5'-O5'-PA-O2A
8	G	301	ZH7	O65-C05-O06-C07
8	G	301	ZH7	C30-C31-C44-C46
8	G	301	ZH7	C17-C18-C19-C22
8	G	301	ZH7	C04-C05-O06-C07
5	C	600	ATP	PB-O3A-PA-O2A
8	G	301	ZH7	C17-C18-C19-O20
8	G	301	ZH7	C07-C11-C12-O13
5	A	600	ATP	PB-O3B-PG-O2G
8	G	301	ZH7	C07-C11-C12-C63
8	G	301	ZH7	O15-C14-C16-O58
5	B	600	ATP	PG-O3B-PB-O1B

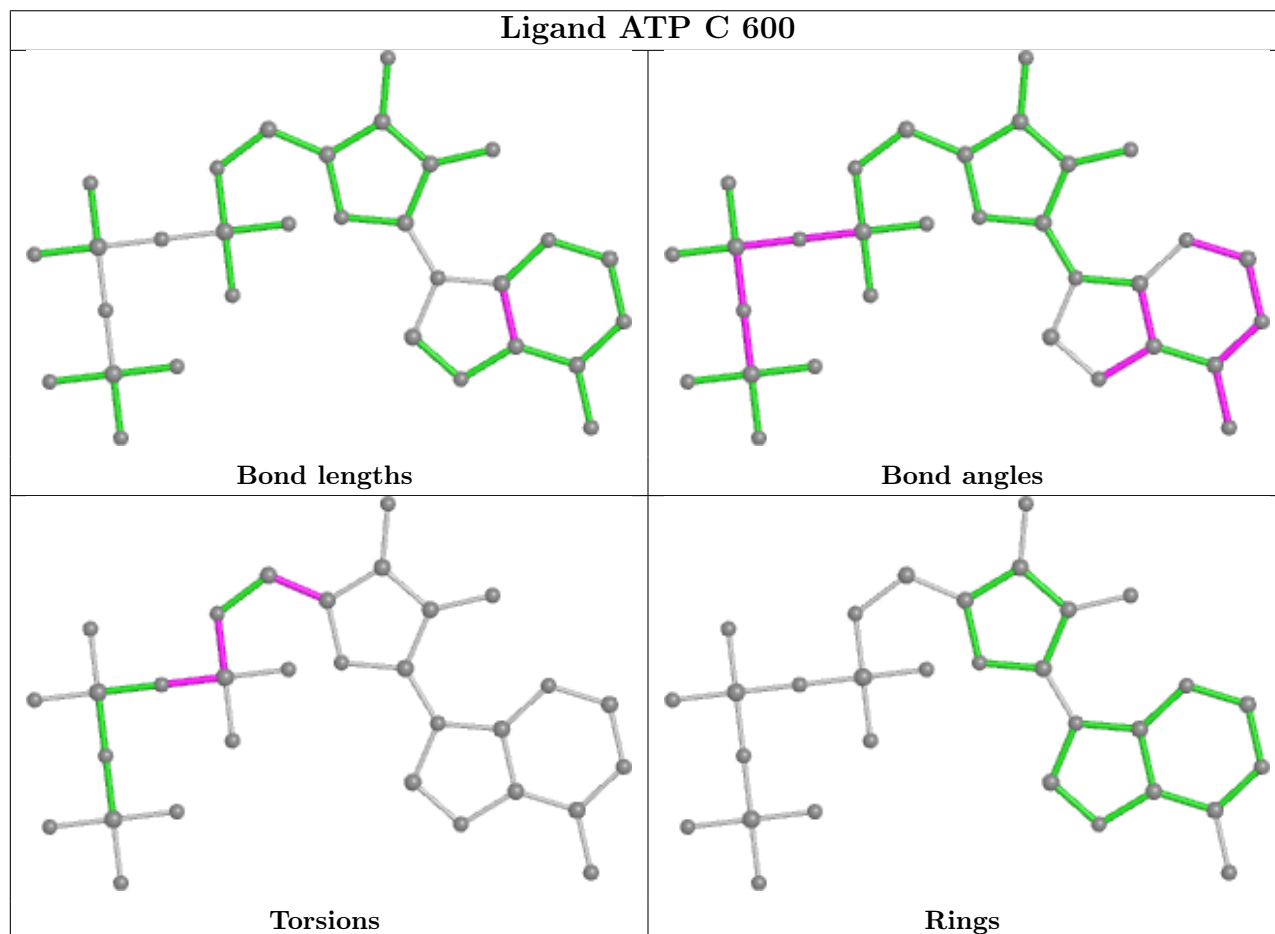
All (1) ring outliers are listed below:

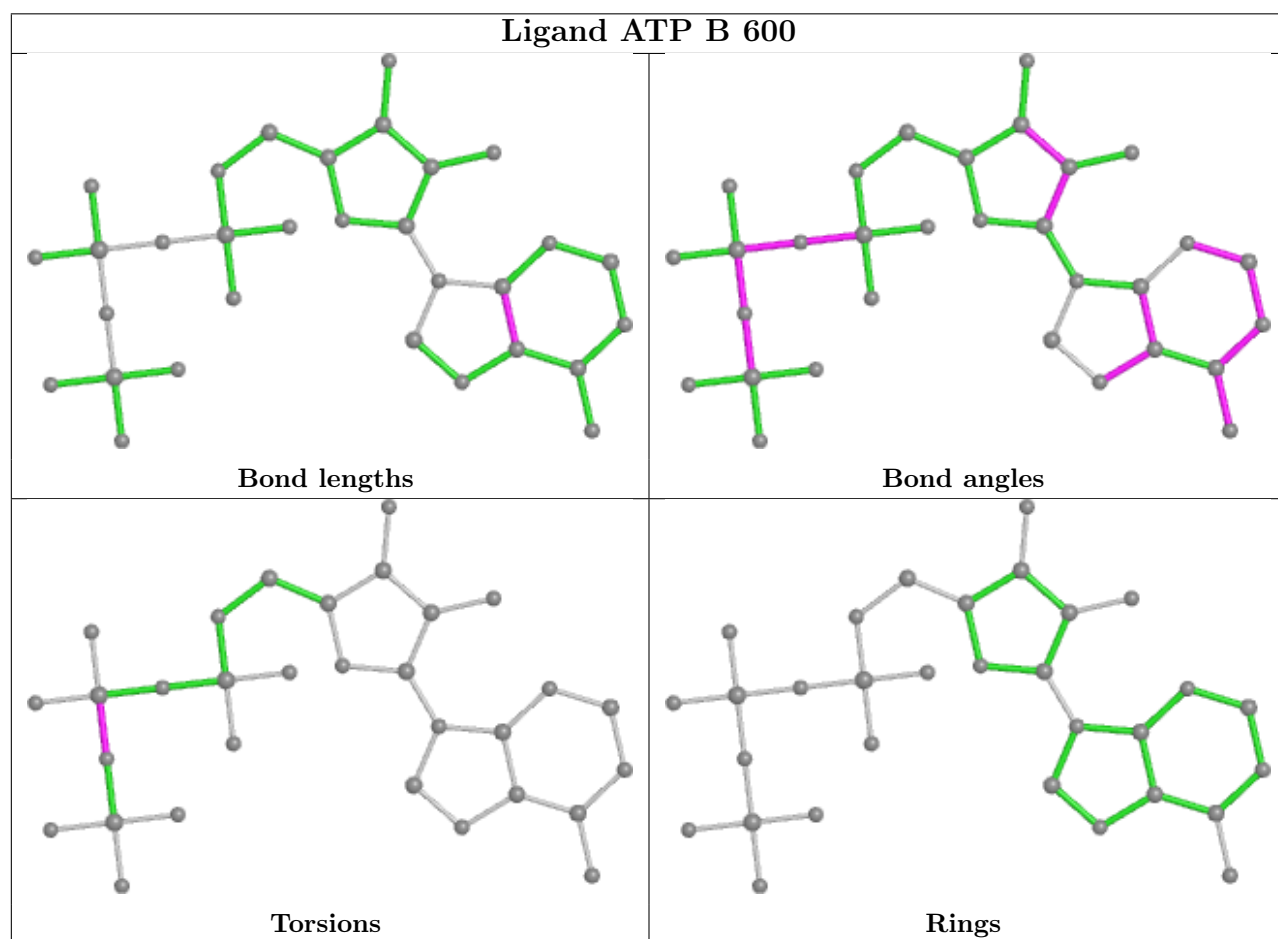
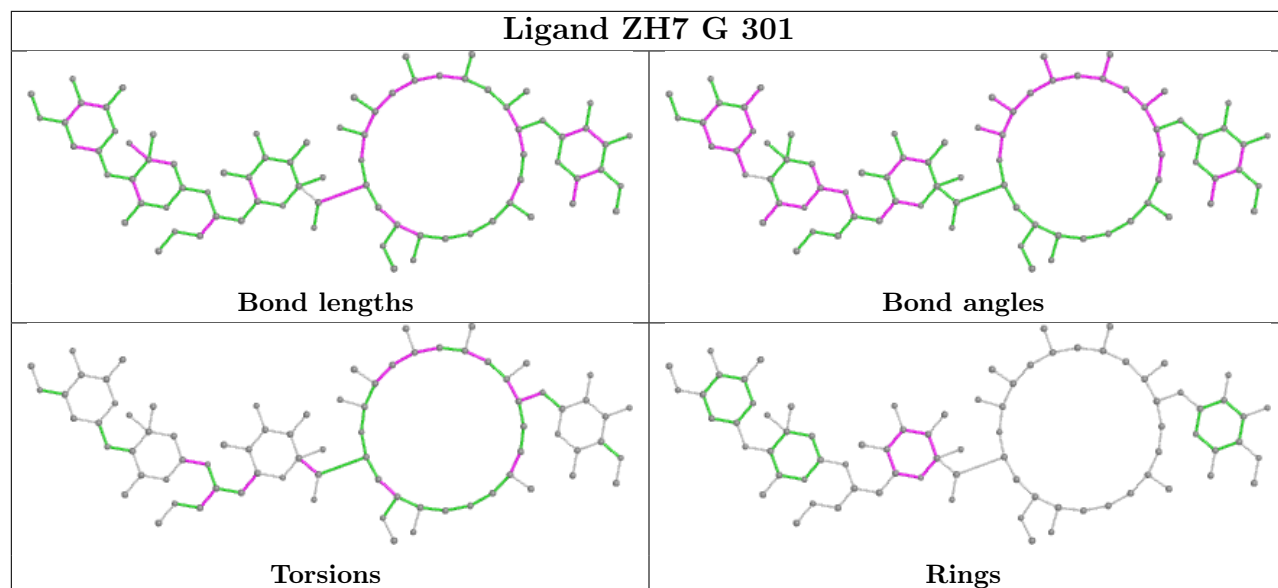
Mol	Chain	Res	Type	Atoms
8	G	301	ZH7	C12-C14-C59-C61-C63-O13

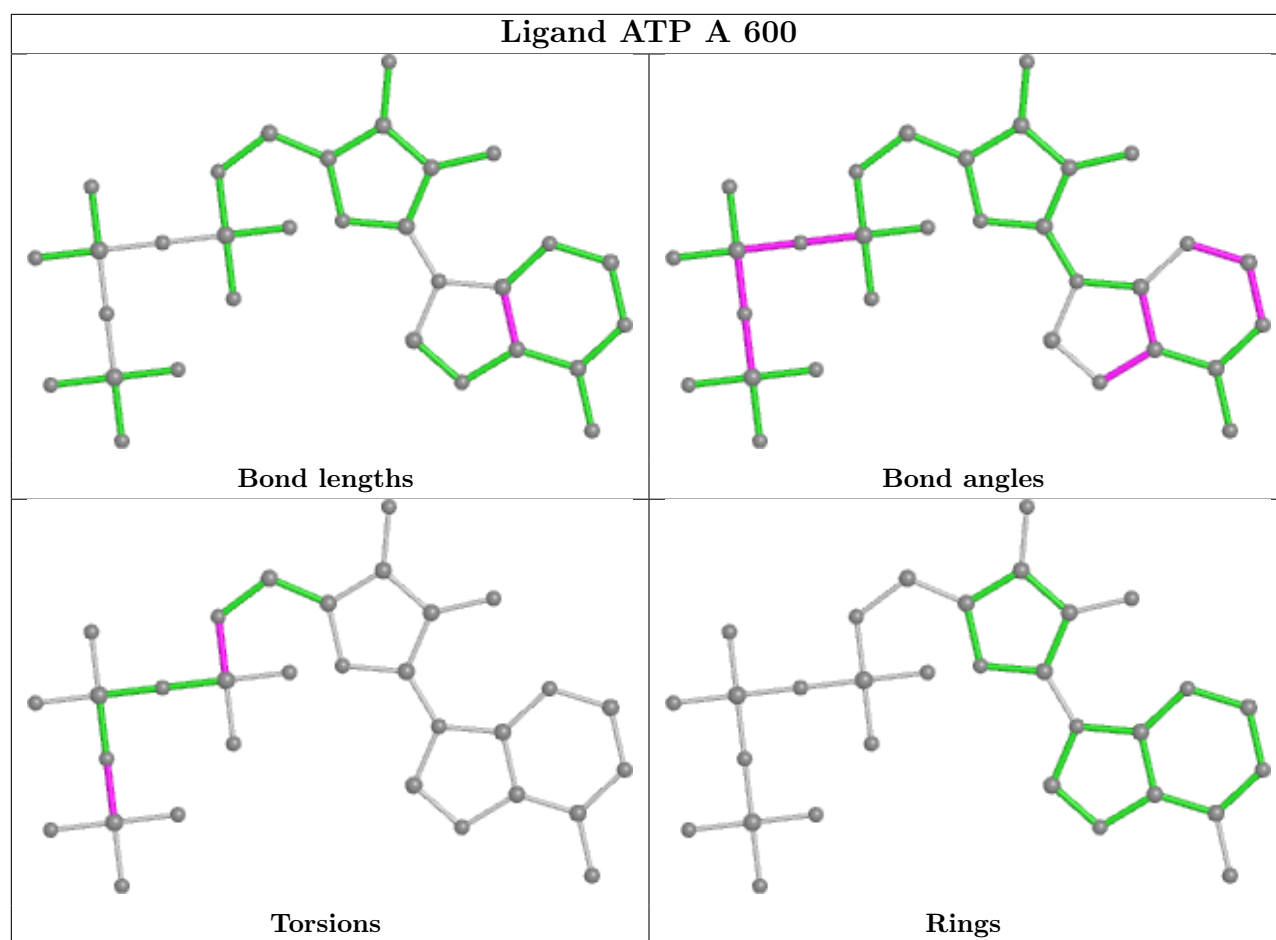
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	600	ATP	1	0
8	G	301	ZH7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

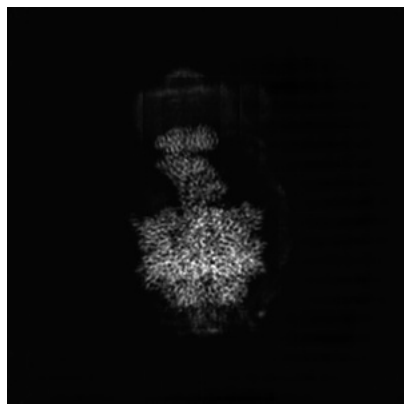
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23764. These allow visual inspection of the internal detail of the map and identification of artifacts.

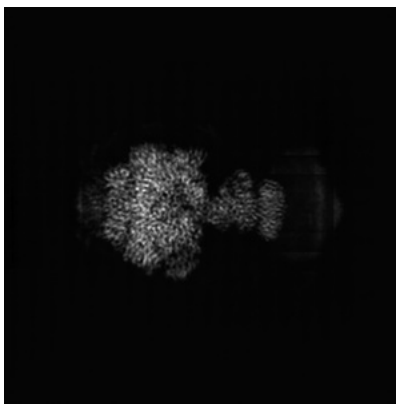
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

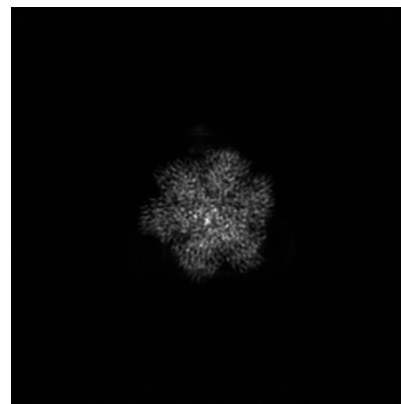
6.1.1 Primary map



X

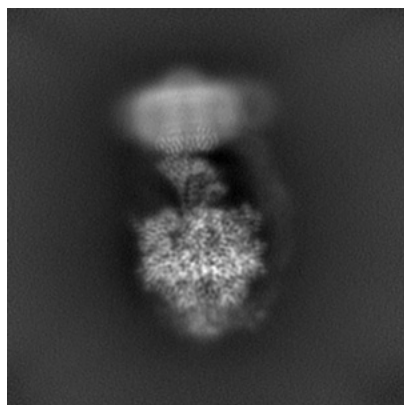


Y

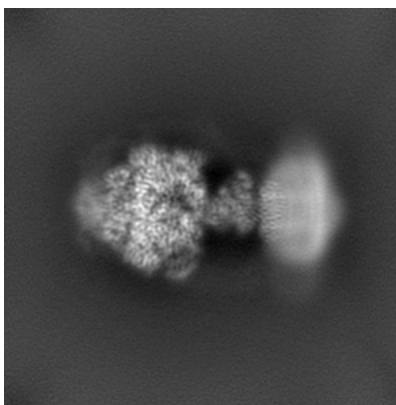


Z

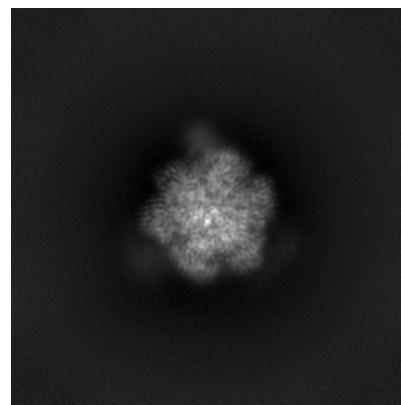
6.1.2 Raw map



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: 128

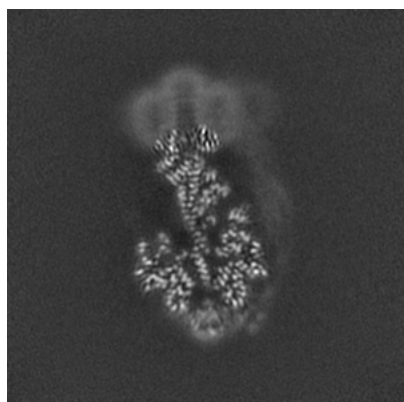


Y Index: 128

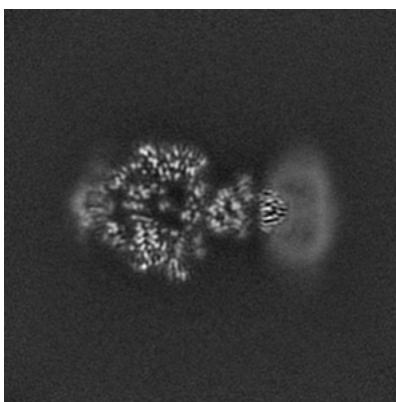


Z Index: 128

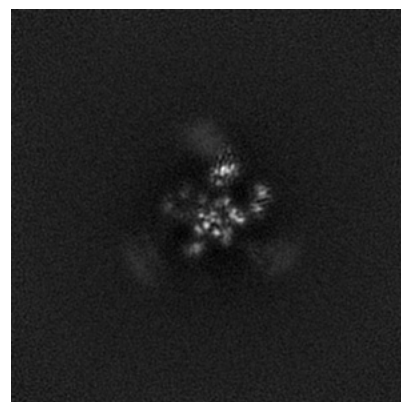
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

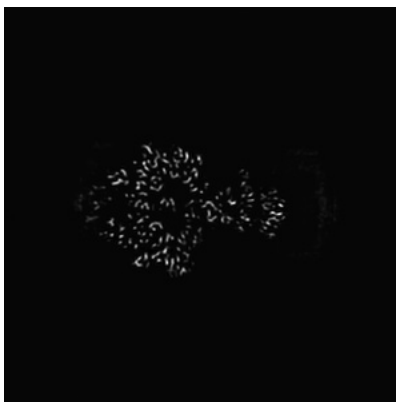
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 126

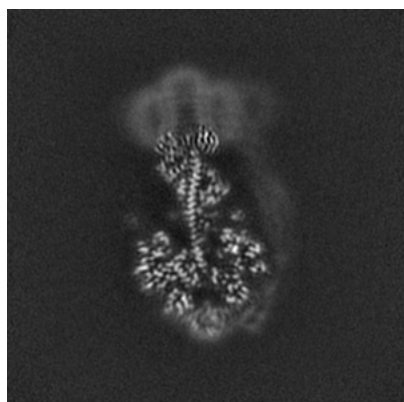


Y Index: 125

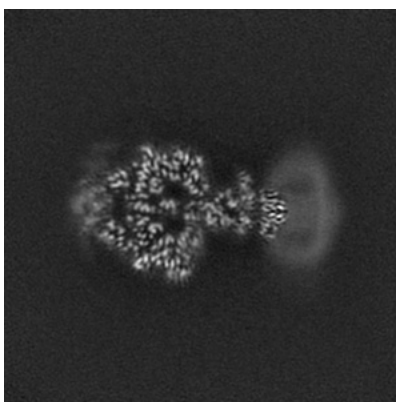


Z Index: 90

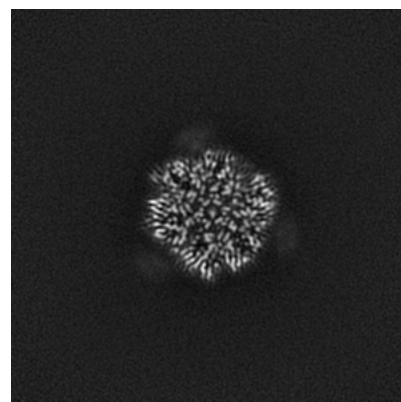
6.3.2 Raw map



X Index: 126



Y Index: 125

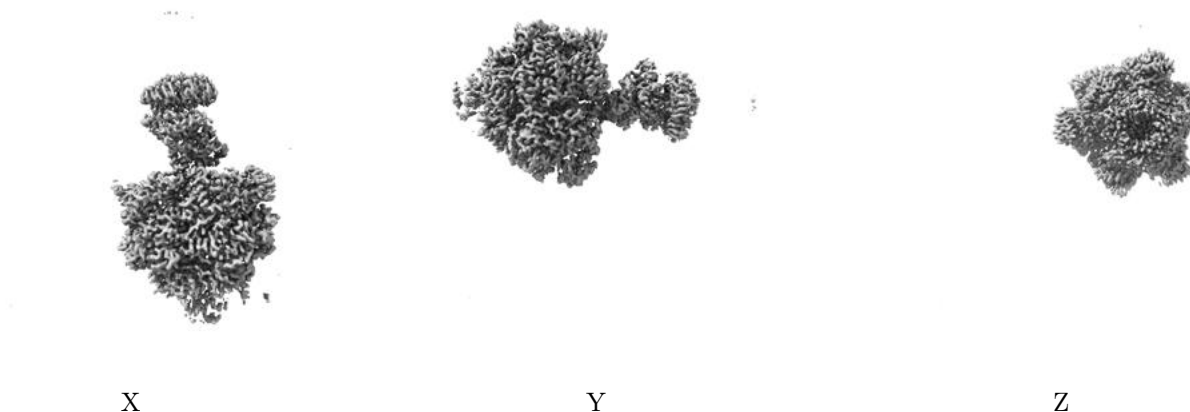


Z Index: 89

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

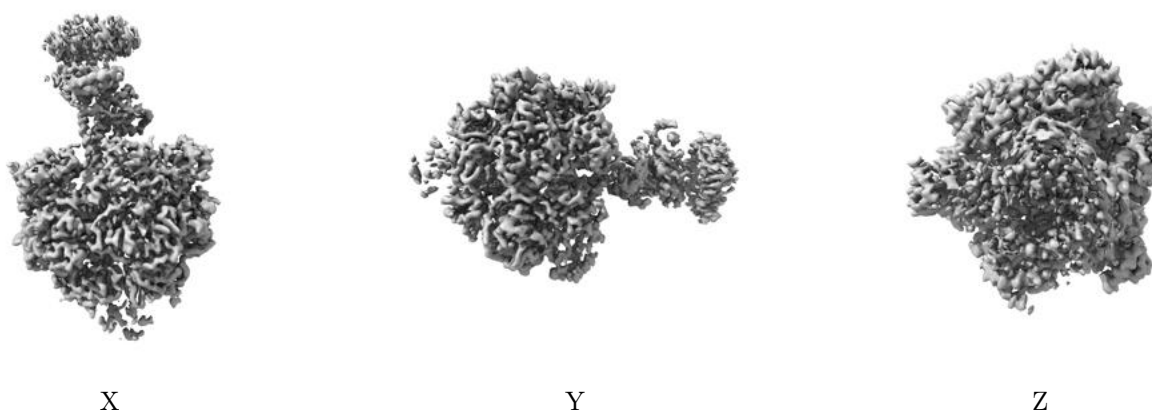
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

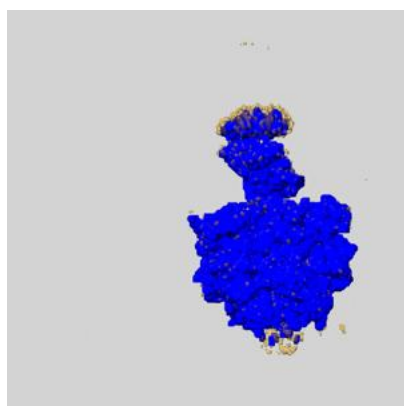
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

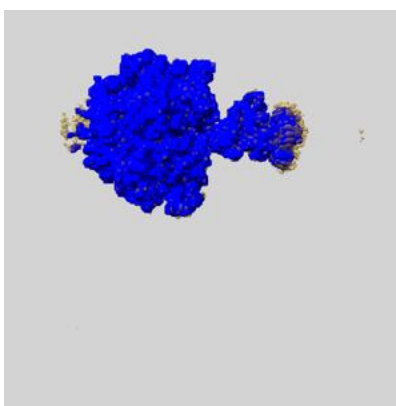
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

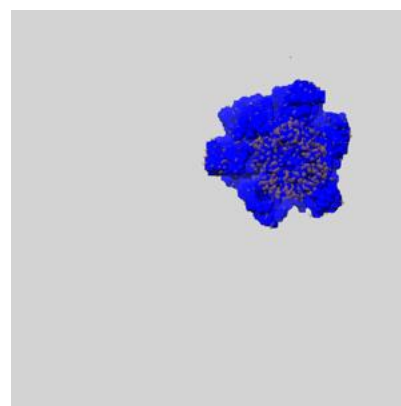
6.5.1 emd_23764_msk_1.map [i](#)



X



Y

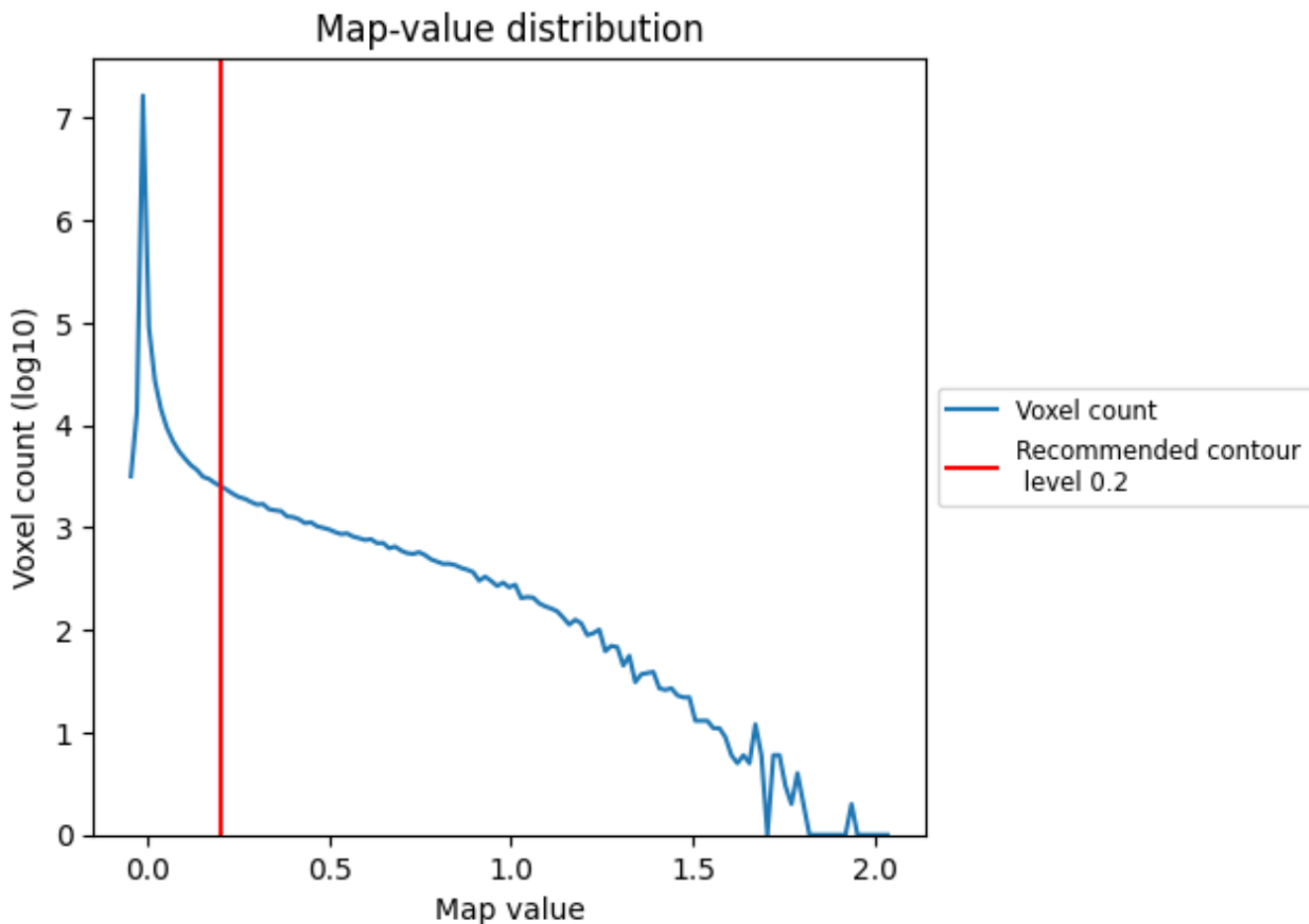


Z

7 Map analysis [i](#)

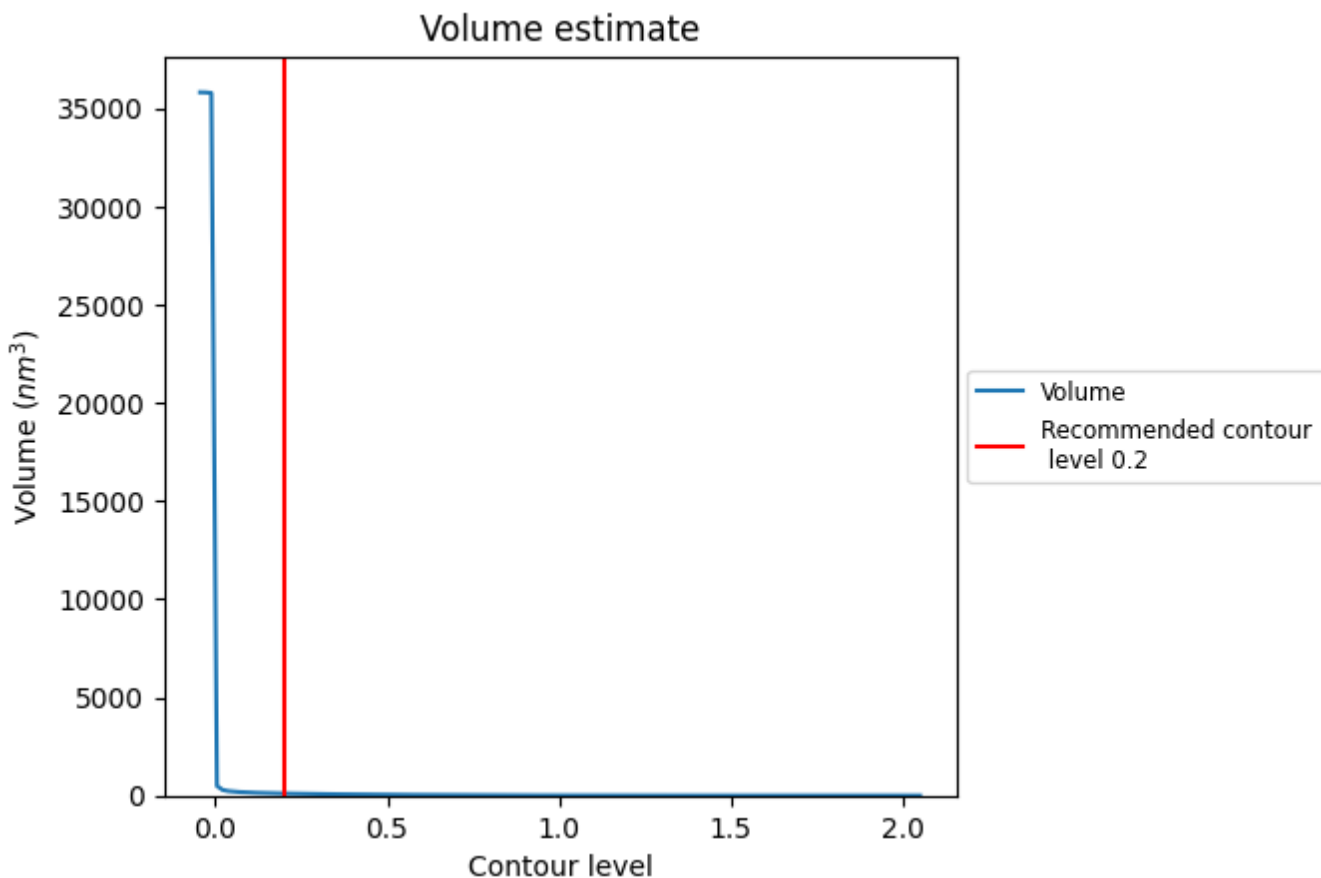
This section contains the results of statistical analysis of the map.

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.

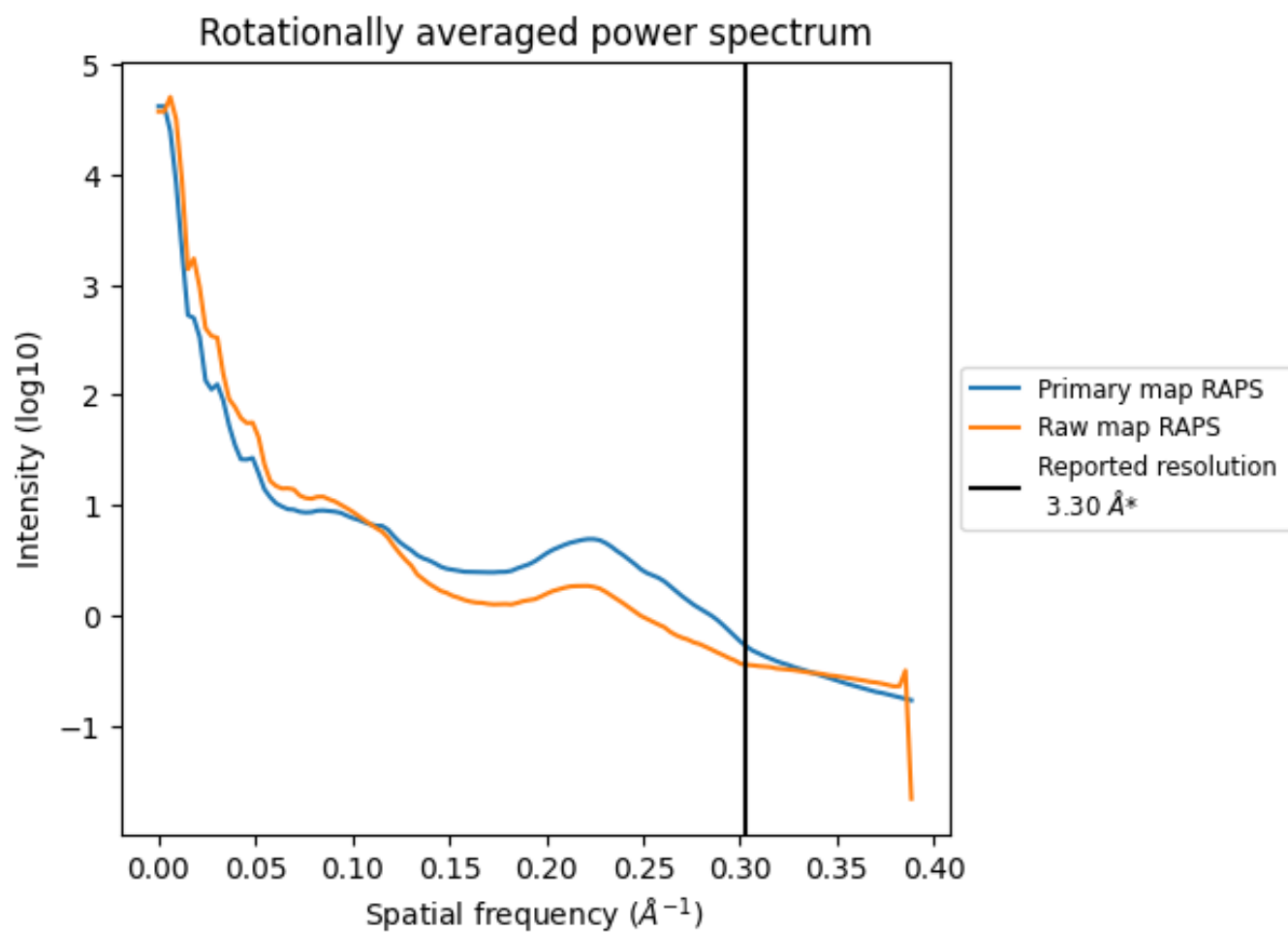
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm^3 ; this corresponds to an approximate mass of 95 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

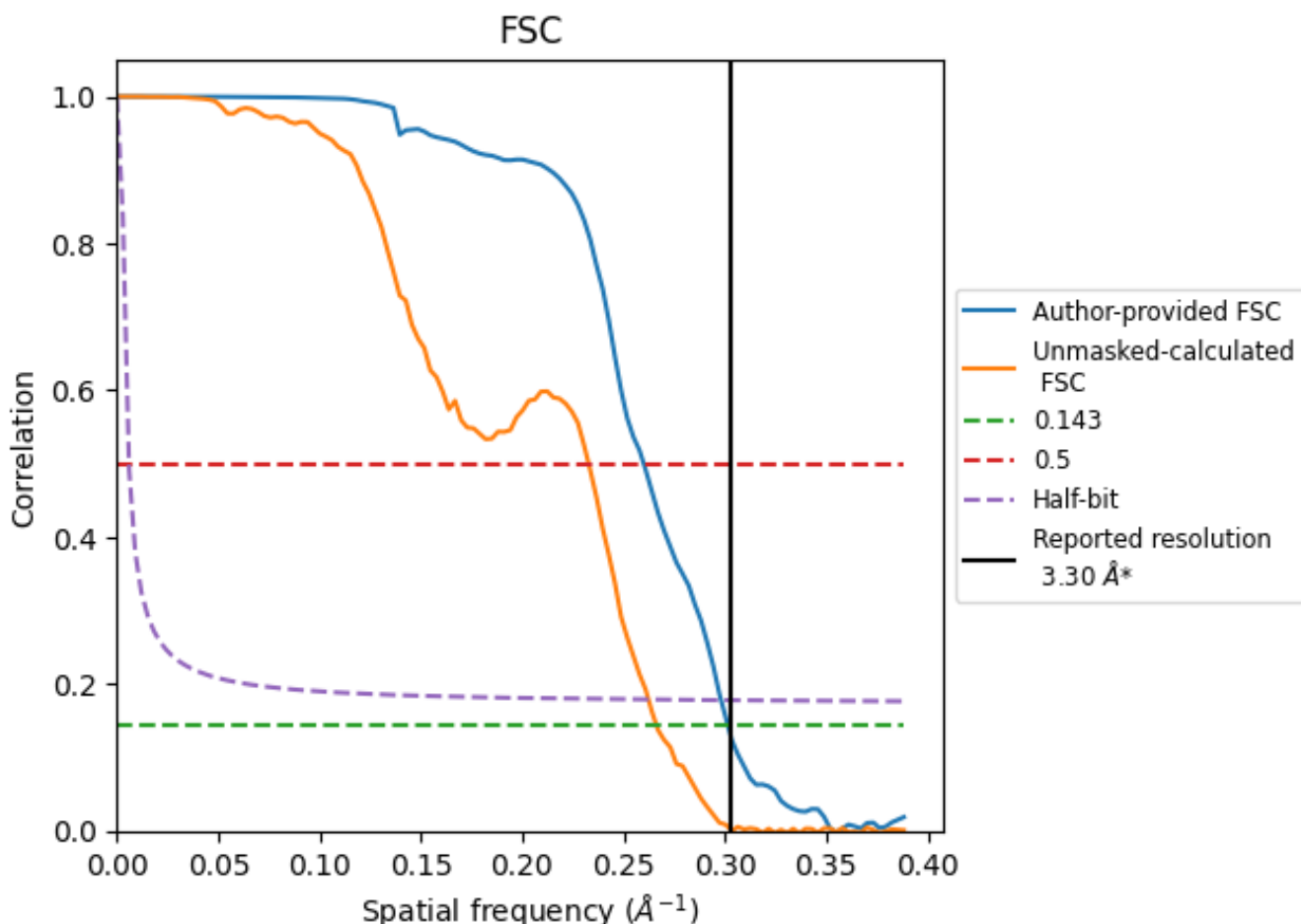


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

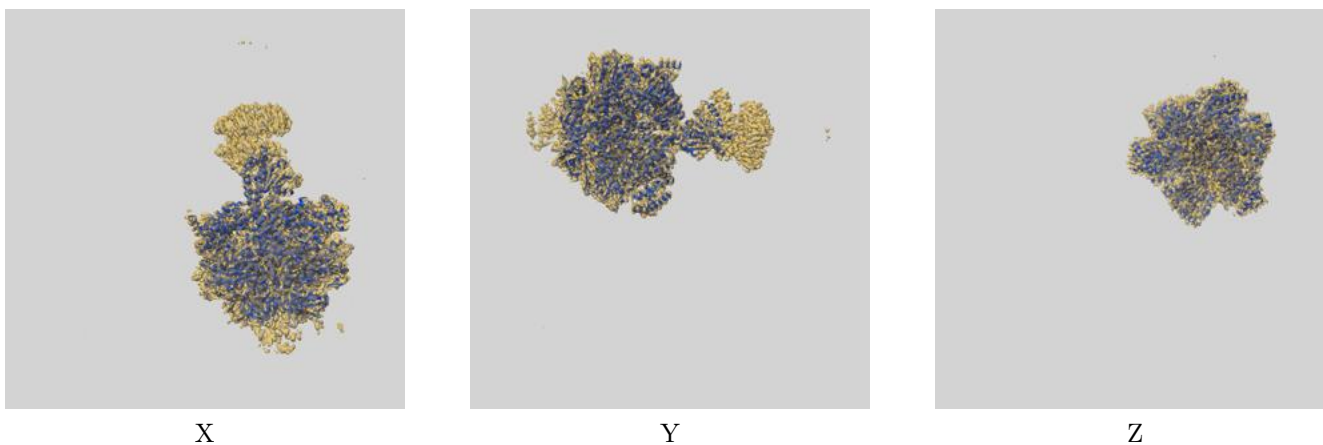
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.85	3.35
Unmasked-calculated*	3.76	4.30	3.81

*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 3.76 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

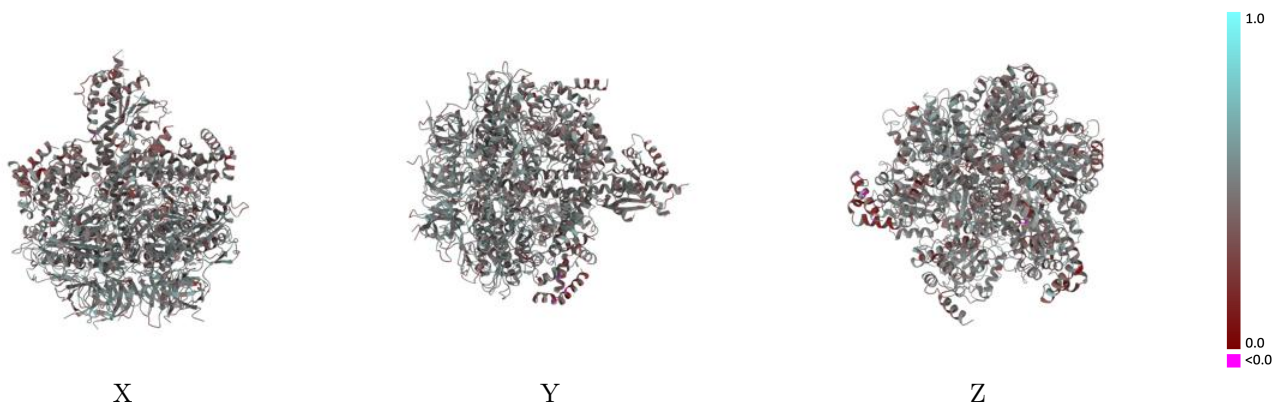
This section contains information regarding the fit between EMDB map EMD-23764 and PDB model 7MD3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



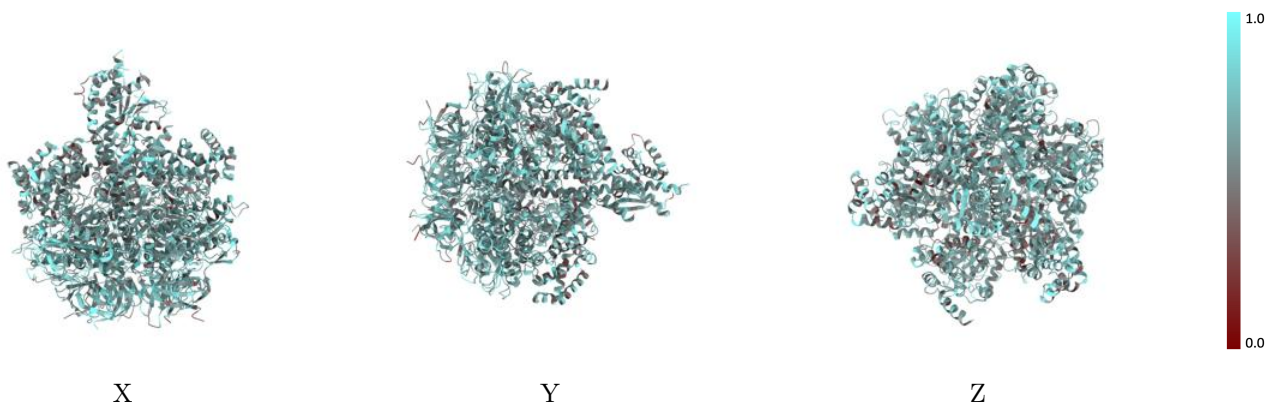
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



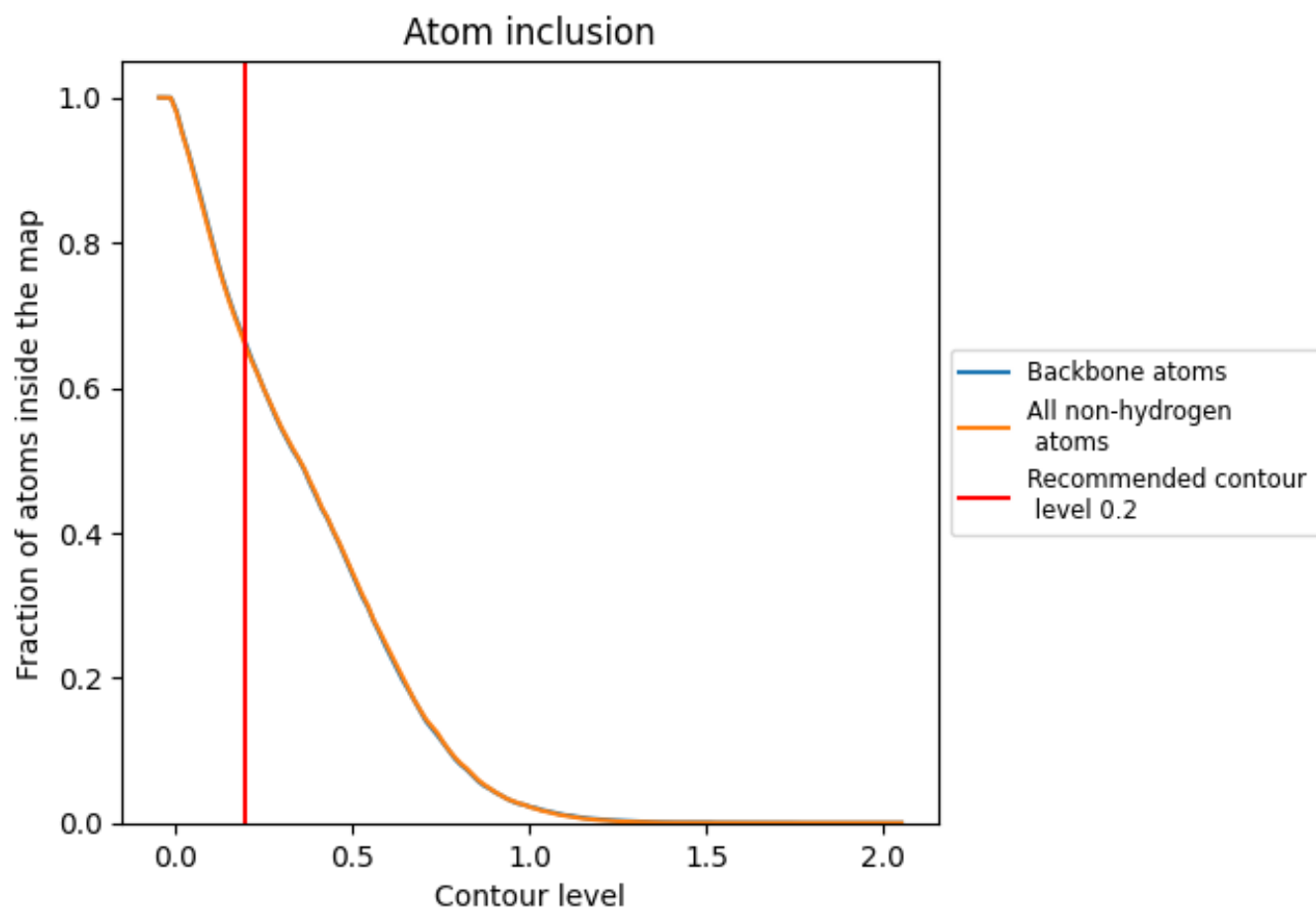
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6571	 0.4600
A	 0.6724	 0.4620
B	 0.6626	 0.4510
C	 0.6791	 0.4700
D	 0.6664	 0.4620
E	 0.6571	 0.4630
F	 0.6798	 0.4750
G	 0.6276	 0.4330
H	 0.6111	 0.3920

