



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:52 PM UTC

PDB ID : 8PSJ / pdb_00008psj
EMDB ID : EMD-17853
Title : Asymmetric unit of the yeast fatty acid synthase in the semi rotated state with ACP at the acetyl transferase domain (FASx sample)
Authors : Singh, K.; Bunzel, G.; Graf, B.; Yip, K.M.; Stark, H.; Chari, A.
Deposited on : 2023-07-13
Resolution : 3.40 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

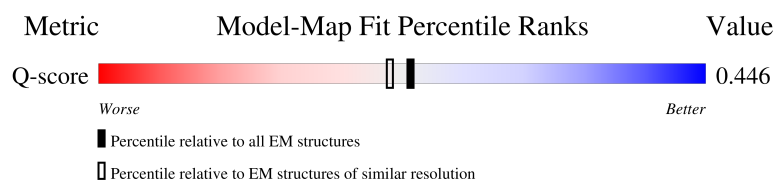
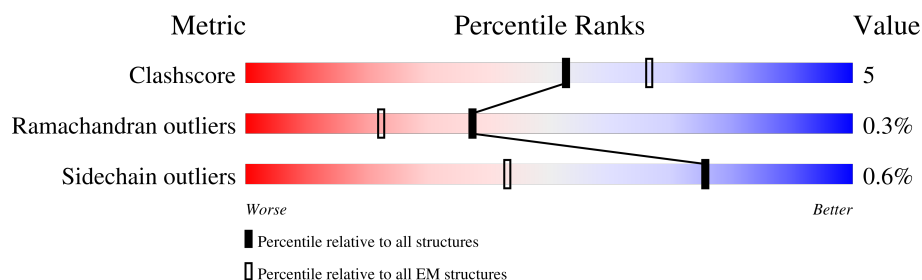
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1887	5% 74% 10% 16%
1	B	1887	6% 91%
2	G	2051	8% 83% 16%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 29695 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.

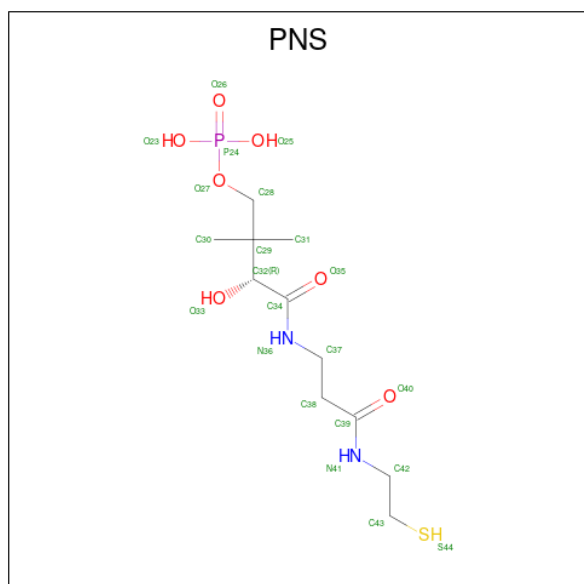
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1589	Total	C	N	O	S	0	0
			12402	7852	2095	2407	48		
1	B	163	Total	C	N	O	S	0	0
			1223	775	205	240	3		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The atoms in the ring are labeled: N1, N3, N5, N10 for nitrogen; C2, C4, C5A, C6, C7, C8, C9 for carbon. Substituents on the ring include a methyl group (C8M) at C8, a methyl group (C7M) at C7, and a ribityl chain at C10. The ribityl chain consists of three carbon atoms (C1, C2, C3) in a chain, with C1 attached to the ring. C2 has a hydroxyl group (OH) attached with a wedge bond, and C3 has a hydroxyl group (OH) attached with a dashed bond. The terminal carbon (C4) is part of a phosphate group, which is shown as a phosphorus atom (P) bonded to four oxygen atoms: one double-bonded (O1P), and three single-bonded (O2P, O3P, O4P). The oxygen atoms are colored red, and the phosphorus atom is colored purple.

Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total 31	C 17	N 4	O 9	P 1	0





Met	ASP	ALA	TRR	S5	T6	R7	P8	L9	T10	L11	S12	H13	G14	S15	L16	E17	H18	V19	L20	L21	V22	P23	T24	A25	I29	A30	S31	Q32	L33	Q34	E35	Q36	F37	N38	K39	I40	L41	P42	E43	P44	T45	E46	G47	F48	A49	A50	D51	D52	E53	P54	T55	T56	F57	A58	E59	L60	V61	G62																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35781	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.059	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	253.19998, 253.19998, 253.19998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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: PNS, FMN

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	1.01	1/12637 (0.0%)	1.52	16/17080 (0.1%)
1	B	1.10	0/1241	1.64	2/1675 (0.1%)
2	G	1.06	0/16383	1.52	31/22229 (0.1%)
All	All	1.04	1/30261 (0.0%)	1.53	49/40984 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1174	TYR	C-O	6.03	1.30	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	662	GLY	CA-C-N	7.22	126.10	120.33
2	G	662	GLY	C-N-CA	7.22	126.10	120.33
1	A	381	GLU	CB-CG-CD	6.20	123.14	112.60
2	G	186	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	1502	ARG	N-CA-C	-6.00	104.65	111.07
1	A	1378	GLU	CB-CG-CD	5.96	122.73	112.60
2	G	781	LEU	CA-C-N	5.62	128.28	120.29
2	G	781	LEU	C-N-CA	5.62	128.28	120.29
2	G	748	THR	CA-CB-OG1	-5.53	101.31	109.60
1	A	1614	VAL	CA-C-O	-5.51	115.30	121.36
1	A	1287	VAL	N-CA-C	-5.50	104.96	110.30
2	G	61	VAL	CA-C-N	5.50	127.20	120.22
2	G	61	VAL	C-N-CA	5.50	127.20	120.22
1	A	852	ARG	N-CA-C	-5.48	105.22	111.14
1	A	1417	SER	CA-C-N	5.45	124.69	120.33
1	A	1417	SER	C-N-CA	5.45	124.69	120.33
2	G	1820	ASP	CA-CB-CG	5.43	118.03	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1276	GLN	N-CA-C	-5.39	105.41	111.28
2	G	230	TYR	N-CA-C	-5.38	104.86	111.75
2	G	1723	GLY	CA-C-O	-5.35	117.65	122.57
1	A	1582	GLY	CA-C-O	-5.34	117.03	122.59
2	G	1103	PHE	CA-C-O	-5.31	115.11	120.84
1	B	262	ASP	CA-C-N	5.30	126.77	120.14
1	B	262	ASP	C-N-CA	5.30	126.77	120.14
2	G	246	LEU	CA-C-N	5.30	127.39	120.28
2	G	246	LEU	C-N-CA	5.30	127.39	120.28
2	G	767	PHE	CB-CA-C	5.28	119.07	109.83
1	A	1326	ILE	CA-C-O	-5.27	114.78	120.36
2	G	24	THR	CA-C-N	5.21	127.27	120.28
2	G	24	THR	C-N-CA	5.21	127.27	120.28
1	A	1316	VAL	CA-C-O	-5.19	116.02	121.41
2	G	1340	PRO	CA-C-N	5.16	127.45	120.38
2	G	1340	PRO	C-N-CA	5.16	127.45	120.38
2	G	168	ASP	CA-C-N	5.16	127.20	120.28
2	G	168	ASP	C-N-CA	5.16	127.20	120.28
1	A	1174	TYR	CA-C-N	5.16	126.30	122.59
1	A	1174	TYR	C-N-CA	5.16	126.30	122.59
2	G	557	LYS	N-CA-C	5.15	116.74	110.41
2	G	56	THR	CB-CA-C	5.13	116.83	109.09
1	A	749	ILE	CA-C-O	-5.11	115.64	120.95
2	G	166	THR	CA-C-N	5.10	127.07	120.44
2	G	166	THR	C-N-CA	5.10	127.07	120.44
2	G	792	PRO	CB-CA-C	-5.07	106.40	111.17
1	A	1388	MET	CA-C-O	-5.06	115.84	121.51
2	G	933	ARG	CA-C-N	5.04	127.35	120.54
2	G	933	ARG	C-N-CA	5.04	127.35	120.54
2	G	637	VAL	N-CA-C	-5.02	105.43	110.30
2	G	621	GLY	CA-C-N	5.01	125.64	120.03
2	G	621	GLY	C-N-CA	5.01	125.64	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12402	0	12349	102	0
1	B	1223	0	1264	22	0
2	G	16018	0	15993	203	0
3	B	21	0	21	2	0
4	G	31	0	19	2	0
All	All	29695	0	29646	317	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 5.

All (317) 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)
1:A:803:MET:HE3	1:A:822:VAL:HG21	1.59	0.84
1:A:688:ILE:HD11	1:A:872:THR:HG21	1.67	0.76
2:G:569:LEU:HB3	2:G:577:ILE:HD11	1.69	0.75
1:B:249:TYR:OH	1:B:288:ASP:OD1	2.07	0.73
1:A:413:LEU:HD22	1:A:451:MET:HG2	1.70	0.72
1:A:1812:THR:OG1	1:A:1841:ARG:NH1	2.23	0.71
2:G:555:LEU:HD11	2:G:557:LYS:HE3	1.73	0.70
3:B:1901:PNS:N41	2:G:163:GLN:O	2.26	0.68
2:G:128:THR:O	2:G:132:MET:HB2	1.92	0.68
2:G:177:TYR:OH	2:G:220:GLU:OE2	2.11	0.68
2:G:553:ASN:HB2	2:G:556:LYS:HE2	1.76	0.68
1:A:756:GLU:N	1:A:756:GLU:OE1	2.28	0.67
1:A:487:ASP:OD2	1:A:674:LYS:HE3	1.93	0.67
1:A:1531:LEU:HD21	1:A:1660:TYR:CE2	2.30	0.66
2:G:1530:LYS:HE2	2:G:1637:LEU:HG	1.79	0.65
2:G:715:GLN:O	2:G:719:ILE:HD12	1.98	0.64
2:G:338:MET:SD	2:G:380:SER:OG	2.56	0.62
1:A:1592:MET:HE2	1:A:1641:ILE:HG23	1.82	0.62
1:A:1248:GLY:O	1:A:1331:GLY:HA2	1.99	0.62
1:A:1483:ASN:OD1	1:A:1484:GLU:N	2.32	0.62
2:G:105:ALA:HB1	2:G:119:THR:HG23	1.81	0.61
2:G:161:GLY:O	2:G:245:GLN:NE2	2.33	0.61
2:G:339:LEU:HD12	2:G:419:ARG:O	2.00	0.61
2:G:1632:ILE:HG22	2:G:1637:LEU:HD21	1.82	0.61
3:B:1901:PNS:H382	2:G:372:ASN:ND2	2.16	0.60
1:A:56:MET:HE3	2:G:1892:ASN:HB3	1.83	0.60
1:B:147:ALA:HB2	1:B:217:PHE:CD2	2.37	0.59
2:G:119:THR:O	2:G:123:ILE:HG12	2.02	0.59
2:G:198:LEU:O	2:G:202:THR:N	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:517:HIS:HB2	2:G:527:VAL:HG11	1.85	0.58
1:A:413:LEU:CD2	1:A:451:MET:HG2	2.32	0.58
2:G:264:ARG:HD3	2:G:456:GLN:HB2	1.84	0.58
1:A:755:THR:OG1	1:A:758:ASN:ND2	2.35	0.58
2:G:241:ILE:HG21	2:G:275:GLN:HE22	1.70	0.57
2:G:13:HIS:HB2	2:G:41:LEU:HD21	1.87	0.57
2:G:1854:MET:HB2	2:G:1969:LEU:HB2	1.86	0.57
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.86	0.57
2:G:1496:LYS:HB2	2:G:2002:LYS:HD2	1.86	0.57
2:G:517:HIS:O	2:G:521:ASP:N	2.38	0.56
1:B:198:PRO:HG3	1:B:212:THR:HG21	1.87	0.56
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.21	0.56
1:A:1759:MET:HE1	1:A:1771:VAL:HG23	1.88	0.55
2:G:324:LEU:HD23	2:G:324:LEU:O	2.06	0.55
1:A:1343:PHE:HB3	1:A:1349:THR:HG23	1.88	0.55
2:G:577:ILE:HG23	2:G:1082:ILE:HD13	1.89	0.55
1:A:529:MET:HE1	1:A:894:ARG:HG2	1.89	0.55
1:A:1022:THR:HG22	1:A:1226:SER:OG	2.07	0.55
2:G:229:ASP:HA	2:G:232:LEU:HB3	1.89	0.55
1:B:256:LEU:HD21	1:B:302:LEU:HD11	1.88	0.54
2:G:56:THR:HG21	2:G:108:LEU:HD22	1.90	0.54
1:B:232:LEU:HD13	1:B:269:LEU:HA	1.90	0.54
2:G:369:SER:O	2:G:487:PRO:HA	2.08	0.54
2:G:228:LYS:O	2:G:232:LEU:HB2	2.07	0.54
1:A:1086:ASP:O	1:A:1089:VAL:HG12	2.08	0.54
2:G:667:LYS:HE2	2:G:697:THR:HB	1.90	0.54
1:A:969:ASN:HB3	1:A:973:ALA:HB3	1.89	0.53
2:G:246:LEU:HD12	2:G:279:THR:HG23	1.90	0.53
2:G:665:LEU:O	2:G:669:LEU:HD13	2.08	0.53
2:G:1129:ALA:HB3	2:G:1180:MET:HB2	1.90	0.53
1:A:21:GLN:HE22	2:G:1808:SER:HA	1.74	0.53
2:G:573:LYS:HG2	2:G:1101:GLU:HA	1.89	0.53
1:B:295:ALA:HB2	1:B:302:LEU:HD12	1.92	0.52
2:G:281:VAL:HG12	2:G:459:VAL:HG11	1.90	0.52
1:B:268:ALA:HB2	1:B:290:MET:HE3	1.91	0.52
2:G:1094:GLU:HG3	2:G:1097:ILE:HD12	1.91	0.52
1:A:841:GLU:OE1	1:A:841:GLU:N	2.43	0.52
2:G:173:LEU:HA	2:G:244:ILE:HD13	1.92	0.52
1:A:501:THR:OG1	1:A:883:ILE:O	2.26	0.52
1:A:1157:ILE:HD11	1:A:1164:SER:HB3	1.92	0.52
2:G:732:TRP:CG	2:G:750:MET:HE3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.09	0.52
2:G:1737:ILE:O	2:G:1833:TYR:OH	2.28	0.52
1:A:1544:THR:O	1:A:1545:SER:HB3	2.10	0.51
2:G:652:ILE:N	2:G:658:MET:HE1	2.26	0.51
2:G:920:GLU:HA	2:G:984:PHE:CE2	2.46	0.51
2:G:245:GLN:HB3	2:G:279:THR:HG21	1.92	0.51
1:A:1764:VAL:HG21	1:A:1883:VAL:HG11	1.92	0.51
1:B:153:VAL:HG21	1:B:266:LEU:HB3	1.92	0.51
2:G:553:ASN:CB	2:G:556:LYS:HE2	2.40	0.51
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.43	0.51
1:A:1541:PHE:CZ	1:A:1557:ILE:HD12	2.45	0.51
1:B:268:ALA:HB2	1:B:290:MET:CE	2.41	0.51
2:G:241:ILE:HA	2:G:244:ILE:HG22	1.92	0.51
2:G:542:GLY:HA3	2:G:546:GLU:OE2	2.11	0.51
2:G:741:HIS:CD2	2:G:855:HIS:ND1	2.79	0.51
2:G:1928:GLN:HB3	2:G:1936:VAL:HG21	1.93	0.51
1:A:61:LEU:HA	1:A:65:TYR:HB2	1.93	0.51
2:G:56:THR:HG22	2:G:112:ASN:ND2	2.26	0.50
1:A:41:THR:HG21	2:G:1663:THR:HG22	1.93	0.50
2:G:1182:VAL:HG22	2:G:1197:LEU:HD13	1.94	0.50
2:G:1628:HIS:NE2	2:G:1636:LYS:HG2	2.26	0.50
1:B:264:VAL:HG12	1:B:290:MET:HE1	1.92	0.50
1:B:228:LEU:HA	1:B:231:ARG:HE	1.77	0.50
2:G:1345:GLY:HA3	2:G:1412:TYR:CD1	2.46	0.50
2:G:1542:LEU:HD13	2:G:1592:LEU:HD12	1.94	0.50
2:G:353:VAL:HG13	2:G:366:VAL:HG23	1.94	0.49
2:G:1156:CYS:SG	2:G:1250:PRO:HD2	2.52	0.49
1:A:1771:VAL:HG22	1:A:1881:VAL:HG22	1.94	0.49
2:G:1149:TRP:HA	2:G:1242:PHE:CE1	2.47	0.49
2:G:234:ILE:N	2:G:235:PRO:CD	2.76	0.49
1:A:1249:SER:HB2	1:A:1332:TYR:CE2	2.48	0.49
1:A:511:TYR:CE1	1:A:882:ASN:HB3	2.47	0.49
2:G:1459:LEU:HD22	2:G:1464:LEU:HD11	1.94	0.49
2:G:694:TYR:HA	2:G:698:LEU:CD1	2.43	0.49
2:G:1129:ALA:CB	2:G:1180:MET:HB2	2.43	0.49
2:G:1260:GLN:N	2:G:1260:GLN:OE1	2.46	0.49
2:G:1320:LEU:HD23	2:G:1367:GLN:HG2	1.95	0.48
1:A:1249:SER:HB3	1:A:1280:ILE:HG23	1.94	0.48
2:G:1755:ILE:HD11	2:G:1762:TYR:CG	2.49	0.48
1:A:1388:MET:HE1	1:A:1396:MET:SD	2.53	0.48
2:G:182:VAL:HG23	2:G:183:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1638:ILE:HD13	2:G:1657:ILE:HG12	1.95	0.48
2:G:1868:GLN:HG3	2:G:1898:TYR:OH	2.14	0.48
1:A:719:GLN:HG3	1:A:1612:ASP:HA	1.95	0.48
1:A:1252:GLY:HA3	1:A:1280:ILE:HG13	1.96	0.48
2:G:1223:MET:SD	2:G:1568:HIS:HD2	2.36	0.48
2:G:338:MET:HB2	2:G:421:LEU:HB2	1.96	0.48
2:G:1151:HIS:NE2	2:G:1155:LEU:HD12	2.30	0.47
2:G:1663:THR:OG1	2:G:1803:THR:O	2.23	0.47
1:A:767:ALA:HA	1:A:821:GLN:O	2.15	0.47
2:G:210:THR:C	2:G:212:GLY:H	2.22	0.47
1:A:49:PRO:HD3	2:G:1781:LEU:HD11	1.97	0.47
1:A:1114:TYR:CE1	1:A:1337:GLU:HG3	2.50	0.47
2:G:621:GLY:HA2	2:G:630:MET:CE	2.45	0.47
2:G:176:LEU:HD21	2:G:248:HIS:CE1	2.50	0.47
2:G:1008:GLN:OE1	2:G:1024:ARG:NH1	2.48	0.47
1:A:739:GLN:O	1:A:798:ASN:ND2	2.44	0.47
2:G:1086:LEU:HD12	2:G:1090:TYR:HB2	1.97	0.47
2:G:1583:MET:HE3	2:G:1583:MET:HA	1.97	0.47
1:A:487:ASP:CG	1:A:674:LYS:HE3	2.40	0.46
2:G:56:THR:HG22	2:G:112:ASN:HD22	1.80	0.46
2:G:598:THR:HA	2:G:599:PRO:HA	1.77	0.46
2:G:764:MET:HA	2:G:797:ASP:OD2	2.15	0.46
2:G:1265:MET:HE3	2:G:1269:LEU:HD12	1.96	0.46
2:G:54:PRO:HG3	2:G:60:LEU:HD13	1.96	0.46
1:A:697:LEU:HB3	1:A:726:GLY:HA2	1.96	0.46
1:A:1370:THR:O	1:A:1373:ARG:NH1	2.41	0.46
1:A:46:GLU:OE1	1:A:54:ALA:N	2.49	0.46
1:A:1694:TYR:OH	2:G:1001:ASP:OD2	2.23	0.46
1:A:41:THR:O	1:A:76:ARG:NH1	2.39	0.46
1:A:1812:THR:HG1	1:A:1841:ARG:HH11	1.60	0.46
2:G:1681:TYR:O	2:G:1688:GLN:HG3	2.16	0.46
1:A:34:VAL:O	1:A:38:ASP:HB3	2.15	0.46
2:G:1325:PHE:O	2:G:1328:VAL:HB	2.15	0.46
2:G:1669:GLN:N	2:G:1669:GLN:OE1	2.49	0.46
2:G:433:VAL:HG13	2:G:485:ARG:HH22	1.80	0.46
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	1.96	0.46
2:G:80:PHE:HA	2:G:83:VAL:HG12	1.98	0.46
2:G:538:ASP:O	2:G:759:ARG:NH2	2.49	0.46
2:G:669:LEU:O	2:G:674:TYR:HB2	2.16	0.46
2:G:1201:VAL:HG11	2:G:1226:ASN:HB2	1.98	0.46
2:G:1546:THR:HG1	2:G:1620:THR:H	1.61	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:VAL:HG21	1:A:910:THR:HG22	1.98	0.46
2:G:1784:MET:SD	2:G:1784:MET:C	2.98	0.46
1:A:22:PHE:HA	2:G:1977:HIS:ND1	2.30	0.45
2:G:820:CYS:SG	2:G:857:ILE:HG21	2.56	0.45
2:G:919:TYR:CD2	2:G:954:VAL:HG22	2.51	0.45
1:A:1759:MET:HE3	1:A:1769:VAL:HG12	1.98	0.45
2:G:783:GLY:O	2:G:793:PRO:HA	2.16	0.45
2:G:1269:LEU:HD13	2:G:1560:LEU:O	2.16	0.45
2:G:716:VAL:HG11	2:G:730:LEU:HG	1.99	0.45
2:G:1150:ARG:HH12	2:G:1184:ILE:HG21	1.82	0.45
1:A:1266:LYS:O	1:A:1267:ASP:C	2.59	0.45
2:G:203:LEU:HG	2:G:204:ASP:OD1	2.17	0.45
1:A:1106:ILE:HA	1:A:1188:GLN:NE2	2.32	0.45
2:G:713:ILE:HD11	2:G:732:TRP:CZ3	2.51	0.45
1:A:1246:CYS:HA	1:A:1299:LYS:O	2.16	0.45
2:G:391:LEU:HD23	2:G:394:ARG:HH11	1.81	0.45
2:G:597:MET:HE2	2:G:802:GLY:HA2	1.99	0.45
2:G:695:ILE:HD11	2:G:726:PHE:HB3	1.99	0.45
2:G:802:GLY:O	2:G:805:VAL:HG22	2.17	0.45
1:A:1808:SER:O	1:A:1841:ARG:NH1	2.45	0.45
2:G:847:ARG:HG3	2:G:851:GLY:HA2	1.97	0.45
2:G:930:MET:HE3	2:G:943:TRP:CG	2.52	0.45
2:G:100:ASP:HB3	2:G:548:PHE:CD2	2.51	0.45
2:G:631:THR:OG1	2:G:665:LEU:HD11	2.17	0.45
1:A:1677:VAL:O	1:A:1680:ARG:N	2.50	0.45
1:A:1685:TYR:OH	2:G:993:GLN:NE2	2.50	0.45
1:A:1851:LEU:HD12	1:A:1851:LEU:N	2.32	0.45
2:G:173:LEU:HD23	2:G:219:LEU:HD11	2.00	0.45
2:G:103:ALA:HA	2:G:545:GLN:HB2	1.99	0.44
2:G:597:MET:HA	4:G:2101:FMN:N5	2.32	0.44
1:A:1292:ILE:HG22	1:A:1294:SER:HB3	1.99	0.44
1:B:260:ARG:O	1:B:264:VAL:HG23	2.17	0.44
2:G:9:LEU:HD21	2:G:34:GLN:HB2	1.99	0.44
2:G:1398:ARG:HB3	2:G:1403:VAL:HG21	2.00	0.44
2:G:1290:PHE:HB3	2:G:1329:VAL:HG13	1.99	0.44
1:A:861:GLN:N	1:A:861:GLN:OE1	2.50	0.44
1:A:1021:VAL:HG11	1:A:1597:LEU:HD11	1.99	0.44
2:G:587:ILE:HG13	2:G:589:ARG:H	1.83	0.44
2:G:2036:GLU:N	2:G:2037:PRO:CD	2.81	0.44
1:A:826:MET:HE1	1:A:847:GLU:HG2	1.99	0.44
1:A:1326:ILE:HG12	1:A:1388:MET:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.52	0.44
1:B:163:LEU:HD21	1:B:270:SER:CB	2.48	0.43
2:G:179:THR:HB	2:G:180:TYR:CD2	2.53	0.43
2:G:821:ILE:HG23	2:G:1055:HIS:CE1	2.53	0.43
2:G:1630:GLY:O	2:G:1631:MET:SD	2.76	0.43
2:G:1286:LYS:HD2	2:G:1374:THR:O	2.18	0.43
2:G:1734:SER:O	2:G:1750:LYS:NZ	2.51	0.43
2:G:1663:THR:HA	2:G:1803:THR:O	2.18	0.43
1:A:768:ILE:HD11	1:A:806:VAL:HG21	2.01	0.43
1:A:1064:ASN:OD1	1:A:1073:THR:OG1	2.35	0.43
1:A:1772:ASP:O	1:A:1814:SER:OG	2.36	0.43
2:G:31:SER:HA	2:G:34:GLN:HB3	2.00	0.43
2:G:210:THR:H	2:G:230:TYR:HE1	1.66	0.43
1:A:1352:THR:HG23	1:A:1365:MET:HE1	2.00	0.43
2:G:1594:GLU:HA	2:G:1598:ALA:HB3	2.01	0.43
1:A:665:LYS:NZ	1:A:912:GLU:OE2	2.52	0.43
1:A:1557:ILE:HA	1:A:1560:MET:HE3	2.01	0.43
1:B:140:ILE:HG21	1:B:256:LEU:HD23	2.00	0.43
1:B:250:LEU:HD12	1:B:256:LEU:HD12	2.00	0.43
2:G:58:ALA:HA	2:G:95:TYR:CZ	2.53	0.43
2:G:227:ASP:C	2:G:229:ASP:H	2.26	0.43
2:G:236:ILE:O	2:G:240:LEU:HD13	2.18	0.43
2:G:241:ILE:CG2	2:G:275:GLN:HE22	2.31	0.43
2:G:751:LEU:HD23	2:G:794:MET:HE1	1.99	0.43
1:A:823:ILE:HD11	1:A:909:LEU:HD21	2.01	0.43
1:A:1857:LYS:O	1:A:1861:GLU:HG2	2.19	0.43
2:G:1381:VAL:HG13	2:G:1422:THR:HA	2.01	0.43
2:G:1638:ILE:HD13	2:G:1657:ILE:CG1	2.49	0.43
1:A:31:THR:HG23	2:G:2011:ILE:HG21	2.00	0.43
2:G:114:THR:HA	2:G:118:LYS:HE2	2.00	0.43
2:G:163:GLN:HG3	2:G:427:PHE:CE2	2.54	0.43
2:G:1430:VAL:HB	2:G:1527:LEU:HD11	2.00	0.43
1:A:37:LYS:HB3	1:A:65:TYR:HE1	1.84	0.42
1:A:989:GLN:HA	1:A:989:GLN:OE1	2.18	0.42
1:A:1403:ILE:HD11	1:A:1661:LEU:HB2	2.00	0.42
2:G:203:LEU:O	2:G:204:ASP:HB2	2.18	0.42
2:G:246:LEU:HD23	2:G:296:VAL:HG22	2.01	0.42
2:G:1353:LEU:HG	2:G:1411:PHE:HB2	2.01	0.42
2:G:1605:VAL:HG22	2:G:1657:ILE:HD12	2.00	0.42
2:G:1697:HIS:CD2	2:G:1825:GLU:HB3	2.53	0.42
2:G:1846:GLU:HG2	2:G:1847:LEU:HD12	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:TYR:CE1	1:A:764:ASP:HA	2.54	0.42
1:A:1251:MET:HE3	1:A:1251:MET:O	2.19	0.42
1:A:1354:GLU:O	1:A:1358:HIS:ND1	2.50	0.42
2:G:694:TYR:HA	2:G:698:LEU:HD13	2.02	0.42
2:G:1632:ILE:O	2:G:1632:ILE:HG23	2.18	0.42
2:G:229:ASP:O	2:G:233:SER:N	2.37	0.42
2:G:1632:ILE:HG22	2:G:1637:LEU:CD2	2.50	0.42
1:A:45:VAL:HA	1:A:79:LEU:O	2.19	0.42
1:A:952:GLU:OE1	1:A:952:GLU:HA	2.20	0.42
1:A:992:PHE:CE2	1:A:1399:PRO:HG3	2.55	0.42
2:G:36:GLN:O	2:G:40:ILE:HG12	2.19	0.42
2:G:713:ILE:HD11	2:G:732:TRP:CE3	2.55	0.42
2:G:1889:VAL:HB	2:G:1977:HIS:HB2	2.02	0.42
1:A:1400:ILE:HG22	1:A:1658:PRO:HB3	2.01	0.42
2:G:45:THR:HG22	2:G:53:GLU:OE2	2.20	0.42
2:G:583:PHE:HA	2:G:764:MET:HG2	2.02	0.42
2:G:1263:LYS:HE2	2:G:1339:PHE:O	2.20	0.42
1:A:1004:ILE:HG13	1:A:1005:ALA:N	2.34	0.42
1:B:290:MET:HA	1:B:293:LYS:HE2	2.01	0.42
2:G:591:PRO:O	2:G:592:LEU:HD23	2.19	0.42
1:A:677:TYR:CD1	1:A:677:TYR:N	2.84	0.42
2:G:767:PHE:HB2	2:G:796:PHE:CD2	2.54	0.42
2:G:1383:ASN:HB2	2:G:1419:PHE:CE1	2.55	0.42
2:G:1892:ASN:HD21	2:G:1899:VAL:HG23	1.84	0.42
1:A:1117:GLU:O	1:A:1180:ARG:HA	2.19	0.42
2:G:229:ASP:O	2:G:230:TYR:C	2.61	0.42
2:G:310:CYS:O	2:G:432:LEU:HD22	2.19	0.42
2:G:706:LYS:NZ	4:G:2101:FMN:O2'	2.49	0.42
1:A:23:ALA:O	2:G:1982:MET:HE1	2.19	0.42
1:A:1443:LEU:HD23	1:A:1443:LEU:HA	1.92	0.42
2:G:180:TYR:O	2:G:184:VAL:HG12	2.19	0.42
2:G:1949:LYS:O	2:G:1953:VAL:HG23	2.20	0.42
1:A:1008:GLU:N	1:A:1008:GLU:OE1	2.53	0.41
2:G:234:ILE:HA	2:G:237:SER:OG	2.20	0.41
2:G:1528:GLU:OE2	2:G:1633:ASN:ND2	2.42	0.41
2:G:1625:SER:OG	2:G:1641:GLU:OE2	2.36	0.41
1:A:773:ALA:HB2	1:A:795:MET:HE3	2.01	0.41
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.55	0.41
2:G:567:PRO:HG2	2:G:1085:LEU:HD11	2.02	0.41
2:G:741:HIS:CE1	2:G:855:HIS:CE1	3.08	0.41
2:G:1013:LYS:HZ1	2:G:1035:TRP:CD1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:PHE:HB2	1:A:1282:THR:OG1	2.21	0.41
2:G:597:MET:N	2:G:601:THR:OG1	2.49	0.41
2:G:649:ILE:HG21	2:G:666:ILE:HD11	2.02	0.41
2:G:663:ILE:HB	2:G:664:PRO:HD3	2.03	0.41
2:G:1783:LEU:HD23	2:G:1783:LEU:HA	1.92	0.41
1:A:710:PHE:HB2	1:A:736:PRO:HB3	2.01	0.41
1:A:1520:ALA:O	1:A:1523:ARG:N	2.54	0.41
1:A:1759:MET:HE1	1:A:1771:VAL:CG2	2.51	0.41
1:B:163:LEU:HD21	1:B:270:SER:HB2	2.02	0.41
2:G:148:ALA:HB1	2:G:153:ASN:HB2	2.03	0.41
2:G:229:ASP:C	2:G:231:LEU:N	2.74	0.41
2:G:1237:PRO:HG2	2:G:1261:ARG:HD2	2.01	0.41
2:G:1551:GLU:N	2:G:1552:PRO:CD	2.84	0.41
2:G:1858:ASN:HB3	2:G:1861:ARG:HD2	2.03	0.41
2:G:1992:LEU:O	2:G:1996:ILE:N	2.53	0.41
1:A:443:SER:HA	1:A:447:LEU:HD23	2.03	0.41
1:A:679:LEU:HD12	1:A:704:VAL:O	2.21	0.41
1:A:706:THR:HB	1:A:737:PHE:HB3	2.02	0.41
1:A:1305:CYS:HB2	1:A:1645:GLY:HA2	2.02	0.41
1:B:151:LEU:HD21	1:B:206:LEU:HD22	2.02	0.41
1:B:250:LEU:HA	1:B:254:TRP:HD1	1.86	0.41
2:G:106:ALA:HA	2:G:535:ILE:HD11	2.03	0.41
2:G:404:GLN:HA	2:G:407:ILE:HD12	2.02	0.41
2:G:1138:TRP:NE1	2:G:1142:LEU:HD11	2.36	0.41
1:A:1232:TYR:O	1:A:1233:GLU:C	2.63	0.41
1:A:1682:LYS:HD3	2:G:992:GLU:O	2.20	0.41
2:G:741:HIS:CD2	2:G:855:HIS:CE1	3.09	0.41
2:G:1561:ASN:O	2:G:1562:PRO:C	2.64	0.41
2:G:1789:PHE:CD1	2:G:1817:SER:HB2	2.57	0.40
1:A:1811:GLY:HA2	1:A:1878:ALA:HB1	2.03	0.40
1:B:187:LEU:HD22	1:B:201:PRO:HG2	2.03	0.40
2:G:270:ALA:O	2:G:459:VAL:HA	2.21	0.40
2:G:1547:PRO:HD3	2:G:1584:PHE:CE1	2.56	0.40
2:G:1979:THR:HA	2:G:1982:MET:HE3	2.03	0.40
1:B:154:LEU:O	1:B:158:LYS:HB2	2.21	0.40
2:G:313:ALA:O	2:G:315:PRO:HD3	2.22	0.40
2:G:2023:LYS:HD2	2:G:2045:TRP:CD1	2.57	0.40
1:B:152:HIS:ND1	1:B:168:MET:HE1	2.36	0.40
1:A:1673:TYR:O	1:A:1676:LYS:N	2.54	0.40
2:G:131:ILE:HG13	2:G:183:LEU:HD21	2.04	0.40
2:G:159:ILE:HA	2:G:271:THR:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1752:PHE:CE1	2:G:1836:MET:HE2	2.57	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	1583/1887 (84%)	1458 (92%)	119 (8%)	6 (0%)	30	59
1	B	161/1887 (8%)	146 (91%)	14 (9%)	1 (1%)	21	50
2	G	2032/2051 (99%)	1870 (92%)	157 (8%)	5 (0%)	43	71
All	All	3776/5825 (65%)	3474 (92%)	290 (8%)	12 (0%)	37	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	LYS
2	G	526	ARG
1	A	726	GLY
1	A	877	LEU
1	A	1337	GLU
1	A	1545	SER
1	A	1608	ASN
1	A	1783	ASN
2	G	77	VAL
2	G	313	ALA
2	G	1661	VAL
2	G	802	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1341/1566 (86%)	1335 (100%)	6 (0%)	84	83
1	B	135/1566 (9%)	126 (93%)	9 (7%)	15	41
2	G	1775/1789 (99%)	1770 (100%)	5 (0%)	86	84
All	All	3251/4921 (66%)	3231 (99%)	20 (1%)	76	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	GLU
1	A	938	GLU
1	A	1096	SER
1	A	1210	PRO
1	A	1255	SER
1	A	1751	GLU
1	B	232	LEU
1	B	233	ILE
1	B	236	LYS
1	B	237	MET
1	B	242	THR
1	B	243	ILE
1	B	244	THR
1	B	248	LYS
1	B	277	LEU
2	G	336	SER
2	G	626	SER
2	G	1380	SER
2	G	1467	GLU
2	G	1641	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	32	GLN
1	A	379	ASN
1	A	467	GLN
1	A	506	ASN
1	A	527	GLN
1	A	618	ASN
1	A	669	ASN
1	A	758	ASN
1	A	830	HIS
1	A	987	ASN
1	A	989	GLN
1	A	1112	ASN
1	A	1146	HIS
1	A	1147	GLN
1	A	1188	GLN
1	A	1433	HIS
1	A	1505	GLN
1	A	1549	ASN
1	A	1601	ASN
1	A	1608	ASN
1	A	1843	ASN
1	A	1877	GLN
1	B	183	GLN
2	G	34	GLN
2	G	36	GLN
2	G	38	ASN
2	G	224	ASN
2	G	248	HIS
2	G	365	GLN
2	G	440	ASN
2	G	640	GLN
2	G	718	ASN
2	G	723	HIS
2	G	993	GLN
2	G	998	GLN
2	G	1055	HIS
2	G	1061	GLN
2	G	1078	HIS
2	G	1186	ASN
2	G	1352	HIS
2	G	1355	ASN
2	G	1451	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	1512	HIS
2	G	1535	ASN
2	G	1568	HIS
2	G	1872	GLN
2	G	1890	ASN
2	G	1912	ASN
2	G	1983	ASN
2	G	2044	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PNS	B	1901	1	15,20,21	0.61	0	18,26,29	1.56	5 (27%)
4	FMN	G	2101	-	33,33,33	1.42	5 (15%)	48,50,50	1.54	9 (18%)

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
3	PNS	B	1901	1	-	7/24/26/27	-
4	FMN	G	2101	-	-	5/18/18/18	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2101	FMN	C8-C7	3.56	1.49	1.40
4	G	2101	FMN	C9A-C5A	3.36	1.46	1.41
4	G	2101	FMN	C4-N3	-2.94	1.33	1.38
4	G	2101	FMN	C2-N3	-2.73	1.33	1.39
4	G	2101	FMN	C5A-N5	-2.66	1.34	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2101	FMN	C4-C4A-N5	4.10	123.88	118.21
3	B	1901	PNS	C37-C38-C39	3.53	118.27	112.39
4	G	2101	FMN	C4A-C10-N10	3.04	120.84	116.48
4	G	2101	FMN	O2P-P-O5'	-2.96	98.96	106.67
3	B	1901	PNS	C42-N41-C39	2.88	128.18	122.82
4	G	2101	FMN	C10-C4A-N5	-2.84	119.00	124.81
3	B	1901	PNS	O40-C39-C38	-2.81	116.93	122.02
4	G	2101	FMN	C4A-C10-N1	-2.72	117.92	124.59
4	G	2101	FMN	C10-N1-C2	2.41	122.08	116.85
4	G	2101	FMN	O4'-C4'-C5'	-2.32	104.88	109.99
3	B	1901	PNS	C38-C39-N41	2.16	120.27	116.34
3	B	1901	PNS	C43-C42-N41	2.15	117.19	112.31
4	G	2101	FMN	O4'-C4'-C3'	2.14	114.26	109.25
4	G	2101	FMN	O3P-P-O2P	2.02	115.38	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1901	PNS	N36-C37-C38-C39
3	B	1901	PNS	C38-C39-N41-C42
3	B	1901	PNS	O40-C39-N41-C42
4	G	2101	FMN	C2'-C3'-C4'-C5'
3	B	1901	PNS	C29-C32-C34-N36

Continued on next page...

Continued from previous page...

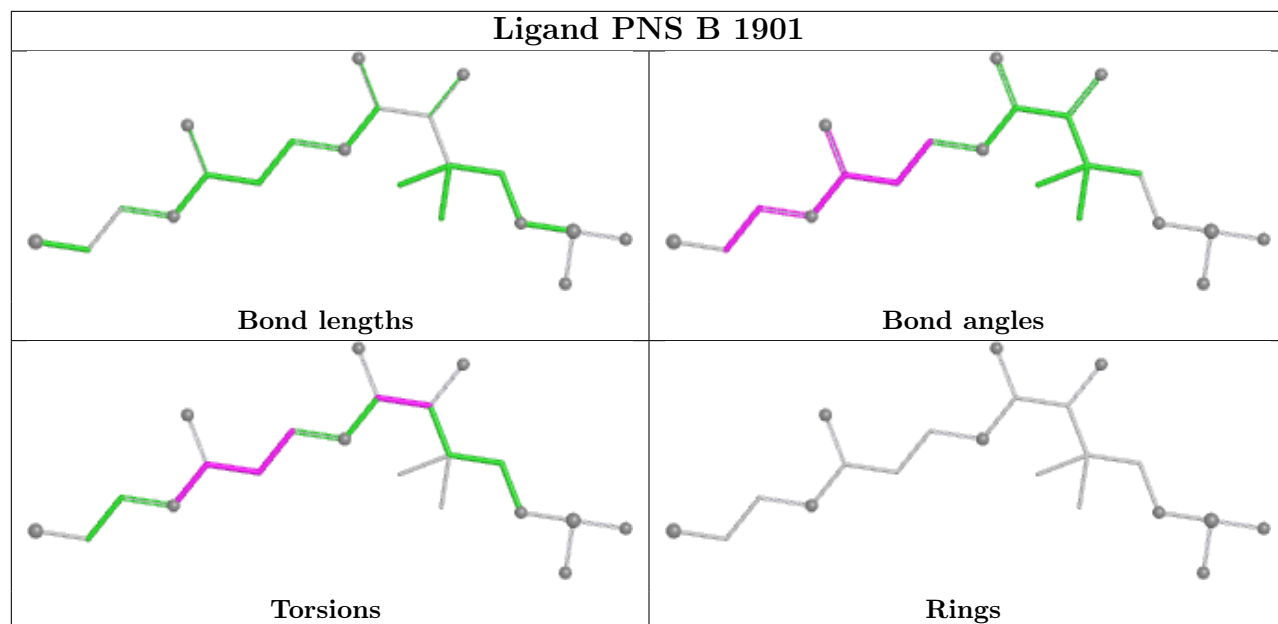
Mol	Chain	Res	Type	Atoms
4	G	2101	FMN	C2'-C3'-C4'-O4'
4	G	2101	FMN	C4'-C5'-O5'-P
3	B	1901	PNS	C37-C38-C39-O40
3	B	1901	PNS	C29-C32-C34-O35
4	G	2101	FMN	O3'-C3'-C4'-C5'
4	G	2101	FMN	C5'-O5'-P-O1P
3	B	1901	PNS	C37-C38-C39-N41

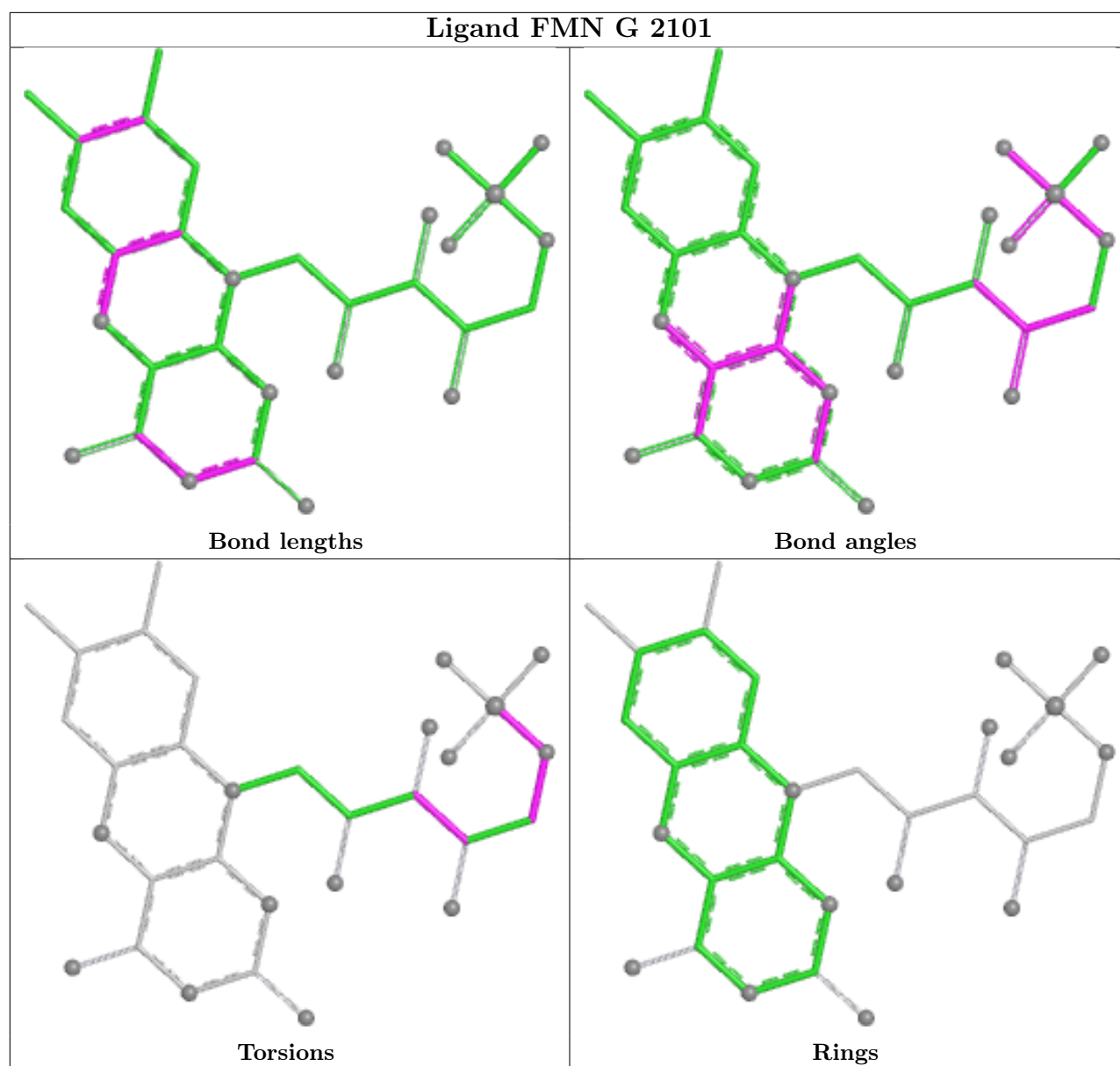
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1901	PNS	2	0
4	G	2101	FMN	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

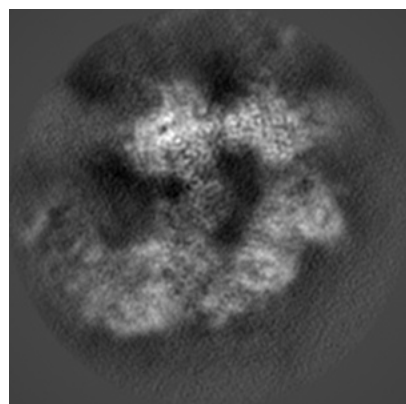
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17853. These allow visual inspection of the internal detail of the map and identification of artifacts.

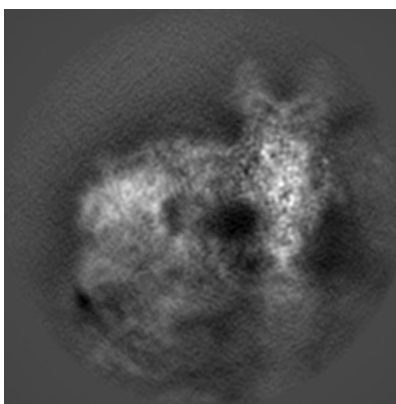
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

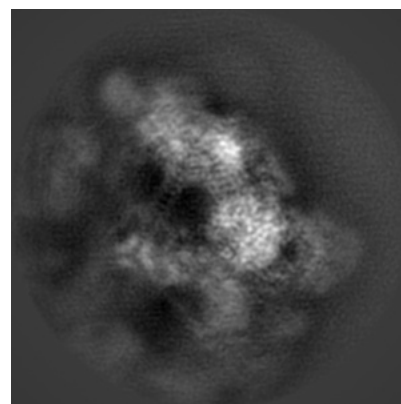
6.1.1 Primary map



X

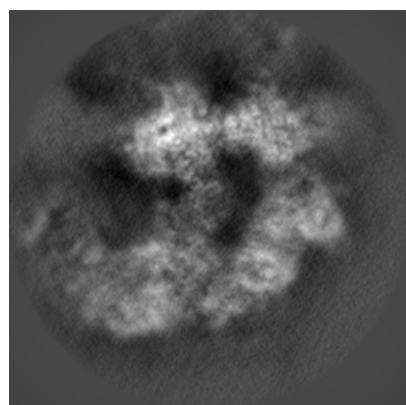


Y

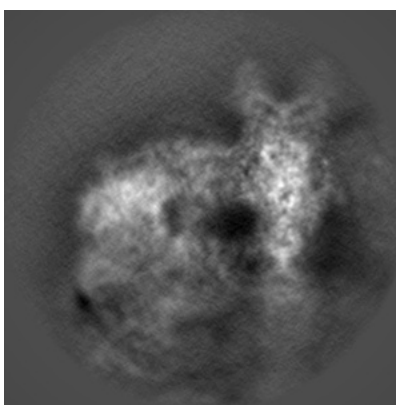


Z

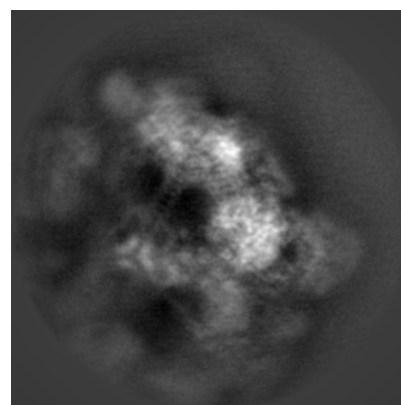
6.1.2 Raw map



X



Y

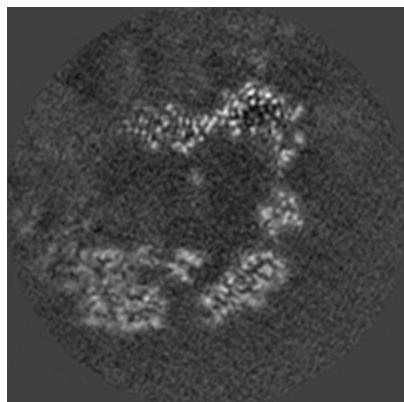


Z

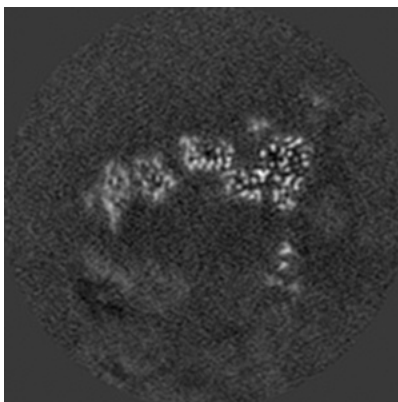
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

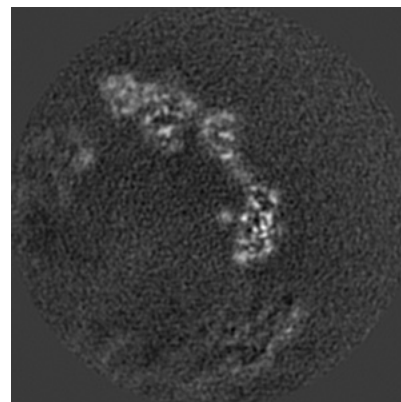
6.2.1 Primary map



X Index: 120

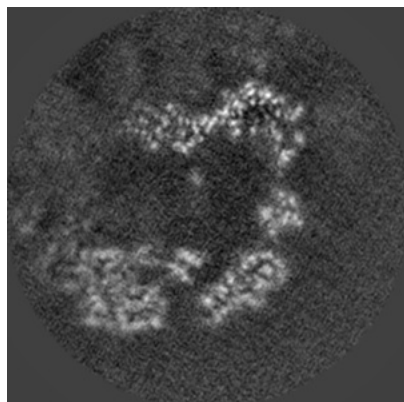


Y Index: 120

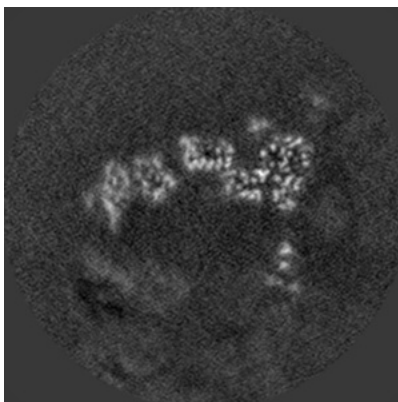


Z Index: 120

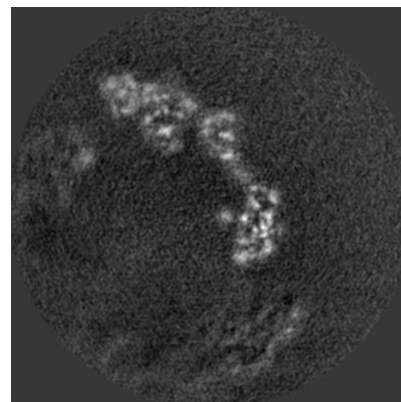
6.2.2 Raw map



X Index: 120



Y Index: 120

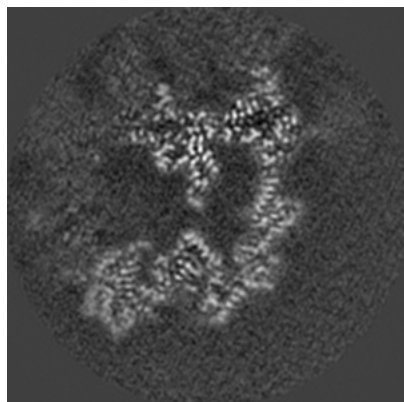


Z Index: 120

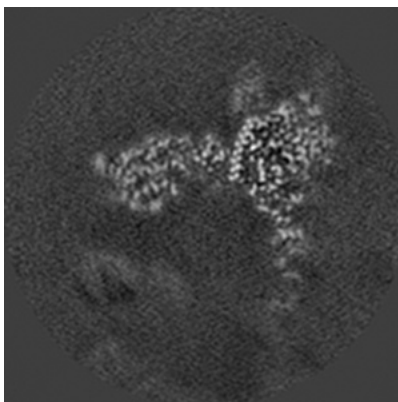
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

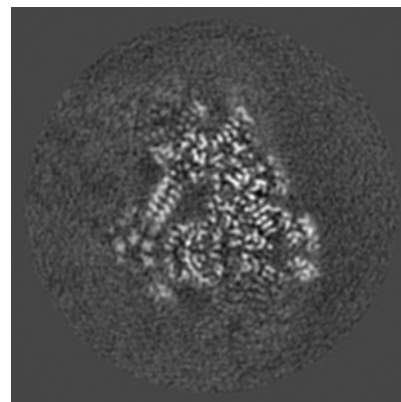
6.3.1 Primary map



X Index: 129

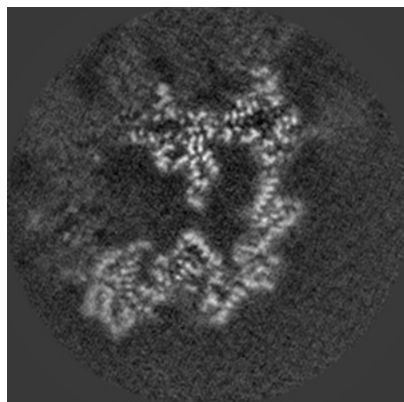


Y Index: 107

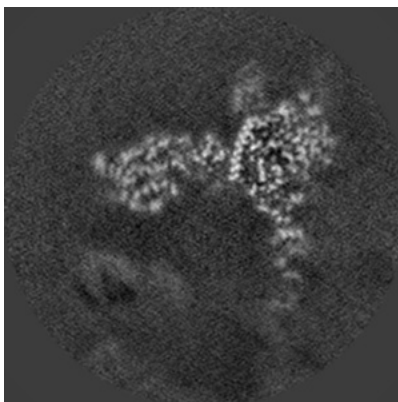


Z Index: 167

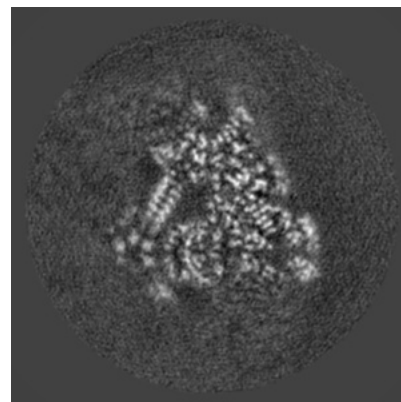
6.3.2 Raw map



X Index: 129



Y Index: 107

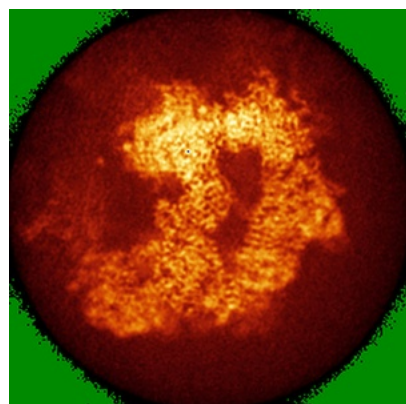


Z Index: 167

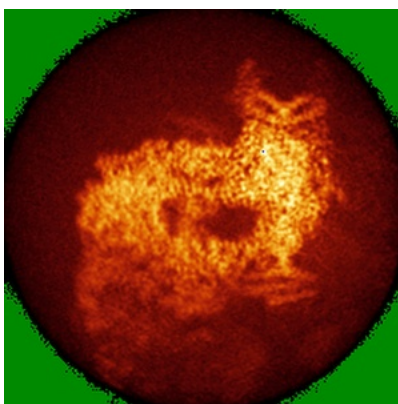
The images above show the largest variance slices of the map in three orthogonal directions.

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

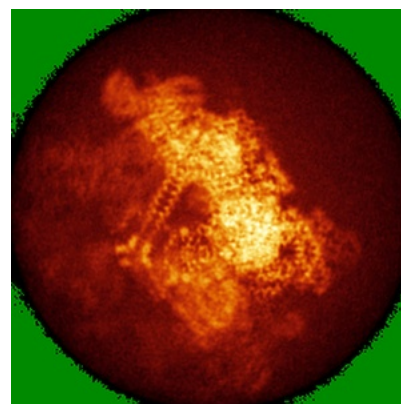
6.4.1 Primary map



X

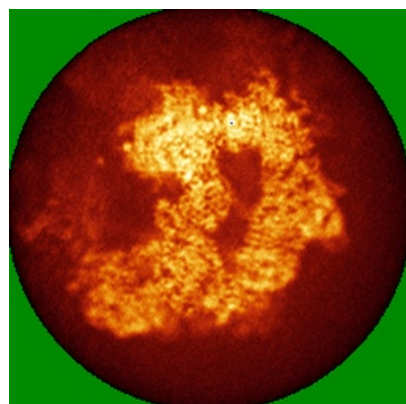


Y

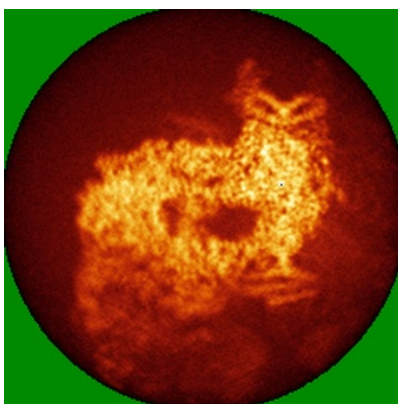


Z

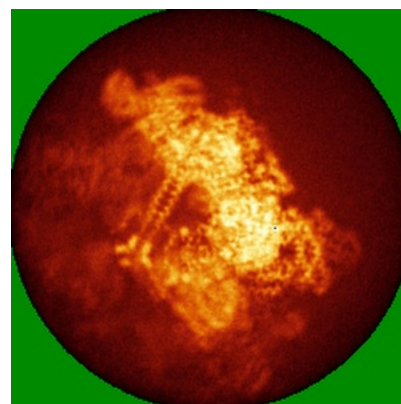
6.4.2 Raw map



X



Y



Z

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

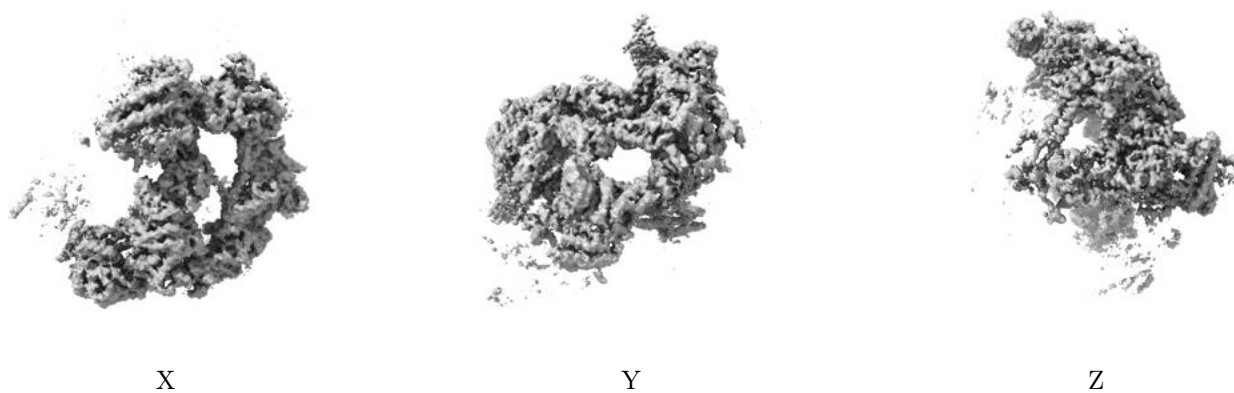
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

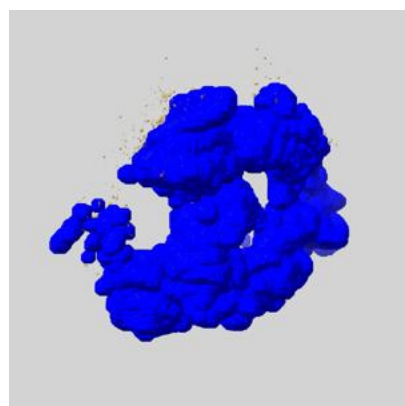
6.6 Mask visualisation [i](#)

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

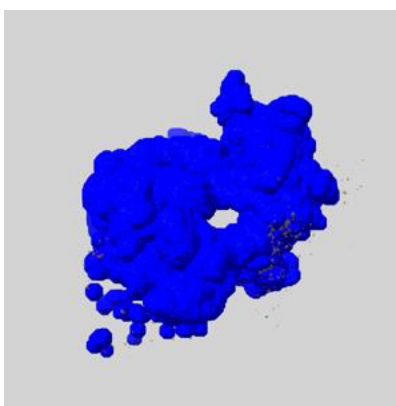
A mask typically either:

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

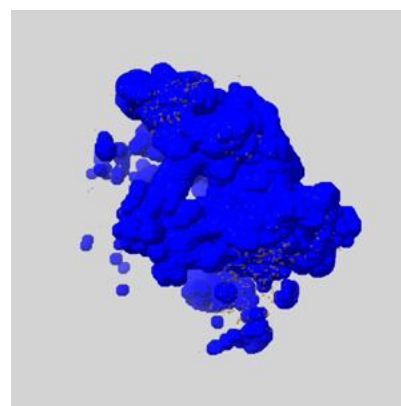
6.6.1 emd_17853_msk_1.map [i](#)



X



Y

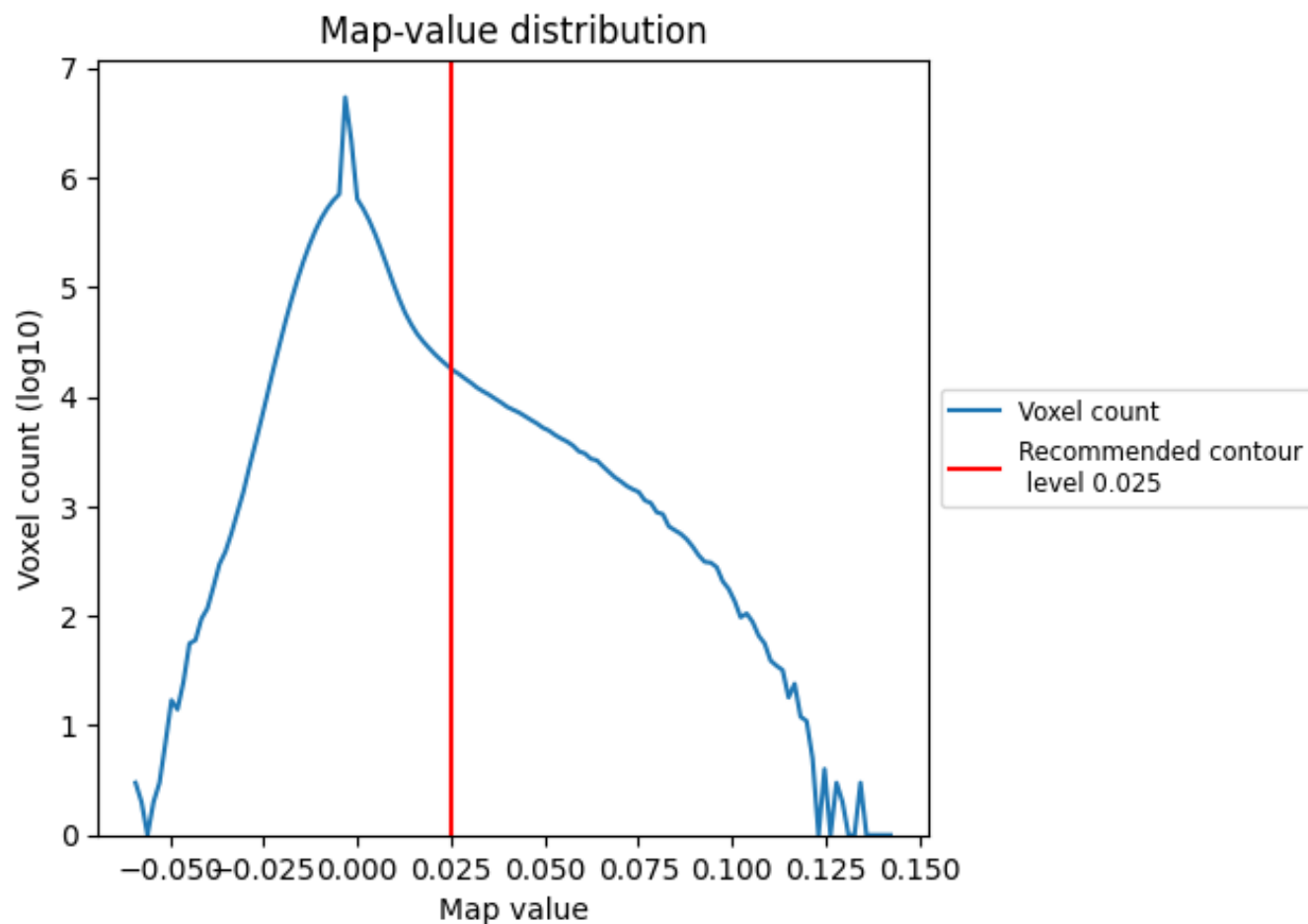


Z

7 Map analysis [i](#)

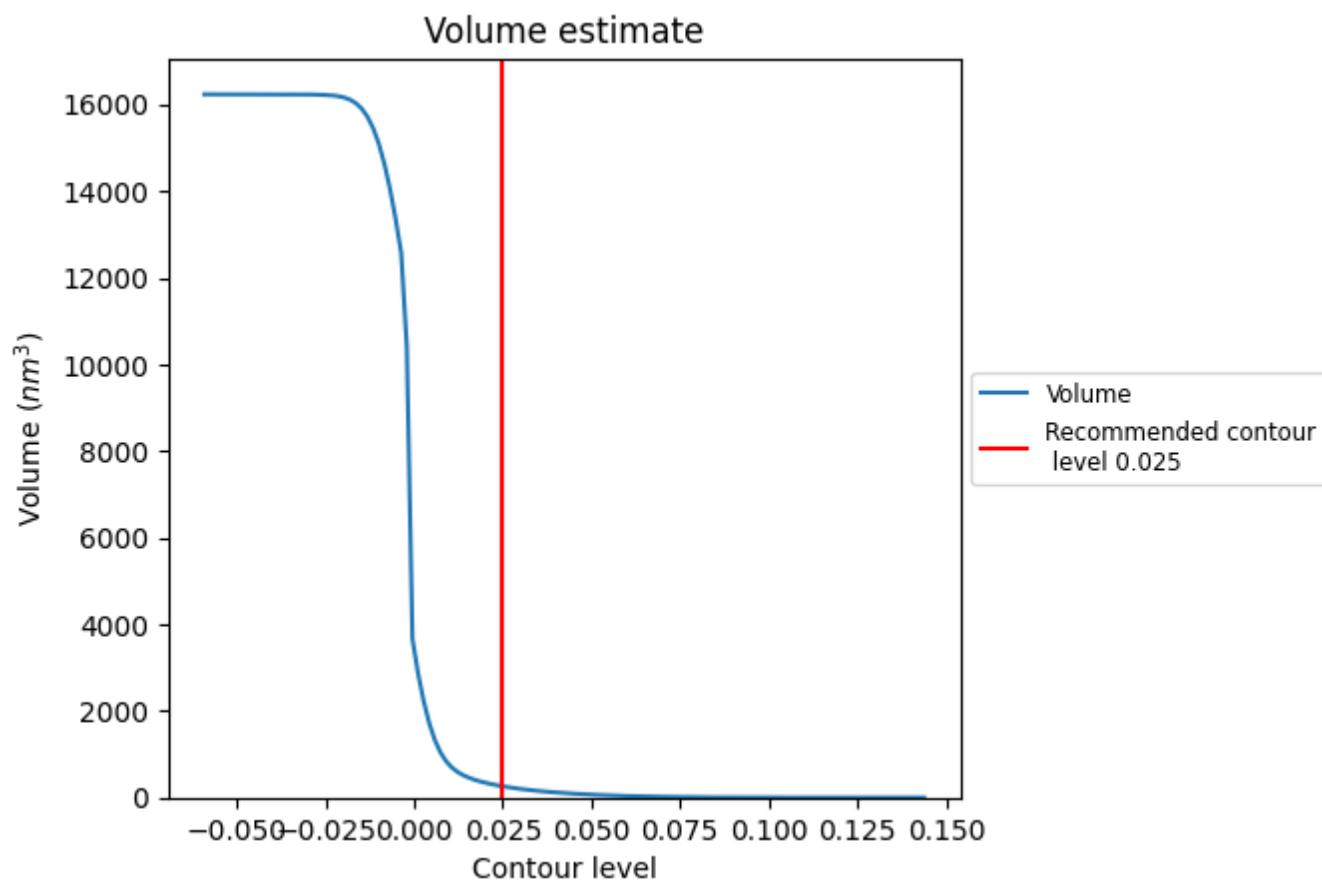
This section contains the results of statistical analysis of the map.

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.

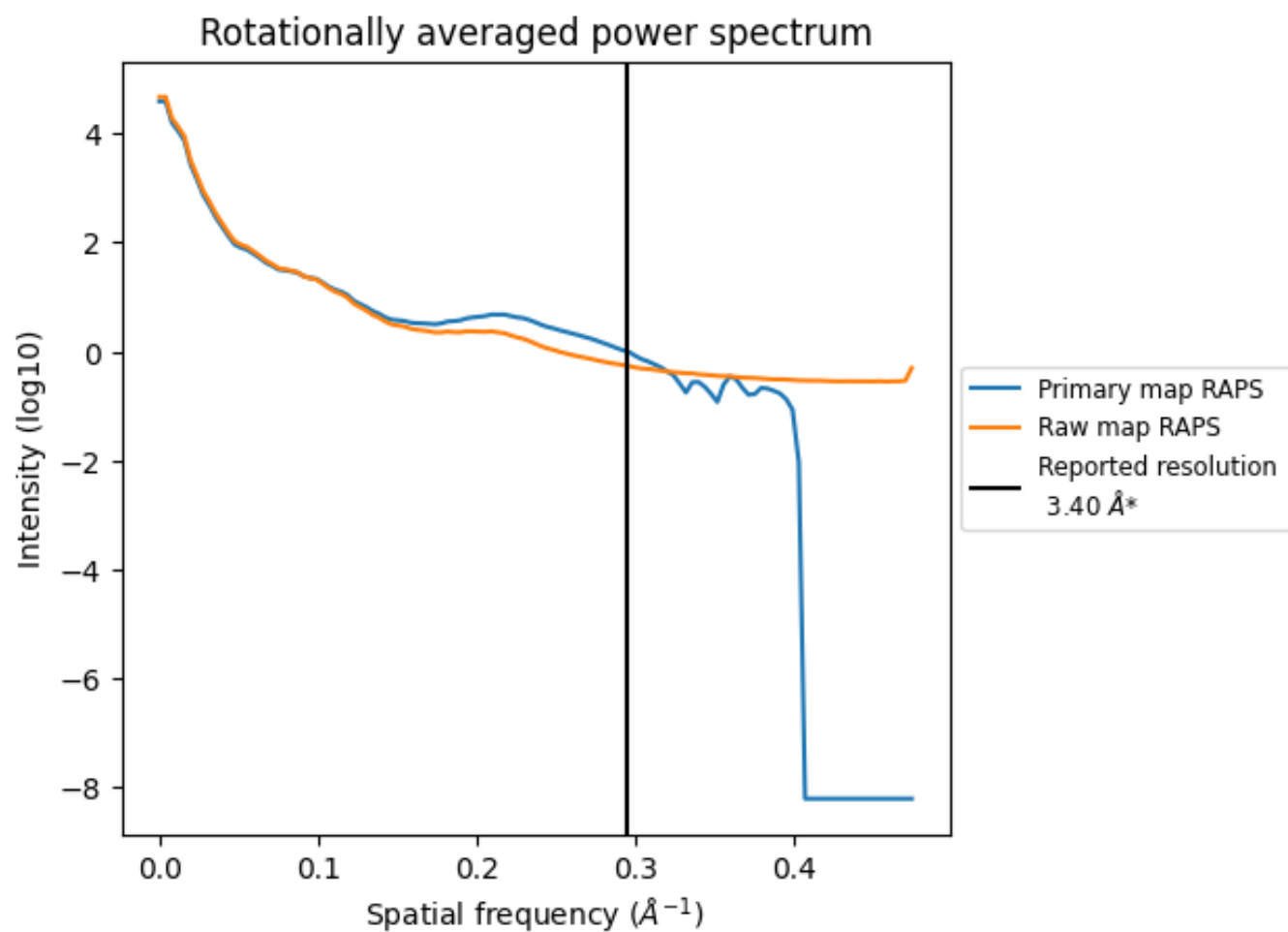
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm³; this corresponds to an approximate mass of 234 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

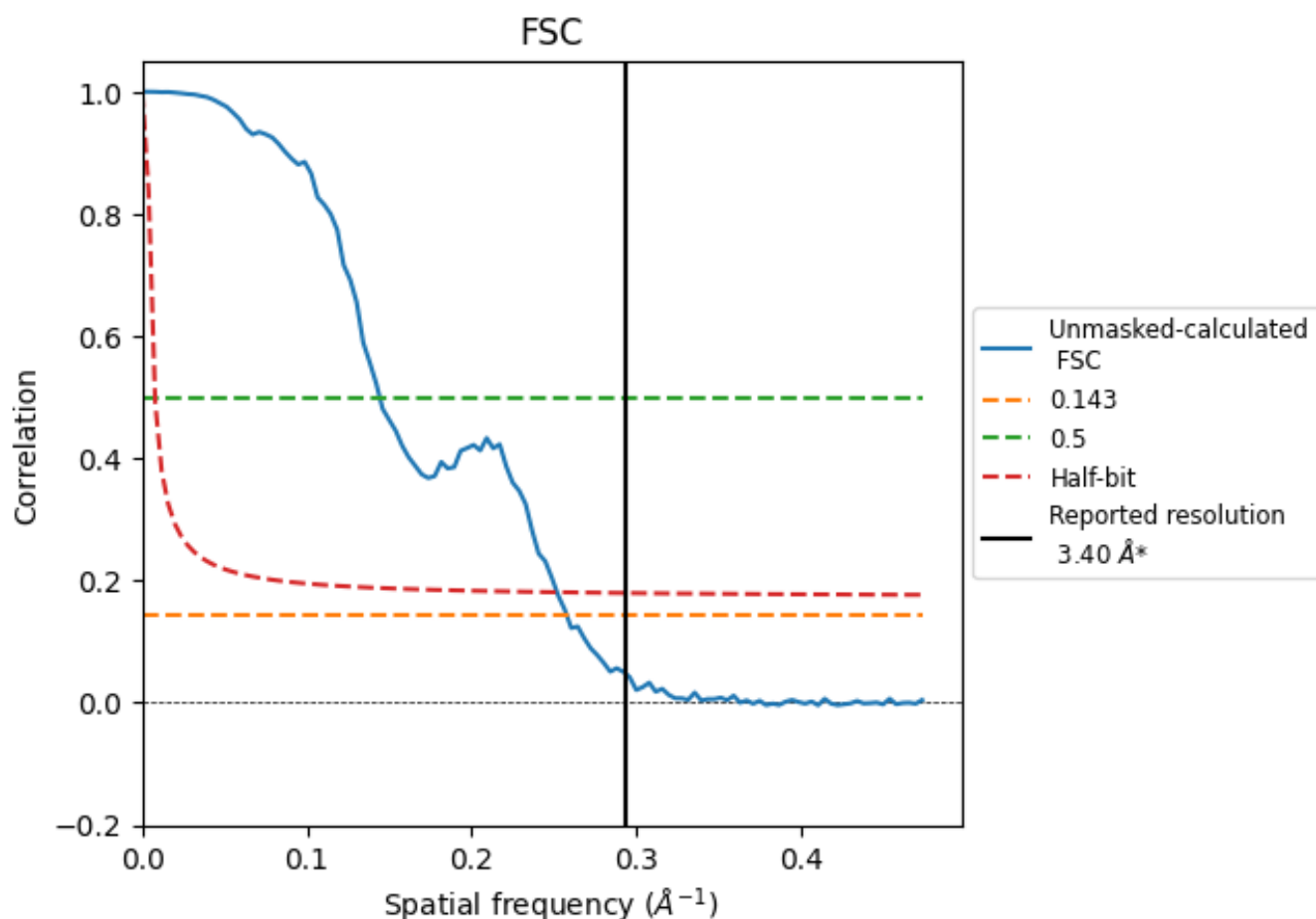


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

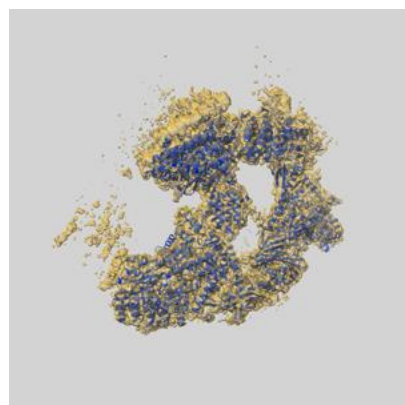
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	6.93	3.97

*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 3.88 differs from the reported value 3.4 by more than 10 %

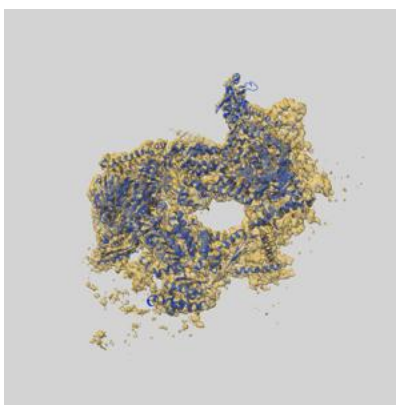
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17853 and PDB model 8PSJ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



X



Y



Z

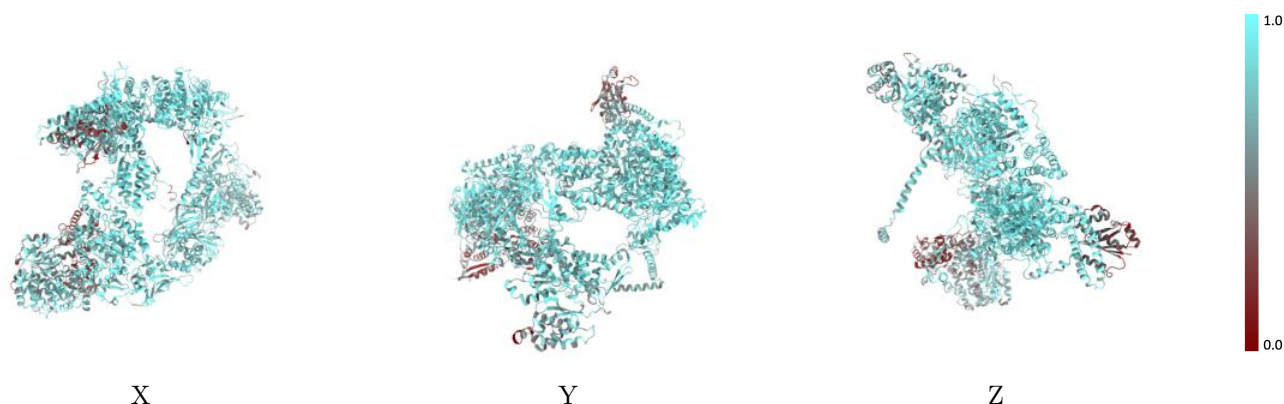
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



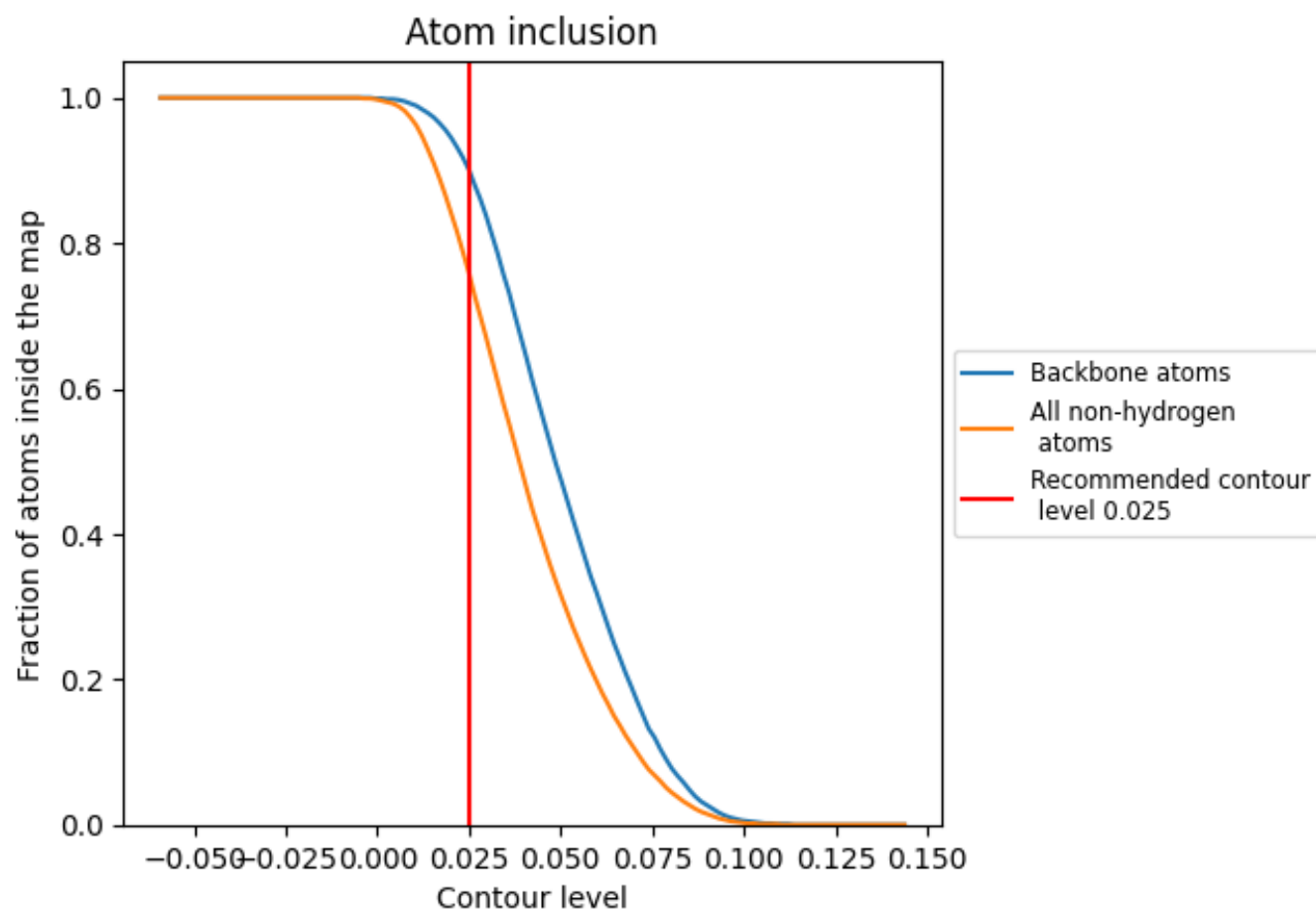
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.4460
A	0.8070	0.5030
B	0.2780	0.2560
G	0.7590	0.4160

