



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:13 PM UTC

PDB ID : 8PSL / pdb_00008psl
EMDB ID : EMD-17855
Title : Asymmetric unit of the yeast fatty acid synthase in the semi non-rotated state with ACP at the ketosynthase domain (FASx sample)
Authors : Singh, K.; Bunzel, G.; Graf, B.; Yip, K.M.; Stark, H.; Chari, A.
Deposited on : 2023-07-13
Resolution : 3.70 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

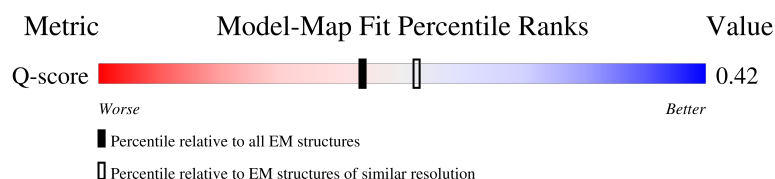
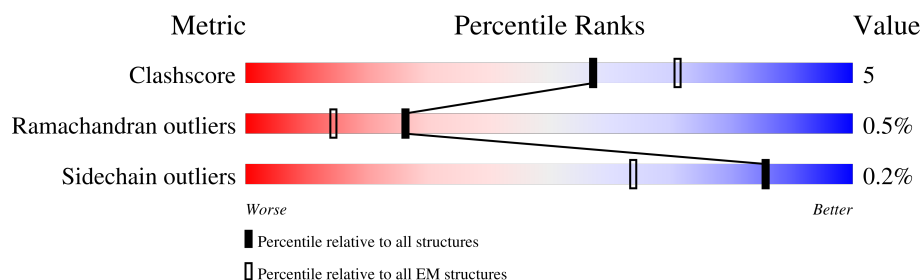
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	
1	B	1887	
2	G	2051	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 29610 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.

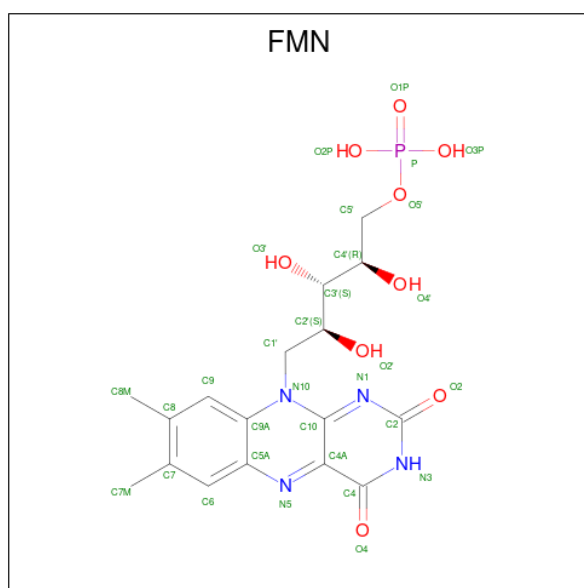
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1579	Total	C	N	O	S	0	0
			12346	7817	2084	2398	47		
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	2035	Total	C	N	O	S	0	0
			16010	10261	2662	3031	56		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

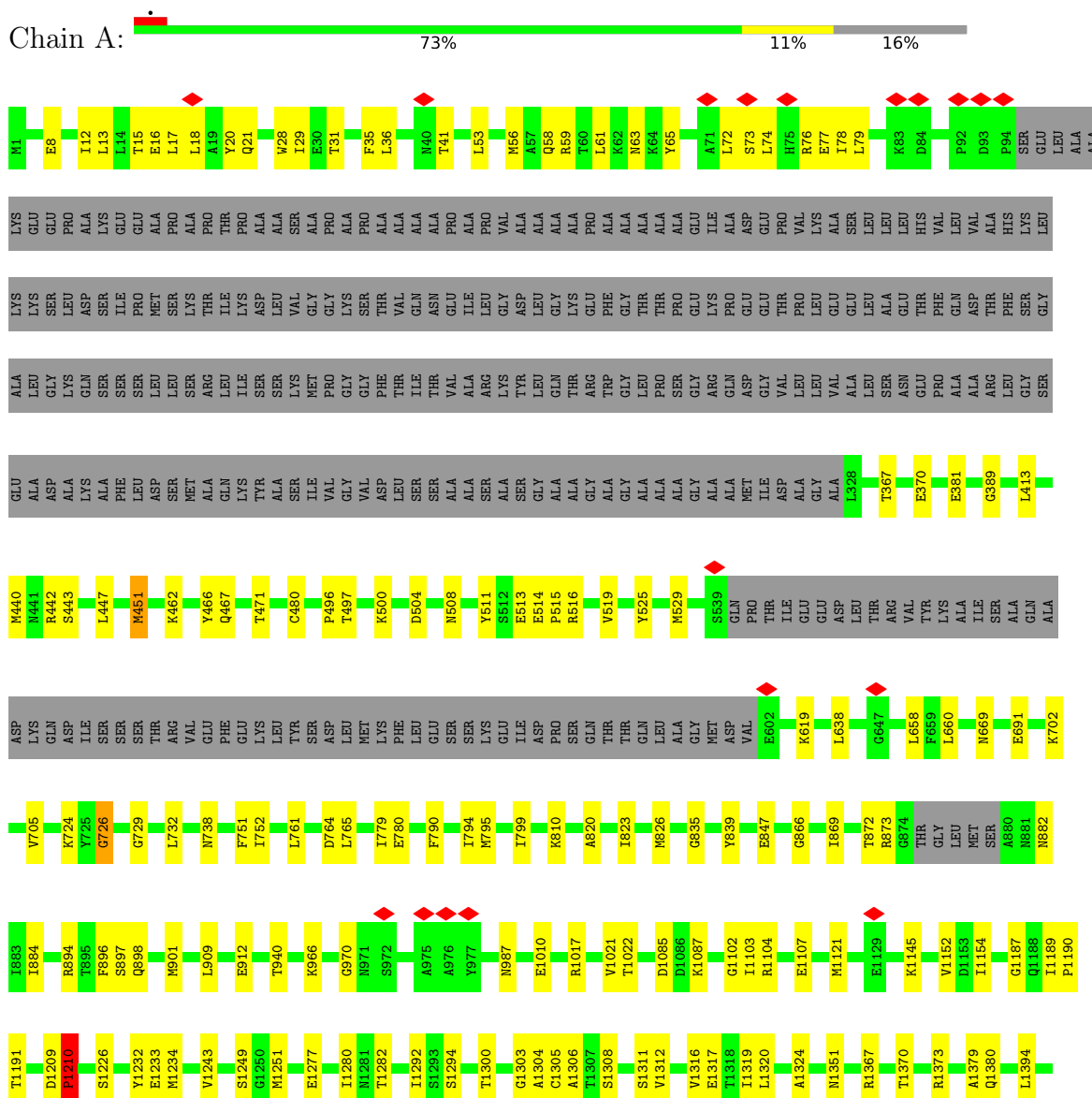


Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			31	17	4	9	1	

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: Fatty acid synthase subunit alpha



- Molecule 2: Fatty acid synthase subunit beta

[illegible]

C94	V296	K573	P795	P1057	H1307	L1527	L1729	Q1872	R1962
W9	I300	F583	F796	D1079	C1308	L1532	M1736	Y1873	G1963
T128	T301	P591	L800	G1080	D1316	M1532	I1737	V1874	F1964
M132	L303	L592	G802	L1086	I1327	P1536	I1741	E1876	L1969
A133	I306	G596	S803	D1092	G1330	I1539	V1742	R1877	V1970
K134	P320	M597	M806	D1093	W1331	A1540	D1743	V1878	G1971
L145	T598	P599	D816	K1096	I1334	V1541	G1744	K1745	I1972
V149	S322	V602	A817	E1101	I1335	L1542	K1746	R1881	H1977
L156	I323	A628	X318	V1109	I1338	D1559	K1747	L1885	K1986
F160	M338	T646	K819	ASP	F1339	R1567	T1748	V1886	P1987
L187	K355	T846	D829	VAL	P1340	S1585	E1749	I1887	K1993
F209	K358	N650	T835	GLN	V1343	L1592	K1751	E1888	V2001
T210	V366	L651	T840	SER	L1347	W1596	K1768	V1889	R2005
Q211	S369	Y653	I843	GLN	L1350	R1604	P1779	Q1896	I2011
G212	L370	M658	H855	VAL	Y1357	L1620	T1782	V1899	F2019
L213	V378	L659	A858	SER	L1366	A1621	L1783	A1906	F2026
D227	G381	I663	M863	VAL	T1374	K1623	A1787	T1911	T2033
K228	Y387	P664	E867	A1129	T1375	H1628	E1790	L1914	E2036
T234	S400	Q677	D913	W1138	V1381	V1629	A1805	N1915	P2037
P235	V423	I681	L914	L1142	V1390	G1630	S1808	F1916	I2038
G242	H428	G682	L926	N1148	V1406	R1635	A1813	L1919	K2039
Q245	L246	P686	M930	H1151	Y1412	T1642	L1815	Q1920	E2040
A253	L432	G704	S961	F1154	F1419	R1643	V1821	L1924	Q2050
K254	P434	K706	K962	L1155	T1422	E1645	L1827	I1925	SER
F258	T439	T733	T963	D1162	F1423	D1646	V1828	E1926	
G261	Q456	R736	L964	F1165	K1425	L1651	Y1833	L1927	
E262	R469	G739	Q993	T1171	V1430	E1658	P1843	Q1928	
S265	C482	H740	P1014	S1177	V1443	G1668	R1844	K1929	
S274	I483	H741	D1022	M1180	S1446	Q1689	D1845	S1930	
T279	L486	Y754	R1024	Q1202	L1459	Q1672	E1846	L1931	
I283	W490	I763	I1027	W1270	L1464	A1686	P1859	S1932	
T286	L502	F767	K1031	K1286	T1470	F1698	G1860	L1933	
S288	L512	G768	D1032	V1304	E1471	I1706	R1861	E1937	
W289	I547	S769	V1048	G1305	V1472	K1725	V1862	G1938	
F293		M794	L1054	N1306	K1496		A1864	H1939	
							F1866	I1944	
							E1869	P1955	
							A1870	R1956	
							L1871	P1957	
								L1958	
								K1959	
								L1960	
								E1961	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20373	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	0.131	Depositor
Minimum map value	-0.059	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	253.19998, 253.19998, 253.19998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 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	1.02	1/12579 (0.0%)	1.51	11/17001 (0.1%)
1	B	1.02	0/1241	1.67	6/1675 (0.4%)
2	G	1.07	1/16375 (0.0%)	1.53	12/22218 (0.1%)
All	All	1.05	2/30195 (0.0%)	1.52	29/40894 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1121	MET	CG-SD	5.82	1.95	1.80
2	G	56	THR	N-CA	5.76	1.50	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	GLU	CB-CG-CD	10.57	130.57	112.60
1	A	1317	GLU	CB-CG-CD	6.83	124.22	112.60
1	A	780	GLU	CB-CG-CD	6.71	124.00	112.60
1	A	1582	GLY	CA-C-O	-6.68	117.25	122.52
1	B	272	GLU	CA-C-N	-6.57	113.04	119.87
1	B	272	GLU	C-N-CA	-6.57	113.04	119.87
2	G	432	LEU	CA-C-N	5.66	124.86	120.33
2	G	432	LEU	C-N-CA	5.66	124.86	120.33
1	A	1300	THR	CB-CA-C	5.57	115.68	110.17
2	G	628	ALA	CA-C-N	5.34	125.87	119.94
2	G	628	ALA	C-N-CA	5.34	125.87	119.94
1	A	1312	VAL	CA-C-O	-5.32	115.74	121.27
2	G	599	PRO	N-CA-CB	-5.29	96.79	102.60
2	G	795	PRO	CB-CA-C	-5.25	104.22	111.21
1	A	1715	TYR	CA-C-O	-5.24	115.32	120.82
1	A	1316	VAL	CA-C-O	-5.21	115.85	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1308	CYS	CA-C-N	5.21	127.26	120.28
2	G	1308	CYS	C-N-CA	5.21	127.26	120.28
1	B	190	LEU	CA-C-N	5.16	125.81	120.03
1	B	190	LEU	C-N-CA	5.16	125.81	120.03
1	A	1705	PRO	N-CA-C	-5.13	106.40	113.53
2	G	1585	SER	CA-C-N	5.06	127.06	120.28
2	G	1585	SER	C-N-CA	5.06	127.06	120.28
2	G	160	PHE	CA-C-N	5.05	125.70	120.60
2	G	160	PHE	C-N-CA	5.05	125.70	120.60
1	A	724	LYS	CA-C-O	-5.03	115.52	120.80
1	B	179	LYS	CA-C-N	5.02	127.00	120.28
1	B	179	LYS	C-N-CA	5.02	127.00	120.28
1	A	1673	TYR	N-CA-C	-5.01	105.51	110.97

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	12346	0	12279	120	0
1	B	1223	0	1265	17	0
2	G	16010	0	15989	160	0
3	G	31	0	19	2	0
All	All	29610	0	29552	285	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 (285) 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:G:706:LYS:NZ	3:G:2101:FMN:O2'	2.09	0.86
1:A:497:THR:HG22	1:A:515:PRO:HA	1.66	0.78
1:A:823:ILE:HD11	1:A:909:LEU:HD21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1773:VAL:HG12	1:A:1879:VAL:HG12	1.69	0.75
2:G:456:GLN:O	2:G:469:ARG:NH1	2.20	0.74
1:A:1379:ALA:O	1:A:1584:PRO:HA	1.93	0.68
2:G:1154:PHE:O	2:G:1171:ARG:NH1	2.28	0.67
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.76	0.67
2:G:1642:THR:HB	2:G:1651:LEU:HB2	1.78	0.66
2:G:2039:LYS:HE2	2:G:2039:LYS:HA	1.77	0.65
2:G:1742:VAL:HB	2:G:1747:LYS:HE3	1.79	0.65
1:A:15:THR:HG21	2:G:1993:LYS:HG3	1.80	0.64
1:A:987:ASN:HD21	2:G:993:GLN:HE22	1.46	0.63
2:G:145:LEU:HD12	2:G:547:ILE:HA	1.80	0.63
2:G:1783:LEU:HD21	2:G:1828:VAL:HG12	1.81	0.63
1:A:1303:GLY:O	1:A:1305:CYS:N	2.33	0.62
1:A:500:LYS:HB2	1:A:514:GLU:HG2	1.80	0.62
2:G:1623:LYS:NZ	2:G:1644:ASN:O	2.32	0.62
1:A:1021:VAL:HG11	1:A:1597:LEU:HD11	1.82	0.62
1:A:1319:ILE:HA	1:A:1324:ALA:O	1.99	0.62
2:G:1875:VAL:HG21	2:G:1888:ILE:HD11	1.80	0.61
1:A:61:LEU:HA	1:A:65:TYR:HB2	1.80	0.61
2:G:653:TYR:HA	2:G:659:LEU:HD11	1.82	0.61
2:G:211:GLN:NE2	2:G:227:ASP:OD1	2.34	0.60
1:A:1021:VAL:HG11	1:A:1597:LEU:CD1	2.31	0.60
1:A:1560:MET:HE1	1:A:1652:GLN:HE22	1.66	0.60
2:G:1443:VAL:O	2:G:1446:SER:OG	2.20	0.59
1:A:795:MET:O	1:A:799:ILE:HD12	2.02	0.59
2:G:768:GLY:HA3	2:G:800:LEU:HG	1.84	0.59
2:G:128:THR:HG22	2:G:132:MET:HE1	1.84	0.58
2:G:1419:PHE:O	2:G:1422:THR:OG1	2.20	0.58
2:G:1821:VAL:HG13	2:G:2001:VAL:HG12	1.84	0.58
1:A:1107:GLU:OE1	1:A:1191:THR:OG1	2.21	0.58
2:G:1889:VAL:HB	2:G:1977:HIS:HB2	1.84	0.58
2:G:338:MET:HE2	2:G:423:VAL:HG21	1.86	0.57
2:G:1022:ASP:OD2	2:G:1024:ARG:NH1	2.38	0.57
2:G:23:PRO:HD2	2:G:86:LEU:HD22	1.86	0.57
1:A:59:ARG:HB3	2:G:1896:GLN:HE22	1.69	0.57
2:G:90:GLU:OE2	2:G:94:CYS:SG	2.58	0.57
1:A:12:ILE:O	1:A:16:GLU:HG2	2.04	0.56
2:G:1335:ILE:O	2:G:1338:ILE:HG12	2.05	0.56
1:A:53:LEU:HD13	1:A:56:MET:SD	2.45	0.56
1:A:367:THR:O	1:A:370:GLU:HG3	2.05	0.56
2:G:646:THR:HG22	2:G:1165:PHE:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:736:ARG:NH1	2:G:829:ASP:OD2	2.38	0.55
1:A:529:MET:HE1	1:A:894:ARG:HG2	1.88	0.55
1:B:201:PRO:O	1:B:204:THR:OG1	2.22	0.55
1:A:31:THR:HG23	2:G:2011:ILE:HG21	1.89	0.54
1:A:413:LEU:HD11	1:A:451:MET:SD	2.46	0.54
1:A:619:LYS:HE3	1:A:669:ASN:HB3	1.89	0.54
2:G:1782:THR:HG23	2:G:1813:ALA:HB2	1.88	0.54
1:A:29:ILE:HD12	2:G:1891:TYR:HB3	1.89	0.54
2:G:653:TYR:CZ	2:G:686:PRO:HA	2.43	0.54
1:A:13:LEU:HD23	2:G:2019:PHE:CZ	2.43	0.54
2:G:1151:HIS:NE2	2:G:1155:LEU:HD12	2.23	0.54
1:A:658:LEU:HD21	1:A:912:GLU:HB3	1.91	0.53
1:A:497:THR:HA	1:A:516:ARG:H	1.73	0.53
2:G:1129:ALA:HB3	2:G:1180:MET:HB2	1.91	0.53
2:G:246:LEU:HD13	2:G:296:VAL:HG23	1.90	0.53
2:G:754:TYR:OH	2:G:795:PRO:O	2.25	0.53
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.44	0.53
2:G:646:THR:HG22	2:G:1165:PHE:CE2	2.44	0.53
2:G:1532:ASN:HA	2:G:1630:GLY:HA2	1.91	0.53
1:A:462:LYS:HE2	1:A:466:TYR:CE2	2.44	0.52
1:A:884:ILE:HD11	1:A:940:THR:HA	1.92	0.52
2:G:646:THR:HB	2:G:677:GLN:HB2	1.92	0.52
2:G:733:THR:HA	2:G:768:GLY:O	2.09	0.52
2:G:961:SER:OG	2:G:962:LYS:N	2.41	0.52
1:A:1303:GLY:O	1:A:1306:ALA:N	2.42	0.52
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	1.90	0.52
1:A:795:MET:HE1	1:A:839:TYR:CD1	2.44	0.52
2:G:1459:LEU:HD22	2:G:1464:LEU:HD11	1.91	0.52
1:A:1249:SER:HB3	1:A:1280:ILE:HG23	1.91	0.52
2:G:482:CYS:HA	2:G:486:LEU:HB2	1.92	0.51
2:G:816:ASP:HA	2:G:819:LYS:HD2	1.92	0.51
2:G:1430:VAL:HG13	2:G:1527:LEU:HD13	1.92	0.51
1:A:1758:ASN:HA	1:A:1763:LYS:HG2	1.92	0.51
1:A:751:PHE:CZ	1:A:761:LEU:HD11	2.45	0.51
1:A:35:PHE:CD2	2:G:1663:THR:HG21	2.45	0.51
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.24	0.51
1:A:389:GLY:O	1:A:738:ASN:ND2	2.38	0.51
1:A:500:LYS:HD3	1:A:514:GLU:CD	2.36	0.50
1:A:1542:HIS:N	1:A:1553:GLU:OE2	2.37	0.50
2:G:1357:TYR:HD1	2:G:1406:VAL:HG12	1.76	0.50
2:G:1928:GLN:HB3	2:G:1936:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:680:THR:HA	2:G:704:GLY:O	2.11	0.50
1:A:1209:ASP:C	1:A:1209:ASP:OD1	2.54	0.50
2:G:926:LEU:HD22	2:G:930:MET:HE3	1.92	0.50
2:G:355:LYS:O	2:G:358:SER:OG	2.28	0.49
2:G:1381:VAL:HG23	2:G:1390:VAL:HG22	1.94	0.49
2:G:1585:SER:HB3	2:G:1651:LEU:HD11	1.93	0.49
2:G:757:ILE:HG23	2:G:763:ILE:HG21	1.94	0.49
1:A:467:GLN:NE2	1:A:471:THR:OG1	2.45	0.49
1:A:1102:GLY:O	1:A:1104:ARG:NH1	2.46	0.49
1:B:168:MET:O	1:B:206:LEU:HB2	2.13	0.49
2:G:433:VAL:N	2:G:434:PRO:HD2	2.27	0.49
2:G:1621:ALA:N	2:G:1645:GLU:OE2	2.45	0.49
1:A:751:PHE:CE2	1:A:761:LEU:HD11	2.47	0.49
1:A:1351:ASN:C	1:A:1351:ASN:OD1	2.55	0.49
1:B:151:LEU:HD11	1:B:168:MET:HE1	1.94	0.49
1:A:790:PHE:CE1	1:A:794:ILE:HD11	2.47	0.49
2:G:843:ILE:HD12	2:G:1057:PRO:HA	1.94	0.49
2:G:1381:VAL:HG13	2:G:1422:THR:HA	1.94	0.49
2:G:754:TYR:CD2	2:G:794:MET:SD	3.06	0.49
1:A:1187:GLY:O	1:A:1379:ALA:HA	2.12	0.48
1:A:1277:GLU:HA	1:A:1282:THR:HG21	1.94	0.48
1:A:1647:GLY:O	1:A:1648:GLN:HB2	2.14	0.48
2:G:1086:LEU:HG	2:G:1092:ASP:HA	1.96	0.48
1:A:1022:THR:HG22	1:A:1226:SER:OG	2.13	0.48
2:G:1779:PRO:O	2:G:1783:LEU:HD23	2.13	0.48
2:G:245:GLN:HB3	2:G:279:THR:HG21	1.94	0.48
2:G:1620:THR:HG23	2:G:1645:GLU:OE1	2.14	0.48
2:G:490:TRP:CH2	2:G:512:LEU:HD21	2.49	0.48
2:G:739:GLY:HA2	2:G:1054:LEU:HD23	1.96	0.48
2:G:2037:PRO:O	2:G:2041:ILE:HG12	2.13	0.48
2:G:234:ILE:N	2:G:235:PRO:CD	2.77	0.48
2:G:1027:ILE:HG23	2:G:1031:LYS:HE3	1.96	0.48
1:B:143:GLU:HB3	1:B:260:ARG:HE	1.78	0.48
2:G:1177:SER:OG	2:G:1567:ARG:NH1	2.46	0.48
2:G:1270:TRP:HE1	2:G:1559:ASP:HA	1.79	0.48
2:G:156:LEU:HD12	2:G:502:LEU:HG	1.95	0.47
2:G:573:LYS:HG2	2:G:1101:GLU:HA	1.96	0.47
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.95	0.47
1:B:151:LEU:HD12	1:B:151:LEU:C	2.39	0.47
2:G:1539:ILE:HD11	2:G:1628:HIS:HB2	1.97	0.47
1:A:511:TYR:CZ	1:A:882:ASN:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:TYR:O	1:A:529:MET:HG2	2.13	0.47
1:A:1604:ILE:HG12	1:A:1632:LYS:HG2	1.97	0.47
2:G:283:ILE:O	2:G:286:THR:HG22	2.13	0.47
1:A:691:GLU:HG3	1:A:898:GLN:HB3	1.96	0.47
1:A:1251:MET:HE1	1:A:1585:LYS:HD2	1.97	0.47
1:A:1541:PHE:HD2	1:A:1576:PHE:CZ	2.33	0.47
2:G:296:VAL:HG22	2:G:300:ILE:HG12	1.97	0.47
2:G:1542:LEU:HD11	2:G:1596:TRP:CD1	2.50	0.47
2:G:1334:ILE:HD11	2:G:1406:VAL:HG21	1.97	0.47
1:A:1010:GLU:O	1:A:1449:LYS:NZ	2.40	0.47
1:B:271:ASN:HB2	1:B:290:MET:HE1	1.97	0.47
2:G:682:GLY:HA3	3:G:2101:FMN:O2	2.14	0.47
2:G:2026:PHE:CE2	2:G:2041:ILE:HG21	2.49	0.47
1:A:1557:ILE:O	1:A:1558:ASN:C	2.58	0.46
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.50	0.46
2:G:652:ILE:H	2:G:658:MET:CE	2.28	0.46
2:G:1286:LYS:HG3	2:G:1375:THR:HG22	1.97	0.46
1:A:36:LEU:O	1:A:76:ARG:NH2	2.48	0.46
2:G:145:LEU:O	2:G:149:VAL:HG23	2.16	0.46
2:G:913:ASP:OD1	2:G:914:LEU:N	2.47	0.46
1:B:238:PRO:HD3	1:B:277:LEU:HB2	1.97	0.46
2:G:1014:PRO:HG2	2:G:1032:ASP:HB2	1.96	0.46
2:G:1536:PRO:HB3	2:G:1629:VAL:HG22	1.97	0.46
1:A:1189:ILE:HG23	1:A:1190:PRO:HD2	1.97	0.46
1:A:1367:ARG:O	1:A:1370:THR:HG22	2.16	0.46
1:A:1531:LEU:HD21	1:A:1660:TYR:CE2	2.51	0.46
1:A:1555:ALA:HB2	1:A:1621:PHE:CZ	2.50	0.46
1:A:1849:VAL:HB	1:A:1867:VAL:HG23	1.97	0.46
2:G:187:LEU:HD11	2:G:296:VAL:HG21	1.98	0.46
2:G:369:SER:HB2	2:G:428:HIS:HB2	1.98	0.46
2:G:583:PHE:HD2	2:G:591:PRO:HA	1.80	0.46
2:G:1079:ASP:OD1	2:G:1080:GLY:N	2.49	0.46
1:A:18:LEU:HD11	2:G:1815:LEU:HD23	1.96	0.46
1:A:58:GLN:HB3	1:A:78:ILE:HD13	1.97	0.45
1:A:1669:ARG:O	1:A:1672:GLU:HG3	2.16	0.45
2:G:596:GLY:HA3	2:G:650:ASN:CB	2.46	0.45
2:G:1663:THR:O	2:G:1663:THR:HG23	2.17	0.45
1:B:147:ALA:HB2	1:B:217:PHE:CD1	2.52	0.45
1:A:1394:LEU:HA	1:A:1673:TYR:CD1	2.51	0.45
2:G:1138:TRP:O	2:G:1142:LEU:HG	2.16	0.45
2:G:1805:ALA:HB2	2:G:2011:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1782:THR:HG22	2:G:1827:LEU:HD21	1.99	0.45
1:A:872:THR:HA	1:A:896:PHE:O	2.17	0.45
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.47	0.45
1:A:13:LEU:HD22	2:G:2026:PHE:HE1	1.81	0.45
1:A:442:ARG:HD3	1:A:726:GLY:O	2.17	0.45
1:A:1232:TYR:O	1:A:1233:GLU:C	2.60	0.45
1:A:966:LYS:O	1:A:970:GLY:N	2.50	0.44
1:B:168:MET:HE3	1:B:207:GLU:HA	1.99	0.44
1:A:826:MET:HE1	1:A:847:GLU:HG3	1.98	0.44
1:A:1541:PHE:HD2	1:A:1576:PHE:CE2	2.36	0.44
2:G:599:PRO:O	2:G:602:VAL:HG22	2.18	0.44
2:G:1725:LYS:O	2:G:1729:ILE:HG12	2.17	0.44
2:G:598:THR:HA	2:G:599:PRO:HA	1.82	0.44
2:G:253:ALA:O	2:G:258:PHE:N	2.48	0.44
2:G:1672:GLN:O	2:G:1672:GLN:HG2	2.18	0.44
1:A:705:VAL:HG12	1:A:732:LEU:HD11	2.00	0.44
1:A:1791:PHE:CD1	1:A:1816:LYS:HE3	2.52	0.44
1:A:20:TYR:HB3	2:G:2033:THR:HG21	2.00	0.44
1:A:1560:MET:HE1	1:A:1652:GLN:NE2	2.33	0.44
2:G:803:SER:HA	2:G:806:MET:HE3	1.99	0.44
1:A:496:PRO:HG2	1:A:519:VAL:HG12	2.00	0.44
1:B:267:VAL:HG11	1:B:294:TYR:HB2	2.00	0.44
1:A:13:LEU:HD23	2:G:2019:PHE:CE2	2.53	0.44
1:A:1568:GLU:OE2	1:A:1568:GLU:HA	2.17	0.44
2:G:274:SER:O	2:G:483:ILE:HG12	2.18	0.44
1:A:1704:ALA:HB1	1:A:1705:PRO:HD2	1.99	0.43
2:G:1955:PRO:HB2	2:G:1957:PRO:HD2	2.00	0.43
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.33	0.43
1:A:72:LEU:HB3	1:A:74:LEU:HD13	1.99	0.43
1:A:1490:THR:HA	1:A:1493:ILE:HG22	2.00	0.43
2:G:48:PHE:HB2	2:G:55:THR:HG22	2.00	0.43
2:G:1859:PRO:HG3	2:G:1871:LEU:HD22	2.01	0.43
1:A:1305:CYS:HB2	1:A:1645:GLY:HA2	2.00	0.43
1:A:77:GLU:HB3	1:A:79:LEU:HD11	2.00	0.43
2:G:1347:LEU:HD12	2:G:1350:LEU:HB2	2.01	0.43
1:A:1189:ILE:H	1:A:1380:GLN:HE21	1.66	0.43
2:G:1101:GLU:OE1	2:G:1148:ASN:HA	2.19	0.43
2:G:1736:MET:HB3	2:G:1751:ILE:HD12	2.01	0.43
1:A:779:ILE:N	1:A:835:GLY:O	2.52	0.43
1:A:1145:LYS:HA	1:A:1152:VAL:HG11	2.01	0.43
2:G:1878:VAL:HG22	2:G:1944:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:234:ILE:N	2:G:235:PRO:HD3	2.34	0.43
1:A:513:GLU:CD	1:A:873:ARG:HH21	2.27	0.43
1:A:1209:ASP:O	1:A:1210:PRO:C	2.62	0.43
2:G:242:GLY:HA3	2:G:303:LEU:CD1	2.49	0.43
2:G:817:ALA:HA	2:G:1048:VAL:HG21	2.01	0.43
1:A:1154:ILE:HG13	1:A:1154:ILE:O	2.18	0.42
2:G:370:LEU:HB2	2:G:378:VAL:HB	1.99	0.42
1:A:1292:ILE:HG22	1:A:1294:SER:HB3	2.01	0.42
1:A:1017:ARG:HE	1:A:1320:LEU:HD22	1.83	0.42
1:A:1085:ASP:OD2	1:A:1087:LYS:HG2	2.19	0.42
2:G:1542:LEU:HD13	2:G:1592:LEU:HD22	2.02	0.42
2:G:262:GLU:O	2:G:265:SER:OG	2.32	0.42
2:G:293:PHE:HA	2:G:296:VAL:HG12	2.02	0.42
2:G:767:PHE:HB2	2:G:796:PHE:CD2	2.55	0.42
1:A:500:LYS:HB2	1:A:514:GLU:CG	2.49	0.42
1:A:638:LEU:O	1:A:660:LEU:HD21	2.20	0.42
1:A:1710:LEU:O	1:A:1711:GLU:C	2.62	0.42
2:G:261:GLY:N	2:G:287:ASP:O	2.49	0.42
2:G:835:THR:HG22	2:G:840:THR:HB	2.01	0.42
1:A:8:GLU:O	1:A:12:ILE:HG12	2.19	0.42
1:A:440:MET:HA	1:A:480:CYS:SG	2.60	0.41
1:B:222:GLY:O	1:B:226:SER:OG	2.12	0.41
2:G:863:MET:O	2:G:867:GLU:HG2	2.20	0.41
2:G:254:LYS:HG3	2:G:289:TRP:CH2	2.55	0.41
2:G:366:VAL:HG12	2:G:381:GLY:HA3	2.02	0.41
2:G:1737:ILE:O	2:G:1833:TYR:OH	2.32	0.41
1:A:497:THR:C	1:A:516:ARG:HG3	2.45	0.41
2:G:1304:VAL:HG23	2:G:1306:ASN:HB2	2.01	0.41
1:A:702:LYS:HE3	1:A:729:GLY:O	2.19	0.41
2:G:1686:ALA:HB1	2:G:1790:GLU:HG3	2.03	0.41
1:A:17:LEU:O	1:A:21:GLN:HB2	2.21	0.41
1:A:764:ASP:OD1	1:A:810:LYS:NZ	2.47	0.41
1:A:1234:MET:HE1	1:A:1243:VAL:HG13	2.03	0.41
1:A:1615:ASP:C	1:A:1615:ASP:OD1	2.64	0.41
1:A:897:SER:O	1:A:898:GLN:C	2.63	0.41
1:A:752:ILE:HA	1:A:761:LEU:HD13	2.02	0.41
1:A:765:LEU:O	1:A:820:ALA:HB2	2.20	0.41
2:G:1604:ARG:HA	2:G:1658:GLU:HB2	2.02	0.41
2:G:1698:PHE:CD2	2:G:1706:ILE:HB	2.55	0.41
2:G:1863:ALA:HB3	2:G:1866:PHE:HB2	2.02	0.41
1:A:28:TRP:CZ3	1:A:31:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:SER:O	1:B:229:LEU:HD23	2.20	0.41
2:G:323:ILE:HD12	2:G:387:TYR:CE2	2.56	0.41
2:G:592:LEU:HD22	2:G:801:PHE:HE2	1.86	0.41
2:G:741:HIS:CD2	2:G:855:HIS:ND1	2.88	0.41
2:G:1635:ARG:HG2	2:G:1658:GLU:HA	2.01	0.41
1:A:869:ILE:HA	1:A:901:MET:CE	2.51	0.41
1:A:1103:ILE:HA	1:A:1187:GLY:HA2	2.03	0.41
1:B:213:PHE:O	1:B:217:PHE:HB3	2.21	0.41
1:B:233:ILE:O	1:B:237:MET:HB2	2.20	0.41
2:G:228:LYS:HA	2:G:228:LYS:HD2	1.91	0.41
2:G:246:LEU:HG	2:G:279:THR:HG23	2.03	0.41
2:G:1327:ILE:O	2:G:1331:TRP:HB2	2.21	0.41
2:G:1470:THR:HG22	2:G:1472:VAL:HG23	2.02	0.41
1:B:176:VAL:HG22	1:B:179:LYS:HB2	2.03	0.41
1:B:192:LYS:HB3	1:B:224:GLN:NE2	2.36	0.41
2:G:1343:VAL:HG12	2:G:1412:TYR:HE2	1.86	0.41
1:A:504:ASP:OD1	1:A:508:ASN:N	2.49	0.40
1:A:1308:SER:O	1:A:1311:SER:HB3	2.21	0.40
1:B:251:GLN:HG2	1:B:261:GLN:HE22	1.86	0.40
2:G:45:THR:HG22	2:G:53:GLU:OE2	2.21	0.40
2:G:209:PHE:CE2	2:G:213:LEU:HD22	2.57	0.40
2:G:1093:ASP:OD2	2:G:1096:LYS:HG3	2.20	0.40
2:G:1698:PHE:HD2	2:G:1706:ILE:HB	1.86	0.40
1:A:41:THR:HG21	2:G:1663:THR:HB	2.02	0.40
1:A:443:SER:HA	1:A:447:LEU:HD23	2.02	0.40
1:A:1444:ASN:HD21	1:A:1446:LYS:HE2	1.86	0.40
2:G:149:VAL:CG2	2:G:156:LEU:HD23	2.51	0.40
2:G:302:VAL:O	2:G:306:ILE:HG12	2.21	0.40
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.83	0.40
2:G:1423:PHE:CD2	2:G:1425:LYS:HG3	2.56	0.40
1:A:1460:LYS:HG3	1:A:1773:VAL:HG23	2.03	0.40
2:G:37:PHE:CZ	2:G:41:LEU:HD13	2.56	0.40
2:G:306:ILE:HD13	2:G:439:ILE:HD13	2.03	0.40
2:G:320:PRO:HA	2:G:321:PRO:HD3	1.98	0.40
1:A:1370:THR:O	1:A:1373:ARG:NH1	2.44	0.40
2:G:963:THR:OG1	2:G:964:LEU:N	2.54	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	1569/1887 (83%)	1447 (92%)	112 (7%)	10 (1%)	21	52
1	B	161/1887 (8%)	148 (92%)	12 (8%)	1 (1%)	21	52
2	G	2031/2051 (99%)	1874 (92%)	150 (7%)	7 (0%)	36	65
All	All	3761/5825 (65%)	3469 (92%)	274 (7%)	18 (0%)	26	56

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1304	ALA
1	A	1545	SER
2	G	769	SER
1	A	726	GLY
1	A	866	GLY
2	G	1162	ASP
1	A	1711	GLU
2	G	858	ALA
2	G	1527	LEU
1	A	63	ASN
1	B	252	THR
2	G	1808	SER
1	A	73	SER
1	A	1412	ASP
1	A	1611	ALA
2	G	1027	ILE
1	A	1210	PRO
2	G	1843	PRO

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	1336/1566 (85%)	1334 (100%)	2 (0%)	88	88
1	B	135/1566 (9%)	131 (97%)	4 (3%)	36	57
2	G	1774/1789 (99%)	1773 (100%)	1 (0%)	88	88
All	All	3245/4921 (66%)	3238 (100%)	7 (0%)	85	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	MET
1	A	1210	PRO
1	B	236	LYS
1	B	237	MET
1	B	276	ARG
1	B	280	GLU
2	G	816	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	40	ASN
1	A	344	GLN
1	A	467	GLN
1	A	475	GLN
1	A	506	ASN
1	A	527	GLN
1	A	618	ASN
1	A	758	ASN
1	A	777	GLN
1	A	854	HIS
1	A	983	GLN
1	A	987	ASN
1	A	1000	GLN
1	A	1063	HIS
1	A	1100	HIS
1	A	1442	ASN
1	A	1458	GLN
1	A	1542	HIS

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Mol	Chain	Res	Type
1	A	1652	GLN
1	A	1794	GLN
1	A	1852	HIS
1	B	184	ASN
1	B	261	GLN
2	G	112	ASN
2	G	155	GLN
2	G	163	GLN
2	G	330	ASN
2	G	343	ASN
2	G	354	ASN
2	G	440	ASN
2	G	456	GLN
2	G	640	GLN
2	G	677	GLN
2	G	747	HIS
2	G	878	ASN
2	G	1078	HIS
2	G	1217	ASN
2	G	1434	HIS
2	G	1595	ASN
2	G	1619	ASN
2	G	1659	GLN
2	G	1858	ASN
2	G	1896	GLN
2	G	1920	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	FMN	G	2101	-	33,33,33	1.41	6 (18%)	48,50,50	1.77	11 (22%)

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	FMN	G	2101	-	-	2/18/18/18	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2101	FMN	C5A-N5	-3.36	1.33	1.39
3	G	2101	FMN	C9A-C5A	3.26	1.46	1.41
3	G	2101	FMN	C8-C7	2.95	1.48	1.40
3	G	2101	FMN	C6-C5A	-2.59	1.36	1.40
3	G	2101	FMN	C4-N3	-2.25	1.34	1.38
3	G	2101	FMN	C9-C8	-2.06	1.36	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2101	FMN	O5'-P-O1P	-4.31	94.80	106.44
3	G	2101	FMN	O2P-P-O5'	3.45	115.67	106.67
3	G	2101	FMN	O4'-C4'-C3'	3.34	117.06	109.25
3	G	2101	FMN	O4'-C4'-C5'	-3.25	102.83	109.99
3	G	2101	FMN	C9A-N10-C10	-2.91	116.31	120.75
3	G	2101	FMN	C4A-C10-N10	2.88	120.60	116.48
3	G	2101	FMN	O3P-P-O5'	-2.62	99.84	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2101	FMN	O3'-C3'-C4'	2.57	114.77	108.93
3	G	2101	FMN	C1'-C2'-C3'	2.54	116.54	109.66
3	G	2101	FMN	O2-C2-N1	-2.46	117.71	121.80
3	G	2101	FMN	C7M-C7-C8	2.21	125.28	120.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

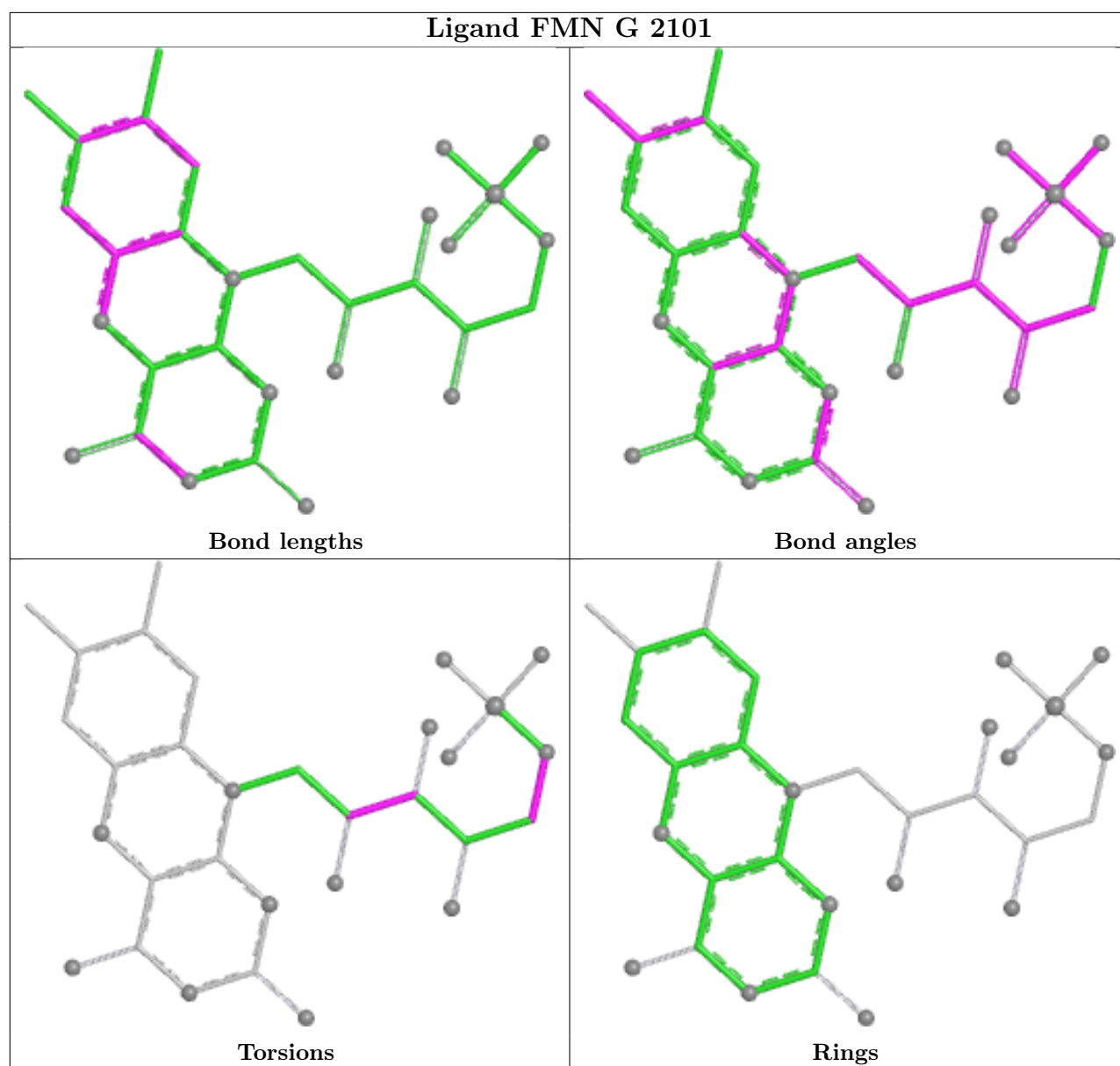
Mol	Chain	Res	Type	Atoms
3	G	2101	FMN	C4'-C5'-O5'-P
3	G	2101	FMN	O2'-C2'-C3'-C4'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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.

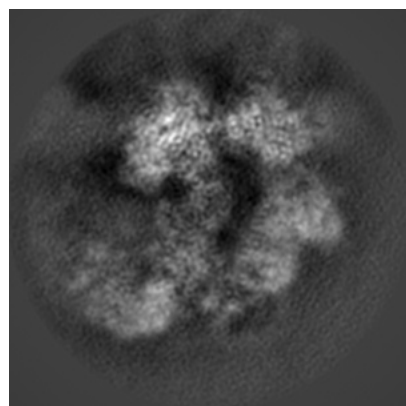
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17855. These allow visual inspection of the internal detail of the map and identification of artifacts.

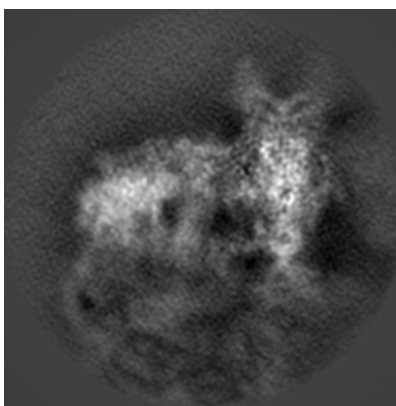
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

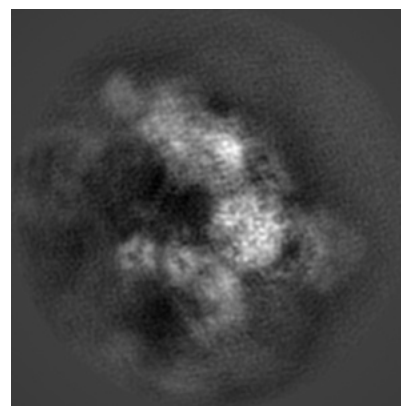
6.1.1 Primary map



X

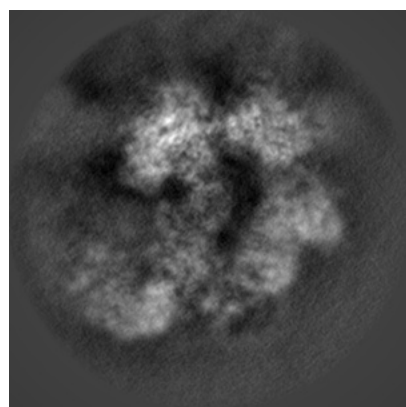


Y

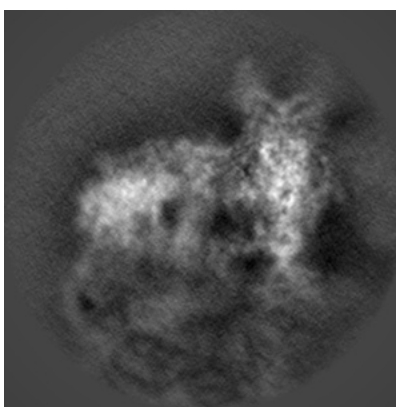


Z

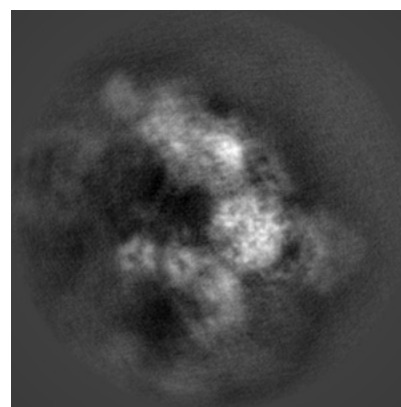
6.1.2 Raw map



X



Y

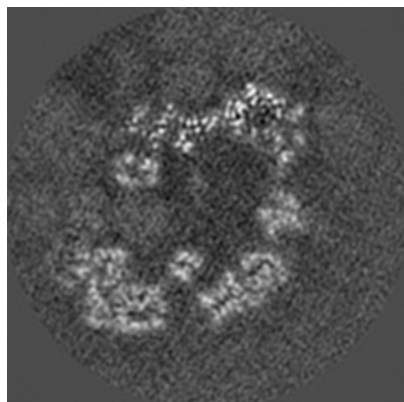


Z

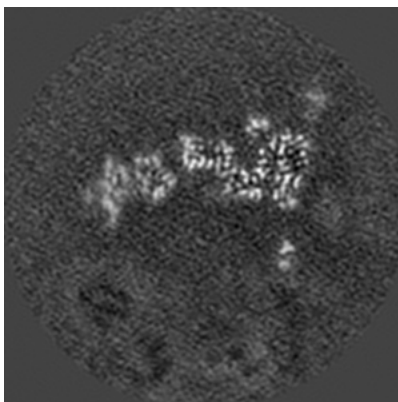
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

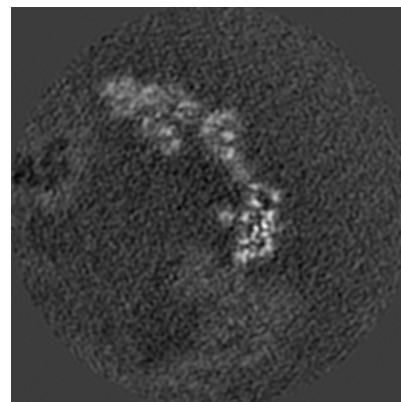
6.2.1 Primary map



X Index: 120

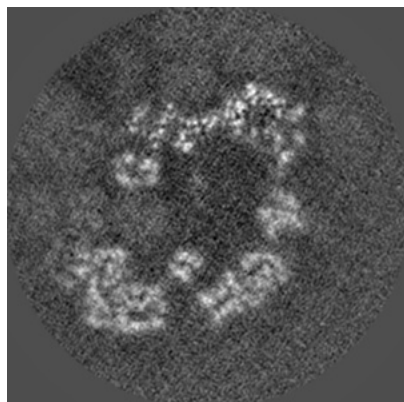


Y Index: 120

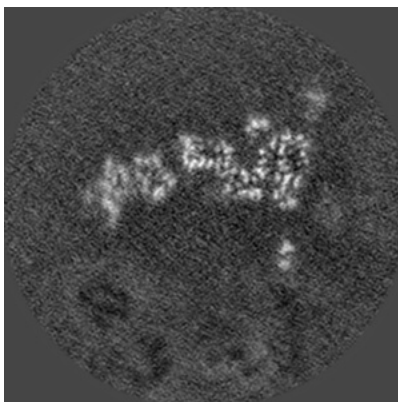


Z Index: 120

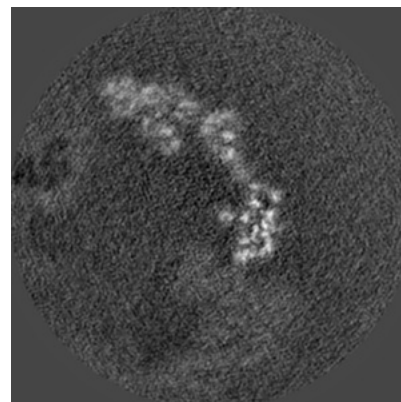
6.2.2 Raw map



X Index: 120



Y Index: 120

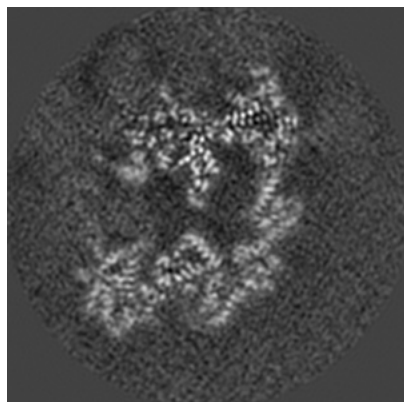


Z Index: 120

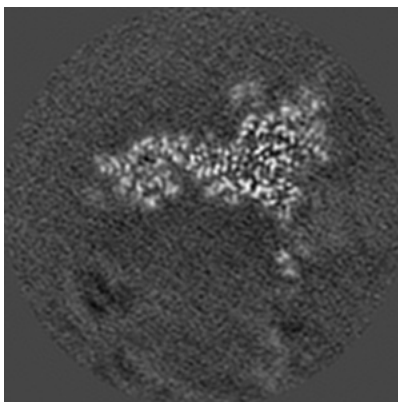
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

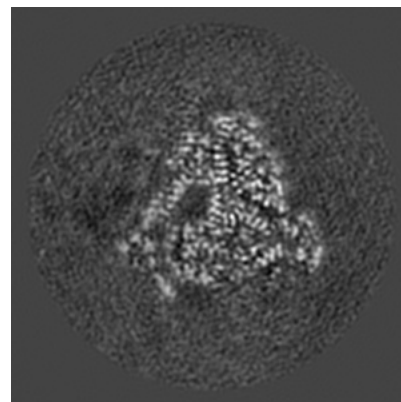
6.3.1 Primary map



X Index: 129

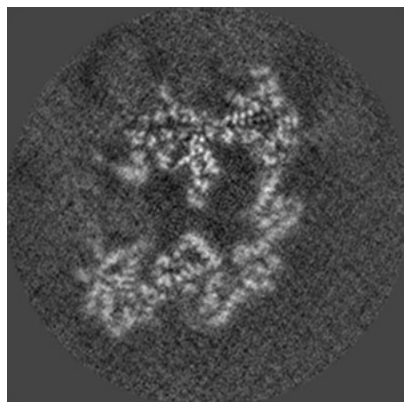


Y Index: 111

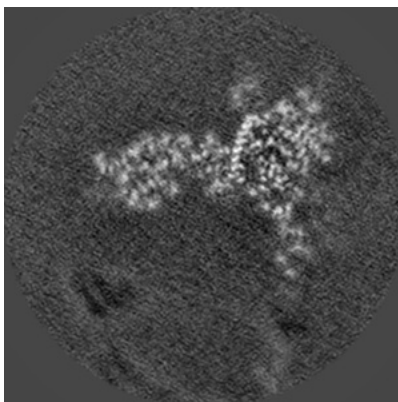


Z Index: 171

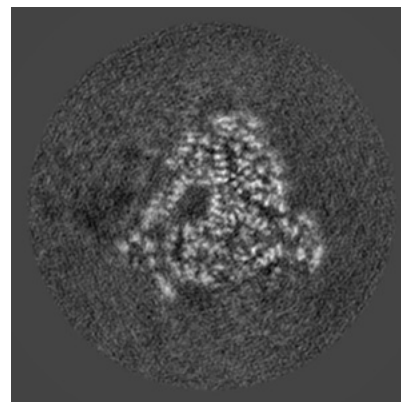
6.3.2 Raw map



X Index: 129



Y Index: 109

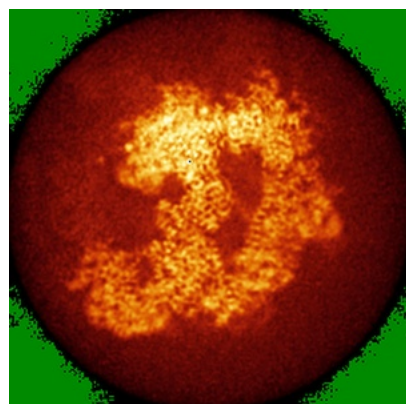


Z Index: 171

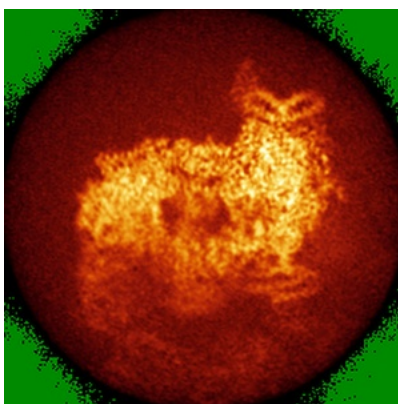
The images above show the largest variance slices of the map in three orthogonal directions.

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

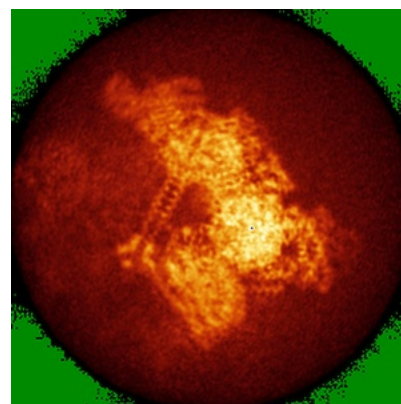
6.4.1 Primary map



X

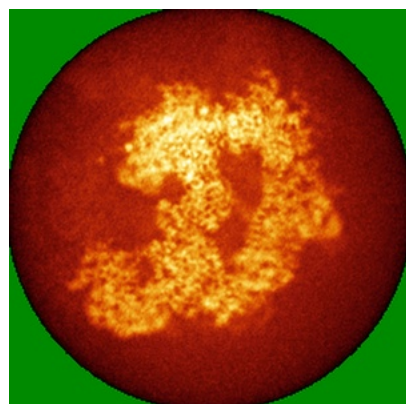


Y

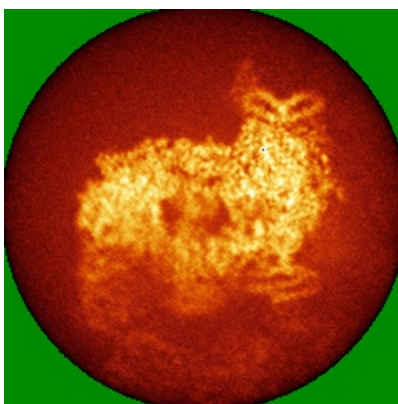


Z

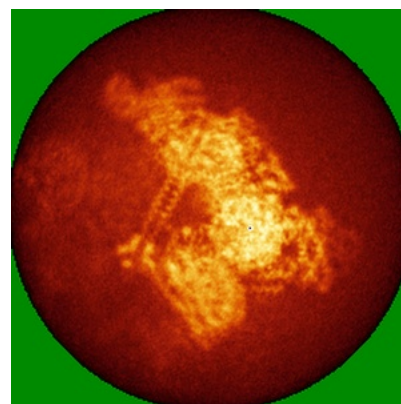
6.4.2 Raw map



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](#)

This section was not generated.

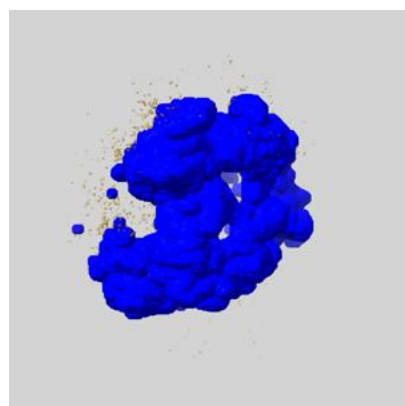
6.6 Mask visualisation [i](#)

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

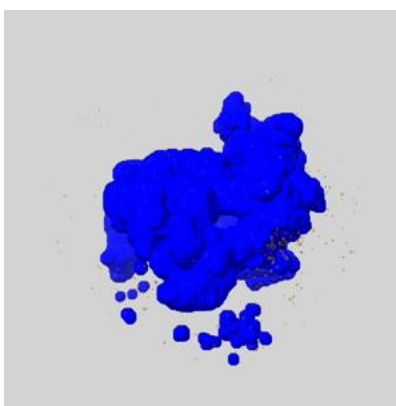
A mask typically either:

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

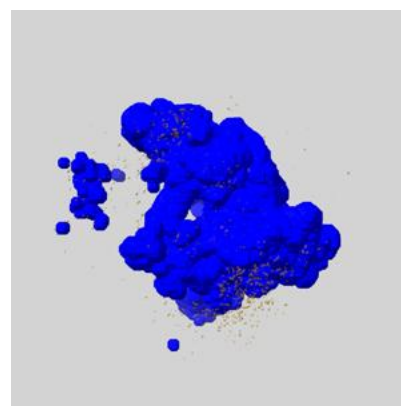
6.6.1 emd_17855_msk_1.map [i](#)



X



Y

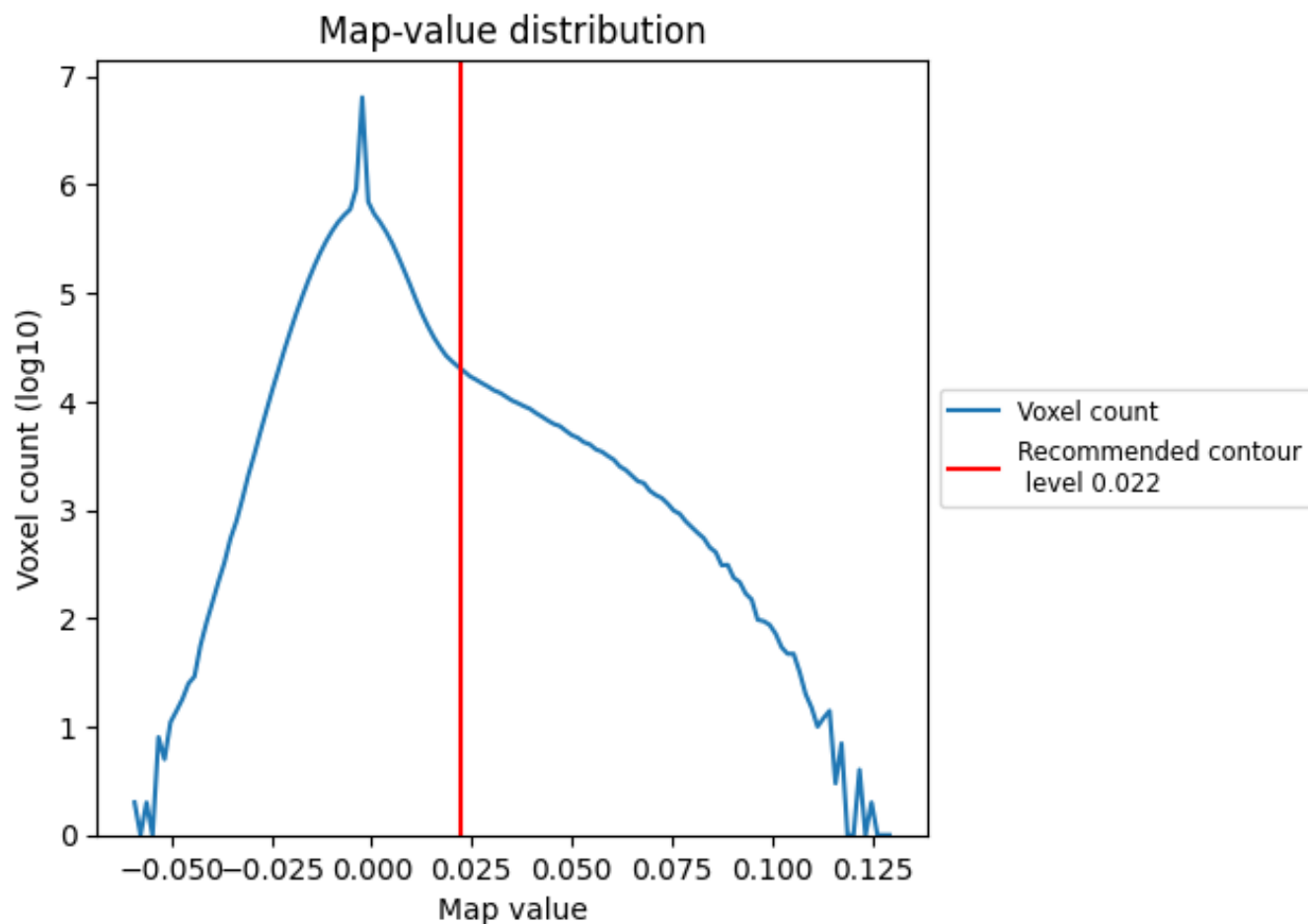


Z

7 Map analysis [i](#)

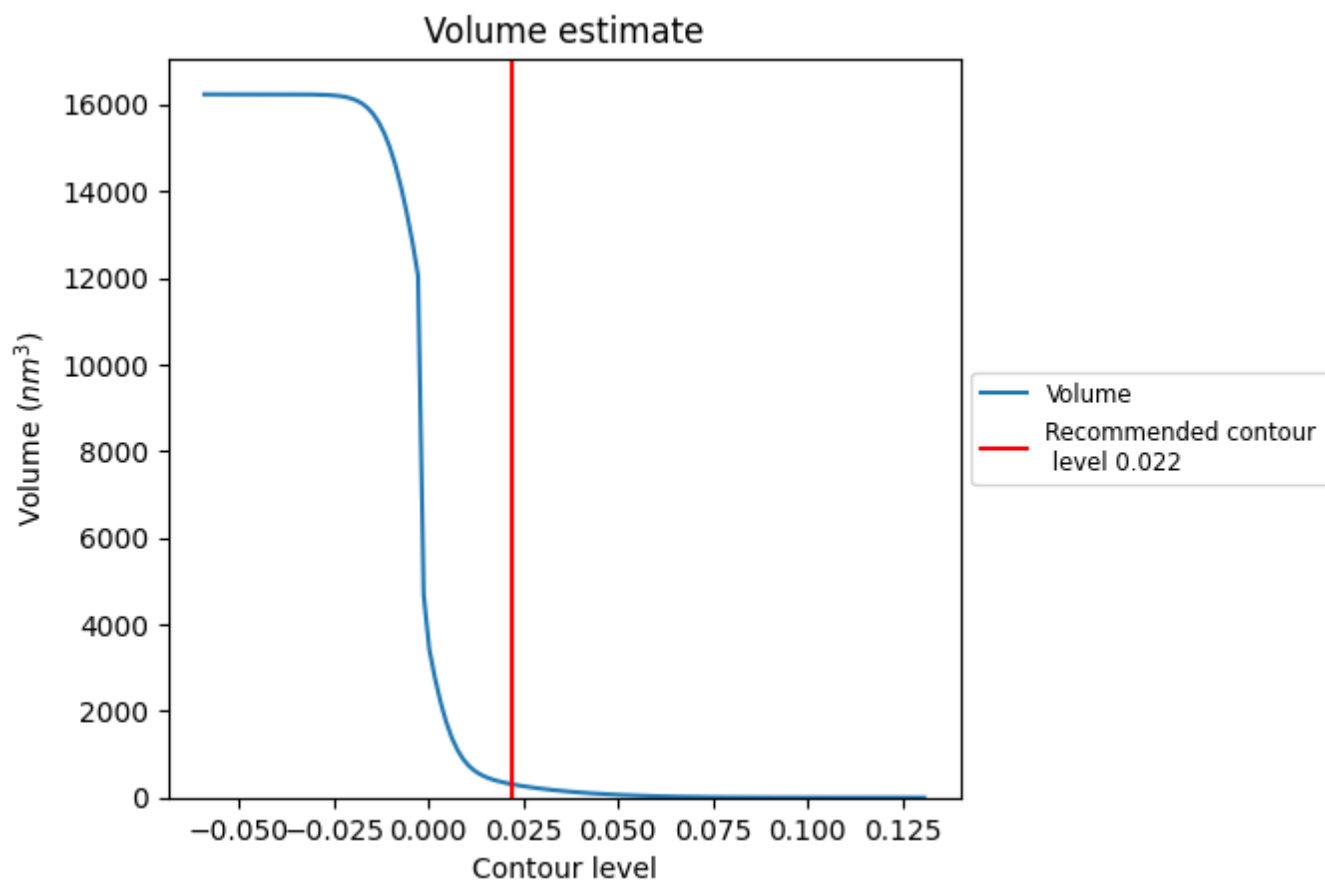
This section contains the results of statistical analysis of the map.

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.

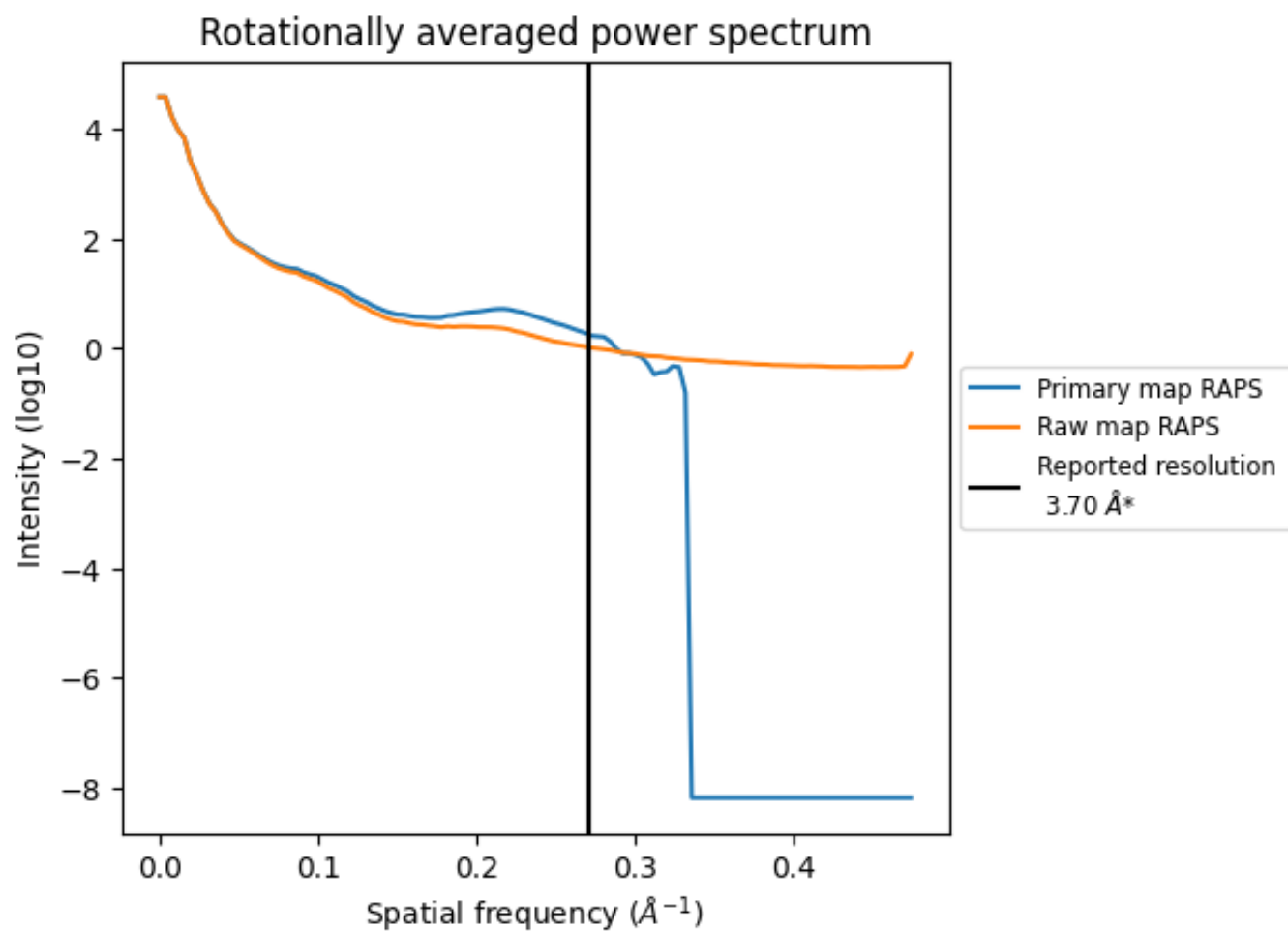
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 279 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 ⓘ

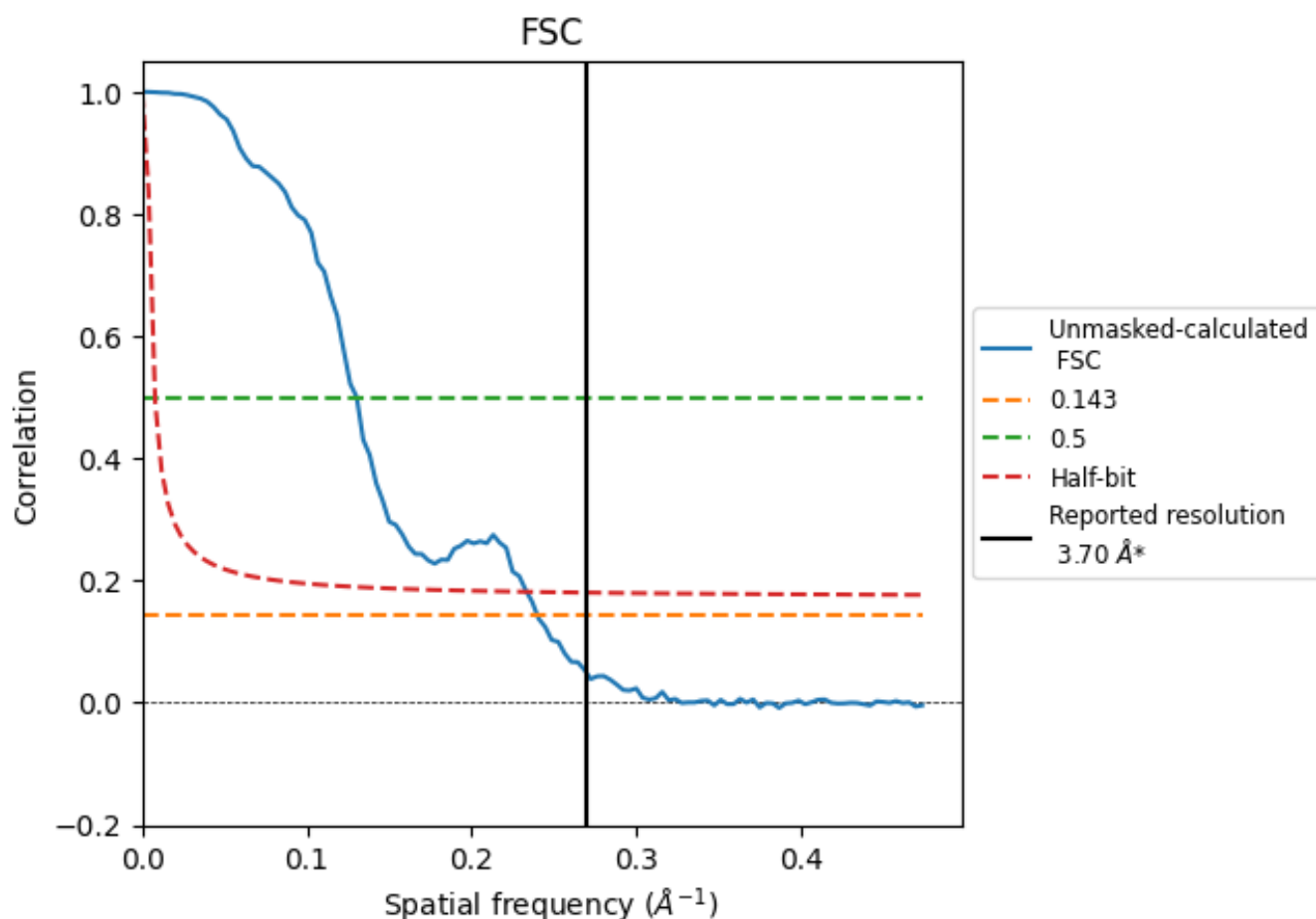


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.67	4.28

*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 4.16 differs from the reported value 3.7 by more than 10 %

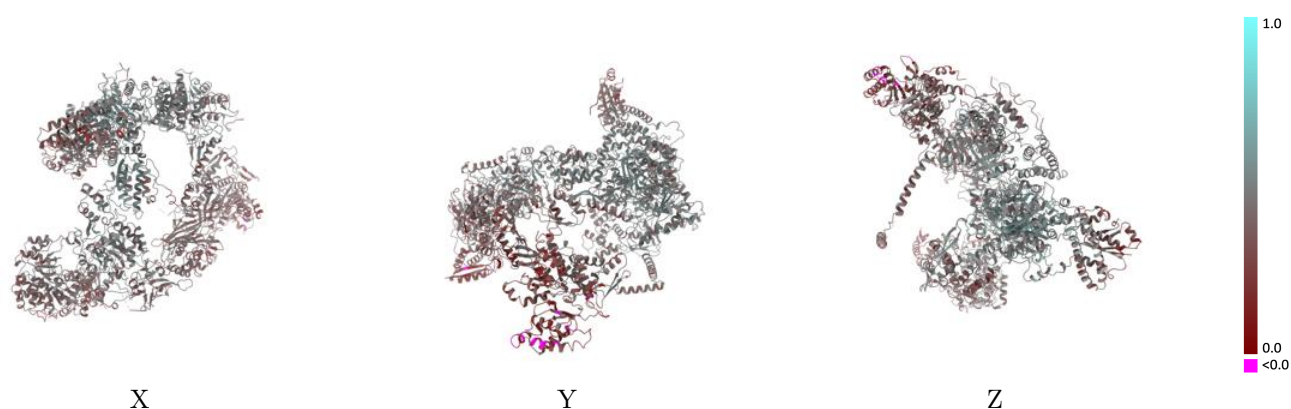
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17855 and PDB model 8PSL. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

This section was not generated.

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

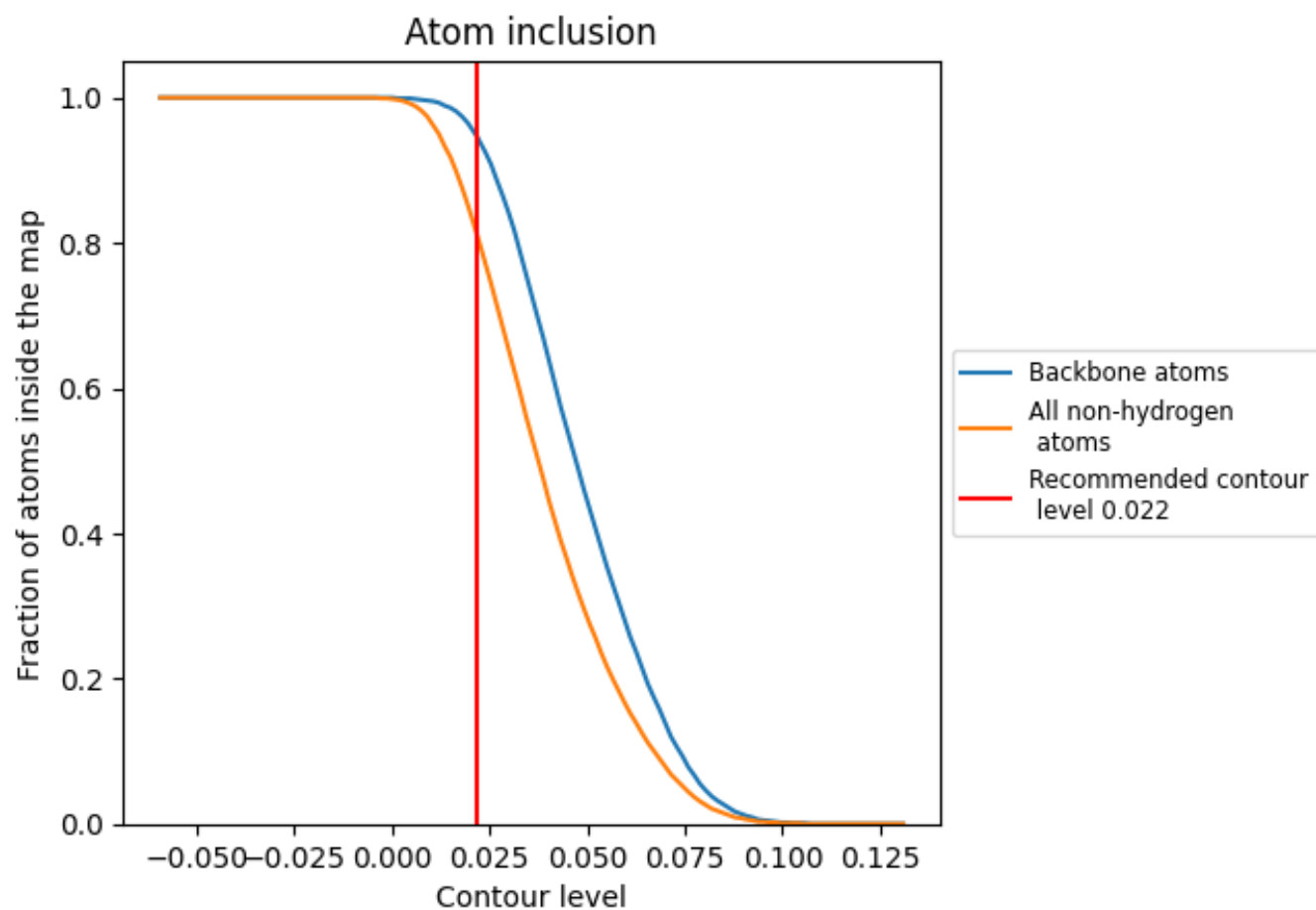


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.4200
A	0.8120	0.4650
B	0.7930	0.3870
G	0.8060	0.3880

