Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 03:55 pm GMT

PDB ID	:	8PSK
EMDB ID	:	EMD-17854
Title	:	Asymmetric unit of the yeast fatty acid synthase in the 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	:	2.80 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:

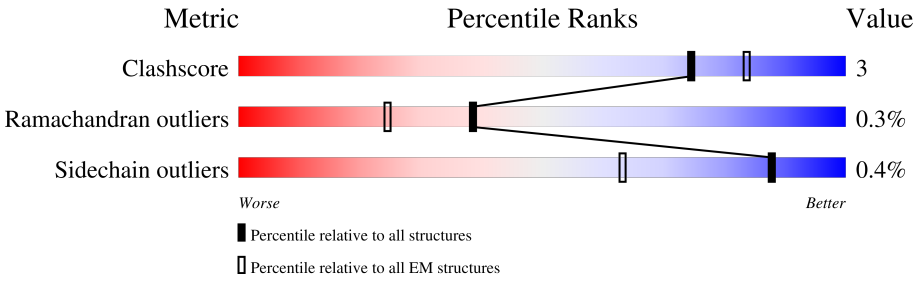
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1887	9% 77% 7% 16%
1	B	1887	8% 91%
2	G	2051	7% 90% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29604 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.

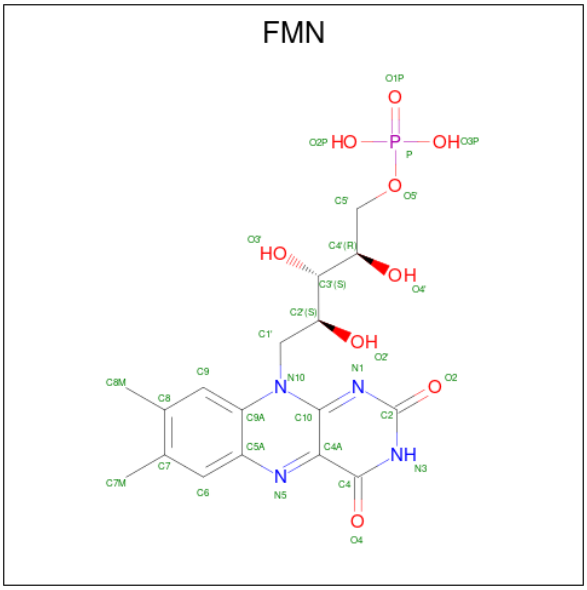
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

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	2034	Total	C	N	O	S	0	0
			16004	10258	2661	3029	56		

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



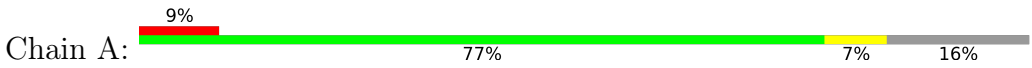
Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			31	17	4	9	1	

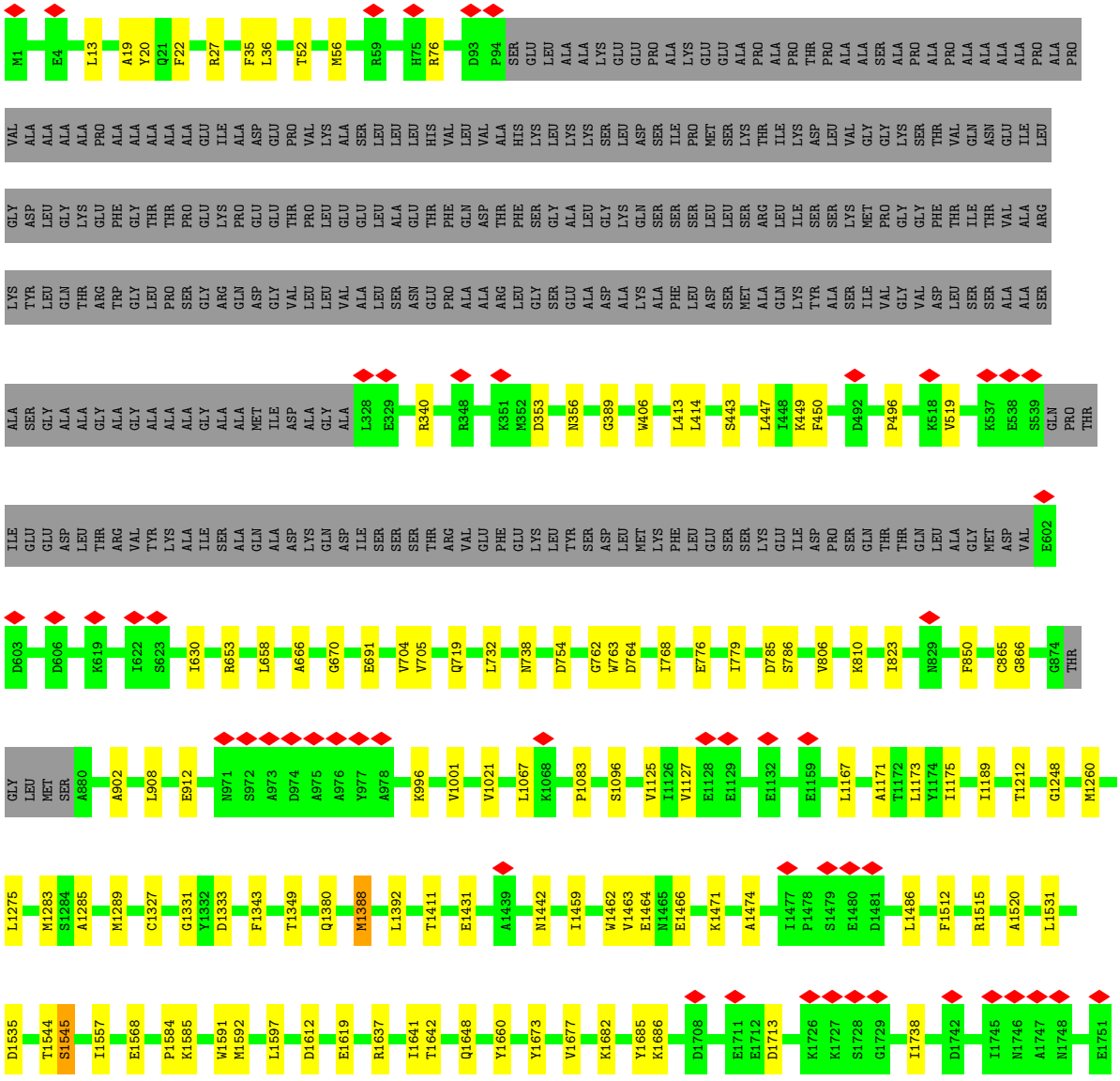
3 Residue-property plots (i)

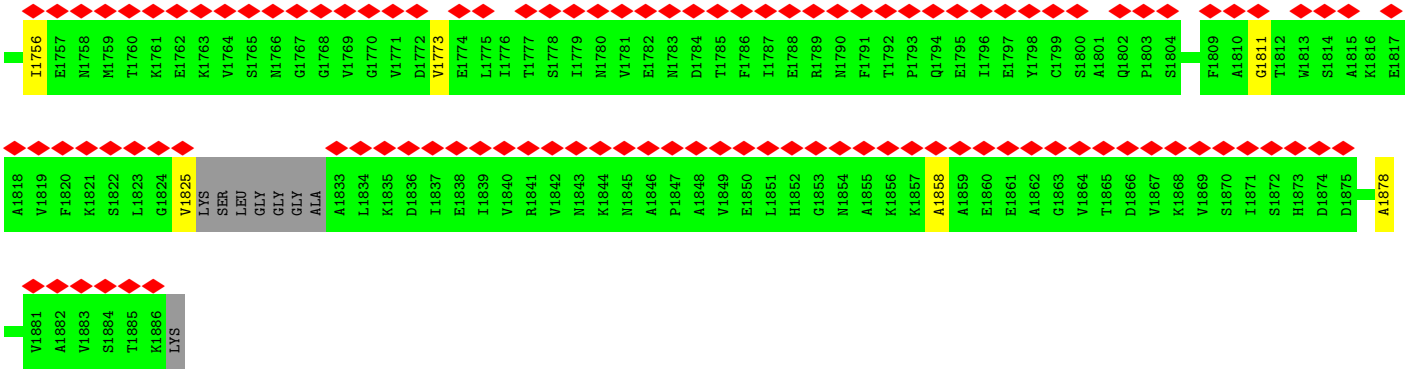
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Fatty acid synthase subunit alpha

Chain A:

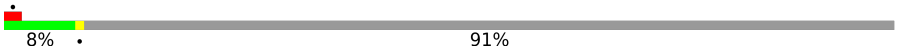


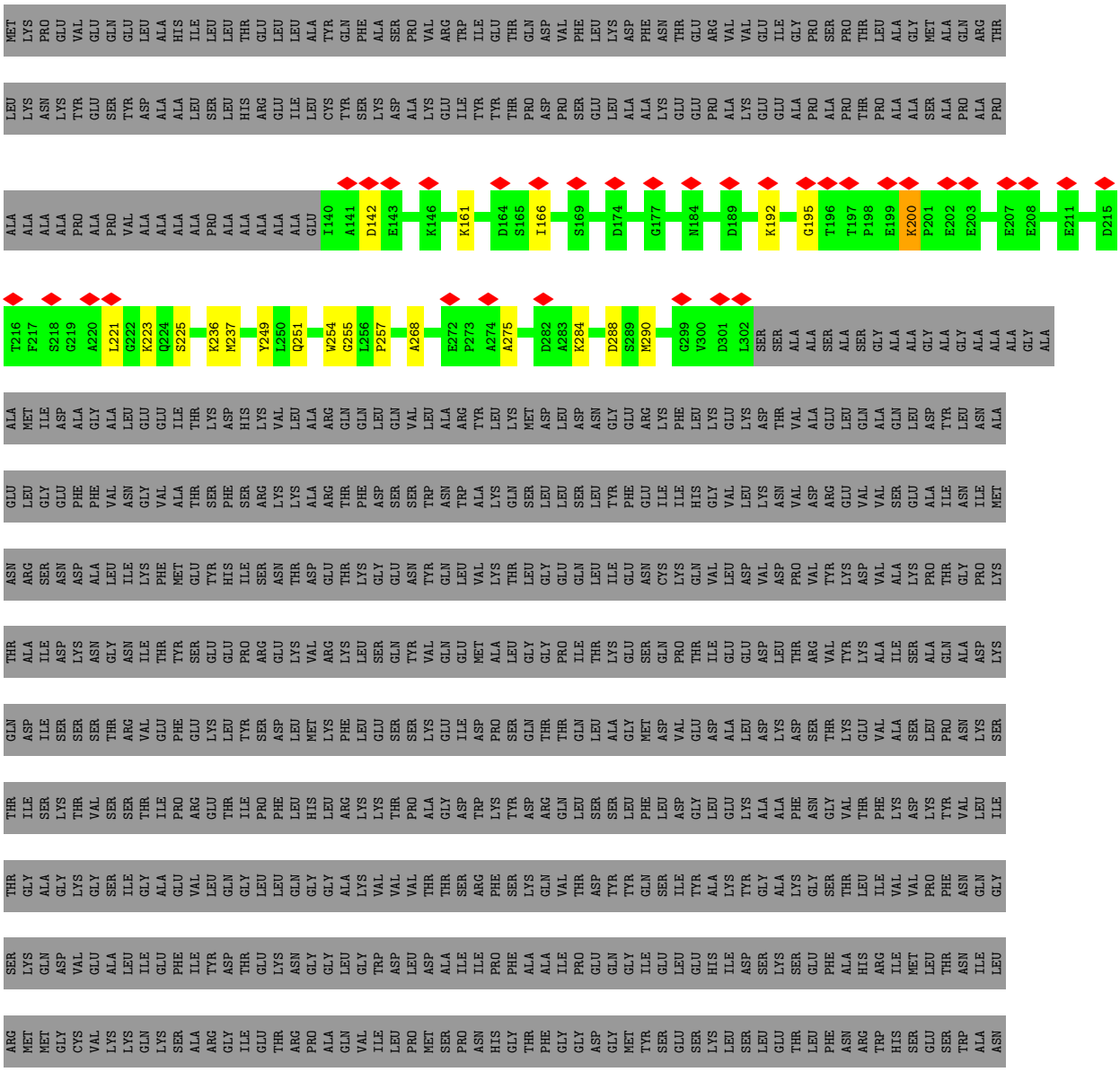




• Molecule 1: Fatty acid synthase subunit alpha

Chain B:





GLN LEU THR VAL CYS GLY ALA ILE ILE GLY TRP THR ARG GLY THR GLY LEU MET SER ALA ASN ASN ILE ILE ALA GLU GLY ILE GLU LYS MET GLY VAL ARG THR PHE SER GLN LYS GLU MET ALA PHE ASN LEU LEU LEU GLY LEU LEU THR PRO GLU VAL VAL GLU LEU CYS GLN LYS SER

PRO VAL MET ALA ASP LEU ASN GLY GLY LEU GLN PHE VAL PRO GLU LEU LYS GLU PHE THR ALA LYS LEU ARG LYS GLU LEU GLU THR SER GLU VAL ARG LYS ALA VAL SER ILE GLU THR ALA LEU GLU HIS LYS VAL VAL ASN GLY ASN SER ALA ASP ALA ALA ALA TYR ALA GLN VAL

GLU ILE GLN PRO ARG ALA ASN ILE GLN LEU ASP PHE PRO GLU LEU LYS PRO TYR LYS GLN VAL LYS GLN ILE ALA PRO ALA GLU LEU GLU GLY GLU LEU LEU ASP LEU GLU ARG THR ARG TRP GLU MET GLU

ALA PHE GLY GLU PHE SER LEU GLU GLY CYS VAL GLU MET ALA TRP ILE MET GLY PHE ILE SER TYR HIS ASN GLY ASN LEU LYS GLY ARG PRO TYR THR GLY TRP VAL ASP SER LYS THR LYS GLU PRO VAL ASP ASP LYS ASP VAL LYS ALA LEU GLU THR SER ILE LEU LEU GLU HIS

SER GLY ILE ARG LEU ILE GLU PRO GLU LEU PHE ASN GLY TYR ASN PRO GLU LYS LYS GLU MET ILE GLN GLU VAL ILE VAL GLU GLU ASP LEU GLU PRO PHE GLU ALA SER LYS GLU THR ALA GLU GLN PHE LYS HIS GLN HIS GLY ASP LYS VAL ASP ILE PHE GLU GLU ILE LEU PRO GLU THR

GLY GLU TYR SER VAL LYS LEU LEU LYS GLY ALA THR LEU TYR ILE PRO LYS ALA LEU ARG PHE ASP ARG LEU VAL ALA GLY GLN ILE PRO THR GLY TRP ASN ALA LYS THR TYR GLY ILE SER ASP ASP ILE SER GLN VAL ASP PRO ILE THR LEU PHE VAL LEU VAL SER VAL VAL

GLU ALA PHE ILE ALA SER GLY ILE THR ASP PRO TYR GLU MET TYR LYS TYR VAL HIS VAL SER GLU VAL GLY ASN CYS SER GLY SER GLY MET GLY GLY VAL SER ALA LEU ARG GLY MET PHE LYS ASP ARG PHE LYS ASP GLU PRO VAL GLN ASN ASP ILE LEU GLN GLU SER PHE ILE

ASN THR MET SER ALA TRP VAL ASN MET LEU LEU ILE SER SER SER GLY PRO ILE LYS THR PRO VAL GLY ALA CYS ALA THR SER VAL GLU SER VAL ASP ILE GLY VAL GLU THR ILE LEU SER GLY LYS ALA ARG ILE CYS ILE VAL GLY GLY TYR ASP ASP PHE GLN GLU GLU GLY SER

PHE GLU PHE GLY ASN MET LYS ALA THR SER ASN THR LEU GLU GLU PHE GLU HIS GLY ARG THR PRO ALA GLU MET SER ARG PRO ALA THR THR THR ARG ASN GLY PHE MET GLU ALA GLN GLY ALA ILE GLN ILE ILE MET GLN ALA ASP LEU ALA LEU LYS MET GLY VAL PRO ILE

TYR GLY ILE VAL ALA MET ALA ALA THR ALA THR ASP LYS ILE GLY ARG SER VAL PRO ALA PRO GLY LYS GLY ILE LEU THR THR ALA ARG GLU HIS HIS SER SER VAL LYS TYR ALA SER PRO ASN LEU ASN MET LYS TYR ARG LYS ARG GLN LEU VAL THR ARG GLU GLU ALA GLN ILE LYS

ASP TRP VAL GLU ASN GLU LEU GLU ALA LEU LYS LEU GLU ALA GLU GLU ILE PRO SER GLU ASP GLN ASN GLU PHE LEU LEU GLU ARG THR ARG GLU ILE HIS ASN GLU ALA GLU SER GLN LEU ARG ALA ALA GLN GLN GLN TRP GLY ASN ASP PHE TYR LYS ARG GLN LEU VAL LYS ARG ASP PRO ARG ILE ALA

PRO LEU ARG GLY ALA LEU ALA THR TYR GLY LEU THR LEU ASP ASP LEU GLY VAL ALA SER PHE HIS GLY THR SER THR LYS ALA ASN ASP LYS ASN GLU LYS HIS LEU GLY ARG SER GLU GLY ASN PRO VAL ILE GLY PHE GLN LYS PHE LEU

THR GLY HIS PRO LYS GLY ALA ALA GLY ALA TRP MET MET ASN GLY ALA LEU GLN ILE LEU ASN SER GLY ILE ILE PRO GLY ASN ARG ASN ALA ASP ASN ARG LYS ILE LEU GLU GLN PHE GLU TYR VAL LEU TYR PRO SER LYS THR ILE ASP GLY VAL ARG ALA VAL SER

ILE THR SER PHE GLY PHE GLY GLN LYS GLY GLY GLN ALA ILE VAL VAL HIS PRO ASP TYR LEU TYR GLY ALA ILE THR GLU ASP ARG TYR ASN GLU TYR VAL ALA LYS VAL SER ALA ARG GLU LYS SER ALA TYR LYS PHE PHE HIS ASN GLY MET ILE TYR ASN LYS LEU GLU ASN VAL

LYS GLU HIS ALA PRO TYR THR ASP GLU LEU GLU GLU ASP VAL TYR LEU ASP PRO LEU ALA ARG VAL SER LYS ASP LYS LYS SER GLY SER LEU THR PHE ASN SER LYS ASN ILE GLN SER LYS ASP SER TYR ILE ASN ALA ASN THR ILE GLU GLU THR ALA LYS MET ILE GLU THR

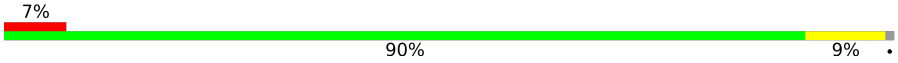
LYS GLU LYS VAL SER GLY VAL GLY VAL ASP VAL GLU LEU ILE THR SER ILE GLU ASN ASP THR PHE THR PRO GLN GLU ILE GLU TYR CYS SER ALA GLN PRO SER VAL GLN SER SER PHE ALA GLY THR TRP SER ALA LYS GLU ASN ALA VAL PHE

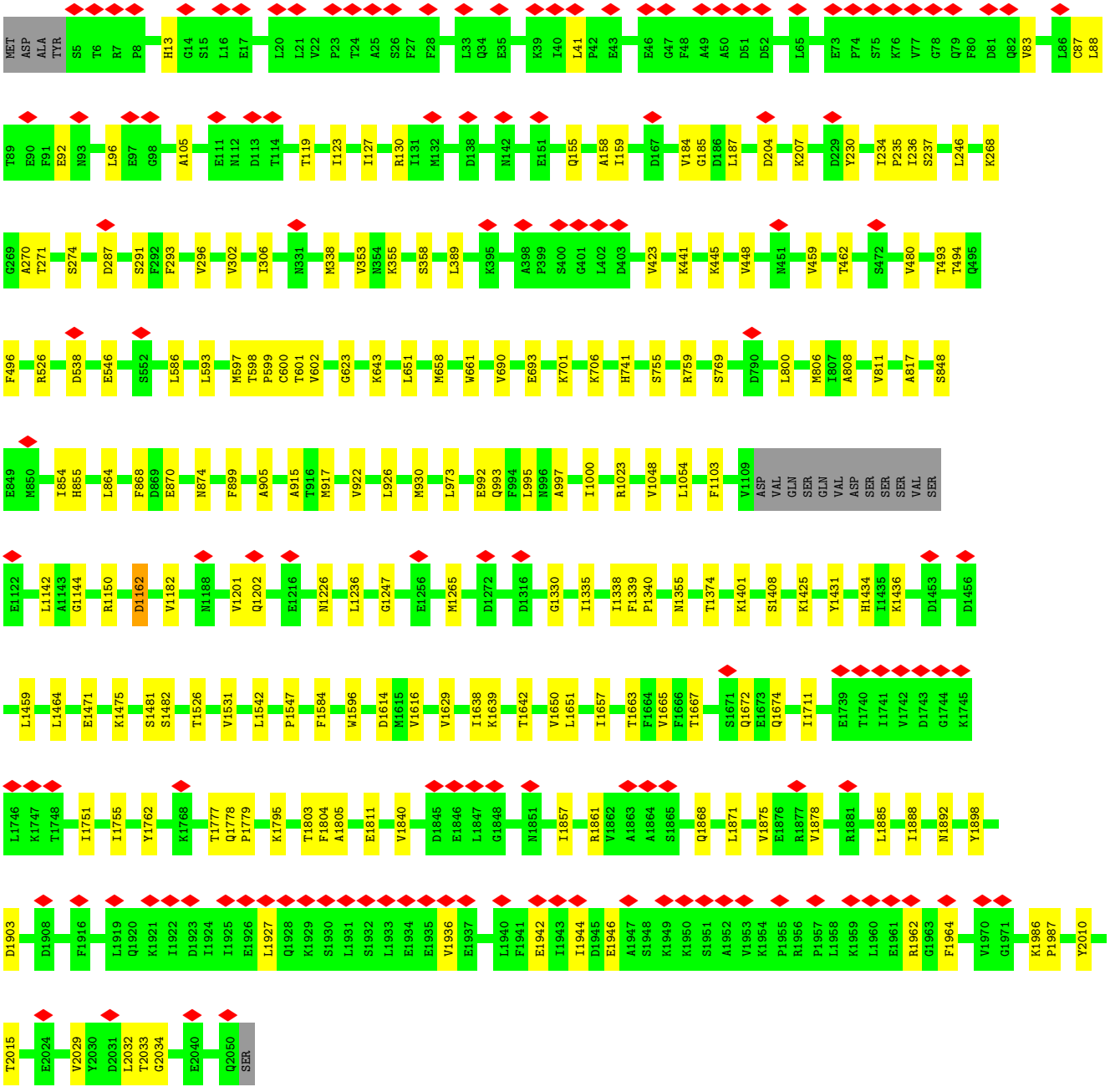
LYS SER LEU GLY GLY GLY ALA ALA LEU LYS ASP ILE GLU ILE VAL ARG VAL ASN ASN LYS ASN ALA PRO ALA VAL GLU LEU HIS GLY ASN ALA LYS LYS ALA ALA GLU GLU ALA GLY VAL THR ASP VAL LYS VAL SER ILE SER HIS ASP ASP LEU GLN ALA VAL ALA

VAL ALA VAL SER THR LYS LYS

• Molecule 2: Fatty acid synthase subunit beta

Chain G:




MET ASP ALA TYR S5 T6 R7 P8 H13 G14 S15 L16 E17 L20 L21 V22 P23 T24 A25 S26 F27 F28 L33 Q34 E35 K39 I40 L41 P42 E43 E46 G47 F48 A49 A50 D51 D52 L65 E73 P74 S75 K76 V77 G78 Q79 F80 D81 Q82 V83 L86 C87 L88
T89 E90 F91 E92 N93 L96 E97 G98 A105 E111 N112 D113 T114 T119 I123 I127 R130 I131 M132 D138 N142 E151 Q155 A158 I159 D167 V184 G185 D186 L187 D204 K207 D229 Y230 I234 P235 I236 S237 L246 K268
G269 A270 T271 S274 D287 S291 F292 F293 V296 V302 I306 N331 M338 V353 N354 K355 S358 L389 K395 A398 P399 S400 G401 L402 D403 V423 K441 K445 V448 N451 V459 T462 S472 V480 T493 T494 Q495
F496 R526 D538 E546 S552 L586 L593 M597 T598 P599 C600 T601 V602 G623 K643 L651 M658 W661 V690 E693 K701 K706 H741 S755 R759 S769 D790 L800 M806 I807 A808 V811 A817 S848
E849 M850 I854 H855 L864 F868 D869 E870 N874 F899 A905 A915 T916 M917 V922 L926 M930 L973 E992 Q993 F994 L995 N996 A997 I1000 R1023 V1048 L1054 F1103 V1109 ASP VAL GLN SER GLN VAL ASP SER SER SER VAL SER
E1122 L1142 A1143 G1144 R1150 D1162 V1182 N1188 V1201 Q1202 E1216 N1226 L1236 G1247 E1256 M1265 D1272 D1316 G1330 I1335 I1338 F1339 P1340 N1355 T1374 K1401 S1408 K1425 Y1431 H1434 I1435 K1436 D1453 D1456
L1459 L1464 E1471 K1475 S1481 S1482 T1526 V1531 L1542 P1547 F1584 W1596 D1614 M1615 V1616 V1629 I1638 K1639 T1642 V1650 L1651 I1657 T1663 F1664 V1665 F1666 T1667 S1671 Q1672 E1673 Q1674 I1711 E1739 T1740 I1741 V1742 D1743 G1744 K1745
L1746 K1747 T1748 I1751 I1755 Y1762 K1768 T1777 Q1778 P1779 K1795 T1803 F1804 A1805 E1811 V1840 D1845 E1846 L1847 G1848 N1851 I1857 R1861 V1862 A1863 A1864 S1865 Q1868 L1871 V1875 E1876 R1877 V1878 R1881 L1885 I1888 N1892 Y1898
D1903 D1908 F1916 L1919 Q1920 K1921 I1922 D1923 I1924 I1925 E1926 L1927 Q1928 K1929 S1930 L1931 S1932 L1933 E1934 E1935 V1936 E1937 L1940 F1941 E1942 I1943 I1944 D1945 E1946 A1947 S1948 K1949 K1950 S1951 A1952 V1953 K1954 P1955 R1956 P1957 L1958 K1959 L1960 E1961 R1962 G1963 F1964 V1970 G1971 K1986 P1987 Y2010
T2015 E2024 V2029 Y2030 D2031 L2032 T2033 G2034 E2040 Q2050 SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252925	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 ($e^-/Å^2$)	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	0.234	Depositor
Minimum map value	-0.108	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	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

5.1 Standard geometry

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	0.68	0/12579	0.83	2/17001 (0.0%)
1	B	0.67	0/1241	0.79	0/1675
2	G	0.64	0/16369	0.80	0/22210
All	All	0.66	0/30189	0.81	2/40886 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1515	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	1388	MET	CG-SD-CE	-5.68	91.11	100.20

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	12346	0	12279	69	0
1	B	1223	0	1265	9	0
2	G	16004	0	15984	109	0
3	G	31	0	19	4	0
All	All	29604	0	29547	178	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 3.

All (178) 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:1557:ILE:HD11	1:A:1642:THR:HG21	1.72	0.70
2:G:246:LEU:HD13	2:G:296:VAL:HG23	1.76	0.66
2:G:643:LYS:HG3	2:G:1162:ASP:O	1.95	0.66
2:G:287:ASP:OD1	2:G:291:SER:OG	2.14	0.66
2:G:1616:VAL:HG22	2:G:1650:VAL:HG21	1.78	0.65
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.32	0.65
2:G:526:ARG:NH2	2:G:546:GLU:OE2	2.32	0.60
2:G:293:PHE:HA	2:G:296:VAL:HG12	1.83	0.59
2:G:597:MET:HA	3:G:2101:FMN:N5	2.18	0.58
2:G:1638:ILE:HD13	2:G:1657:ILE:HG12	1.85	0.58
2:G:997:ALA:HA	2:G:1000:ILE:HD12	1.87	0.57
1:B:221:LEU:O	1:B:225:SER:OG	2.21	0.56
1:A:785:ASP:CG	1:A:786:SER:H	2.09	0.56
2:G:1054:LEU:HB2	3:G:2101:FMN:HM72	1.87	0.56
2:G:538:ASP:O	2:G:759:ARG:NH2	2.38	0.56
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.42	0.55
1:A:1685:TYR:OH	2:G:993:GLN:NE2	2.40	0.55
1:A:443:SER:HA	1:A:447:LEU:HD23	1.89	0.55
1:A:1431:GLU:HG3	1:A:1520:ALA:HB2	1.88	0.55
1:A:20:TYR:CD1	2:G:2033:THR:HB	2.42	0.54
2:G:355:LYS:O	2:G:358:SER:OG	2.25	0.54
1:A:1411:THR:HA	1:A:1648:GLN:O	2.08	0.54
1:A:764:ASP:OD1	1:A:810:LYS:NZ	2.41	0.54
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.89	0.54
2:G:306:ILE:HD11	2:G:480:VAL:HG22	1.89	0.53
2:G:1425:LYS:HE3	2:G:1471:GLU:OE2	2.09	0.53
1:A:1167:LEU:HD12	1:A:1171:ALA:HB1	1.91	0.52
2:G:1927:LEU:HG	2:G:1936:VAL:HG12	1.91	0.52
1:A:13:LEU:HD11	2:G:2029:VAL:HG21	1.91	0.52
1:A:719:GLN:HG3	1:A:1612:ASP:HA	1.91	0.52
1:A:1260:MET:CE	1:A:1275:LEU:HA	2.39	0.52
2:G:1878:VAL:HG22	2:G:1944:ILE:HG12	1.92	0.52
1:B:200:LYS:O	1:B:200:LYS:HD2	2.10	0.51
2:G:1811:GLU:OE1	2:G:2010:TYR:OH	2.22	0.51
1:A:1544:THR:O	1:A:1545:SER:HB3	2.11	0.51
2:G:1638:ILE:HD13	2:G:1657:ILE:CG1	2.41	0.51
2:G:1751:ILE:HG23	2:G:1840:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:LEU:HD21	1:A:1660:TYR:CE1	2.47	0.50
2:G:83:VAL:O	2:G:87:CYS:SG	2.53	0.50
2:G:905:ALA:HA	2:G:917:MET:SD	2.51	0.50
1:A:1442:ASN:ND2	1:A:1512:PHE:O	2.44	0.50
2:G:1471:GLU:N	2:G:1471:GLU:OE1	2.45	0.50
2:G:1663:THR:HA	2:G:1803:THR:O	2.11	0.50
1:A:35:PHE:CD1	2:G:1663:THR:HG21	2.47	0.49
1:A:1459:ILE:O	1:A:1463:VAL:HG23	2.13	0.49
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.46	0.49
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.13	0.49
1:B:251:GLN:O	1:B:255:GLY:HA2	2.13	0.49
2:G:13:HIS:ND1	2:G:41:LEU:HD21	2.27	0.49
2:G:600:CYS:SG	2:G:806:MET:HG2	2.53	0.49
2:G:706:LYS:NZ	3:G:2101:FMN:O2'	2.46	0.49
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.95	0.48
1:B:249:TYR:CE1	1:B:284:LYS:HD2	2.48	0.48
1:A:1285:ALA:O	1:A:1289:MET:HG3	2.13	0.48
2:G:1355:ASN:ND2	2:G:1408:SER:OG	2.45	0.48
2:G:1868:GLN:HG3	2:G:1898:TYR:OH	2.14	0.48
1:A:658:LEU:HD21	1:A:912:GLU:HB3	1.95	0.47
2:G:593:LEU:O	2:G:800:LEU:HA	2.14	0.47
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.49	0.47
2:G:1144:GLY:HA3	2:G:1150:ARG:HH21	1.79	0.47
1:A:1021:VAL:HG11	1:A:1597:LEU:HD11	1.97	0.47
2:G:1142:LEU:HD22	2:G:1182:VAL:HG11	1.96	0.47
2:G:808:ALA:HB3	2:G:811:VAL:HG23	1.96	0.47
2:G:1459:LEU:HD22	2:G:1464:LEU:HD11	1.97	0.47
2:G:597:MET:HB2	2:G:601:THR:HG23	1.97	0.47
2:G:1431:TYR:CE1	2:G:1526:THR:HG22	2.49	0.47
1:A:1343:PHE:HB3	1:A:1349:THR:HG23	1.96	0.47
2:G:1434:HIS:HB3	2:G:1436:LYS:HE3	1.97	0.47
1:A:630:ILE:O	1:A:653:ARG:NH2	2.47	0.46
1:A:1388:MET:HE3	1:A:1392:LEU:HG	1.96	0.46
1:B:142:ASP:HA	1:B:257:PRO:HG2	1.97	0.46
2:G:234:ILE:HG13	2:G:235:PRO:HD3	1.97	0.46
1:A:1682:LYS:HE3	2:G:992:GLU:O	2.16	0.45
2:G:586:LEU:HD11	2:G:701:LYS:HD2	1.98	0.45
2:G:462:THR:HA	2:G:493:THR:HG21	1.96	0.45
3:G:2101:FMN:O4'	3:G:2101:FMN:H9	2.15	0.45
1:A:52:THR:CG2	2:G:1667:THR:HG23	2.46	0.45
2:G:602:VAL:HG11	2:G:623:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1335:ILE:O	2:G:1338:ILE:HG12	2.16	0.45
2:G:338:MET:HE2	2:G:423:VAL:HG21	1.99	0.45
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.15	0.45
1:A:1825:VAL:HG11	1:A:1858:ALA:HB1	1.99	0.45
1:A:449:LYS:HE2	1:A:1568:GLU:HB3	1.98	0.45
1:A:850:PHE:HZ	1:A:866:GLY:HA3	1.82	0.45
2:G:1547:PRO:HD3	2:G:1584:PHE:CZ	2.52	0.45
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.80	0.45
1:A:996:LYS:HB2	1:A:1001:VAL:HG13	1.99	0.44
1:B:254:TRP:HE1	1:B:288:ASP:HA	1.82	0.44
2:G:159:ILE:HA	2:G:271:THR:O	2.17	0.44
2:G:270:ALA:O	2:G:459:VAL:HA	2.17	0.44
2:G:302:VAL:HG23	2:G:448:VAL:HG11	1.99	0.44
2:G:817:ALA:HA	2:G:1048:VAL:HG21	1.99	0.44
1:A:1592:MET:HE2	1:A:1641:ILE:HG23	1.99	0.44
2:G:441:LYS:O	2:G:445:LYS:HD3	2.18	0.44
1:A:754:ASP:O	1:A:762:GLY:N	2.50	0.44
2:G:651:LEU:HD22	2:G:658:MET:SD	2.57	0.44
1:A:776:GLU:HB3	1:A:779:ILE:HD12	1.99	0.44
1:A:1212:THR:OG1	1:A:1283:MET:HG3	2.18	0.44
1:A:1535:ASP:OD1	1:A:1637:ARG:NH1	2.49	0.44
2:G:598:THR:HA	2:G:599:PRO:HA	1.75	0.44
1:A:19:ALA:O	1:A:22:PHE:HB3	2.18	0.44
2:G:1614:ASP:HB3	2:G:1650:VAL:HG23	1.99	0.44
2:G:1542:LEU:HD11	2:G:1596:TRP:CD1	2.53	0.44
2:G:1986:LYS:HB3	2:G:1987:PRO:HD3	1.99	0.44
1:A:691:GLU:HB2	1:A:902:ALA:HB2	2.00	0.44
2:G:926:LEU:HD22	2:G:930:MET:CE	2.48	0.44
1:A:27:ARG:HH21	2:G:2015:THR:HA	1.82	0.43
1:A:1811:GLY:HA2	1:A:1878:ALA:HB1	2.00	0.43
2:G:230:TYR:CZ	2:G:236:ILE:HD11	2.52	0.43
2:G:234:ILE:N	2:G:235:PRO:CD	2.81	0.43
2:G:1236:LEU:HB2	2:G:1265:MET:HG3	2.00	0.43
2:G:1672:GLN:HG3	2:G:1777:THR:HG23	2.00	0.43
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.53	0.43
2:G:864:LEU:HD23	2:G:899:PHE:HB2	2.00	0.43
2:G:1857:ILE:HG21	2:G:1871:LEU:HD11	2.01	0.43
2:G:1475:LYS:HB2	2:G:1481:SER:HB3	2.00	0.43
2:G:204:ASP:OD1	2:G:207:LYS:HD3	2.19	0.43
2:G:1861:ARG:NH2	2:G:1964:PHE:O	2.52	0.43
2:G:155:GLN:HG3	2:G:268:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ALA:O	1:A:670:GLY:HA2	2.19	0.43
1:A:1189:ILE:H	1:A:1380:GLN:HE21	1.67	0.43
1:A:1474:ALA:HB2	1:A:1486:LEU:HD21	2.01	0.43
2:G:88:LEU:HD21	2:G:130:ARG:HD2	2.00	0.43
2:G:1629:VAL:HG11	2:G:1639:LYS:HG2	2.01	0.43
2:G:158:ALA:O	2:G:270:ALA:HA	2.18	0.43
1:A:1464:GLU:HG3	1:A:1773:VAL:HG22	2.00	0.42
1:A:1713:ASP:HB3	1:A:1738:ILE:HG21	2.01	0.42
1:A:56:MET:HE3	2:G:1892:ASN:HB3	2.01	0.42
1:B:223:LYS:HE2	1:B:223:LYS:HA	2.01	0.42
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.94	0.42
1:A:1686:LYS:HD2	2:G:915:ALA:HB1	2.01	0.42
1:B:268:ALA:HA	1:B:290:MET:SD	2.59	0.42
2:G:123:ILE:O	2:G:127:ILE:HG12	2.19	0.42
1:A:27:ARG:NH2	2:G:2032:LEU:HD21	2.34	0.42
1:A:413:LEU:HD23	1:A:450:PHE:CE2	2.55	0.42
2:G:353:VAL:HG12	2:G:389:LEU:HD11	2.01	0.42
1:A:389:GLY:O	1:A:738:ASN:ND2	2.48	0.42
2:G:1531:VAL:HG11	2:G:1795:LYS:HA	2.01	0.42
2:G:915:ALA:HA	2:G:1000:ILE:HD11	2.02	0.42
2:G:1755:ILE:HD11	2:G:1762:TYR:CG	2.55	0.42
1:A:496:PRO:HG2	1:A:519:VAL:HG12	2.02	0.42
2:G:1642:THR:HB	2:G:1651:LEU:HB3	2.02	0.42
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	2.02	0.42
1:A:704:VAL:HG23	1:A:763:TRP:CZ3	2.55	0.42
1:A:768:ILE:HD11	1:A:806:VAL:HG21	2.02	0.42
1:A:823:ILE:HD13	1:A:865:CYS:HB3	2.02	0.42
2:G:741:HIS:CD2	2:G:855:HIS:ND1	2.87	0.42
2:G:926:LEU:HD22	2:G:930:MET:HE1	2.02	0.42
1:A:865:CYS:SG	1:A:908:LEU:HD13	2.60	0.41
1:A:406:TRP:CD2	1:A:1619:GLU:HG3	2.55	0.41
1:A:705:VAL:HG12	1:A:732:LEU:HD11	2.02	0.41
2:G:1674:GLN:NE2	2:G:1711:ILE:O	2.52	0.41
2:G:92:GLU:HA	2:G:96:LEU:HB2	2.03	0.41
2:G:690:VAL:O	2:G:693:GLU:HG3	2.20	0.41
1:A:1260:MET:HE2	1:A:1275:LEU:HA	2.02	0.41
1:B:161:LYS:HB2	1:B:166:ILE:HD11	2.02	0.41
2:G:494:THR:HA	2:G:496:PHE:CE2	2.55	0.41
2:G:1103:PHE:O	2:G:1247:GLY:HA3	2.21	0.41
2:G:187:LEU:HD11	2:G:296:VAL:HG21	2.03	0.41
1:A:36:LEU:O	1:A:76:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:870:GLU:O	2:G:874:ASN:ND2	2.53	0.41
2:G:658:MET:HA	2:G:661:TRP:NE1	2.36	0.41
2:G:922:VAL:HG21	2:G:995:LEU:HD11	2.02	0.41
2:G:1875:VAL:HG21	2:G:1888:ILE:HD11	2.02	0.41
1:A:1127:VAL:CG2	1:A:1173:LEU:HD13	2.50	0.41
2:G:105:ALA:HB1	2:G:119:THR:CG2	2.51	0.41
2:G:1201:VAL:HG11	2:G:1226:ASN:HB2	2.02	0.41
1:A:1021:VAL:HG11	1:A:1597:LEU:CD1	2.51	0.40
1:A:1471:LYS:HB2	1:A:1756:ILE:HD11	2.03	0.40
1:A:1462:TRP:CH2	1:A:1466:GLU:HG3	2.56	0.40
2:G:234:ILE:HA	2:G:237:SER:OG	2.21	0.40
1:A:353:ASP:HB3	1:A:356:ASN:HB2	2.03	0.40
1:A:1067:LEU:HD23	1:A:1083:PRO:HG3	2.04	0.40
2:G:184:VAL:O	2:G:187:LEU:N	2.54	0.40
2:G:1885:LEU:O	2:G:1903:ASP:N	2.53	0.40
1:A:1125:VAL:HG11	1:A:1175:ILE:HD12	2.03	0.40
2:G:755:SER:O	2:G:759:ARG:HG2	2.21	0.40
2:G:973:LEU:HD23	2:G:973:LEU:HA	1.95	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%)	1514 (96%)	53 (3%)	2 (0%)	48 77
1	B	161/1887 (8%)	145 (90%)	14 (9%)	2 (1%)	11 34
2	G	2030/2051 (99%)	1921 (95%)	103 (5%)	6 (0%)	37 67
All	All	3760/5825 (64%)	3580 (95%)	170 (4%)	10 (0%)	38 67

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1545	SER
1	A	1585	LYS
1	B	275	ALA
2	G	274	SER
2	G	769	SER
2	G	1162	ASP
2	G	1482	SER
2	G	2034	GLY
1	B	195	GLY
2	G	185	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	1336/1566 (85%)	1332 (100%)	4 (0%)	91 97
1	B	135/1566 (9%)	131 (97%)	4 (3%)	36 70
2	G	1773/1789 (99%)	1767 (100%)	6 (0%)	91 97
All	All	3244/4921 (66%)	3230 (100%)	14 (0%)	88 96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	ARG
1	A	1096	SER
1	A	1327	CYS
1	A	1333	ASP
1	B	192	LYS
1	B	200	LYS
1	B	236	LYS
1	B	237	MET
2	G	1023	ARG
2	G	1202	GLN
2	G	1401	LYS
2	G	1942	GLU
2	G	1946	GLU

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Mol	Chain	Res	Type
2	G	1962	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	379	ASN
1	A	524	GLN
1	A	989	GLN
1	A	1272	ASN
1	A	1380	GLN
1	A	1563	HIS
1	A	1695	ASN
1	A	1758	ASN
1	A	1780	ASN
1	B	214	GLN
1	B	251	GLN
2	G	93	ASN
2	G	346	GLN
2	G	354	ASN
2	G	440	ASN
2	G	715	GLN
2	G	718	ASN
2	G	747	HIS
2	G	993	GLN
2	G	1088	GLN
2	G	1217	ASN
2	G	1241	ASN
2	G	1352	HIS
2	G	1355	ASN
2	G	1564	HIS
2	G	1581	HIS
2	G	1595	ASN
2	G	1851	ASN
2	G	1872	GLN
2	G	1890	ASN

5.3.3 RNA

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)

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	1.28	3 (9%)	48,50,50	1.15	5 (10%)

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	-	-	5/18/18/18	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2101	FMN	C9A-C5A	3.96	1.47	1.41
3	G	2101	FMN	C5A-N5	-2.77	1.34	1.39
3	G	2101	FMN	C8-C7	2.45	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2101	FMN	C4-C4A-N5	3.10	122.65	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2101	FMN	C4A-C10-N10	2.53	120.18	116.48
3	G	2101	FMN	C10-N1-C2	2.36	121.62	116.90
3	G	2101	FMN	C4A-C10-N1	-2.26	119.50	124.73
3	G	2101	FMN	C10-C4A-N5	-2.07	120.46	124.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2101	FMN	C2'-C3'-C4'-C5'
3	G	2101	FMN	O3'-C3'-C4'-C5'
3	G	2101	FMN	O3'-C3'-C4'-O4'
3	G	2101	FMN	C2'-C3'-C4'-O4'
3	G	2101	FMN	C4'-C5'-O5'-P

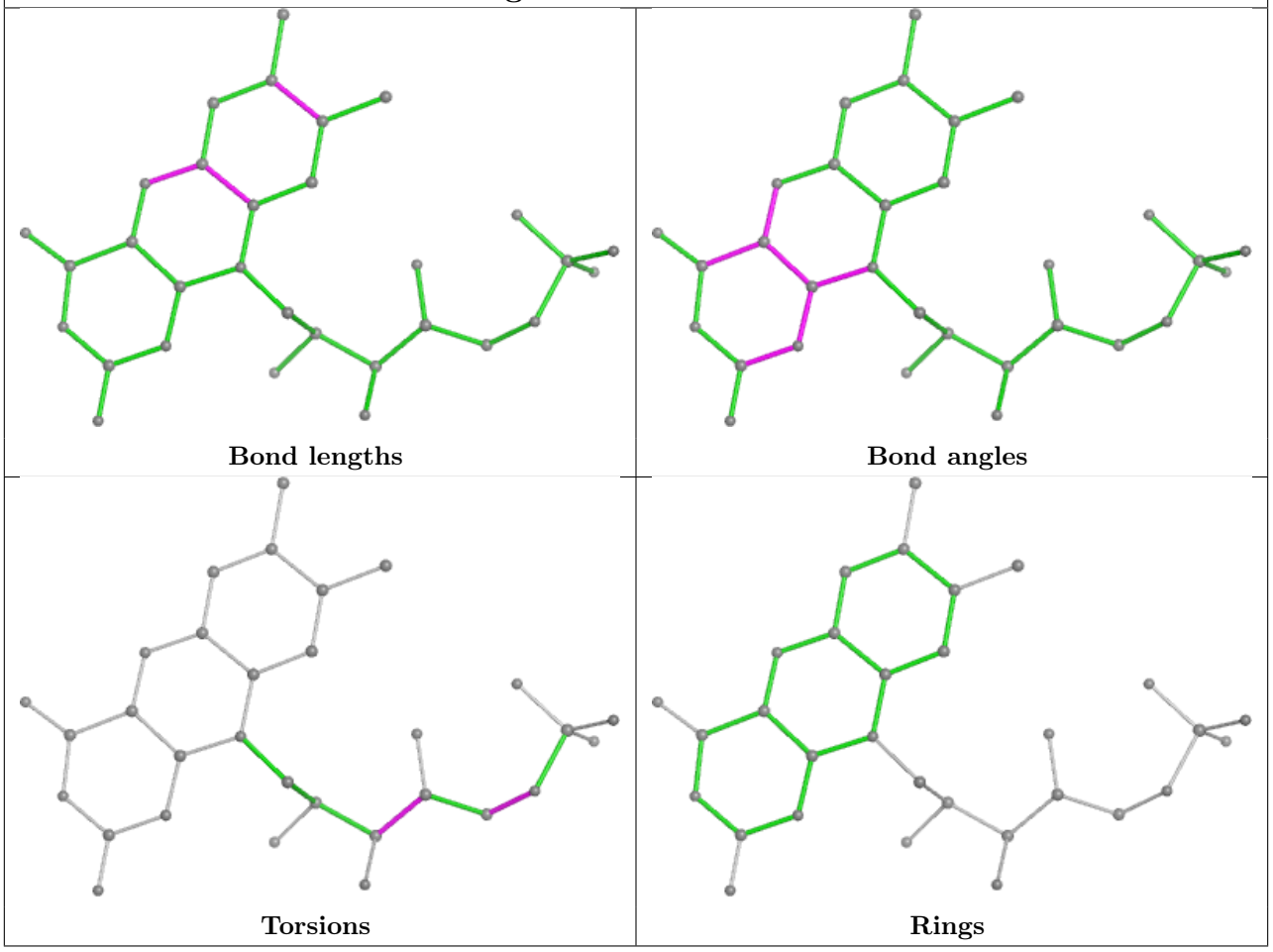
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2101	FMN	4	0

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

Ligand FMN G 2101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

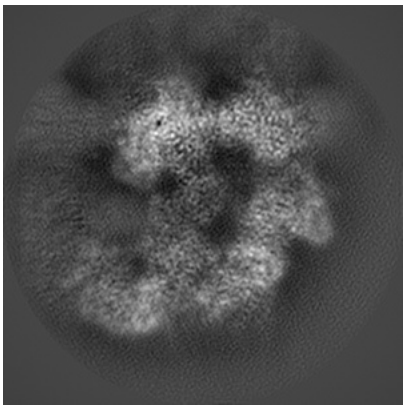
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17854. These allow visual inspection of the internal detail of the map and identification of artifacts.

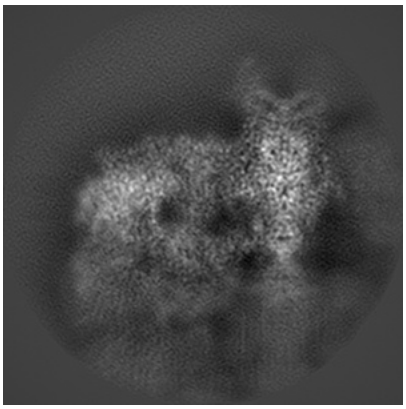
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

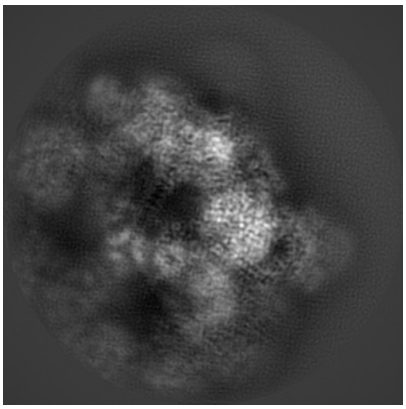
6.1.1 Primary map



X

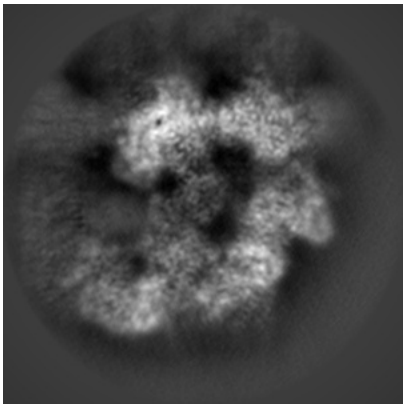


Y

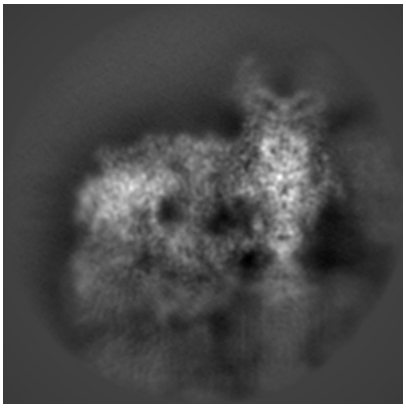


Z

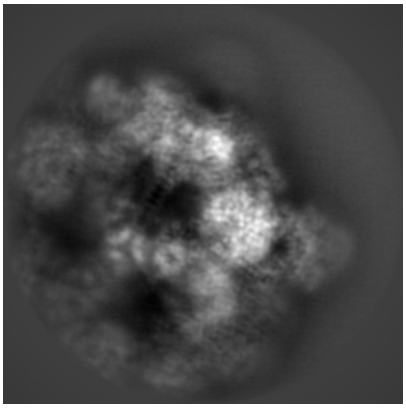
6.1.2 Raw map



X



Y

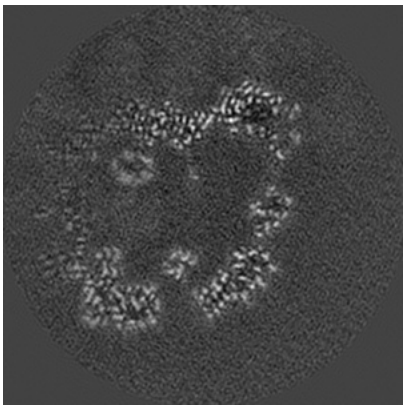


Z

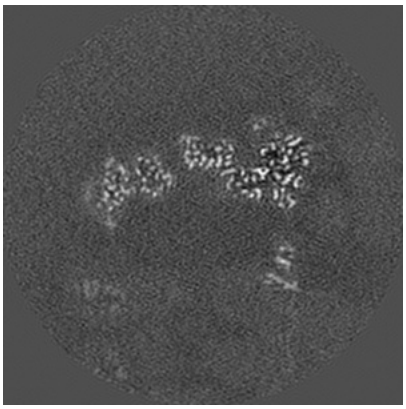
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

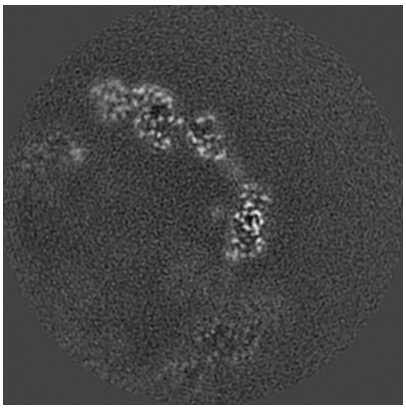
6.2.1 Primary map



X Index: 120

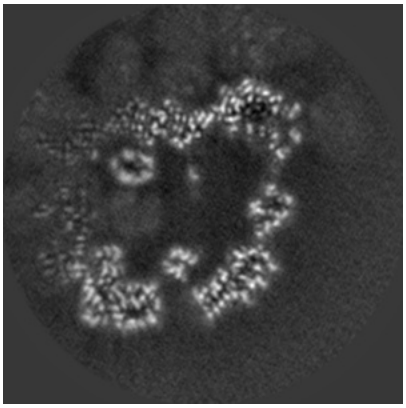


Y Index: 120

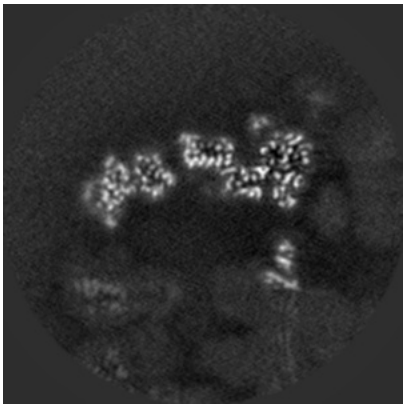


Z Index: 120

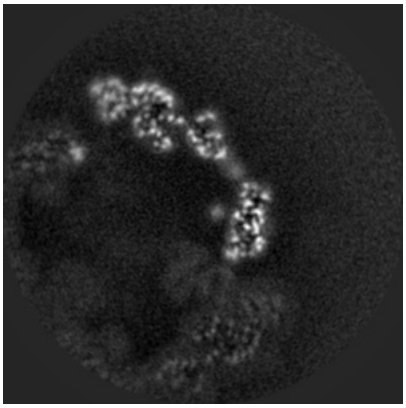
6.2.2 Raw map



X Index: 120



Y Index: 120

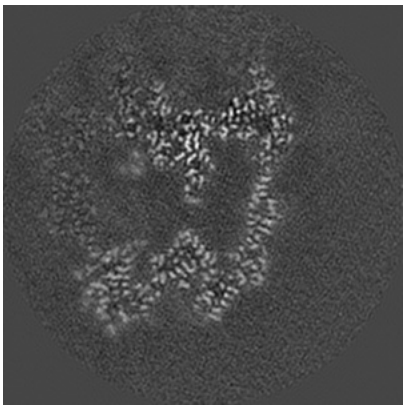


Z Index: 120

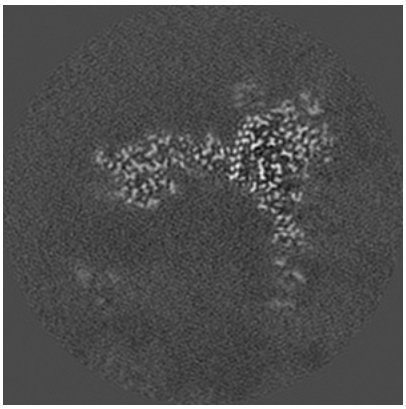
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

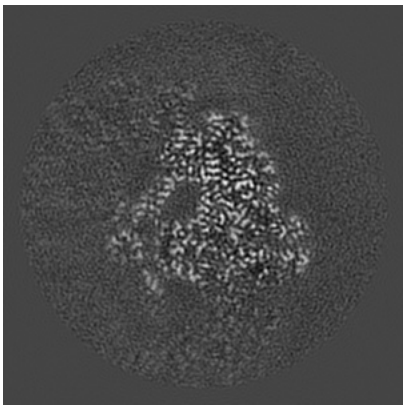
6.3.1 Primary map



X Index: 129

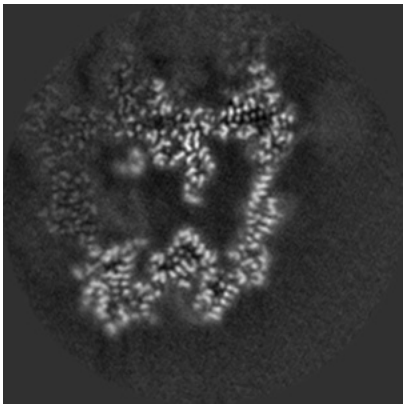


Y Index: 107

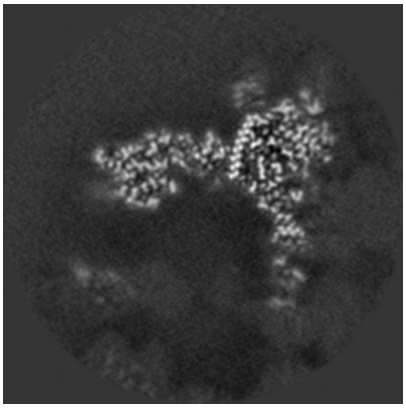


Z Index: 171

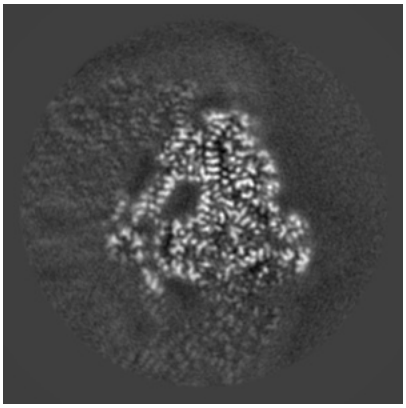
6.3.2 Raw map



X Index: 129



Y Index: 107

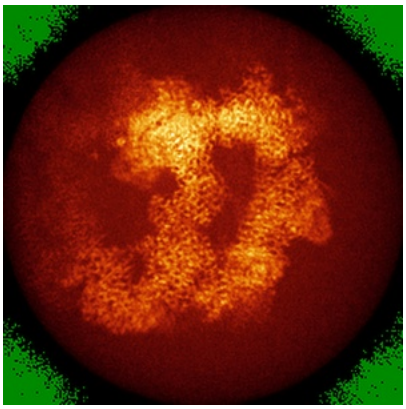


Z Index: 171

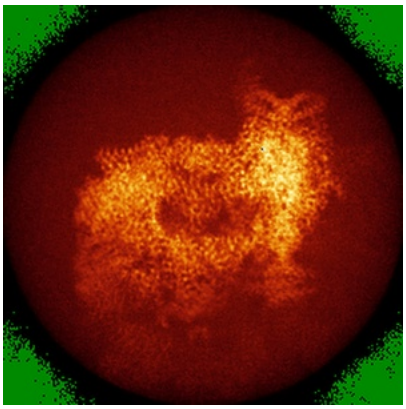
The images above show the largest variance slices of the map in three orthogonal directions.

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

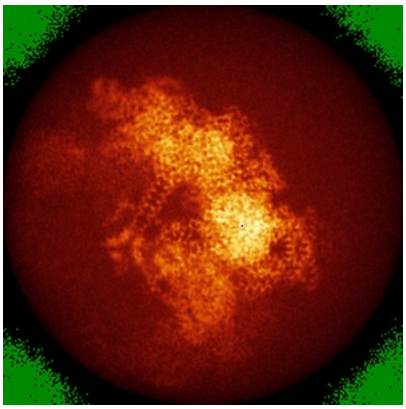
6.4.1 Primary map



X

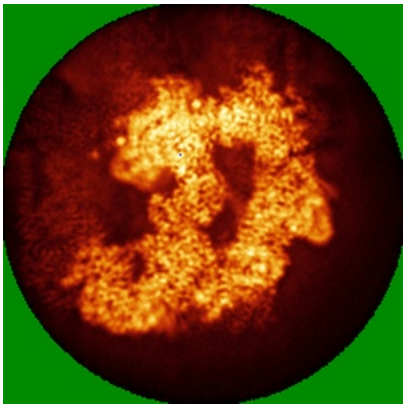


Y

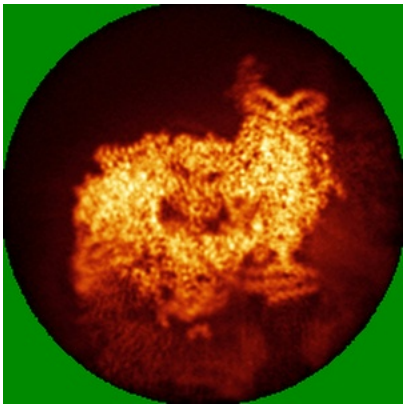


Z

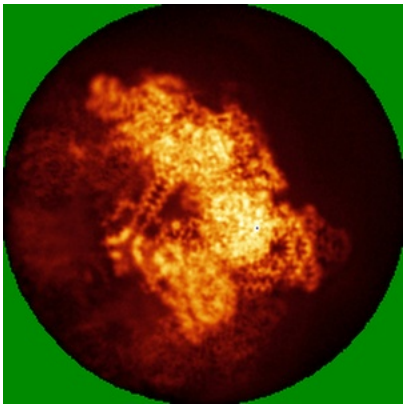
6.4.2 Raw map



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.

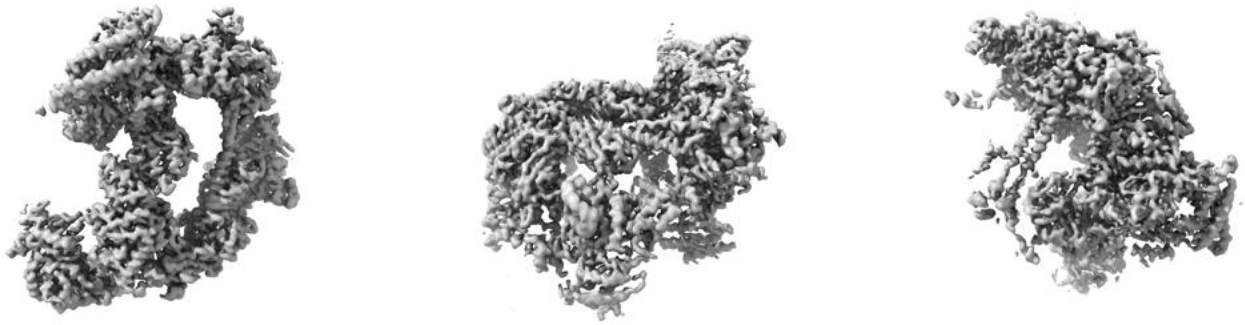
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

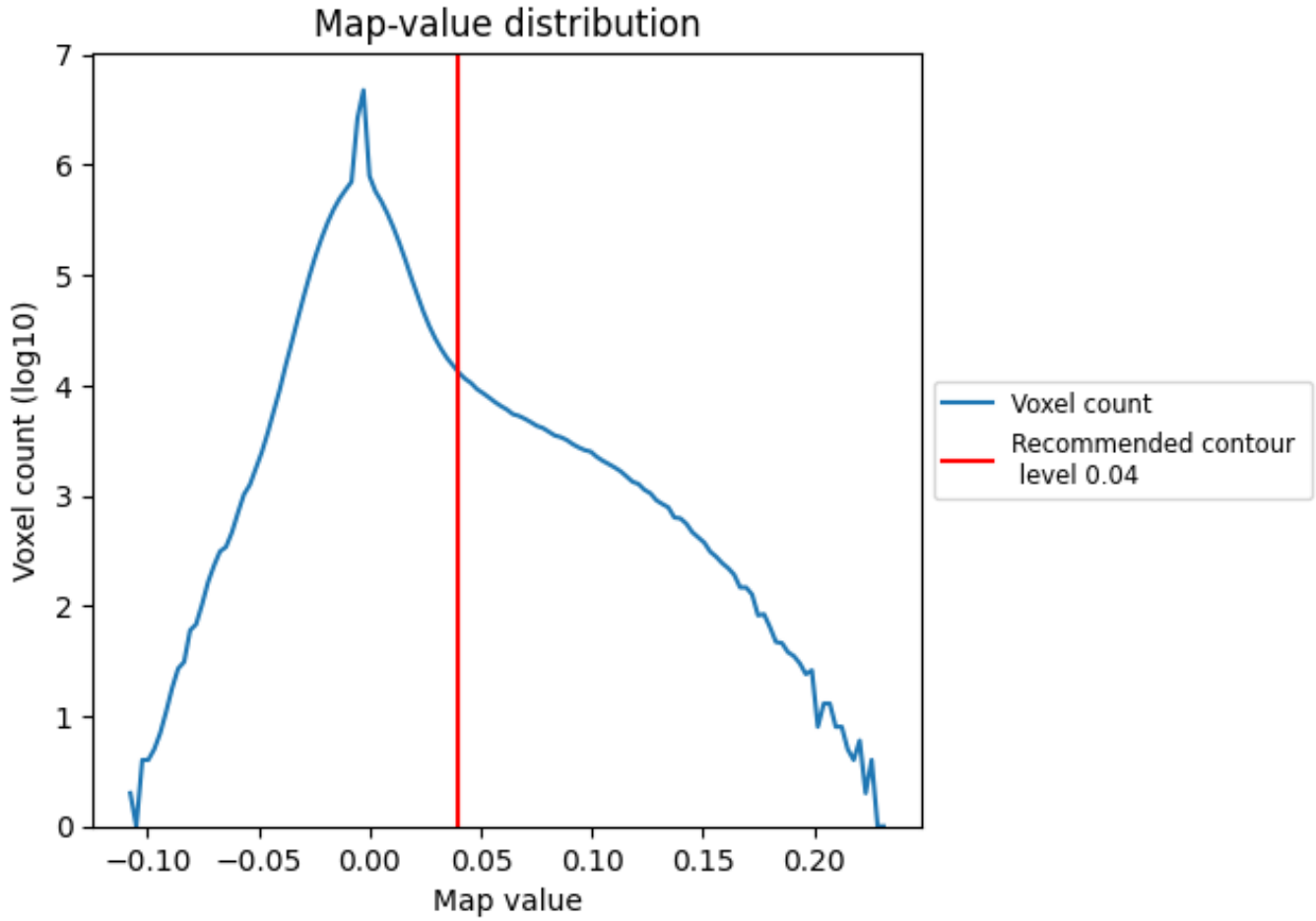
6.6 Mask visualisation (i)

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

7 Map analysis

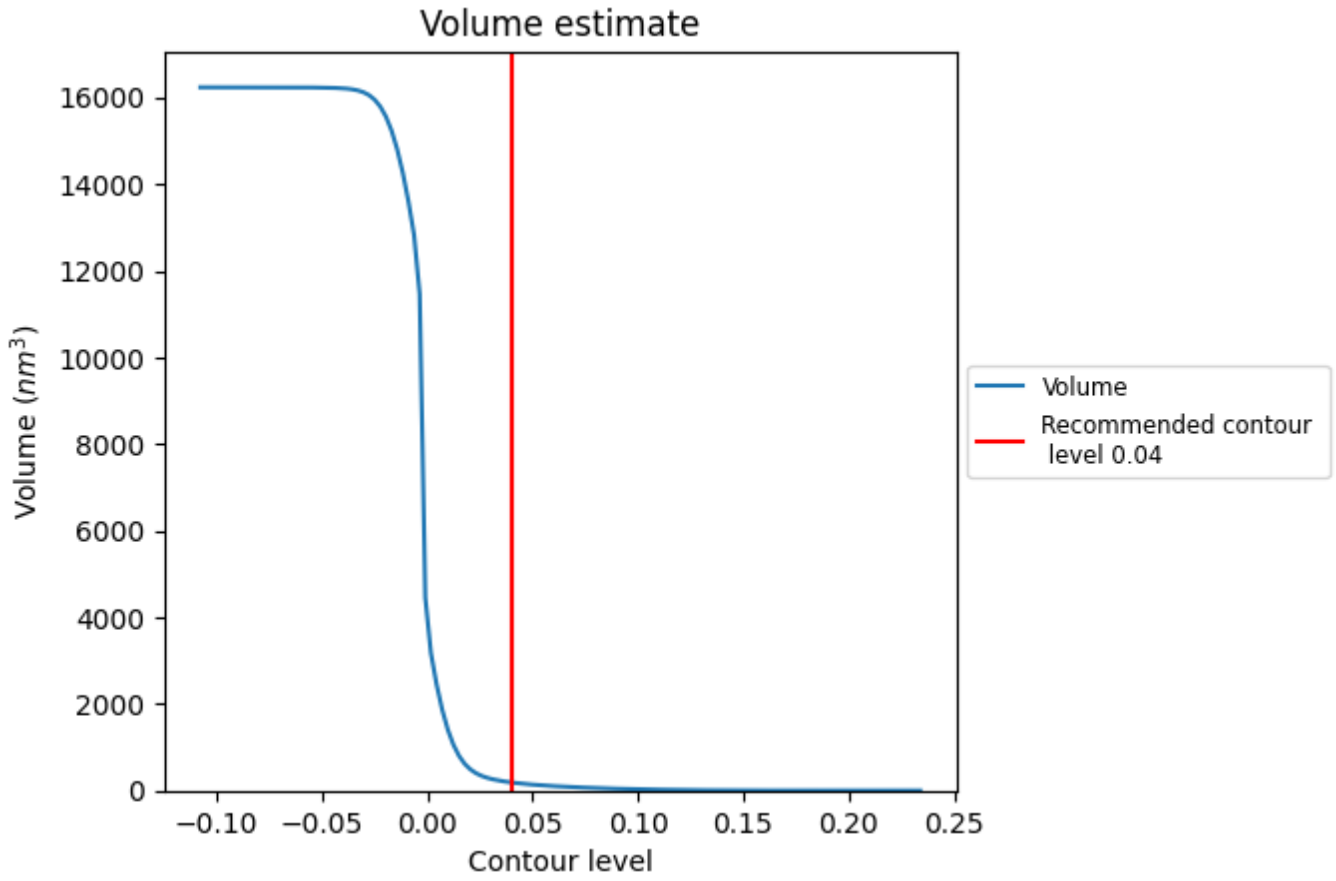
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

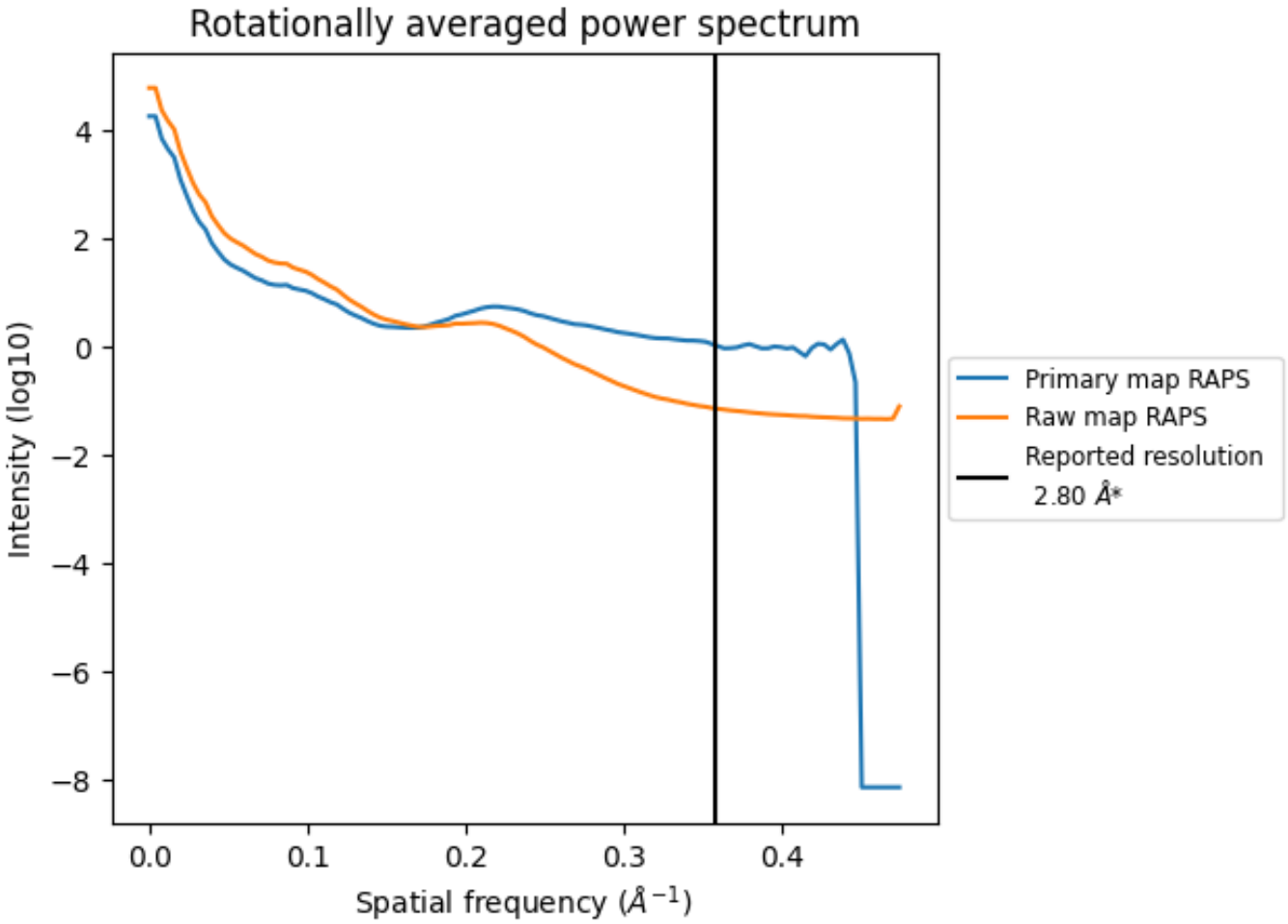
7.2 Volume estimate



The volume at the recommended contour level is 186 nm^3; this corresponds to an approximate mass of 168 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)

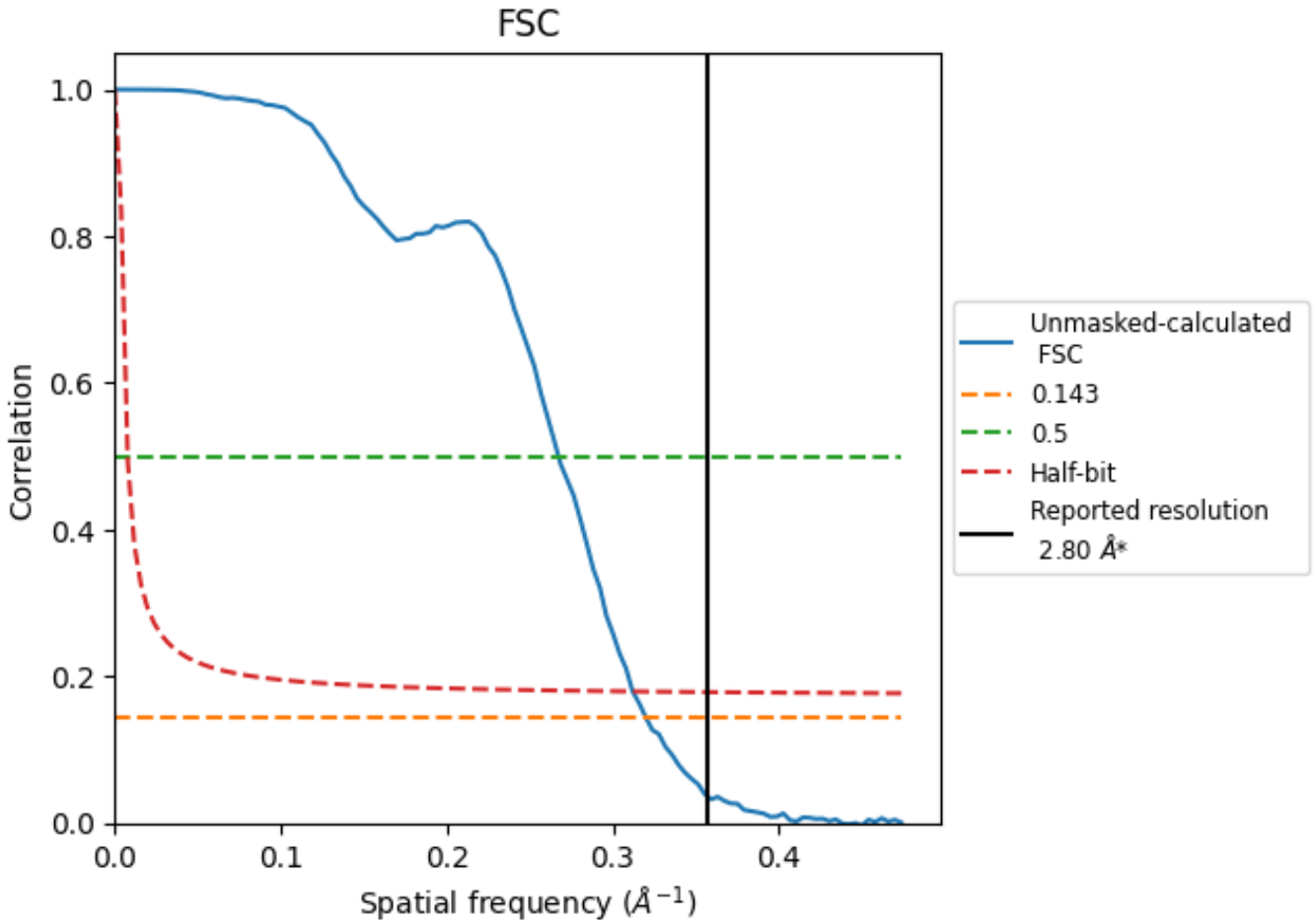


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

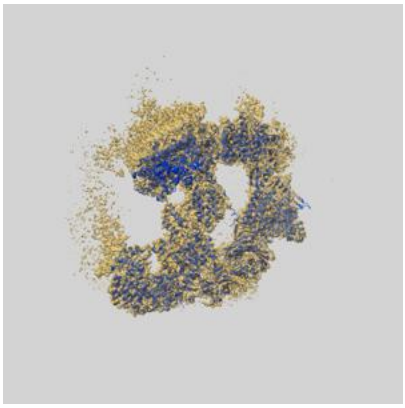
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.74	3.21

*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 3.12 differs from the reported value 2.8 by more than 10 %

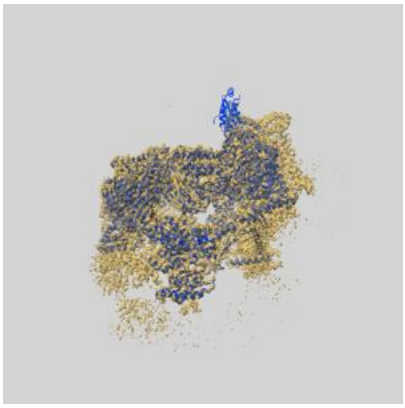
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17854 and PDB model 8PSK. Per-residue inclusion information can be found in section 3 on page 4.

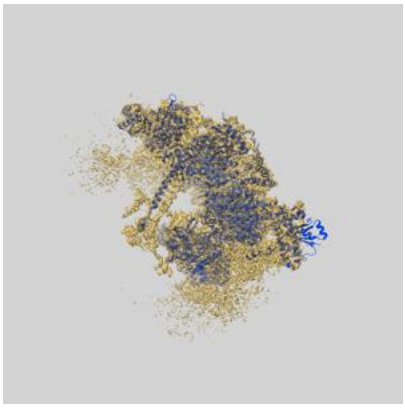
9.1 Map-model overlay



X



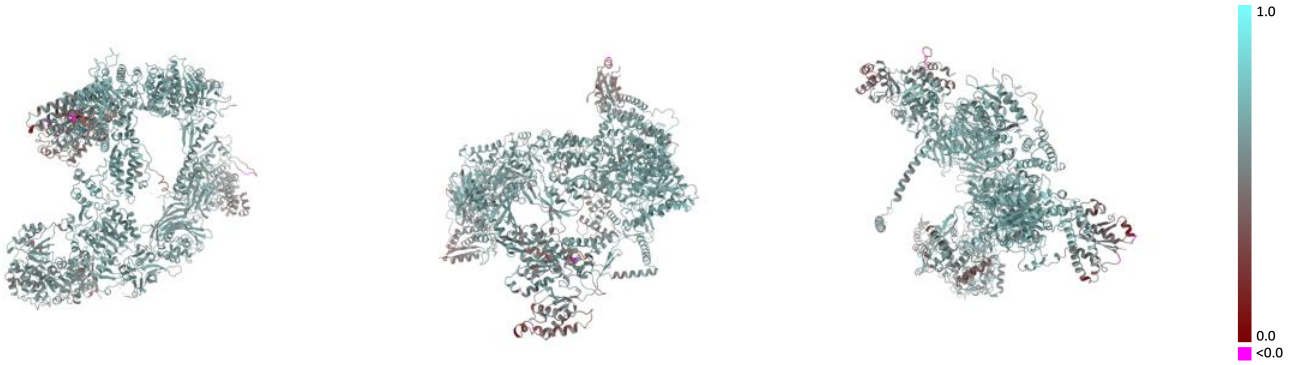
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

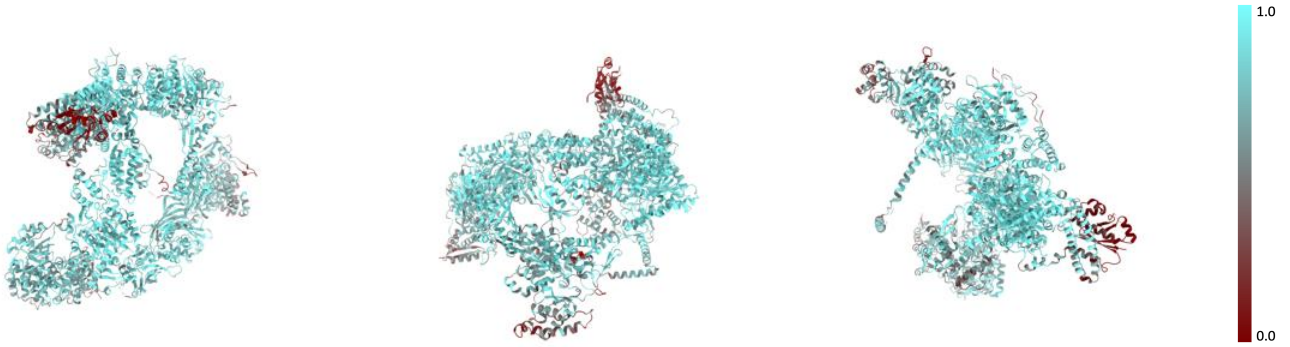
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

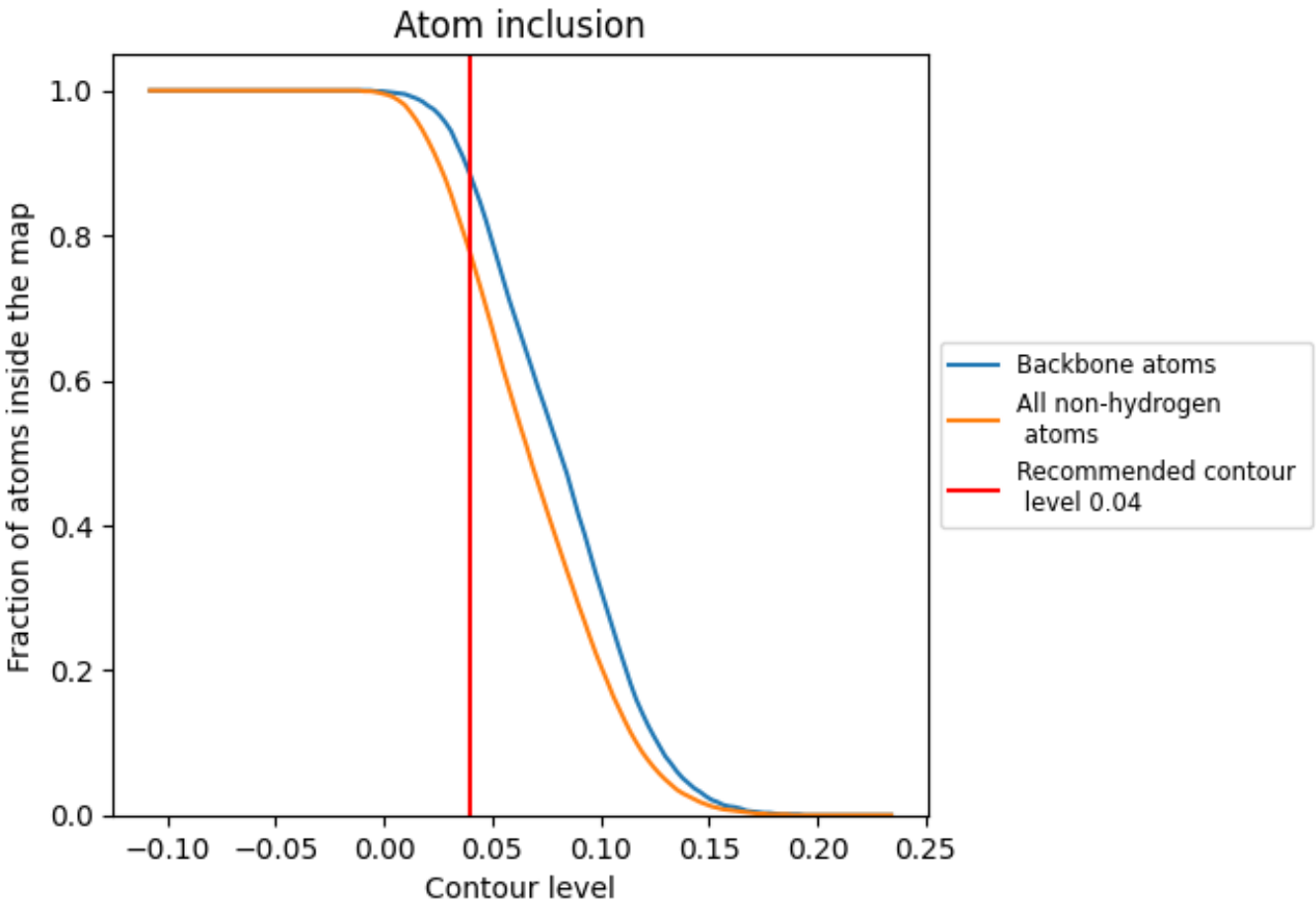
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 77% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.5780
A	0.7840	0.5980
B	0.5730	0.4710
G	0.7810	0.5700