Full wwPDB EM Validation Report ⓘ

Nov 15, 2023 – 03:39 am GMT

PDB ID	:	8PRV
EMDB ID	:	EMD-17839
Title	:	Asymmetric unit of the yeast fatty acid synthase in the non-rotated state with ACP at the ketosreductase domain (FASamn sample)
Authors	:	Singh, K.; Bunzel, G.; Graf, B.; Yip, K.M.; Stark, H.; Chari, A.
Deposited on	:	2023-07-12
Resolution	:	2.90 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:

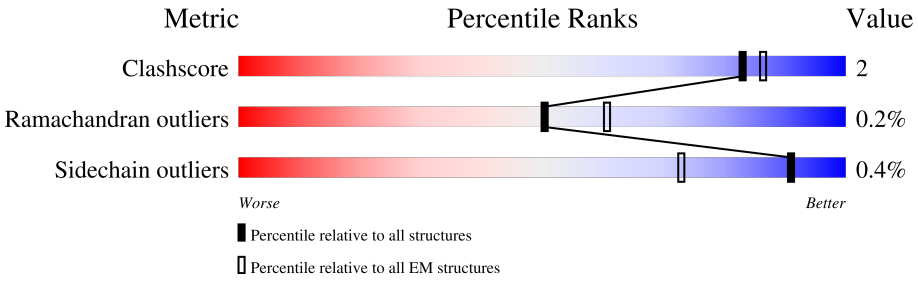
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	78% 5% 16%
1	B	1887	8% 91%
2	G	2051	91% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29814 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.

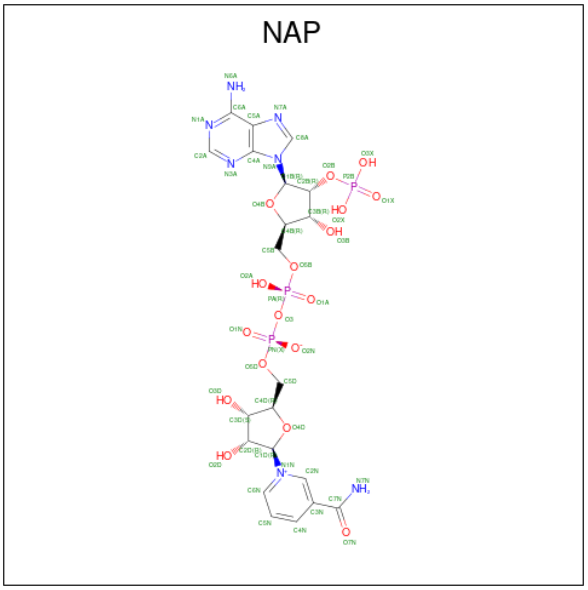
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1584	Total	C	N	O	S	0	0
			12379	7837	2089	2405	48		
1	B	163	Total	C	N	O	S	0	0
			1222	775	205	239	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
			16010	10261	2661	3032	56		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	

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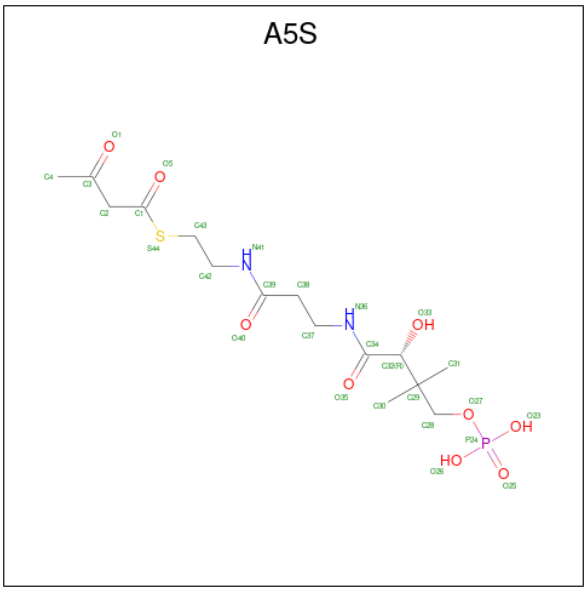
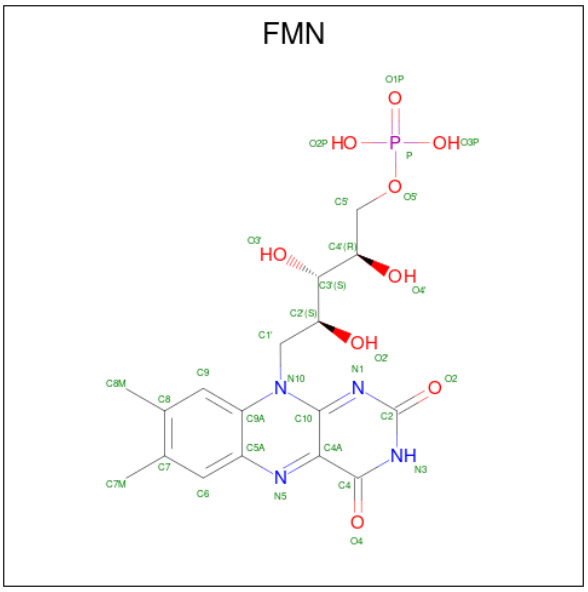
Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 4 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] 3-oxidanylidenebutanethioate (three-letter code: A5S) (formula: $C_{15}H_{27}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



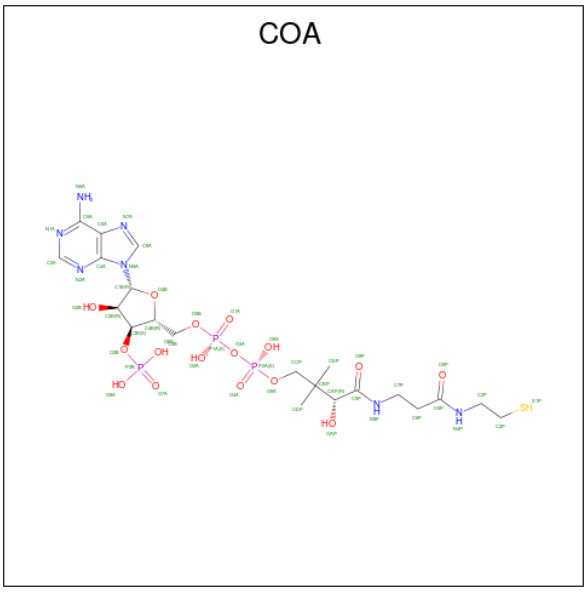
Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	N	O	P	S	0
			28	15	2	9	1	1	

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



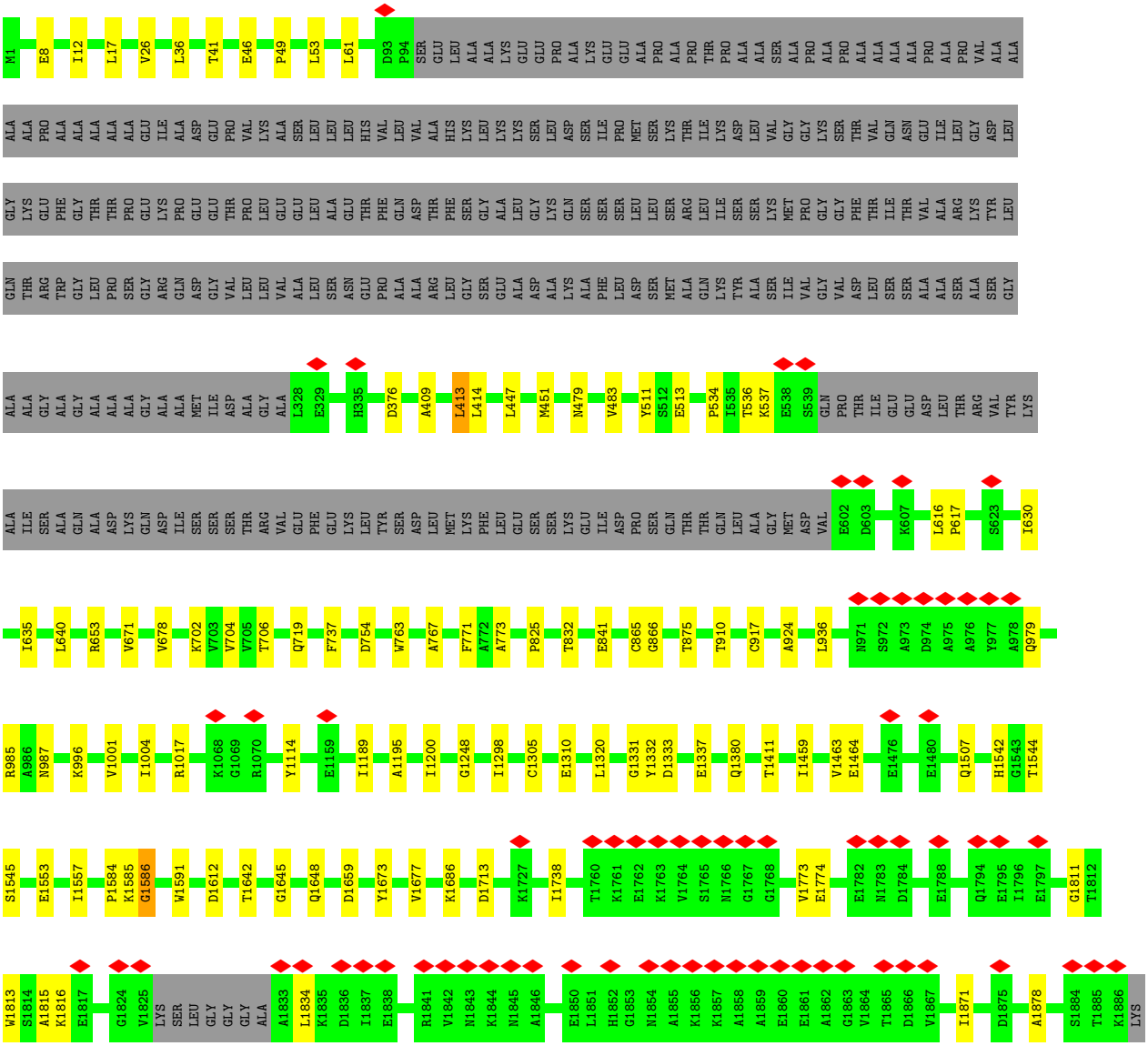
Mol	Chain	Residues	Atoms						AltConf
6	G	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

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.

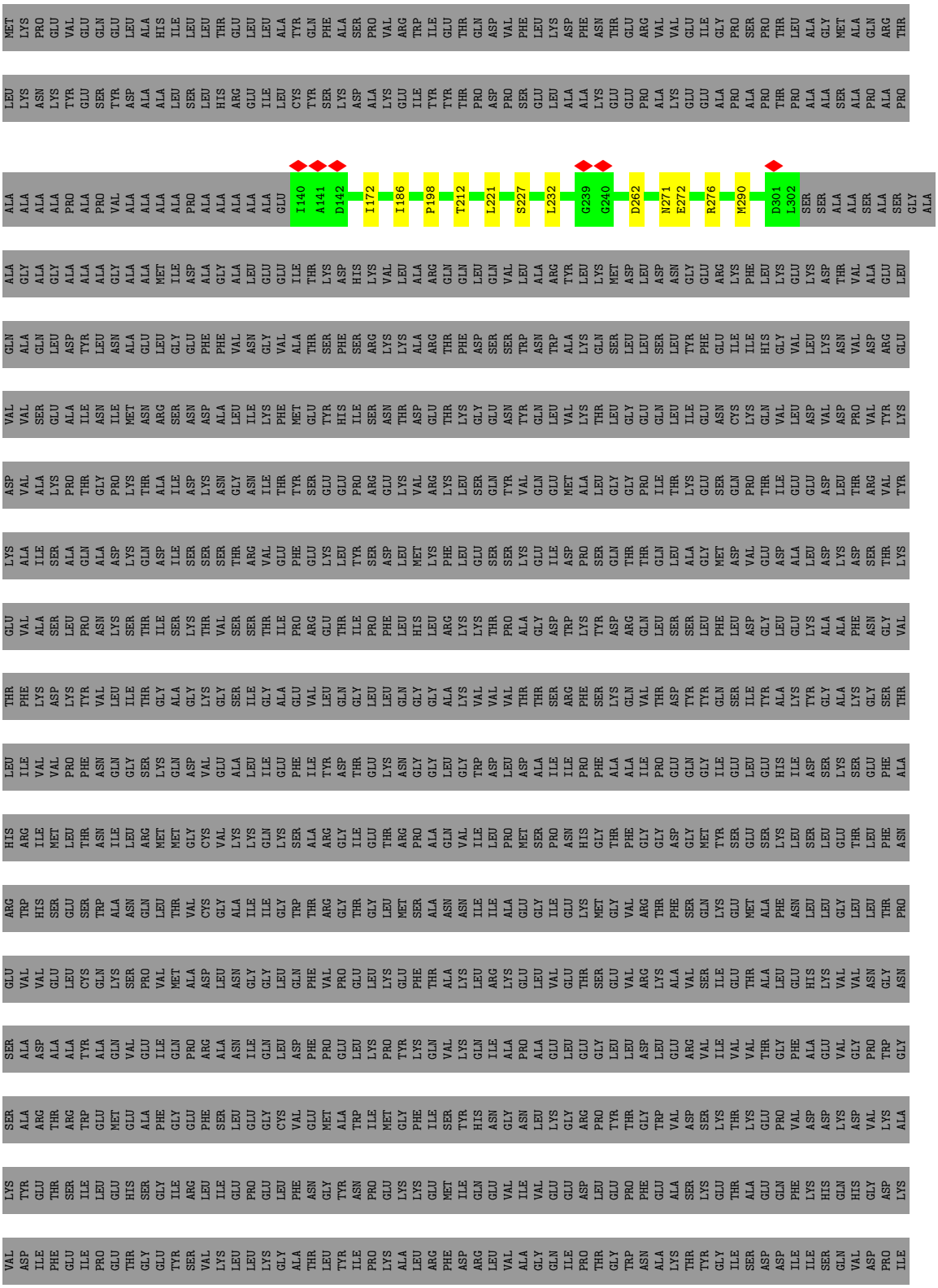
- Molecule 1: Fatty acid synthase subunit alpha

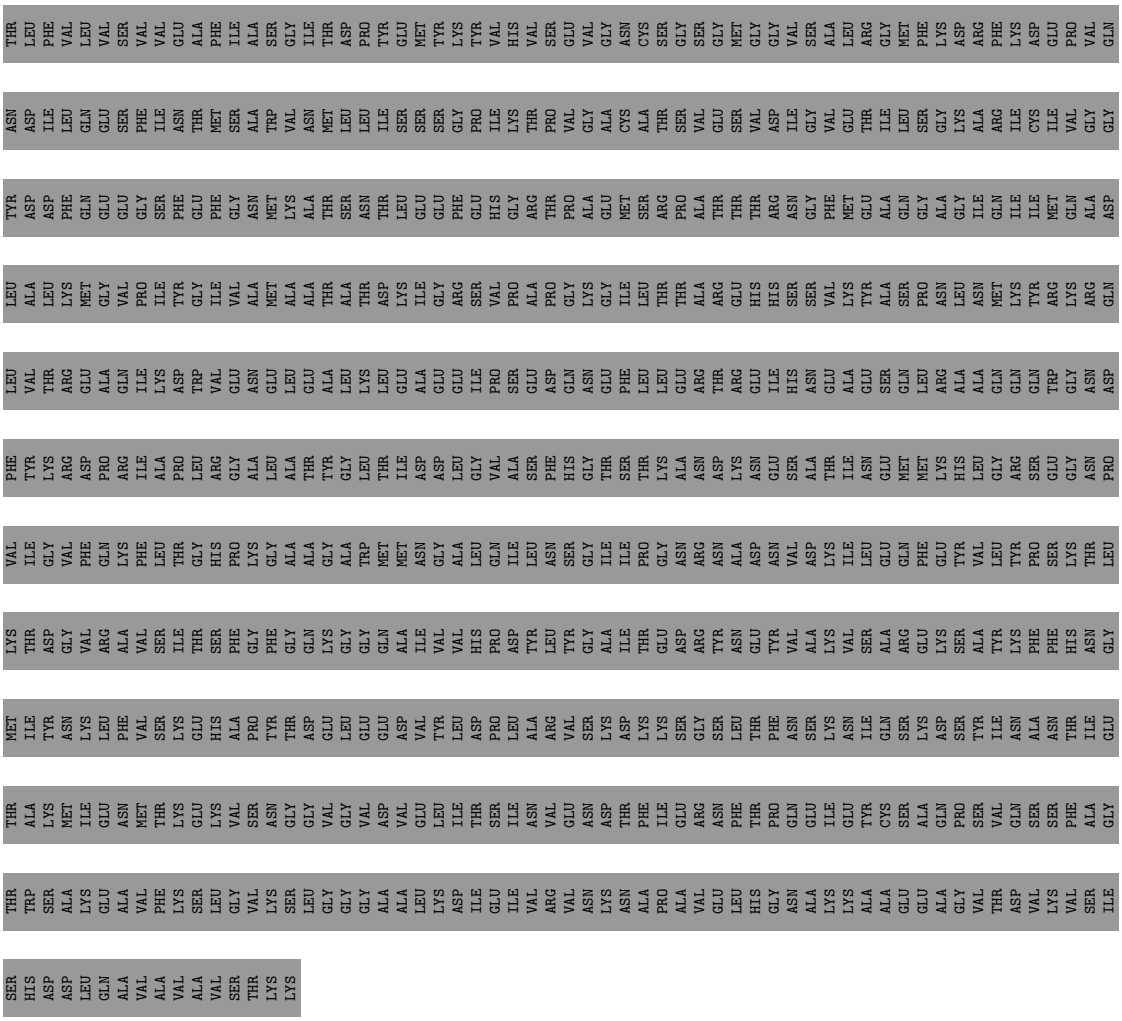
Chain A:



• Molecule 1: Fatty acid synthase subunit alpha

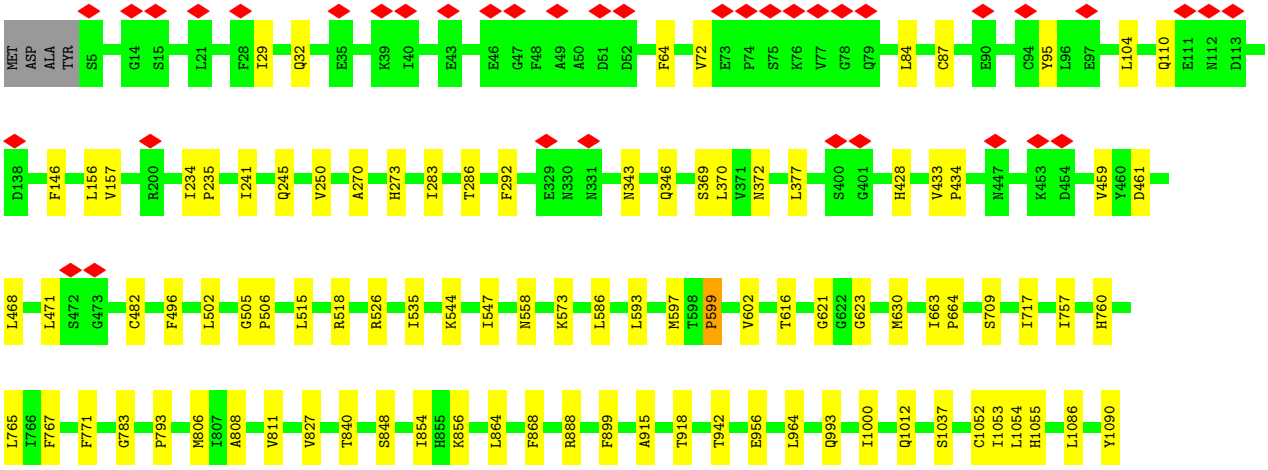
Chain B: 8% 91%

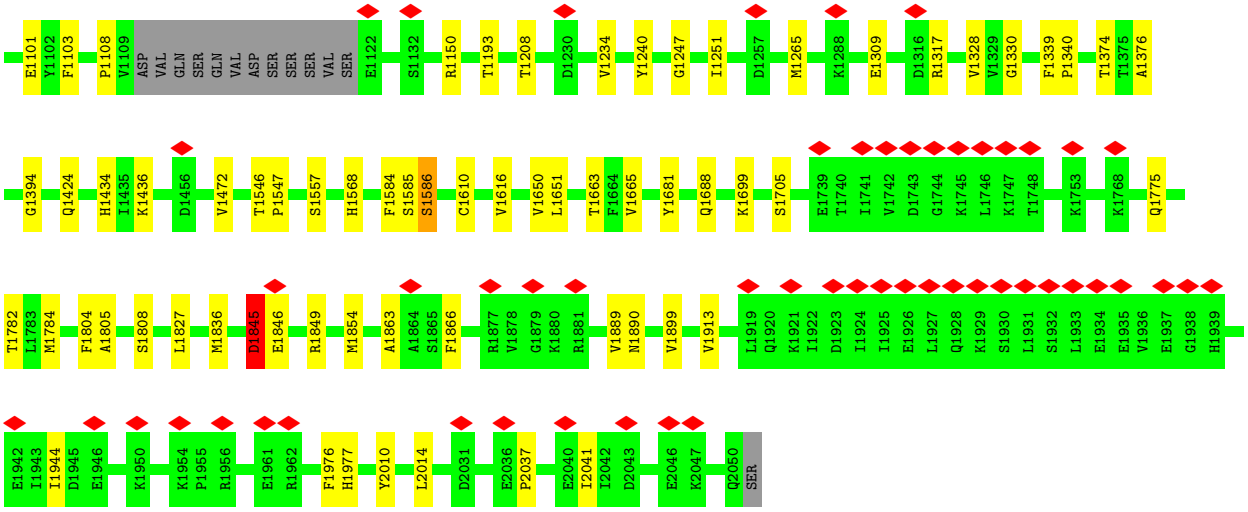




• Molecule 2: Fatty acid synthase subunit beta

Chain G:




E1101 Y1102 F1103 P1108 V1109 ASP VAL GLN SER GLN VAL ASP SER SER SER VAL SER E1122 S1132 R1150 T1193 T1208 D1230 V1234 Y1240 G1247 I1251 D1257 M1265 K1288 E1309 D1316 R1317 V1328 V1329 G1330 F1339 P1340 T1374 T1375 A1376
G1394 Q1424 H1434 I1435 K1436 D1456 V1472 T1546 P1547 S1557 H1568 F1584 S1585 S1586 C1610 V1616 V1650 L1651 T1663 F1664 V1665 Y1681 Q1688 K1699 S1705 E1739 T1740 I1741 V1742 D1743 G1744 K1745 L1746 K1747 T1748 K1753 K1768 Q1775
T1782 L1783 M1784 F1804 A1805 S1808 L1827 M1836 D1845 E1846 R1849 M1854 A1863 A1864 S1865 F1866 R1877 V1878 G1879 K1880 R1881 V1889 N1890 V1899 V1913 L1919 Q1920 K1921 I1922 D1923 I1924 I1925 E1926 L1927 Q1928 K1929 S1930 L1931 S1932 L1933 E1934 E1935 V1936 E1937 G1938 H1939
E1942 I1943 I1944 D1945 E1946 K1950 K1954 P1955 R1956 E1961 R1962 F1976 H1977 Y2010 L2014 D2031 E2036 P2037 E2040 I2041 I2042 D2043 E2046 K2047 Q2050 SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83949	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	0.312	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	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: NAP, COA, FMN, J8W, A5S

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	0.70	2/12613 (0.0%)	0.86	0/17048
1	B	0.72	0/1240	0.80	0/1674
2	G	0.68	2/16362 (0.0%)	0.84	4/22199 (0.0%)
All	All	0.69	4/30215 (0.0%)	0.85	4/40921 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1845	ASP	CG-OD1	13.40	1.56	1.25
2	G	1845	ASP	CG-OD2	-10.32	1.01	1.25
1	A	1310	GLU	CD-OE2	6.83	1.33	1.25
1	A	841	GLU	CD-OE2	5.45	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1845	ASP	CB-CG-OD1	-22.55	98.01	118.30
2	G	1845	ASP	CB-CG-OD2	12.96	129.97	118.30
2	G	1845	ASP	OD1-CG-OD2	-8.28	107.57	123.30
2	G	599	PRO	N-CA-CB	-5.58	96.47	102.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1845	ASP	Sidechain

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	12379	0	12315	55	0
1	B	1222	0	1262	6	0
2	G	16010	0	15979	88	0
3	A	48	0	25	1	0
3	G	48	0	25	0	0
4	B	28	0	0	0	0
5	G	31	0	19	2	0
6	G	48	0	32	0	0
All	All	29814	0	29657	140	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 2.

All (140) 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:376:ASP:OD1	1:B:276:ARG:NH1	2.23	0.72
1:A:1815:ALA:HB2	1:A:1871:ILE:HD11	1.73	0.71
1:A:1189:ILE:H	1:A:1380:GLN:HE21	1.43	0.66
1:A:987:ASN:HD21	2:G:993:GLN:HE22	1.46	0.64
2:G:1546:THR:HG21	2:G:1616:VAL:HG11	1.82	0.62
1:A:1686:LYS:HD2	2:G:915:ALA:HB1	1.82	0.61
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.36	0.61
2:G:95:TYR:HB3	2:G:104:LEU:HD11	1.82	0.61
2:G:827:VAL:HG11	2:G:840:THR:HG22	1.83	0.59
2:G:1616:VAL:HG22	2:G:1650:VAL:HG21	1.85	0.59
1:A:1464:GLU:HG3	1:A:1773:VAL:HG12	1.83	0.58
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	1.84	0.58
2:G:597:MET:HA	5:G:2101:FMN:N5	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ILE:O	1:A:653:ARG:NH2	2.37	0.57
1:A:1463:VAL:HB	1:A:1773:VAL:HG11	1.87	0.56
2:G:915:ALA:HA	2:G:1000:ILE:HD11	1.87	0.56
1:A:8:GLU:O	1:A:12:ILE:HD12	2.06	0.56
2:G:1854:MET:HE1	2:G:1976:PHE:HB2	1.88	0.55
2:G:346:GLN:HA	2:G:377:LEU:HD11	1.87	0.54
2:G:621:GLY:HA2	2:G:630:MET:CE	2.38	0.54
2:G:461:ASP:OD1	2:G:482:CYS:SG	2.60	0.54
1:A:41:THR:HG21	2:G:1663:THR:HG22	1.88	0.54
1:A:413:LEU:CD1	1:A:451:MET:HG2	2.39	0.53
2:G:283:ILE:O	2:G:286:THR:HG22	2.08	0.53
1:A:704:VAL:HG23	1:A:763:TRP:CZ3	2.44	0.52
1:A:1774:GLU:HG3	1:A:1813:TRP:HD1	1.74	0.52
1:B:172:ILE:HD11	1:B:186:ILE:HB	1.91	0.52
2:G:64:PHE:HE2	2:G:87:CYS:HG	1.57	0.52
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.91	0.52
2:G:468:LEU:HA	2:G:471:LEU:HD23	1.92	0.51
1:A:536:THR:HG22	1:A:635:ILE:HB	1.93	0.51
2:G:808:ALA:HB3	2:G:811:VAL:HG23	1.93	0.50
2:G:1376:ALA:HA	2:G:1394:GLY:HA2	1.93	0.50
2:G:1150:ARG:HD3	2:G:1193:THR:HG21	1.93	0.50
2:G:1309:GLU:O	2:G:1317:ARG:NH2	2.44	0.50
2:G:2037:PRO:O	2:G:2041:ILE:HG12	2.12	0.50
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.27	0.50
1:A:706:THR:HB	1:A:737:PHE:HB3	1.93	0.50
2:G:864:LEU:HD23	2:G:899:PHE:HB2	1.94	0.49
2:G:157:VAL:HG11	2:G:496:PHE:CZ	2.48	0.49
2:G:573:LYS:HG2	2:G:1101:GLU:HA	1.94	0.49
1:A:771:PHE:CE1	1:A:825:PRO:HB3	2.48	0.49
2:G:29:ILE:O	2:G:32:GLN:HB3	2.13	0.49
2:G:110:GLN:HB3	2:G:535:ILE:HD13	1.95	0.49
1:A:1542:HIS:N	1:A:1553:GLU:OE2	2.40	0.49
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.76	0.49
2:G:1547:PRO:HD3	2:G:1584:PHE:CZ	2.48	0.48
2:G:806:MET:SD	2:G:1055:HIS:HD2	2.36	0.48
1:A:1557:ILE:HD11	1:A:1642:THR:HG21	1.95	0.48
2:G:593:LEU:CB	2:G:616:THR:OG1	2.62	0.48
2:G:234:ILE:N	2:G:235:PRO:CD	2.76	0.48
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.96	0.48
1:A:1004:ILE:HD11	1:A:1659:ASP:HB3	1.96	0.48
1:A:49:PRO:N	2:G:1784:MET:HE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:VAL:HG21	1:A:910:THR:HG22	1.95	0.47
1:A:1017:ARG:HG3	1:A:1320:LEU:HD22	1.96	0.47
1:A:875:THR:HB	3:A:1901:NAP:O1N	2.15	0.47
2:G:1546:THR:HG21	2:G:1616:VAL:CG1	2.45	0.47
2:G:1845:ASP:CG	2:G:1846:GLU:N	2.69	0.47
2:G:856:LYS:HD3	2:G:1052:CYS:HB3	1.96	0.46
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.16	0.46
1:A:979:GLN:HG3	2:G:964:LEU:HD22	1.98	0.46
1:A:1114:TYR:CE1	1:A:1337:GLU:HG3	2.51	0.46
2:G:241:ILE:HG23	2:G:506:PRO:HG3	1.97	0.46
1:A:413:LEU:HD13	1:A:451:MET:HG2	1.97	0.46
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.50	0.46
1:A:832:THR:HG22	1:A:936:LEU:HB3	1.97	0.46
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.51	0.46
1:A:719:GLN:HG3	1:A:1612:ASP:HA	1.98	0.45
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.97	0.45
1:A:1411:THR:HA	1:A:1648:GLN:O	2.17	0.45
1:A:1713:ASP:HB3	1:A:1738:ILE:HG21	1.98	0.45
2:G:602:VAL:HG11	2:G:623:GLY:HA3	1.98	0.45
2:G:1863:ALA:HB3	2:G:1866:PHE:HB2	1.98	0.45
1:A:678:VAL:HG22	1:A:767:ALA:HB3	1.99	0.45
1:A:1811:GLY:HA2	1:A:1878:ALA:HB1	1.99	0.45
1:A:26:VAL:HB	2:G:1890:ASN:HD22	1.81	0.44
1:A:1459:ILE:O	1:A:1463:VAL:HG23	2.17	0.44
1:A:996:LYS:HB2	1:A:1001:VAL:HG13	1.98	0.44
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.17	0.44
2:G:1234:VAL:HG12	2:G:1265:MET:HG2	1.98	0.44
2:G:1699:LYS:HE3	2:G:1705:SER:HB2	1.99	0.44
2:G:1845:ASP:OD1	2:G:1849:ARG:HB2	2.18	0.44
2:G:245:GLN:HG2	2:G:505:GLY:HA2	2.00	0.44
2:G:717:ILE:HG23	2:G:760:HIS:CE1	2.52	0.44
2:G:1037:SER:HB2	2:G:1053:ILE:HG12	2.00	0.44
2:G:156:LEU:HD22	2:G:502:LEU:HG	1.99	0.44
1:A:46:GLU:OE2	1:A:53:LEU:N	2.49	0.43
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.91	0.43
1:A:36:LEU:HD22	1:A:61:LEU:HD21	2.01	0.43
2:G:767:PHE:HD2	2:G:771:PHE:CE2	2.36	0.43
2:G:1103:PHE:O	2:G:1247:GLY:HA3	2.18	0.43
2:G:1208:THR:HB	2:G:1568:HIS:CE1	2.54	0.43
1:A:1544:THR:O	1:A:1545:SER:HB3	2.19	0.43
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:270:ALA:O	2:G:459:VAL:HA	2.18	0.43
2:G:146:PHE:HE1	2:G:547:ILE:HG23	1.83	0.43
1:A:865:CYS:HB2	1:A:917:CYS:SG	2.59	0.43
1:B:221:LEU:HD21	1:B:262:ASP:HB3	2.00	0.43
2:G:593:LEU:HB2	2:G:616:THR:OG1	2.19	0.43
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	2.01	0.42
2:G:369:SER:HB2	2:G:428:HIS:HB2	2.01	0.42
2:G:273:HIS:HE1	2:G:370:LEU:HD13	1.84	0.42
2:G:526:ARG:HA	2:G:558:ASN:ND2	2.34	0.42
2:G:1054:LEU:HB2	5:G:2101:FMN:HM72	2.01	0.42
1:A:616:LEU:N	1:A:617:PRO:CD	2.82	0.42
2:G:1434:HIS:HB3	2:G:1436:LYS:HE3	2.00	0.42
2:G:1775:GLN:HG3	2:G:1836:MET:HE3	2.02	0.42
1:A:1305:CYS:HB2	1:A:1645:GLY:HA2	2.02	0.42
2:G:433:VAL:N	2:G:434:PRO:CD	2.82	0.42
1:A:409:ALA:HB1	1:A:447:LEU:HD22	2.02	0.42
2:G:1240:TYR:HB3	2:G:1251:ILE:HG23	2.02	0.42
2:G:372:ASN:HB3	2:G:515:LEU:HD21	2.02	0.42
2:G:918:THR:HA	2:G:993:GLN:O	2.21	0.41
2:G:942:THR:HB	2:G:1012:GLN:HB2	2.01	0.41
2:G:1889:VAL:HB	2:G:1977:HIS:HB2	2.02	0.41
1:A:479:ASN:O	1:A:483:VAL:HG22	2.20	0.41
2:G:1328:VAL:HG22	2:G:1557:SER:HA	2.02	0.41
1:A:534:PRO:HA	1:A:537:LYS:HE2	2.03	0.41
2:G:1913:VAL:HG21	2:G:1944:ILE:HG22	2.03	0.41
2:G:1586:SER:HB2	2:G:1610:CYS:SG	2.61	0.41
1:A:1585:LYS:O	1:A:1586:GLY:C	2.60	0.41
1:B:198:PRO:HG3	1:B:212:THR:HG21	2.03	0.41
2:G:72:VAL:HG21	2:G:84:LEU:HD22	2.02	0.41
2:G:1681:TYR:O	2:G:1688:GLN:HG3	2.21	0.41
1:A:1816:LYS:HB3	1:A:1834:LEU:HD12	2.03	0.41
2:G:757:ILE:HG21	2:G:765:LEU:HD22	2.02	0.41
2:G:783:GLY:O	2:G:793:PRO:HA	2.21	0.41
2:G:1086:LEU:HD12	2:G:1090:TYR:HB2	2.03	0.41
2:G:1585:SER:HB3	2:G:1651:LEU:HD22	2.03	0.41
1:A:511:TYR:OH	1:A:513:GLU:OE2	2.36	0.40
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.56	0.40
1:B:232:LEU:HD13	1:B:272:GLU:HG3	2.03	0.40
2:G:250:VAL:CG2	2:G:292:PHE:CE2	3.04	0.40
2:G:1424:GLN:HB3	2:G:1472:VAL:HG12	2.02	0.40
1:A:640:LEU:HD23	1:A:924:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ARG:HG2	2:G:956:GLU:HB3	2.02	0.40
1:B:271:ASN:HB2	1:B:290:MET:HE2	2.04	0.40
2:G:586:LEU:HD13	2:G:1108:PRO:HD3	2.03	0.40
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.51	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	1576/1887 (84%)	1500 (95%)	72 (5%)	4 (0%)	41 71
1	B	161/1887 (8%)	155 (96%)	6 (4%)	0	100 100
2	G	2029/2051 (99%)	1904 (94%)	122 (6%)	3 (0%)	51 82
All	All	3766/5825 (65%)	3559 (94%)	200 (5%)	7 (0%)	50 78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	888	ARG
2	G	343	ASN
1	A	773	ALA
1	A	1298	ILE
2	G	544	LYS
1	A	866	GLY
1	A	1586	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	1340/1566 (86%)	1334 (100%)	6 (0%)	91 97
1	B	134/1566 (9%)	133 (99%)	1 (1%)	84 95
2	G	1772/1788 (99%)	1767 (100%)	5 (0%)	92 98
All	All	3246/4920 (66%)	3234 (100%)	12 (0%)	91 97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	413	LEU
1	A	702	LYS
1	A	754	ASP
1	A	1332	TYR
1	A	1333	ASP
1	A	1507	GLN
1	B	227	SER
2	G	518	ARG
2	G	599	PRO
2	G	709	SER
2	G	1586	SER
2	G	1845	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	A	411	GLN
1	A	527	GLN
1	A	1380	GLN
1	A	1695	ASN
1	B	292	GLN
2	G	79	GLN
2	G	102	HIS
2	G	110	GLN
2	G	245	GLN
2	G	440	ASN
2	G	747	HIS
2	G	760	HIS

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Mol	Chain	Res	Type
2	G	993	GLN
2	G	1055	HIS
2	G	1178	GLN
2	G	1355	ASN
2	G	1581	HIS
2	G	1851	ASN
2	G	1890	ASN
2	G	2020	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
2	J8W	G	1808	2	10,11,12	1.67	1 (10%)	9,13,15	1.24	1 (11%)

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
2	J8W	G	1808	2	-	3/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1808	J8W	OG-C2	4.58	1.46	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1808	J8W	OG-C2-C1	2.01	116.81	111.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1808	J8W	C1-C2-OG-CB
2	G	1808	J8W	O7-C2-OG-CB
2	G	1808	J8W	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	NAP	G	2102	-	45,52,52	1.23	6 (13%)	56,80,80	1.29	4 (7%)
6	COA	G	2103	-	41,50,50	0.68	1 (2%)	52,75,75	0.70	1 (1%)
4	A5S	B	1901	1	23,27,27	0.97	2 (8%)	34,37,37	1.91	11 (32%)
5	FMN	G	2101	-	33,33,33	1.33	3 (9%)	48,50,50	1.49	10 (20%)
3	NAP	A	1901	-	45,52,52	1.13	4 (8%)	56,80,80	1.44	12 (21%)

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	NAP	G	2102	-	-	11/31/67/67	0/5/5/5
6	COA	G	2103	-	-	17/44/64/64	0/3/3/3
4	A5S	B	1901	1	-	9/33/34/34	-
5	FMN	G	2101	-	-	1/18/18/18	0/3/3/3
3	NAP	A	1901	-	-	3/31/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2102	NAP	C5A-C4A	3.11	1.49	1.40
5	G	2101	FMN	C9A-C5A	3.05	1.46	1.41
3	G	2102	NAP	C2A-N3A	2.85	1.36	1.32
4	B	1901	A5S	C1-S44	-2.82	1.69	1.76
3	A	1901	NAP	P2B-O2B	2.60	1.64	1.59
6	G	2103	COA	P3B-O3B	2.59	1.64	1.59
3	G	2102	NAP	O4D-C1D	2.57	1.44	1.41
3	A	1901	NAP	C4A-N3A	-2.44	1.32	1.35
5	G	2101	FMN	C5A-N5	-2.38	1.34	1.39
3	G	2102	NAP	O4B-C1B	2.35	1.44	1.41
3	G	2102	NAP	C6A-C5A	2.32	1.51	1.43
5	G	2101	FMN	C9-C8	-2.32	1.36	1.39
3	G	2102	NAP	P2B-O2B	2.28	1.63	1.59
3	A	1901	NAP	C2D-C1D	-2.27	1.50	1.53
3	A	1901	NAP	C3N-C7N	-2.04	1.47	1.50
4	B	1901	A5S	O33-C32	2.02	1.46	1.42

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1901	A5S	C2-C1-S44	4.83	119.71	113.69
4	B	1901	A5S	C37-C38-C39	-4.56	104.76	112.36
3	G	2102	NAP	C3N-C7N-N7N	4.22	122.81	117.75
3	G	2102	NAP	N3A-C2A-N1A	-3.94	122.51	128.68
4	B	1901	A5S	C43-S44-C1	3.66	113.26	101.87
3	A	1901	NAP	PN-O3-PA	-3.52	120.74	132.83
5	G	2101	FMN	C4A-C10-N10	3.39	121.43	116.48
5	G	2101	FMN	C4-C4A-N5	3.36	123.02	118.23
3	G	2102	NAP	C4A-C5A-N7A	-3.06	106.21	109.40
4	B	1901	A5S	O27-C28-C29	3.04	115.43	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1901	NAP	N3A-C2A-N1A	-2.98	124.02	128.68
4	B	1901	A5S	C31-C29-C32	2.94	113.91	108.82
4	B	1901	A5S	C31-C29-C28	-2.87	103.55	108.23
3	G	2102	NAP	O7N-C7N-N7N	-2.80	118.61	122.58
3	A	1901	NAP	O7N-C7N-N7N	-2.71	118.72	122.58
5	G	2101	FMN	O2-C2-N1	-2.68	117.38	121.83
3	A	1901	NAP	O3X-P2B-O2X	2.65	117.75	107.64
5	G	2101	FMN	C10-C4A-N5	-2.60	119.35	124.86
5	G	2101	FMN	C10-N1-C2	2.53	121.97	116.90
3	A	1901	NAP	C1B-N9A-C4A	-2.50	122.25	126.64
5	G	2101	FMN	C9A-C5A-N5	2.43	125.07	122.43
4	B	1901	A5S	O23-P24-O25	-2.43	101.18	110.68
5	G	2101	FMN	C7M-C7-C6	-2.40	115.05	119.49
5	G	2101	FMN	C4A-C10-N1	-2.34	119.29	124.73
6	G	2103	COA	C5A-C6A-N6A	2.26	123.79	120.35
3	A	1901	NAP	O2N-PN-O1N	2.26	123.41	112.24
4	B	1901	A5S	O23-P24-O27	2.26	112.73	106.73
3	A	1901	NAP	N6A-C6A-N1A	2.25	123.24	118.57
5	G	2101	FMN	C5A-C9A-N10	-2.23	115.65	117.95
5	G	2101	FMN	C4'-C3'-C2'	-2.23	108.73	113.36
3	A	1901	NAP	O3B-C3B-C4B	-2.16	104.80	111.05
4	B	1901	A5S	O33-C32-C29	2.08	115.15	110.25
3	A	1901	NAP	C2N-C3N-C4N	2.08	120.61	118.26
4	B	1901	A5S	O5-C1-C2	-2.07	119.77	123.35
4	B	1901	A5S	C30-C29-C28	2.06	111.60	108.23
3	A	1901	NAP	O2X-P2B-O1X	2.03	118.63	110.68
3	A	1901	NAP	O4D-C4D-C3D	2.01	109.10	105.11
3	A	1901	NAP	O3B-C3B-C2B	2.00	116.85	111.17

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	NAP	O4D-C1D-N1N-C2N
3	G	2102	NAP	C5B-O5B-PA-O1A
3	G	2102	NAP	C5D-O5D-PN-O3
3	G	2102	NAP	C5D-O5D-PN-O1N
3	G	2102	NAP	C5D-O5D-PN-O2N
4	B	1901	A5S	C28-O27-P24-O23
4	B	1901	A5S	C28-O27-P24-O25
4	B	1901	A5S	C28-O27-P24-O26
6	G	2103	COA	OAP-CAP-CBP-CCP

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Mol	Chain	Res	Type	Atoms
6	G	2103	COA	C9P-CAP-CBP-CCP
6	G	2103	COA	C9P-CAP-CBP-CDP
6	G	2103	COA	OAP-CAP-CBP-CEP
6	G	2103	COA	C9P-CAP-CBP-CEP
6	G	2103	COA	O9P-C9P-CAP-CBP
6	G	2103	COA	N8P-C9P-CAP-CBP
6	G	2103	COA	O9P-C9P-CAP-OAP
6	G	2103	COA	N8P-C9P-CAP-OAP
6	G	2103	COA	S1P-C2P-C3P-N4P
6	G	2103	COA	OAP-CAP-CBP-CDP
4	B	1901	A5S	O33-C32-C34-N36
3	G	2102	NAP	C4B-C5B-O5B-PA
5	G	2101	FMN	C4'-C5'-O5'-P
3	G	2102	NAP	C2B-O2B-P2B-O3X
6	G	2103	COA	C3B-O3B-P3B-O9A
6	G	2103	COA	C5B-O5B-P1A-O3A
3	G	2102	NAP	C5B-O5B-PA-O2A
4	B	1901	A5S	O27-C28-C29-C30
6	G	2103	COA	CEP-CBP-CCP-O6A
3	G	2102	NAP	PA-O3-PN-O1N
3	G	2102	NAP	PA-O3-PN-O2N
4	B	1901	A5S	C1-C2-C3-C4
4	B	1901	A5S	C1-C2-C3-O1
4	B	1901	A5S	O33-C32-C34-O35
6	G	2103	COA	C3B-O3B-P3B-O7A
3	G	2102	NAP	O4B-C4B-C5B-O5B
3	A	1901	NAP	C2B-O2B-P2B-O2X
3	G	2102	NAP	C5B-O5B-PA-O3
6	G	2103	COA	O5P-C5P-C6P-C7P
6	G	2103	COA	C5B-O5B-P1A-O1A
3	A	1901	NAP	O4B-C4B-C5B-O5B
4	B	1901	A5S	C28-C29-C32-C34

There are no ring outliers.

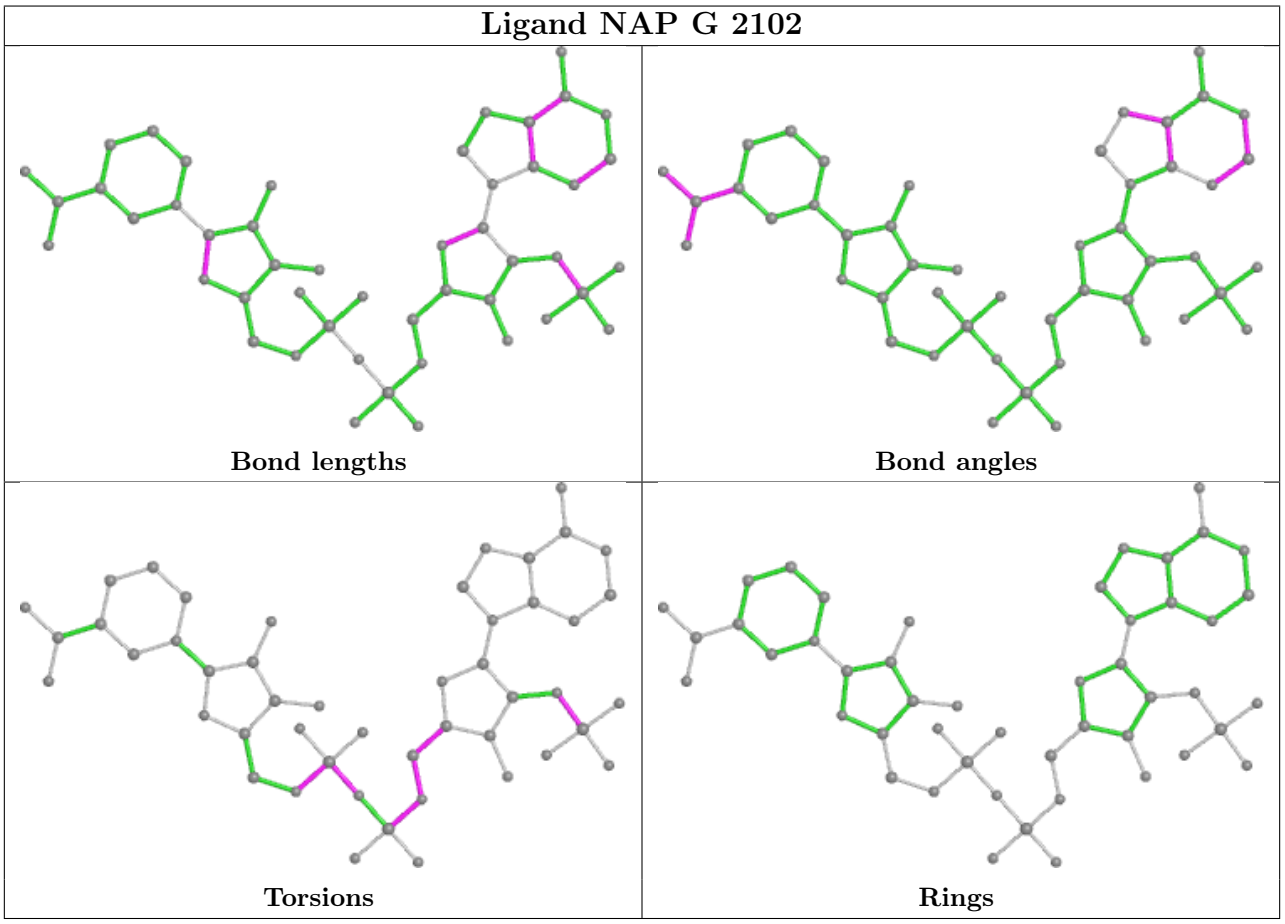
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2101	FMN	2	0
3	A	1901	NAP	1	0

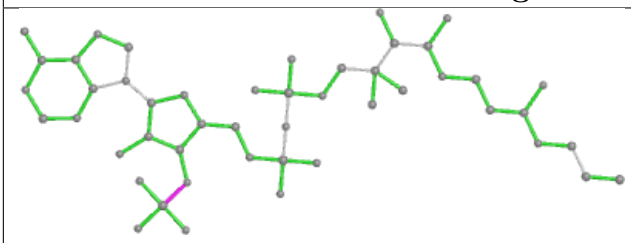
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

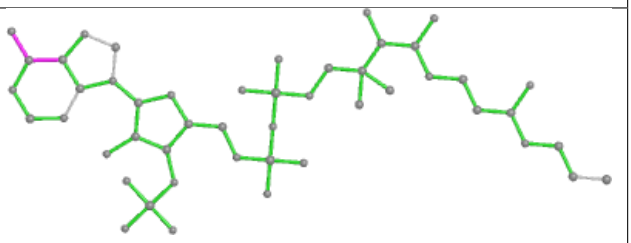
Ligand NAP G 2102



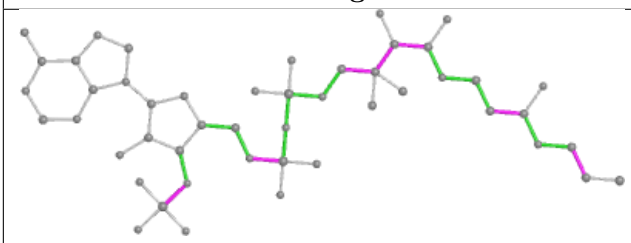
Ligand COA G 2103



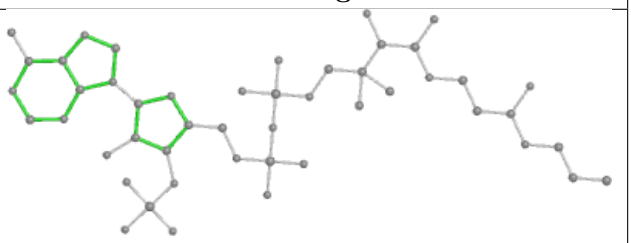
Bond lengths



Bond angles

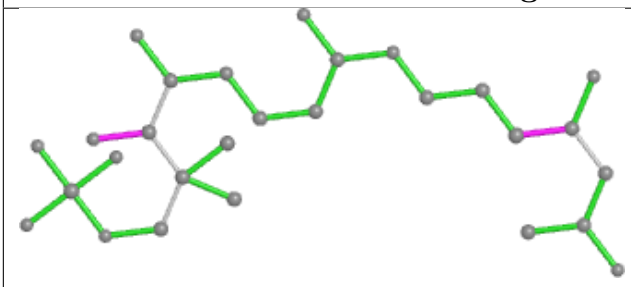


Torsions

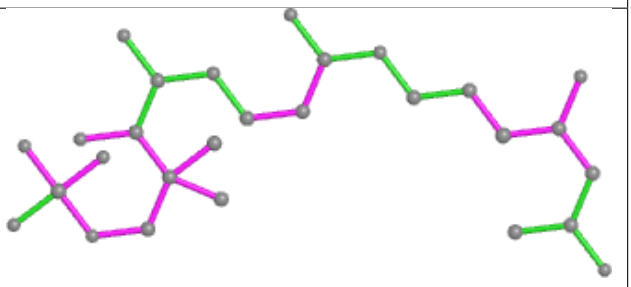


Rings

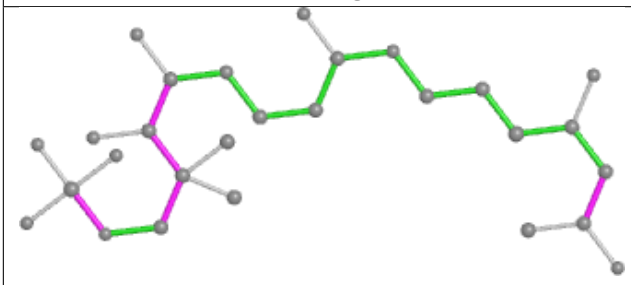
Ligand A5S B 1901



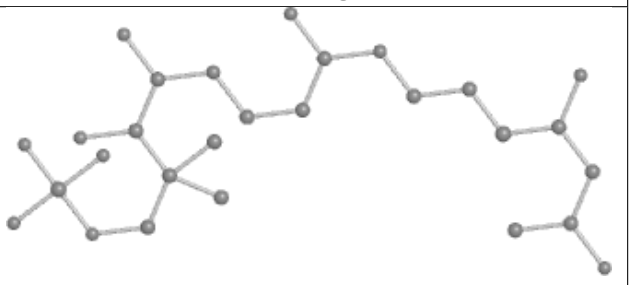
Bond lengths



Bond angles

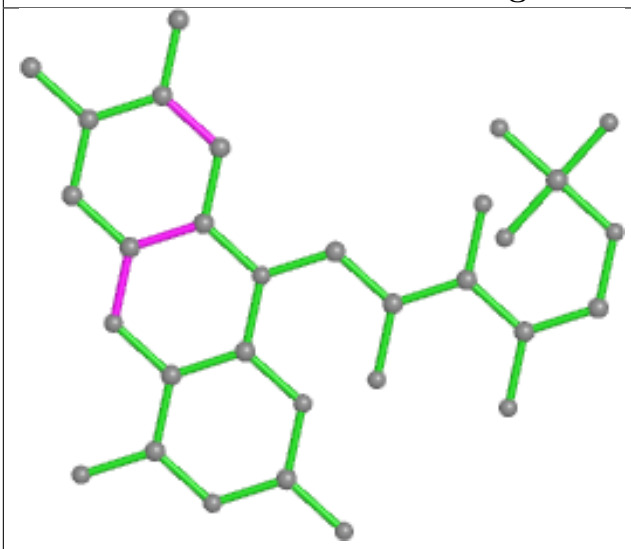


Torsions

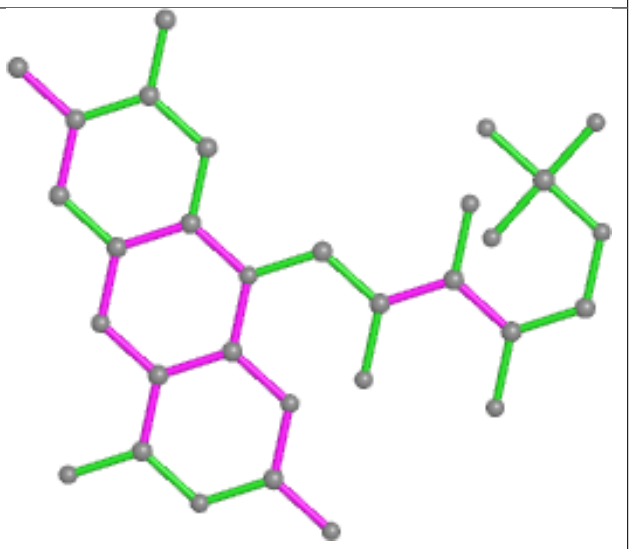


Rings

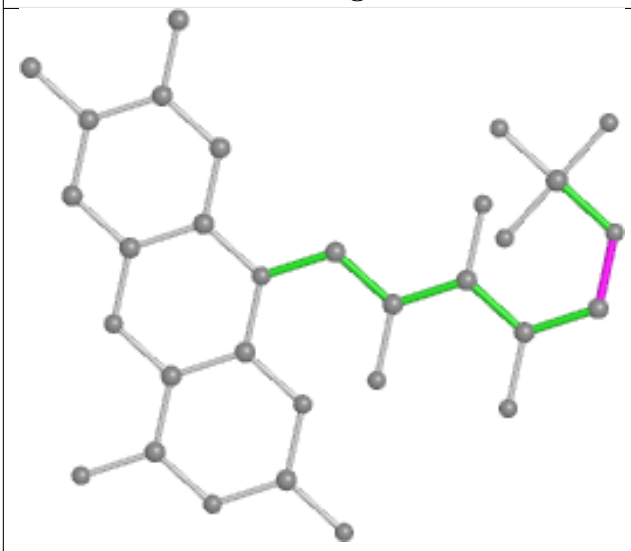
Ligand FMN G 2101



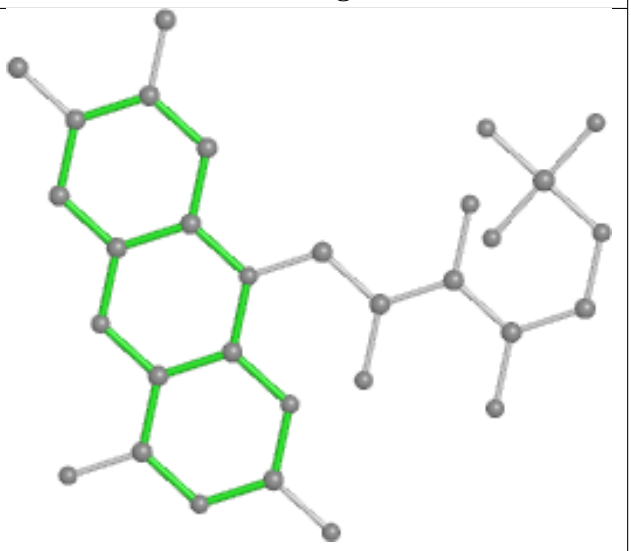
Bond lengths



Bond angles

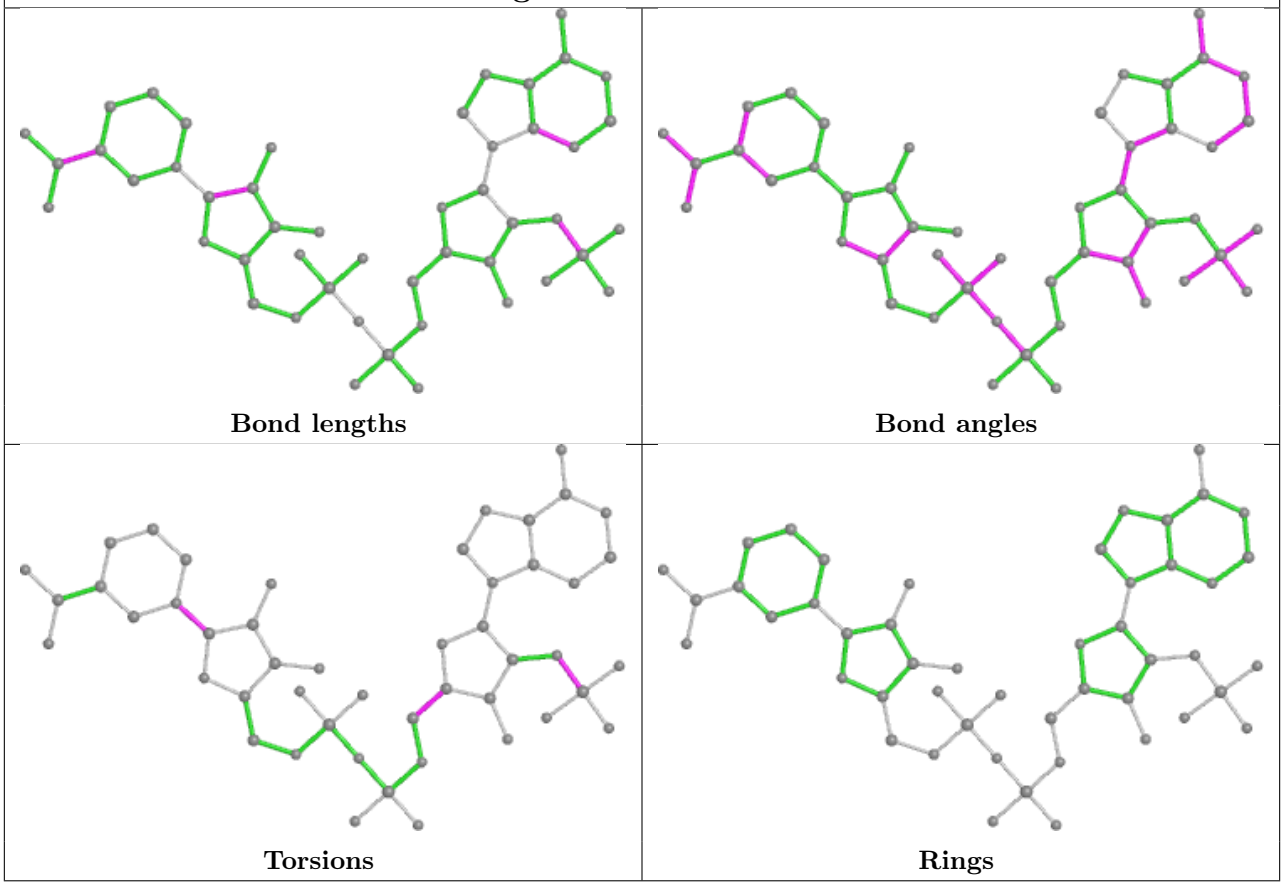


Torsions



Rings

Ligand NAP A 1901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

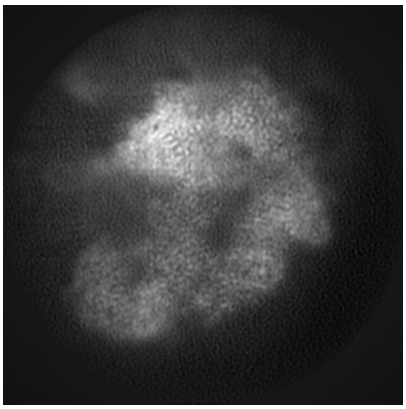
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17839. These allow visual inspection of the internal detail of the map and identification of artifacts.

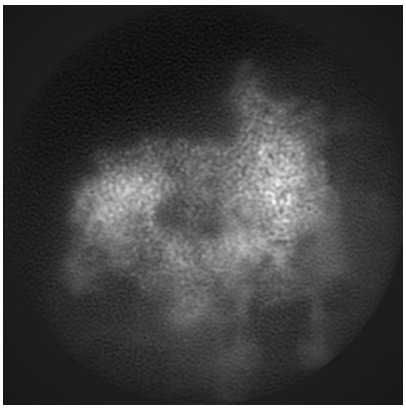
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

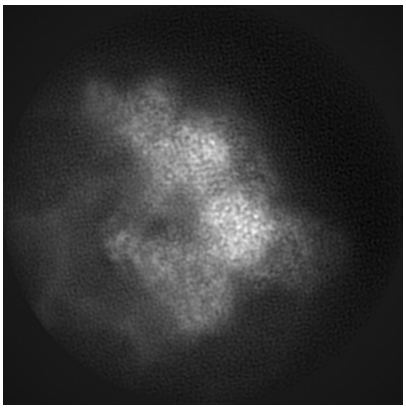
6.1.1 Primary map



X

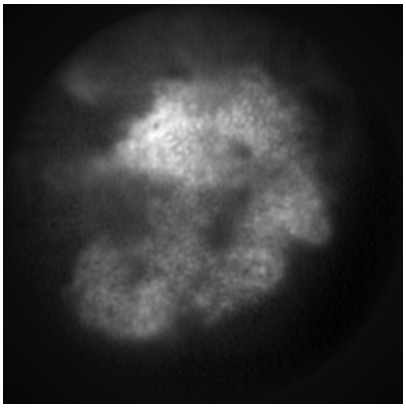


Y

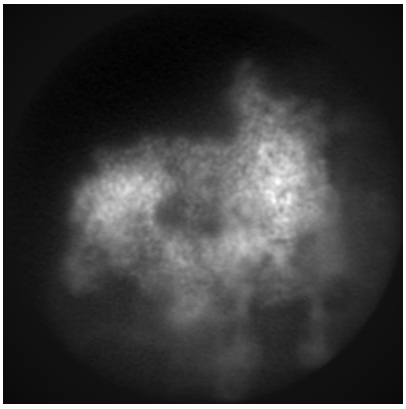


Z

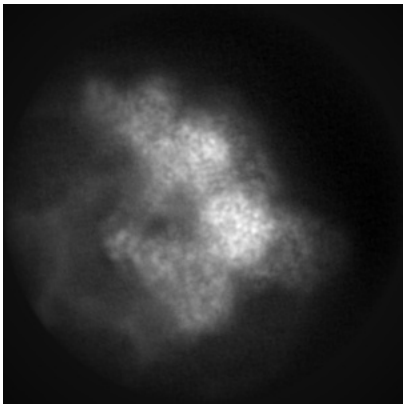
6.1.2 Raw map



X



Y

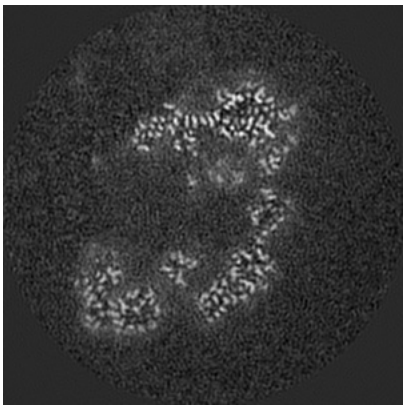


Z

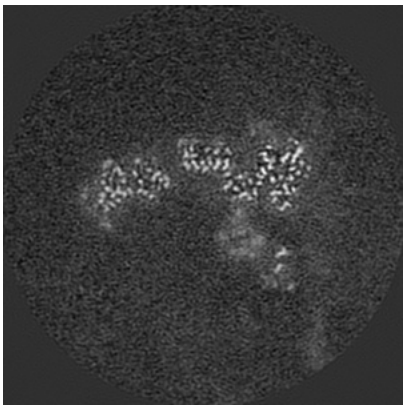
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

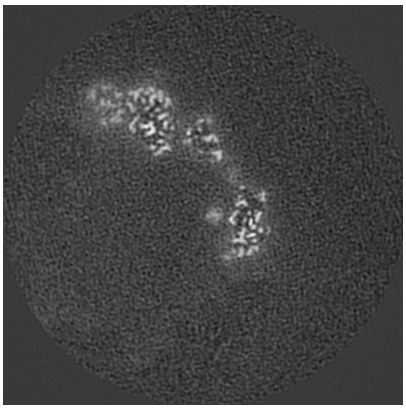
6.2.1 Primary map



X Index: 120

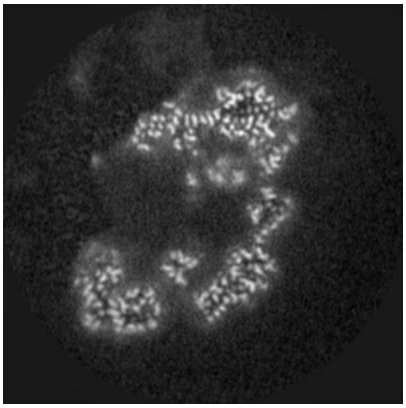


Y Index: 120

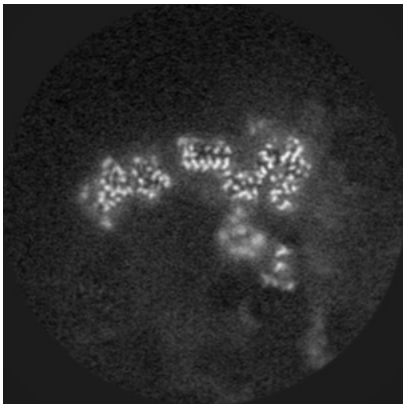


Z Index: 120

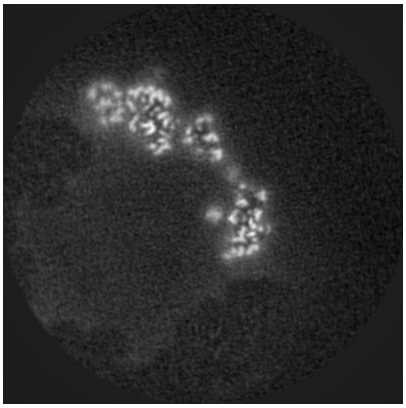
6.2.2 Raw map



X Index: 120



Y Index: 120

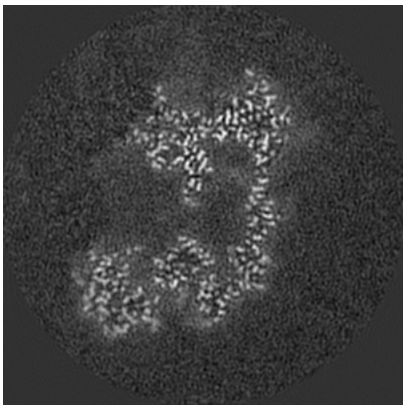


Z Index: 120

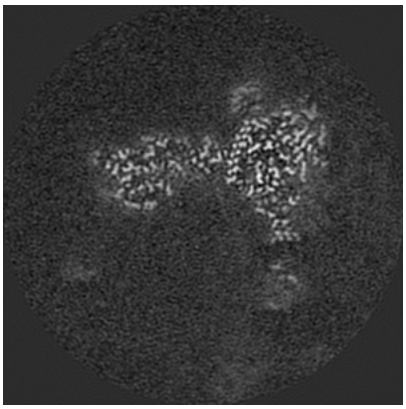
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

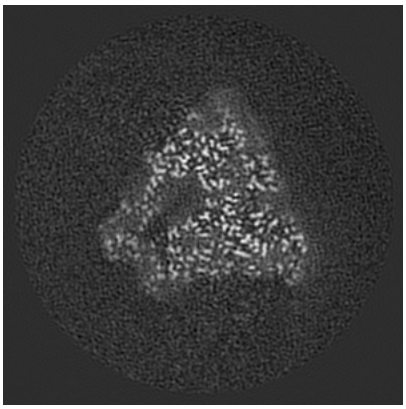
6.3.1 Primary map



X Index: 126

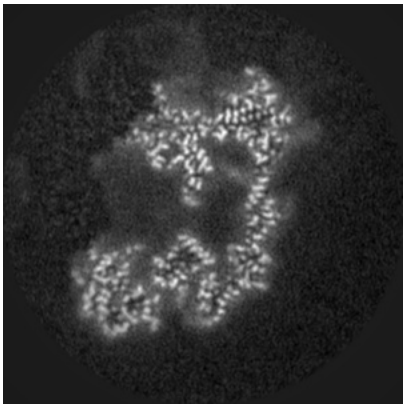


Y Index: 106

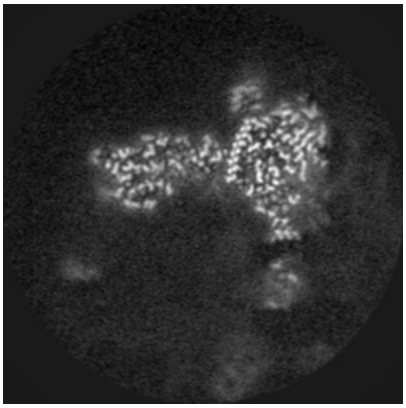


Z Index: 163

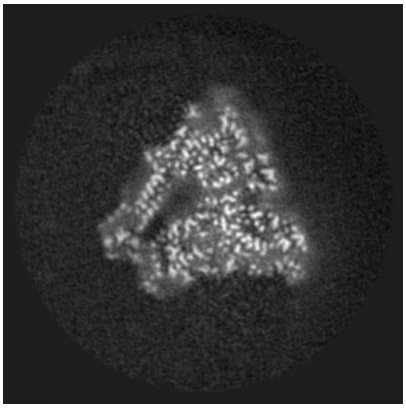
6.3.2 Raw map



X Index: 126



Y Index: 106

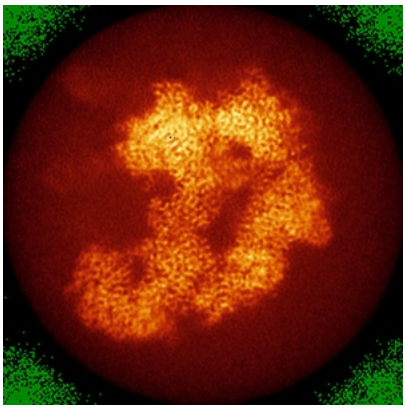


Z Index: 164

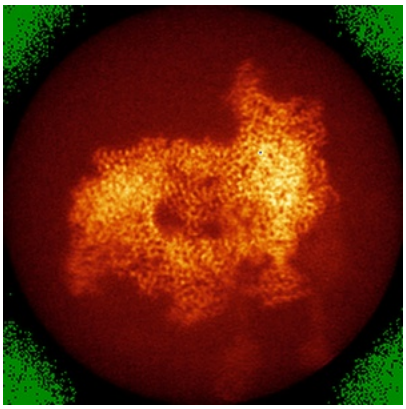
The images above show the largest variance slices of the map in three orthogonal directions.

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

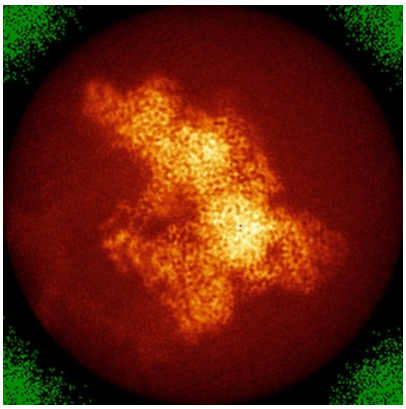
6.4.1 Primary map



X

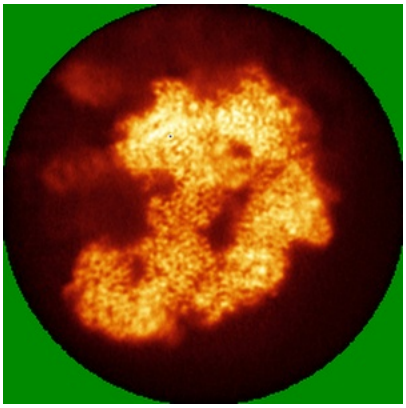


Y

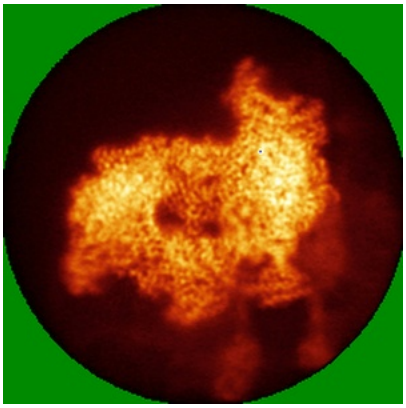


Z

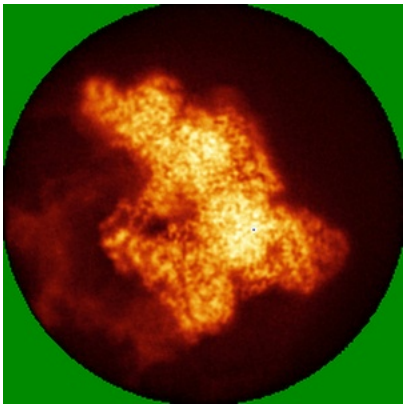
6.4.2 Raw map



X



Y



Z

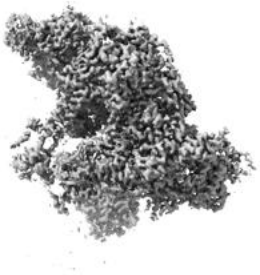
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

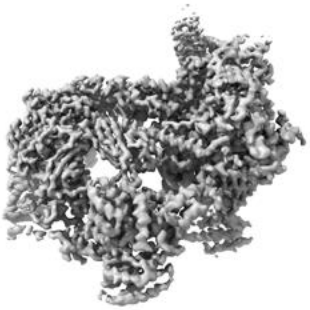


Z

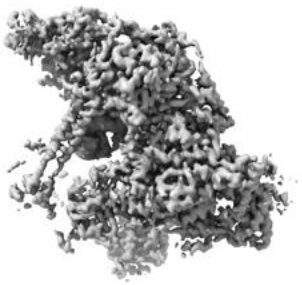
The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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.

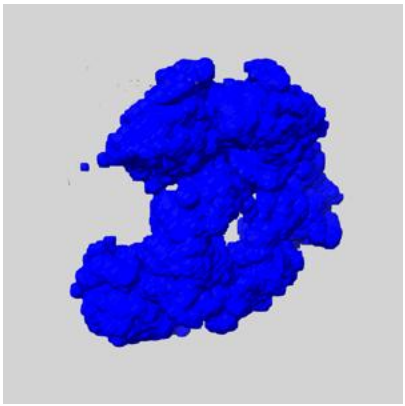
6.6 Mask visualisation

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

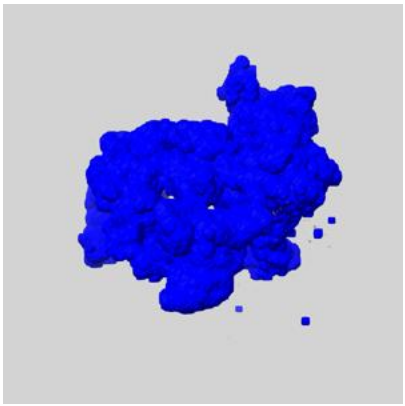
A mask typically either:

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

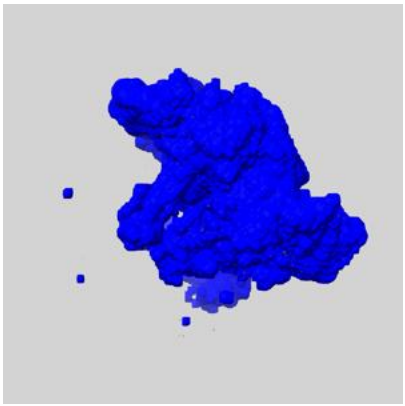
6.6.1 emd_17839_msk_1.map



X



Y

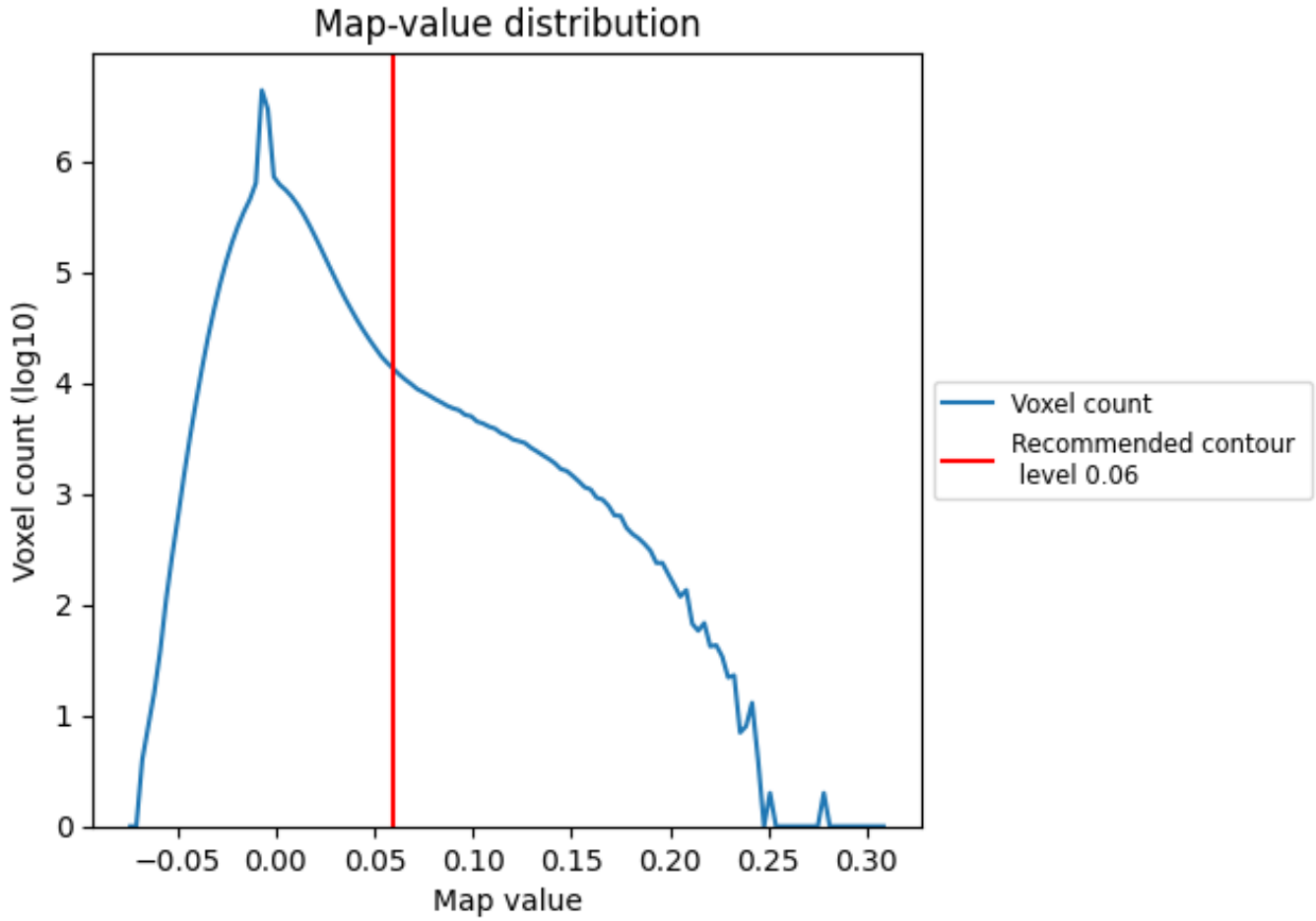


Z

7 Map analysis

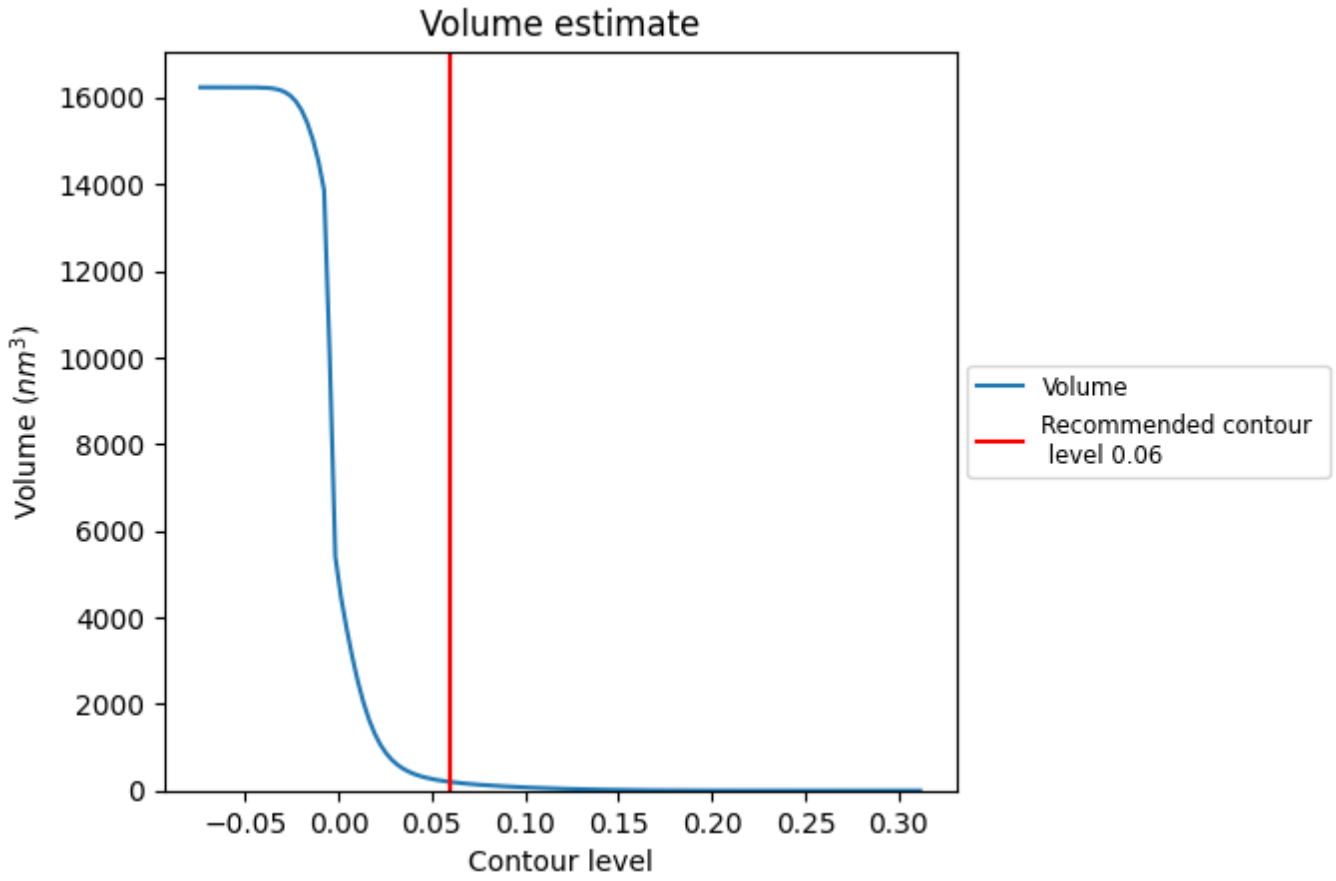
This section contains the results of statistical analysis of the map.

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.

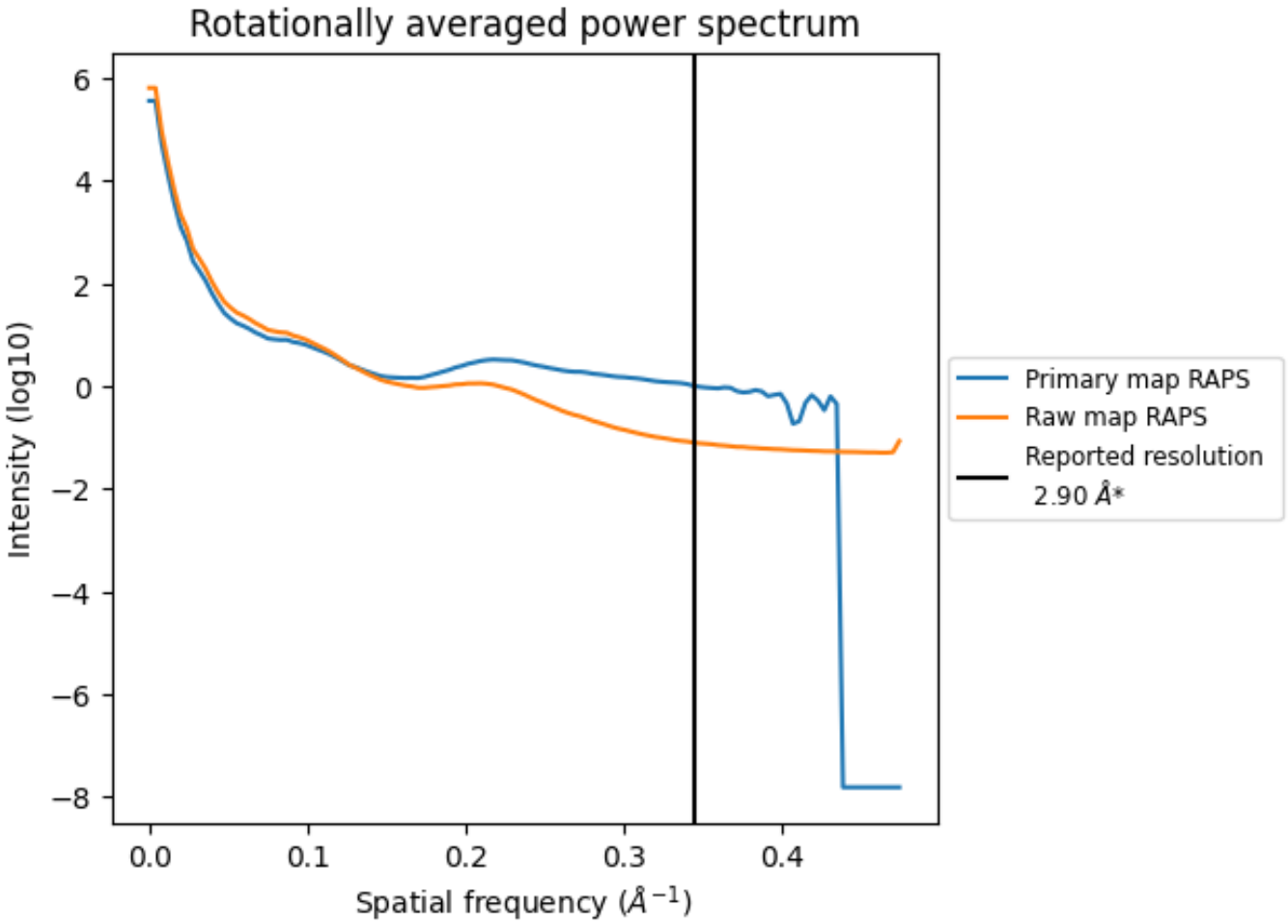
7.2 Volume estimate



The volume at the recommended contour level is 199 nm^3; this corresponds to an approximate mass of 180 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)

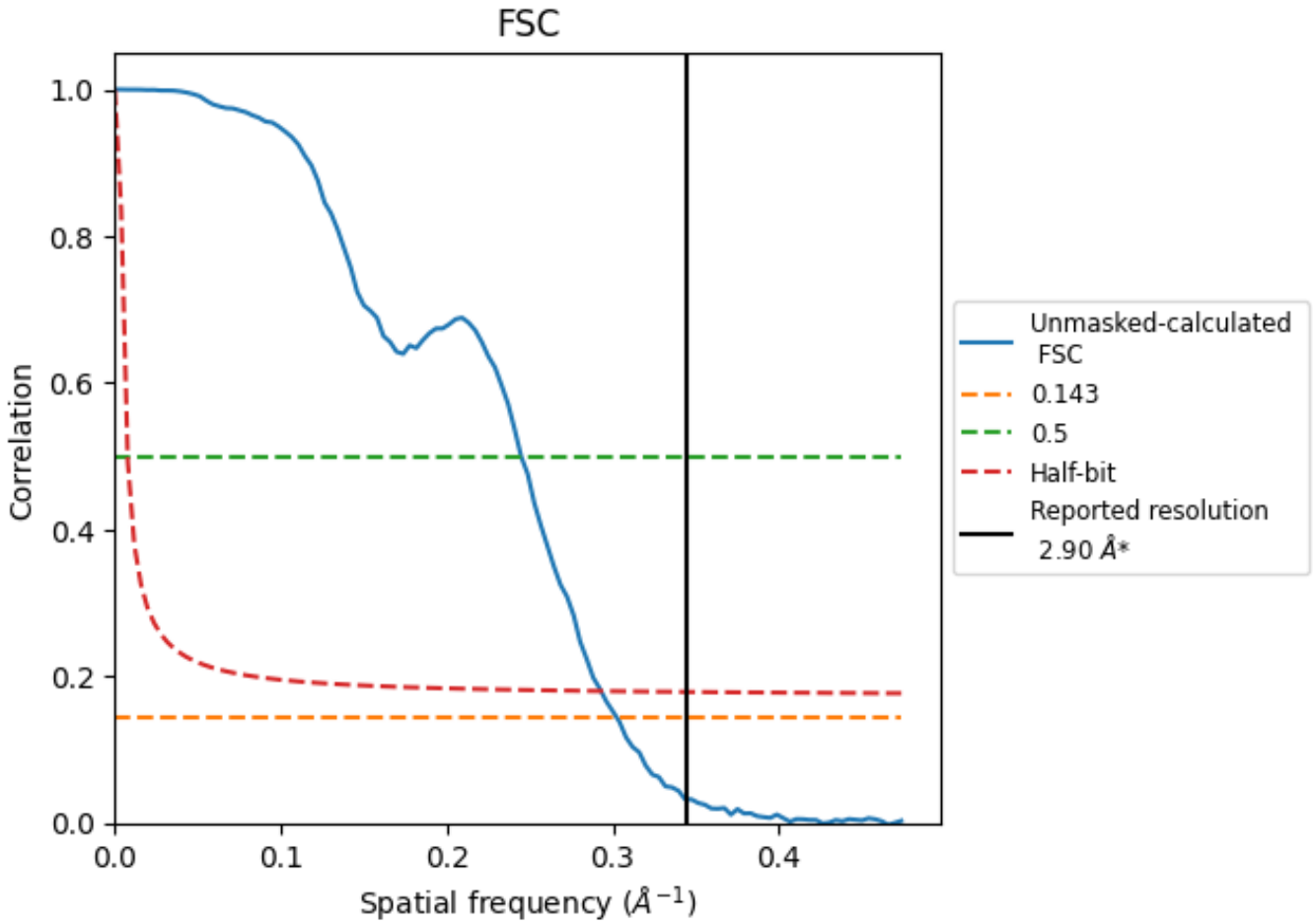


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

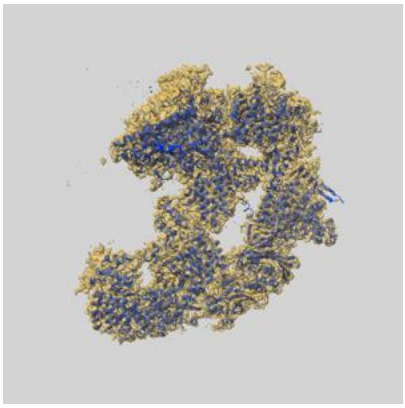
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.31	4.08	3.41

*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 3.31 differs from the reported value 2.9 by more than 10 %

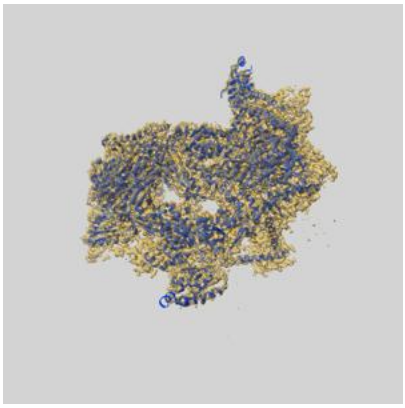
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17839 and PDB model 8PRV. Per-residue inclusion information can be found in section 3 on page 6.

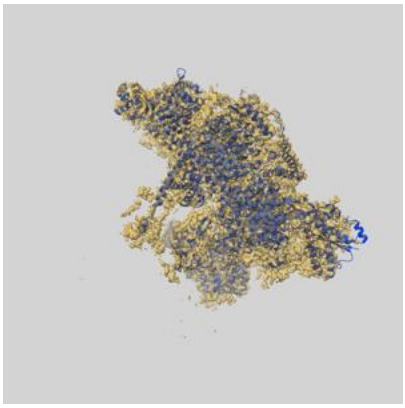
9.1 Map-model overlay



X



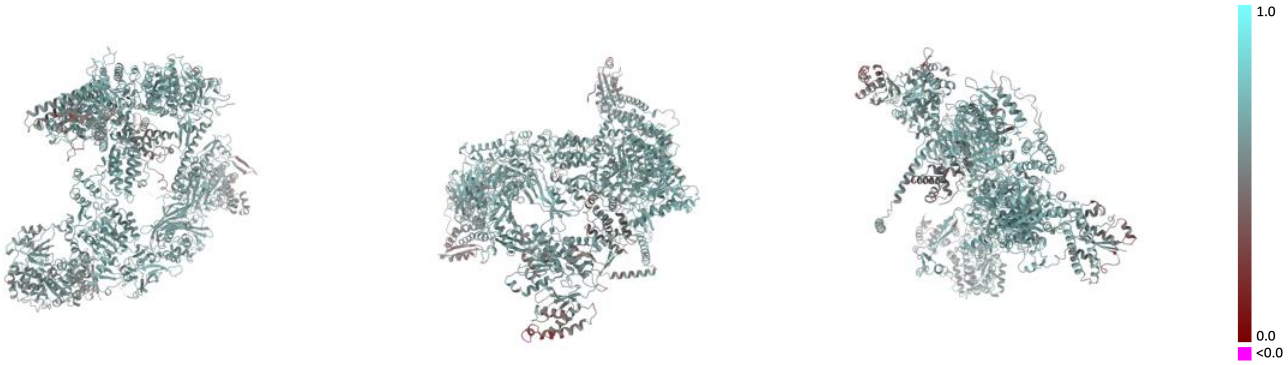
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

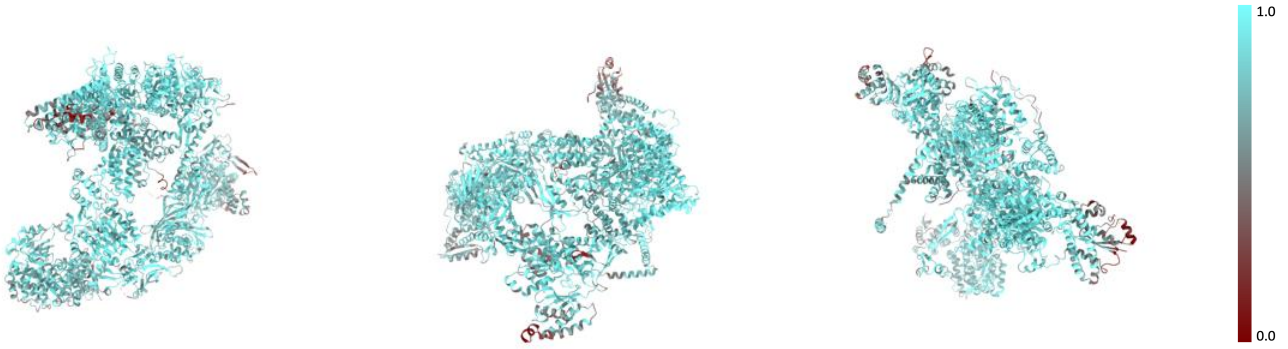
9.2 Q-score mapped to coordinate model (i)



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.

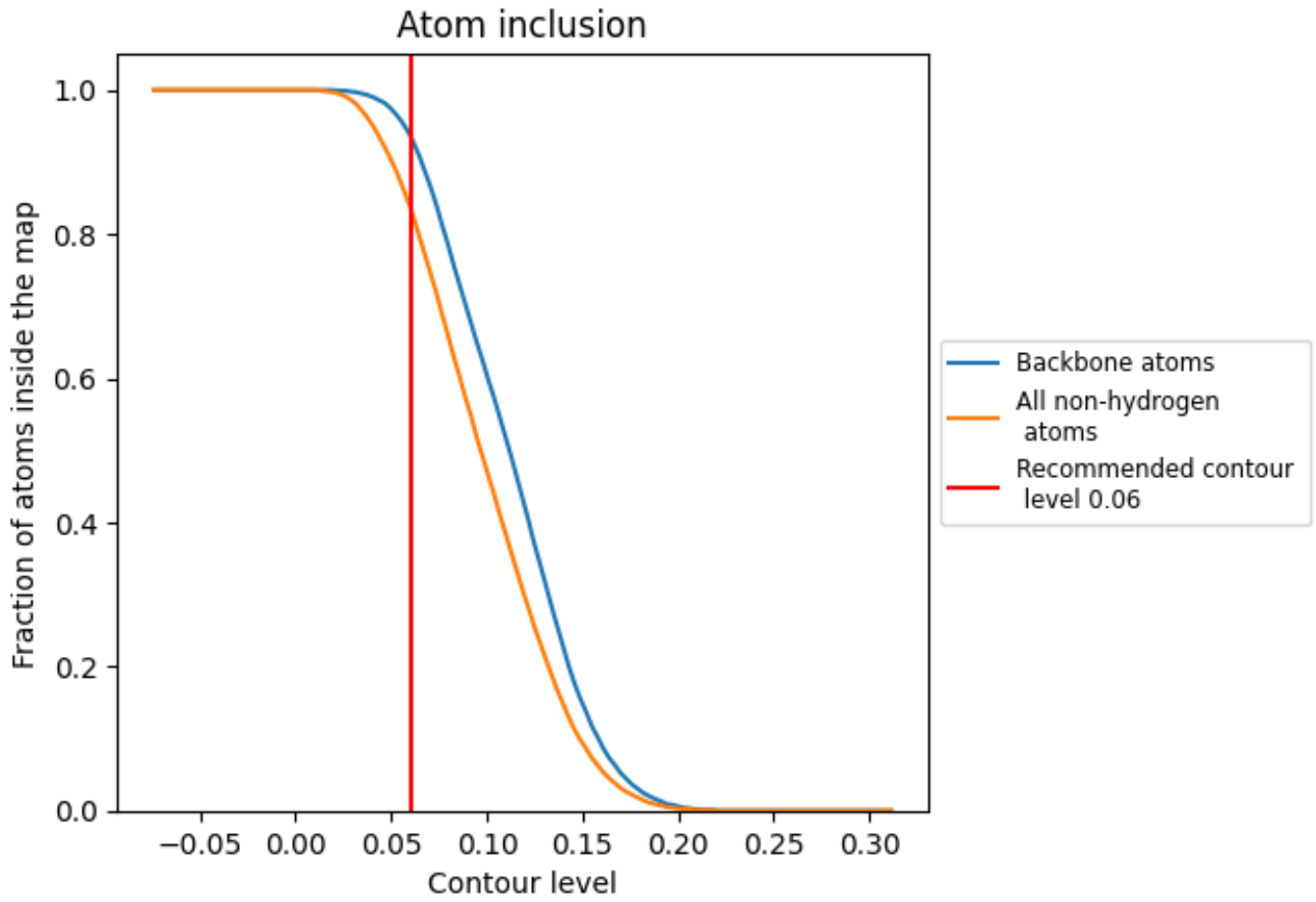
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8370	0.5810
A	0.8610	0.6020
B	0.7830	0.4840
G	0.8220	0.5730