Full wwPDB EM Validation Report

Mar 19, 2026 – 09:49 PM UTC

PDB ID	:	8VYK / pdb_00008vyk
EMDB ID	:	EMD-43663
Title	:	Structure of full-length human cardiac sodium channel - Class-II.
Authors	:	Biswas, R.; Chinthalapudi, K.
Deposited on	:	2024-02-08
Resolution	:	3.90 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:

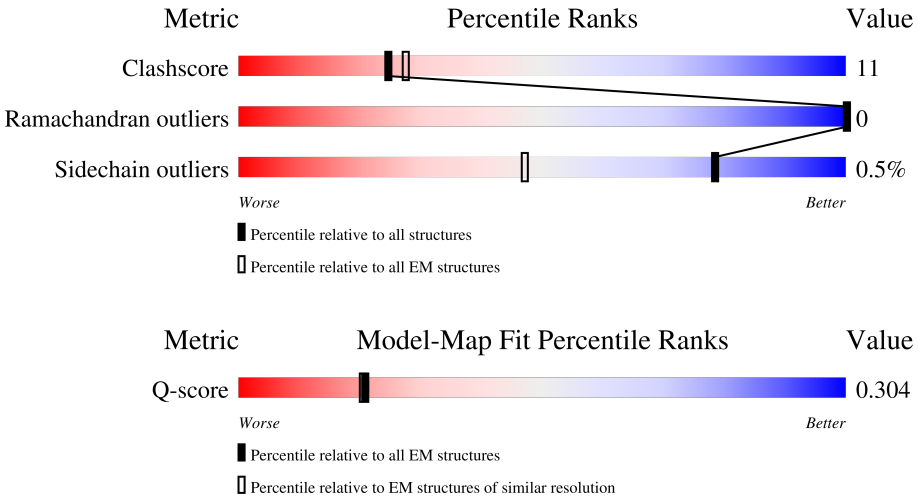
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	2016	52% 17% 31%
2	B	5	40% 40% 20%
3	C	2	100%
3	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	E	2	50% 50%

2 Entry composition

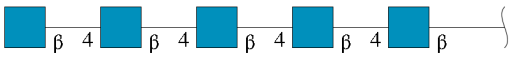
There are 6 unique types of molecules in this entry. The entry contains 11721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sodium channel protein type 5 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1395	11216	7374	1789	1964	89	1	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	5	70	40	5	25	0	0

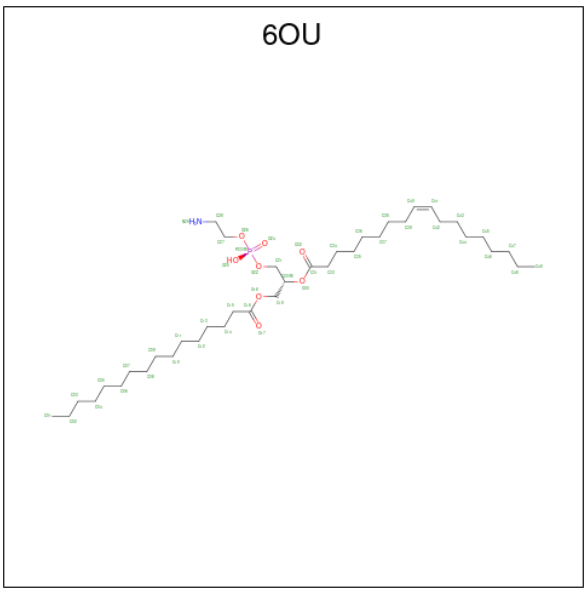
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	2	28	16	2	10	0	0
3	D	2	28	16	2	10	0	0
3	E	2	28	16	2	10	0	0

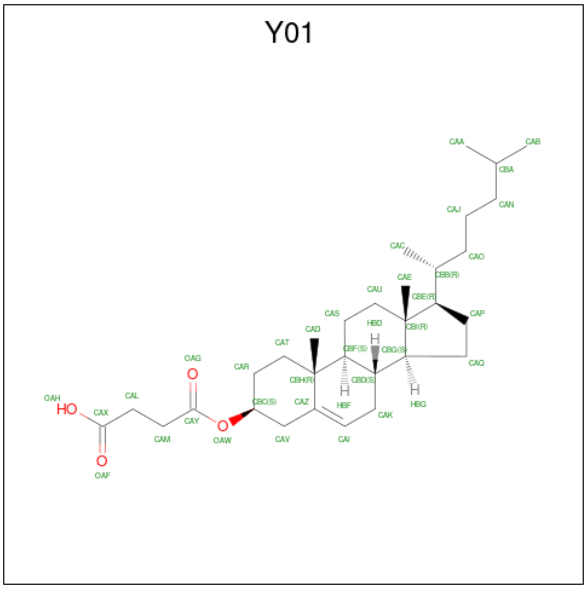
- Molecule 4 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: $C_{39}H_{76}NO_8P$) (labeled as

"Ligand of Interest" by depositor).



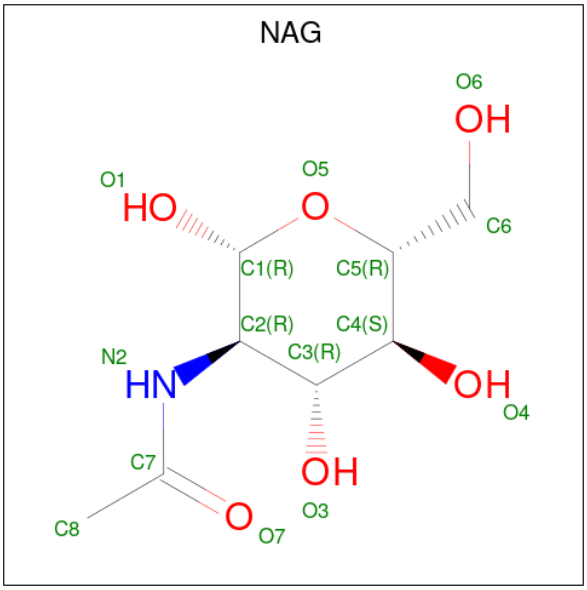
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O P 31 22 8 1	0
4	A	1	Total C N O P 40 30 1 8 1	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 35 31 4	0
5	A	1	Total C O 28 27 1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0

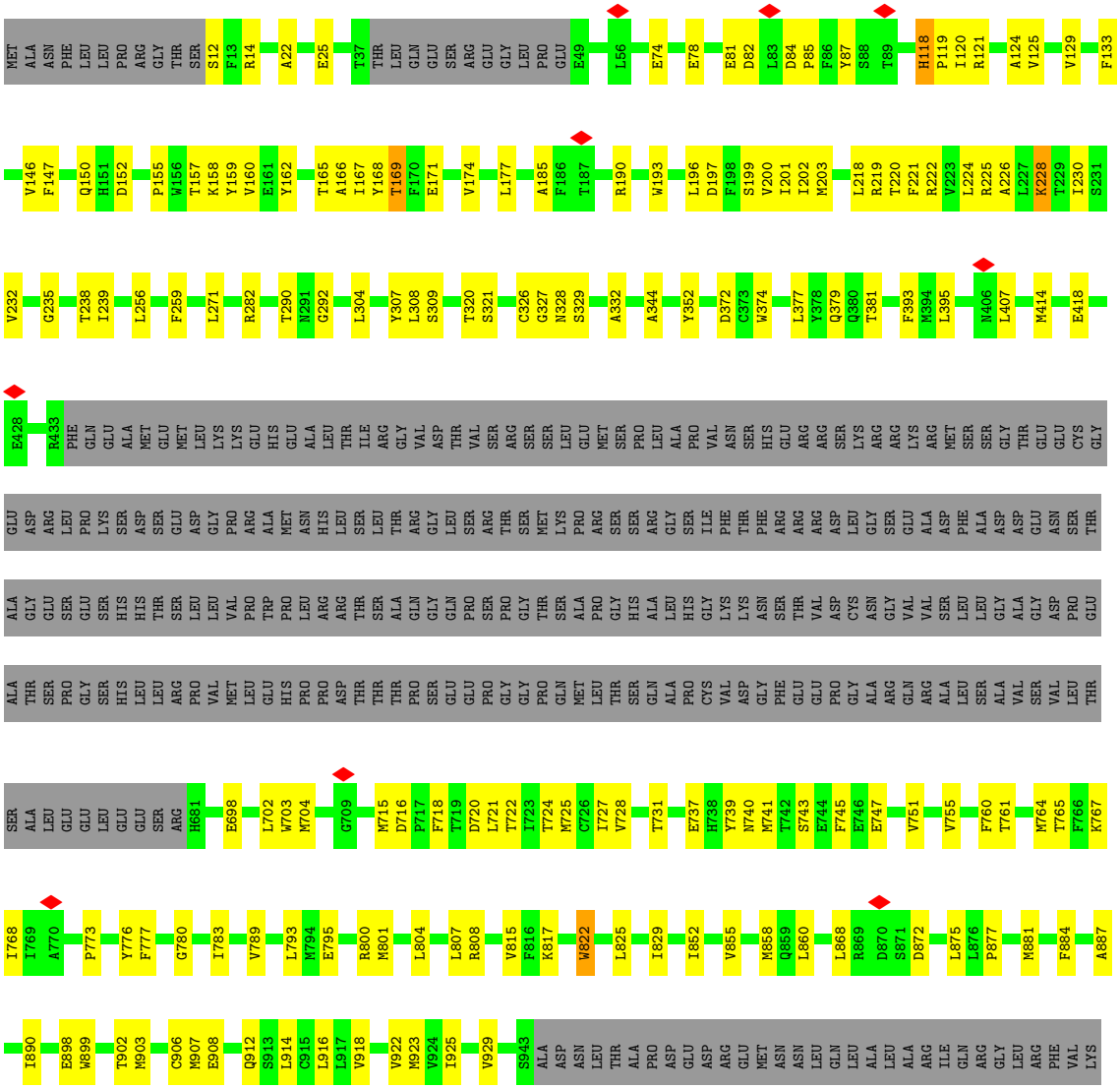
3 Residue-property plots (i)

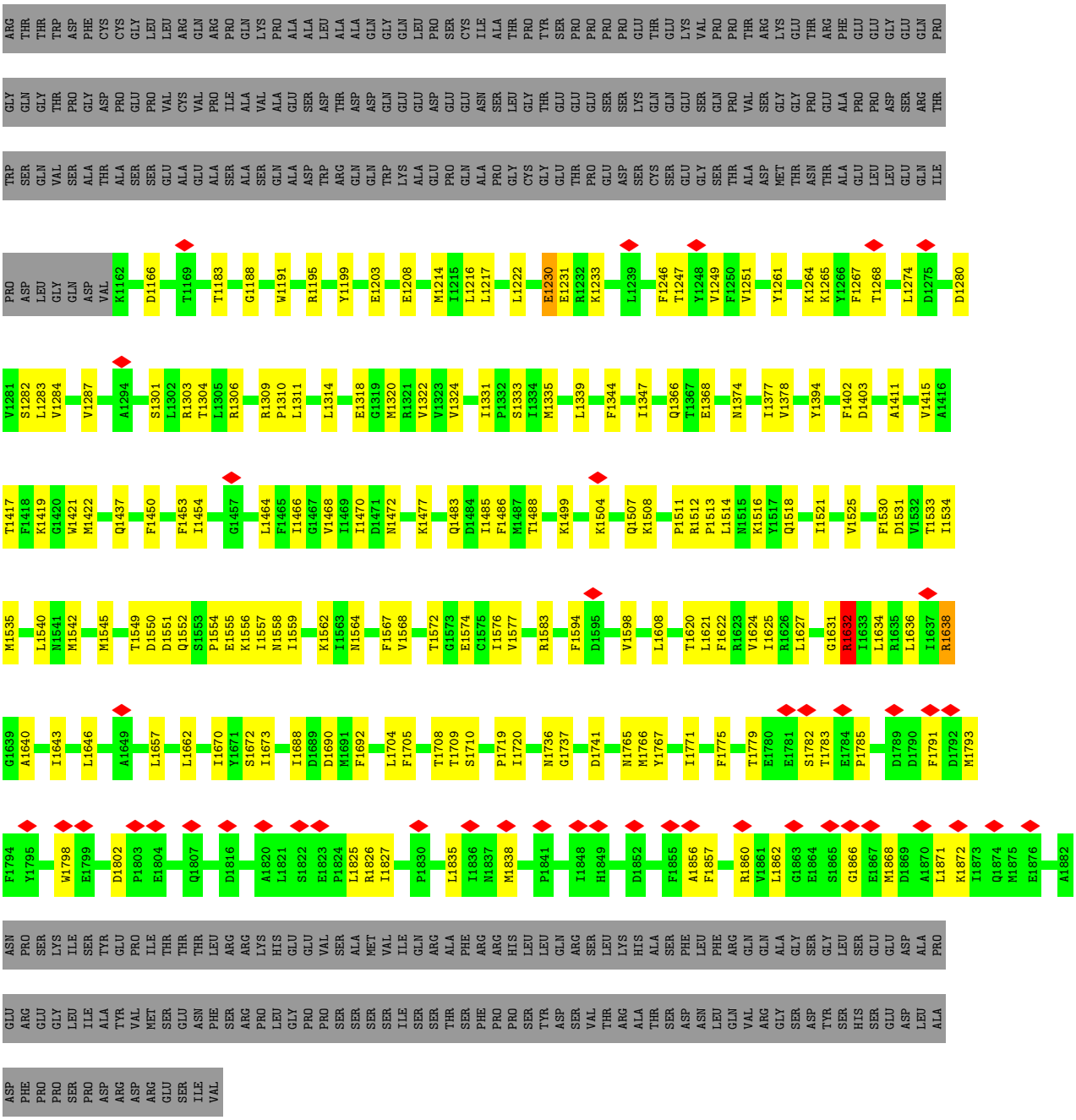
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium channel protein type 5 subunit alpha

Chain A:

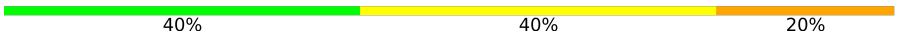






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

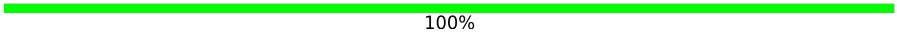
Chain B:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	30.051	Depositor
Minimum map value	-19.726	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	230.144, 230.144, 230.144	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.899, 0.899, 0.899	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6OU, NAG, Y01

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	0.19	0/11492	0.55	5/15579 (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
1	A	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	THR	N-CA-C	-6.92	103.82	111.36
1	A	1542	MET	CA-CB-CG	6.91	127.93	114.10
1	A	1230	GLU	CA-CB-CG	5.71	125.52	114.10
1	A	737	GLU	CA-CB-CG	5.35	124.79	114.10
1	A	822	TRP	C-N-CD	-5.25	103.47	125.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1632	ARG	Sidechain
1	A	1638	ARG	Sidechain
1	A	167	ILE	Mainchain
1	A	168	TYR	Mainchain

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	11216	0	11357	244	0
2	B	70	0	61	2	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
4	A	71	0	0	0	0
5	A	238	0	339	8	0
6	A	42	0	39	0	0
All	All	11721	0	11871	250	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 11.

All (250) 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:1514:LEU:HD23	1:A:1516:LYS:H	1.35	0.89
1:A:1378:VAL:HG23	1:A:1437:GLN:HG3	1.60	0.82
1:A:1621:LEU:O	1:A:1625:ILE:HD12	1.84	0.77
1:A:326:CYS:SG	1:A:327:GLY:N	2.58	0.77
1:A:118:HIS:ND1	1:A:119:PRO:HD2	2.01	0.75
1:A:222:ARG:HH11	1:A:225:ARG:HH22	1.32	0.75
1:A:162:TYR:O	1:A:165:THR:OG1	2.03	0.74
1:A:1835:LEU:HA	1:A:1838:MET:HE2	1.69	0.74
1:A:804:LEU:HB3	1:A:807:LEU:HD23	1.70	0.73
1:A:702:LEU:HD23	1:A:703:TRP:H	1.52	0.73
1:A:1247:THR:O	1:A:1251:VAL:HG23	1.89	0.72
1:A:1191:TRP:HZ2	1:A:1195:ARG:HH21	1.35	0.72
1:A:1208:GLU:OE2	1:A:1208:GLU:N	2.19	0.71
1:A:1417:THR:HG22	1:A:1419:LYS:HG2	1.72	0.70
1:A:1549:THR:HG22	1:A:1550:ASP:H	1.54	0.70
1:A:166:ALA:O	1:A:169:THR:OG1	2.08	0.70
1:A:1555:GLU:O	1:A:1559:ILE:HG12	1.92	0.70
1:A:1572:THR:O	1:A:1576:ILE:HG13	1.91	0.70
1:A:238:THR:HG23	1:A:239:ILE:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:MET:HG2	1:A:718:PHE:HB3	1.75	0.69
1:A:1545:MET:HE2	1:A:1545:MET:HA	1.74	0.68
1:A:197:ASP:O	1:A:200:VAL:HB	1.93	0.67
1:A:1333:SER:OG	1:A:1472:ASN:ND2	2.22	0.66
1:A:121:ARG:O	1:A:125:VAL:HG23	1.96	0.65
1:A:728:VAL:O	1:A:731:THR:HG22	1.97	0.65
1:A:724:THR:HA	1:A:727:ILE:HD12	1.79	0.65
1:A:1199:TYR:O	1:A:1203:GLU:HG2	1.96	0.65
1:A:1464:LEU:O	1:A:1468:VAL:HG23	1.96	0.65
1:A:1280:ASP:O	1:A:1284:VAL:HG23	1.96	0.64
1:A:1166:ASP:O	1:A:1195:ARG:NH2	2.30	0.64
1:A:1511:PRO:HG3	1:A:1583:ARG:HG3	1.80	0.64
1:A:271:LEU:HD21	1:A:1627:LEU:HD11	1.80	0.63
1:A:133:PHE:HZ	1:A:171:GLU:HG3	1.63	0.63
1:A:235:GLY:O	1:A:239:ILE:HG12	2.00	0.62
1:A:256:LEU:HD13	1:A:1643:ILE:HD11	1.82	0.61
1:A:22:ALA:HA	1:A:25:GLU:HG2	1.81	0.61
1:A:764:MET:HG3	1:A:765:THR:HG23	1.83	0.61
1:A:1283:LEU:O	1:A:1287:VAL:HG12	2.02	0.60
1:A:1688:ILE:HD12	1:A:1719:PRO:HG2	1.83	0.60
1:A:868:LEU:HD13	1:A:877:PRO:HG2	1.84	0.60
1:A:1531:ASP:O	1:A:1535:MET:HG2	2.02	0.59
1:A:219:ARG:O	1:A:219:ARG:NH1	2.36	0.59
1:A:222:ARG:H	1:A:222:ARG:HD3	1.67	0.59
1:A:1741:ASP:OD1	1:A:1741:ASP:N	2.36	0.59
1:A:185:ALA:HA	1:A:190:ARG:NH1	2.17	0.59
1:A:290:THR:HG23	1:A:292:GLY:H	1.69	0.58
1:A:124:ALA:HB2	1:A:177:LEU:HD11	1.86	0.58
1:A:12:SER:N	1:A:81:GLU:OE1	2.36	0.58
1:A:372:ASP:OD2	1:A:898:GLU:HA	2.05	0.57
1:A:1222:LEU:HD21	1:A:1673:ILE:HG21	1.86	0.57
1:A:125:VAL:O	1:A:129:VAL:HG22	2.05	0.57
1:A:133:PHE:CZ	1:A:171:GLU:HG3	2.39	0.57
1:A:1344:PHE:O	1:A:1347:ILE:HG22	2.05	0.57
1:A:203:MET:SD	1:A:203:MET:N	2.78	0.56
1:A:773:PRO:HA	1:A:776:TYR:HB2	1.86	0.56
1:A:890:ILE:HD11	1:A:902:THR:OG1	2.04	0.56
1:A:1554:PRO:O	1:A:1557:ILE:HG22	2.04	0.56
1:A:1785:PRO:HB2	1:A:1868:MET:HB2	1.86	0.56
1:A:1419:LYS:HE3	1:A:1710:SER:O	2.06	0.56
1:A:1552:GLN:HB3	1:A:1556:LYS:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1690:ASP:N	1:A:1690:ASP:OD1	2.38	0.56
1:A:414:MET:HE2	1:A:1775:PHE:CE1	2.40	0.56
1:A:1783:THR:HB	1:A:1866:GLY:HA2	1.88	0.56
1:A:872:ASP:O	1:A:875:LEU:HD22	2.06	0.56
1:A:1450:PHE:O	1:A:1454:ILE:HG22	2.06	0.55
1:A:1318:GLU:O	1:A:1322:VAL:HG23	2.06	0.55
1:A:155:PRO:O	1:A:158:LYS:HG2	2.07	0.54
1:A:698:GLU:HG3	1:A:773:PRO:HD2	1.89	0.54
1:A:1736:ASN:CG	1:A:1737:GLY:H	2.15	0.54
1:A:741:MET:HB3	1:A:745:PHE:CD1	2.42	0.54
1:A:1310:PRO:HB2	1:A:1670:ILE:HD11	1.89	0.54
1:A:741:MET:HB3	1:A:745:PHE:HD1	1.72	0.54
1:A:1574:GLU:HA	1:A:1577:VAL:HG22	1.90	0.54
1:A:379:GLN:HG2	1:A:1692:PHE:CE2	2.43	0.53
1:A:1564:ASN:O	1:A:1568:VAL:HG12	2.08	0.53
1:A:722:THR:O	1:A:725:MET:HG2	2.08	0.53
1:A:199:SER:HA	1:A:202:ILE:HD12	1.89	0.53
1:A:219:ARG:HG2	1:A:222:ARG:HE	1.73	0.53
1:A:760:PHE:HZ	1:A:817:LYS:HD3	1.73	0.53
1:A:1767:TYR:O	1:A:1771:ILE:HG22	2.09	0.53
1:A:860:LEU:HD22	1:A:914:LEU:HD21	1.90	0.52
1:A:881:MET:HE3	1:A:890:ILE:HG21	1.91	0.52
1:A:1594:PHE:O	1:A:1598:VAL:HG22	2.10	0.52
1:A:1485:ILE:HG23	1:A:1486:PHE:HD1	1.76	0.52
1:A:768:ILE:HG12	1:A:776:TYR:CE1	2.46	0.51
1:A:414:MET:O	1:A:418:GLU:HG2	2.11	0.51
1:A:739:TYR:HB3	1:A:1403:ASP:OD1	2.09	0.51
1:A:795:GLU:HG3	1:A:808:ARG:HE	1.76	0.51
1:A:800:ARG:HG3	1:A:801:MET:HG2	1.93	0.51
1:A:760:PHE:CZ	1:A:817:LYS:HD3	2.47	0.50
1:A:1620:THR:O	1:A:1624:VAL:HG23	2.12	0.50
1:A:1608:LEU:HD23	1:A:1625:ILE:HG21	1.92	0.50
1:A:1485:ILE:HG12	1:A:1486:PHE:CD1	2.47	0.50
1:A:1540:LEU:HB3	1:A:1567:PHE:HZ	1.77	0.50
1:A:1559:ILE:HA	1:A:1562:LYS:HG2	1.94	0.50
2:B:2:NAG:H4	2:B:3:NAG:H83	1.94	0.50
1:A:776:TYR:HD2	1:A:777:PHE:CE1	2.29	0.50
1:A:320:THR:OG1	1:A:321:SER:N	2.44	0.50
1:A:1282:SER:HB2	1:A:1309:ARG:HH22	1.76	0.50
1:A:219:ARG:CG	1:A:222:ARG:HE	2.25	0.49
1:A:222:ARG:HH11	1:A:225:ARG:NH2	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:CZ	1:A:224:LEU:HD12	2.47	0.49
1:A:741:MET:HG3	1:A:745:PHE:HB2	1.94	0.49
1:A:721:LEU:O	1:A:724:THR:HB	2.12	0.49
1:A:918:VAL:O	1:A:922:VAL:HG23	2.13	0.49
1:A:1504:LYS:HG2	1:A:1871:LEU:HD11	1.93	0.49
1:A:1534:ILE:HB	1:A:1535:MET:HE2	1.94	0.49
1:A:235:GLY:O	1:A:238:THR:HG22	2.12	0.49
1:A:1183:THR:HA	1:A:1188:GLY:HA3	1.95	0.49
1:A:169:THR:HG22	1:A:201:ILE:HD11	1.94	0.49
1:A:761:THR:HG22	1:A:789:VAL:HG22	1.94	0.49
1:A:1798:TRP:O	1:A:1802:ASP:N	2.45	0.49
1:A:795:GLU:HG3	1:A:808:ARG:NE	2.29	0.48
1:A:804:LEU:O	1:A:807:LEU:HB2	2.13	0.48
1:A:1736:ASN:CG	1:A:1737:GLY:N	2.71	0.48
1:A:256:LEU:HB2	1:A:1643:ILE:HD11	1.96	0.48
1:A:1558:ASN:O	1:A:1562:LYS:HG2	2.14	0.48
1:A:1838:MET:HE3	1:A:1860:ARG:HH22	1.76	0.48
1:A:222:ARG:HD3	1:A:222:ARG:N	2.29	0.48
1:A:702:LEU:CD2	1:A:703:TRP:H	2.22	0.48
1:A:282:ARG:O	1:A:307:TYR:OH	2.29	0.47
1:A:1415:VAL:HG13	1:A:1421:TRP:HE3	1.78	0.47
1:A:1608:LEU:HG	1:A:1622:PHE:HE1	1.79	0.47
1:A:1499:LYS:O	1:A:1499:LYS:HD3	2.13	0.47
1:A:152:ASP:N	1:A:152:ASP:OD1	2.47	0.47
1:A:795:GLU:OE2	1:A:807:LEU:HB3	2.14	0.47
1:A:1791:PHE:HB3	1:A:1872:LYS:HE3	1.96	0.47
1:A:1504:LYS:HE3	1:A:1871:LEU:HD21	1.97	0.47
1:A:14:ARG:NH1	1:A:74:GLU:O	2.44	0.46
1:A:304:LEU:HD23	1:A:308:LEU:HD23	1.96	0.46
1:A:1550:ASP:O	1:A:1552:GLN:HG3	2.14	0.46
1:A:718:PHE:O	1:A:722:THR:HG23	2.15	0.46
1:A:1368:GLU:N	1:A:1368:GLU:OE2	2.48	0.46
1:A:1477:LYS:NZ	1:A:1483:GLN:OE1	2.48	0.46
1:A:85:PRO:HB2	1:A:87:TYR:HD1	1.81	0.46
1:A:740:ASN:ND2	1:A:740:ASN:O	2.49	0.46
1:A:1512:ARG:N	1:A:1513:PRO:HD3	2.30	0.46
1:A:1301:SER:O	1:A:1304:THR:HG22	2.15	0.46
1:A:157:THR:HA	1:A:160:VAL:HG12	1.98	0.45
1:A:716:ASP:O	1:A:720:ASP:HB2	2.16	0.45
1:A:925:ILE:O	1:A:929:VAL:HG23	2.17	0.45
1:A:159:TYR:O	1:A:162:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:SER:O	1:A:309:SER:OG	2.33	0.45
1:A:328:ASN:HB2	2:B:1:NAG:N2	2.31	0.45
1:A:329:SER:HB3	1:A:332:ALA:HB2	1.98	0.45
1:A:308:LEU:HD13	1:A:308:LEU:HA	1.84	0.45
1:A:789:VAL:O	1:A:793:LEU:HG	2.16	0.45
1:A:1231:GLU:O	1:A:1233:LYS:NZ	2.49	0.45
1:A:1366:GLN:HB2	1:A:1394:TYR:CE1	2.52	0.45
1:A:1466:ILE:O	1:A:1470:ILE:HG22	2.16	0.45
1:A:379:GLN:HG2	1:A:1692:PHE:HE2	1.81	0.45
1:A:1331:ILE:O	1:A:1335:MET:HG2	2.16	0.45
1:A:1765:ASN:C	1:A:1765:ASN:HD22	2.25	0.45
1:A:1320:MET:O	1:A:1324:VAL:HG22	2.17	0.45
1:A:899:TRP:CD1	1:A:923:MET:HE1	2.52	0.45
1:A:1826:ARG:HD2	1:A:1857:PHE:HB2	1.99	0.45
1:A:1540:LEU:HB3	1:A:1567:PHE:CZ	2.52	0.45
5:A:2107:Y01:HAP1	5:A:2107:Y01:HAO2	1.49	0.45
1:A:82:ASP:O	1:A:84:ASP:N	2.49	0.44
1:A:374:TRP:HZ3	1:A:1709:THR:HG21	1.82	0.44
1:A:1303:ARG:HB3	1:A:1306:ARG:HH12	1.82	0.44
5:A:2104:Y01:HAP1	5:A:2104:Y01:HAO1	1.59	0.44
1:A:743:SER:C	1:A:745:PHE:H	2.25	0.44
1:A:1264:LYS:NZ	1:A:1268:THR:HG21	2.32	0.44
1:A:1518:GLN:HA	1:A:1521:ILE:HB	1.99	0.44
1:A:150:GLN:NE2	5:A:2107:Y01:HAT1	2.32	0.44
1:A:777:PHE:HD2	1:A:783:ILE:HG12	1.82	0.44
1:A:395:LEU:HD12	1:A:395:LEU:HA	1.82	0.44
1:A:887:ALA:O	1:A:890:ILE:HG22	2.16	0.44
1:A:193:TRP:HA	1:A:196:LEU:HG	1.98	0.44
1:A:218:LEU:HD12	1:A:219:ARG:H	1.83	0.44
1:A:226:ALA:HB3	1:A:852:ILE:HD11	1.98	0.44
1:A:1485:ILE:HG23	1:A:1486:PHE:CD1	2.53	0.44
1:A:1216:LEU:HD23	1:A:1216:LEU:HA	1.86	0.44
1:A:1608:LEU:O	1:A:1608:LEU:HD12	2.18	0.44
1:A:1705:PHE:O	1:A:1708:THR:HG22	2.17	0.43
1:A:1793:MET:HE1	1:A:1825:LEU:HD12	2.00	0.43
1:A:751:VAL:O	1:A:755:VAL:HG23	2.17	0.43
1:A:1314:LEU:HD12	1:A:1320:MET:HB3	2.00	0.43
5:A:2104:Y01:HAN1	5:A:2104:Y01:HBB	1.75	0.43
1:A:703:TRP:C	1:A:704:MET:HG3	2.43	0.43
1:A:715:MET:HE3	1:A:718:PHE:HB3	2.01	0.43
1:A:815:VAL:HG11	1:A:1347:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:ILE:HD12	1:A:1347:ILE:HA	1.81	0.43
1:A:1199:TYR:HE1	1:A:1261:TYR:CE1	2.36	0.43
1:A:822:TRP:HZ2	1:A:1339:LEU:HD13	1.83	0.43
1:A:1477:LYS:HZ3	1:A:1483:GLN:HA	1.84	0.43
1:A:1550:ASP:OD1	1:A:1550:ASP:C	2.61	0.43
1:A:381:THR:HG21	1:A:393:PHE:CZ	2.53	0.43
1:A:907:MET:HG3	1:A:912:GLN:HG3	1.99	0.43
1:A:1779:THR:HB	1:A:1782:SER:HB2	1.99	0.43
1:A:120:ILE:H	1:A:120:ILE:HG12	1.61	0.43
1:A:159:TYR:HA	1:A:162:TYR:CD2	2.53	0.43
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.71	0.43
1:A:1657:LEU:HD22	1:A:1766:MET:HG2	2.01	0.43
1:A:1827:ILE:HG12	1:A:1835:LEU:HD13	2.00	0.43
1:A:230:ILE:C	1:A:232:VAL:H	2.27	0.42
1:A:776:TYR:HB3	1:A:777:PHE:CD1	2.54	0.42
1:A:352:TYR:OH	1:A:907:MET:HB3	2.18	0.42
1:A:174:VAL:O	1:A:177:LEU:HG	2.19	0.42
1:A:228:LYS:C	1:A:230:ILE:N	2.77	0.42
1:A:903:MET:HE3	1:A:916:LEU:HD22	2.00	0.42
1:A:1785:PRO:CB	1:A:1868:MET:HB2	2.50	0.42
5:A:2108:Y01:HAC1	5:A:2108:Y01:HAP1	1.76	0.42
1:A:767:LYS:HE3	1:A:776:TYR:CE1	2.55	0.42
1:A:884:PHE:HE2	5:A:2107:Y01:HAP2	1.85	0.42
1:A:906:CYS:C	1:A:908:GLU:H	2.27	0.42
1:A:1217:LEU:HG	1:A:1246:PHE:HZ	1.85	0.42
1:A:1550:ASP:OD1	1:A:1551:ASP:N	2.53	0.42
1:A:407:LEU:HD13	1:A:1646:LEU:HD13	2.01	0.42
1:A:1374:ASN:HD21	1:A:1377:ILE:HG13	1.85	0.42
1:A:1634:LEU:HD23	1:A:1634:LEU:HA	1.87	0.42
1:A:308:LEU:HD12	1:A:344:ALA:CB	2.50	0.41
1:A:1214:MET:HE1	1:A:1249:VAL:HG21	2.02	0.41
1:A:352:TYR:CZ	1:A:907:MET:HB3	2.55	0.41
1:A:715:MET:HE3	1:A:718:PHE:CB	2.50	0.41
1:A:1230:GLU:O	1:A:1230:GLU:CD	2.63	0.41
1:A:852:ILE:O	1:A:855:VAL:HG12	2.20	0.41
1:A:1318:GLU:HG2	1:A:1488:THR:HG22	2.01	0.41
1:A:1402:PHE:HE1	1:A:1411:ALA:HB3	1.85	0.41
1:A:14:ARG:HH21	1:A:78:GLU:HG3	1.85	0.41
1:A:747:GLU:O	1:A:751:VAL:HG22	2.21	0.41
1:A:780:GLY:HA2	1:A:783:ILE:HD12	2.02	0.41
1:A:1265:LYS:C	1:A:1267:PHE:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:O	1:A:328:ASN:OD1	2.39	0.41
1:A:1838:MET:HE3	1:A:1838:MET:HB2	1.88	0.41
1:A:118:HIS:CD2	1:A:120:ILE:HD11	2.56	0.41
1:A:146:VAL:HG12	1:A:147:PHE:HD1	1.85	0.41
1:A:259:PHE:CE1	1:A:1636:LEU:HD11	2.55	0.41
1:A:825:LEU:HD12	1:A:825:LEU:HA	1.73	0.41
1:A:868:LEU:HD23	1:A:868:LEU:HA	1.88	0.41
1:A:1507:GLN:HB3	1:A:1508:LYS:H	1.67	0.41
1:A:1640:ALA:O	1:A:1643:ILE:HG22	2.20	0.41
1:A:1672:SER:HB2	1:A:1704:LEU:HD12	2.03	0.41
1:A:1856:ALA:O	1:A:1860:ARG:HG3	2.21	0.41
1:A:825:LEU:O	1:A:829:ILE:HG12	2.20	0.40
1:A:1453:PHE:CD1	1:A:1453:PHE:C	2.98	0.40
1:A:1720:ILE:O	1:A:1720:ILE:HG22	2.22	0.40
1:A:1785:PRO:HA	1:A:1862:LEU:HD23	2.03	0.40
1:A:1403:ASP:OD1	1:A:1403:ASP:O	2.39	0.40
1:A:1422:MET:HA	1:A:1422:MET:HE3	2.02	0.40
1:A:414:MET:HE3	1:A:414:MET:HB2	1.89	0.40
5:A:2102:Y01:HAC2	5:A:2102:Y01:HAJ2	1.74	0.40
1:A:222:ARG:N	1:A:222:ARG:CD	2.85	0.40
1:A:377:LEU:O	1:A:381:THR:HG22	2.20	0.40
1:A:1521:ILE:O	1:A:1525:VAL:HG13	2.21	0.40
1:A:220:THR:HG23	5:A:2103:Y01:HAQ2	2.02	0.40
1:A:1274:LEU:HD21	1:A:1311:LEU:HG	2.03	0.40
1:A:1530:PHE:O	1:A:1533:THR:OG1	2.32	0.40
1:A:1631:GLY:O	1:A:1632:ARG:HG2	2.22	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	1312/2016 (65%)	1215 (93%)	97 (7%)	0	100 100

There are no Ramachandran outliers to report.

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	1232/1763 (70%)	1226 (100%)	6 (0%)	81 82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	228	LYS
1	A	858	MET
1	A	1632	ARG
1	A	1638	ARG
1	A	1662	LEU

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

Mol	Chain	Res	Type
1	A	90	GLN
1	A	144	ASN
1	A	803	ASN
1	A	834	ASN
1	A	1366	GLN
1	A	1383	GLN
1	A	1437	GLN
1	A	1475	GLN
1	A	1552	GLN
1	A	1558	ASN
1	A	1695	GLN
1	A	1699	ASN

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Mol	Chain	Res	Type
1	A	1765	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

11 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.71	1 (7%)	17,19,21	0.93	1 (5%)
2	NAG	B	2	2	14,14,15	0.51	0	17,19,21	0.42	0
2	NAG	B	3	2	14,14,15	0.34	0	17,19,21	0.35	0
2	NAG	B	4	2	14,14,15	0.28	0	17,19,21	0.47	0
2	NAG	B	5	2	14,14,15	0.38	0	17,19,21	0.36	0
3	NAG	C	1	3	14,14,15	0.39	0	17,19,21	0.34	0
3	NAG	C	2	3	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	D	1	3	14,14,15	0.76	1 (7%)	17,19,21	0.50	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	E	1	3,1	14,14,15	0.23	0	17,19,21	0.54	0
3	NAG	E	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.03	1 (5%)

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	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	B	3	2	-	2/6/23/26	0/1/1/1
2	NAG	B	4	2	-	0/6/23/26	0/1/1/1
2	NAG	B	5	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.64	1.39	1.43
3	E	2	NAG	O5-C1	2.45	1.47	1.43
2	B	1	NAG	C1-C2	2.06	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C1-O5-C5	3.75	117.22	112.19
2	B	1	NAG	C1-O5-C5	3.40	116.74	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	3	NAG	C8-C7-N2-C2
2	B	3	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	5	NAG	O5-C5-C6-O6
2	B	5	NAG	C4-C5-C6-O6

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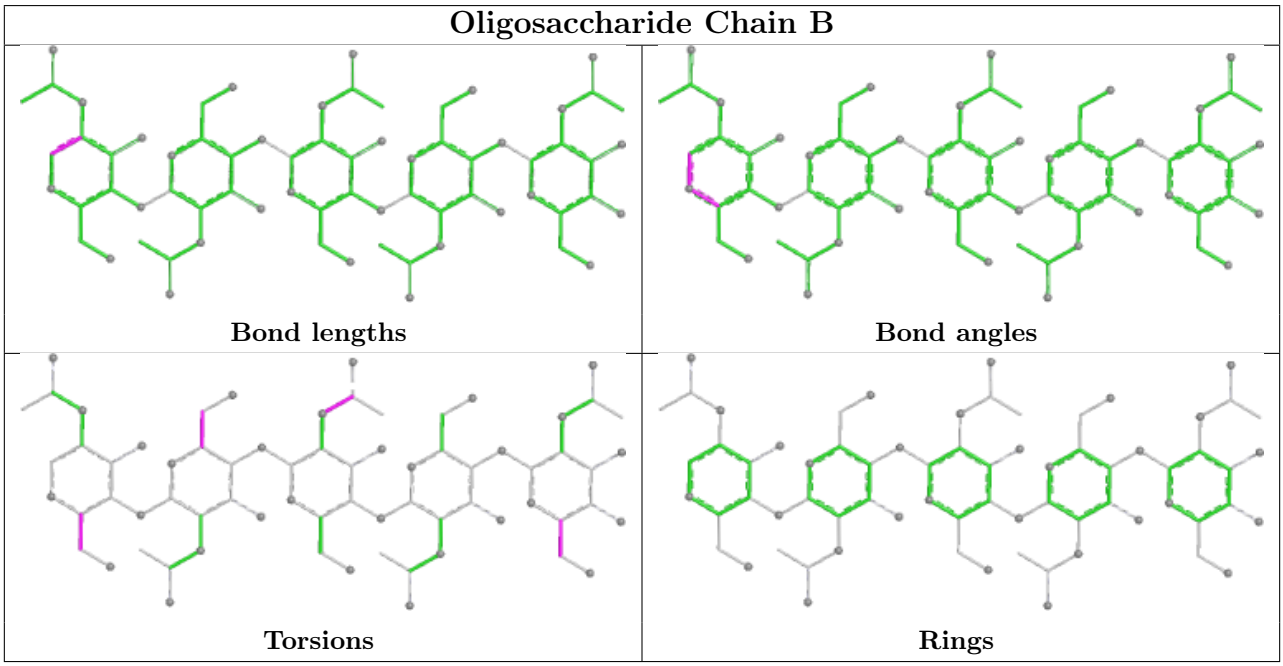
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C3-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	E	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C1-C2-N2-C7
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

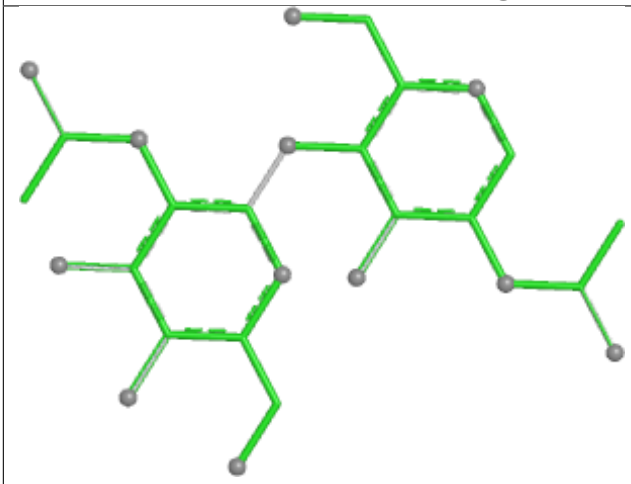
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	B	3	NAG	1	0
2	B	1	NAG	1	0

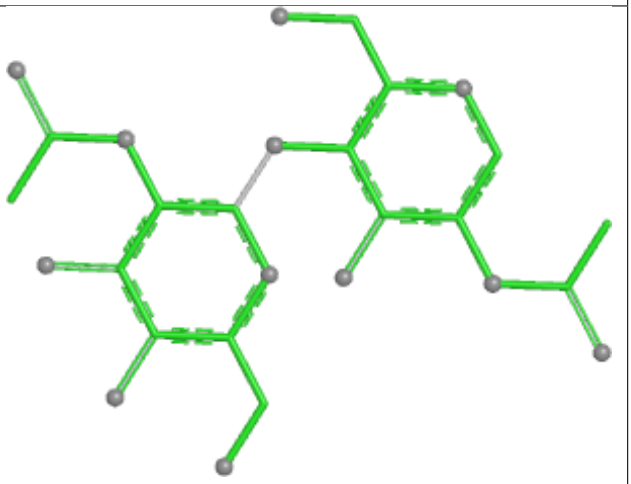
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



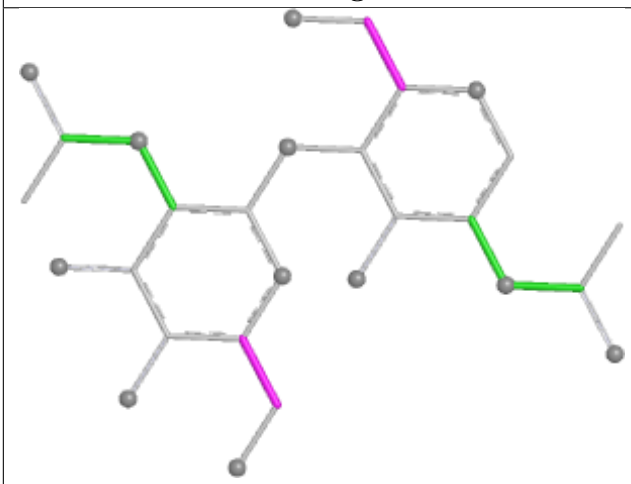
Oligosaccharide Chain C



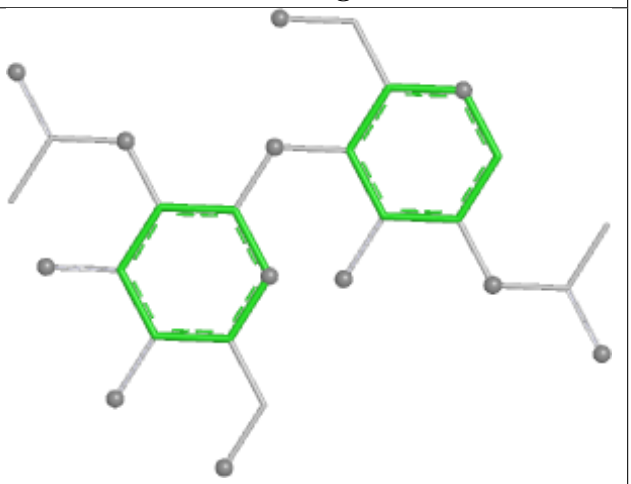
Bond lengths



Bond angles

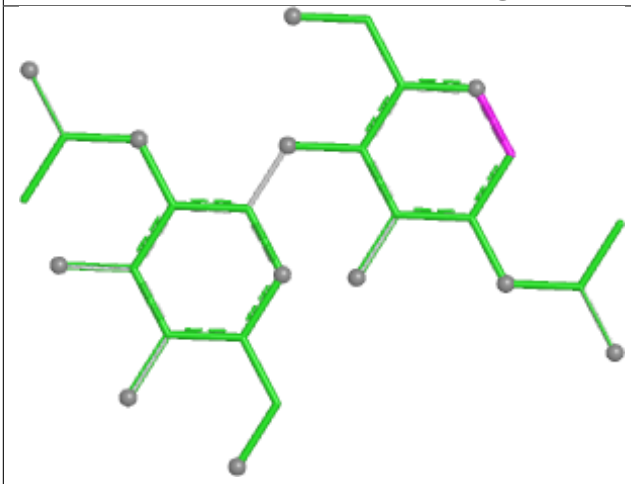


Torsions

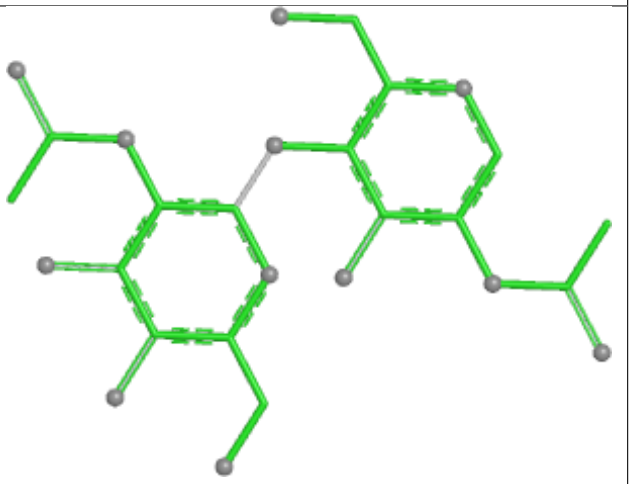


Rings

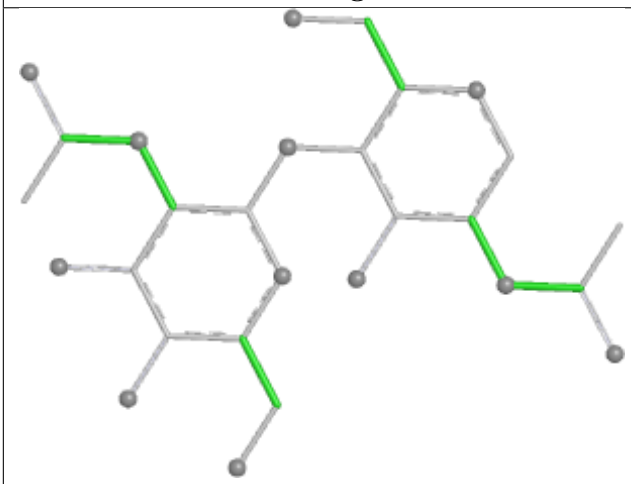
Oligosaccharide Chain D



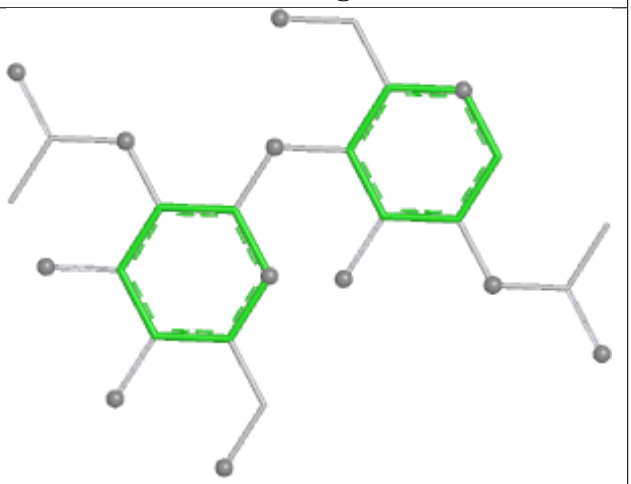
Bond lengths



Bond angles

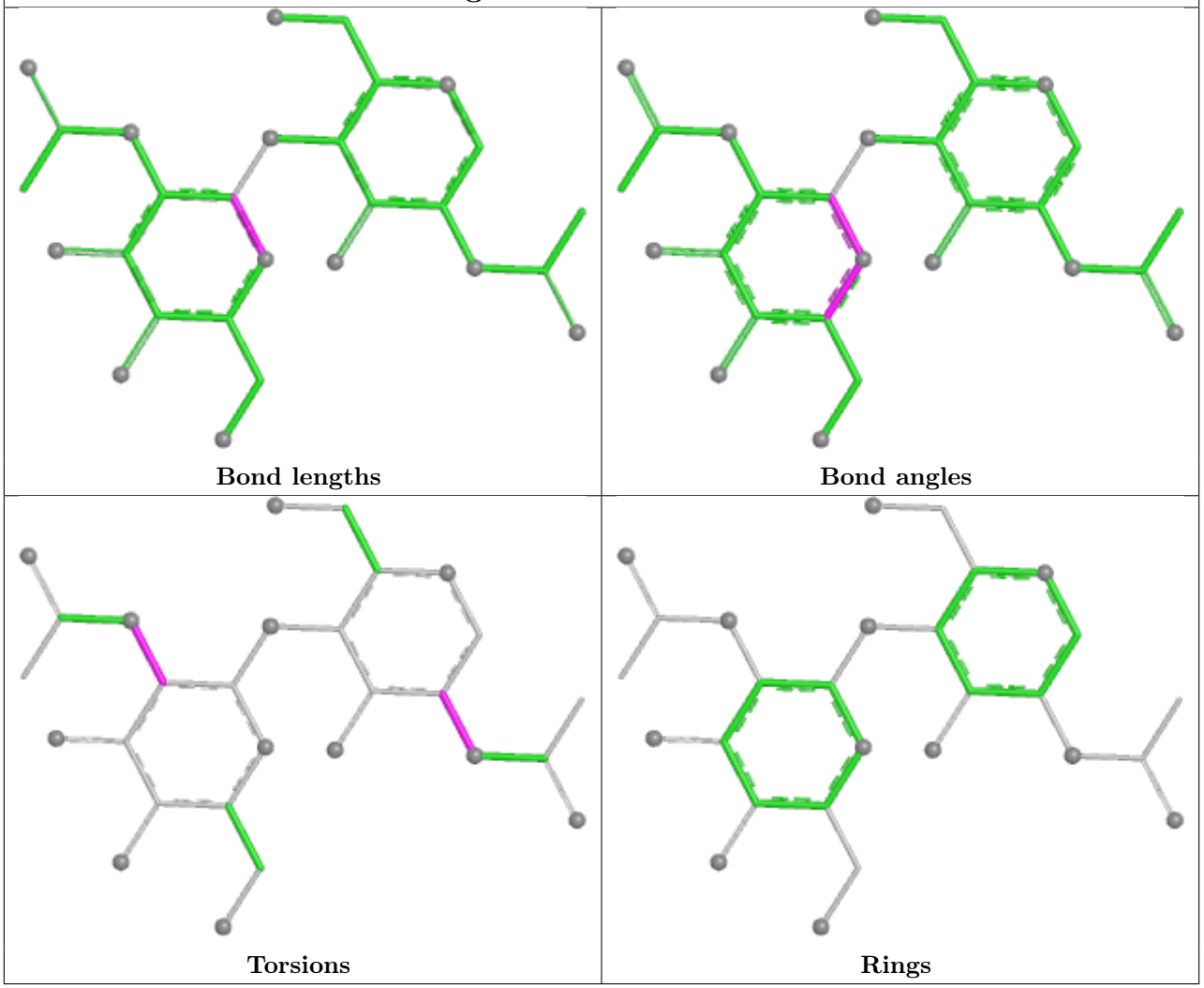


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
5	Y01	A	2107	-	38,38,38	0.56	0	57,57,57	0.57	0
5	Y01	A	2103	-	38,38,38	0.55	0	57,57,57	0.67	0
5	Y01	A	2102	-	38,38,38	0.54	0	57,57,57	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	6OU	A	2101	-	30,30,48	0.72	1 (3%)	33,35,53	1.08	2 (6%)
5	Y01	A	2108	-	31,31,38	0.40	0	48,48,57	0.88	1 (2%)
6	NAG	A	2109	1	14,14,15	0.21	0	17,19,21	0.43	0
5	Y01	A	2105	-	38,38,38	0.56	0	57,57,57	0.55	0
5	Y01	A	2106	-	38,38,38	0.55	0	57,57,57	0.86	2 (3%)
6	NAG	A	2110	1	14,14,15	0.24	0	17,19,21	0.39	0
5	Y01	A	2104	-	38,38,38	0.55	0	57,57,57	0.58	0
4	6OU	A	2112	-	39,39,48	0.53	0	42,44,53	0.51	0
6	NAG	A	2111	1	14,14,15	0.29	0	17,19,21	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	Y01	A	2107	-	-	12/19/77/77	0/4/4/4
5	Y01	A	2103	-	-	10/19/77/77	0/4/4/4
5	Y01	A	2102	-	-	11/19/77/77	0/4/4/4
4	6OU	A	2101	-	-	16/32/32/52	-
5	Y01	A	2108	-	-	5/10/68/77	0/4/4/4
6	NAG	A	2109	1	-	2/6/23/26	0/1/1/1
5	Y01	A	2105	-	-	7/19/77/77	0/4/4/4
5	Y01	A	2106	-	-	9/19/77/77	0/4/4/4
6	NAG	A	2110	1	-	2/6/23/26	0/1/1/1
5	Y01	A	2104	-	-	7/19/77/77	0/4/4/4
4	6OU	A	2112	-	-	6/43/43/52	-
6	NAG	A	2111	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2101	6OU	P23-O26	2.54	1.64	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2101	6OU	O26-P23-O22	-4.88	93.95	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2108	Y01	CBI-CBE-CBB	3.40	124.74	119.50
5	A	2106	Y01	CAV-CAZ-CAI	-2.32	117.42	120.57
5	A	2106	Y01	CAD-CBH-CBF	-2.18	109.22	111.66
4	A	2101	6OU	O25-P23-O24	2.10	119.00	110.83

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2103	Y01	OAG-CAY-OAW-CBC
5	A	2103	Y01	CAM-CAY-OAW-CBC
5	A	2106	Y01	OAG-CAY-OAW-CBC
5	A	2106	Y01	CAM-CAY-OAW-CBC
5	A	2107	Y01	OAG-CAY-OAW-CBC
5	A	2107	Y01	CAM-CAY-OAW-CBC
5	A	2108	Y01	CAO-CBB-CBE-CBI
5	A	2103	Y01	CAR-CBC-OAW-CAY
5	A	2107	Y01	CAV-CBC-OAW-CAY
4	A	2101	6OU	O17-C16-O18-C19
4	A	2112	6OU	O17-C16-O18-C19
5	A	2106	Y01	CAC-CBB-CBE-CAP
5	A	2106	Y01	CAC-CBB-CBE-CBI
4	A	2112	6OU	C15-C16-O18-C19
5	A	2104	Y01	CAC-CBB-CBE-CAP
5	A	2107	Y01	CAC-CBB-CBE-CAP
4	A	2101	6OU	C15-C16-O18-C19
5	A	2107	Y01	CAJ-CAO-CBB-CAC
5	A	2108	Y01	CAC-CBB-CBE-CAP
5	A	2106	Y01	CAO-CBB-CBE-CAP
5	A	2106	Y01	CAO-CBB-CBE-CBI
6	A	2111	NAG	O5-C5-C6-O6
5	A	2102	Y01	CAJ-CAO-CBB-CAC
5	A	2104	Y01	CAC-CBB-CBE-CBI
5	A	2107	Y01	CAC-CBB-CBE-CBI
5	A	2104	Y01	CAO-CBB-CBE-CAP
5	A	2107	Y01	CAO-CBB-CBE-CAP
5	A	2108	Y01	CAO-CBB-CBE-CAP
5	A	2104	Y01	CAO-CBB-CBE-CBI
5	A	2107	Y01	CAO-CBB-CBE-CBI
5	A	2105	Y01	CAJ-CAO-CBB-CAC
5	A	2105	Y01	CAJ-CAO-CBB-CBE
4	A	2101	6OU	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	A	2103	Y01	CAO-CBB-CBE-CBI
6	A	2111	NAG	C4-C5-C6-O6
4	A	2101	6OU	C13-C14-C15-C16
6	A	2109	NAG	O5-C5-C6-O6
6	A	2111	NAG	C8-C7-N2-C2
6	A	2111	NAG	O7-C7-N2-C2
6	A	2110	NAG	O5-C5-C6-O6
5	A	2102	Y01	CAJ-CAO-CBB-CBE
5	A	2103	Y01	CAV-CBC-OAW-CAY
5	A	2108	Y01	CAC-CBB-CBE-CBI
5	A	2108	Y01	CAN-CAJ-CAO-CBB
5	A	2102	Y01	CAN-CAJ-CAO-CBB
5	A	2103	Y01	CAC-CBB-CBE-CBI
5	A	2103	Y01	CAC-CBB-CBE-CAP
5	A	2103	Y01	CAO-CBB-CBE-CAP
5	A	2102	Y01	CAO-CBB-CBE-CBI
6	A	2109	NAG	C4-C5-C6-O6
4	A	2101	6OU	C33-C34-C35-C36
4	A	2112	6OU	C19-C20-C21-O22
5	A	2107	Y01	CAR-CBC-OAW-CAY
5	A	2102	Y01	CAC-CBB-CBE-CBI
4	A	2101	6OU	O30-C20-C21-O22
5	A	2102	Y01	CAO-CBB-CBE-CAP
5	A	2106	Y01	CAX-CAL-CAM-CAY
4	A	2101	6OU	C38-C39-C40-C41
5	A	2102	Y01	CAC-CBB-CBE-CAP
4	A	2112	6OU	O30-C20-C21-O22
4	A	2101	6OU	O18-C19-C20-C21
5	A	2102	Y01	CAM-CAY-OAW-CBC
4	A	2101	6OU	O18-C19-C20-O30
4	A	2101	6OU	C10-C11-C12-C13
5	A	2107	Y01	CAX-CAL-CAM-CAY
5	A	2102	Y01	OAG-CAY-OAW-CBC
4	A	2101	6OU	C21-O22-P23-O24
5	A	2104	Y01	CAN-CAJ-CAO-CBB
4	A	2112	6OU	C11-C12-C13-C14
5	A	2105	Y01	CAM-CAL-CAX-OAF
4	A	2101	6OU	C19-C20-C21-O22
5	A	2106	Y01	CAM-CAL-CAX-OAF
4	A	2101	6OU	C34-C35-C36-C37
5	A	2104	Y01	CAM-CAL-CAX-OAF
5	A	2106	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
5	A	2104	Y01	CAM-CAL-CAX-OAH
5	A	2105	Y01	CAM-CAL-CAX-OAH
5	A	2107	Y01	CAM-CAL-CAX-OAF
6	A	2110	NAG	C4-C5-C6-O6
5	A	2102	Y01	CAM-CAL-CAX-OAF
5	A	2102	Y01	CAM-CAL-CAX-OAH
5	A	2105	Y01	CAO-CBB-CBE-CAP
4	A	2112	6OU	C20-C21-O22-P23
4	A	2101	6OU	C14-C15-C16-O18
5	A	2107	Y01	CAM-CAL-CAX-OAH
5	A	2105	Y01	CAC-CBB-CBE-CBI
5	A	2103	Y01	CAM-CAL-CAX-OAF
4	A	2101	6OU	C14-C15-C16-O17
5	A	2105	Y01	CAX-CAL-CAM-CAY
5	A	2103	Y01	CAM-CAL-CAX-OAH
4	A	2101	6OU	C11-C12-C13-C14

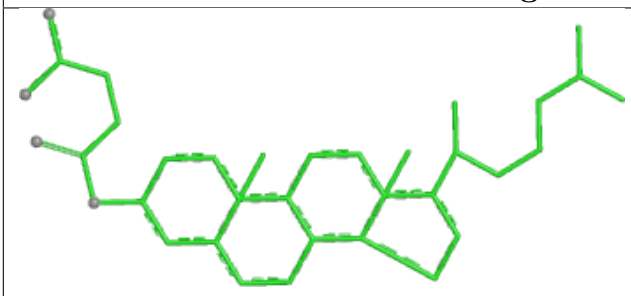
There are no ring outliers.

5 monomers are involved in 8 short contacts:

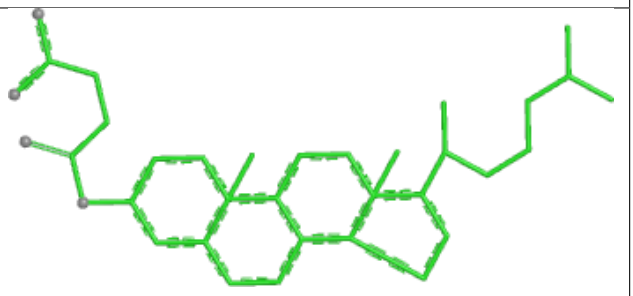
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2107	Y01	3	0
5	A	2103	Y01	1	0
5	A	2102	Y01	1	0
5	A	2108	Y01	1	0
5	A	2104	Y01	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

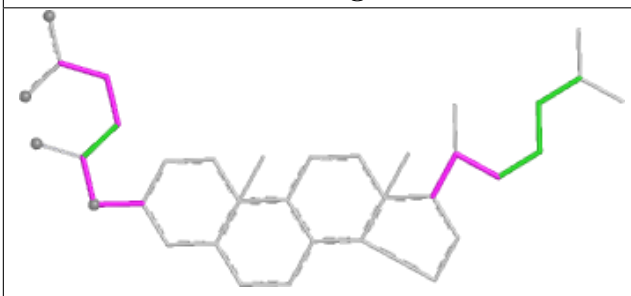
Ligand Y01 A 2107



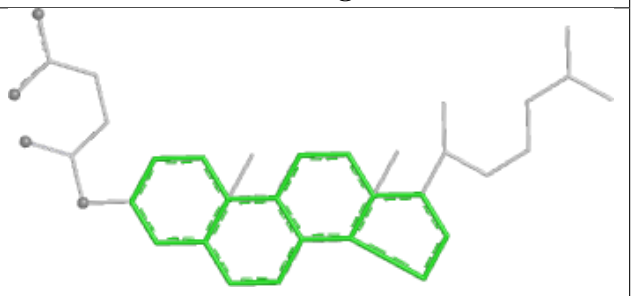
Bond lengths



Bond angles

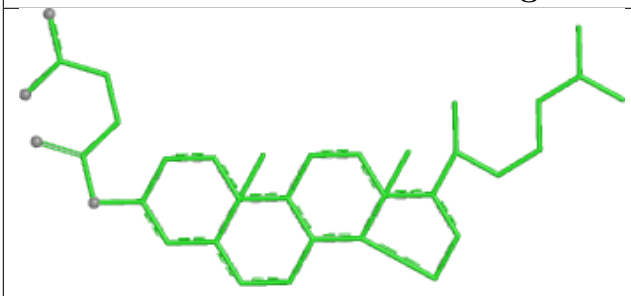


Torsions



Rings

Ligand Y01 A 2103



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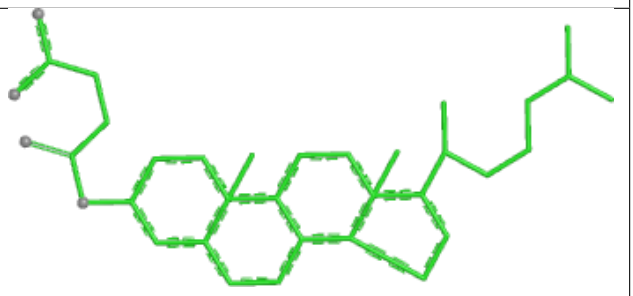

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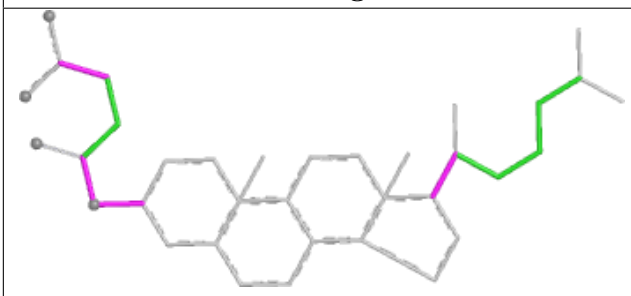
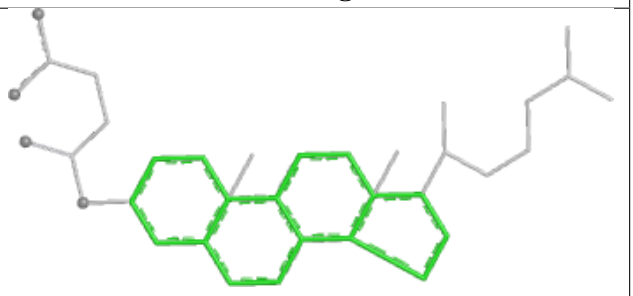
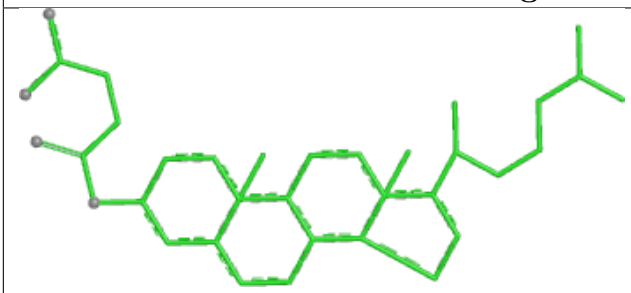


Torsions



Rings

Ligand Y01 A 2102



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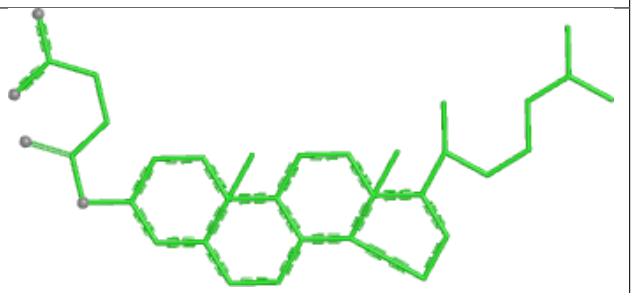
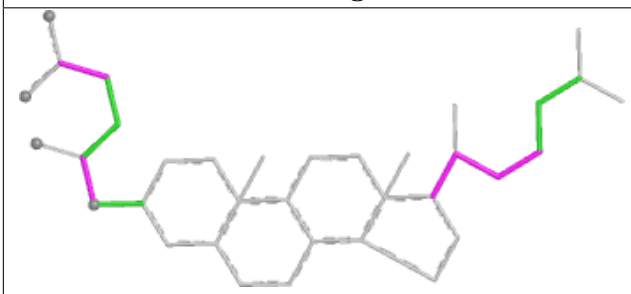
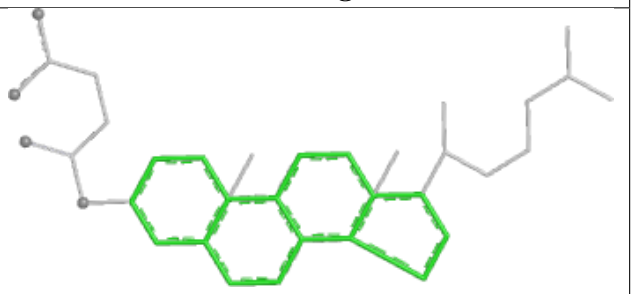


Bond angles

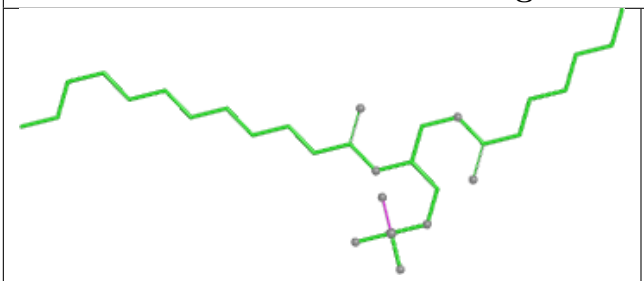


Torsions



Rings

Ligand 6OU A 2101



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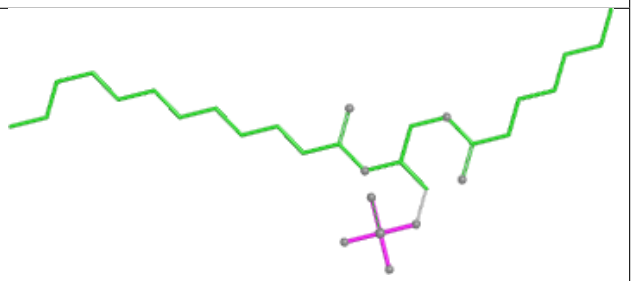
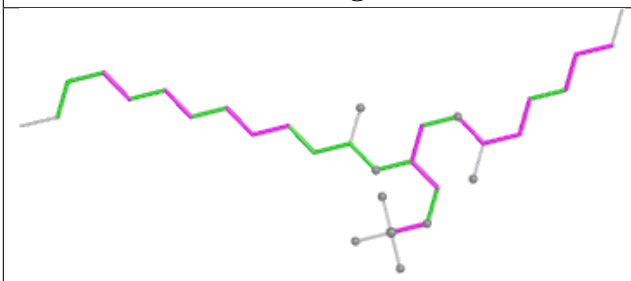


Bond angles



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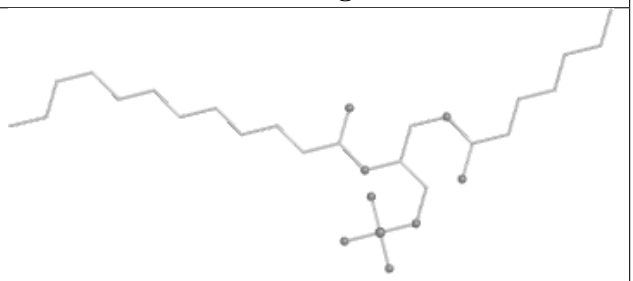
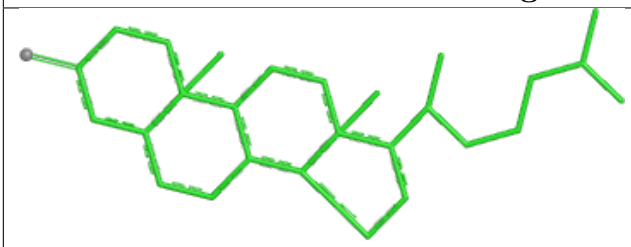
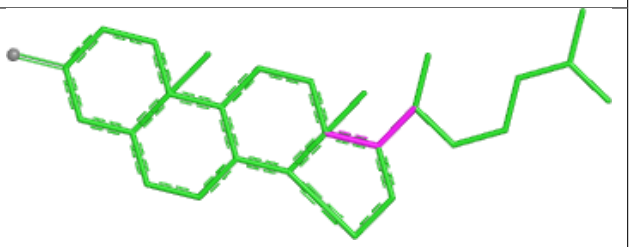


Rings

Ligand Y01 A 2108



Bond lengths



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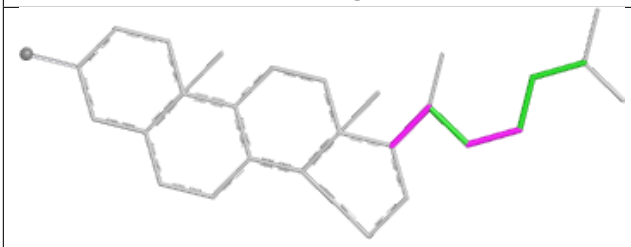

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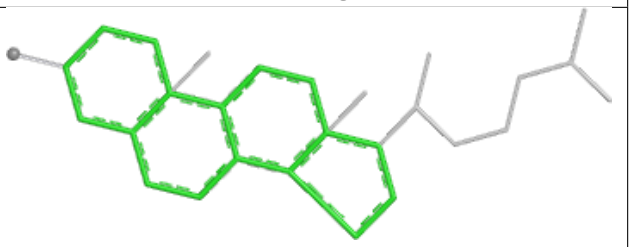
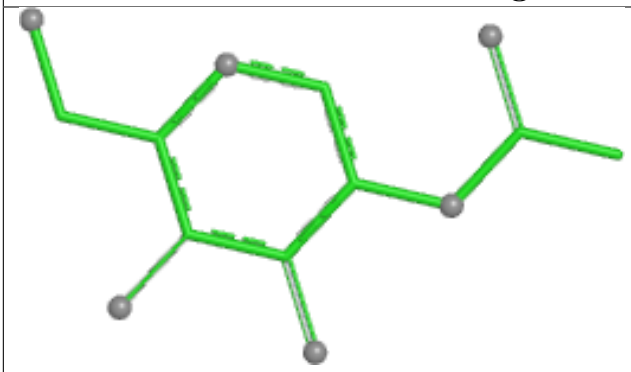


Rings

Ligand NAG A 2109



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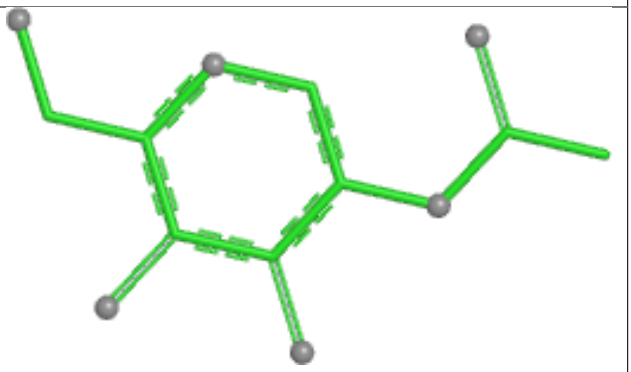
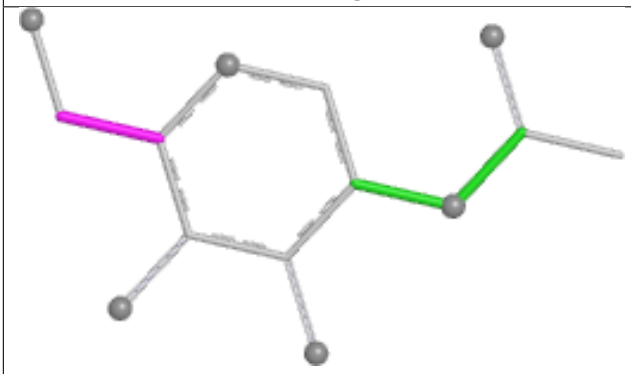


Bond angles



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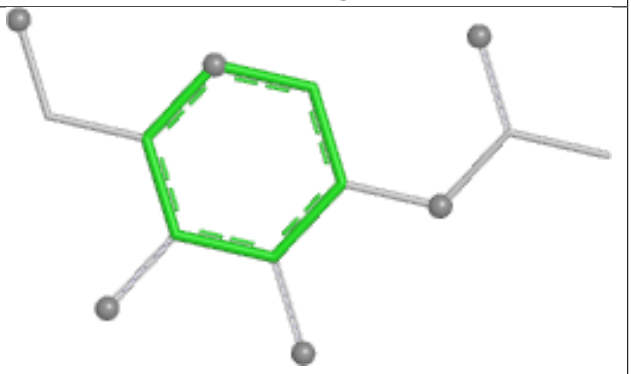
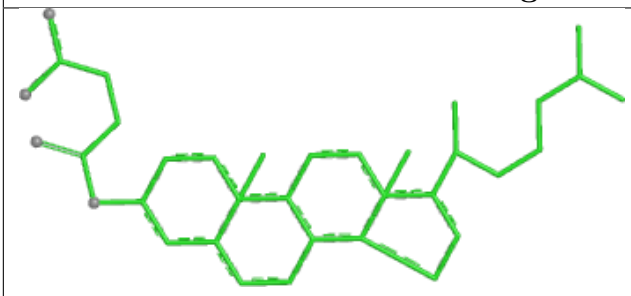
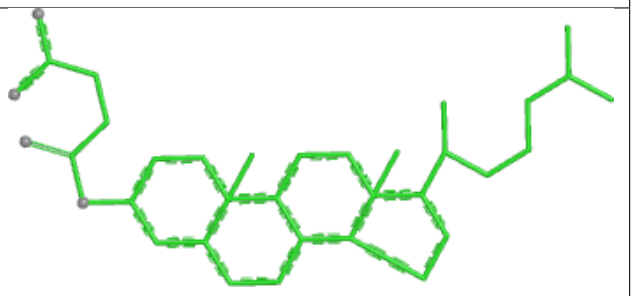


Rings

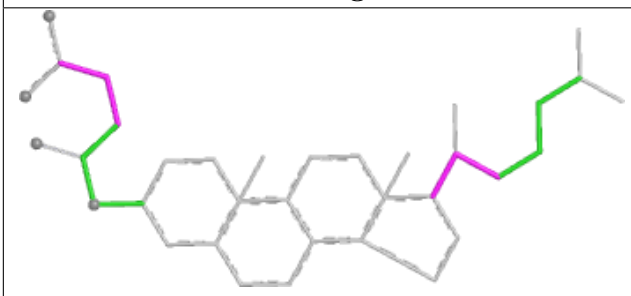
Ligand Y01 A 2105



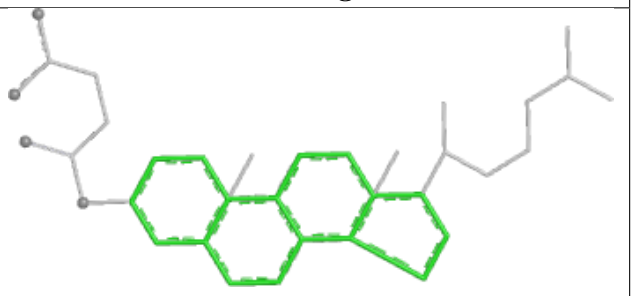
Bond lengths



Bond angles

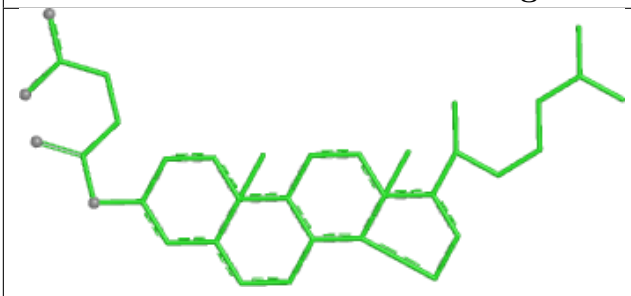


Torsions

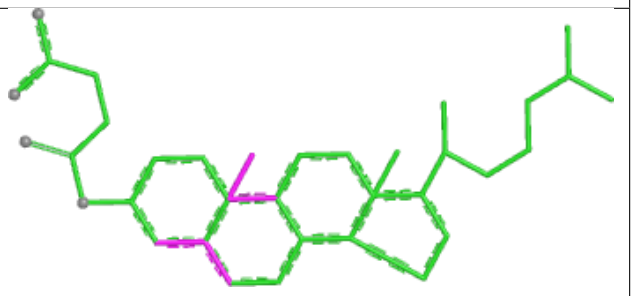


Rings

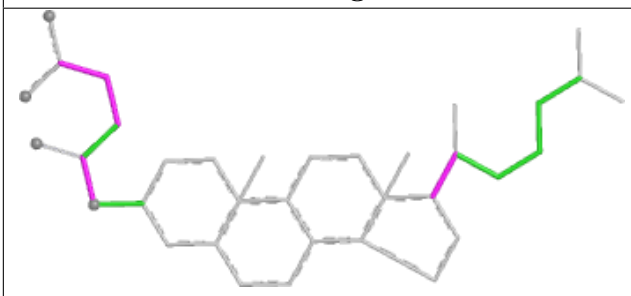
Ligand Y01 A 2106



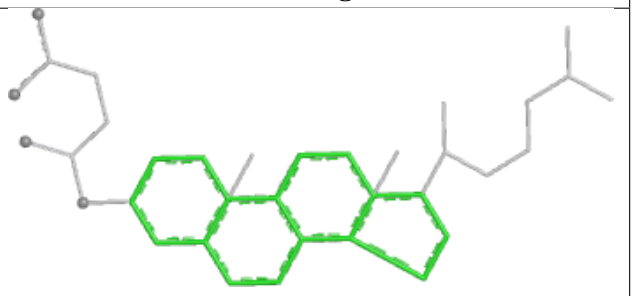
Bond lengths



Bond angles

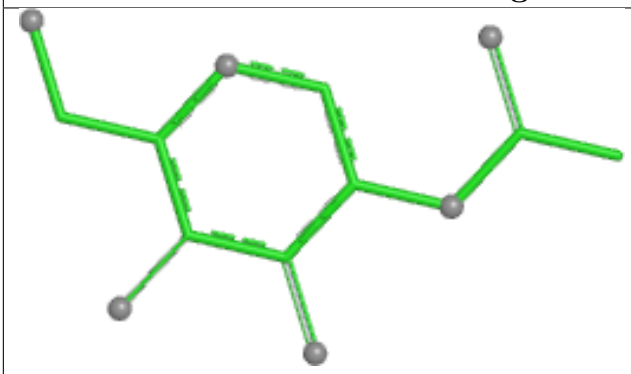


Torsions

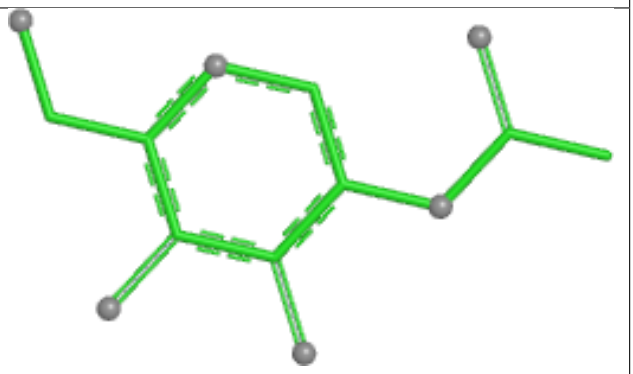


Rings

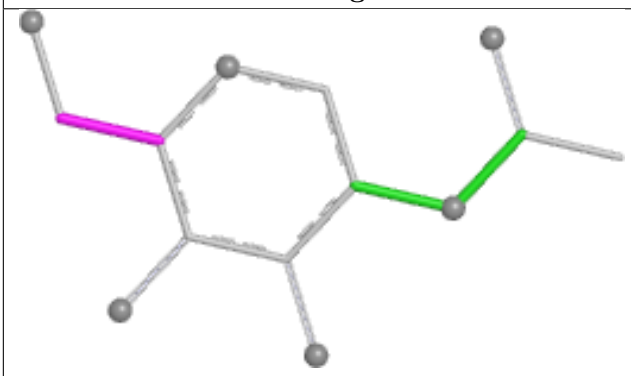
Ligand NAG A 2110



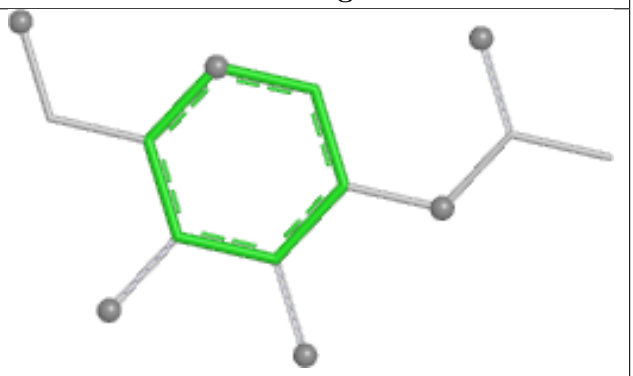
Bond lengths



Bond angles

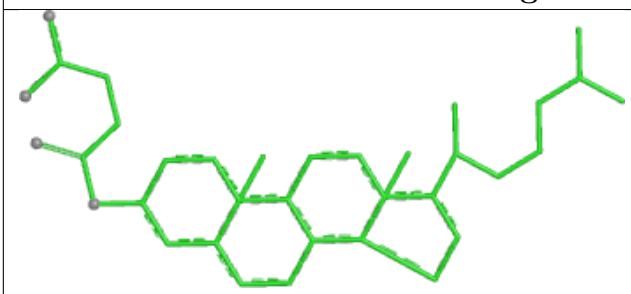


Torsions

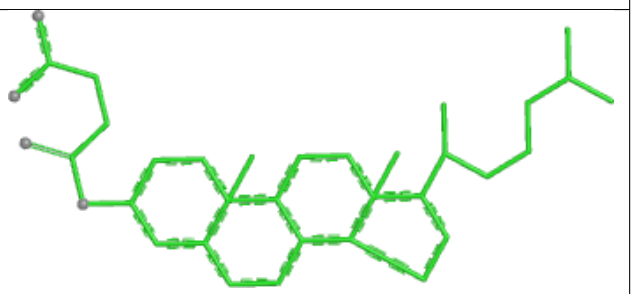


Rings

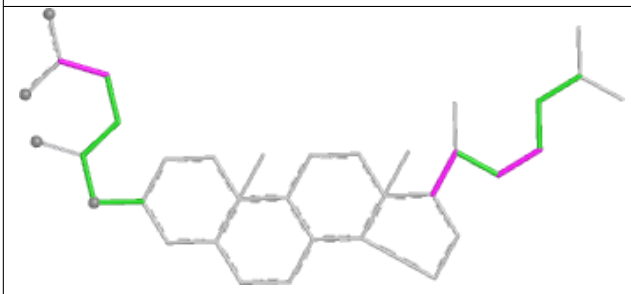
Ligand Y01 A 2104



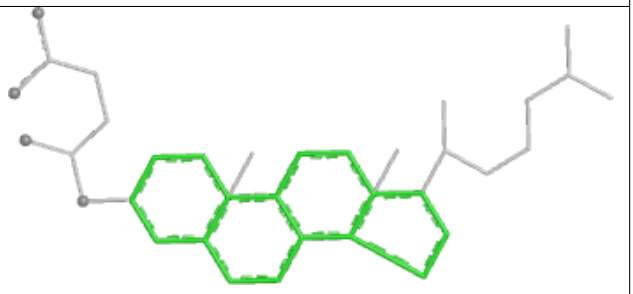
Bond lengths



Bond angles

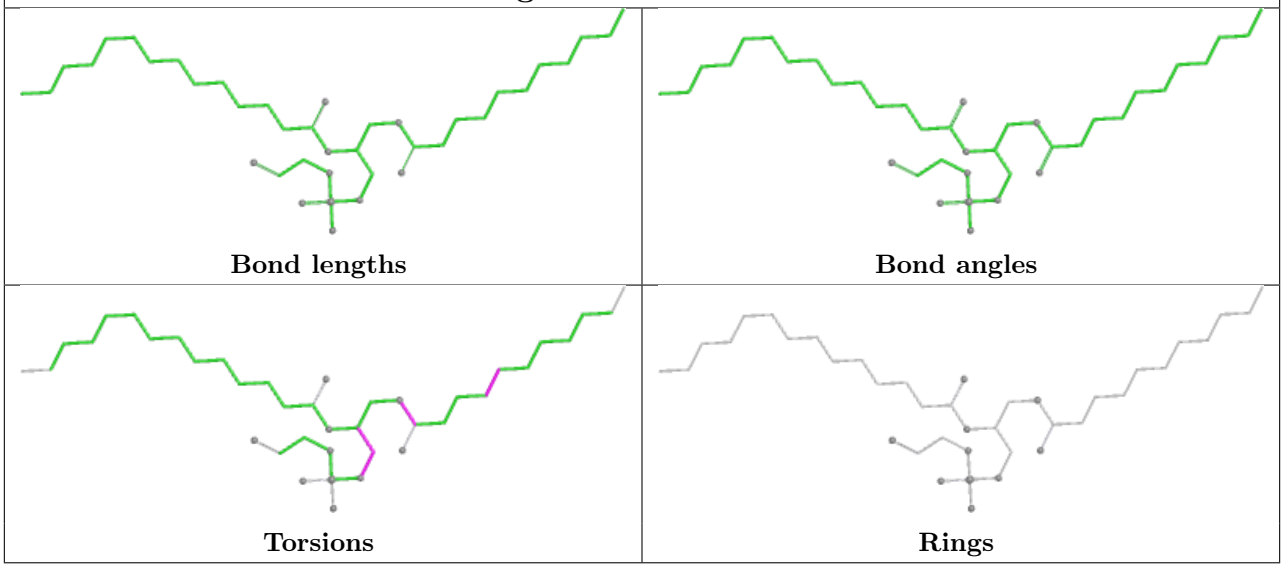


Torsions

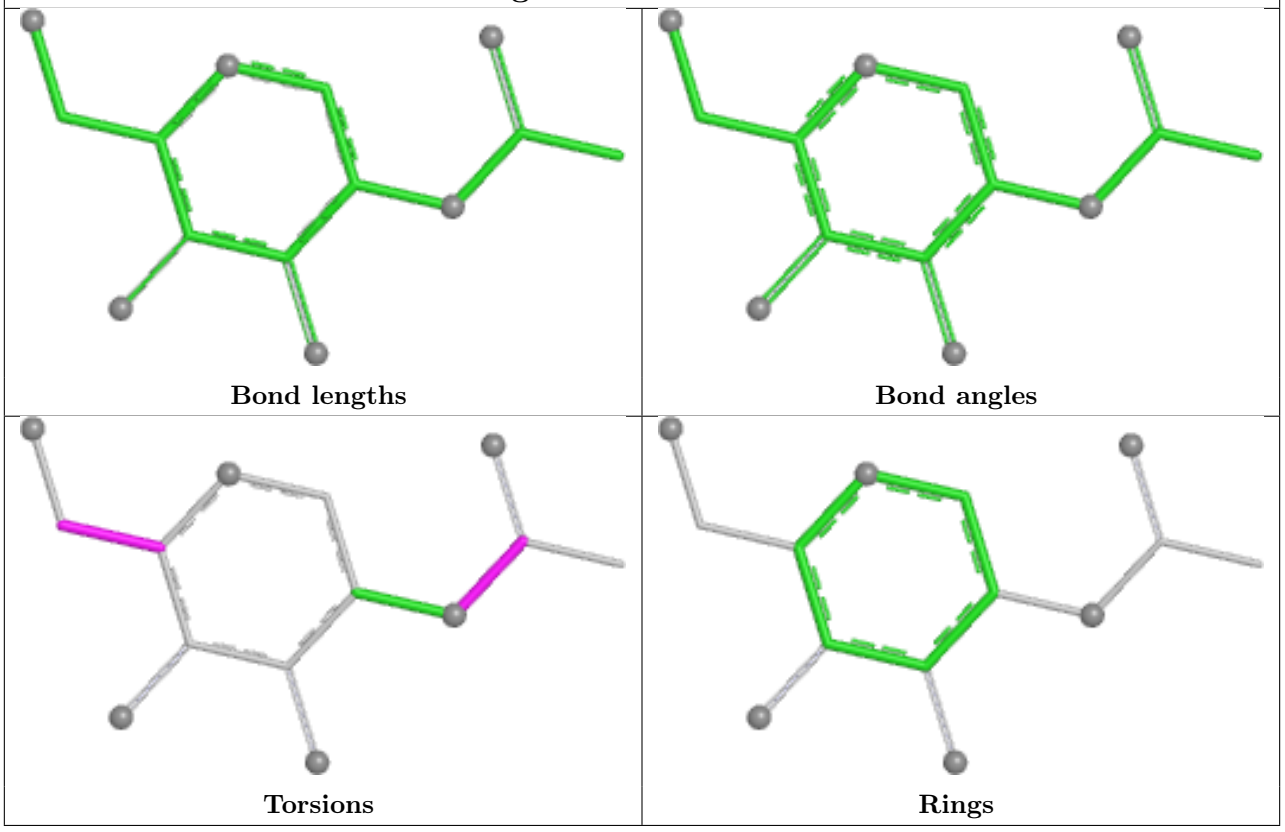


Rings

Ligand 6OU A 2112



Ligand NAG A 2111



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.

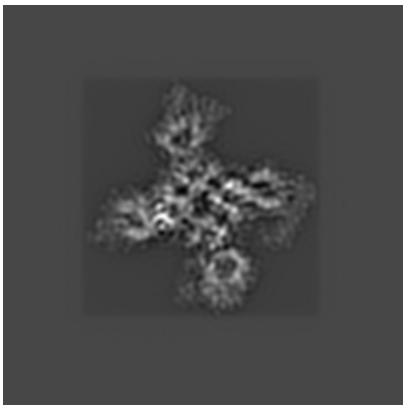
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43663. These allow visual inspection of the internal detail of the map and identification of artifacts.

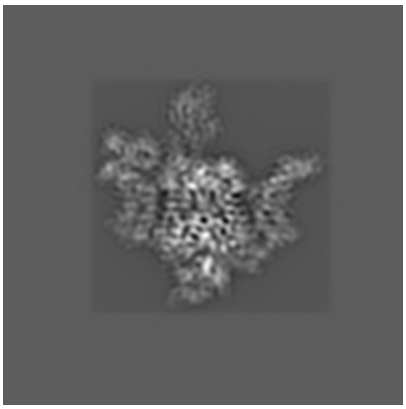
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

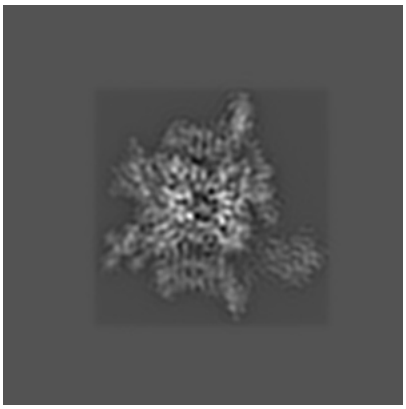
6.1.1 Primary map



X

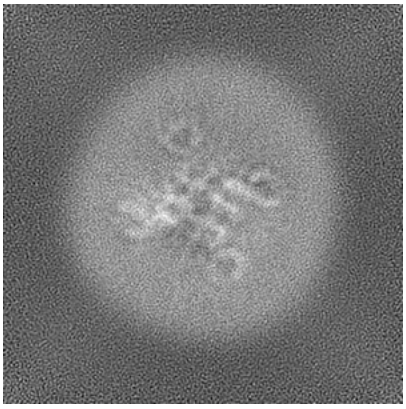


Y

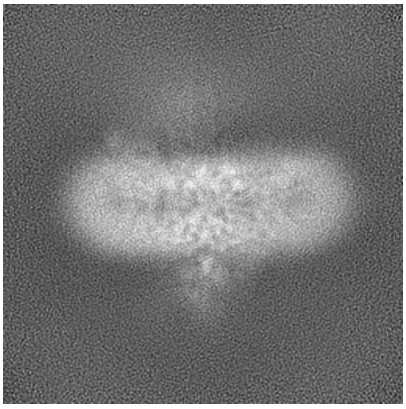


Z

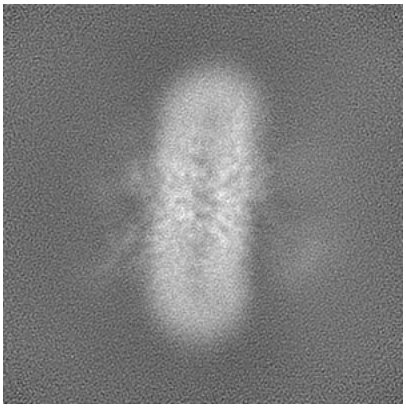
6.1.2 Raw map



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: 128

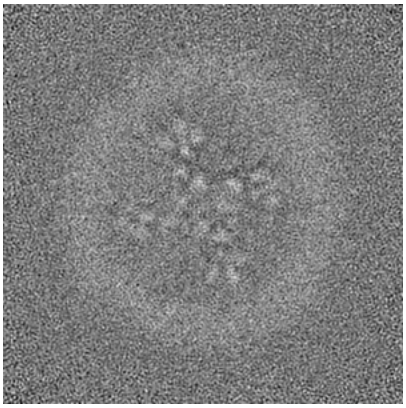


Y Index: 128

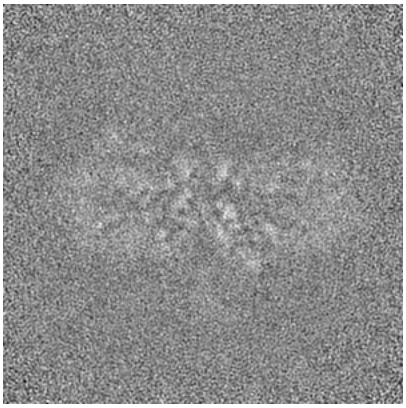


Z Index: 128

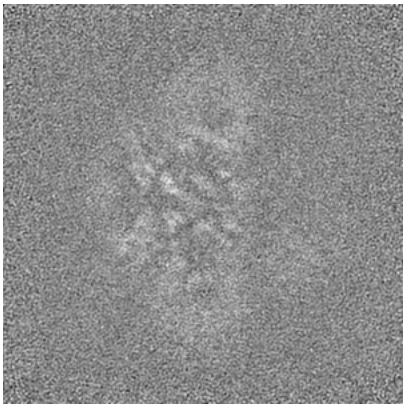
6.2.2 Raw map



X Index: 128



Y Index: 128

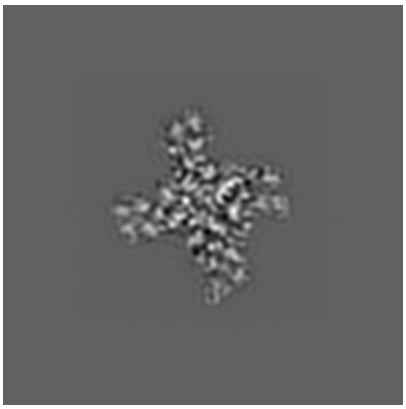


Z Index: 128

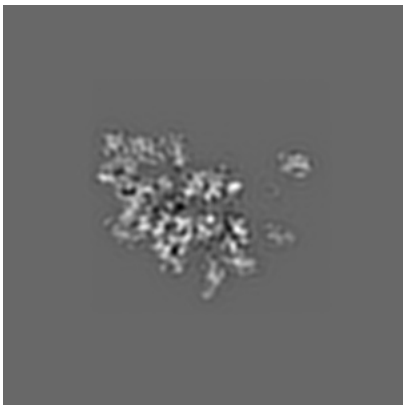
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 115

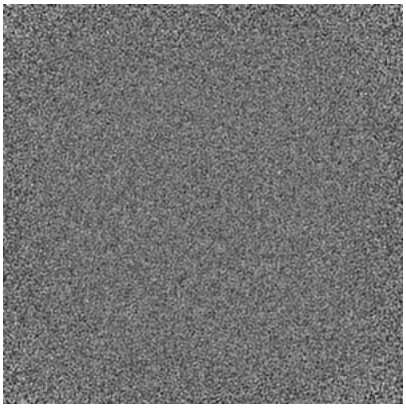


Y Index: 134

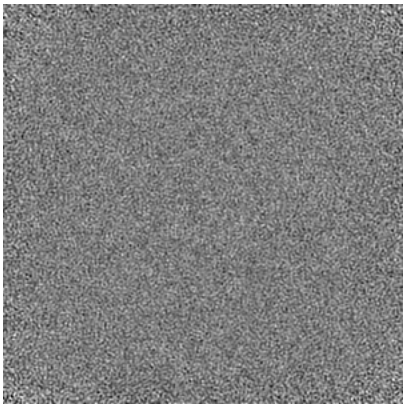


Z Index: 130

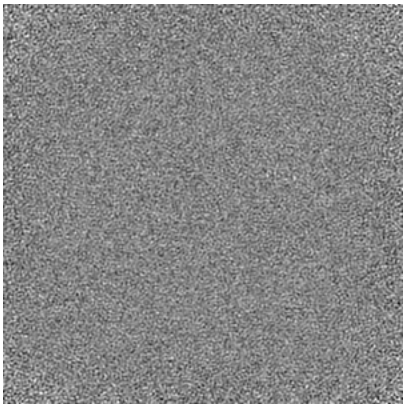
6.3.2 Raw map



X Index: 0



Y Index: 0

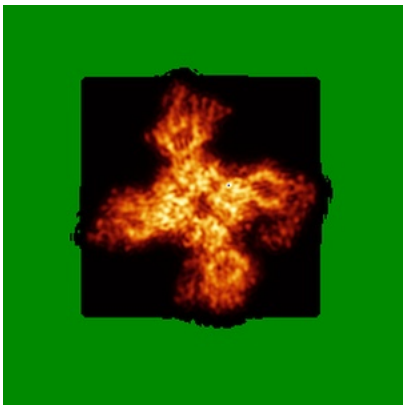


Z Index: 0

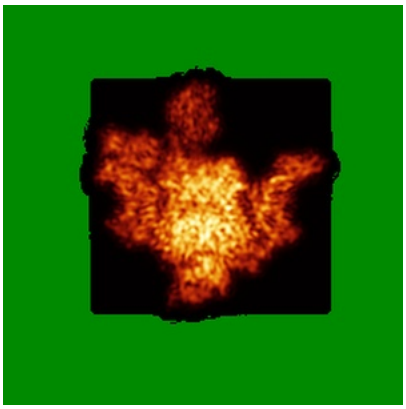
The images above show the largest variance slices of the map in three orthogonal directions.

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

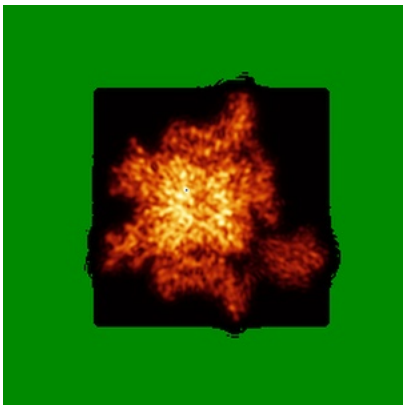
6.4.1 Primary map



X

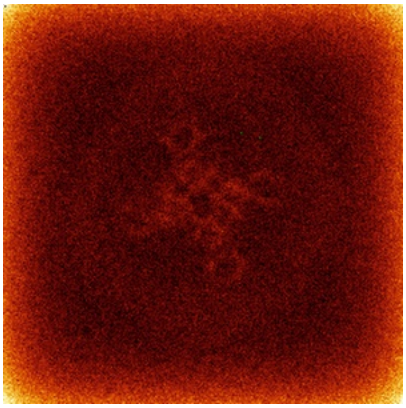


Y

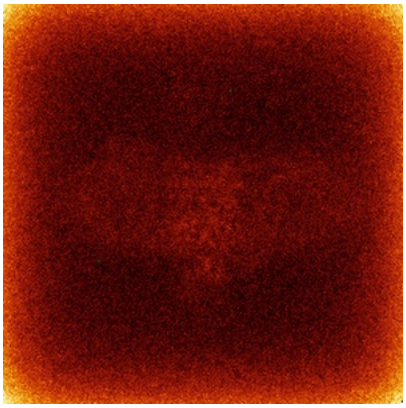


Z

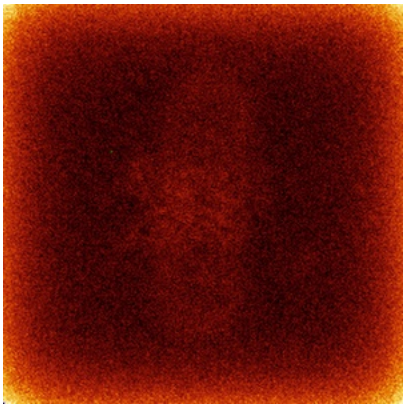
6.4.2 Raw map



X



Y

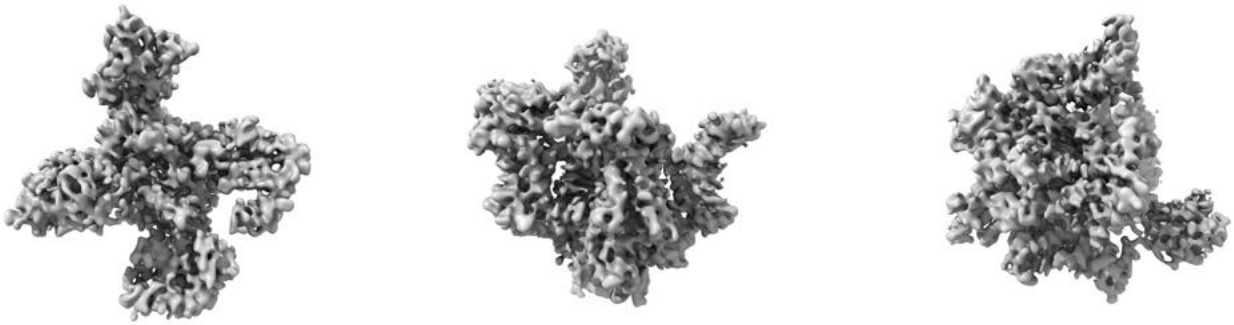


Z

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)

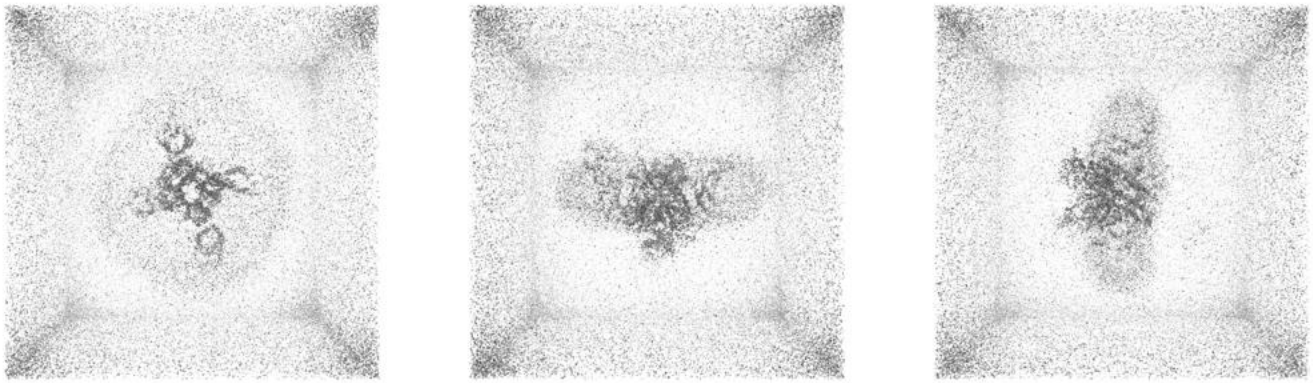
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. 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.

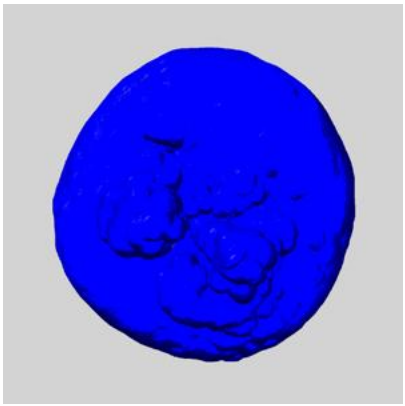
6.6 Mask visualisation (i)

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

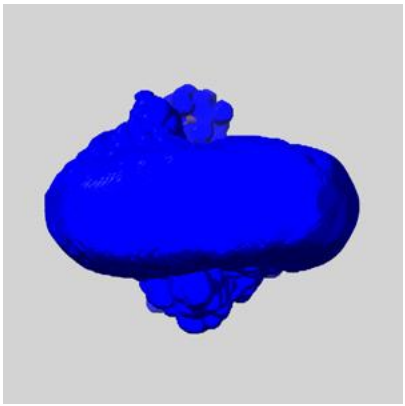
A mask typically either:

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

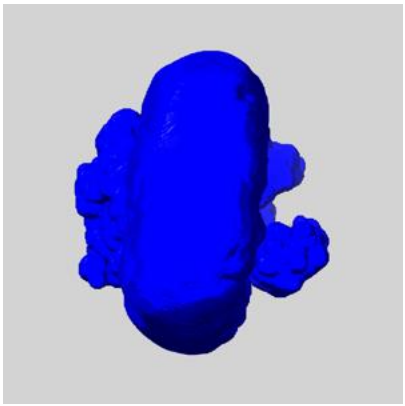
6.6.1 emd_43663_msk_1.map (i)



X



Y

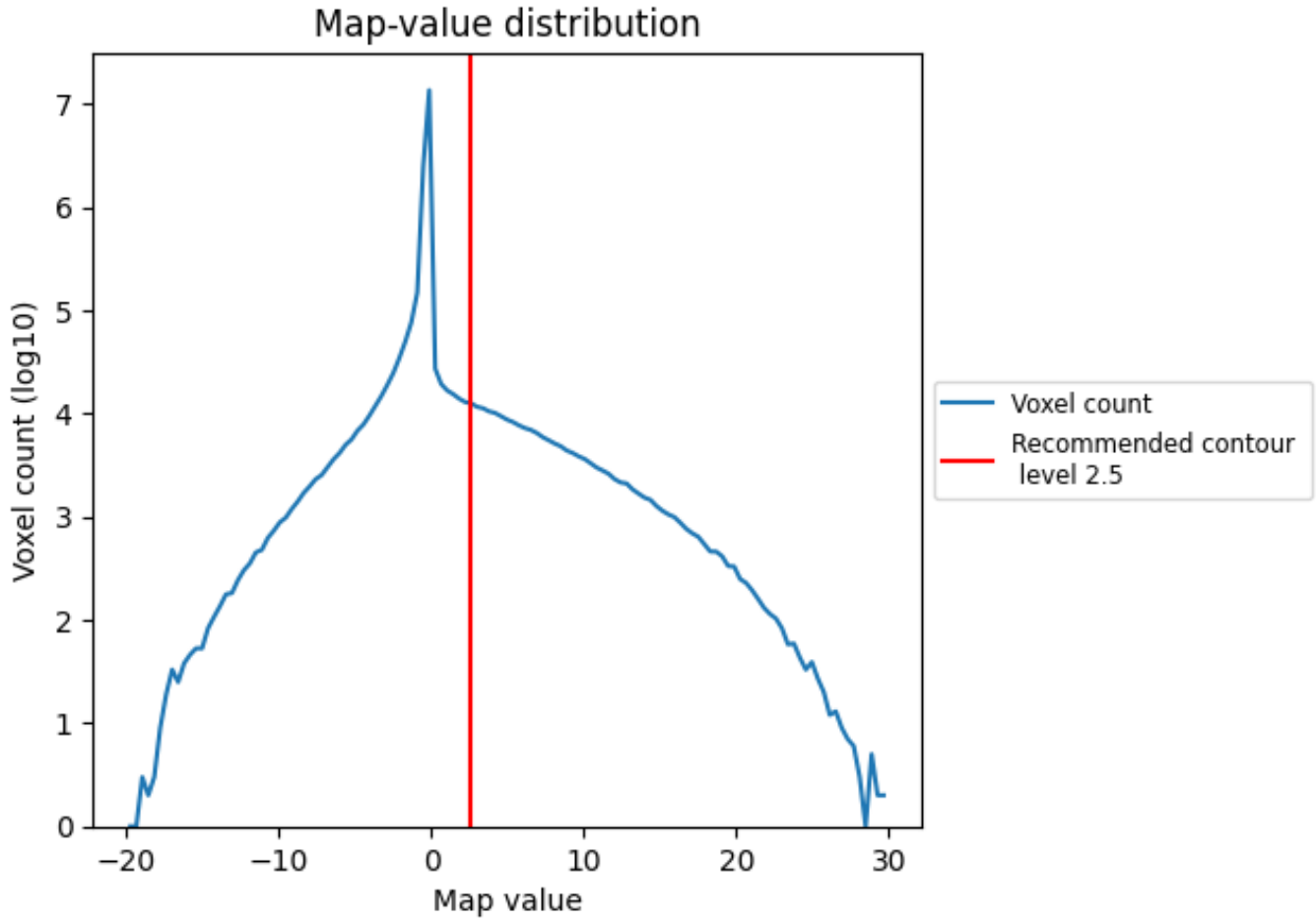


Z

7 Map analysis

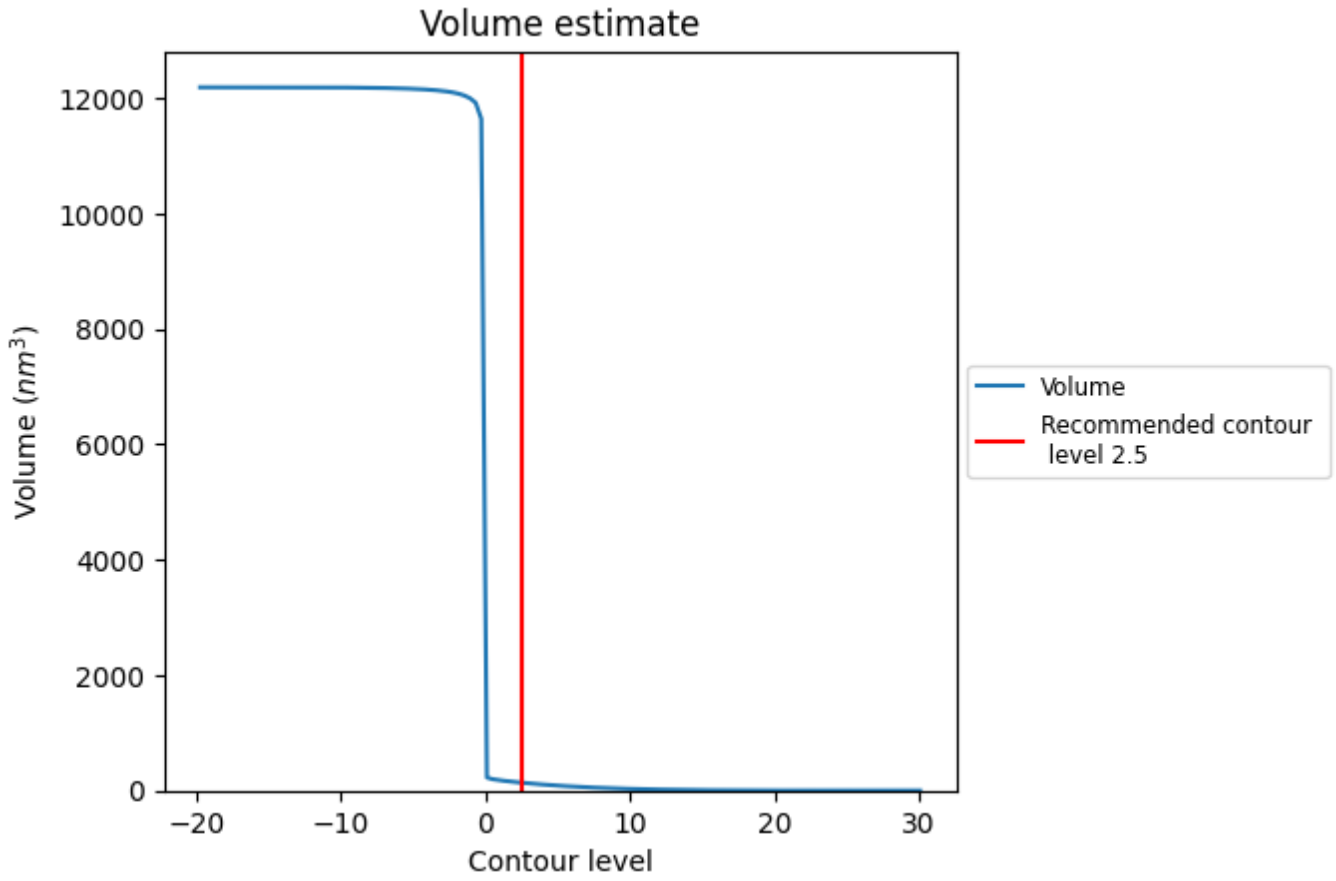
This section contains the results of statistical analysis of the map.

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.

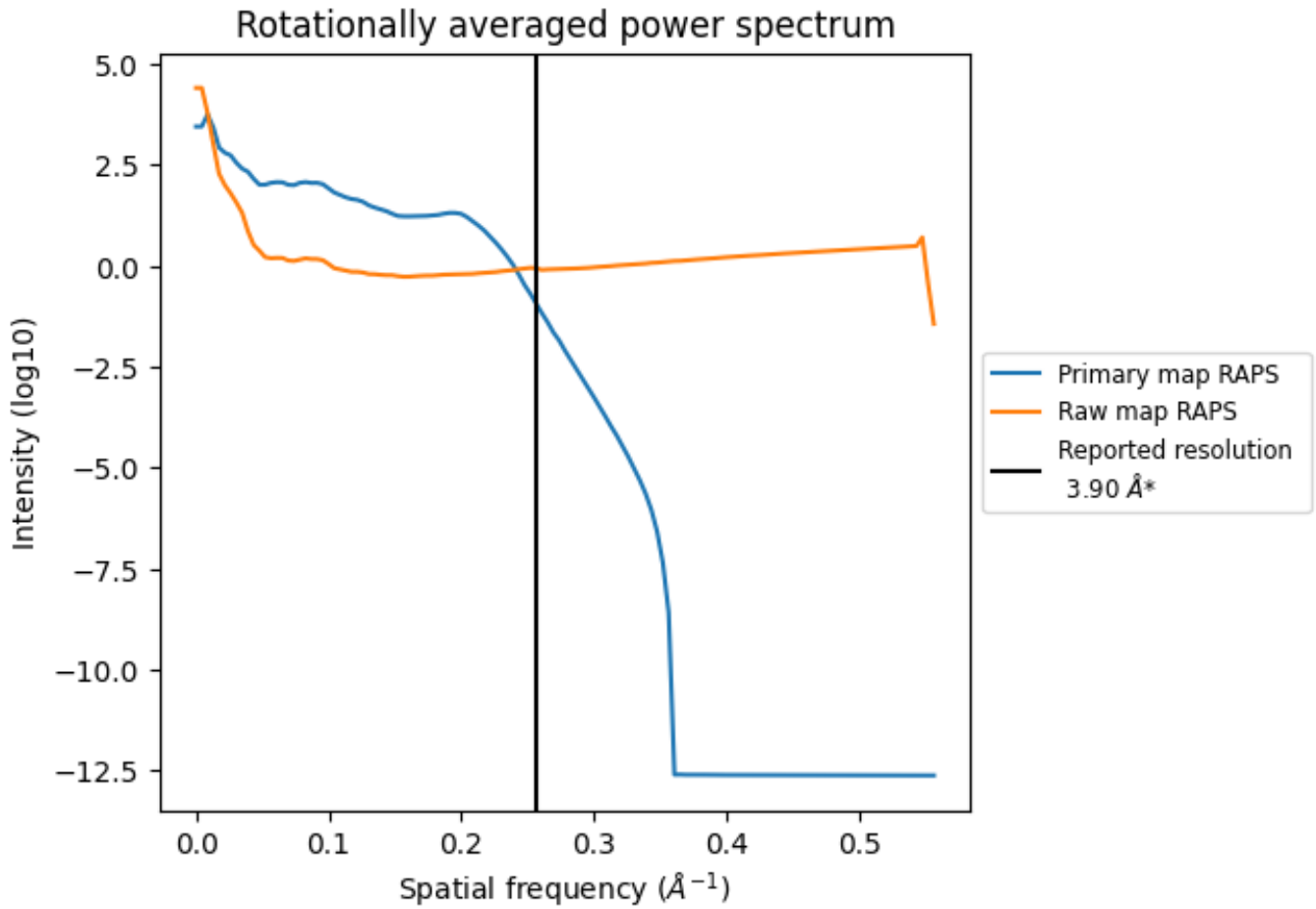
7.2 Volume estimate



The volume at the recommended contour level is 137 nm^3; this corresponds to an approximate mass of 123 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)

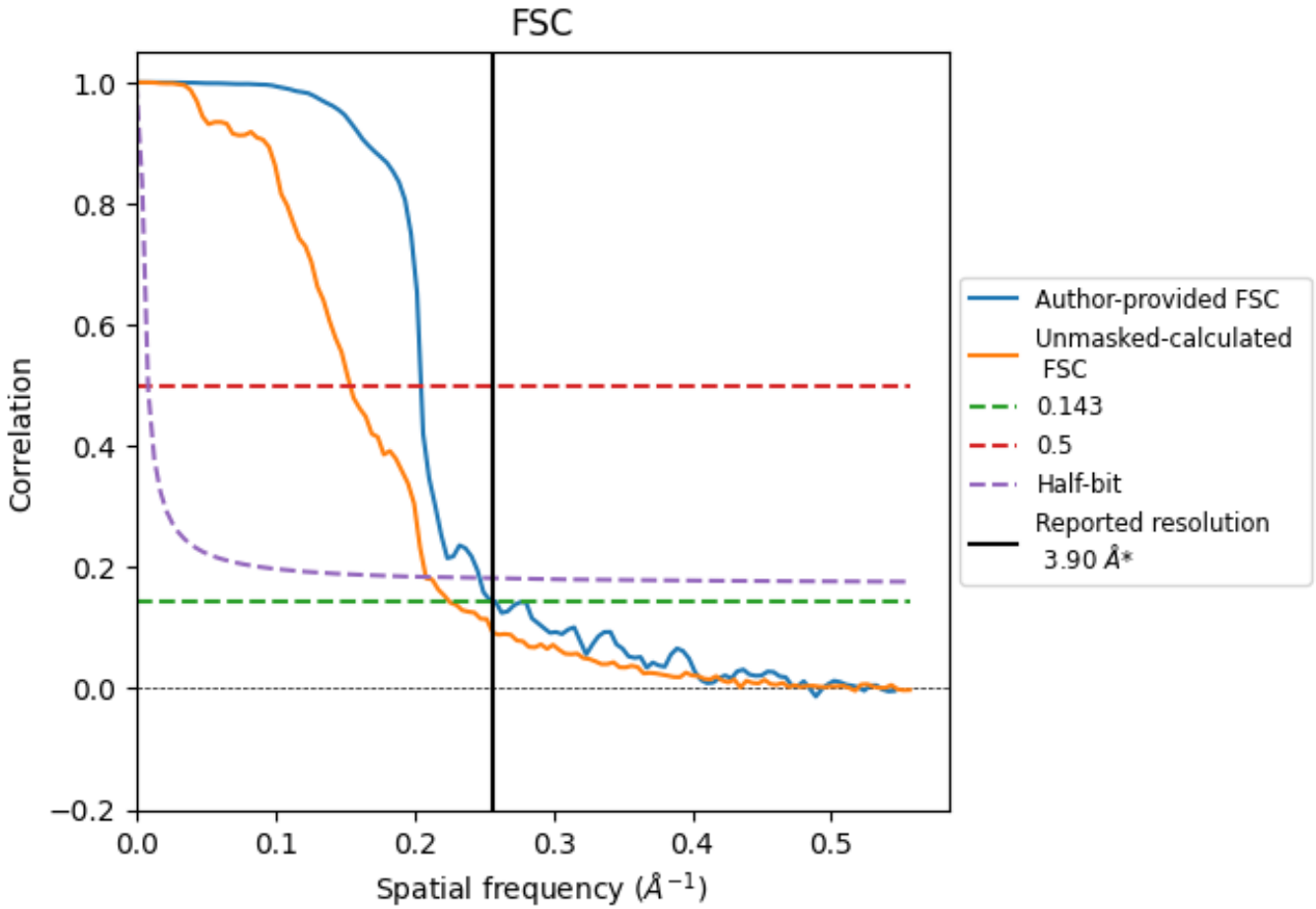


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

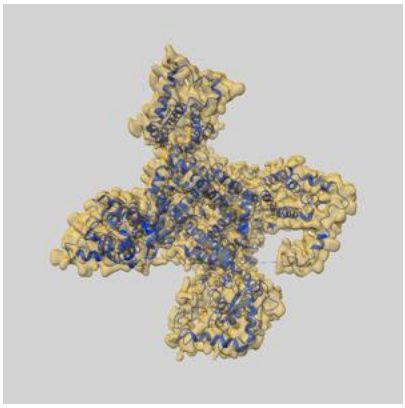
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.87	4.88	4.05
Unmasked-calculated*	4.44	6.50	4.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.9 by more than 10 %

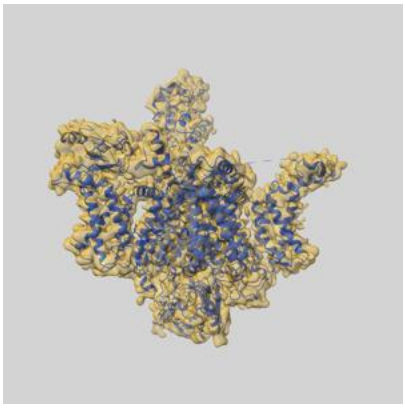
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43663 and PDB model 8VYK. Per-residue inclusion information can be found in section 3 on page 7.

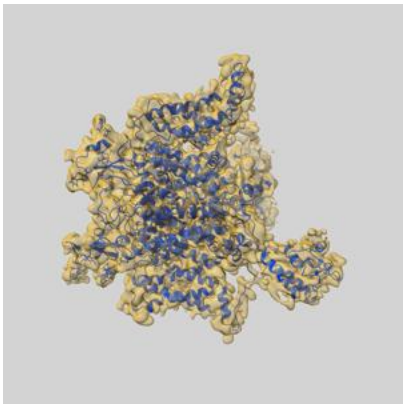
9.1 Map-model overlay



X



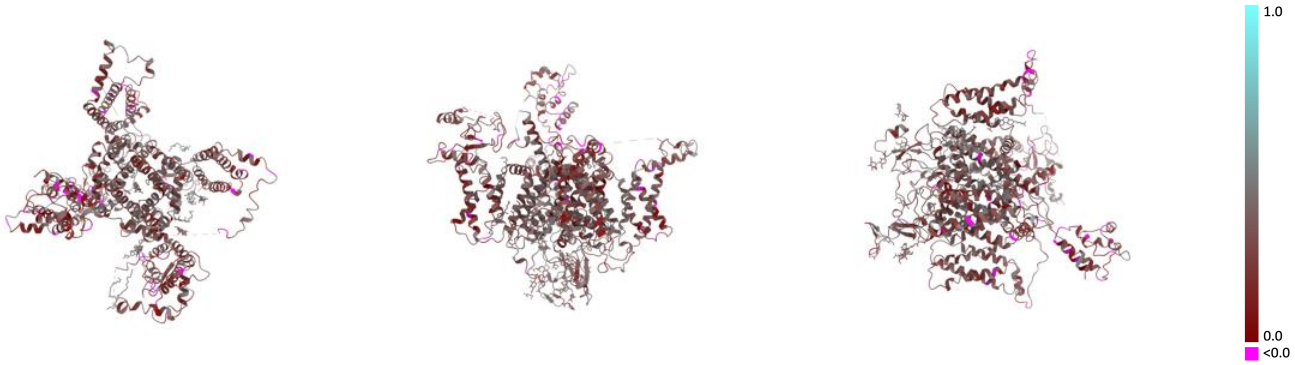
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

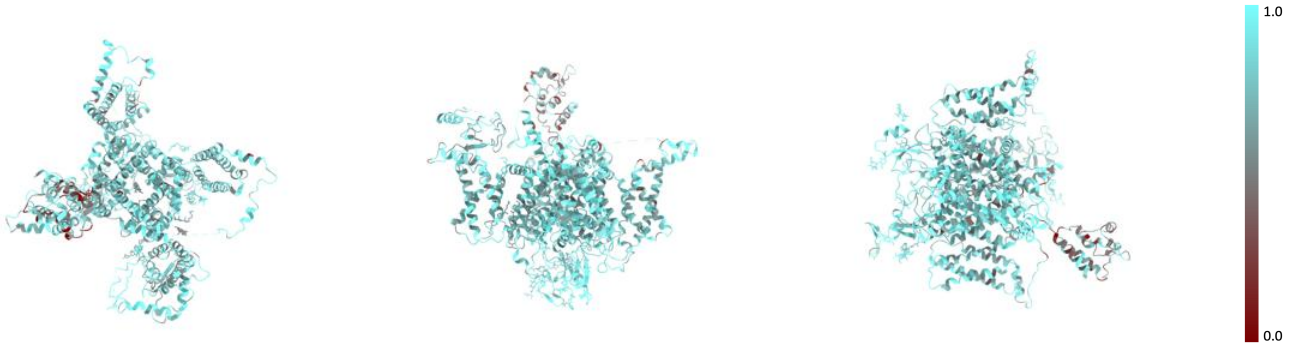
9.2 Q-score mapped to coordinate model (i)



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.

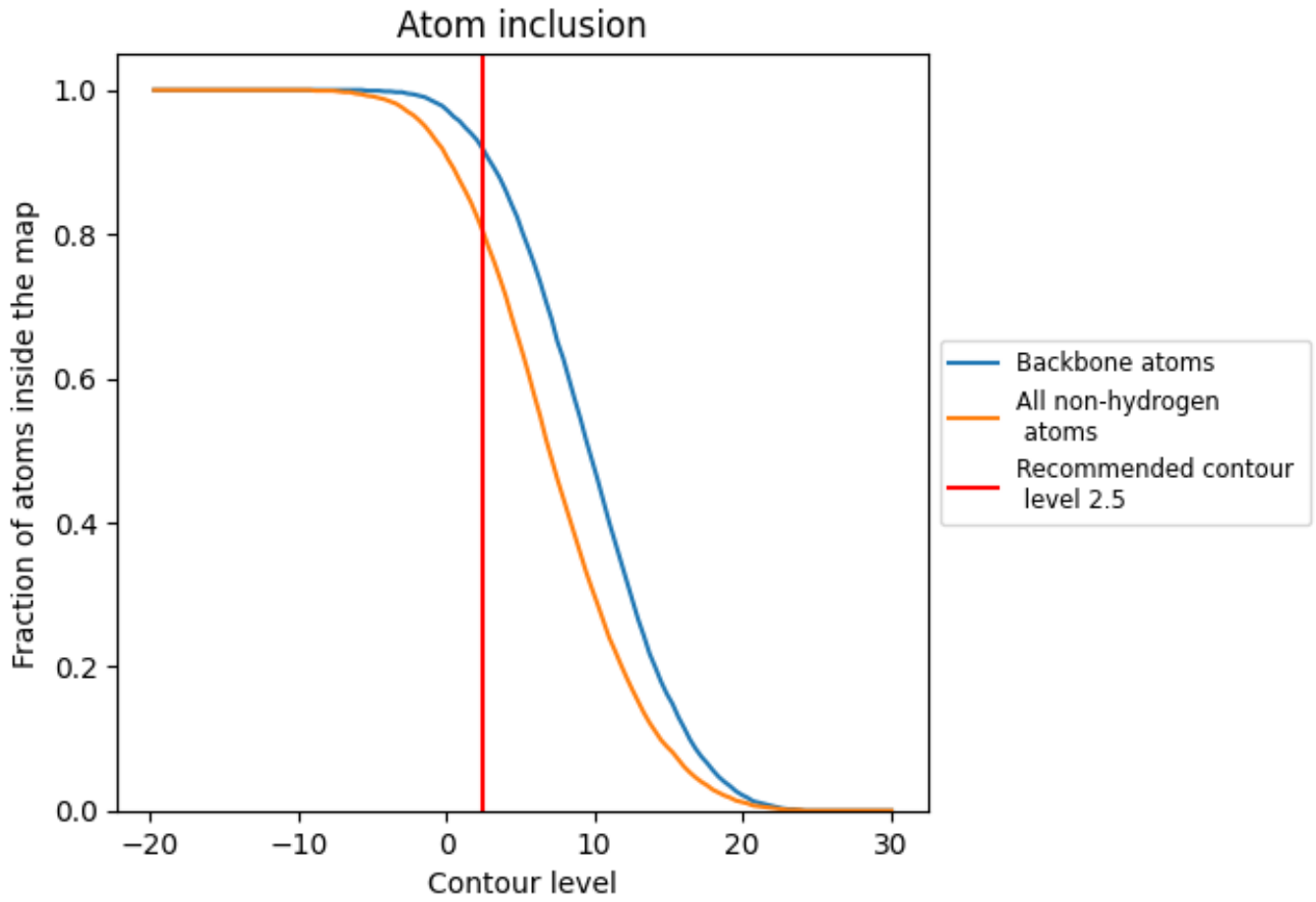
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 80% 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 (2.5) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8020	0.3040
A	0.8010	0.3030
B	0.8570	0.3560
C	0.8570	0.3940
D	0.8930	0.3840
E	0.9290	0.3200