



Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 12:26 PM EDT

PDB ID : 9PE4 / pdb_00009pe4
EMDB ID : EMD-71553
Title : Structure of beta-1,3-glucan synthase from *Saccharomyces cerevisiae* (ScFks1) at the catalytically less relevant L2 state
Authors : Ren, Z.; Lee, S.Y.
Deposited on : 2025-07-01
Resolution : 2.69 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

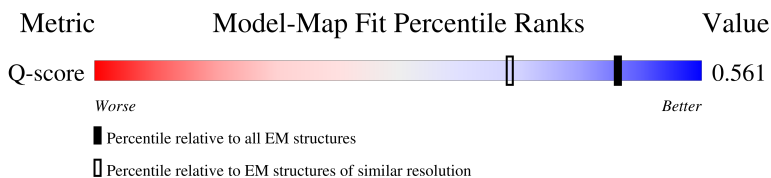
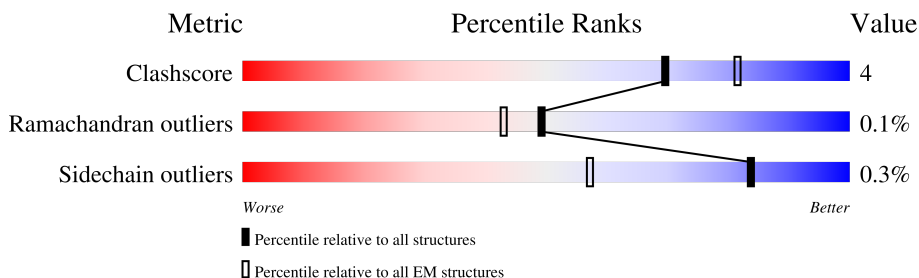
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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	9309 (2.19 - 3.19)

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

Mol	Chain	Length	Quality of chain
1	A	1931	 72% 7% 21%
2	G	197	 23% 73%
3	D	3	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25996 atoms, of which 12946 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 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1524	Total	C	H	N	O	S	0	0
			24110	7945	11945	2052	2099	69		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1877	LEU	-	expression tag	UNP P38631
A	1878	GLU	-	expression tag	UNP P38631
A	1879	VAL	-	expression tag	UNP P38631
A	1880	LEU	-	expression tag	UNP P38631
A	1881	PHE	-	expression tag	UNP P38631
A	1882	GLN	-	expression tag	UNP P38631
A	1883	GLY	-	expression tag	UNP P38631
A	1884	PRO	-	expression tag	UNP P38631
A	1885	ALA	-	expression tag	UNP P38631
A	1886	ALA	-	expression tag	UNP P38631
A	1887	ALA	-	expression tag	UNP P38631
A	1888	GLY	-	expression tag	UNP P38631
A	1889	SER	-	expression tag	UNP P38631
A	1890	ALA	-	expression tag	UNP P38631
A	1891	GLY	-	expression tag	UNP P38631
A	1892	SER	-	expression tag	UNP P38631
A	1893	ALA	-	expression tag	UNP P38631
A	1894	ALA	-	expression tag	UNP P38631
A	1895	GLY	-	expression tag	UNP P38631
A	1896	SER	-	expression tag	UNP P38631
A	1897	GLY	-	expression tag	UNP P38631
A	1898	GLU	-	expression tag	UNP P38631
A	1899	PHE	-	expression tag	UNP P38631
A	1900	ASP	-	expression tag	UNP P38631
A	1901	TYR	-	expression tag	UNP P38631
A	1902	LYS	-	expression tag	UNP P38631
A	1903	ASP	-	expression tag	UNP P38631
A	1904	HIS	-	expression tag	UNP P38631

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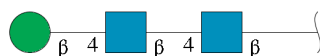
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1905	ASP	-	expression tag	UNP P38631
A	1906	GLY	-	expression tag	UNP P38631
A	1907	ASP	-	expression tag	UNP P38631
A	1908	TYR	-	expression tag	UNP P38631
A	1909	LYS	-	expression tag	UNP P38631
A	1910	ASP	-	expression tag	UNP P38631
A	1911	HIS	-	expression tag	UNP P38631
A	1912	ASP	-	expression tag	UNP P38631
A	1913	ILE	-	expression tag	UNP P38631
A	1914	ASP	-	expression tag	UNP P38631
A	1915	TYR	-	expression tag	UNP P38631
A	1916	LYS	-	expression tag	UNP P38631
A	1917	ASP	-	expression tag	UNP P38631
A	1918	ASP	-	expression tag	UNP P38631
A	1919	ASP	-	expression tag	UNP P38631
A	1920	ASP	-	expression tag	UNP P38631
A	1921	LYS	-	expression tag	UNP P38631
A	1922	HIS	-	expression tag	UNP P38631
A	1923	HIS	-	expression tag	UNP P38631
A	1924	HIS	-	expression tag	UNP P38631
A	1925	HIS	-	expression tag	UNP P38631
A	1926	HIS	-	expression tag	UNP P38631
A	1927	HIS	-	expression tag	UNP P38631
A	1928	HIS	-	expression tag	UNP P38631
A	1929	HIS	-	expression tag	UNP P38631
A	1930	HIS	-	expression tag	UNP P38631
A	1931	HIS	-	expression tag	UNP P38631

- Molecule 2 is a protein called YMR295C.

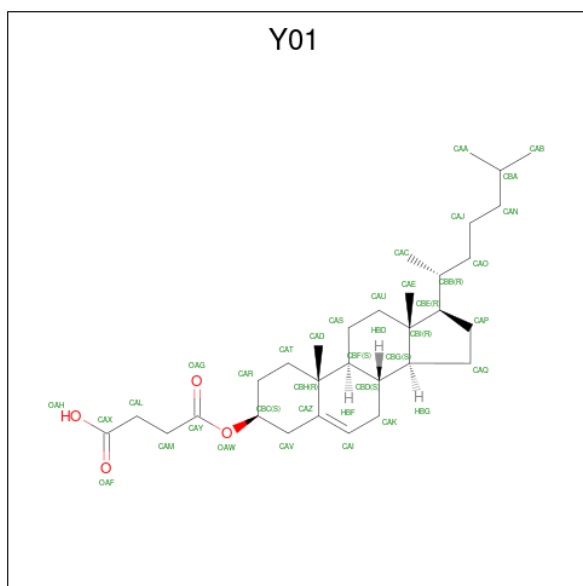
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	53	Total	C	H	N	O	0	0
			791	264	378	74	75		

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

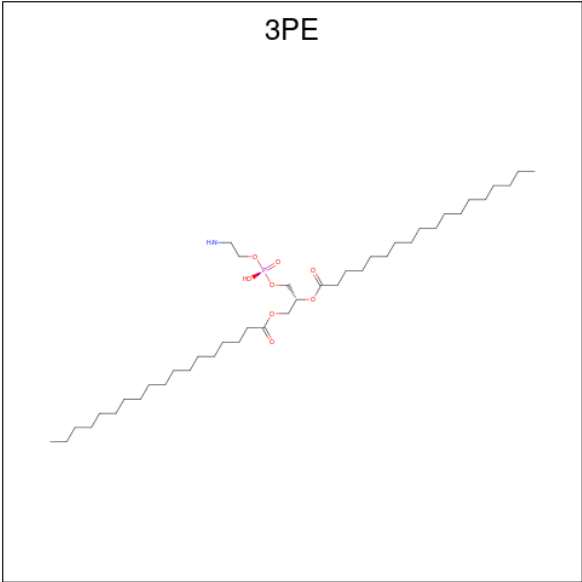


Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	3	Total	C	H	N	O	0	0
			67	22	28	2	15		

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).

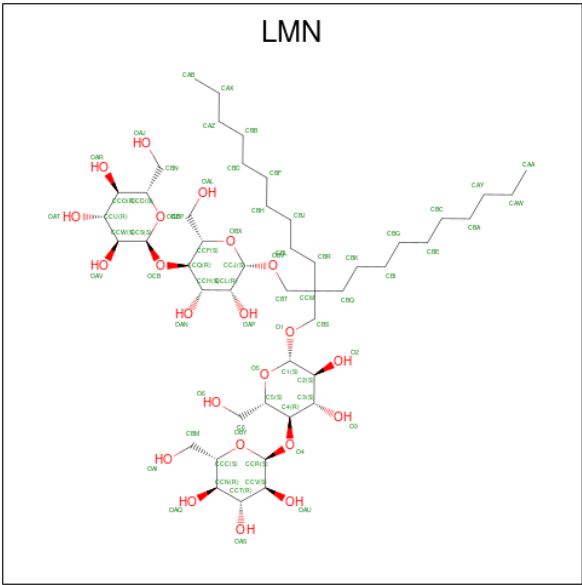
[illegible]

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			125	39	76	1	8	1	

- Molecule 6 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
6	A	1	157	47	88	22	0
6	A	1	157	47	88	22	0

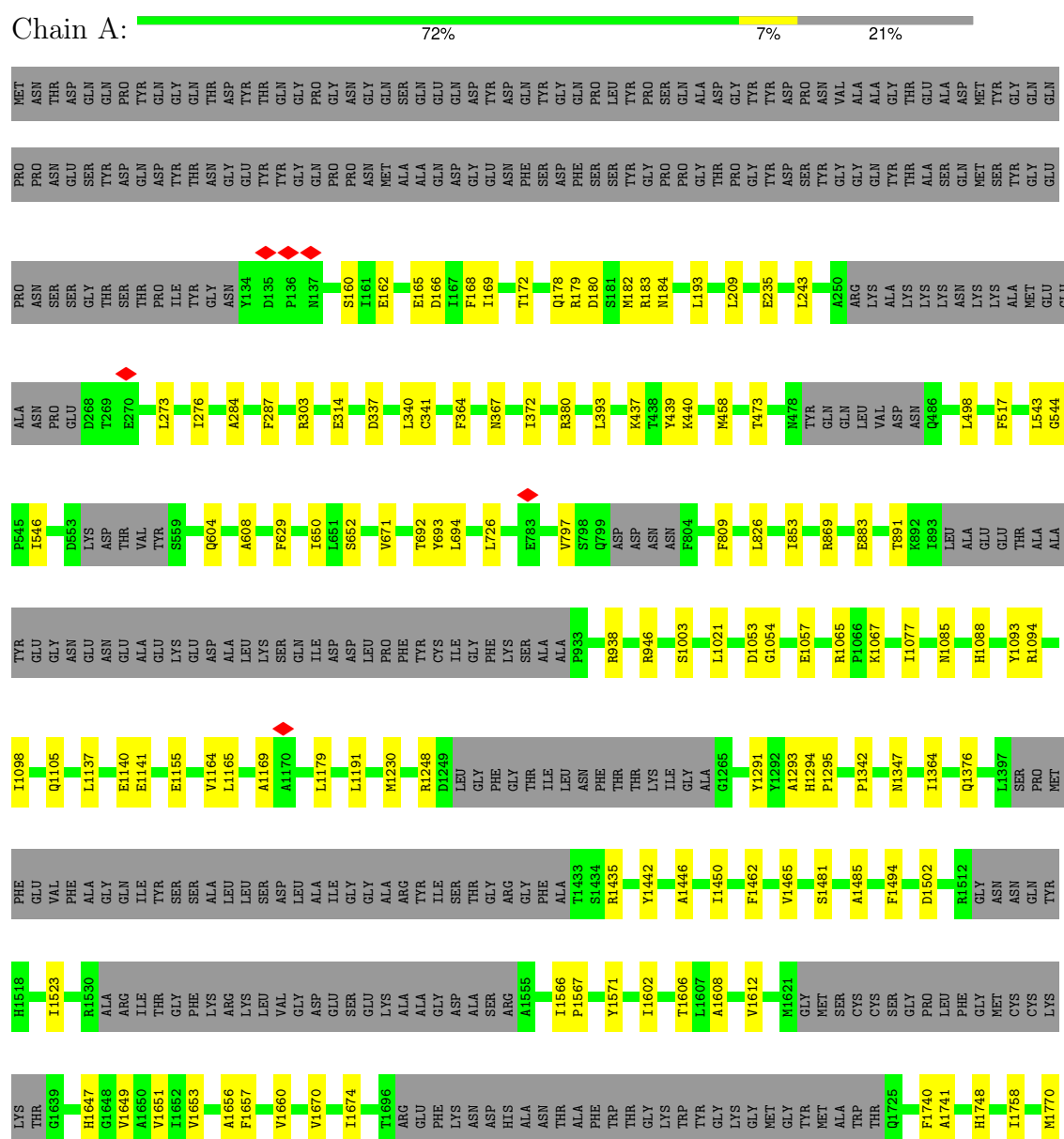
- Molecule 7 is water.

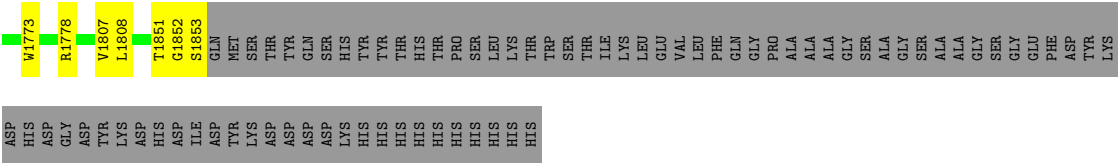
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	

3 Residue-property plots

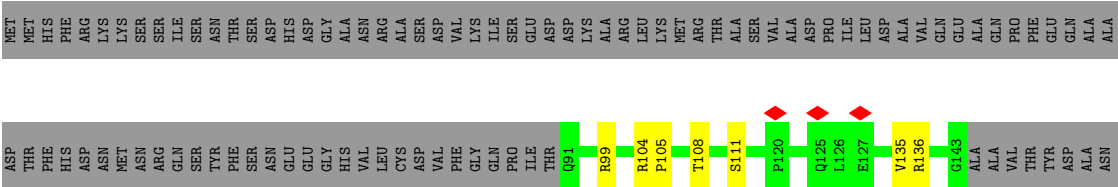
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 1,3-beta-glucan synthase component FKS1





• Molecule 2: YMR295C



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117759	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.285	Depositor
Minimum map value	-0.747	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.103	Depositor
Map size (\AA)	264.64, 264.64, 264.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, LMN, Y01, 3PE

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	0.13	0/12491	0.28	0/16970
2	G	0.10	0/426	0.25	0/583
All	All	0.13	0/12917	0.28	0/17553

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12165	11945	11938	82	0
2	G	413	378	377	7	0
3	D	39	28	34	0	0
4	A	245	343	343	12	0
5	A	49	76	75	0	0
6	A	138	176	176	2	0
7	A	1	0	0	0	0
All	All	13050	12946	12943	94	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 4.

All (94) 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)
4:A:2008:Y01:HAE1	6:A:2009:LMN:HABB	1.72	0.72
1:A:437:LYS:NZ	1:A:439:TYR:O	2.25	0.68
1:A:1191:LEU:HD21	1:A:1230:MET:SD	2.34	0.67
1:A:364:PHE:CE1	1:A:393:LEU:HD21	2.34	0.63
1:A:1105:GLN:NE2	1:A:1155:GLU:OE2	2.33	0.62
1:A:1057:GLU:OE2	1:A:1065:ARG:NH1	2.34	0.61
1:A:1748:HIS:CD2	1:A:1807:VAL:HG11	2.37	0.60
1:A:1852:GLY:O	1:A:1853:SER:C	2.46	0.58
1:A:303:ARG:NH2	1:A:337:ASP:OD1	2.37	0.57
1:A:340:LEU:HD12	1:A:341:CYS:N	2.18	0.57
1:A:726:LEU:HD12	1:A:826:LEU:HD12	1.85	0.57
4:A:2002:Y01:HAC1	4:A:2002:Y01:HAU2	1.87	0.57
1:A:1169:ALA:HB2	1:A:1248:ARG:HE	1.70	0.56
1:A:883:GLU:OE1	1:A:946:ARG:NE	2.38	0.56
1:A:473:THR:HG21	1:A:652:SER:OG	2.06	0.55
1:A:726:LEU:CD1	1:A:826:LEU:HD12	2.36	0.55
1:A:172:THR:HG21	1:A:182:MET:SD	2.48	0.53
1:A:1137:LEU:HD12	1:A:1141:GLU:OE1	2.09	0.53
1:A:671:VAL:HG12	1:A:671:VAL:O	2.10	0.51
1:A:1770:MET:HE1	1:A:1773:TRP:CZ3	2.46	0.51
1:A:650:ILE:HG21	1:A:1347:ASN:O	2.11	0.51
2:G:108:THR:O	2:G:111:SER:OG	2.24	0.50
1:A:193:LEU:HD23	1:A:209:LEU:HD12	1.93	0.50
1:A:1435:ARG:NH1	1:A:1502:ASP:OD2	2.45	0.50
4:A:2003:Y01:HAU2	4:A:2003:Y01:HAC1	1.94	0.49
4:A:2001:Y01:HAC1	4:A:2001:Y01:HAU2	1.94	0.49
1:A:543:LEU:C	1:A:543:LEU:HD23	2.38	0.49
4:A:2004:Y01:HAC1	4:A:2004:Y01:HAU2	1.95	0.49
1:A:273:LEU:HD12	1:A:287:PHE:CE2	2.48	0.48
4:A:2008:Y01:HAE1	6:A:2009:LMN:CAB	2.41	0.48
1:A:235:GLU:OE1	1:A:235:GLU:N	2.42	0.48
1:A:273:LEU:HD12	1:A:287:PHE:HE2	1.78	0.48
1:A:1612:VAL:HG11	1:A:1653:VAL:HG21	1.96	0.48
1:A:166:ASP:OD1	2:G:104:ARG:NH2	2.46	0.48
1:A:1294:HIS:HB3	1:A:1295:PRO:HD3	1.96	0.48
1:A:1442:TYR:O	1:A:1446:ALA:HB2	2.13	0.47
1:A:797:VAL:HG12	1:A:797:VAL:O	2.14	0.47
1:A:1602:ILE:O	1:A:1606:THR:HG22	2.13	0.47
4:A:2006:Y01:HAC1	4:A:2006:Y01:HAU2	1.96	0.47
1:A:182:MET:HE2	2:G:105:PRO:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASN:OD1	1:A:1094:ARG:NH2	2.41	0.47
1:A:1494:PHE:HA	1:A:1758:ILE:HG22	1.96	0.47
1:A:1651:VAL:HG22	1:A:1741:ALA:HA	1.96	0.47
4:A:2008:Y01:HAC1	4:A:2008:Y01:HAU2	1.97	0.47
1:A:1462:PHE:CE1	1:A:1670:VAL:HG12	2.49	0.47
1:A:1808:LEU:C	1:A:1808:LEU:HD23	2.40	0.47
1:A:853:ILE:HG23	1:A:1021:LEU:HD11	1.97	0.47
1:A:179:ARG:O	1:A:182:MET:HG2	2.16	0.46
1:A:1053:ASP:OD1	1:A:1054:GLY:N	2.47	0.46
1:A:692:THR:HG23	1:A:693:TYR:N	2.31	0.46
1:A:372:ILE:O	1:A:372:ILE:HG23	2.16	0.45
1:A:1656:ALA:O	1:A:1660:VAL:HG23	2.17	0.45
1:A:182:MET:HE2	2:G:105:PRO:HG3	1.99	0.45
1:A:498:LEU:CD2	1:A:546:ILE:HG21	2.47	0.45
1:A:179:ARG:HA	1:A:182:MET:HG2	2.00	0.44
1:A:1523:ILE:HD12	1:A:1523:ILE:H	1.83	0.44
1:A:165:GLU:OE1	2:G:136:ARG:NH2	2.51	0.44
1:A:166:ASP:HB3	2:G:135:VAL:HG13	2.00	0.43
1:A:1465:VAL:HG12	1:A:1670:VAL:HG22	2.00	0.43
1:A:169:ILE:O	1:A:172:THR:HG22	2.18	0.43
1:A:1342:PRO:HB2	1:A:1851:THR:HB	1.99	0.43
1:A:1179:LEU:HD13	1:A:1376:GLN:HB2	2.00	0.43
1:A:1566:ILE:HB	1:A:1567:PRO:HD3	2.00	0.43
1:A:367:ASN:O	1:A:380:ARG:NH2	2.52	0.43
1:A:178:GLN:NE2	1:A:314:GLU:OE1	2.52	0.42
1:A:1077:ILE:N	1:A:1077:ILE:HD12	2.34	0.42
1:A:458:MET:HE1	1:A:629:PHE:CZ	2.54	0.42
1:A:1003:SER:OG	1:A:1085:ASN:OD1	2.35	0.42
1:A:1649:VAL:O	1:A:1653:VAL:HG23	2.20	0.42
1:A:694:LEU:HD11	1:A:1364:ILE:HG22	2.01	0.42
1:A:1291:TYR:O	1:A:1295:PRO:HD2	2.19	0.42
1:A:604:GLN:HA	1:A:608:ALA:HB3	2.02	0.42
1:A:160:SER:OG	1:A:162:GLU:OE1	2.38	0.42
1:A:182:MET:HG3	1:A:183:ARG:N	2.34	0.42
1:A:276:ILE:HG23	1:A:284:ALA:HB1	2.02	0.42
1:A:543:LEU:HD23	1:A:544:GLY:N	2.35	0.42
1:A:1462:PHE:CE1	1:A:1674:ILE:HB	2.54	0.41
1:A:1481:SER:O	1:A:1485:ALA:HB2	2.20	0.41
4:A:2007:Y01:HAE2	4:A:2007:Y01:HAC1	2.02	0.41
1:A:243:LEU:HD21	1:A:1140:GLU:HG3	2.03	0.41
1:A:1093:TYR:CD1	1:A:1098:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:ILE:HD12	1:A:1523:ILE:N	2.35	0.41
1:A:1647:HIS:HB3	1:A:1740:PHE:CE2	2.55	0.41
4:A:2001:Y01:OAG	4:A:2001:Y01:HAV1	2.21	0.41
1:A:440:LYS:O	1:A:517:PHE:HB2	2.21	0.41
1:A:1067:LYS:O	2:G:99:ARG:NH2	2.54	0.41
1:A:1660:VAL:HG22	4:A:2007:Y01:CAE	2.50	0.41
1:A:869:ARG:CB	1:A:1778:ARG:HD2	2.51	0.40
1:A:1446:ALA:HA	1:A:1450:ILE:HB	2.04	0.40
4:A:2003:Y01:HAC1	4:A:2003:Y01:CAU	2.51	0.40
1:A:168:PHE:HB3	1:A:182:MET:HE3	2.03	0.40
1:A:1164:VAL:HG12	1:A:1165:LEU:N	2.37	0.40
1:A:891:THR:OG1	1:A:938:ARG:NH1	2.55	0.40
1:A:1608:ALA:HB1	1:A:1657:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1500/1931 (78%)	1471 (98%)	28 (2%)	1 (0%)	48	73
2	G	51/197 (26%)	50 (98%)	1 (2%)	0	100	100
All	All	1551/2128 (73%)	1521 (98%)	29 (2%)	1 (0%)	49	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1293	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1263/1663 (76%)	1259 (100%)	4 (0%)	86	94
2	G	40/167 (24%)	40 (100%)	0	100	100
All	All	1303/1830 (71%)	1299 (100%)	4 (0%)	84	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	ASP
1	A	809	PHE
1	A	1088	HIS
1	A	1571	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	274	ASN
1	A	295	GLN
1	A	363	HIS
1	A	700	ASN
1	A	1005	GLN
1	A	1105	GLN
1	A	1142	GLN
1	A	1145	ASN
1	A	1146	HIS
1	A	1269	GLN
1	A	1305	GLN
1	A	1668	ASN
1	A	1748	HIS
1	A	1767	HIS

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 ⓘ

3 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	$\# Z > 2$
3	NAG	D	1	3	14,14,15	0.29	0	17,19,21	0.45	0
3	NAG	D	2	3	14,14,15	0.20	0	17,19,21	0.52	0
3	BMA	D	3	3	11,11,12	0.74	0	15,15,17	0.77	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
3	NAG	D	1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

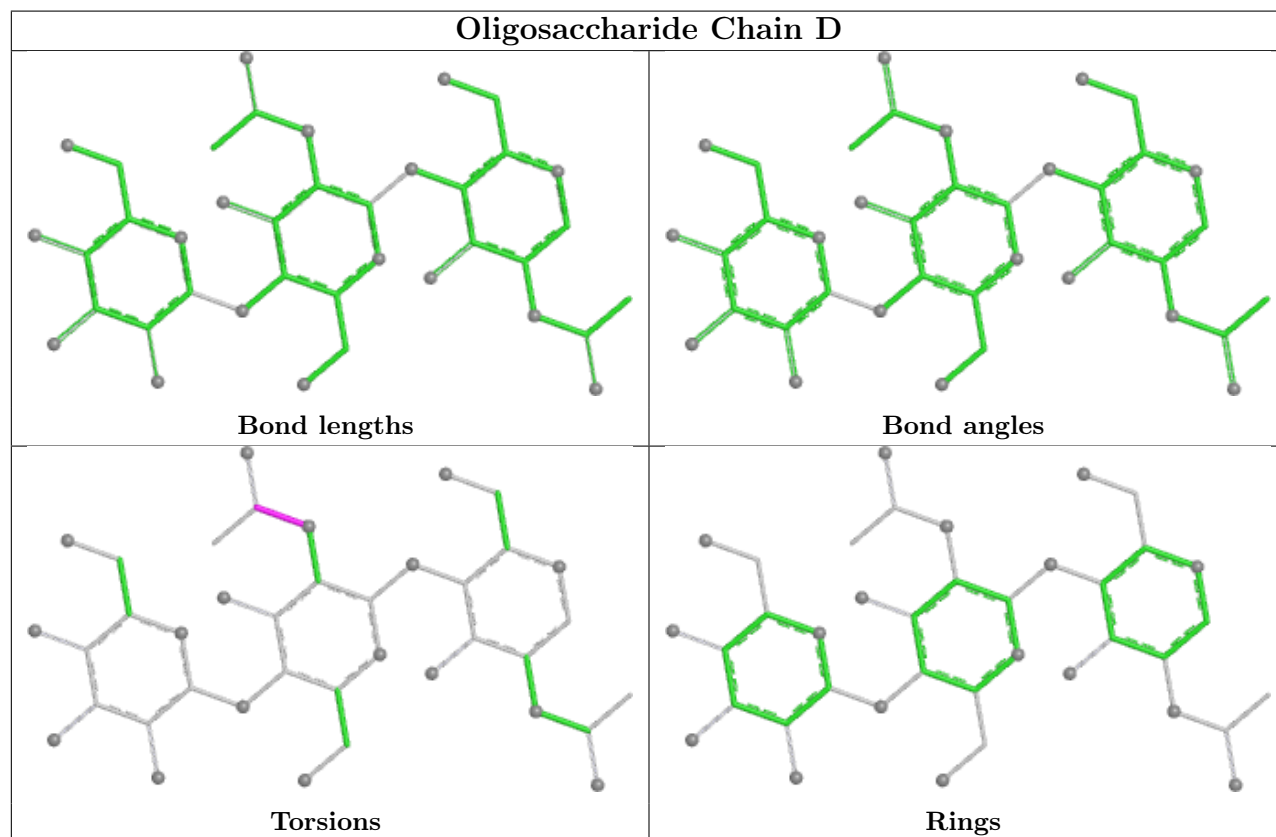
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

10 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
4	Y01	A	2008	-	38,38,38	1.11	3 (7%)	57,57,57	2.68	14 (24%)
4	Y01	A	2001	-	38,38,38	1.12	2 (5%)	57,57,57	2.26	14 (24%)
4	Y01	A	2002	-	38,38,38	1.10	3 (7%)	57,57,57	2.58	12 (21%)
6	LMN	A	2010	-	72,72,72	0.15	0	92,98,98	0.60	3 (3%)
4	Y01	A	2003	-	38,38,38	1.11	2 (5%)	57,57,57	2.44	17 (29%)
4	Y01	A	2007	-	38,38,38	1.12	2 (5%)	57,57,57	2.35	15 (26%)
4	Y01	A	2004	-	38,38,38	1.11	3 (7%)	57,57,57	2.43	16 (28%)
6	LMN	A	2009	-	72,72,72	0.12	0	92,98,98	0.27	0
4	Y01	A	2006	-	38,38,38	1.15	4 (10%)	57,57,57	2.68	17 (29%)
5	3PE	A	2005	-	48,48,50	0.48	0	51,53,55	0.45	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
4	Y01	A	2008	-	-	8/19/77/77	0/4/4/4
4	Y01	A	2001	-	-	5/19/77/77	0/4/4/4
4	Y01	A	2002	-	-	7/19/77/77	0/4/4/4
6	LMN	A	2010	-	-	14/50/130/130	0/4/4/4
4	Y01	A	2003	-	-	12/19/77/77	0/4/4/4
4	Y01	A	2007	-	-	10/19/77/77	0/4/4/4
4	Y01	A	2004	-	-	5/19/77/77	0/4/4/4
6	LMN	A	2009	-	-	11/50/130/130	0/4/4/4
4	Y01	A	2006	-	-	9/19/77/77	0/4/4/4
5	3PE	A	2005	-	-	14/52/52/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	Y01	OAW-CAY	3.40	1.43	1.34
4	A	2007	Y01	OAW-CAY	3.33	1.43	1.34
4	A	2004	Y01	OAW-CAY	3.33	1.43	1.34
4	A	2002	Y01	OAW-CAY	3.29	1.43	1.34
4	A	2008	Y01	OAW-CAY	3.29	1.43	1.34
4	A	2003	Y01	OAW-CAY	3.28	1.43	1.34
4	A	2006	Y01	OAW-CAY	3.23	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	Y01	OAH-CAX	-2.86	1.21	1.30
4	A	2002	Y01	OAH-CAX	-2.86	1.21	1.30
4	A	2008	Y01	OAH-CAX	-2.85	1.21	1.30
4	A	2006	Y01	OAH-CAX	-2.84	1.21	1.30
4	A	2003	Y01	OAH-CAX	-2.83	1.21	1.30
4	A	2007	Y01	OAH-CAX	-2.82	1.21	1.30
4	A	2004	Y01	OAH-CAX	-2.82	1.21	1.30
4	A	2006	Y01	CAS-CBF	2.18	1.57	1.53
4	A	2002	Y01	CAK-CAI	2.17	1.54	1.50
4	A	2008	Y01	CAK-CAI	2.15	1.54	1.50
4	A	2004	Y01	CAK-CAI	2.07	1.54	1.50
4	A	2006	Y01	CAK-CAI	2.02	1.54	1.50

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2007	Y01	CAT-CBH-CBF	-10.57	94.75	108.74
4	A	2001	Y01	CAT-CBH-CBF	-9.82	95.75	108.74
4	A	2004	Y01	CAT-CBH-CBF	-9.63	96.00	108.74
4	A	2003	Y01	CAT-CBH-CBF	-9.56	96.09	108.74
4	A	2006	Y01	CAT-CBH-CBF	-9.38	96.32	108.74
4	A	2002	Y01	CAV-CAZ-CAI	8.91	132.64	120.57
4	A	2008	Y01	CAT-CBH-CBF	-8.11	98.00	108.74
4	A	2008	Y01	CBH-CAZ-CAI	-7.30	112.27	122.93
4	A	2006	Y01	CAV-CAZ-CAI	7.21	130.34	120.57
4	A	2004	Y01	CAV-CAZ-CAI	7.17	130.29	120.57
4	A	2003	Y01	CAV-CAZ-CAI	7.16	130.27	120.57
4	A	2002	Y01	CAT-CBH-CBF	-7.12	99.31	108.74
4	A	2001	Y01	CAV-CAZ-CAI	6.72	129.68	120.57
4	A	2008	Y01	CAV-CAZ-CAI	6.65	129.59	120.57
4	A	2002	Y01	CBH-CAZ-CAI	-6.53	113.39	122.93
4	A	2006	Y01	CBH-CBF-CBD	-6.51	103.20	112.71
4	A	2007	Y01	CAV-CAZ-CAI	6.36	129.18	120.57
4	A	2008	Y01	CBC-CAV-CAZ	6.33	120.80	111.45
4	A	2002	Y01	CBH-CBF-CBD	-5.66	104.45	112.71
4	A	2002	Y01	CBF-CBH-CAZ	-5.47	101.64	109.65
4	A	2004	Y01	CBH-CBF-CBD	-5.47	104.72	112.71
4	A	2003	Y01	CBH-CBF-CBD	-5.36	104.88	112.71
4	A	2006	Y01	CBD-CAK-CAI	-5.28	105.44	112.76
4	A	2008	Y01	CBH-CBF-CBD	-5.21	105.10	112.71
4	A	2002	Y01	CAD-CBH-CAZ	5.13	116.23	108.38
4	A	2008	Y01	CBF-CBH-CAZ	-4.91	102.47	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2006	Y01	CAK-CBD-CBF	-4.75	104.23	109.72
4	A	2008	Y01	CAD-CBH-CAZ	4.74	115.62	108.38
4	A	2002	Y01	CAD-CBH-CBF	4.42	116.62	111.66
4	A	2001	Y01	CBH-CBF-CBD	-4.33	106.38	112.71
4	A	2006	Y01	CAD-CBH-CBF	4.23	116.41	111.66
4	A	2006	Y01	CAV-CAZ-CBH	-4.22	111.02	116.42
4	A	2006	Y01	CAU-CAS-CBF	4.16	120.20	113.14
4	A	2007	Y01	OAW-CAY-CAM	4.11	120.38	111.48
4	A	2008	Y01	CAD-CBH-CBF	4.10	116.26	111.66
4	A	2002	Y01	OAW-CAY-CAM	4.08	120.31	111.48
4	A	2007	Y01	CAD-CBH-CAZ	4.06	114.59	108.38
4	A	2004	Y01	CAK-CBD-CBF	-4.06	105.03	109.72
4	A	2004	Y01	OAW-CAY-CAM	4.00	120.14	111.48
4	A	2004	Y01	CAD-CBH-CBF	3.98	116.12	111.66
4	A	2006	Y01	OAW-CAY-CAM	3.87	119.84	111.48
4	A	2003	Y01	CAD-CBH-CBF	3.83	115.96	111.66
4	A	2003	Y01	OAW-CAY-CAM	3.80	119.70	111.48
4	A	2003	Y01	CAK-CBD-CBF	-3.76	105.37	109.72
4	A	2006	Y01	CAU-CBI-CBE	-3.75	111.08	116.60
4	A	2008	Y01	OAW-CAY-CAM	3.73	119.56	111.48
4	A	2004	Y01	CBH-CAZ-CAI	-3.73	117.48	122.93
4	A	2006	Y01	CAK-CBD-CBG	3.70	116.18	110.93
4	A	2001	Y01	CAD-CBH-CBF	3.66	115.77	111.66
4	A	2001	Y01	CBH-CAZ-CAI	-3.64	117.61	122.93
4	A	2003	Y01	CAU-CBI-CBE	-3.61	111.29	116.60
4	A	2003	Y01	CBH-CAZ-CAI	-3.55	117.75	122.93
4	A	2004	Y01	CAU-CBI-CBE	-3.51	111.44	116.60
4	A	2008	Y01	CAU-CBI-CBE	-3.50	111.45	116.60
4	A	2003	Y01	CAV-CAZ-CBH	-3.48	111.97	116.42
4	A	2001	Y01	OAW-CAY-CAM	3.45	118.95	111.48
4	A	2001	Y01	CAU-CBI-CBE	-3.41	111.58	116.60
4	A	2008	Y01	CAR-CBC-CAV	3.39	115.68	110.97
4	A	2007	Y01	CAU-CBI-CBE	-3.28	111.77	116.60
4	A	2004	Y01	CAV-CAZ-CBH	-3.28	112.22	116.42
4	A	2002	Y01	CAK-CBD-CBG	3.27	115.56	110.93
4	A	2003	Y01	CAU-CAS-CBF	3.26	118.67	113.14
4	A	2007	Y01	CBF-CBH-CAZ	3.22	114.36	109.65
4	A	2006	Y01	CAS-CBF-CBD	3.21	116.25	111.78
4	A	2007	Y01	CAP-CBE-CBB	-3.20	107.33	112.18
4	A	2002	Y01	CBI-CBE-CBB	-3.20	114.56	119.50
4	A	2007	Y01	CAV-CAZ-CBH	-3.19	112.33	116.42
4	A	2007	Y01	CBH-CAZ-CAI	-3.05	118.48	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	Y01	CAU-CBI-CBE	-3.03	112.13	116.60
4	A	2008	Y01	CBF-CBD-CBG	-3.03	105.13	109.09
4	A	2007	Y01	CBF-CBD-CBG	-2.97	105.21	109.09
4	A	2006	Y01	CBI-CBE-CBB	-2.95	114.94	119.50
4	A	2006	Y01	CBH-CAZ-CAI	-2.94	118.64	122.93
4	A	2004	Y01	CAD-CBH-CAZ	2.93	112.86	108.38
4	A	2003	Y01	CBI-CBE-CBB	-2.92	114.98	119.50
4	A	2001	Y01	CAV-CAZ-CBH	-2.91	112.70	116.42
4	A	2008	Y01	CAK-CBD-CBG	2.89	115.02	110.93
4	A	2006	Y01	CAD-CBH-CAT	2.84	113.76	109.43
4	A	2001	Y01	CAD-CBH-CAZ	2.80	112.66	108.38
4	A	2003	Y01	CAD-CBH-CAZ	2.79	112.65	108.38
4	A	2001	Y01	CBI-CBE-CBB	-2.74	115.27	119.50
4	A	2004	Y01	CAU-CAS-CBF	2.69	117.71	113.14
4	A	2002	Y01	CBF-CBD-CBG	-2.69	105.58	109.09
4	A	2007	Y01	CAT-CBH-CAZ	-2.68	104.12	108.74
4	A	2001	Y01	CAR-CBC-CAV	-2.63	107.31	110.97
4	A	2003	Y01	CAS-CBF-CBD	2.63	115.45	111.78
4	A	2007	Y01	CAD-CBH-CBF	2.51	114.48	111.66
4	A	2004	Y01	CAS-CBF-CBD	2.48	115.25	111.78
6	A	2010	LMN	CBR-CCM-CBQ	-2.40	105.50	109.96
4	A	2007	Y01	CAS-CBF-CBH	-2.39	110.14	113.08
4	A	2003	Y01	CAS-CBF-CBH	-2.28	110.28	113.08
4	A	2001	Y01	CAC-CBB-CBE	-2.24	109.52	112.88
4	A	2003	Y01	CAC-CBB-CAO	-2.23	106.89	110.34
6	A	2010	LMN	CBT-OBV-CCJ	2.21	118.93	113.31
4	A	2003	Y01	CBD-CAK-CAI	-2.20	109.72	112.76
4	A	2006	Y01	CAD-CBH-CAZ	2.18	111.72	108.38
4	A	2004	Y01	CAP-CBE-CBB	-2.18	108.88	112.18
6	A	2010	LMN	OBX-CCJ-OBV	-2.18	104.90	110.04
4	A	2007	Y01	CBH-CBF-CBD	-2.17	109.54	112.71
4	A	2006	Y01	CAS-CAU-CBI	2.15	116.36	112.74
4	A	2003	Y01	CAC-CBB-CBE	-2.13	109.69	112.88
4	A	2001	Y01	OAW-CBC-CAV	2.09	112.34	108.04
4	A	2004	Y01	CBD-CAK-CAI	-2.09	109.87	112.76
4	A	2007	Y01	CAP-CAQ-CBG	-2.08	101.06	105.14
4	A	2008	Y01	CBG-CBI-CBE	-2.07	97.72	100.10
4	A	2004	Y01	CBI-CBE-CBB	-2.06	116.31	119.50
4	A	2001	Y01	CAU-CAS-CBF	2.04	116.61	113.14
4	A	2004	Y01	CAS-CBF-CBH	-2.02	110.60	113.08

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2002	Y01	OAG-CAY-OAW-CBC
4	A	2004	Y01	OAG-CAY-OAW-CBC
4	A	2004	Y01	CAM-CAY-OAW-CBC
4	A	2006	Y01	CAM-CAY-OAW-CBC
4	A	2007	Y01	CAM-CAY-OAW-CBC
5	A	2005	3PE	C11-O13-P-O14
5	A	2005	3PE	O13-C11-C12-N
5	A	2005	3PE	C22-C21-O21-C2
6	A	2010	LMN	OBX-CCJ-OBV-CBT
4	A	2001	Y01	CAV-CBC-OAW-CAY
4	A	2007	Y01	OAG-CAY-OAW-CBC
5	A	2005	3PE	O22-C21-O21-C2
4	A	2002	Y01	CAM-CAY-OAW-CBC
4	A	2006	Y01	OAG-CAY-OAW-CBC
6	A	2010	LMN	CCF-CCQ-OCB-CCS
4	A	2003	Y01	CAJ-CAO-CBB-CBE
4	A	2003	Y01	CAJ-CAO-CBB-CAC
6	A	2009	LMN	OBX-CCJ-OBV-CBT
4	A	2006	Y01	CAJ-CAO-CBB-CBE
5	A	2005	3PE	C32-C31-O31-C3
4	A	2007	Y01	CAV-CBC-OAW-CAY
4	A	2008	Y01	CAJ-CAO-CBB-CBE
6	A	2010	LMN	C3-C4-O4-CCR
4	A	2008	Y01	CAN-CAJ-CAO-CBB
4	A	2006	Y01	CAJ-CAO-CBB-CAC
5	A	2005	3PE	O32-C31-O31-C3
4	A	2008	Y01	CAX-CAL-CAM-CAY
4	A	2008	Y01	CAJ-CAO-CBB-CAC
4	A	2004	Y01	CAO-CAJ-CAN-CBA
4	A	2006	Y01	CAO-CAJ-CAN-CBA
6	A	2010	LMN	CCL-CCJ-OBV-CBT
4	A	2003	Y01	CAJ-CAN-CBA-CAB
4	A	2008	Y01	CAJ-CAN-CBA-CAB
4	A	2002	Y01	CAJ-CAN-CBA-CAA
4	A	2007	Y01	CAR-CBC-OAW-CAY
4	A	2003	Y01	CAJ-CAN-CBA-CAA
4	A	2008	Y01	CAJ-CAN-CBA-CAA
6	A	2010	LMN	C5-C4-O4-CCR
4	A	2002	Y01	CAN-CAJ-CAO-CBB
4	A	2001	Y01	CAJ-CAN-CBA-CAB
4	A	2008	Y01	CAM-CAY-OAW-CBC
6	A	2010	LMN	CBH-CBJ-CBL-CBR

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Mol	Chain	Res	Type	Atoms
4	A	2001	Y01	CAJ-CAN-CBA-CAA
6	A	2010	LMN	OAJ-CBN-CCD-OBZ
5	A	2005	3PE	C35-C36-C37-C38
6	A	2009	LMN	OAL-CBP-CCF-OBX
4	A	2007	Y01	CAO-CAJ-CAN-CBA
6	A	2010	LMN	OAI-CBM-CCC-OBY
4	A	2002	Y01	CAJ-CAN-CBA-CAB
6	A	2009	LMN	OAI-CBM-CCC-OBY
5	A	2005	3PE	C2A-C2B-C2C-C2D
6	A	2010	LMN	CCH-CCQ-OCB-CCS
6	A	2009	LMN	OAJ-CBN-CCD-OBZ
6	A	2010	LMN	CBI-CBK-CBQ-CCM
4	A	2008	Y01	OAG-CAY-OAW-CBC
4	A	2001	Y01	CAN-CAJ-CAO-CBB
4	A	2002	Y01	CAV-CBC-OAW-CAY
4	A	2002	Y01	CAR-CBC-OAW-CAY
4	A	2007	Y01	CAJ-CAO-CBB-CAC
4	A	2003	Y01	CAM-CAY-OAW-CBC
5	A	2005	3PE	C21-C22-C23-C24
5	A	2005	3PE	C39-C3A-C3B-C3C
4	A	2004	Y01	CAJ-CAN-CBA-CAA
6	A	2010	LMN	OBV-CBT-CCM-CBR
4	A	2003	Y01	OAG-CAY-OAW-CBC
6	A	2009	LMN	OBZ-CCS-OCB-CCQ
4	A	2004	Y01	CAJ-CAN-CBA-CAB
4	A	2003	Y01	CAV-CBC-OAW-CAY
6	A	2009	LMN	C5-C4-O4-CCR
5	A	2005	3PE	C27-C28-C29-C2A
4	A	2007	Y01	CAM-CAL-CAX-OAF
4	A	2007	Y01	CAM-CAL-CAX-OAH
6	A	2009	LMN	CCW-CCS-OCB-CCQ
6	A	2009	LMN	C3-C4-O4-CCR
4	A	2003	Y01	CAR-CBC-OAW-CAY
6	A	2010	LMN	CAB-CAX-CAZ-CBB
4	A	2006	Y01	CAM-CAL-CAX-OAF
4	A	2003	Y01	CAO-CAJ-CAN-CBA
4	A	2003	Y01	CAM-CAL-CAX-OAH
4	A	2006	Y01	CAN-CAJ-CAO-CBB
5	A	2005	3PE	C36-C37-C38-C39
6	A	2010	LMN	CBG-CBI-CBK-CBQ
4	A	2003	Y01	CAM-CAL-CAX-OAF
4	A	2006	Y01	CAX-CAL-CAM-CAY

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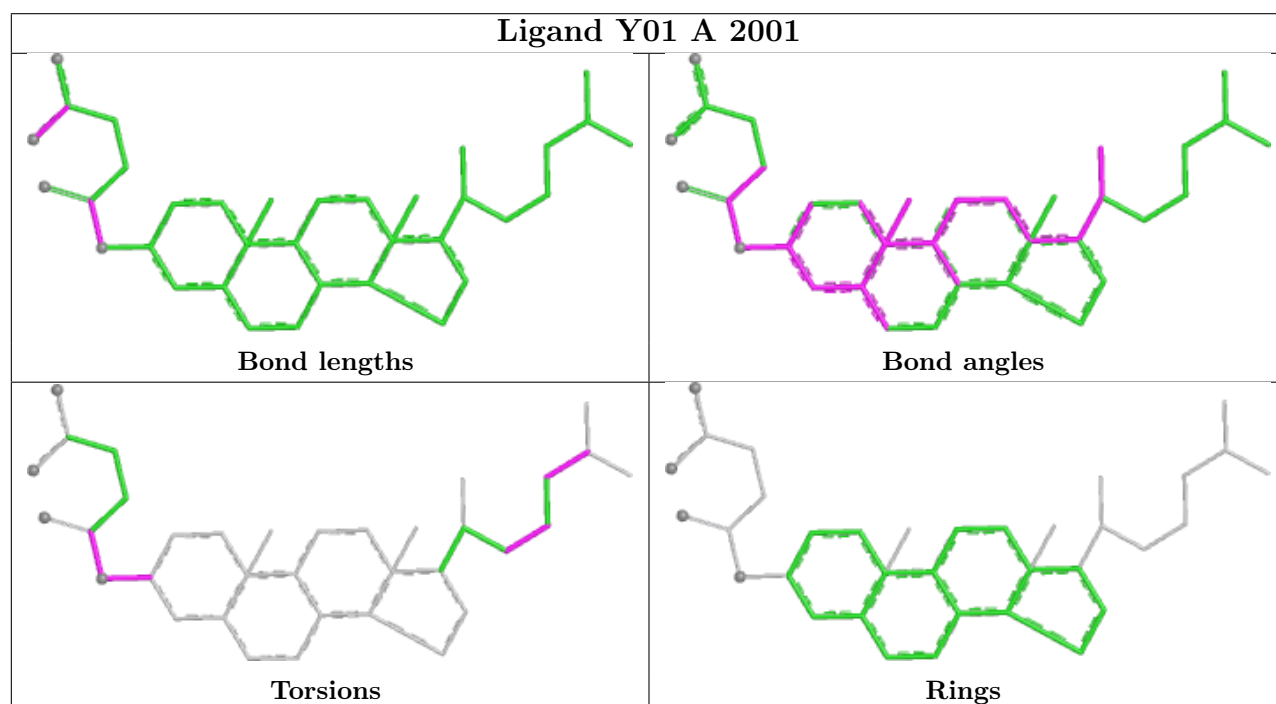
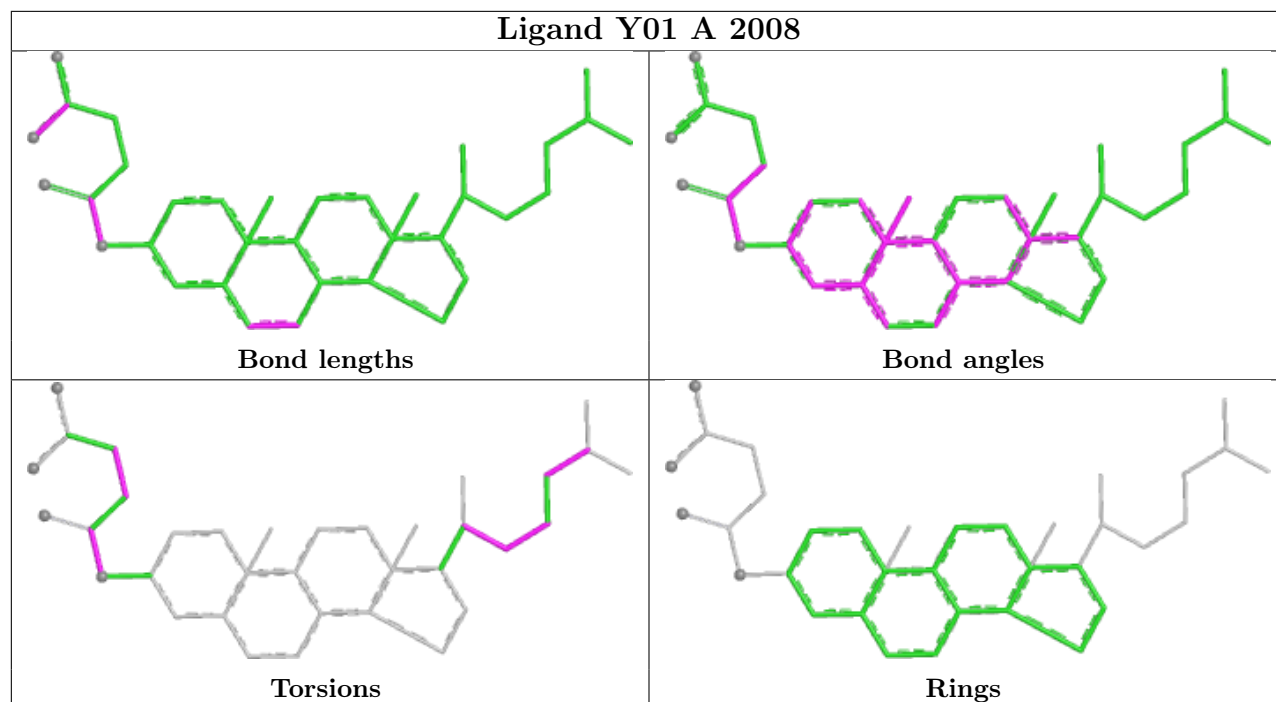
Mol	Chain	Res	Type	Atoms
5	A	2005	3PE	C28-C29-C2A-C2B
4	A	2006	Y01	CAM-CAL-CAX-OAH
4	A	2007	Y01	CAL-CAM-CAY-OAW
6	A	2009	LMN	OBV-CBT-CCM-CBR
6	A	2010	LMN	OBV-CBT-CCM-CBQ
4	A	2001	Y01	OAG-CAY-OAW-CBC
5	A	2005	3PE	C33-C34-C35-C36
6	A	2009	LMN	CBG-CBI-CBK-CBQ
4	A	2003	Y01	CAC-CBB-CBE-CBI
4	A	2007	Y01	CAL-CAM-CAY-OAG
6	A	2009	LMN	C4-C5-C6-O6

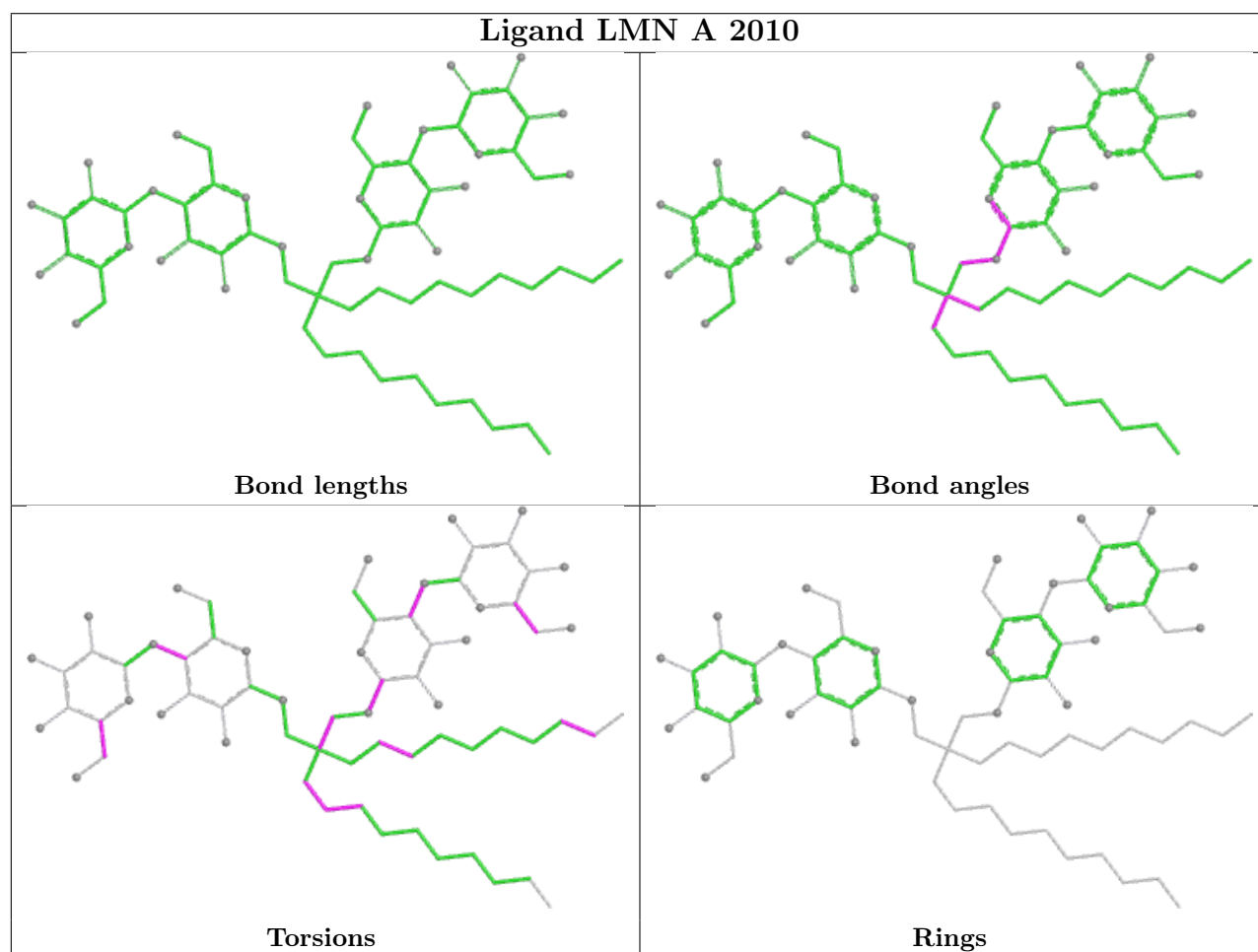
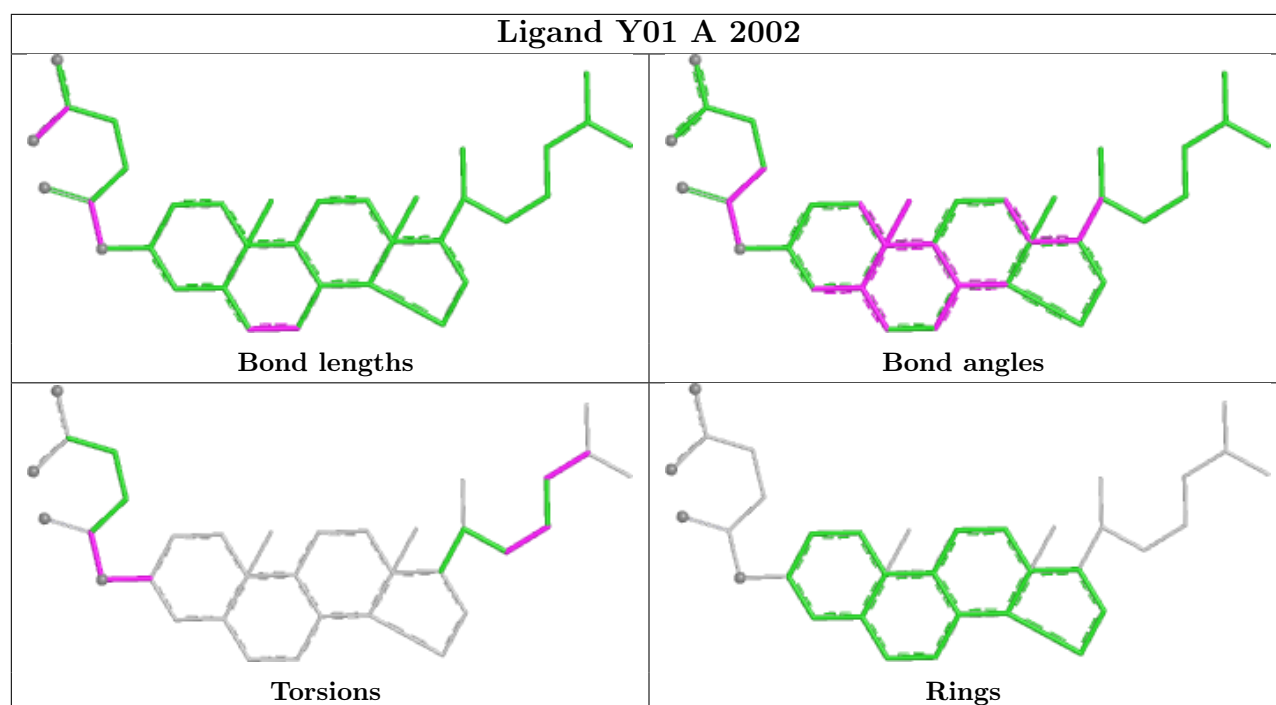
There are no ring outliers.

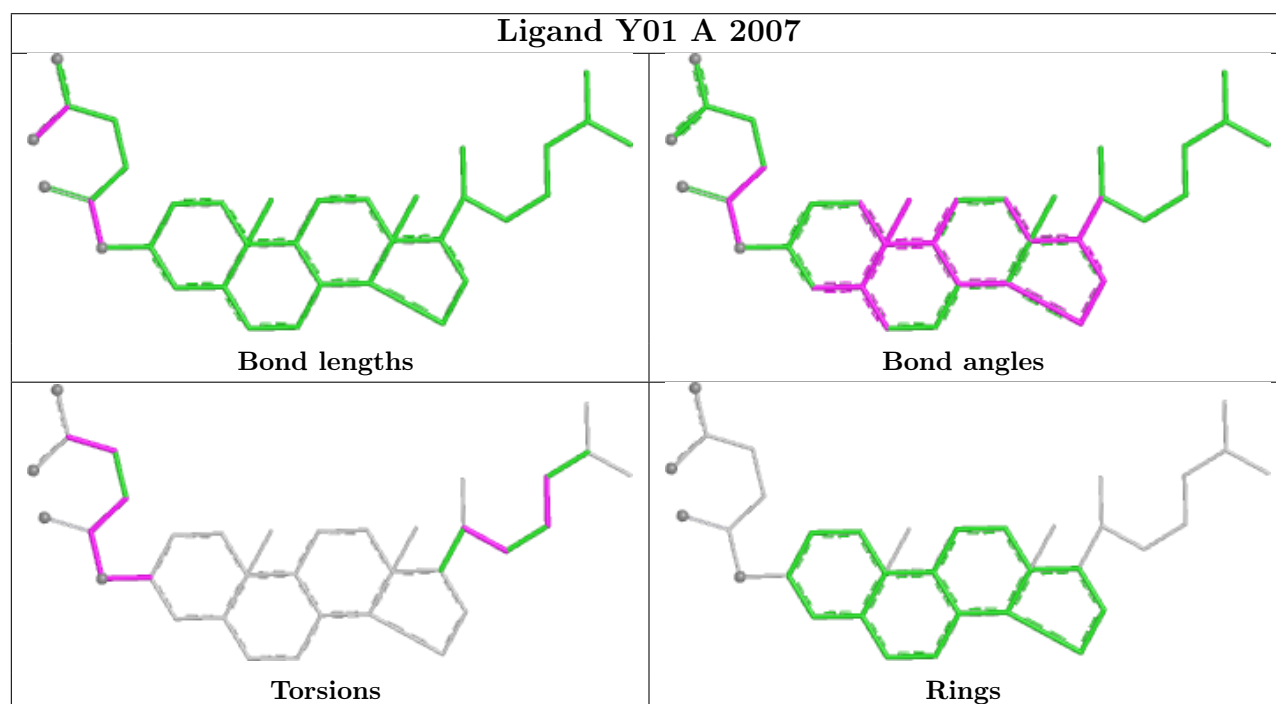
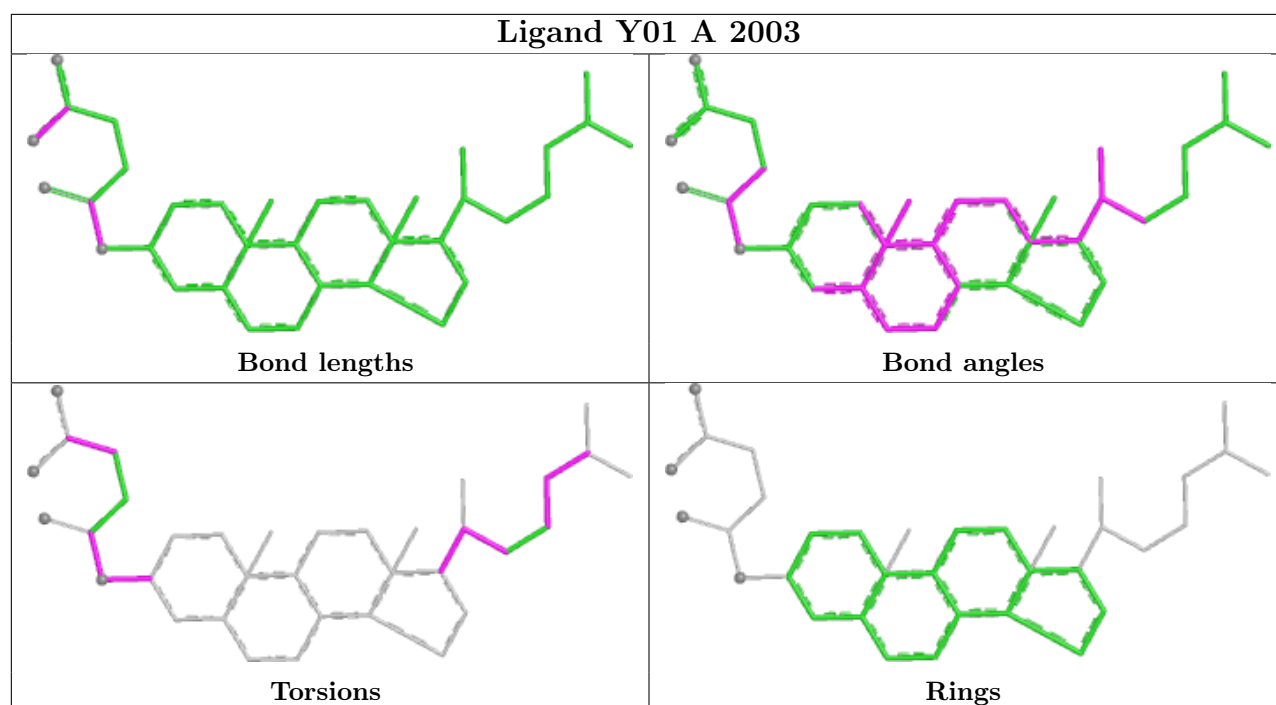
8 monomers are involved in 12 short contacts:

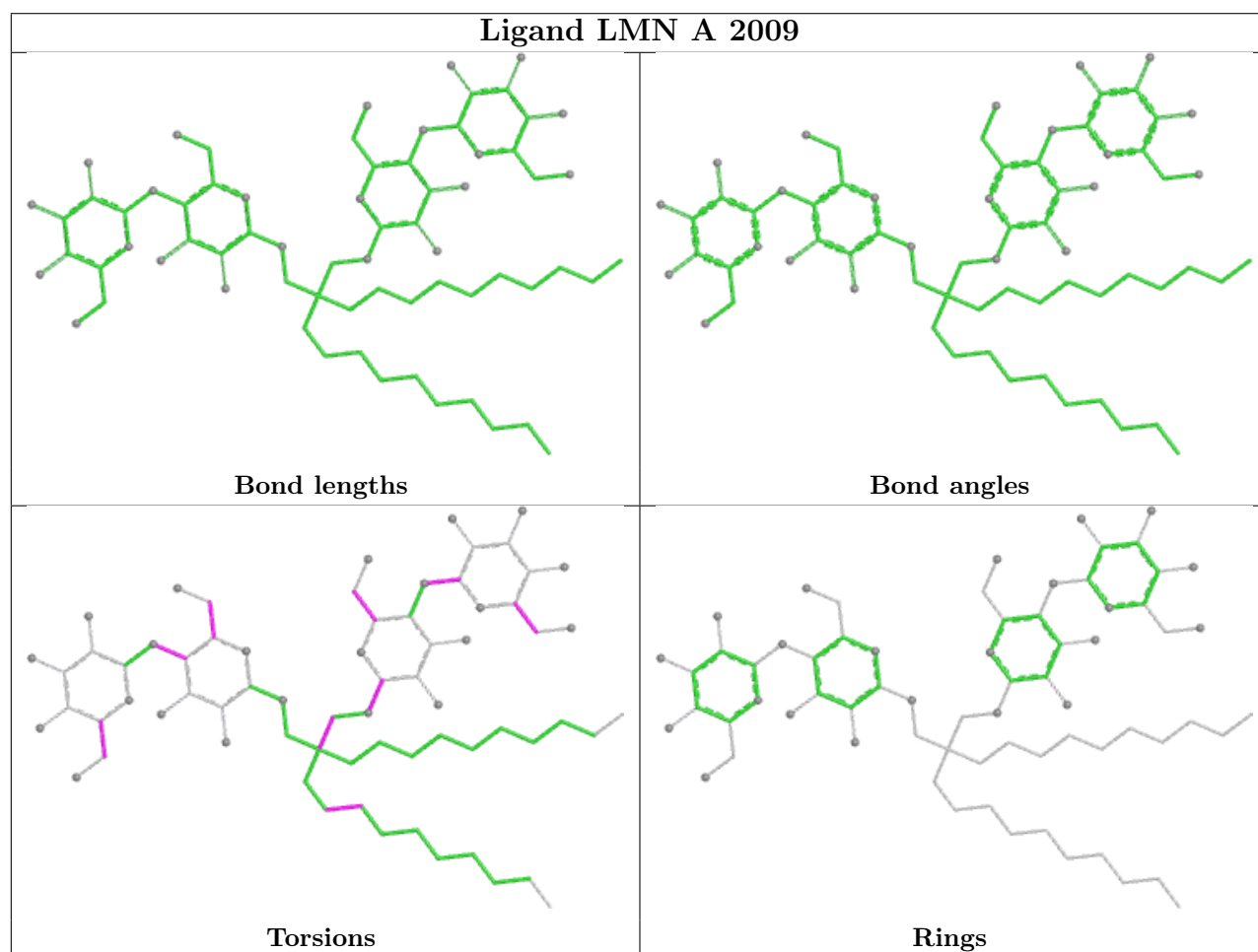
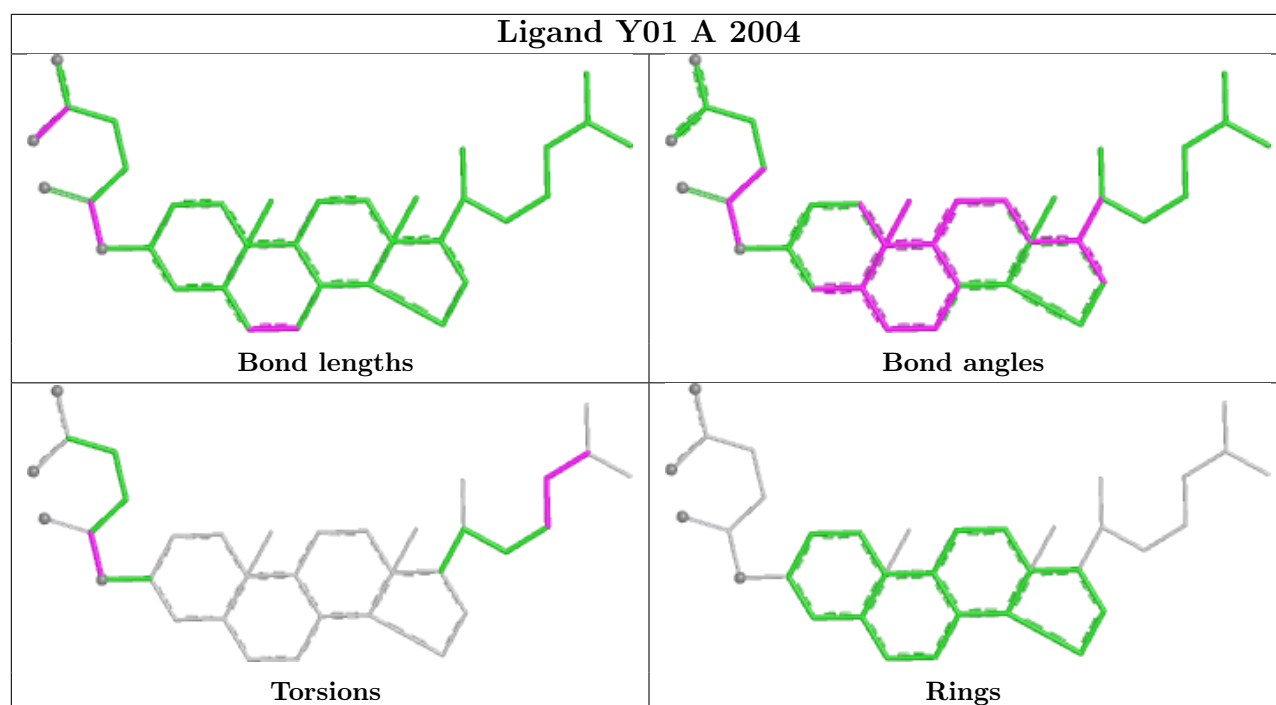
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2008	Y01	3	0
4	A	2001	Y01	2	0
4	A	2002	Y01	1	0
4	A	2003	Y01	2	0
4	A	2007	Y01	2	0
4	A	2004	Y01	1	0
6	A	2009	LMN	2	0
4	A	2006	Y01	1	0

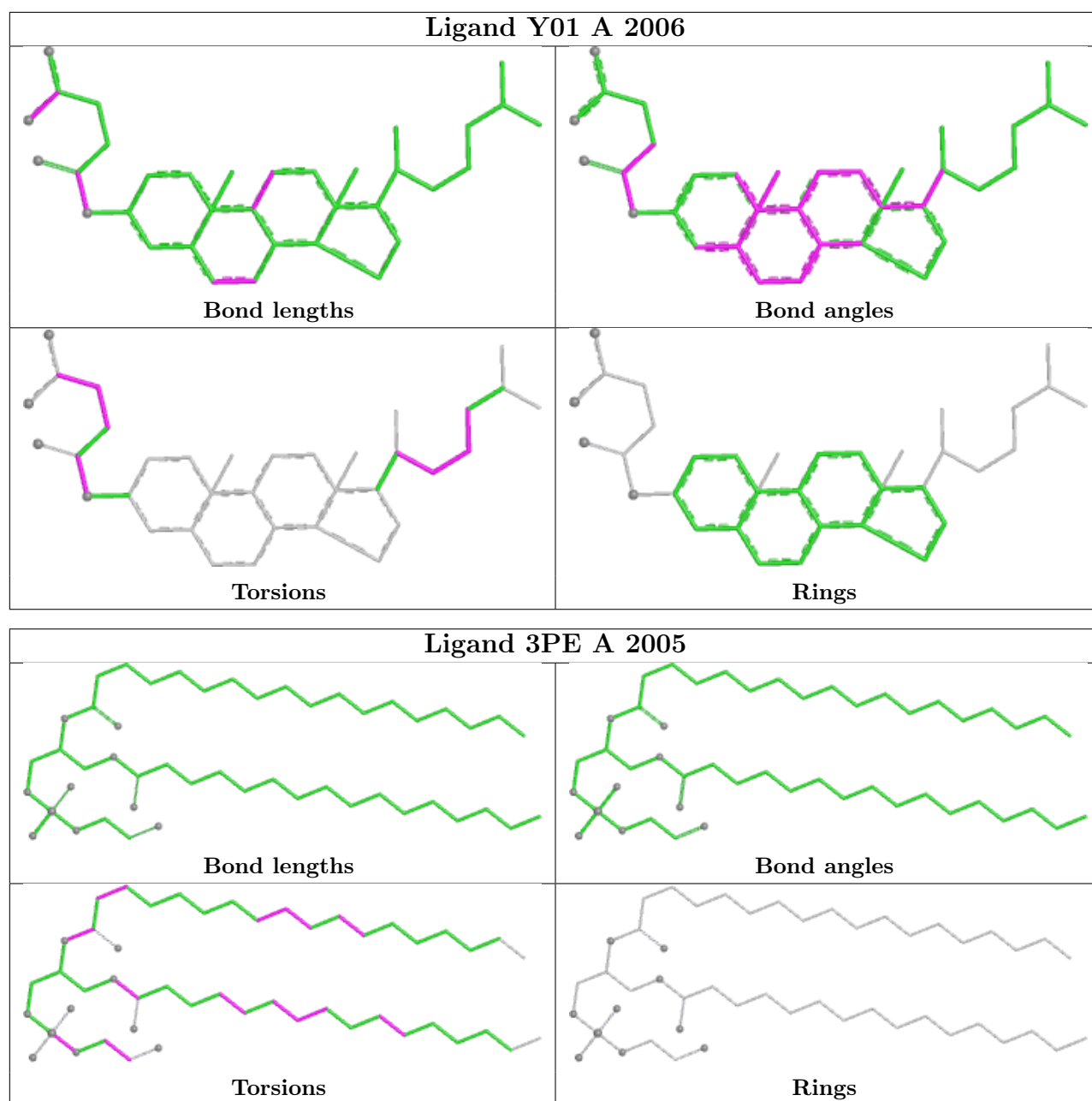
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

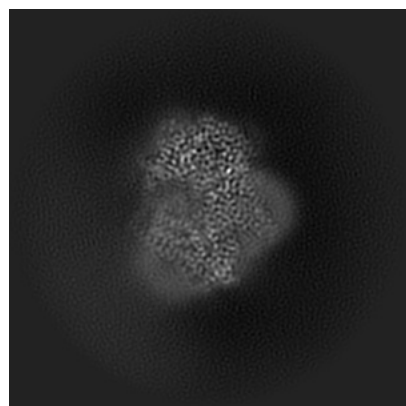
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71553. These allow visual inspection of the internal detail of the map and identification of artifacts.

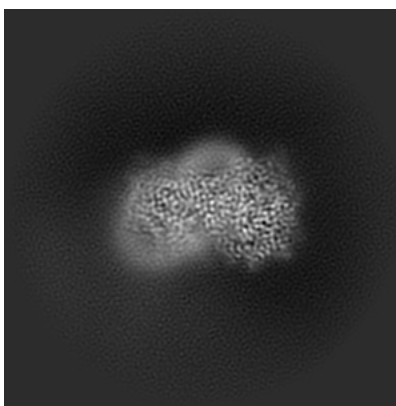
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

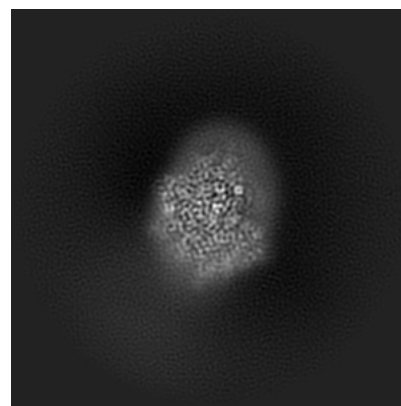
6.1.1 Primary map



X

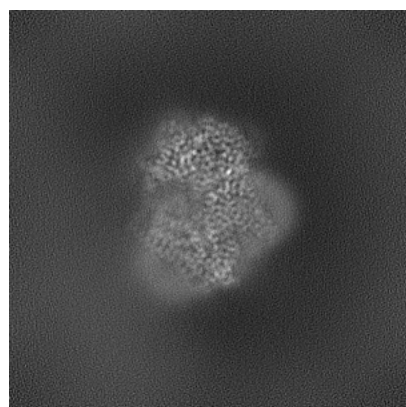


Y

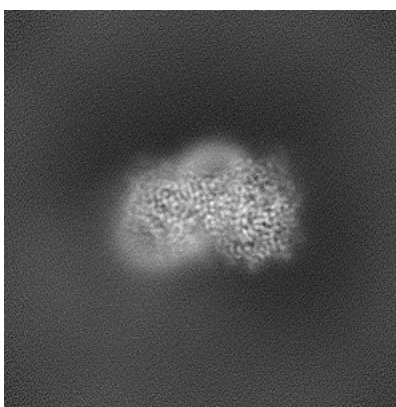


Z

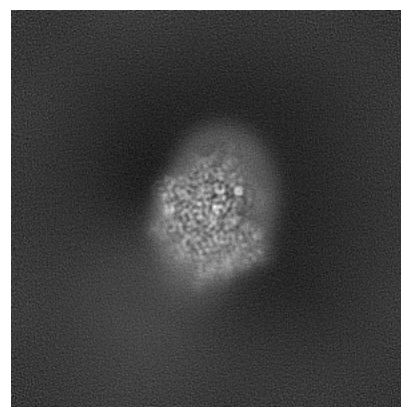
6.1.2 Raw map



X



Y

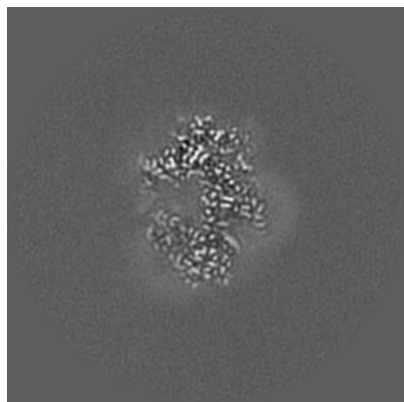


Z

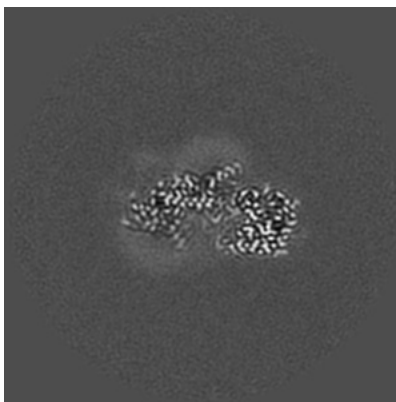
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

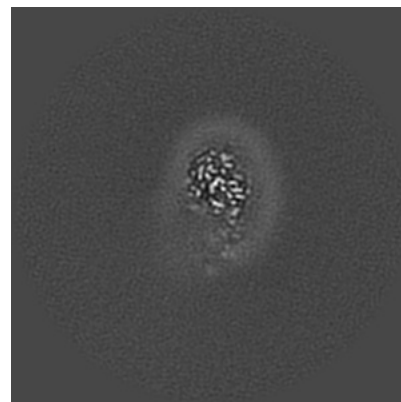
6.2.1 Primary map



X Index: 160

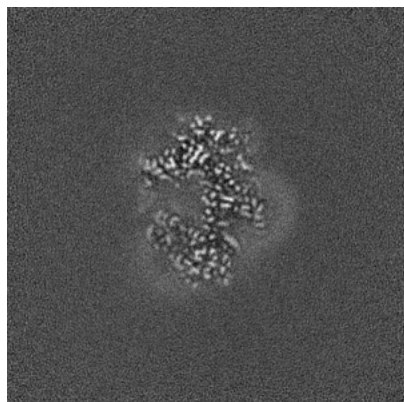


Y Index: 160

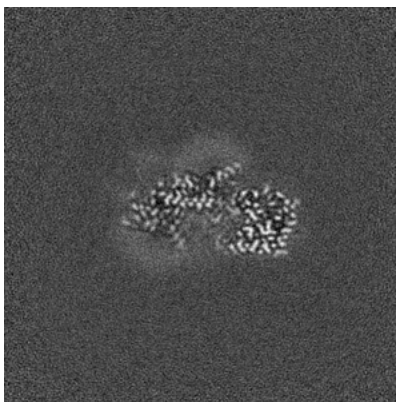


Z Index: 160

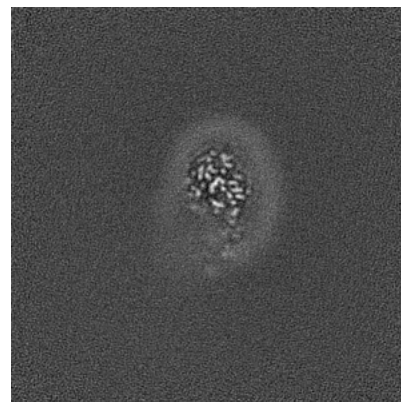
6.2.2 Raw map



X Index: 160



Y Index: 160

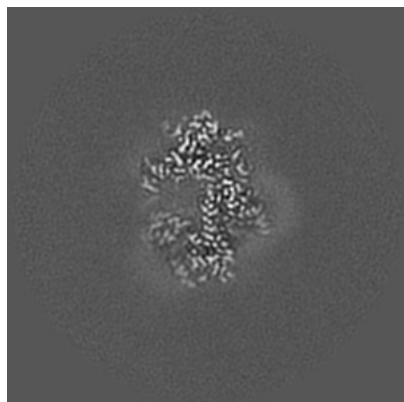


Z Index: 160

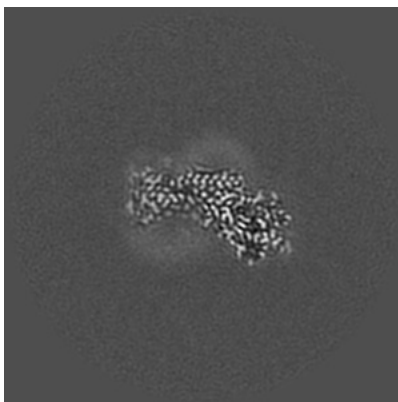
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

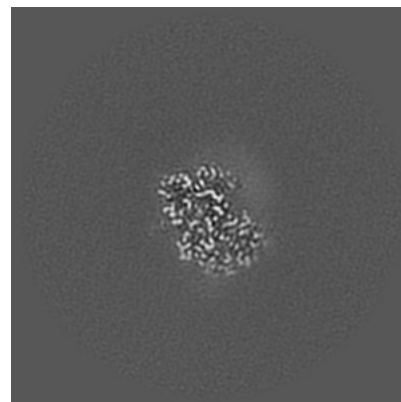
6.3.1 Primary map



X Index: 163

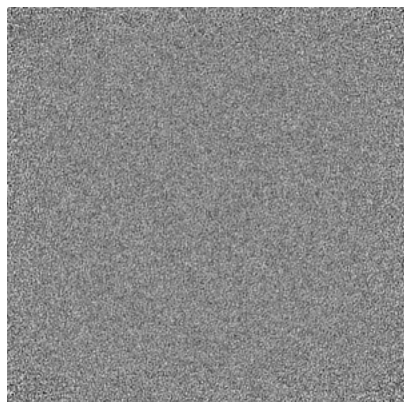


Y Index: 174

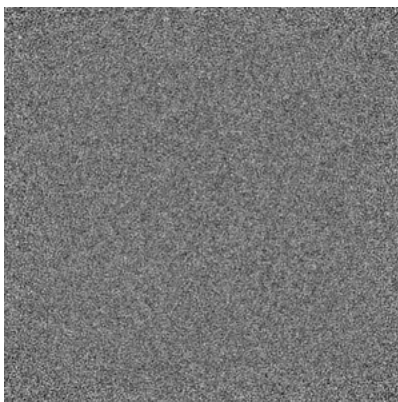


Z Index: 193

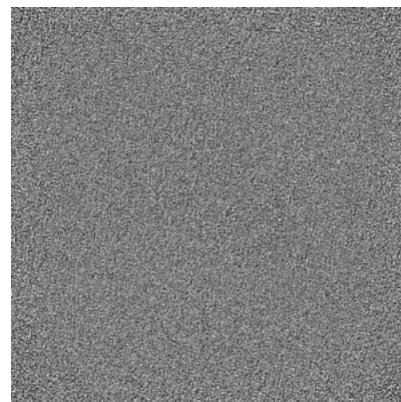
6.3.2 Raw map



X Index: 0



Y Index: 0

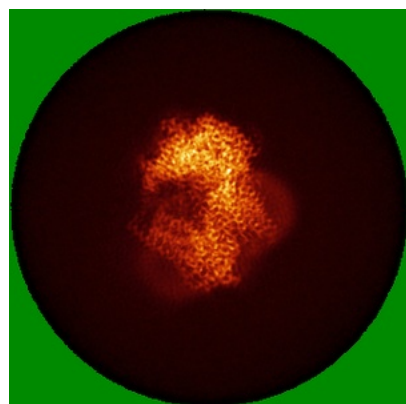


Z Index: 0

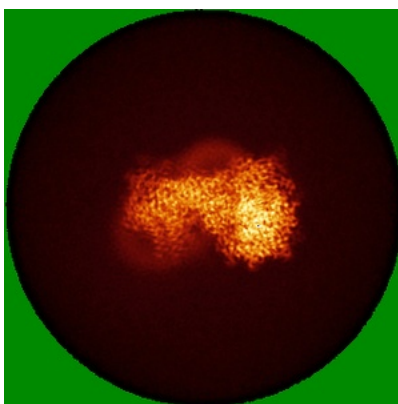
The images above show the largest variance slices of the map in three orthogonal directions.

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

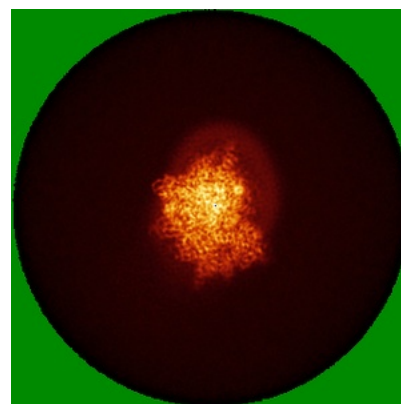
6.4.1 Primary map



X

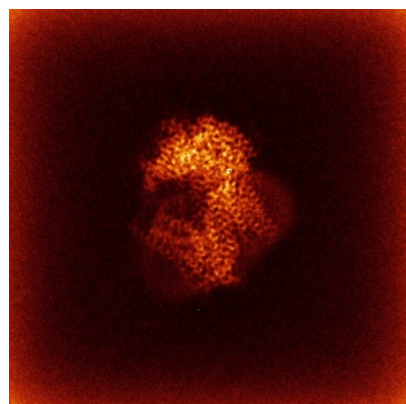


Y

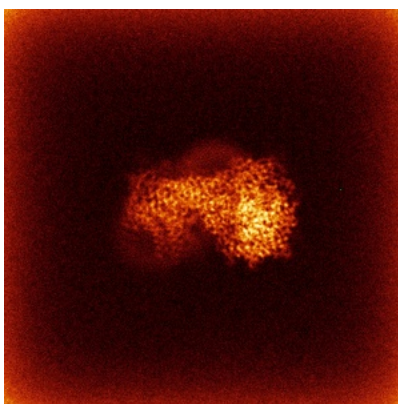


Z

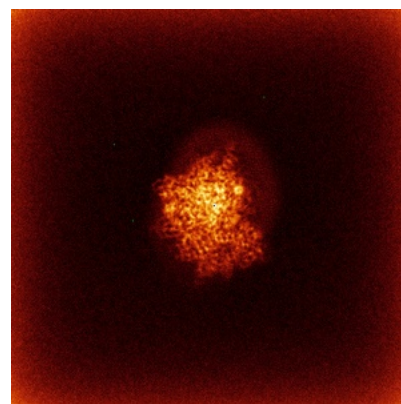
6.4.2 Raw map



X



Y

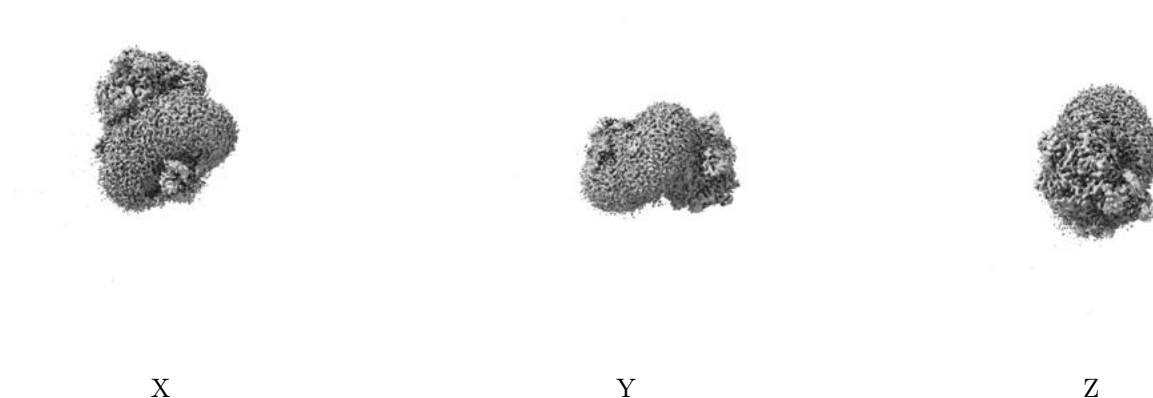


Z

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.

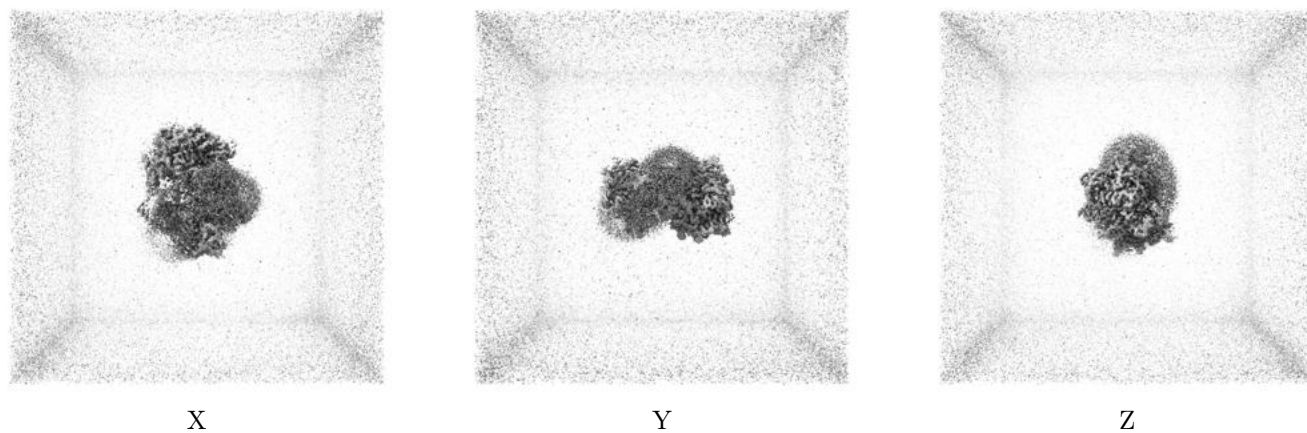
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.103. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

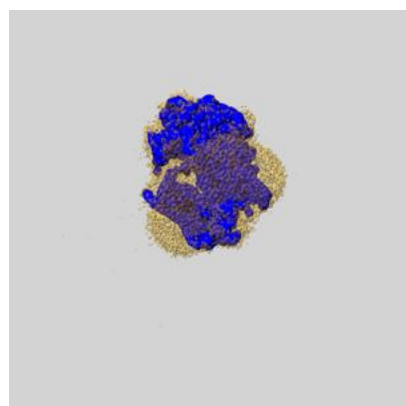
6.6 Mask visualisation [i](#)

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

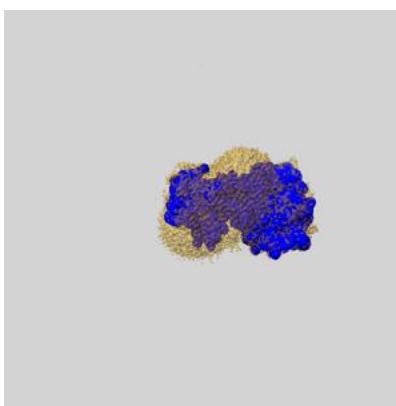
A mask typically either:

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

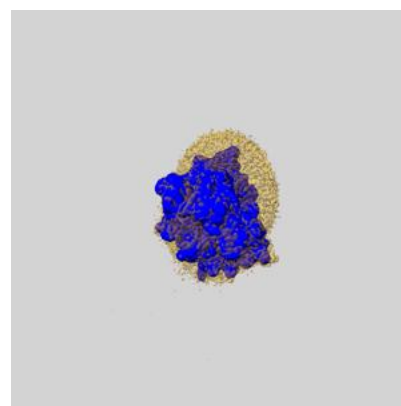
6.6.1 emd_71553_msk_1.map [i](#)



X



Y

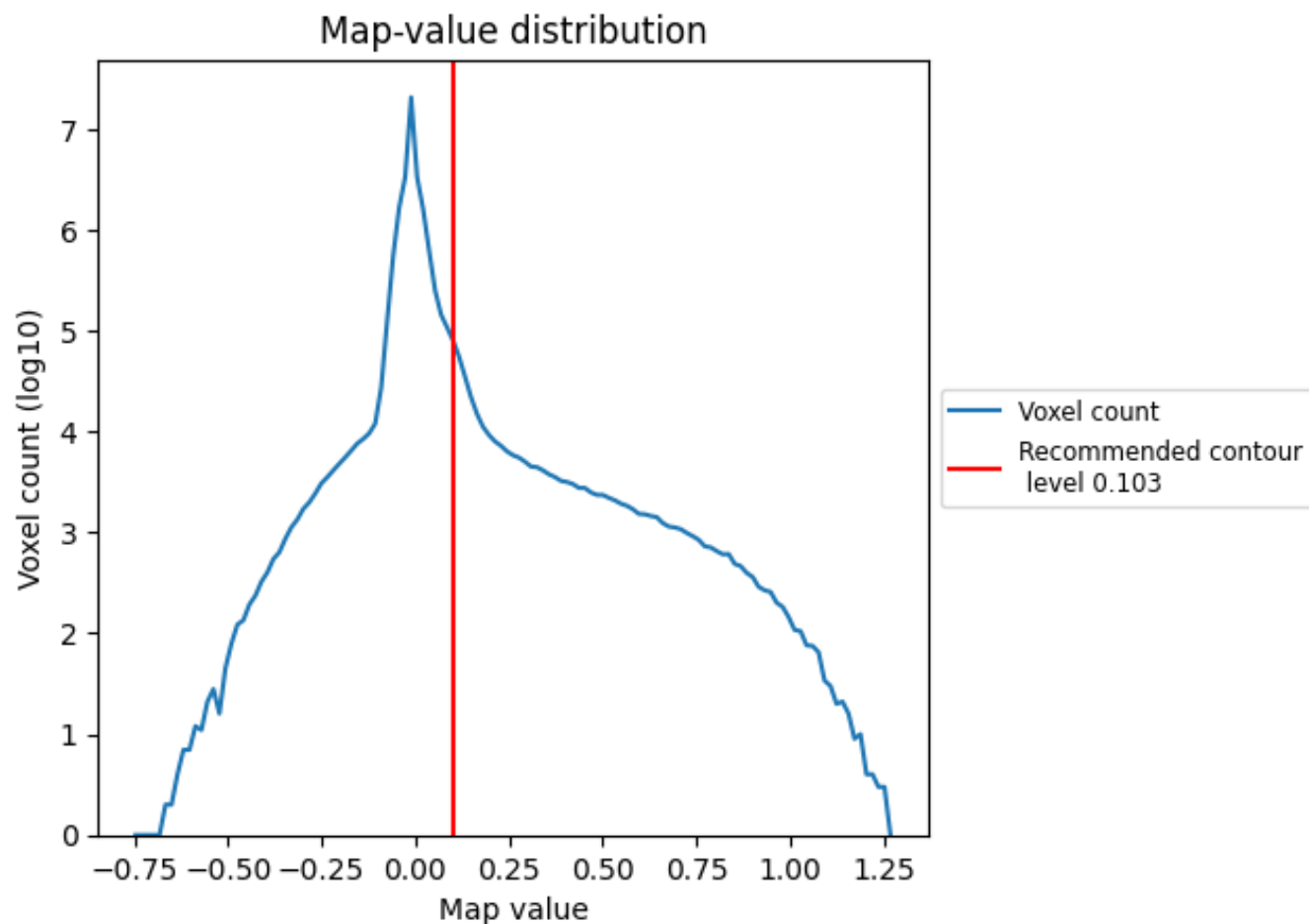


Z

7 Map analysis [i](#)

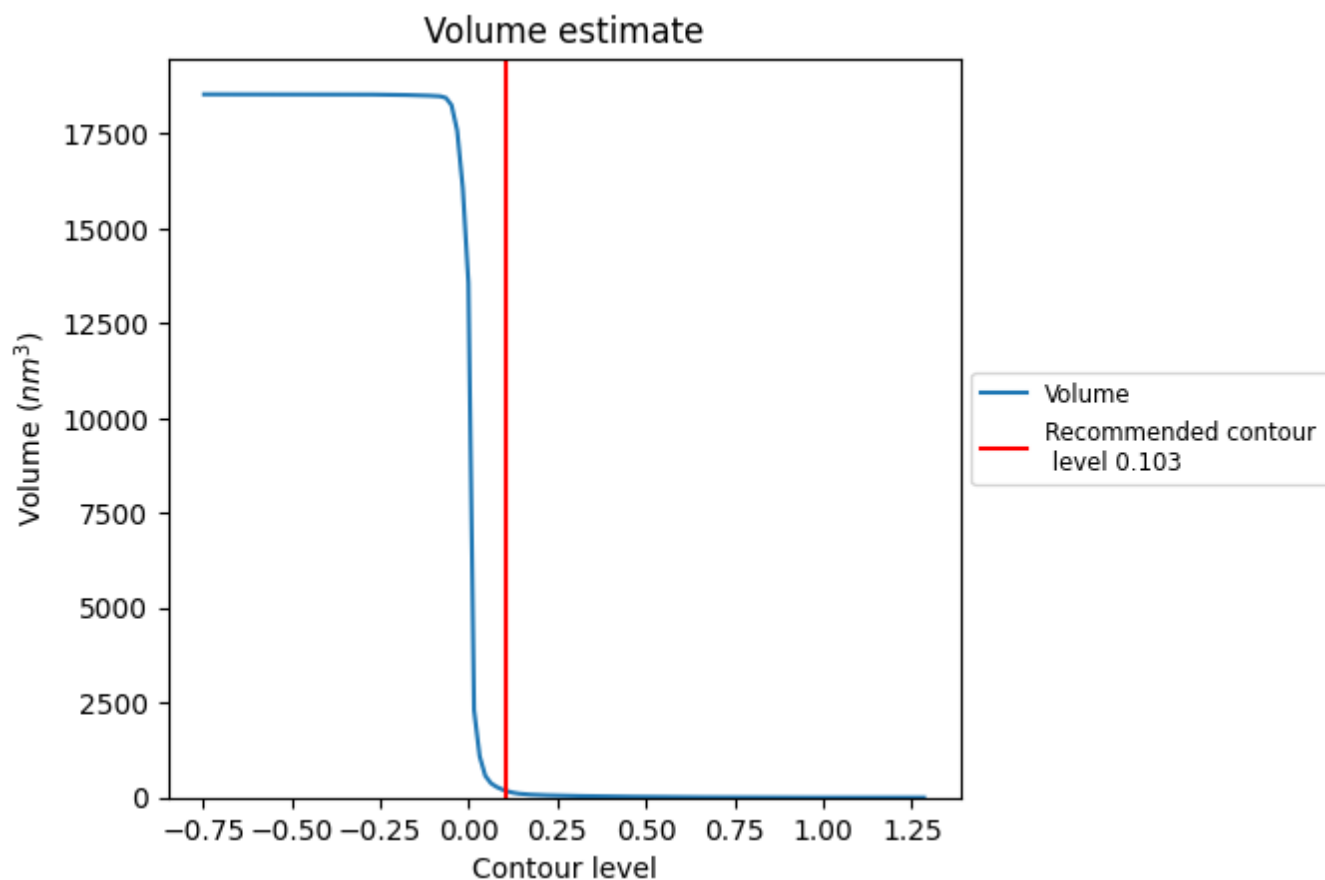
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

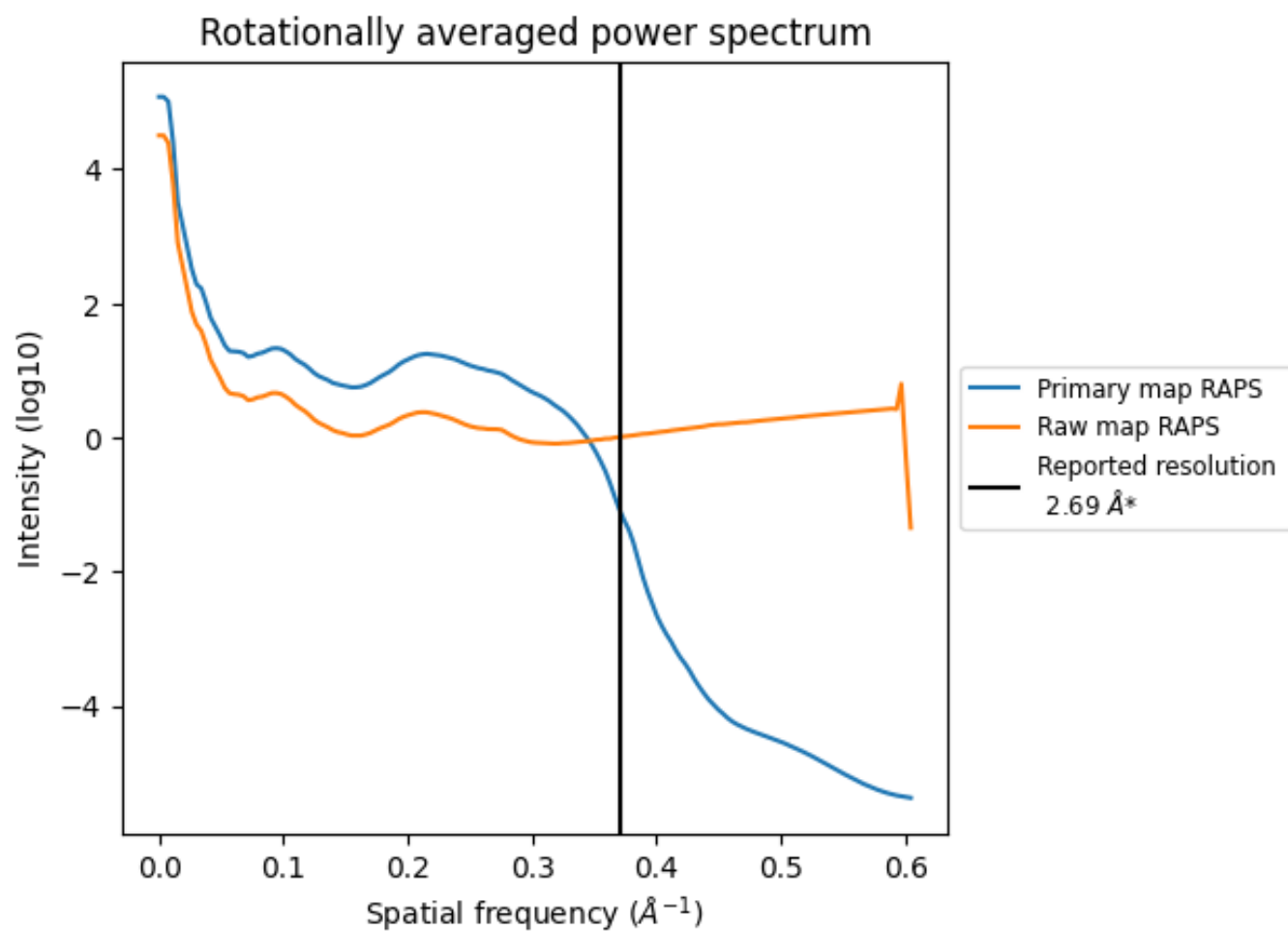
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm^3 ; this corresponds to an approximate mass of 169 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

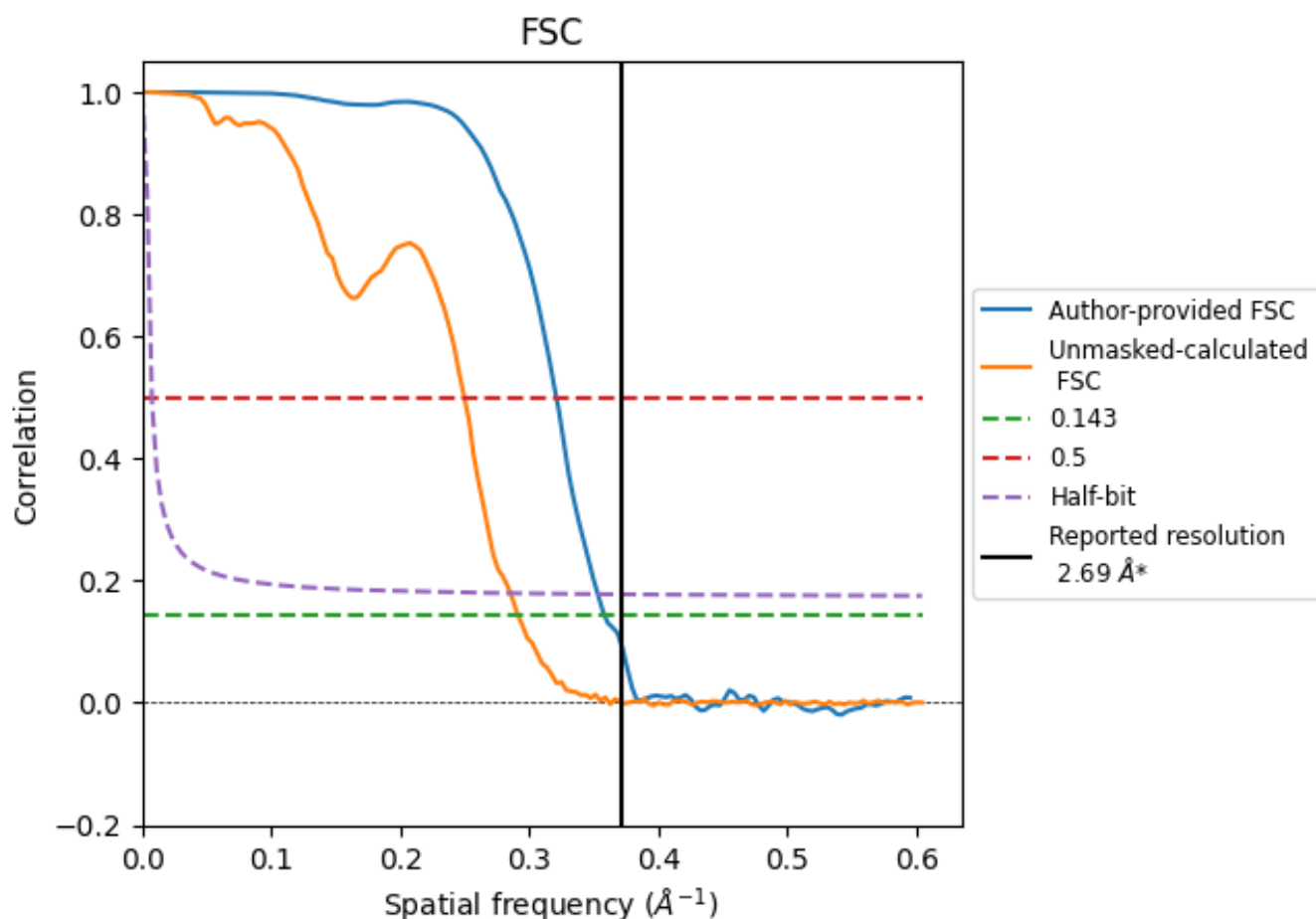


*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.372 \AA^{-1}

8.2 Resolution estimates [i](#)

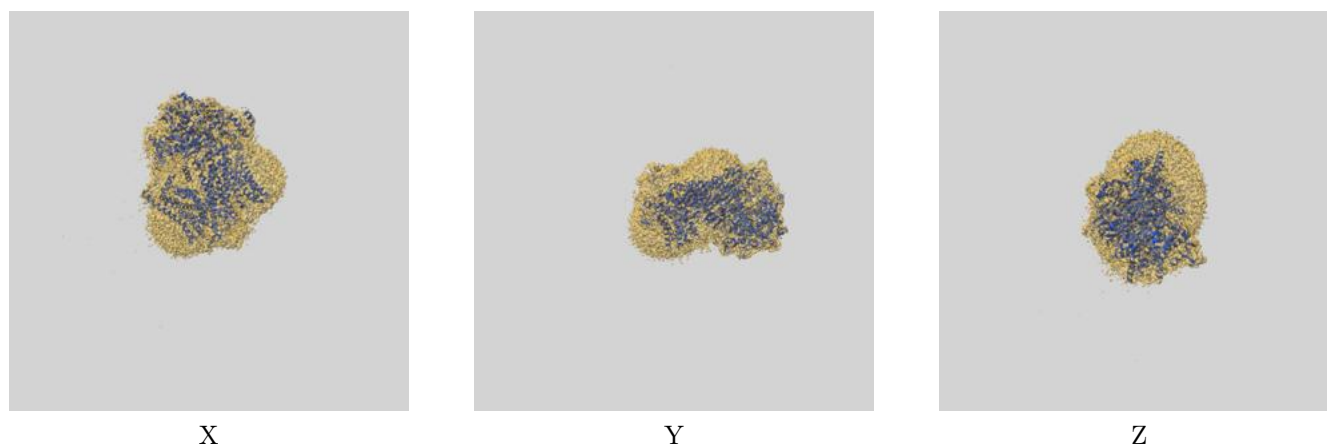
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.79	3.12	2.83
Unmasked-calculated*	3.43	4.01	3.51

*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 3.43 differs from the reported value 2.69 by more than 10 %

9 Map-model fit [i](#)

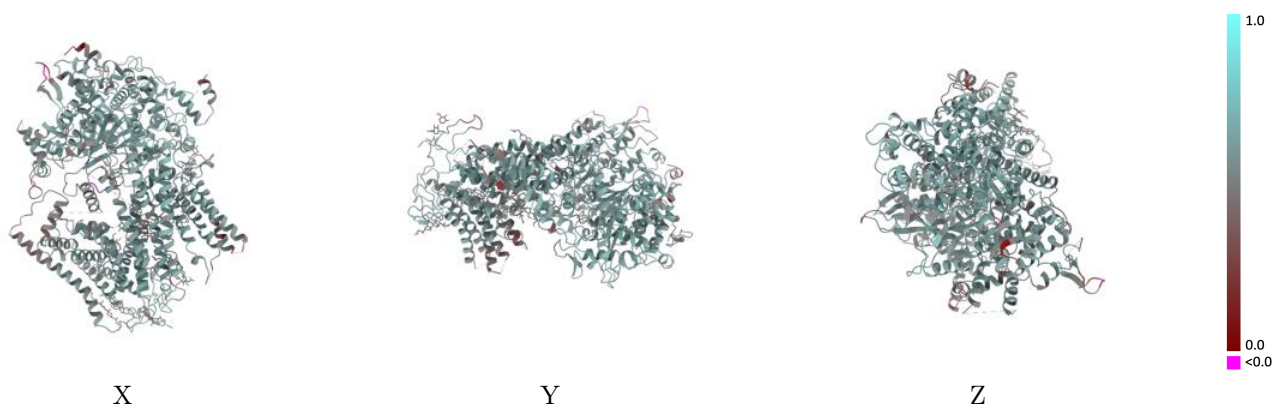
This section contains information regarding the fit between EMDB map EMD-71553 and PDB model 9PE4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



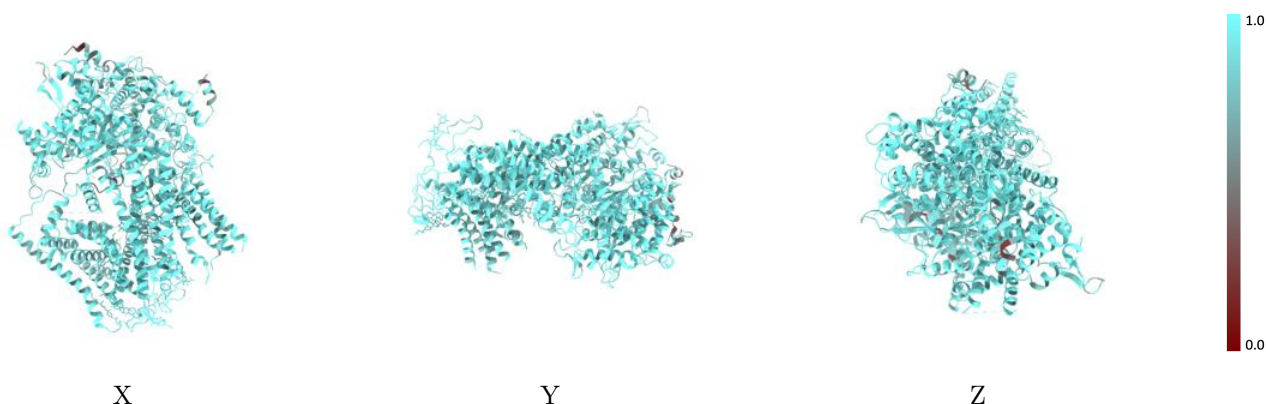
The images above show the 3D surface view of the map at the recommended contour level 0.103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



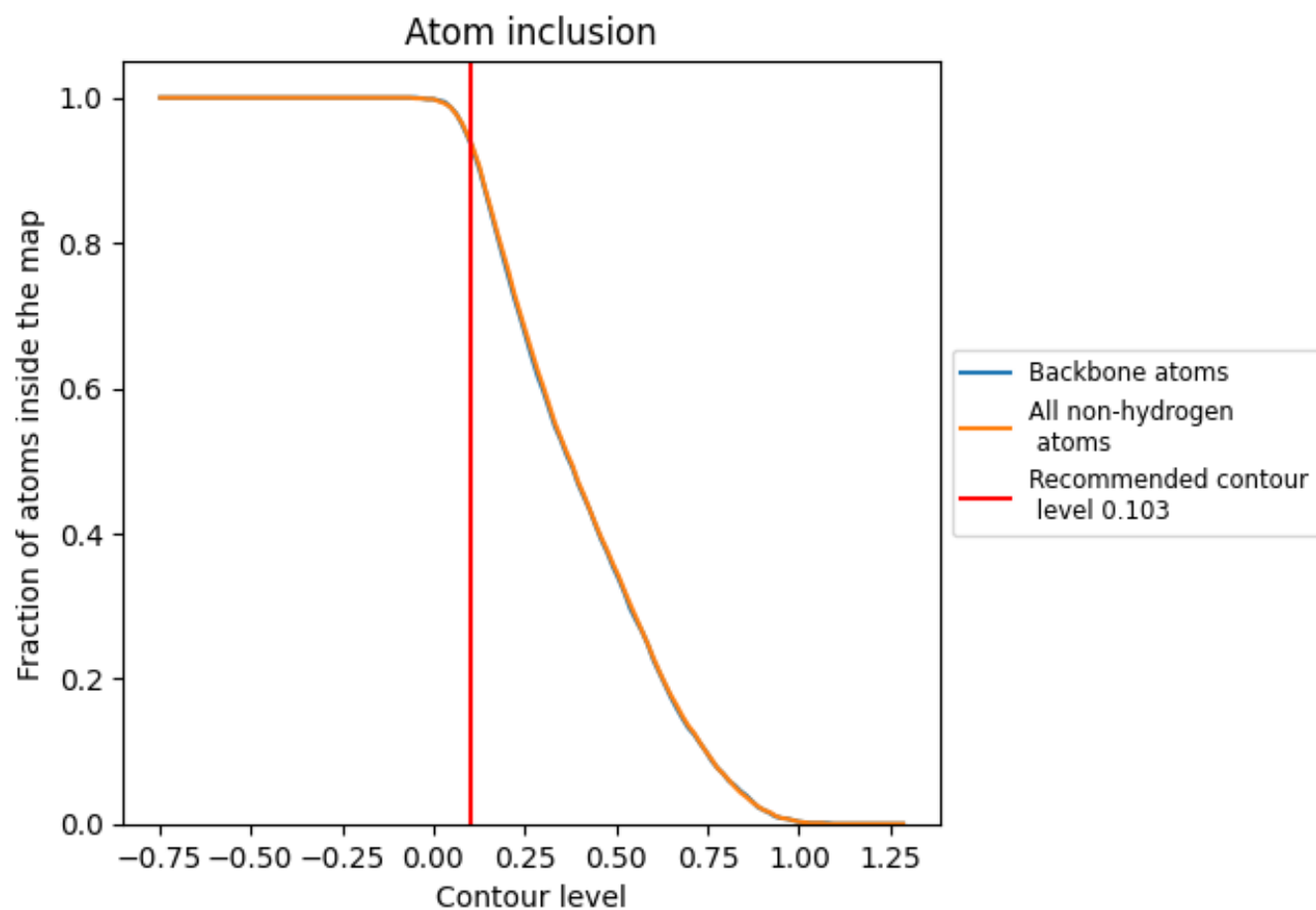
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.103).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9380	<div></div> 0.5610
A	<div></div> 0.9490	<div></div> 0.5630
D	<div></div> 0.9740	<div></div> 0.4400
G	<div></div> 0.7390	<div></div> 0.5150

