



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 08:14 PM JST

PDB ID : 7CM3
EMDB ID : EMD-30400
Title : Cryo-EM structure of human NALCN in complex with FAM155A
Authors : Wu, J.; Yan, Z.; Ke, M.
Deposited on : 2020-07-24
Resolution : 3.10 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

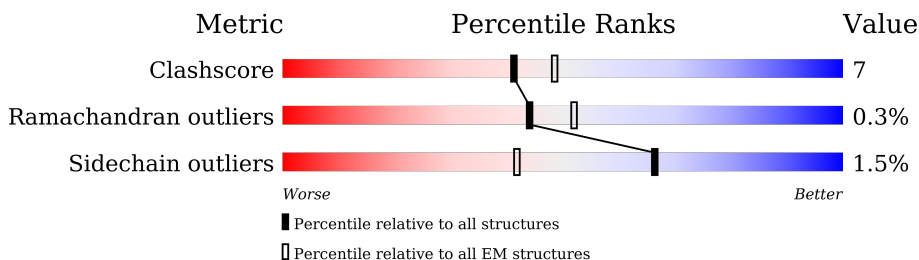
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1765	
2	B	485	
3	C	2	
4	D	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12418 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 leak channel non-selective protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1278	10442	6905	1698	1757	82	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1739	LEU	-	expression tag	UNP Q8IZF0
A	1740	GLU	-	expression tag	UNP Q8IZF0
A	1741	ASP	-	expression tag	UNP Q8IZF0
A	1742	GLU	-	expression tag	UNP Q8IZF0
A	1743	VAL	-	expression tag	UNP Q8IZF0
A	1744	ASP	-	expression tag	UNP Q8IZF0
A	1745	ALA	-	expression tag	UNP Q8IZF0
A	1746	GLY	-	expression tag	UNP Q8IZF0
A	1747	SER	-	expression tag	UNP Q8IZF0
A	1748	ASP	-	expression tag	UNP Q8IZF0
A	1749	TYR	-	expression tag	UNP Q8IZF0
A	1750	LYS	-	expression tag	UNP Q8IZF0
A	1751	ASP	-	expression tag	UNP Q8IZF0
A	1752	ASP	-	expression tag	UNP Q8IZF0
A	1753	ASP	-	expression tag	UNP Q8IZF0
A	1754	ASP	-	expression tag	UNP Q8IZF0
A	1755	LYS	-	expression tag	UNP Q8IZF0
A	1756	GLY	-	expression tag	UNP Q8IZF0
A	1757	SER	-	expression tag	UNP Q8IZF0
A	1758	ASP	-	expression tag	UNP Q8IZF0
A	1759	TYR	-	expression tag	UNP Q8IZF0
A	1760	LYS	-	expression tag	UNP Q8IZF0
A	1761	ASP	-	expression tag	UNP Q8IZF0
A	1762	ASP	-	expression tag	UNP Q8IZF0
A	1763	ASP	-	expression tag	UNP Q8IZF0
A	1764	ASP	-	expression tag	UNP Q8IZF0
A	1765	LYS	-	expression tag	UNP Q8IZF0

- Molecule 2 is a protein called Transmembrane protein FAM155A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	182	1483	934	243	292	14	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	459	LEU	-	expression tag	UNP B1AL88
B	460	GLU	-	expression tag	UNP B1AL88
B	461	ASP	-	expression tag	UNP B1AL88
B	462	GLU	-	expression tag	UNP B1AL88
B	463	VAL	-	expression tag	UNP B1AL88
B	464	ASP	-	expression tag	UNP B1AL88
B	465	ALA	-	expression tag	UNP B1AL88
B	466	GLY	-	expression tag	UNP B1AL88
B	467	SER	-	expression tag	UNP B1AL88
B	468	ASP	-	expression tag	UNP B1AL88
B	469	TYR	-	expression tag	UNP B1AL88
B	470	LYS	-	expression tag	UNP B1AL88
B	471	ASP	-	expression tag	UNP B1AL88
B	472	ASP	-	expression tag	UNP B1AL88
B	473	ASP	-	expression tag	UNP B1AL88
B	474	ASP	-	expression tag	UNP B1AL88
B	475	LYS	-	expression tag	UNP B1AL88
B	476	GLY	-	expression tag	UNP B1AL88
B	477	SER	-	expression tag	UNP B1AL88
B	478	ASP	-	expression tag	UNP B1AL88
B	479	TYR	-	expression tag	UNP B1AL88
B	480	LYS	-	expression tag	UNP B1AL88
B	481	ASP	-	expression tag	UNP B1AL88
B	482	ASP	-	expression tag	UNP B1AL88
B	483	ASP	-	expression tag	UNP B1AL88
B	484	ASP	-	expression tag	UNP B1AL88
B	485	LYS	-	expression tag	UNP B1AL88

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



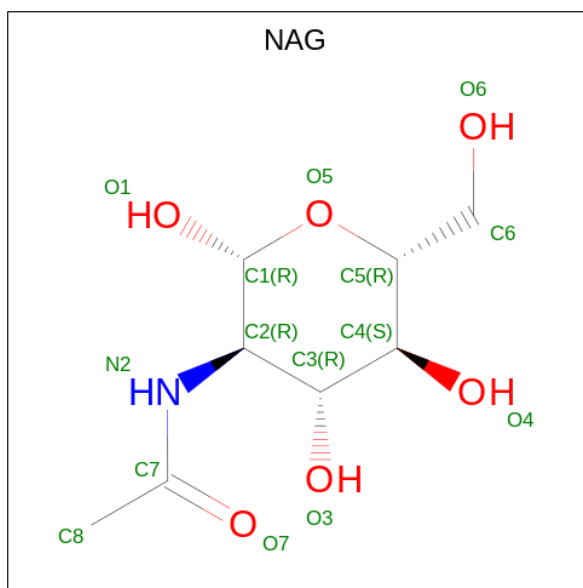
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	2	28	16	2	10	0	0

- Molecule 4 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.



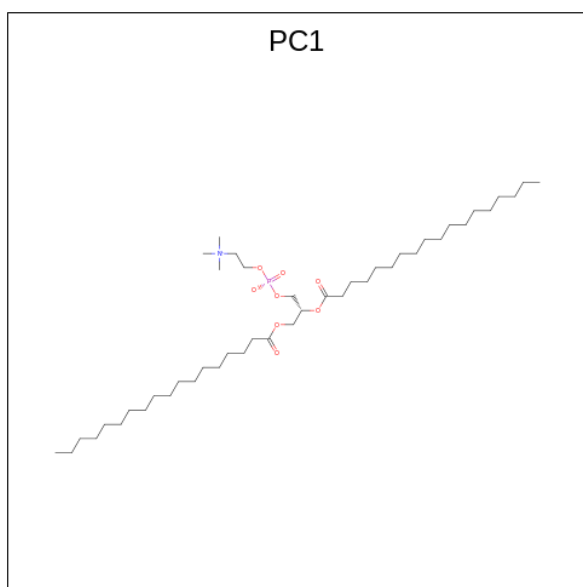
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	3	39	22	2	15	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).

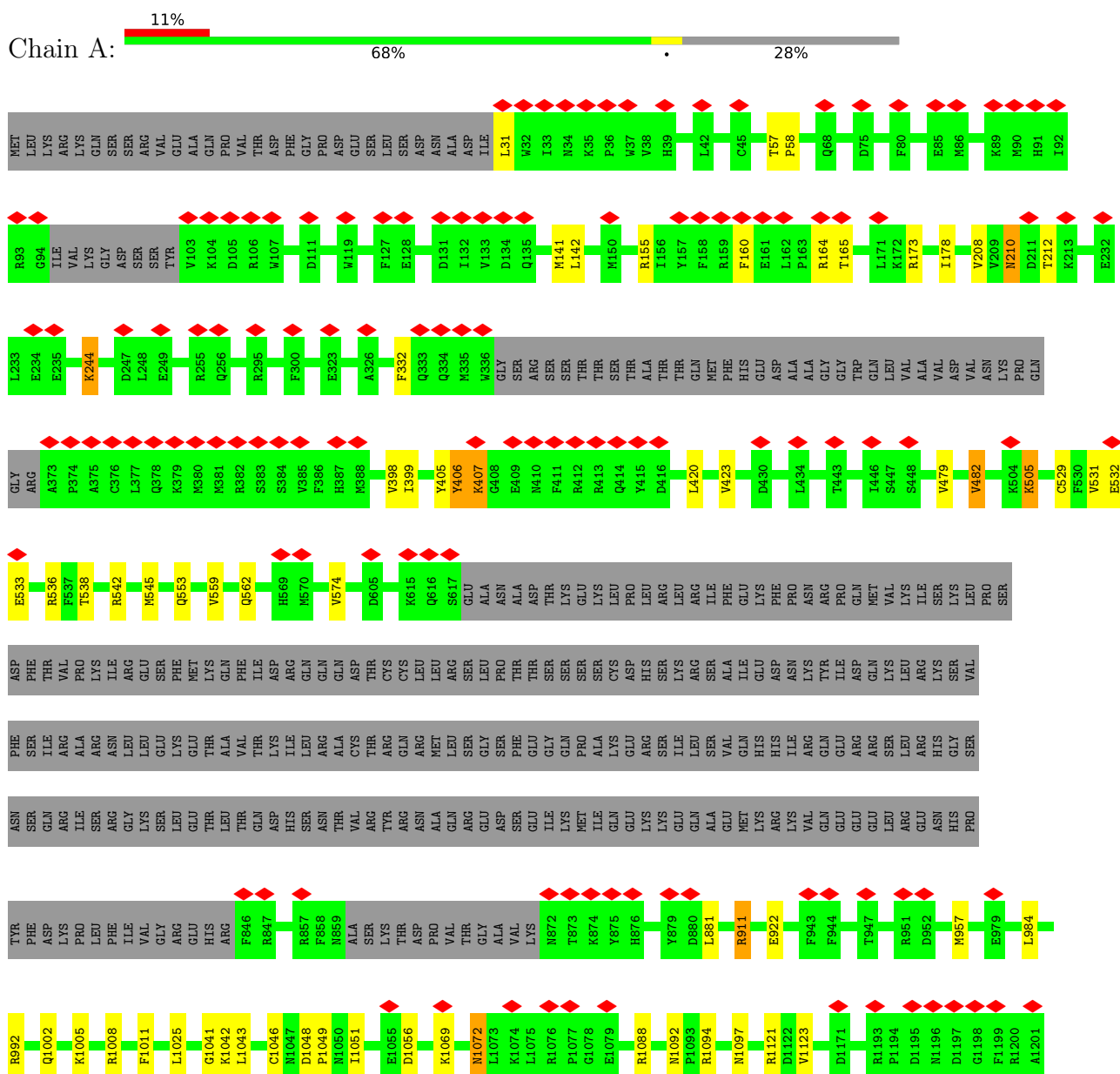


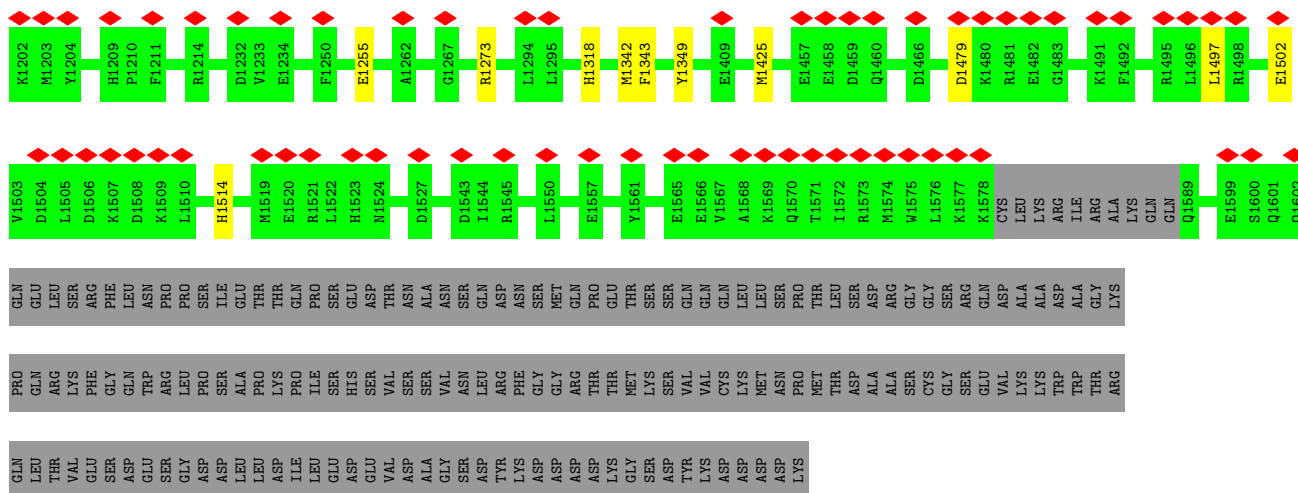
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0
6	A	1	Total 398	301	9	78	10	0

3 Residue-property plots i

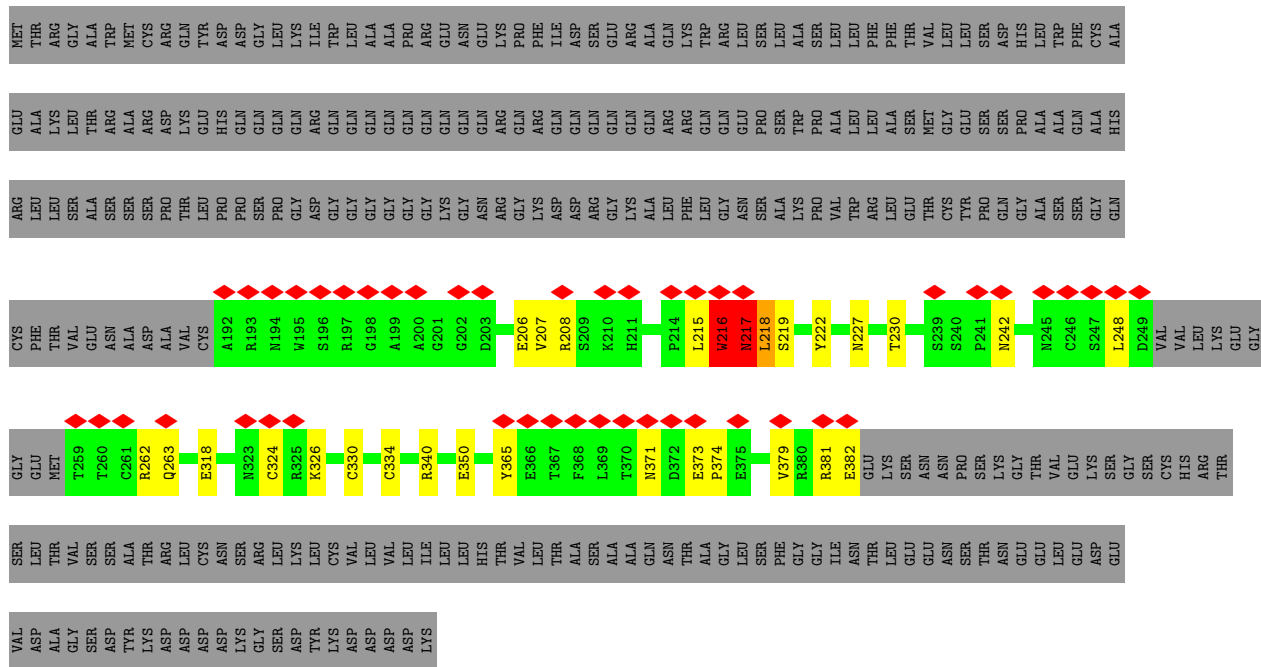
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





• Molecule 2: Transmembrane protein FAM155A



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



• Molecule 4: 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, Not provided	
Number of particles used	65177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.067	Depositor
Minimum map value	-2.153	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.7	Depositor
Map size (\AA)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, BMA, NAG

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	0.71	0/10714	0.87	0/14526
2	B	0.72	0/1522	0.86	0/2065
All	All	0.71	0/12236	0.87	0/16591

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	10442	0	10629	102	0
2	B	1483	0	1360	58	0
3	C	28	0	25	1	0
4	D	39	0	34	2	0
5	A	14	0	13	0	0
5	B	14	0	13	13	0
6	A	398	0	548	83	0
All	All	12418	0	12622	184	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 7.

All (184) 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:1273:ARG:HH22	6:A:1804:PC1:C13	1.49	1.25
1:A:574:VAL:CG1	6:A:1806:PC1:H271	1.68	1.22
1:A:1425:MET:CE	6:A:1809:PC1:H352	1.68	1.22
1:A:545:MET:HE1	6:A:1805:PC1:H12	1.27	1.13
1:A:574:VAL:HG12	6:A:1806:PC1:H271	1.16	1.12
1:A:1273:ARG:NH2	6:A:1804:PC1:H132	1.67	1.08
2:B:217:ASN:O	5:B:501:NAG:H2	1.54	1.08
1:A:984:LEU:HD22	6:A:1809:PC1:H11	1.25	1.07
1:A:1273:ARG:HH22	6:A:1804:PC1:H132	1.14	1.02
6:A:1807:PC1:C12	6:A:1807:PC1:H11	1.90	1.01
1:A:1425:MET:HE3	6:A:1809:PC1:C35	1.90	1.00
1:A:1342:MET:HB3	6:A:1808:PC1:C3A	1.92	0.99
1:A:1425:MET:HE3	6:A:1809:PC1:H352	0.95	0.94
2:B:215:LEU:HD12	2:B:216:TRP:H	1.32	0.93
1:A:141:MET:HE1	6:A:1806:PC1:H362	1.50	0.93
6:A:1810:PC1:H231	6:A:1811:PC1:C15	1.99	0.93
2:B:218:LEU:HD22	5:B:501:NAG:H81	1.48	0.92
1:A:1273:ARG:NH2	6:A:1804:PC1:C13	2.30	0.92
2:B:216:TRP:CZ3	2:B:248:LEU:CD1	2.53	0.92
6:A:1807:PC1:H11	6:A:1807:PC1:H121	1.50	0.92
2:B:216:TRP:CH2	2:B:248:LEU:HD12	2.06	0.90
2:B:216:TRP:CZ3	2:B:248:LEU:HD12	2.07	0.89
1:A:545:MET:HE1	6:A:1805:PC1:C1	2.02	0.87
6:A:1806:PC1:H32	6:A:1806:PC1:H221	1.57	0.87
1:A:545:MET:CE	6:A:1805:PC1:O22	2.22	0.87
1:A:399:ILE:HG22	6:A:1811:PC1:H381	1.55	0.87
2:B:218:LEU:HB2	5:B:501:NAG:C8	2.06	0.86
2:B:218:LEU:HB2	5:B:501:NAG:H82	1.57	0.86
2:B:215:LEU:HD12	2:B:216:TRP:CE3	2.11	0.85
6:A:1807:PC1:H11	6:A:1807:PC1:C11	2.06	0.85
1:A:1002:GLN:HE21	6:A:1807:PC1:H12	1.40	0.85
1:A:1273:ARG:HH22	6:A:1804:PC1:H131	1.39	0.85
6:A:1806:PC1:H32	6:A:1806:PC1:C22	2.08	0.84
1:A:406:TYR:CE1	1:A:1041:GLY:CA	2.62	0.82
2:B:218:LEU:HA	5:B:501:NAG:O7	1.79	0.82
1:A:1425:MET:CE	6:A:1809:PC1:C35	2.51	0.82
1:A:406:TYR:CE1	1:A:1041:GLY:HA3	2.14	0.82
1:A:1342:MET:CB	6:A:1808:PC1:C3A	2.57	0.82
2:B:215:LEU:CD1	2:B:216:TRP:H	1.92	0.82
1:A:957:MET:CE	6:A:1809:PC1:H2D2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1810:PC1:H231	6:A:1811:PC1:H152	1.62	0.79
2:B:218:LEU:HD12	2:B:219:SER:N	1.98	0.79
2:B:216:TRP:CZ3	2:B:248:LEU:HG	2.18	0.78
2:B:216:TRP:HZ3	2:B:248:LEU:HG	1.47	0.78
2:B:216:TRP:HZ3	2:B:248:LEU:CD1	1.97	0.77
6:A:1810:PC1:H231	6:A:1811:PC1:H151	1.66	0.77
1:A:141:MET:HE1	6:A:1806:PC1:H232	1.67	0.77
1:A:574:VAL:HG12	6:A:1806:PC1:C27	2.08	0.77
2:B:218:LEU:HD22	5:B:501:NAG:C8	2.15	0.77
1:A:141:MET:CE	6:A:1806:PC1:H362	2.15	0.76
2:B:216:TRP:HZ3	2:B:248:LEU:CG	1.99	0.76
1:A:545:MET:HE2	6:A:1805:PC1:O22	1.83	0.76
2:B:217:ASN:O	5:B:501:NAG:C2	2.34	0.75
2:B:262:ARG:NH1	2:B:262:ARG:HB3	2.04	0.73
2:B:216:TRP:CZ3	2:B:248:LEU:CG	2.72	0.72
1:A:542:ARG:NH1	6:A:1805:PC1:O14	2.23	0.72
1:A:1318:HIS:HD2	6:A:1804:PC1:C21	2.02	0.72
2:B:218:LEU:CD2	5:B:501:NAG:H81	2.21	0.71
2:B:222:TYR:HD1	2:B:227:ASN:O	1.72	0.71
1:A:957:MET:HE1	6:A:1809:PC1:H2D2	1.71	0.70
1:A:406:TYR:HE1	1:A:1041:GLY:HA3	1.51	0.69
1:A:1343:PHE:CD2	6:A:1807:PC1:C2E	2.75	0.69
6:A:1804:PC1:H32	6:A:1804:PC1:O12	1.92	0.69
1:A:574:VAL:HG11	6:A:1806:PC1:H271	1.69	0.68
2:B:215:LEU:HD12	2:B:216:TRP:N	2.06	0.68
1:A:984:LEU:HD22	6:A:1809:PC1:C1	2.14	0.67
2:B:218:LEU:HD12	2:B:218:LEU:C	2.13	0.67
1:A:545:MET:CE	6:A:1805:PC1:H12	2.15	0.67
1:A:553:GLN:HA	1:A:553:GLN:OE1	1.97	0.65
1:A:1343:PHE:CE2	6:A:1807:PC1:C2E	2.79	0.65
1:A:1025:LEU:HD21	6:A:1810:PC1:H2G1	1.78	0.65
1:A:957:MET:HE3	6:A:1809:PC1:H2D2	1.77	0.64
1:A:1072:ASN:O	1:A:1072:ASN:ND2	2.25	0.64
1:A:332:PHE:CE2	6:A:1802:PC1:O32	2.51	0.64
1:A:406:TYR:CE1	1:A:1041:GLY:HA2	2.33	0.63
1:A:1318:HIS:CD2	6:A:1804:PC1:C21	2.82	0.62
2:B:218:LEU:HA	5:B:501:NAG:C7	2.30	0.62
1:A:142:LEU:HD12	1:A:142:LEU:O	2.01	0.61
6:A:1806:PC1:H221	6:A:1806:PC1:C3	2.30	0.61
6:A:1802:PC1:O13	6:A:1802:PC1:H153	2.01	0.61
6:A:1806:PC1:C38	6:A:1806:PC1:H281	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:NAG:O7	4:D:1:NAG:O3	2.20	0.60
2:B:262:ARG:HB3	2:B:262:ARG:HH11	1.67	0.60
1:A:141:MET:HE1	6:A:1806:PC1:C23	2.31	0.59
2:B:216:TRP:CE3	2:B:216:TRP:N	2.70	0.59
1:A:332:PHE:HE2	6:A:1802:PC1:O32	1.85	0.59
1:A:1051:ILE:HG23	1:A:1056:ASP:HB2	1.84	0.59
1:A:1425:MET:HE1	6:A:1809:PC1:C35	2.32	0.59
1:A:545:MET:CE	6:A:1805:PC1:C1	2.76	0.58
1:A:57:THR:HG23	1:A:529:CYS:HB2	1.86	0.58
1:A:881:LEU:HD13	6:A:1807:PC1:O22	2.04	0.58
2:B:340:ARG:HG3	2:B:340:ARG:NH2	2.19	0.58
1:A:57:THR:HG21	1:A:538:THR:O	2.03	0.58
1:A:1069:LYS:HA	1:A:1069:LYS:HE2	1.85	0.58
2:B:218:LEU:HD13	5:B:501:NAG:H81	1.86	0.58
1:A:210:ASN:HB3	1:A:244:LYS:HD2	1.85	0.58
1:A:545:MET:SD	6:A:1805:PC1:O22	2.62	0.58
2:B:373:GLU:O	2:B:373:GLU:HG3	2.03	0.57
6:A:1807:PC1:H121	6:A:1807:PC1:C1	2.31	0.57
2:B:340:ARG:HG3	2:B:340:ARG:HH21	1.68	0.57
1:A:398:VAL:HG21	1:A:482:VAL:HG12	1.86	0.57
6:A:1802:PC1:O13	6:A:1802:PC1:H142	2.04	0.57
2:B:216:TRP:HE3	2:B:216:TRP:C	2.09	0.56
2:B:216:TRP:CH2	2:B:248:LEU:CD1	2.83	0.56
6:A:1806:PC1:C38	6:A:1806:PC1:H262	2.34	0.56
2:B:215:LEU:CG	2:B:216:TRP:H	2.18	0.56
2:B:262:ARG:O	2:B:262:ARG:HG2	2.06	0.56
2:B:371:ASN:O	2:B:371:ASN:ND2	2.38	0.56
2:B:216:TRP:O	2:B:217:ASN:HB2	2.07	0.55
1:A:1343:PHE:HD2	6:A:1807:PC1:C2E	2.19	0.55
2:B:206:GLU:HA	2:B:222:TYR:O	2.07	0.54
1:A:406:TYR:O	1:A:407:LYS:HB3	2.08	0.54
1:A:1094:ARG:HG2	1:A:1094:ARG:O	2.05	0.54
1:A:1342:MET:HB2	6:A:1808:PC1:C3A	2.37	0.54
1:A:31:LEU:HD23	1:A:31:LEU:N	2.22	0.54
1:A:1011:PHE:CZ	6:A:1803:PC1:H272	2.43	0.54
1:A:1425:MET:CE	6:A:1809:PC1:H341	2.37	0.53
2:B:218:LEU:CB	5:B:501:NAG:C8	2.82	0.53
2:B:216:TRP:CE3	2:B:216:TRP:C	2.82	0.52
2:B:215:LEU:CG	2:B:216:TRP:N	2.73	0.52
6:A:1807:PC1:C11	6:A:1807:PC1:C1	2.85	0.52
2:B:216:TRP:CE3	2:B:217:ASN:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:LEU:CG	5:B:501:NAG:H81	2.39	0.52
2:B:263:GLN:OE1	2:B:263:GLN:N	2.41	0.51
1:A:533:GLU:HG2	1:A:533:GLU:O	2.11	0.51
6:A:1810:PC1:C23	6:A:1811:PC1:H151	2.39	0.51
6:A:1808:PC1:O12	6:A:1808:PC1:H121	2.11	0.50
1:A:142:LEU:HD12	1:A:142:LEU:C	2.31	0.50
1:A:1043:LEU:HD22	1:A:1123:VAL:HG12	1.93	0.50
1:A:178:ILE:CD1	6:A:1802:PC1:H3C1	2.43	0.49
1:A:1425:MET:CE	6:A:1809:PC1:C34	2.90	0.49
1:A:1479:ASP:N	1:A:1479:ASP:OD1	2.44	0.49
1:A:173:ARG:HG2	1:A:173:ARG:HH11	1.77	0.48
1:A:1121:ARG:HH21	1:A:1121:ARG:HG2	1.79	0.48
2:B:340:ARG:HH21	2:B:340:ARG:CG	2.26	0.48
2:B:215:LEU:HG	2:B:216:TRP:N	2.28	0.48
1:A:57:THR:CG2	1:A:58:PRO:HD2	2.43	0.48
1:A:1048:ASP:OD2	1:A:1088:ARG:NH1	2.42	0.47
1:A:881:LEU:HD13	6:A:1807:PC1:C21	2.44	0.47
1:A:881:LEU:CD1	6:A:1807:PC1:O22	2.63	0.47
1:A:1002:GLN:NE2	6:A:1807:PC1:H12	2.20	0.47
2:B:330:CYS:SG	2:B:374:PRO:O	2.73	0.47
1:A:531:VAL:HG12	1:A:533:GLU:H	1.80	0.47
2:B:207:VAL:HG13	2:B:207:VAL:O	2.15	0.46
2:B:216:TRP:N	2:B:216:TRP:CD2	2.84	0.45
2:B:318:GLU:H	2:B:318:GLU:CD	2.16	0.45
1:A:1049:PRO:HD2	3:C:1:NAG:H83	1.98	0.45
1:A:399:ILE:HG22	6:A:1811:PC1:C38	2.37	0.45
2:B:324:CYS:SG	2:B:326:LYS:O	2.74	0.45
1:A:57:THR:HG23	1:A:58:PRO:HD2	1.98	0.45
1:A:420:LEU:HA	1:A:423:VAL:HG12	1.98	0.45
6:A:1806:PC1:H122	6:A:1806:PC1:O14	2.17	0.45
1:A:1343:PHE:HE2	6:A:1807:PC1:C2E	2.27	0.44
1:A:1425:MET:HE1	6:A:1809:PC1:H341	1.99	0.44
6:A:1807:PC1:H143	6:A:1807:PC1:H111	1.77	0.44
1:A:479:VAL:O	1:A:482:VAL:HG13	2.17	0.44
6:A:1810:PC1:H252	6:A:1810:PC1:H221	1.74	0.43
1:A:405:TYR:CE2	6:A:1811:PC1:O14	2.72	0.43
2:B:216:TRP:CH2	2:B:248:LEU:CG	3.01	0.43
2:B:218:LEU:CD1	5:B:501:NAG:H81	2.47	0.43
1:A:1349:TYR:CE1	6:A:1809:PC1:H3D1	2.54	0.43
1:A:208:VAL:O	1:A:208:VAL:HG23	2.19	0.42
2:B:381:ARG:HD2	2:B:382:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:HD3	1:A:559:VAL:HG13	2.02	0.42
1:A:505:LYS:HG2	6:A:1802:PC1:H12	2.01	0.42
1:A:1497:LEU:O	1:A:1502:GLU:HA	2.19	0.42
2:B:379:VAL:O	2:B:379:VAL:HG22	2.19	0.42
1:A:155:ARG:HD2	1:A:155:ARG:HA	1.79	0.42
1:A:1042:LYS:N	1:A:1042:LYS:HD2	2.35	0.42
6:A:1805:PC1:H392	6:A:1805:PC1:H362	1.74	0.42
1:A:911:ARG:N	1:A:911:ARG:HD3	2.35	0.41
1:A:1005:LYS:HG3	1:A:1008:ARG:NH1	2.36	0.41
1:A:164:ARG:NE	1:A:164:ARG:HA	2.36	0.41
1:A:1092:ASN:ND2	1:A:1097:ASN:HB2	2.36	0.41
1:A:532:GLU:HA	1:A:532:GLU:OE1	2.20	0.41
1:A:984:LEU:CD2	6:A:1809:PC1:H11	2.19	0.41
4:D:2:NAG:O7	4:D:2:NAG:O3	2.36	0.41
2:B:208:ARG:H	2:B:208:ARG:HG2	1.66	0.41
1:A:332:PHE:CZ	6:A:1802:PC1:O32	2.74	0.40
1:A:922:GLU:CD	1:A:992:ARG:HH12	2.24	0.40
2:B:262:ARG:HB3	2:B:262:ARG:CZ	2.51	0.40
1:A:141:MET:CE	6:A:1806:PC1:H231	2.51	0.40
1:A:210:ASN:C	1:A:212:THR:H	2.24	0.40
2:B:206:GLU:HG2	2:B:208:ARG:HH11	1.87	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	1266/1765 (72%)	1213 (96%)	51 (4%)	2 (0%)	47 79
2	B	178/485 (37%)	157 (88%)	19 (11%)	2 (1%)	14 46
All	All	1444/2250 (64%)	1370 (95%)	70 (5%)	4 (0%)	44 73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	216	TRP
2	B	217	ASN
1	A	406	TYR
1	A	407	LYS

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	1153/1592 (72%)	1141 (99%)	12 (1%)	76	90
2	B	168/421 (40%)	160 (95%)	8 (5%)	25	58
All	All	1321/2013 (66%)	1301 (98%)	20 (2%)	66	85

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	PHE
1	A	165	THR
1	A	210	ASN
1	A	244	LYS
1	A	482	VAL
1	A	505	LYS
1	A	562	GLN
1	A	911	ARG
1	A	1046	CYS
1	A	1072	ASN
1	A	1255	GLU
1	A	1514	HIS
2	B	216	TRP
2	B	217	ASN
2	B	218	LEU
2	B	230	THR
2	B	242	ASN
2	B	334	CYS
2	B	350	GLU

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Mol	Chain	Res	Type
2	B	365	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	ASN
1	A	451	HIS
1	A	1318	HIS
2	B	291	GLN
2	B	371	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

5 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	C	1	3,1	14,14,15	1.21	1 (7%)	17,19,21	0.72	0
3	NAG	C	2	3	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	D	1	4,1	14,14,15	0.79	0	17,19,21	2.72	5 (29%)
4	NAG	D	2	4	14,14,15	0.47	0	17,19,21	0.96	2 (11%)
4	BMA	D	3	4	11,11,12	0.31	0	15,15,17	0.80	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	-3.80	1.37	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	-6.31	113.91	122.90
4	D	1	NAG	C4-C3-C2	-6.10	102.08	111.02
4	D	1	NAG	O5-C1-C2	-3.92	105.09	111.29
4	D	1	NAG	C1-C2-N2	3.60	116.63	110.49
4	D	1	NAG	O4-C4-C3	-3.05	103.30	110.35
4	D	2	NAG	C4-C3-C2	-2.35	107.58	111.02
4	D	2	NAG	C2-N2-C7	-2.11	119.90	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

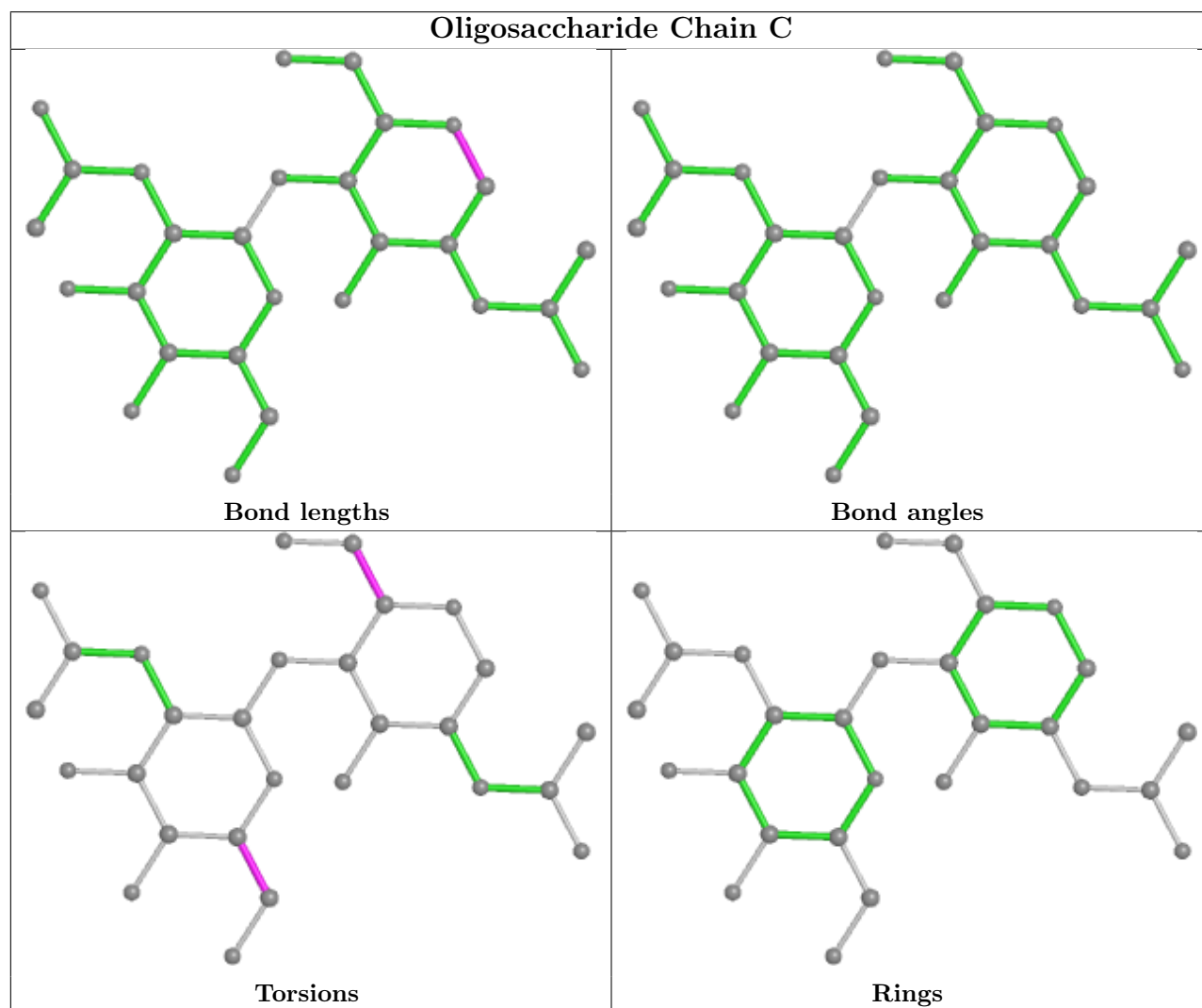
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6

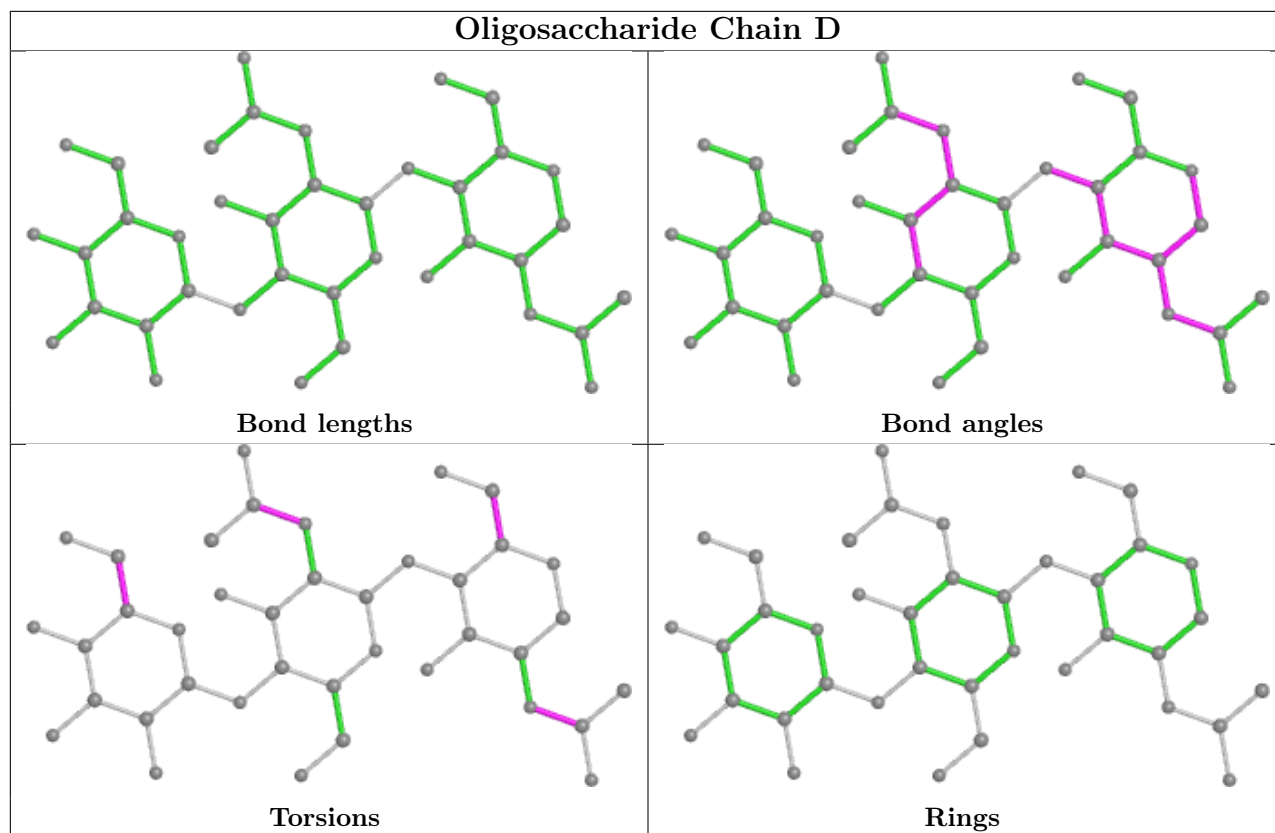
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	D	2	NAG	1	0
3	C	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.





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	$\# Z > 2$
6	PC1	A	1807	-	42,42,53	0.60	0	48,50,61	0.73	2 (4%)
5	NAG	B	501	2	14,14,15	0.45	0	17,19,21	0.44	0
6	PC1	A	1805	-	37,37,53	0.39	0	41,42,61	0.51	1 (2%)
6	PC1	A	1808	-	23,23,53	0.56	0	25,27,61	0.93	1 (4%)
6	PC1	A	1810	-	49,49,53	0.51	0	55,57,61	0.61	0
6	PC1	A	1806	-	37,37,53	0.83	2 (5%)	43,45,61	1.06	2 (4%)
6	PC1	A	1811	-	40,40,53	0.50	0	46,48,61	0.80	1 (2%)
6	PC1	A	1803	-	35,35,53	0.36	0	41,43,61	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PC1	A	1802	-	44,44,53	0.48	0	50,52,61	0.59	1 (2%)
5	NAG	A	1801	1	14,14,15	0.32	0	17,19,21	1.19	2 (11%)
6	PC1	A	1809	-	46,46,53	0.55	0	52,54,61	0.70	1 (1%)
6	PC1	A	1804	-	35,35,53	0.66	1 (2%)	40,42,61	0.54	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
6	PC1	A	1807	-	-	22/46/46/57	-
5	NAG	B	501	2	-	3/6/23/26	0/1/1/1
6	PC1	A	1805	-	-	19/39/39/57	-
6	PC1	A	1808	-	-	13/25/25/57	-
6	PC1	A	1810	-	-	25/53/53/57	-
6	PC1	A	1806	-	-	23/41/41/57	-
6	PC1	A	1811	-	-	21/44/44/57	-
6	PC1	A	1803	-	-	7/39/39/57	-
6	PC1	A	1802	-	-	22/48/48/57	-
5	NAG	A	1801	1	-	0/6/23/26	0/1/1/1
6	PC1	A	1809	-	-	31/50/50/57	-
6	PC1	A	1804	-	-	26/38/38/57	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1806	PC1	O22-C21	-2.58	1.14	1.22
6	A	1804	PC1	O21-C21	-2.15	1.34	1.42
6	A	1806	PC1	C22-C21	-2.10	1.44	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1806	PC1	O21-C21-C22	4.96	122.19	111.50
5	A	1801	NAG	C1-O5-C5	3.31	116.68	112.19
6	A	1809	PC1	O13-P-O14	-2.76	98.30	109.07
6	A	1811	PC1	O21-C21-C22	2.68	117.27	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1808	PC1	O21-C2-C3	-2.67	100.18	109.56
6	A	1802	PC1	O21-C21-C22	2.53	116.95	111.50
6	A	1807	PC1	O21-C21-C22	2.42	116.72	111.50
6	A	1807	PC1	O13-P-O14	-2.40	99.68	109.07
6	A	1805	PC1	O12-P-O14	2.36	119.94	110.68
6	A	1806	PC1	O21-C21-O22	-2.25	118.26	123.70
5	A	1801	NAG	C4-C3-C2	-2.10	107.95	111.02

There are no chirality outliers.

All (212) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1802	PC1	C11-O13-P-O12
6	A	1802	PC1	C11-O13-P-O11
6	A	1802	PC1	C1-O11-P-O12
6	A	1802	PC1	C1-O11-P-O14
6	A	1802	PC1	O13-C11-C12-N
6	A	1803	PC1	O22-C21-O21-C2
6	A	1803	PC1	C22-C21-O21-C2
6	A	1804	PC1	C11-O13-P-O14
6	A	1804	PC1	C1-O11-P-O14
6	A	1804	PC1	C1-O11-P-O13
6	A	1804	PC1	O13-C11-C12-N
6	A	1804	PC1	C1-C2-O21-C21
6	A	1804	PC1	C3-C2-O21-C21
6	A	1805	PC1	C1-O11-P-O14
6	A	1806	PC1	C11-O13-P-O14
6	A	1806	PC1	C1-O11-P-O14
6	A	1806	PC1	O13-C11-C12-N
6	A	1806	PC1	O22-C21-O21-C2
6	A	1807	PC1	C1-O11-P-O14
6	A	1807	PC1	O13-C11-C12-N
6	A	1807	PC1	O22-C21-O21-C2
6	A	1807	PC1	C22-C21-O21-C2
6	A	1808	PC1	C11-O13-P-O11
6	A	1808	PC1	C1-O11-P-O12
6	A	1808	PC1	C1-O11-P-O13
6	A	1808	PC1	C12-C11-O13-P
6	A	1808	PC1	O13-C11-C12-N
6	A	1809	PC1	C1-O11-P-O12
6	A	1809	PC1	C1-O11-P-O14
6	A	1809	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
6	A	1809	PC1	C22-C21-O21-C2
6	A	1810	PC1	C11-O13-P-O12
6	A	1810	PC1	C11-O13-P-O14
6	A	1810	PC1	C11-O13-P-O11
6	A	1810	PC1	C1-O11-P-O13
6	A	1810	PC1	C22-C21-O21-C2
6	A	1811	PC1	C1-O11-P-O14
6	A	1811	PC1	C22-C21-O21-C2
6	A	1802	PC1	O32-C31-O31-C3
6	A	1806	PC1	O32-C31-O31-C3
6	A	1806	PC1	C32-C31-O31-C3
6	A	1810	PC1	O22-C21-O21-C2
6	A	1811	PC1	O22-C21-O21-C2
6	A	1802	PC1	C32-C31-O31-C3
6	A	1805	PC1	C32-C31-O31-C3
6	A	1806	PC1	C22-C21-O21-C2
6	A	1805	PC1	O32-C31-O31-C3
6	A	1808	PC1	O11-C1-C2-O21
6	A	1809	PC1	C3B-C3C-C3D-C3E
6	A	1811	PC1	C31-C32-C33-C34
6	A	1802	PC1	C31-C32-C33-C34
6	A	1805	PC1	C21-C22-C23-C24
6	A	1806	PC1	C31-C32-C33-C34
6	A	1807	PC1	C21-C22-C23-C24
6	A	1807	PC1	C31-C32-C33-C34
6	A	1809	PC1	C21-C22-C23-C24
6	A	1809	PC1	C31-C32-C33-C34
6	A	1810	PC1	C21-C22-C23-C24
6	A	1811	PC1	C21-C22-C23-C24
6	A	1808	PC1	C34-C35-C36-C37
6	A	1811	PC1	C25-C26-C27-C28
6	A	1805	PC1	C36-C37-C38-C39
6	A	1802	PC1	C1-O11-P-O13
6	A	1807	PC1	C1-O11-P-O13
6	A	1809	PC1	C1-O11-P-O13
6	A	1811	PC1	C1-O11-P-O13
6	A	1810	PC1	C22-C23-C24-C25
6	A	1804	PC1	C36-C37-C38-C39
6	A	1802	PC1	C24-C25-C26-C27
6	A	1806	PC1	C27-C28-C29-C2A
6	A	1806	PC1	C33-C34-C35-C36
6	A	1807	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
6	A	1811	PC1	C22-C23-C24-C25
6	A	1803	PC1	C33-C34-C35-C36
6	A	1805	PC1	C22-C23-C24-C25
6	A	1809	PC1	C2A-C2B-C2C-C2D
6	A	1804	PC1	C33-C34-C35-C36
6	A	1805	PC1	C38-C39-C3A-C3B
6	A	1805	PC1	C39-C3A-C3B-C3C
6	A	1806	PC1	C22-C23-C24-C25
6	A	1807	PC1	C37-C38-C39-C3A
6	A	1807	PC1	C35-C36-C37-C38
6	A	1809	PC1	C3A-C3B-C3C-C3D
6	A	1805	PC1	C35-C36-C37-C38
6	A	1807	PC1	C26-C27-C28-C29
6	A	1807	PC1	C27-C28-C29-C2A
6	A	1804	PC1	C3C-C3D-C3E-C3F
6	A	1804	PC1	C3D-C3E-C3F-C3G
6	A	1810	PC1	C32-C31-O31-C3
6	A	1805	PC1	C22-C21-O21-C2
6	A	1809	PC1	C28-C29-C2A-C2B
6	A	1802	PC1	C37-C38-C39-C3A
6	A	1806	PC1	C24-C25-C26-C27
6	A	1811	PC1	C32-C31-O31-C3
6	A	1810	PC1	O32-C31-O31-C3
6	A	1804	PC1	C3F-C3G-C3H-C3I
6	A	1808	PC1	C31-C32-C33-C34
6	A	1804	PC1	C39-C3A-C3B-C3C
6	A	1805	PC1	C32-C33-C34-C35
6	A	1809	PC1	C33-C34-C35-C36
6	A	1809	PC1	C37-C38-C39-C3A
6	A	1807	PC1	O11-C1-C2-O21
6	A	1805	PC1	O22-C21-O21-C2
6	A	1811	PC1	O32-C31-O31-C3
6	A	1810	PC1	C36-C37-C38-C39
5	B	501	NAG	O5-C5-C6-O6
6	A	1811	PC1	C35-C36-C37-C38
6	A	1810	PC1	C25-C26-C27-C28
6	A	1806	PC1	C11-O13-P-O11
6	A	1807	PC1	O11-C1-C2-C3
6	A	1809	PC1	C23-C24-C25-C26
6	A	1802	PC1	C3A-C3B-C3C-C3D
6	A	1804	PC1	C38-C39-C3A-C3B
6	A	1809	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	A	1809	PC1	C25-C26-C27-C28
6	A	1807	PC1	C38-C39-C3A-C3B
6	A	1809	PC1	C1-C2-C3-O31
6	A	1802	PC1	C25-C26-C27-C28
6	A	1804	PC1	C32-C33-C34-C35
6	A	1805	PC1	C24-C25-C26-C27
6	A	1806	PC1	C26-C27-C28-C29
6	A	1808	PC1	C37-C38-C39-C3A
6	A	1809	PC1	C38-C39-C3A-C3B
5	B	501	NAG	C1-C2-N2-C7
6	A	1802	PC1	C36-C37-C38-C39
6	A	1810	PC1	C2E-C2F-C2G-C2H
6	A	1810	PC1	O11-C1-C2-O21
6	A	1805	PC1	C28-C29-C2A-C2B
6	A	1805	PC1	C3A-C3B-C3C-C3D
6	A	1811	PC1	C29-C2A-C2B-C2C
6	A	1810	PC1	O11-C1-C2-C3
6	A	1802	PC1	C3D-C3E-C3F-C3G
6	A	1808	PC1	C32-C33-C34-C35
6	A	1807	PC1	C29-C2A-C2B-C2C
6	A	1805	PC1	C2A-C2B-C2C-C2D
6	A	1809	PC1	C39-C3A-C3B-C3C
6	A	1807	PC1	C25-C26-C27-C28
6	A	1807	PC1	C1-C2-C3-O31
6	A	1809	PC1	O11-C1-C2-O21
6	A	1807	PC1	C32-C33-C34-C35
6	A	1810	PC1	C2C-C2D-C2E-C2F
6	A	1808	PC1	O11-C1-C2-C3
6	A	1802	PC1	C33-C34-C35-C36
6	A	1804	PC1	C2-C1-O11-P
6	A	1804	PC1	C34-C35-C36-C37
6	A	1807	PC1	C2B-C2C-C2D-C2E
6	A	1810	PC1	C2A-C2B-C2C-C2D
6	A	1809	PC1	C2B-C2C-C2D-C2E
6	A	1804	PC1	C1-C2-C3-O31
6	A	1809	PC1	O21-C2-C3-O31
6	A	1804	PC1	C32-C31-O31-C3
6	A	1806	PC1	C32-C33-C34-C35
6	A	1810	PC1	C29-C2A-C2B-C2C
6	A	1804	PC1	C11-O13-P-O11
6	A	1802	PC1	C11-O13-P-O14
6	A	1806	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
6	A	1806	PC1	C1-O11-P-O12
6	A	1808	PC1	C11-O13-P-O14
6	A	1810	PC1	C1-O11-P-O12
6	A	1810	PC1	C1-O11-P-O14
6	A	1811	PC1	C1-O11-P-O12
6	A	1809	PC1	O11-C1-C2-C3
6	A	1805	PC1	C27-C28-C29-C2A
6	A	1803	PC1	C12-C11-O13-P
6	A	1806	PC1	C12-C11-O13-P
6	A	1811	PC1	C12-C11-O13-P
6	A	1809	PC1	C11-C12-N-C15
6	A	1803	PC1	O13-C11-C12-N
6	A	1811	PC1	O13-C11-C12-N
6	A	1804	PC1	O21-C2-C3-O31
6	A	1806	PC1	C3-C2-O21-C21
6	A	1804	PC1	O32-C31-O31-C3
6	A	1809	PC1	C11-C12-N-C14
6	A	1803	PC1	C11-O13-P-O11
6	A	1809	PC1	C11-O13-P-O11
6	A	1806	PC1	C28-C29-C2A-C2B
6	A	1808	PC1	O31-C31-C32-C33
6	A	1809	PC1	C22-C23-C24-C25
6	A	1809	PC1	C36-C37-C38-C39
6	A	1811	PC1	C1-C2-C3-O31
6	A	1805	PC1	C31-C32-C33-C34
6	A	1804	PC1	C11-C12-N-C14
6	A	1809	PC1	C11-C12-N-C13
6	A	1806	PC1	C1-O11-P-O13
6	A	1809	PC1	O32-C31-O31-C3
6	A	1811	PC1	C11-C12-N-C14
6	A	1810	PC1	C38-C39-C3A-C3B
6	A	1804	PC1	C3E-C3F-C3G-C3H
6	A	1807	PC1	C28-C29-C2A-C2B
6	A	1811	PC1	C23-C24-C25-C26
6	A	1805	PC1	O11-C1-C2-O21
6	A	1802	PC1	C21-C22-C23-C24
6	A	1804	PC1	O11-C1-C2-O21
6	A	1802	PC1	O31-C31-C32-C33
6	A	1811	PC1	O21-C2-C3-O31
6	A	1810	PC1	C2F-C2G-C2H-C2I
6	A	1802	PC1	O32-C31-C32-C33
5	B	501	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	A	1804	PC1	C11-C12-N-C15
6	A	1802	PC1	C22-C23-C24-C25
6	A	1802	PC1	C3B-C3C-C3D-C3E
6	A	1807	PC1	O31-C31-C32-C33
6	A	1810	PC1	C2B-C2C-C2D-C2E
6	A	1803	PC1	C11-O13-P-O14
6	A	1804	PC1	C11-C12-N-C13
6	A	1806	PC1	C11-C12-N-C13
6	A	1810	PC1	O21-C21-C22-C23
6	A	1811	PC1	C11-C12-N-C13
6	A	1811	PC1	C11-C12-N-C15
6	A	1810	PC1	O22-C21-C22-C23
6	A	1809	PC1	C32-C31-O31-C3
6	A	1806	PC1	C25-C26-C27-C28

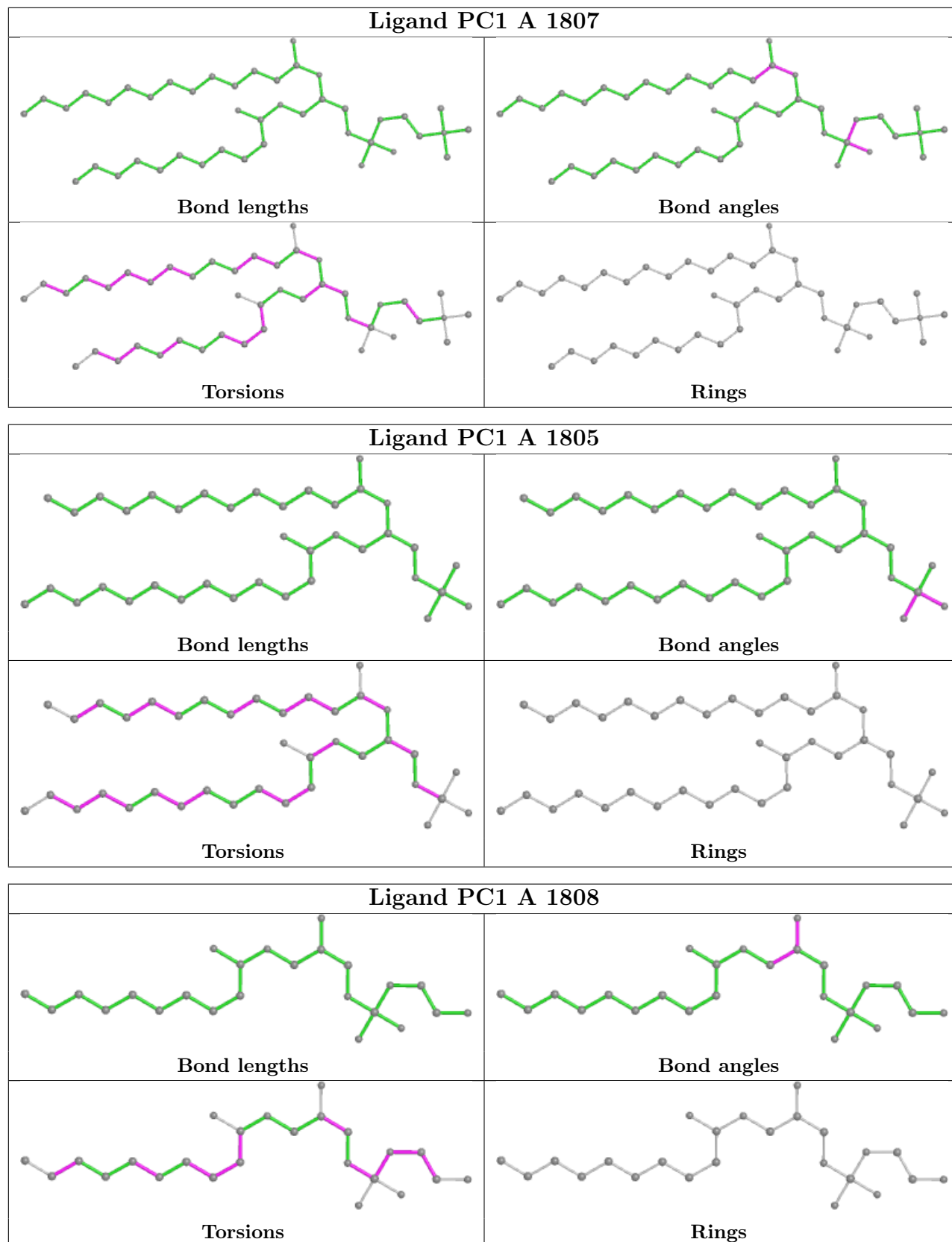
There are no ring outliers.

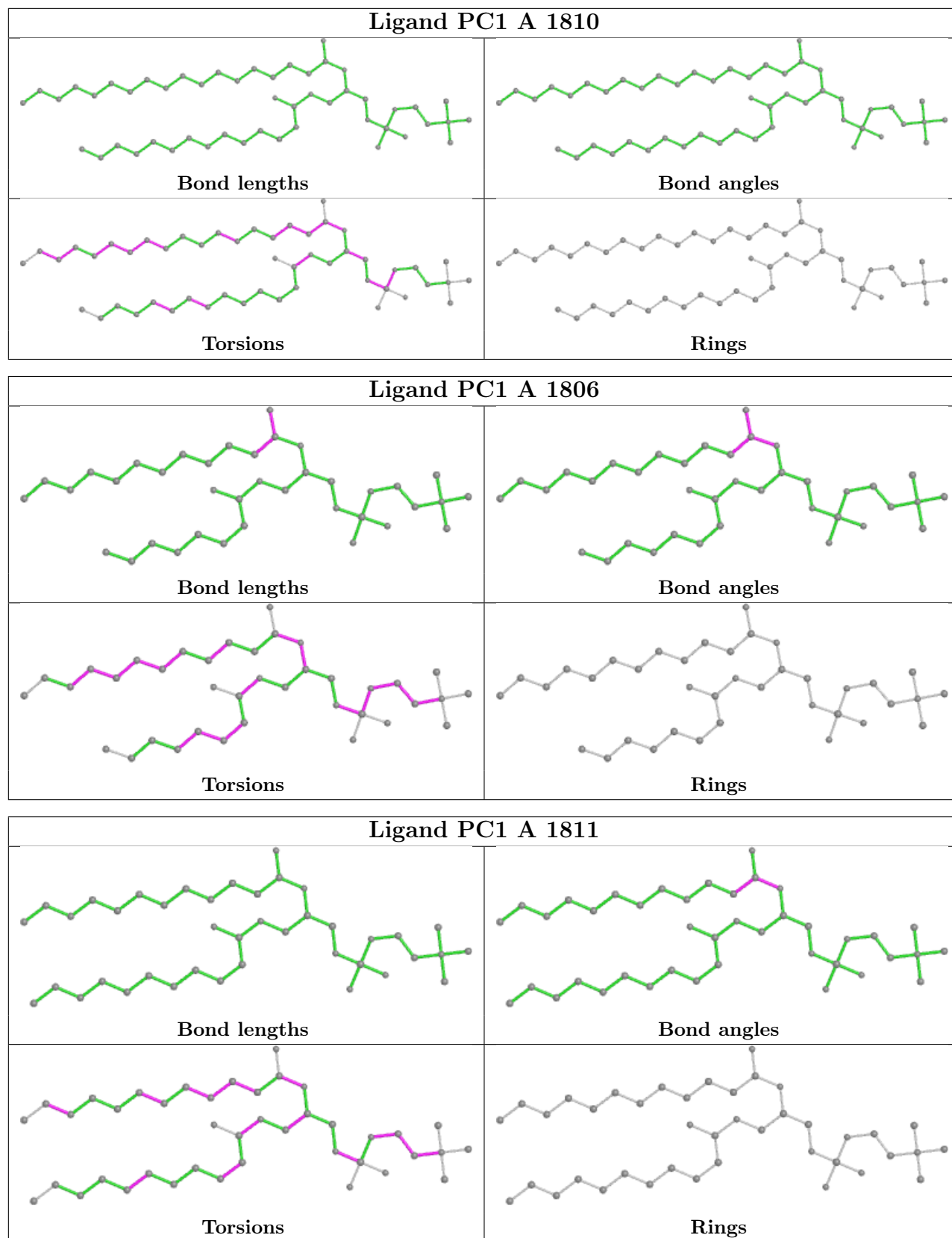
11 monomers are involved in 96 short contacts:

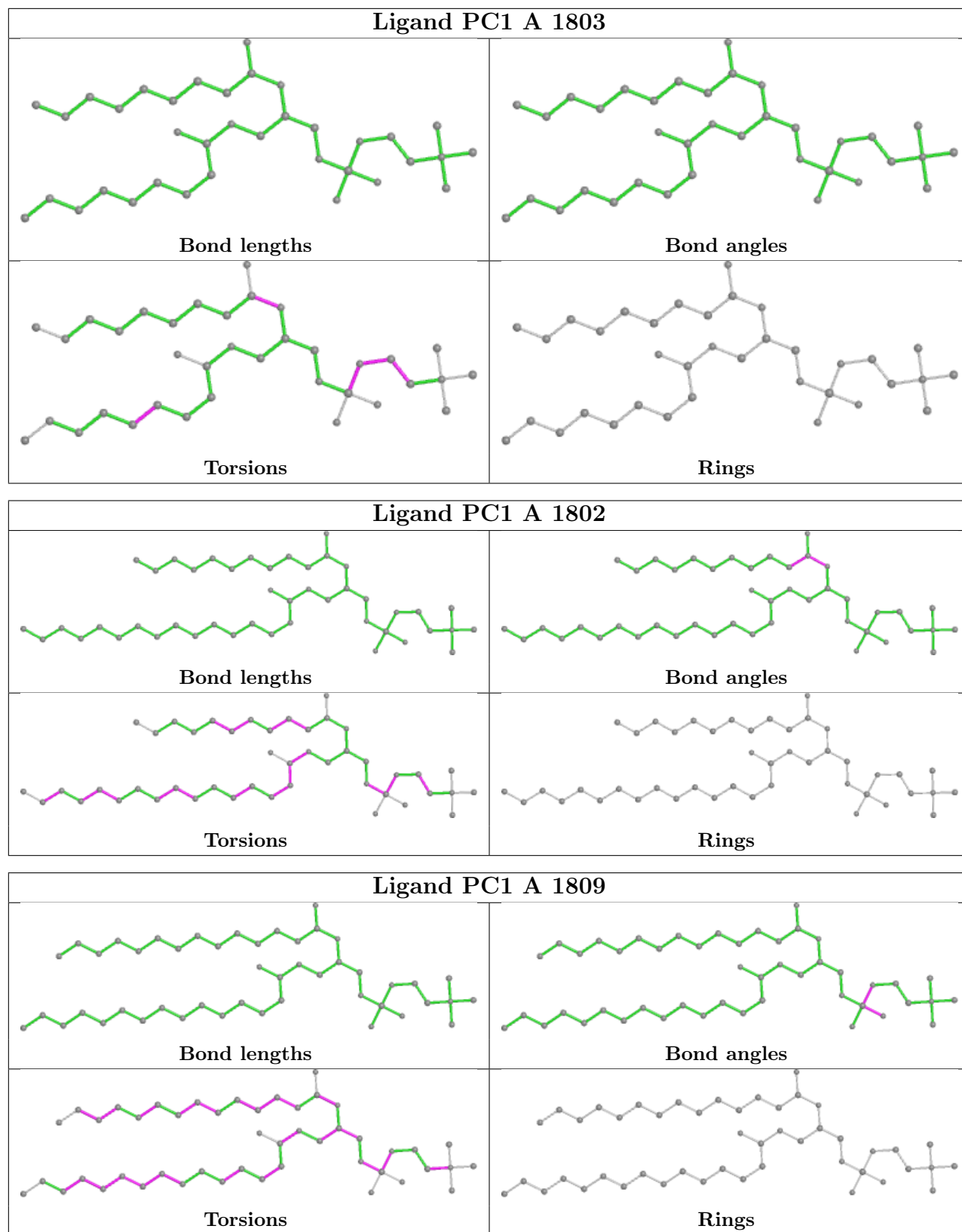
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1807	PC1	15	0
5	B	501	NAG	13	0
6	A	1805	PC1	9	0
6	A	1808	PC1	4	0
6	A	1810	PC1	6	0
6	A	1806	PC1	15	0
6	A	1811	PC1	7	0
6	A	1803	PC1	1	0
6	A	1802	PC1	7	0
6	A	1809	PC1	15	0
6	A	1804	PC1	8	0

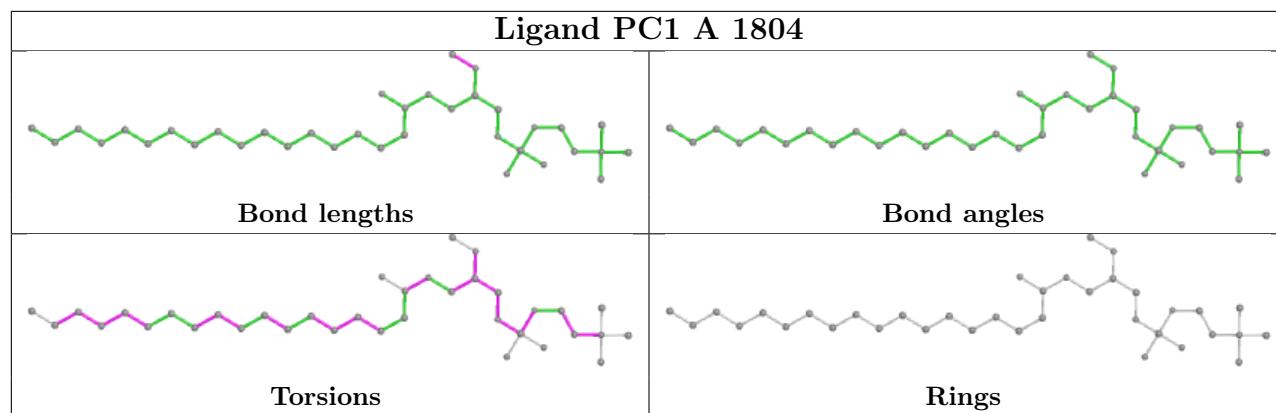
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

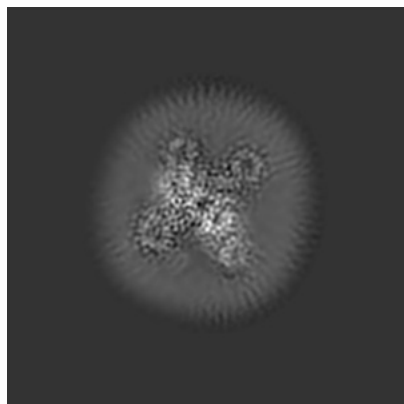
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30400. These allow visual inspection of the internal detail of the map and identification of artifacts.

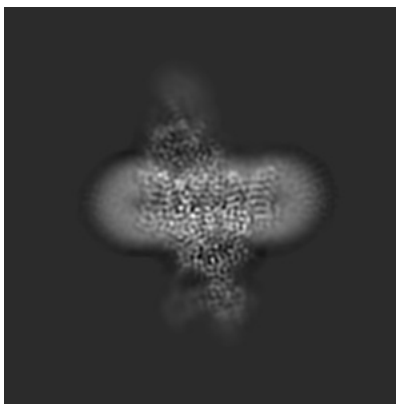
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

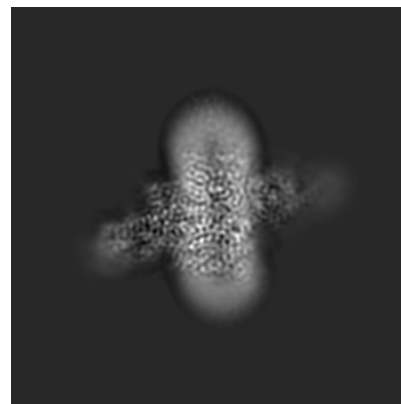
6.1.1 Primary map



X

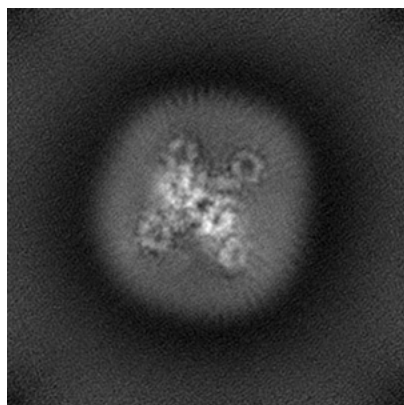


Y

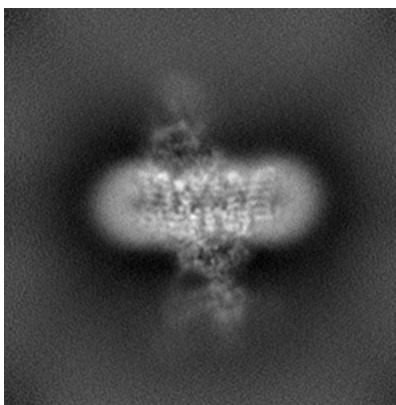


Z

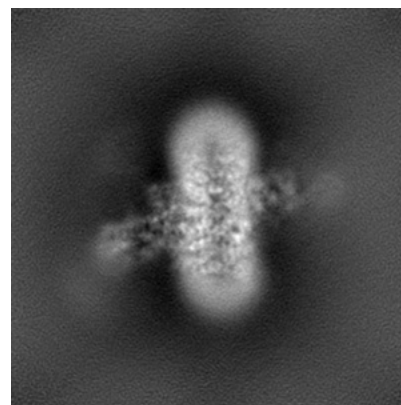
6.1.2 Raw map



X



Y

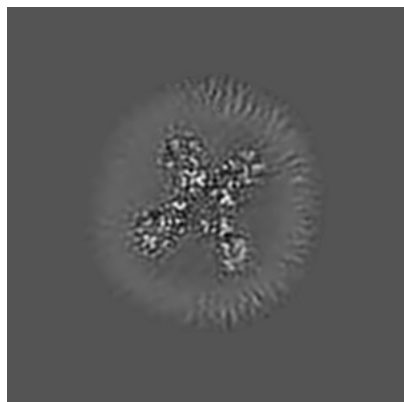


Z

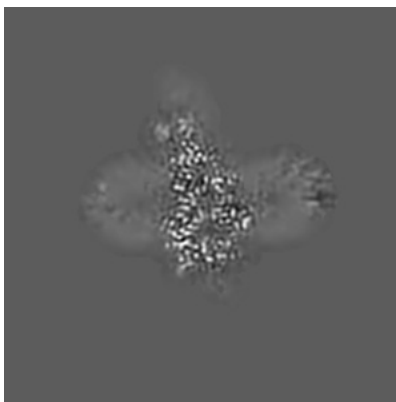
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

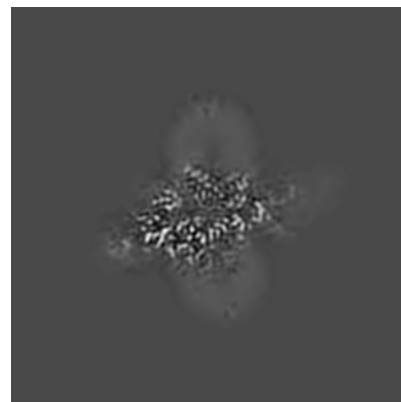
6.2.1 Primary map



X Index: 120

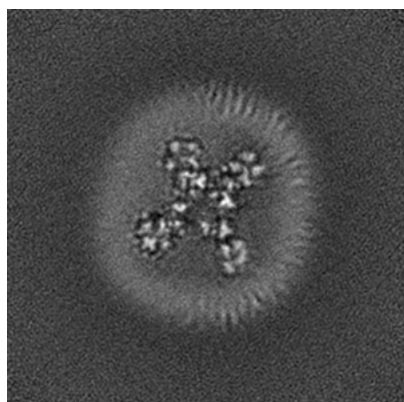


Y Index: 120

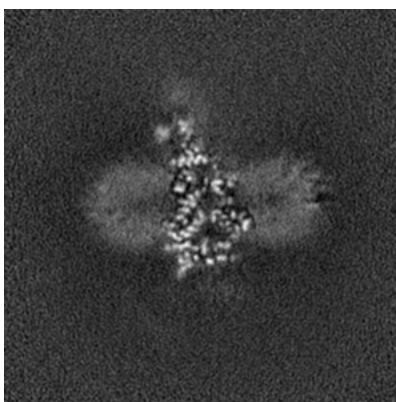


Z Index: 120

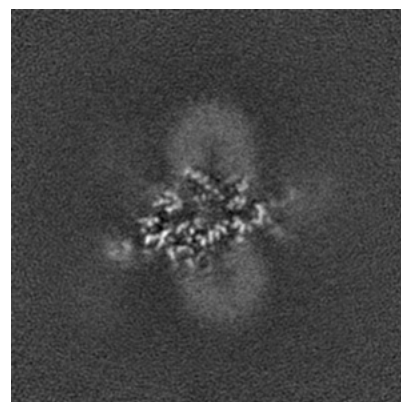
6.2.2 Raw map



X Index: 120



Y Index: 120

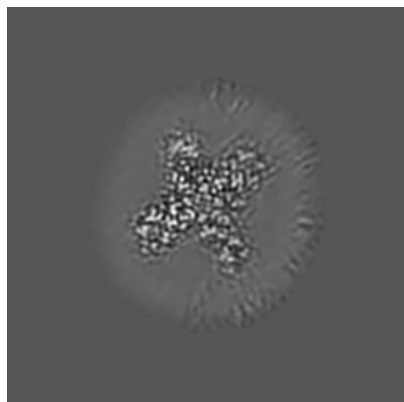


Z Index: 120

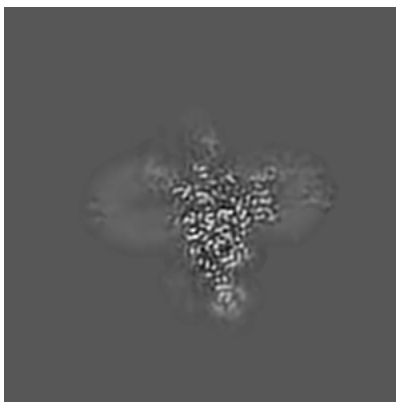
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

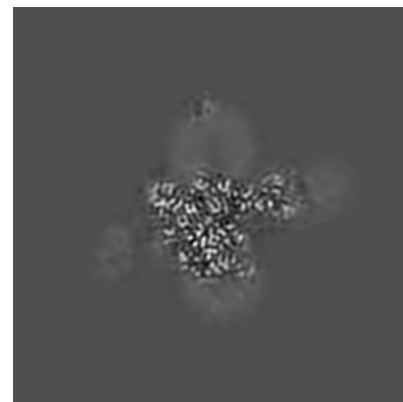
6.3.1 Primary map



X Index: 114

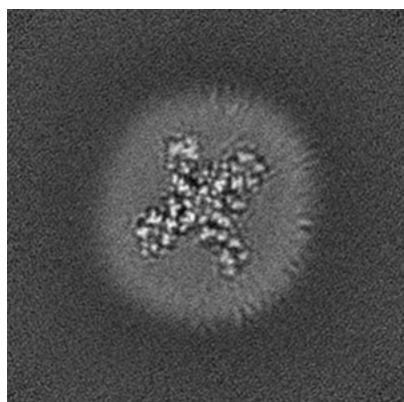


Y Index: 108

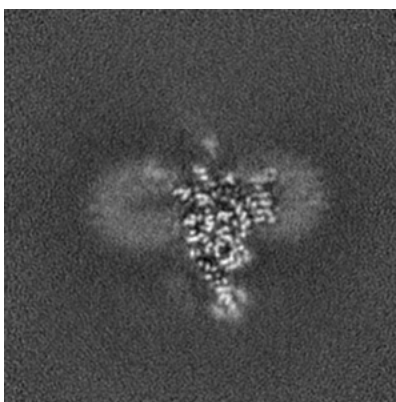


Z Index: 110

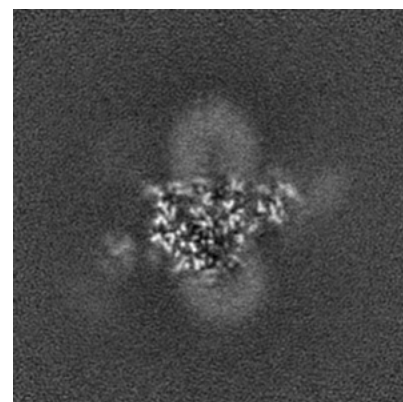
6.3.2 Raw map



X Index: 114



Y Index: 108



Z Index: 115

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

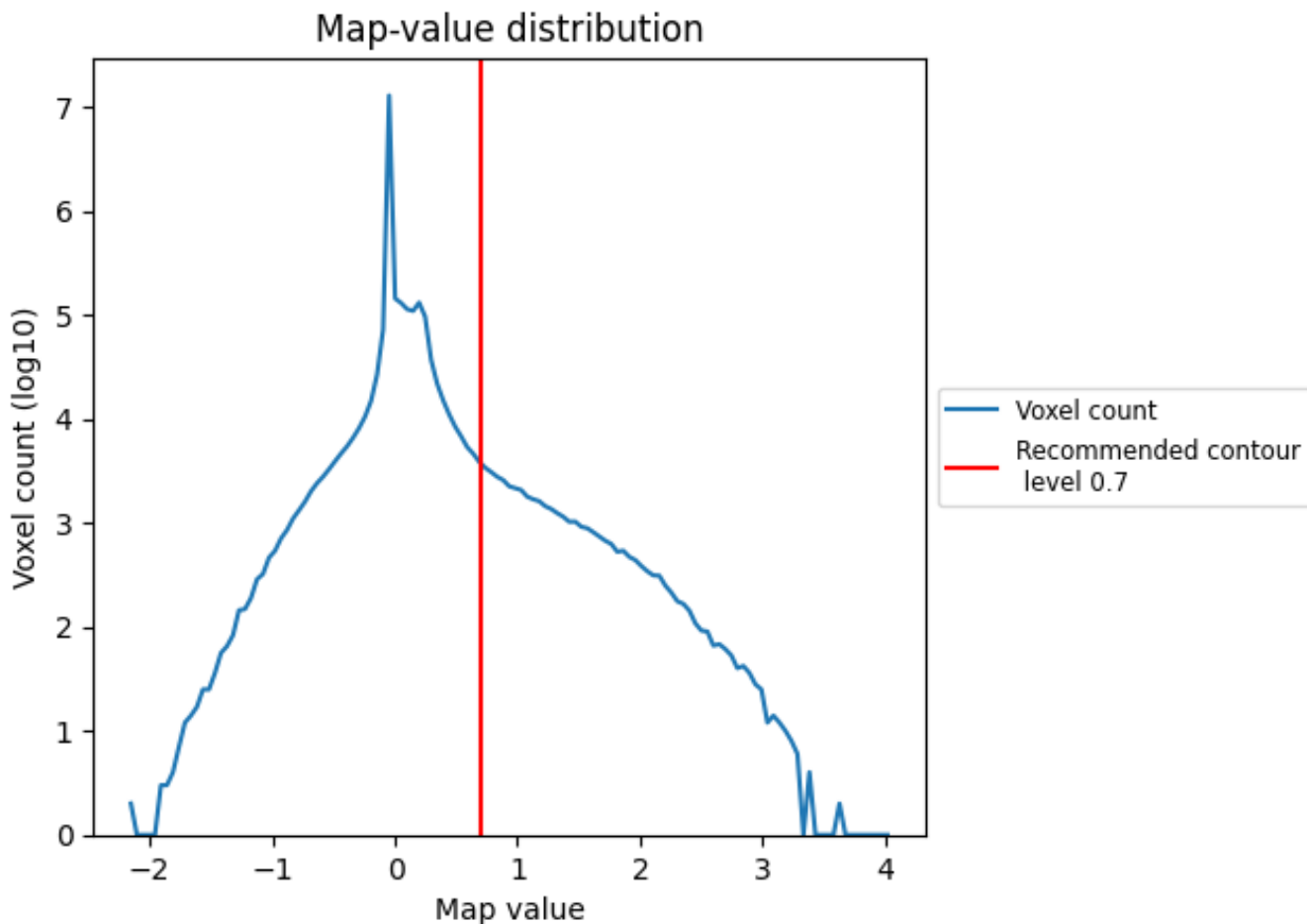
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

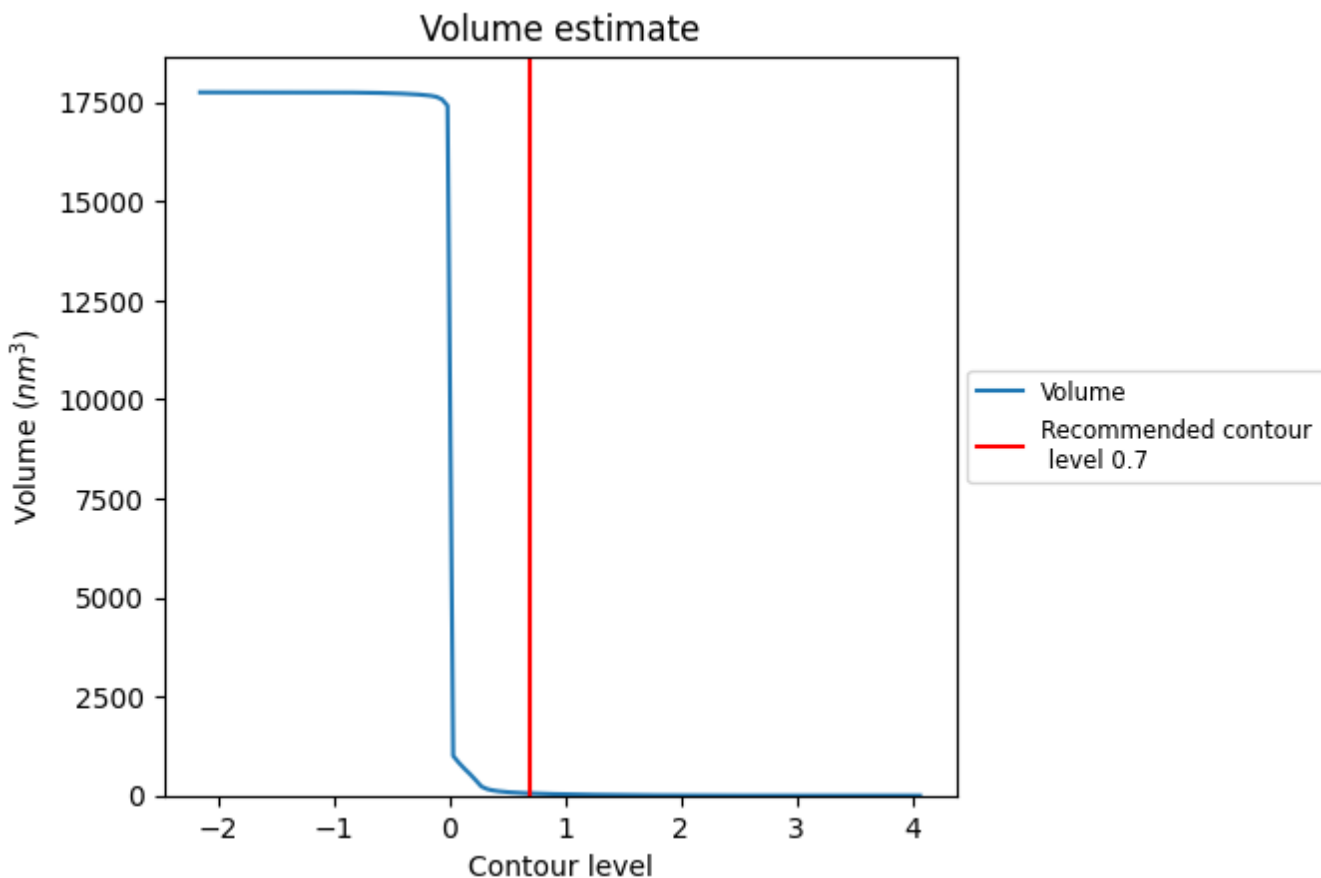
This section contains the results of statistical analysis of the map.

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.

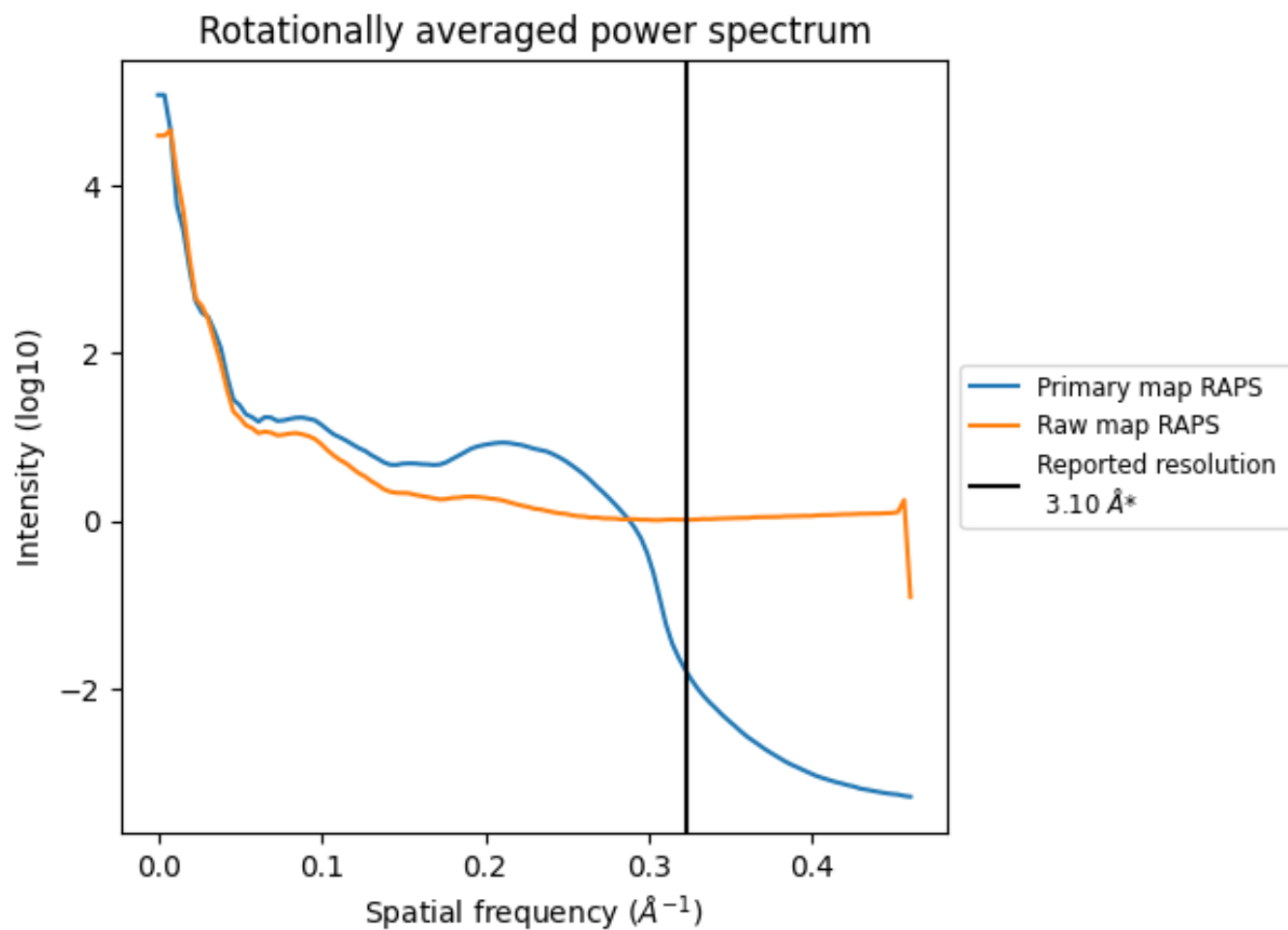
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 55 nm³; this corresponds to an approximate mass of 50 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

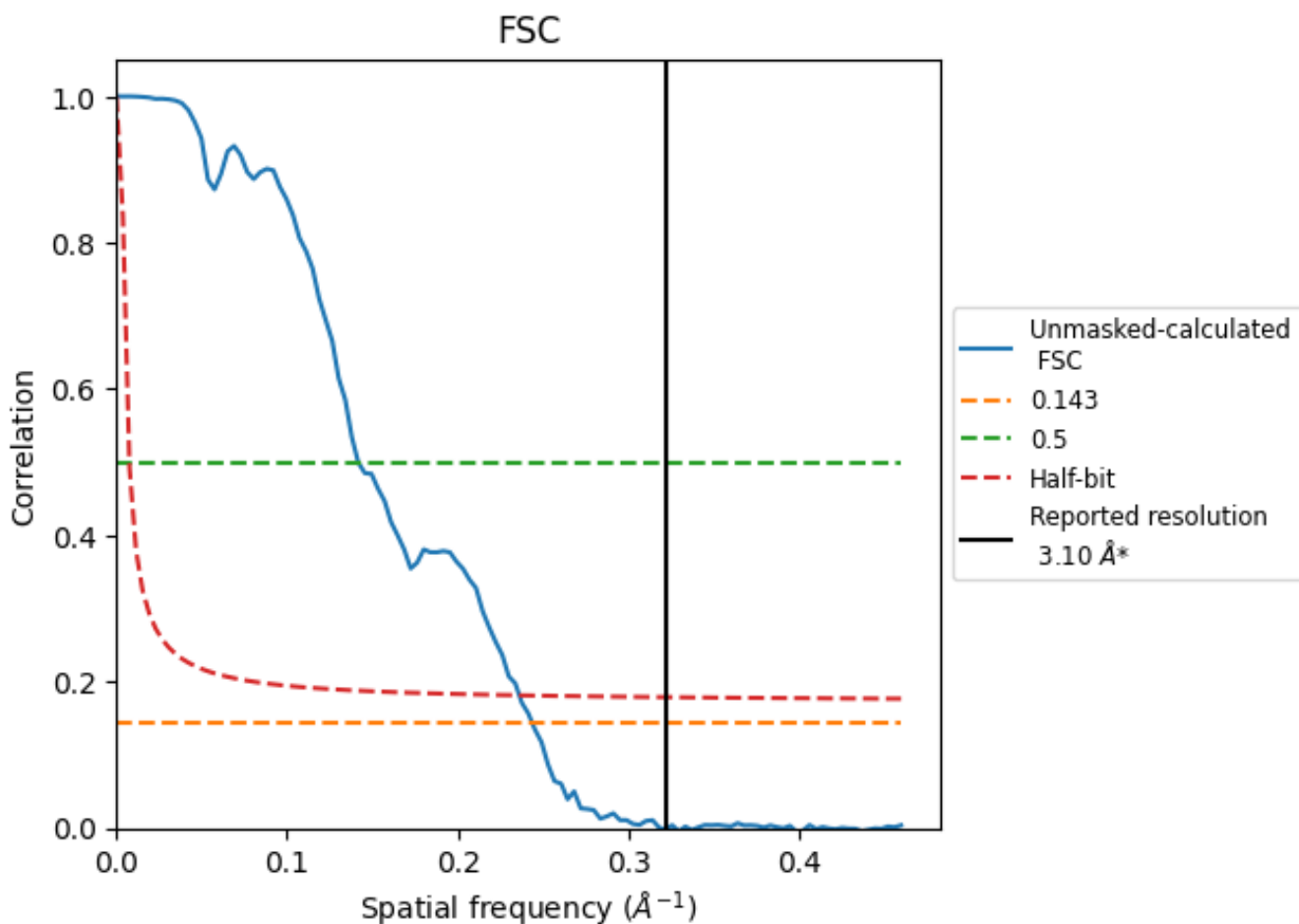


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

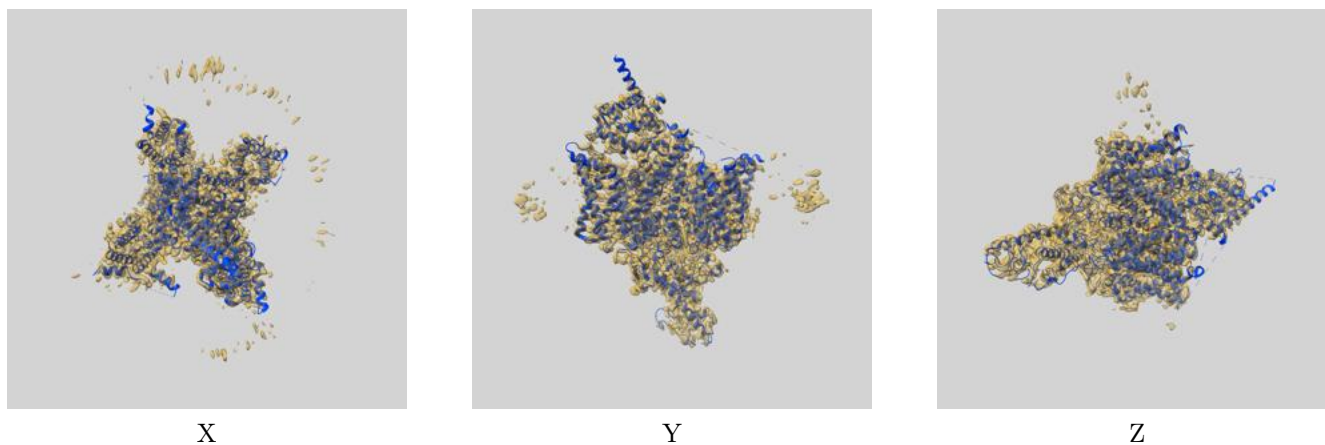
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.10	7.06	4.23

*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 4.10 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

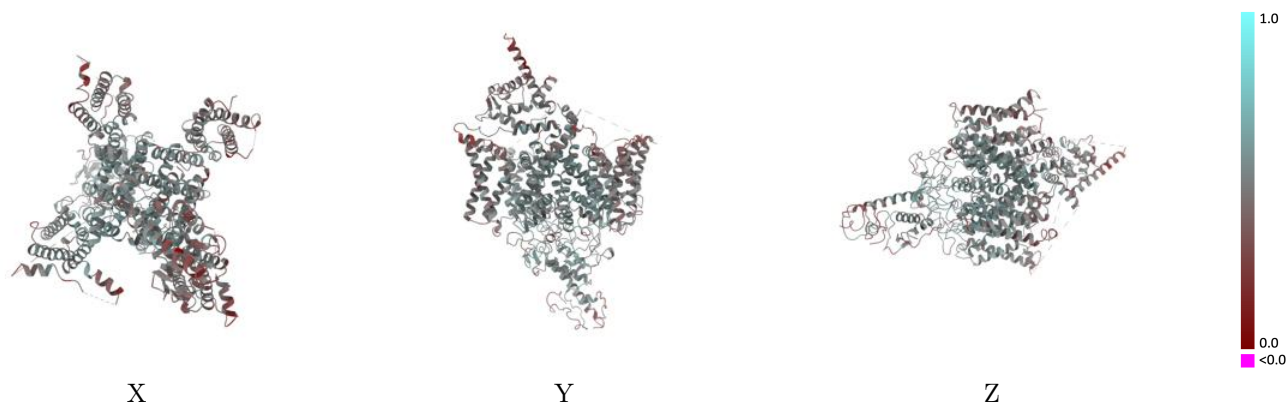
This section contains information regarding the fit between EMDB map EMD-30400 and PDB model 7CM3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



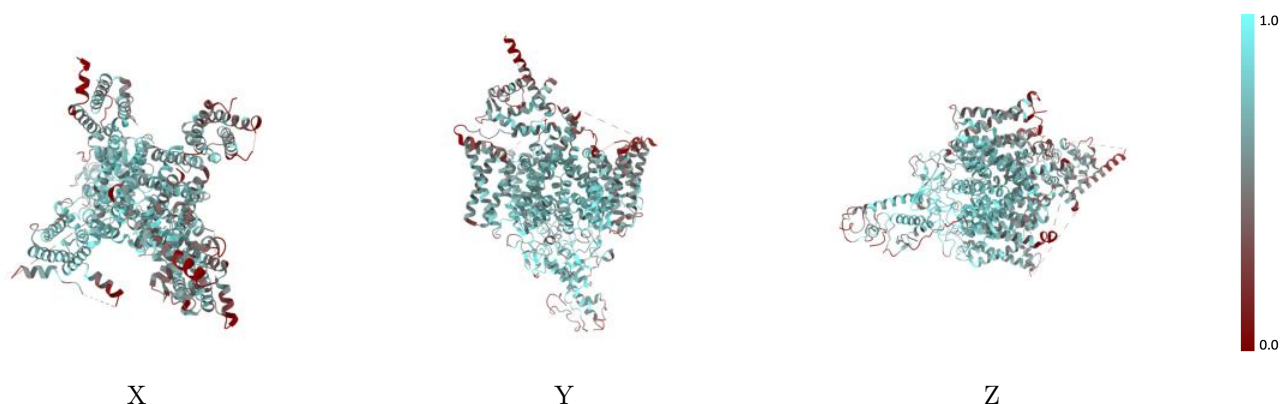
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



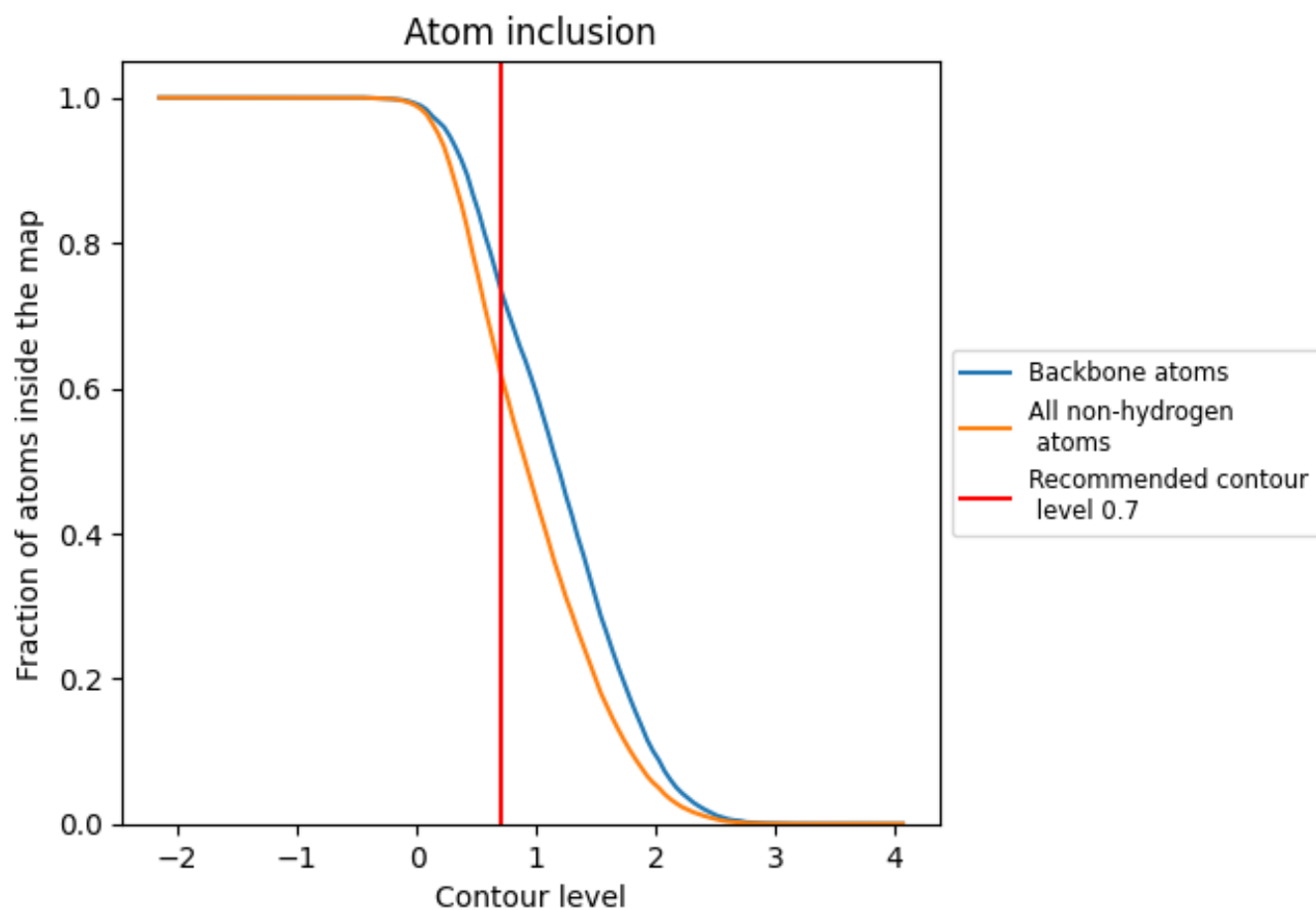
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.7).











9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6217	 0.4850
A	 0.6287	 0.4900
B	 0.5863	 0.4510
C	 0.4643	 0.4810
D	 0.1795	 0.4010

