



Full wwPDB EM Validation Report ⓘ

Apr 3, 2023 – 10:16 AM EDT

PDB ID : 8F0P
EMDB ID : EMD-28776
Title : Structure of VSD4-NaV1.7-NaVPas channel chimera bound to the hybrid inhibitor GNE-1305
Authors : Kschonsak, M.; Jao, C.C.; Arthur, C.P.; Rohou, A.L.; Bergeron, P.; Ortwine, D.; McKerall, S.J.; Hackos, D.H.; Deng, L.; Chen, J.; Sutherlin, D.; Dragovich, P.S.; Volgraf, M.; Wright, M.R.; Payandeh, J.; Ciferri, C.; Tellis, J.C.
Deposited on : 2022-11-03
Resolution : 2.20 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.dev50
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) : 2.32.2

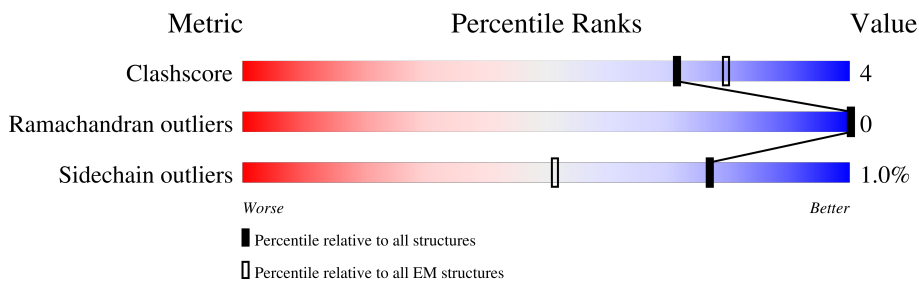
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	1608	 63% 6% 31%
2	B	5	 40% 40% 20%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium channel protein PaFPC1, Sodium channel protein type 9 subunit alpha chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1116	9119	6104	1436	1517	62	0	0

There are 63 discrepancies between the modelled and reference sequences:

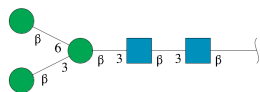
Chain	Residue	Modelled	Actual	Comment	Reference
A	-54	MET	-	initiating methionine	UNP D0E0C2
A	-53	TRP	-	expression tag	UNP D0E0C2
A	-52	SER	-	expression tag	UNP D0E0C2
A	-51	HIS	-	expression tag	UNP D0E0C2
A	-50	PRO	-	expression tag	UNP D0E0C2
A	-49	GLN	-	expression tag	UNP D0E0C2
A	-48	PHE	-	expression tag	UNP D0E0C2
A	-47	GLU	-	expression tag	UNP D0E0C2
A	-46	LYS	-	expression tag	UNP D0E0C2
A	-45	GLY	-	expression tag	UNP D0E0C2
A	-44	GLY	-	expression tag	UNP D0E0C2
A	-43	GLY	-	expression tag	UNP D0E0C2
A	-42	SER	-	expression tag	UNP D0E0C2
A	-41	GLY	-	expression tag	UNP D0E0C2
A	-40	GLY	-	expression tag	UNP D0E0C2
A	-39	GLY	-	expression tag	UNP D0E0C2
A	-38	SER	-	expression tag	UNP D0E0C2
A	-37	GLY	-	expression tag	UNP D0E0C2
A	-36	GLY	-	expression tag	UNP D0E0C2
A	-35	SER	-	expression tag	UNP D0E0C2
A	-34	ALA	-	expression tag	UNP D0E0C2
A	-33	TRP	-	expression tag	UNP D0E0C2
A	-32	SER	-	expression tag	UNP D0E0C2
A	-31	HIS	-	expression tag	UNP D0E0C2
A	-30	PRO	-	expression tag	UNP D0E0C2
A	-29	GLN	-	expression tag	UNP D0E0C2
A	-28	PHE	-	expression tag	UNP D0E0C2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLU	-	expression tag	UNP D0E0C2
A	-26	LYS	-	expression tag	UNP D0E0C2
A	-25	GLY	-	expression tag	UNP D0E0C2
A	-24	GLY	-	expression tag	UNP D0E0C2
A	-23	SER	-	expression tag	UNP D0E0C2
A	-22	GLY	-	expression tag	UNP D0E0C2
A	-21	GLY	-	expression tag	UNP D0E0C2
A	-20	ASP	-	expression tag	UNP D0E0C2
A	-19	TYR	-	expression tag	UNP D0E0C2
A	-18	LYS	-	expression tag	UNP D0E0C2
A	-17	ASP	-	expression tag	UNP D0E0C2
A	-16	ASP	-	expression tag	UNP D0E0C2
A	-15	ASP	-	expression tag	UNP D0E0C2
A	-14	ASP	-	expression tag	UNP D0E0C2
A	-13	LYS	-	expression tag	UNP D0E0C2
A	-12	GLY	-	expression tag	UNP D0E0C2
A	-11	GLY	-	expression tag	UNP D0E0C2
A	-10	SER	-	expression tag	UNP D0E0C2
A	-9	GLY	-	expression tag	UNP D0E0C2
A	-8	GLY	-	expression tag	UNP D0E0C2
A	-7	ASP	-	expression tag	UNP D0E0C2
A	-6	TYR	-	expression tag	UNP D0E0C2
A	-5	LYS	-	expression tag	UNP D0E0C2
A	-4	ASP	-	expression tag	UNP D0E0C2
A	-3	ASP	-	expression tag	UNP D0E0C2
A	-2	ASP	-	expression tag	UNP D0E0C2
A	-1	ASP	-	expression tag	UNP D0E0C2
A	0	LYS	-	expression tag	UNP D0E0C2
A	270	SER	PHE	conflict	UNP D0E0C2
A	274	LEU	VAL	conflict	UNP D0E0C2
A	275	ILE	LEU	conflict	UNP D0E0C2
A	279	LEU	ILE	conflict	UNP D0E0C2
A	280	PHE	TYR	conflict	UNP D0E0C2
A	283	ASN	VAL	conflict	UNP D0E0C2
A	285	LYS	THR	conflict	UNP D0E0C2
A	286	HIS	GLN	conflict	UNP D0E0C2

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranos e-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucofuranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucofuranose.



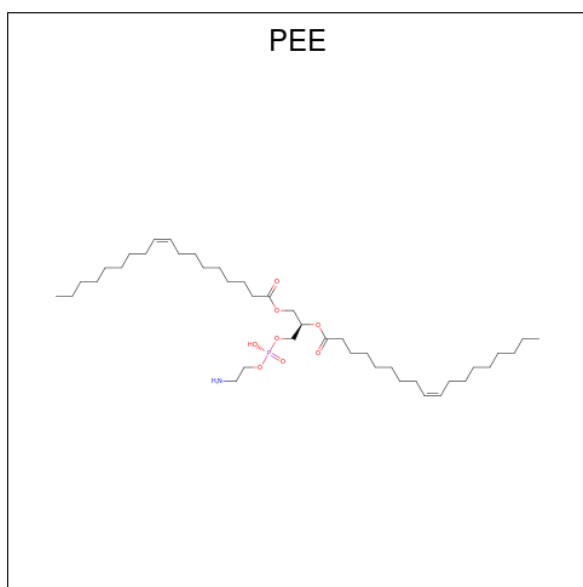
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	5	61	34	2	25	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



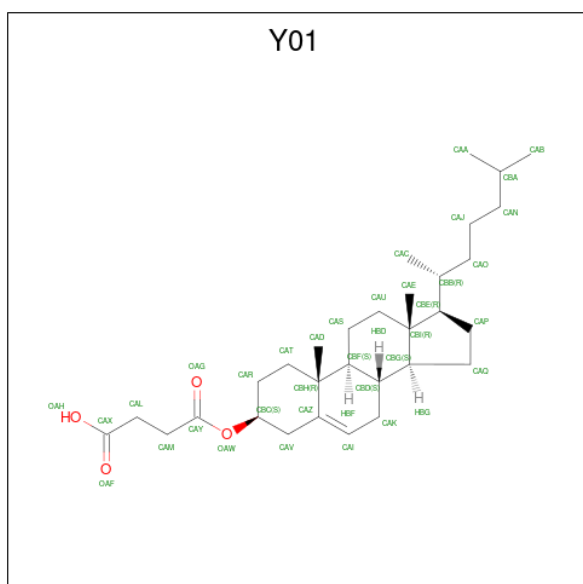
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0

- Molecule 4 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



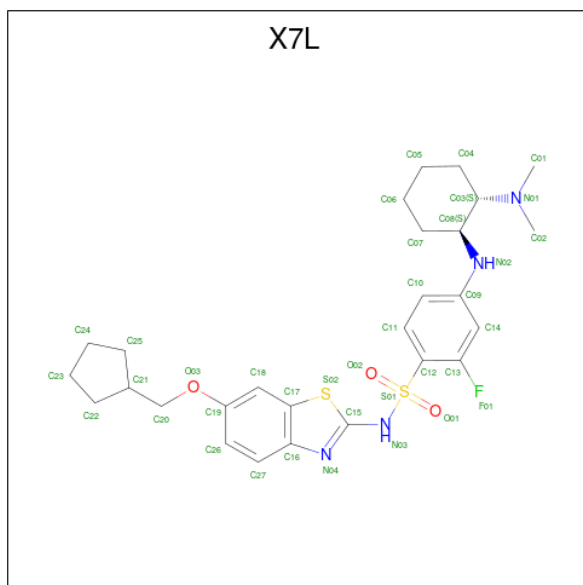
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	42	32	1	8	1	0
4	A	1	47	37	1	8	1	0
4	A	1	42	32	1	8	1	0
4	A	1	41	31	1	8	1	0
4	A	1	39	29	1	8	1	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



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

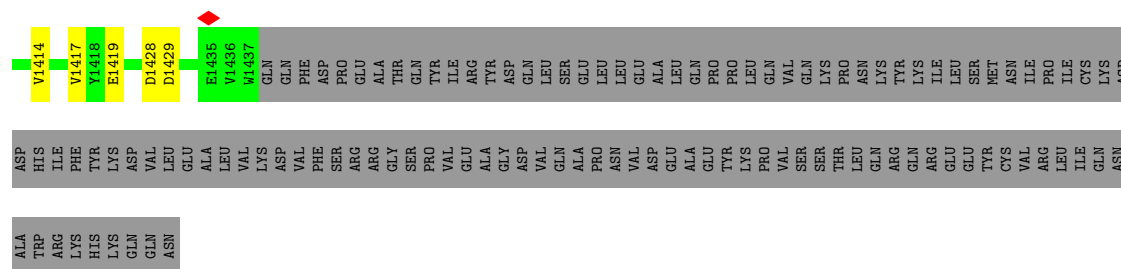
- Molecule 6 is N-[6-(cyclopentylmethoxy)-1,3-benzothiazol-2-yl]-4-[[[(1S,2S)-2-(dimethylamino)cyclohexyl]amino]-2-fluorobenzene-1-sulfonamide (three-letter code: X7L) (formula: $C_{27}H_{35}FN_4O_3S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
6	A	1	37	27	1	4	3	2	0

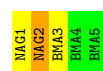
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
7	A	111	111	111	0



- Molecule 2: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 40% 40% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1201168	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; micrographs with CTFfit of 6.0 Å or better were selected	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	21.512	Depositor
Minimum map value	-8.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	112.292, 118.158, 100.56	wwPDB
Map dimensions	120, 141, 134	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.838, 0.838, 0.838	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: X7L, NAG, Y01, PEE, BMA

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	0.28	0/9371	0.50	0/12739

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9119	0	9209	65	0
2	B	61	0	52	1	0
3	A	42	0	39	0	0
4	A	211	0	301	3	0
5	A	35	0	49	1	0
6	A	37	0	0	1	0
7	A	111	0	0	2	0
All	All	9616	0	9650	67	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 (67) 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:412:LEU:HD11	1:A:737:ILE:HD11	1.69	0.74
1:A:148:ILE:O	1:A:152:ILE:HD12	1.89	0.72
1:A:205:ASP:OD1	1:A:233:ARG:NH1	2.27	0.68
1:A:144:TYR:O	1:A:148:ILE:HD12	1.95	0.66
1:A:872:LEU:CD1	7:A:1709:HOH:O	2.45	0.63
1:A:886:LEU:O	1:A:890:THR:HG23	1.99	0.62
1:A:1428:ASP:OD1	1:A:1429:ASP:N	2.33	0.61
1:A:1163:ILE:HG22	1:A:1223:SER:OG	2.00	0.60
1:A:926:ASP:OD1	1:A:957:ARG:NE	2.36	0.59
1:A:872:LEU:HD13	7:A:1709:HOH:O	2.03	0.59
1:A:206:PHE:CE2	1:A:210:LEU:HD11	2.39	0.58
1:A:671:MET:CE	1:A:679:LEU:HB2	2.34	0.57
1:A:323:ILE:HD12	1:A:323:ILE:N	2.21	0.56
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.72	0.55
1:A:1197:HIS:O	1:A:1201:VAL:HG23	2.07	0.54
1:A:1384:ARG:NH2	4:A:1604:PEE:O4	2.38	0.53
1:A:523:LEU:O	1:A:527:VAL:HG13	2.09	0.53
1:A:901:PHE:HB3	1:A:930:VAL:HG22	1.91	0.52
1:A:1254:ILE:O	1:A:1258:PHE:N	2.40	0.52
1:A:915:LYS:H	1:A:915:LYS:CD	2.23	0.51
1:A:671:MET:HE2	1:A:679:LEU:HB2	1.92	0.51
1:A:855:ASN:O	1:A:859:GLN:HG3	2.11	0.49
1:A:228:ALA:HB2	1:A:661:GLN:HG2	1.93	0.48
1:A:872:LEU:HD11	1:A:890:THR:HG22	1.94	0.48
1:A:1384:ARG:HE	4:A:1604:PEE:H7	1.78	0.48
1:A:258:LEU:O	1:A:262:VAL:HG23	2.13	0.48
1:A:554:GLY:O	1:A:558:PHE:CD2	2.67	0.47
1:A:1119:ARG:NE	1:A:1123:GLU:OE2	2.47	0.47
1:A:141:ILE:HA	1:A:144:TYR:CD2	2.50	0.47
1:A:1291:ALA:HB2	1:A:1417:VAL:HG21	1.97	0.46
1:A:180:VAL:O	1:A:184:VAL:HG22	2.16	0.46
1:A:327:LEU:HD23	1:A:387:SER:HB3	1.98	0.46
1:A:148:ILE:HG22	1:A:152:ILE:CD1	2.45	0.46
1:A:733:LEU:O	1:A:737:ILE:HG23	2.15	0.46
1:A:542:ASP:O	1:A:542:ASP:CG	2.54	0.46
1:A:1121:LYS:NZ	1:A:1121:LYS:HB3	2.30	0.45
1:A:371:LEU:HD23	1:A:399:VAL:HG11	1.99	0.45
1:A:524:PHE:O	1:A:527:VAL:HG22	2.17	0.45
1:A:164:THR:O	1:A:167:ILE:HG13	2.17	0.45
1:A:1325:ARG:HG3	1:A:1380:ASN:O	2.17	0.45
1:A:671:MET:HE1	1:A:679:LEU:HB2	1.99	0.44
1:A:935:LEU:C	1:A:935:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:PHE:O	1:A:409:ASN:ND2	2.45	0.44
1:A:844:ASN:O	1:A:848:VAL:HG13	2.17	0.44
1:A:1015:ASN:O	1:A:1017:THR:N	2.50	0.44
1:A:1144:MET:O	1:A:1144:MET:SD	2.76	0.44
1:A:935:LEU:HD23	1:A:935:LEU:O	2.18	0.44
1:A:688:LEU:C	1:A:688:LEU:HD13	2.39	0.43
5:A:1609:Y01:HAC1	5:A:1609:Y01:HAU2	2.01	0.43
2:B:2:NAG:O7	2:B:2:NAG:O3	2.36	0.43
1:A:206:PHE:CZ	1:A:210:LEU:HD11	2.54	0.43
1:A:1414:VAL:O	1:A:1417:VAL:HG22	2.19	0.43
1:A:137:MET:CE	1:A:186:ALA:HB3	2.49	0.43
1:A:1159:ILE:HD12	1:A:1159:ILE:N	2.34	0.42
1:A:1368:CYS:HB2	1:A:1381:CYS:HB3	1.77	0.42
1:A:674:PHE:HB3	1:A:675:PRO:HD2	2.01	0.42
1:A:1171:ALA:O	1:A:1175:SER:OG	2.35	0.42
1:A:264:LEU:HB2	1:A:1285:ILE:HD12	2.02	0.41
1:A:690:SER:O	1:A:693:ILE:HG22	2.20	0.41
1:A:1138:ARG:NH1	1:A:1419:GLU:OE2	2.52	0.41
1:A:1247:GLY:HA3	6:A:1610:X7L:C19	2.51	0.41
1:A:208:VAL:HG13	1:A:230:ARG:HA	2.01	0.41
1:A:1366:GLU:N	1:A:1366:GLU:CD	2.74	0.41
1:A:963:SER:O	4:A:1605:PEE:N	2.53	0.41
1:A:1282:ALA:O	1:A:1286:ARG:HB2	2.22	0.40
1:A:330:ASN:OD1	1:A:330:ASN:N	2.54	0.40
1:A:1140:VAL:O	1:A:1143:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1104/1608 (69%)	1084 (98%)	20 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	989/1415 (70%)	979 (99%)	10 (1%)	76 86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	330	ASN
1	A	532	ASN
1	A	593	PHE
1	A	737	ILE
1	A	969	GLN
1	A	1010	LYS
1	A	1063	TRP
1	A	1108	VAL
1	A	1183	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	742	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
2	NAG	B	1	2,1	14,14,15	0.55	0	17,19,21	0.87	1 (5%)
2	NAG	B	2	2	14,14,15	0.91	2 (14%)	17,19,21	0.43	0
2	BMA	B	3	2	11,11,12	0.88	0	15,15,17	1.21	1 (6%)
2	BMA	B	4	2	11,11,12	0.63	0	15,15,17	0.84	0
2	BMA	B	5	2	11,11,12	0.60	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1
2	BMA	B	5	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	2.60	1.47	1.43
2	B	2	NAG	C1-C2	2.11	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	2.67	115.81	112.19
2	B	3	BMA	O5-C1-C2	-2.13	107.49	110.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

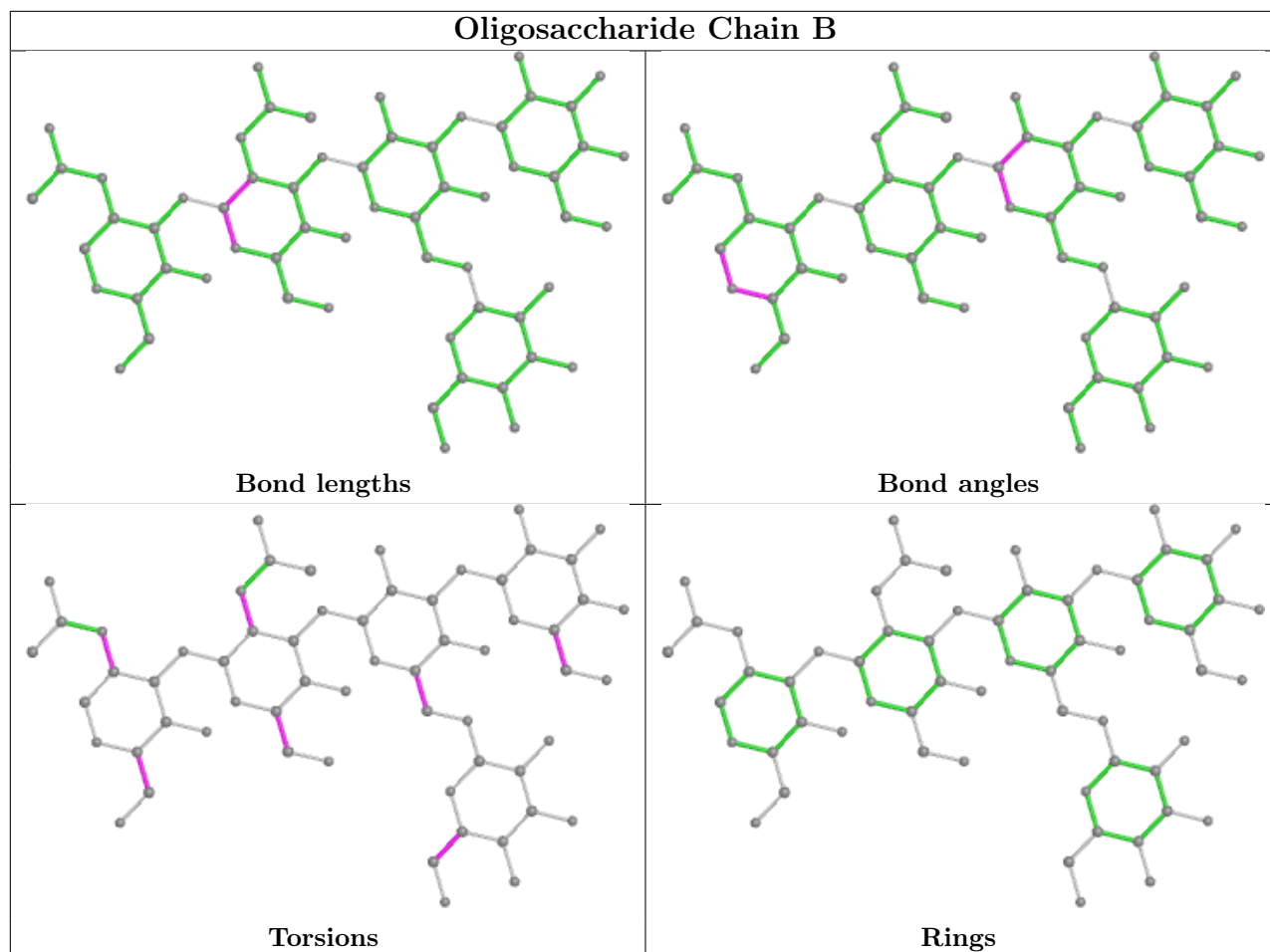
Mol	Chain	Res	Type	Atoms
2	B	4	BMA	C4-C5-C6-O6
2	B	5	BMA	O5-C5-C6-O6
2	B	4	BMA	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
2	B	1	NAG	C4-C5-C6-O6
2	B	5	BMA	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	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](#)

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$
3	NAG	A	1602	1	14,14,15	0.27	0	17,19,21	0.56	0
4	PEE	A	1604	-	41,41,50	0.86	2 (4%)	43,46,55	1.11	5 (11%)
3	NAG	A	1603	1	14,14,15	0.31	0	17,19,21	0.66	0
4	PEE	A	1607	-	40,40,50	0.82	2 (5%)	43,45,55	1.08	5 (11%)
5	Y01	A	1609	-	38,38,38	0.76	0	57,57,57	1.16	5 (8%)
4	PEE	A	1608	-	38,38,50	0.73	1 (2%)	41,43,55	0.97	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	X7L	A	1610	-	38,41,41	1.09	4 (10%)	50,59,59	1.56	8 (16%)
3	NAG	A	1601	1	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
4	PEE	A	1606	-	41,41,50	0.71	1 (2%)	44,46,55	1.01	5 (11%)
4	PEE	A	1605	-	46,46,50	0.81	2 (4%)	49,51,55	1.01	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1602	1	-	0/6/23/26	0/1/1/1
4	PEE	A	1604	-	-	21/45/45/54	-
3	NAG	A	1603	1	-	3/6/23/26	0/1/1/1
4	PEE	A	1607	-	-	20/44/44/54	-
5	Y01	A	1609	-	-	8/19/77/77	0/4/4/4
4	PEE	A	1608	-	-	16/42/42/54	-
6	X7L	A	1610	-	-	7/22/42/42	0/5/5/5
3	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
4	PEE	A	1606	-	-	21/45/45/54	-
4	PEE	A	1605	-	-	19/50/50/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1605	PEE	C18-C19	3.24	1.50	1.31
4	A	1608	PEE	C18-C19	3.20	1.50	1.31
4	A	1604	PEE	C18-C19	3.20	1.50	1.31
4	A	1606	PEE	C18-C19	3.18	1.50	1.31
4	A	1605	PEE	C39-C38	3.05	1.49	1.31
4	A	1607	PEE	C39-C38	3.04	1.49	1.31
4	A	1604	PEE	C39-C38	2.96	1.48	1.31
4	A	1607	PEE	C18-C19	2.77	1.50	1.29
6	A	1610	X7L	C03-N01	2.16	1.53	1.48
6	A	1610	X7L	O02-S01	2.08	1.45	1.43
6	A	1610	X7L	C08-N02	2.07	1.48	1.45
6	A	1610	X7L	O01-S01	2.01	1.45	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1610	X7L	C14-C13-C12	-5.09	120.15	123.10
6	A	1610	X7L	C09-C14-C13	3.73	121.81	118.76
5	A	1609	Y01	OAW-CBC-CAR	-3.71	99.37	108.33
6	A	1610	X7L	O03-C19-C18	-3.46	112.25	123.96
4	A	1604	PEE	C2-O2-C10	3.45	126.28	117.79
4	A	1605	PEE	C2-O2-C10	3.18	125.62	117.79
4	A	1606	PEE	C2-O2-C10	3.07	125.35	117.79
5	A	1609	Y01	CAS-CBF-CBD	2.97	116.03	111.75
4	A	1608	PEE	O2-C2-C1	2.96	119.11	108.40
6	A	1610	X7L	C17-C16-N04	2.94	114.89	108.04
4	A	1607	PEE	C2-O2-C10	2.84	124.80	117.79
4	A	1604	PEE	O2-C10-C11	-2.79	105.48	111.50
4	A	1605	PEE	O2-C10-C11	-2.76	105.55	111.50
4	A	1607	PEE	O2-C2-C1	2.73	118.27	108.40
4	A	1605	PEE	O2-C2-C1	2.71	118.23	108.40
4	A	1606	PEE	O2-C10-C11	-2.59	105.92	111.50
4	A	1607	PEE	O2-C10-C11	-2.56	105.99	111.50
4	A	1606	PEE	O2-C2-C1	2.54	117.60	108.40
6	A	1610	X7L	F01-C13-C12	2.52	121.41	118.89
5	A	1609	Y01	CAT-CBH-CBF	-2.51	105.22	108.73
5	A	1609	Y01	OAW-CBC-CAV	2.43	113.10	108.12
4	A	1607	PEE	C17-C18-C19	-2.43	111.75	131.07
4	A	1608	PEE	O2-C10-C11	-2.37	106.39	111.50
4	A	1604	PEE	O4P-P-O1P	-2.36	99.85	109.07
6	A	1610	X7L	C10-C09-C14	-2.24	116.99	119.65
4	A	1604	PEE	O2-C10-O4	2.23	129.09	123.70
4	A	1605	PEE	O4P-P-O1P	-2.21	100.44	109.07
4	A	1606	PEE	O2-C10-O4	2.20	129.02	123.70
4	A	1604	PEE	O2-C2-C1	2.18	116.29	108.40
4	A	1607	PEE	O4P-P-O1P	-2.17	100.60	109.07
4	A	1608	PEE	O4P-P-O1P	-2.16	100.63	109.07
3	A	1601	NAG	C1-O5-C5	2.13	115.08	112.19
4	A	1606	PEE	O4P-P-O1P	-2.04	101.10	109.07
6	A	1610	X7L	C18-C17-S02	2.02	129.14	125.10
5	A	1609	Y01	CAT-CAR-CBC	-2.01	106.89	110.33
6	A	1610	X7L	C16-C17-S02	-2.01	109.19	111.85
4	A	1605	PEE	O2-C10-O4	2.01	128.55	123.70

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1604	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
4	A	1605	PEE	C1-O3P-P-O1P
4	A	1606	PEE	C4-O4P-P-O3P
4	A	1606	PEE	C4-O4P-P-O2P
4	A	1606	PEE	C4-O4P-P-O1P
4	A	1607	PEE	C17-C18-C19-C20
4	A	1607	PEE	C11-C10-O2-C2
4	A	1607	PEE	C1-O3P-P-O2P
4	A	1607	PEE	O4P-C4-C5-N
4	A	1608	PEE	C1-O3P-P-O1P
4	A	1608	PEE	O4P-C4-C5-N
4	A	1607	PEE	O4-C10-O2-C2
4	A	1605	PEE	C37-C38-C39-C40
4	A	1607	PEE	C37-C38-C39-C40
5	A	1609	Y01	CAM-CAY-OAW-CBC
5	A	1609	Y01	CAJ-CAO-CBB-CBE
5	A	1609	Y01	OAG-CAY-OAW-CBC
3	A	1603	NAG	C8-C7-N2-C2
3	A	1603	NAG	O7-C7-N2-C2
5	A	1609	Y01	CAJ-CAO-CBB-CAC
6	A	1610	X7L	C11-C12-S01-O02
4	A	1606	PEE	C23-C24-C25-C26
5	A	1609	Y01	CAR-CBC-OAW-CAY
6	A	1610	X7L	C11-C12-S01-O01
5	A	1609	Y01	CAN-CAJ-CAO-CBB
4	A	1608	PEE	C10-C11-C12-C13
4	A	1607	PEE	C1-O3P-P-O4P
4	A	1608	PEE	C1-O3P-P-O4P
6	A	1610	X7L	C11-C12-S01-N03
4	A	1608	PEE	C31-C30-O3-C3
4	A	1607	PEE	C39-C40-C41-C42
4	A	1608	PEE	C11-C12-C13-C14
5	A	1609	Y01	CAV-CBC-OAW-CAY
4	A	1604	PEE	C37-C38-C39-C40
4	A	1605	PEE	C12-C13-C14-C15
4	A	1608	PEE	O5-C30-O3-C3
4	A	1608	PEE	C30-C31-C32-C33
4	A	1605	PEE	C17-C18-C19-C20
4	A	1604	PEE	C31-C32-C33-C34
4	A	1604	PEE	C12-C13-C14-C15
4	A	1604	PEE	C17-C18-C19-C20
4	A	1605	PEE	C11-C12-C13-C14
4	A	1607	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	A	1605	PEE	C11-C10-O2-C2
6	A	1610	X7L	C13-C12-S01-O02
4	A	1604	PEE	C11-C10-O2-C2
4	A	1606	PEE	O3P-C1-C2-C3
4	A	1607	PEE	C14-C15-C16-C17
4	A	1604	PEE	C21-C22-C23-C24
4	A	1605	PEE	C15-C16-C17-C18
4	A	1606	PEE	C16-C17-C18-C19
4	A	1605	PEE	O3P-C1-C2-O2
4	A	1605	PEE	O4-C10-O2-C2
6	A	1610	X7L	C13-C12-S01-O01
4	A	1608	PEE	C31-C32-C33-C34
4	A	1606	PEE	C31-C30-O3-C3
4	A	1604	PEE	O4-C10-O2-C2
4	A	1607	PEE	C31-C32-C33-C34
4	A	1606	PEE	C21-C22-C23-C24
4	A	1606	PEE	C10-C11-C12-C13
4	A	1605	PEE	C31-C32-C33-C34
4	A	1605	PEE	C36-C37-C38-C39
4	A	1604	PEE	C14-C15-C16-C17
6	A	1610	X7L	C13-C12-S01-N03
4	A	1604	PEE	C38-C39-C40-C41
4	A	1605	PEE	O3P-C1-C2-C3
6	A	1610	X7L	O03-C20-C21-C25
4	A	1604	PEE	C33-C34-C35-C36
4	A	1604	PEE	C1-C2-O2-C10
4	A	1606	PEE	O5-C30-O3-C3
4	A	1606	PEE	O3P-C1-C2-O2
4	A	1608	PEE	C13-C14-C15-C16
4	A	1604	PEE	C20-C21-C22-C23
4	A	1608	PEE	C22-C23-C24-C25
4	A	1608	PEE	C4-O4P-P-O3P
4	A	1607	PEE	C1-O3P-P-O1P
4	A	1608	PEE	C1-O3P-P-O2P
4	A	1607	PEE	C12-C13-C14-C15
4	A	1606	PEE	C1-C2-C3-O3
4	A	1608	PEE	O2-C2-C3-O3
4	A	1606	PEE	C33-C34-C35-C36
4	A	1605	PEE	C14-C15-C16-C17
4	A	1605	PEE	C13-C14-C15-C16
4	A	1605	PEE	C44-C45-C46-C47
4	A	1604	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
4	A	1606	PEE	C1-O3P-P-O4P
4	A	1607	PEE	C4-O4P-P-O3P
4	A	1605	PEE	C16-C17-C18-C19
3	A	1603	NAG	O5-C5-C6-O6
4	A	1606	PEE	C32-C33-C34-C35
4	A	1604	PEE	C11-C12-C13-C14
5	A	1609	Y01	CAX-CAL-CAM-CAY
4	A	1607	PEE	O3-C30-C31-C32
4	A	1607	PEE	C30-C31-C32-C33
4	A	1605	PEE	O3-C30-C31-C32
4	A	1605	PEE	C38-C39-C40-C41
4	A	1606	PEE	C35-C36-C37-C38
4	A	1607	PEE	C16-C17-C18-C19
4	A	1605	PEE	C42-C43-C44-C45
4	A	1606	PEE	O2-C2-C3-O3
4	A	1604	PEE	O3-C30-C31-C32
4	A	1608	PEE	C18-C19-C20-C21
4	A	1604	PEE	O5-C30-O3-C3
4	A	1604	PEE	C31-C30-O3-C3
4	A	1606	PEE	C13-C14-C15-C16
4	A	1607	PEE	C1-C2-C3-O3
4	A	1604	PEE	C4-O4P-P-O1P
4	A	1606	PEE	C1-O3P-P-O1P
4	A	1607	PEE	C4-O4P-P-O1P
4	A	1604	PEE	O5-C30-C31-C32
4	A	1604	PEE	C16-C17-C18-C19
4	A	1607	PEE	C5-C4-O4P-P
4	A	1606	PEE	O3-C30-C31-C32
4	A	1606	PEE	C11-C12-C13-C14
4	A	1608	PEE	C23-C24-C25-C26

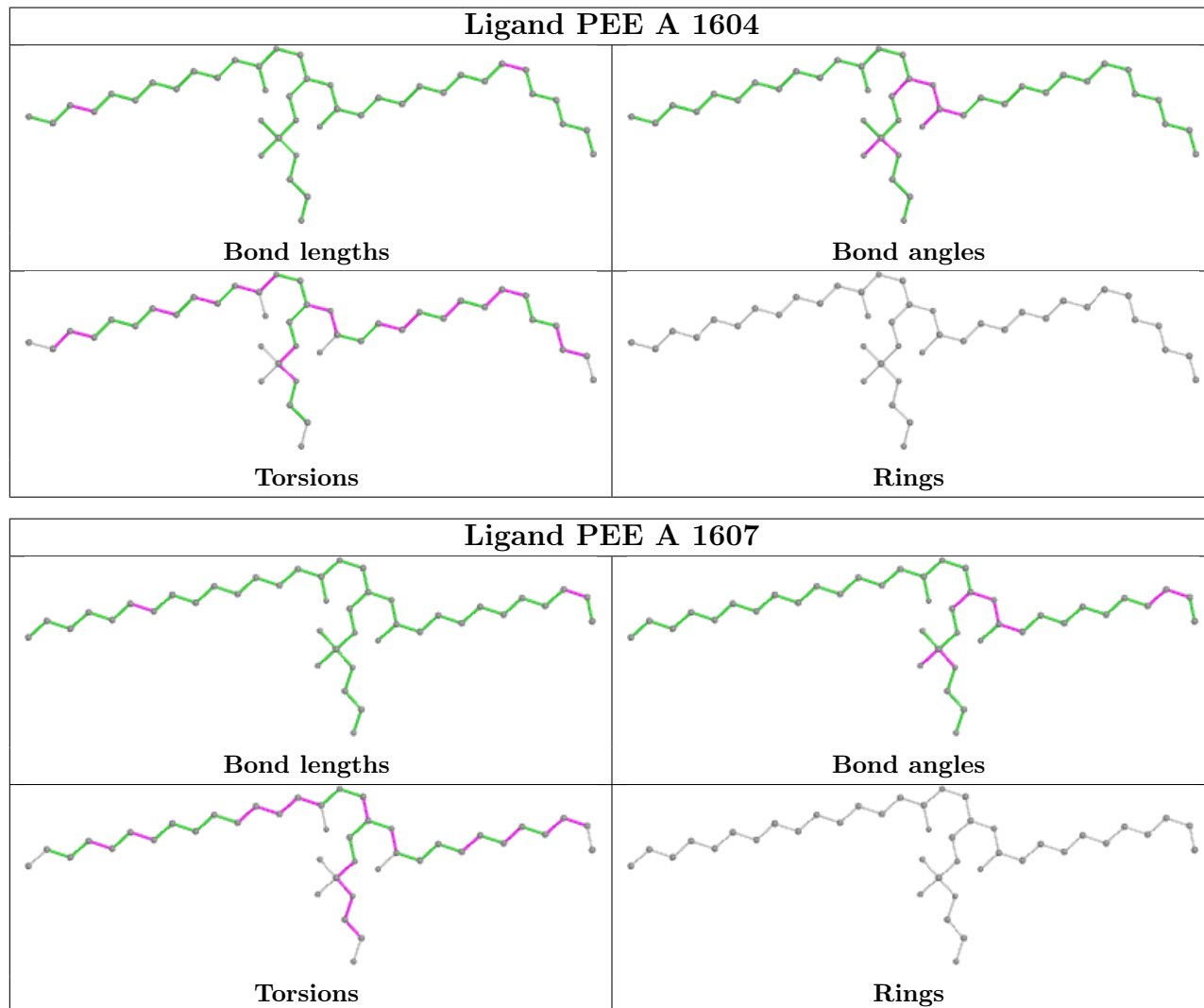
There are no ring outliers.

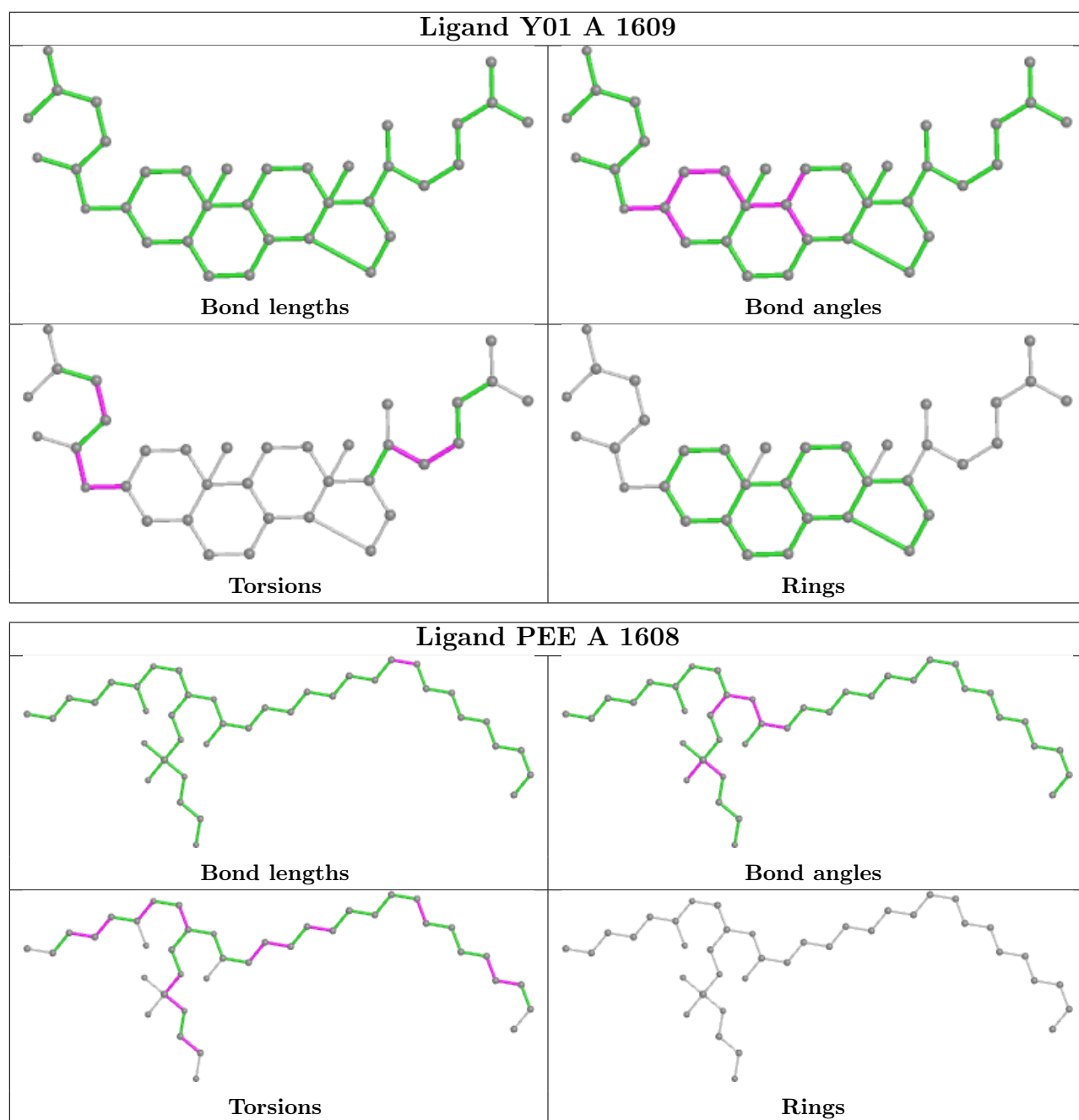
4 monomers are involved in 5 short contacts:

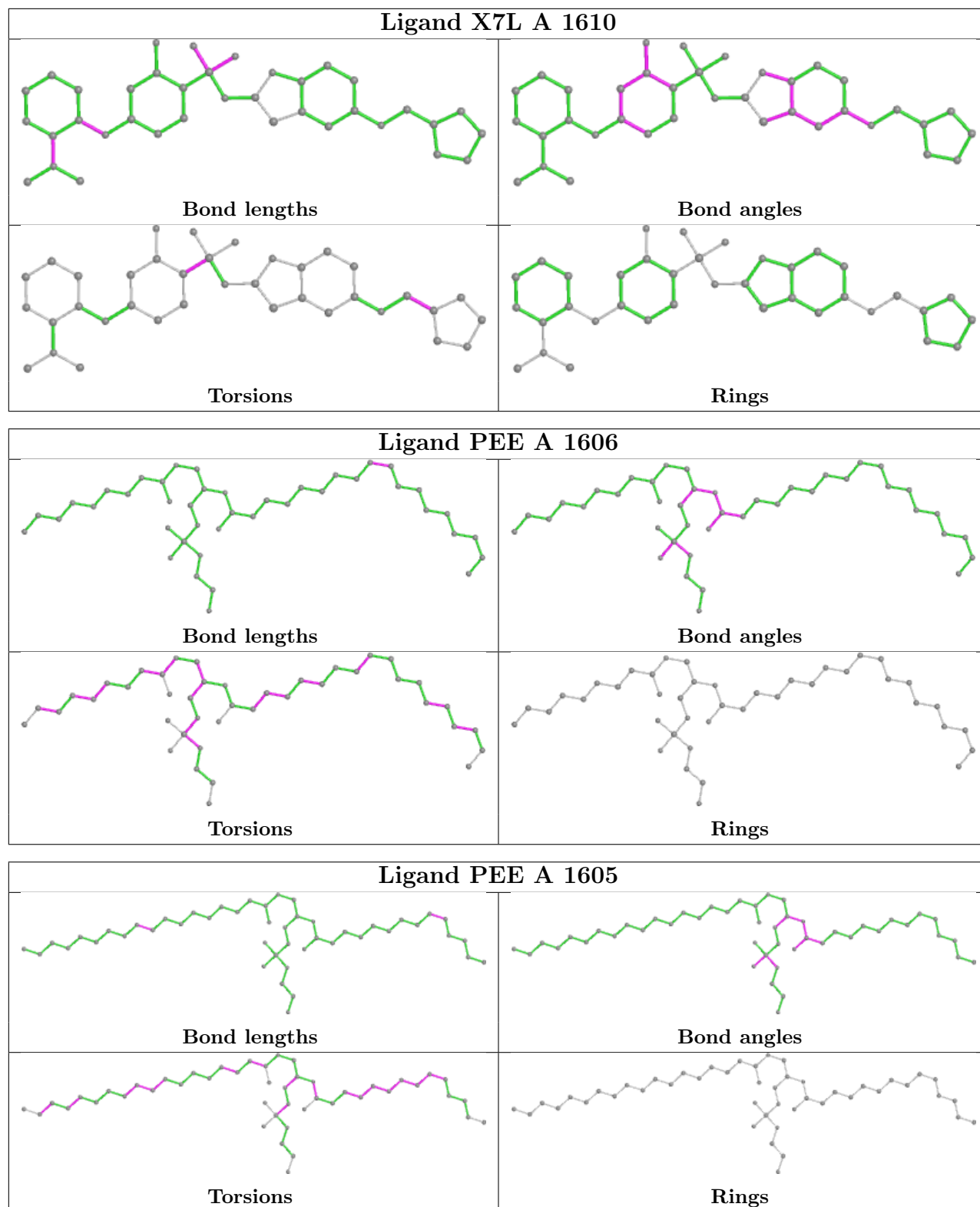
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1604	PEE	2	0
5	A	1609	Y01	1	0
6	A	1610	X7L	1	0
4	A	1605	PEE	1	0

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

There are no chain breaks in this entry.

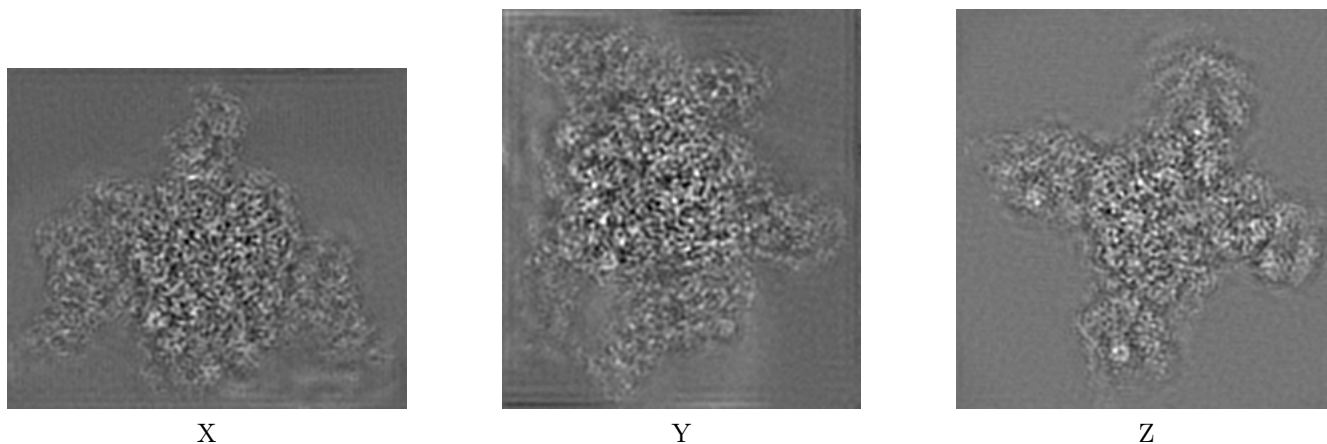
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28776. These allow visual inspection of the internal detail of the map and identification of artifacts.

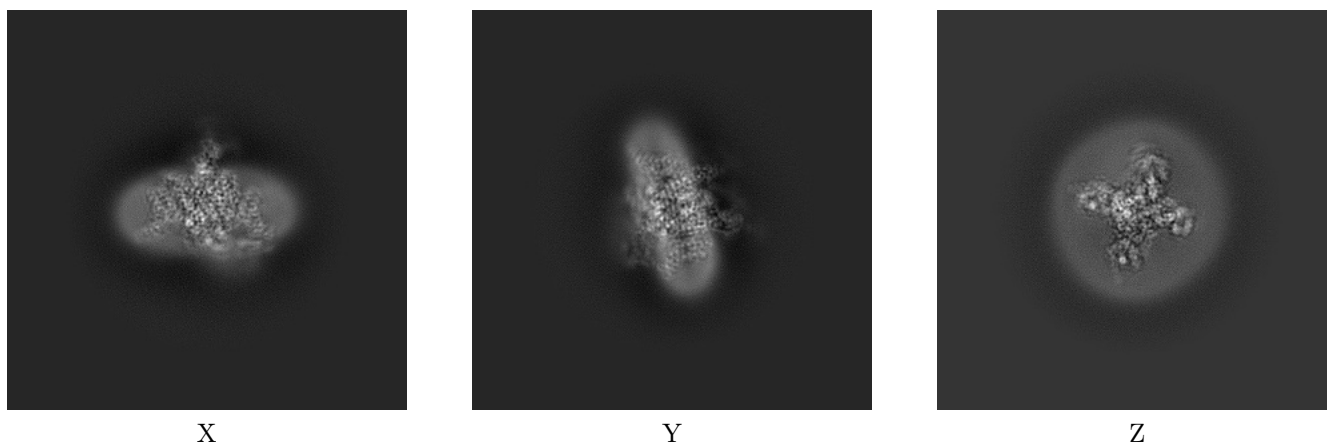
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



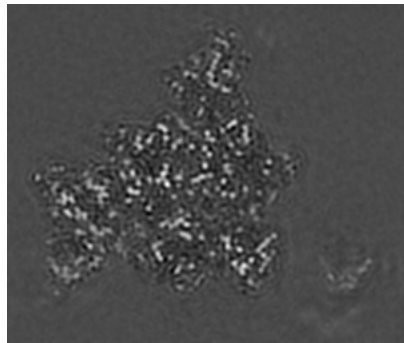
6.1.2 Raw map



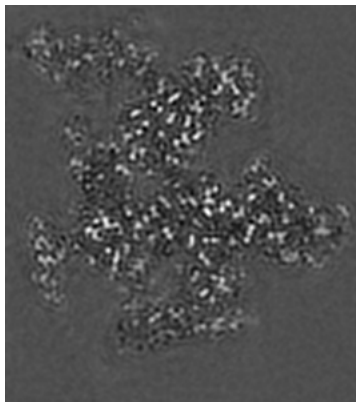
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

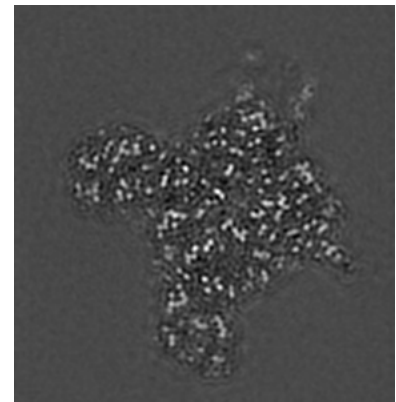
6.2.1 Primary map



X Index: 67

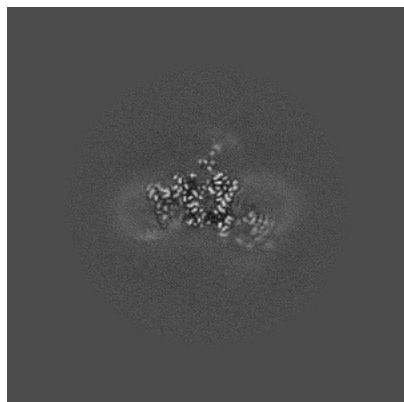


Y Index: 70

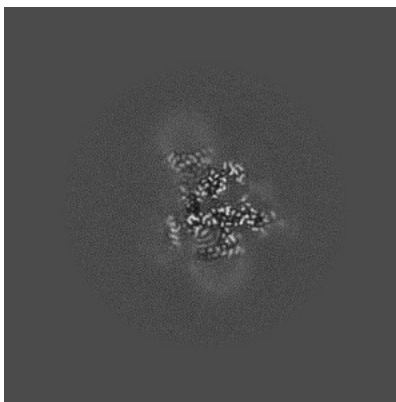


Z Index: 60

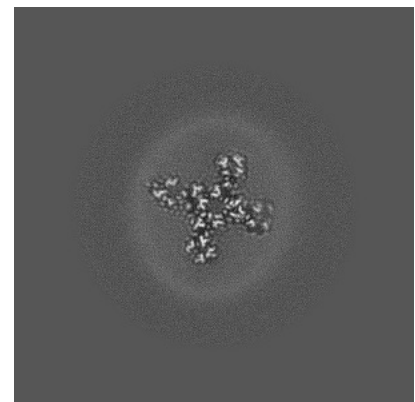
6.2.2 Raw map



X Index: 200



Y Index: 200

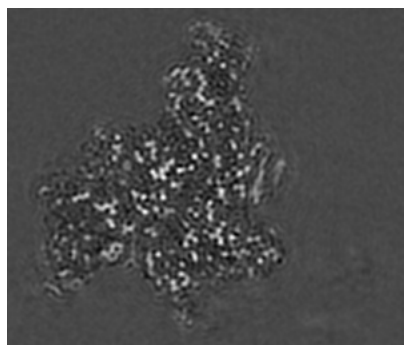


Z Index: 200

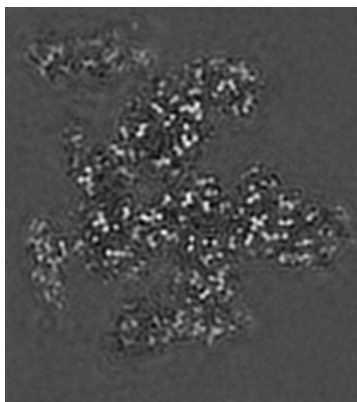
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

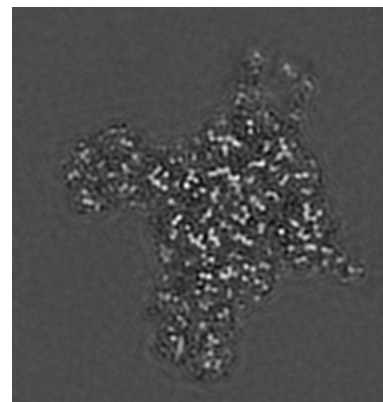
6.3.1 Primary map



X Index: 63

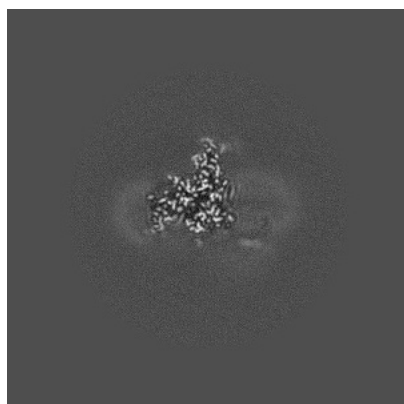


Y Index: 71

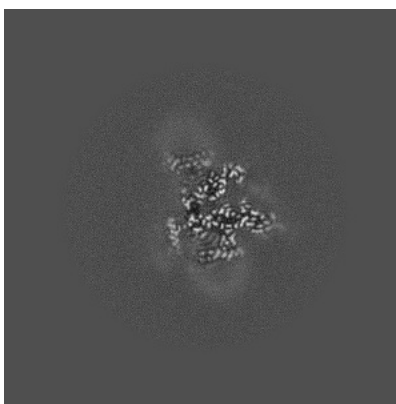


Z Index: 57

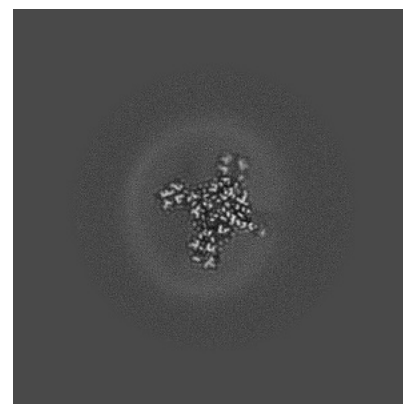
6.3.2 Raw map



X Index: 192



Y Index: 201

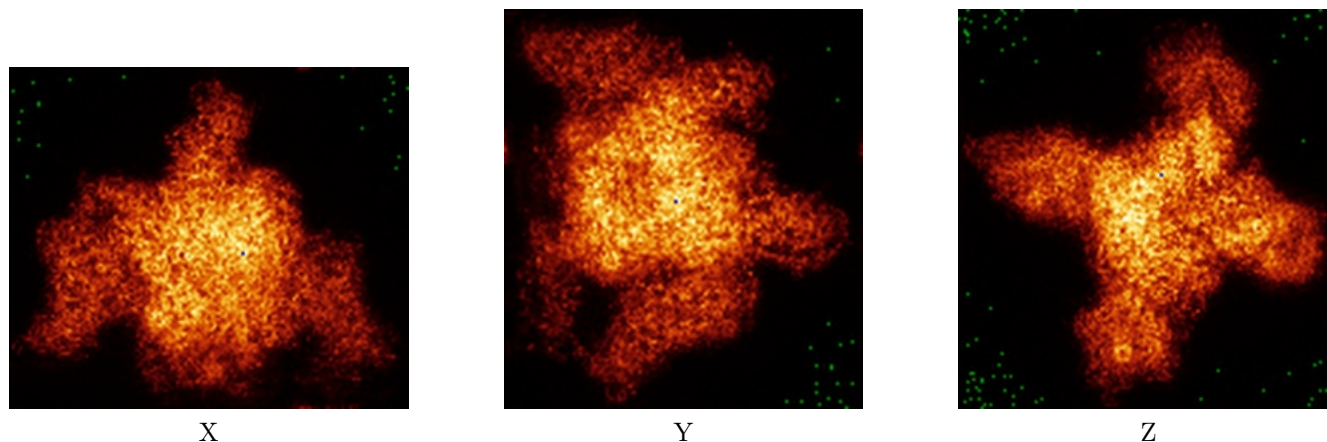


Z Index: 211

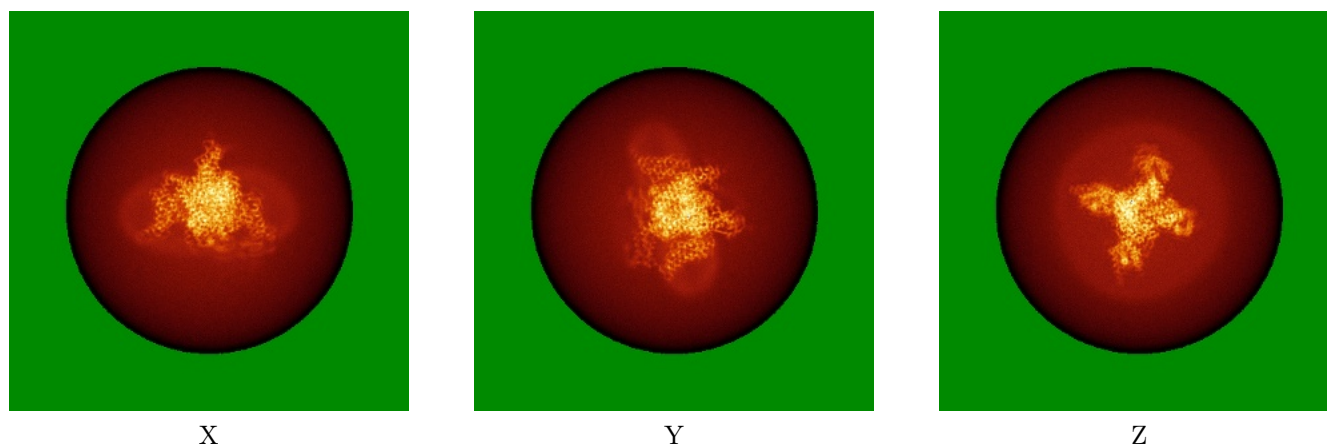
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

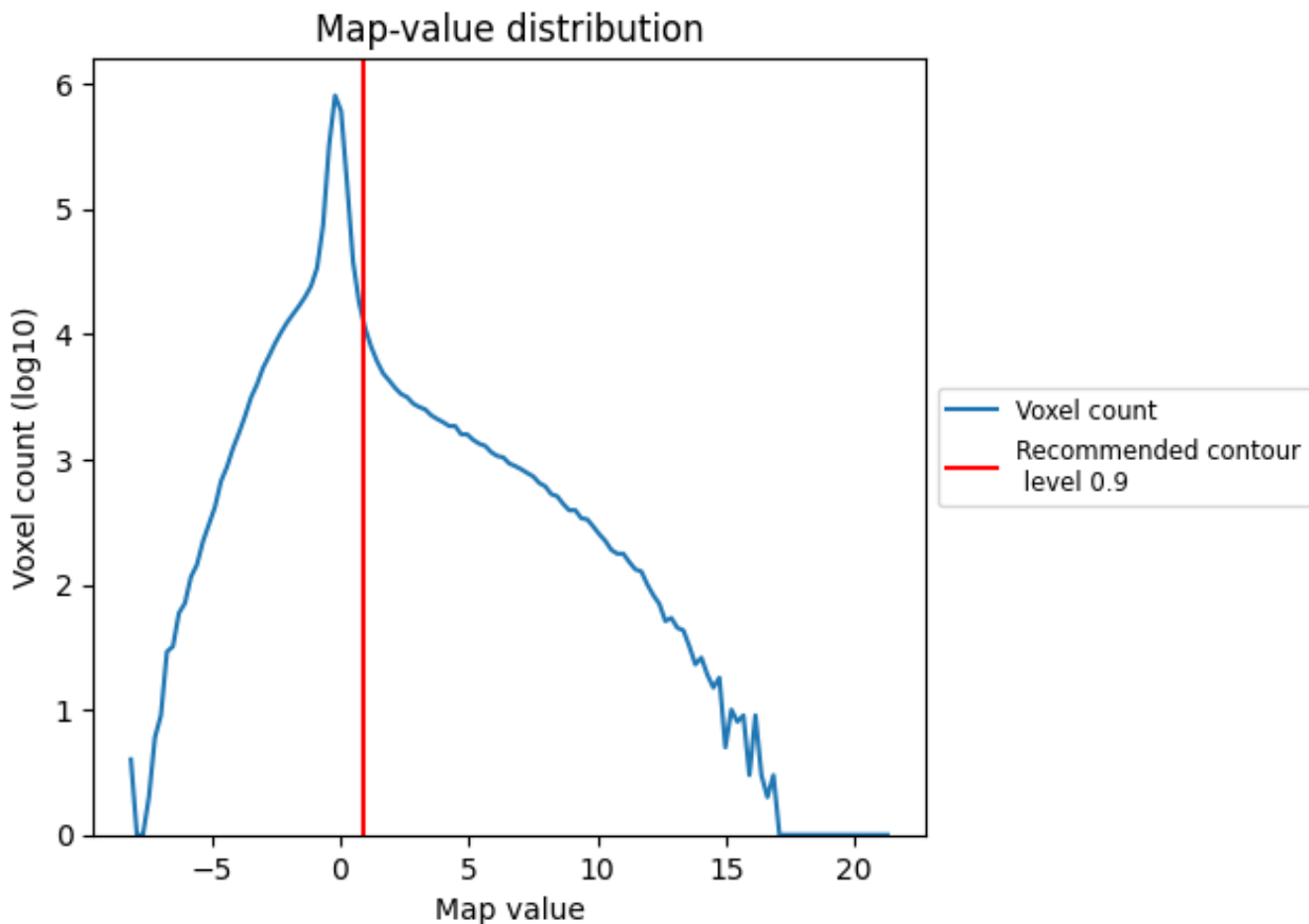
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

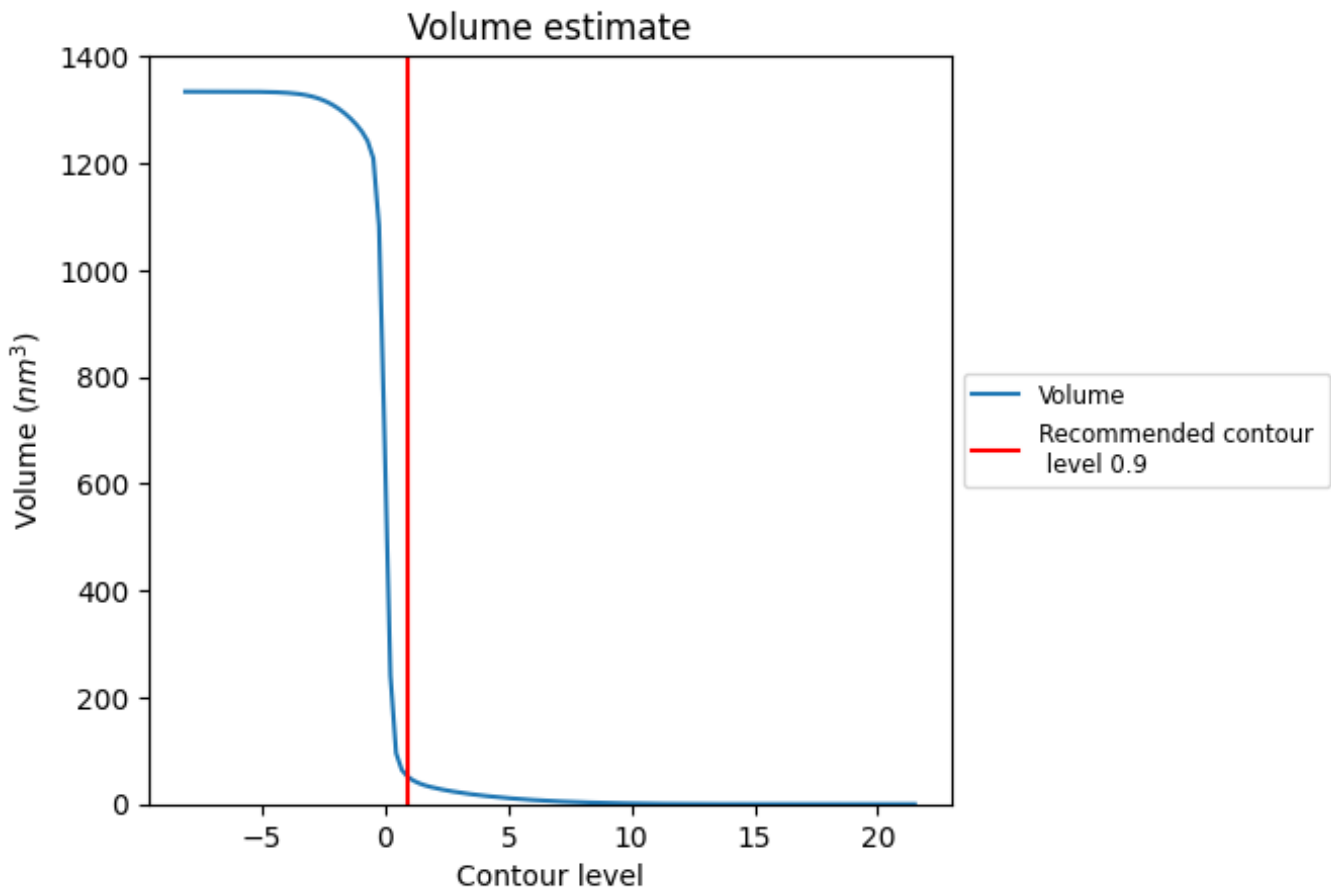
This section contains the results of statistical analysis of the map.

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 52 nm³; this corresponds to an approximate mass of 47 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.

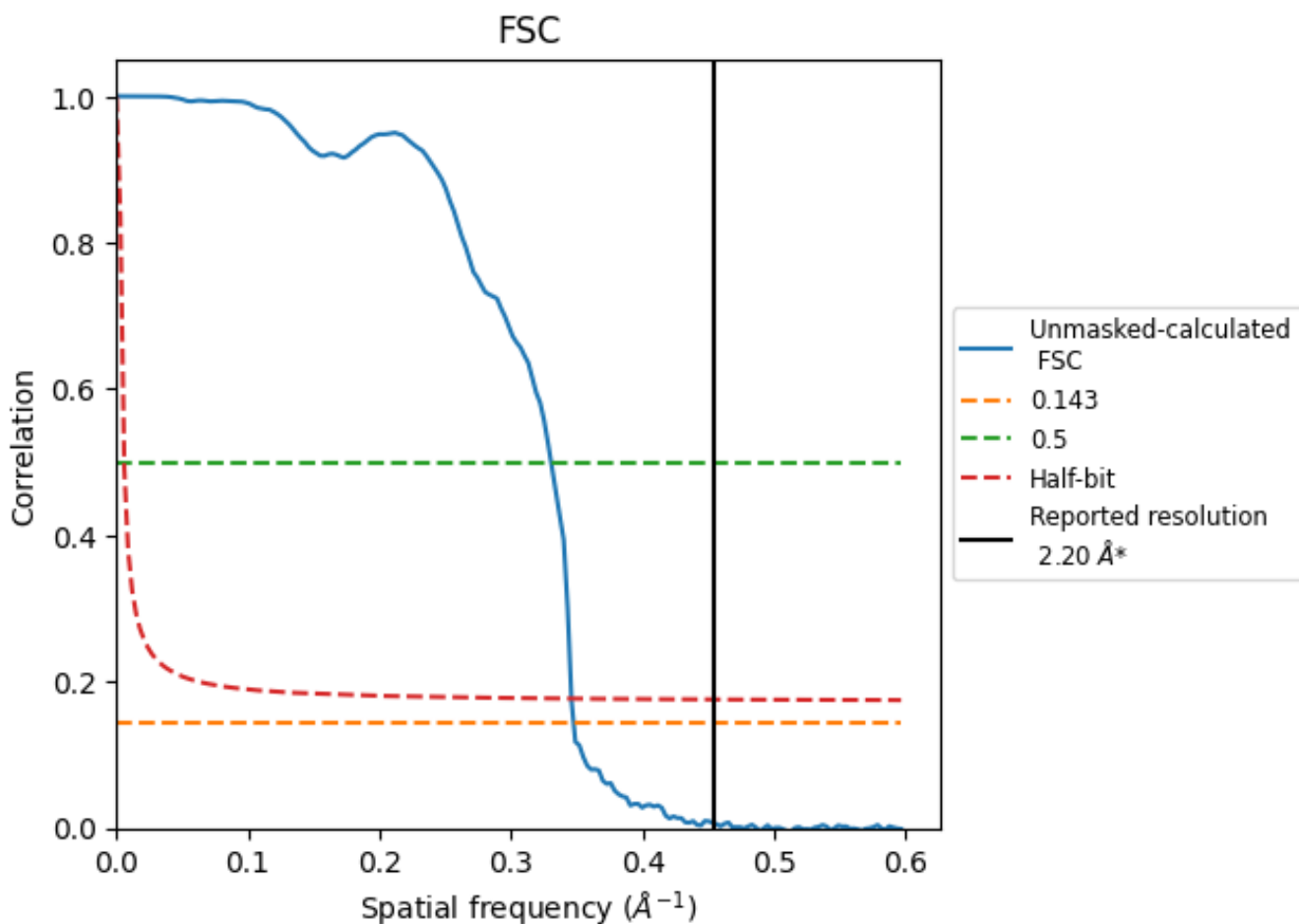
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

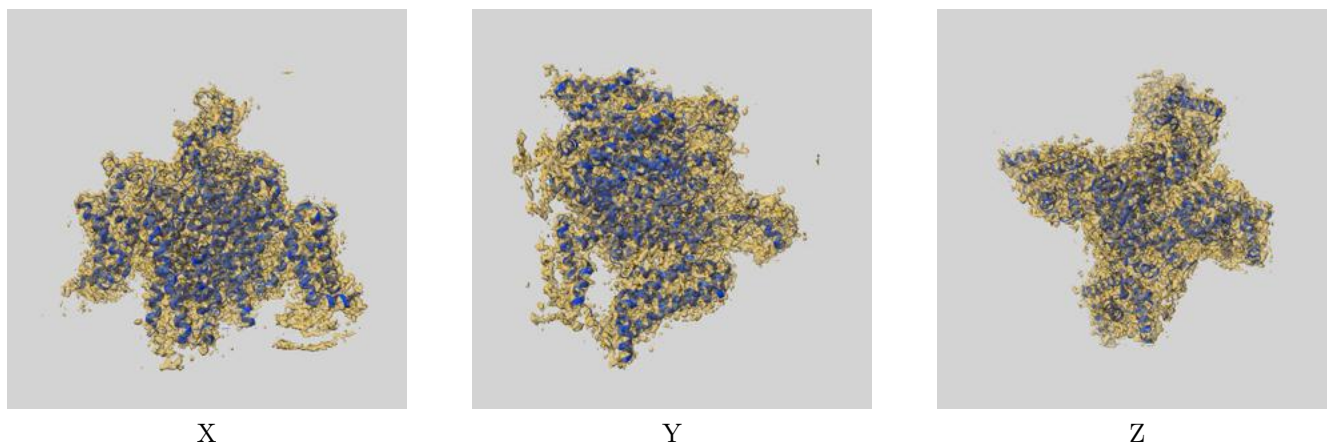
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.03	2.89

*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 2.88 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

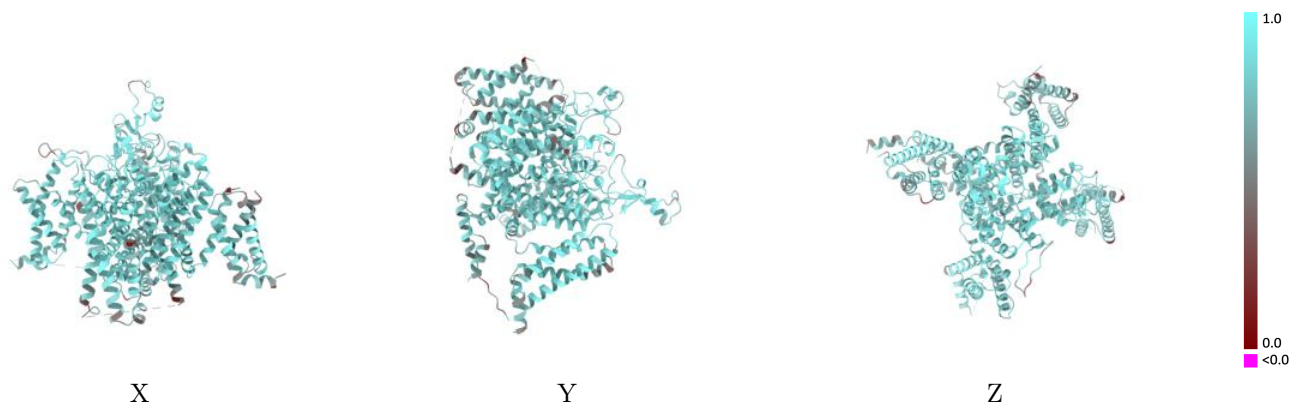
This section contains information regarding the fit between EMDB map EMD-28776 and PDB model 8F0P. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



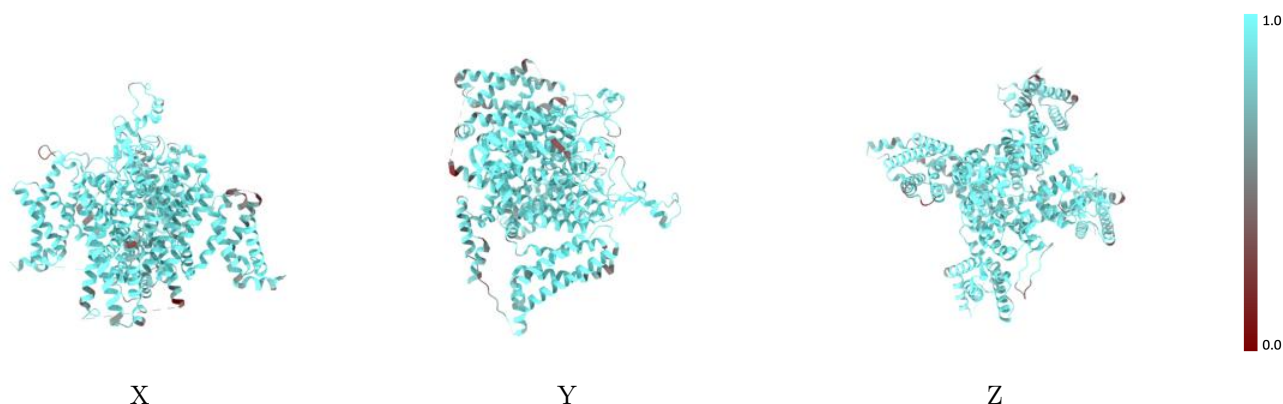
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



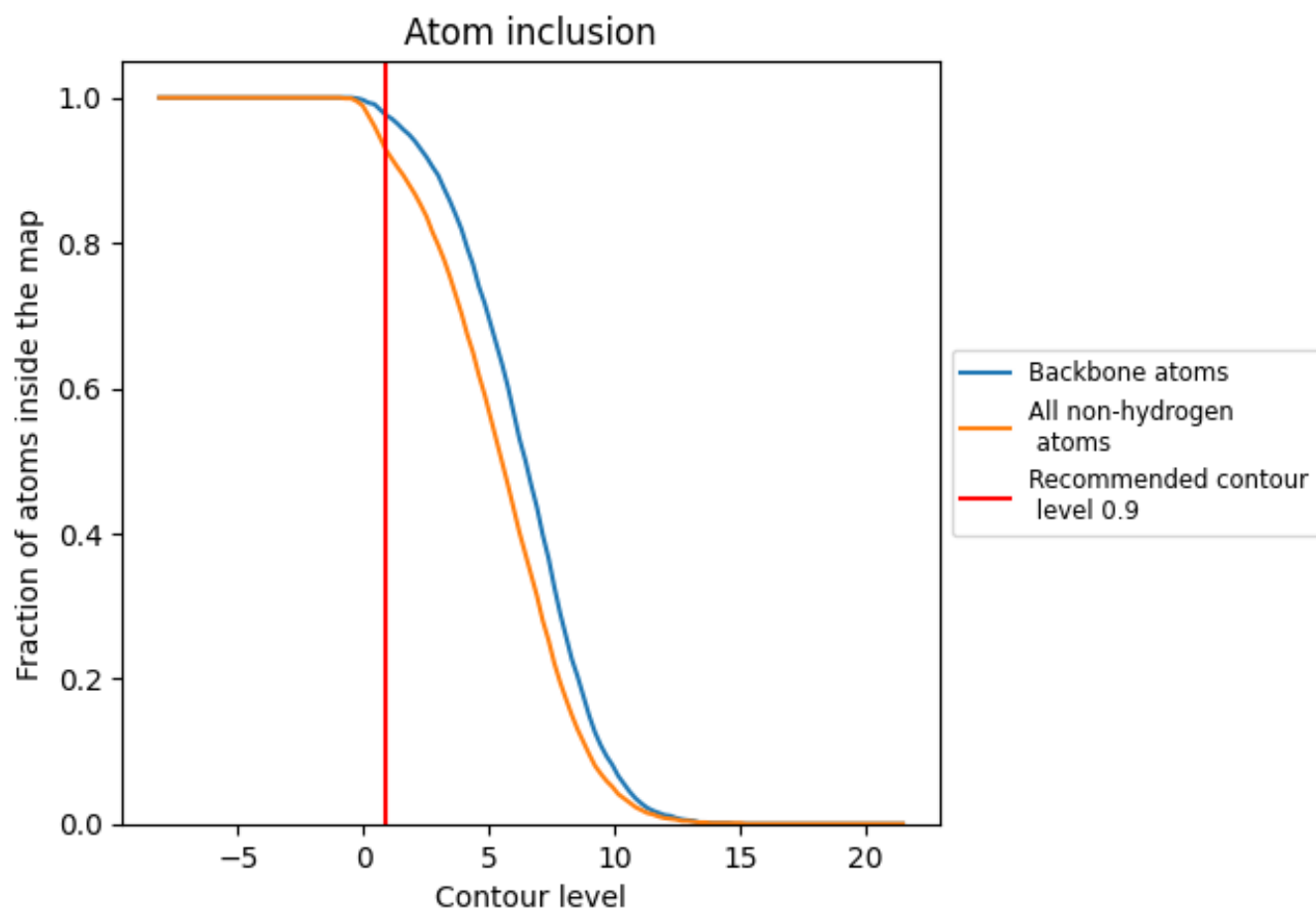
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).


9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.7760
A	 0.9280	 0.7770
B	 0.9020	 0.6170

