



Full wwPDB EM Validation Report ⓘ

Jan 24, 2024 – 12:50 pm GMT

PDB ID : 8QQ0
EMDB ID : EMD-18571
Title : SARS-CoV-2 S protein bound to neutralising antibody UZGENT_A3
Authors : Remaut, H.; Reiter, D.; Vandekerckhove, L.; Acar, D.D.; Witkowski, W.; Gerlo, S.
Deposited on : 2023-10-03
Resolution : 3.50 Å(reported)
Based on initial model : 7K8V

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

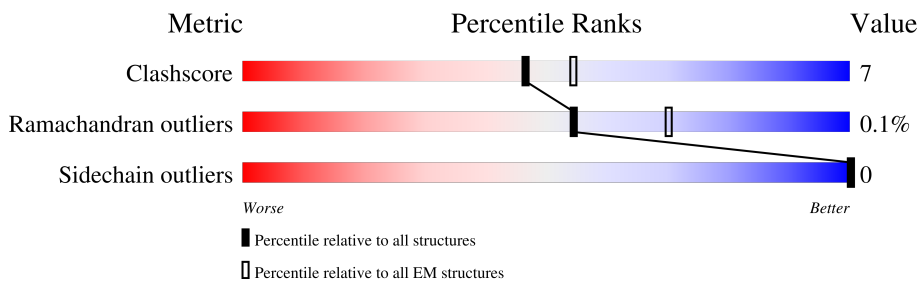
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	1288	
2	D	216	
3	E	229	
4	B	2	
4	a	2	
5	F	3	
5	c	3	
5	e	3	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5677 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 Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	484	3751	2431	612	693	15	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	engineered mutation	UNP P10104
A	1238	GLY	-	insertion	UNP P10104
A	1239	ARG	-	insertion	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	PRO	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	SER	-	expression tag	UNP P10104
A	1259	ALA	-	expression tag	UNP P10104
A	1260	TRP	-	expression tag	UNP P10104
A	1261	SER	-	expression tag	UNP P10104
A	1262	HIS	-	expression tag	UNP P10104
A	1263	PRO	-	expression tag	UNP P10104
A	1264	GLN	-	expression tag	UNP P10104
A	1265	PHE	-	expression tag	UNP P10104
A	1266	GLU	-	expression tag	UNP P10104
A	1267	LYS	-	expression tag	UNP P10104
A	1268	GLY	-	expression tag	UNP P10104
A	1269	GLY	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	GLY	-	expression tag	UNP P10104
A	1273	GLY	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	GLY	-	expression tag	UNP P10104
A	1278	GLY	-	expression tag	UNP P10104
A	1279	SER	-	expression tag	UNP P10104
A	1280	ALA	-	expression tag	UNP P10104
A	1281	TRP	-	expression tag	UNP P10104
A	1282	SER	-	expression tag	UNP P10104
A	1283	HIS	-	expression tag	UNP P10104
A	1284	PRO	-	expression tag	UNP P10104
A	1285	GLN	-	expression tag	UNP P10104
A	1286	PHE	-	expression tag	UNP P10104
A	1287	GLU	-	expression tag	UNP P10104
A	1288	LYS	-	expression tag	UNP P10104

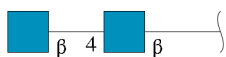
- Molecule 2 is a protein called IgG light chain - FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	111	814	507	137	167	3	0	0

- Molecule 3 is a protein called IgG heavy chain - FAB.

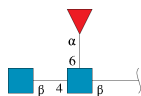
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	120	928	588	160	175	5	0	0

- Molecule 4 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		
4	a	2	28	16	2	10	0	0
4	B	2	28	16	2	10	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	c	3	38	22	2	14	0	0
5	F	3	38	22	2	14	0	0
5	e	3	38	22	2	14	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]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	114237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	94.670	Depositor
Minimum map value	-59.580	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	13.1	Depositor
Map size (\AA)	449.27997, 449.27997, 449.27997	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.78, 0.78, 0.78	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: FUC, 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	0.33	0/3849	0.50	0/5248
2	D	0.31	0/834	0.51	0/1136
3	E	0.30	0/953	0.49	0/1300
All	All	0.32	0/5636	0.50	0/7684

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	52	GLU	Peptide

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	3751	0	3531	41	0
2	D	814	0	769	17	0
3	E	928	0	885	14	0
4	B	28	0	25	1	0
4	a	28	0	25	0	0
5	F	38	0	34	0	0
5	c	38	0	34	0	0
5	e	38	0	34	0	0
6	A	14	0	13	0	0
All	All	5677	0	5350	72	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 (72) 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:226:LEU:HD23	1:A:227:VAL:HG23	1.65	0.77
1:A:291:CYS:O	1:A:292:ALA:N	2.20	0.75
3:E:67:ARG:HH11	3:E:85:ARG:HB3	1.53	0.73
1:A:457:ARG:NH1	1:A:459:SER:O	2.21	0.72
2:D:56:ARG:NH1	2:D:60:VAL:O	2.22	0.71
3:E:13:LYS:HA	3:E:13:LYS:HE3	1.77	0.65
1:A:68:ILE:HD13	1:A:79:PHE:HD1	1.64	0.63
2:D:11:SER:OG	2:D:108:THR:OG1	2.16	0.62
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.63	0.61
1:A:328:ARG:NH1	1:A:533:LEU:HB2	2.16	0.60
1:A:131:CYS:HB2	1:A:133:PHE:CE1	2.37	0.59
3:E:110:ASP:OD1	3:E:111:CYS:N	2.35	0.59
1:A:353:TRP:O	1:A:466:ARG:NH1	2.36	0.59
1:A:231:ILE:HG13	1:A:232:GLY:H	1.68	0.58
3:E:61:THR:HG22	3:E:63:LYS:H	1.69	0.58
1:A:457:ARG:NH2	1:A:467:ASP:OD1	2.36	0.58
2:D:52:GLU:O	2:D:54:THR:N	2.37	0.57
1:A:231:ILE:HD12	1:A:233:ILE:HG12	1.85	0.57
1:A:287:ASP:OD2	1:A:288:ALA:N	2.37	0.57
2:D:61:PRO:HB2	2:D:63:ARG:HG2	1.85	0.57
2:D:53:VAL:HG11	2:D:68:LYS:HB2	1.89	0.55
1:A:458:LYS:H	1:A:458:LYS:HD2	1.72	0.55
3:E:67:ARG:HD2	3:E:85:ARG:HB3	1.88	0.54
1:A:64:TRP:CD1	1:A:266:TYR:HE1	2.25	0.54
1:A:274:THR:HG23	1:A:291:CYS:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG21	1:A:387:LEU:HD21	1.90	0.54
1:A:433:VAL:HG22	1:A:512:VAL:HG22	1.90	0.54
3:E:94:TYR:O	3:E:115:GLY:HA2	2.08	0.54
1:A:409:GLN:OE1	1:A:418:ILE:HG22	2.09	0.53
2:D:63:ARG:NH2	2:D:84:ASP:OD2	2.42	0.53
2:D:65:SER:O	2:D:76:THR:OG1	2.26	0.52
1:A:80:ASP:N	1:A:80:ASP:OD1	2.42	0.51
1:A:458:LYS:HD2	1:A:458:LYS:N	2.24	0.51
1:A:81:ASN:O	1:A:239:GLN:NE2	2.44	0.51
1:A:328:ARG:HH12	1:A:533:LEU:HB2	1.76	0.50
1:A:328:ARG:HD3	1:A:532:ASN:O	2.12	0.50
2:D:92:SER:OG	2:D:93:TYR:N	2.43	0.50
3:E:73:ASP:OD2	3:E:76:ILE:HG12	2.12	0.49
2:D:56:ARG:HH11	2:D:60:VAL:HG13	1.77	0.49
1:A:418:ILE:HG13	1:A:422:ASN:HD22	1.78	0.49
3:E:97:ALA:HB1	3:E:109:LEU:HD22	1.94	0.49
1:A:102:ARG:HG3	1:A:141:LEU:HD12	1.95	0.48
1:A:119:ILE:HG23	1:A:128:ILE:HG12	1.95	0.48
3:E:39:GLN:HB2	3:E:45:LEU:HD23	1.97	0.47
1:A:159:VAL:HG23	1:A:160:TYR:CD1	2.47	0.47
2:D:44:LYS:HE2	2:D:44:LYS:HB3	1.70	0.47
2:D:56:ARG:NH2	2:D:62:ASP:OD1	2.48	0.47
1:A:167:THR:O	1:A:167:THR:HG22	2.17	0.45
1:A:210:ILE:HG21	1:A:217:PRO:HG3	1.98	0.45
3:E:100:VAL:HB	3:E:101:PRO:HD3	1.98	0.44
2:D:4:LEU:HD23	2:D:22:CYS:SG	2.58	0.44
1:A:444:LYS:O	1:A:499:PRO:HD3	2.18	0.43
3:E:97:ALA:CB	3:E:109:LEU:HD22	2.49	0.43
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.83	0.43
1:A:444:LYS:HE2	1:A:444:LYS:HB3	1.79	0.43
3:E:35:HIS:CG	3:E:109:LEU:HD21	2.54	0.43
1:A:493:GLN:HG3	1:A:494:SER:N	2.33	0.43
4:B:1:NAG:H4	4:B:2:NAG:H2	1.76	0.43
2:D:49:MET:HB3	2:D:50:ILE:HD12	2.01	0.43
2:D:65:SER:OG	2:D:76:THR:OG1	2.27	0.43
2:D:64:PHE:CD1	2:D:77:VAL:HG22	2.54	0.42
1:A:296:LEU:O	1:A:299:THR:OG1	2.35	0.42
1:A:96:GLU:HA	1:A:96:GLU:OE2	2.19	0.41
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.86	0.41
3:E:12:LYS:HB3	3:E:16:ALA:HB3	2.02	0.41
1:A:474:GLN:OE1	1:A:479:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:TYR:HB2	3:E:108:TRP:CD1	2.55	0.41
1:A:106:PHE:HB3	1:A:235:ILE:HD13	2.03	0.41
1:A:480:CYS:O	1:A:483:VAL:HG12	2.20	0.41
1:A:403:ARG:NH1	1:A:504:GLY:O	2.54	0.41
1:A:190:ARG:HG2	1:A:207:HIS:CD2	2.56	0.40
2:D:16:GLN:O	2:D:80:LEU:HD13	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	466/1288 (36%)	422 (91%)	44 (9%)	0	100	100
2	D	109/216 (50%)	99 (91%)	9 (8%)	1 (1%)	17	56
3	E	118/229 (52%)	104 (88%)	14 (12%)	0	100	100
All	All	693/1733 (40%)	625 (90%)	67 (10%)	1 (0%)	54	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	53	VAL

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	402/1116 (36%)	402 (100%)	0	100	100
2	D	88/181 (49%)	88 (100%)	0	100	100
3	E	98/196 (50%)	98 (100%)	0	100	100
All	All	588/1493 (39%)	588 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	422	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](#)

13 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
4	NAG	B	1	1,4	14,14,15	0.94	1 (7%)	17,19,21	0.87	1 (5%)
4	NAG	B	2	4	14,14,15	0.37	0	17,19,21	0.37	0
5	NAG	F	1	1,5	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	F	2	5	14,14,15	0.28	0	17,19,21	0.41	0
5	FUC	F	3	5	10,10,11	0.81	0	14,14,16	1.03	1 (7%)
4	NAG	a	1	1,4	14,14,15	0.22	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	a	2	4	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	c	1	1,5	14,14,15	0.27	0	17,19,21	0.49	0
5	NAG	c	2	5	14,14,15	0.27	0	17,19,21	0.39	0
5	FUC	c	3	5	10,10,11	0.77	0	14,14,16	0.92	0
5	NAG	e	1	3,5	14,14,15	0.31	0	17,19,21	0.46	0
5	NAG	e	2	5	14,14,15	0.58	1 (7%)	17,19,21	0.88	2 (11%)
5	FUC	e	3	5	10,10,11	0.67	0	14,14,16	0.94	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	NAG	B	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
4	NAG	a	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	1/6/23/26	0/1/1/1
5	FUC	c	3	5	-	-	0/1/1/1
5	NAG	e	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	4/6/23/26	0/1/1/1
5	FUC	e	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	O5-C1	-3.38	1.38	1.43
5	e	2	NAG	O5-C1	-2.01	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C3-C4-C5	2.22	114.20	110.24
5	e	2	NAG	C1-O5-C5	2.11	115.05	112.19
5	e	2	NAG	C3-C4-C5	2.07	113.94	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3	FUC	C1-O5-C5	2.04	117.41	112.78

There are no chirality outliers.

All (21) torsion outliers are listed below:

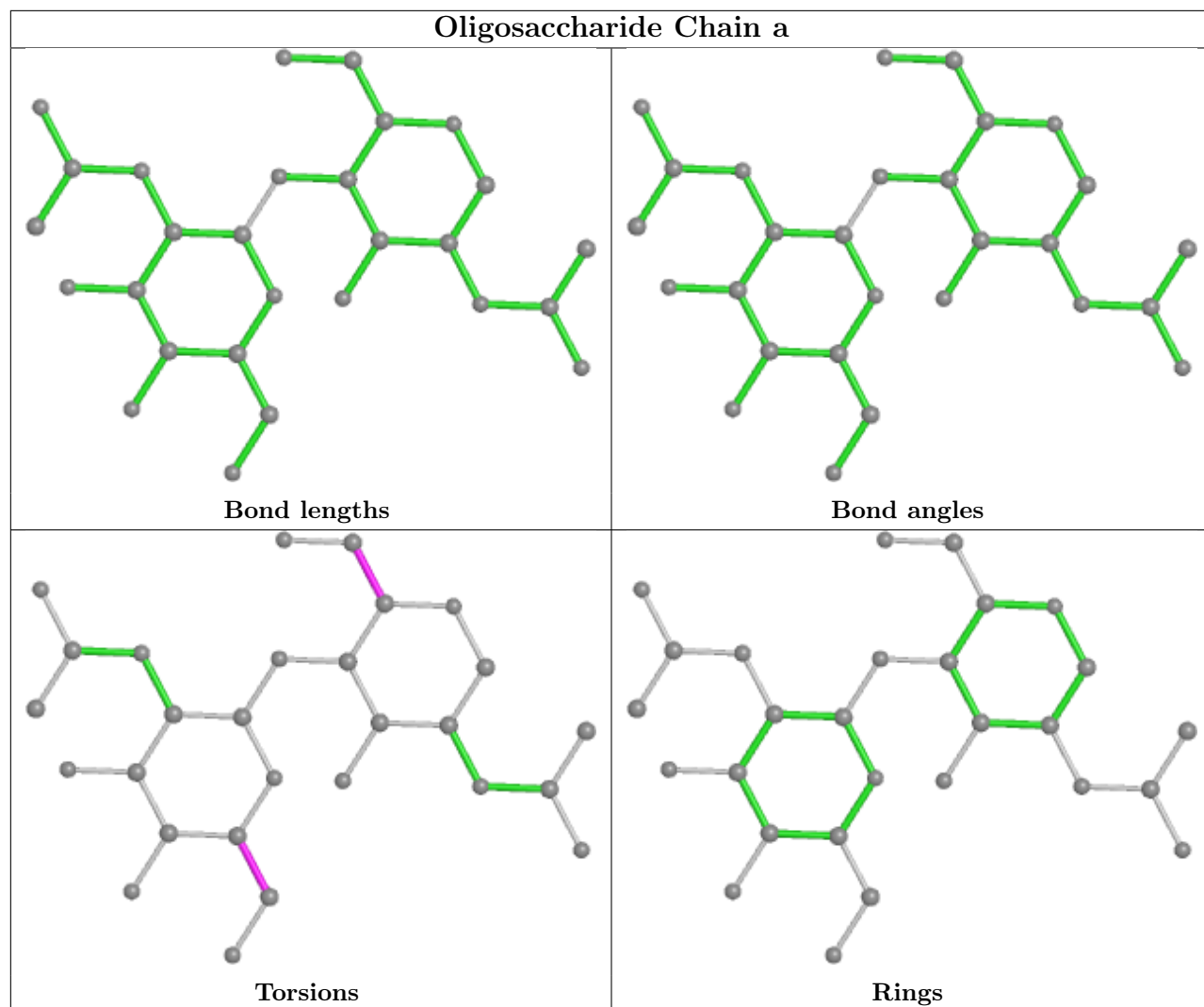
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	e	2	NAG	C8-C7-N2-C2
5	e	2	NAG	O7-C7-N2-C2
4	a	2	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	e	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C1-C2-N2-C7
5	e	2	NAG	O5-C5-C6-O6
4	B	1	NAG	C1-C2-N2-C7
4	a	1	NAG	C4-C5-C6-O6
4	B	1	NAG	C3-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7
5	e	1	NAG	C4-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6

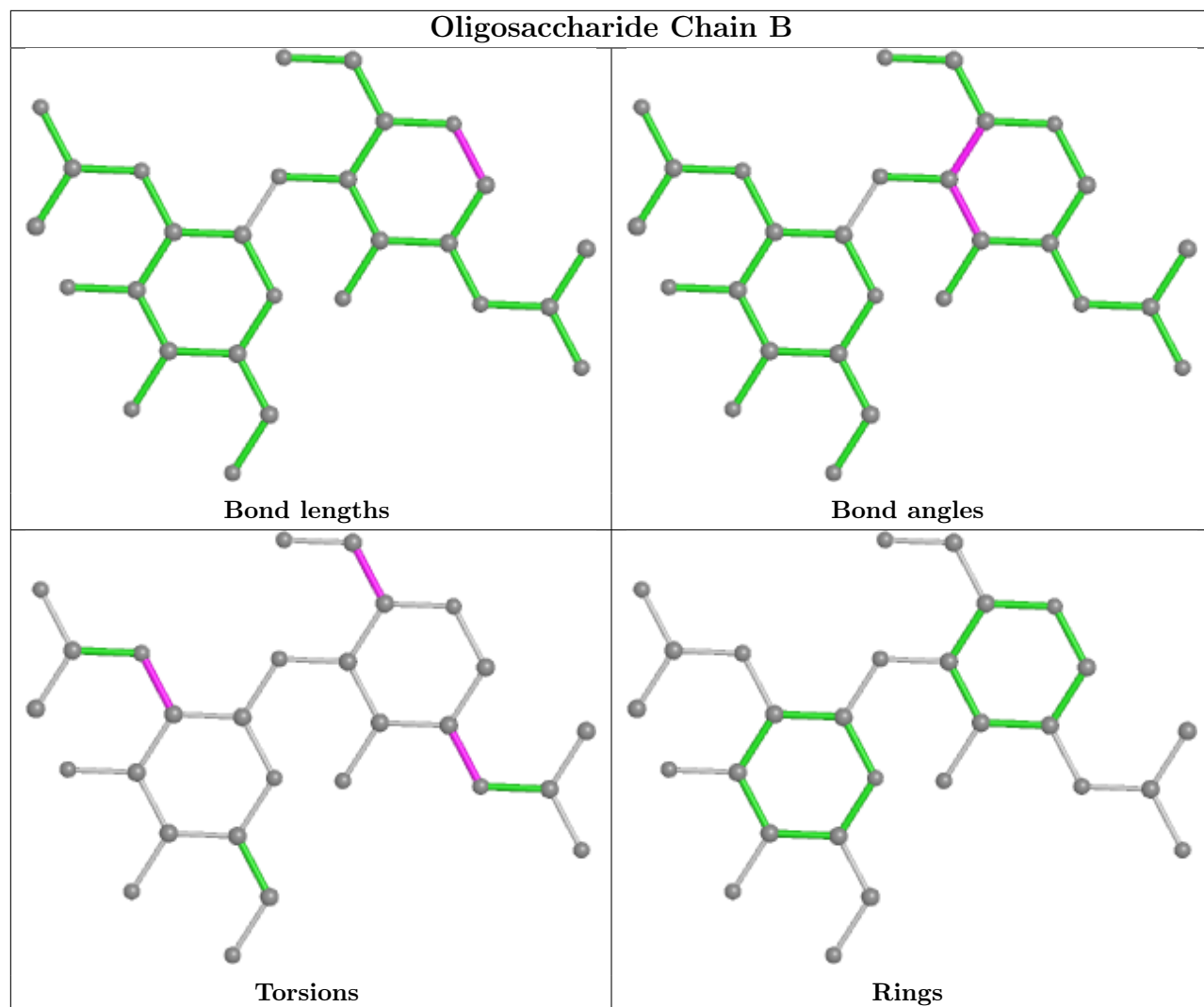
There are no ring outliers.

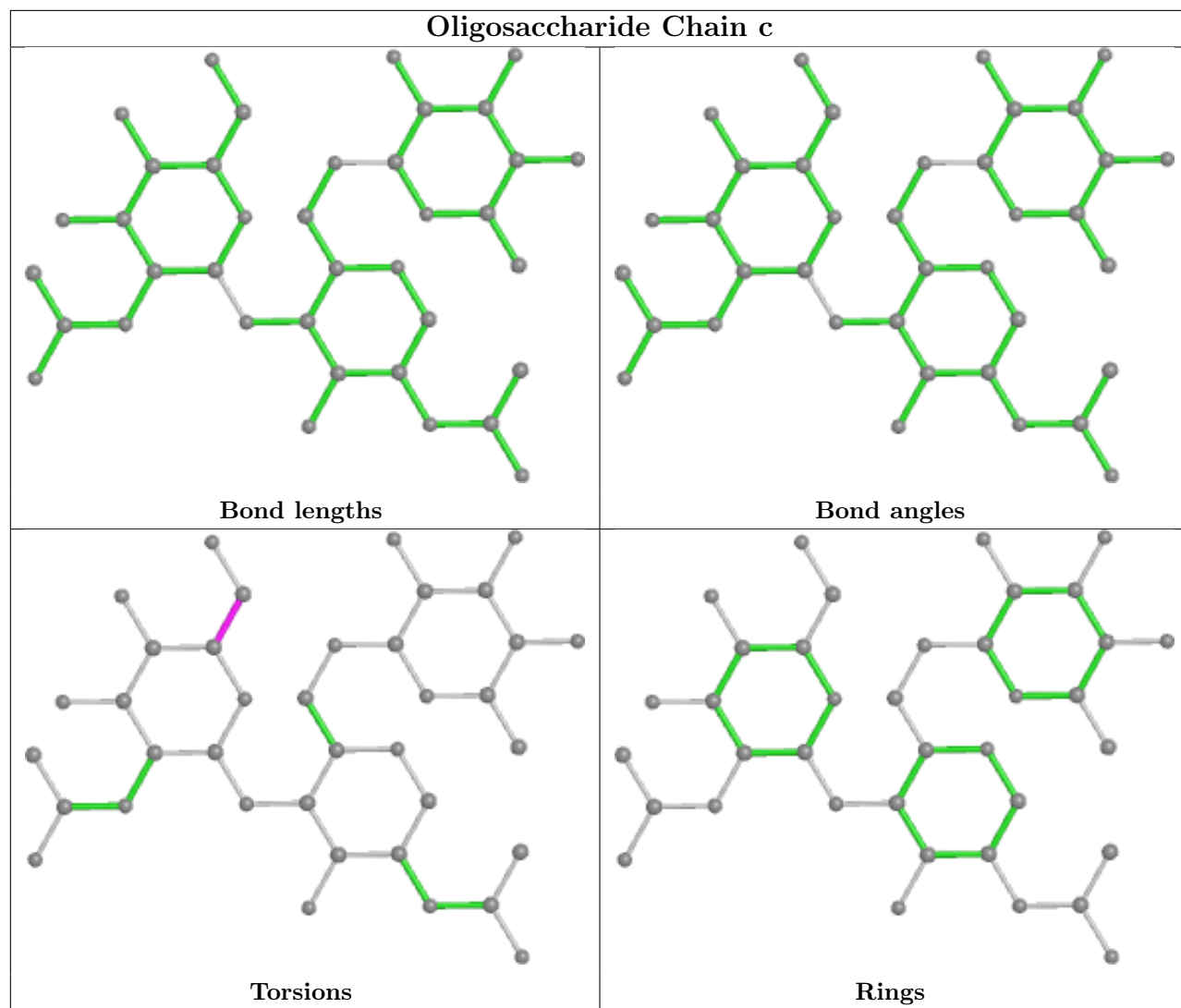
2 monomers are involved in 1 short contact:

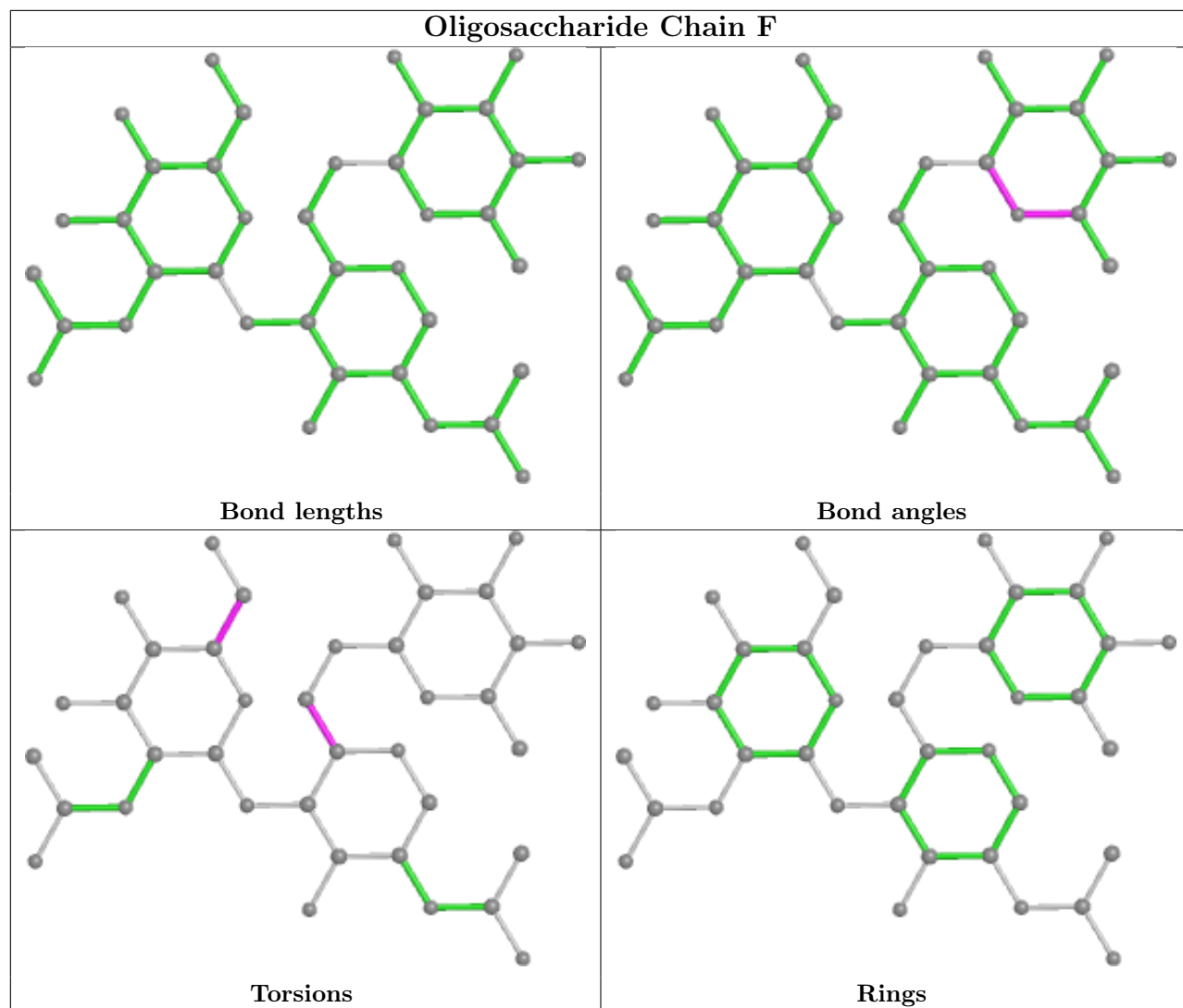
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	NAG	1	0
4	B	1	NAG	1	0

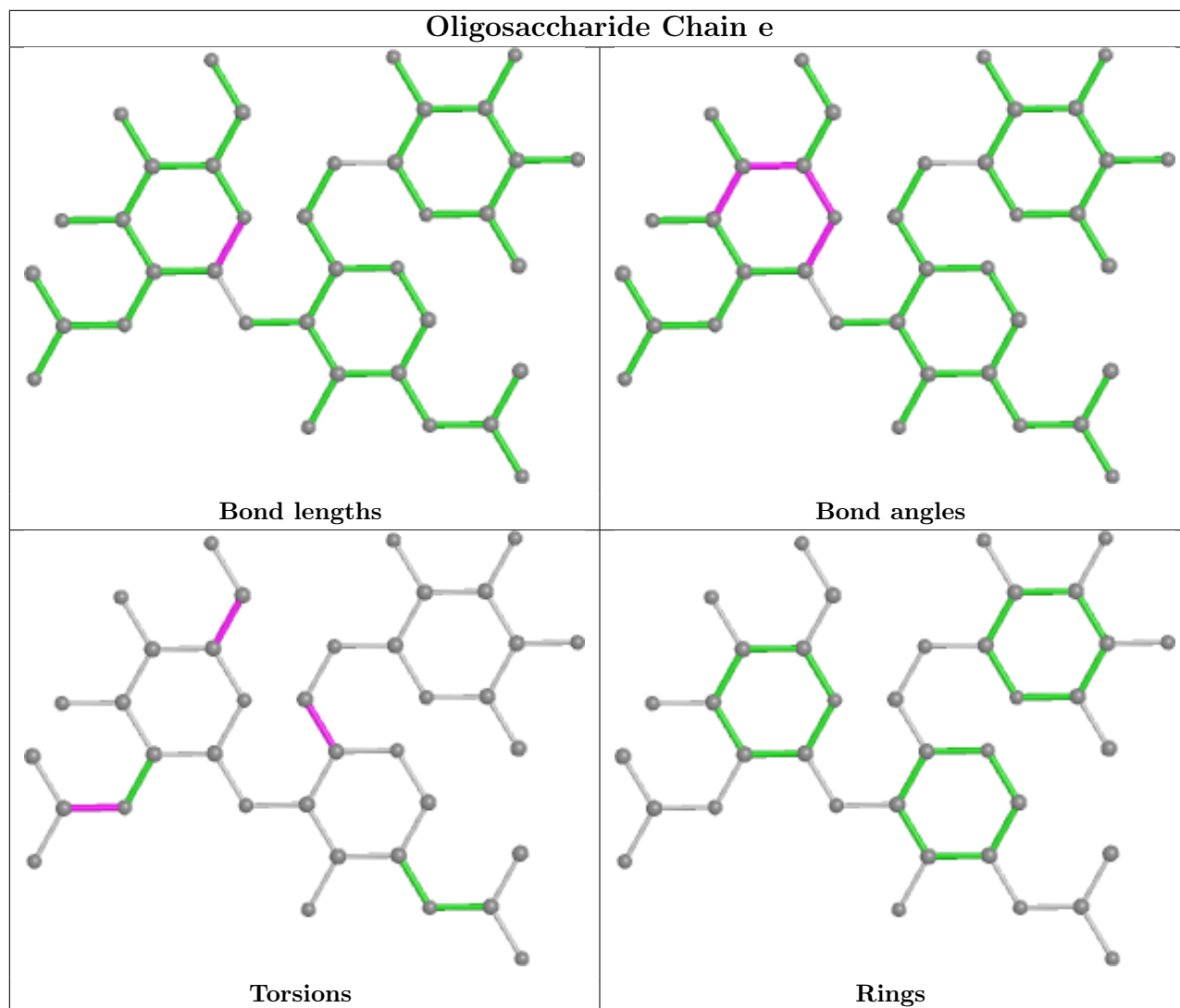
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	NAG	A	1301	1	14,14,15	0.62	1 (7%)	17,19,21	0.96	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1301	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1301	NAG	O5-C1	-2.07	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1301	NAG	C1-O5-C5	2.59	115.69	112.19
6	A	1301	NAG	C3-C4-C5	2.01	113.83	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1301	NAG	O5-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	A	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	291:CYS	C	292:ALA	N	3.04

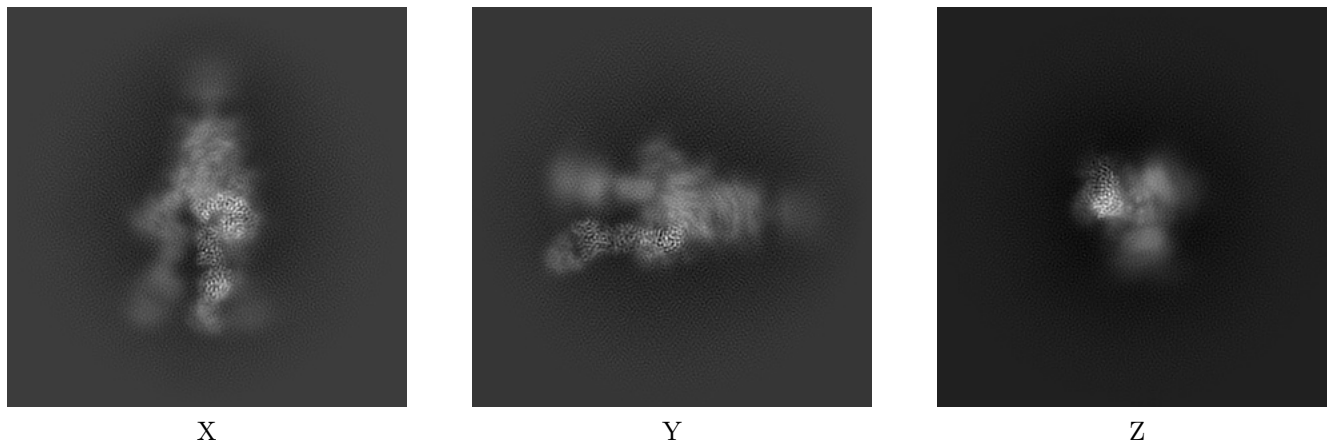
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18571. These allow visual inspection of the internal detail of the map and identification of artifacts.

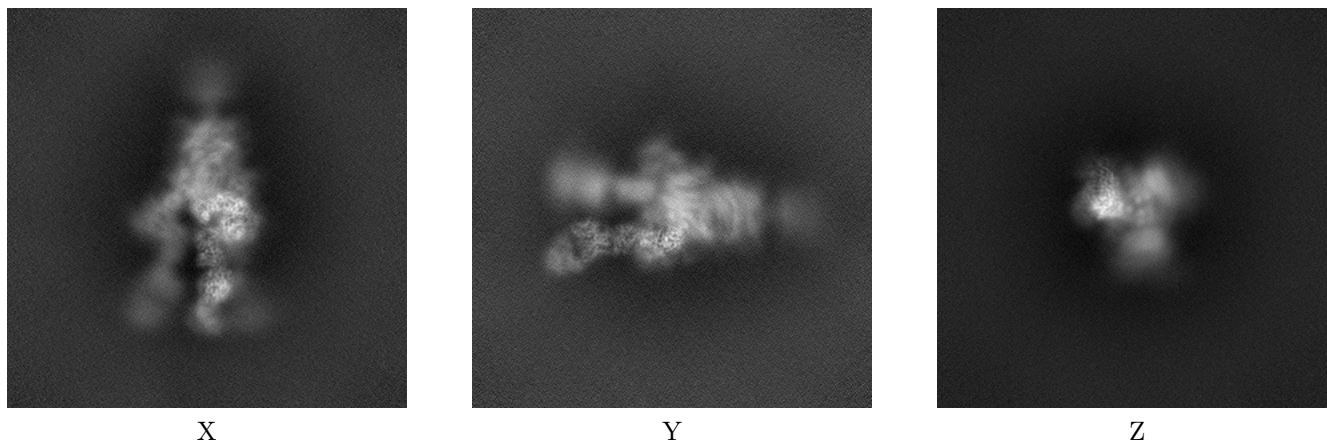
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



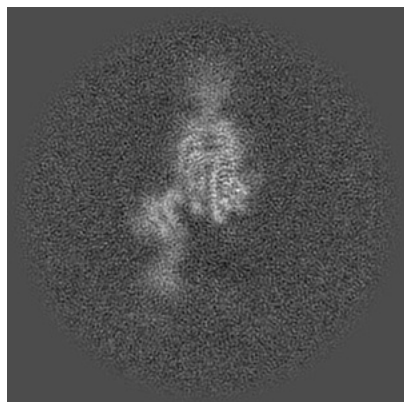
6.1.2 Raw map



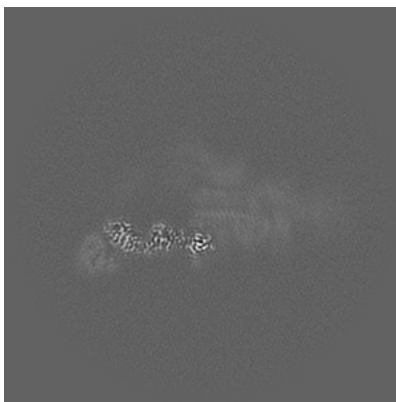
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

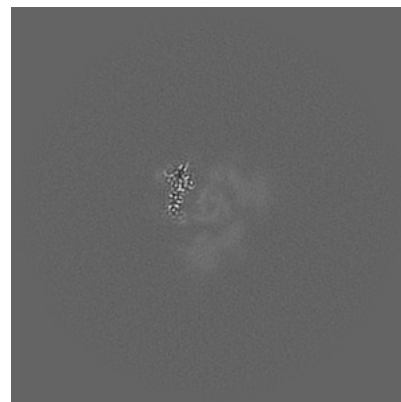
6.2.1 Primary map



X Index: 288



Y Index: 288



Z Index: 288

6.2.2 Raw map



X Index: 288



Y Index: 288

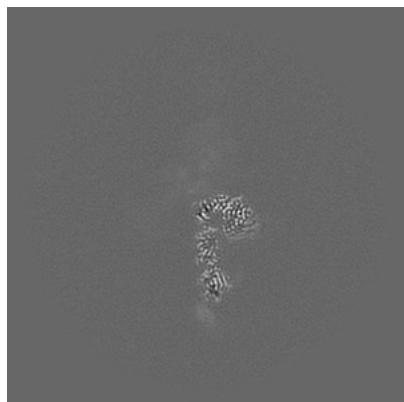


Z Index: 288

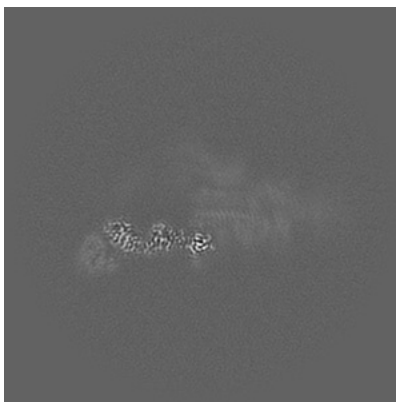
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

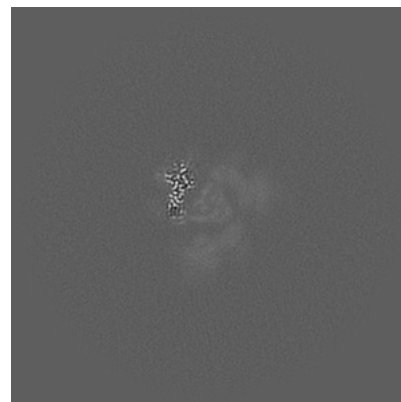
6.3.1 Primary map



X Index: 237



Y Index: 288



Z Index: 286

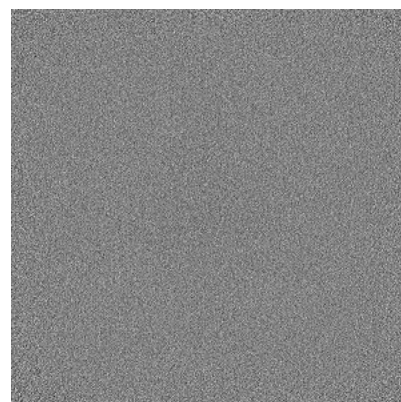
6.3.2 Raw map



X Index: 237



Y Index: 288

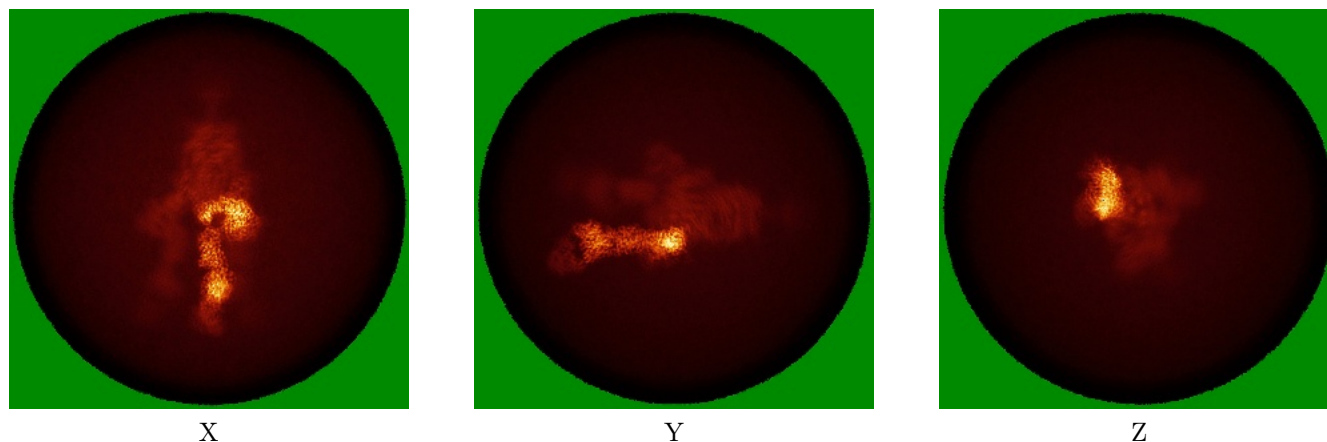


Z Index: 0

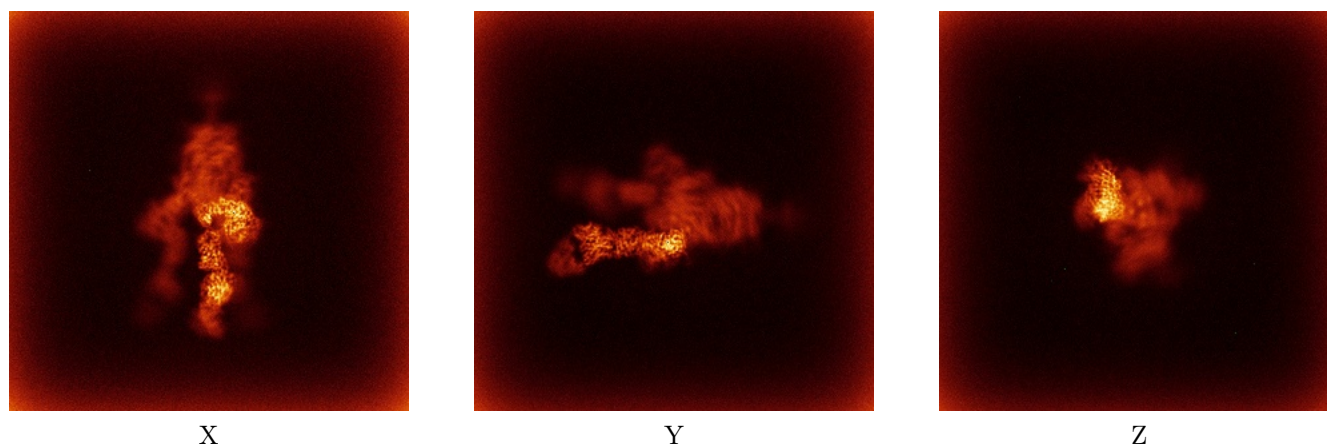
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



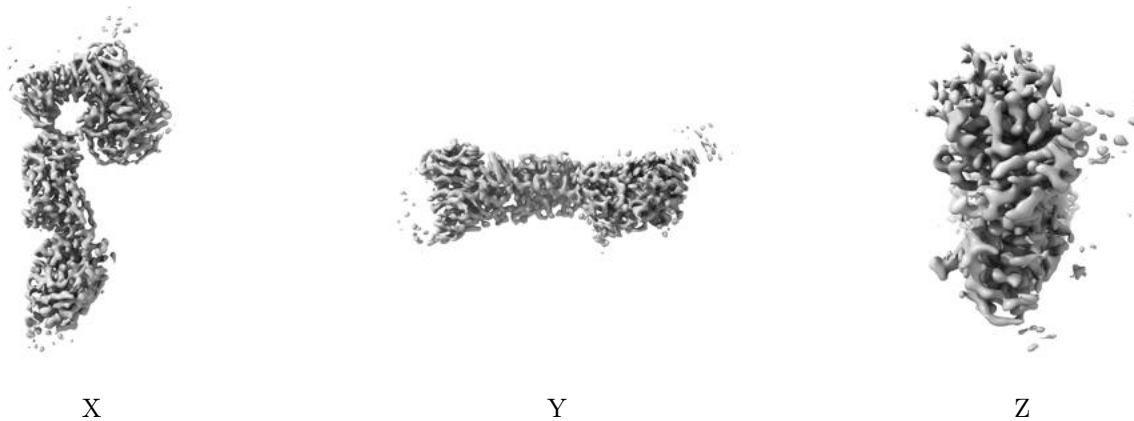
6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 13.1. 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.

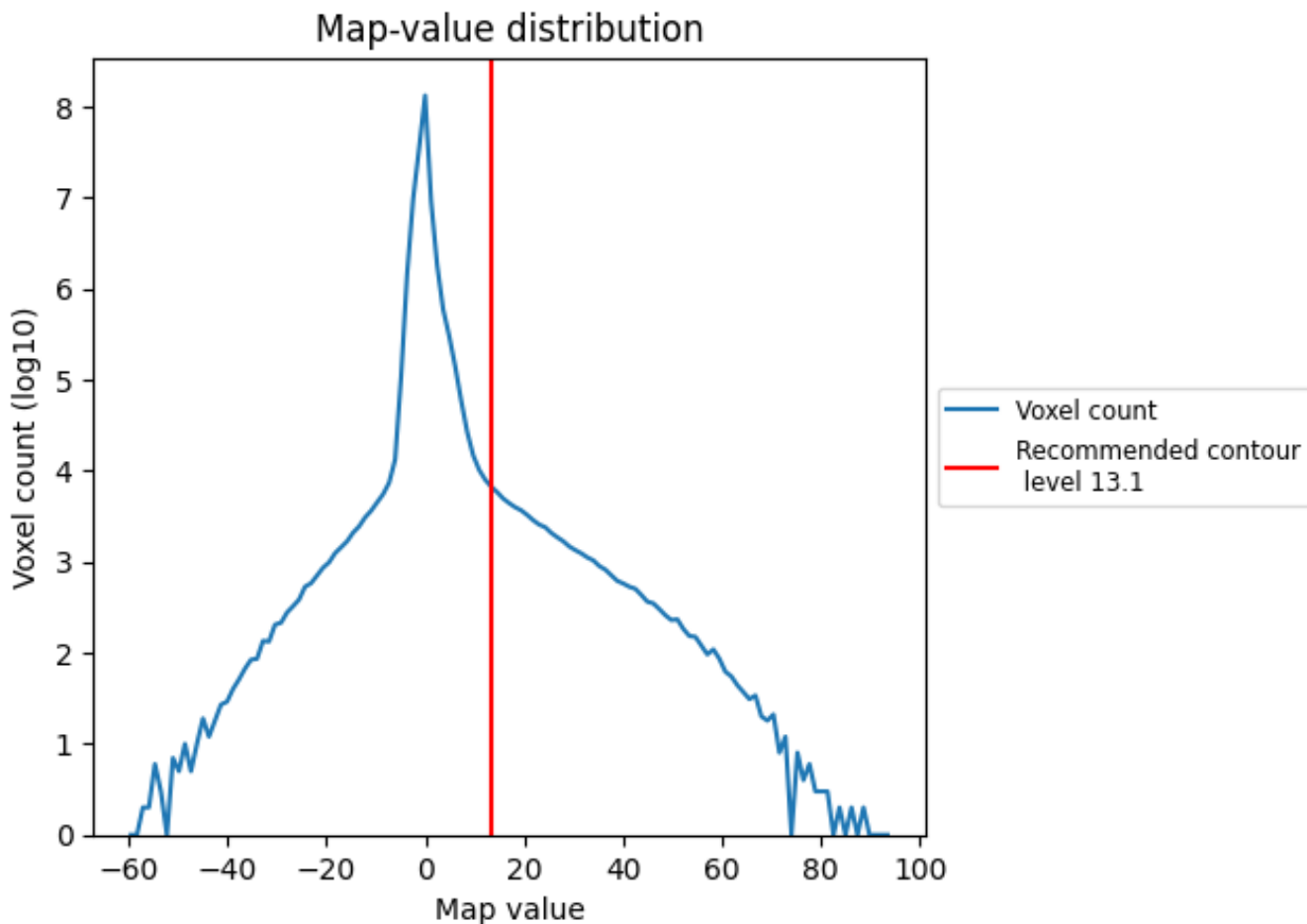
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

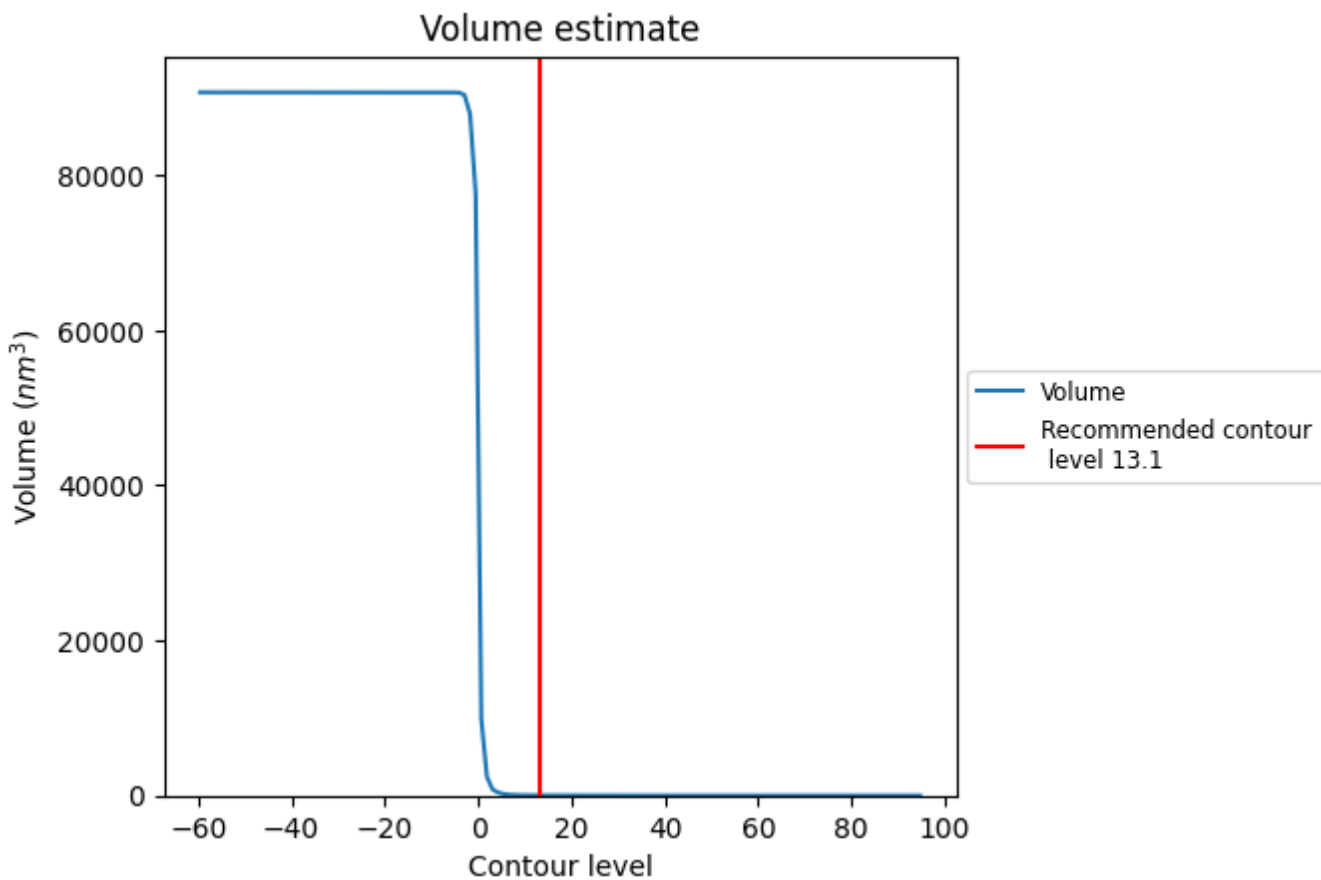
This section contains the results of statistical analysis of the map.

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.

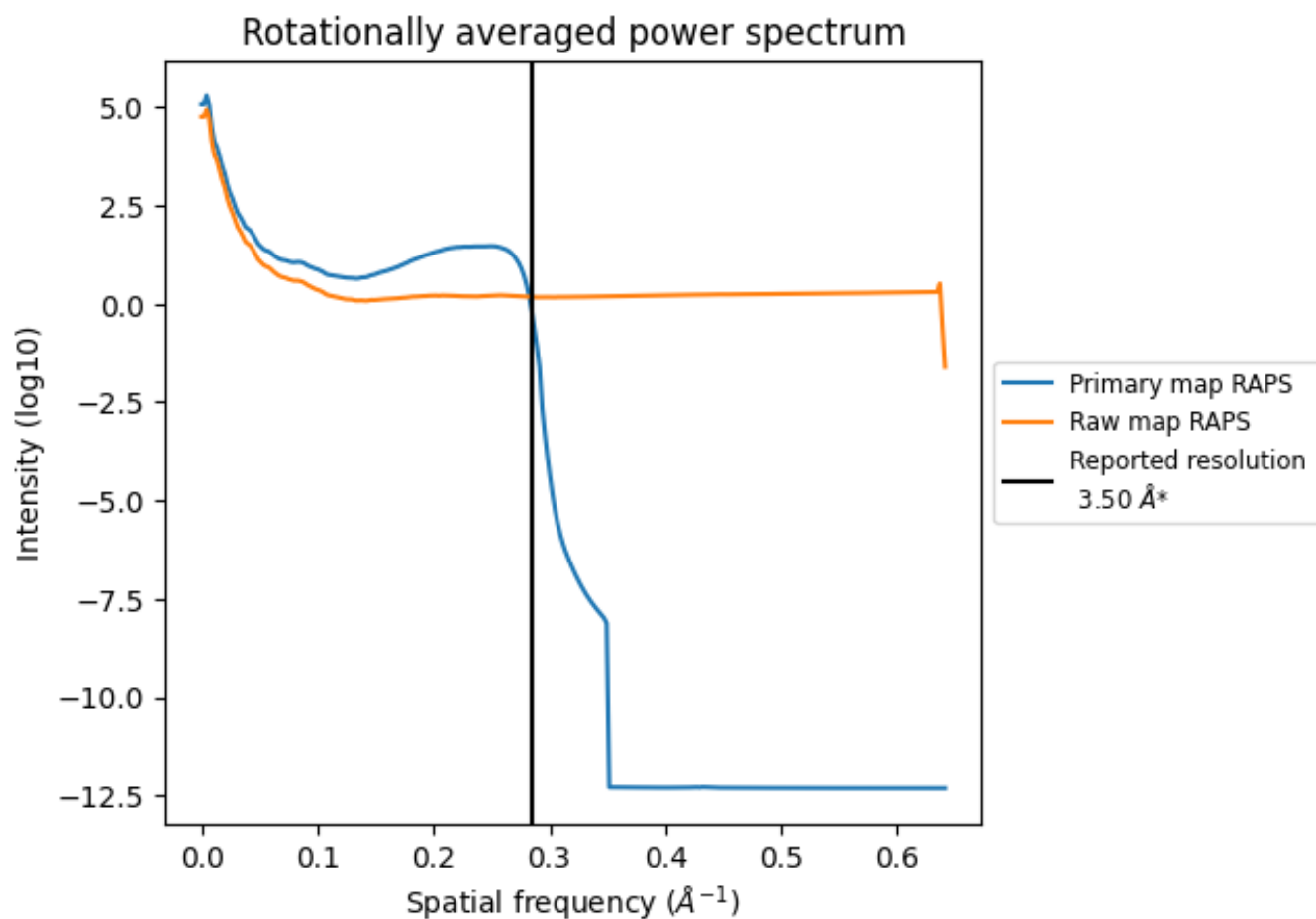
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29 nm^3 ; this corresponds to an approximate mass of 27 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

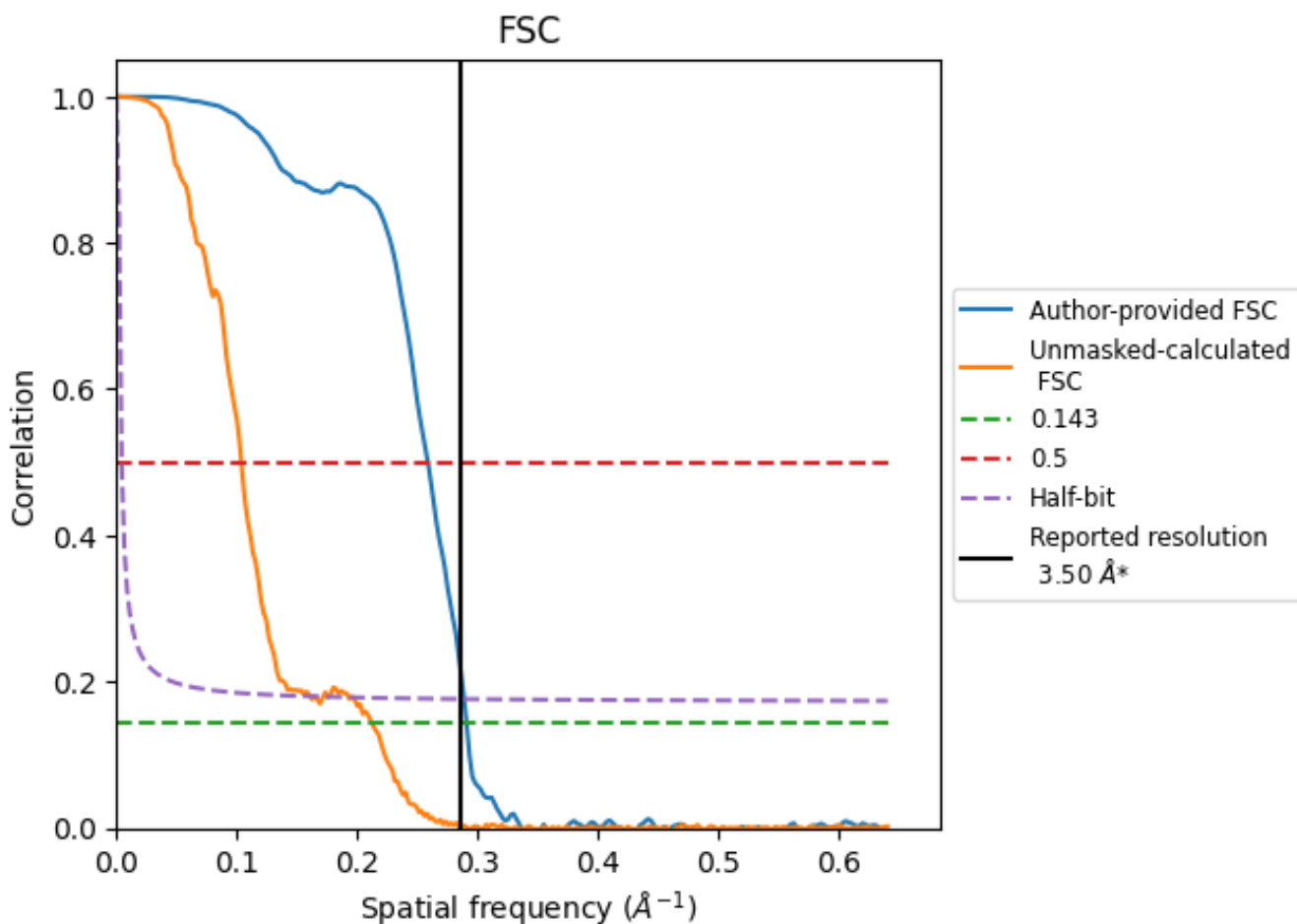


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

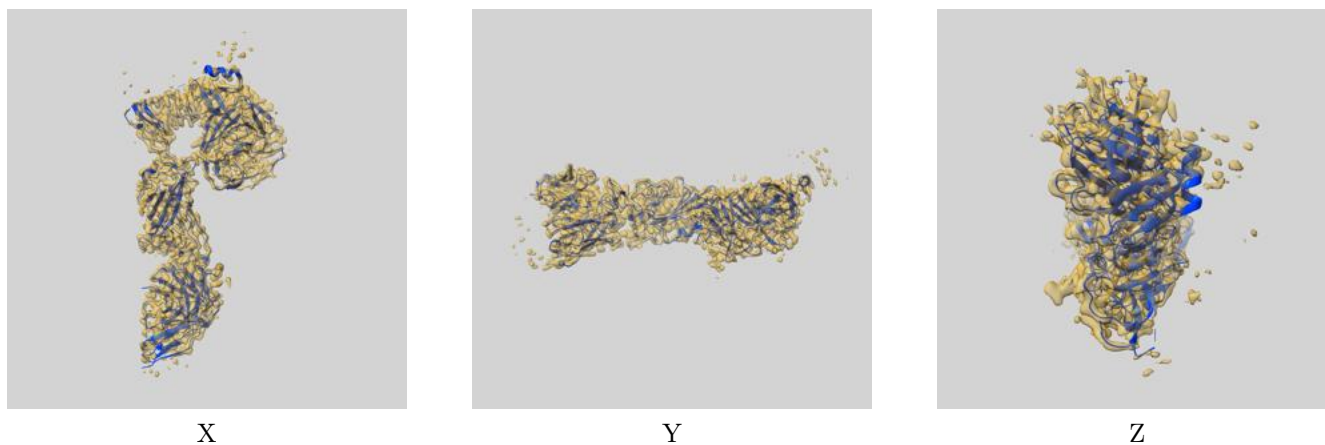
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.86	3.46
Unmasked-calculated*	4.71	9.63	6.21

*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 4.71 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

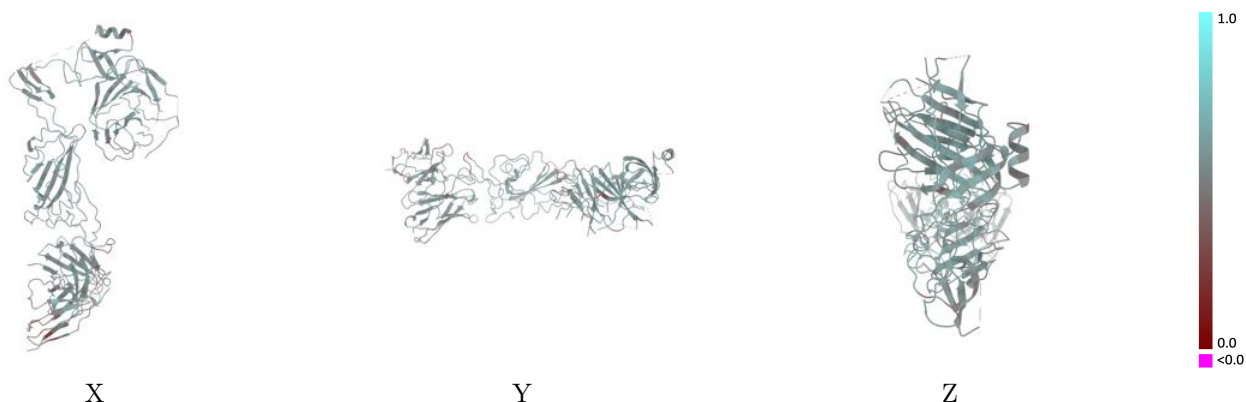
This section contains information regarding the fit between EMDB map EMD-18571 and PDB model 8QQ0. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



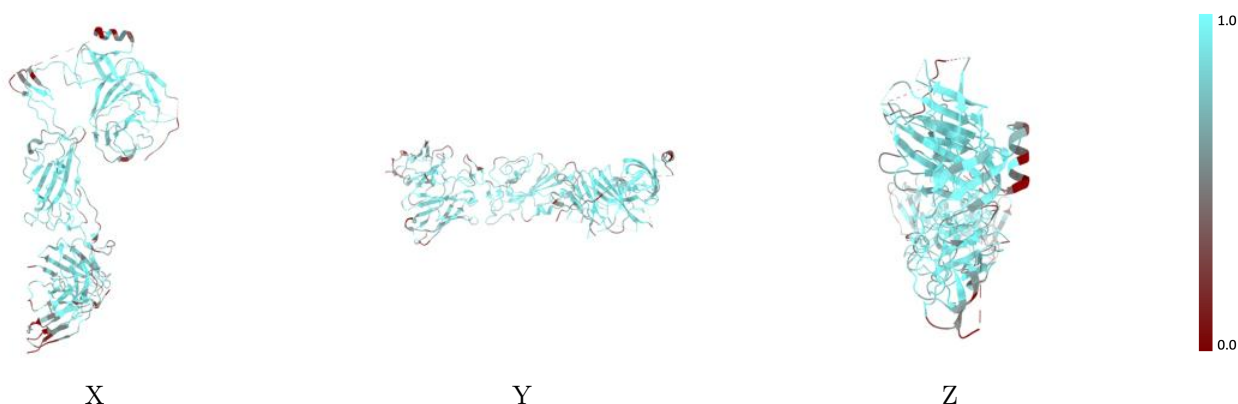
The images above show the 3D surface view of the map at the recommended contour level 13.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



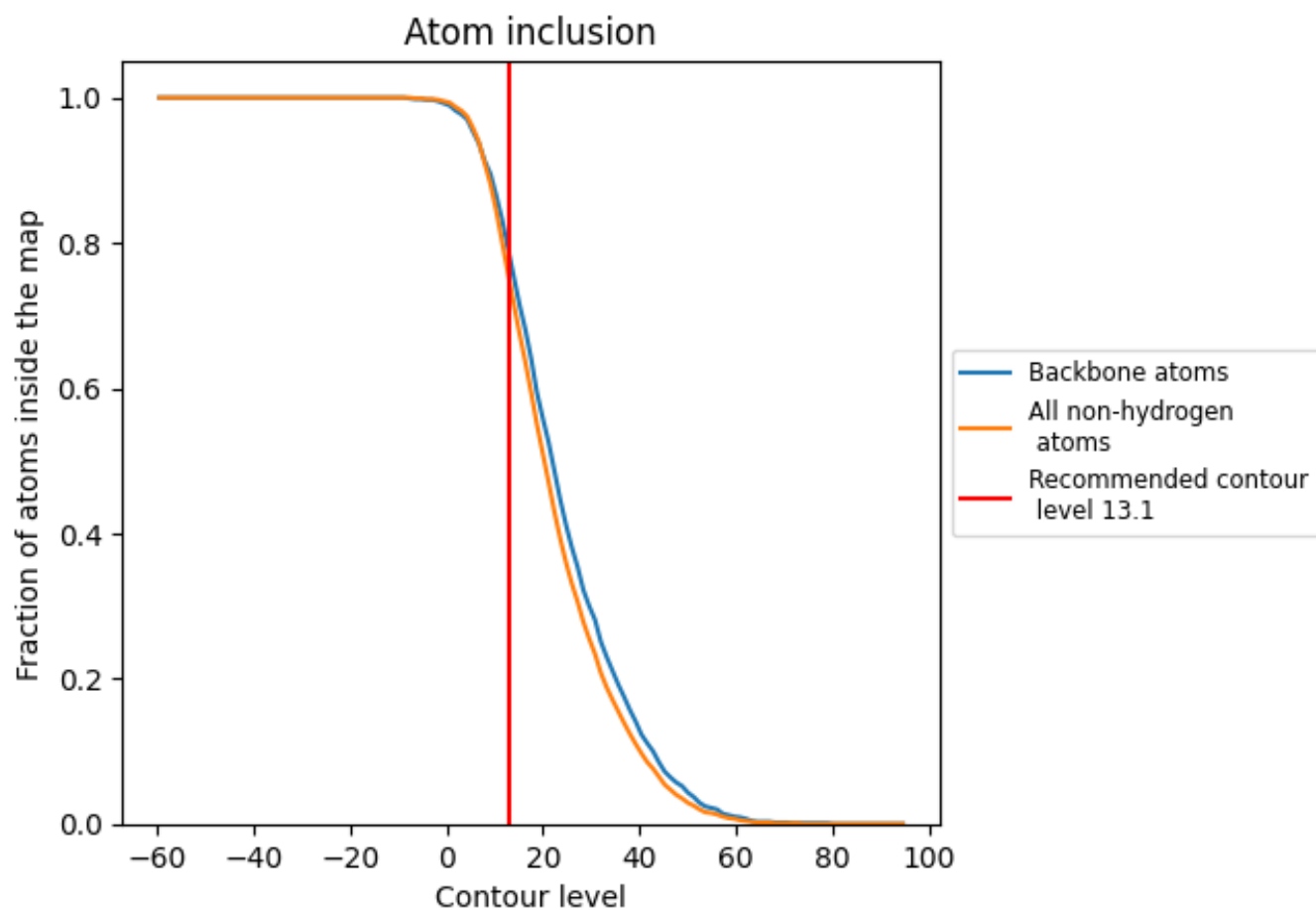
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (13.1).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (13.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.5340
A	 0.7740	 0.5460
B	 0.2140	 0.3960
D	 0.6610	 0.4990
E	 0.7690	 0.5290
F	 0.6320	 0.4750
a	 0.1790	 0.4100
c	 0.2100	 0.5200
e	 0.3680	 0.4480

