



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 04:52 AM UTC

PDB ID : 6ZB5 / pdb_00006zb5
EMDB ID : EMD-11145
Title : SARS CoV-2 Spike protein, Closed conformation, C3 symmetry
Authors : Toelzer, C.; Gupta, K.; Yadav, S.K.N.; Burucu, U.; Schaffitzel, C.; Berger, I.
Deposited on : 2020-06-07
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

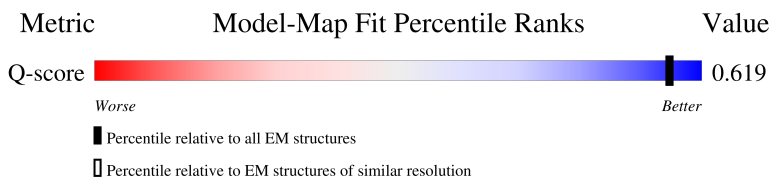
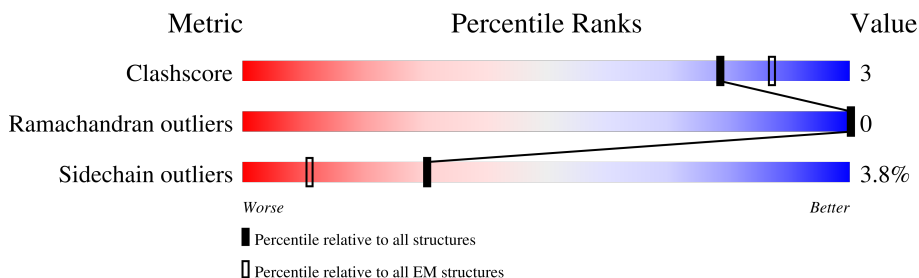
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	1259	 76% 6% 18%
1	B	1259	 75% 6% 18%
1	C	1259	 76% 6% 18%
2	D	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%

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
3	NAG	B	1307	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24499 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1032	Total	C	N	O	S	0	0
			8025	5128	1339	1520	38		
1	B	1032	Total	C	N	O	S	0	0
			8025	5128	1339	1520	38		
1	A	1032	Total	C	N	O	S	0	0
			8025	5128	1339	1520	38		

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	675J	ALA	ARG	conflict	UNP P0DTC2
C	1211	SER	-	expression tag	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	ARG	-	expression tag	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	VAL	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	ARG	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	SER	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	ILE	-	expression tag	UNP P0DTC2
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	GLU	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	ARG	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1234	ALA	-	expression tag	UNP P0DTC2
C	1235	TYR	-	expression tag	UNP P0DTC2
C	1236	VAL	-	expression tag	UNP P0DTC2
C	1237	ARG	-	expression tag	UNP P0DTC2
C	1238	LYS	-	expression tag	UNP P0DTC2
C	1239	ASP	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	TRP	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	LEU	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	THR	-	expression tag	UNP P0DTC2
C	1248	PHE	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
B	675J	ALA	ARG	conflict	UNP P0DTC2
B	1211	SER	-	expression tag	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	ARG	-	expression tag	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	VAL	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	ARG	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	SER	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	ILE	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	ARG	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLN	-	expression tag	UNP P0DTC2
B	1234	ALA	-	expression tag	UNP P0DTC2
B	1235	TYR	-	expression tag	UNP P0DTC2
B	1236	VAL	-	expression tag	UNP P0DTC2
B	1237	ARG	-	expression tag	UNP P0DTC2
B	1238	LYS	-	expression tag	UNP P0DTC2
B	1239	ASP	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	TRP	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	LEU	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	THR	-	expression tag	UNP P0DTC2
B	1248	PHE	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
A	675J	ALA	ARG	conflict	UNP P0DTC2
A	1211	SER	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	ARG	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	VAL	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	SER	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2

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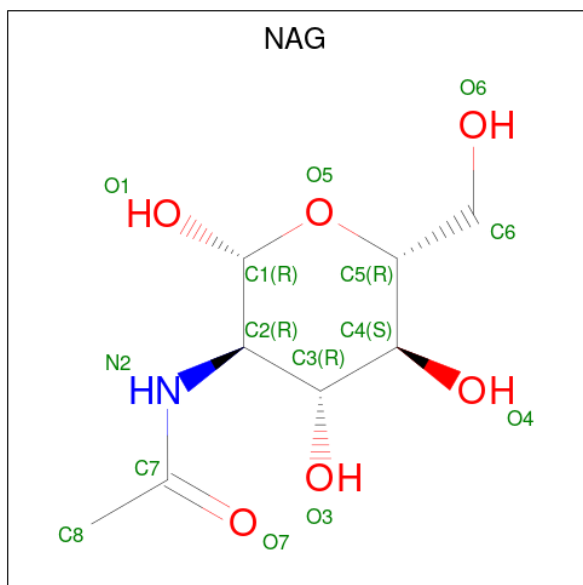
Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

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



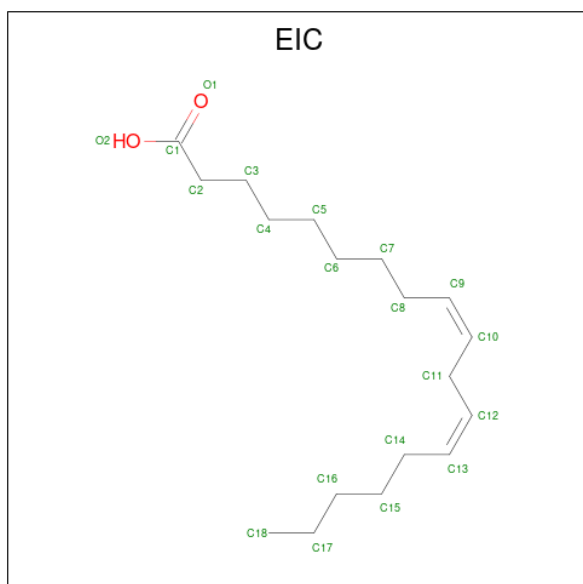
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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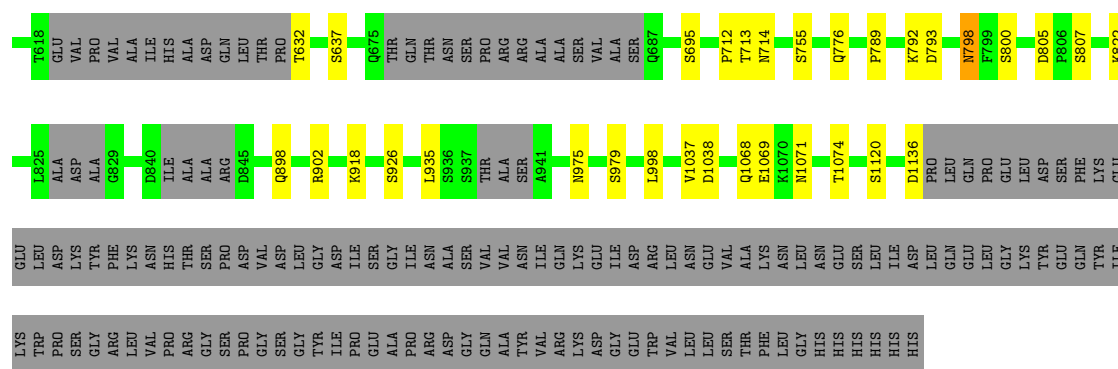
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C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

- Molecule 4 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

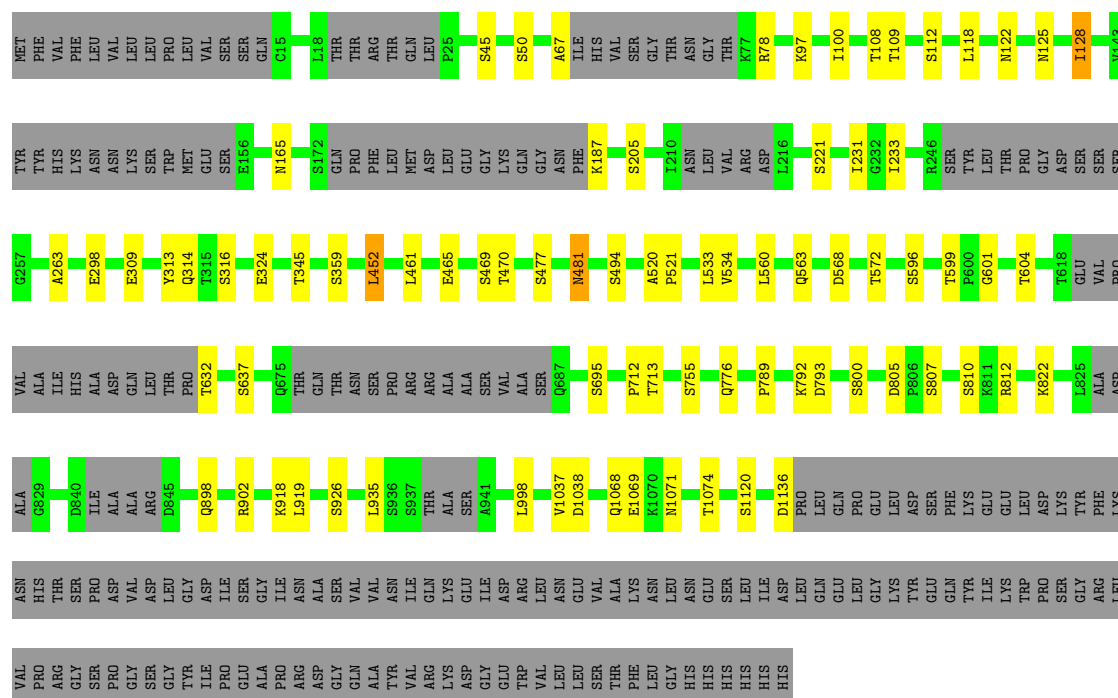


Mol	Chain	Residues	Atoms			AltConf
4	C	1	Total 20	C 18	O 2	0
4	B	1	Total 20	C 18	O 2	0
4	B	1	Total 20	C 18	O 2	0



• Molecule 1: Spike glycoprotein

Chain A: 76% 6% 18%



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

Chain D: 50% 50%



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

Chain E: 100%

MAG1
MAG2

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

Chain F:

100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	217815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.316	Depositor
Minimum map value	-0.197	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	230.99998, 230.99998, 230.99998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: NAG, EIC

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	0/8203	0.40	0/11155
1	B	0.33	0/8203	0.44	4/11155 (0.0%)
1	C	0.33	0/8203	0.40	1/11155 (0.0%)
All	All	0.33	0/24609	0.41	5/33465 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	798	ASN	CA-CB-CG	15.42	128.02	112.60
1	B	798	ASN	CB-CG-ND2	5.63	124.84	116.40
1	B	311	GLY	N-CA-C	5.03	116.81	110.38
1	C	311	GLY	N-CA-C	5.02	116.81	110.38
1	B	798	ASN	CB-CA-C	-5.02	102.61	110.79

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	8025	0	7802	36	0
1	B	8025	0	7801	47	0
1	C	8025	0	7802	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	4	0
2	E	28	0	25	9	0
2	F	28	0	25	2	0
3	A	84	0	78	11	0
3	B	112	0	104	16	0
3	C	84	0	78	6	0
4	B	40	0	62	0	0
4	C	20	0	31	0	0
All	All	24499	0	23833	134	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 3.

All (134) 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:B:165:ASN:HD21	3:B:1303:NAG:C1	1.06	1.68
1:B:165:ASN:ND2	3:B:1303:NAG:C1	1.84	1.37
1:B:714:ASN:HD21	2:E:1:NAG:C1	1.46	1.29
1:B:714:ASN:ND2	2:E:1:NAG:C1	2.06	1.17
3:A:2104:NAG:H83	3:A:2104:NAG:H3	1.30	1.08
1:C:164:ASN:HD21	3:C:1402:NAG:H61	1.19	1.08
1:C:165:ASN:ND2	3:C:1402:NAG:C1	2.19	1.06
1:A:165:ASN:HD21	3:A:2103:NAG:C1	1.70	1.03
1:C:919:LEU:HD11	2:D:1:NAG:H5	1.40	1.02
1:A:1071:ASN:ND2	3:A:2106:NAG:C1	2.23	1.01
1:C:165:ASN:HD21	3:C:1402:NAG:C1	1.75	0.98
1:A:1071:ASN:HD21	3:A:2106:NAG:C1	1.81	0.93
1:C:165:ASN:ND2	3:C:1402:NAG:O5	2.01	0.92
1:A:165:ASN:ND2	3:A:2103:NAG:C1	2.42	0.83
1:C:100:ILE:HD11	1:C:263:ALA:HB2	1.61	0.83
1:A:100:ILE:HD11	1:A:263:ALA:HB2	1.61	0.83
1:B:568:ASP:OD2	1:B:572:THR:OG1	1.99	0.81
1:B:100:ILE:HD11	1:B:263:ALA:HB2	1.61	0.81
1:A:568:ASP:OD2	1:A:572:THR:OG1	1.99	0.80
1:C:568:ASP:OD2	1:C:572:THR:OG1	1.99	0.80
1:B:1071:ASN:ND2	3:B:1305:NAG:C1	2.47	0.78
1:B:234:ASN:CG	3:B:1307:NAG:C1	2.60	0.75
1:C:919:LEU:CD1	2:D:1:NAG:H5	2.18	0.73
1:B:789:PRO:O	1:B:792:LYS:NZ	2.23	0.71
1:C:789:PRO:O	1:C:792:LYS:NZ	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASN:ND2	3:C:1402:NAG:H61	2.01	0.71
2:E:1:NAG:H62	2:E:2:NAG:HN2	1.56	0.70
1:C:599:THR:HG22	1:C:601:GLY:H	1.57	0.70
1:A:599:THR:HG22	1:A:601:GLY:H	1.57	0.69
1:B:599:THR:HG22	1:B:601:GLY:H	1.57	0.69
1:A:789:PRO:O	1:A:792:LYS:NZ	2.24	0.69
1:A:100:ILE:CD1	1:A:263:ALA:HB2	2.23	0.69
1:B:100:ILE:CD1	1:B:263:ALA:HB2	2.23	0.69
1:C:100:ILE:CD1	1:C:263:ALA:HB2	2.23	0.68
2:E:2:NAG:H61	2:E:2:NAG:H2	1.74	0.68
1:A:67:ALA:CB	1:A:263:ALA:HB3	2.27	0.65
1:C:714:ASN:HD21	2:D:1:NAG:C1	2.10	0.65
1:C:67:ALA:CB	1:C:263:ALA:HB3	2.27	0.64
1:B:67:ALA:CB	1:B:263:ALA:HB3	2.27	0.64
1:B:1071:ASN:HD22	3:B:1305:NAG:C1	2.13	0.61
1:B:234:ASN:ND2	3:B:1307:NAG:C1	2.64	0.60
1:A:1071:ASN:HD22	3:A:2106:NAG:C1	2.10	0.60
1:B:714:ASN:ND2	2:E:1:NAG:O5	2.25	0.59
1:A:324:GLU:OE2	1:A:534:VAL:HG21	2.03	0.58
1:A:822:LYS:NZ	1:A:935:LEU:O	2.36	0.58
1:B:324:GLU:OE2	1:B:534:VAL:HG21	2.03	0.58
1:C:324:GLU:OE2	1:C:534:VAL:HG21	2.03	0.58
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.86	0.57
1:C:822:LYS:NZ	1:C:935:LEU:O	2.36	0.57
1:C:461:LEU:HD22	1:C:465:GLU:HB3	1.87	0.56
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.86	0.56
1:B:108:THR:HG23	3:B:1307:NAG:H61	1.86	0.56
3:A:2104:NAG:O6	3:A:2104:NAG:O4	2.21	0.56
2:F:1:NAG:H61	2:F:2:NAG:H82	1.88	0.56
1:A:461:LEU:HD22	1:A:465:GLU:HB3	1.87	0.56
3:A:2104:NAG:H3	3:A:2104:NAG:C8	2.09	0.56
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.86	0.56
1:B:461:LEU:HD22	1:B:465:GLU:HB3	1.87	0.55
1:B:822:LYS:NZ	1:B:935:LEU:O	2.36	0.55
1:C:805:ASP:O	1:C:805:ASP:OD2	2.27	0.54
1:B:805:ASP:O	1:B:805:ASP:OD2	2.26	0.53
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.90	0.53
1:A:805:ASP:OD2	1:A:805:ASP:O	2.26	0.53
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.90	0.53
1:B:108:THR:CG2	3:B:1307:NAG:H61	2.39	0.53
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:NAG:H2	2:E:2:NAG:C6	2.40	0.52
1:C:309:GLU:O	1:C:313:TYR:OH	2.28	0.52
1:C:560:LEU:N	1:C:563:GLN:OE1	2.42	0.52
1:A:309:GLU:O	1:A:313:TYR:OH	2.28	0.52
1:A:231:ILE:HD12	1:A:233:ILE:HG12	1.92	0.52
3:B:1301:NAG:H83	3:B:1301:NAG:O3	2.09	0.52
1:C:714:ASN:ND2	2:D:1:NAG:C1	2.73	0.51
1:B:108:THR:HG21	3:B:1307:NAG:H62	1.92	0.51
1:B:560:LEU:N	1:B:563:GLN:OE1	2.42	0.51
1:C:231:ILE:HD12	1:C:233:ILE:HG12	1.92	0.51
1:C:805:ASP:O	1:C:807:SER:N	2.44	0.50
1:B:1071:ASN:HD21	3:B:1305:NAG:C1	2.20	0.50
1:A:919:LEU:HD11	2:F:1:NAG:H5	1.93	0.50
1:B:314:GLN:OE1	1:B:596:SER:OG	2.27	0.50
1:A:122:ASN:OD1	1:A:125:ASN:N	2.44	0.50
1:B:231:ILE:HD12	1:B:233:ILE:HG12	1.92	0.50
1:B:1071:ASN:ND2	3:B:1305:NAG:N2	2.60	0.50
1:A:805:ASP:O	1:A:807:SER:N	2.44	0.50
1:B:714:ASN:CG	2:E:1:NAG:C1	2.83	0.49
3:B:1304:NAG:O6	3:B:1304:NAG:O4	2.18	0.48
1:A:108:THR:HG22	1:A:109:THR:HG23	1.95	0.48
1:B:805:ASP:O	1:B:807:SER:N	2.44	0.48
1:A:314:GLN:OE1	1:A:596:SER:OG	2.27	0.48
1:B:309:GLU:O	1:B:313:TYR:OH	2.28	0.48
1:A:67:ALA:C	1:A:78:ARG:HE	2.21	0.48
3:A:2105:NAG:C3	3:A:2105:NAG:H82	2.42	0.48
1:C:122:ASN:OD1	1:C:125:ASN:N	2.44	0.48
1:B:234:ASN:OD1	3:B:1307:NAG:O5	2.32	0.48
1:B:67:ALA:C	1:B:78:ARG:HE	2.21	0.47
1:C:67:ALA:C	1:C:78:ARG:HE	2.21	0.47
1:C:108:THR:HG22	1:C:109:THR:HG23	1.95	0.47
1:B:108:THR:HG22	1:B:109:THR:HG23	1.95	0.47
1:B:108:THR:HG21	3:B:1307:NAG:C6	2.44	0.47
1:B:793:ASP:O	1:B:793:ASP:OD1	2.33	0.47
1:B:898:GLN:OE1	1:B:902:ARG:NH2	2.46	0.47
1:B:122:ASN:OD1	1:B:125:ASN:N	2.44	0.46
1:C:118:LEU:O	1:C:128:ILE:O	2.34	0.46
1:C:793:ASP:O	1:C:793:ASP:OD1	2.33	0.46
2:E:2:NAG:C6	2:E:2:NAG:C2	2.93	0.46
1:A:560:LEU:N	1:A:563:GLN:OE1	2.42	0.46
1:C:898:GLN:OE1	1:C:902:ARG:NH2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ASP:OD1	1:A:793:ASP:O	2.33	0.45
1:B:118:LEU:O	1:B:128:ILE:O	2.34	0.45
1:A:118:LEU:O	1:A:128:ILE:O	2.34	0.45
1:B:108:THR:CG2	3:B:1307:NAG:C6	2.94	0.45
1:C:314:GLN:OE1	1:C:596:SER:OG	2.27	0.45
1:B:975:ASN:O	1:B:979:SER:OG	2.18	0.44
1:A:898:GLN:OE1	1:A:902:ARG:NH2	2.46	0.44
1:A:1071:ASN:ND2	3:A:2106:NAG:N2	2.66	0.43
1:C:67:ALA:HB2	1:C:263:ALA:HB3	2.00	0.43
1:A:452:LEU:HD23	1:A:494:SER:OG	2.19	0.43
1:C:452:LEU:HD23	1:C:494:SER:OG	2.18	0.43
3:A:2105:NAG:H82	3:A:2105:NAG:H3	2.01	0.43
1:B:452:LEU:HD23	1:B:494:SER:OG	2.18	0.43
1:B:481:ASN:OD1	1:B:481:ASN:N	2.53	0.42
1:A:481:ASN:OD1	1:A:481:ASN:N	2.53	0.42
1:C:481:ASN:OD1	1:C:481:ASN:N	2.53	0.42
1:B:1037:VAL:HG12	1:B:1038:ASP:OD2	2.20	0.42
1:C:1037:VAL:HG12	1:C:1038:ASP:OD2	2.20	0.42
1:C:164:ASN:HD21	3:C:1402:NAG:C6	2.09	0.42
2:E:2:NAG:O7	2:E:2:NAG:O3	2.31	0.42
1:A:67:ALA:HB2	1:A:263:ALA:HB3	2.00	0.41
1:B:712:PRO:HA	1:B:1068:GLN:O	2.21	0.41
1:A:712:PRO:HA	1:A:1068:GLN:O	2.21	0.41
1:A:1037:VAL:HG12	1:A:1038:ASP:OD2	2.20	0.41
1:C:712:PRO:HA	1:C:1068:GLN:O	2.21	0.40
1:B:67:ALA:C	1:B:78:ARG:HB2	2.47	0.40
1:A:810:SER:O	1:A:812:ARG:N	2.52	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	1008/1259 (80%)	932 (92%)	76 (8%)	0	100	100
1	B	1008/1259 (80%)	931 (92%)	77 (8%)	0	100	100
1	C	1008/1259 (80%)	932 (92%)	76 (8%)	0	100	100
All	All	3024/3777 (80%)	2795 (92%)	229 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	887/1095 (81%)	854 (96%)	33 (4%)	30	55
1	B	887/1095 (81%)	853 (96%)	34 (4%)	29	54
1	C	887/1095 (81%)	854 (96%)	33 (4%)	30	55
All	All	2661/3285 (81%)	2561 (96%)	100 (4%)	30	54

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	45	SER
1	C	50	SER
1	C	97	LYS
1	C	112	SER
1	C	128	ILE
1	C	187	LYS
1	C	205	SER
1	C	221	SER
1	C	298	GLU
1	C	316	SER
1	C	345	THR
1	C	359	SER
1	C	452	LEU
1	C	469	SER
1	C	470	THR

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Mol	Chain	Res	Type
1	C	477	SER
1	C	481	ASN
1	C	533	LEU
1	C	604	THR
1	C	632	THR
1	C	637	SER
1	C	695	SER
1	C	713	THR
1	C	755	SER
1	C	776	GLN
1	C	800	SER
1	C	918	LYS
1	C	926	SER
1	C	998	LEU
1	C	1069	GLU
1	C	1074	THR
1	C	1120	SER
1	C	1136	ASP
1	B	45	SER
1	B	50	SER
1	B	97	LYS
1	B	112	SER
1	B	128	ILE
1	B	187	LYS
1	B	205	SER
1	B	221	SER
1	B	240	THR
1	B	298	GLU
1	B	316	SER
1	B	345	THR
1	B	359	SER
1	B	469	SER
1	B	470	THR
1	B	477	SER
1	B	481	ASN
1	B	533	LEU
1	B	604	THR
1	B	632	THR
1	B	637	SER
1	B	695	SER
1	B	713	THR
1	B	755	SER

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Mol	Chain	Res	Type
1	B	776	GLN
1	B	798	ASN
1	B	800	SER
1	B	918	LYS
1	B	926	SER
1	B	998	LEU
1	B	1069	GLU
1	B	1074	THR
1	B	1120	SER
1	B	1136	ASP
1	A	45	SER
1	A	50	SER
1	A	97	LYS
1	A	112	SER
1	A	128	ILE
1	A	187	LYS
1	A	205	SER
1	A	221	SER
1	A	298	GLU
1	A	316	SER
1	A	345	THR
1	A	359	SER
1	A	452	LEU
1	A	469	SER
1	A	470	THR
1	A	477	SER
1	A	481	ASN
1	A	533	LEU
1	A	604	THR
1	A	632	THR
1	A	637	SER
1	A	695	SER
1	A	713	THR
1	A	755	SER
1	A	776	GLN
1	A	800	SER
1	A	918	LYS
1	A	926	SER
1	A	998	LEU
1	A	1069	GLU
1	A	1074	THR
1	A	1120	SER

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Mol	Chain	Res	Type
1	A	1136	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	ASN
1	C	137	ASN
1	C	164	ASN
1	C	165	ASN
1	C	331	ASN
1	C	448	ASN
1	C	474	GLN
1	C	687	GLN
1	C	714	ASN
1	C	850	GLN
1	C	916	ASN
1	C	1007	GLN
1	C	1045	HIS
1	B	30	ASN
1	B	137	ASN
1	B	165	ASN
1	B	331	ASN
1	B	474	GLN
1	B	687	GLN
1	B	714	ASN
1	B	916	ASN
1	B	1007	GLN
1	B	1045	HIS
1	B	1071	ASN
1	A	30	ASN
1	A	137	ASN
1	A	165	ASN
1	A	331	ASN
1	A	474	GLN
1	A	687	GLN
1	A	850	GLN
1	A	916	ASN
1	A	1007	GLN
1	A	1045	HIS
1	A	1071	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	D	1	2	14,14,15	0.41	0	17,19,21	2.06	6 (35%)
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	E	1	2	14,14,15	0.33	0	17,19,21	0.87	1 (5%)
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.95	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.39	0	17,19,21	0.82	0
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.58	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	D	1	2	-	6/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C4-C3-C2	-4.53	104.38	111.02
2	D	1	NAG	O5-C5-C6	3.57	114.61	107.66
2	D	1	NAG	C2-N2-C7	-2.95	118.94	122.90
2	D	1	NAG	C3-C4-C5	2.71	115.14	110.23
2	D	1	NAG	O4-C4-C5	-2.54	103.07	109.32
2	D	1	NAG	C6-C5-C4	-2.51	106.86	113.02
2	E	1	NAG	O5-C1-C2	-2.32	107.70	111.29
2	E	2	NAG	C1-O5-C5	2.19	115.12	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 15 short contacts:

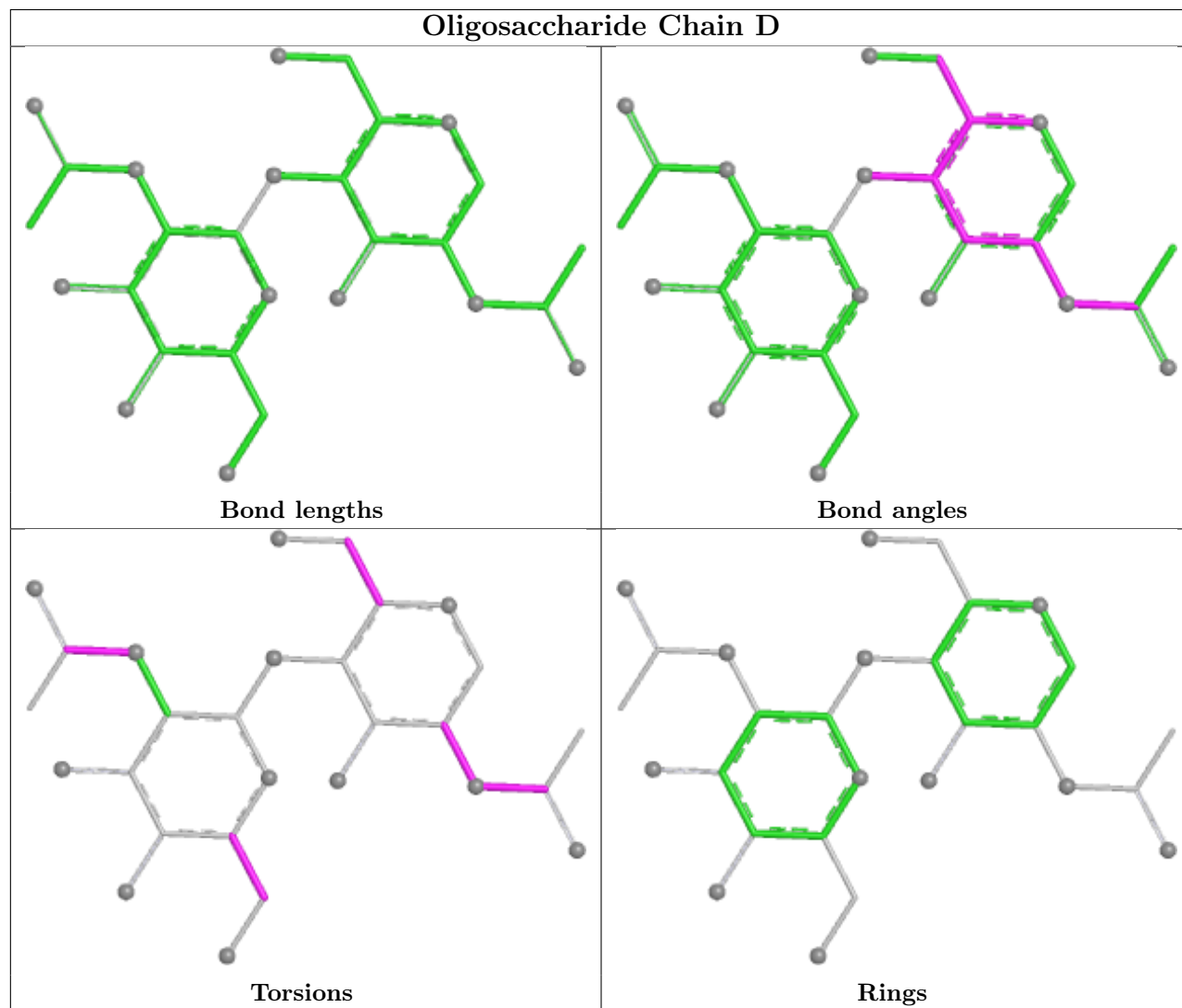
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	2	0
2	D	1	NAG	4	0
2	E	2	NAG	5	0
2	F	2	NAG	1	0

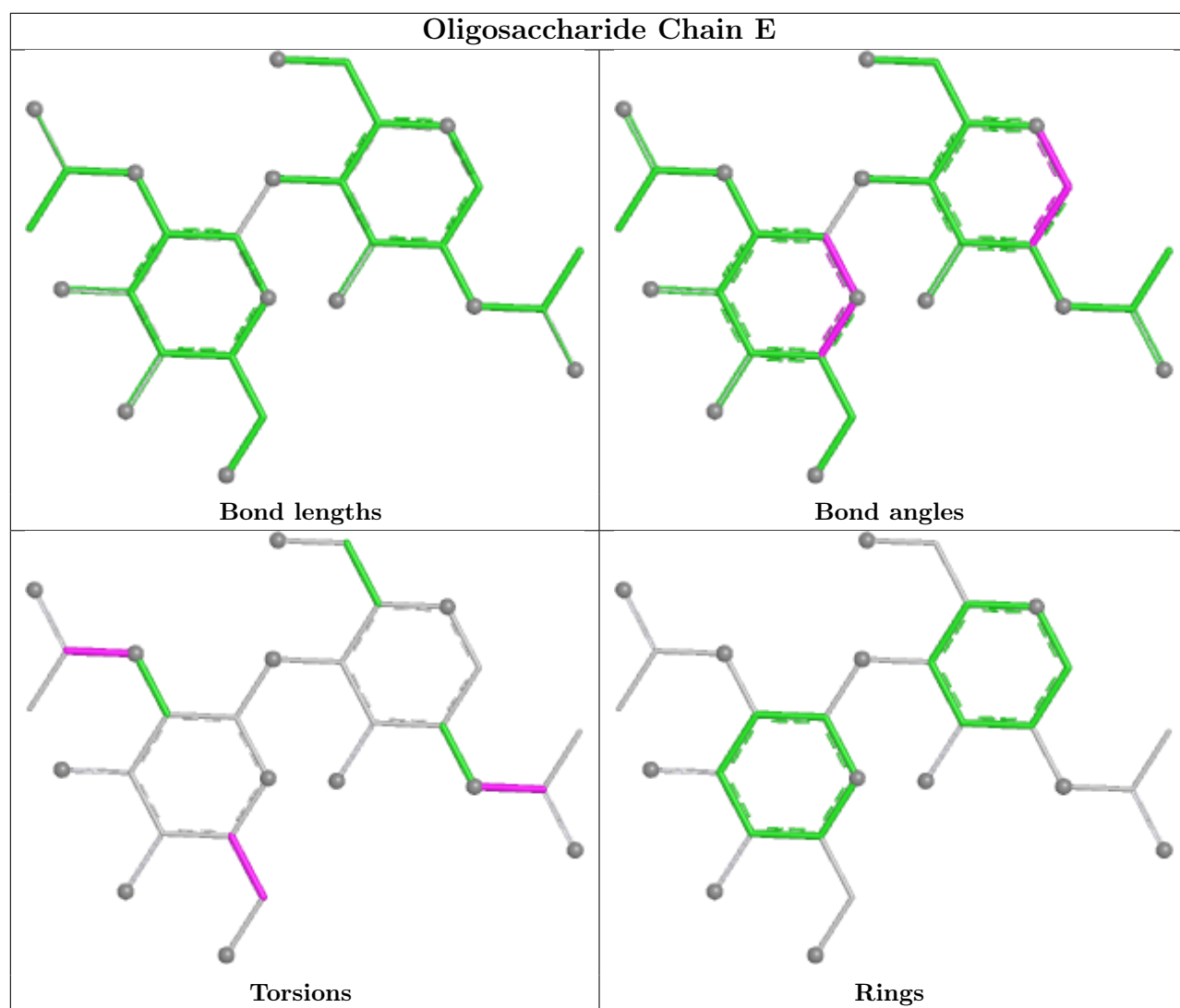
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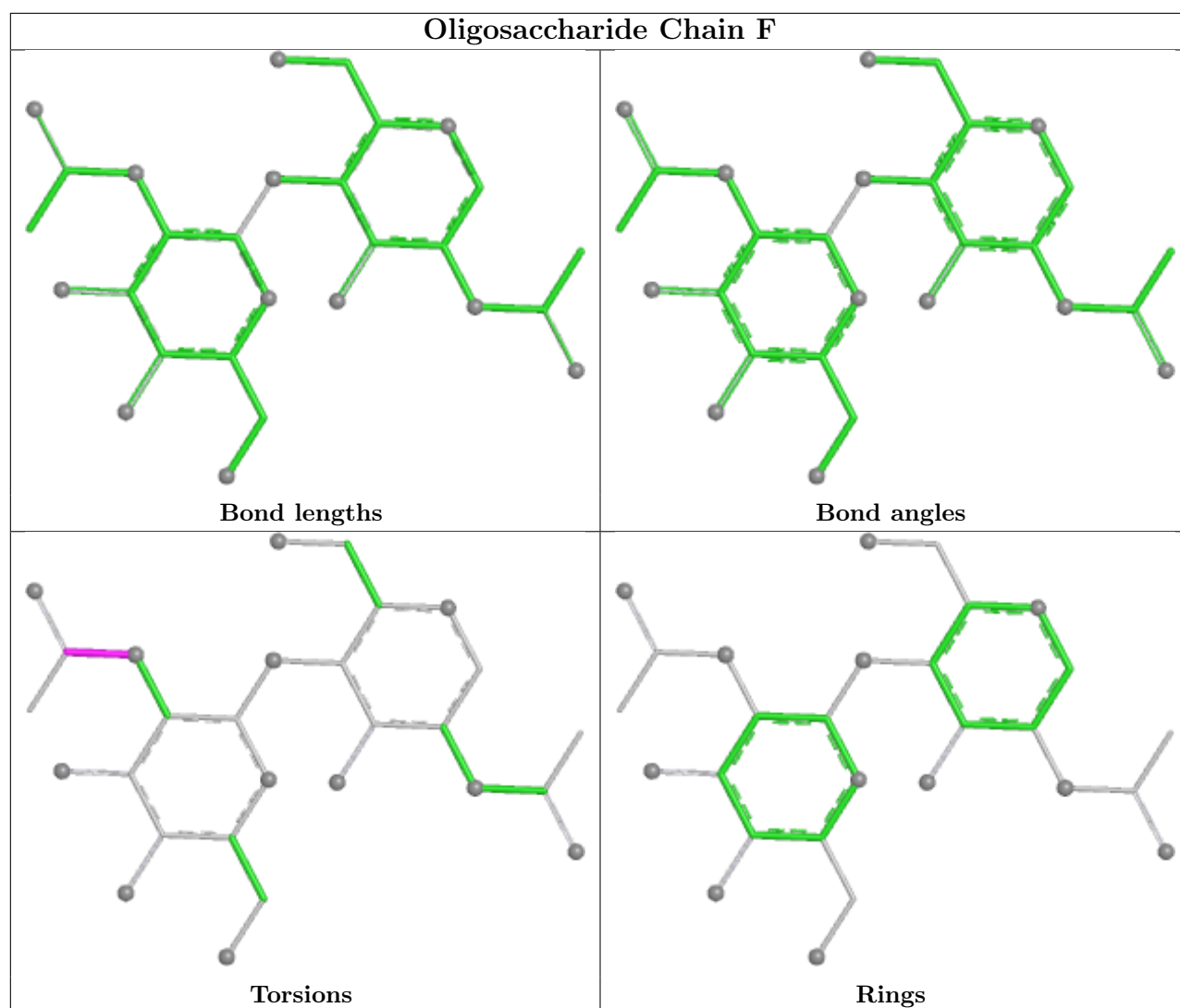
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	5	0

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](#)

23 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	C	1404	1	14,14,15	0.38	0	17,19,21	0.88	0
3	NAG	C	1406	-	14,14,15	1.87	5 (35%)	17,19,21	1.14	1 (5%)
4	EIC	B	1309	-	19,19,19	0.57	0	19,19,19	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1303	-	14,14,15	0.38	0	17,19,21	0.75	0
3	NAG	B	1307	-	14,14,15	0.37	0	17,19,21	0.78	0
4	EIC	B	1310	-	19,19,19	0.53	0	19,19,19	0.95	1 (5%)
3	NAG	B	1301	1	14,14,15	0.40	0	17,19,21	1.07	1 (5%)
3	NAG	B	1305	-	14,14,15	0.30	0	17,19,21	0.66	0
3	NAG	A	2103	-	14,14,15	0.42	0	17,19,21	1.82	5 (29%)
3	NAG	C	1405	1	14,14,15	0.40	0	17,19,21	1.27	2 (11%)
3	NAG	B	1304	1	14,14,15	0.40	0	17,19,21	0.92	0
3	NAG	A	2101	-	14,14,15	1.85	4 (28%)	17,19,21	1.12	1 (5%)
3	NAG	A	2106	-	14,14,15	0.36	0	17,19,21	0.67	0
3	NAG	C	1403	1	14,14,15	0.38	0	17,19,21	0.83	0
3	NAG	B	1302	1	14,14,15	0.40	0	17,19,21	1.05	2 (11%)
3	NAG	A	2105	1	14,14,15	0.36	0	17,19,21	1.14	2 (11%)
3	NAG	A	2104	1	14,14,15	0.39	0	17,19,21	0.79	0
3	NAG	C	1402	-	14,14,15	0.37	0	17,19,21	0.72	0
3	NAG	A	2102	1	14,14,15	0.28	0	17,19,21	0.82	0
4	EIC	C	1407	-	19,19,19	0.56	0	19,19,19	0.94	0
3	NAG	C	1401	1	14,14,15	0.41	0	17,19,21	1.26	2 (11%)
3	NAG	B	1306	1	14,14,15	0.35	0	17,19,21	0.87	1 (5%)
3	NAG	B	1308	1	14,14,15	0.32	0	17,19,21	1.94	3 (17%)

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	C	1404	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1406	-	-	2/6/23/26	0/1/1/1
4	EIC	B	1309	-	-	7/17/17/17	-
3	NAG	B	1303	-	-	4/6/23/26	0/1/1/1
3	NAG	B	1307	-	-	1/6/23/26	0/1/1/1
4	EIC	B	1310	-	-	10/17/17/17	-
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
3	NAG	A	2103	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2101	-	-	1/6/23/26	0/1/1/1
3	NAG	A	2106	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2105	1	-	5/6/23/26	0/1/1/1
3	NAG	A	2104	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1402	-	-	4/6/23/26	0/1/1/1
3	NAG	A	2102	1	-	2/6/23/26	0/1/1/1
4	EIC	C	1407	-	-	6/17/17/17	-
3	NAG	C	1401	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1406	NAG	C7-N2	3.90	1.46	1.34
3	C	1406	NAG	O5-C1	3.88	1.50	1.43
3	A	2101	NAG	C7-N2	3.85	1.46	1.34
3	A	2101	NAG	O5-C1	3.83	1.50	1.43
3	C	1406	NAG	C2-N2	2.30	1.50	1.46
3	A	2101	NAG	C2-N2	2.25	1.50	1.46
3	C	1406	NAG	C3-C2	-2.11	1.48	1.52
3	A	2101	NAG	C3-C2	-2.06	1.48	1.52
3	C	1406	NAG	O7-C7	-2.01	1.18	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1308	NAG	C1-O5-C5	6.48	120.87	112.19
3	A	2103	NAG	C2-N2-C7	-4.24	117.21	122.90
3	C	1401	NAG	O5-C1-C2	-3.71	105.55	111.29
3	A	2103	NAG	C1-C2-N2	3.28	115.60	110.43
3	A	2103	NAG	O5-C1-C2	-3.16	106.40	111.29
3	A	2103	NAG	C4-C3-C2	-2.90	106.76	111.02
3	B	1308	NAG	O5-C1-C2	2.79	115.61	111.29
3	B	1301	NAG	C1-O5-C5	2.72	115.83	112.19
3	B	1302	NAG	C1-O5-C5	2.70	115.81	112.19
3	A	2105	NAG	O5-C1-C2	-2.66	107.18	111.29
3	B	1308	NAG	C4-C3-C2	-2.64	107.14	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1306	NAG	C1-O5-C5	-2.60	108.70	112.19
3	C	1405	NAG	C1-O5-C5	2.60	115.67	112.19
3	C	1401	NAG	C2-N2-C7	-2.50	119.55	122.90
3	C	1405	NAG	C2-N2-C7	-2.46	119.61	122.90
3	A	2105	NAG	C2-N2-C7	-2.42	119.66	122.90
3	B	1302	NAG	O5-C5-C6	2.32	112.19	107.66
3	A	2103	NAG	O5-C5-C6	2.27	112.08	107.66
3	A	2101	NAG	C1-C2-N2	-2.23	106.93	110.43
4	B	1310	EIC	C3-C2-C1	-2.14	108.91	114.51
3	C	1406	NAG	C2-N2-C7	-2.06	120.15	122.90

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1401	NAG	C8-C7-N2-C2
3	C	1401	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1308	NAG	C8-C7-N2-C2
3	B	1308	NAG	O7-C7-N2-C2
3	A	2102	NAG	C8-C7-N2-C2
3	A	2102	NAG	O7-C7-N2-C2
3	A	2104	NAG	C3-C2-N2-C7
3	A	2104	NAG	C8-C7-N2-C2
3	A	2104	NAG	O7-C7-N2-C2
3	C	1403	NAG	C8-C7-N2-C2
3	C	1403	NAG	O7-C7-N2-C2
3	C	1403	NAG	O5-C5-C6-O6
3	B	1304	NAG	C8-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	C	1406	NAG	O5-C5-C6-O6
3	A	2104	NAG	O5-C5-C6-O6
3	A	2105	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1403	NAG	C4-C5-C6-O6
3	C	1402	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	A	2103	NAG	O5-C5-C6-O6
3	C	1406	NAG	C4-C5-C6-O6
3	A	2105	NAG	C8-C7-N2-C2
3	A	2103	NAG	C4-C5-C6-O6
3	A	2105	NAG	C4-C5-C6-O6
3	C	1402	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	A	2105	NAG	O7-C7-N2-C2
3	C	1401	NAG	C4-C5-C6-O6
3	C	1404	NAG	O5-C5-C6-O6
4	B	1310	EIC	C1-C2-C3-C4
3	A	2104	NAG	C4-C5-C6-O6
3	C	1405	NAG	C4-C5-C6-O6
3	C	1401	NAG	O5-C5-C6-O6
3	C	1404	NAG	C4-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	A	2106	NAG	O5-C5-C6-O6
4	B	1309	EIC	C2-C3-C4-C5
3	B	1302	NAG	C4-C5-C6-O6
4	B	1310	EIC	C2-C3-C4-C5
3	B	1304	NAG	C4-C5-C6-O6
4	B	1310	EIC	C14-C15-C16-C17
3	C	1405	NAG	O5-C5-C6-O6
4	B	1309	EIC	C3-C4-C5-C6
4	C	1407	EIC	C3-C4-C5-C6
3	C	1402	NAG	C8-C7-N2-C2
4	B	1310	EIC	C6-C7-C8-C9
4	B	1310	EIC	C4-C5-C6-C7
3	A	2106	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1402	NAG	O7-C7-N2-C2
3	B	1305	NAG	O5-C5-C6-O6
4	B	1310	EIC	C3-C4-C5-C6
3	A	2101	NAG	C4-C5-C6-O6
4	B	1309	EIC	C7-C8-C9-C10
4	B	1310	EIC	C12-C13-C14-C15
4	B	1309	EIC	O1-C1-C2-C3
4	B	1309	EIC	O2-C1-C2-C3
4	C	1407	EIC	C9-C10-C11-C12

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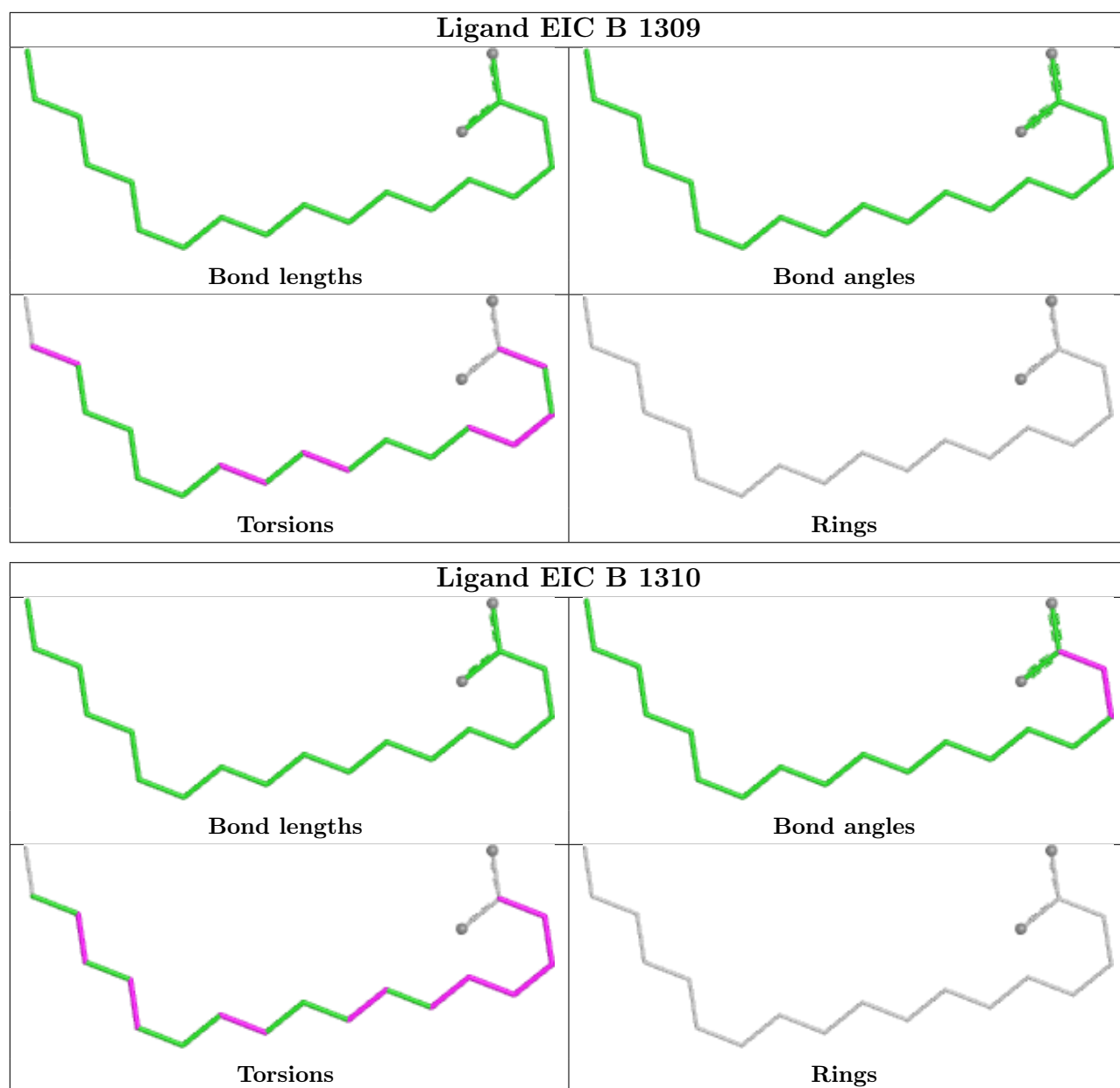
Mol	Chain	Res	Type	Atoms
4	B	1309	EIC	C9-C10-C11-C12
4	B	1310	EIC	C9-C10-C11-C12
4	B	1310	EIC	O2-C1-C2-C3
3	A	2105	NAG	C3-C2-N2-C7
4	C	1407	EIC	O2-C1-C2-C3
4	B	1310	EIC	O1-C1-C2-C3
4	C	1407	EIC	O1-C1-C2-C3
4	C	1407	EIC	C2-C3-C4-C5
4	C	1407	EIC	C6-C7-C8-C9
4	B	1309	EIC	C15-C16-C17-C18

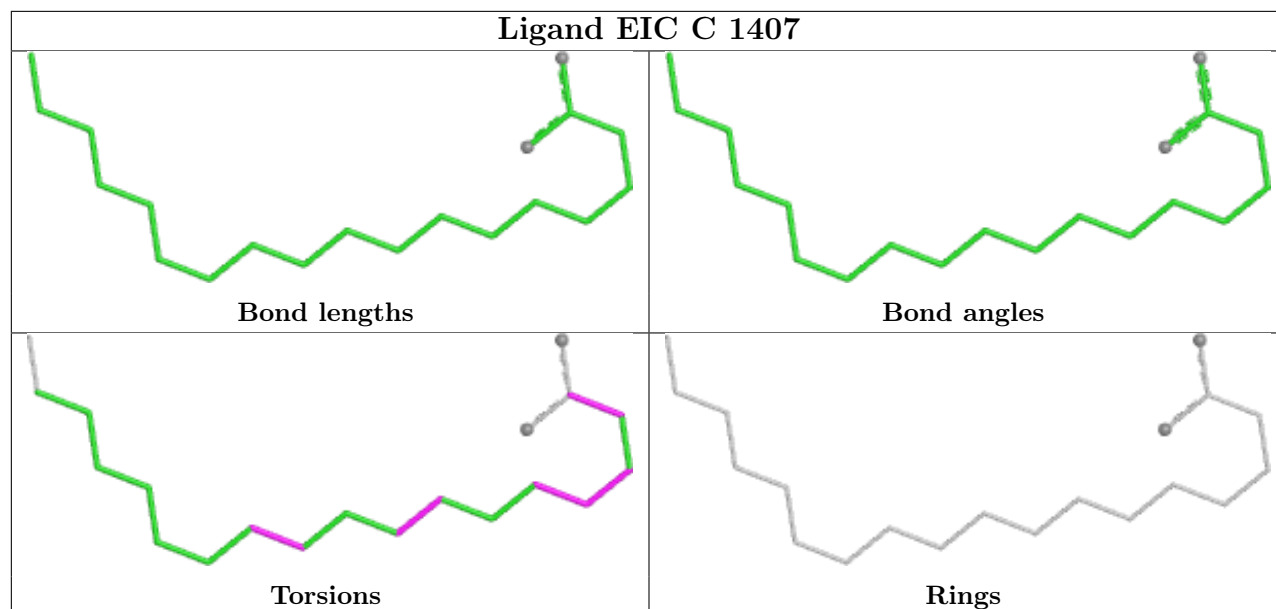
There are no ring outliers.

10 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1303	NAG	2	0
3	B	1307	NAG	8	0
3	B	1301	NAG	1	0
3	B	1305	NAG	4	0
3	A	2103	NAG	2	0
3	B	1304	NAG	1	0
3	A	2106	NAG	4	0
3	A	2105	NAG	2	0
3	A	2104	NAG	3	0
3	C	1402	NAG	6	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.

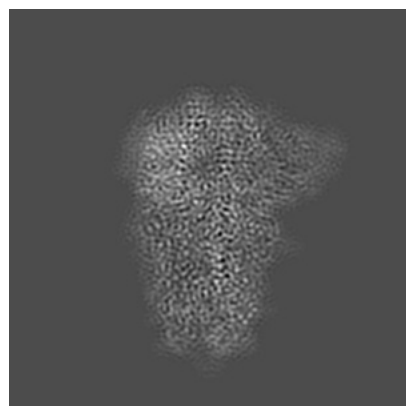
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11145. These allow visual inspection of the internal detail of the map and identification of artifacts.

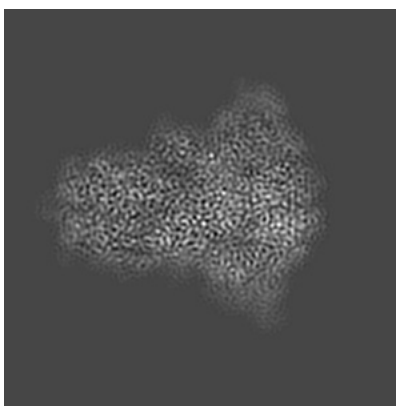
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

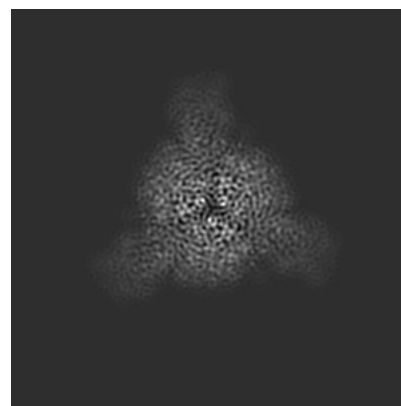
6.1.1 Primary map



X

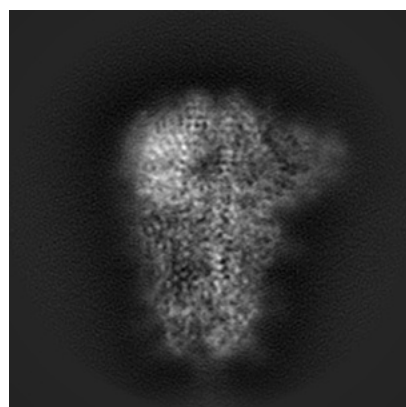


Y

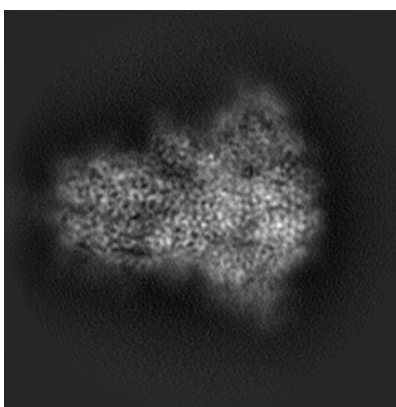


Z

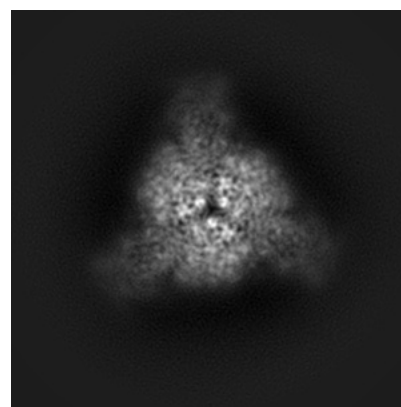
6.1.2 Raw map



X



Y

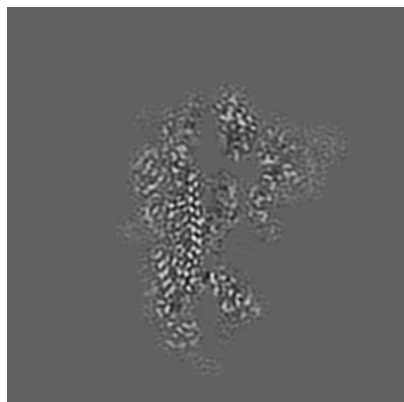


Z

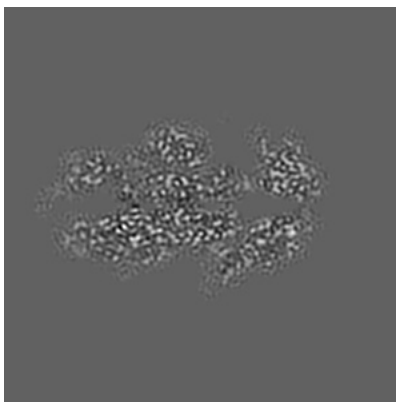
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

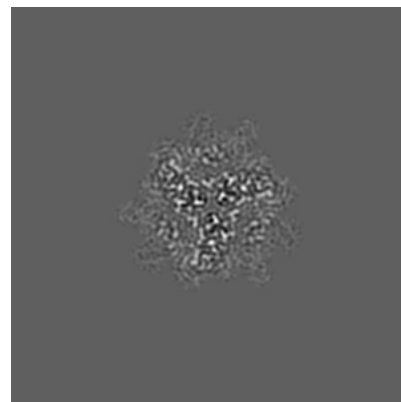
6.2.1 Primary map



X Index: 110

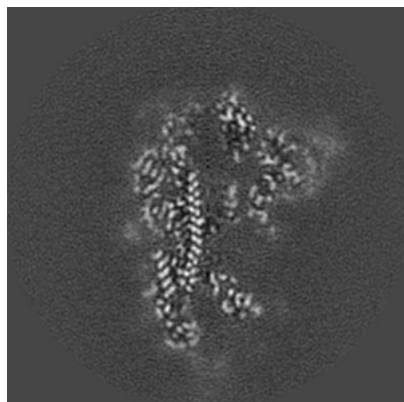


Y Index: 110

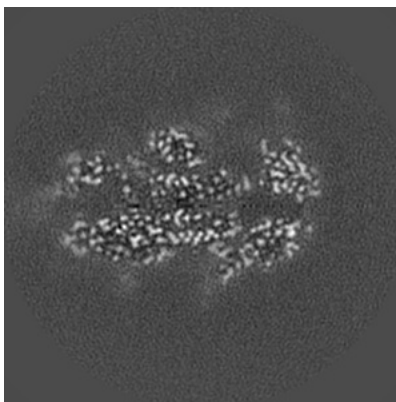


Z Index: 110

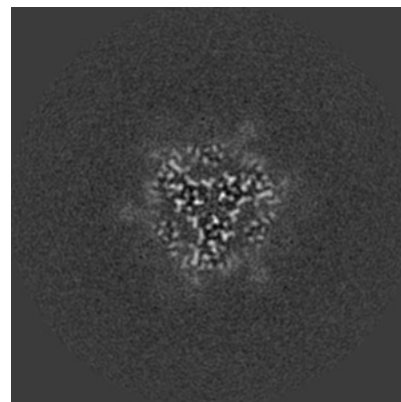
6.2.2 Raw map



X Index: 110



Y Index: 110

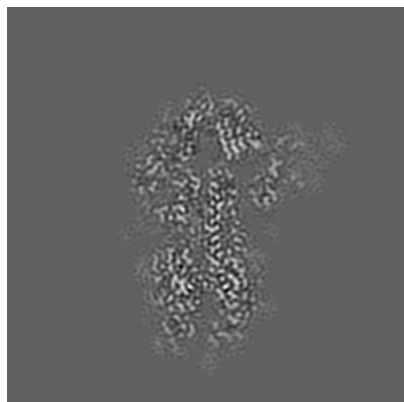


Z Index: 110

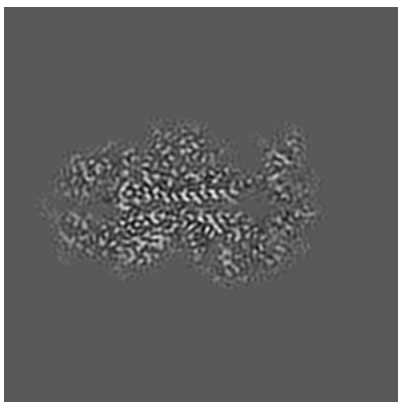
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

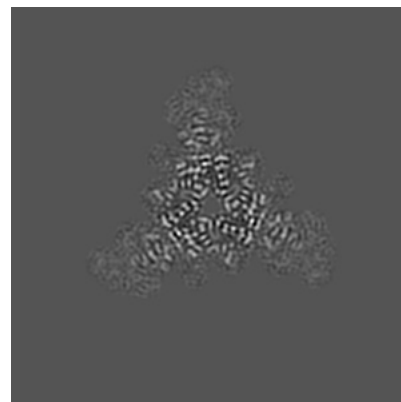
6.3.1 Primary map



X Index: 116

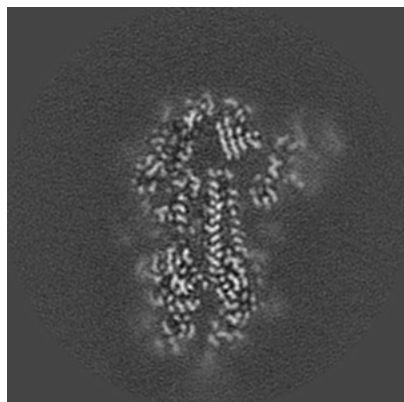


Y Index: 115

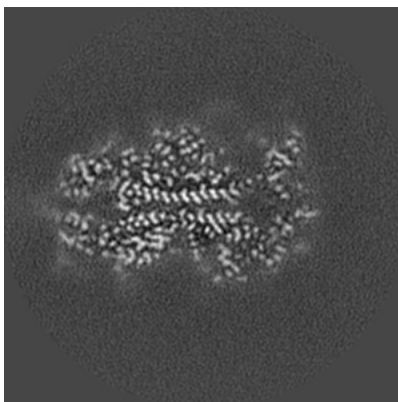


Z Index: 150

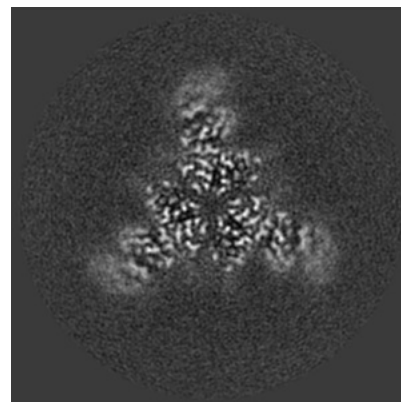
6.3.2 Raw map



X Index: 116



Y Index: 115

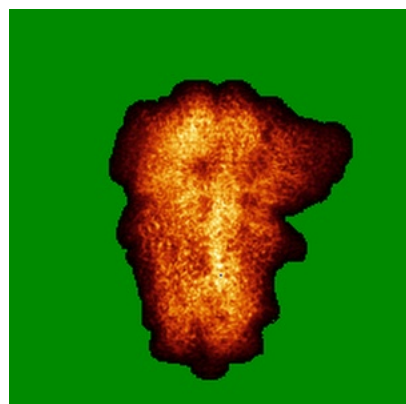


Z Index: 144

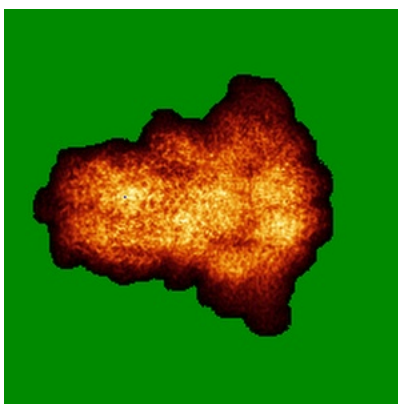
The images above show the largest variance slices of the map in three orthogonal directions.

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

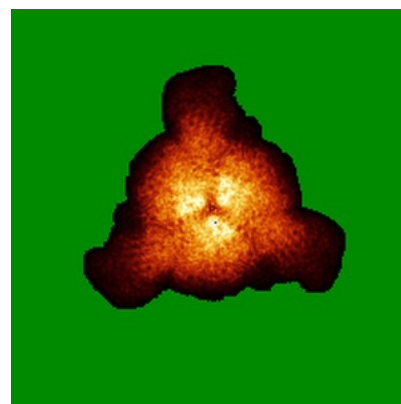
6.4.1 Primary map



X

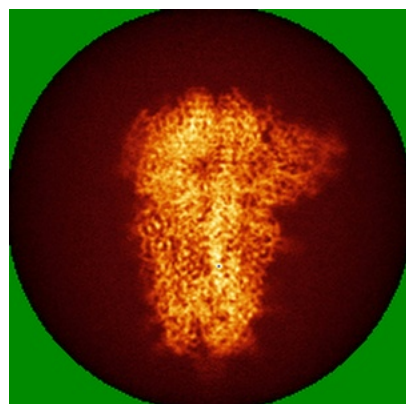


Y

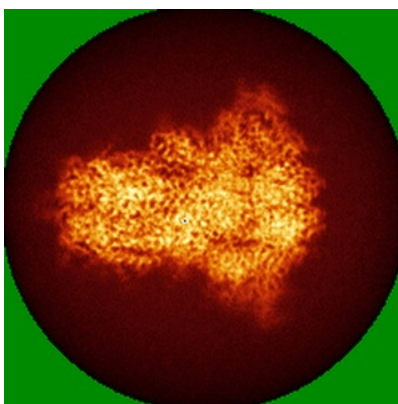


Z

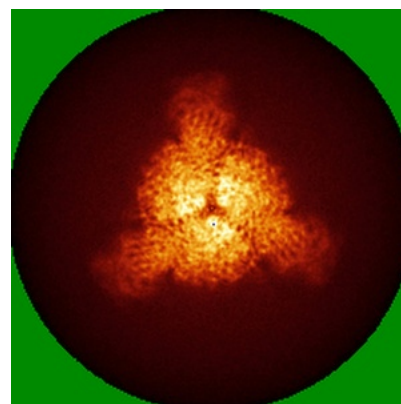
6.4.2 Raw map



X



Y

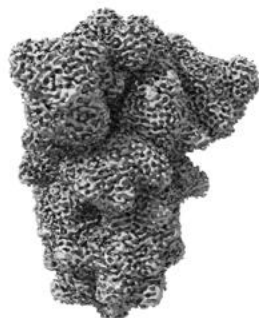


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



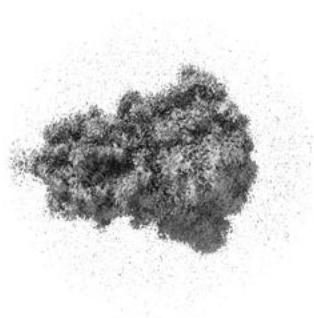
Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

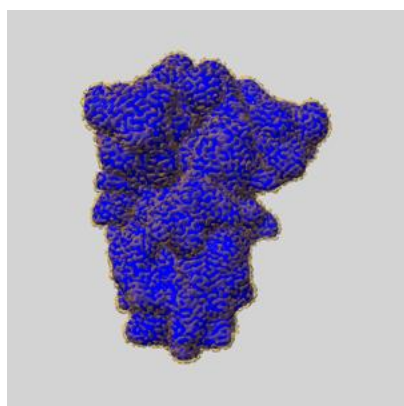
6.6 Mask visualisation [i](#)

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

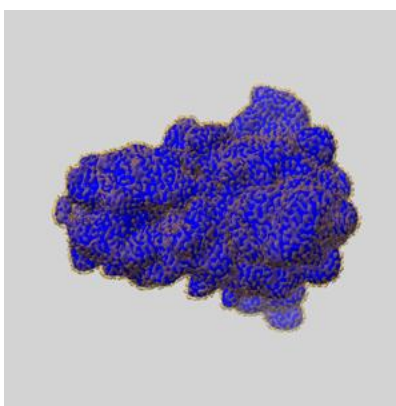
A mask typically either:

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

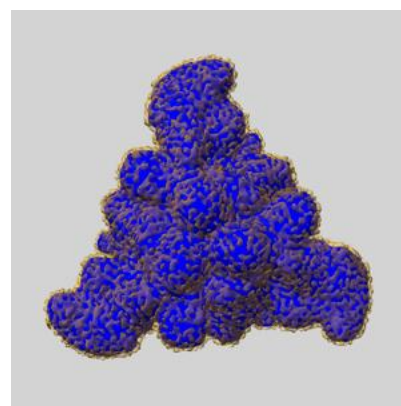
6.6.1 emd_11145_msk_1.map [i](#)



X



Y

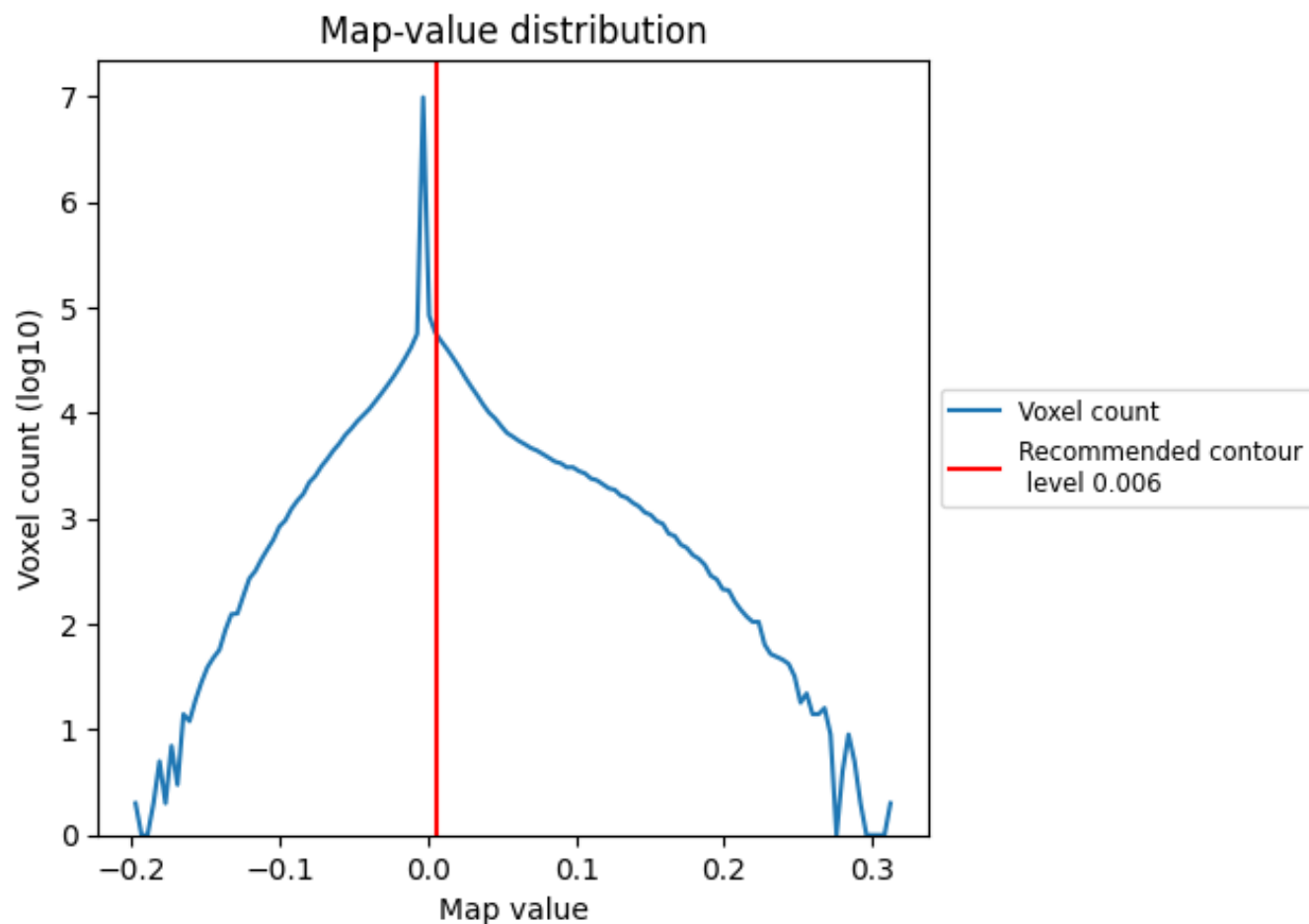


Z

7 Map analysis [i](#)

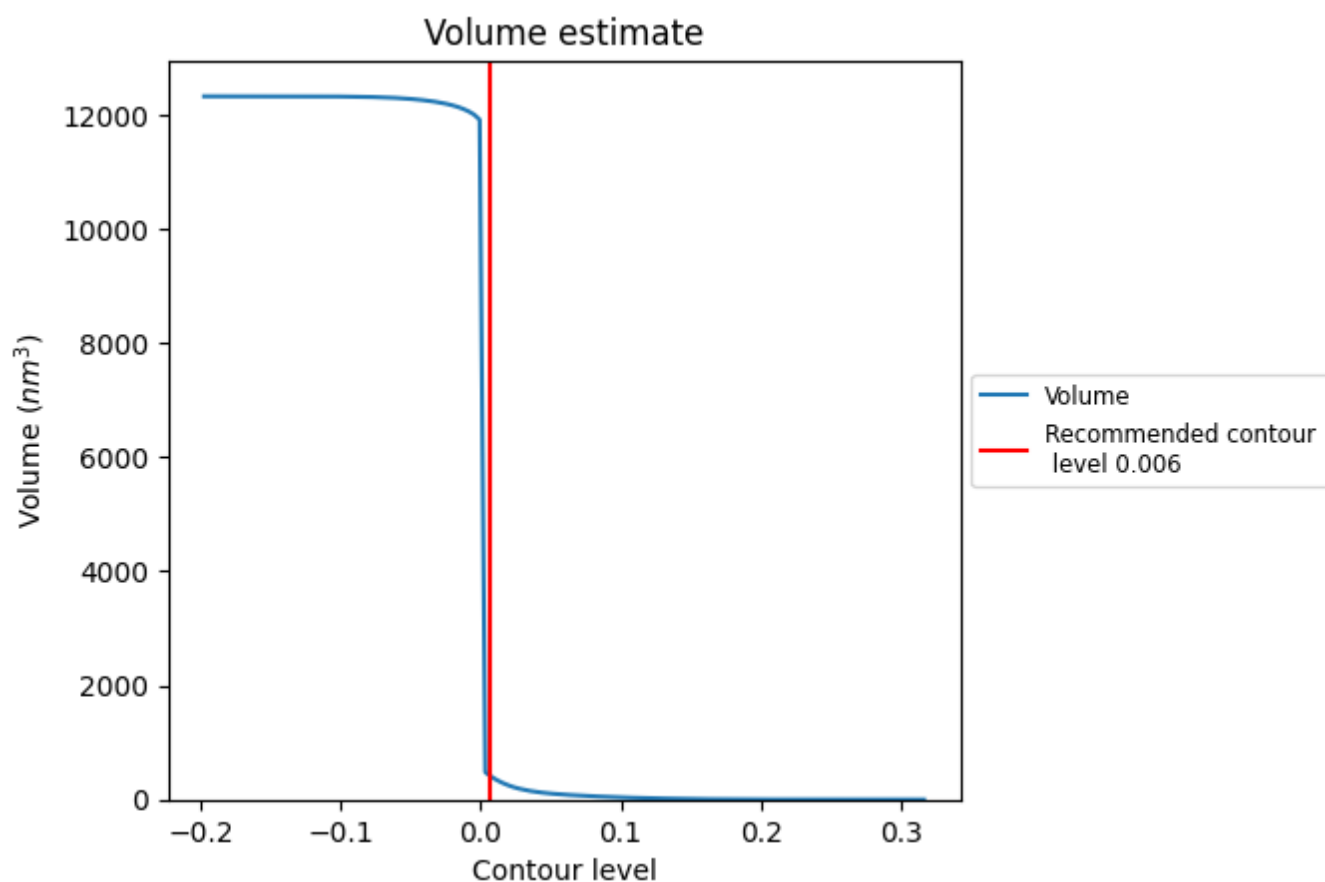
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

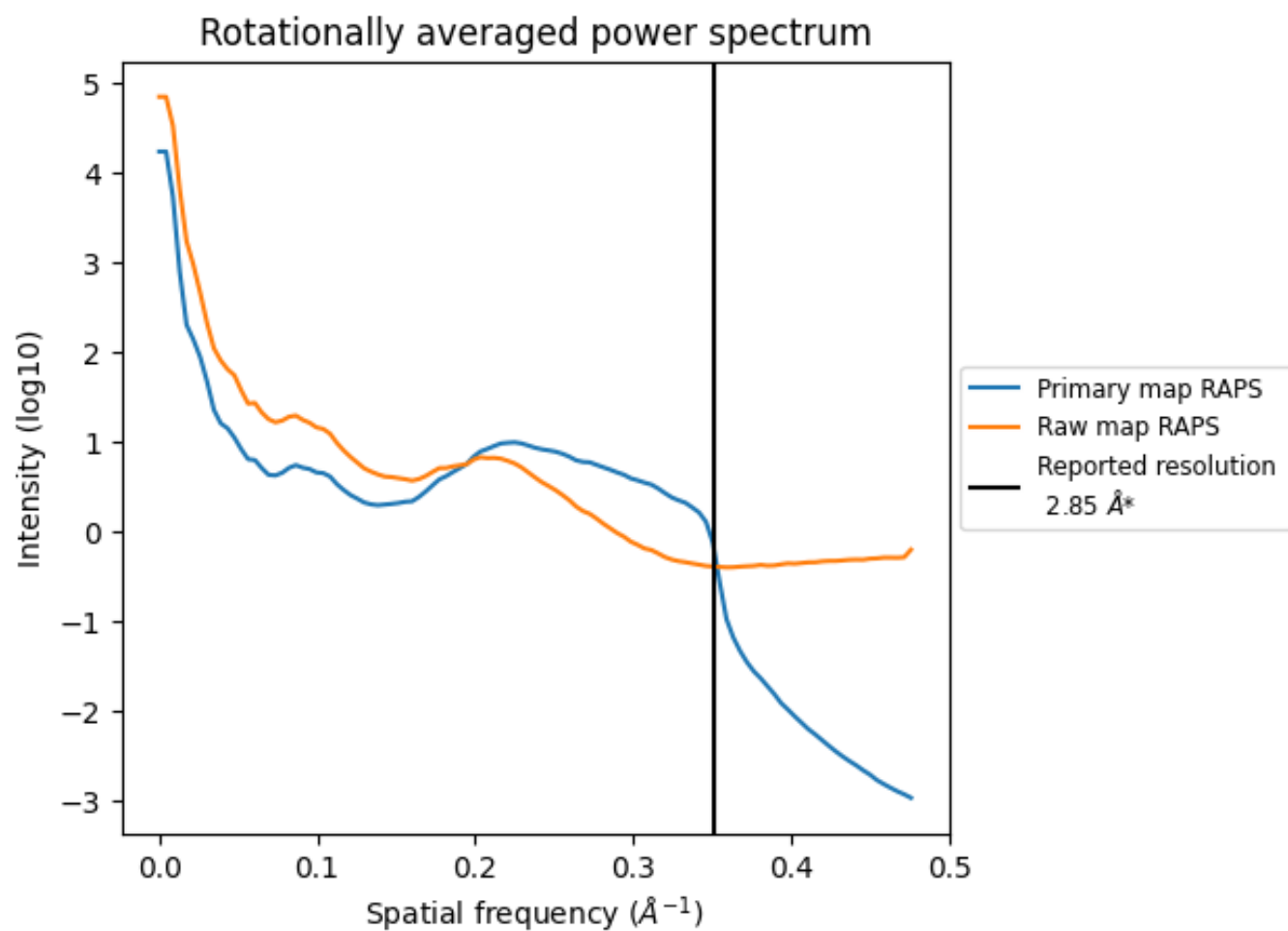
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm^3 ; this corresponds to an approximate mass of 387 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

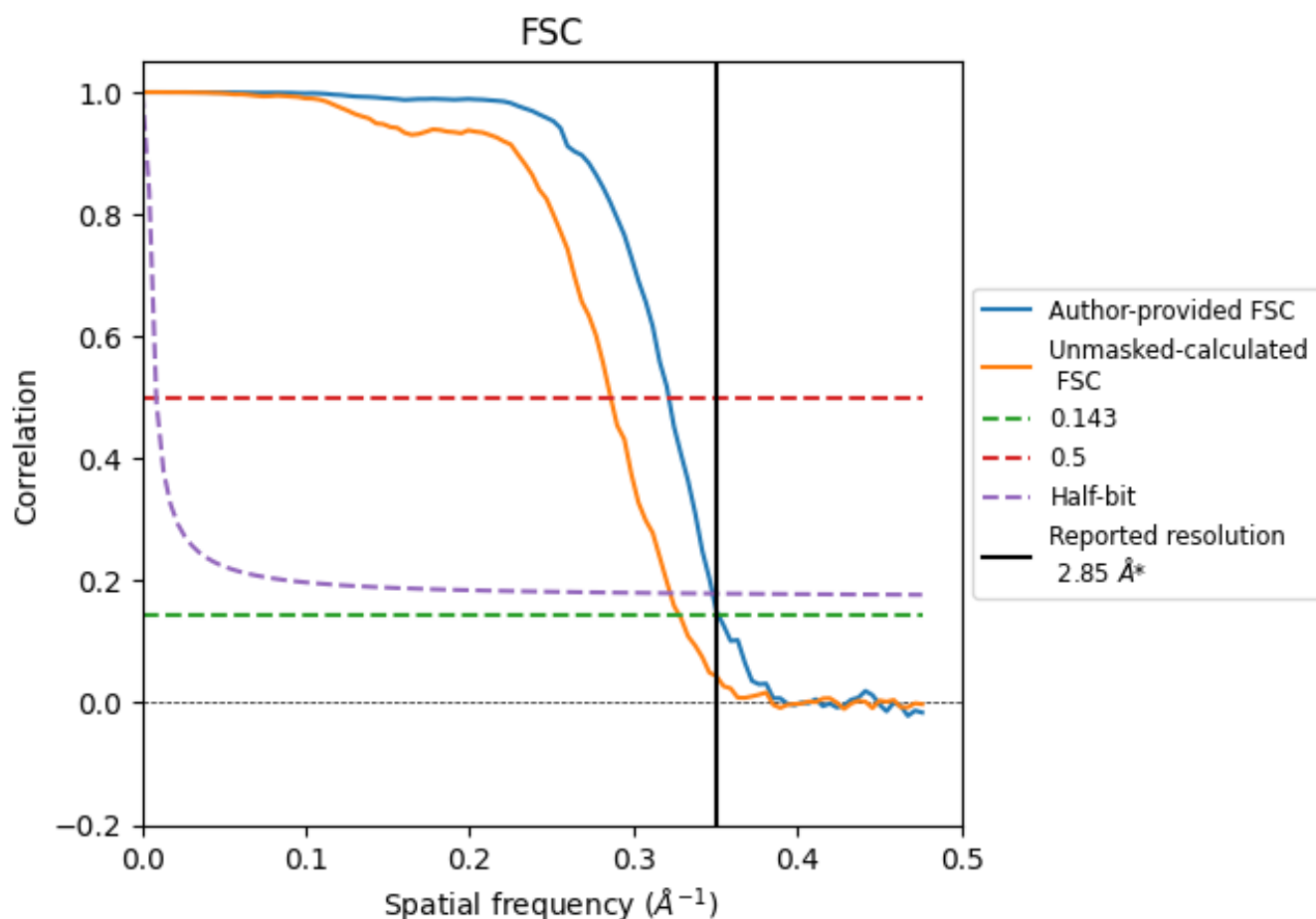


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

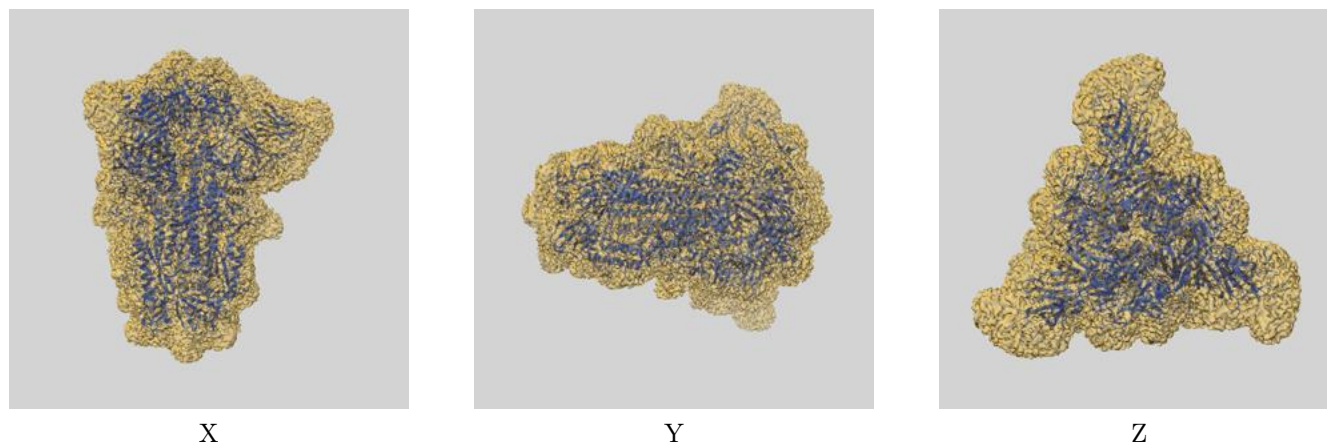
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.84	3.11	2.87
Unmasked-calculated*	3.05	3.50	3.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

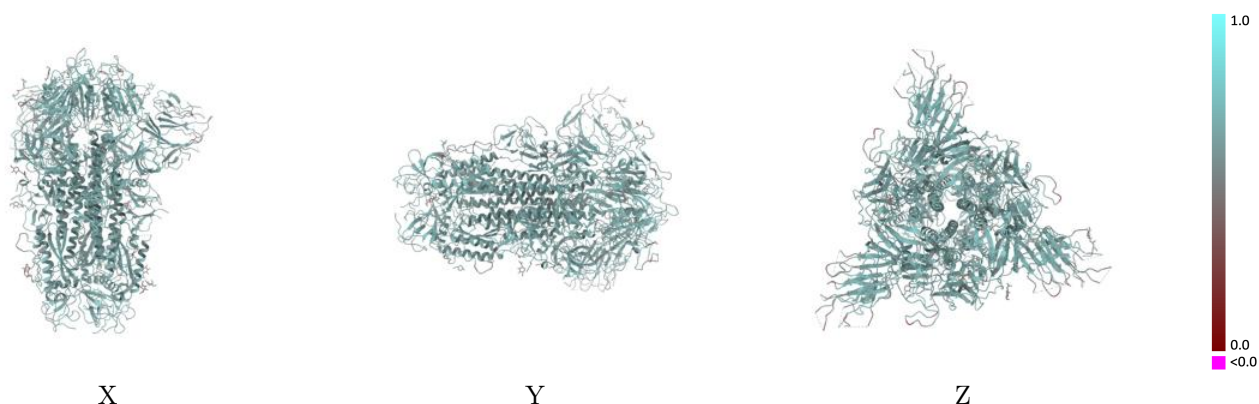
This section contains information regarding the fit between EMDB map EMD-11145 and PDB model 6ZB5. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



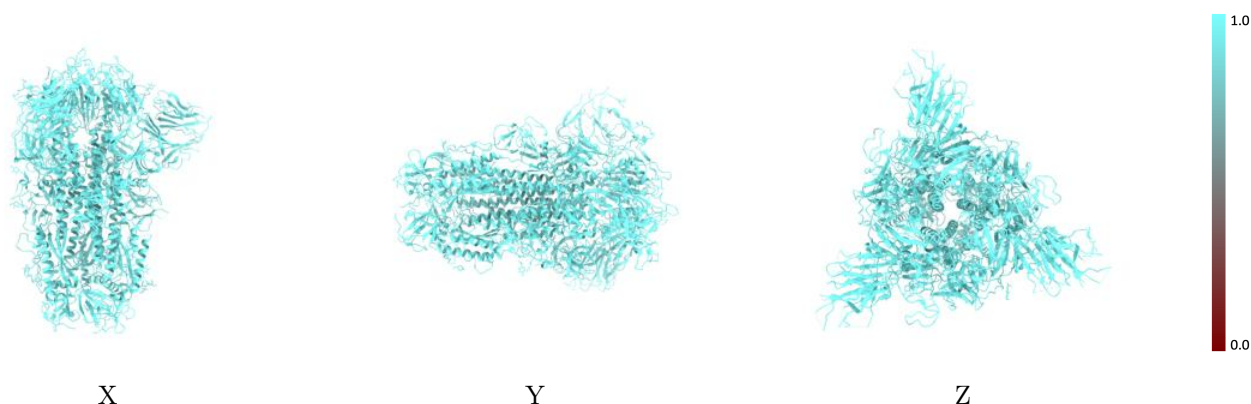
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



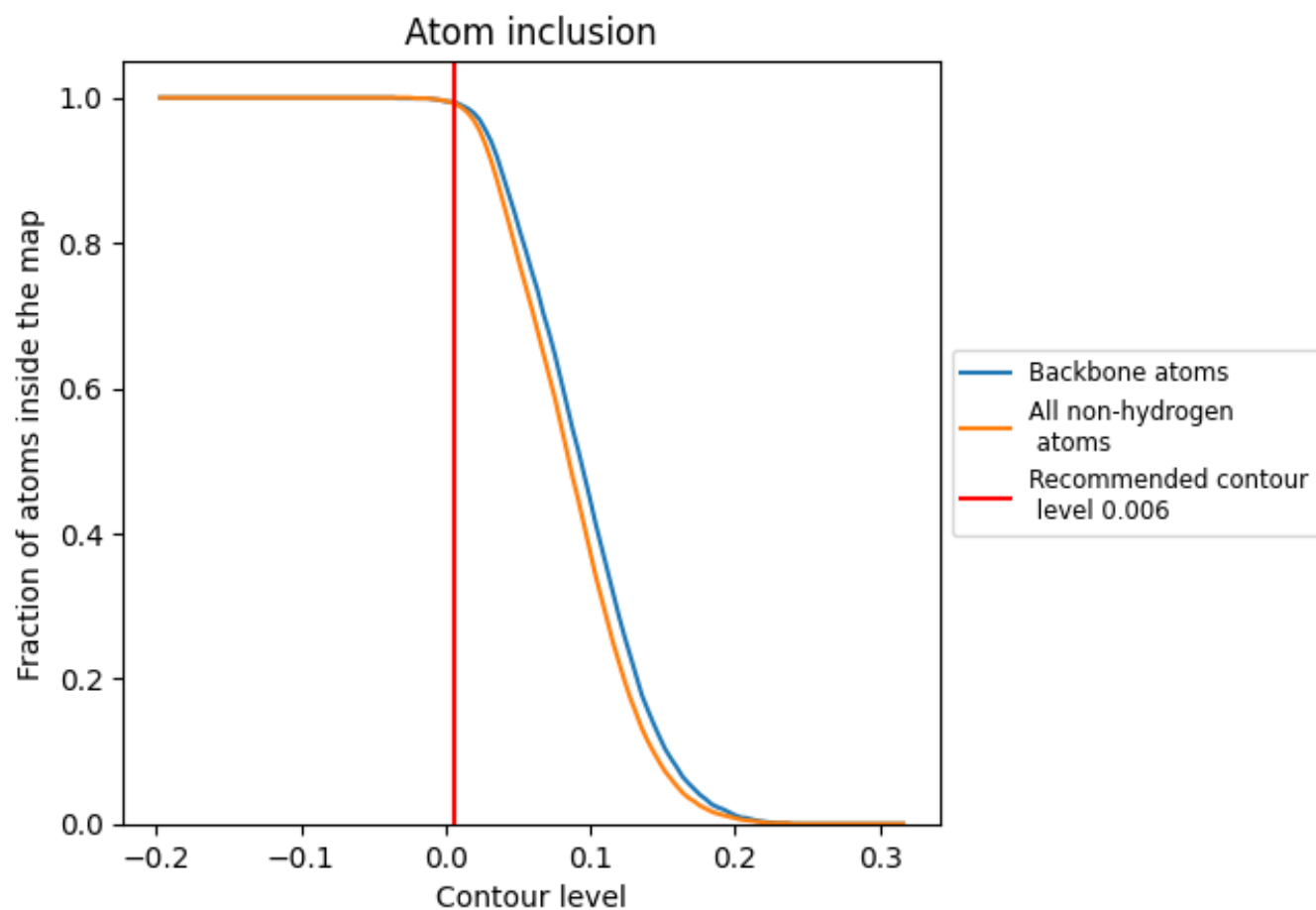
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9920	0.6190
A	0.9920	0.6200
B	0.9920	0.6180
C	0.9920	0.6200
D	0.9290	0.4360
E	0.9290	0.5230
F	1.0000	0.5850

1.0

0.0

<0.0