Full wwPDB EM Validation Report ⓘ

Jan 7, 2025 – 08:17 PM JST

PDB ID	:	8JYP
EMDB ID	:	EMD-36729
Title	:	Structure of SARS-CoV-2 XBB.1.5 spike RBD in complex with ACE2
Authors	:	Yajima, H.; Anraku, Y.; Kita, S.; Kimura, K.; Sasaki, J.; Sasaki-Tabata, K.; Maenaka, K.; Hashiguchi, T.
Deposited on	:	2023-07-03
Resolution	:	3.38 Å(reported)
Based on initial model	:	8IOV

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:

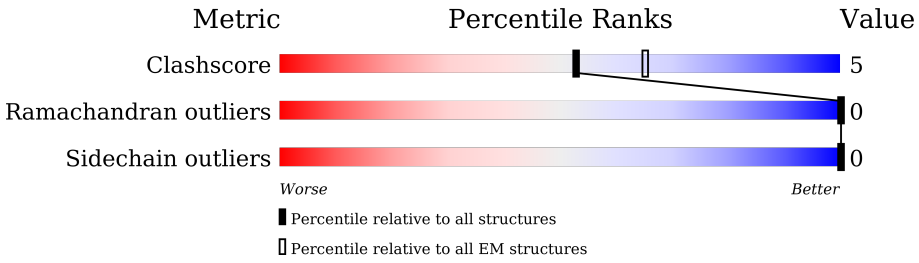
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	1245	14% · 84%
2	D	608	· 84% 14% ·
3	B	2	100%
4	C	3	33% 67% 33%
5	E	5	60% 60% 40%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6627 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
			Total	C	N	O	S		
1	A	199	1581	1020	266	287	8	0	0

There are 109 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	MET	-	expression tag	UNP P0DTC2
A	9	GLY	-	expression tag	UNP P0DTC2
A	10	CYS	-	expression tag	UNP P0DTC2
A	11	VAL	-	expression tag	UNP P0DTC2
A	12	ALA	-	expression tag	UNP P0DTC2
A	13	GLU	-	expression tag	UNP P0DTC2
A	14	THR	-	expression tag	UNP P0DTC2
A	15	GLY	-	expression tag	UNP P0DTC2
A	16	SER	-	expression tag	UNP P0DTC2
A	17	SER	-	expression tag	UNP P0DTC2
A	18	GLN	-	expression tag	UNP P0DTC2
A	19	CYS	-	expression tag	UNP P0DTC2
A	20	VAL	-	expression tag	UNP P0DTC2
A	21	ASN	-	expression tag	UNP P0DTC2
A	22	LEU	-	expression tag	UNP P0DTC2
A	23	ILE	-	expression tag	UNP P0DTC2
A	24	THR	-	expression tag	UNP P0DTC2
A	25	ARG	-	expression tag	UNP P0DTC2
A	26	THR	-	expression tag	UNP P0DTC2
A	27	GLN	-	expression tag	UNP P0DTC2
A	28	SER	-	expression tag	UNP P0DTC2
A	84	ALA	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	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	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1211	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2
A	1243	THR	-	expression tag	UNP P0DTC2
A	1244	LYS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		

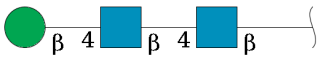
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	618	GLY	-	expression tag	UNP Q9BYF1
D	619	THR	-	expression tag	UNP Q9BYF1
D	620	LYS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
D	622	HIS	-	expression tag	UNP Q9BYF1
D	623	HIS	-	expression tag	UNP Q9BYF1
D	624	HIS	-	expression tag	UNP Q9BYF1
D	625	HIS	-	expression tag	UNP Q9BYF1
D	626	HIS	-	expression tag	UNP Q9BYF1

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

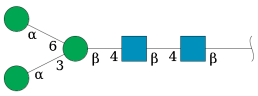
Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

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



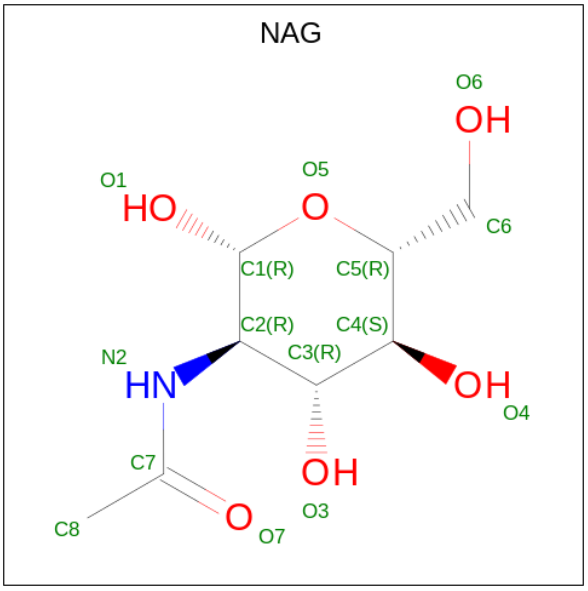
Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



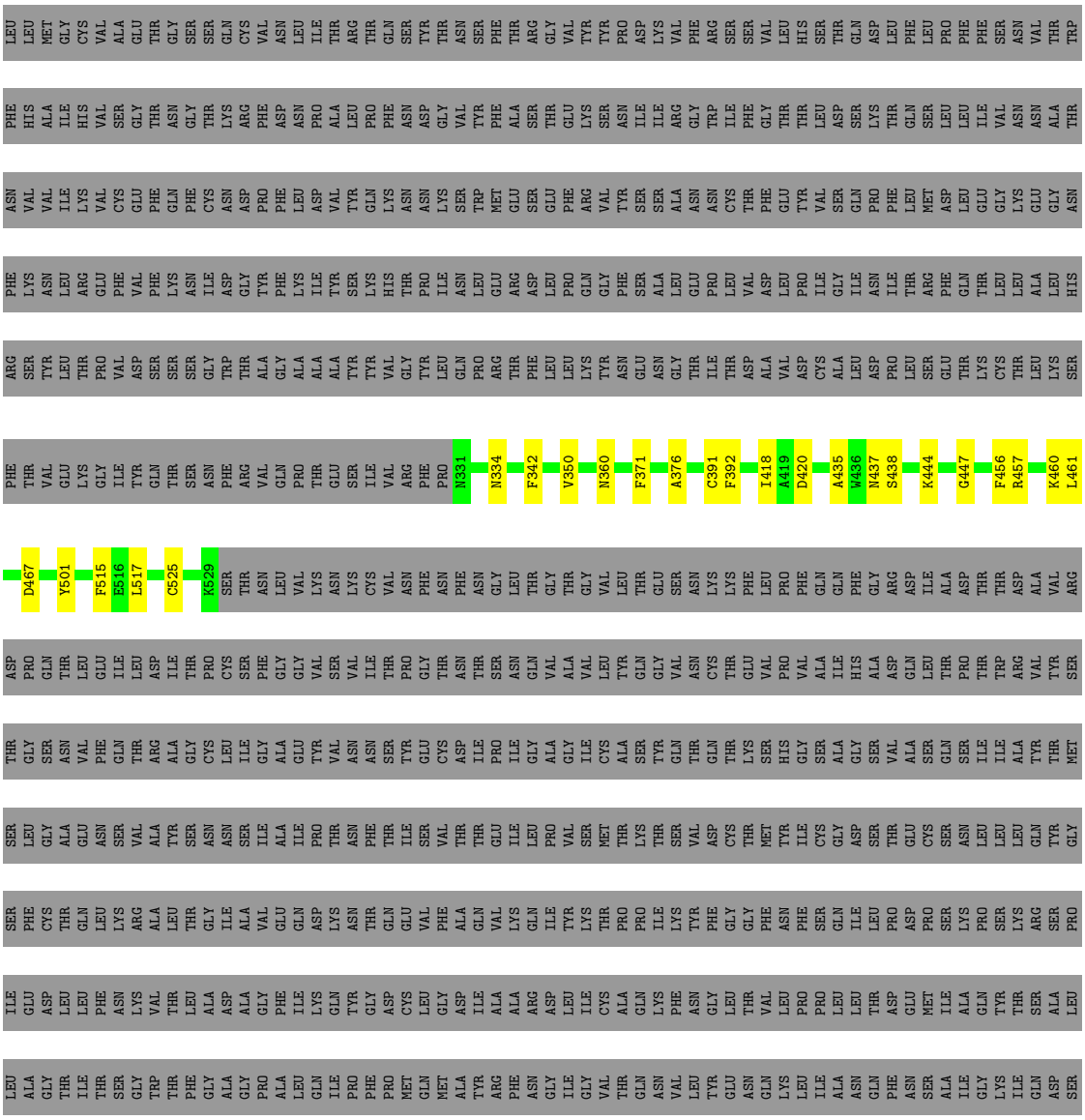
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 14 8 1 5	0
6	D	1	Total C N O 14 8 1 5	0
6	D	1	Total C N O 14 8 1 5	0
6	D	1	Total C N O 14 8 1 5	0

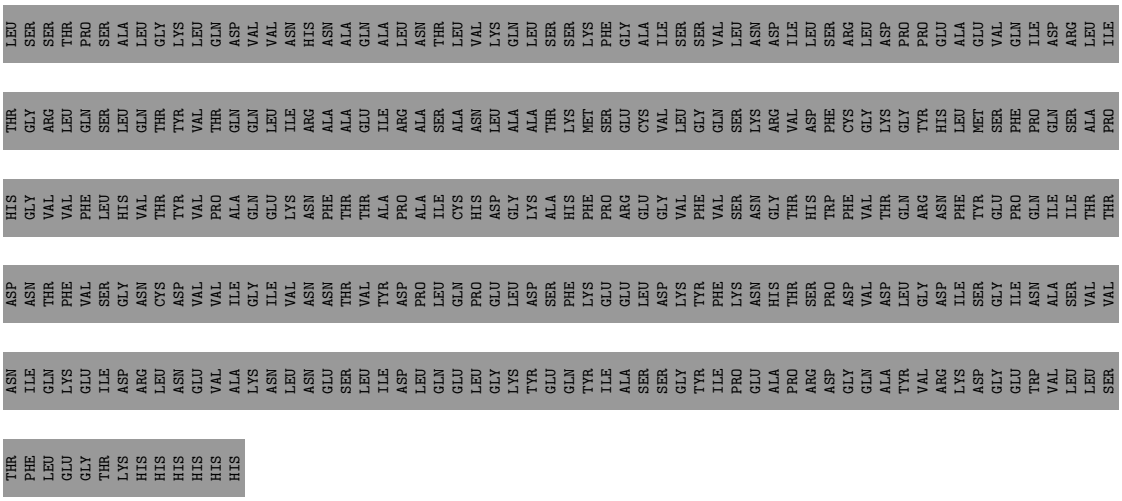
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

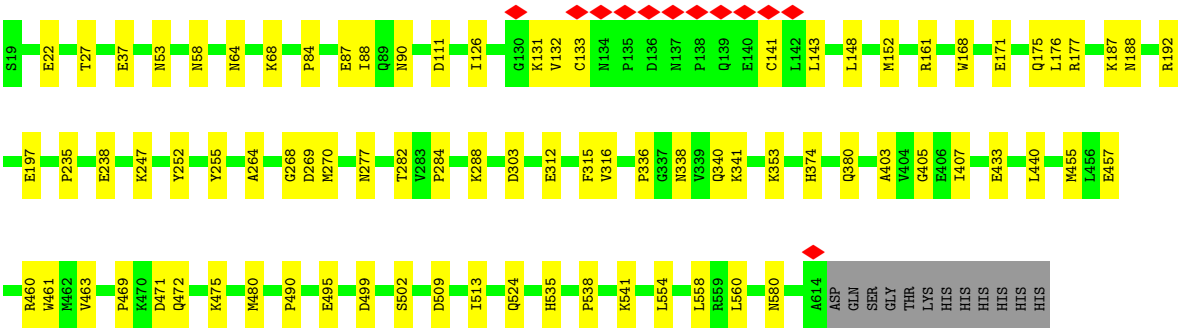
Chain A:





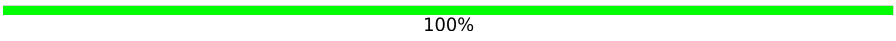
• Molecule 2: Processed angiotensin-converting enzyme 2

Chain D:



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

Chain B:

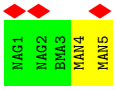


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:


NAG1
NAG2
BMA3
MAN4
MAN5

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.490	Depositor
Minimum map value	-0.212	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	385.91998, 385.91998, 385.91998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.005, 1.005, 1.005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, 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	0.27	0/1630	0.48	0/2220
2	D	0.26	0/4999	0.44	0/6792
All	All	0.26	0/6629	0.45	0/9012

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1581	0	1515	16	0
2	D	4862	0	4633	53	0
3	B	28	0	25	0	0
4	C	39	0	34	1	0
5	E	61	0	52	0	0
6	A	14	0	13	0	0
6	D	42	0	39	0	0
All	All	6627	0	6311	66	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 5.

All (66) 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:501:TYR:HE1	2:D:353:LYS:HD3	1.49	0.75
1:A:350:VAL:HG21	1:A:418:ILE:HD11	1.73	0.69
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.75	0.68
1:A:376:ALA:HB3	1:A:435:ALA:HB3	1.79	0.65
2:D:268:GLY:O	2:D:277:ASN:ND2	2.32	0.63
2:D:284:PRO:HG3	2:D:440:LEU:HD13	1.82	0.62
2:D:53:ASN:O	2:D:58:ASN:ND2	2.34	0.60
2:D:90:ASN:OD1	4:C:1:NAG:N2	2.35	0.60
2:D:338:ASN:O	2:D:341:LYS:NZ	2.34	0.60
2:D:171:GLU:O	2:D:175:GLN:NE2	2.35	0.60
2:D:37:GLU:HB3	2:D:353:LYS:HE2	1.84	0.60
1:A:420:ASP:HB2	1:A:460:LYS:HG3	1.83	0.60
1:A:334:ASN:ND2	1:A:360:ASN:O	2.37	0.58
2:D:457:GLU:HG2	2:D:513:ILE:HD13	1.85	0.58
2:D:131:LYS:HB3	2:D:143:LEU:HD23	1.86	0.57
1:A:501:TYR:CE1	2:D:353:LYS:HD3	2.37	0.56
2:D:252:TYR:HB3	2:D:255:TYR:HD2	1.70	0.56
2:D:161:ARG:HH22	2:D:268:GLY:H	1.52	0.55
2:D:374:HIS:ND1	2:D:405:GLY:O	2.41	0.54
2:D:264:ALA:HB3	2:D:490:PRO:HD3	1.89	0.53
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.41	0.53
2:D:247:LYS:HG3	2:D:282:THR:HG23	1.91	0.53
2:D:177:ARG:NH1	2:D:495:GLU:O	2.42	0.52
1:A:444:LYS:HG3	1:A:447:GLY:H	1.74	0.51
2:D:538:PRO:HG2	2:D:541:LYS:HE3	1.93	0.51
2:D:460:ARG:HA	2:D:463:VAL:HG12	1.93	0.50
2:D:64:ASN:O	2:D:68:LYS:HG2	2.12	0.50
2:D:303:ASP:OD1	2:D:303:ASP:N	2.45	0.50
1:A:392:PHE:CD1	1:A:517:LEU:HD21	2.47	0.49
2:D:312:GLU:O	2:D:316:VAL:HG23	2.13	0.49
2:D:288:LYS:HG3	2:D:433:GLU:HG3	1.95	0.48
2:D:269:ASP:OD1	2:D:269:ASP:N	2.46	0.47
2:D:187:LYS:NZ	2:D:509:ASP:OD2	2.46	0.47
2:D:457:GLU:OE2	2:D:461:TRP:NE1	2.48	0.47
2:D:53:ASN:HB3	2:D:58:ASN:HD21	1.80	0.47
2:D:403:ALA:O	2:D:407:ILE:HG23	2.15	0.47
2:D:126:ILE:HG21	2:D:176:LEU:HD21	1.96	0.46
2:D:152:MET:O	2:D:161:ARG:NH1	2.41	0.46
2:D:111:ASP:N	2:D:111:ASP:OD1	2.48	0.46
2:D:315:PHE:CE2	2:D:380:GLN:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:535:HIS:NE2	2:D:541:LYS:O	2.49	0.46
1:A:392:PHE:HD2	1:A:515:PHE:HB3	1.81	0.46
2:D:524:GLN:OE1	2:D:580:ASN:N	2.46	0.45
2:D:161:ARG:NH2	2:D:268:GLY:H	2.13	0.45
2:D:53:ASN:HB3	2:D:58:ASN:ND2	2.33	0.44
1:A:460:LYS:HG2	1:A:461:LEU:H	1.81	0.44
2:D:336:PRO:HB2	2:D:340:GLN:HB3	1.99	0.43
1:A:342:PHE:HB3	1:A:371:PHE:CE2	2.53	0.43
2:D:168:TRP:HB3	2:D:270:MET:HE1	1.99	0.43
2:D:235:PRO:HA	2:D:238:GLU:HG2	2.01	0.42
1:A:391:CYS:CB	1:A:525:CYS:HA	2.47	0.42
2:D:472:GLN:HB3	2:D:475:LYS:HE3	2.02	0.41
1:A:437:ASN:OD1	1:A:438:SER:N	2.54	0.41
2:D:315:PHE:CD2	2:D:380:GLN:HG3	2.56	0.41
2:D:84:PRO:HB2	2:D:87:GLU:OE1	2.21	0.41
2:D:455:MET:HE1	2:D:480:MET:HB2	2.03	0.41
1:A:456:PHE:CE1	2:D:27:THR:HG23	2.55	0.41
2:D:197:GLU:OE1	2:D:197:GLU:N	2.54	0.41
2:D:554:LEU:O	2:D:558:LEU:HG	2.21	0.41
2:D:133:CYS:HB3	2:D:141:CYS:HA	2.03	0.41
2:D:188:ASN:O	2:D:192:ARG:HD3	2.20	0.41
2:D:22:GLU:OE1	2:D:88:ILE:HG13	2.21	0.40
2:D:560:LEU:HD23	2:D:560:LEU:HA	1.92	0.40
2:D:469:PRO:HB2	2:D:471:ASP:OD1	2.22	0.40
2:D:132:VAL:HG12	2:D:148:LEU:HD11	2.02	0.40
2:D:499:ASP:O	2:D:502:SER:OG	2.29	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	197/1245 (16%)	189 (96%)	8 (4%)	0	100	100
2	D	594/608 (98%)	582 (98%)	12 (2%)	0	100	100
All	All	791/1853 (43%)	771 (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	172/1083 (16%)	172 (100%)	0	100	100
2	D	526/537 (98%)	526 (100%)	0	100	100
All	All	698/1620 (43%)	698 (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. There are no such sidechains identified.

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)

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1	2,3	14,14,15	0.31	0	17,19,21	0.43	0
3	NAG	B	2	3	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	C	1	4,2	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	C	2	4	14,14,15	0.19	0	17,19,21	0.43	0
4	BMA	C	3	4	11,11,12	0.58	0	15,15,17	0.76	0
5	NAG	E	1	2,5	14,14,15	0.58	0	17,19,21	0.63	0
5	NAG	E	2	5	14,14,15	0.19	0	17,19,21	0.48	0
5	BMA	E	3	5	11,11,12	0.56	0	15,15,17	0.82	0
5	MAN	E	4	5	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
5	MAN	E	5	5	11,11,12	0.66	0	15,15,17	1.00	2 (13%)

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	B	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
4	NAG	C	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	4	MAN	O2-C2-C3	-2.35	105.43	110.14
5	E	4	MAN	C1-O5-C5	2.20	115.17	112.19
5	E	5	MAN	O2-C2-C3	-2.19	105.76	110.14

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	5	MAN	C1-O5-C5	2.14	115.10	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

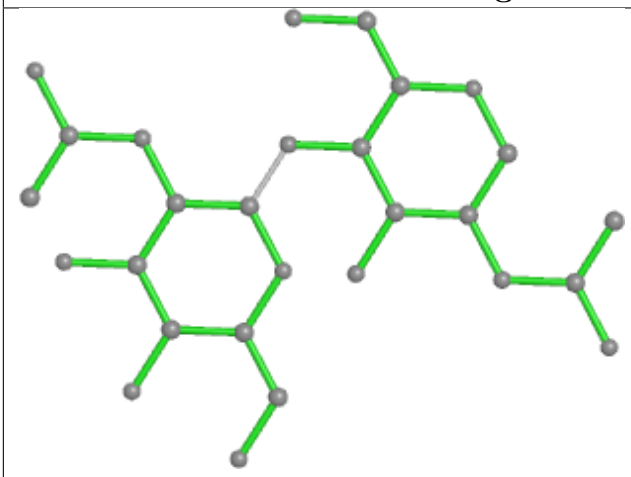
There are no ring outliers.

1 monomer is involved in 1 short contact:

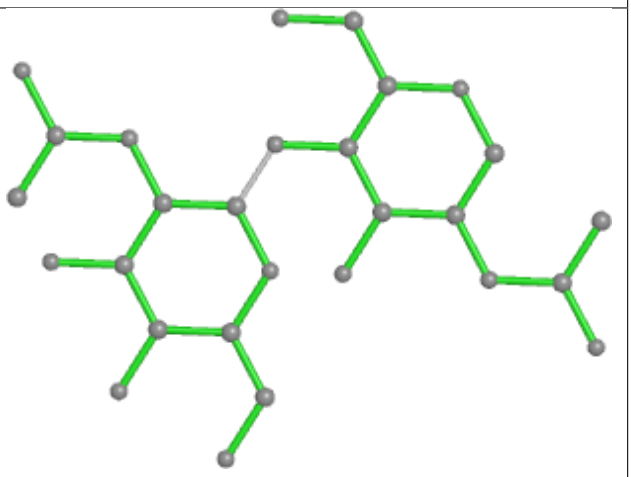
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	NAG	1	0

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

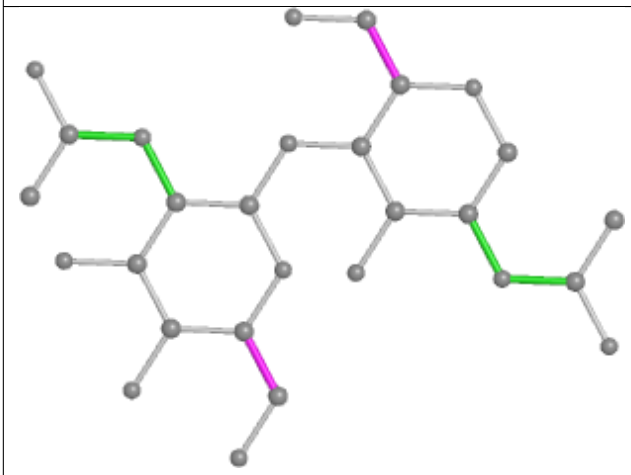
Oligosaccharide Chain B



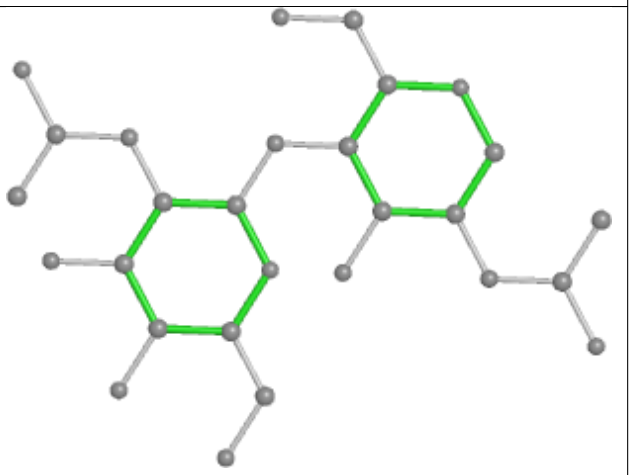
Bond lengths



Bond angles

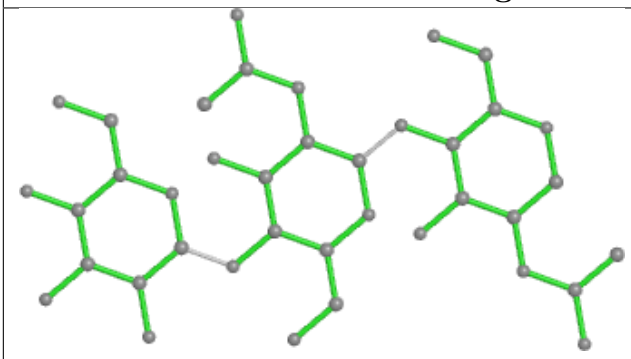


Torsions

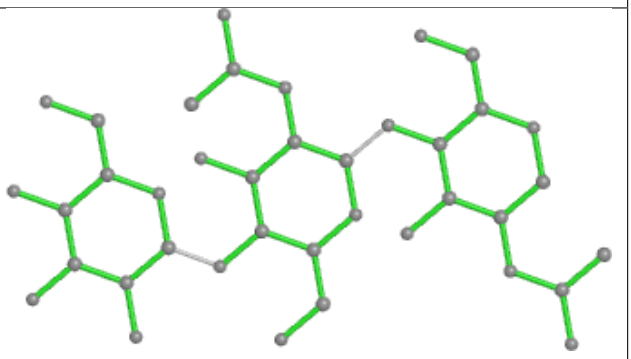


Rings

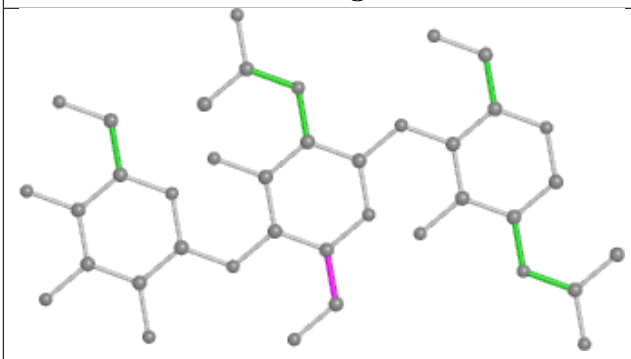
Oligosaccharide Chain C



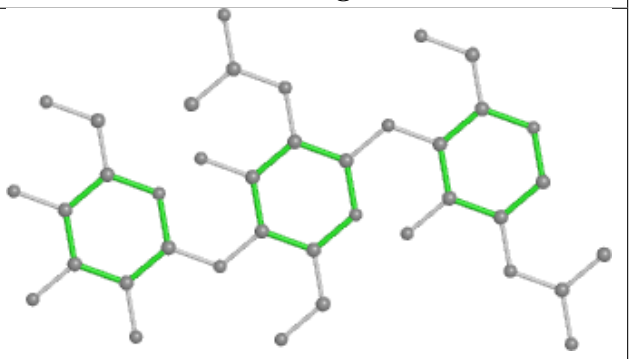
Bond lengths



Bond angles

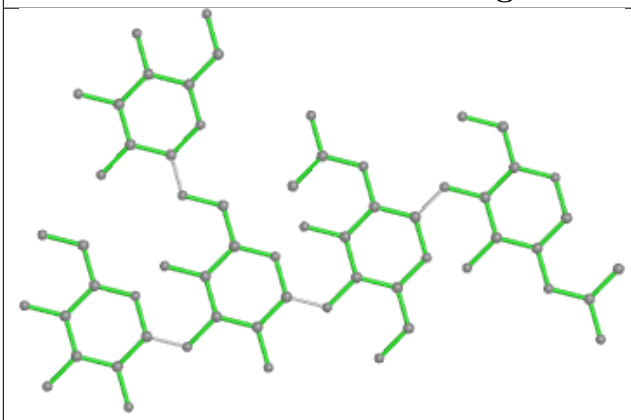


Torsions

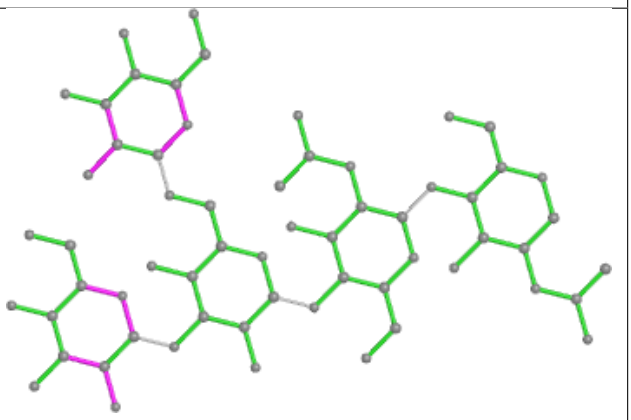


Rings

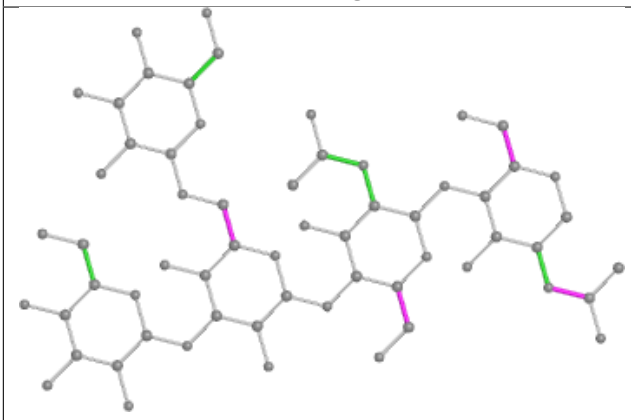
Oligosaccharide Chain E



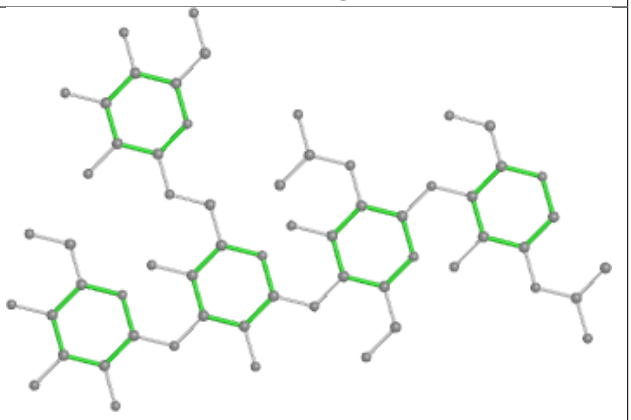
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	D	703	2	14,14,15	0.25	0	17,19,21	0.57	0
6	NAG	D	702	2	14,14,15	0.21	0	17,19,21	0.33	0
6	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.36	0
6	NAG	D	701	2	14,14,15	0.26	0	17,19,21	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	703	2	-	2/6/23/26	0/1/1/1
6	NAG	D	702	2	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
6	NAG	D	701	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

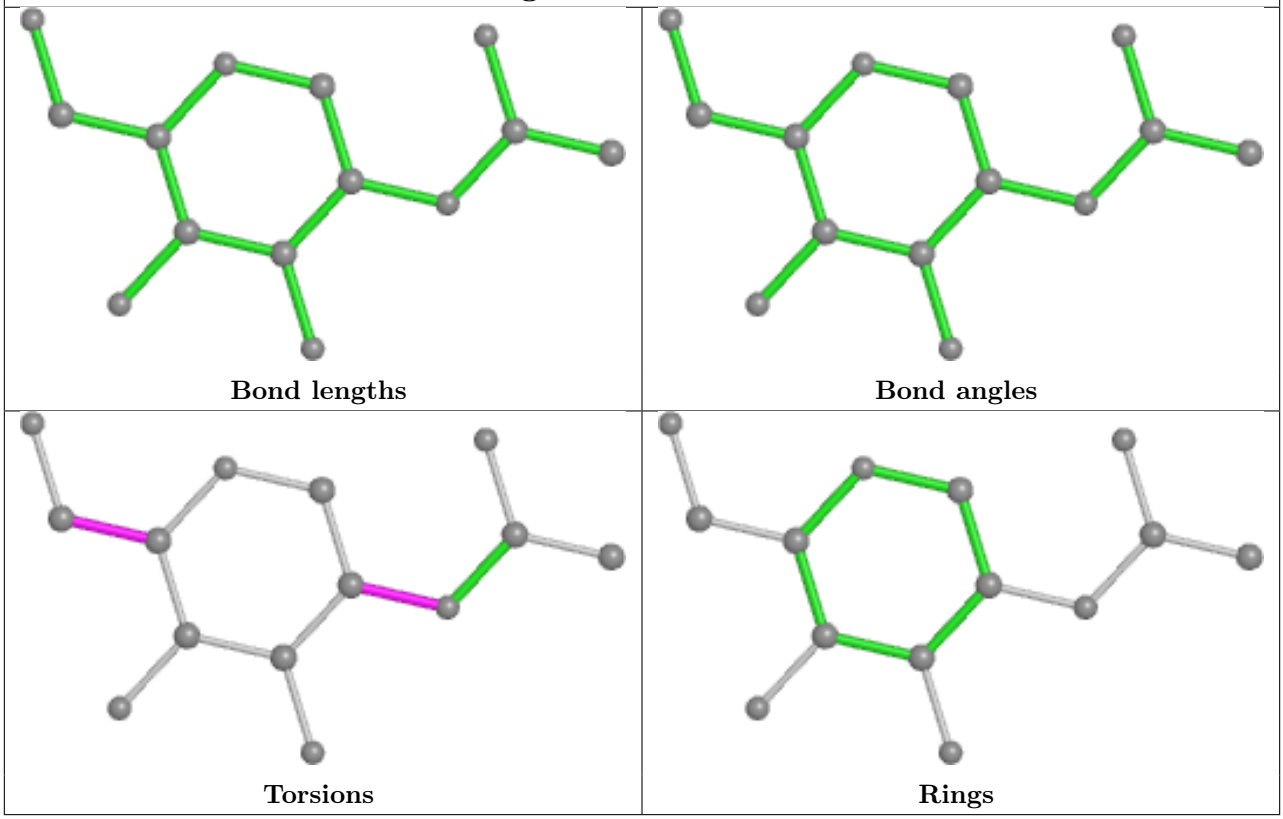
Mol	Chain	Res	Type	Atoms
6	D	702	NAG	O5-C5-C6-O6
6	A	1301	NAG	C8-C7-N2-C2
6	A	1301	NAG	O7-C7-N2-C2
6	A	1301	NAG	O5-C5-C6-O6
6	D	702	NAG	C4-C5-C6-O6
6	D	703	NAG	C3-C2-N2-C7
6	D	703	NAG	C4-C5-C6-O6

There are no ring outliers.

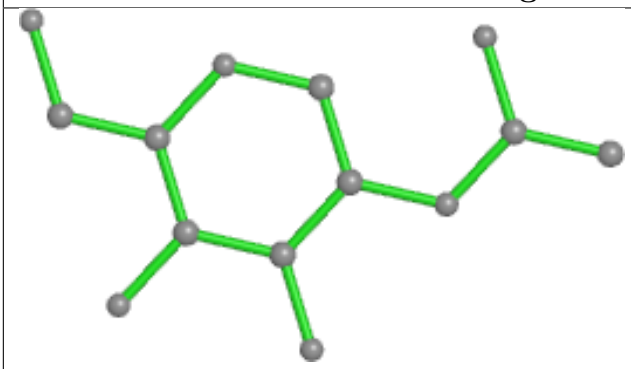
No monomer is involved in short contacts.

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

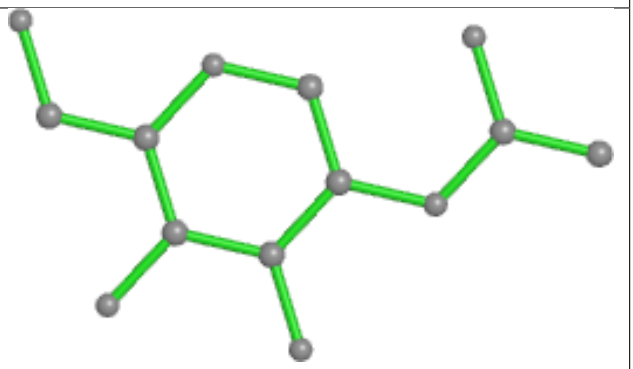
Ligand NAG D 703



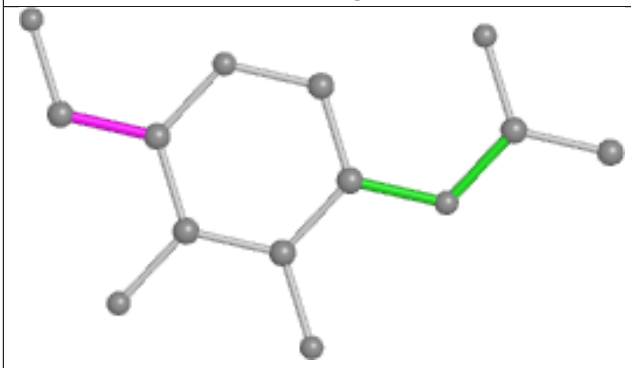
Ligand NAG D 702



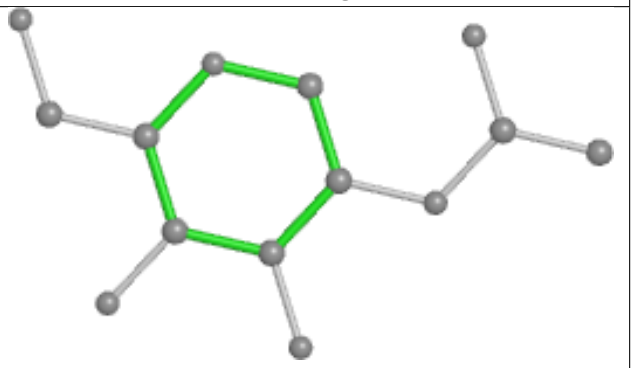
Bond lengths



Bond angles

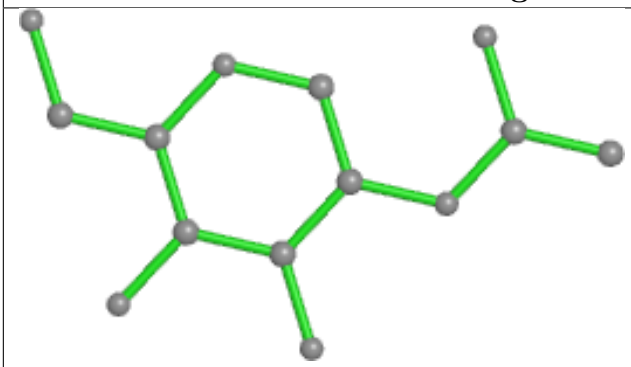


Torsions

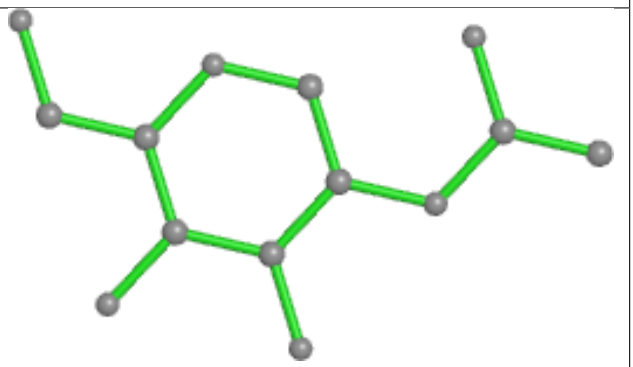


Rings

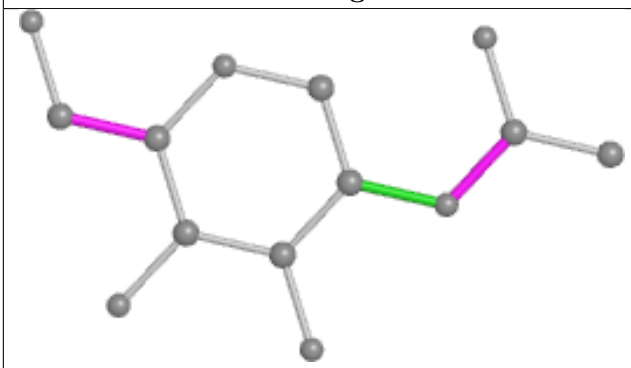
Ligand NAG A 1301



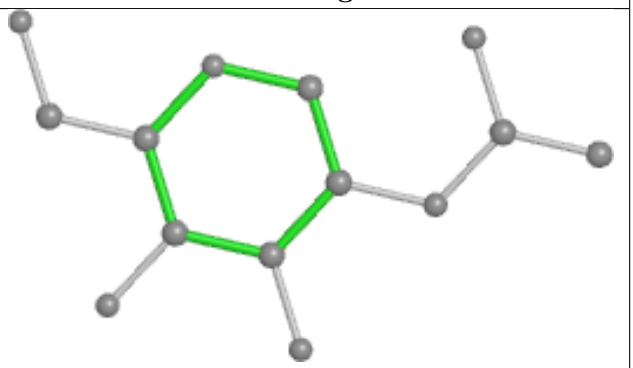
Bond lengths



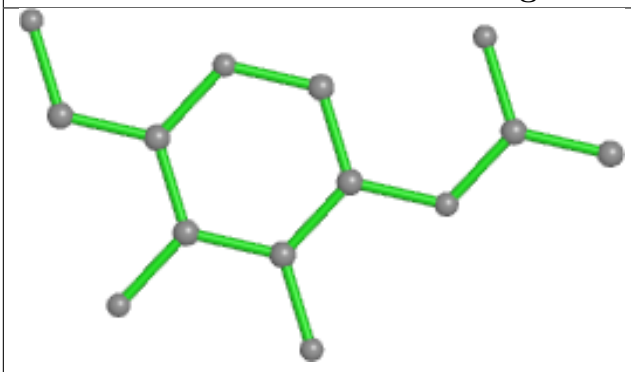
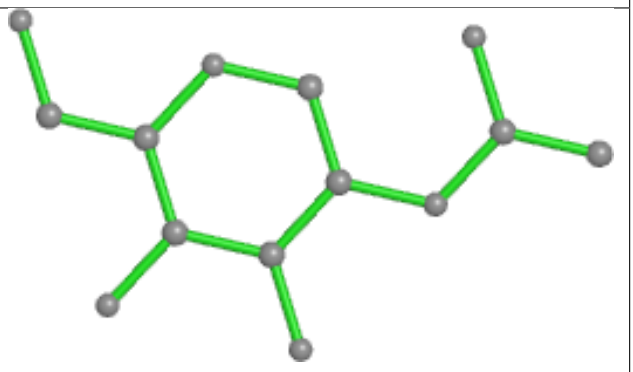
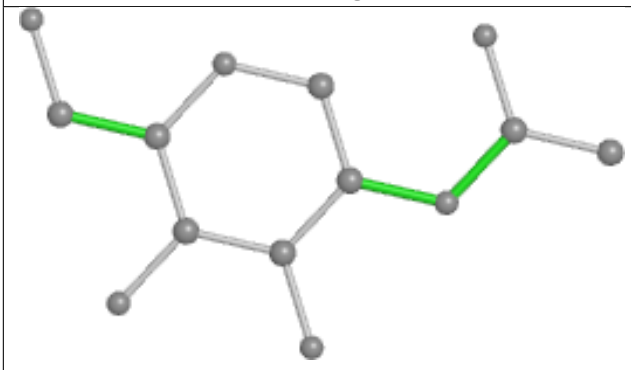
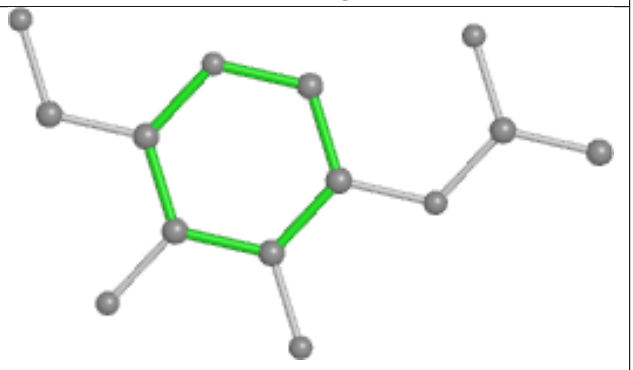
Bond angles



Torsions



Rings

Ligand NAG D 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

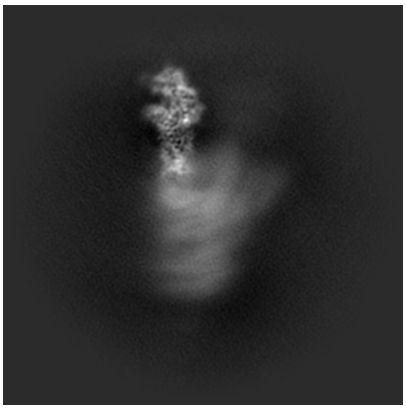
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36729. These allow visual inspection of the internal detail of the map and identification of artifacts.

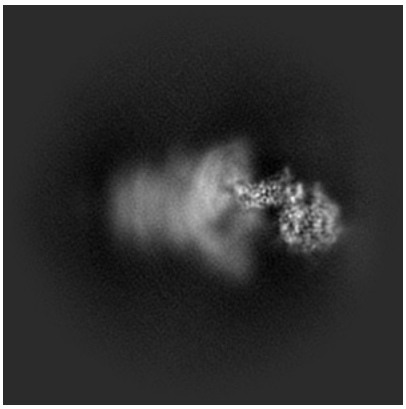
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

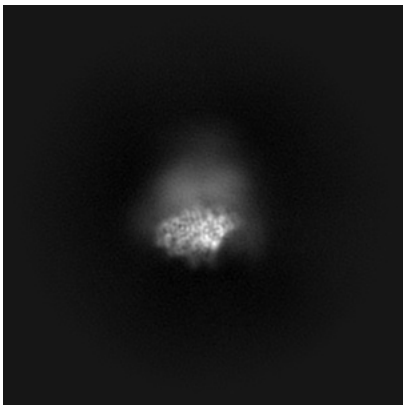
6.1.1 Primary map



X

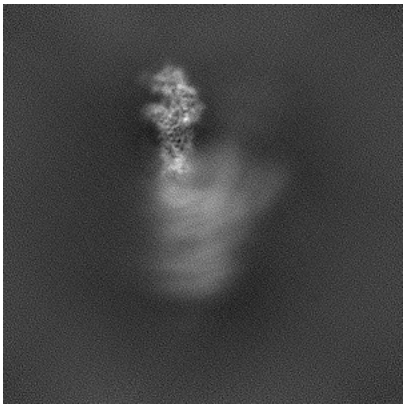


Y

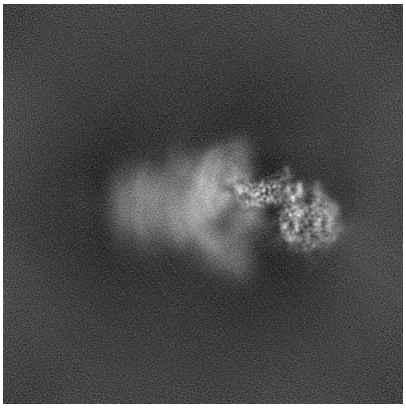


Z

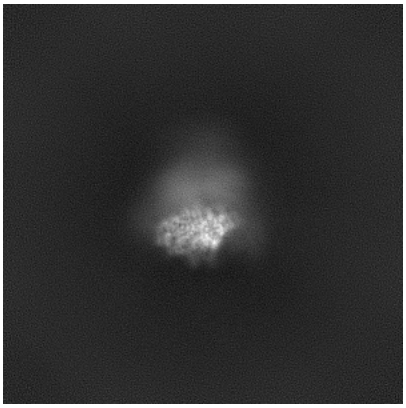
6.1.2 Raw map



X



Y

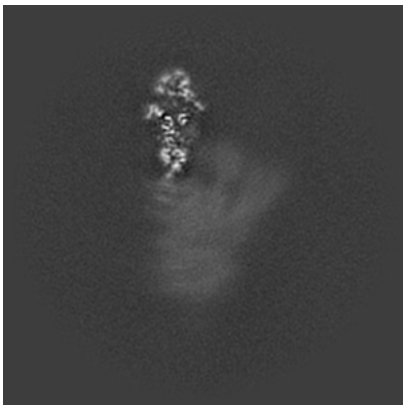


Z

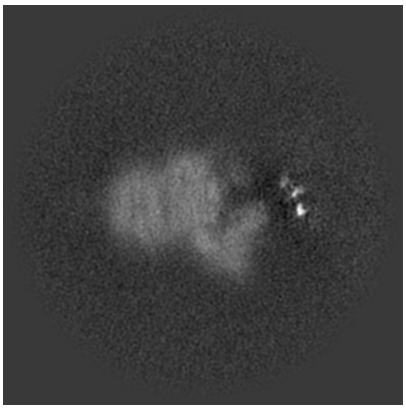
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

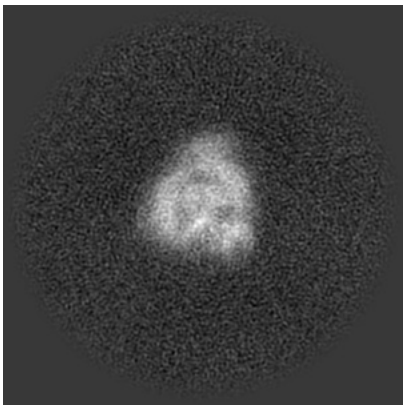
6.2.1 Primary map



X Index: 192

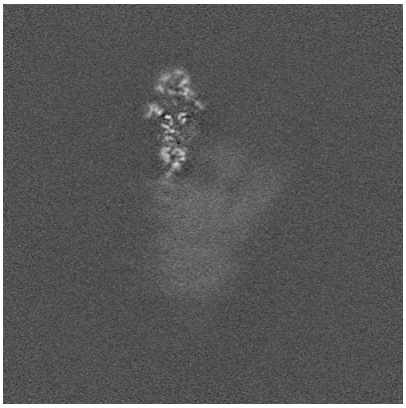


Y Index: 192

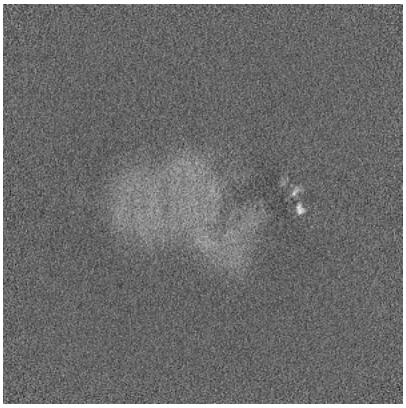


Z Index: 192

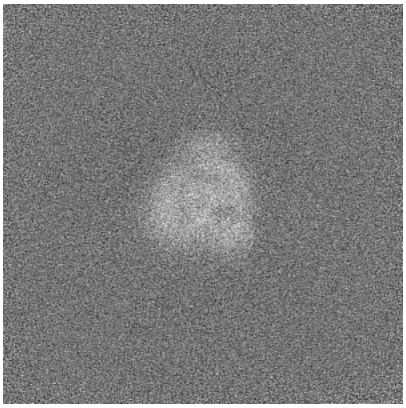
6.2.2 Raw map



X Index: 192



Y Index: 192

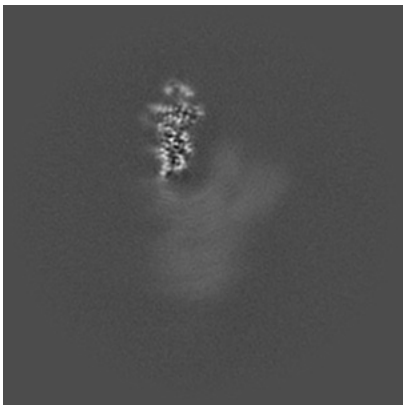


Z Index: 192

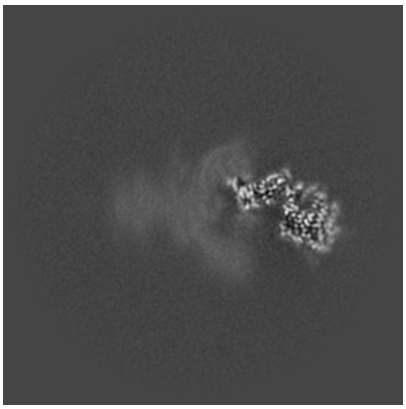
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

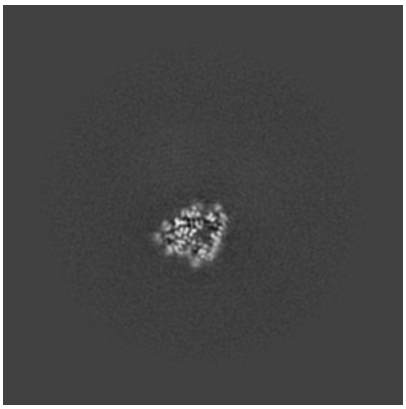
6.3.1 Primary map



X Index: 203

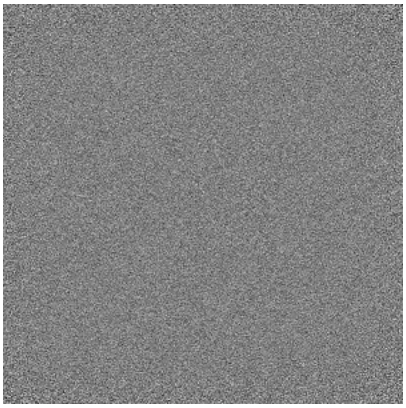


Y Index: 170

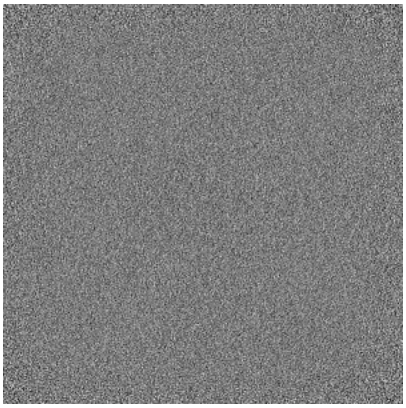


Z Index: 282

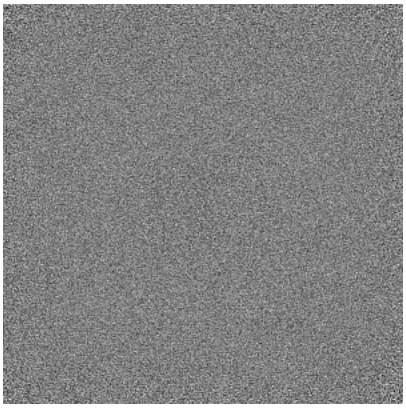
6.3.2 Raw map



X Index: 0



Y Index: 0

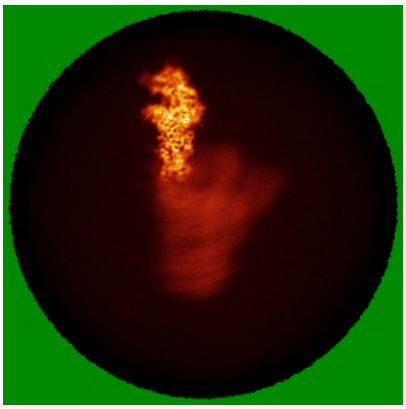


Z Index: 0

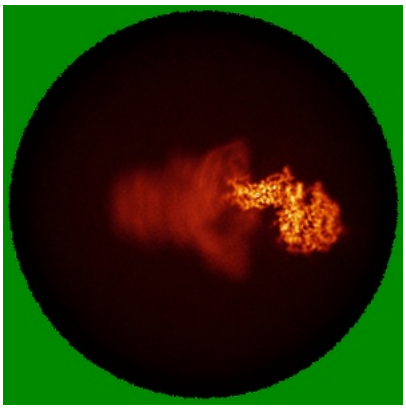
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

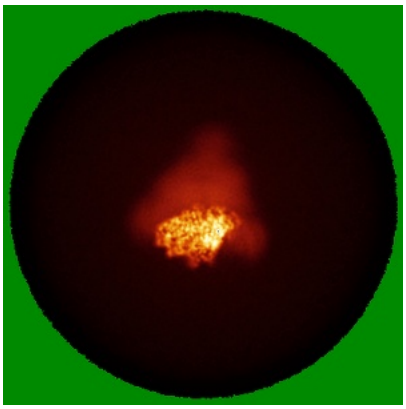
6.4.1 Primary map



X

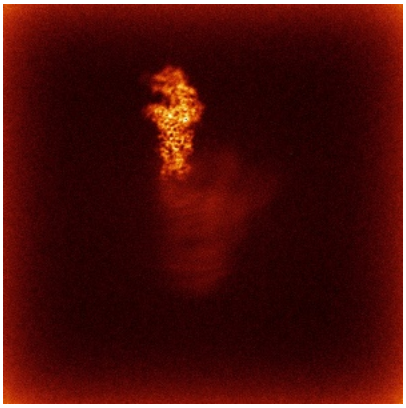


Y

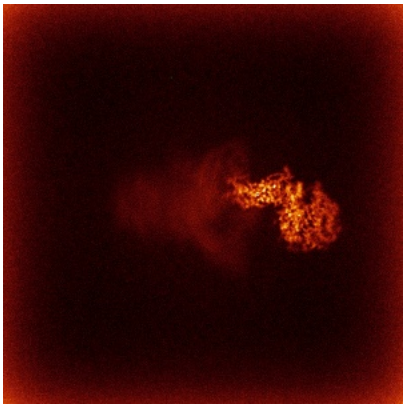


Z

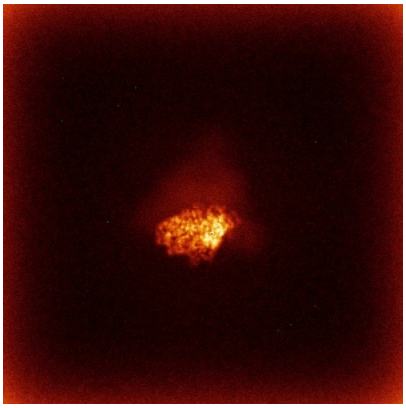
6.4.2 Raw map



X



Y

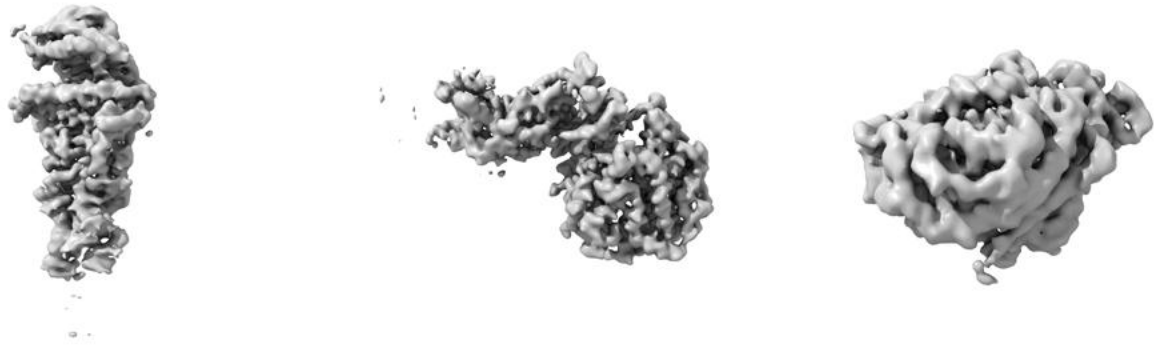


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

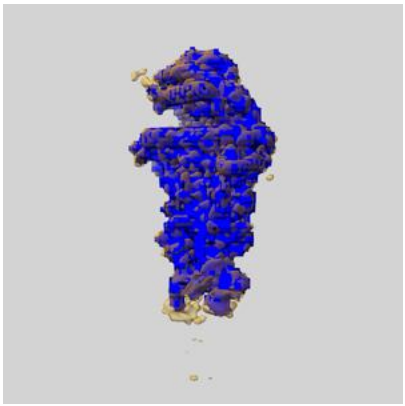
6.6 Mask visualisation (i)

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

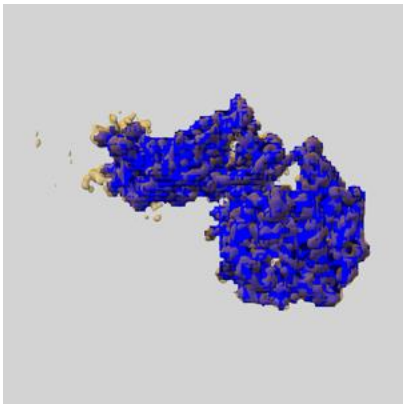
A mask typically either:

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

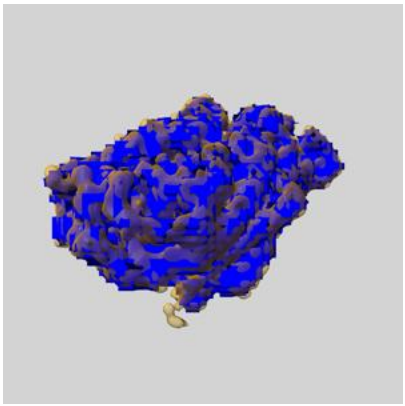
6.6.1 emd_36729_msk_1.map (i)



X



Y

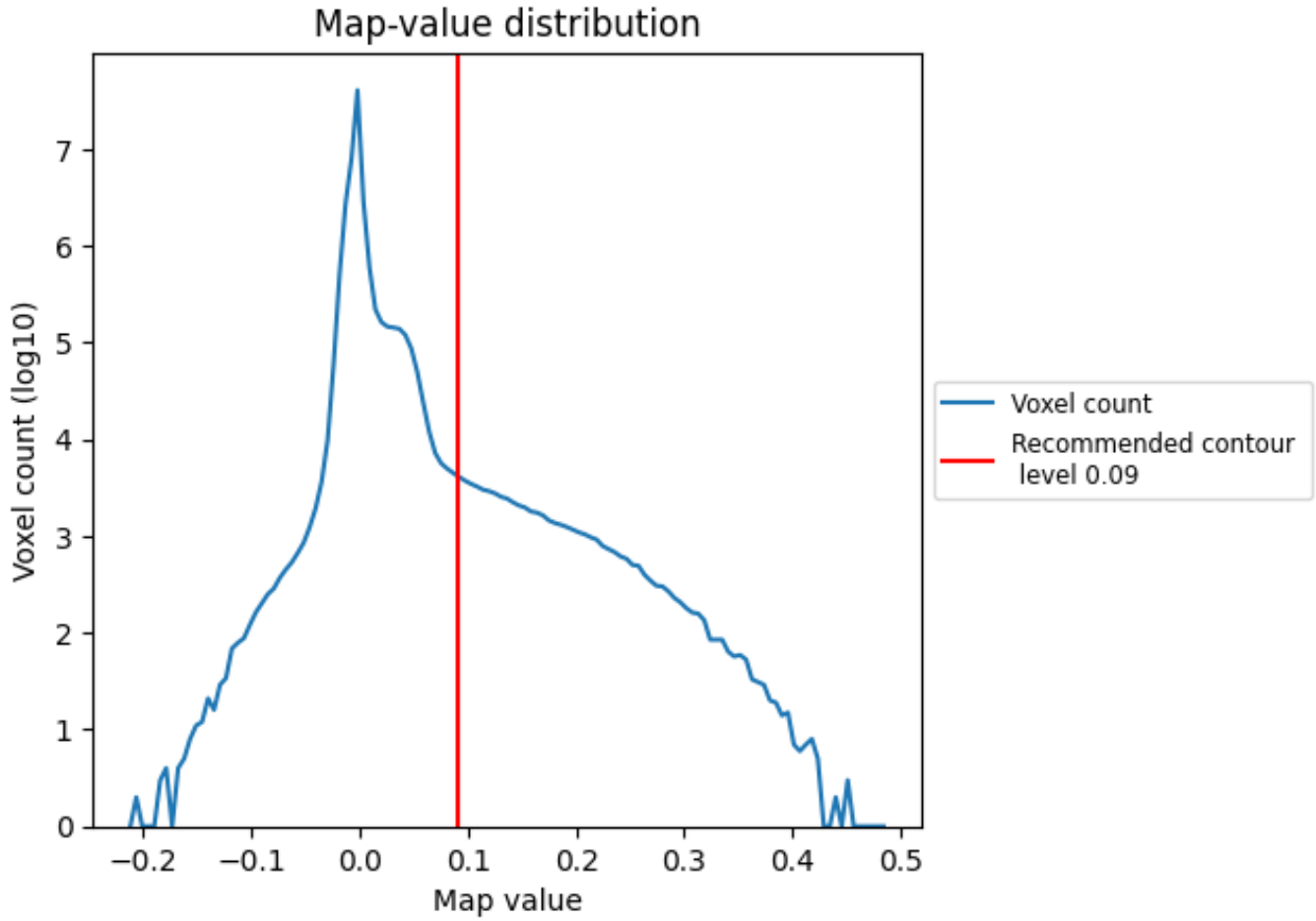


Z

7 Map analysis

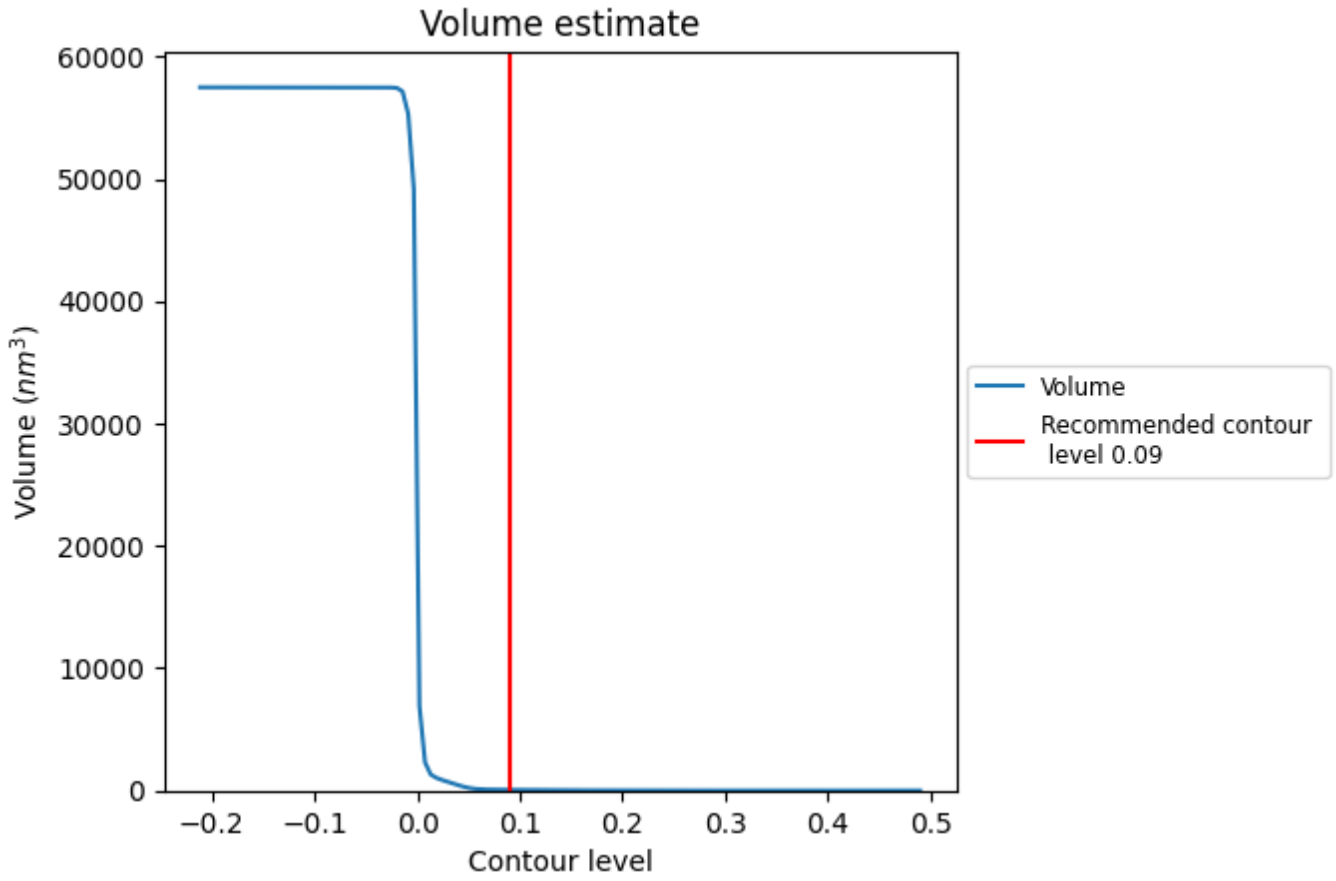
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

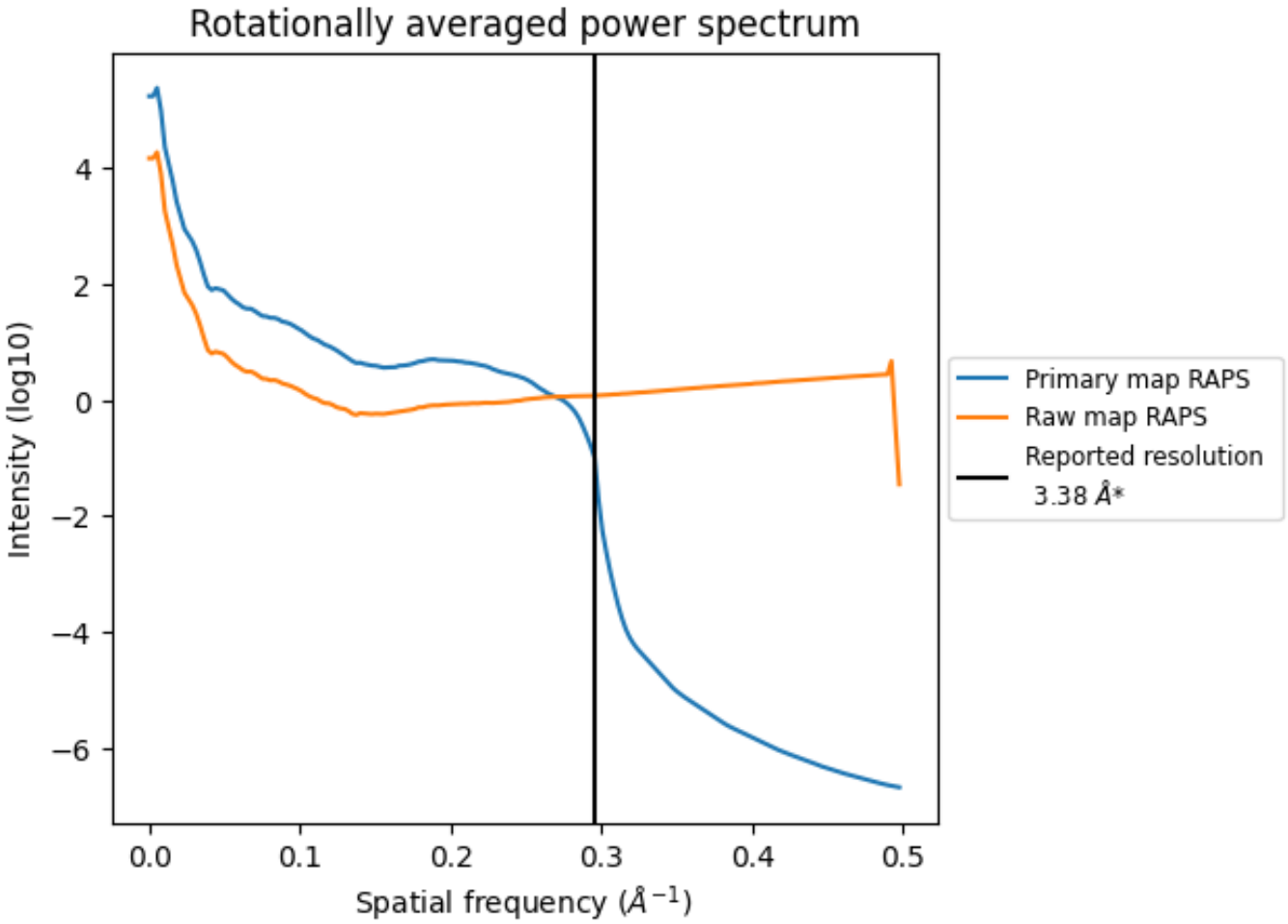
7.2 Volume estimate



The volume at the recommended contour level is 61 nm^3; this corresponds to an approximate mass of 55 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)

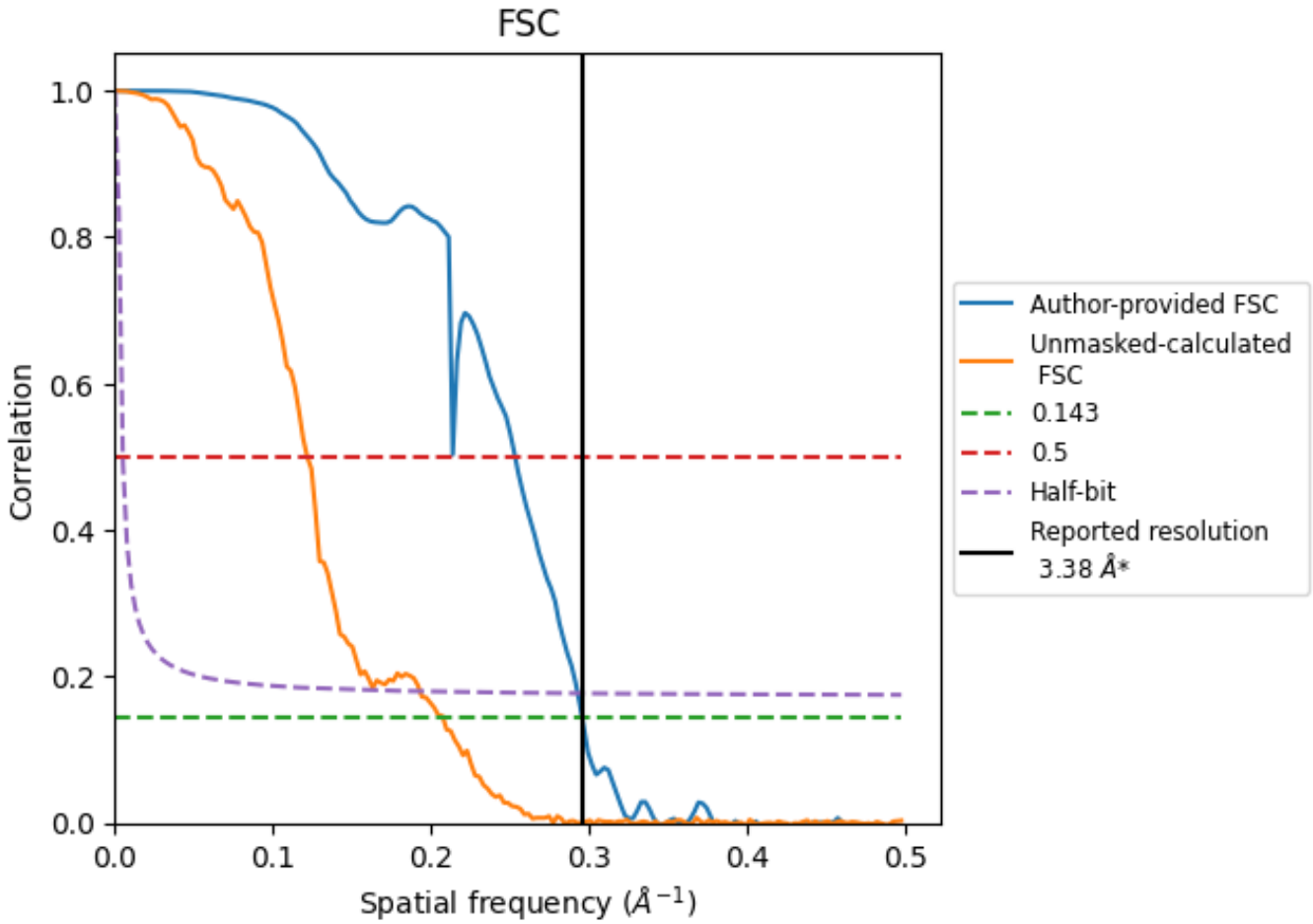


*Reported resolution corresponds to spatial frequency of 0.296 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.296 Å^{-1}

8.2 Resolution estimates (i)

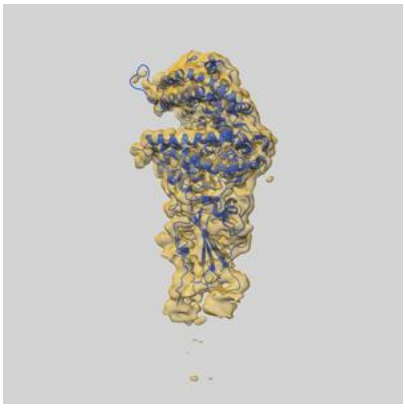
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	3.38	3.95	3.42
Unmasked-calculated*	4.81	8.22	5.18

*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 4.81 differs from the reported value 3.38 by more than 10 %

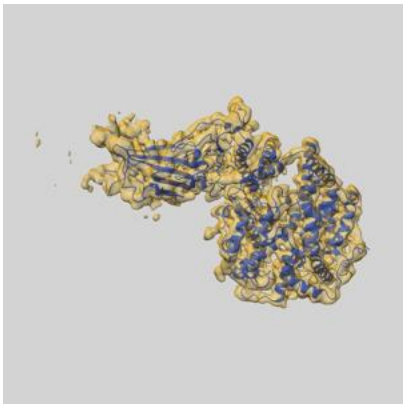
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36729 and PDB model 8JYP. Per-residue inclusion information can be found in section 3 on page 8.

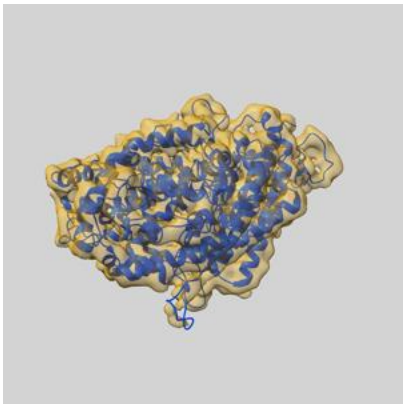
9.1 Map-model overlay



X



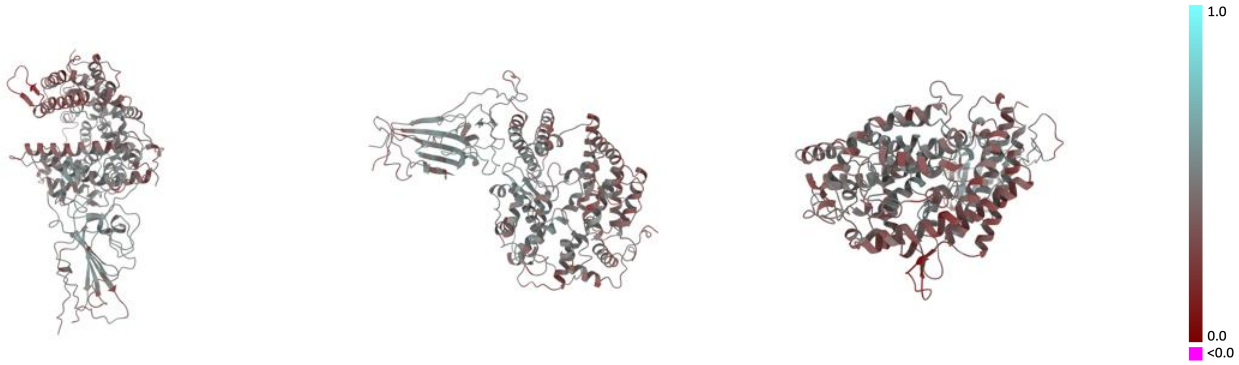
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

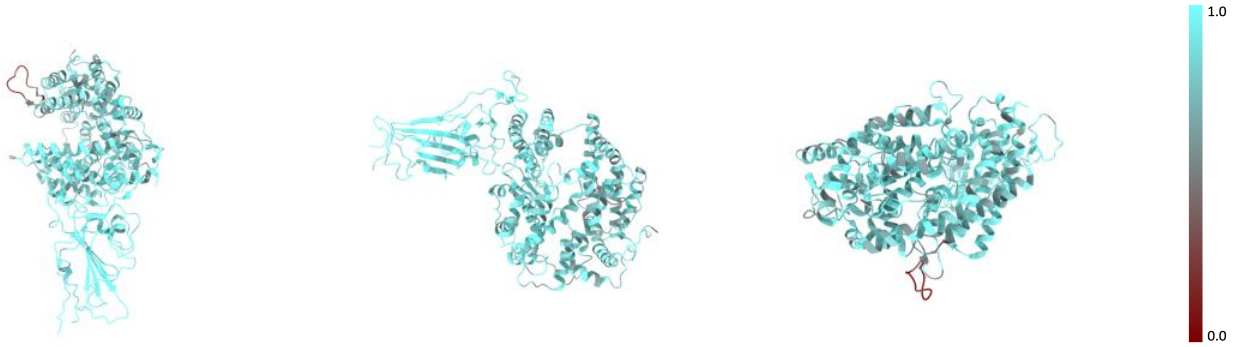
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

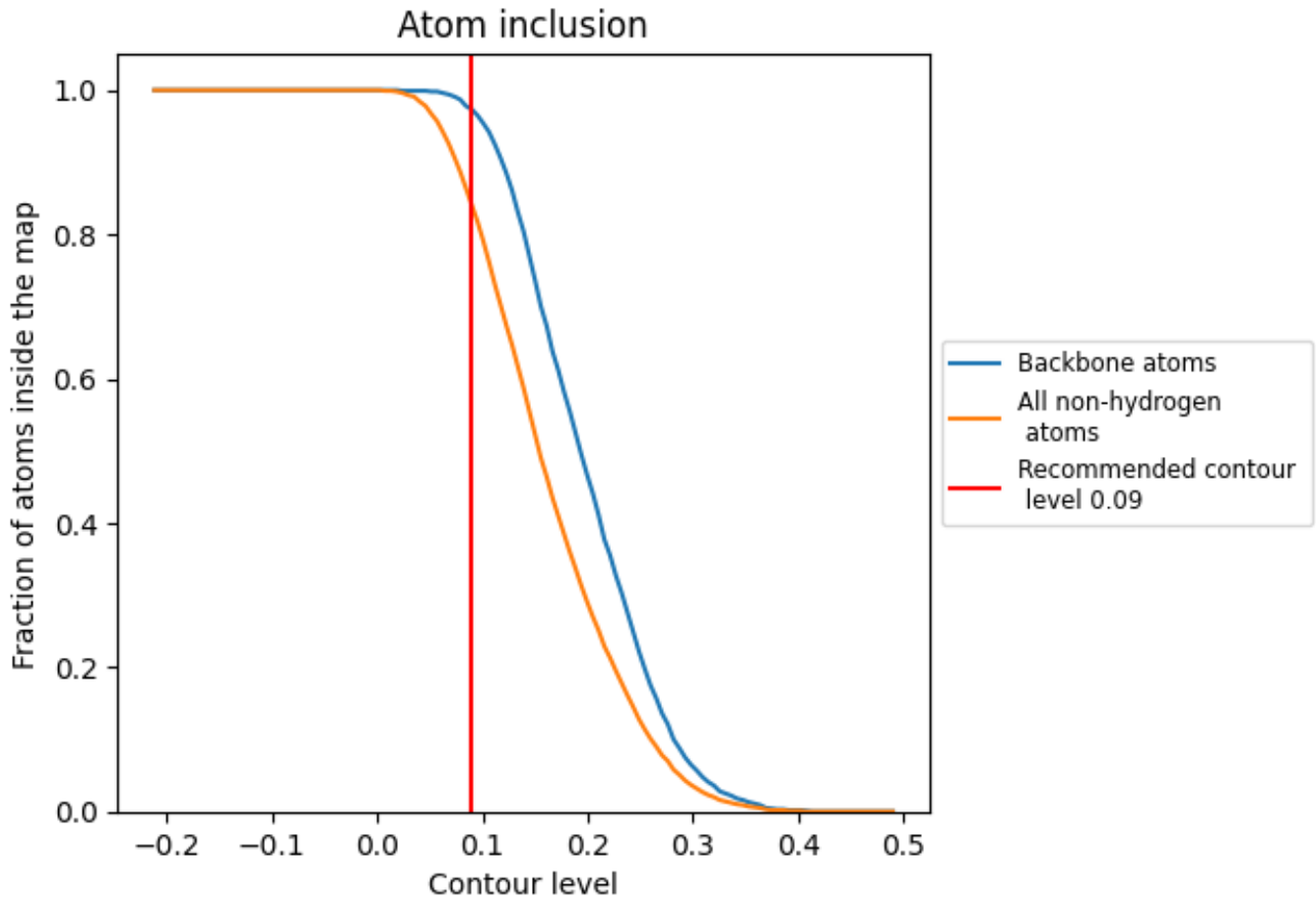
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 84% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.4300
A	0.9300	0.4710
B	0.6070	0.4150
C	0.6150	0.4290
D	0.8220	0.4170
E	0.3440	0.4400