Full wwPDB EM Validation Report

Apr 17, 2025 – 04:47 PM EDT

PDB ID	:	9BLK / pdb_00009blk
EMDB ID	:	EMD-44658
Title	:	HCoV-OC43 Spike glycoprotein
Authors	:	Torrents de la Pena, A.; Sewall, L.M.; Ward, A.B.
Deposited on	:	2024-04-30
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

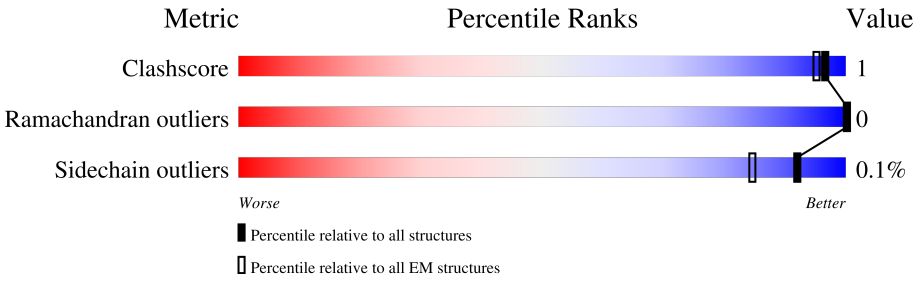
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	1363	7% 82% . 14%
1	B	1363	7% 82% . 14%
1	C	1363	7% 82% . 14%
2	D	3	67% 100%
2	F	3	67% 100%
2	H	3	67% 100%
3	E	2	50% 100%
3	G	2	50% 100%

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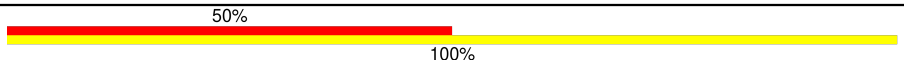
Mol	Chain	Length	Quality of chain
3	I	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28035 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	A	1173	Total	C	N	O	S	0	0
			9138	5826	1503	1748	61		
1	B	1173	Total	C	N	O	S	0	0
			9138	5826	1503	1748	61		
1	C	1173	Total	C	N	O	S	0	0
			9138	5826	1503	1748	61		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	VAL	ASP	conflict	UNP Q696P8
A	505	SER	GLY	conflict	UNP Q696P8
A	507	LEU	-	insertion	UNP Q696P8
A	532	HIS	ASP	conflict	UNP Q696P8
A	712	UNK	-	insertion	UNP Q696P8
A	768	ARG	GLY	conflict	UNP Q696P8
A	1237	THR	ILE	conflict	UNP Q696P8
A	1244	ARG	LYS	conflict	UNP Q696P8
A	1315	GLY	CYS	conflict	UNP Q696P8
A	1364	HIS	-	expression tag	UNP Q696P8
A	1365	HIS	-	expression tag	UNP Q696P8
A	1366	HIS	-	expression tag	UNP Q696P8
A	1367	HIS	-	expression tag	UNP Q696P8
A	1368	HIS	-	expression tag	UNP Q696P8
A	1369	HIS	-	expression tag	UNP Q696P8
A	1370	HIS	-	expression tag	UNP Q696P8
A	1371	HIS	-	expression tag	UNP Q696P8
B	152	VAL	ASP	conflict	UNP Q696P8
B	505	SER	GLY	conflict	UNP Q696P8
B	507	LEU	-	insertion	UNP Q696P8
B	532	HIS	ASP	conflict	UNP Q696P8
B	712	UNK	-	insertion	UNP Q696P8
B	768	ARG	GLY	conflict	UNP Q696P8
B	1237	THR	ILE	conflict	UNP Q696P8

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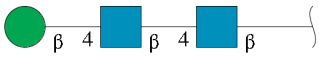
Chain	Residue	Modelled	Actual	Comment	Reference
B	1244	ARG	LYS	conflict	UNP Q696P8
B	1315	GLY	CYS	conflict	UNP Q696P8
B	1364	HIS	-	expression tag	UNP Q696P8
B	1365	HIS	-	expression tag	UNP Q696P8
B	1366	HIS	-	expression tag	UNP Q696P8
B	1367	HIS	-	expression tag	UNP Q696P8
B	1368	HIS	-	expression tag	UNP Q696P8
B	1369	HIS	-	expression tag	UNP Q696P8
B	1370	HIS	-	expression tag	UNP Q696P8
B	1371	HIS	-	expression tag	UNP Q696P8
C	152	VAL	ASP	conflict	UNP Q696P8
C	505	SER	GLY	conflict	UNP Q696P8
C	507	LEU	-	insertion	UNP Q696P8
C	532	HIS	ASP	conflict	UNP Q696P8
C	712	UNK	-	insertion	UNP Q696P8
C	768	ARG	GLY	conflict	UNP Q696P8
C	1237	THR	ILE	conflict	UNP Q696P8
C	1244	ARG	LYS	conflict	UNP Q696P8
C	1315	GLY	CYS	conflict	UNP Q696P8
C	1364	HIS	-	expression tag	UNP Q696P8
C	1365	HIS	-	expression tag	UNP Q696P8
C	1366	HIS	-	expression tag	UNP Q696P8
C	1367	HIS	-	expression tag	UNP Q696P8
C	1368	HIS	-	expression tag	UNP Q696P8
C	1369	HIS	-	expression tag	UNP Q696P8
C	1370	HIS	-	expression tag	UNP Q696P8
C	1371	HIS	-	expression tag	UNP Q696P8

- Molecule 2 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.

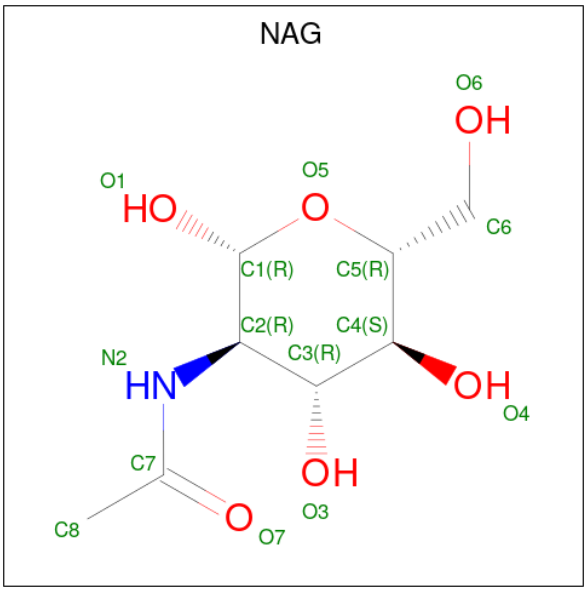


Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	H	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	E	2	Total C N O 28 16 2 10	0	0
3	G	2	Total C N O 28 16 2 10	0	0
3	I	2	Total C N O 28 16 2 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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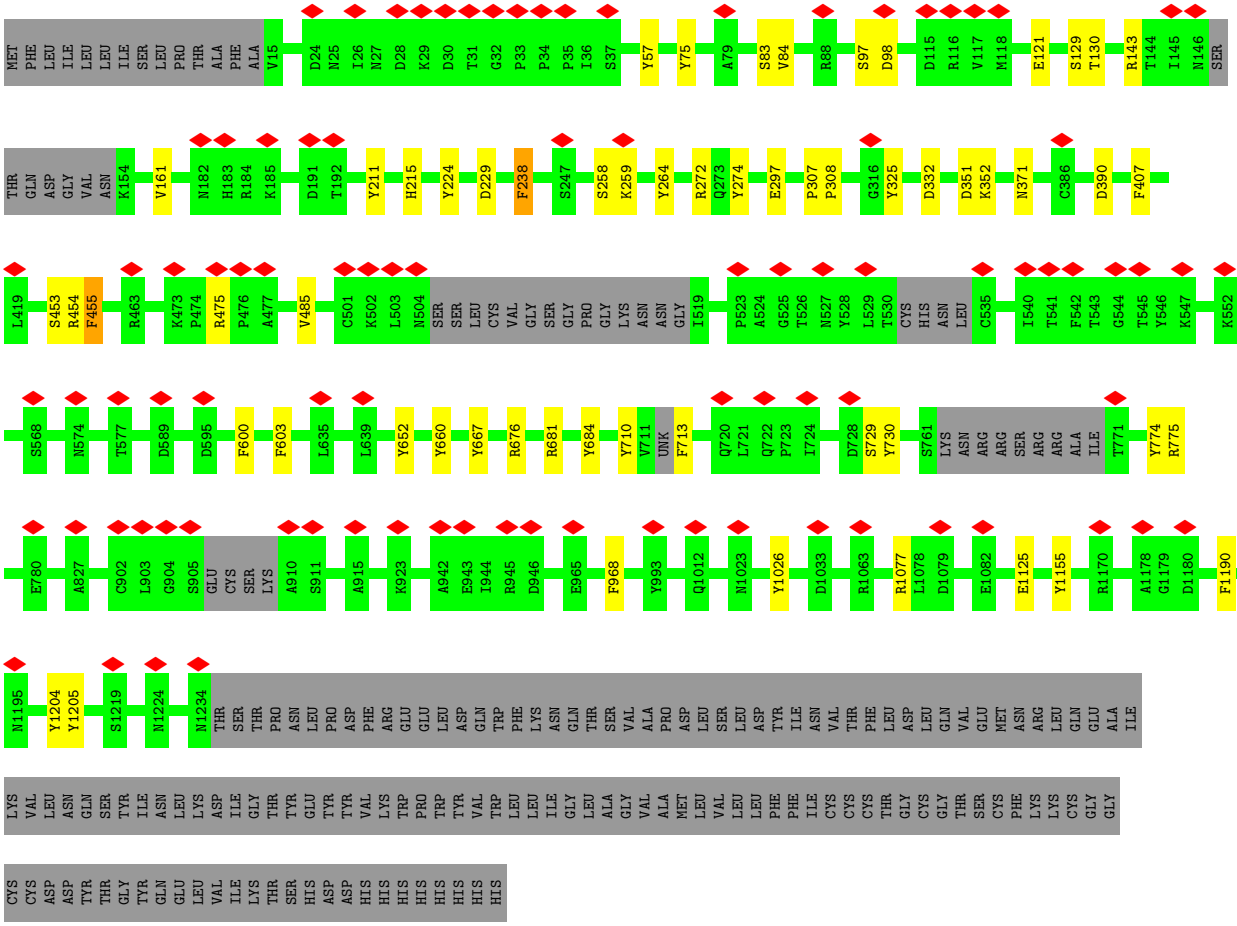
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

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.

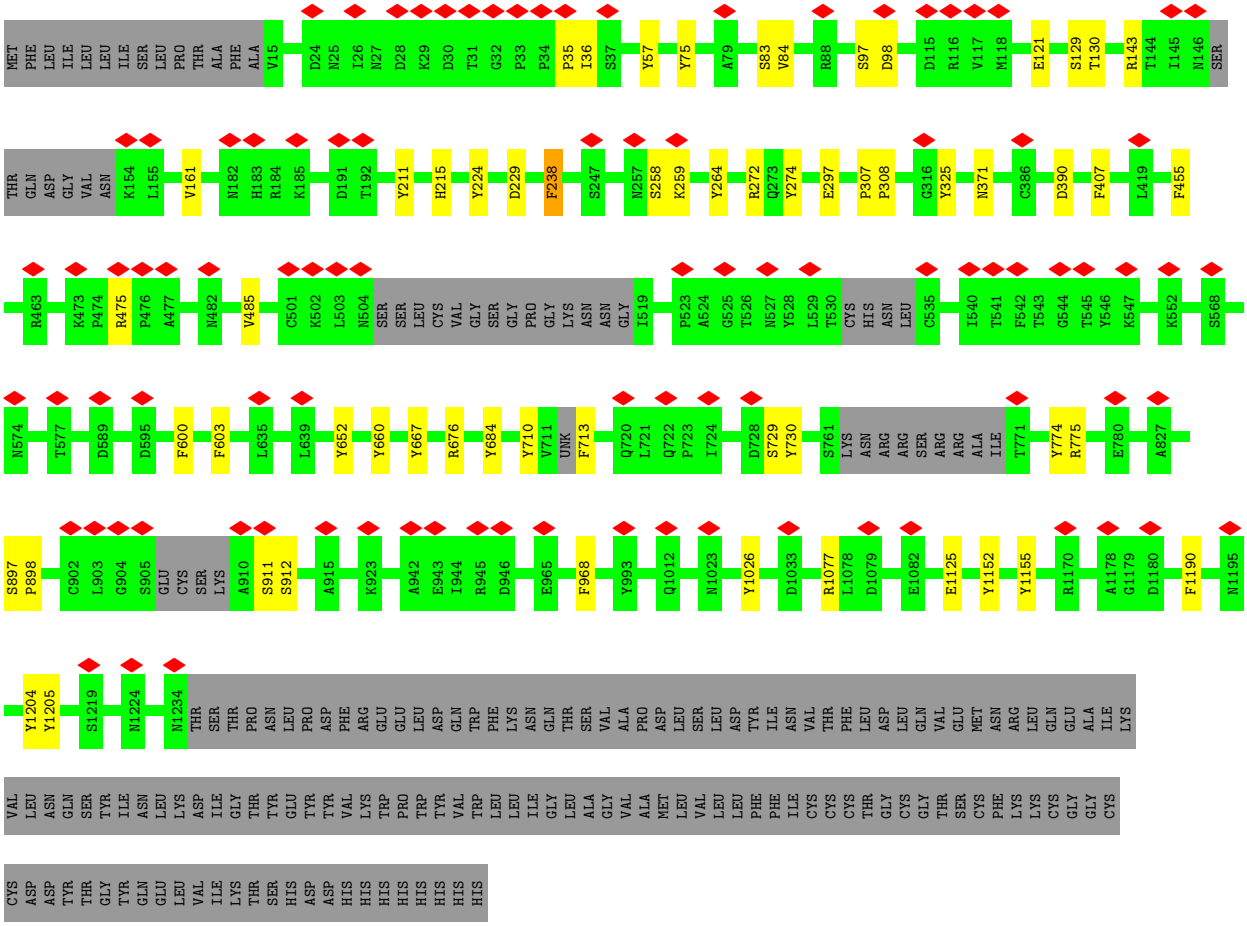
• Molecule 1: Spike glycoprotein

Chain A:



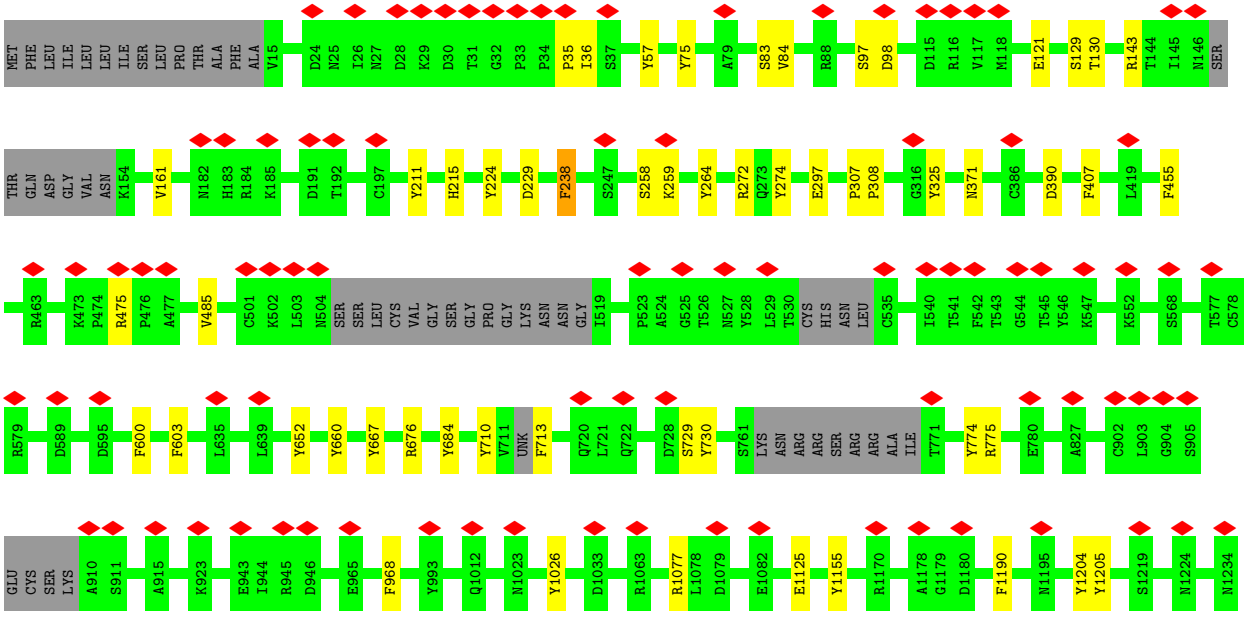
• Molecule 1: Spike glycoprotein

Chain B:



• Molecule 1: Spike glycoprotein

Chain C:



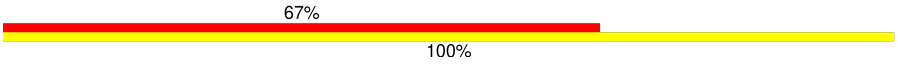
THR SER THR PRO ASN LEU PRO ASP PHE ARG GLU GLU LEU ASP GLN TRP PHE LYS ASN GLN THR SER VAL ALA PRO ASP LEU SER LEU ASP TYR ILE ASN VAL THR PHE LEU ASP LEU GLN VAL GLU MET ASN ARG LEU GLN GLU ALA ILE LYS VAL LEU ASN GLN SER TYR ILE ASN LEU

LYS ASP ILE GLY THR TYR GLU TYR TYR VAL LYS TRP PRO TRP TYR VAL TRP LEU LEU ILE GLY LEU ALA GLY VAL ALA MET LEU LEU VAL LEU LEU PHE PHE ILE CYS CYS CYS THR GLY CYS GLY THR SER CYS PHE LYS LYS CYS GLY GLY CYS CYS ASP ASP TYR THR GLY TYR GLN GLU

LEU VAL ILE LYS THR SER HIS ASP ASP HIS HIS HIS HIS HIS HIS HIS HIS

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

Chain D:



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

Chain F:

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

Chain H:

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

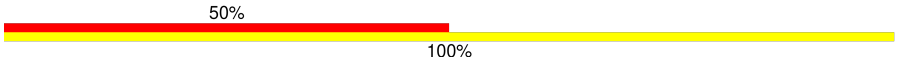
Chain E:

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

Chain G:

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

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	18599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.800	Depositor
Minimum map value	-0.534	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	367.616, 367.616, 367.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.718, 0.718, 0.718	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.13	30/9346 (0.3%)	0.96	21/12725 (0.2%)
1	B	1.12	29/9346 (0.3%)	0.96	21/12725 (0.2%)
1	C	1.12	29/9346 (0.3%)	0.96	20/12725 (0.2%)
All	All	1.12	88/28038 (0.3%)	0.96	62/38175 (0.2%)

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	968	PHE	CB-CG	-7.28	1.39	1.51
1	C	968	PHE	CB-CG	-7.28	1.39	1.51
1	A	968	PHE	CB-CG	-7.21	1.39	1.51
1	A	274	TYR	CD1-CE1	-7.15	1.28	1.39
1	B	274	TYR	CD1-CE1	-7.13	1.28	1.39
1	C	274	TYR	CD1-CE1	-7.12	1.28	1.39
1	B	713	PHE	CG-CD2	6.74	1.48	1.38
1	C	713	PHE	CG-CD2	6.73	1.48	1.38
1	A	274	TYR	CG-CD1	-6.71	1.30	1.39
1	A	713	PHE	CG-CD2	6.71	1.48	1.38
1	C	224	TYR	CB-CG	-6.66	1.41	1.51
1	A	224	TYR	CB-CG	-6.65	1.41	1.51
1	B	224	TYR	CB-CG	-6.63	1.41	1.51
1	C	274	TYR	CG-CD1	-6.62	1.30	1.39
1	B	274	TYR	CG-CD1	-6.59	1.30	1.39
1	B	485	VAL	CB-CG1	-6.24	1.39	1.52
1	A	485	VAL	CB-CG1	-6.24	1.39	1.52
1	C	390	ASP	CB-CG	-6.18	1.38	1.51
1	B	390	ASP	CB-CG	-6.17	1.38	1.51
1	C	485	VAL	CB-CG1	-6.16	1.40	1.52
1	A	390	ASP	CB-CG	-6.11	1.39	1.51
1	C	485	VAL	CB-CG2	-6.10	1.40	1.52
1	B	485	VAL	CB-CG2	-6.10	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	VAL	CB-CG2	-6.08	1.40	1.52
1	A	455	PHE	CB-CG	-6.08	1.41	1.51
1	A	713	PHE	CG-CD1	6.05	1.47	1.38
1	B	455	PHE	CB-CG	-6.05	1.41	1.51
1	C	455	PHE	CB-CG	-6.04	1.41	1.51
1	B	713	PHE	CG-CD1	6.02	1.47	1.38
1	C	713	PHE	CG-CD1	6.01	1.47	1.38
1	A	1190	PHE	CB-CG	-5.95	1.41	1.51
1	C	1125	GLU	CD-OE1	-5.94	1.19	1.25
1	C	1190	PHE	CB-CG	-5.94	1.41	1.51
1	A	238	PHE	CB-CG	-5.94	1.41	1.51
1	B	1190	PHE	CB-CG	-5.92	1.41	1.51
1	B	1125	GLU	CD-OE1	-5.89	1.19	1.25
1	B	238	PHE	CB-CG	-5.88	1.41	1.51
1	C	238	PHE	CB-CG	-5.86	1.41	1.51
1	A	1125	GLU	CD-OE1	-5.83	1.19	1.25
1	C	667	TYR	CE2-CZ	-5.80	1.31	1.38
1	A	667	TYR	CE2-CZ	-5.78	1.31	1.38
1	B	600	PHE	CB-CG	-5.78	1.41	1.51
1	B	667	TYR	CE2-CZ	-5.76	1.31	1.38
1	C	600	PHE	CB-CG	-5.73	1.41	1.51
1	A	652	TYR	CG-CD2	-5.72	1.31	1.39
1	A	600	PHE	CB-CG	-5.72	1.41	1.51
1	C	652	TYR	CG-CD2	-5.70	1.31	1.39
1	B	652	TYR	CG-CD2	-5.70	1.31	1.39
1	A	264	TYR	CG-CD1	-5.51	1.31	1.39
1	C	264	TYR	CG-CD1	-5.50	1.31	1.39
1	B	264	TYR	CG-CD1	-5.43	1.32	1.39
1	B	297	GLU	CD-OE1	-5.39	1.19	1.25
1	A	297	GLU	CD-OE1	-5.39	1.19	1.25
1	C	297	GLU	CD-OE1	-5.38	1.19	1.25
1	A	121	GLU	CD-OE1	-5.29	1.19	1.25
1	A	274	TYR	CE1-CZ	-5.29	1.31	1.38
1	B	274	TYR	CE1-CZ	-5.25	1.31	1.38
1	C	121	GLU	CD-OE1	-5.25	1.19	1.25
1	C	274	TYR	CE1-CZ	-5.24	1.31	1.38
1	B	684	TYR	CG-CD1	-5.24	1.32	1.39
1	B	121	GLU	CD-OE1	-5.23	1.19	1.25
1	B	1204	TYR	CB-CG	-5.22	1.43	1.51
1	A	1204	TYR	CG-CD2	-5.22	1.32	1.39
1	B	215	HIS	CB-CG	-5.21	1.40	1.50
1	B	1204	TYR	CG-CD2	-5.21	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1204	TYR	CB-CG	-5.20	1.43	1.51
1	A	215	HIS	CB-CG	-5.19	1.40	1.50
1	B	667	TYR	CD2-CE2	-5.18	1.31	1.39
1	C	215	HIS	CB-CG	-5.18	1.40	1.50
1	B	1026	TYR	CB-CG	-5.17	1.43	1.51
1	C	1204	TYR	CG-CD2	-5.15	1.32	1.39
1	C	667	TYR	CD2-CE2	-5.15	1.31	1.39
1	A	1026	TYR	CB-CG	-5.15	1.44	1.51
1	A	1204	TYR	CB-CG	-5.13	1.44	1.51
1	C	684	TYR	CG-CD1	-5.13	1.32	1.39
1	A	407	PHE	CB-CG	-5.11	1.42	1.51
1	A	1155	TYR	CE2-CZ	-5.11	1.31	1.38
1	B	1125	GLU	CG-CD	-5.11	1.44	1.51
1	A	667	TYR	CD2-CE2	-5.11	1.31	1.39
1	A	684	TYR	CG-CD1	-5.10	1.32	1.39
1	C	407	PHE	CB-CG	-5.10	1.42	1.51
1	C	1026	TYR	CB-CG	-5.09	1.44	1.51
1	C	1125	GLU	CG-CD	-5.06	1.44	1.51
1	C	1155	TYR	CE2-CZ	-5.05	1.31	1.38
1	B	1155	TYR	CE2-CZ	-5.04	1.31	1.38
1	A	1125	GLU	CG-CD	-5.02	1.44	1.51
1	B	407	PHE	CB-CG	-5.01	1.42	1.51
1	A	667	TYR	CB-CG	-5.01	1.44	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	272	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	A	272	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	272	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	C	475	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	1077	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	475	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	475	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	1077	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	C	1077	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	B	676	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	676	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	676	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	775	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	775	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	775	ARG	NE-CZ-NH2	-6.91	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	667	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	C	325	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	C	1205	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	C	667	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	A	667	TYR	CB-CG-CD2	-6.49	117.10	121.00
1	A	325	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	B	325	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	A	1205	TYR	CB-CG-CD1	-6.37	117.17	121.00
1	B	1205	TYR	CB-CG-CD1	-6.36	117.18	121.00
1	B	660	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	C	660	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	A	660	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	B	143	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	143	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	774	TYR	CB-CG-CD2	-5.44	117.73	121.00
1	A	272	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	272	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	272	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	143	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	774	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	B	603	PHE	CB-CG-CD1	5.35	124.55	120.80
1	C	603	PHE	CB-CG-CD1	5.33	124.53	120.80
1	C	274	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	A	774	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	968	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	C	57	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	274	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	A	603	PHE	CB-CG-CD1	5.31	124.52	120.80
1	B	75	TYR	CA-CB-CG	5.30	123.47	113.40
1	C	75	TYR	CA-CB-CG	5.30	123.46	113.40
1	A	75	TYR	CA-CB-CG	5.28	123.42	113.40
1	A	710	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	B	57	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	57	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	968	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	C	710	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	274	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	C	211	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	C	603	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	C	968	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	B	603	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	A	211	TYR	CB-CG-CD2	-5.17	117.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	710	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	B	211	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	603	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	B	1152	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	681	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	9138	0	8841	18	0
1	B	9138	0	8841	11	0
1	C	9138	0	8841	9	0
2	D	39	0	34	0	0
2	F	39	0	34	0	0
2	H	39	0	34	0	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
4	A	140	0	130	0	0
4	B	140	0	130	0	0
4	C	140	0	130	0	0
All	All	28035	0	27090	38	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 1.

All (38) 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:351:ASP:OD1	1:A:352:LYS:N	1.99	0.95
1:A:453:SER:HB2	1:A:455:PHE:HE2	1.57	0.69
1:A:351:ASP:CG	1:A:352:LYS:H	1.98	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:SER:HB2	1:A:455:PHE:CE2	2.38	0.58
1:A:454:ARG:O	1:A:455:PHE:CG	2.57	0.57
1:B:229:ASP:OD1	1:B:229:ASP:N	2.43	0.52
1:B:729:SER:OG	1:B:730:TYR:N	2.42	0.52
1:C:729:SER:OG	1:C:730:TYR:N	2.42	0.52
1:A:729:SER:OG	1:A:730:TYR:N	2.42	0.51
1:A:229:ASP:OD1	1:A:229:ASP:N	2.43	0.51
1:C:229:ASP:OD1	1:C:229:ASP:N	2.43	0.50
1:A:129:SER:OG	1:A:130:THR:N	2.47	0.47
1:A:161:VAL:HG11	1:A:238:PHE:CE1	2.50	0.47
1:C:161:VAL:HG11	1:C:238:PHE:CE1	2.50	0.46
1:B:161:VAL:HG11	1:B:238:PHE:CE1	2.50	0.46
1:B:129:SER:OG	1:B:130:THR:N	2.47	0.45
1:C:129:SER:OG	1:C:130:THR:N	2.47	0.45
1:A:83:SER:OG	1:A:84:VAL:N	2.49	0.45
1:C:83:SER:OG	1:C:84:VAL:N	2.49	0.45
1:B:83:SER:OG	1:B:84:VAL:N	2.49	0.45
1:A:351:ASP:CG	1:A:352:LYS:N	2.59	0.44
1:B:35:PRO:O	1:B:36:ILE:C	2.56	0.43
1:A:258:SER:OG	1:A:259:LYS:N	2.51	0.43
1:A:454:ARG:C	1:A:455:PHE:CG	2.92	0.43
1:C:258:SER:OG	1:C:259:LYS:N	2.51	0.43
1:B:258:SER:OG	1:B:259:LYS:N	2.51	0.42
1:C:35:PRO:O	1:C:36:ILE:C	2.56	0.42
1:C:307:PRO:HA	1:C:308:PRO:HD3	1.89	0.42
1:A:332:ASP:OD1	1:A:332:ASP:N	2.48	0.42
1:A:454:ARG:O	1:A:455:PHE:CD2	2.72	0.42
1:B:307:PRO:HA	1:B:308:PRO:HD3	1.90	0.42
1:A:454:ARG:C	1:A:455:PHE:CD2	2.93	0.42
1:B:97:SER:OG	1:B:98:ASP:N	2.53	0.41
1:C:97:SER:OG	1:C:98:ASP:N	2.53	0.41
1:A:97:SER:OG	1:A:98:ASP:N	2.53	0.41
1:B:911:SER:OG	1:B:912:SER:N	2.54	0.41
1:B:897:SER:N	1:B:898:PRO:HD2	2.37	0.40
1:A:307:PRO:HA	1:A:308:PRO:HD3	1.90	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	1159/1363 (85%)	1128 (97%)	31 (3%)	0	100	100
1	B	1159/1363 (85%)	1128 (97%)	31 (3%)	0	100	100
1	C	1159/1363 (85%)	1128 (97%)	31 (3%)	0	100	100
All	All	3477/4089 (85%)	3384 (97%)	93 (3%)	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	1021/1190 (86%)	1020 (100%)	1 (0%)	92	98
1	B	1021/1190 (86%)	1020 (100%)	1 (0%)	92	98
1	C	1021/1190 (86%)	1020 (100%)	1 (0%)	92	98
All	All	3063/3570 (86%)	3060 (100%)	3 (0%)	92	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	ASN
1	B	371	ASN
1	C	371	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
1	A	418	GLN
1	B	248	HIS
1	B	418	GLN
1	C	248	HIS
1	C	418	GLN

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)

15 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	1,2	14,14,15	2.05	5 (35%)	17,19,21	0.84	0
2	NAG	D	2	2	14,14,15	2.01	6 (42%)	17,19,21	0.96	2 (11%)
2	BMA	D	3	2	11,11,12	1.88	5 (45%)	15,15,17	0.67	0
3	NAG	E	1	3,1	14,14,15	2.10	4 (28%)	17,19,21	1.11	1 (5%)
3	NAG	E	2	3	14,14,15	1.95	5 (35%)	17,19,21	0.92	1 (5%)
2	NAG	F	1	1,2	14,14,15	2.05	4 (28%)	17,19,21	0.85	0
2	NAG	F	2	2	14,14,15	2.01	6 (42%)	17,19,21	0.97	2 (11%)
2	BMA	F	3	2	11,11,12	1.86	5 (45%)	15,15,17	0.67	0
3	NAG	G	1	3,1	14,14,15	2.11	4 (28%)	17,19,21	1.12	1 (5%)
3	NAG	G	2	3	14,14,15	1.95	4 (28%)	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	H	1	1,2	14,14,15	2.04	5 (35%)	17,19,21	0.84	0
2	NAG	H	2	2	14,14,15	2.01	6 (42%)	17,19,21	0.97	2 (11%)
2	BMA	H	3	2	11,11,12	1.88	5 (45%)	15,15,17	0.67	0
3	NAG	I	1	3,1	14,14,15	2.10	4 (28%)	17,19,21	1.11	1 (5%)
3	NAG	I	2	3	14,14,15	1.94	4 (28%)	17,19,21	0.93	1 (5%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	5.89	1.60	1.52
3	G	1	NAG	C1-C2	5.89	1.60	1.52
3	I	1	NAG	C1-C2	5.87	1.60	1.52
2	D	1	NAG	C1-C2	5.79	1.60	1.52
2	F	1	NAG	C1-C2	5.72	1.60	1.52
2	H	1	NAG	C1-C2	5.67	1.60	1.52
3	G	2	NAG	C1-C2	4.49	1.58	1.52
3	I	2	NAG	C1-C2	4.49	1.58	1.52
2	D	2	NAG	C1-C2	4.47	1.58	1.52
2	H	2	NAG	C1-C2	4.45	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	4.43	1.58	1.52
2	F	2	NAG	C1-C2	4.42	1.58	1.52
2	D	3	BMA	O5-C5	3.24	1.49	1.43
2	F	3	BMA	O5-C5	3.22	1.49	1.43
2	H	3	BMA	O5-C5	3.18	1.49	1.43
3	E	2	NAG	O5-C5	3.17	1.49	1.43
3	I	2	NAG	O5-C5	3.14	1.49	1.43
3	G	2	NAG	O5-C5	3.14	1.49	1.43
2	F	2	NAG	O5-C5	3.01	1.49	1.43
2	D	2	NAG	O5-C5	3.00	1.49	1.43
2	H	2	NAG	O5-C5	2.98	1.49	1.43
2	D	3	BMA	C2-C3	2.80	1.56	1.52
2	H	3	BMA	C2-C3	2.80	1.56	1.52
2	F	3	BMA	C2-C3	2.73	1.56	1.52
2	H	1	NAG	O5-C5	2.65	1.48	1.43
2	H	3	BMA	C1-C2	2.63	1.58	1.52
2	F	3	BMA	C1-C2	2.60	1.58	1.52
2	F	1	NAG	O5-C5	2.60	1.48	1.43
2	D	3	BMA	C1-C2	2.60	1.58	1.52
2	H	2	NAG	C4-C5	2.57	1.58	1.53
2	D	1	NAG	O5-C5	2.57	1.48	1.43
2	F	2	NAG	C4-C5	2.55	1.58	1.53
2	D	2	NAG	C4-C5	2.54	1.58	1.53
2	H	2	NAG	C3-C2	2.49	1.57	1.52
2	F	2	NAG	C3-C2	2.48	1.57	1.52
2	D	2	NAG	C3-C2	2.47	1.57	1.52
3	I	2	NAG	C3-C2	2.44	1.57	1.52
3	G	2	NAG	C3-C2	2.42	1.57	1.52
3	E	2	NAG	C3-C2	2.42	1.57	1.52
2	H	3	BMA	C4-C5	2.39	1.58	1.53
2	F	3	BMA	C4-C5	2.35	1.58	1.53
3	G	2	NAG	C4-C5	2.34	1.58	1.53
2	D	3	BMA	C4-C5	2.34	1.58	1.53
3	I	2	NAG	C4-C5	2.33	1.58	1.53
3	I	1	NAG	O5-C5	2.31	1.47	1.43
3	E	2	NAG	C4-C5	2.30	1.57	1.53
3	I	1	NAG	C4-C5	2.28	1.57	1.53
3	G	1	NAG	C4-C5	2.28	1.57	1.53
2	F	2	NAG	C4-C3	2.27	1.58	1.52
3	E	1	NAG	C3-C2	2.26	1.57	1.52
3	G	1	NAG	C3-C2	2.26	1.57	1.52
2	H	1	NAG	O5-C1	2.26	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O5-C1	2.26	1.47	1.43
3	E	1	NAG	O5-C5	2.24	1.47	1.43
3	G	1	NAG	O5-C5	2.24	1.47	1.43
3	E	1	NAG	C4-C5	2.24	1.57	1.53
3	I	1	NAG	C3-C2	2.24	1.57	1.52
2	H	2	NAG	C4-C3	2.23	1.58	1.52
2	D	2	NAG	C4-C3	2.23	1.58	1.52
2	D	1	NAG	O5-C1	2.22	1.47	1.43
2	D	2	NAG	C2-N2	2.17	1.49	1.46
2	H	2	NAG	C2-N2	2.14	1.49	1.46
2	F	2	NAG	C2-N2	2.13	1.49	1.46
2	D	3	BMA	O5-C1	2.11	1.47	1.43
2	H	3	BMA	O5-C1	2.09	1.47	1.43
2	H	1	NAG	C3-C2	2.07	1.56	1.52
2	F	3	BMA	O5-C1	2.05	1.47	1.43
2	F	1	NAG	C3-C2	2.03	1.56	1.52
3	E	2	NAG	O5-C1	2.02	1.47	1.43
2	D	1	NAG	C3-C2	2.02	1.56	1.52
2	H	1	NAG	C4-C5	2.02	1.57	1.53
2	D	1	NAG	C4-C5	2.00	1.57	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	C1-O5-C5	2.56	115.62	112.19
3	G	1	NAG	C1-O5-C5	2.54	115.59	112.19
3	I	1	NAG	C1-O5-C5	2.53	115.58	112.19
2	F	2	NAG	C8-C7-N2	2.39	120.08	116.12
2	D	2	NAG	C8-C7-N2	2.39	120.07	116.12
2	H	2	NAG	C8-C7-N2	2.38	120.06	116.12
3	I	2	NAG	C8-C7-N2	2.17	119.72	116.12
3	G	2	NAG	C8-C7-N2	2.14	119.67	116.12
3	E	2	NAG	C8-C7-N2	2.12	119.63	116.12
2	D	2	NAG	O7-C7-C8	-2.04	118.42	122.05
2	F	2	NAG	O7-C7-C8	-2.03	118.43	122.05
2	H	2	NAG	O7-C7-C8	-2.02	118.45	122.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	BMA	O5-C5-C6-O6

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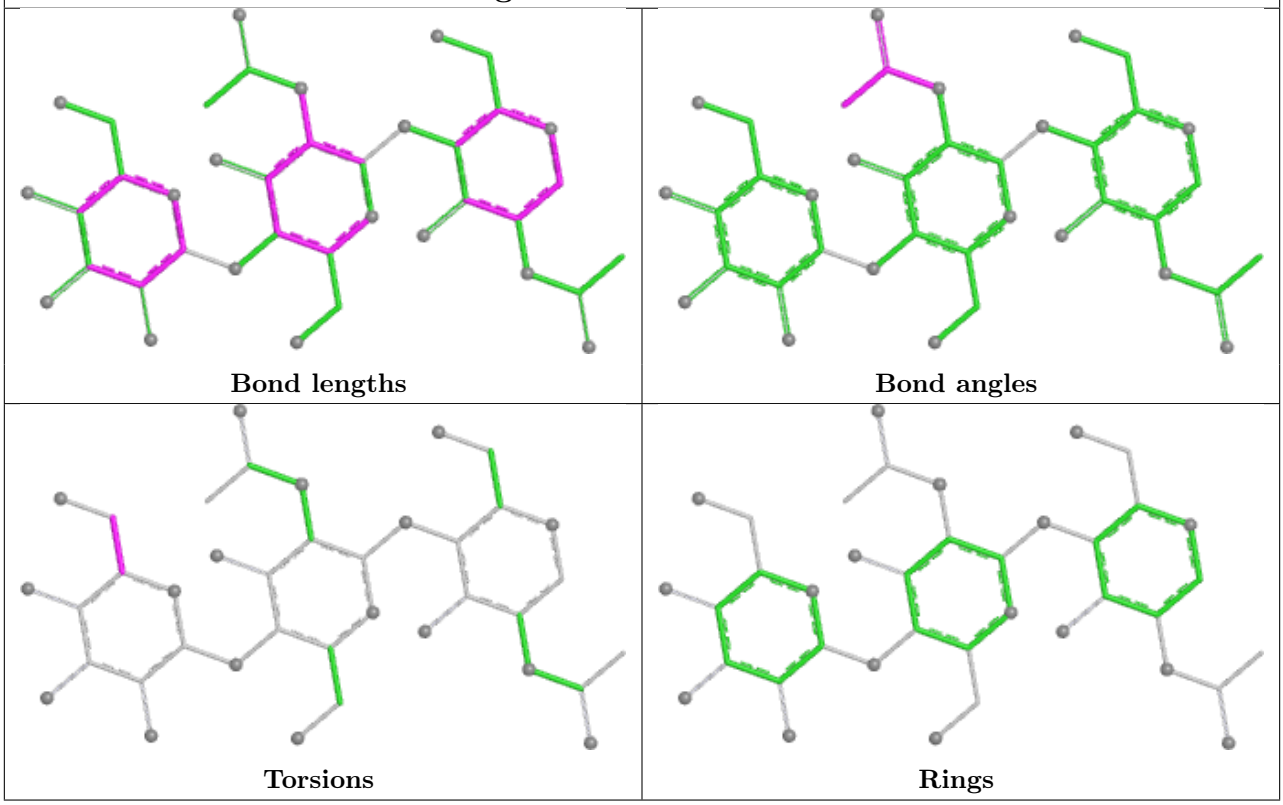
Mol	Chain	Res	Type	Atoms
2	F	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6

There are no ring outliers.

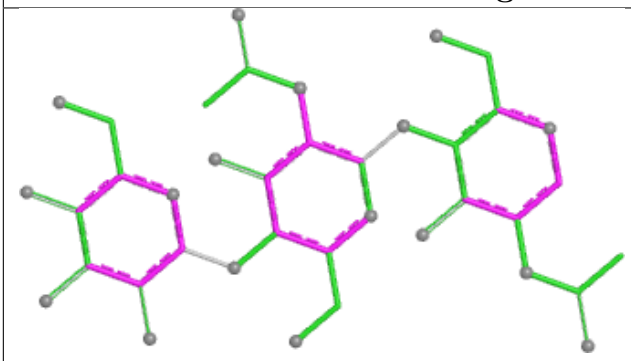
No monomer is involved in short contacts.

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

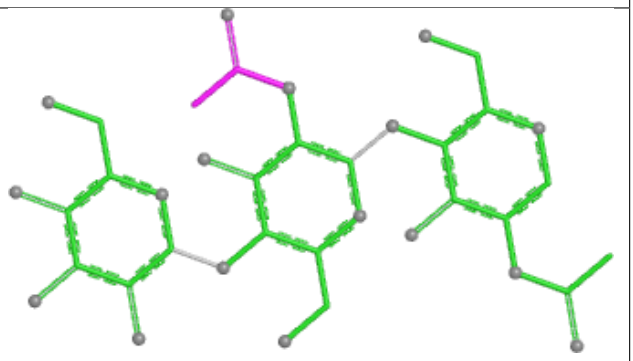
Oligosaccharide Chain D



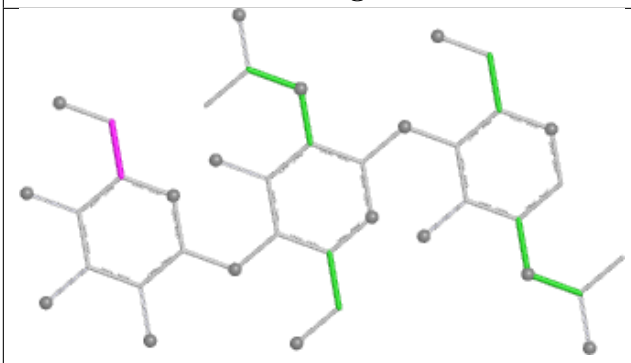
Oligosaccharide Chain F



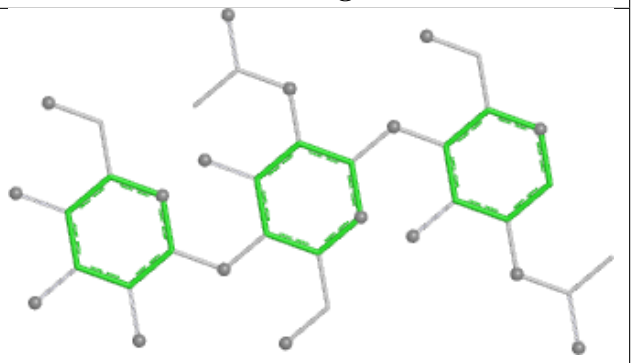
Bond lengths



Bond angles

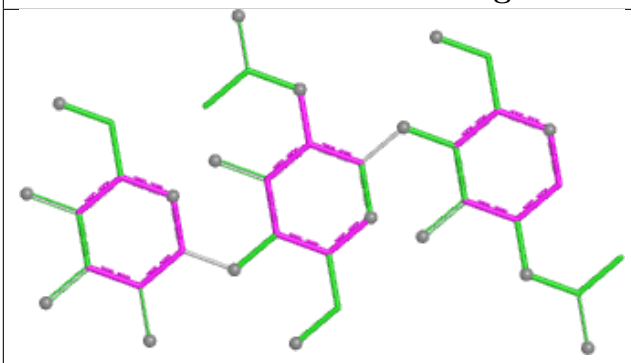


Torsions

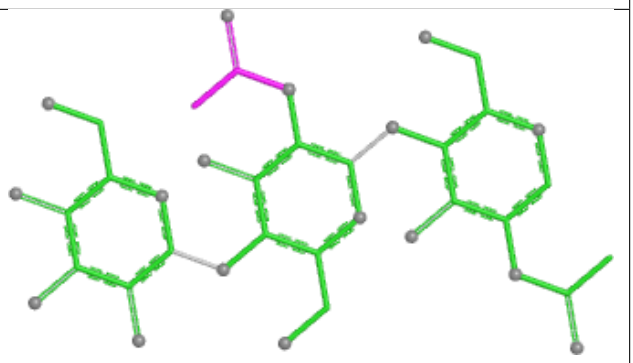


Rings

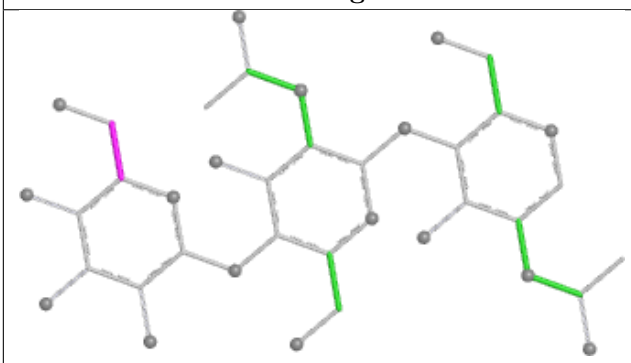
Oligosaccharide Chain H



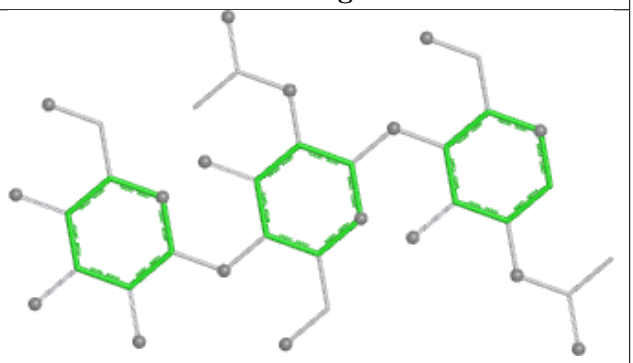
Bond lengths



Bond angles

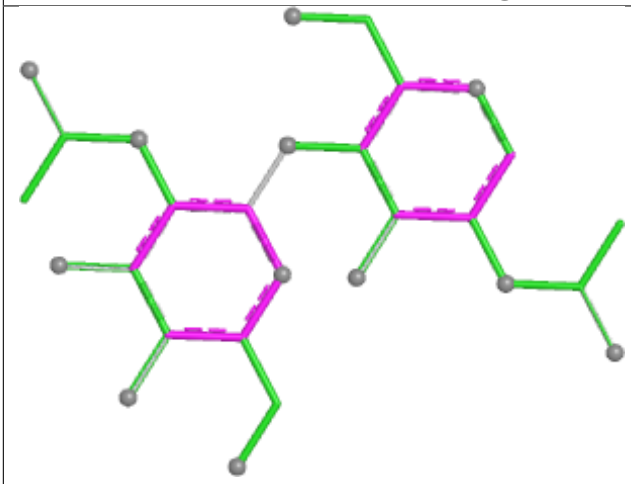


Torsions

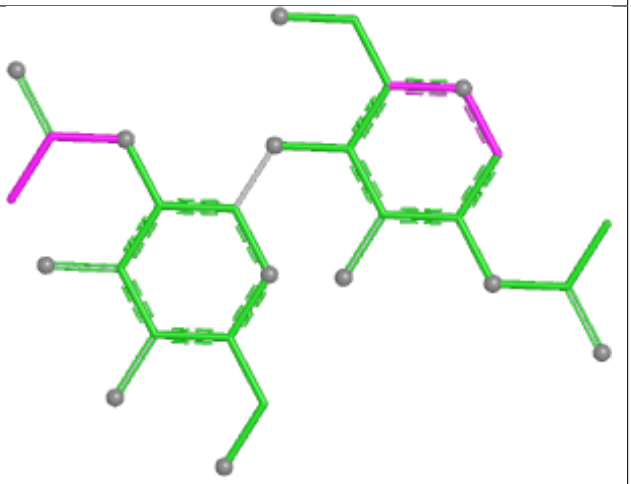


Rings

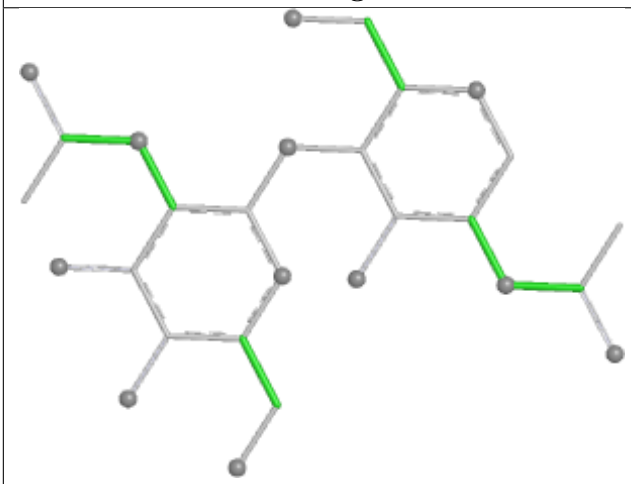
Oligosaccharide Chain E



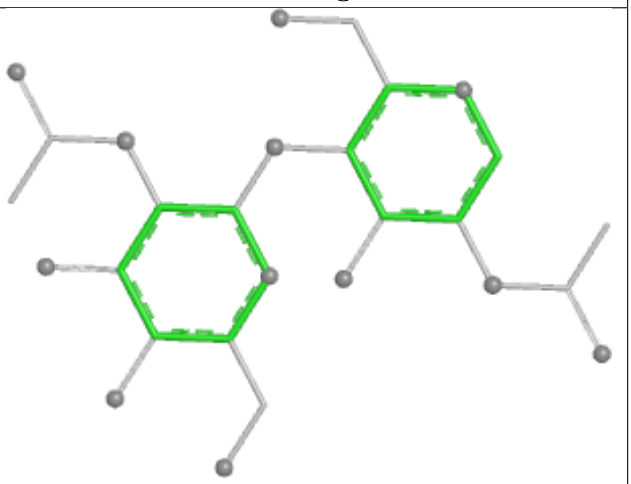
Bond lengths



Bond angles

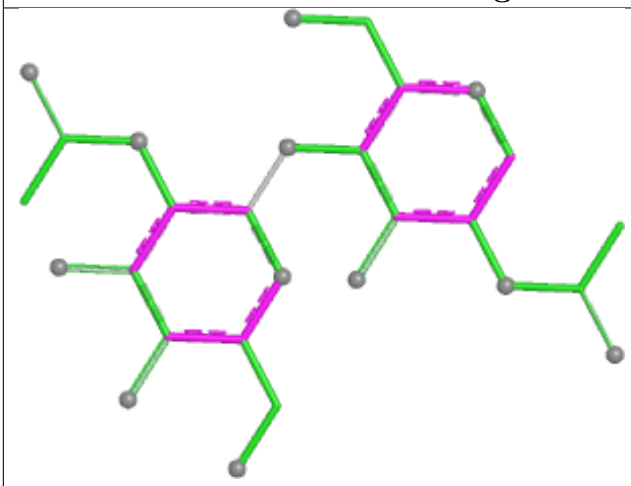


Torsions

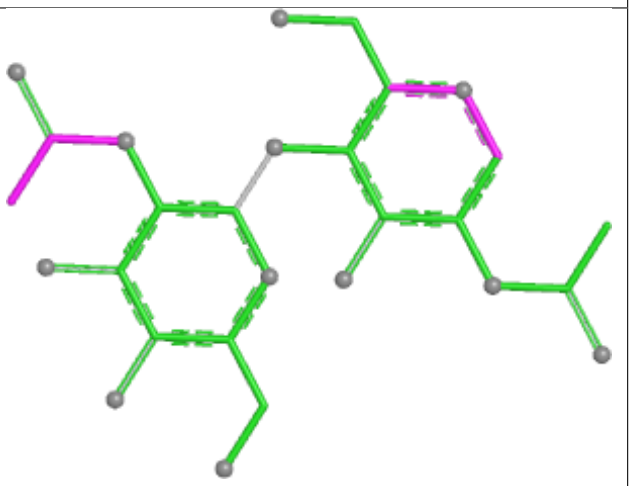


Rings

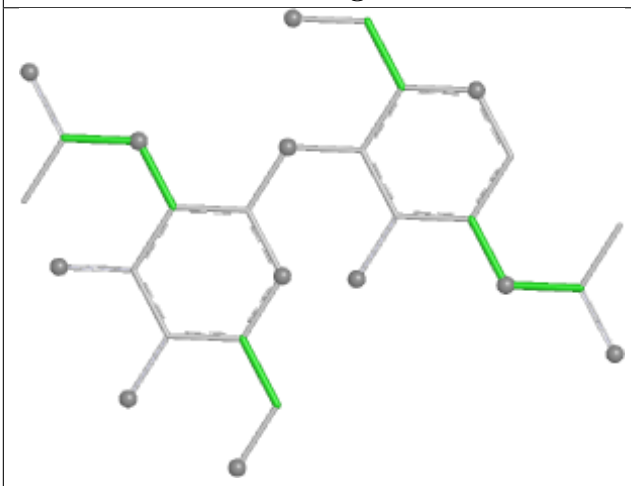
Oligosaccharide Chain G



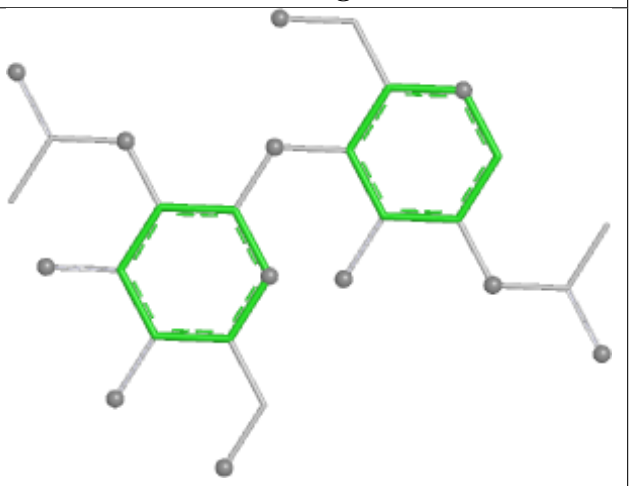
Bond lengths



Bond angles

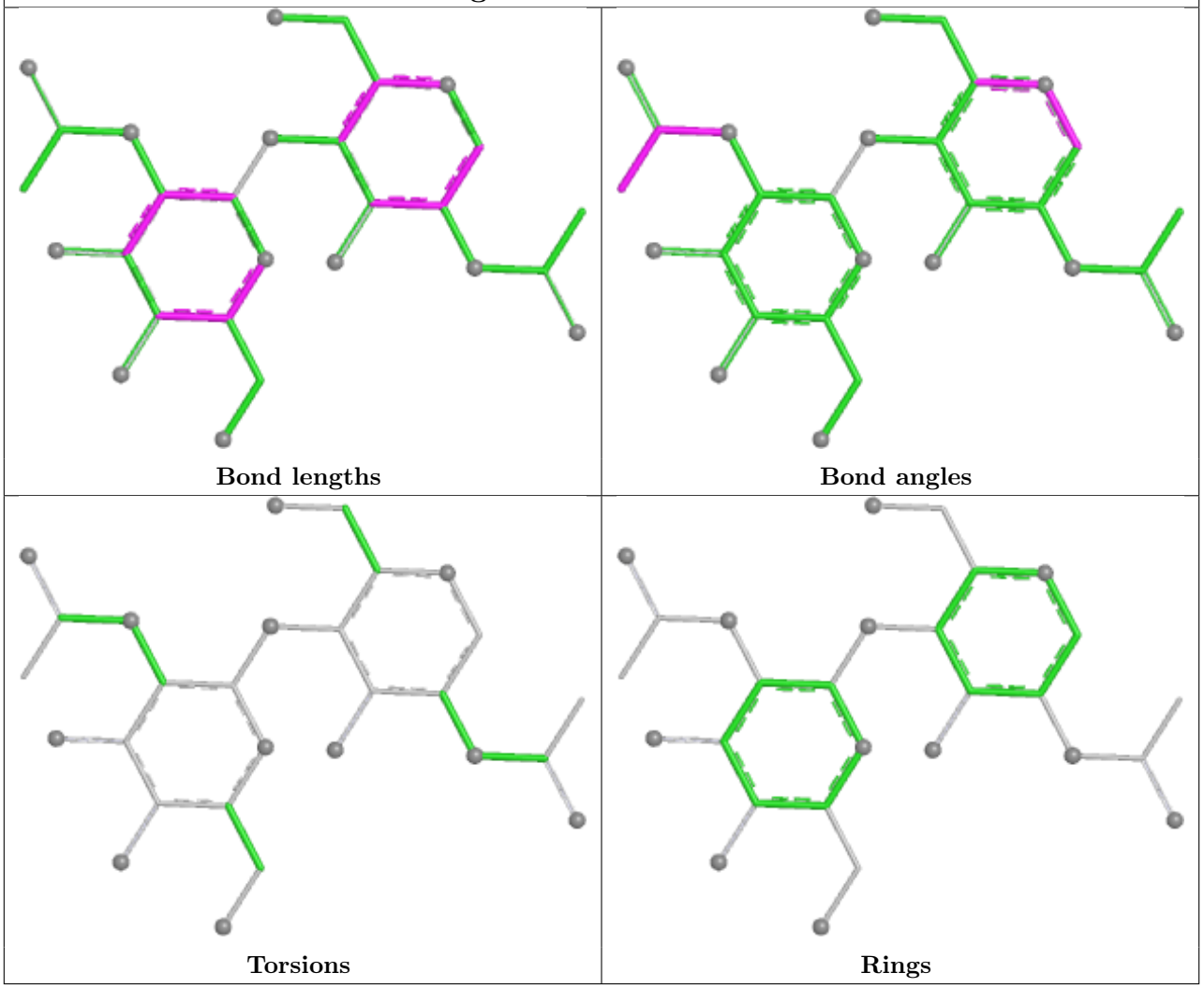


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

30 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	$\#\|Z\| > 2$
4	NAG	B	1406	1	14,14,15	2.20	6 (42%)	17,19,21	1.05	2 (11%)
4	NAG	A	1406	1	14,14,15	2.21	6 (42%)	17,19,21	1.05	2 (11%)
4	NAG	C	1405	1	14,14,15	2.17	5 (35%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1410	1	14,14,15	2.25	5 (35%)	17,19,21	0.89	0
4	NAG	A	1404	1	14,14,15	2.08	5 (35%)	17,19,21	1.09	1 (5%)
4	NAG	B	1409	1	14,14,15	2.29	4 (28%)	17,19,21	1.16	2 (11%)
4	NAG	A	1409	1	14,14,15	2.30	5 (35%)	17,19,21	1.15	2 (11%)
4	NAG	C	1402	1	14,14,15	2.14	5 (35%)	17,19,21	1.00	0
4	NAG	C	1403	1	14,14,15	2.05	5 (35%)	17,19,21	1.19	2 (11%)
4	NAG	C	1404	1	14,14,15	2.08	5 (35%)	17,19,21	1.08	1 (5%)
4	NAG	A	1407	1	14,14,15	2.22	5 (35%)	17,19,21	0.96	1 (5%)
4	NAG	B	1408	1	14,14,15	2.21	4 (28%)	17,19,21	1.02	0
4	NAG	B	1401	1	14,14,15	2.24	4 (28%)	17,19,21	0.92	0
4	NAG	A	1408	1	14,14,15	2.21	5 (35%)	17,19,21	1.02	0
4	NAG	B	1407	1	14,14,15	2.22	5 (35%)	17,19,21	0.95	1 (5%)
4	NAG	A	1402	1	14,14,15	2.16	5 (35%)	17,19,21	1.01	0
4	NAG	C	1409	1	14,14,15	2.29	5 (35%)	17,19,21	1.15	2 (11%)
4	NAG	C	1406	1	14,14,15	2.20	6 (42%)	17,19,21	1.06	2 (11%)
4	NAG	C	1401	1	14,14,15	2.24	4 (28%)	17,19,21	0.92	0
4	NAG	B	1410	1	14,14,15	2.24	5 (35%)	17,19,21	0.90	0
4	NAG	A	1410	1	14,14,15	2.27	5 (35%)	17,19,21	0.89	0
4	NAG	B	1405	1	14,14,15	2.18	5 (35%)	17,19,21	0.86	0
4	NAG	C	1408	1	14,14,15	2.22	4 (28%)	17,19,21	1.02	0
4	NAG	C	1407	1	14,14,15	2.23	5 (35%)	17,19,21	0.96	1 (5%)
4	NAG	A	1405	1	14,14,15	2.18	5 (35%)	17,19,21	0.85	0
4	NAG	B	1403	1	14,14,15	2.07	5 (35%)	17,19,21	1.19	2 (11%)
4	NAG	A	1403	1	14,14,15	2.07	6 (42%)	17,19,21	1.18	2 (11%)
4	NAG	B	1402	1	14,14,15	2.14	5 (35%)	17,19,21	1.01	0
4	NAG	B	1404	1	14,14,15	2.07	5 (35%)	17,19,21	1.09	1 (5%)
4	NAG	A	1401	1	14,14,15	2.25	4 (28%)	17,19,21	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1406	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1405	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	1/6/23/26	0/1/1/1

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1401	NAG	C1-C2	6.25	1.60	1.52
4	A	1409	NAG	C1-C2	6.19	1.60	1.52
4	B	1401	NAG	C1-C2	6.17	1.60	1.52
4	C	1401	NAG	C1-C2	6.16	1.60	1.52
4	B	1409	NAG	C1-C2	6.12	1.60	1.52
4	C	1409	NAG	C1-C2	6.10	1.60	1.52
4	A	1402	NAG	C1-C2	5.97	1.60	1.52
4	C	1402	NAG	C1-C2	5.93	1.60	1.52
4	B	1402	NAG	C1-C2	5.92	1.60	1.52
4	A	1410	NAG	C1-C2	5.90	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1406	NAG	C1-C2	5.88	1.60	1.52
4	C	1408	NAG	C1-C2	5.88	1.60	1.52
4	B	1405	NAG	C1-C2	5.87	1.60	1.52
4	C	1405	NAG	C1-C2	5.86	1.60	1.52
4	C	1406	NAG	C1-C2	5.86	1.60	1.52
4	A	1405	NAG	C1-C2	5.84	1.60	1.52
4	B	1408	NAG	C1-C2	5.84	1.60	1.52
4	B	1410	NAG	C1-C2	5.84	1.60	1.52
4	C	1410	NAG	C1-C2	5.83	1.60	1.52
4	A	1408	NAG	C1-C2	5.80	1.60	1.52
4	B	1406	NAG	C1-C2	5.79	1.60	1.52
4	C	1407	NAG	C1-C2	5.49	1.59	1.52
4	B	1407	NAG	C1-C2	5.48	1.59	1.52
4	A	1407	NAG	C1-C2	5.46	1.59	1.52
4	A	1404	NAG	C1-C2	5.40	1.59	1.52
4	C	1404	NAG	C1-C2	5.35	1.59	1.52
4	B	1404	NAG	C1-C2	5.33	1.59	1.52
4	B	1403	NAG	C1-C2	5.25	1.59	1.52
4	A	1403	NAG	C1-C2	5.24	1.59	1.52
4	C	1403	NAG	C1-C2	5.19	1.59	1.52
4	C	1407	NAG	O5-C5	3.60	1.50	1.43
4	A	1410	NAG	O5-C5	3.59	1.50	1.43
4	B	1407	NAG	O5-C5	3.57	1.50	1.43
4	A	1407	NAG	O5-C5	3.57	1.50	1.43
4	C	1410	NAG	O5-C5	3.55	1.50	1.43
4	C	1408	NAG	O5-C5	3.53	1.50	1.43
4	B	1410	NAG	O5-C5	3.53	1.50	1.43
4	C	1405	NAG	O5-C5	3.49	1.50	1.43
4	A	1405	NAG	O5-C5	3.49	1.50	1.43
4	B	1405	NAG	O5-C5	3.48	1.50	1.43
4	A	1408	NAG	O5-C5	3.47	1.50	1.43
4	B	1408	NAG	O5-C5	3.46	1.50	1.43
4	B	1409	NAG	O5-C5	3.39	1.50	1.43
4	C	1409	NAG	O5-C5	3.36	1.50	1.43
4	A	1409	NAG	O5-C5	3.36	1.50	1.43
4	C	1401	NAG	O5-C5	3.20	1.49	1.43
4	A	1401	NAG	O5-C5	3.17	1.49	1.43
4	B	1406	NAG	O5-C5	3.13	1.49	1.43
4	B	1401	NAG	O5-C5	3.10	1.49	1.43
4	C	1406	NAG	O5-C5	3.10	1.49	1.43
4	B	1404	NAG	O5-C5	3.09	1.49	1.43
4	C	1404	NAG	O5-C5	3.08	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1406	NAG	O5-C5	3.07	1.49	1.43
4	A	1404	NAG	O5-C5	3.03	1.49	1.43
4	B	1403	NAG	O5-C5	2.96	1.49	1.43
4	C	1403	NAG	O5-C5	2.96	1.49	1.43
4	A	1403	NAG	O5-C5	2.95	1.49	1.43
4	C	1409	NAG	O5-C1	2.82	1.48	1.43
4	B	1408	NAG	O5-C1	2.80	1.48	1.43
4	B	1409	NAG	O5-C1	2.79	1.48	1.43
4	A	1409	NAG	O5-C1	2.78	1.48	1.43
4	C	1408	NAG	O5-C1	2.77	1.48	1.43
4	A	1408	NAG	O5-C1	2.75	1.48	1.43
4	C	1407	NAG	O5-C1	2.74	1.48	1.43
4	B	1407	NAG	O5-C1	2.72	1.48	1.43
4	A	1407	NAG	O5-C1	2.70	1.48	1.43
4	C	1410	NAG	O5-C1	2.65	1.48	1.43
4	A	1410	NAG	O5-C1	2.62	1.48	1.43
4	B	1401	NAG	O5-C1	2.60	1.48	1.43
4	B	1410	NAG	O5-C1	2.59	1.48	1.43
4	A	1403	NAG	C3-C2	2.57	1.57	1.52
4	A	1402	NAG	O5-C5	2.57	1.48	1.43
4	C	1403	NAG	C3-C2	2.55	1.57	1.52
4	B	1403	NAG	C3-C2	2.54	1.57	1.52
4	A	1405	NAG	O5-C1	2.54	1.48	1.43
4	B	1406	NAG	C2-N2	2.53	1.50	1.46
4	B	1402	NAG	O5-C5	2.52	1.48	1.43
4	C	1401	NAG	O5-C1	2.51	1.47	1.43
4	A	1401	NAG	O5-C1	2.50	1.47	1.43
4	C	1402	NAG	O5-C5	2.49	1.48	1.43
4	B	1405	NAG	O5-C1	2.48	1.47	1.43
4	C	1405	NAG	O5-C1	2.47	1.47	1.43
4	C	1406	NAG	C2-N2	2.47	1.50	1.46
4	A	1406	NAG	O5-C1	2.43	1.47	1.43
4	A	1402	NAG	C3-C2	2.41	1.57	1.52
4	C	1402	NAG	O5-C1	2.41	1.47	1.43
4	A	1402	NAG	O5-C1	2.41	1.47	1.43
4	A	1407	NAG	C4-C5	2.39	1.58	1.53
4	C	1402	NAG	C3-C2	2.39	1.57	1.52
4	A	1406	NAG	C2-N2	2.39	1.50	1.46
4	B	1402	NAG	O5-C1	2.37	1.47	1.43
4	C	1406	NAG	O5-C1	2.36	1.47	1.43
4	C	1404	NAG	O5-C1	2.35	1.47	1.43
4	B	1407	NAG	C4-C5	2.35	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1406	NAG	O5-C1	2.35	1.47	1.43
4	A	1410	NAG	C4-C5	2.35	1.58	1.53
4	B	1404	NAG	O5-C1	2.34	1.47	1.43
4	B	1402	NAG	C3-C2	2.34	1.57	1.52
4	A	1404	NAG	O5-C1	2.33	1.47	1.43
4	B	1401	NAG	C3-C2	2.32	1.57	1.52
4	C	1404	NAG	C3-C2	2.32	1.57	1.52
4	B	1404	NAG	C3-C2	2.31	1.57	1.52
4	A	1404	NAG	C3-C2	2.31	1.57	1.52
4	C	1407	NAG	C3-C2	2.31	1.57	1.52
4	A	1409	NAG	C3-C2	2.30	1.57	1.52
4	C	1401	NAG	C3-C2	2.30	1.57	1.52
4	C	1407	NAG	C4-C5	2.29	1.57	1.53
4	B	1410	NAG	C4-C5	2.29	1.57	1.53
4	C	1408	NAG	C3-C2	2.29	1.57	1.52
4	B	1407	NAG	C3-C2	2.28	1.57	1.52
4	B	1408	NAG	C3-C2	2.28	1.57	1.52
4	A	1408	NAG	C3-C2	2.28	1.57	1.52
4	C	1410	NAG	C4-C5	2.28	1.57	1.53
4	A	1407	NAG	C3-C2	2.27	1.57	1.52
4	A	1403	NAG	O5-C1	2.26	1.47	1.43
4	A	1401	NAG	C3-C2	2.26	1.57	1.52
4	C	1409	NAG	C3-C2	2.25	1.57	1.52
4	B	1409	NAG	C3-C2	2.24	1.57	1.52
4	C	1403	NAG	O5-C1	2.24	1.47	1.43
4	B	1403	NAG	O5-C1	2.23	1.47	1.43
4	C	1410	NAG	C3-C2	2.22	1.57	1.52
4	A	1410	NAG	C3-C2	2.19	1.57	1.52
4	B	1410	NAG	C3-C2	2.18	1.57	1.52
4	A	1404	NAG	C4-C5	2.18	1.57	1.53
4	A	1405	NAG	C4-C5	2.17	1.57	1.53
4	A	1406	NAG	C3-C2	2.16	1.57	1.52
4	B	1403	NAG	C2-N2	2.15	1.49	1.46
4	B	1406	NAG	C3-C2	2.15	1.57	1.52
4	C	1405	NAG	C4-C5	2.15	1.57	1.53
4	C	1404	NAG	C4-C5	2.14	1.57	1.53
4	B	1405	NAG	C4-C5	2.14	1.57	1.53
4	C	1403	NAG	C2-N2	2.13	1.49	1.46
4	B	1404	NAG	C4-C5	2.13	1.57	1.53
4	A	1403	NAG	C2-N2	2.12	1.49	1.46
4	C	1406	NAG	C3-C2	2.10	1.56	1.52
4	A	1405	NAG	C3-C2	2.09	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1405	NAG	C3-C2	2.05	1.56	1.52
4	A	1408	NAG	C4-C5	2.05	1.57	1.53
4	B	1405	NAG	C3-C2	2.05	1.56	1.52
4	B	1402	NAG	C2-N2	2.05	1.49	1.46
4	A	1403	NAG	C4-C5	2.04	1.57	1.53
4	B	1406	NAG	C4-C5	2.03	1.57	1.53
4	C	1406	NAG	C4-C5	2.01	1.57	1.53
4	C	1402	NAG	C2-N2	2.01	1.49	1.46
4	A	1402	NAG	C2-N2	2.01	1.49	1.46
4	A	1409	NAG	C4-C5	2.00	1.57	1.53
4	C	1409	NAG	C4-C5	2.00	1.57	1.53
4	A	1406	NAG	C4-C5	2.00	1.57	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1409	NAG	C8-C7-N2	2.90	120.93	116.12
4	A	1409	NAG	C8-C7-N2	2.86	120.86	116.12
4	C	1409	NAG	C8-C7-N2	2.84	120.84	116.12
4	C	1406	NAG	C8-C7-N2	2.83	120.81	116.12
4	A	1406	NAG	C8-C7-N2	2.81	120.78	116.12
4	B	1406	NAG	C8-C7-N2	2.78	120.72	116.12
4	C	1403	NAG	C8-C7-N2	2.71	120.62	116.12
4	A	1403	NAG	C8-C7-N2	2.69	120.58	116.12
4	B	1403	NAG	C8-C7-N2	2.68	120.57	116.12
4	C	1409	NAG	O7-C7-C8	-2.39	117.79	122.05
4	A	1409	NAG	O7-C7-C8	-2.38	117.81	122.05
4	B	1409	NAG	O7-C7-C8	-2.38	117.82	122.05
4	B	1404	NAG	C8-C7-N2	2.25	119.85	116.12
4	A	1404	NAG	C8-C7-N2	2.22	119.80	116.12
4	B	1403	NAG	O7-C7-C8	-2.21	118.13	122.05
4	C	1403	NAG	O7-C7-C8	-2.20	118.14	122.05
4	C	1404	NAG	C8-C7-N2	2.19	119.75	116.12
4	C	1407	NAG	O7-C7-C8	-2.15	118.22	122.05
4	A	1407	NAG	O7-C7-C8	-2.15	118.23	122.05
4	A	1403	NAG	O7-C7-C8	-2.14	118.24	122.05
4	B	1407	NAG	O7-C7-C8	-2.13	118.27	122.05
4	B	1406	NAG	O7-C7-C8	-2.11	118.31	122.05
4	A	1406	NAG	O7-C7-C8	-2.10	118.32	122.05
4	C	1406	NAG	O7-C7-C8	-2.09	118.33	122.05

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1405	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	A	1409	NAG	O5-C5-C6-O6
4	B	1409	NAG	O5-C5-C6-O6
4	C	1409	NAG	O5-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1406	NAG	O5-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

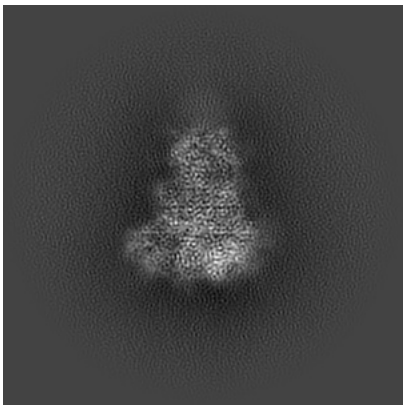
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44658. These allow visual inspection of the internal detail of the map and identification of artifacts.

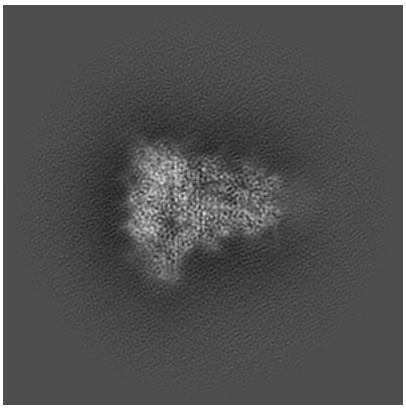
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

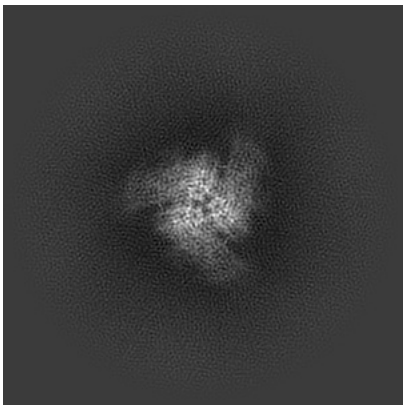
6.1.1 Primary map



X

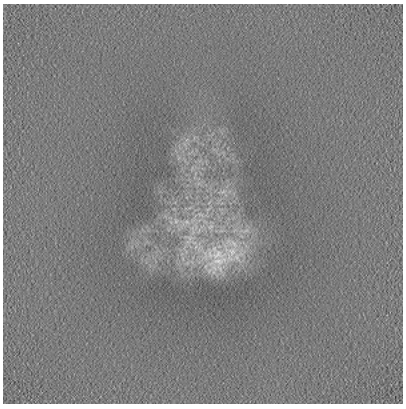


Y

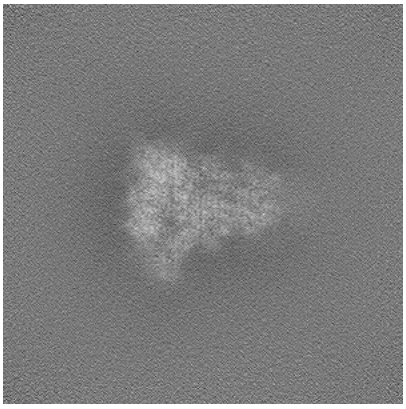


Z

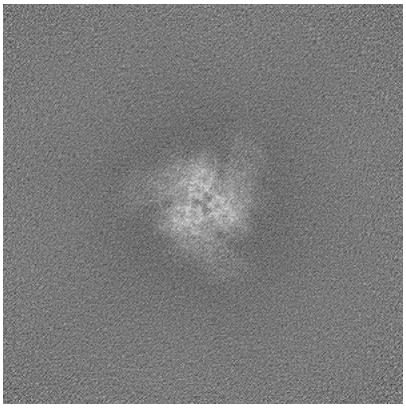
6.1.2 Raw map



X



Y

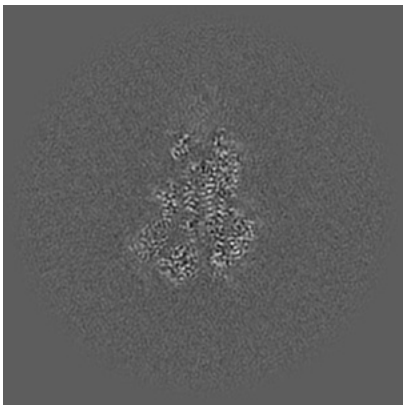


Z

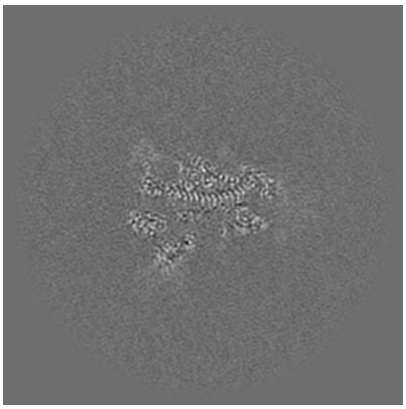
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

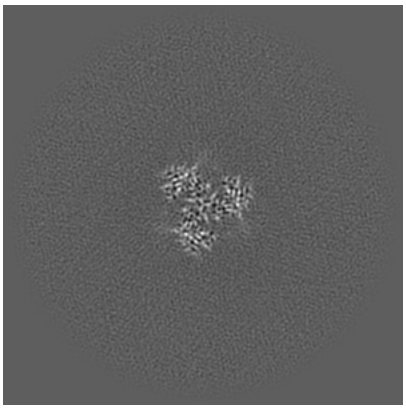
6.2.1 Primary map



X Index: 256

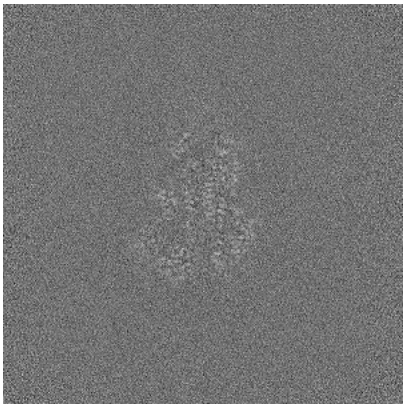


Y Index: 256

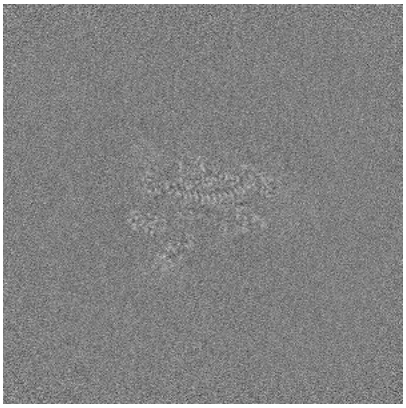


Z Index: 256

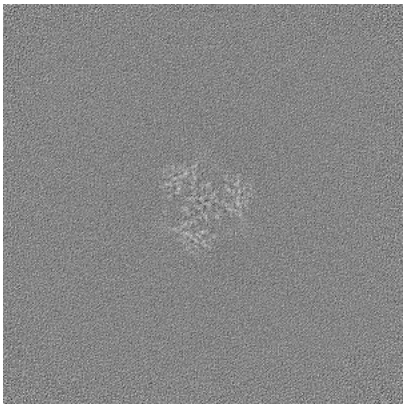
6.2.2 Raw map



X Index: 256



Y Index: 256

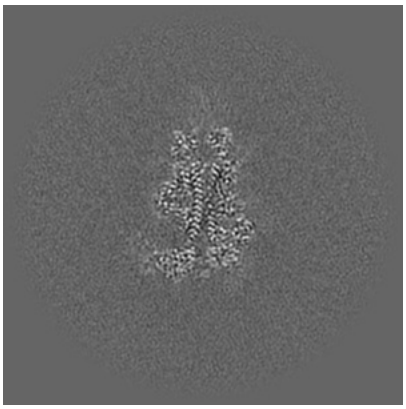


Z Index: 256

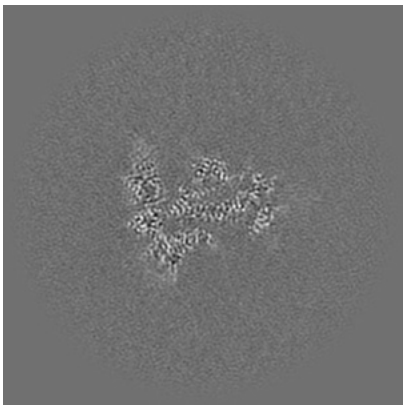
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

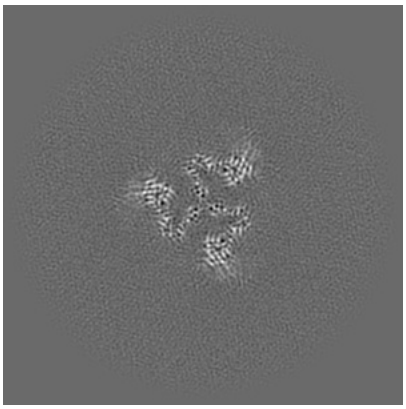
6.3.1 Primary map



X Index: 248

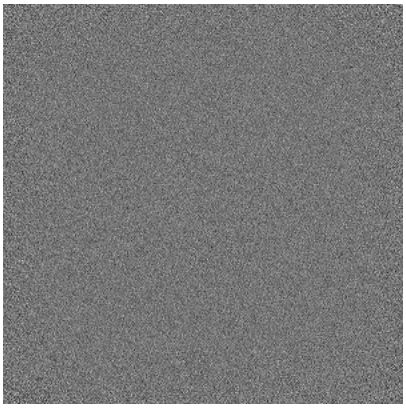


Y Index: 269

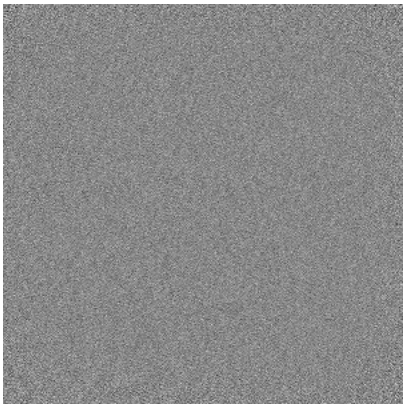


Z Index: 221

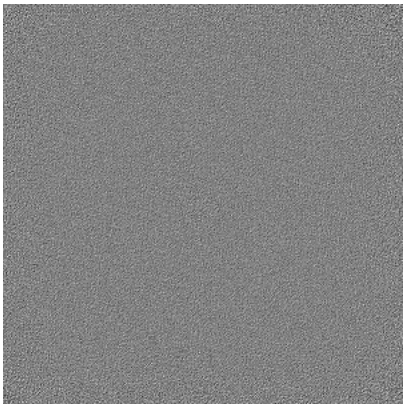
6.3.2 Raw map



X Index: 0



Y Index: 0

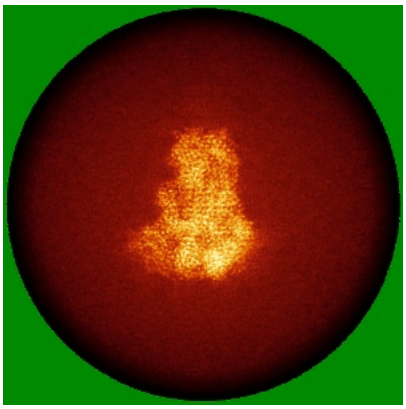


Z Index: 0

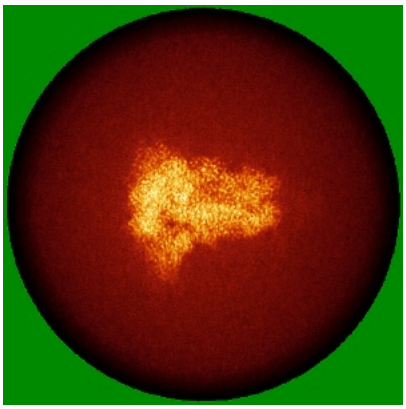
The images above show the largest variance slices of the map in three orthogonal directions.

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

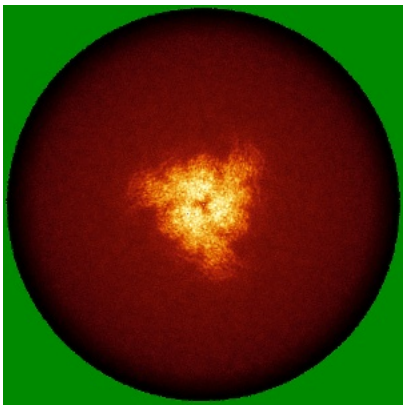
6.4.1 Primary map



X

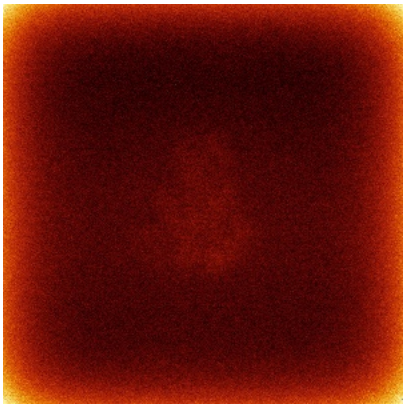


Y

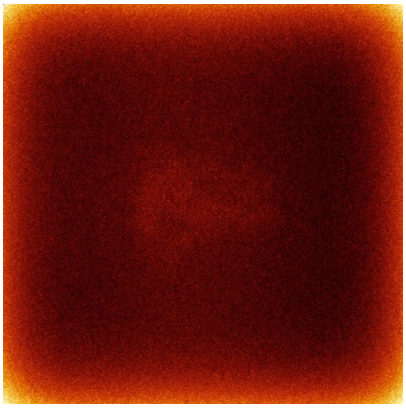


Z

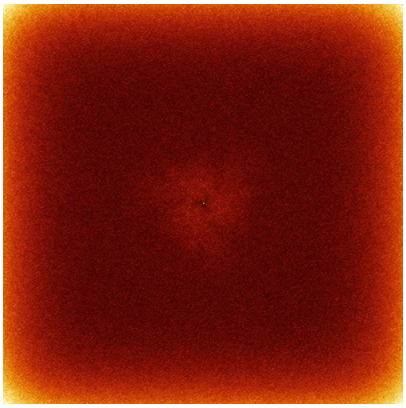
6.4.2 Raw map



X



Y

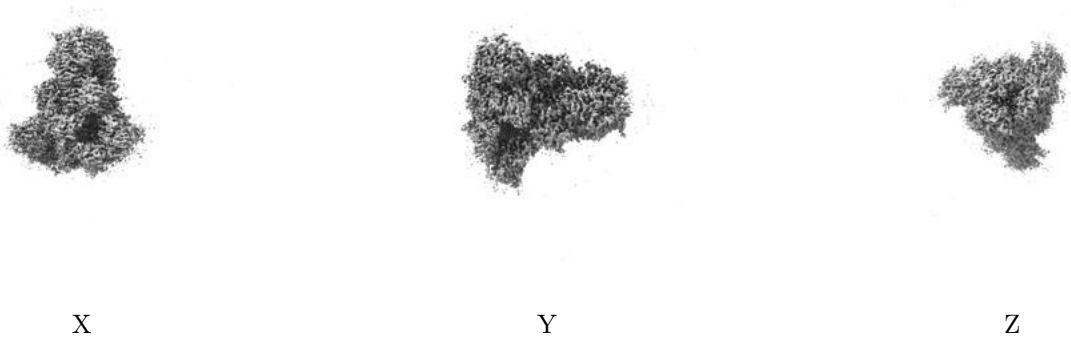


Z

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)

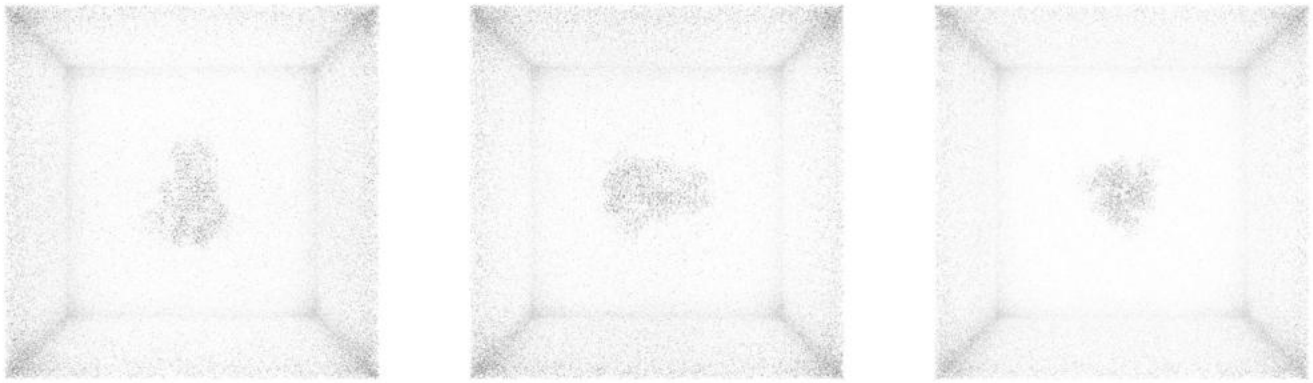
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

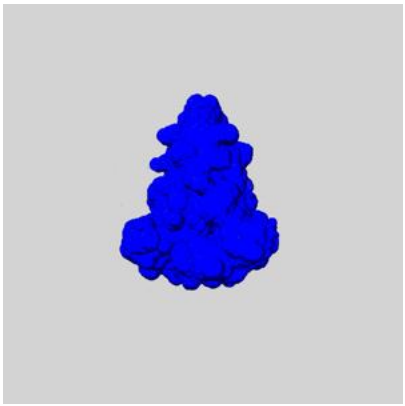
6.6 Mask visualisation

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

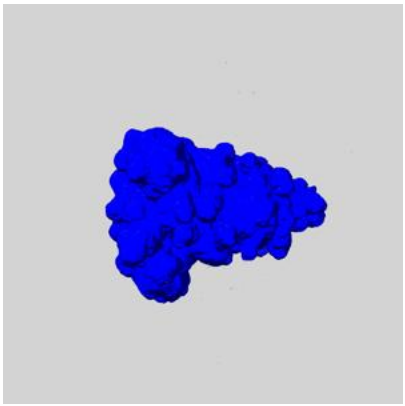
A mask typically either:

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

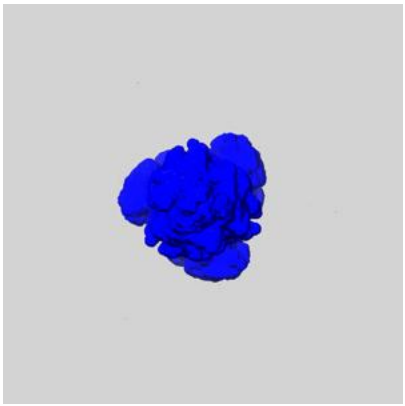
6.6.1 emd_44658_msk_1.map



X



Y

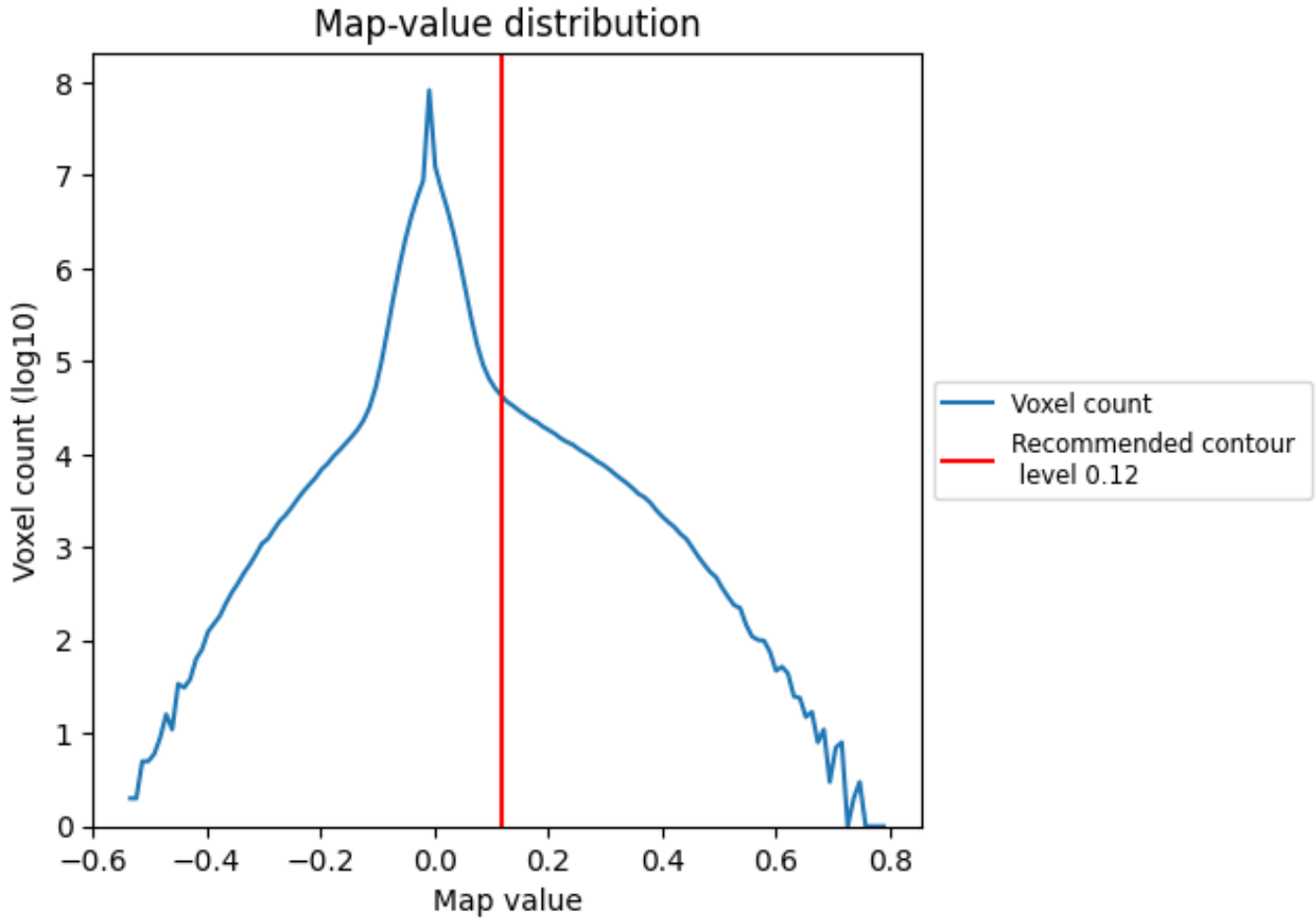


Z

7 Map analysis

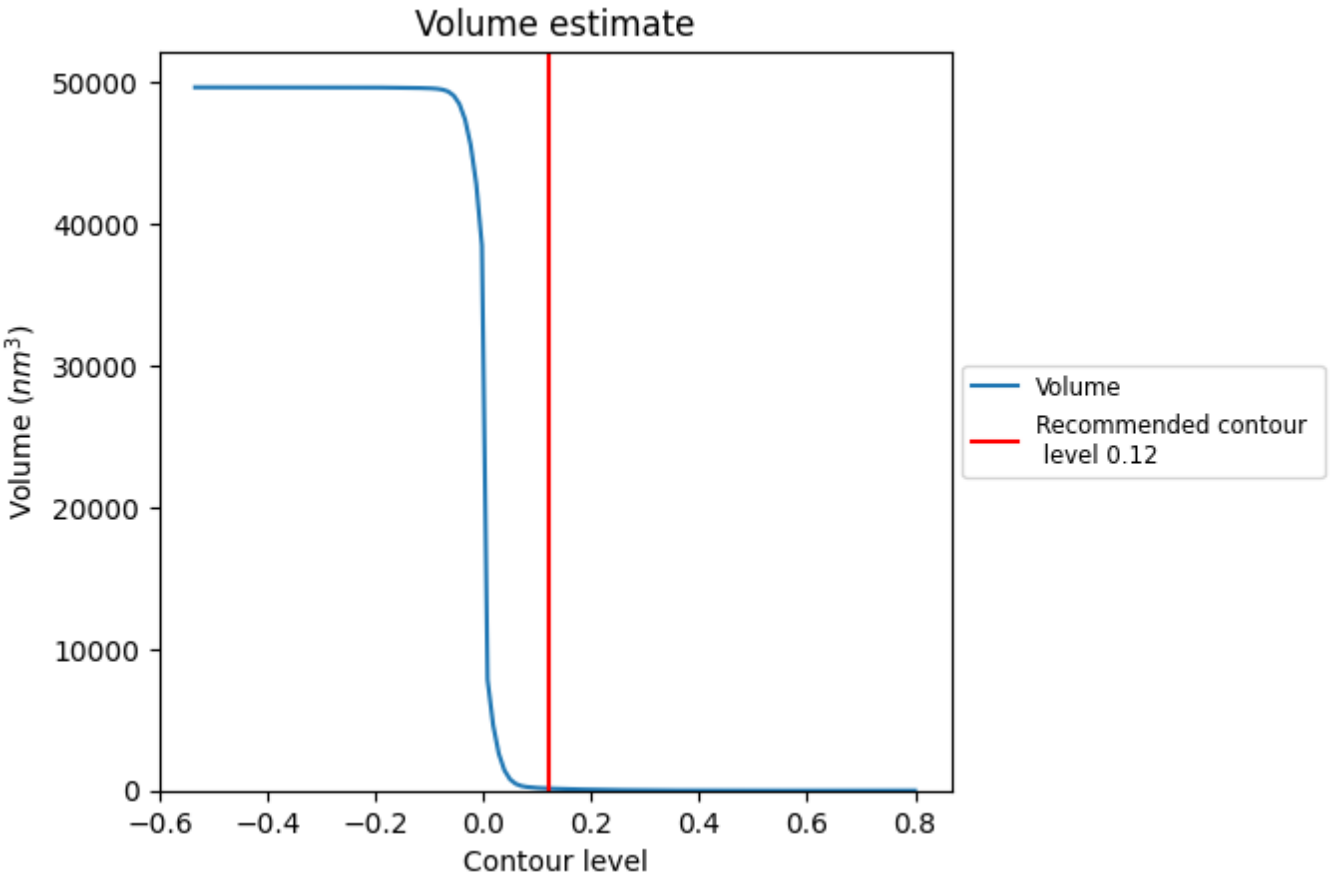
This section contains the results of statistical analysis of the map.

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.

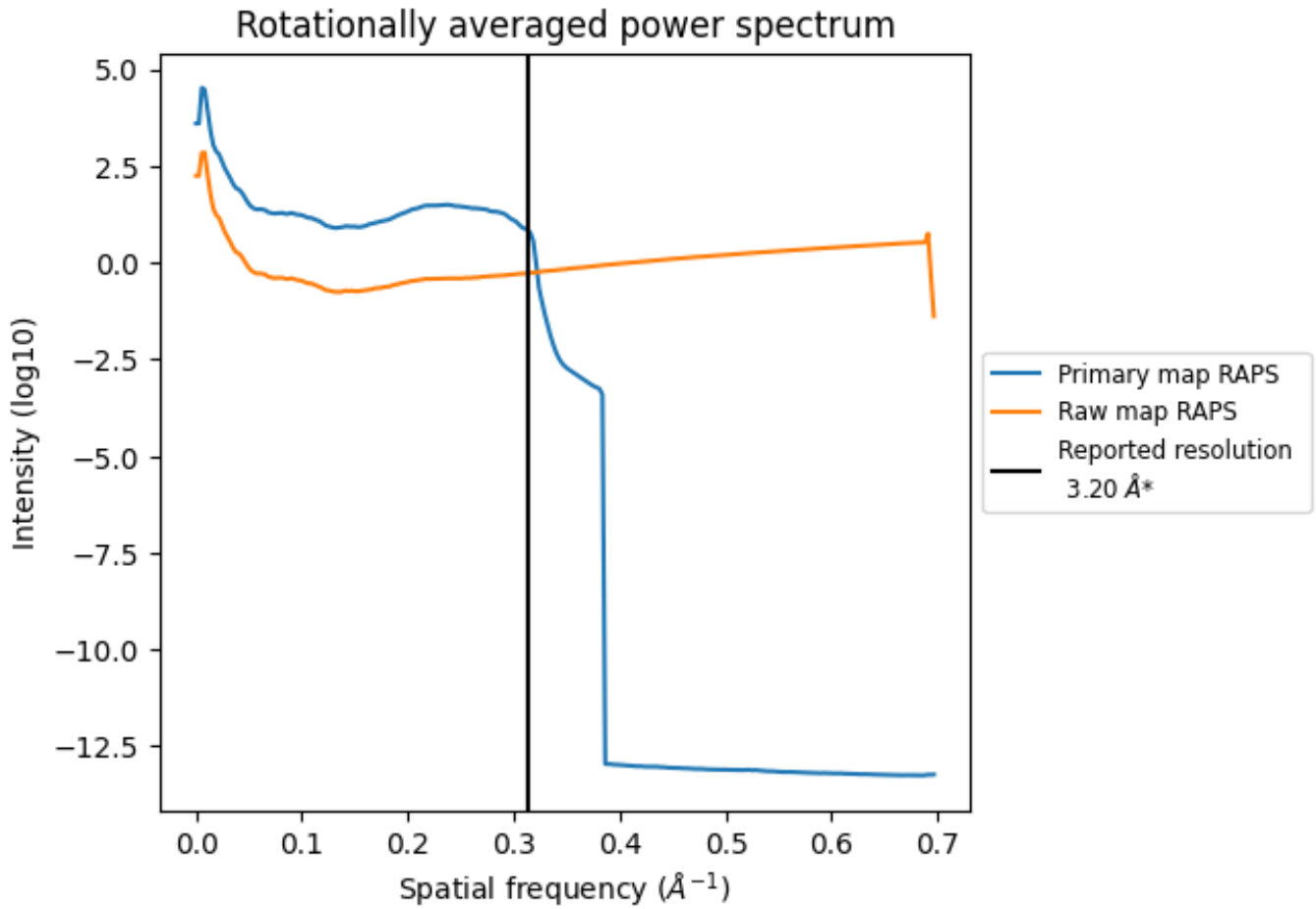
7.2 Volume estimate



The volume at the recommended contour level is 149 nm^3; this corresponds to an approximate mass of 134 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)

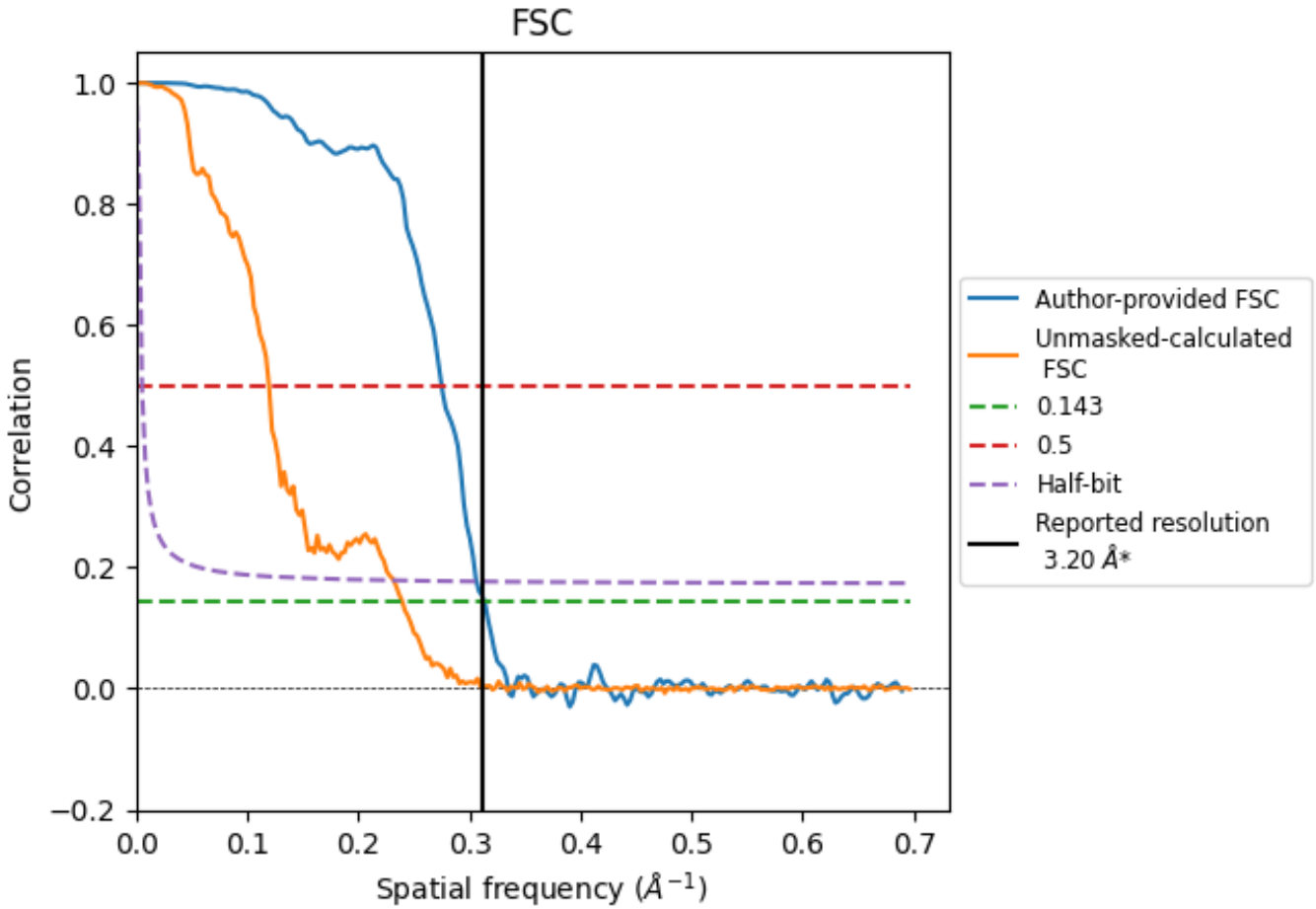


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

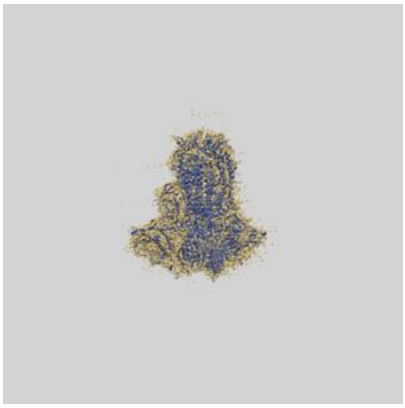
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.64	3.26
Unmasked-calculated*	4.17	8.36	4.31

*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 4.17 differs from the reported value 3.2 by more than 10 %

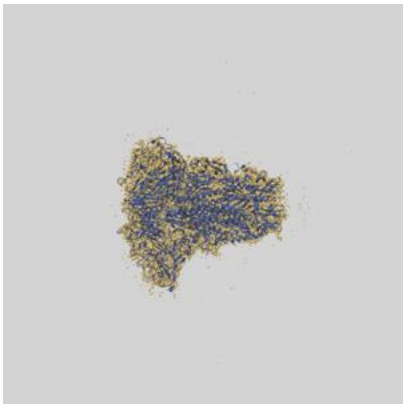
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44658 and PDB model 9BLK. Per-residue inclusion information can be found in section 3 on page 9.

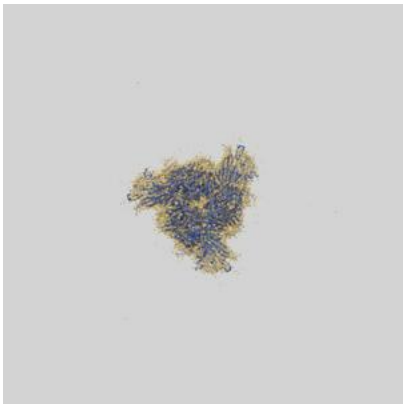
9.1 Map-model overlay



X



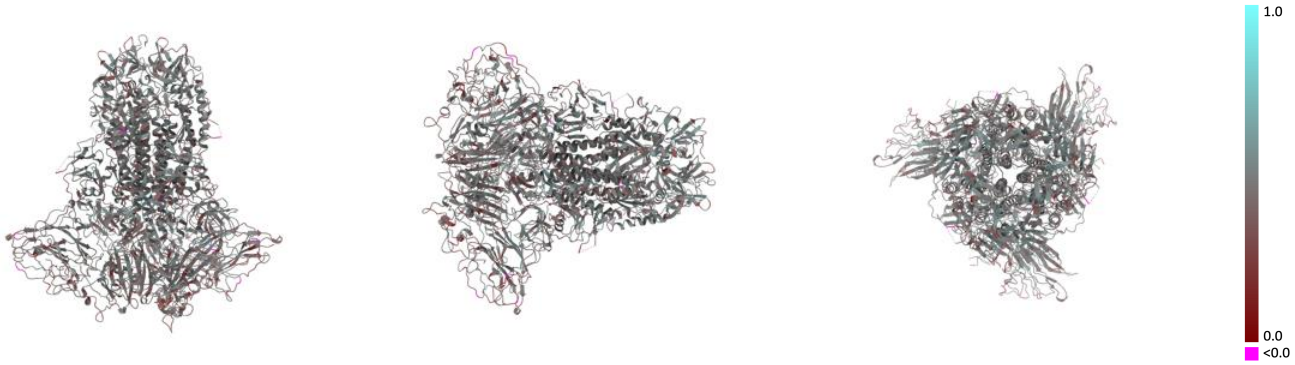
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

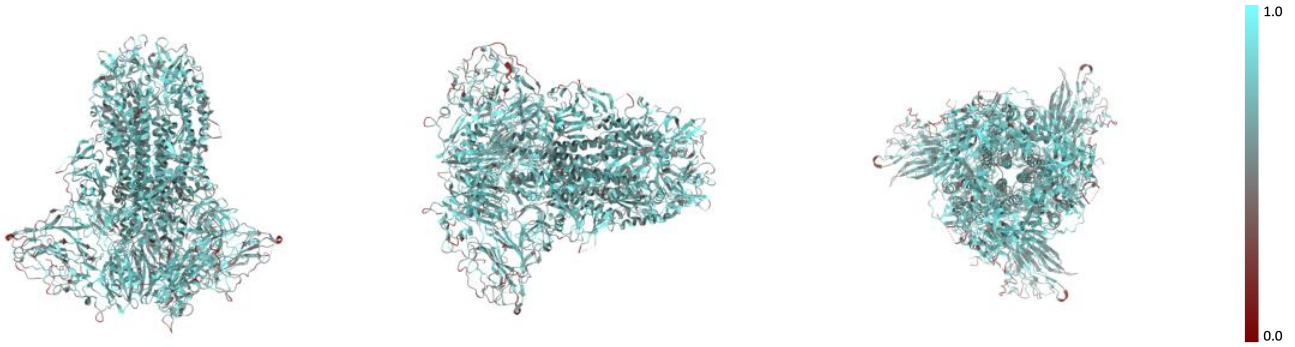
9.2 Q-score mapped to coordinate model (i)



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.

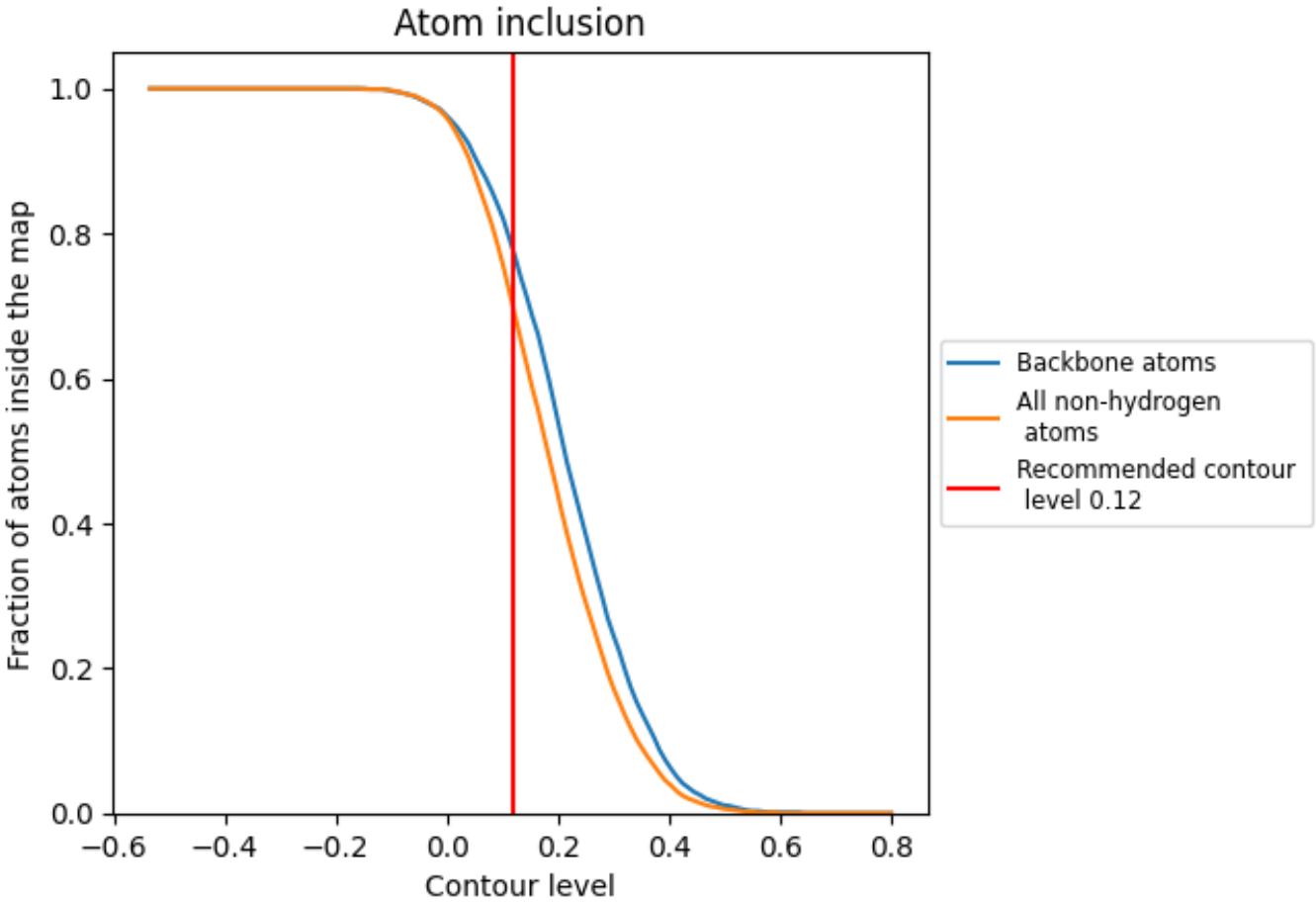
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.4450
A	0.6990	0.4460
B	0.6980	0.4460
C	0.7000	0.4460
D	0.3080	0.3500
E	0.3210	0.3190
F	0.3080	0.3390
G	0.2860	0.3170
H	0.3330	0.3450
I	0.2860	0.3150