



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:24 AM UTC

PDB ID : 8JX9 / pdb_00008jx9
EMDB ID : EMD-36693
Title : rat megalin bodyA
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-30
Resolution : 3.80 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

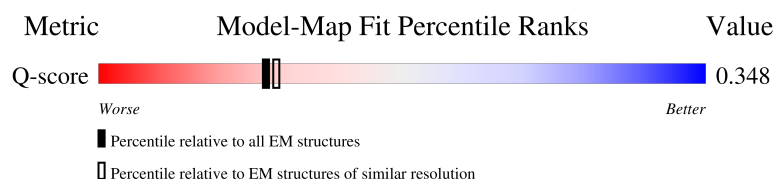
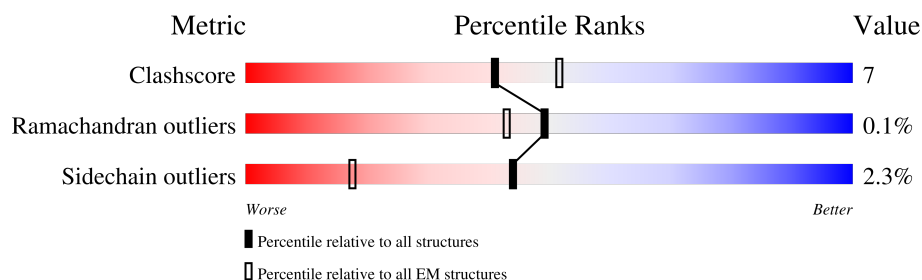
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



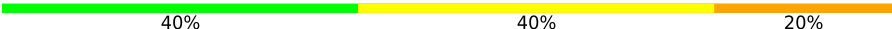
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4660	 7% 7% 92%
1	B	4660	 19% 77%
2	O	5	 80% 20%
3	C	3	 67% 33% 67%

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Mol	Chain	Length	Quality of chain
3	D	3	 67% 33%
4	E	5	 40% 40% 60%
4	H	5	 20% 60% 20% 20%
4	I	5	 40% 40% 20%
5	F	2	 100%
5	G	2	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11822 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.

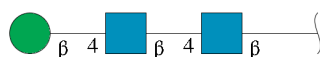
- Molecule 1 is a protein called LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2904	1844	493	549	18		
1	B	1077	Total	C	N	O	S	0	0
			8455	5100	1537	1687	131		

- Molecule 2 is a protein called ligand.

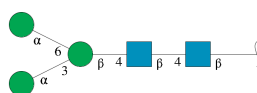
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 3 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
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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.



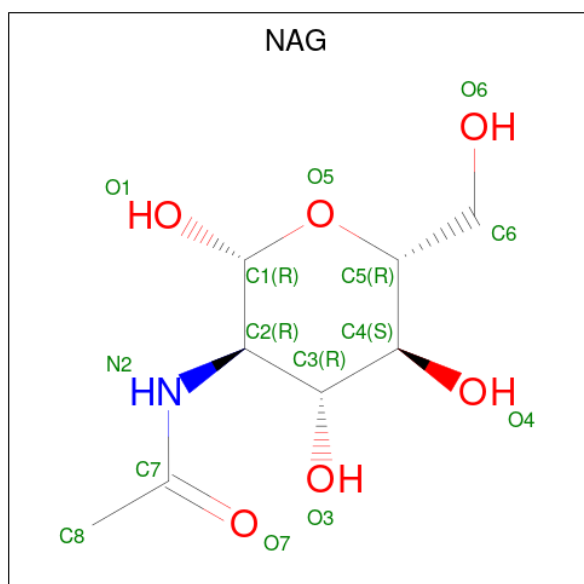
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	5	Total	C	N	O	0	0
			61	34	2	25		
4	H	5	Total	C	N	O	0	0
			61	34	2	25		
4	I	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 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
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



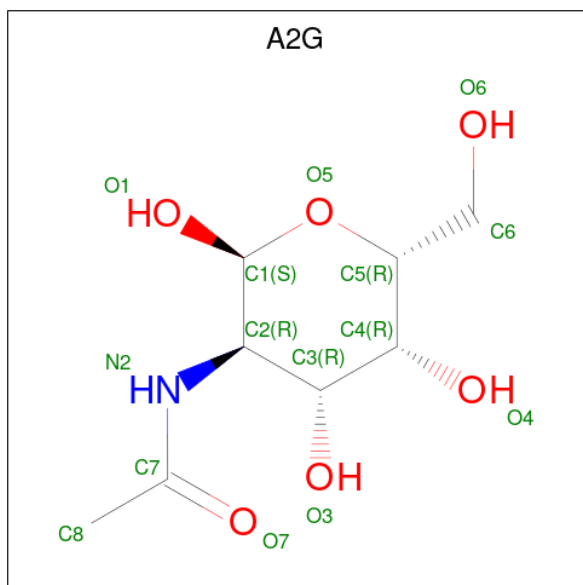
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 7 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	B	20	Total	Ca	0
			20	20	







V4339	C4340	S4341	H4342	L4343	C4344	L4345	L4346	R4347	P4348	G4349	O4350	Y4351	S4352	C4353	A4354	C4355	P4356	O4357	G4358	S4359	D4360	F4361	V4362	T4363	O4364	S4365	T4366	V4367	O4368	C4369	D4370	A4371	A4372	S4373	E4374	L4375	P4376	V4377	T4378	M4379	P4380	F4381	P4382	C4383	R4384	C4385	M4386	H4387	O4388	M4389	C4390	C4391	Y4392	F4393	D4394	E4395	M4396	L4398
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P4399	K4400	C4401	K4402	C4403	S4404	S4405	G4406	Y4407	S4408	G4409	E4410	Y4411	C4412	E4413	V4414	C4415	LEU	SER	ARG	GLY	ILE	PRO	ASN	GLY	THR	THR	ASP	ALA	VAL	LEU	THR	PHE	GLN	GLY	THR	ILE	ILE	VAL	GLY	ALA	LEU	VAL	GLY	LEU	VAL	GLY	THR	GLN	THR
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PRO	VAL	ILE	PHE	GLU	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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GLY	TYR	THR	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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● Molecule 1: LDL receptor related protein 2



MET	GLU	ARG	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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GLY	CYS	PRO	ASP	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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THR	LEU	CYS	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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CYS	ASP	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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THR	SER	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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CYS	GLU	ASN	PRO	ASP	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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ASN	ARG	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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TYR	LEU	VAL	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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PHE	MET	ASP	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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PRO	HIS	PRO	PHE	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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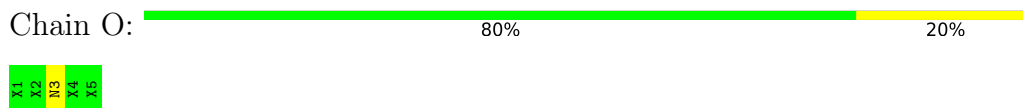
PRO	CYS	GLY	ASN	GLY	ALA	THR	GLY	ASN	PRO	LEU	SER	THR	GLY	ASN	GLY	VAL	THR	ALA	PHE	GLY	GLY	ALA	THR	GLN	ARG	SER	THR	ASP	GLY	PRO	GLY	ASN	PRO	GLN	THR	ILE	ILE	ARG	ASP	ARG	GLY	HIS	VAL	PHE	GLU	VAL	THR	GLN
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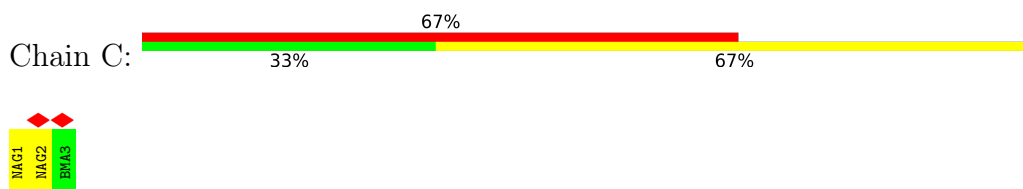




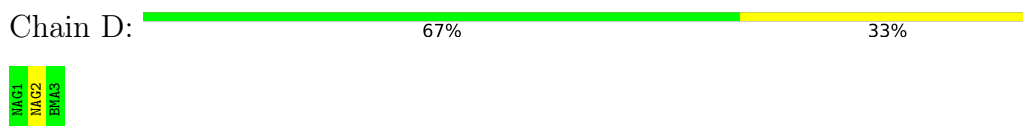
- Molecule 2: ligand



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



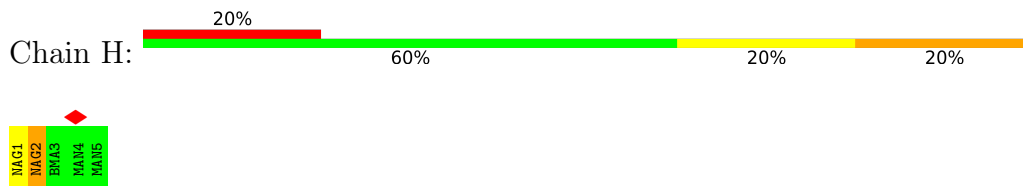
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



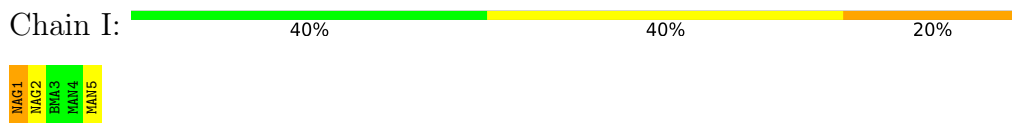
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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



- Molecule 4: 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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.411, 1.411, 1.411	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, A2G, BMA, CA, MAN

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	0.11	0/2981	0.32	0/4047
1	B	0.18	0/8659	0.44	2/11737 (0.0%)
2	O	0.19	0/7	0.52	0/8
All	All	0.16	0/11647	0.42	2/15792 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3871	ASP	N-CA-C	-5.84	102.94	111.17
1	B	3872	GLY	N-CA-C	5.11	118.94	110.97

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	2904	0	2797	27	0
1	B	8455	0	7529	127	0
2	O	28	0	12	1	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0
4	E	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	61	0	52	1	0
4	I	61	0	52	1	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
6	B	28	0	26	1	0
7	B	70	0	60	11	0
8	B	20	0	0	0	0
All	All	11822	0	10698	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1225:THR:OG1	7:B:4703:A2G:C1	1.90	1.19
1:B:3799:THR:OG1	7:B:4706:A2G:C1	1.92	1.18
1:B:1225:THR:CB	7:B:4703:A2G:C1	2.26	1.12
1:B:1225:THR:HB	7:B:4703:A2G:C1	1.83	1.08
1:B:3799:THR:CB	7:B:4706:A2G:C1	2.36	1.03
1:B:3799:THR:HB	7:B:4706:A2G:C1	2.02	0.89
1:B:1225:THR:HB	7:B:4703:A2G:O5	1.83	0.79
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.46	0.78
1:B:3146:MET:SD	1:B:3151:SER:HB3	2.27	0.74
1:B:3009:ARG:HG2	1:B:3011:SER:H	1.56	0.70
1:B:3082:PHE:N	1:B:3090:ILE:O	2.24	0.70
1:B:3123:ARG:HG2	1:B:3150:ARG:HH11	1.58	0.69
1:B:3790:SER:OG	1:B:3793:ARG:NH2	2.26	0.68
1:B:3082:PHE:HB2	1:B:3092:MET:HG3	1.75	0.66
1:B:3799:THR:HB	7:B:4706:A2G:O5	1.95	0.66
1:A:4129:SER:O	1:A:4130:ASN:ND2	2.30	0.64
1:B:3425:THR:HG22	1:B:3432:VAL:HG22	1.80	0.64
1:B:3270:ARG:HH12	1:B:3597:GLU:HG2	1.63	0.63
1:B:3366:ILE:HD11	1:B:3369:PRO:HB3	1.80	0.62
1:B:3799:THR:HB	7:B:4706:A2G:C5	2.30	0.62
1:B:3867:ASN:ND2	1:B:3869:CYS:O	2.33	0.61
1:A:4310:VAL:HG12	1:A:4311:LEU:HG	1.80	0.61
1:A:4179:LYS:HA	1:A:4357:GLN:HB2	1.83	0.59
1:B:3123:ARG:HG2	1:B:3150:ARG:NH1	2.16	0.59
1:B:1225:THR:HG1	7:B:4703:A2G:C1	2.14	0.59
1:B:3210:TYR:OH	1:B:3764:SER:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3122:SER:O	1:B:3123:ARG:C	2.46	0.58
1:B:3283:SER:HB3	1:B:3484:ILE:HD11	1.84	0.58
1:B:3146:MET:O	1:B:3149:LYS:NZ	2.37	0.58
1:B:3605:ASN:ND2	1:B:3623:ASP:OD2	2.36	0.58
1:B:3025:ASP:OD1	1:B:3025:ASP:N	2.37	0.57
1:B:3805:PHE:N	1:B:3813:VAL:O	2.37	0.57
1:A:4289:VAL:HG11	1:A:4317:LEU:HD22	1.88	0.56
1:B:3096:CYS:HA	1:B:3108:GLU:HG3	1.87	0.56
1:B:3849:PHE:O	1:B:3856:CYS:HB2	2.06	0.56
1:B:3074:GLU:OE1	1:B:3083:ARG:NH2	2.39	0.55
1:B:3870:VAL:O	1:B:3871:ASP:C	2.48	0.55
1:B:1254:HIS:N	1:B:1263:GLU:OE2	2.40	0.54
1:B:3289:LEU:HD21	1:B:3339:TRP:HB2	1.88	0.54
1:A:4093:TRP:CE2	1:A:4325:GLN:HB3	2.43	0.53
1:B:3600:GLU:HB2	1:B:3609:ILE:O	2.09	0.53
1:B:3862:ILE:HG22	1:B:3863:CYS:SG	2.49	0.53
1:B:3038:GLN:HG2	1:B:3046:CYS:HB3	1.91	0.52
1:B:3083:ARG:HA	1:B:3089:CYS:HB3	1.92	0.52
4:I:1:NAG:H62	4:I:2:NAG:C7	2.40	0.52
1:B:1225:THR:CB	7:B:4703:A2G:O5	2.51	0.52
1:B:3238:ARG:NH1	1:B:3464:GLN:O	2.42	0.52
1:B:3671:ASP:N	1:B:3671:ASP:OD1	2.43	0.51
1:B:3805:PHE:HE2	1:B:3830:ASP:HA	1.75	0.51
1:B:3150:ARG:O	1:B:3151:SER:HB2	2.10	0.51
1:B:3015:ASP:N	1:B:3026:GLU:OE1	2.42	0.51
1:B:3039:PHE:HD2	1:B:3047:ILE:HD11	1.76	0.51
1:B:3123:ARG:CG	1:B:3150:ARG:HH11	2.24	0.51
1:B:3791:ASP:OD1	1:B:3791:ASP:N	2.37	0.51
1:B:3901:GLY:O	1:B:3904:LEU:HD22	2.10	0.51
1:B:3344:VAL:HG11	1:B:3653:SER:HB2	1.92	0.51
1:B:3016:ARG:NH2	1:B:3044:GLY:O	2.44	0.50
1:B:2965:ARG:HH12	1:B:2966:ARG:NH2	2.09	0.50
1:A:4085:HIS:O	1:A:4108:LEU:N	2.38	0.50
1:B:3203:LEU:HD22	1:B:3456:ILE:HD11	1.94	0.50
1:B:3662:CYS:SG	1:B:3667:ASP:HB3	2.52	0.50
1:B:3842:THR:OG1	1:B:3843:TYR:N	2.46	0.49
1:B:3079:LEU:HD22	1:B:3080:HIS:H	1.77	0.48
1:B:3505:ARG:HH11	1:B:3506:ASP:H	1.59	0.48
1:A:4148:GLY:HA3	1:A:4191:ALA:HA	1.95	0.48
1:B:3448:ASN:OD1	6:B:4701:NAG:N2	2.47	0.48
1:A:4384:ARG:HB3	1:A:4411:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3000:PHE:N	1:B:3008:VAL:O	2.47	0.48
1:B:3207:ASN:HB2	1:B:3210:TYR:HB2	1.94	0.48
1:A:4087:GLN:HB2	1:A:4108:LEU:HD13	1.95	0.48
1:A:4162:ASP:HB3	1:A:4165:SER:HB2	1.95	0.48
1:B:3016:ARG:N	1:B:3026:GLU:OE1	2.42	0.47
1:B:3326:ARG:HH12	2:O:3:ASN:HB3	1.77	0.47
1:B:3621:CYS:SG	1:B:3626:ASP:HB3	2.55	0.47
1:B:3658:VAL:HG23	1:B:3693:ARG:HB3	1.96	0.47
1:B:3135:PHE:HZ	1:B:3150:ARG:NH2	2.12	0.47
1:B:2936:MET:SD	1:B:2940:ASP:HB3	2.55	0.47
1:B:3736:PRO:HD2	1:B:3739:TRP:CE3	2.49	0.47
1:B:3416:THR:HG21	1:B:3457:HIS:HA	1.96	0.46
1:B:3258:LEU:HA	1:B:3258:LEU:HD23	1.67	0.46
1:B:3083:ARG:HG2	1:B:3083:ARG:HH11	1.81	0.46
1:B:1247:ASN:O	1:B:1250:GLU:HG3	2.16	0.46
1:B:2969:PRO:HD2	1:B:2972:TRP:HE1	1.80	0.46
1:B:3291:ALA:HA	1:B:3325:PRO:HD2	1.97	0.46
1:A:4061:PRO:HG3	1:A:4089:ILE:HG12	1.98	0.46
1:B:3009:ARG:HE	1:B:3009:ARG:H	1.64	0.46
1:B:3720:PRO:HA	1:B:3728:ARG:HH12	1.79	0.46
1:B:3131:THR:N	1:B:3134:SER:O	2.40	0.46
1:A:4086:ILE:HG22	1:A:4107:VAL:HG12	1.98	0.46
1:B:2993:ARG:HG3	1:B:2995:CYS:H	1.80	0.46
1:B:3296:LEU:HD22	1:B:3309:ILE:HD11	1.97	0.46
1:B:3840:ASN:OD1	1:B:3842:THR:HG22	2.17	0.45
1:B:3659:ASP:OD2	1:B:3708:ARG:NE	2.50	0.45
1:B:3170:GLU:HB3	1:B:3177:ILE:HG23	1.98	0.45
1:B:3670:ILE:HA	1:B:3673:CYS:HB2	1.99	0.45
1:B:3123:ARG:HG3	1:B:3123:ARG:O	2.17	0.44
1:B:3885:CYS:HB3	1:B:3898:CYS:HB3	1.81	0.44
1:B:2917:ASN:N	1:B:2935:ASP:OD2	2.40	0.44
1:B:3112:GLY:O	1:B:3114:ASN:N	2.44	0.44
1:B:3280:ASP:OD2	1:B:3283:SER:OG	2.31	0.44
1:A:4218:ASN:ND2	1:A:4220:GLU:OE2	2.36	0.44
1:A:4108:LEU:HD12	1:A:4146:PRO:HD2	1.98	0.44
1:B:3351:ILE:HD12	1:B:3358:LYS:HB3	1.99	0.44
1:A:4102:VAL:HG22	1:A:4121:TYR:CE1	2.52	0.44
1:B:3068:HIS:HD1	1:B:3068:HIS:C	2.26	0.44
1:B:3081:GLN:N	1:B:3092:MET:SD	2.92	0.43
1:B:3799:THR:HG22	1:B:3800:CYS:N	2.33	0.43
1:A:4121:TYR:OH	1:A:4379:MET:SD	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3421:THR:HG21	1:B:3434:LYS:HD2	2.00	0.43
1:B:3891:PHE:HE1	1:B:3921:HIS:HD1	1.67	0.43
1:B:2988:GLN:NE2	1:B:2989:ASN:OD1	2.46	0.43
1:A:4213:GLU:HG2	1:A:4224:VAL:HG22	2.01	0.43
1:B:3049:ARG:HD3	1:B:3049:ARG:O	2.19	0.43
1:B:1230:MET:HE2	1:B:1230:MET:HB3	1.87	0.43
1:B:3013:ARG:HG2	1:B:3014:CYS:N	2.33	0.43
1:B:3417:ILE:HD12	1:B:3417:ILE:N	2.34	0.43
1:A:4123:PRO:HB3	1:A:4125:PHE:CZ	2.54	0.43
1:B:3091:GLU:OE1	1:B:3093:GLY:N	2.47	0.43
4:H:1:NAG:O6	4:H:2:NAG:N2	2.52	0.43
1:B:3126:HIS:ND1	1:B:3152:CYS:HB2	2.34	0.42
1:B:1248:THR:HG23	1:B:1249:TRP:HD1	1.83	0.42
1:B:3080:HIS:H	1:B:3092:MET:HE1	1.84	0.42
1:B:3149:LYS:HA	1:B:3149:LYS:HD3	1.94	0.42
1:B:3556:ARG:CG	1:B:3822:ARG:HH12	2.32	0.42
1:B:3269:HIS:CE1	1:B:3270:ARG:HG3	2.54	0.42
1:B:3918:LYS:HG2	1:B:3919:GLU:H	1.85	0.42
1:B:3013:ARG:HG2	1:B:3014:CYS:SG	2.60	0.42
1:B:3080:HIS:N	1:B:3092:MET:HE1	2.35	0.42
1:B:3245:TRP:CE2	1:B:3254:GLU:HB2	2.55	0.42
1:B:3744:THR:OG1	1:B:3746:ASP:OD1	2.36	0.42
1:B:3805:PHE:CE2	1:B:3830:ASP:HA	2.55	0.42
1:A:4084:GLU:OE2	1:A:4085:HIS:HB2	2.20	0.41
1:A:4096:GLU:OE2	1:A:4121:TYR:OH	2.26	0.41
1:A:4299:GLN:NE2	1:A:4305:GLU:O	2.38	0.41
1:B:3556:ARG:HE	1:B:3822:ARG:HH12	1.68	0.41
1:A:4116:ALA:HA	1:A:4143:LEU:HD12	2.02	0.41
1:B:3592:GLU:C	1:B:3606:LYS:HZ1	2.28	0.41
1:B:3213:ASN:HB2	1:B:3224:ILE:HG13	2.02	0.41
1:A:4259:ILE:HD12	1:A:4266:ARG:HB2	2.02	0.41
1:B:2958:VAL:HA	1:B:2966:ARG:HD2	2.01	0.41
1:B:3132:ILE:HG23	1:B:3133:THR:HG23	2.01	0.41
1:B:3392:GLU:OE1	1:B:3401:ARG:NH2	2.49	0.41
1:A:4142:TYR:HB3	1:B:3793:ARG:HG2	2.02	0.41
1:A:4375:LEU:H	1:A:4375:LEU:HD23	1.85	0.41
1:B:3618:VAL:N	1:B:3627:GLU:OE2	2.54	0.41
1:B:3861:TRP:HB3	1:B:3868:ASP:OD2	2.20	0.41
1:B:3030:SER:O	1:B:3031:TYR:C	2.64	0.41
1:B:3083:ARG:HG2	1:B:3083:ARG:NH1	2.36	0.41
1:A:4238:ILE:HG12	1:A:4246:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3122:SER:HA	1:B:3150:ARG:CZ	2.50	0.40
1:A:4215:ALA:HB2	1:A:4222:ARG:HA	2.03	0.40
1:B:3000:PHE:HD2	1:B:3013:ARG:NH2	2.19	0.40
1:B:3139:CYS:SG	1:B:3145:LEU:HD22	2.61	0.40
1:B:3505:ARG:H	1:B:3505:ARG:HD3	1.86	0.40
1:B:3761:CYS:HB3	1:B:3765:GLU:HB2	2.04	0.40
1:B:3887:SER:OG	1:B:3888:PRO:HD3	2.21	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	359/4660 (8%)	334 (93%)	25 (7%)	0	100	100
1	B	1073/4660 (23%)	985 (92%)	87 (8%)	1 (0%)	48	79
2	O	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1433/9325 (15%)	1320 (92%)	112 (8%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3123	ARG

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	320/4089 (8%)	309 (97%)	11 (3%)	32	55
1	B	965/4089 (24%)	947 (98%)	18 (2%)	50	66
2	O	1/1 (100%)	1 (100%)	0	100	100
All	All	1286/8179 (16%)	1257 (98%)	29 (2%)	44	63

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4062	GLU
1	A	4090	ASP
1	A	4102	VAL
1	A	4194	VAL
1	A	4256	ILE
1	A	4279	LEU
1	A	4313	VAL
1	A	4320	VAL
1	A	4359	SER
1	A	4387	HIS
1	A	4412	CYS
1	B	1271	THR
1	B	3118	ASP
1	B	3131	THR
1	B	3172	VAL
1	B	3317	ASN
1	B	3373	THR
1	B	3408	SER
1	B	3416	THR
1	B	3478	CYS
1	B	3515	SER
1	B	3534	CYS
1	B	3683	HIS
1	B	3774	ILE
1	B	3791	ASP
1	B	3844	CYS
1	B	3870	VAL
1	B	3894	ASP
1	B	3897	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4087	GLN
1	A	4195	ASN
1	B	2954	GLN
1	B	3066	GLN
1	B	3086	ASN
1	B	3171	ASN
1	B	3602	GLN
1	B	3614	GLN
1	B	3691	ASN
1	B	3714	GLN
1	B	3722	HIS
1	B	3732	HIS
1	B	3733	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

25 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	C	1	1,3	14,14,15	0.44	0	17,19,21	2.41	3 (17%)
3	NAG	C	2	3	14,14,15	0.53	0	17,19,21	1.17	1 (5%)
3	BMA	C	3	3	11,11,12	0.23	0	15,15,17	0.73	0
3	NAG	D	1	1,3	14,14,15	0.38	0	17,19,21	0.86	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	1.14	1 (5%)
3	BMA	D	3	3	11,11,12	0.24	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1	1,4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.73	0
4	BMA	E	3	4	11,11,12	0.26	0	15,15,17	1.02	2 (13%)
4	MAN	E	4	4	11,11,12	0.22	0	15,15,17	0.50	0
4	MAN	E	5	4	11,11,12	0.24	0	15,15,17	0.50	0
5	NAG	F	1	1,5	14,14,15	0.37	0	17,19,21	1.09	1 (5%)
5	NAG	F	2	5	14,14,15	0.31	0	17,19,21	1.16	2 (11%)
5	NAG	G	1	1,5	14,14,15	0.32	0	17,19,21	1.43	1 (5%)
5	NAG	G	2	5	14,14,15	0.33	0	17,19,21	0.87	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.34	0	17,19,21	0.63	0
4	NAG	H	2	4	14,14,15	0.31	0	17,19,21	0.97	1 (5%)
4	BMA	H	3	4	11,11,12	0.28	0	15,15,17	0.75	0
4	MAN	H	4	4	11,11,12	0.25	0	15,15,17	0.57	0
4	MAN	H	5	4	11,11,12	0.22	0	15,15,17	0.55	0
4	NAG	I	1	1,4	14,14,15	0.35	0	17,19,21	1.13	2 (11%)
4	NAG	I	2	4	14,14,15	0.33	0	17,19,21	0.55	0
4	BMA	I	3	4	11,11,12	0.27	0	15,15,17	0.94	0
4	MAN	I	4	4	11,11,12	0.23	0	15,15,17	0.50	0
4	MAN	I	5	4	11,11,12	0.40	0	15,15,17	1.04	1 (6%)

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

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

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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	8.13	123.08	112.19
5	G	1	NAG	C1-O5-C5	5.14	119.08	112.19
3	C	1	NAG	O4-C4-C5	-4.19	98.99	109.32
4	I	1	NAG	C1-O5-C5	3.58	116.98	112.19
3	C	2	NAG	C1-O5-C5	3.11	116.35	112.19
3	D	2	NAG	O5-C1-C2	-3.02	106.61	111.29
5	F	2	NAG	O5-C1-C2	-2.77	107.00	111.29
5	G	2	NAG	C1-O5-C5	2.64	115.73	112.19
5	F	1	NAG	C1-O5-C5	-2.57	108.74	112.19
4	I	5	MAN	C1-C2-C3	2.42	113.16	109.64
3	C	1	NAG	C6-C5-C4	-2.31	107.35	113.02
4	E	3	BMA	C1-O5-C5	2.29	115.25	112.19
4	E	3	BMA	C1-C2-C3	2.25	112.93	109.64
4	I	1	NAG	C1-C2-N2	-2.18	107.00	110.43
4	H	2	NAG	O5-C1-C2	-2.08	108.07	111.29
5	F	2	NAG	C2-N2-C7	2.02	125.61	122.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2

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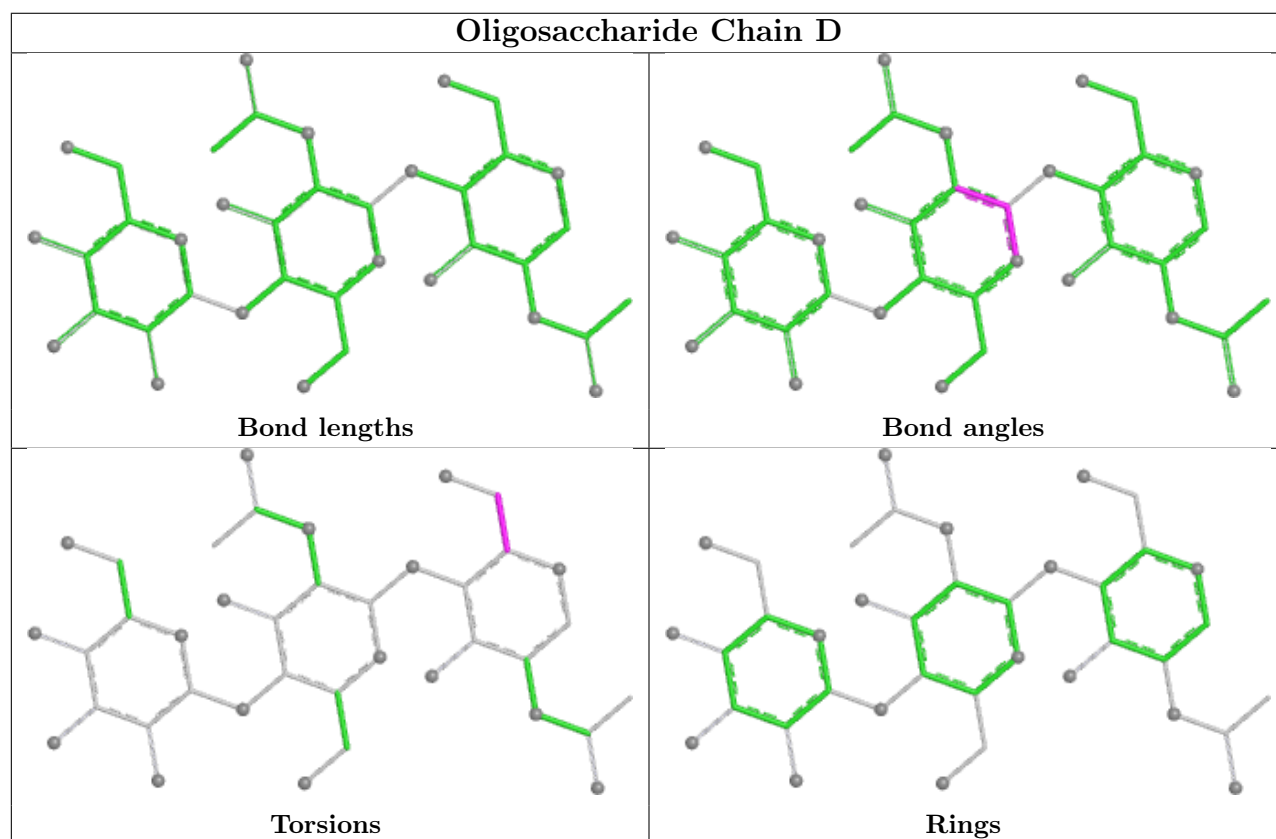
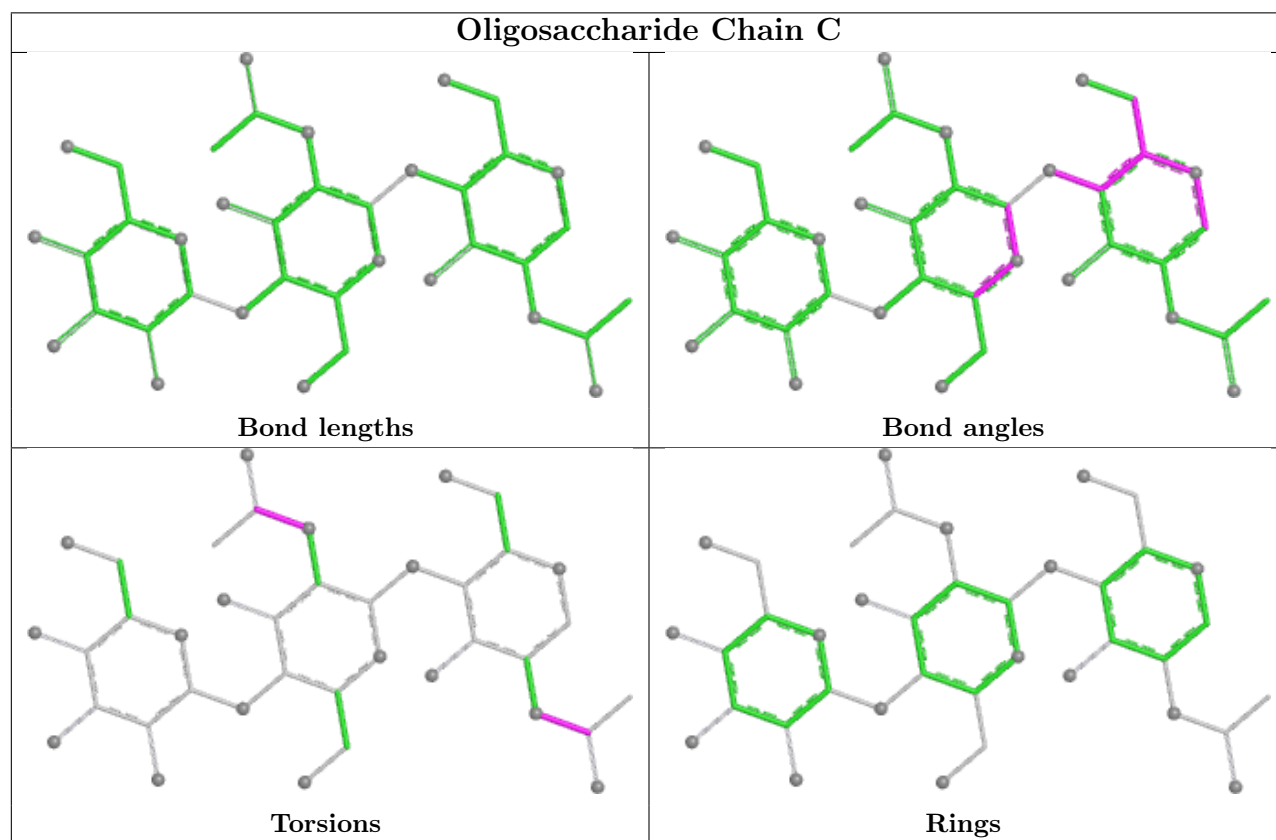
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
5	F	2	NAG	C1-C2-N2-C7
4	I	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
4	I	3	BMA	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
4	I	1	NAG	C3-C2-N2-C7
4	H	1	NAG	O5-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
4	I	2	NAG	O7-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C3-C2-N2-C7
4	H	3	BMA	O5-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C4-C5-C6-O6

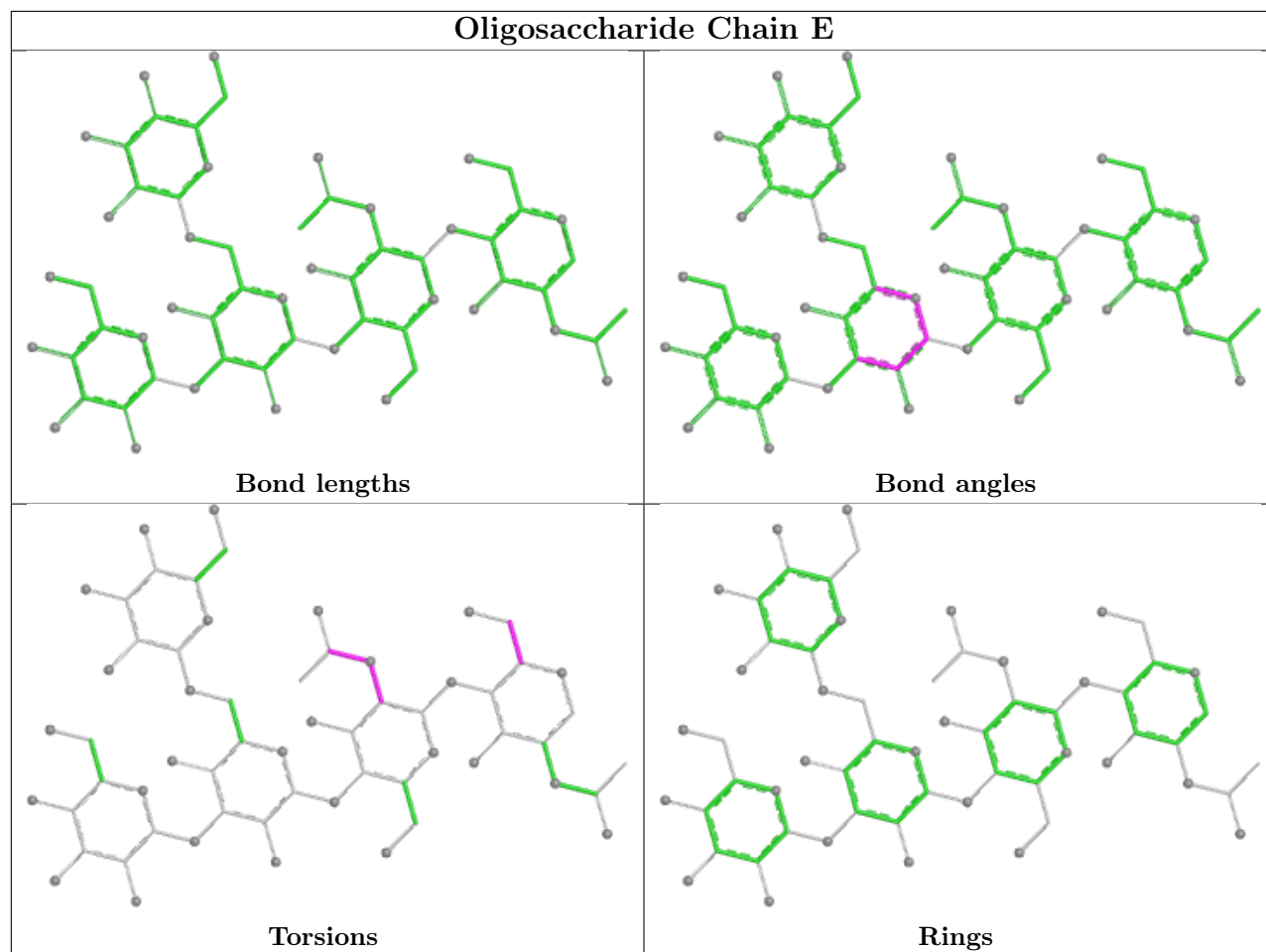
There are no ring outliers.

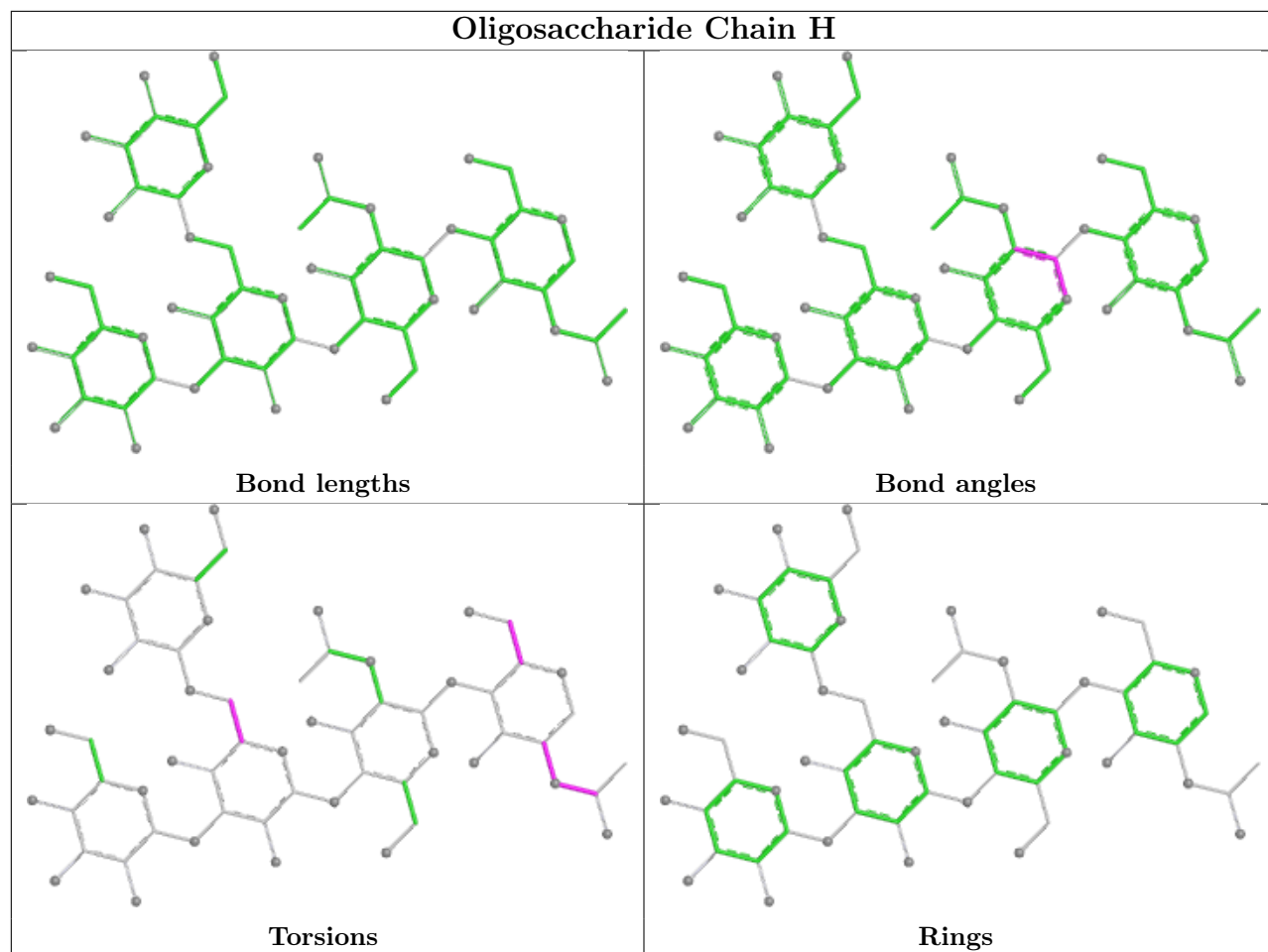
6 monomers are involved in 3 short contacts:

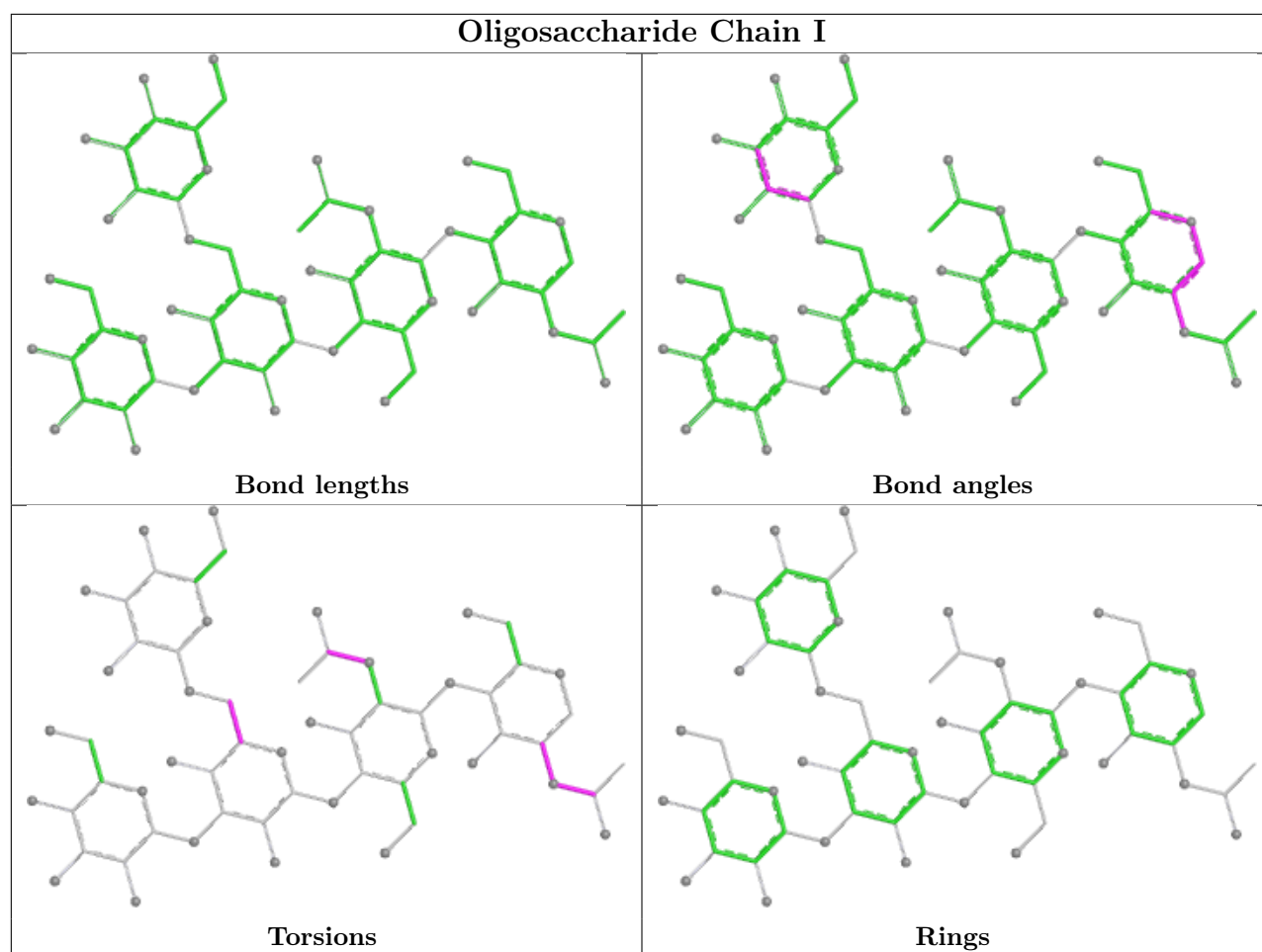
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
4	I	1	NAG	1	0
4	E	2	NAG	1	0
4	H	1	NAG	1	0
4	E	1	NAG	1	0
4	I	2	NAG	1	0

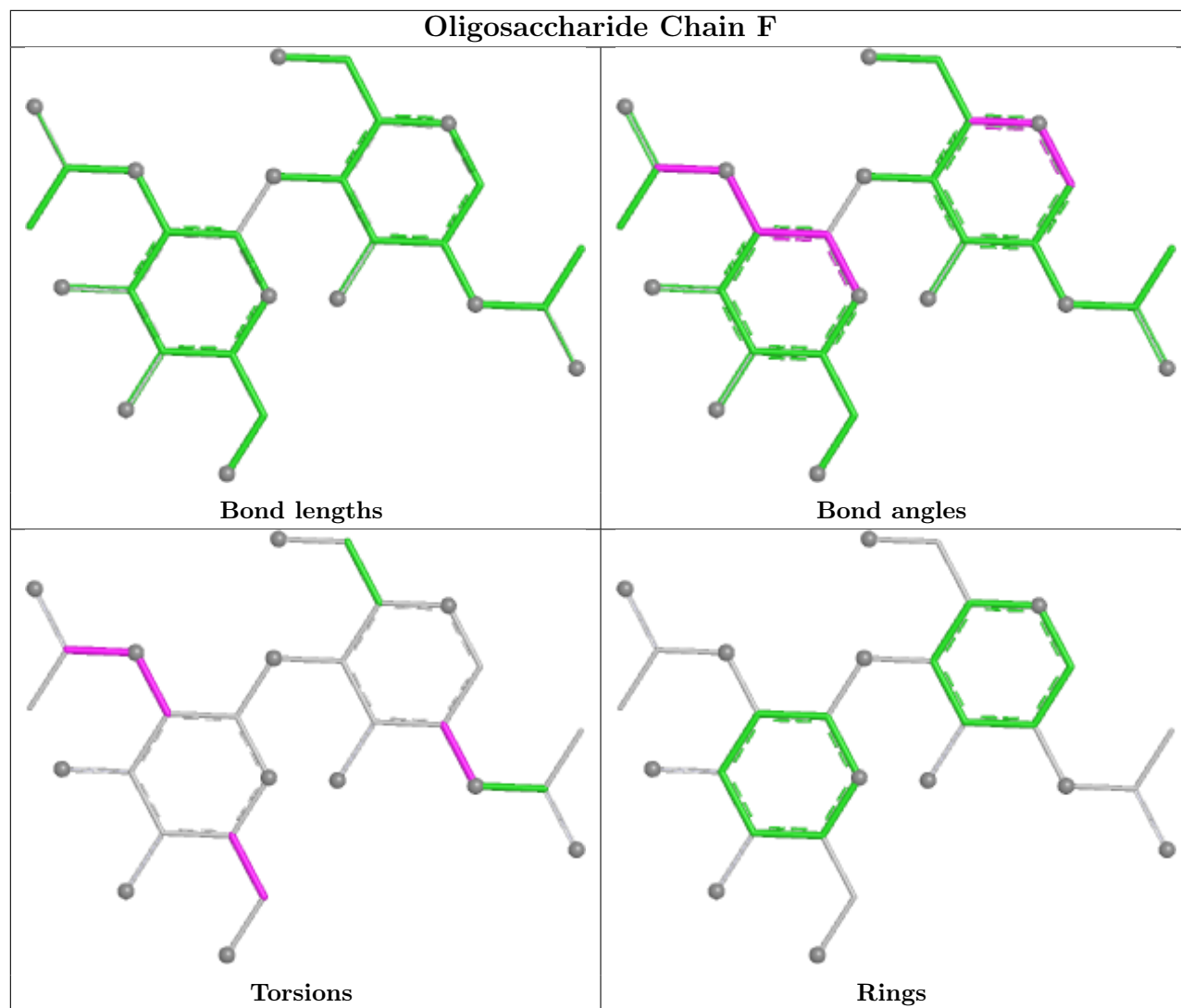
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

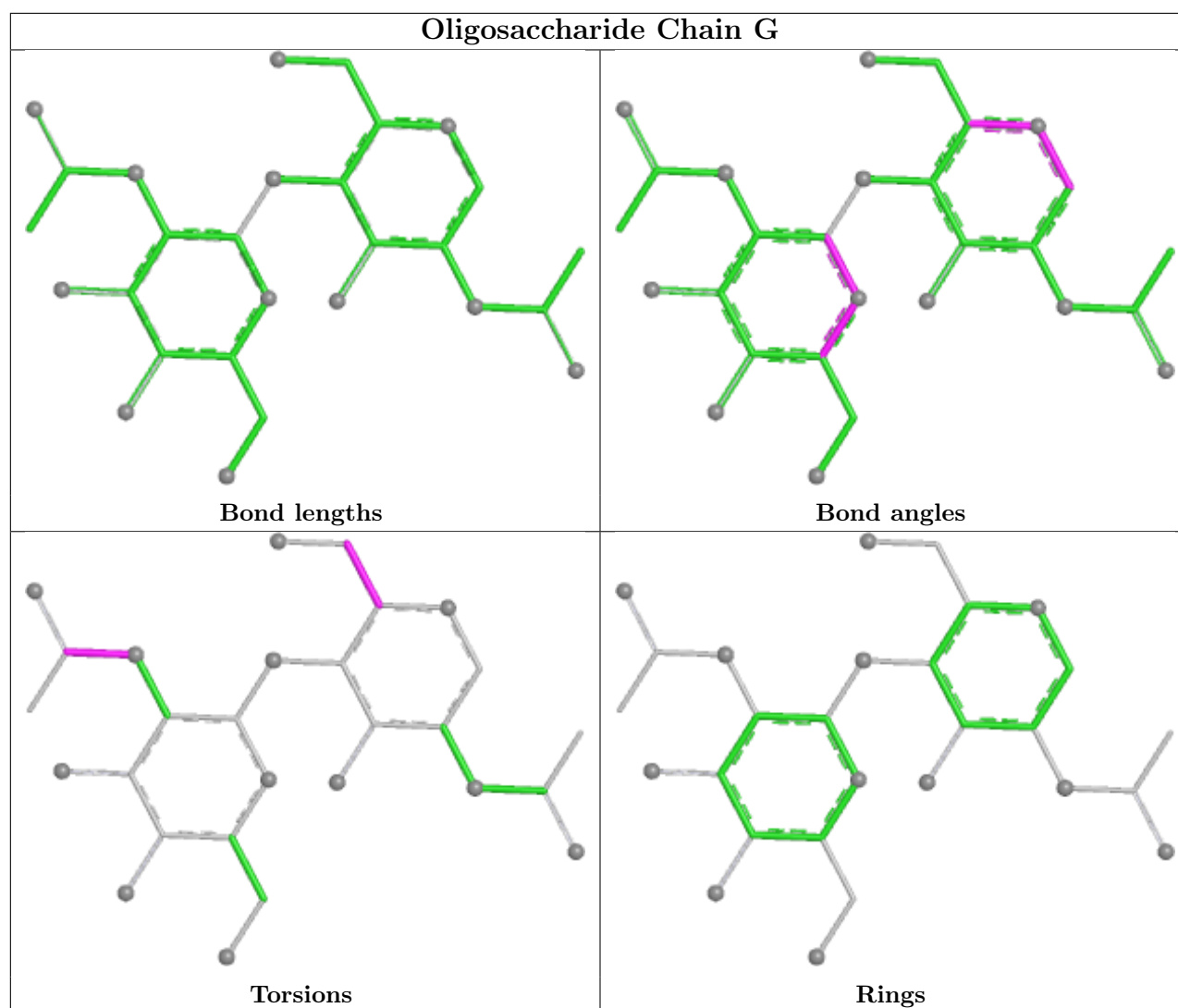












5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 20 are monoatomic - leaving 7 for Mogul analysis.

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	B	4702	1	14,14,15	0.34	0	17,19,21	0.66	0
7	A2G	B	4705	1	14,14,15	0.41	0	17,19,21	0.69	1 (5%)
7	A2G	B	4703	-	14,14,15	0.43	0	17,19,21	1.60	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	A2G	B	4707	1	14,14,15	0.40	0	17,19,21	0.39	0
7	A2G	B	4706	-	14,14,15	0.41	0	17,19,21	2.23	3 (17%)
6	NAG	B	4701	1	14,14,15	0.41	0	17,19,21	1.18	1 (5%)
7	A2G	B	4704	1	14,14,15	0.41	0	17,19,21	0.64	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
6	NAG	B	4702	1	-	1/6/23/26	0/1/1/1
7	A2G	B	4705	1	-	0/6/23/26	0/1/1/1
7	A2G	B	4703	-	-	0/6/23/26	0/1/1/1
7	A2G	B	4707	1	-	0/6/23/26	0/1/1/1
7	A2G	B	4706	-	-	0/6/23/26	0/1/1/1
6	NAG	B	4701	1	-	3/6/23/26	0/1/1/1
7	A2G	B	4704	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4706	A2G	O5-C1-C2	8.06	123.76	111.29
7	B	4703	A2G	C1-C2-N2	5.11	118.48	110.43
6	B	4701	NAG	C1-O5-C5	3.74	117.20	112.19
7	B	4706	A2G	C1-O5-C5	3.54	116.93	112.19
7	B	4703	A2G	O5-C1-C2	2.93	115.83	111.29
7	B	4705	A2G	O5-C1-C2	-2.43	107.54	111.29
7	B	4706	A2G	C1-C2-N2	2.33	114.10	110.43
7	B	4703	A2G	C1-O5-C5	2.30	115.27	112.19
7	B	4704	A2G	O5-C1-C2	-2.26	107.79	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	4701	NAG	C3-C2-N2-C7
6	B	4701	NAG	O7-C7-N2-C2
6	B	4701	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	B	4702	NAG	O5-C5-C6-O6
7	B	4704	A2G	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4703	A2G	6	0
7	B	4706	A2G	5	0
6	B	4701	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

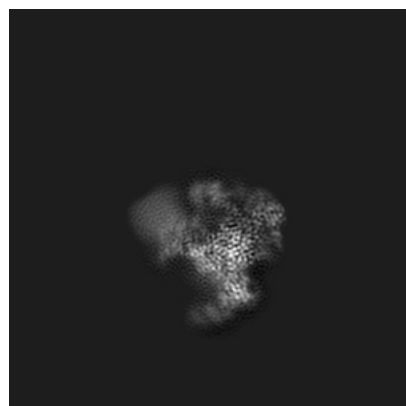
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36693. These allow visual inspection of the internal detail of the map and identification of artifacts.

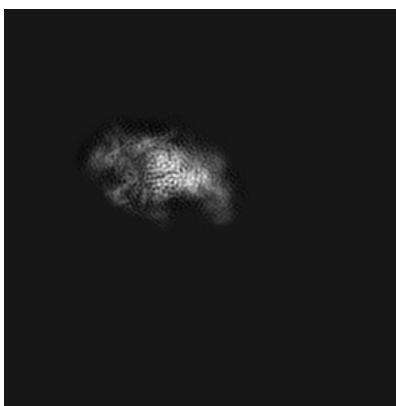
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

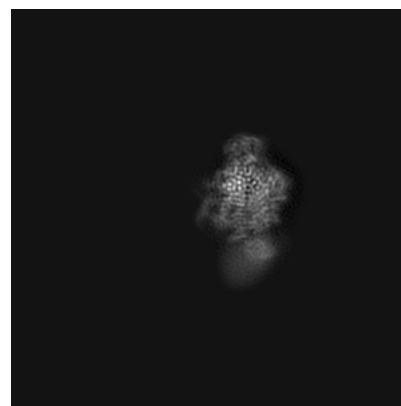
6.1.1 Primary map



X

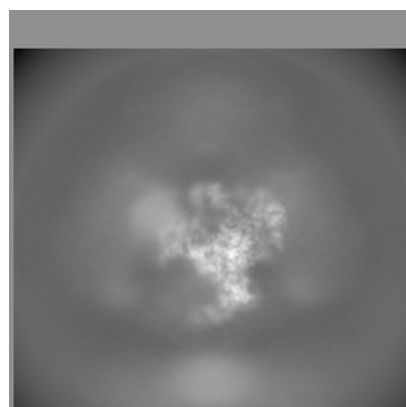


Y

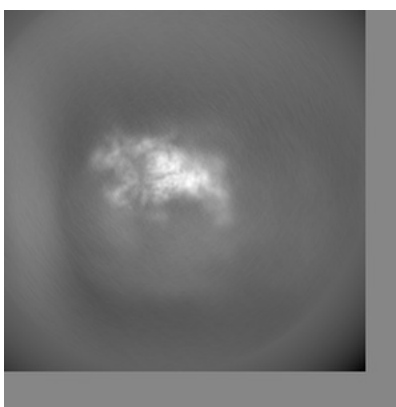


Z

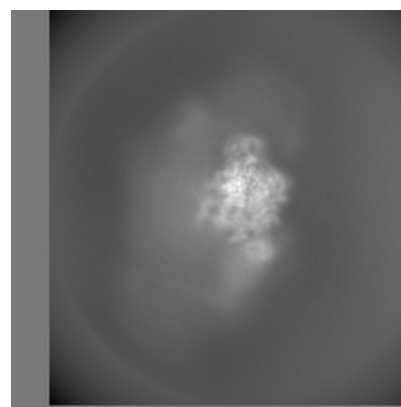
6.1.2 Raw map



X



Y

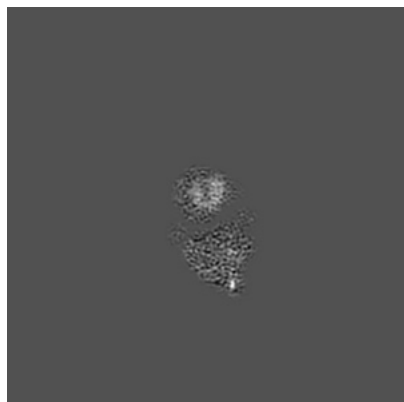


Z

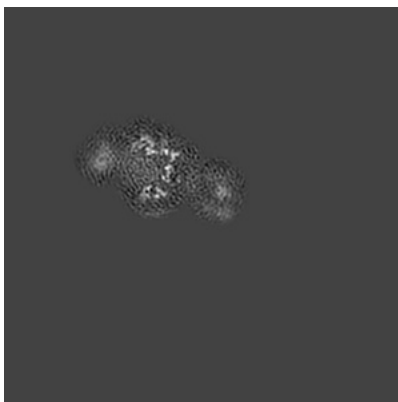
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

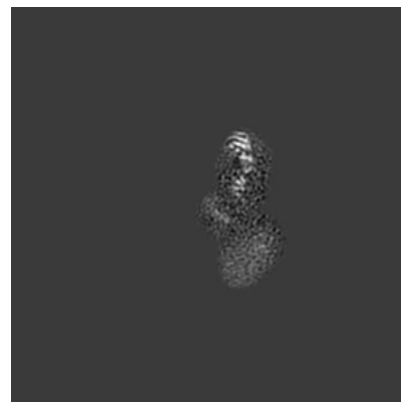
6.2.1 Primary map



X Index: 130

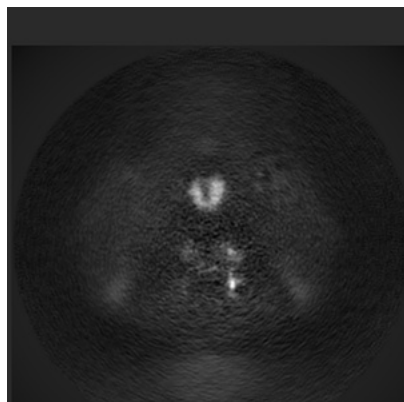


Y Index: 130

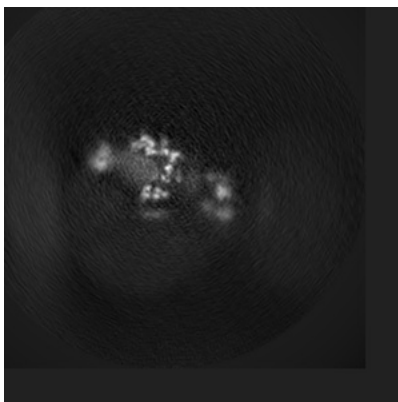


Z Index: 130

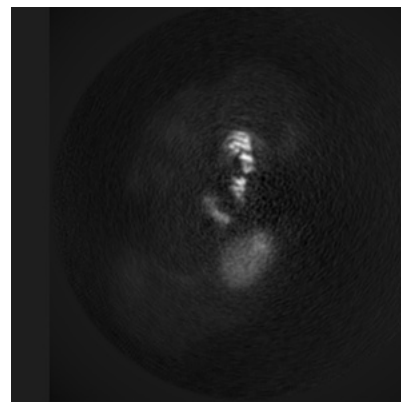
6.2.2 Raw map



X Index: 130



Y Index: 130

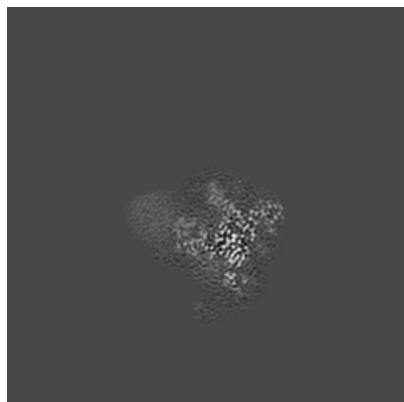


Z Index: 130

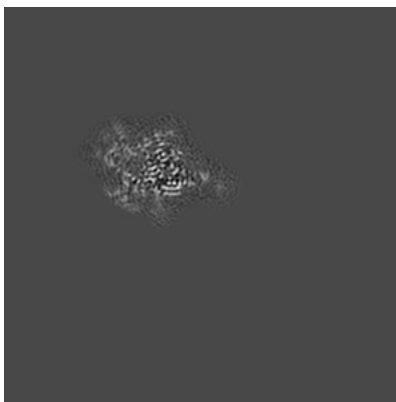
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

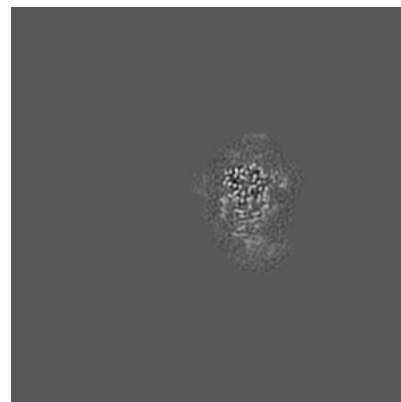
6.3.1 Primary map



X Index: 148

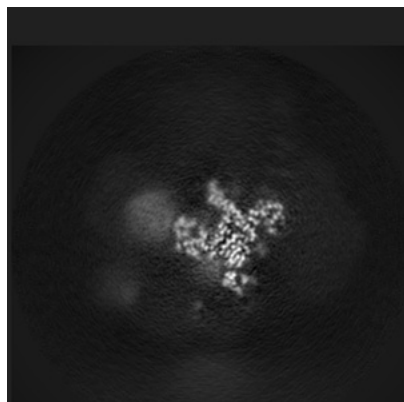


Y Index: 145

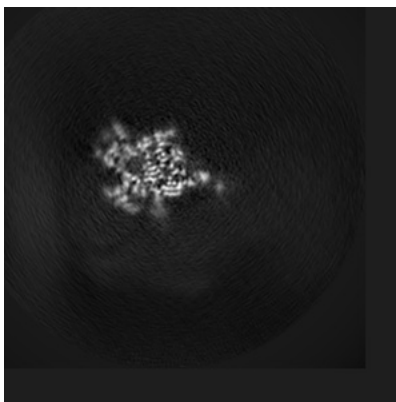


Z Index: 105

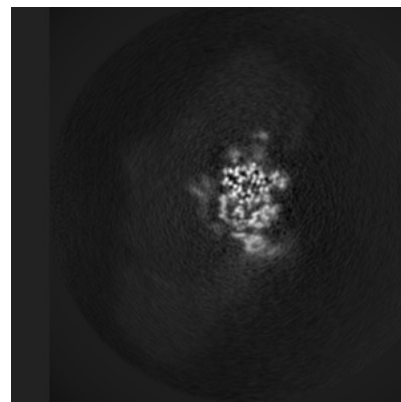
6.3.2 Raw map



X Index: 148



Y Index: 145

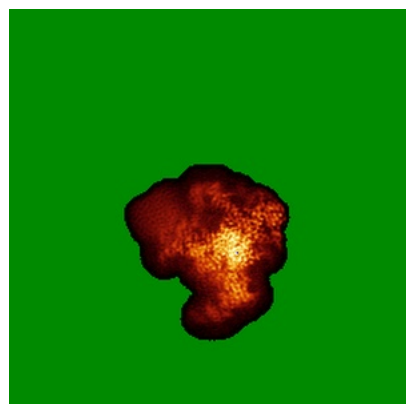


Z Index: 104

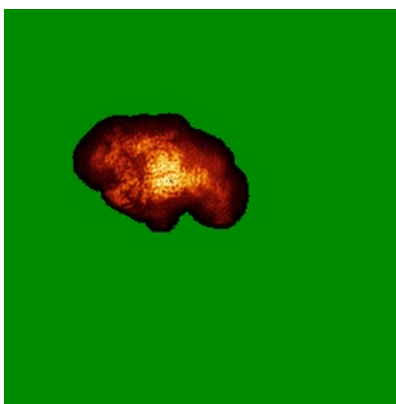
The images above show the largest variance slices of the map in three orthogonal directions.

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

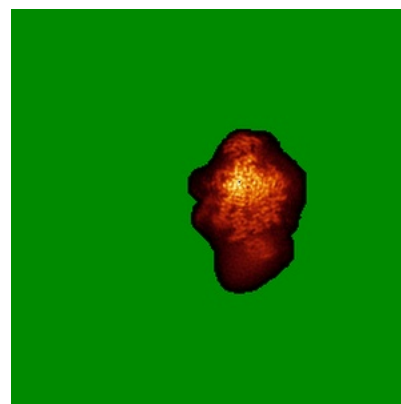
6.4.1 Primary map



X

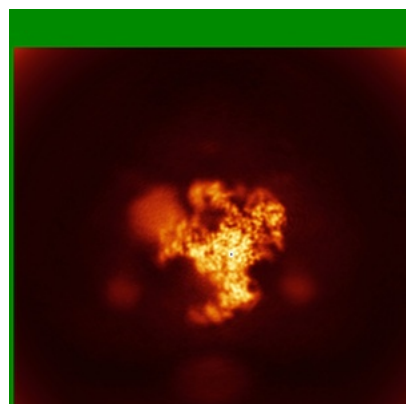


Y

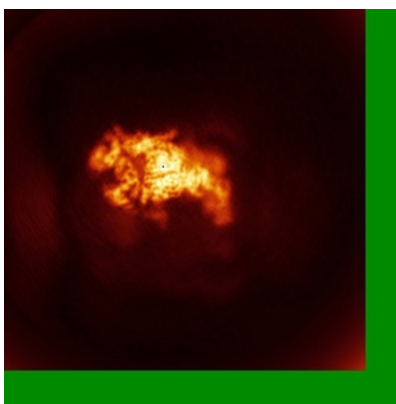


Z

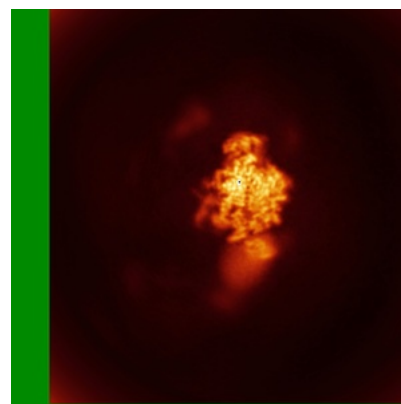
6.4.2 Raw map



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.

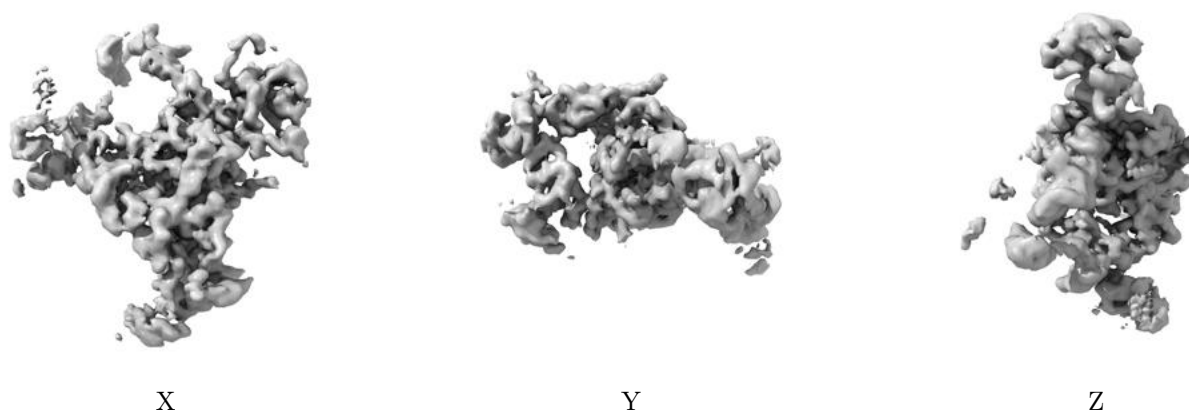
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

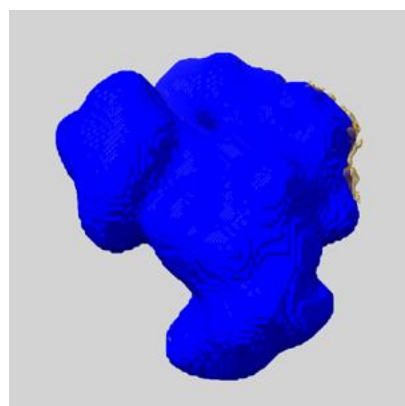
6.6 Mask visualisation [i](#)

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

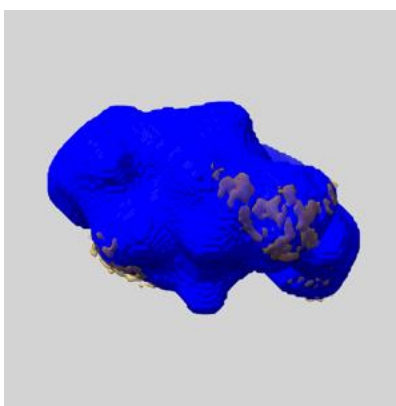
A mask typically either:

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

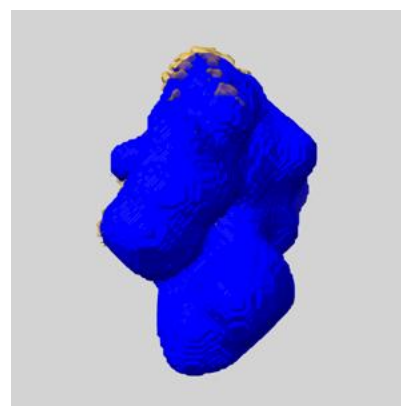
6.6.1 emd_36693_msk_1.map [i](#)



X



Y

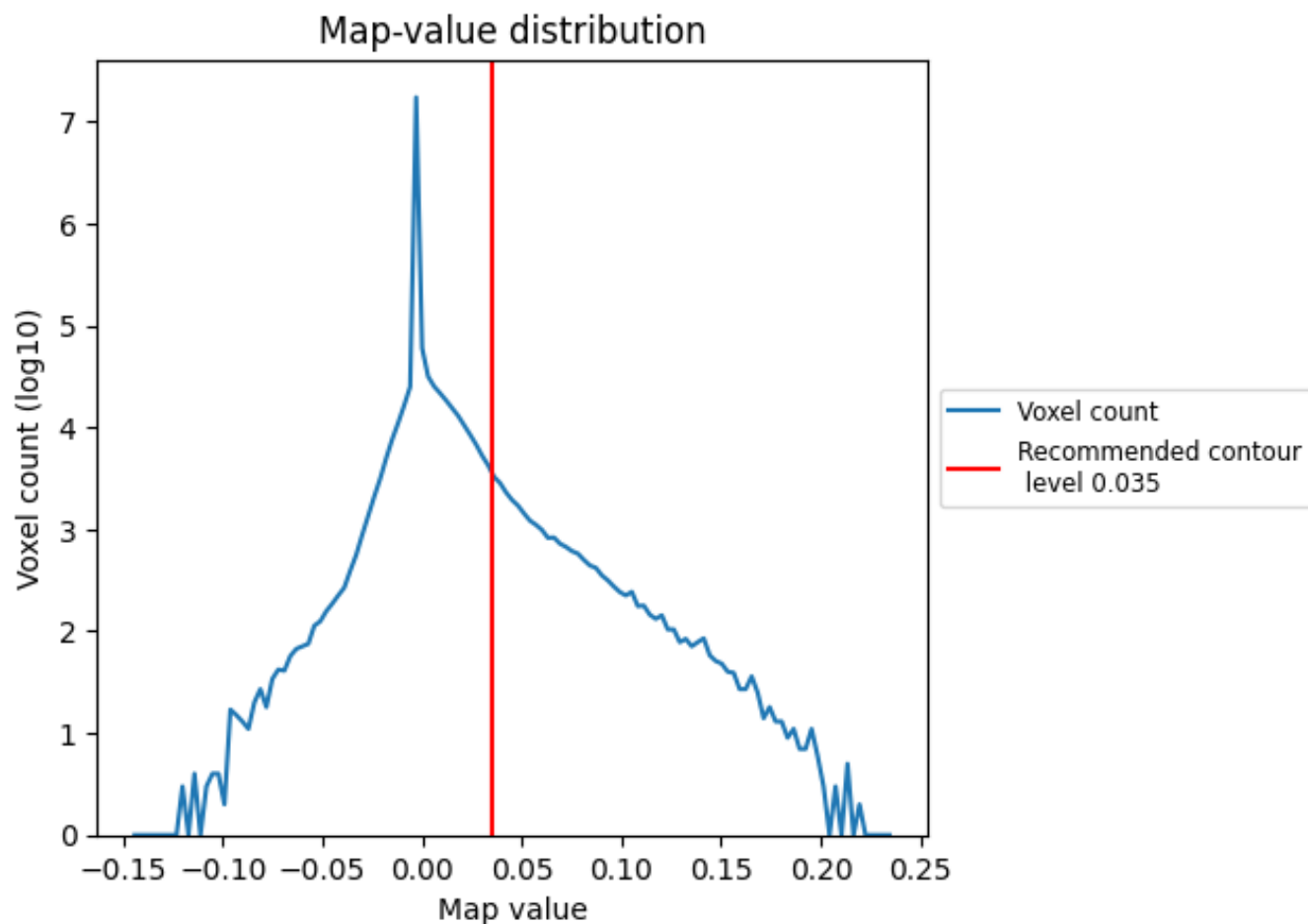


Z

7 Map analysis [i](#)

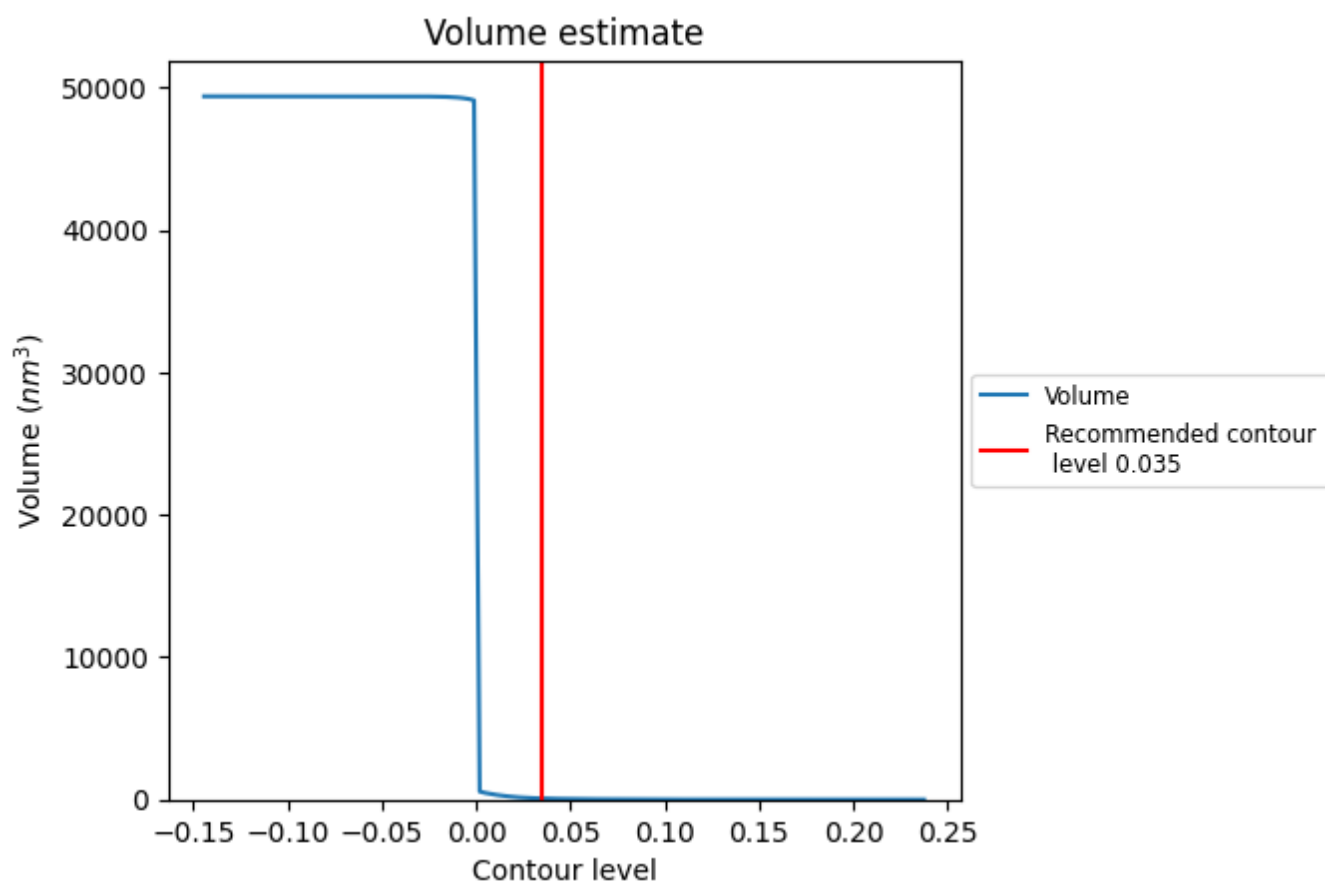
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

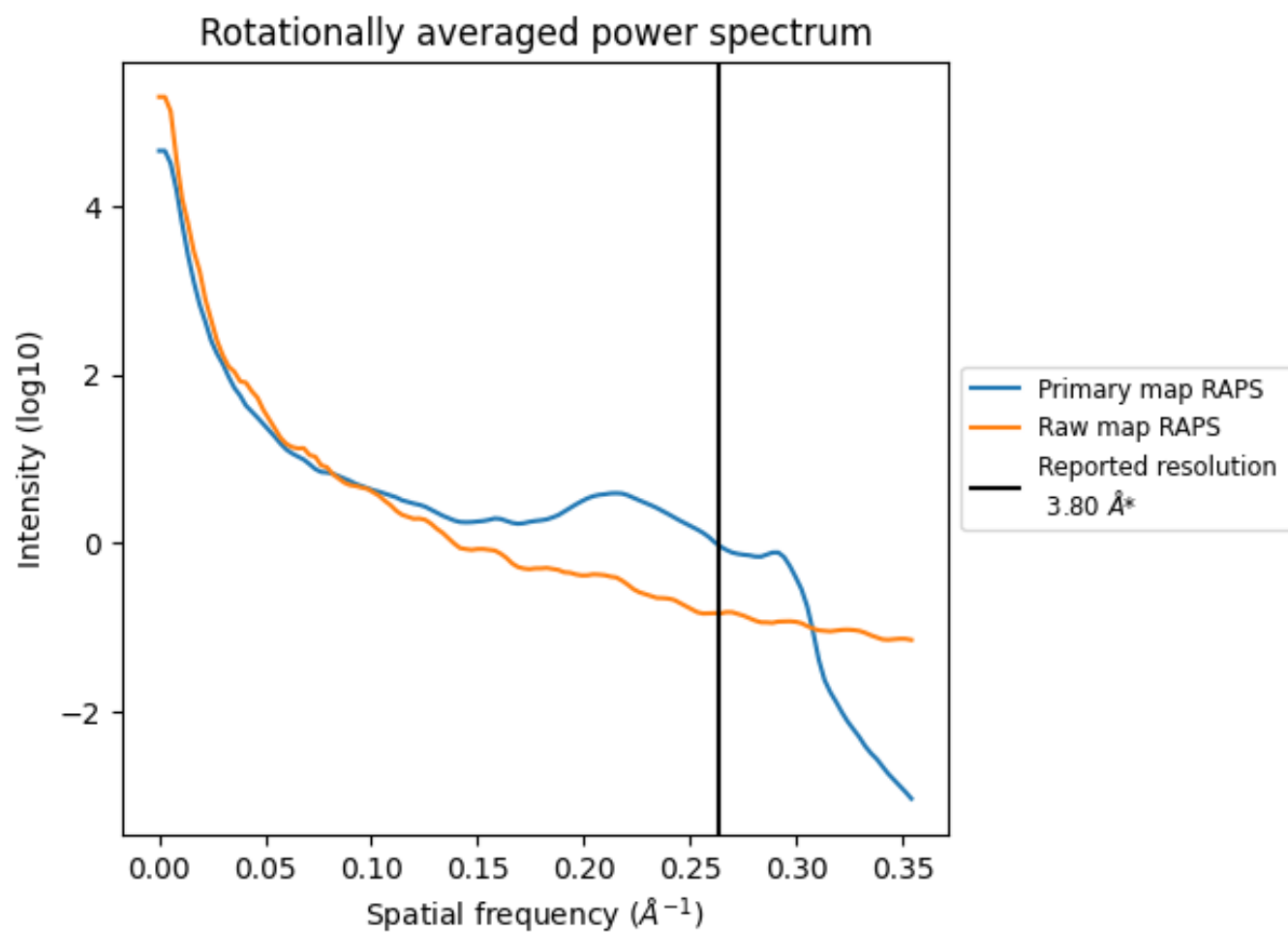
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm³; this corresponds to an approximate mass of 70 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

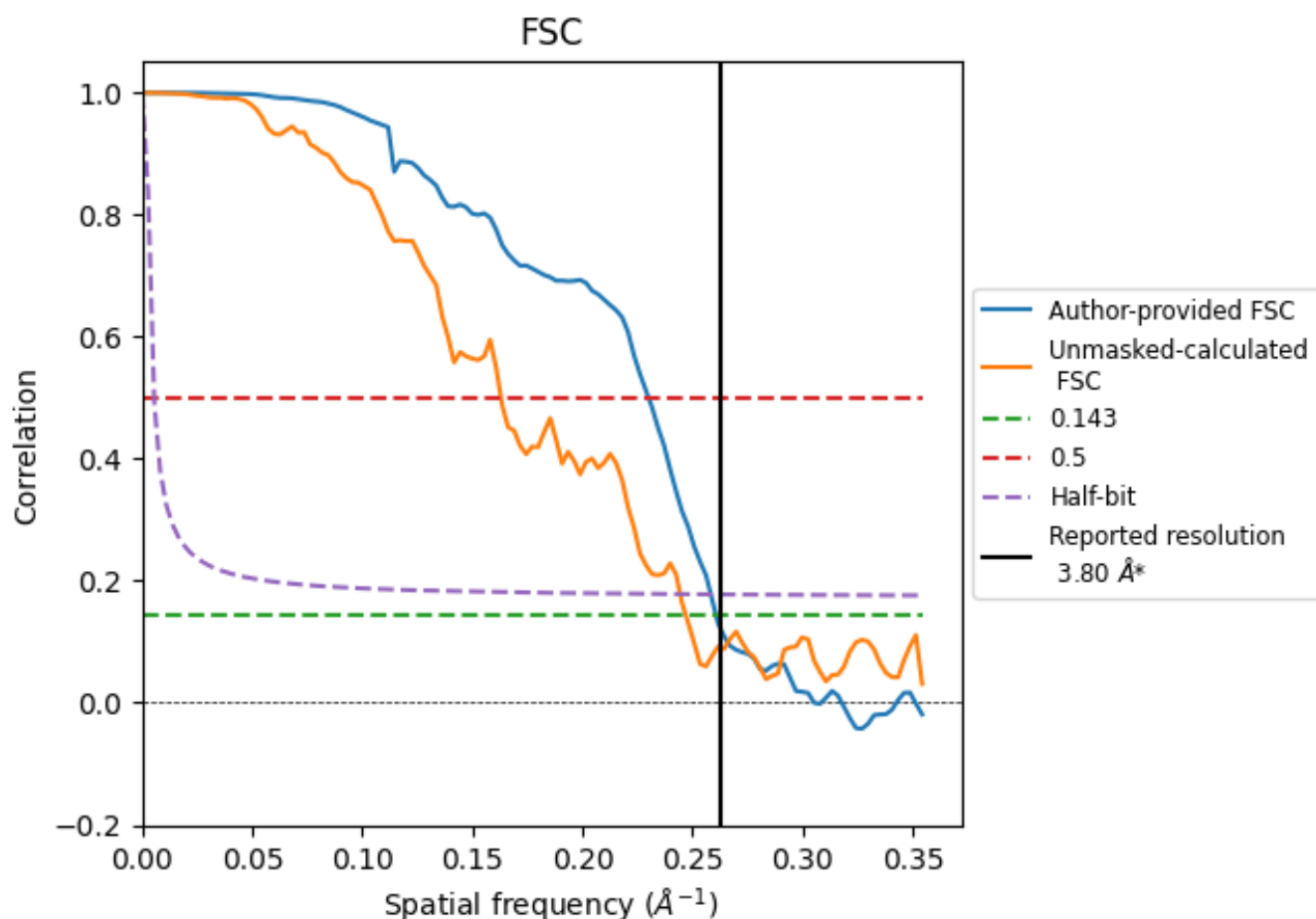


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

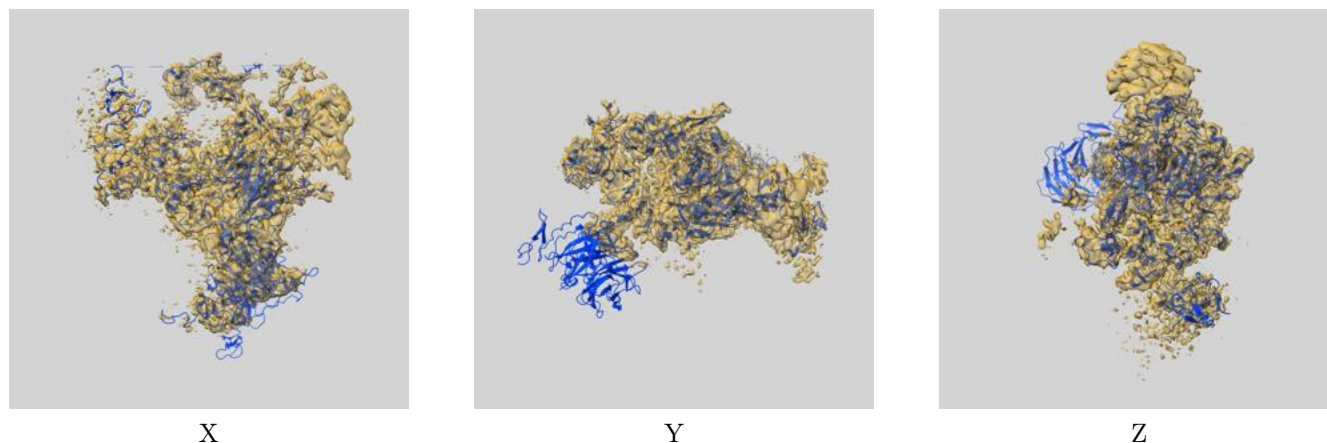
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.35	3.87
Unmasked-calculated*	4.05	6.13	4.09

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

9 Map-model fit [i](#)

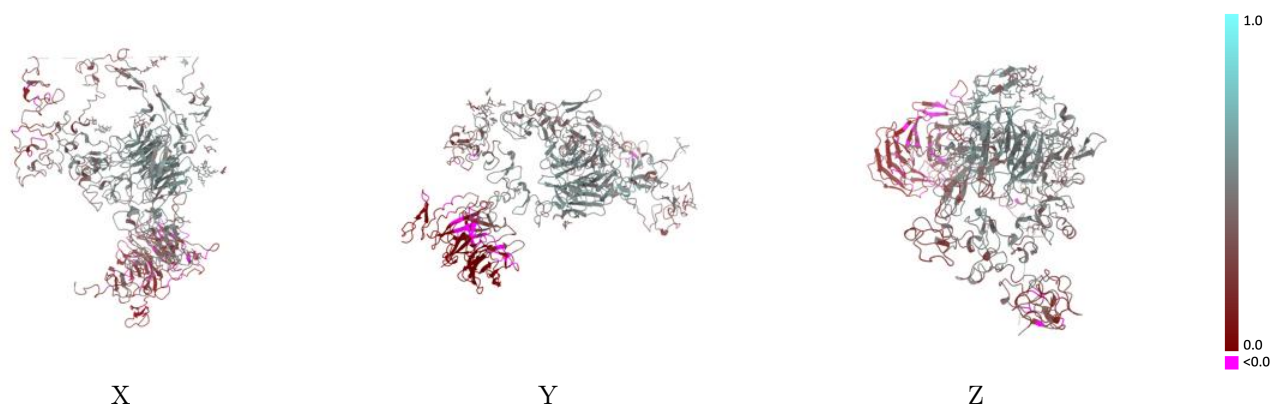
This section contains information regarding the fit between EMDB map EMD-36693 and PDB model 8JX9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



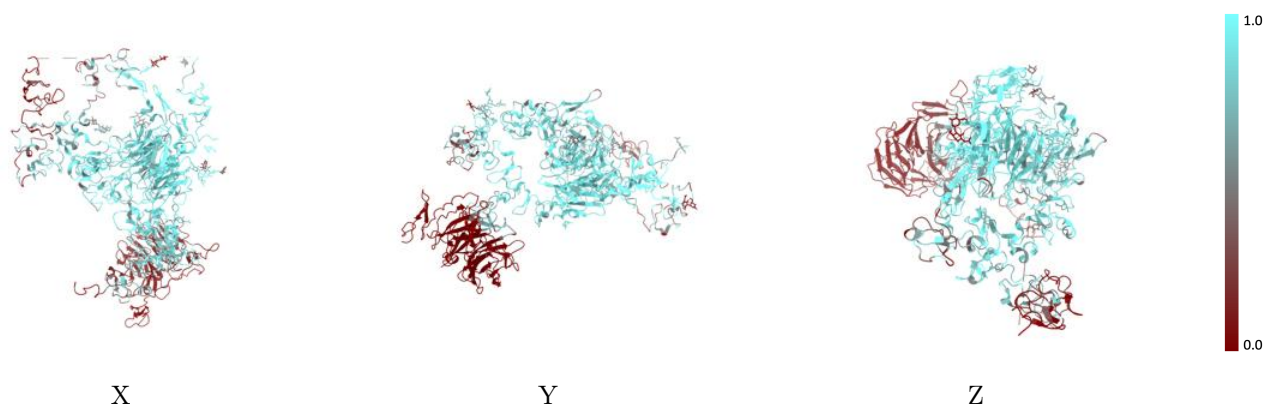
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



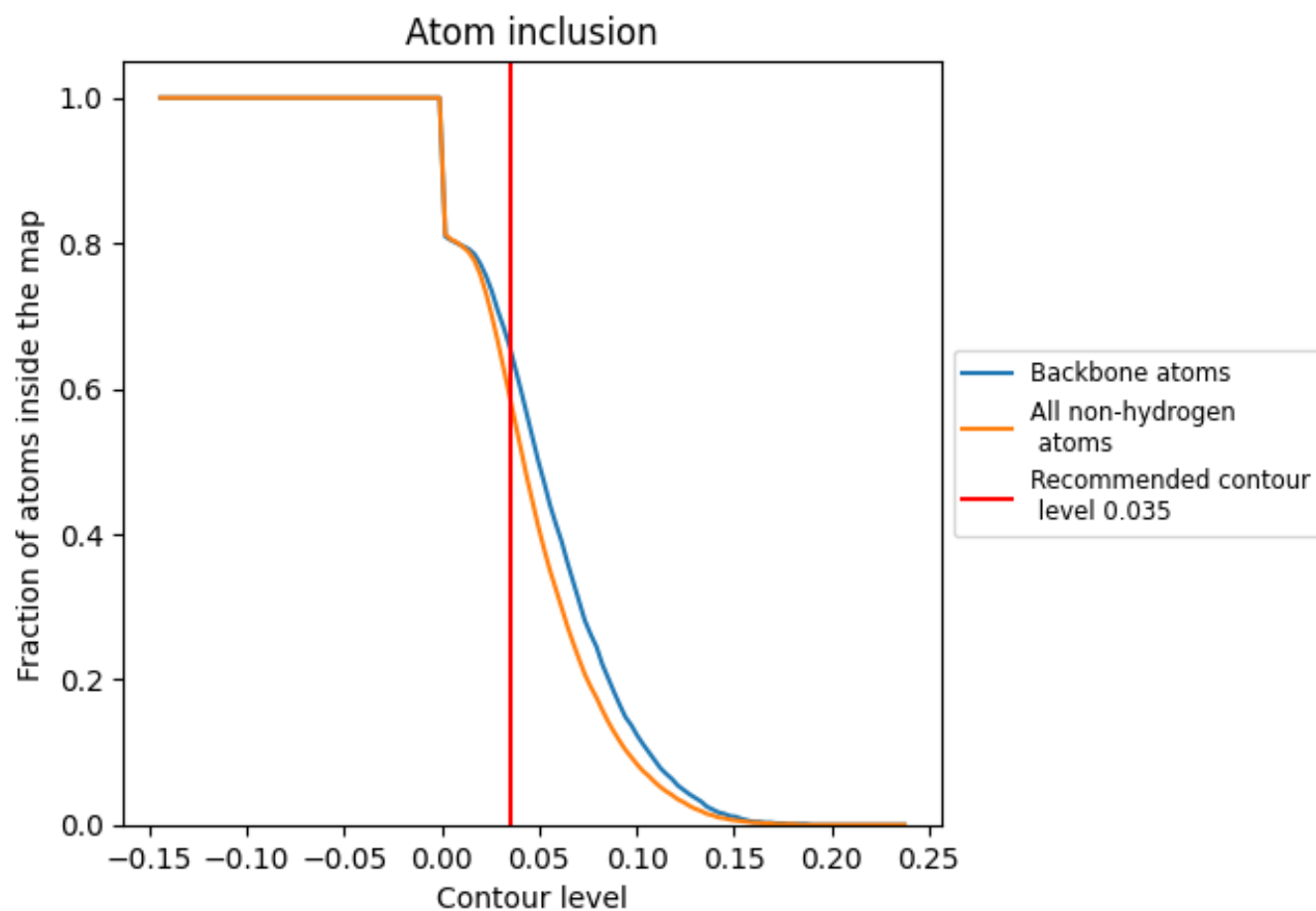
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5900	 0.3480
A	 0.0930	 0.0690
B	 0.7560	 0.4390
C	 0.3330	 0.3370
D	 0.7950	 0.5070
E	 0.6890	 0.4650
F	 0.5360	 0.4360
G	 0.5710	 0.4210
H	 0.5250	 0.3520
I	 0.7380	 0.4320
O	 1.0000	 0.5960

