



Full wwPDB EM Validation Report ⓘ

Jul 7, 2026 – 04:15 PM EDT

PDB ID : 9NPR / pdb_00009npr
EMDB ID : EMD-49630
Title : RAVV glycoprotein in complex with hNPC1-C
Authors : Ye, G.; Bu, F.; Liu, B.; Li, F.
Deposited on : 2025-03-11
Resolution : 3.53 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:

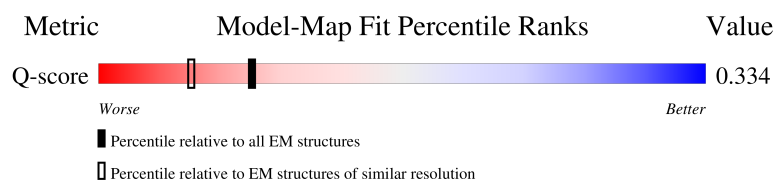
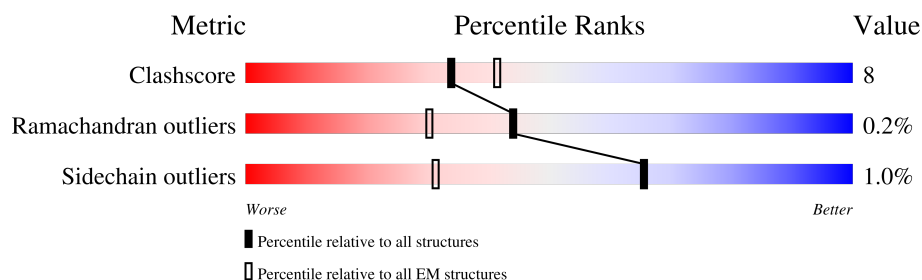
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

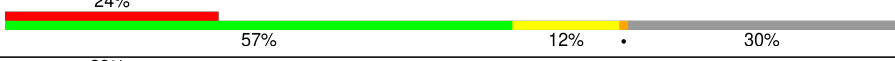
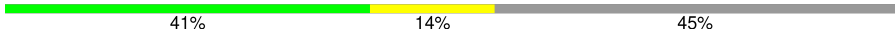
The reported resolution of this entry is 3.53 Å.

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.



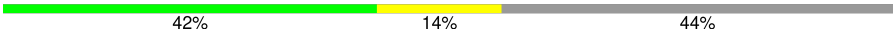
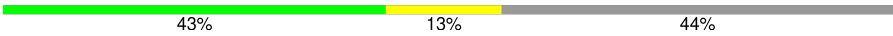
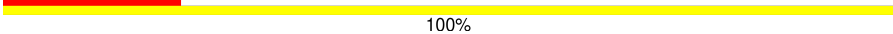
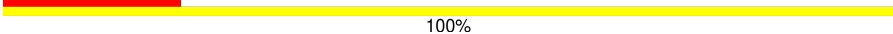
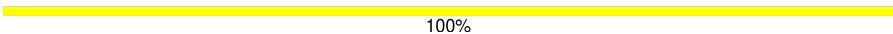
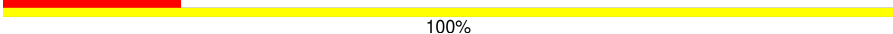
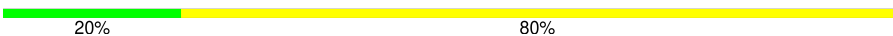
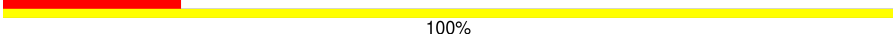
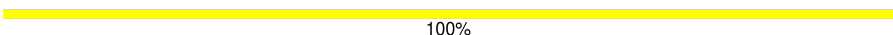
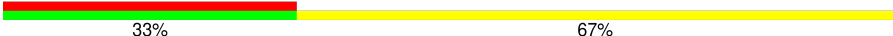
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12947 (3.03 - 4.02)

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	G	280	
1	H	280	
1	I	280	
2	A	256	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	256	
2	C	256	
3	D	247	
3	E	247	
3	F	247	
4	K	5	
4	L	5	
4	M	5	
4	Q	5	
4	R	5	
4	S	5	
5	N	3	
5	O	3	
5	P	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11006 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 NPC intracellular cholesterol transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	194	Total	C	N	O	S	0	0
			1591	1036	253	298	4		
1	H	195	Total	C	N	O	S	0	0
			1598	1040	254	300	4		
1	I	194	Total	C	N	O	S	0	0
			1591	1036	253	298	4		

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	351	MET	-	expression tag	UNP O15118
G	352	ASP	-	expression tag	UNP O15118
G	353	ALA	-	expression tag	UNP O15118
G	354	MET	-	expression tag	UNP O15118
G	355	LYS	-	expression tag	UNP O15118
G	356	ARG	-	expression tag	UNP O15118
G	357	GLY	-	expression tag	UNP O15118
G	358	LEU	-	expression tag	UNP O15118
G	359	CYS	-	expression tag	UNP O15118
G	360	CYS	-	expression tag	UNP O15118
G	361	VAL	-	expression tag	UNP O15118
G	362	LEU	-	expression tag	UNP O15118
G	363	LEU	-	expression tag	UNP O15118
G	364	LEU	-	expression tag	UNP O15118
G	365	CYS	-	expression tag	UNP O15118
G	366	GLY	-	expression tag	UNP O15118
G	367	ALA	-	expression tag	UNP O15118
G	368	VAL	-	expression tag	UNP O15118
G	369	PHE	-	expression tag	UNP O15118
G	370	VAL	-	expression tag	UNP O15118
G	371	SER	-	expression tag	UNP O15118
G	372	ALA	-	expression tag	UNP O15118
G	373	SER	-	expression tag	UNP O15118
G	621	GLY	-	expression tag	UNP O15118

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	622	SER	-	expression tag	UNP O15118
G	623	TRP	-	expression tag	UNP O15118
G	624	SER	-	expression tag	UNP O15118
G	625	HIS	-	expression tag	UNP O15118
G	626	PRO	-	expression tag	UNP O15118
G	627	GLN	-	expression tag	UNP O15118
G	628	PHE	-	expression tag	UNP O15118
G	629	GLU	-	expression tag	UNP O15118
G	630	LYS	-	expression tag	UNP O15118
H	351	MET	-	expression tag	UNP O15118
H	352	ASP	-	expression tag	UNP O15118
H	353	ALA	-	expression tag	UNP O15118
H	354	MET	-	expression tag	UNP O15118
H	355	LYS	-	expression tag	UNP O15118
H	356	ARG	-	expression tag	UNP O15118
H	357	GLY	-	expression tag	UNP O15118
H	358	LEU	-	expression tag	UNP O15118
H	359	CYS	-	expression tag	UNP O15118
H	360	CYS	-	expression tag	UNP O15118
H	361	VAL	-	expression tag	UNP O15118
H	362	LEU	-	expression tag	UNP O15118
H	363	LEU	-	expression tag	UNP O15118
H	364	LEU	-	expression tag	UNP O15118
H	365	CYS	-	expression tag	UNP O15118
H	366	GLY	-	expression tag	UNP O15118
H	367	ALA	-	expression tag	UNP O15118
H	368	VAL	-	expression tag	UNP O15118
H	369	PHE	-	expression tag	UNP O15118
H	370	VAL	-	expression tag	UNP O15118
H	371	SER	-	expression tag	UNP O15118
H	372	ALA	-	expression tag	UNP O15118
H	373	SER	-	expression tag	UNP O15118
H	621	GLY	-	expression tag	UNP O15118
H	622	SER	-	expression tag	UNP O15118
H	623	TRP	-	expression tag	UNP O15118
H	624	SER	-	expression tag	UNP O15118
H	625	HIS	-	expression tag	UNP O15118
H	626	PRO	-	expression tag	UNP O15118
H	627	GLN	-	expression tag	UNP O15118
H	628	PHE	-	expression tag	UNP O15118
H	629	GLU	-	expression tag	UNP O15118
H	630	LYS	-	expression tag	UNP O15118

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	351	MET	-	expression tag	UNP O15118
I	352	ASP	-	expression tag	UNP O15118
I	353	ALA	-	expression tag	UNP O15118
I	354	MET	-	expression tag	UNP O15118
I	355	LYS	-	expression tag	UNP O15118
I	356	ARG	-	expression tag	UNP O15118
I	357	GLY	-	expression tag	UNP O15118
I	358	LEU	-	expression tag	UNP O15118
I	359	CYS	-	expression tag	UNP O15118
I	360	CYS	-	expression tag	UNP O15118
I	361	VAL	-	expression tag	UNP O15118
I	362	LEU	-	expression tag	UNP O15118
I	363	LEU	-	expression tag	UNP O15118
I	364	LEU	-	expression tag	UNP O15118
I	365	CYS	-	expression tag	UNP O15118
I	366	GLY	-	expression tag	UNP O15118
I	367	ALA	-	expression tag	UNP O15118
I	368	VAL	-	expression tag	UNP O15118
I	369	PHE	-	expression tag	UNP O15118
I	370	VAL	-	expression tag	UNP O15118
I	371	SER	-	expression tag	UNP O15118
I	372	ALA	-	expression tag	UNP O15118
I	373	SER	-	expression tag	UNP O15118
I	621	GLY	-	expression tag	UNP O15118
I	622	SER	-	expression tag	UNP O15118
I	623	TRP	-	expression tag	UNP O15118
I	624	SER	-	expression tag	UNP O15118
I	625	HIS	-	expression tag	UNP O15118
I	626	PRO	-	expression tag	UNP O15118
I	627	GLN	-	expression tag	UNP O15118
I	628	PHE	-	expression tag	UNP O15118
I	629	GLU	-	expression tag	UNP O15118
I	630	LYS	-	expression tag	UNP O15118

- Molecule 2 is a protein called Envelope glycoprotein RAVV GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	142	Total 1112	C 706	N 195	O 205	S 6	0	0
2	B	143	Total 1118	C 709	N 196	O 207	S 6	0	0
2	C	143	Total 1118	C 709	N 196	O 207	S 6	0	0

- Molecule 3 is a protein called Envelope glycoprotein RAVV GP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	99	Total	C	N	O	S	0	0
			792	507	137	146	2		
3	E	101	Total	C	N	O	S	0	0
			805	514	139	150	2		
3	F	100	Total	C	N	O	S	0	0
			798	510	138	148	2		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	589	ILE	HIS	conflict	UNP Q1PDC7
D	638	SER	-	expression tag	UNP Q1PDC7
D	639	GLY	-	expression tag	UNP Q1PDC7
D	640	TYR	-	expression tag	UNP Q1PDC7
D	641	ILE	-	expression tag	UNP Q1PDC7
D	642	PRO	-	expression tag	UNP Q1PDC7
D	643	GLU	-	expression tag	UNP Q1PDC7
D	644	ALA	-	expression tag	UNP Q1PDC7
D	645	PRO	-	expression tag	UNP Q1PDC7
D	646	ARG	-	expression tag	UNP Q1PDC7
D	647	ASP	-	expression tag	UNP Q1PDC7
D	648	GLY	-	expression tag	UNP Q1PDC7
D	649	GLN	-	expression tag	UNP Q1PDC7
D	650	ALA	-	expression tag	UNP Q1PDC7
D	651	TYR	-	expression tag	UNP Q1PDC7
D	652	VAL	-	expression tag	UNP Q1PDC7
D	653	ARG	-	expression tag	UNP Q1PDC7
D	654	LYS	-	expression tag	UNP Q1PDC7
D	655	ASP	-	expression tag	UNP Q1PDC7
D	656	GLY	-	expression tag	UNP Q1PDC7
D	657	GLU	-	expression tag	UNP Q1PDC7
D	658	TRP	-	expression tag	UNP Q1PDC7
D	659	VAL	-	expression tag	UNP Q1PDC7
D	660	LEU	-	expression tag	UNP Q1PDC7
D	661	LEU	-	expression tag	UNP Q1PDC7
D	662	SER	-	expression tag	UNP Q1PDC7
D	663	THR	-	expression tag	UNP Q1PDC7
D	664	PHE	-	expression tag	UNP Q1PDC7
D	665	LEU	-	expression tag	UNP Q1PDC7
D	666	GLY	-	expression tag	UNP Q1PDC7
D	667	HIS	-	expression tag	UNP Q1PDC7
D	668	HIS	-	expression tag	UNP Q1PDC7

Continued on next page...

Continued from previous page...

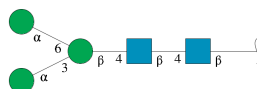
Chain	Residue	Modelled	Actual	Comment	Reference
D	669	HIS	-	expression tag	UNP Q1PDC7
D	670	HIS	-	expression tag	UNP Q1PDC7
D	671	HIS	-	expression tag	UNP Q1PDC7
D	672	HIS	-	expression tag	UNP Q1PDC7
E	589	ILE	HIS	conflict	UNP Q1PDC7
E	638	SER	-	expression tag	UNP Q1PDC7
E	639	GLY	-	expression tag	UNP Q1PDC7
E	640	TYR	-	expression tag	UNP Q1PDC7
E	641	ILE	-	expression tag	UNP Q1PDC7
E	642	PRO	-	expression tag	UNP Q1PDC7
E	643	GLU	-	expression tag	UNP Q1PDC7
E	644	ALA	-	expression tag	UNP Q1PDC7
E	645	PRO	-	expression tag	UNP Q1PDC7
E	646	ARG	-	expression tag	UNP Q1PDC7
E	647	ASP	-	expression tag	UNP Q1PDC7
E	648	GLY	-	expression tag	UNP Q1PDC7
E	649	GLN	-	expression tag	UNP Q1PDC7
E	650	ALA	-	expression tag	UNP Q1PDC7
E	651	TYR	-	expression tag	UNP Q1PDC7
E	652	VAL	-	expression tag	UNP Q1PDC7
E	653	ARG	-	expression tag	UNP Q1PDC7
E	654	LYS	-	expression tag	UNP Q1PDC7
E	655	ASP	-	expression tag	UNP Q1PDC7
E	656	GLY	-	expression tag	UNP Q1PDC7
E	657	GLU	-	expression tag	UNP Q1PDC7
E	658	TRP	-	expression tag	UNP Q1PDC7
E	659	VAL	-	expression tag	UNP Q1PDC7
E	660	LEU	-	expression tag	UNP Q1PDC7
E	661	LEU	-	expression tag	UNP Q1PDC7
E	662	SER	-	expression tag	UNP Q1PDC7
E	663	THR	-	expression tag	UNP Q1PDC7
E	664	PHE	-	expression tag	UNP Q1PDC7
E	665	LEU	-	expression tag	UNP Q1PDC7
E	666	GLY	-	expression tag	UNP Q1PDC7
E	667	HIS	-	expression tag	UNP Q1PDC7
E	668	HIS	-	expression tag	UNP Q1PDC7
E	669	HIS	-	expression tag	UNP Q1PDC7
E	670	HIS	-	expression tag	UNP Q1PDC7
E	671	HIS	-	expression tag	UNP Q1PDC7
E	672	HIS	-	expression tag	UNP Q1PDC7
F	589	ILE	HIS	conflict	UNP Q1PDC7
F	638	SER	-	expression tag	UNP Q1PDC7

Continued on next page...

Continued from previous page...

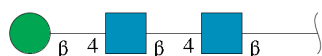
Chain	Residue	Modelled	Actual	Comment	Reference
F	639	GLY	-	expression tag	UNP Q1PDC7
F	640	TYR	-	expression tag	UNP Q1PDC7
F	641	ILE	-	expression tag	UNP Q1PDC7
F	642	PRO	-	expression tag	UNP Q1PDC7
F	643	GLU	-	expression tag	UNP Q1PDC7
F	644	ALA	-	expression tag	UNP Q1PDC7
F	645	PRO	-	expression tag	UNP Q1PDC7
F	646	ARG	-	expression tag	UNP Q1PDC7
F	647	ASP	-	expression tag	UNP Q1PDC7
F	648	GLY	-	expression tag	UNP Q1PDC7
F	649	GLN	-	expression tag	UNP Q1PDC7
F	650	ALA	-	expression tag	UNP Q1PDC7
F	651	TYR	-	expression tag	UNP Q1PDC7
F	652	VAL	-	expression tag	UNP Q1PDC7
F	653	ARG	-	expression tag	UNP Q1PDC7
F	654	LYS	-	expression tag	UNP Q1PDC7
F	655	ASP	-	expression tag	UNP Q1PDC7
F	656	GLY	-	expression tag	UNP Q1PDC7
F	657	GLU	-	expression tag	UNP Q1PDC7
F	658	TRP	-	expression tag	UNP Q1PDC7
F	659	VAL	-	expression tag	UNP Q1PDC7
F	660	LEU	-	expression tag	UNP Q1PDC7
F	661	LEU	-	expression tag	UNP Q1PDC7
F	662	SER	-	expression tag	UNP Q1PDC7
F	663	THR	-	expression tag	UNP Q1PDC7
F	664	PHE	-	expression tag	UNP Q1PDC7
F	665	LEU	-	expression tag	UNP Q1PDC7
F	666	GLY	-	expression tag	UNP Q1PDC7
F	667	HIS	-	expression tag	UNP Q1PDC7
F	668	HIS	-	expression tag	UNP Q1PDC7
F	669	HIS	-	expression tag	UNP Q1PDC7
F	670	HIS	-	expression tag	UNP Q1PDC7
F	671	HIS	-	expression tag	UNP Q1PDC7
F	672	HIS	-	expression tag	UNP Q1PDC7

- 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	K	5	Total	C	N	O	0	0
			61	34	2	25		
4	L	5	Total	C	N	O	0	0
			61	34	2	25		
4	M	5	Total	C	N	O	0	0
			61	34	2	25		
4	Q	5	Total	C	N	O	0	0
			61	34	2	25		
4	R	5	Total	C	N	O	0	0
			61	34	2	25		
4	S	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 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.

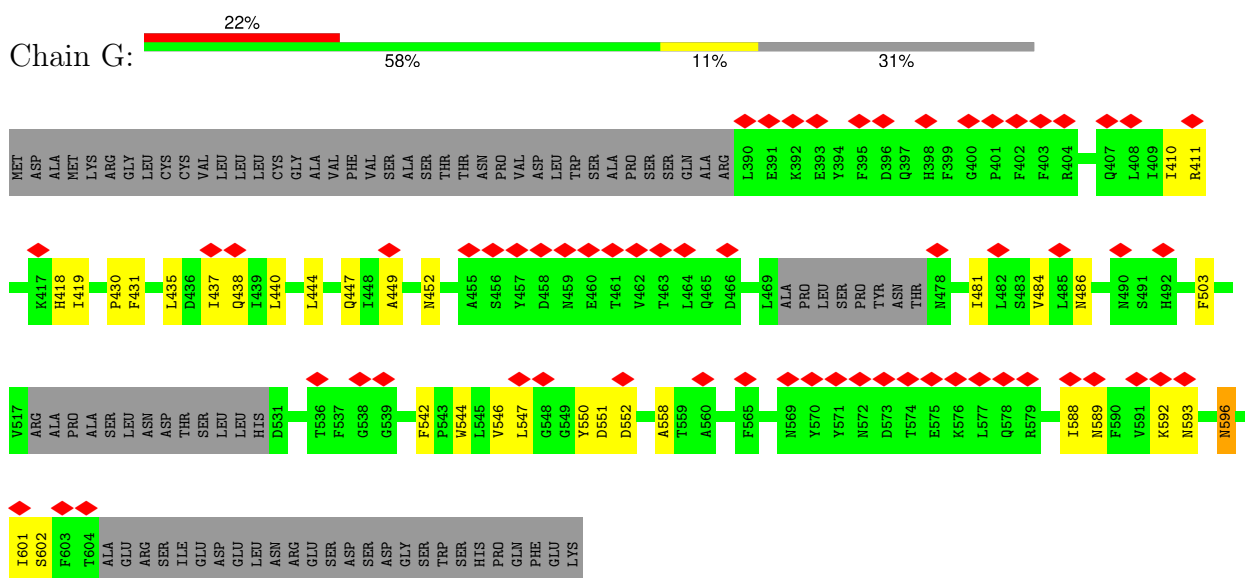


Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	P	3	Total	C	N	O	0	0
			39	22	2	15		

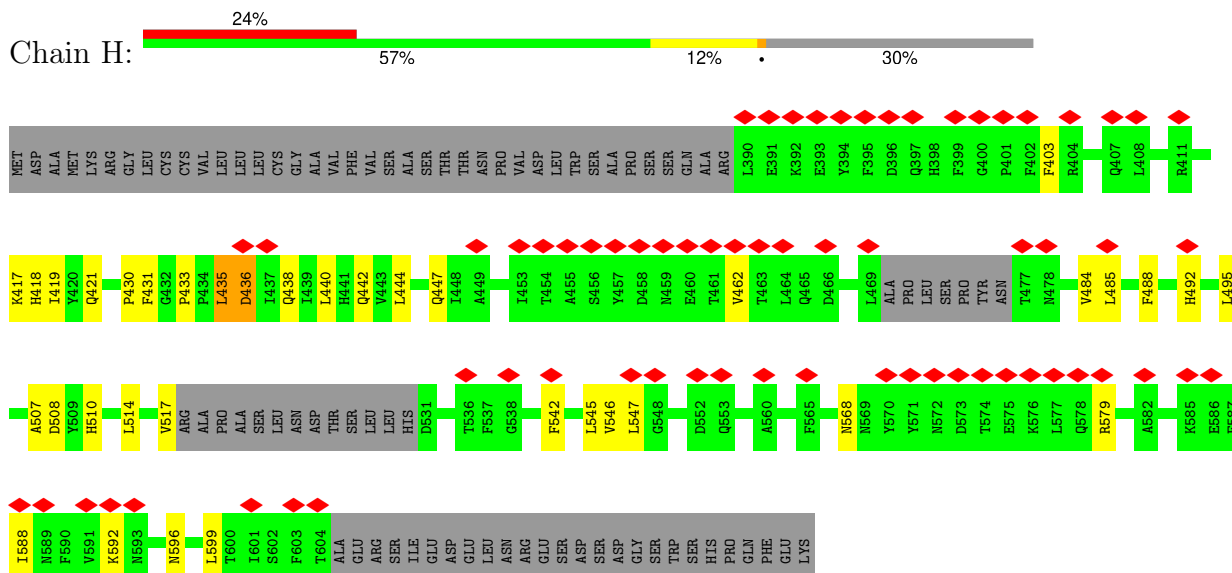
3 Residue-property plots

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.

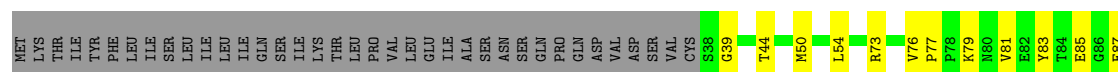
- Molecule 1: NPC intracellular cholesterol transporter 1



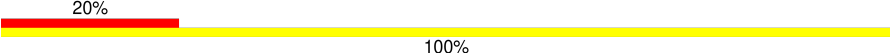
- Molecule 1: NPC intracellular cholesterol transporter 1



- Molecule 1: NPC intracellular cholesterol transporter 1

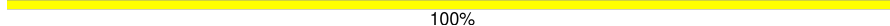


- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain S: 



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

Chain N: 



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

Chain O: 



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

Chain P: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116624	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.513	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.078	Depositor
Map size ($\text{\AA}$)	283.30664, 283.30664, 283.30664	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.88533324, 0.88533324, 0.88533324	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	G	0.15	0/1639	0.38	0/2238
1	H	0.19	0/1646	0.35	0/2248
1	I	0.30	0/1639	0.48	0/2238
2	A	0.16	0/1140	0.40	0/1545
2	B	0.16	0/1146	0.40	0/1553
2	C	0.14	0/1146	0.37	0/1553
3	D	0.17	0/805	0.40	0/1087
3	E	0.17	0/818	0.41	0/1105
3	F	0.14	0/811	0.38	0/1095
All	All	0.19	0/10790	0.40	0/14662

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1591	0	1499	23	0
1	H	1598	0	1506	24	0
1	I	1591	0	1499	24	0
2	A	1112	0	1098	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1118	0	1103	30	0
2	C	1118	0	1103	26	0
3	D	792	0	786	23	0
3	E	805	0	798	15	0
3	F	798	0	790	18	0
4	K	61	0	52	0	0
4	L	61	0	52	0	0
4	M	61	0	52	0	0
4	Q	61	0	52	0	0
4	R	61	0	52	0	0
4	S	61	0	52	0	0
5	N	39	0	34	0	0
5	O	39	0	34	0	0
5	P	39	0	34	0	0
All	All	11006	0	10596	178	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 8.

All (178) 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)
3:F:469:ASP:N	3:F:569:SER:HG	1.67	0.90
1:I:390:LEU:N	1:I:550:TYR:HH	1.75	0.85
1:G:503:PHE:O	2:A:129:ASN:ND2	2.19	0.76
2:A:112:ASN:HD21	3:E:578:THR:HB	1.57	0.69
2:B:87:GLU:OE1	3:E:560:ARG:NH2	2.26	0.69
1:I:467:ILE:HG21	1:I:579:ARG:HG2	1.75	0.67
3:E:528:ALA:N	3:E:531:SER:HG	1.93	0.67
2:A:76:VAL:HG21	2:A:137:LEU:HD11	1.78	0.66
2:C:164:ASN:HB2	3:F:563:ALA:HB1	1.78	0.66
3:D:592:ASP:OD1	2:C:44:THR:OG1	2.14	0.65
1:H:431:PHE:HB3	1:H:435:LEU:HD21	1.79	0.64
1:H:419:ILE:HA	1:H:430:PRO:HA	1.80	0.63
1:G:550:TYR:HB3	1:G:558:ALA:HB2	1.81	0.62
2:A:82:GLU:HA	2:A:149:VAL:HA	1.80	0.62
2:C:87:GLU:OE2	3:F:560:ARG:NH2	2.32	0.62
2:A:138:HIS:HE1	2:A:140:TRP:HB2	1.65	0.62
2:C:76:VAL:HG21	2:C:137:LEU:HD11	1.82	0.62
2:C:87:GLU:O	2:C:116:TYR:OH	2.18	0.62
1:H:444:LEU:HD21	1:H:492:HIS:HA	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:503:PHE:O	2:B:129:ASN:ND2	2.24	0.62
1:I:437:ILE:HG13	1:I:438:GLN:N	2.16	0.61
3:F:518:ILE:HD13	3:F:549:ILE:HD11	1.82	0.61
2:B:88:GLU:HG3	2:B:118:LYS:HB2	1.82	0.60
1:I:596:ASN:ND2	1:I:599:LEU:O	2.34	0.60
3:E:474:PHE:CE1	3:E:555:LEU:HD11	2.37	0.60
1:H:447:GLN:HE22	1:H:485:LEU:HG	1.66	0.60
2:A:87:GLU:OE2	3:D:560:ARG:NH2	2.35	0.60
1:G:419:ILE:HA	1:G:430:PRO:HA	1.84	0.59
3:D:579:GLU:HG3	3:D:581:ARG:H	1.67	0.59
2:A:180:SER:O	3:D:550:LYS:NZ	2.35	0.59
1:G:437:ILE:HD12	1:G:438:GLN:HE22	1.68	0.58
1:H:418:HIS:CE1	1:H:436:ASP:HA	2.39	0.58
2:B:82:GLU:OE1	3:F:578:THR:OG1	2.20	0.58
2:A:87:GLU:HA	3:D:518:ILE:HG22	1.86	0.57
3:D:581:ARG:HA	3:D:581:ARG:HE	1.69	0.57
1:G:481:ILE:O	1:G:486:ASN:ND2	2.31	0.56
2:B:65:GLU:N	2:B:65:GLU:OE1	2.38	0.56
1:G:596:ASN:C	1:G:596:ASN:HD22	2.11	0.56
1:H:510:HIS:HB2	1:H:514:LEU:HB2	1.87	0.56
2:A:172:LYS:HE3	2:A:172:LYS:HA	1.88	0.56
2:B:130:PRO:HG2	2:B:131:HIS:ND1	2.21	0.56
2:B:148:ARG:NH1	3:F:576:VAL:O	2.39	0.55
2:B:112:ASN:ND2	3:F:579:GLU:OE1	2.38	0.55
2:A:172:LYS:HB3	2:A:176:ARG:HH12	1.71	0.55
2:C:39:GLY:HA2	3:F:593:PHE:HZ	1.72	0.55
1:G:418:HIS:O	1:G:431:PHE:N	2.40	0.54
2:B:99:ASP:HB3	2:B:105:LEU:HD21	1.89	0.54
3:D:541:GLU:N	3:D:541:GLU:OE1	2.41	0.54
1:I:423:TYR:OH	2:B:63:PRO:O	2.26	0.53
2:C:138:HIS:HE1	2:C:140:TRP:HB2	1.73	0.53
2:C:112:ASN:ND2	3:F:582:THR:OG1	2.40	0.53
2:A:138:HIS:CE1	2:A:140:TRP:HB2	2.43	0.53
3:D:576:VAL:O	2:C:148:ARG:NH1	2.42	0.52
1:H:588:ILE:O	1:H:592:LYS:NZ	2.39	0.52
3:E:517:ARG:HH22	3:E:548:LEU:HD23	1.74	0.52
2:C:167:ALA:O	3:F:472:PRO:HD2	2.10	0.52
2:A:164:ASN:HB2	3:D:563:ALA:HB1	1.91	0.52
1:I:440:LEU:HG	1:I:485:LEU:HD21	1.92	0.52
1:G:418:HIS:ND1	1:G:435:LEU:O	2.41	0.52
1:I:542:PHE:HB2	1:I:545:LEU:HG	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:437:ILE:HG13	1:I:438:GLN:H	1.74	0.52
1:H:444:LEU:HD22	1:H:495:LEU:HD13	1.92	0.51
2:A:88:GLU:O	3:D:517:ARG:NH1	2.40	0.51
3:E:533:ILE:HD12	3:E:534:PRO:HD2	1.92	0.51
2:C:54:LEU:HD13	2:C:162:GLU:HB3	1.92	0.51
2:A:93:TYR:HB3	2:A:95:ILE:HG13	1.93	0.51
2:A:81:VAL:O	2:A:150:ALA:N	2.44	0.51
1:G:546:VAL:HG13	1:G:547:LEU:HG	1.93	0.50
3:E:474:PHE:HE1	3:E:555:LEU:HD11	1.76	0.50
2:A:76:VAL:HG23	2:A:135:ILE:HD11	1.92	0.50
2:C:81:VAL:HG23	3:F:585:LEU:HD13	1.94	0.50
2:C:106:LEU:HD22	2:C:154:MET:HB2	1.93	0.49
1:H:442:GLN:HB3	1:H:599:LEU:HD23	1.94	0.49
3:D:516:LEU:HB3	3:D:549:ILE:HB	1.94	0.49
1:G:419:ILE:HG22	1:G:430:PRO:HB3	1.95	0.49
1:I:544:TRP:HB3	1:I:555:TYR:HB3	1.93	0.49
3:E:532:TRP:HA	3:F:572:LEU:HD21	1.95	0.49
2:C:130:PRO:HG2	2:C:131:HIS:ND1	2.28	0.48
2:A:104:SER:OG	2:A:156:ARG:NH2	2.47	0.48
2:B:50:MET:HG2	2:B:85:GLU:HG3	1.95	0.48
2:A:143:PHE:CZ	3:D:570:LEU:HD23	2.48	0.48
1:G:437:ILE:HG13	1:G:438:GLN:OE1	2.14	0.48
1:H:462:VAL:HG21	1:H:579:ARG:HG2	1.96	0.48
1:H:546:VAL:HG13	1:H:547:LEU:HG	1.96	0.48
2:C:50:MET:HG2	2:C:85:GLU:HG3	1.96	0.48
2:C:138:HIS:CE1	2:C:140:TRP:HB2	2.49	0.48
1:H:542:PHE:HB2	1:H:545:LEU:HG	1.96	0.48
2:A:79:LYS:NZ	3:D:574:LEU:O	2.33	0.48
3:D:537:GLY:O	2:B:73:ARG:NH2	2.47	0.48
2:C:50:MET:HE2	2:C:168:MET:HE1	1.96	0.47
1:I:504:PHE:HA	2:B:129:ASN:HB3	1.96	0.47
1:I:547:LEU:HD12	1:I:558:ALA:HB3	1.96	0.47
2:A:57:GLN:O	2:A:58:LYS:HG2	2.15	0.47
2:B:53:THR:OG1	2:B:87:GLU:OE2	2.26	0.47
1:H:440:LEU:HB3	1:H:495:LEU:HD21	1.96	0.46
2:B:143:PHE:CZ	3:E:570:LEU:HD23	2.50	0.46
3:E:587:ASN:O	3:E:591:ILE:HG13	2.16	0.46
1:I:431:PHE:CD1	1:I:435:LEU:HD22	2.51	0.46
1:G:410:ILE:HG22	1:G:601:ILE:HA	1.97	0.46
1:I:437:ILE:HG21	2:B:130:PRO:HB2	1.98	0.45
1:H:421:GLN:HG3	2:C:127:GLY:HA2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:PHE:CD2	1:H:435:LEU:HD11	2.51	0.45
1:H:419:ILE:HG22	1:H:430:PRO:HB3	1.97	0.45
2:B:106:LEU:HD13	2:B:154:MET:HG3	1.98	0.45
1:I:443:VAL:HA	1:I:446:LEU:HB3	1.98	0.45
2:B:97:VAL:HG12	2:B:105:LEU:HD12	1.98	0.45
1:G:411:ARG:NH2	1:G:602:SER:OG	2.50	0.45
1:G:588:ILE:O	1:G:592:LYS:NZ	2.43	0.45
2:A:56:GLY:HA3	3:D:560:ARG:HH12	1.81	0.45
1:H:417:LYS:HE3	1:H:433:PRO:HD3	1.98	0.44
1:H:507:ALA:HA	1:H:510:HIS:NE2	2.33	0.44
1:I:516:CYS:N	1:I:533:CYS:SG	2.90	0.44
3:F:551:ASN:OD1	3:F:556:VAL:N	2.50	0.44
2:A:81:VAL:HG13	2:A:150:ALA:HB3	1.99	0.44
2:B:81:VAL:HG13	2:B:150:ALA:HB3	1.99	0.44
3:E:474:PHE:CZ	3:E:555:LEU:HD11	2.53	0.44
1:H:484:VAL:HG12	1:H:488:PHE:HE2	1.82	0.44
2:B:81:VAL:O	2:B:150:ALA:N	2.44	0.44
2:B:88:GLU:OE1	2:B:88:GLU:N	2.44	0.44
2:C:77:PRO:HB2	2:C:79:LYS:HE3	1.99	0.44
2:C:172:LYS:HA	2:C:172:LYS:HD3	1.86	0.44
1:I:494:VAL:HA	1:I:497:HIS:HB2	2.00	0.44
2:C:99:ASP:OD1	2:C:103:LYS:N	2.51	0.44
1:G:503:PHE:HB2	2:A:70:TRP:HB2	2.00	0.44
1:I:436:ASP:O	1:I:437:ILE:C	2.61	0.44
3:D:494:TYR:HE1	3:D:558:ARG:HH22	1.66	0.44
2:B:99:ASP:OD1	2:B:103:LYS:N	2.51	0.44
3:E:532:TRP:CD1	3:F:568:LYS:HZ2	2.36	0.43
1:G:589:ASN:OD1	1:G:593:ASN:ND2	2.52	0.43
1:H:508:ASP:OD1	1:H:508:ASP:N	2.52	0.43
3:D:472:PRO:HA	3:D:494:TYR:HA	2.00	0.43
3:D:517:ARG:HD3	3:D:517:ARG:H	1.82	0.43
3:D:580:GLU:N	3:D:580:GLU:OE1	2.51	0.43
1:G:542:PHE:HB3	1:G:544:TRP:CD1	2.54	0.43
2:A:120:LYS:HE2	2:A:120:LYS:HB2	1.87	0.43
2:B:116:TYR:CD1	2:B:117:PRO:HD2	2.54	0.43
1:H:418:HIS:O	1:H:431:PHE:N	2.44	0.43
1:I:467:ILE:O	1:I:570:TYR:OH	2.36	0.43
3:D:518:ILE:HD13	3:D:549:ILE:HD11	2.01	0.43
2:B:74:THR:HG23	2:B:133:GLN:HB2	1.99	0.43
3:E:534:PRO:HD3	3:F:571:GLU:HG2	2.01	0.42
2:C:83:TYR:OH	2:C:146:TYR:O	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:83:TYR:OH	2:A:146:TYR:O	2.27	0.42
2:A:99:ASP:OD1	2:A:102:GLY:N	2.47	0.42
1:G:551:ASP:OD1	1:G:551:ASP:N	2.52	0.42
2:C:81:VAL:O	2:C:150:ALA:N	2.52	0.42
1:H:596:ASN:HD22	1:H:599:LEU:HD12	1.83	0.42
3:D:475:ASN:OD1	3:D:476:THR:N	2.50	0.42
1:H:403:PHE:HD1	1:H:568:ASN:HA	1.85	0.42
2:B:47:VAL:HG12	2:B:169:ILE:HG12	2.00	0.42
2:C:73:ARG:HB3	2:C:137:LEU:HD12	2.02	0.42
1:G:449:ALA:HA	1:G:452:ASN:HB3	2.01	0.42
1:I:433:PRO:N	1:I:434:PRO:HD2	2.34	0.42
1:I:514:LEU:HD21	1:I:543:PRO:HB3	2.00	0.42
2:B:72:PHE:HB3	2:B:133:GLN:O	2.20	0.41
2:A:49:LEU:O	2:A:83:TYR:HB2	2.20	0.41
1:G:596:ASN:O	1:G:596:ASN:ND2	2.46	0.41
2:A:99:ASP:HB3	2:A:105:LEU:HD11	2.02	0.41
2:C:103:LYS:HE3	2:C:103:LYS:HB3	1.93	0.41
2:B:174:VAL:HG22	3:E:476:THR:HB	2.03	0.41
2:A:43:LYS:HB3	2:A:43:LYS:HE2	1.73	0.41
3:F:469:ASP:N	3:F:569:SER:OG	2.44	0.41
1:G:440:LEU:HD23	1:G:440:LEU:HA	1.92	0.41
1:G:444:LEU:HD12	1:G:447:GLN:HE21	1.85	0.41
1:I:437:ILE:HD13	2:B:130:PRO:HB2	2.03	0.41
2:A:112:ASN:C	2:A:112:ASN:HD22	2.29	0.41
3:D:470:GLU:H	3:D:470:GLU:CD	2.29	0.41
1:I:432:GLY:C	1:I:434:PRO:HD2	2.46	0.40
1:G:484:VAL:N	1:G:546:VAL:HG21	2.37	0.40
3:D:528:ALA:HB3	3:D:531:SER:HB3	2.02	0.40
3:F:469:ASP:N	3:F:469:ASP:OD1	2.52	0.40
1:H:514:LEU:HA	1:H:517:VAL:HG23	2.02	0.40
2:B:80:ASN:OD1	2:B:155:TYR:OH	2.38	0.40
2:B:150:ALA:HB3	2:B:165:ILE:HD11	2.03	0.40
2:C:117:PRO:HG2	3:F:519:TRP:CE2	2.57	0.40
1:I:444:LEU:O	1:I:448:ILE:HG12	2.22	0.40
2:A:61:ASP:O	2:A:93:TYR:OH	2.33	0.40
3:E:552:GLN:O	3:E:553:ASN:ND2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	G	188/280 (67%)	175 (93%)	12 (6%)	1 (0%)	24	58
1	H	189/280 (68%)	176 (93%)	12 (6%)	1 (0%)	24	58
1	I	188/280 (67%)	172 (92%)	16 (8%)	0	100	100
2	A	140/256 (55%)	131 (94%)	9 (6%)	0	100	100
2	B	141/256 (55%)	133 (94%)	8 (6%)	0	100	100
2	C	141/256 (55%)	134 (95%)	7 (5%)	0	100	100
3	D	91/247 (37%)	86 (94%)	5 (6%)	0	100	100
3	E	93/247 (38%)	92 (99%)	1 (1%)	0	100	100
3	F	92/247 (37%)	89 (97%)	3 (3%)	0	100	100
All	All	1263/2349 (54%)	1188 (94%)	73 (6%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	552	ASP
1	H	436	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	176/250 (70%)	175 (99%)	1 (1%)	78	80
1	H	177/250 (71%)	175 (99%)	2 (1%)	65	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	176/250 (70%)	170 (97%)	6 (3%)	32	58
2	A	121/228 (53%)	121 (100%)	0	100	100
2	B	122/228 (54%)	122 (100%)	0	100	100
2	C	122/228 (54%)	122 (100%)	0	100	100
3	D	86/219 (39%)	85 (99%)	1 (1%)	63	73
3	E	88/219 (40%)	87 (99%)	1 (1%)	65	74
3	F	87/219 (40%)	87 (100%)	0	100	100
All	All	1155/2091 (55%)	1144 (99%)	11 (1%)	65	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	596	ASN
1	H	435	LEU
1	H	438	GLN
1	I	436	ASP
1	I	438	GLN
1	I	439	ILE
1	I	440	LEU
1	I	441	HIS
1	I	442	GLN
3	D	581	ARG
3	E	581	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	442	GLN
1	G	447	GLN
1	G	490	ASN
1	G	581	GLN
1	G	593	ASN
1	G	596	ASN
1	G	598	ASN
1	H	581	GLN
1	I	407	GLN
1	I	438	GLN
1	I	442	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	57	GLN
2	A	112	ASN
2	A	131	HIS
2	A	138	HIS
2	B	48	HIS
2	B	57	GLN
3	E	552	GLN
3	E	553	ASN
2	C	42	GLN
2	C	112	ASN
2	C	123	HIS
2	C	126	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](#)

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	K	1	1,4	14,14,15	0.79	0	17,19,21	1.85	6 (35%)
4	NAG	K	2	4	14,14,15	0.72	0	17,19,21	1.49	3 (17%)
4	BMA	K	3	4	11,11,12	0.83	0	15,15,17	2.47	6 (40%)
4	MAN	K	4	4	11,11,12	0.63	0	15,15,17	1.48	1 (6%)
4	MAN	K	5	4	11,11,12	0.76	0	15,15,17	1.30	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	L	1	1,4	14,14,15	0.67	0	17,19,21	1.90	2 (11%)
4	NAG	L	2	4	14,14,15	0.76	1 (7%)	17,19,21	2.03	5 (29%)
4	BMA	L	3	4	11,11,12	0.81	0	15,15,17	2.41	4 (26%)
4	MAN	L	4	4	11,11,12	0.67	0	15,15,17	1.25	1 (6%)
4	MAN	L	5	4	11,11,12	0.75	0	15,15,17	1.14	1 (6%)
4	NAG	M	1	1,4	14,14,15	0.66	0	17,19,21	1.93	2 (11%)
4	NAG	M	2	4	14,14,15	0.74	0	17,19,21	2.06	5 (29%)
4	BMA	M	3	4	11,11,12	0.81	0	15,15,17	2.42	4 (26%)
4	MAN	M	4	4	11,11,12	0.70	0	15,15,17	1.13	1 (6%)
4	MAN	M	5	4	11,11,12	0.69	0	15,15,17	1.13	1 (6%)
5	NAG	N	1	2,5	14,14,15	0.72	0	17,19,21	1.03	2 (11%)
5	NAG	N	2	5	14,14,15	0.71	0	17,19,21	0.88	1 (5%)
5	BMA	N	3	5	11,11,12	0.84	0	15,15,17	2.20	3 (20%)
5	NAG	O	1	2,5	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
5	NAG	O	2	5	14,14,15	0.71	0	17,19,21	0.86	0
5	BMA	O	3	5	11,11,12	0.86	0	15,15,17	2.20	3 (20%)
5	NAG	P	1	2,5	14,14,15	0.70	0	17,19,21	0.89	1 (5%)
5	NAG	P	2	5	14,14,15	0.71	0	17,19,21	0.87	0
5	BMA	P	3	5	11,11,12	0.85	0	15,15,17	2.19	3 (20%)
4	NAG	Q	1	3,4	14,14,15	0.69	0	17,19,21	1.77	3 (17%)
4	NAG	Q	2	4	14,14,15	0.77	0	17,19,21	1.64	3 (17%)
4	BMA	Q	3	4	11,11,12	0.85	0	15,15,17	2.09	3 (20%)
4	MAN	Q	4	4	11,11,12	0.69	0	15,15,17	1.28	1 (6%)
4	MAN	Q	5	4	11,11,12	0.77	0	15,15,17	1.22	1 (6%)
4	NAG	R	1	3,4	14,14,15	0.83	0	17,19,21	2.17	6 (35%)
4	NAG	R	2	4	14,14,15	0.77	0	17,19,21	0.85	0
4	BMA	R	3	4	11,11,12	0.84	0	15,15,17	2.16	3 (20%)
4	MAN	R	4	4	11,11,12	0.72	0	15,15,17	1.08	1 (6%)
4	MAN	R	5	4	11,11,12	0.77	0	15,15,17	1.21	1 (6%)
4	NAG	S	1	3,4	14,14,15	0.88	1 (7%)	17,19,21	2.01	4 (23%)
4	NAG	S	2	4	14,14,15	0.75	0	17,19,21	1.09	2 (11%)
4	BMA	S	3	4	11,11,12	0.89	0	15,15,17	2.08	4 (26%)
4	MAN	S	4	4	11,11,12	0.63	0	15,15,17	1.41	1 (6%)
4	MAN	S	5	4	11,11,12	0.69	0	15,15,17	1.61	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
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	1/2/19/22	1/1/1/1
4	MAN	K	5	4	-	2/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	1/2/19/22	0/1/1/1
4	MAN	L	4	4	-	2/2/19/22	1/1/1/1
4	MAN	L	5	4	-	1/2/19/22	1/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	1/2/19/22	1/1/1/1
4	MAN	M	5	4	-	1/2/19/22	1/1/1/1
5	NAG	N	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	1/2/19/22	0/1/1/1
5	NAG	O	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	NAG	P	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	1/2/19/22	0/1/1/1
4	NAG	Q	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	1/2/19/22	0/1/1/1
4	MAN	Q	4	4	-	2/2/19/22	1/1/1/1
4	MAN	Q	5	4	-	0/2/19/22	0/1/1/1
4	NAG	R	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1
4	BMA	R	3	4	-	1/2/19/22	0/1/1/1
4	MAN	R	4	4	-	0/2/19/22	0/1/1/1
4	MAN	R	5	4	-	1/2/19/22	0/1/1/1
4	NAG	S	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	BMA	S	3	4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	S	4	4	-	2/2/19/22	1/1/1/1
4	MAN	S	5	4	-	2/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	2	NAG	C1-C2	2.05	1.55	1.52
4	S	1	NAG	C1-C2	2.03	1.55	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	3	BMA	C1-O5-C5	7.53	122.28	112.19
4	L	3	BMA	C1-O5-C5	7.48	122.20	112.19
4	K	3	BMA	C1-O5-C5	7.27	121.93	112.19
4	M	1	NAG	C1-O5-C5	7.03	121.61	112.19
5	N	3	BMA	C1-O5-C5	6.80	121.30	112.19
5	P	3	BMA	C1-O5-C5	6.75	121.24	112.19
5	O	3	BMA	C1-O5-C5	6.67	121.12	112.19
4	L	1	NAG	C1-O5-C5	6.64	121.08	112.19
4	R	3	BMA	C1-O5-C5	6.52	120.92	112.19
4	Q	3	BMA	C1-O5-C5	6.51	120.91	112.19
4	S	3	BMA	C1-O5-C5	5.71	119.84	112.19
4	M	2	NAG	C1-O5-C5	5.64	119.75	112.19
4	L	2	NAG	C1-O5-C5	5.58	119.66	112.19
4	S	5	MAN	C1-O5-C5	5.26	119.24	112.19
4	S	1	NAG	O5-C1-C2	-5.13	103.35	111.29
4	K	4	MAN	C1-O5-C5	5.03	118.93	112.19
4	R	1	NAG	C1-O5-C5	4.96	118.83	112.19
4	S	4	MAN	C1-O5-C5	4.59	118.33	112.19
4	Q	2	NAG	O5-C1-C2	-4.56	104.24	111.29
4	R	1	NAG	C2-N2-C7	4.51	128.95	122.90
4	S	1	NAG	C1-C2-N2	4.49	117.50	110.43
4	Q	1	NAG	C2-N2-C7	4.14	128.44	122.90
4	Q	4	MAN	C1-O5-C5	4.11	117.69	112.19
4	K	2	NAG	O5-C1-C2	-4.11	104.94	111.29
4	L	4	MAN	C1-O5-C5	3.89	117.41	112.19
4	K	1	NAG	C1-O5-C5	3.85	117.35	112.19
4	K	5	MAN	C1-O5-C5	3.78	117.26	112.19
4	Q	1	NAG	O4-C4-C3	-3.51	102.09	110.38
4	R	1	NAG	O5-C1-C2	3.45	116.62	111.29
4	Q	5	MAN	C1-O5-C5	3.38	116.72	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	5	MAN	C1-O5-C5	3.34	116.66	112.19
4	M	4	MAN	C1-O5-C5	3.34	116.66	112.19
4	M	5	MAN	C1-O5-C5	3.31	116.62	112.19
4	L	5	MAN	C1-O5-C5	3.27	116.57	112.19
4	Q	1	NAG	O5-C1-C2	-3.24	106.28	111.29
4	L	2	NAG	O5-C1-C2	3.21	116.26	111.29
4	S	3	BMA	C3-C4-C5	3.14	115.92	110.23
4	K	1	NAG	C3-C4-C5	-3.12	104.58	110.23
4	K	3	BMA	C3-C4-C5	3.07	115.79	110.23
4	M	2	NAG	O5-C1-C2	2.94	115.84	111.29
4	Q	2	NAG	C4-C3-C2	2.93	115.32	111.02
4	R	4	MAN	C1-O5-C5	2.87	116.03	112.19
4	L	3	BMA	C3-C4-C5	2.83	115.36	110.23
4	S	1	NAG	C4-C3-C2	2.81	115.13	111.02
4	M	2	NAG	C3-C4-C5	-2.79	105.18	110.23
4	K	3	BMA	C2-C3-C4	2.76	115.72	110.86
4	L	2	NAG	C3-C4-C5	-2.74	105.26	110.23
4	Q	2	NAG	O4-C4-C3	-2.70	104.01	110.38
4	R	1	NAG	C1-C2-N2	-2.66	106.24	110.43
4	L	2	NAG	C2-N2-C7	2.65	126.46	122.90
5	O	3	BMA	C3-C4-C5	2.61	114.96	110.23
5	P	3	BMA	C2-C3-C4	2.55	115.34	110.86
5	N	3	BMA	C2-C3-C4	2.55	115.34	110.86
5	O	1	NAG	O5-C1-C2	-2.54	107.36	111.29
4	M	3	BMA	C3-C4-C5	2.54	114.84	110.23
5	O	3	BMA	C2-C3-C4	2.50	115.26	110.86
4	K	1	NAG	C2-N2-C7	2.49	126.24	122.90
4	K	1	NAG	O4-C4-C3	-2.49	104.52	110.38
4	L	1	NAG	C4-C3-C2	-2.48	107.38	111.02
4	K	2	NAG	O4-C4-C3	-2.45	104.59	110.38
4	M	2	NAG	C2-N2-C7	2.44	126.17	122.90
4	R	3	BMA	C3-C4-C5	2.38	114.55	110.23
4	K	1	NAG	O4-C4-C5	2.38	115.19	109.32
4	R	3	BMA	C2-C3-C4	2.36	115.02	110.86
4	Q	3	BMA	C2-C3-C4	2.35	114.99	110.86
5	P	1	NAG	O5-C1-C2	-2.34	107.67	111.29
4	S	1	NAG	C2-N2-C7	2.32	126.00	122.90
5	N	1	NAG	O4-C4-C3	-2.31	104.94	110.38
4	M	2	NAG	O4-C4-C5	2.29	114.96	109.32
5	N	2	NAG	O5-C1-C2	-2.28	107.76	111.29
5	N	1	NAG	O5-C1-C2	-2.28	107.76	111.29
5	P	3	BMA	C3-C4-C5	2.25	114.31	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	1	NAG	C3-C4-C5	-2.24	106.17	110.23
4	S	3	BMA	C2-C3-C4	2.24	114.80	110.86
4	S	3	BMA	O4-C4-C3	-2.24	105.10	110.38
4	K	2	NAG	C4-C3-C2	2.23	114.29	111.02
5	N	3	BMA	C3-C4-C5	2.23	114.28	110.23
4	M	3	BMA	C2-C3-C4	2.20	114.73	110.86
4	L	2	NAG	O4-C4-C5	2.20	114.74	109.32
4	K	3	BMA	O3-C3-C2	-2.19	105.59	110.05
4	K	3	BMA	O5-C5-C4	2.17	116.10	110.83
4	S	2	NAG	O5-C1-C2	-2.16	107.95	111.29
4	L	3	BMA	C2-C3-C4	2.15	114.64	110.86
4	L	3	BMA	O4-C4-C3	-2.15	105.31	110.38
4	K	1	NAG	C6-C5-C4	2.12	118.21	113.02
4	R	1	NAG	O5-C5-C4	-2.11	105.69	110.83
4	Q	3	BMA	C3-C4-C5	2.10	114.05	110.23
4	M	3	BMA	O3-C3-C2	-2.08	105.81	110.05
4	S	2	NAG	O4-C4-C3	-2.04	105.57	110.38
4	M	1	NAG	C4-C3-C2	-2.01	108.07	111.02
4	K	3	BMA	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	4	MAN	O5-C5-C6-O6
4	K	5	MAN	O5-C5-C6-O6
4	L	4	MAN	O5-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
4	K	5	MAN	C4-C5-C6-O6
4	L	4	MAN	C4-C5-C6-O6
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	S	1	NAG	C8-C7-N2-C2
4	S	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
4	S	4	MAN	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

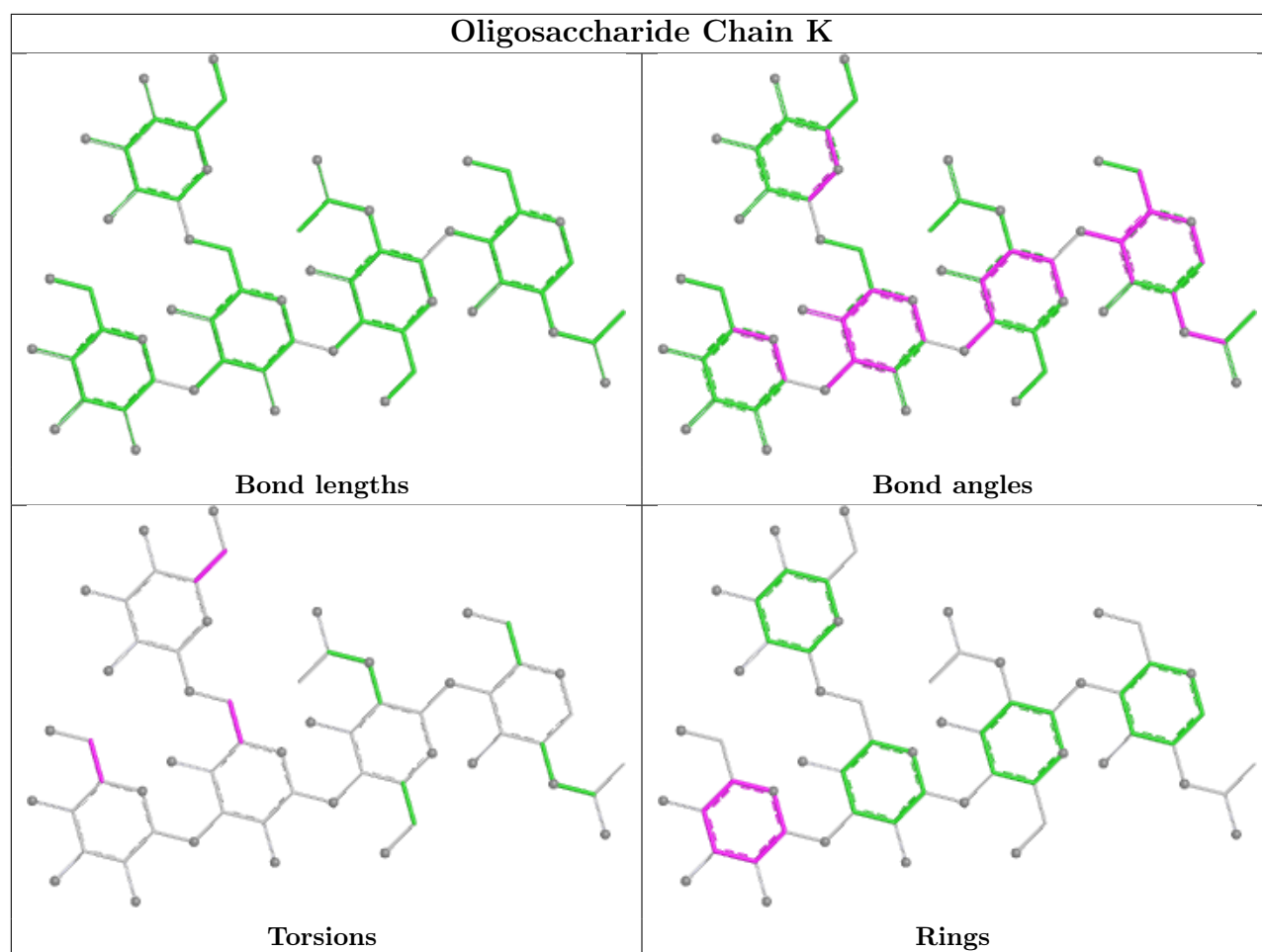
Mol	Chain	Res	Type	Atoms
4	Q	4	MAN	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	S	4	MAN	O5-C5-C6-O6
4	M	5	MAN	O5-C5-C6-O6
4	S	5	MAN	C4-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
4	K	4	MAN	O5-C5-C6-O6
4	Q	3	BMA	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	M	4	MAN	O5-C5-C6-O6
4	R	5	MAN	O5-C5-C6-O6
4	L	3	BMA	O5-C5-C6-O6
4	L	5	MAN	O5-C5-C6-O6
4	R	3	BMA	O5-C5-C6-O6
4	S	5	MAN	O5-C5-C6-O6
4	Q	1	NAG	C1-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7
5	N	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6

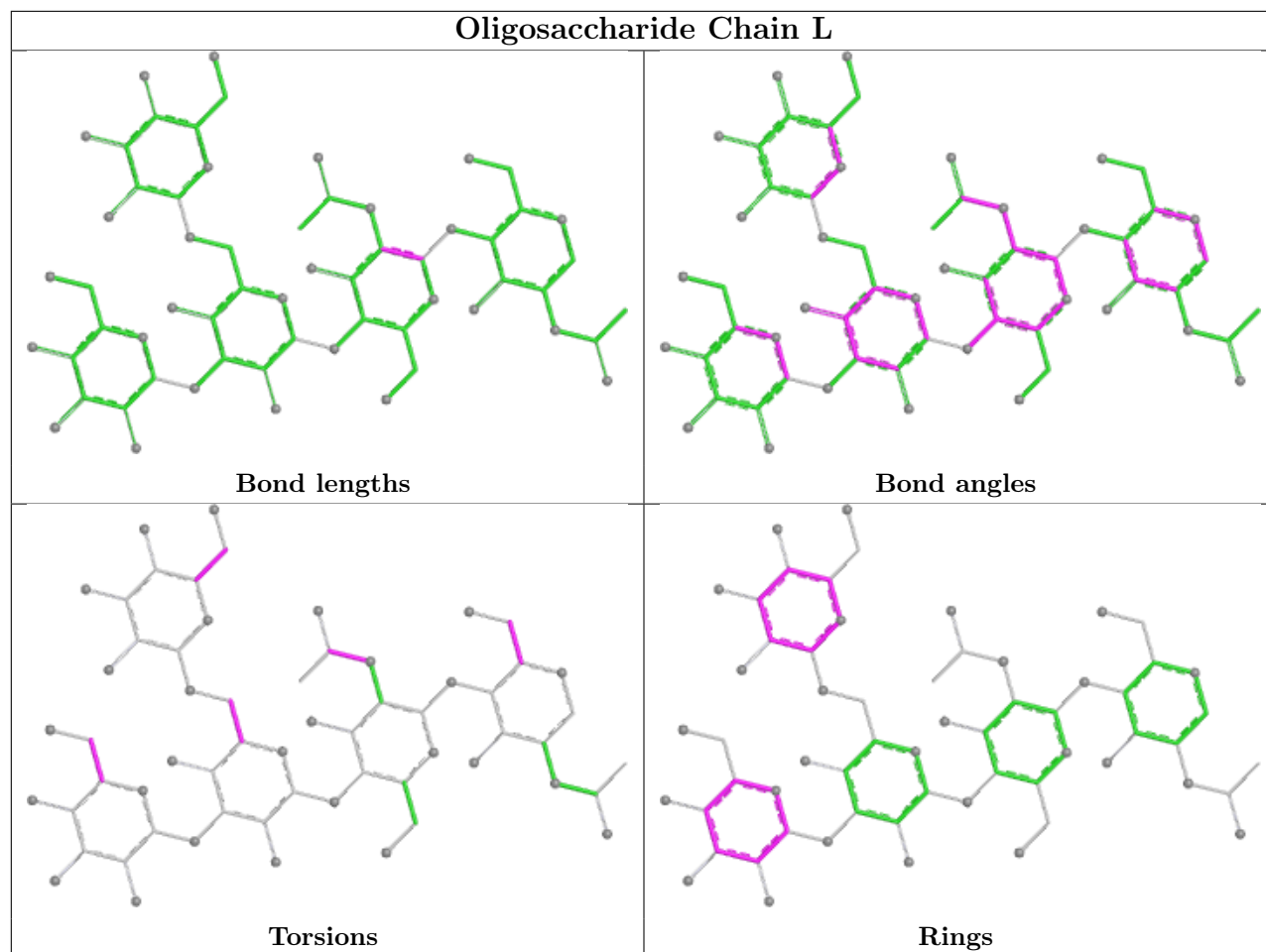
All (8) ring outliers are listed below:

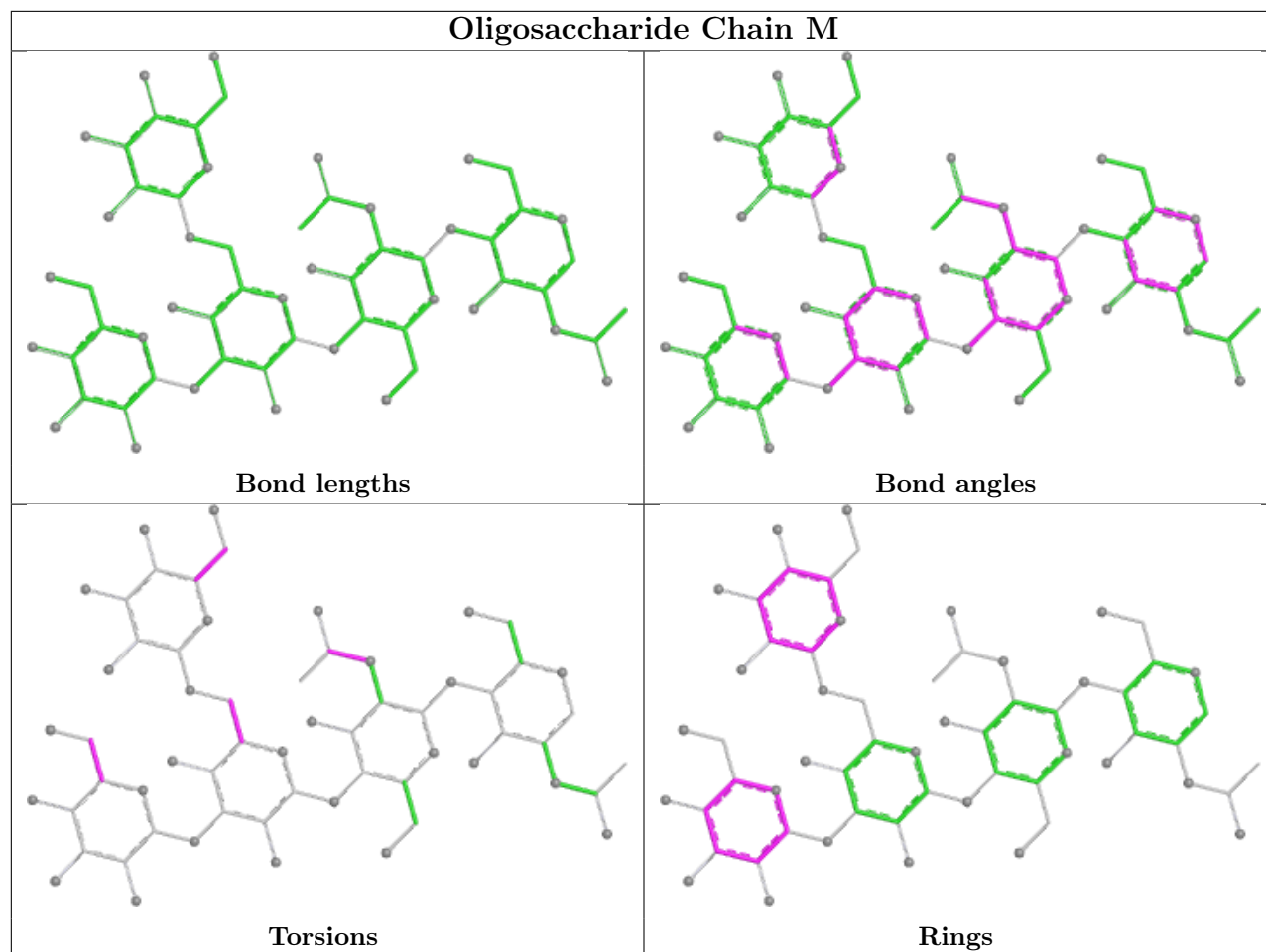
Mol	Chain	Res	Type	Atoms
4	L	5	MAN	C1-C2-C3-C4-C5-O5
4	S	5	MAN	C1-C2-C3-C4-C5-O5
4	M	4	MAN	C1-C2-C3-C4-C5-O5
4	M	5	MAN	C1-C2-C3-C4-C5-O5
4	L	4	MAN	C1-C2-C3-C4-C5-O5
4	Q	4	MAN	C1-C2-C3-C4-C5-O5
4	K	4	MAN	C1-C2-C3-C4-C5-O5
4	S	4	MAN	C1-C2-C3-C4-C5-O5

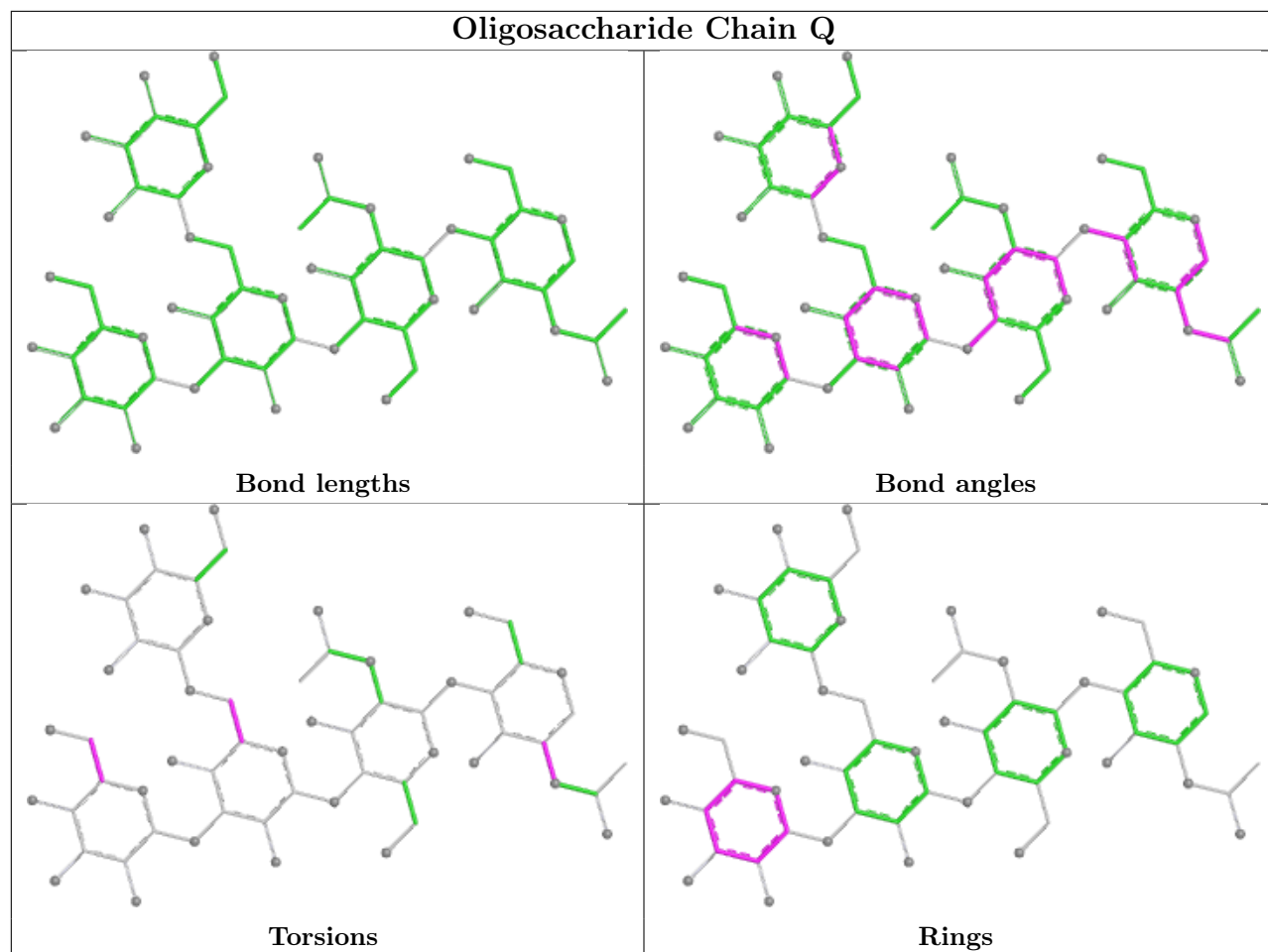
No monomer is involved in short contacts.

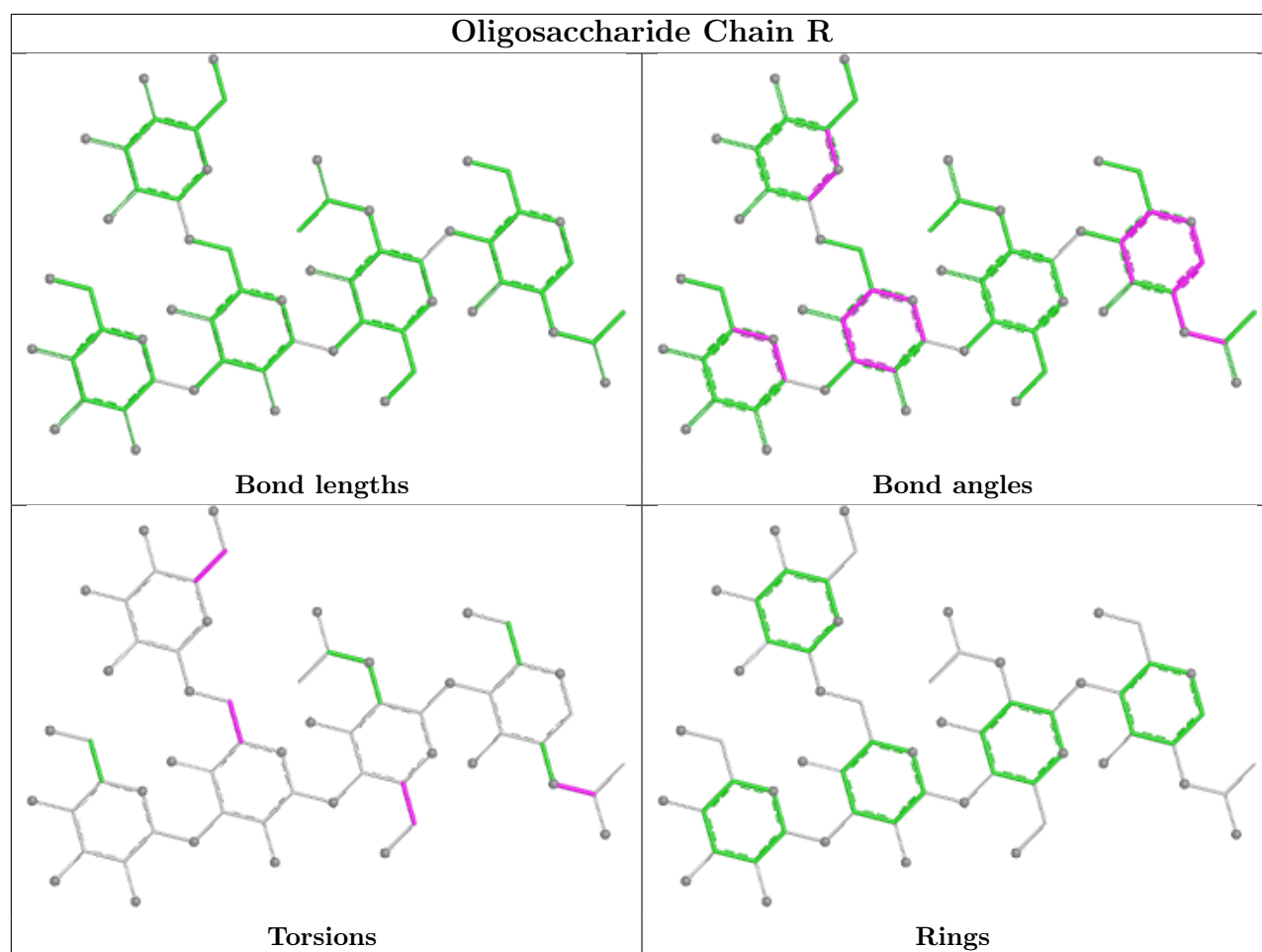
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



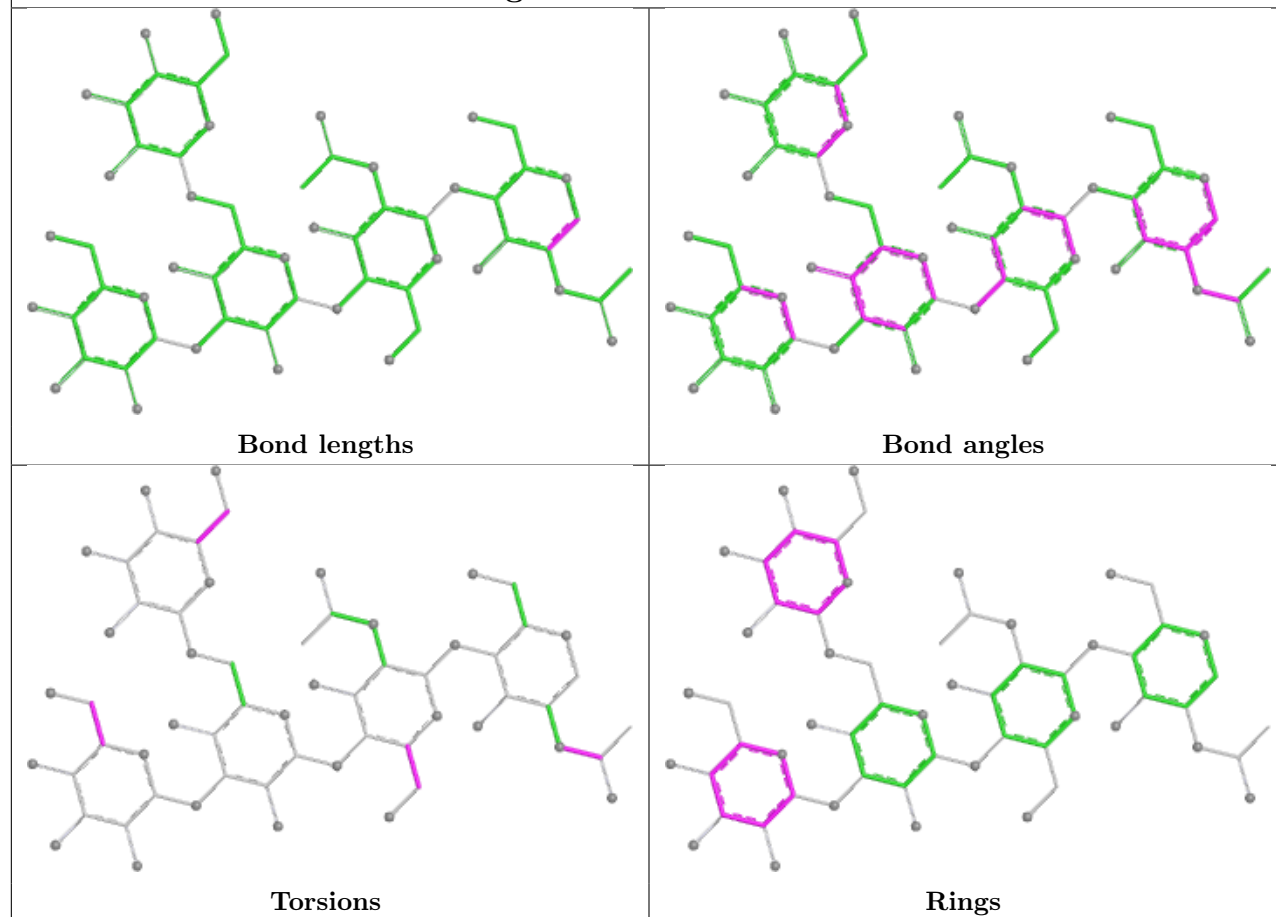




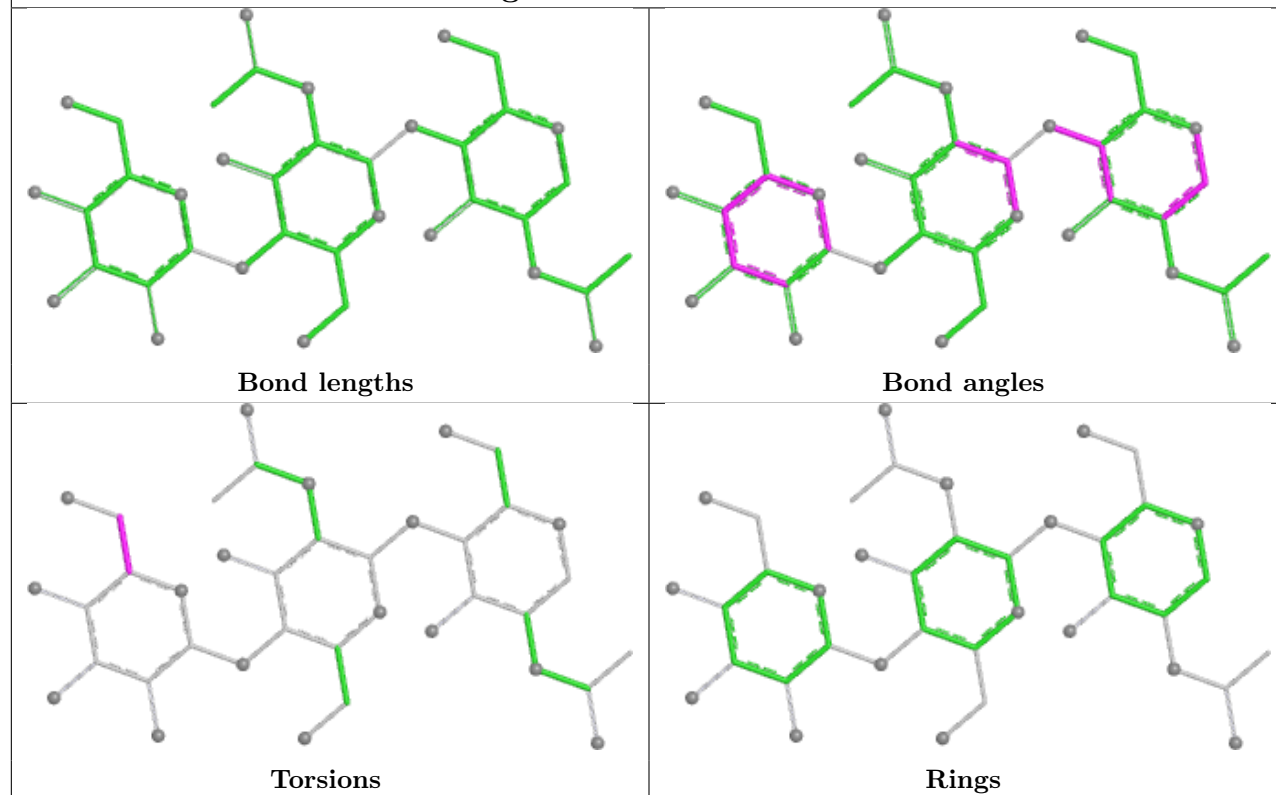


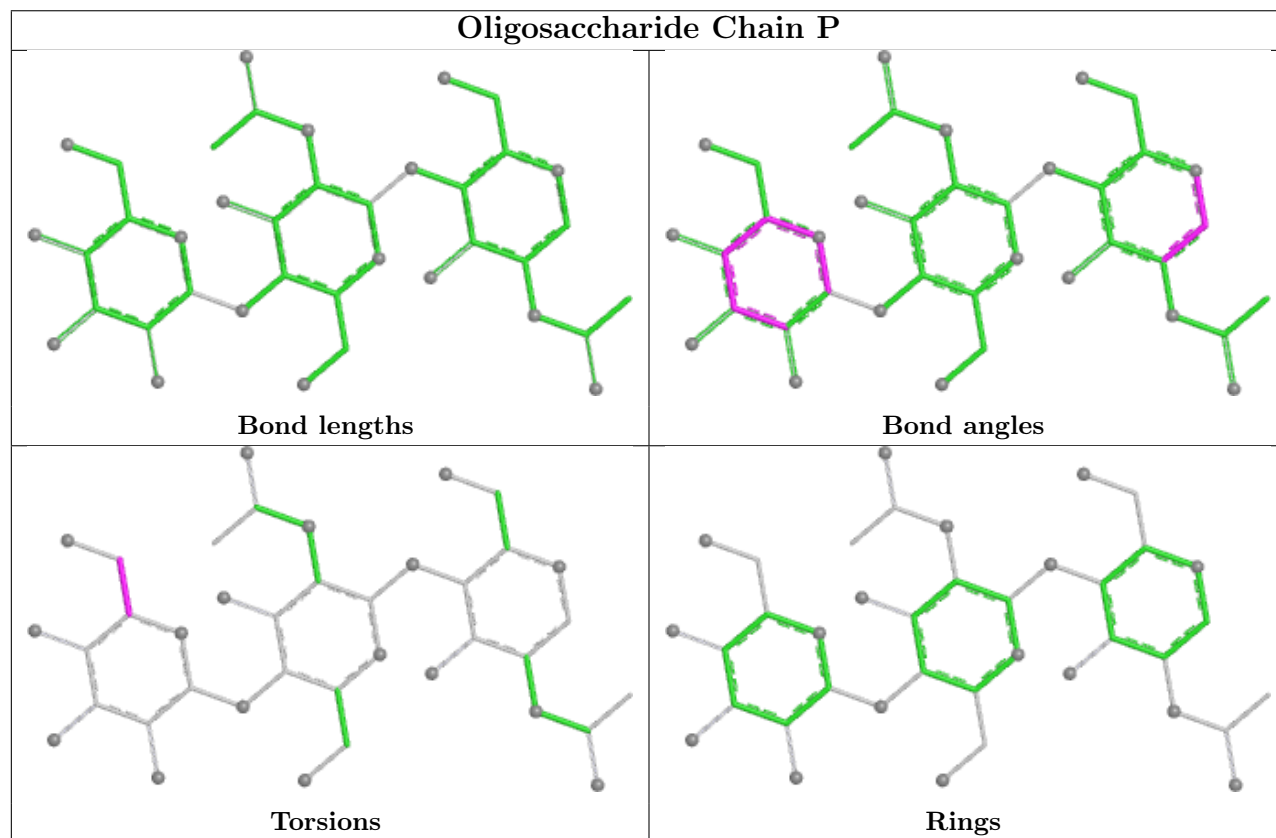
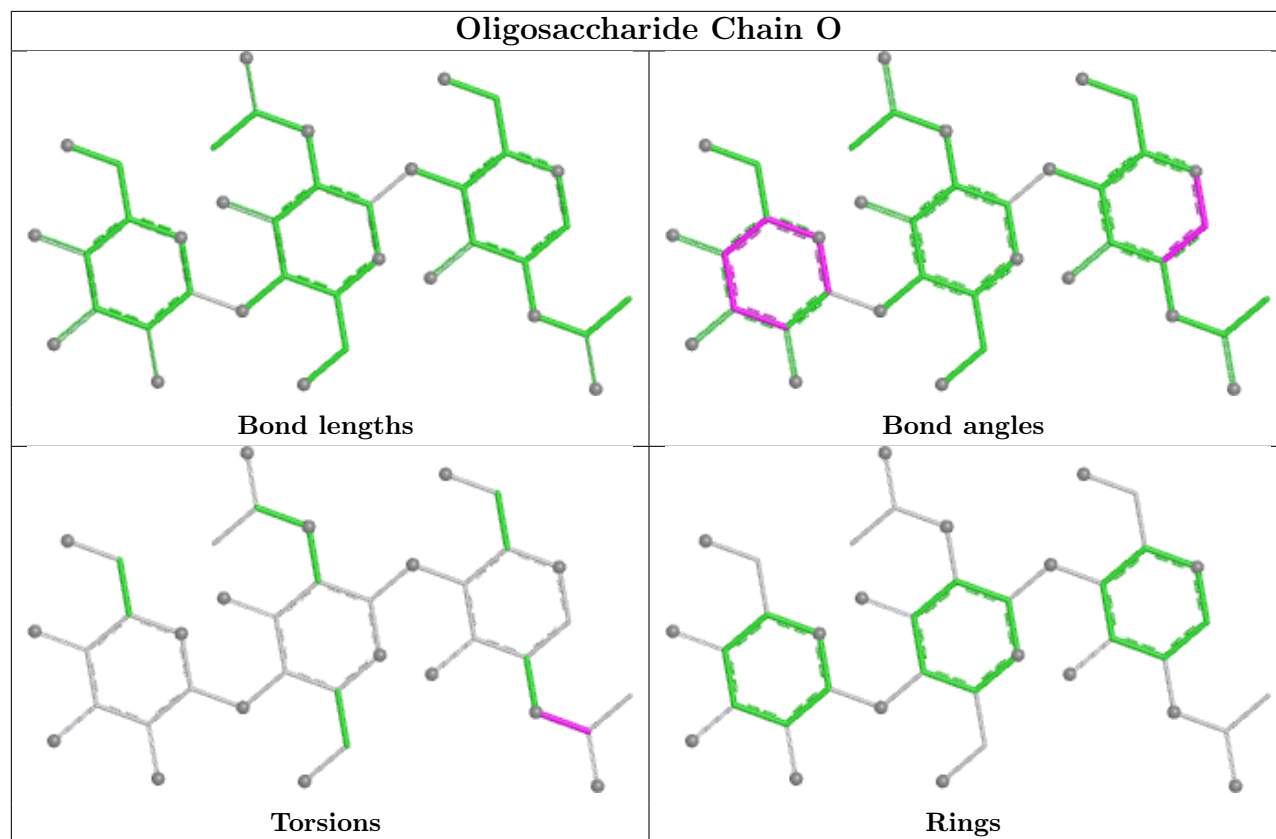


Oligosaccharide Chain S



Oligosaccharide Chain N





5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

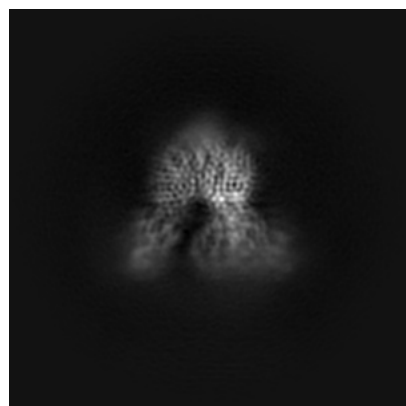
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49630. These allow visual inspection of the internal detail of the map and identification of artifacts.

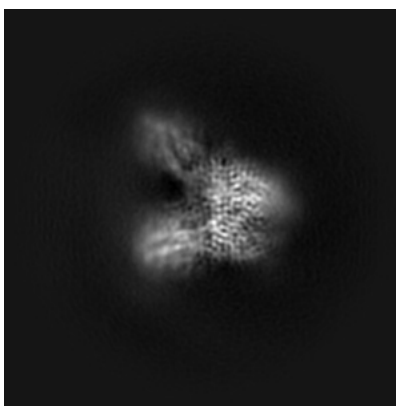
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

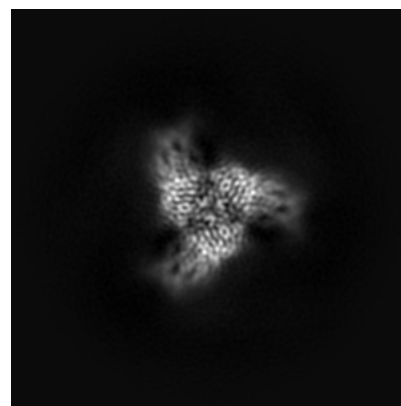
6.1.1 Primary map



X

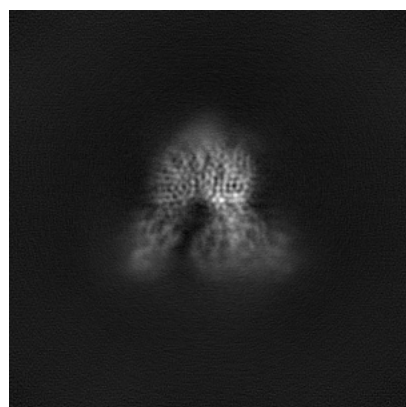


Y

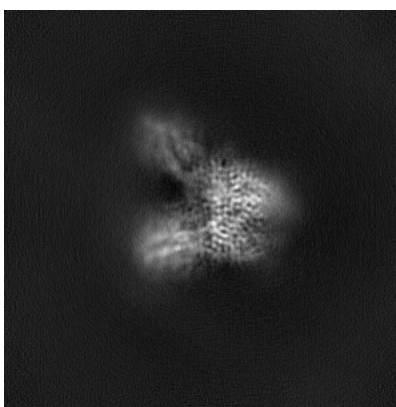


Z

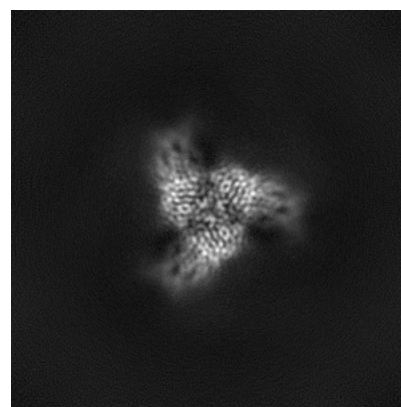
6.1.2 Raw map



X



Y

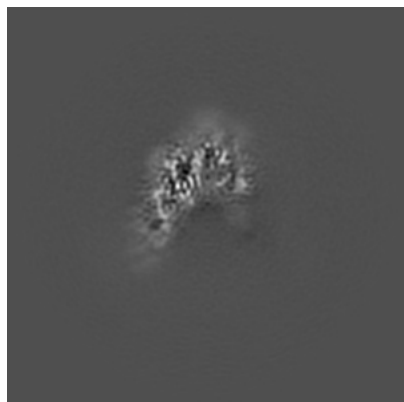


Z

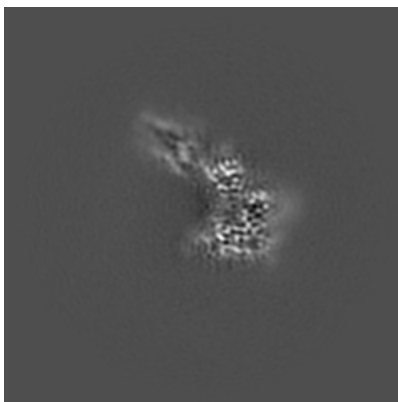
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

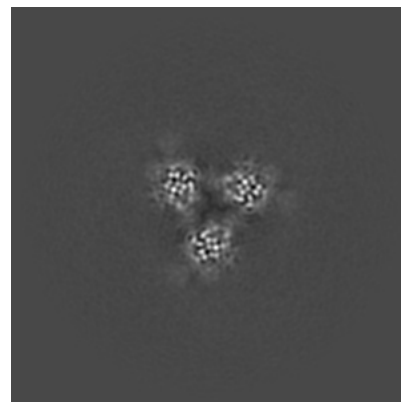
6.2.1 Primary map



X Index: 160

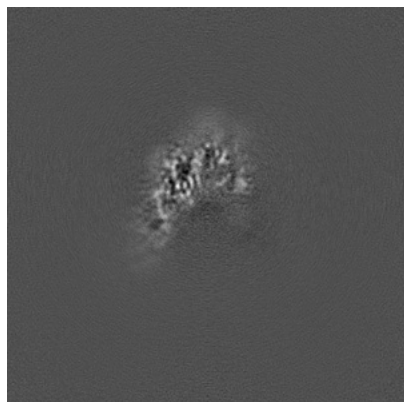


Y Index: 160

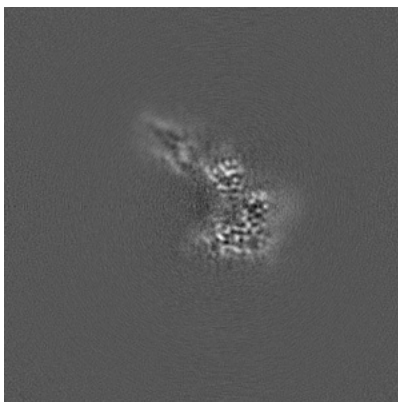


Z Index: 160

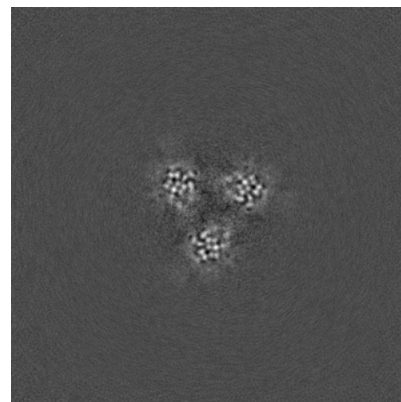
6.2.2 Raw map



X Index: 160



Y Index: 160

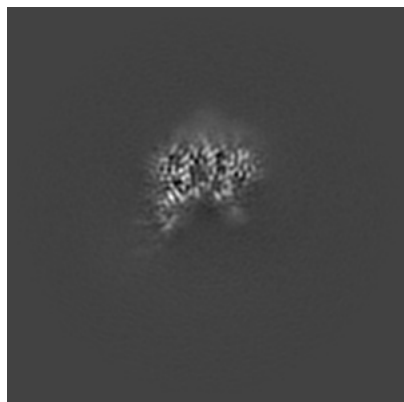


Z Index: 160

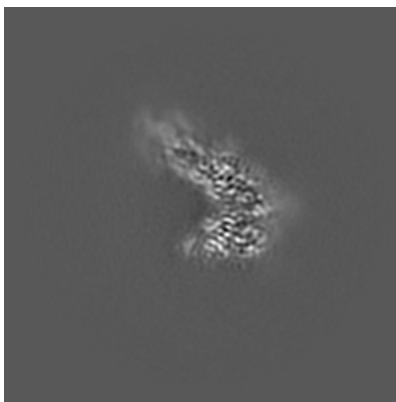
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

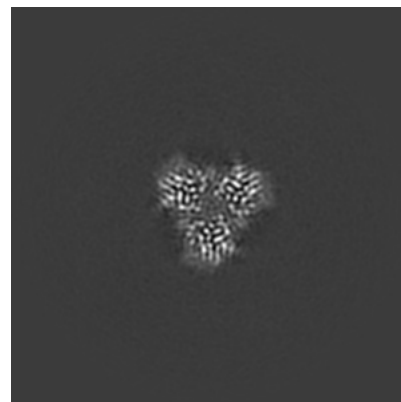
6.3.1 Primary map



X Index: 168

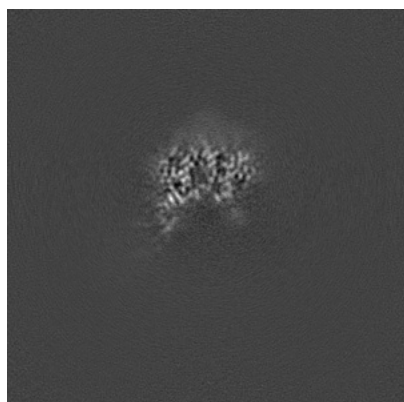


Y Index: 167

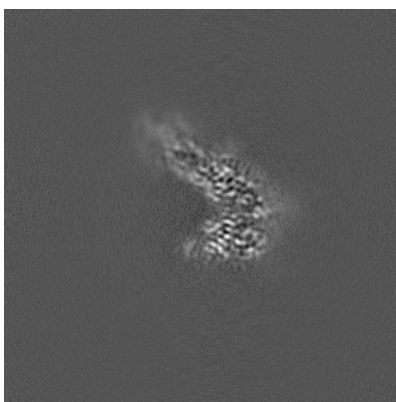


Z Index: 172

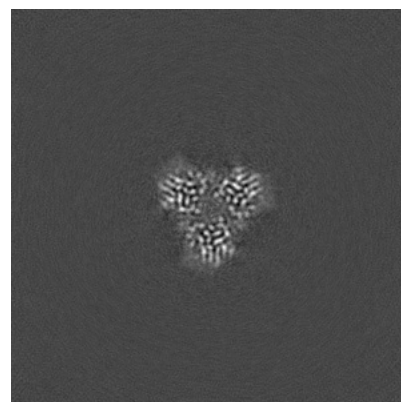
6.3.2 Raw map



X Index: 168



Y Index: 167

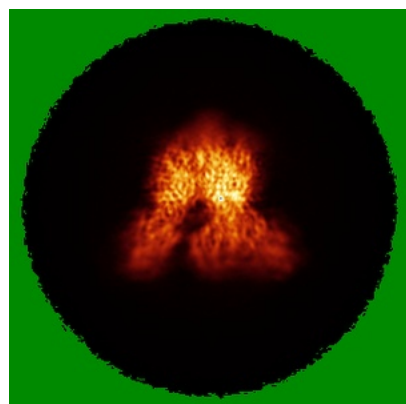


Z Index: 172

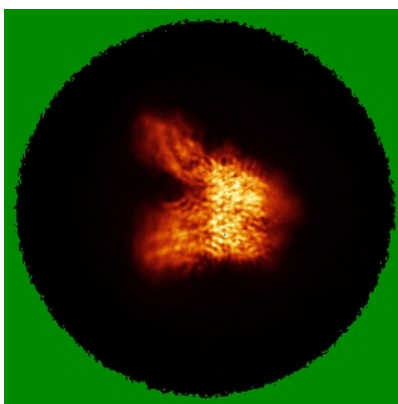
The images above show the largest variance slices of the map in three orthogonal directions.

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

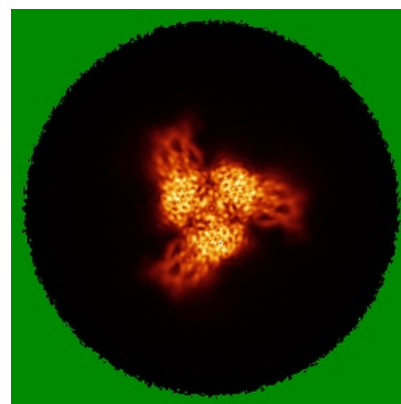
6.4.1 Primary map



X

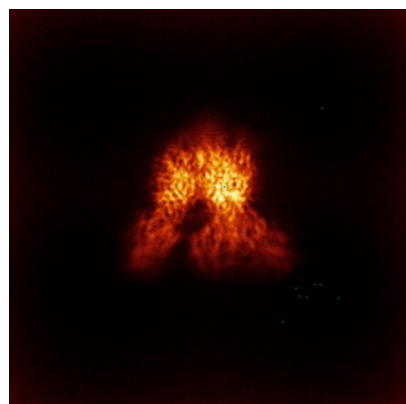


Y

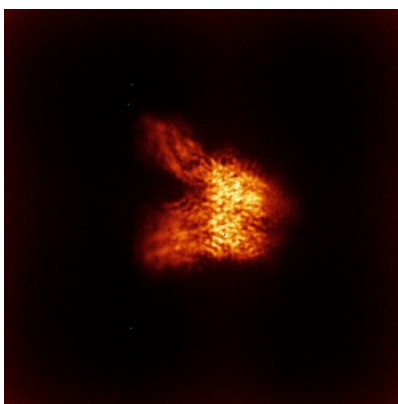


Z

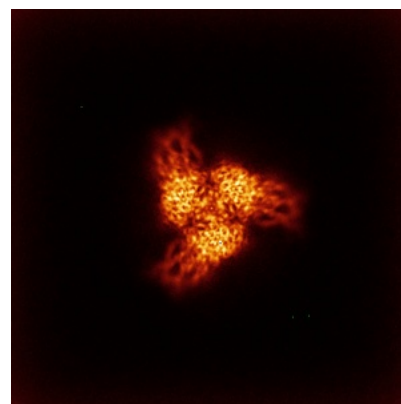
6.4.2 Raw map



X



Y

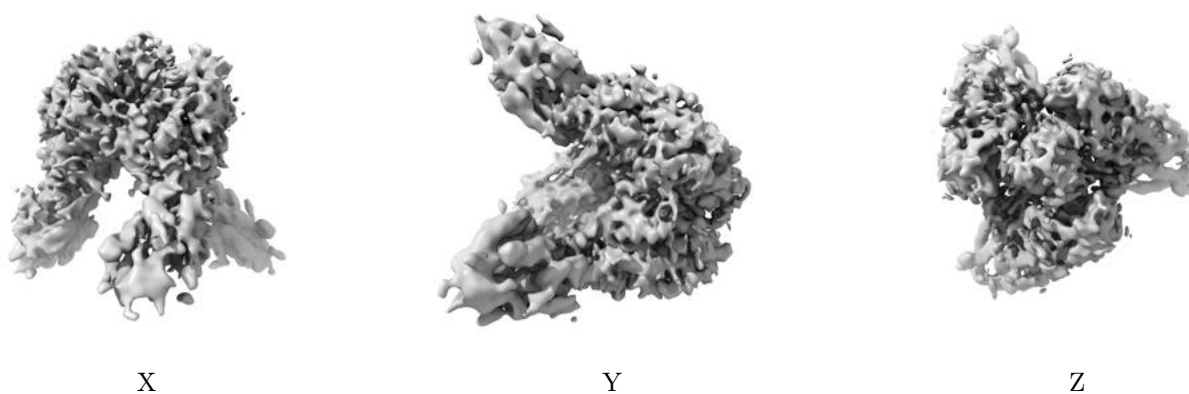


Z

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.

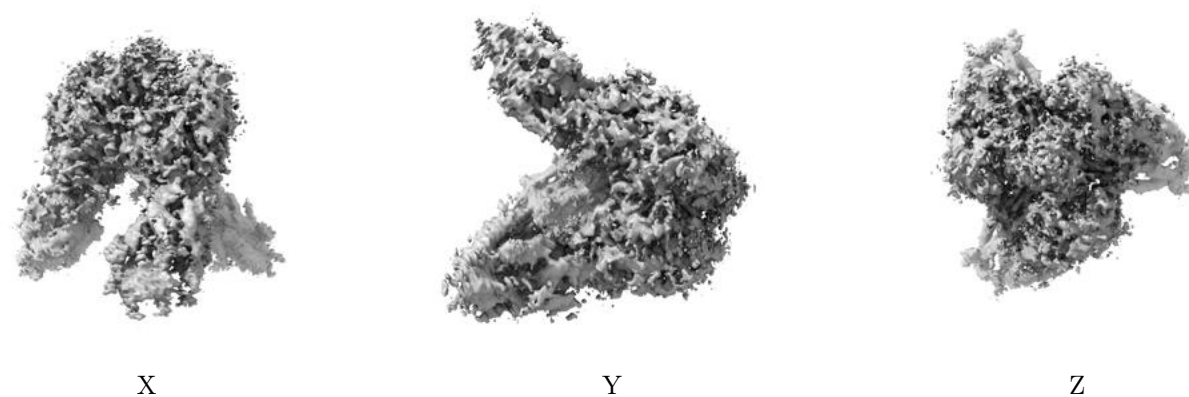
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.078. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

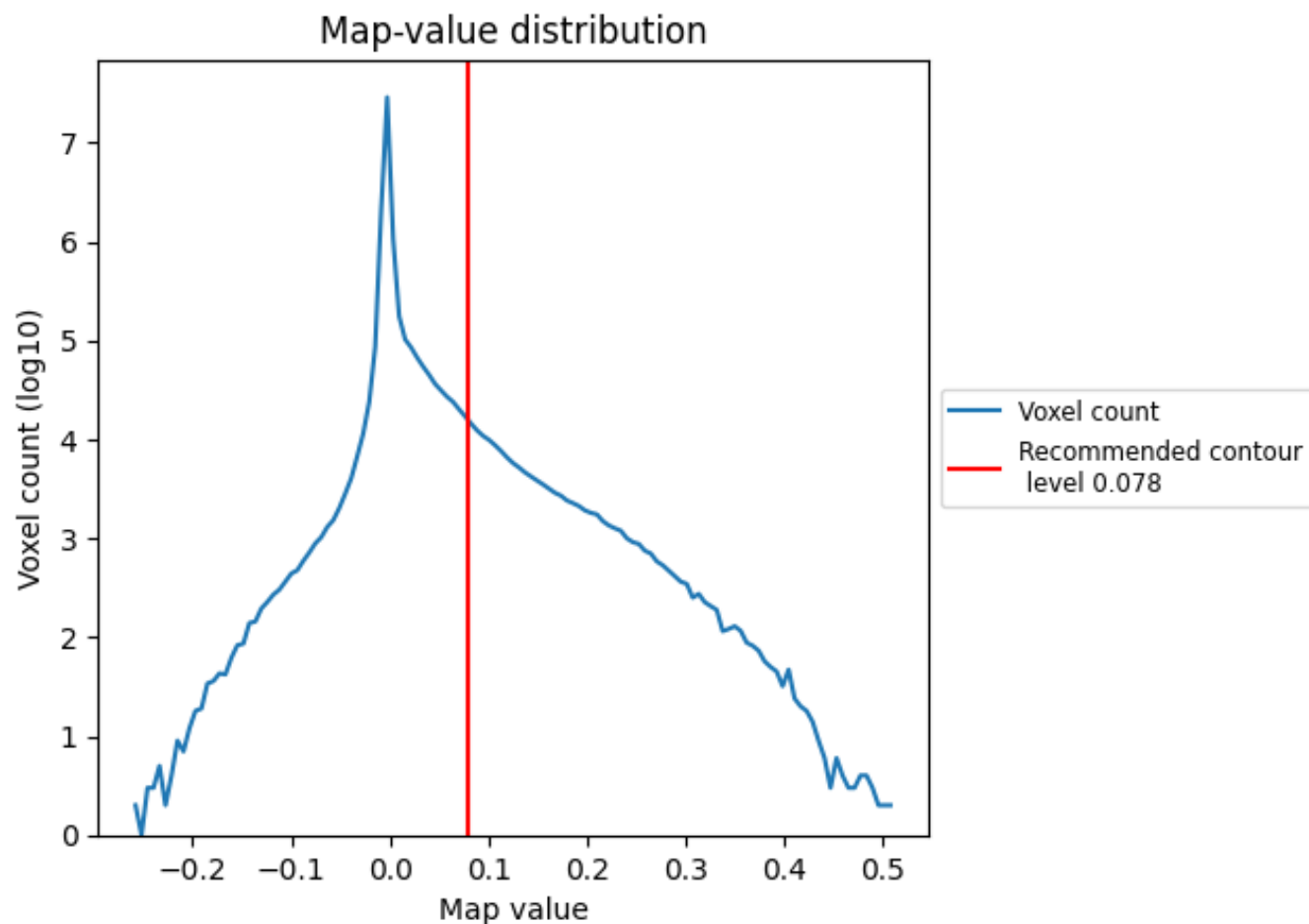
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

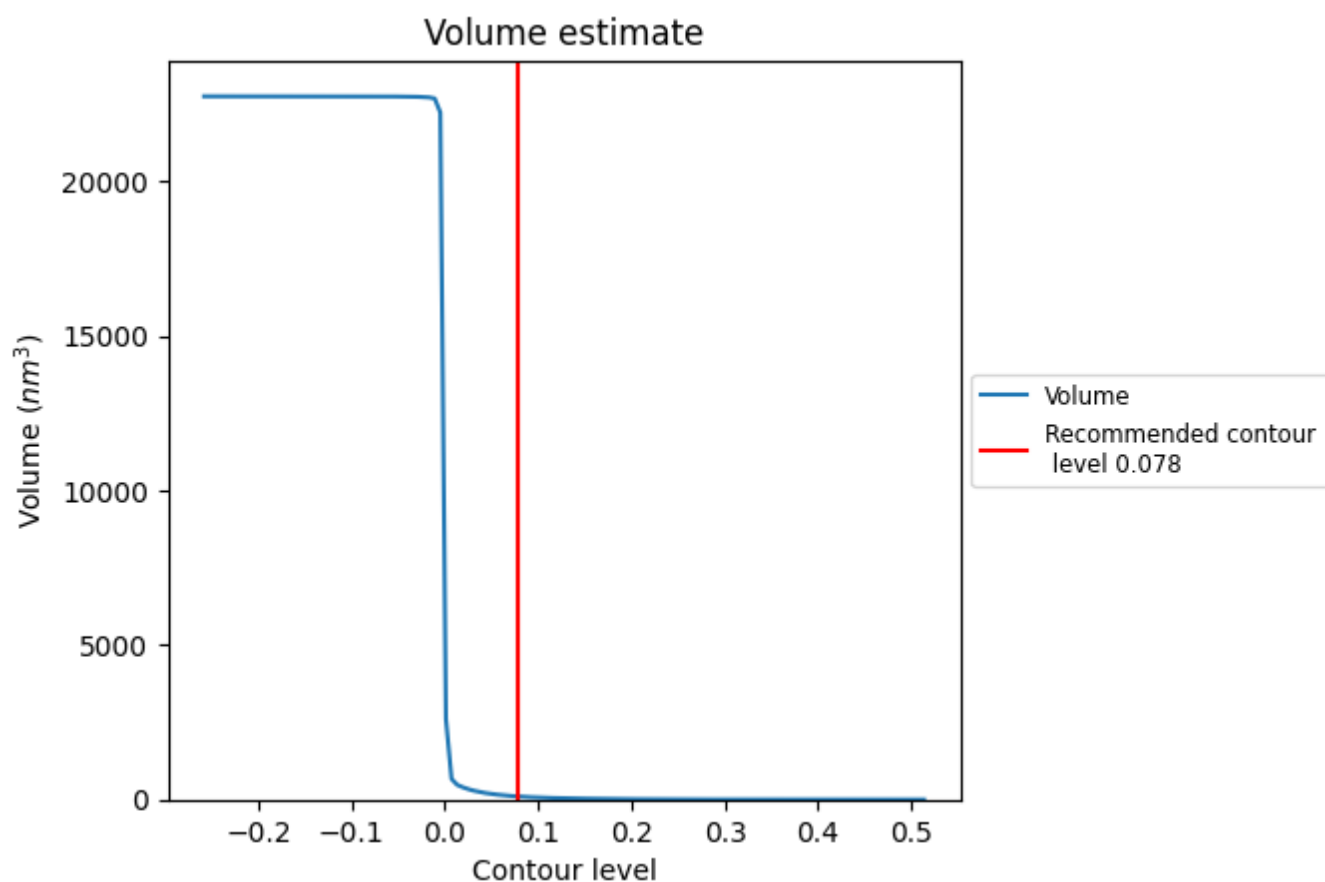
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

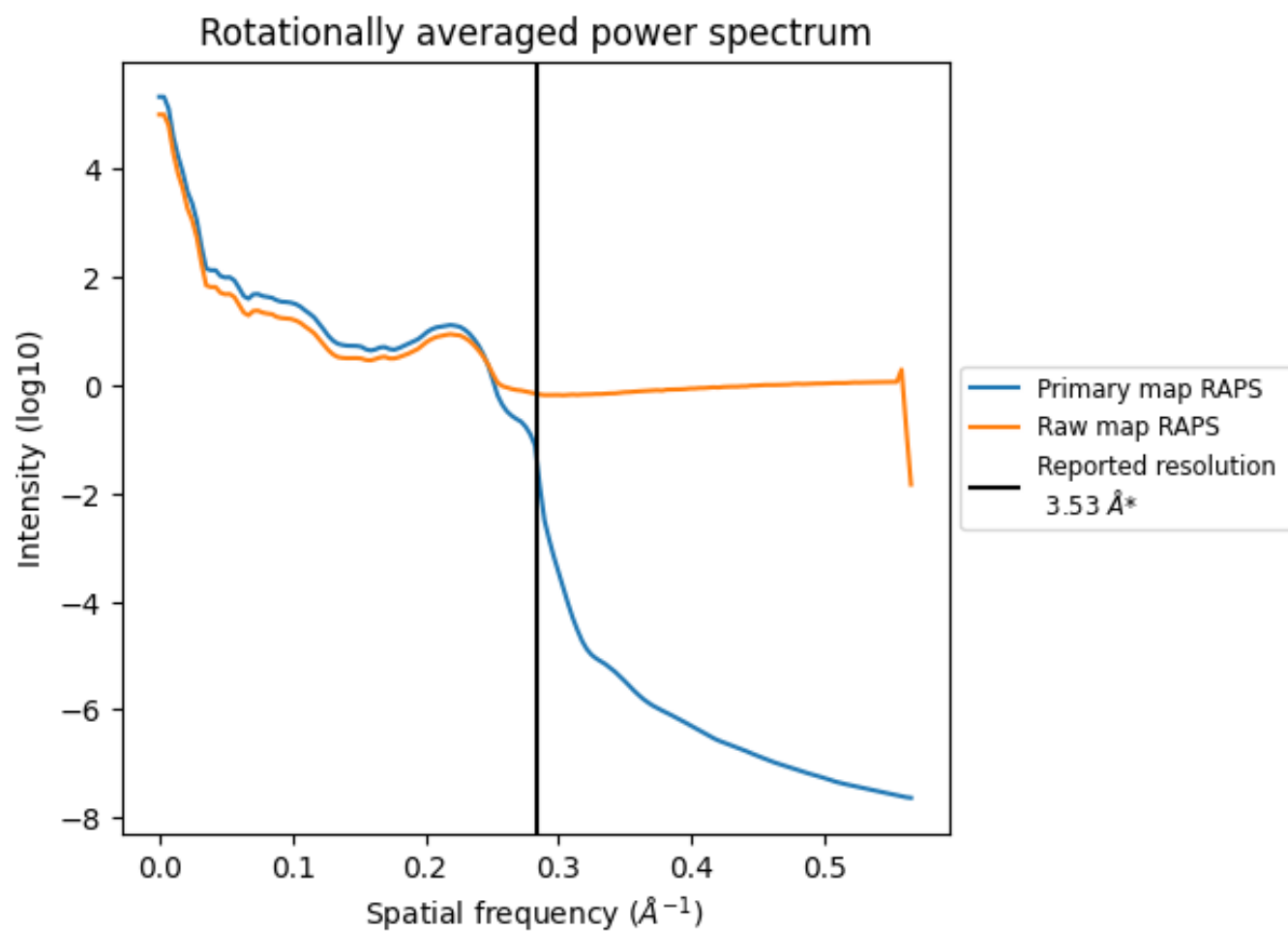
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 91 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 ⓘ

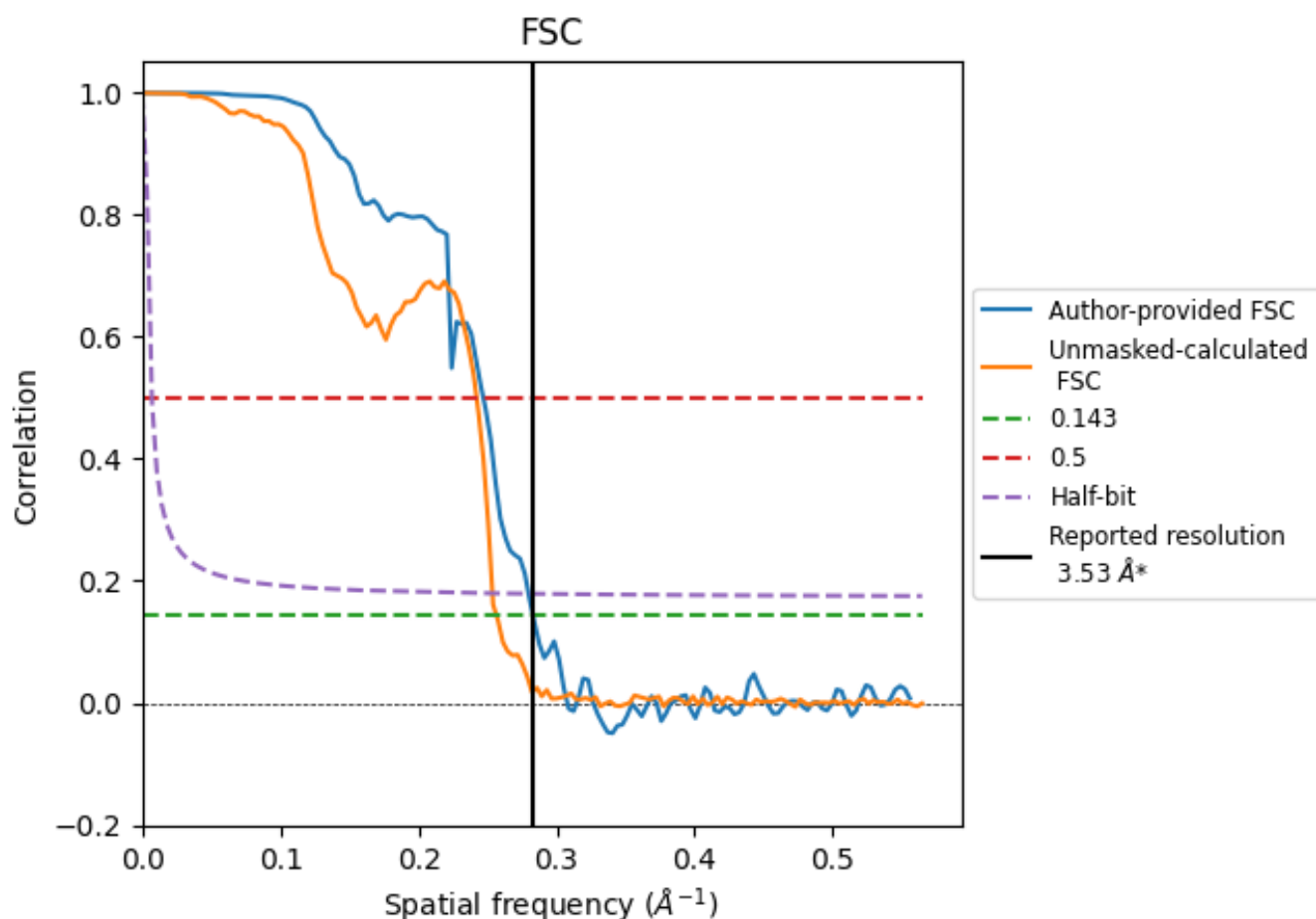


*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.283 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

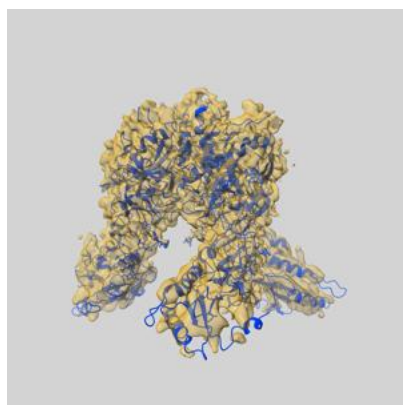
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.53	4.05	3.57
Unmasked-calculated*	3.90	4.13	3.94

*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 3.90 differs from the reported value 3.53 by more than 10 %

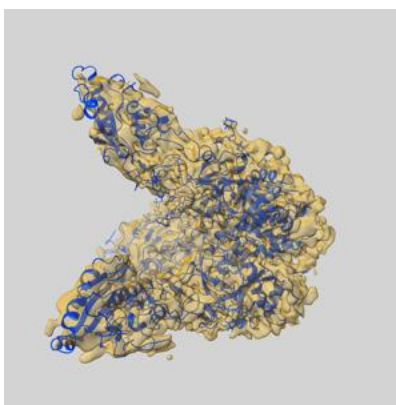
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49630 and PDB model 9NPR. Per-residue inclusion information can be found in section 3 on page 11.

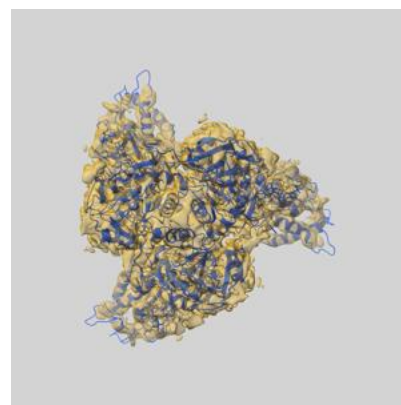
9.1 Map-model overlay [i](#)



X



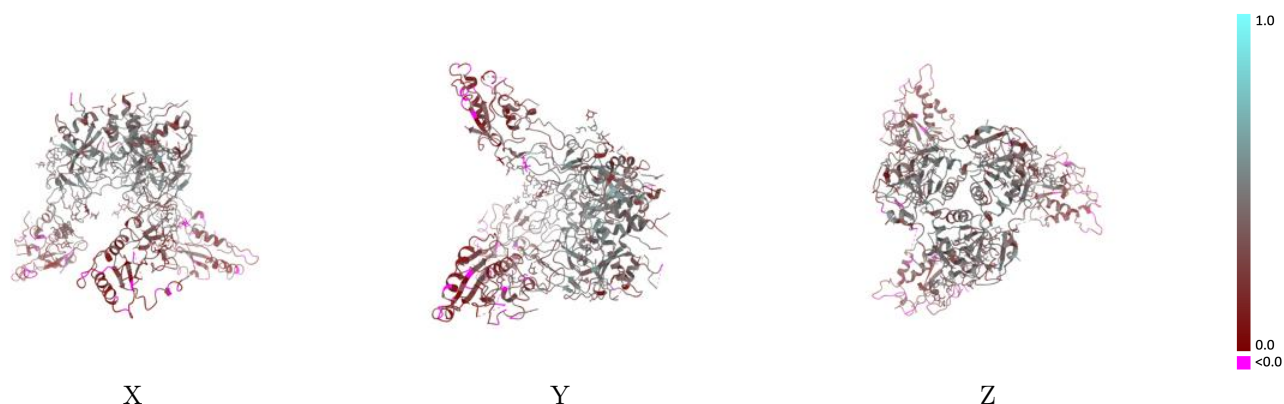
Y



Z

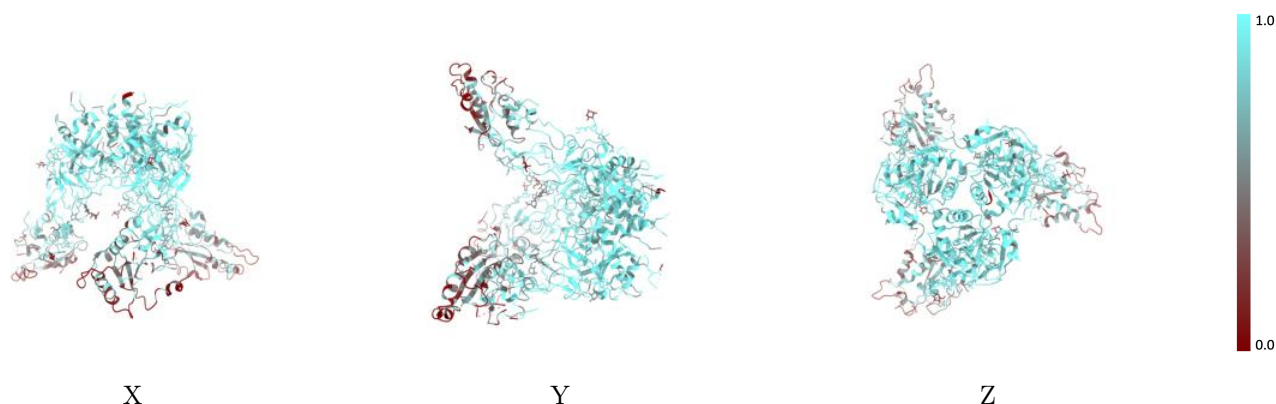
The images above show the 3D surface view of the map at the recommended contour level 0.078 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



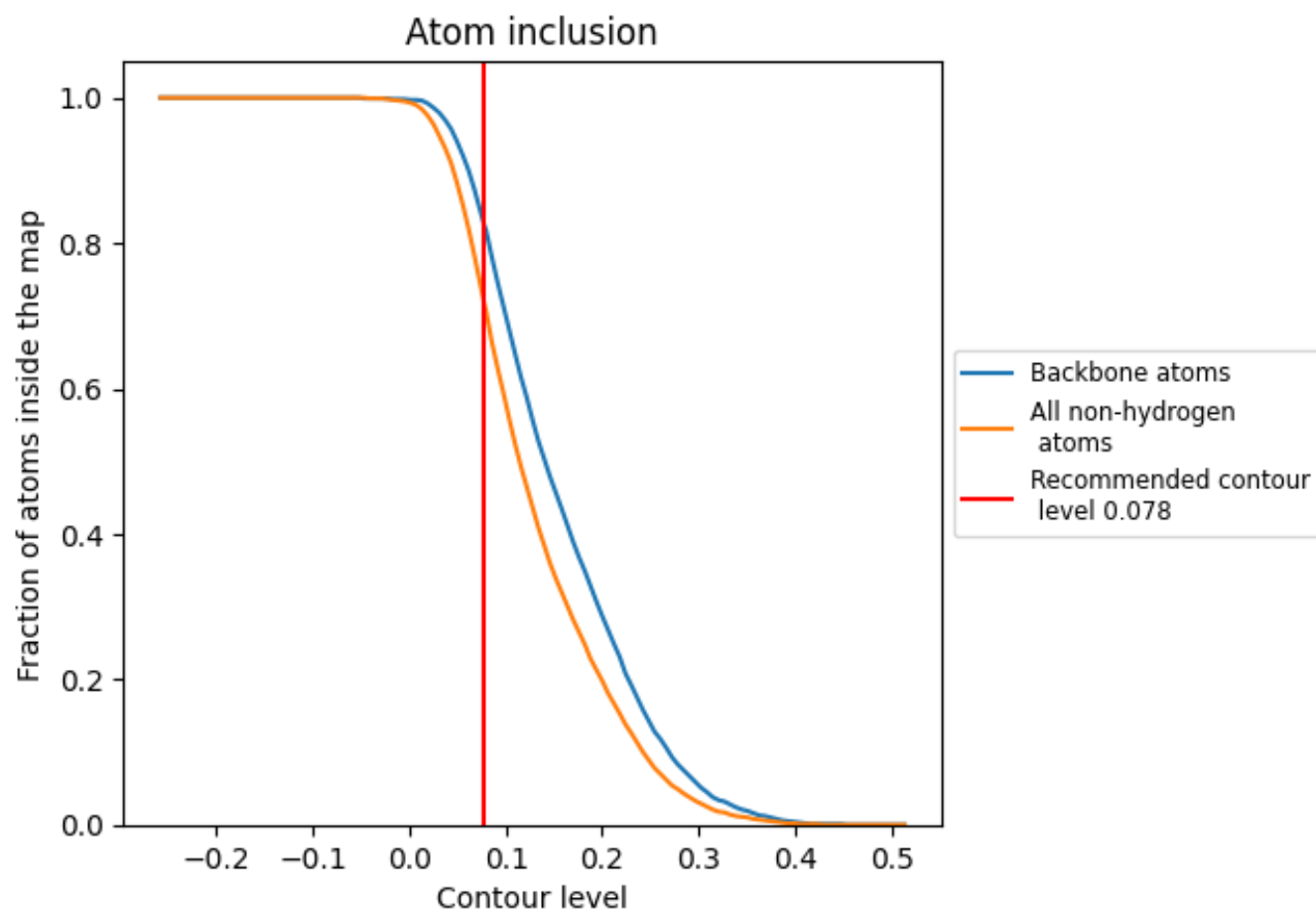
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.078).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.078) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.3340
A	 0.8890	 0.4410
B	 0.8830	 0.4400
C	 0.8840	 0.4410
D	 0.8530	 0.4070
E	 0.8500	 0.3880
F	 0.8370	 0.3990
G	 0.5410	 0.2280
H	 0.5410	 0.2240
I	 0.5290	 0.2260
K	 0.5900	 0.2420
L	 0.6720	 0.3550
M	 0.7380	 0.3390
N	 0.5900	 0.3360
O	 0.5130	 0.3880
P	 0.5130	 0.3710
Q	 0.7540	 0.3420
R	 0.7210	 0.3630
S	 0.7380	 0.4100

