Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 10:10 am GMT

PDB ID	:	6S8J
EMDB ID	:	EMD-10124
Title	:	Structure of ZEBOV GP in complex with 5T0180 antibody
Authors	:	Diskin, R.; Cohen-Dvashi, H.
Deposited on	:	2019-07-10
Resolution	:	2.91 Å(reported)
Based on initial model	:	5JQ3

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 (i) 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 (i)) were used in the production of this report:

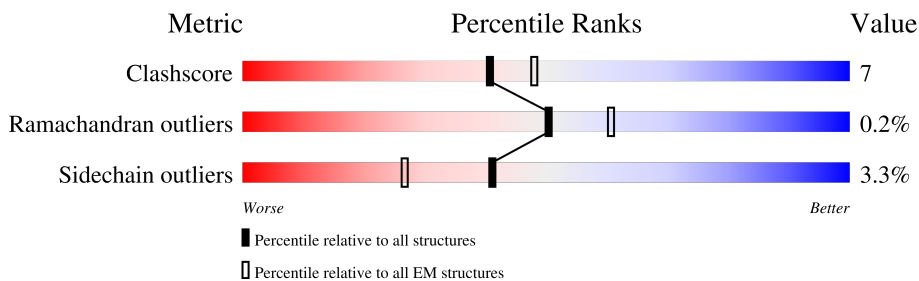|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.91 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		3.3%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	L	218	42% 8% • 50%
1	O	218	42% 7% • 50%
1	U	218	42% 8% • 50%
2	H	231	45% 8% 47%
2	P	231	43% 10% 47%
2	Y	231	45% 8% 47%
3	A	323	50% 7% • 42%
3	C	323	48% 9% • 42%

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Mol	Chain	Length	Quality of chain
3	E	323	48% 8% 42%
4	B	168	54% 11% 35%
4	D	168	54% 10% 35%
4	F	168	55% 9% 35%
5	G	2	100%
5	I	2	100%
5	J	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12391 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 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	110	Total	C	N	O	S	0	0
			816	505	142	167	2		
1	O	110	Total	C	N	O	S	0	0
			816	505	142	167	2		
1	U	110	Total	C	N	O	S	0	0
			816	505	142	167	2		

- Molecule 2 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total	C	N	O	S	0	0
			937	590	165	176	6		
2	P	122	Total	C	N	O	S	0	0
			937	590	165	176	6		
2	Y	122	Total	C	N	O	S	0	0
			937	590	165	176	6		

- Molecule 3 is a protein called Envelope Glycoprotein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	186	Total	C	N	O	S	0	0
			1437	917	244	271	5		
3	C	186	Total	C	N	O	S	0	0
			1437	917	244	271	5		
3	E	186	Total	C	N	O	S	0	0
			1437	917	244	271	5		

- Molecule 4 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	110	Total	C	N	O	S	0	0
			858	548	149	155	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	110	Total	C	N	O	S	0	0
			858	548	149	155	6		
4	F	110	Total	C	N	O	S	0	0
			858	548	149	155	6		

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	633	GLY	-	expression tag	UNP A0A0U3BWW0
B	634	SER	-	expression tag	UNP A0A0U3BWW0
B	635	GLY	-	expression tag	UNP A0A0U3BWW0
B	636	TYR	-	expression tag	UNP A0A0U3BWW0
B	637	ILE	-	expression tag	UNP A0A0U3BWW0
B	638	PRO	-	expression tag	UNP A0A0U3BWW0
B	639	GLU	-	expression tag	UNP A0A0U3BWW0
B	640	ALA	-	expression tag	UNP A0A0U3BWW0
B	641	PRO	-	expression tag	UNP A0A0U3BWW0
B	642	ARG	-	expression tag	UNP A0A0U3BWW0
B	643	ASP	-	expression tag	UNP A0A0U3BWW0
B	644	GLY	-	expression tag	UNP A0A0U3BWW0
B	645	GLN	-	expression tag	UNP A0A0U3BWW0
B	646	ALA	-	expression tag	UNP A0A0U3BWW0
B	647	TYR	-	expression tag	UNP A0A0U3BWW0
B	648	VAL	-	expression tag	UNP A0A0U3BWW0
B	649	ARG	-	expression tag	UNP A0A0U3BWW0
B	650	LYS	-	expression tag	UNP A0A0U3BWW0
B	651	ASP	-	expression tag	UNP A0A0U3BWW0
B	652	GLY	-	expression tag	UNP A0A0U3BWW0
B	653	GLU	-	expression tag	UNP A0A0U3BWW0
B	654	TRP	-	expression tag	UNP A0A0U3BWW0
B	655	VAL	-	expression tag	UNP A0A0U3BWW0
B	656	LEU	-	expression tag	UNP A0A0U3BWW0
B	657	LEU	-	expression tag	UNP A0A0U3BWW0
B	658	SER	-	expression tag	UNP A0A0U3BWW0
B	659	THR	-	expression tag	UNP A0A0U3BWW0
B	660	PHE	-	expression tag	UNP A0A0U3BWW0
B	661	LEU	-	expression tag	UNP A0A0U3BWW0
B	662	GLY	-	expression tag	UNP A0A0U3BWW0
B	663	THR	-	expression tag	UNP A0A0U3BWW0
B	664	HIS	-	expression tag	UNP A0A0U3BWW0
B	665	HIS	-	expression tag	UNP A0A0U3BWW0
B	666	HIS	-	expression tag	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	667	HIS	-	expression tag	UNP A0A0U3BWW0
B	668	HIS	-	expression tag	UNP A0A0U3BWW0
B	669	HIS	-	expression tag	UNP A0A0U3BWW0
D	633	GLY	-	expression tag	UNP A0A0U3BWW0
D	634	SER	-	expression tag	UNP A0A0U3BWW0
D	635	GLY	-	expression tag	UNP A0A0U3BWW0
D	636	TYR	-	expression tag	UNP A0A0U3BWW0
D	637	ILE	-	expression tag	UNP A0A0U3BWW0
D	638	PRO	-	expression tag	UNP A0A0U3BWW0
D	639	GLU	-	expression tag	UNP A0A0U3BWW0
D	640	ALA	-	expression tag	UNP A0A0U3BWW0
D	641	PRO	-	expression tag	UNP A0A0U3BWW0
D	642	ARG	-	expression tag	UNP A0A0U3BWW0
D	643	ASP	-	expression tag	UNP A0A0U3BWW0
D	644	GLY	-	expression tag	UNP A0A0U3BWW0
D	645	GLN	-	expression tag	UNP A0A0U3BWW0
D	646	ALA	-	expression tag	UNP A0A0U3BWW0
D	647	TYR	-	expression tag	UNP A0A0U3BWW0
D	648	VAL	-	expression tag	UNP A0A0U3BWW0
D	649	ARG	-	expression tag	UNP A0A0U3BWW0
D	650	LYS	-	expression tag	UNP A0A0U3BWW0
D	651	ASP	-	expression tag	UNP A0A0U3BWW0
D	652	GLY	-	expression tag	UNP A0A0U3BWW0
D	653	GLU	-	expression tag	UNP A0A0U3BWW0
D	654	TRP	-	expression tag	UNP A0A0U3BWW0
D	655	VAL	-	expression tag	UNP A0A0U3BWW0
D	656	LEU	-	expression tag	UNP A0A0U3BWW0
D	657	LEU	-	expression tag	UNP A0A0U3BWW0
D	658	SER	-	expression tag	UNP A0A0U3BWW0
D	659	THR	-	expression tag	UNP A0A0U3BWW0
D	660	PHE	-	expression tag	UNP A0A0U3BWW0
D	661	LEU	-	expression tag	UNP A0A0U3BWW0
D	662	GLY	-	expression tag	UNP A0A0U3BWW0
D	663	THR	-	expression tag	UNP A0A0U3BWW0
D	664	HIS	-	expression tag	UNP A0A0U3BWW0
D	665	HIS	-	expression tag	UNP A0A0U3BWW0
D	666	HIS	-	expression tag	UNP A0A0U3BWW0
D	667	HIS	-	expression tag	UNP A0A0U3BWW0
D	668	HIS	-	expression tag	UNP A0A0U3BWW0
D	669	HIS	-	expression tag	UNP A0A0U3BWW0
F	633	GLY	-	expression tag	UNP A0A0U3BWW0
F	634	SER	-	expression tag	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	635	GLY	-	expression tag	UNP A0A0U3BWW0
F	636	TYR	-	expression tag	UNP A0A0U3BWW0
F	637	ILE	-	expression tag	UNP A0A0U3BWW0
F	638	PRO	-	expression tag	UNP A0A0U3BWW0
F	639	GLU	-	expression tag	UNP A0A0U3BWW0
F	640	ALA	-	expression tag	UNP A0A0U3BWW0
F	641	PRO	-	expression tag	UNP A0A0U3BWW0
F	642	ARG	-	expression tag	UNP A0A0U3BWW0
F	643	ASP	-	expression tag	UNP A0A0U3BWW0
F	644	GLY	-	expression tag	UNP A0A0U3BWW0
F	645	GLN	-	expression tag	UNP A0A0U3BWW0
F	646	ALA	-	expression tag	UNP A0A0U3BWW0
F	647	TYR	-	expression tag	UNP A0A0U3BWW0
F	648	VAL	-	expression tag	UNP A0A0U3BWW0
F	649	ARG	-	expression tag	UNP A0A0U3BWW0
F	650	LYS	-	expression tag	UNP A0A0U3BWW0
F	651	ASP	-	expression tag	UNP A0A0U3BWW0
F	652	GLY	-	expression tag	UNP A0A0U3BWW0
F	653	GLU	-	expression tag	UNP A0A0U3BWW0
F	654	TRP	-	expression tag	UNP A0A0U3BWW0
F	655	VAL	-	expression tag	UNP A0A0U3BWW0
F	656	LEU	-	expression tag	UNP A0A0U3BWW0
F	657	LEU	-	expression tag	UNP A0A0U3BWW0
F	658	SER	-	expression tag	UNP A0A0U3BWW0
F	659	THR	-	expression tag	UNP A0A0U3BWW0
F	660	PHE	-	expression tag	UNP A0A0U3BWW0
F	661	LEU	-	expression tag	UNP A0A0U3BWW0
F	662	GLY	-	expression tag	UNP A0A0U3BWW0
F	663	THR	-	expression tag	UNP A0A0U3BWW0
F	664	HIS	-	expression tag	UNP A0A0U3BWW0
F	665	HIS	-	expression tag	UNP A0A0U3BWW0
F	666	HIS	-	expression tag	UNP A0A0U3BWW0
F	667	HIS	-	expression tag	UNP A0A0U3BWW0
F	668	HIS	-	expression tag	UNP A0A0U3BWW0
F	669	HIS	-	expression tag	UNP A0A0U3BWW0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total 28	C 16	N 2	O 10	0	0
5	I	2	Total 28	C 16	N 2	O 10	0	0
5	J	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	L	7	Total 7	O 7	0
6	H	11	Total 11	O 11	0
6	A	26	Total 26	O 26	0
6	B	9	Total 9	O 9	0
6	O	13	Total 13	O 13	0
6	U	8	Total 8	O 8	0
6	D	9	Total 9	O 9	0
6	F	10	Total 10	O 10	0
6	C	29	Total 29	O 29	0
6	E	26	Total 26	O 26	0
6	P	8	Total 8	O 8	0
6	Y	7	Total 7	O 7	0

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: Light Chain

Chain L:

• Molecule 1: Light Chain

Chain O:

• Molecule 1: Light Chain

Chain U:

• Molecule 2: Heavy Chain

Chain H: 45%   8%   47%

• Molecule 2: Heavy Chain

Chain P: 43%   10%   47%

• Molecule 2: Heavy Chain

Chain Y: 45%   8%   47%

• Molecule 3: Envelope Glycoprotein 1

Chain A: 50%   7%   •   42%

• Molecule 3: Envelope Glycoprotein 1

Chain C:

48% 9% • 42%

GLU THR GLY ARG S32 G36 H39 N40 S41 Q44 V45 S46 D49 K50 L51 V52 C53 R54 D55 K56 L57 L63 R64 S65 A105 K114 C121 C135 T144 C147 H154 E178 L184 I185 D192 F193 F194 SER SER HIS PRO LEU ARG GLU PRO

VAL ASN ALA THR GLU ASP PRO SER SER GLY Y213 T216 A222 E231 E235 VAL ASP ASN LEU THR VAL GLN LEU GLU SER ARG PHE THR PRO GLN PHE LEU LEU GLN LEU ASN GLU THR ILE TYR THR SER GLY LYS ARG SER ASN THR THR GLY LYS LEU ILE TRP LYS

VAL ASN PRO GLU ILE ASP THR ILE GLY GLU TRP ALA PHE TRP GLU THR LYS LYS ASN LEU THR ARG LYS ILE ARG SER GLU GLU LEU SER PHE THR VAL VAL SER THR HIS HIS GLN ASP THR GLY GLU GLU SER ALA SER SER GLY LYS LEU GLY LEU ILE THR ASN THR ILE ALA

GLY VAL ALA GLY LEU ILE THR GLY GLY ARG ARG THR ARG ARG

• Molecule 3: Envelope Glycoprotein 1

Chain E:

48% 8% • 42%

GLU THR GLY ARG S32 H39 N40 S41 A42 L43 Q44 V45 S46 D49 K50 L51 V52 C53 R54 D55 K56 L57 L63 R64 S65 A105 K114 D117 C121 C135 T144 C147 H154 E178 I185 D192 F193 F194 SER SER HIS PRO LEU ARG GLU PRO

VAL ASN ALA THR GLU ASP PRO SER SER GLY Y213 T216 A222 E231 Y232 E235 VAL ASP ASN LEU THR TYR VAL GLN LEU GLU SER ARG PHE THR PRO GLN PHE LEU LEU GLN LEU ASN GLU THR ILE TYR THR SER GLY LYS ARG SER ASN THR THR GLY LYS LEU LEU ILE TRP

LYS VAL ASN PRO GLU ILE ASP THR ILE GLY GLU TRP ALA PHE TRP GLU THR LYS LYS ASN LEU THR ARG LYS ILE ARG SER GLU GLU LEU SER PHE THR VAL VAL SER THR HIS HIS GLN ASP THR GLY GLU GLU SER ALA SER SER GLY LYS LEU GLY LEU ILE THR ASN THR ILE

ALA GLY VAL ALA GLY LEU ILE THR GLY GLY ARG ARG THR ARG ARG

• Molecule 4: Envelope glycoprotein

Chain B:

54% 11% • 35%

GLU A503 P513 Q521 E545 H549 N550 Q551 I555 L561 K588 R596 W597 T600 C601 H602 I603 L604 D607 C608 C609 I610 E611 P612 HIS ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP GLY SER GLY TYR ILE PRO

GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY TRP VAL LEU LEU SER THR PHE LEU GLY THR HIS HIS HIS HIS HIS HIS

• Molecule 4: Envelope glycoprotein

Chain D:

54% 10% •• 35%

GLU A503 P513 Y517 Q521 H549 N550 Q551 D552 I555 L558 K588 D591 W597 T600 C601 H602 I603 L604 D607 I610 E611 P612 HIS ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP GLY SER GLY TYR ILE

PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY THR HIS HIS HIS HIS HIS HIS

• Molecule 4: Envelope glycoprotein

Chain F:

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

Chain G:

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

Chain I:

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

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	100499	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.900	Depositor
Minimum map value	-4.541	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.194	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	217.344, 217.344, 217.344	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.849, 0.849, 0.849	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

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	L	0.35	0/834	0.59	0/1136
1	O	0.35	0/834	0.59	0/1136
1	U	0.35	0/834	0.59	0/1136
2	H	0.36	0/959	0.66	0/1297
2	P	0.36	0/959	0.66	0/1297
2	Y	0.36	0/959	0.66	0/1297
3	A	0.35	0/1473	0.61	0/2000
3	C	0.35	0/1473	0.61	0/2000
3	E	0.35	0/1473	0.61	0/2000
4	B	0.31	0/879	0.59	1/1198 (0.1%)
4	D	0.31	0/879	0.59	1/1198 (0.1%)
4	F	0.31	0/879	0.59	1/1198 (0.1%)
All	All	0.35	0/12435	0.61	3/16893 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	604	LEU	CB-CG-CD2	6.04	121.27	111.00
4	F	604	LEU	CB-CG-CD2	6.03	121.25	111.00
4	B	604	LEU	CB-CG-CD2	6.01	121.21	111.00

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	L	816	0	777	12	0
1	O	816	0	777	12	0
1	U	816	0	777	12	0
2	H	937	0	908	13	0
2	P	937	0	908	15	0
2	Y	937	0	908	13	0
3	A	1437	0	1377	25	0
3	C	1437	0	1377	28	0
3	E	1437	0	1377	27	0
4	B	858	0	837	16	0
4	D	858	0	837	22	0
4	F	858	0	837	15	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
6	A	26	0	0	0	0
6	B	9	0	0	1	0
6	C	29	0	0	0	0
6	D	9	0	0	1	0
6	E	26	0	0	1	0
6	F	10	0	0	1	0
6	H	11	0	0	1	0
6	L	7	0	0	0	0
6	O	13	0	0	0	0
6	P	8	0	0	1	0
6	U	8	0	0	0	0
6	Y	7	0	0	1	0
All	All	12391	0	11772	179	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 (179) 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:L:19:VAL:HG22	1:L:81:LEU:HD11	1.69	0.74
1:U:19:VAL:HG22	1:U:81:LEU:HD11	1.69	0.74
3:E:52:VAL:HG22	3:E:54:ARG:HD2	1.69	0.74
3:A:52:VAL:HG22	3:A:54:ARG:HD2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:19:VAL:HG22	1:O:81:LEU:HD11	1.69	0.73
3:C:52:VAL:HG22	3:C:54:ARG:HD2	1.69	0.73
2:Y:93:THR:HG23	2:Y:121:THR:HA	1.71	0.73
2:P:93:THR:HG23	2:P:121:THR:HA	1.71	0.72
2:H:93:THR:HG23	2:H:121:THR:HA	1.71	0.71
1:U:18:ARG:HG3	1:U:79:THR:HG22	1.73	0.71
3:E:114:LYS:NZ	2:Y:56:ASP:OD2	2.18	0.71
4:B:603:ILE:HG22	4:B:604:LEU:HD23	1.73	0.70
1:O:18:ARG:HG3	1:O:79:THR:HG22	1.73	0.70
4:F:603:ILE:HG22	4:F:604:LEU:HD23	1.73	0.70
3:A:51:LEU:HD11	4:B:596:ARG:HA	1.73	0.70
1:L:18:ARG:HG3	1:L:79:THR:HG22	1.73	0.69
4:D:603:ILE:HG22	4:D:604:LEU:HD23	1.73	0.69
4:B:597:TRP:NE1	4:D:597:TRP:O	2.26	0.67
4:D:610:ILE:HG23	4:F:601:CYS:HB3	1.75	0.67
1:O:58:PRO:HG2	2:P:110:PRO:HG3	1.78	0.66
2:P:2:VAL:N	6:P:303:HOH:O	2.32	0.62
4:B:549:HIS:HB2	4:B:551:GLN:OE1	2.00	0.61
3:E:49:ASP:OD1	3:E:50:LYS:N	2.34	0.61
4:F:549:HIS:HB2	4:F:551:GLN:OE1	2.00	0.61
3:C:49:ASP:OD1	3:C:50:LYS:N	2.34	0.61
3:C:114:LYS:NZ	2:P:56:ASP:OD2	2.25	0.60
3:A:49:ASP:OD1	3:A:50:LYS:N	2.34	0.60
4:D:549:HIS:HB2	4:D:551:GLN:OE1	2.00	0.60
3:C:39:HIS:CE1	3:C:44:GLN:HB2	2.39	0.58
2:H:56:ASP:OD2	3:A:114:LYS:NZ	2.31	0.58
3:E:39:HIS:CE1	3:E:44:GLN:HB2	2.39	0.57
4:D:558:LEU:HD11	3:C:184:LEU:HD11	1.86	0.57
3:A:39:HIS:CE1	3:A:44:GLN:HB2	2.39	0.57
1:L:81:LEU:HD23	1:L:112:VAL:HG12	1.86	0.57
4:F:611:GLU:N	4:F:611:GLU:OE1	2.37	0.57
1:O:58:PRO:HB2	2:P:109:GLY:HA2	1.86	0.57
4:D:597:TRP:NE1	4:F:597:TRP:O	2.38	0.56
1:O:81:LEU:HD23	1:O:112:VAL:HG12	1.87	0.56
4:D:611:GLU:OE1	4:D:611:GLU:N	2.37	0.56
4:B:611:GLU:N	4:B:611:GLU:OE1	2.37	0.56
1:U:81:LEU:HD23	1:U:112:VAL:HG12	1.86	0.56
4:B:513:PRO:O	4:B:550:ASN:HB2	2.06	0.56
4:F:513:PRO:O	4:F:550:ASN:HB2	2.06	0.56
4:D:513:PRO:O	4:D:550:ASN:HB2	2.06	0.55
4:F:588:LYS:NZ	6:F:802:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:69:ARG:HD3	2:P:89:ARG:HH21	1.72	0.55
2:H:69:ARG:HD3	2:H:89:ARG:HH21	1.72	0.54
3:C:52:VAL:HG22	3:C:54:ARG:CD	2.38	0.54
4:B:610:ILE:HG23	4:D:601:CYS:HB3	1.89	0.54
3:A:52:VAL:HG22	3:A:54:ARG:CD	2.38	0.53
2:Y:69:ARG:HD3	2:Y:89:ARG:HH21	1.72	0.53
4:D:607:ASP:HA	3:C:51:LEU:HD22	1.91	0.53
2:Y:100:ARG:HD3	2:Y:112:ASP:O	2.08	0.53
3:E:39:HIS:CD2	3:E:54:ARG:HH22	2.27	0.53
2:P:100:ARG:HD3	2:P:112:ASP:O	2.08	0.53
2:H:100:ARG:HD3	2:H:112:ASP:O	2.08	0.53
4:B:609:CYS:HB3	4:D:600:THR:HG22	1.90	0.53
3:C:39:HIS:CD2	3:C:54:ARG:HH22	2.27	0.53
3:E:52:VAL:HG22	3:E:54:ARG:CD	2.38	0.52
1:O:66:SER:O	1:O:76:LEU:HD12	2.09	0.52
3:A:39:HIS:CD2	3:A:54:ARG:HH22	2.27	0.52
1:U:66:SER:O	1:U:76:LEU:HD12	2.09	0.52
1:L:66:SER:O	1:L:76:LEU:HD12	2.10	0.52
3:C:57:LEU:HD12	3:C:185:ILE:HD13	1.91	0.52
3:E:57:LEU:HD12	3:E:185:ILE:HD13	1.91	0.52
3:A:57:LEU:HD12	3:A:185:ILE:HD13	1.91	0.51
4:B:610:ILE:HG23	4:D:601:CYS:O	2.11	0.51
2:P:36:TRP:O	2:P:48:VAL:HG12	2.11	0.51
2:Y:36:TRP:O	2:Y:48:VAL:HG12	2.11	0.51
4:D:597:TRP:CE2	4:F:597:TRP:HB3	2.47	0.50
3:A:192:ASP:N	3:A:192:ASP:OD1	2.44	0.50
3:E:105:ALA:O	3:E:135:CYS:HA	2.12	0.50
3:A:105:ALA:O	3:A:135:CYS:HA	2.12	0.50
3:E:192:ASP:N	3:E:192:ASP:OD1	2.44	0.50
3:C:105:ALA:O	3:C:135:CYS:HA	2.12	0.50
3:C:192:ASP:N	3:C:192:ASP:OD1	2.44	0.50
1:L:26:SER:OG	1:L:27:SER:N	2.45	0.49
2:H:36:TRP:O	2:H:48:VAL:HG12	2.11	0.49
3:A:54:ARG:CD	3:A:54:ARG:H	2.26	0.49
3:C:54:ARG:CD	3:C:54:ARG:H	2.26	0.49
3:E:54:ARG:CD	3:E:54:ARG:H	2.26	0.49
1:O:26:SER:OG	1:O:27:SER:N	2.45	0.48
4:D:517:TYR:CZ	3:C:194:PHE:HA	2.48	0.48
4:F:521:GLN:HG2	4:F:521:GLN:O	2.14	0.48
4:F:550:ASN:HA	4:F:555:ILE:HG12	1.95	0.48
1:O:34:TYR:CD2	1:O:94:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:521:GLN:O	4:D:521:GLN:HG2	2.14	0.47
4:D:552:ASP:CG	3:C:41:SER:HB3	2.35	0.47
2:H:85:MET:HE3	2:H:88:LEU:HD21	1.96	0.47
1:U:26:SER:OG	1:U:27:SER:N	2.45	0.47
3:C:54:ARG:HD2	3:C:54:ARG:H	1.80	0.47
1:L:34:TYR:CD2	1:L:94:TYR:HB2	2.49	0.47
3:A:54:ARG:HD2	3:A:54:ARG:H	1.80	0.47
4:B:550:ASN:HA	4:B:555:ILE:HG12	1.95	0.47
4:D:550:ASN:HA	4:D:555:ILE:HG12	1.95	0.47
3:E:54:ARG:HH21	3:E:54:ARG:HG2	1.80	0.47
3:E:54:ARG:HD2	3:E:54:ARG:H	1.79	0.47
4:B:521:GLN:HG2	4:B:521:GLN:O	2.14	0.47
3:C:54:ARG:HG2	3:C:54:ARG:HH21	1.80	0.47
1:U:34:TYR:CD2	1:U:94:TYR:HB2	2.49	0.46
2:P:70:PHE:CZ	2:P:85:MET:HE3	2.50	0.46
3:C:56:LYS:HB3	3:C:56:LYS:HE3	1.63	0.46
2:Y:70:PHE:CZ	2:Y:85:MET:HE3	2.51	0.46
3:A:54:ARG:HH21	3:A:54:ARG:HG2	1.80	0.46
2:H:52:LYS:NZ	6:H:305:HOH:O	2.46	0.45
4:B:588:LYS:NZ	6:B:801:HOH:O	2.49	0.45
3:A:51:LEU:HD22	4:B:607:ASP:HA	1.99	0.45
4:F:552:ASP:OD2	3:E:41:SER:HB3	2.16	0.45
3:A:56:LYS:HE3	3:A:56:LYS:HB3	1.63	0.45
1:U:8:PRO:O	1:U:108:THR:HG22	2.17	0.45
1:L:34:TYR:CE1	1:L:96:SER:HB2	2.52	0.45
2:H:85:MET:HB3	2:H:88:LEU:HD21	1.99	0.44
2:Y:85:MET:HE3	2:Y:88:LEU:HD21	2.00	0.44
3:A:54:ARG:CD	3:A:54:ARG:N	2.81	0.44
3:C:54:ARG:CD	3:C:54:ARG:N	2.81	0.44
2:P:85:MET:HB3	2:P:88:LEU:HD21	2.00	0.44
3:E:54:ARG:CD	3:E:54:ARG:N	2.80	0.44
4:F:561:LEU:HD22	3:E:43:LEU:HD21	1.99	0.44
1:L:8:PRO:O	1:L:108:THR:HG22	2.17	0.44
3:A:57:LEU:HD11	3:A:63:LEU:HD21	1.99	0.44
1:O:97:ARG:O	1:O:97:ARG:HG2	2.17	0.44
2:Y:85:MET:HB3	2:Y:88:LEU:HD21	1.99	0.44
1:O:34:TYR:CE1	1:O:96:SER:HB2	2.52	0.44
3:E:57:LEU:HD11	3:E:63:LEU:HD21	1.99	0.44
1:O:8:PRO:O	1:O:108:THR:HG22	2.17	0.43
2:P:47:TRP:HZ2	2:P:50:ARG:HB2	1.83	0.43
2:Y:100:ARG:O	2:Y:100:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:LEU:HD11	3:C:63:LEU:HD21	1.99	0.43
2:H:70:PHE:CZ	2:H:85:MET:HE3	2.53	0.43
3:A:222:ALA:HA	3:A:231:GLU:O	2.19	0.43
3:A:43:LEU:HD21	4:B:561:LEU:HD22	2.00	0.43
3:C:54:ARG:HD3	3:C:55:ASP:H	1.84	0.43
3:C:121:CYS:HB2	3:C:147:CYS:HB3	1.86	0.43
3:E:222:ALA:HA	3:E:231:GLU:O	2.19	0.43
1:L:97:ARG:O	1:L:97:ARG:HG2	2.17	0.43
4:F:607:ASP:HA	3:E:51:LEU:HD22	2.00	0.43
2:P:85:MET:HE3	2:P:88:LEU:HD21	2.01	0.43
1:L:104:PHE:HE1	2:H:47:TRP:HB2	1.84	0.43
1:U:97:ARG:HG2	1:U:97:ARG:O	2.17	0.43
4:F:596:ARG:HA	3:E:51:LEU:HD11	2.01	0.43
3:C:154:HIS:NE2	3:C:178:GLU:OE1	2.46	0.43
3:A:54:ARG:HD3	3:A:55:ASP:H	1.84	0.43
1:U:34:TYR:CE1	1:U:96:SER:HB2	2.52	0.43
2:H:48:VAL:HG23	2:H:66:VAL:HG11	2.01	0.43
3:C:222:ALA:HA	3:C:231:GLU:O	2.19	0.43
2:H:100:ARG:O	2:H:100:ARG:HG3	2.18	0.43
2:P:48:VAL:HG23	2:P:66:VAL:HG11	2.01	0.42
2:Y:48:VAL:HG23	2:Y:66:VAL:HG11	2.01	0.42
3:E:54:ARG:HD3	3:E:55:ASP:H	1.84	0.42
2:Y:47:TRP:HZ2	2:Y:50:ARG:HB2	1.83	0.42
3:E:56:LYS:HB3	3:E:56:LYS:HE3	1.63	0.42
2:H:47:TRP:HZ2	2:H:50:ARG:HB2	1.83	0.42
3:A:104:TRP:CZ2	4:B:545:GLU:HG2	2.54	0.42
4:D:607:ASP:OD2	4:D:607:ASP:N	2.53	0.42
2:P:100:ARG:HG3	2:P:100:ARG:O	2.18	0.42
2:Y:101:GLY:O	6:Y:301:HOH:O	2.22	0.42
3:A:114:LYS:O	3:A:144:THR:HA	2.20	0.41
3:E:114:LYS:O	3:E:144:THR:HA	2.20	0.41
1:U:94:TYR:OH	3:E:117:ASP:HB3	2.19	0.41
3:C:52:VAL:CG2	3:C:54:ARG:HE	2.34	0.41
3:E:121:CYS:HB2	3:E:147:CYS:HB3	1.86	0.41
3:E:232:TYR:HB2	6:E:426:HOH:O	2.21	0.41
3:E:52:VAL:CG2	3:E:54:ARG:HE	2.34	0.41
3:A:104:TRP:HZ2	4:B:545:GLU:HG2	1.85	0.41
4:D:552:ASP:OD2	3:C:41:SER:HB3	2.21	0.41
4:F:607:ASP:OD2	4:F:607:ASP:N	2.53	0.41
1:U:63:ASP:O	1:U:63:ASP:OD1	2.39	0.41
3:C:114:LYS:O	3:C:144:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:ARG:HA	1:L:79:THR:HA	2.03	0.41
3:A:52:VAL:CG2	3:A:54:ARG:HE	2.34	0.41
4:D:588:LYS:NZ	6:D:803:HOH:O	2.53	0.41
2:P:12:VAL:O	2:P:123:SER:N	2.45	0.41
1:U:58:PRO:HB2	2:Y:109:GLY:HA2	2.04	0.40
3:E:154:HIS:NE2	3:E:178:GLU:OE1	2.46	0.40
1:O:18:ARG:HA	1:O:79:THR:HA	2.03	0.40
3:C:36:GLY:HA2	3:C:45:VAL:HA	2.03	0.40
1:L:63:ASP:OD1	1:L:63:ASP:O	2.39	0.40
3:A:60:THR:HG23	4:D:591:ASP:OD1	2.21	0.40
4:D:517:TYR:CE1	3:C:194:PHE:HA	2.57	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	L	108/218 (50%)	105 (97%)	3 (3%)	0	100	100
1	O	108/218 (50%)	105 (97%)	3 (3%)	0	100	100
1	U	108/218 (50%)	105 (97%)	3 (3%)	0	100	100
2	H	120/231 (52%)	115 (96%)	4 (3%)	1 (1%)	19	49
2	P	120/231 (52%)	115 (96%)	4 (3%)	1 (1%)	19	49
2	Y	120/231 (52%)	115 (96%)	4 (3%)	1 (1%)	19	49
3	A	182/323 (56%)	175 (96%)	7 (4%)	0	100	100
3	C	182/323 (56%)	175 (96%)	7 (4%)	0	100	100
3	E	182/323 (56%)	175 (96%)	7 (4%)	0	100	100
4	B	108/168 (64%)	105 (97%)	3 (3%)	0	100	100
4	D	108/168 (64%)	105 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	108/168 (64%)	105 (97%)	3 (3%)	0	100	100
All	All	1554/2820 (55%)	1500 (96%)	51 (3%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	90	ARG
2	P	90	ARG
2	Y	90	ARG

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	L	89/182 (49%)	85 (96%)	4 (4%)	27	59
1	O	89/182 (49%)	85 (96%)	4 (4%)	27	59
1	U	89/182 (49%)	85 (96%)	4 (4%)	27	59
2	H	99/194 (51%)	98 (99%)	1 (1%)	76	91
2	P	99/194 (51%)	98 (99%)	1 (1%)	76	91
2	Y	99/194 (51%)	98 (99%)	1 (1%)	76	91
3	A	151/273 (55%)	145 (96%)	6 (4%)	31	63
3	C	151/273 (55%)	145 (96%)	6 (4%)	31	63
3	E	151/273 (55%)	145 (96%)	6 (4%)	31	63
4	B	89/140 (64%)	86 (97%)	3 (3%)	37	69
4	D	89/140 (64%)	86 (97%)	3 (3%)	37	69
4	F	89/140 (64%)	86 (97%)	3 (3%)	37	69
All	All	1284/2367 (54%)	1242 (97%)	42 (3%)	41	70

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	SER
1	L	19	VAL
1	L	26	SER
1	L	75	SER
2	H	119	LEU
3	A	46	SER
3	A	54	ARG
3	A	56	LYS
3	A	65	SER
3	A	135	CYS
3	A	216	THR
4	B	600	THR
4	B	601	CYS
4	B	604	LEU
1	O	10	SER
1	O	19	VAL
1	O	26	SER
1	O	75	SER
1	U	10	SER
1	U	19	VAL
1	U	26	SER
1	U	75	SER
4	D	600	THR
4	D	601	CYS
4	D	604	LEU
4	F	600	THR
4	F	601	CYS
4	F	604	LEU
3	C	46	SER
3	C	54	ARG
3	C	56	LYS
3	C	65	SER
3	C	135	CYS
3	C	216	THR
3	E	46	SER
3	E	54	ARG
3	E	56	LYS
3	E	65	SER
3	E	135	CYS
3	E	216	THR
2	P	119	LEU
2	Y	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	82	GLN
3	A	107	ASN
3	A	188	GLN
4	B	516	HIS
1	O	37	GLN
1	O	82	GLN
1	U	37	GLN
1	U	82	GLN
4	D	516	HIS
4	F	516	HIS
3	C	107	ASN
3	C	188	GLN
3	E	107	ASN
3	E	188	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	NAG	G	1	4,5	14,14,15	0.34	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.23	0	17,19,21	0.53	0
5	NAG	I	1	4,5	14,14,15	0.35	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	NAG	I	2	5	14,14,15	0.25	0	17,19,21	0.53	0
5	NAG	J	1	4,5	14,14,15	0.35	0	17,19,21	0.46	0
5	NAG	J	2	5	14,14,15	0.24	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	I	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings
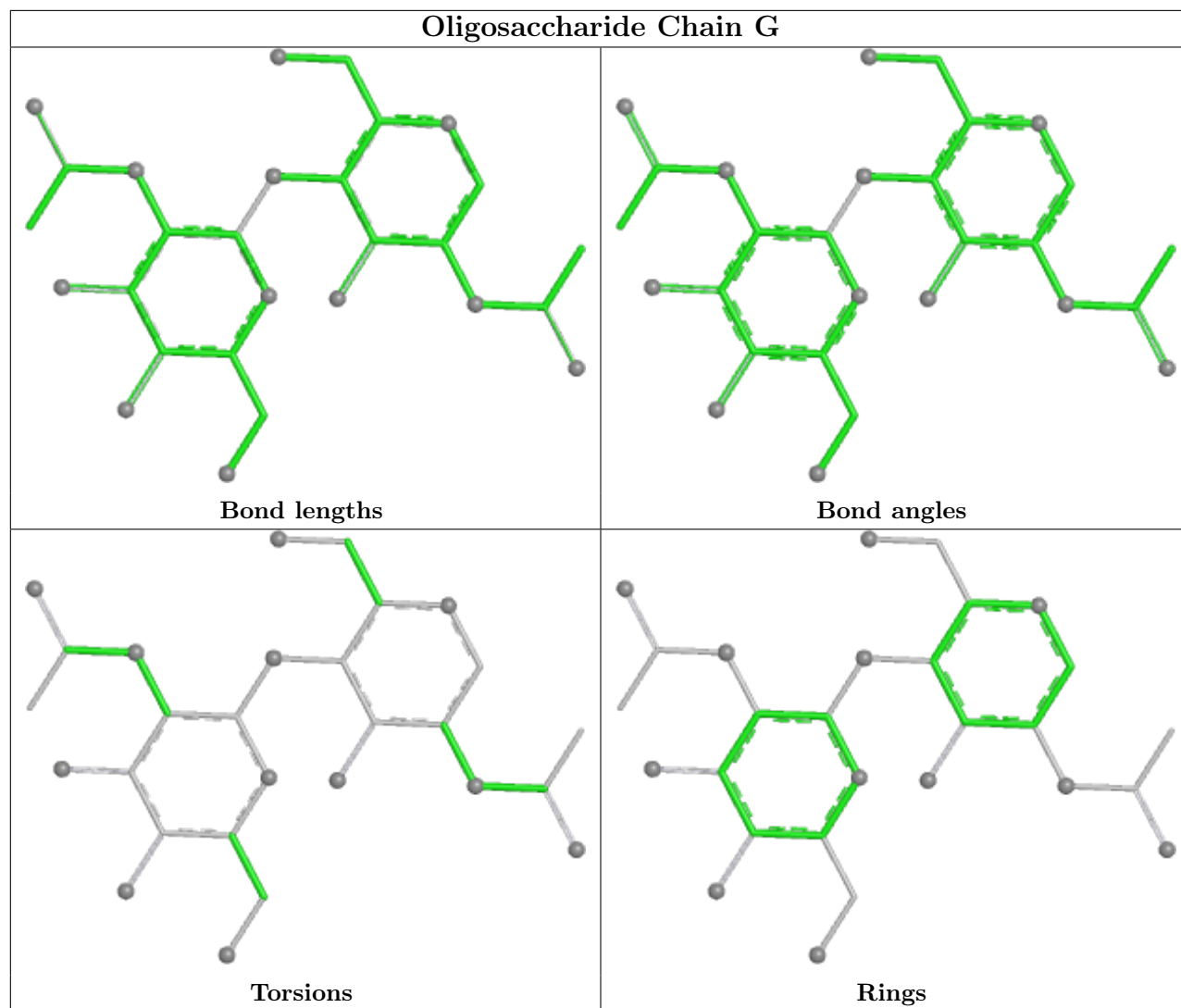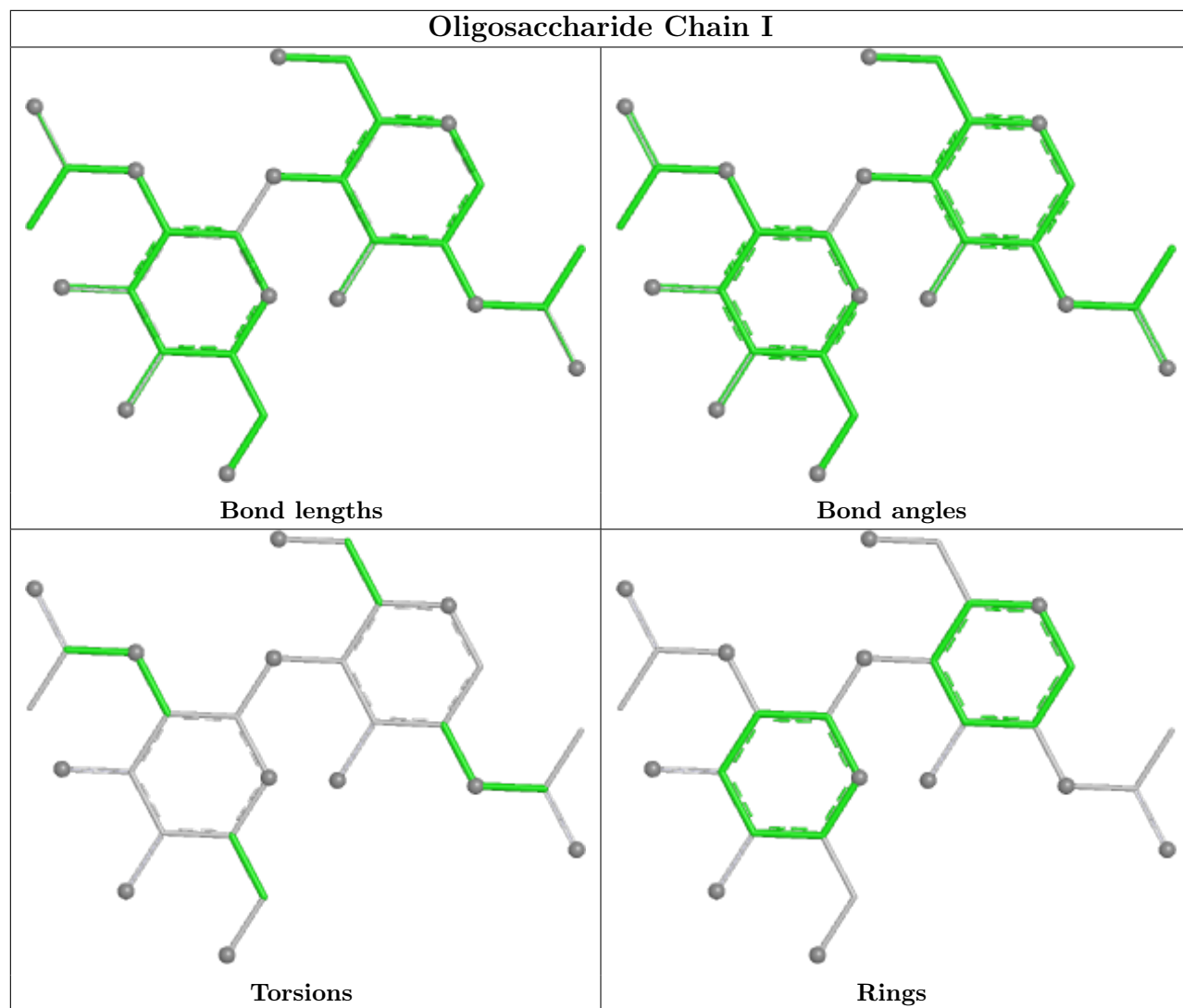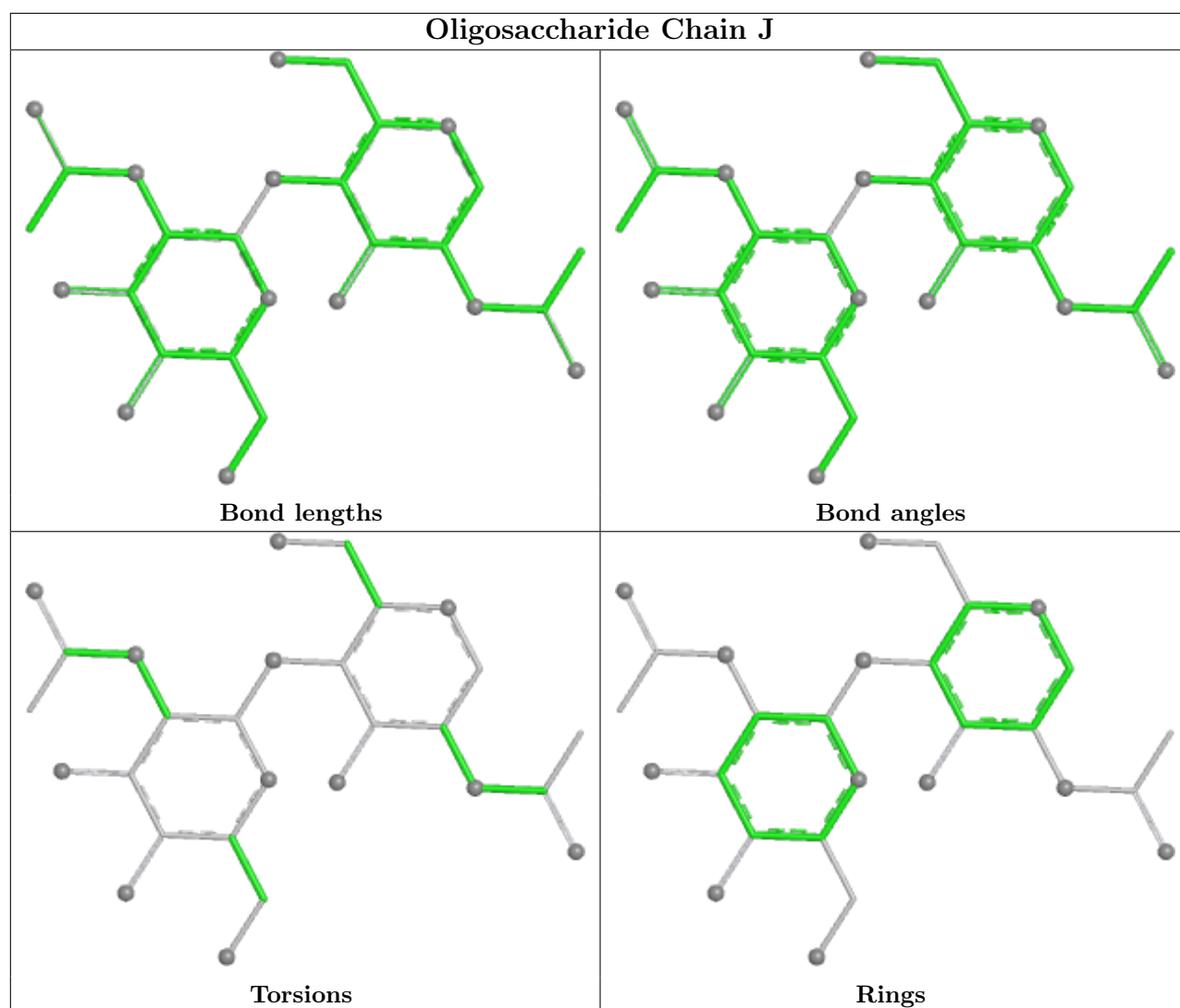
5.6 Ligand geometry ⓘ

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-10124. 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
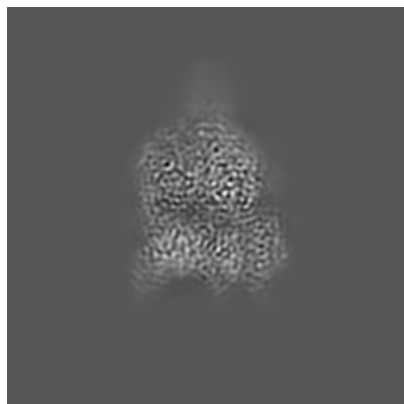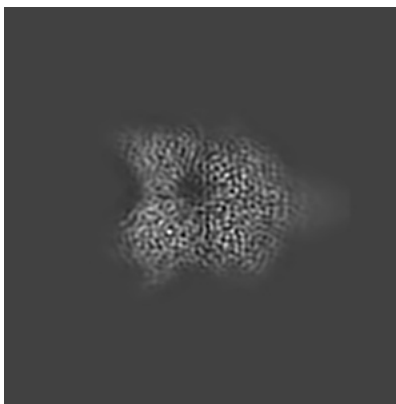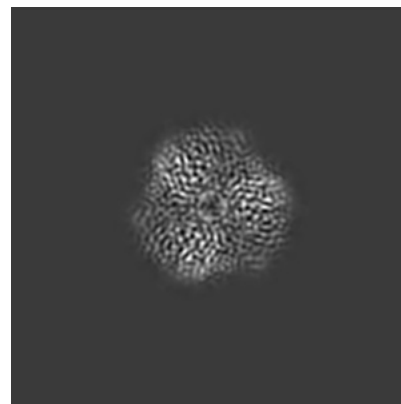
| X | Y | Z |

6.1.2 Raw map

| X | Y | Z |
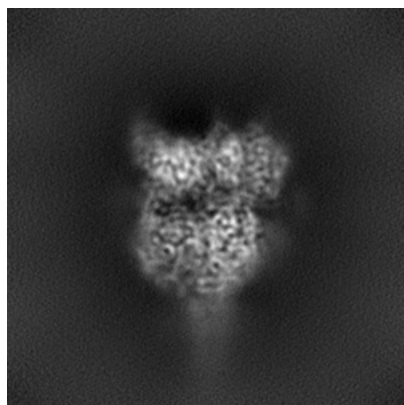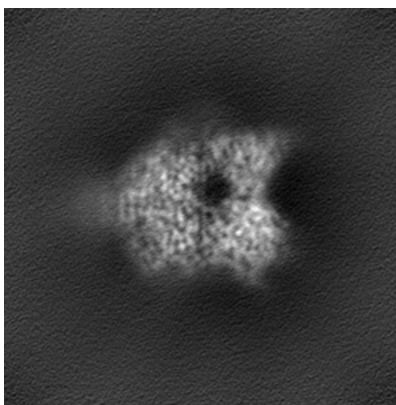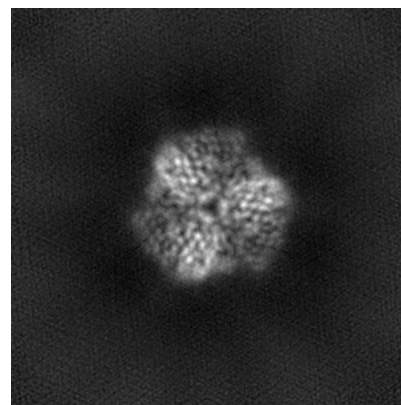
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
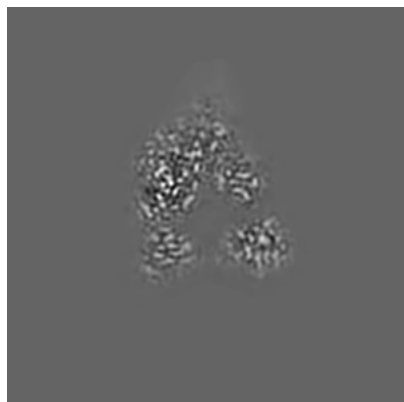
6.2.1 Primary map
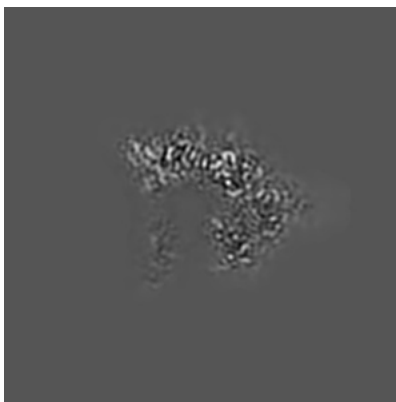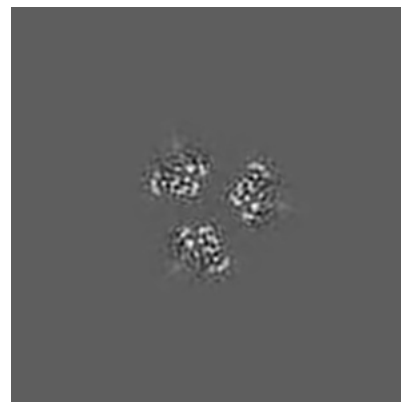
X Index: 128　　　　　Y Index: 128　　　　　Z Index: 128

6.2.2 Raw map
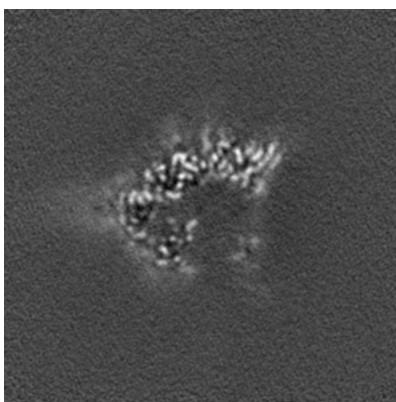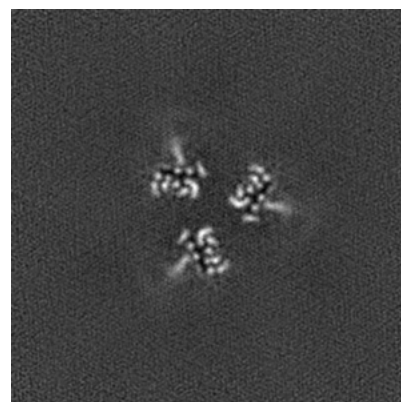
X Index: 128　　　　　Y Index: 128　　　　　Z Index: 128

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
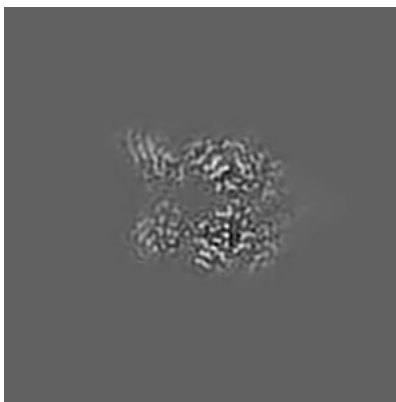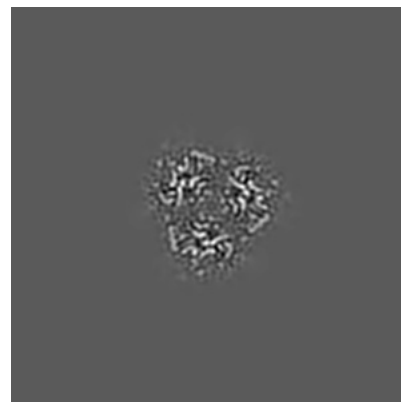
X Index: 114	Y Index: 143	Z Index: 142

6.3.2 Raw map
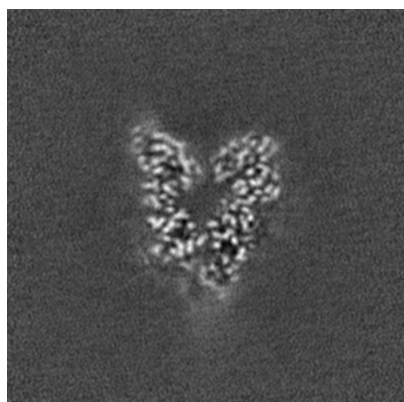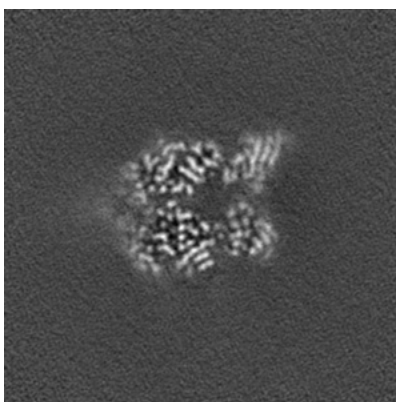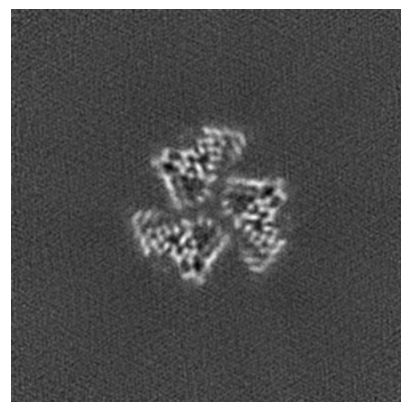
X Index: 114	Y Index: 143	Z Index: 159

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
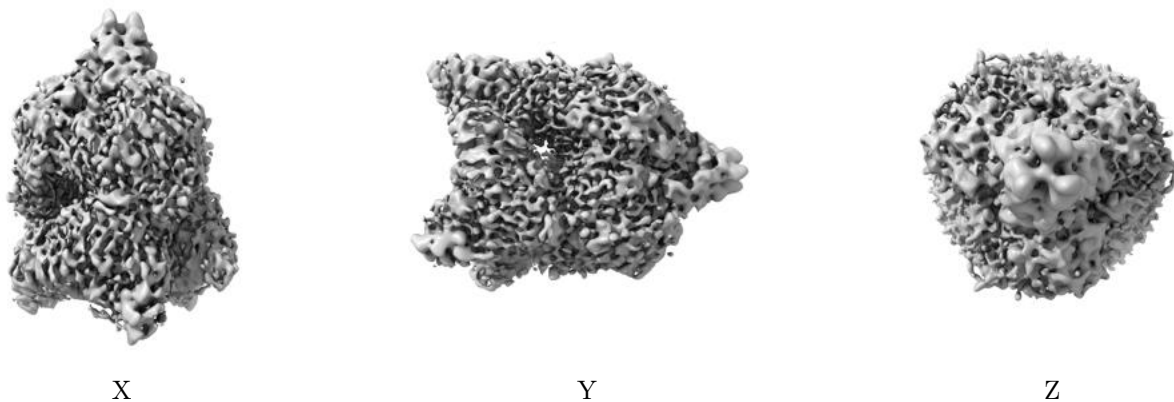
The images above show the 3D surface view of the map at the recommended contour level 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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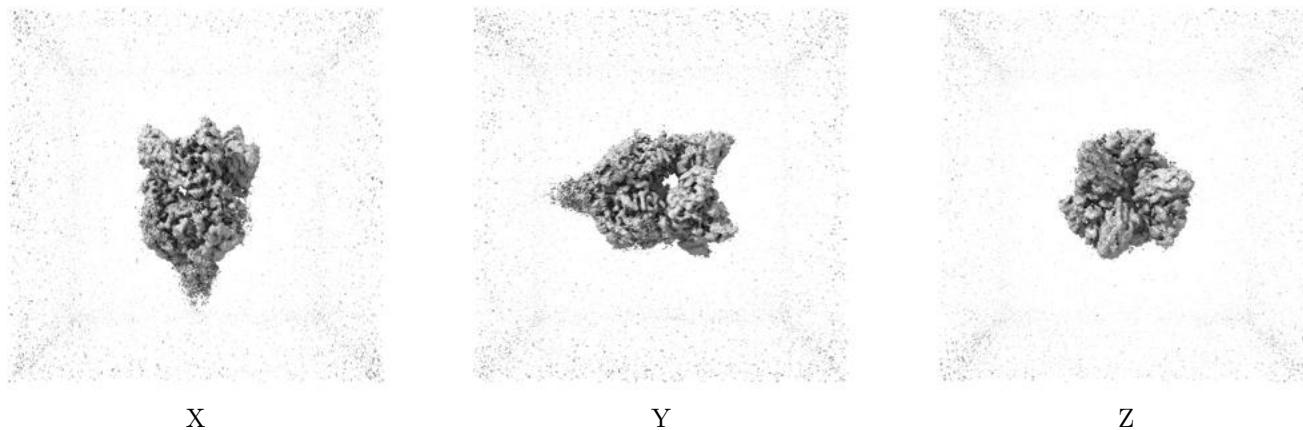
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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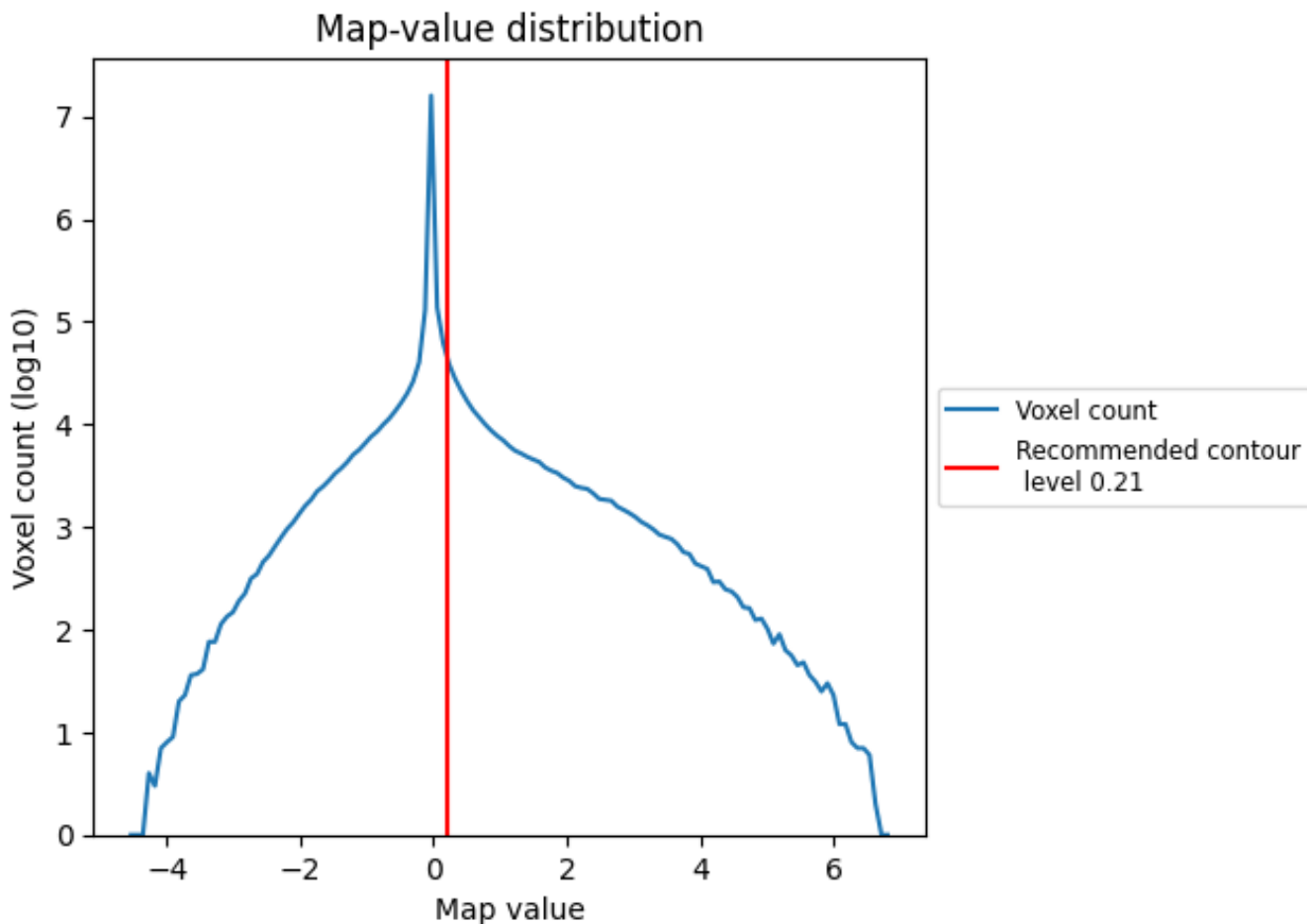
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
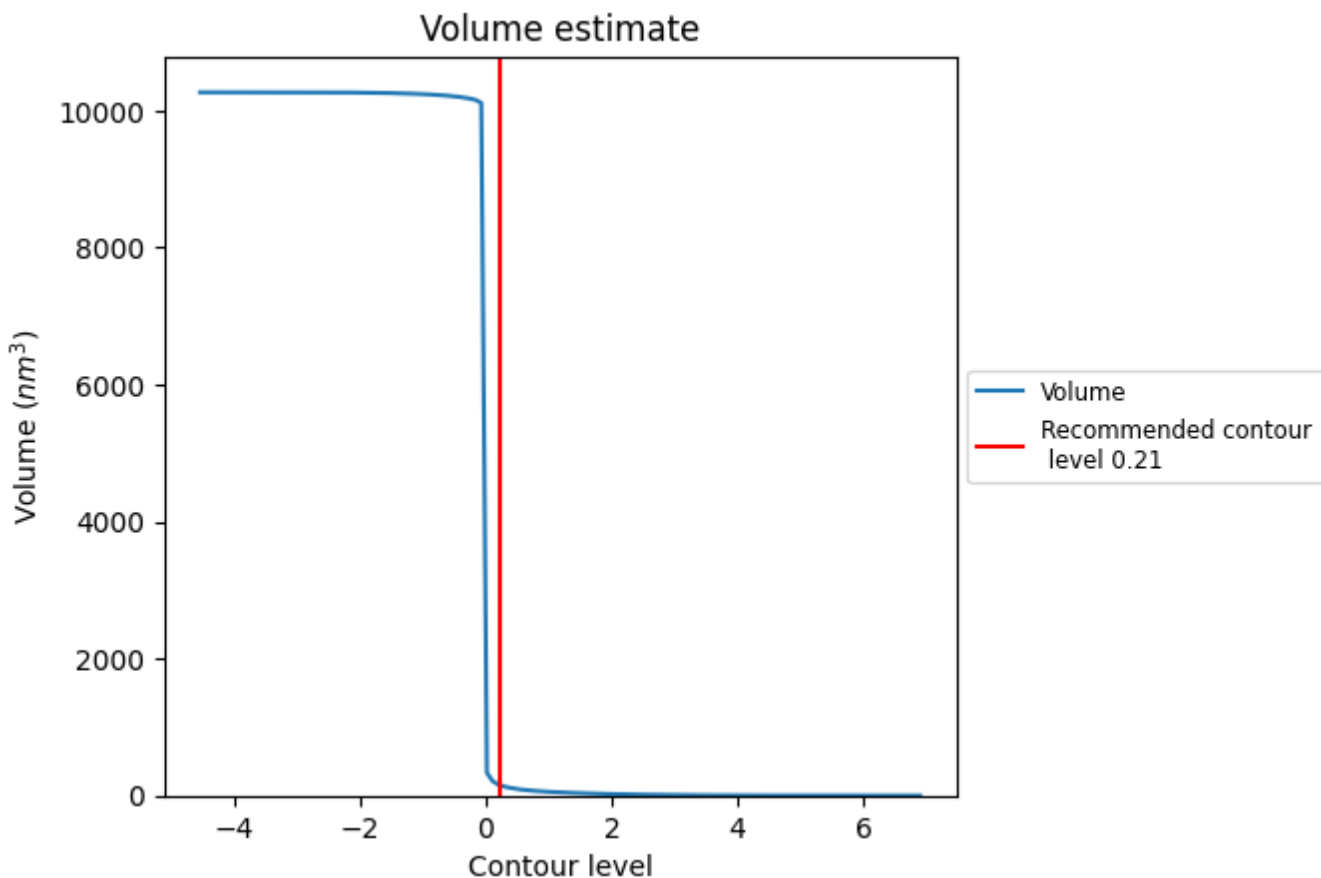
The volume at the recommended contour level is 157 nm^3; this corresponds to an approximate mass of 142 kDa.

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 ⓘ
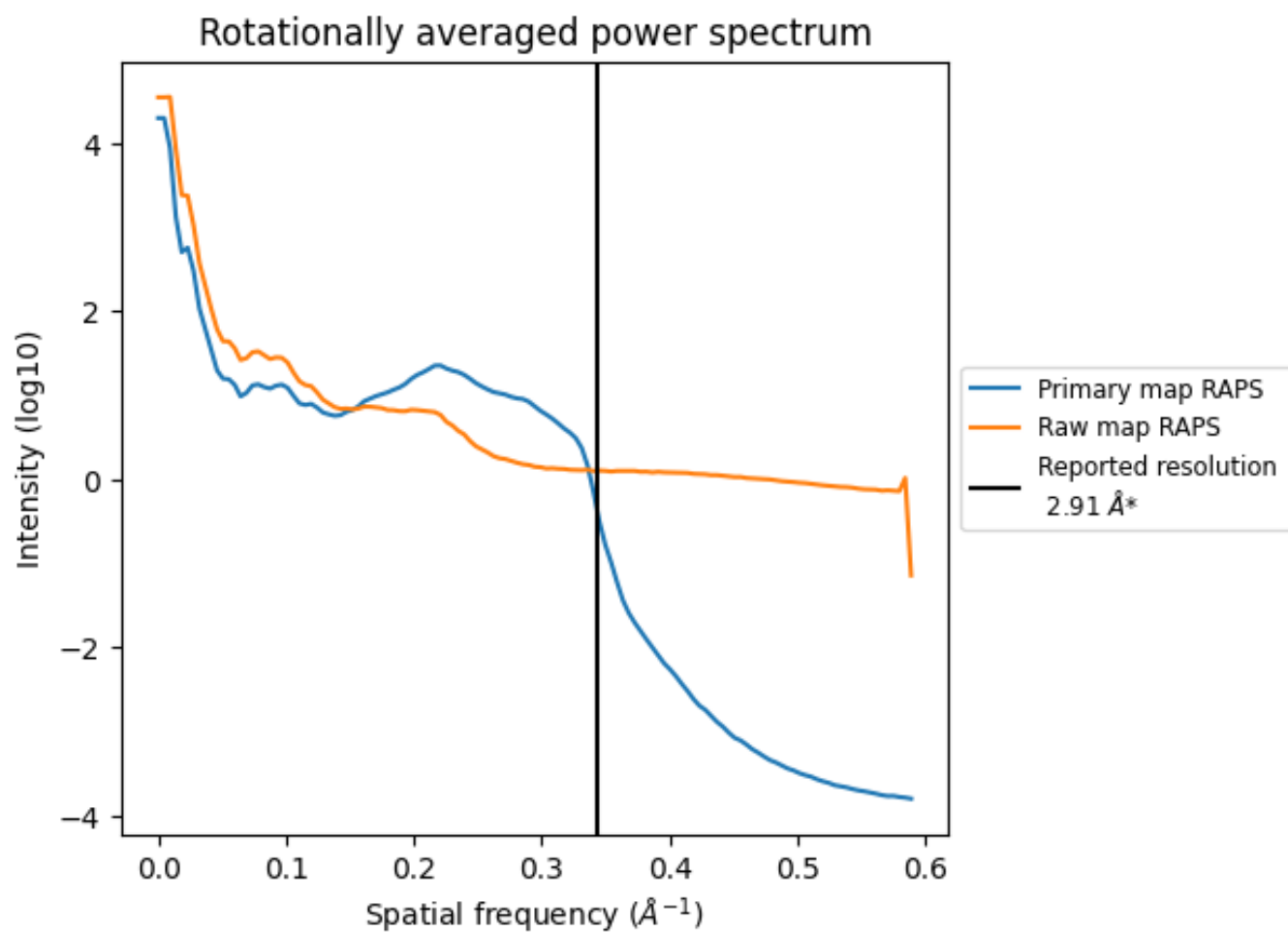
*Reported resolution corresponds to spatial frequency of 0.344 Å^{-1}

8   Fourier-Shell correlation ⓘ

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

8.1   FSC ⓘ
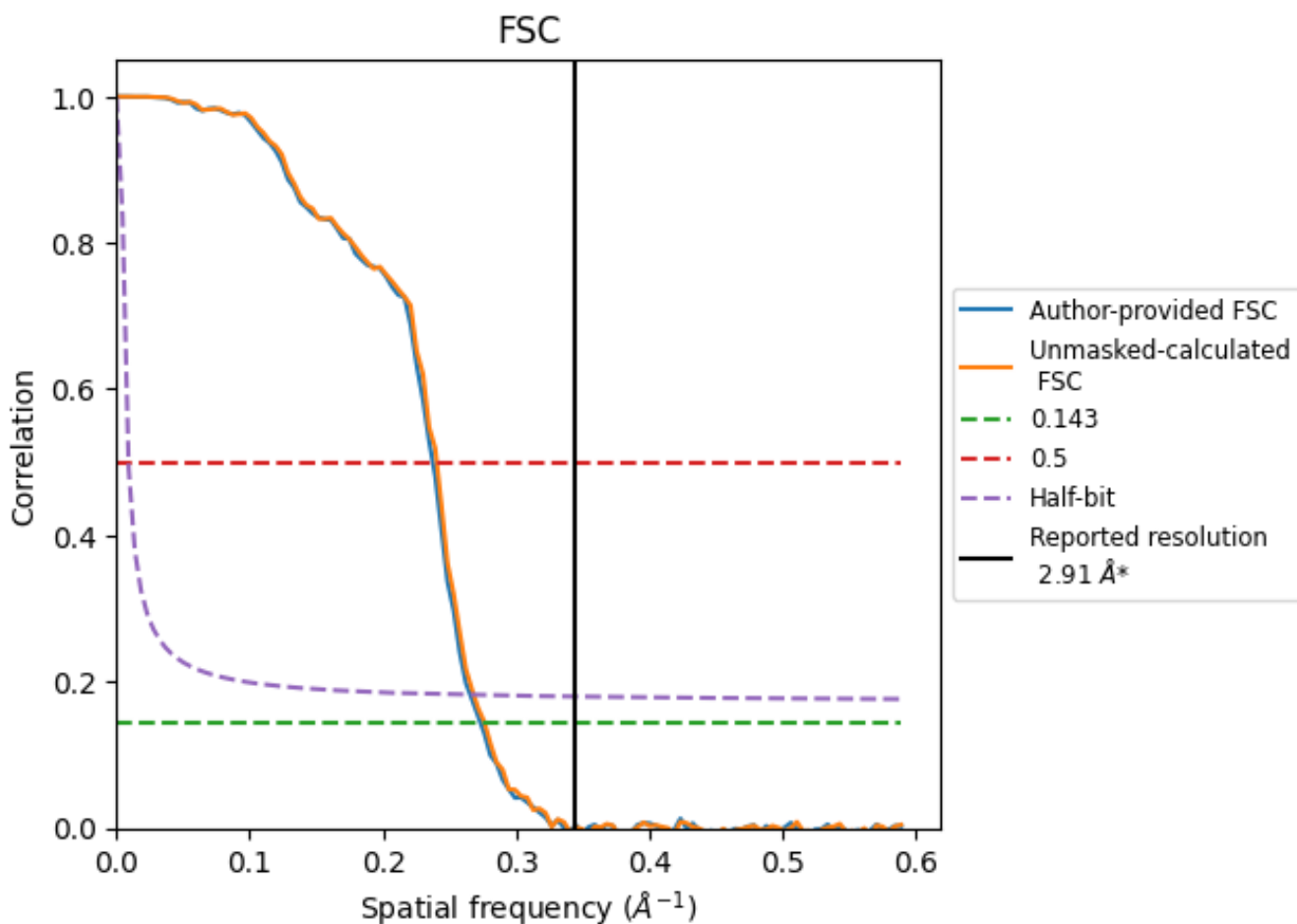
*Reported resolution corresponds to spatial frequency of 0.344 $Å^{-1}$

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	3.66	4.21	3.77
Unmasked-calculated*	3.62	4.16	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 2.91 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 2.91 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10124 and PDB model 6S8J. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay ⓘ

| X | Y | Z |
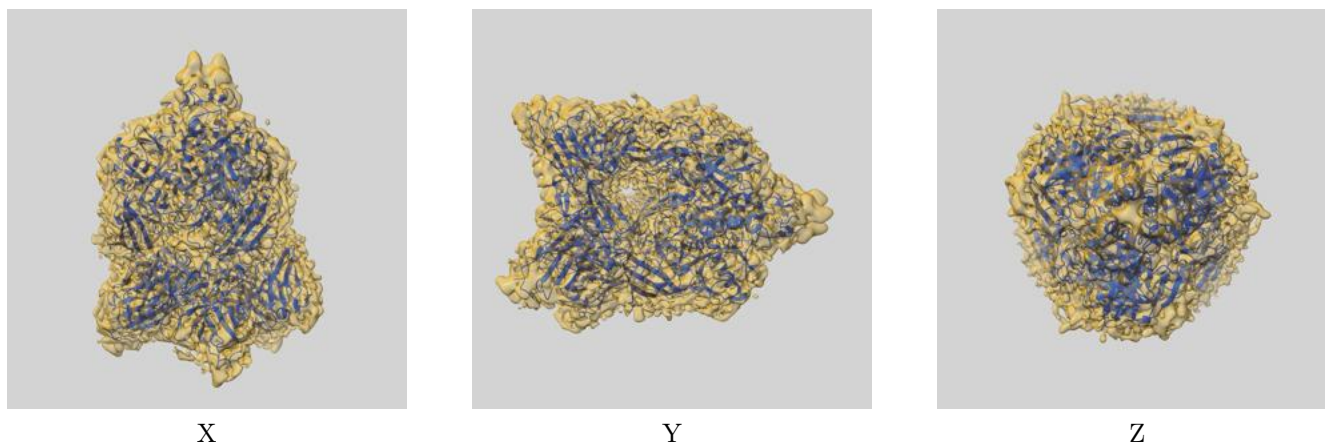
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z

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

9.3　Atom inclusion mapped to coordinate model ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
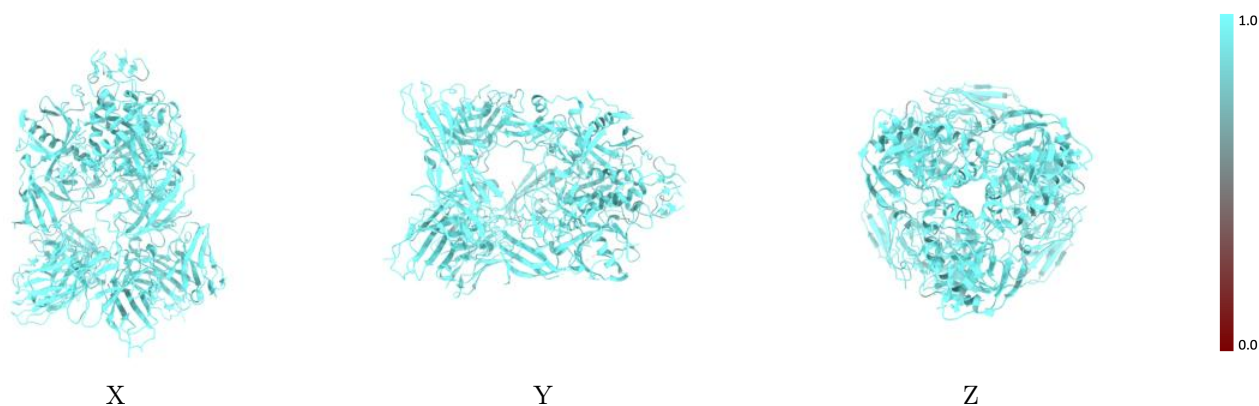
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.21).

9.4 Atom inclusion ⓘ
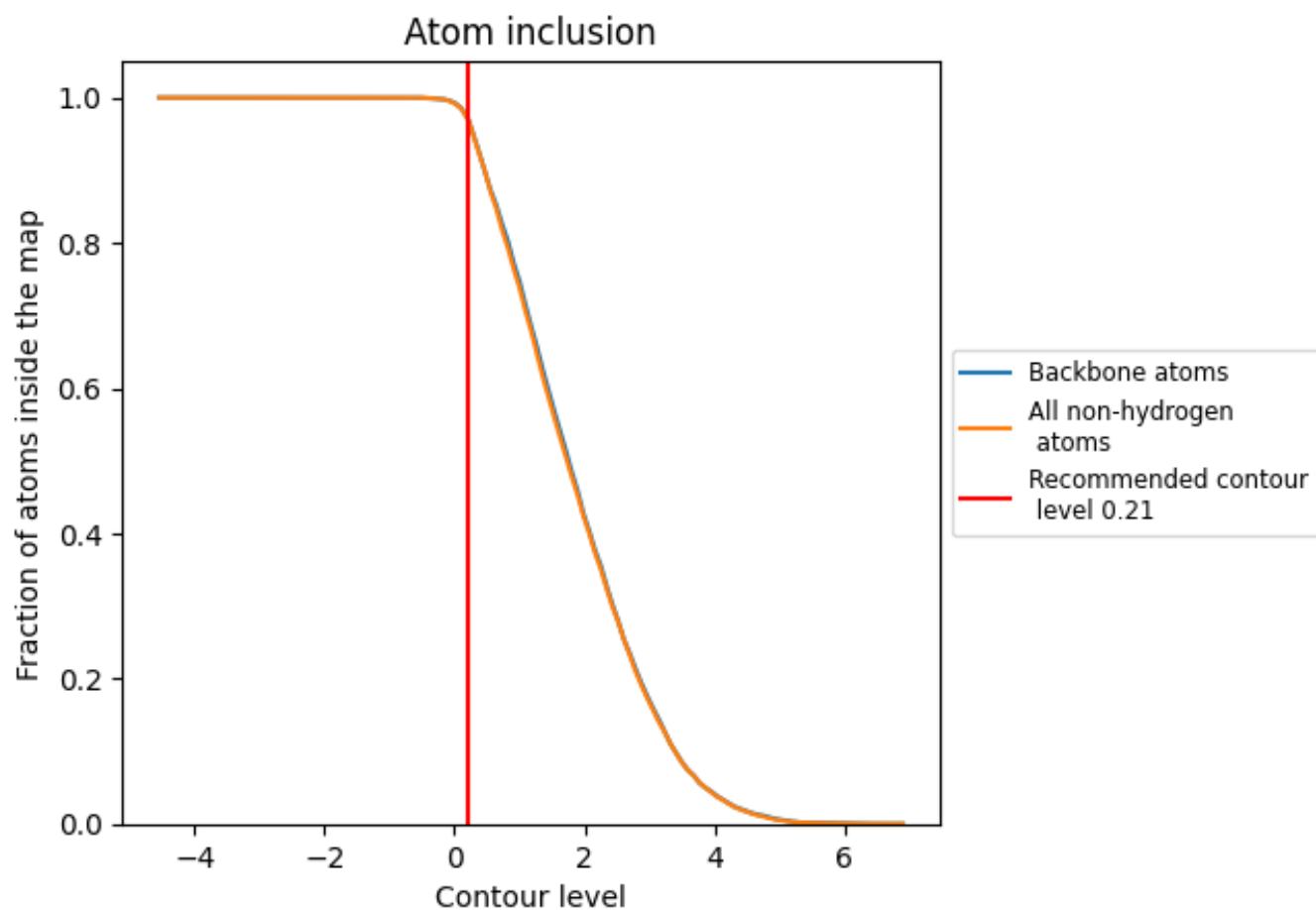
**Atom inclusion**

At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9696	0.5540
A	0.9616	0.5630
B	0.9656	0.5440
C	0.9651	0.5640
D	0.9691	0.5390
E	0.9616	0.5630
F	0.9679	0.5430
G	1.0000	0.5520
H	0.9769	0.5500
I	1.0000	0.5450
J	1.0000	0.5580
L	0.9812	0.5530
O	0.9787	0.5520
P	0.9769	0.5520
U	0.9762	0.5530
Y	0.9769	0.5510

1.0

0.0
<0.0