



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:40 AM UTC

PDB ID : 7UAQ / pdb_00007uaq
EMDB ID : EMD-26430
Title : Structure of the SARS-CoV-2 NTD in complex with C1520, local refinement
Authors : Barnes, C.O.
Deposited on : 2022-03-13
Resolution : 3.10 Å (reported)
Based on initial model : 7RW2

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

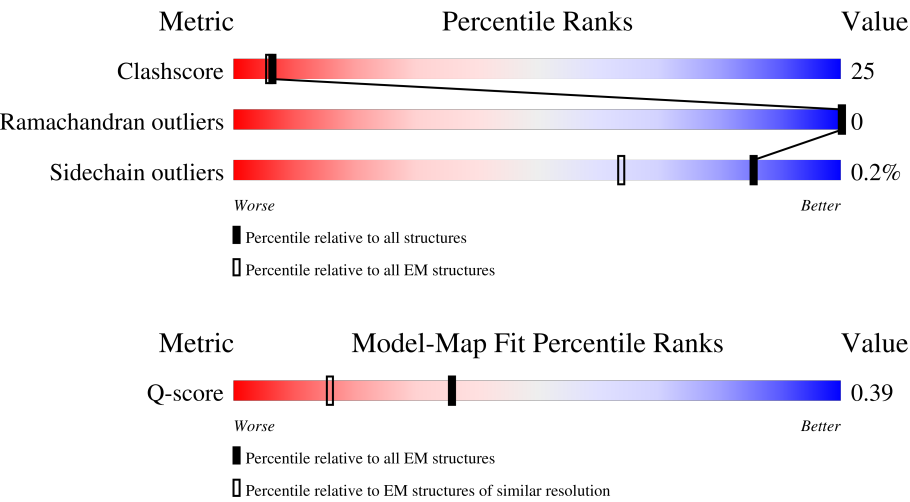
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	1256	14%9%77%
2	H	233	9%23%31%46%
3	L	217	8%28%24%48%
4	B	2	50%50%

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Mol	Chain	Length	Quality of chain
4	C	2	 50%50%
4	D	2	 50%50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4362 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	295	Total	C	N	O	S	0	0
			2392	1550	397	437	8		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	889	PRO	ALA	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	939	PRO	ALA	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1211	SER	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	ARG	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	VAL	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	SER	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called C1520 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	126	Total	C	N	O	S	0	0
			997	631	170	191	5		

- Molecule 3 is a protein called C1520 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	112	Total	C	N	O	S	0	0
			833	512	146	172	3		

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



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

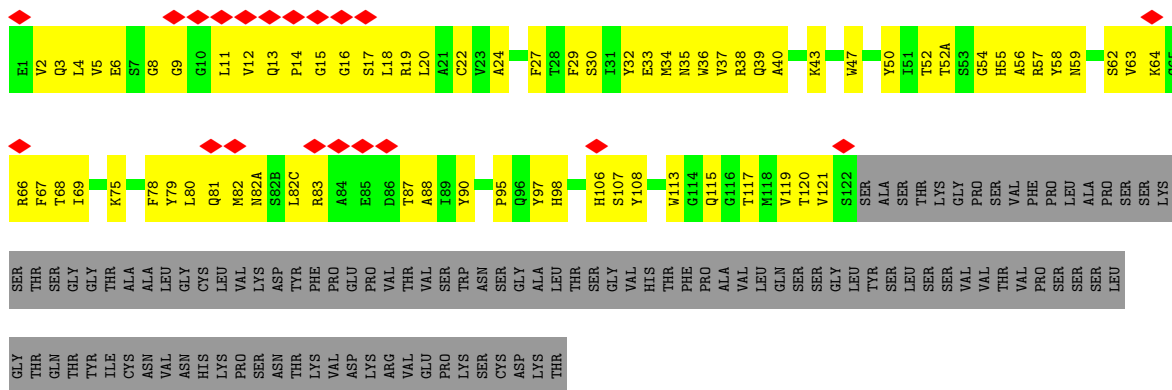
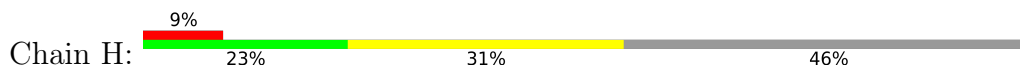
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



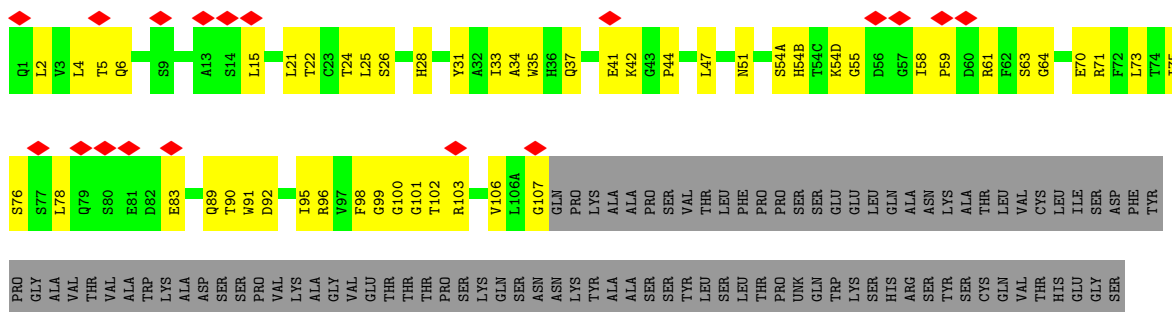
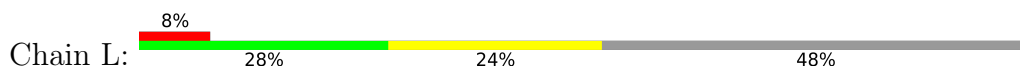
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	L	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 2: C1520 Fab Heavy Chain



- Molecule 3: C1520 Fab Light Chain



THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

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

Chain B:  50% 50%

AG1
AG2

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

Chain C:  50% 50%

AG1
AG2

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

Chain D:  50% 50%

AG1
AG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	614008	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.213	Depositor
Minimum map value	-2.174	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.36	Depositor
Map size (Å)	370.8, 370.8, 370.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	A	0.32	0/2458	0.74	3/3341 (0.1%)
2	H	0.20	0/1024	0.54	0/1389
3	L	0.33	0/850	0.74	1/1153 (0.1%)
All	All	0.30	0/4332	0.70	4/5883 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASN	CB-CA-C	6.27	122.89	110.42
1	A	122	ASN	N-CA-CB	-6.10	101.66	110.45
3	L	101	GLY	CA-C-O	-5.32	117.98	122.29
1	A	165	ASN	N-CA-CB	-5.21	101.68	110.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2392	0	2321	106	0
2	H	997	0	936	70	0
3	L	833	0	785	54	0
4	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	28	0	25	2	0
4	D	28	0	25	1	0
5	A	42	0	39	1	0
5	L	14	0	13	0	0
All	All	4362	0	4169	217	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 25.

All (217) 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:L:51:ASN:HD22	3:L:54(A):SER:HB3	1.27	0.98
1:A:68:ILE:HG12	1:A:262:ALA:HA	1.52	0.92
3:L:59:PRO:HG2	3:L:61:ARG:HG2	1.61	0.83
1:A:96:GLU:OE1	1:A:99:ASN:N	2.16	0.79
3:L:4:LEU:CD1	3:L:99:GLY:HA3	2.13	0.78
1:A:295:PRO:HA	1:A:298:GLU:HG2	1.66	0.78
2:H:47:TRP:CD1	3:L:96:ARG:HB2	2.19	0.77
1:A:290:ASP:HB3	1:A:293:LEU:HD22	1.67	0.76
2:H:18:LEU:HG	2:H:82(C):LEU:HD21	1.70	0.74
1:A:199:GLY:CA	1:A:232:GLY:HA2	2.18	0.74
2:H:107:SER:O	3:L:91:TRP:NE1	2.21	0.74
3:L:4:LEU:HD13	3:L:99:GLY:HA3	1.70	0.74
1:A:126:VAL:HB	1:A:174:PRO:HA	1.70	0.73
1:A:190:ARG:HG2	1:A:207:HIS:HD2	1.54	0.73
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.73	0.70
3:L:6:GLN:OE1	3:L:102:THR:OG1	2.10	0.70
1:A:190:ARG:HG2	1:A:207:HIS:CD2	2.27	0.69
2:H:24:ALA:HB3	2:H:29:PHE:CZ	2.28	0.69
1:A:100:ILE:HG22	1:A:242:LEU:HD22	1.76	0.68
3:L:22:THR:OG1	3:L:70:GLU:OE2	2.10	0.67
1:A:146:HIS:HB2	1:A:149:ASN:OD1	1.95	0.67
2:H:24:ALA:HB3	2:H:29:PHE:HZ	1.60	0.67
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.77	0.67
1:A:231:ILE:HG22	1:A:233:ILE:HG23	1.76	0.67
1:A:108:THR:HA	1:A:236:THR:HG22	1.77	0.66
2:H:87:THR:HB	2:H:121:VAL:H	1.60	0.66
3:L:21:LEU:CD1	3:L:102:THR:HG21	2.26	0.66
2:H:55:HIS:HB3	2:H:57:ARG:HH12	1.62	0.64
2:H:66:ARG:HH11	2:H:83:ARG:HD2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PRO:HG2	1:A:84:LEU:HD21	1.78	0.64
1:A:14:GLN:OE1	1:A:158:ARG:NH1	2.21	0.63
1:A:302:THR:HG21	1:A:315:THR:HA	1.80	0.63
1:A:139:PRO:HB3	1:A:159:VAL:HA	1.80	0.63
2:H:4:LEU:HD13	2:H:24:ALA:HB2	1.80	0.63
1:A:205:SER:HB3	1:A:226:LEU:HD11	1.80	0.63
1:A:176:LEU:HD22	1:A:190:ARG:HD3	1.81	0.63
3:L:24:THR:HA	3:L:70:GLU:HG2	1.79	0.62
3:L:4:LEU:HD21	3:L:100:GLY:H	1.65	0.62
2:H:30:SER:O	2:H:52(A):THR:OG1	2.17	0.61
2:H:37:VAL:HA	2:H:47:TRP:HA	1.82	0.61
3:L:33:ILE:HG22	3:L:90:THR:HG22	1.83	0.61
1:A:199:GLY:HA3	1:A:232:GLY:HA2	1.82	0.61
1:A:109:THR:HA	1:A:237:ARG:HH12	1.65	0.60
2:H:32:TYR:CZ	2:H:98:HIS:HB3	2.36	0.60
3:L:4:LEU:HD11	3:L:99:GLY:HA3	1.83	0.59
3:L:21:LEU:HD11	3:L:102:THR:HG21	1.84	0.59
1:A:122:ASN:OD1	1:A:123:ALA:N	2.33	0.58
1:A:92:PHE:HB3	1:A:192:PHE:HB2	1.86	0.58
2:H:38:ARG:NH2	2:H:90:TYR:OH	2.28	0.57
2:H:3:GLN:HE22	2:H:5:VAL:HB	1.70	0.57
1:A:148:ASN:ND2	4:C:1:NAG:O7	2.37	0.57
1:A:173:GLN:HE21	2:H:55:HIS:CE1	2.23	0.57
1:A:19:THR:HB	1:A:21:ARG:HG2	1.87	0.56
1:A:69:HIS:CG	1:A:70:VAL:H	2.23	0.56
3:L:15:LEU:HD13	3:L:107:GLY:HA3	1.87	0.56
2:H:58:TYR:HE1	2:H:69:ILE:H	1.52	0.56
3:L:102:THR:O	3:L:103:ARG:C	2.49	0.55
1:A:295:PRO:HG3	1:A:319:ARG:HH22	1.70	0.55
2:H:9:GLY:HA2	2:H:119:VAL:HG12	1.88	0.55
3:L:102:THR:O	3:L:102:THR:HG22	2.05	0.55
1:A:177:MET:N	1:A:190:ARG:HH12	2.05	0.55
2:H:97:TYR:HD1	2:H:108:TYR:CE1	2.25	0.55
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.88	0.55
1:A:68:ILE:O	1:A:78:ARG:HD3	2.07	0.55
1:A:277:LEU:HD22	1:A:285:ILE:HD13	1.88	0.55
2:H:67:PHE:CE1	2:H:82:MET:HE1	2.42	0.55
2:H:108:TYR:HB2	3:L:91:TRP:CD1	2.42	0.54
1:A:177:MET:HE1	1:A:179:LEU:HB2	1.90	0.54
3:L:5:THR:H	3:L:24:THR:HB	1.71	0.54
1:A:121:ASN:ND2	1:A:176:LEU:HB2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD23	1:A:259:THR:HA	1.90	0.54
1:A:195:LYS:HZ2	1:A:202:LYS:HD2	1.73	0.54
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.90	0.54
4:D:1:NAG:H83	4:D:1:NAG:H3	1.90	0.53
1:A:119:ILE:CD1	1:A:128:ILE:HD12	2.38	0.53
1:A:300:LYS:HZ1	1:A:306:PHE:C	2.17	0.53
1:A:34:ARG:HH21	1:A:217:PRO:C	2.16	0.53
2:H:38:ARG:HG3	2:H:38:ARG:HH11	1.74	0.52
2:H:62:SER:O	2:H:66:ARG:NH2	2.42	0.52
2:H:64:LYS:HB2	2:H:83:ARG:HH12	1.73	0.51
1:A:198:ASP:O	1:A:200:TYR:HD1	1.94	0.51
3:L:61:ARG:HH22	3:L:78:LEU:HA	1.75	0.51
1:A:200:TYR:HA	1:A:229:LEU:O	2.11	0.50
1:A:69:HIS:CG	1:A:70:VAL:N	2.80	0.50
1:A:112:SER:OG	1:A:113:LYS:N	2.39	0.50
1:A:296:LEU:O	1:A:300:LYS:HG3	2.12	0.50
2:H:15:GLY:N	2:H:82(C):LEU:O	2.35	0.50
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.94	0.50
2:H:113:TRP:CE3	3:L:44:PRO:HG2	2.47	0.50
3:L:55:GLY:O	3:L:58:ILE:HG12	2.12	0.50
1:A:30:ASN:OD1	1:A:59:PHE:HA	2.12	0.50
1:A:106:PHE:HB2	1:A:117:LEU:HD23	1.92	0.50
3:L:61:ARG:NH2	3:L:76:SER:O	2.36	0.50
3:L:54(B):HIS:CE1	3:L:64:GLY:H	2.30	0.49
3:L:31:TYR:O	3:L:71:ARG:NH2	2.45	0.49
3:L:83:GLU:HG3	3:L:106:VAL:HG12	1.95	0.49
1:A:124:THR:C	1:A:174:PRO:HG3	2.38	0.49
1:A:206:LYS:HZ3	1:A:222:ALA:H	1.60	0.49
1:A:109:THR:HG1	1:A:114:THR:HG1	1.50	0.48
2:H:47:TRP:HB3	3:L:98:PHE:HE1	1.78	0.48
1:A:178:ASP:OD1	1:A:179:LEU:N	2.42	0.48
1:A:183:GLN:HE21	3:L:91:TRP:HB2	1.77	0.48
2:H:69:ILE:HD13	2:H:80:LEU:HD12	1.94	0.48
1:A:290:ASP:O	1:A:297:SER:HB2	2.13	0.48
2:H:47:TRP:CZ2	3:L:95:ILE:HA	2.48	0.48
2:H:67:PHE:CD1	2:H:82:MET:HE1	2.48	0.48
2:H:75:LYS:HE2	2:H:75:LYS:HA	1.95	0.48
2:H:13:GLN:OE1	2:H:14:PRO:HD2	2.13	0.48
1:A:295:PRO:O	1:A:299:THR:HG23	2.13	0.48
1:A:299:THR:HA	1:A:302:THR:HG22	1.96	0.47
2:H:33:GLU:O	2:H:95:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HZ3	1:A:212:LEU:HA	1.80	0.47
3:L:34:ALA:HB3	3:L:89:GLN:HE21	1.79	0.47
3:L:25:LEU:HD21	3:L:28:HIS:HB2	1.97	0.47
1:A:295:PRO:HG3	1:A:319:ARG:NH2	2.28	0.47
2:H:6:GLU:HB2	2:H:117:THR:HG23	1.97	0.47
3:L:41:GLU:C	3:L:42:LYS:HD3	2.40	0.47
1:A:18:LEU:O	1:A:18:LEU:HD12	2.14	0.47
3:L:54(B):HIS:NE2	3:L:63:SER:HA	2.30	0.47
1:A:200:TYR:CZ	1:A:230:PRO:HB3	2.49	0.46
1:A:17:ASN:OD1	1:A:19:THR:HG23	2.15	0.46
1:A:121:ASN:ND2	1:A:176:LEU:H	2.14	0.46
1:A:121:ASN:HD22	1:A:176:LEU:H	1.62	0.46
1:A:119:ILE:HD13	1:A:128:ILE:HD12	1.97	0.46
1:A:67:ALA:HB1	1:A:80:ASP:H	1.81	0.46
2:H:35:ASN:HD22	2:H:50:TYR:HB3	1.81	0.46
2:H:56:ALA:O	2:H:57:ARG:HD3	2.16	0.46
2:H:56:ALA:C	2:H:57:ARG:HH11	2.24	0.46
2:H:108:TYR:HB2	3:L:91:TRP:NE1	2.31	0.46
1:A:130:VAL:HG21	1:A:231:ILE:HG23	1.98	0.45
1:A:177:MET:SD	1:A:179:LEU:HB2	2.56	0.45
1:A:120:VAL:HG12	1:A:127:VAL:O	2.17	0.45
2:H:19:ARG:HH22	2:H:81:GLN:HA	1.82	0.45
1:A:69:HIS:O	1:A:78:ARG:HG2	2.17	0.45
1:A:83:VAL:CG1	1:A:237:ARG:HB3	2.47	0.45
2:H:57:ARG:HB3	2:H:59:ASN:OD1	2.17	0.45
1:A:68:ILE:O	1:A:69:HIS:HB3	2.17	0.44
1:A:150:LYS:NZ	2:H:2:VAL:HG13	2.32	0.44
1:A:186:PHE:HA	1:A:210:ILE:O	2.17	0.44
1:A:277:LEU:HD22	1:A:285:ILE:HG21	1.99	0.44
3:L:54(B):HIS:CD2	3:L:54(D):LYS:HD3	2.53	0.44
3:L:51:ASN:ND2	3:L:54(A):SER:HB3	2.11	0.44
2:H:87:THR:HA	2:H:119:VAL:O	2.17	0.44
2:H:36:TRP:CD1	2:H:80:LEU:HD13	2.52	0.44
1:A:281:GLU:OE1	5:A:1303:NAG:H2	2.17	0.44
1:A:50:SER:HB2	1:A:304:LYS:HZ2	1.82	0.44
2:H:52:THR:HG23	2:H:54:GLY:H	1.82	0.44
1:A:118:LEU:HD23	1:A:118:LEU:O	2.17	0.44
1:A:188:ASN:OD1	1:A:190:ARG:NE	2.50	0.43
2:H:34:MET:O	2:H:50:TYR:HB2	2.17	0.43
1:A:33:THR:HA	1:A:58:PHE:CD1	2.53	0.43
1:A:58:PHE:HE2	1:A:288:ALA:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HA	1:A:79:PHE:O	2.18	0.43
1:A:148:ASN:OD1	1:A:149:ASN:N	2.52	0.43
2:H:22:CYS:O	2:H:78:PHE:HB3	2.19	0.43
1:A:14:GLN:O	1:A:158:ARG:HG2	2.19	0.43
2:H:119:VAL:O	2:H:119:VAL:HG23	2.18	0.43
1:A:102:ARG:HE	1:A:243:ALA:HB2	1.84	0.43
1:A:68:ILE:HG13	1:A:69:HIS:H	1.84	0.42
1:A:206:LYS:HD3	1:A:222:ALA:O	2.19	0.42
2:H:19:ARG:NH2	2:H:79:TYR:HB3	2.34	0.42
2:H:97:TYR:HB2	2:H:107:SER:HB2	2.01	0.42
3:L:54(B):HIS:HB3	3:L:54(D):LYS:HD3	2.01	0.42
1:A:153:MET:SD	4:C:1:NAG:H61	2.60	0.42
3:L:25:LEU:HD23	3:L:26:SER:O	2.19	0.42
1:A:295:PRO:O	1:A:298:GLU:HG2	2.20	0.42
1:A:63:THR:HG21	1:A:65:PHE:CZ	2.54	0.42
1:A:119:ILE:HD12	1:A:128:ILE:HD12	2.00	0.42
1:A:183:GLN:NE2	3:L:91:TRP:CE3	2.87	0.42
1:A:290:ASP:HB3	1:A:293:LEU:CD2	2.42	0.42
2:H:35:ASN:HA	2:H:50:TYR:HB2	2.01	0.42
2:H:97:TYR:HB2	2:H:107:SER:CB	2.50	0.42
1:A:83:VAL:HG11	1:A:237:ARG:HE	1.84	0.42
2:H:63:VAL:HG23	2:H:66:ARG:HG2	2.02	0.42
1:A:206:LYS:NZ	1:A:221:SER:HA	2.34	0.42
2:H:64:LYS:HB2	2:H:83:ARG:NH1	2.35	0.42
3:L:21:LEU:HD23	3:L:75:ILE:CD1	2.50	0.42
1:A:149:ASN:OD1	1:A:150:LYS:N	2.53	0.42
3:L:28:HIS:HB3	3:L:31:TYR:CG	2.54	0.42
2:H:47:TRP:HH2	2:H:59:ASN:HB2	1.85	0.42
3:L:92:ASP:HB2	3:L:95:ILE:O	2.20	0.41
1:A:177:MET:CE	1:A:179:LEU:HB2	2.50	0.41
1:A:50:SER:HB2	1:A:304:LYS:NZ	2.35	0.41
2:H:97:TYR:HB2	2:H:107:SER:OG	2.20	0.41
3:L:21:LEU:HD12	3:L:102:THR:HG21	2.00	0.41
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.92	0.41
1:A:152:TRP:HZ3	1:A:245:HIS:HD2	1.68	0.41
1:A:299:THR:HG22	1:A:315:THR:HG22	2.02	0.41
2:H:8:GLY:HA3	2:H:19:ARG:O	2.21	0.41
2:H:11:LEU:HA	2:H:120:THR:O	2.20	0.41
3:L:2:LEU:HA	3:L:26:SER:HB3	2.02	0.41
3:L:35:TRP:CG	3:L:73:LEU:HD12	2.55	0.41
3:L:61:ARG:NH2	3:L:78:LEU:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:O	1:A:241:LEU:N	2.48	0.41
2:H:18:LEU:CD1	2:H:20:LEU:HG	2.51	0.41
1:A:127:VAL:O	1:A:128:ILE:HD13	2.21	0.41
1:A:130:VAL:HG11	1:A:233:ILE:HG21	2.03	0.41
2:H:3:GLN:HE21	2:H:115:GLN:HE22	1.69	0.41
2:H:69:ILE:HD11	2:H:78:PHE:CZ	2.56	0.41
3:L:21:LEU:HD23	3:L:75:ILE:HD13	2.02	0.41
1:A:100:ILE:HB	1:A:263:ALA:HB2	2.03	0.41
1:A:236:THR:HG23	1:A:237:ARG:HG3	2.02	0.41
3:L:2:LEU:HD22	3:L:25:LEU:HG	2.03	0.41
1:A:67:ALA:HB1	1:A:79:PHE:HA	2.03	0.40
2:H:55:HIS:CB	2:H:57:ARG:HH12	2.31	0.40
2:H:58:TYR:CE1	2:H:68:THR:HA	2.56	0.40
2:H:108:TYR:HB2	3:L:91:TRP:HE1	1.85	0.40
1:A:173:GLN:OE1	1:A:173:GLN:HA	2.21	0.40
2:H:12:VAL:HG21	2:H:16:GLY:HA3	2.02	0.40
2:H:47:TRP:HE1	3:L:96:ARG:C	2.29	0.40
3:L:92:ASP:HB2	3:L:95:ILE:HB	2.03	0.40
1:A:194:PHE:HB3	1:A:201:PHE:CZ	2.56	0.40
2:H:39:GLN:O	2:H:88:ALA:HB1	2.21	0.40
2:H:106:HIS:CG	3:L:51:ASN:OD1	2.75	0.40
2:H:2:VAL:HG12	2:H:27:PHE:CD1	2.57	0.40
2:H:17:SER:HA	2:H:82(A):ASN:HA	2.04	0.40
3:L:15:LEU:CD1	3:L:107:GLY:HA3	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	289/1256 (23%)	251 (87%)	38 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	124/233 (53%)	113 (91%)	11 (9%)	0	100	100
3	L	110/217 (51%)	99 (90%)	11 (10%)	0	100	100
All	All	523/1706 (31%)	463 (88%)	60 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/1096 (24%)	266 (100%)	1 (0%)	84	86
2	H	105/198 (53%)	105 (100%)	0	100	100
3	L	91/182 (50%)	91 (100%)	0	100	100
All	All	463/1476 (31%)	462 (100%)	1 (0%)	85	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	207	HIS
1	A	271	GLN
2	H	3	GLN
2	H	55	HIS
2	H	96	GLN
2	H	106	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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$
4	NAG	B	1	1,4	14,14,15	0.78	1 (7%)	17,19,21	0.82	1 (5%)
4	NAG	B	2	4	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	C	1	1,4	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
4	NAG	C	2	4	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	D	1	1,4	14,14,15	0.89	2 (14%)	17,19,21	1.53	3 (17%)
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	4/6/23/26	0/1/1/1
4	NAG	C	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	O5-C1	-2.56	1.39	1.43
4	D	1	NAG	C1-C2	2.46	1.55	1.52
4	D	1	NAG	O5-C1	2.08	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	4.44	128.85	122.90
4	D	1	NAG	C1-O5-C5	3.17	116.44	112.19
4	B	1	NAG	C3-C4-C5	2.32	114.43	110.23
4	D	1	NAG	C1-C2-N2	2.28	114.02	110.43
4	C	1	NAG	O4-C4-C5	2.23	114.82	109.32

There are no chirality outliers.

All (18) torsion outliers are listed below:

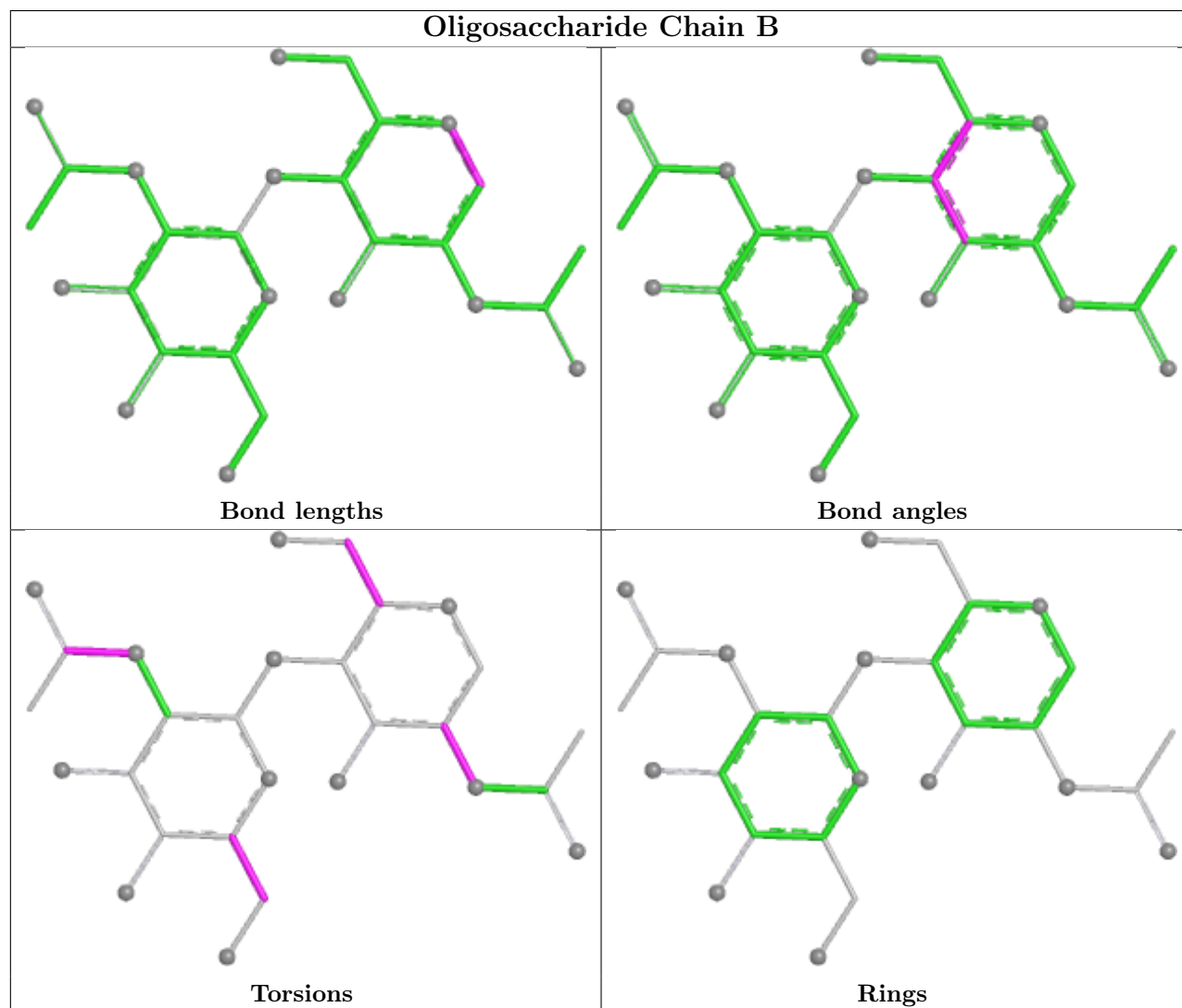
Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	B	1	NAG	C1-C2-N2-C7
4	B	1	NAG	C3-C2-N2-C7
4	D	1	NAG	C1-C2-N2-C7
4	C	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C3-C2-N2-C7

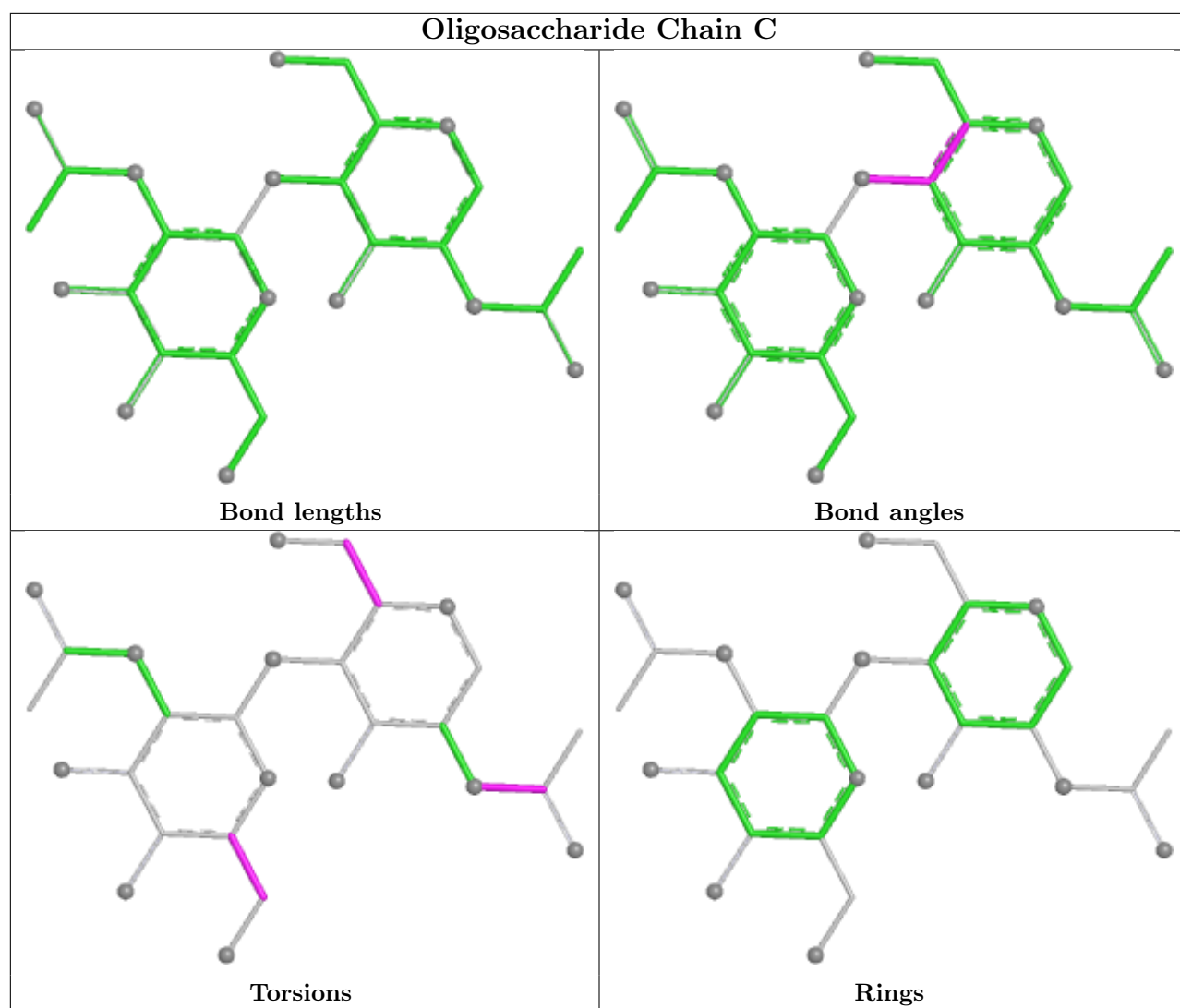
There are no ring outliers.

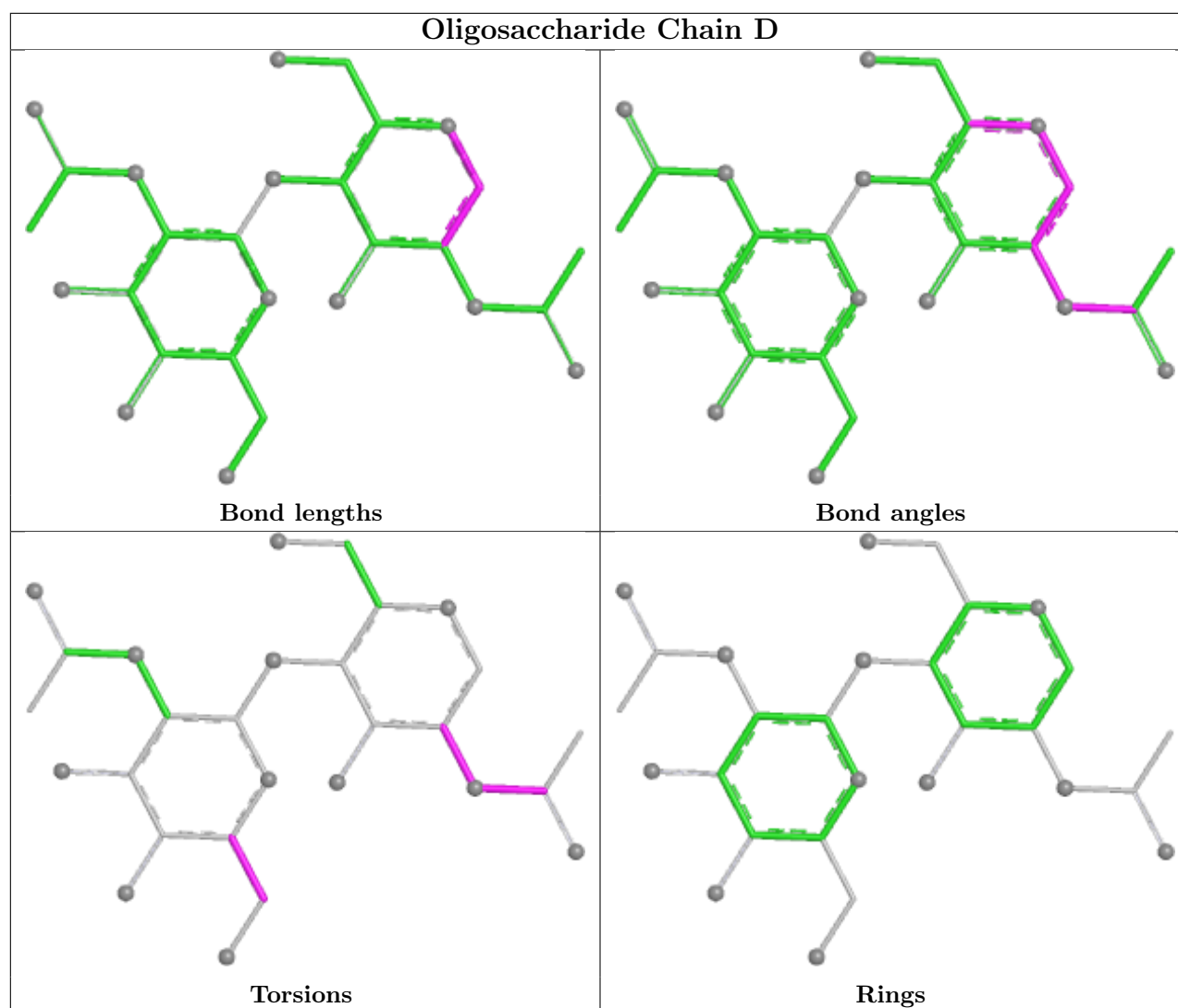
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	C	1	NAG	2	0

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







5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	L	301	3	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
5	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.47	0
5	NAG	A	1302	1	14,14,15	0.31	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1303	1	14,14,15	0.70	1 (7%)	17,19,21	0.67	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	L	301	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1303	NAG	O5-C1	-2.25	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	301	NAG	C1-O5-C5	2.27	115.23	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1303	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1303	NAG	C1-C2-N2-C7
5	L	301	NAG	C4-C5-C6-O6
5	A	1303	NAG	C3-C2-N2-C7
5	L	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1303	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

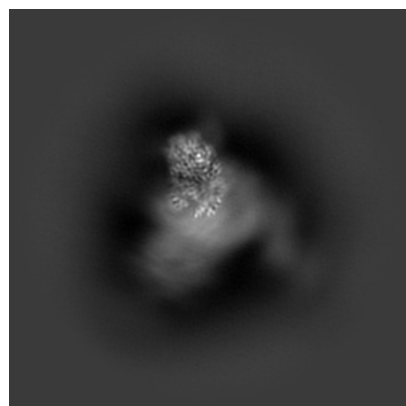
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26430. These allow visual inspection of the internal detail of the map and identification of artifacts.

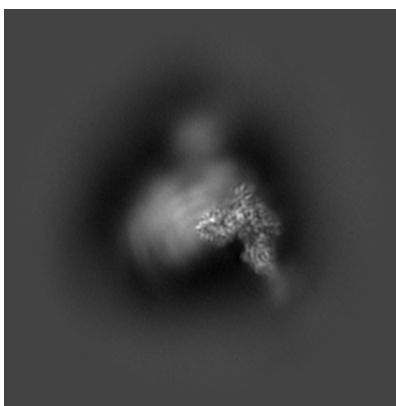
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

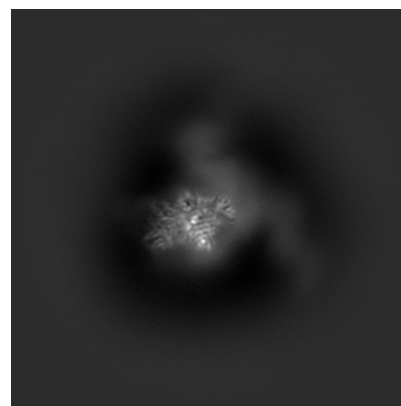
6.1.1 Primary map



X

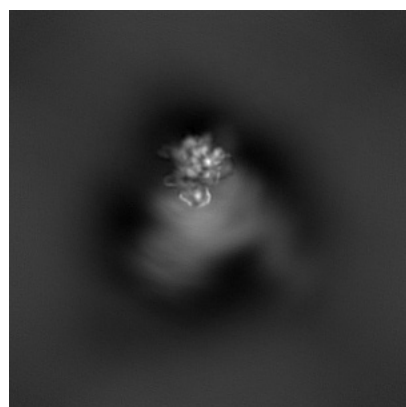


Y

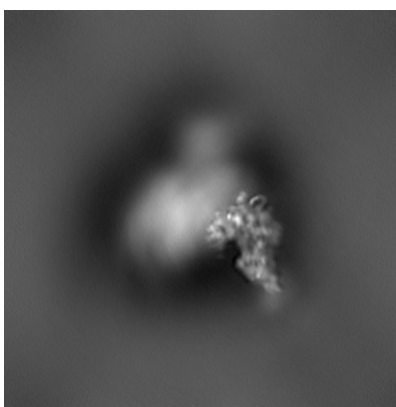


Z

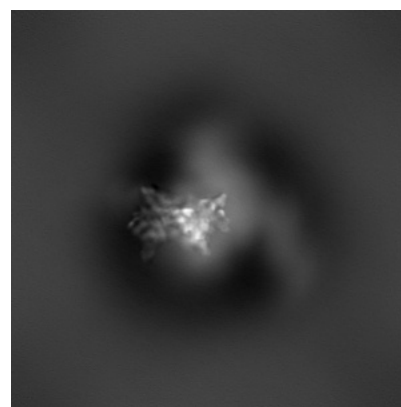
6.1.2 Raw map



X



Y

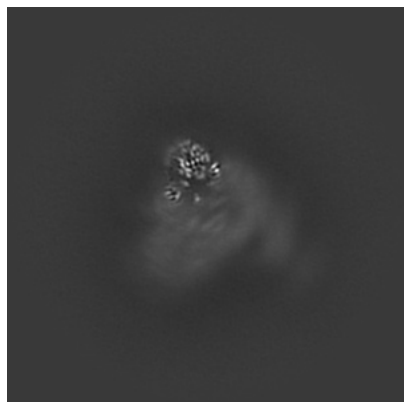


Z

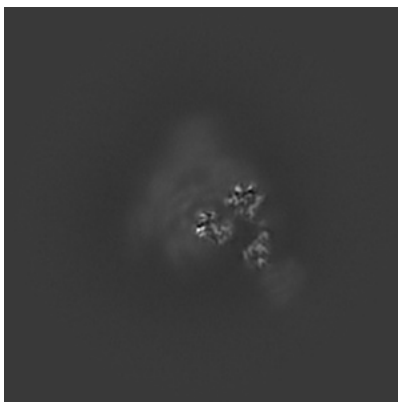
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

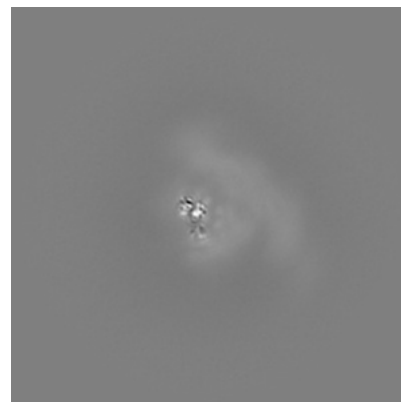
6.2.1 Primary map



X Index: 180

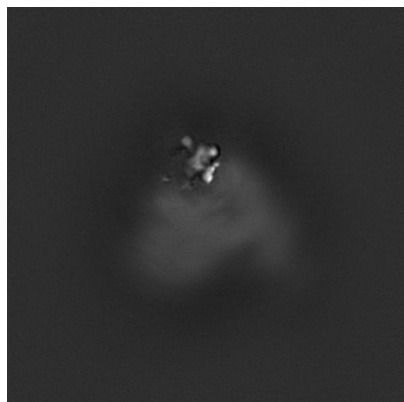


Y Index: 180

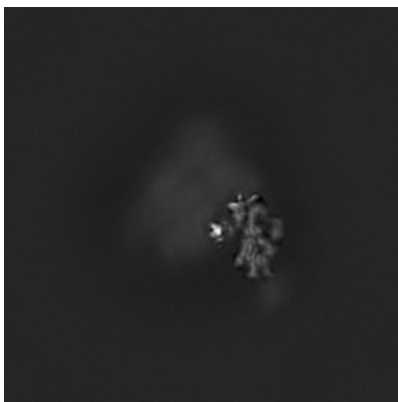


Z Index: 180

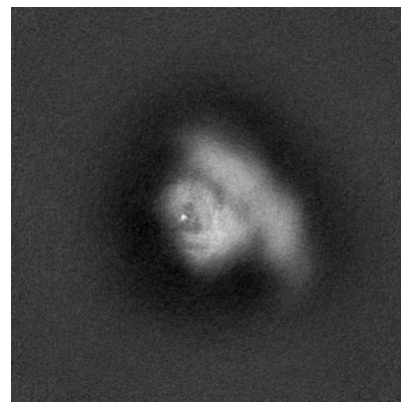
6.2.2 Raw map



X Index: 180



Y Index: 180

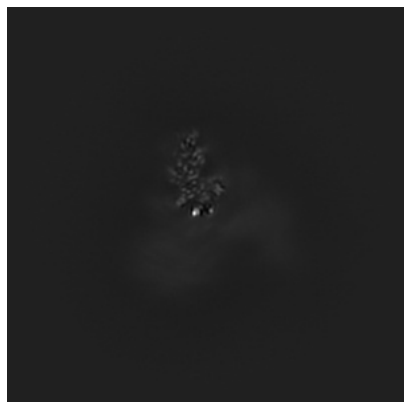


Z Index: 180

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

6.3 Largest variance slices [i](#)

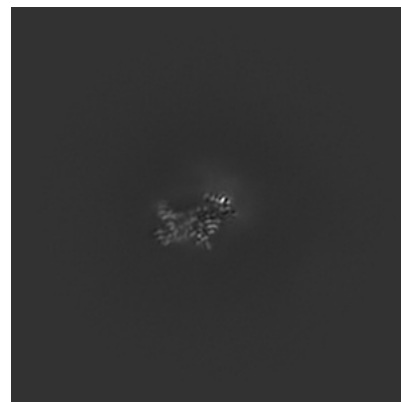
6.3.1 Primary map



X Index: 163

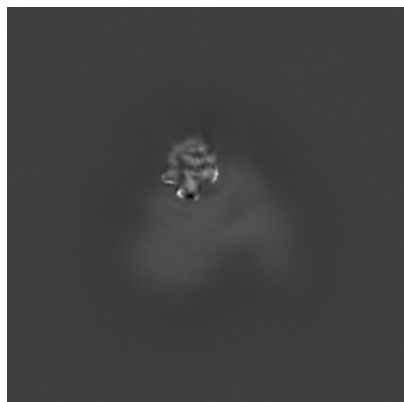


Y Index: 168

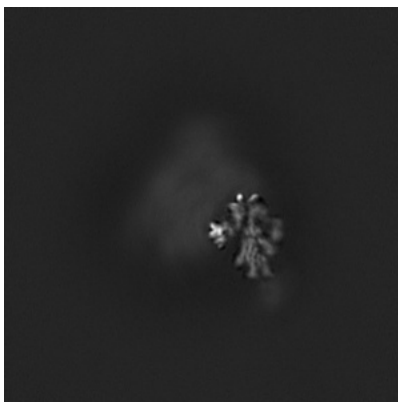


Z Index: 218

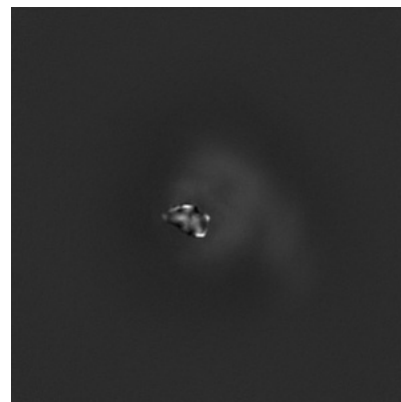
6.3.2 Raw map



X Index: 172



Y Index: 179

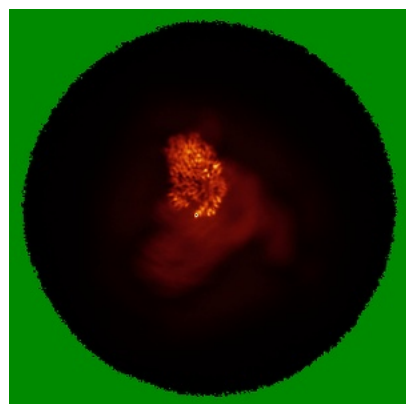


Z Index: 192

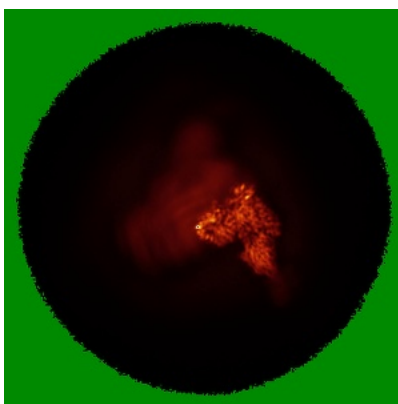
The images above show the largest variance slices of the map in three orthogonal directions.

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

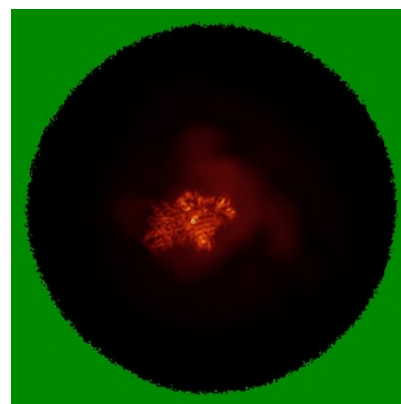
6.4.1 Primary map



X

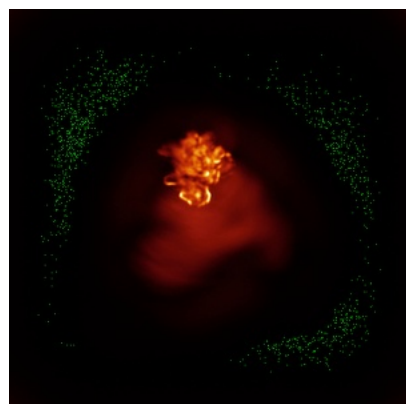


Y

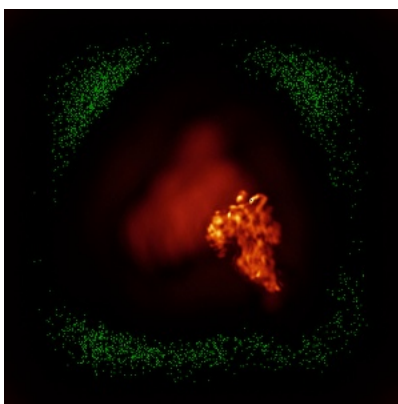


Z

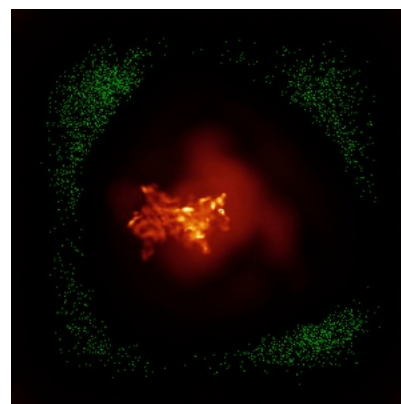
6.4.2 Raw map



X



Y

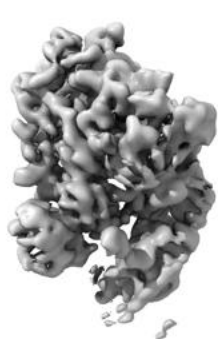


Z

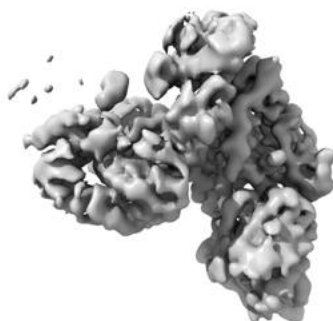
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

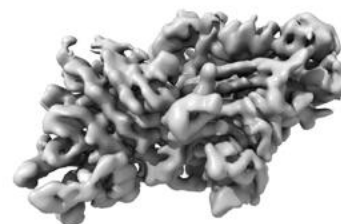
6.5.1 Primary map



X



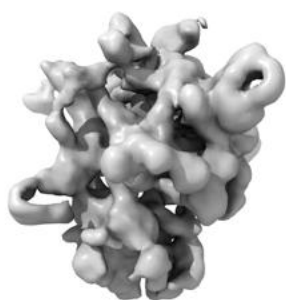
Y



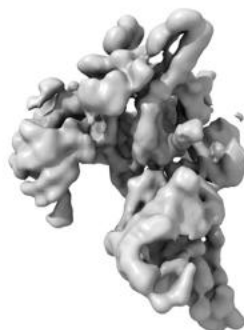
Z

The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

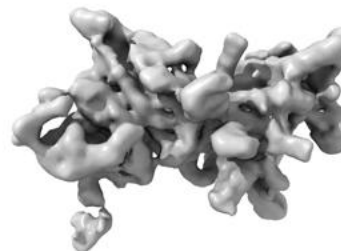
6.5.2 Raw map



X



Y



Z

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

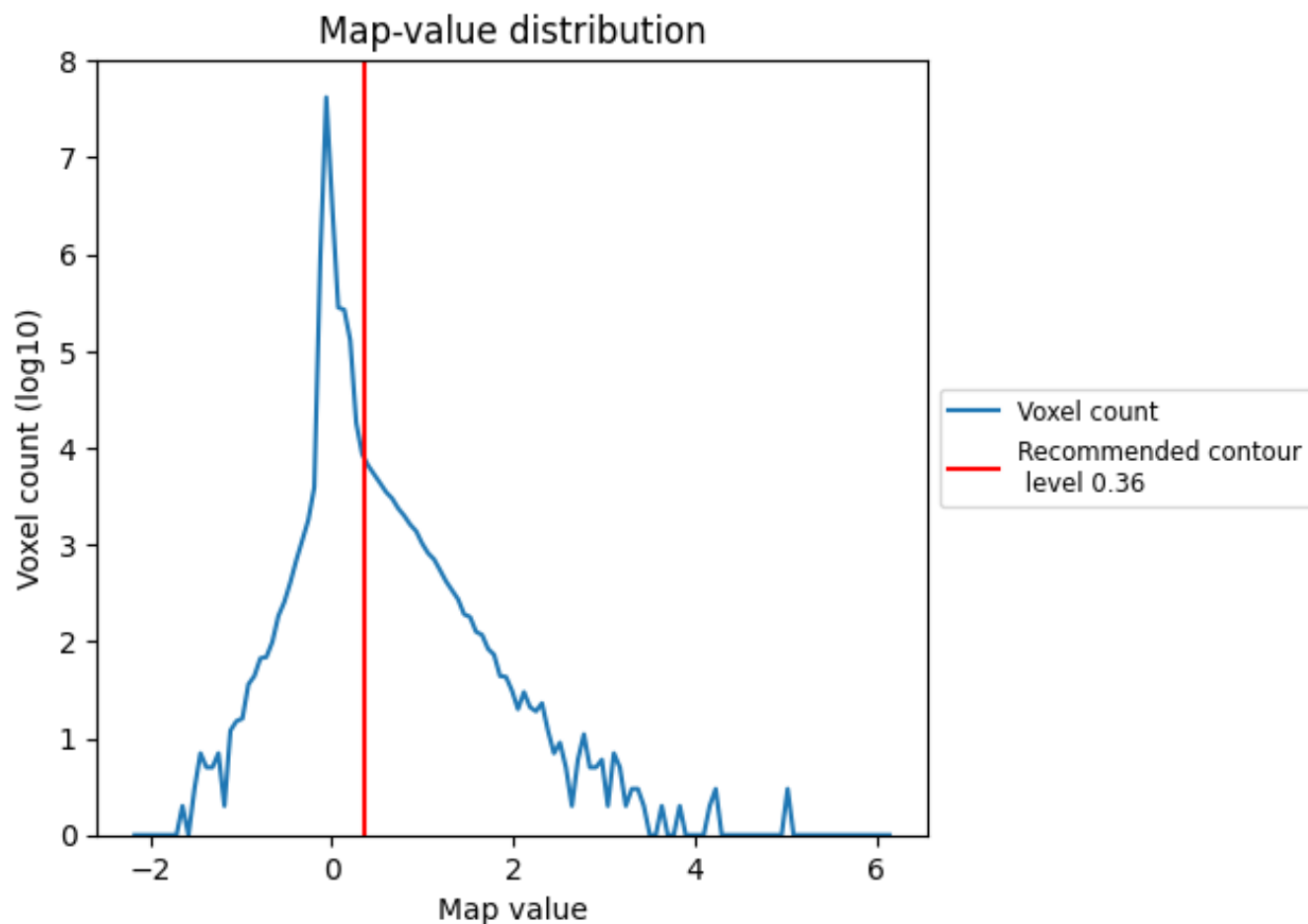
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

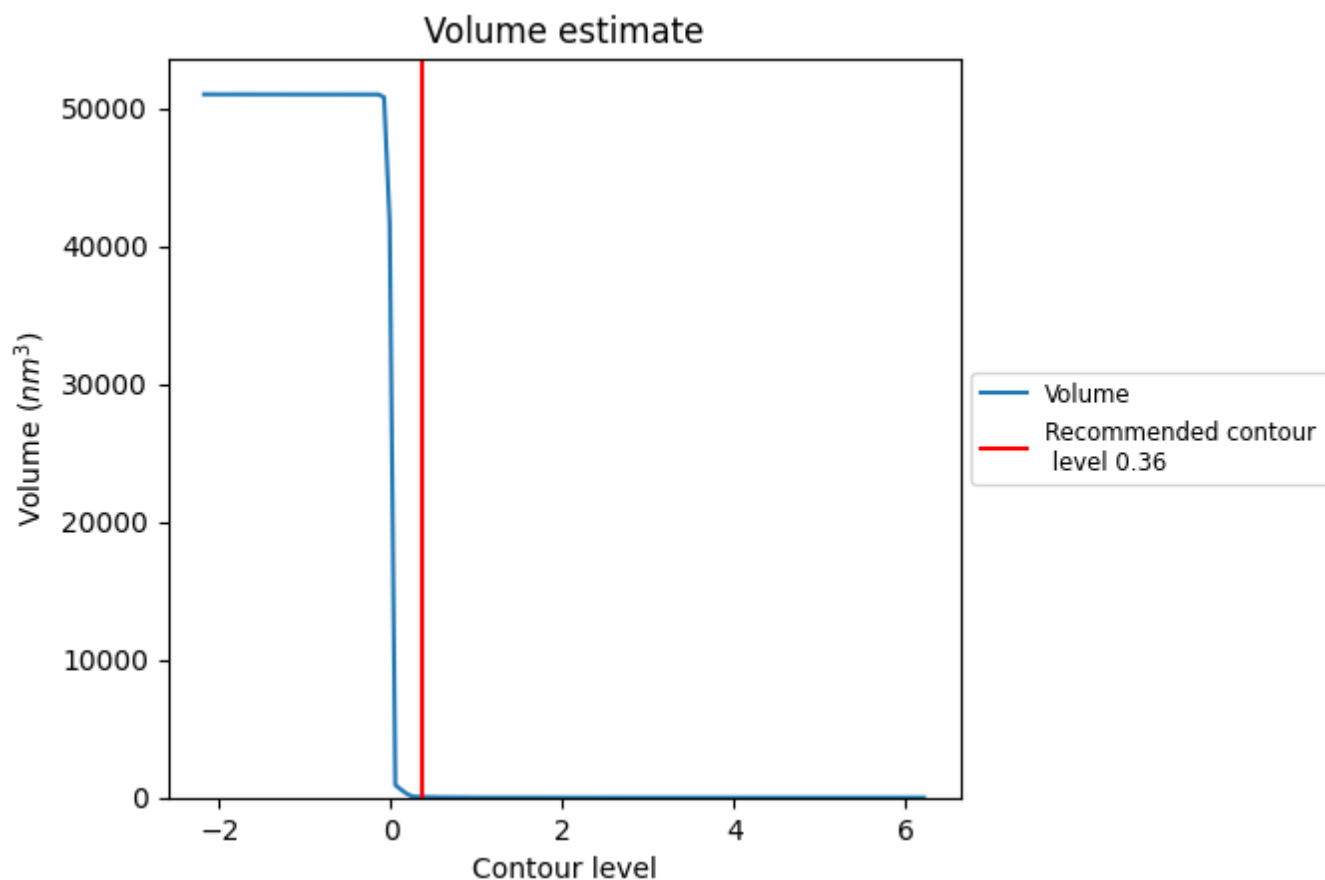
This section contains the results of statistical analysis of the map.

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.

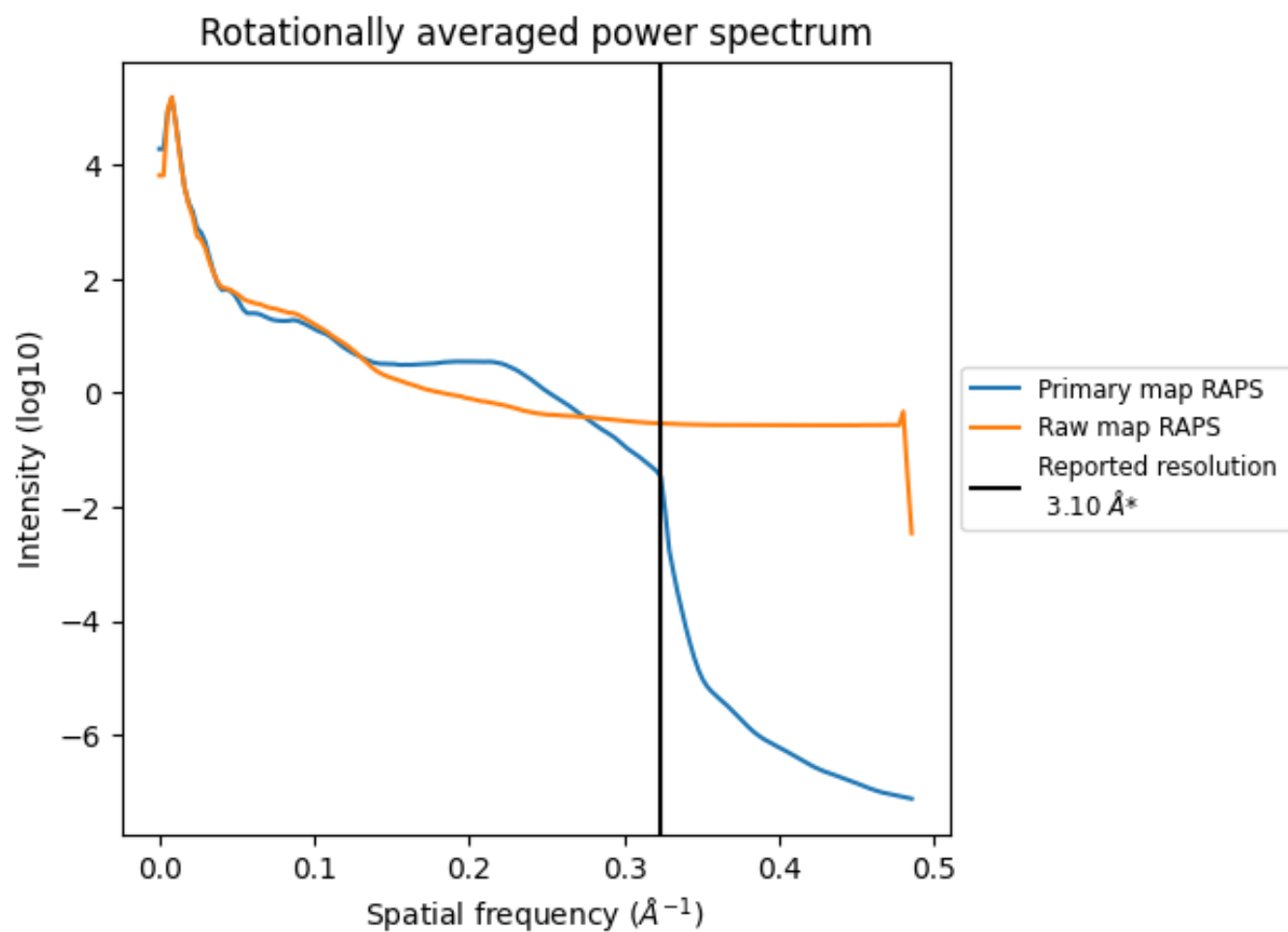
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm^3 ; this corresponds to an approximate mass of 40 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 ⓘ

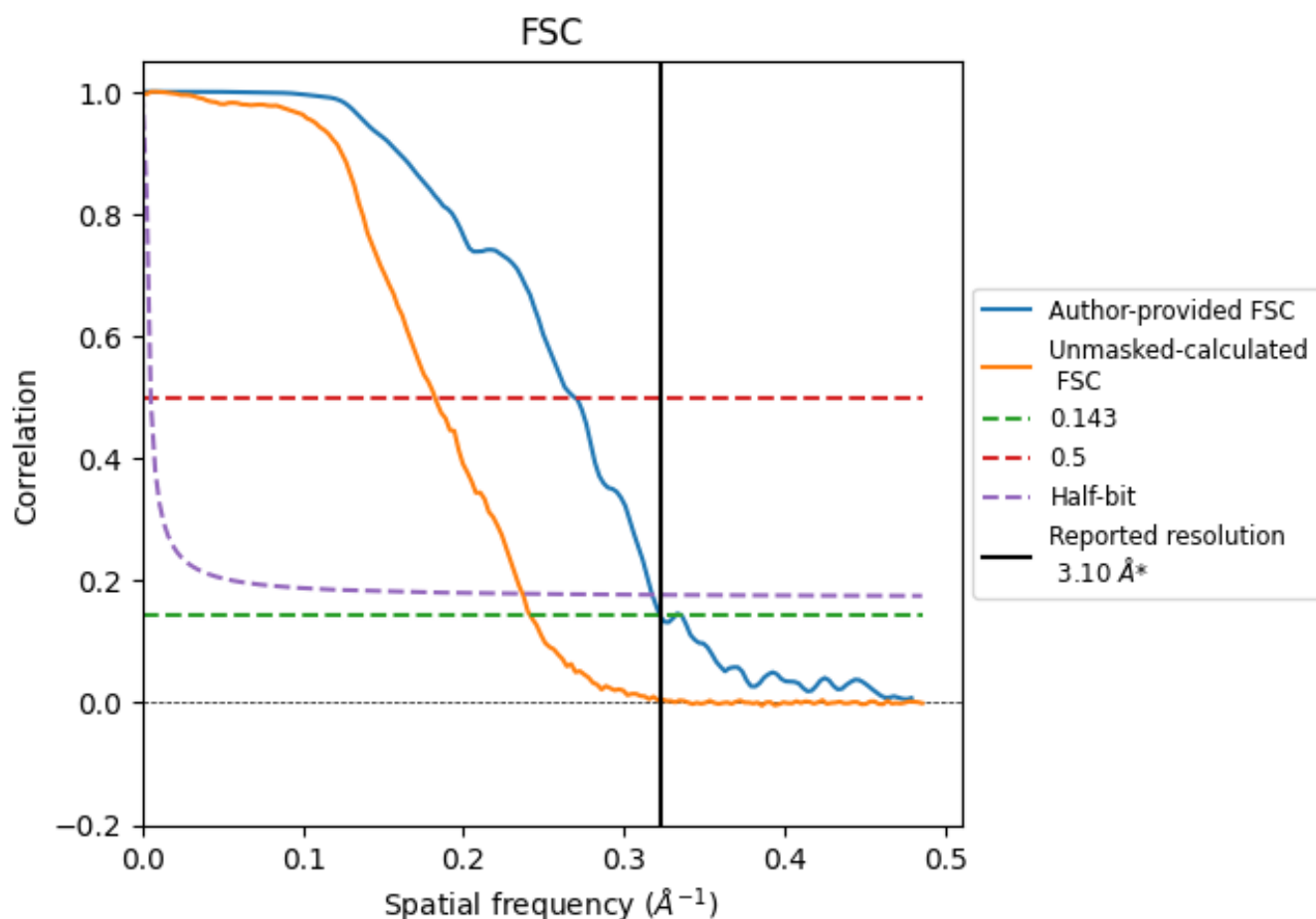


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

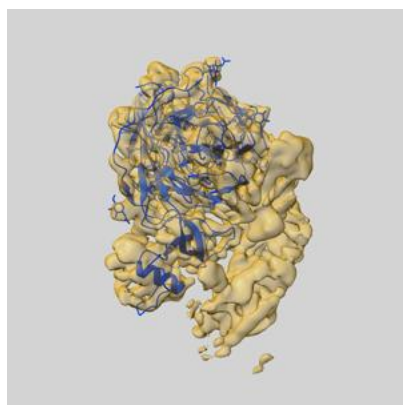
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.72	3.15
Unmasked-calculated*	4.14	5.49	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.1 by more than 10 %

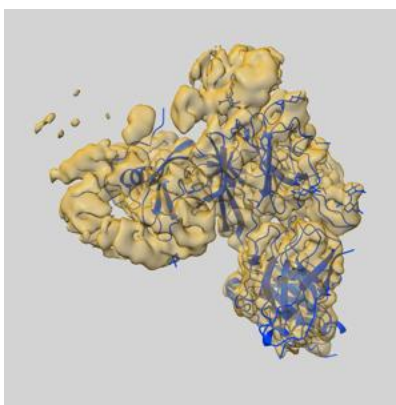
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26430 and PDB model 7UAQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

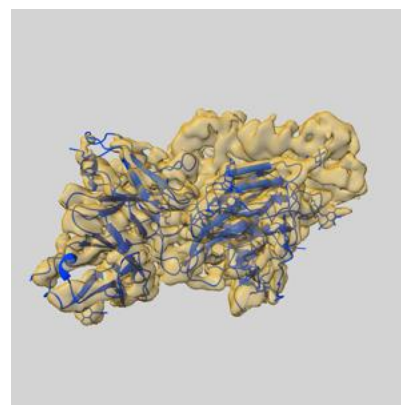
9.1 Map-model overlay [i](#)



X



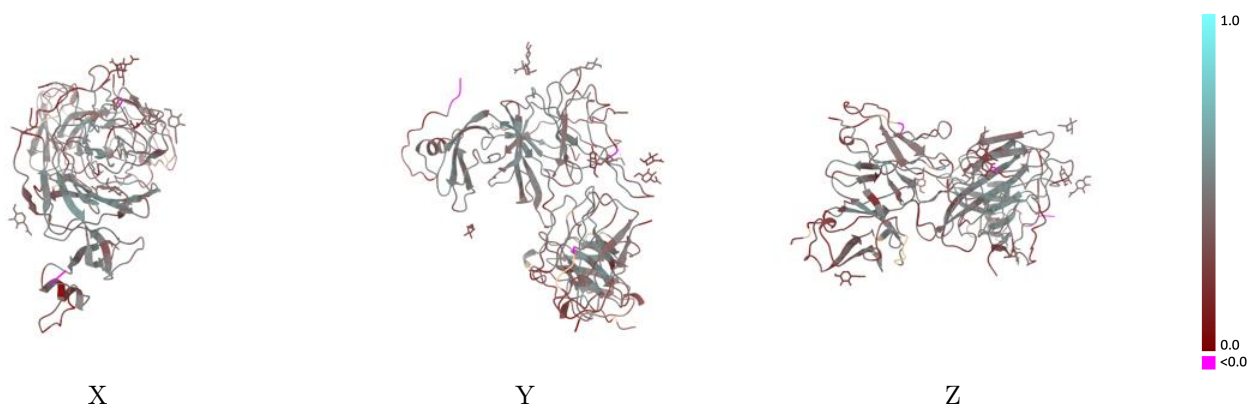
Y



Z

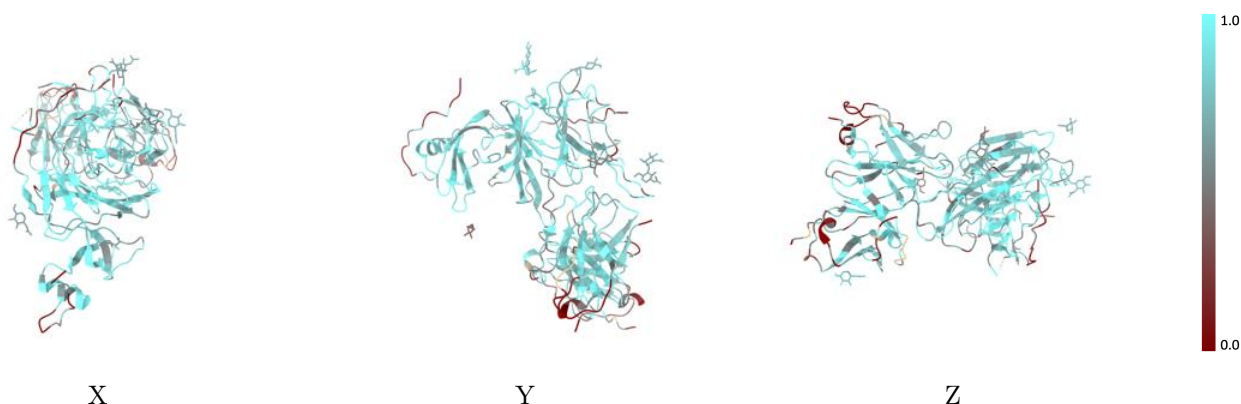
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



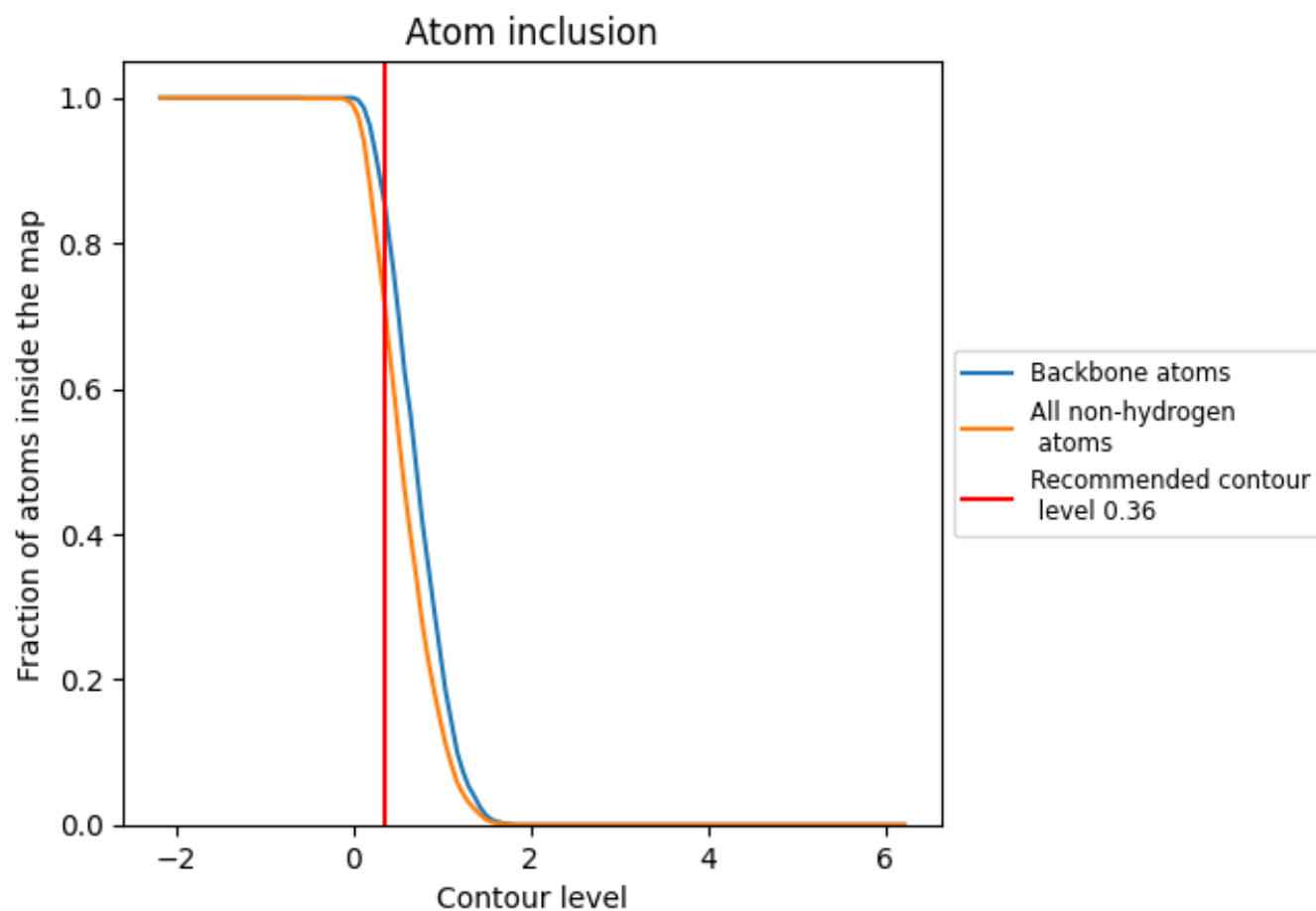
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.3900
A	0.7380	0.4080
B	0.4640	0.2840
C	0.6070	0.2580
D	0.7500	0.3750
H	0.6770	0.3800
L	0.6700	0.3580

1.0

0.0

<0.0