



Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 12:09 PM EST

PDB ID : 7UPX
EMDB ID : EMD-26677
Title : Three RBD-down state of SARS-CoV-2 D614G spike in complex with the SP1-77 neutralizing antibody Fab fragment (local refinement of the RBD and Fab variable domains)
Authors : Zhang, J.; Luo, S.; Kreutzberger, A.; Kirchhausen, T.; Chen, B.; Haynes, B.; Alt, F.
Deposited on : 2022-04-18
Resolution : 3.20 Å (reported)
Based on initial model : 7KRR

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.dev43
Mogul : 1.8.5 (274361), 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) : 2.31.2

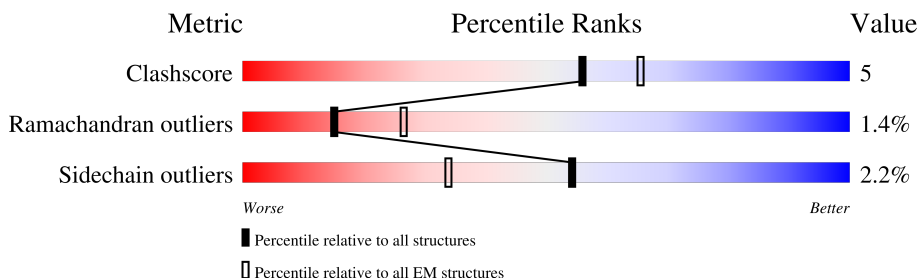
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 $\leq 5\%$. 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	1310	
2	H	451	
3	L	213	
4	B	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4930 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	198	Total	C	N	O	S	0	0
			1569	1007	262	292	8		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	ALA	-	expression tag	UNP P0DTC2
A	1282	TRP	-	expression tag	UNP P0DTC2
A	1283	SER	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	PRO	-	expression tag	UNP P0DTC2
A	1286	GLN	-	expression tag	UNP P0DTC2
A	1287	PHE	-	expression tag	UNP P0DTC2
A	1288	GLU	-	expression tag	UNP P0DTC2
A	1289	LYS	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2
A	1291	GLY	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	SER	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	GLY	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2
A	1297	SER	-	expression tag	UNP P0DTC2
A	1298	GLY	-	expression tag	UNP P0DTC2
A	1299	GLY	-	expression tag	UNP P0DTC2
A	1300	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1301	SER	-	expression tag	UNP P0DTC2
A	1302	ALA	-	expression tag	UNP P0DTC2
A	1303	TRP	-	expression tag	UNP P0DTC2
A	1304	SER	-	expression tag	UNP P0DTC2
A	1305	HIS	-	expression tag	UNP P0DTC2
A	1306	PRO	-	expression tag	UNP P0DTC2
A	1307	GLN	-	expression tag	UNP P0DTC2
A	1308	PHE	-	expression tag	UNP P0DTC2
A	1309	GLU	-	expression tag	UNP P0DTC2
A	1310	LYS	-	expression tag	UNP P0DTC2

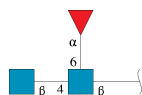
- Molecule 2 is a protein called SP1-77 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	225	Total	C	N	O	S	0	0
			1701	1073	290	331	7		

- Molecule 3 is a protein called SP1-77 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	212	Total	C	N	O	S	0	0
			1622	1010	267	340	5		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

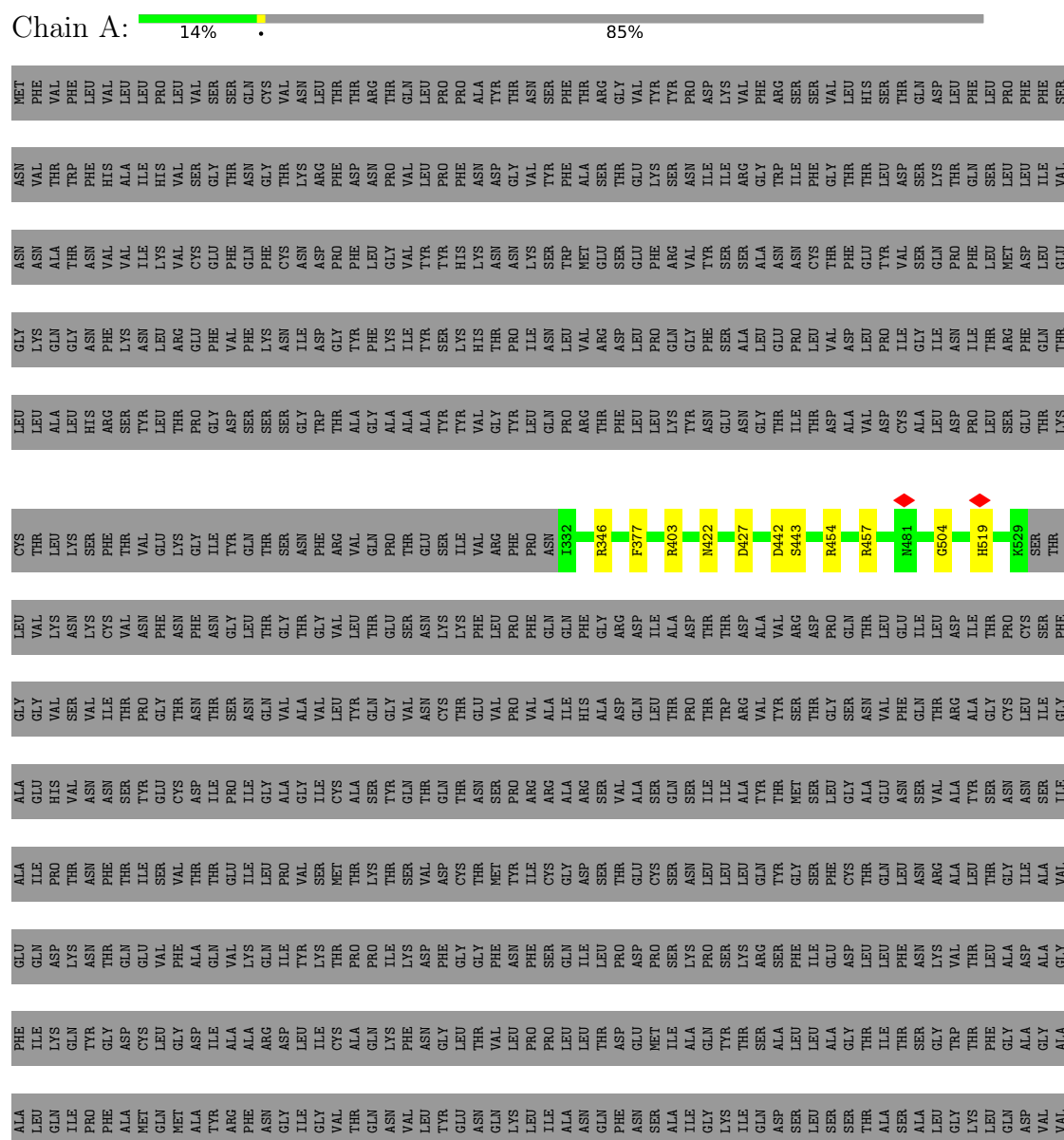


Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	3	Total	C	N	O	0	0
			38	22	2	14		

3 Residue-property plots

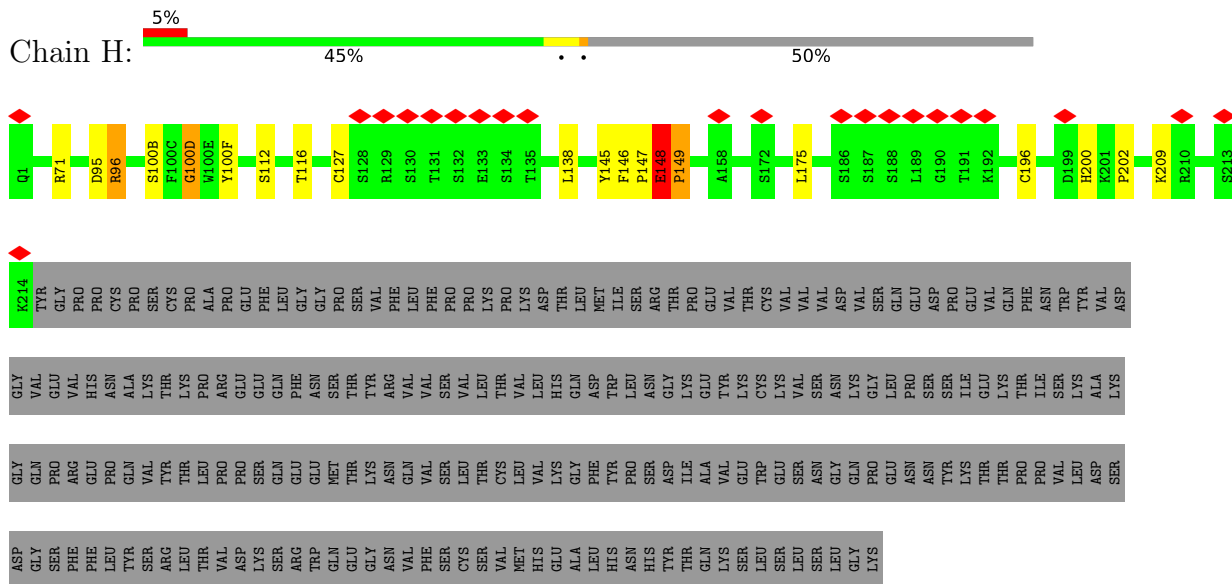
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

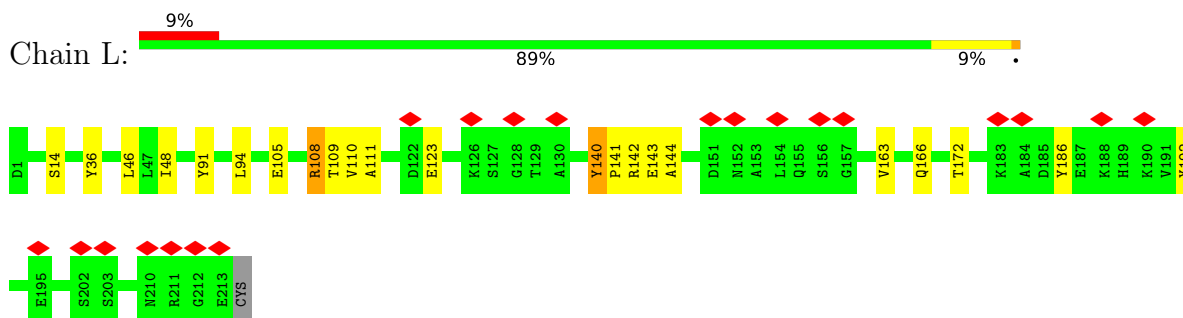


CYS	LEU	VAL	LYS	ILE	ASN
CYS	ASN	ASN	ASN	ARG	ASN
LYS	GLU	ASN	PHE	ALA	ASN
PHE	SER	THR	THR	GLU	ALA
ASP	LEU	VAL	THR	GLN	ALA
GLU	ILE	TYR	ASP	ALA	ALA
ASP	ASP	THR	ASP	ARG	LEU
SER	LEU	PRO	ALA	ALA	ASN
GLU	GLN	LEU	ILE	SER	THR
GLU	GLU	GLN	CYS	ALA	LEU
PRO	GLY	GLU	HIS	ASN	VAL
VAL	GLY	GLU	ASP	LEU	LYS
LEU	LYS	LEU	GLY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

- Molecule 2: SP1-77 Fab heavy chain



- Molecule 3: SP1-77 Fab light chain



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



MAG1
MAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	250319	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 ($e^-/\text{\AA}^2$)	54.91	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.733	Depositor
Minimum map value	-1.387	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	0.71	0/1613	0.95	0/2194
2	H	0.65	0/1744	0.99	0/2379
3	L	0.58	0/1656	0.89	0/2253
All	All	0.65	0/5013	0.95	0/6826

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	A	1569	0	1504	4	0
2	H	1701	0	1655	30	0
3	L	1622	0	1541	20	0
4	B	38	0	34	0	0
All	All	4930	0	4734	50	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 5.

All (50) 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)
2:H:148:GLU:HB3	2:H:149:PRO:CD	1.42	1.44
2:H:148:GLU:CB	2:H:149:PRO:CD	2.19	1.19
2:H:116:THR:HG23	2:H:147:PRO:HG2	1.30	1.11
2:H:148:GLU:CB	2:H:149:PRO:HD2	1.80	1.11
2:H:148:GLU:HB3	2:H:149:PRO:HD3	1.08	1.05
3:L:108:ARG:HH22	3:L:111:ALA:HB2	1.32	0.94
3:L:36:TYR:CE2	3:L:46:LEU:HD13	2.09	0.88
3:L:108:ARG:HH22	3:L:111:ALA:CB	1.90	0.83
3:L:108:ARG:NH2	3:L:111:ALA:HB2	1.97	0.79
3:L:108:ARG:NH2	3:L:111:ALA:CB	2.53	0.71
2:H:147:PRO:HB2	2:H:202:PRO:HG2	1.76	0.66
2:H:71:ARG:HD2	2:H:71:ARG:O	1.98	0.63
2:H:148:GLU:HB2	2:H:149:PRO:HD2	1.77	0.63
2:H:116:THR:HG23	2:H:147:PRO:CG	2.18	0.61
1:A:454:ARG:HD3	1:A:457:ARG:HG3	1.82	0.61
2:H:147:PRO:HB2	2:H:202:PRO:CB	2.34	0.58
3:L:105:GLU:OE2	3:L:140:TYR:OH	2.18	0.58
2:H:145:TYR:HE1	2:H:148:GLU:O	1.86	0.57
2:H:147:PRO:CB	2:H:202:PRO:CB	2.83	0.56
2:H:147:PRO:HB2	2:H:202:PRO:CG	2.36	0.55
3:L:36:TYR:CZ	3:L:46:LEU:HD13	2.42	0.55
2:H:147:PRO:HB2	2:H:202:PRO:HB2	1.90	0.54
3:L:142:ARG:NH1	3:L:163:VAL:HG11	2.24	0.52
2:H:147:PRO:HD2	2:H:200:HIS:HE1	1.73	0.52
3:L:142:ARG:O	3:L:144:ALA:N	2.42	0.52
2:H:147:PRO:CB	2:H:202:PRO:HG2	2.40	0.50
2:H:96:ARG:O	2:H:96:ARG:HG2	2.10	0.50
2:H:146:PHE:CD2	2:H:146:PHE:C	2.85	0.50
2:H:145:TYR:C	2:H:145:TYR:CD1	2.85	0.49
3:L:186:TYR:HA	3:L:192:TYR:OH	2.11	0.49
3:L:140:TYR:CD1	3:L:140:TYR:C	2.85	0.49
2:H:146:PHE:HB3	2:H:147:PRO:HD3	1.93	0.49
3:L:36:TYR:CD2	3:L:46:LEU:HA	2.50	0.47
2:H:100(D):GLY:HA2	3:L:91:TYR:CD1	2.51	0.46
2:H:145:TYR:CE1	2:H:148:GLU:O	2.66	0.45
3:L:108:ARG:NH2	3:L:111:ALA:HB3	2.31	0.44
2:H:146:PHE:HB2	2:H:175:LEU:HD23	1.98	0.44
2:H:147:PRO:CB	2:H:202:PRO:HB2	2.48	0.43
2:H:145:TYR:CD1	2:H:145:TYR:O	2.70	0.43
3:L:36:TYR:CE2	3:L:46:LEU:CD1	2.93	0.43
3:L:108:ARG:HD2	3:L:109:THR:H	1.81	0.43
3:L:110:VAL:HG23	3:L:141:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:140:TYR:O	3:L:140:TYR:CG	2.70	0.43
1:A:442:ASP:OD1	2:H:100(B):SER:OG	2.30	0.43
2:H:146:PHE:O	2:H:146:PHE:CG	2.70	0.42
1:A:346:ARG:NH2	2:H:95:ASP:OD1	2.52	0.42
2:H:112:SER:OG	2:H:146:PHE:CE1	2.73	0.41
3:L:140:TYR:HE2	3:L:166:GLN:NE2	2.19	0.41
2:H:209:LYS:NZ	3:L:123:GLU:OE1	2.43	0.41
1:A:403:ARG:HG2	1:A:504:GLY:O	2.22	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	196/1310 (15%)	185 (94%)	11 (6%)	0	100	100
2	H	223/451 (49%)	206 (92%)	11 (5%)	6 (3%)	5	30
3	L	210/213 (99%)	195 (93%)	12 (6%)	3 (1%)	11	46
All	All	629/1974 (32%)	586 (93%)	34 (5%)	9 (1%)	15	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	148	GLU
2	H	149	PRO
3	L	143	GLU
2	H	96	ARG
2	H	100(F)	TYR
3	L	94	LEU
2	H	127	CYS
2	H	100(D)	GLY
3	L	140	TYR

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	171/1135 (15%)	166 (97%)	5 (3%)	42	74
2	H	189/399 (47%)	186 (98%)	3 (2%)	62	84
3	L	185/188 (98%)	181 (98%)	4 (2%)	52	79
All	All	545/1722 (32%)	533 (98%)	12 (2%)	54	79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	PHE
1	A	422	ASN
1	A	427	ASP
1	A	443	SER
1	A	519	HIS
2	H	138	LEU
2	H	148	GLU
2	H	196	CYS
3	L	14	SER
3	L	48	ILE
3	L	108	ARG
3	L	172	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
3	L	3	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](#)

3 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	4,1	14,14,15	1.25	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	B	2	4	14,14,15	1.19	1 (7%)	17,19,21	0.86	1 (5%)
4	FUC	B	3	4	10,10,11	1.65	2 (20%)	14,14,16	1.05	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	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	FUC	B	3	4	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3	FUC	O5-C1	3.02	1.48	1.43
4	B	2	NAG	O5-C5	2.59	1.48	1.43
4	B	3	FUC	O5-C5	2.41	1.48	1.43
4	B	1	NAG	O5-C5	2.16	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C1-O5-C5	2.67	115.81	112.19
4	B	1	NAG	O5-C5-C6	2.48	111.09	107.20

There are no chirality outliers.

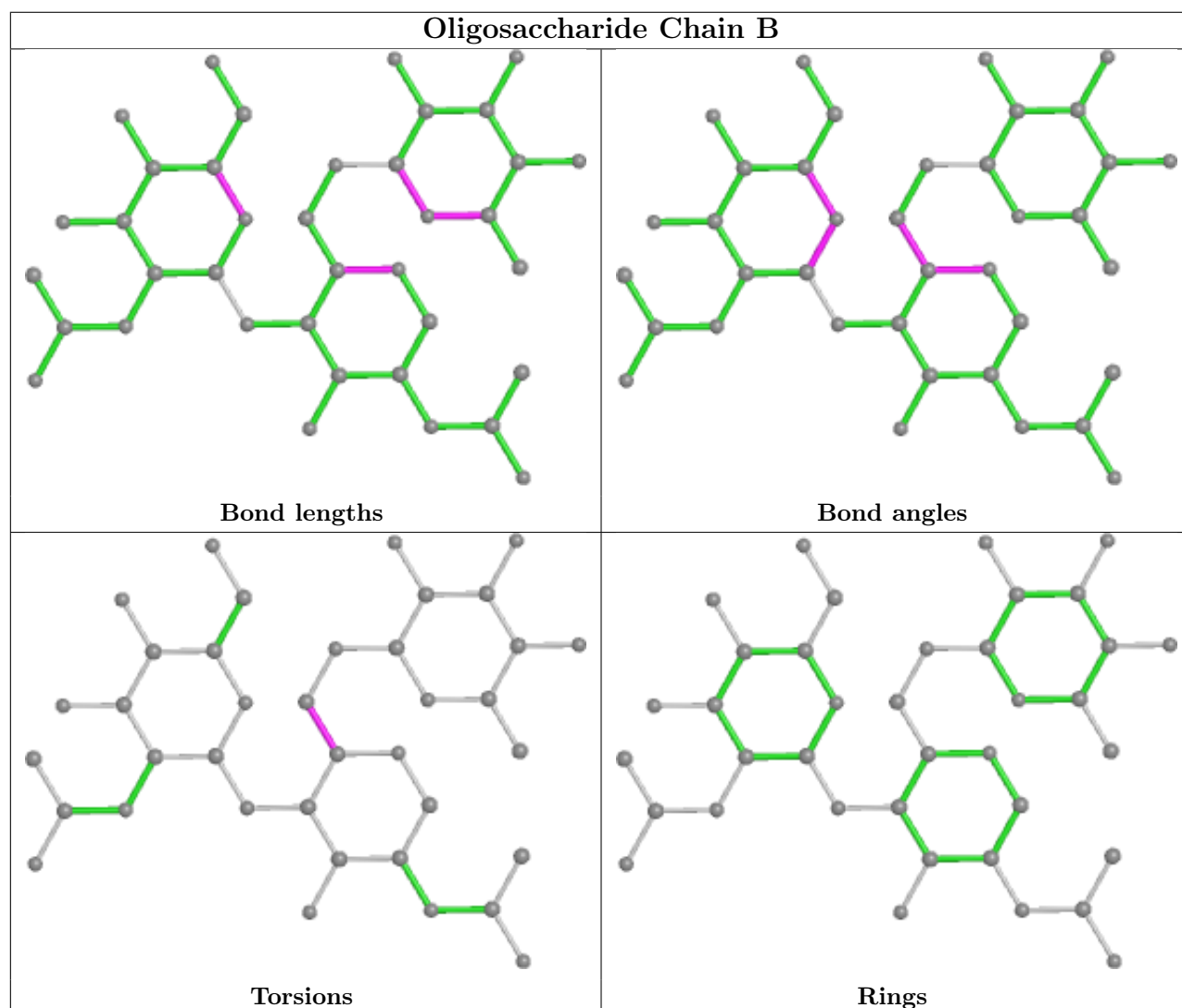
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

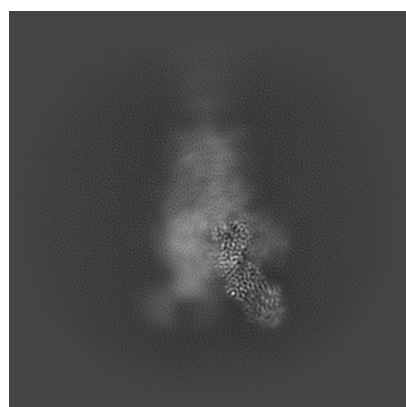
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26677. These allow visual inspection of the internal detail of the map and identification of artifacts.

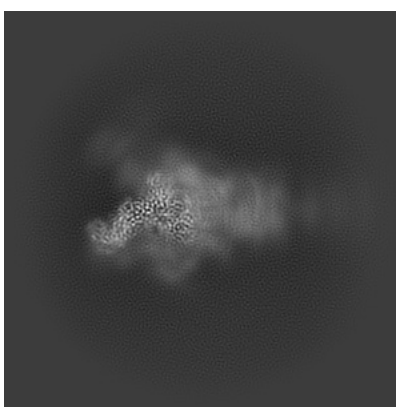
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

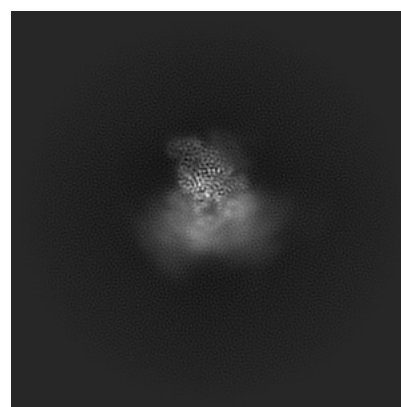
6.1.1 Primary map



X



Y

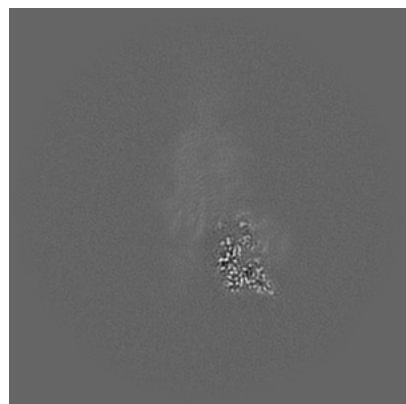


Z

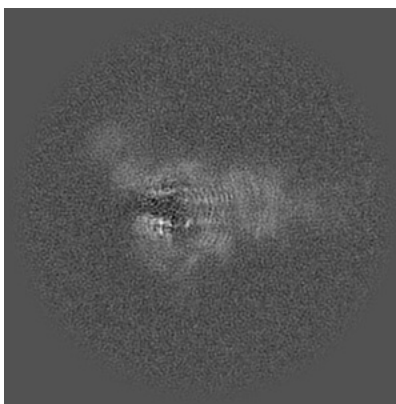
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

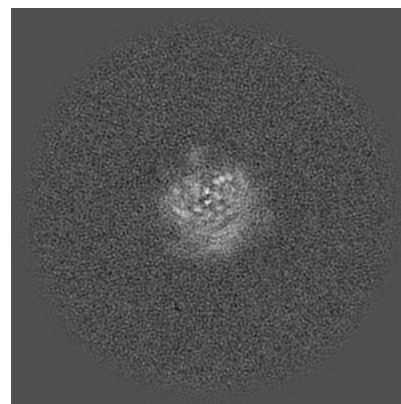
6.2.1 Primary map



X Index: 240



Y Index: 240

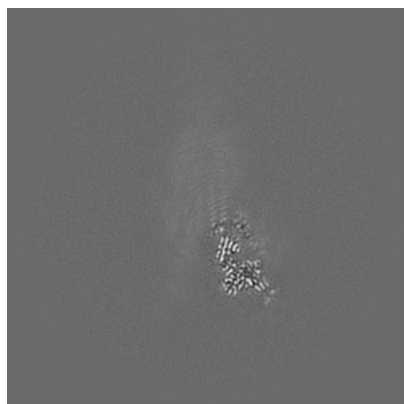


Z Index: 240

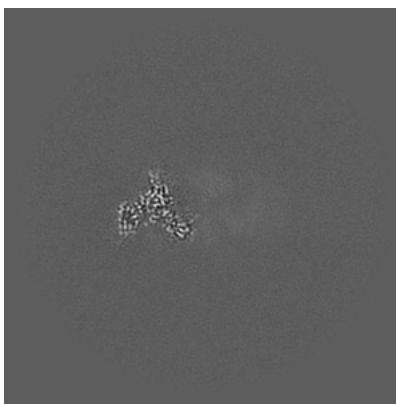
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

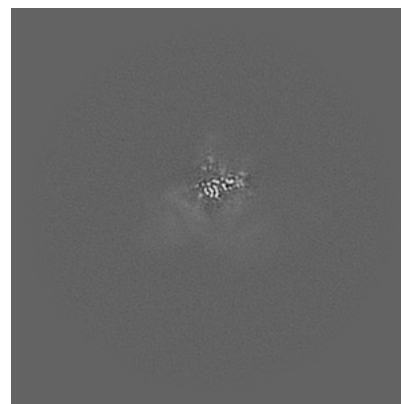
6.3.1 Primary map



X Index: 235



Y Index: 267



Z Index: 178

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

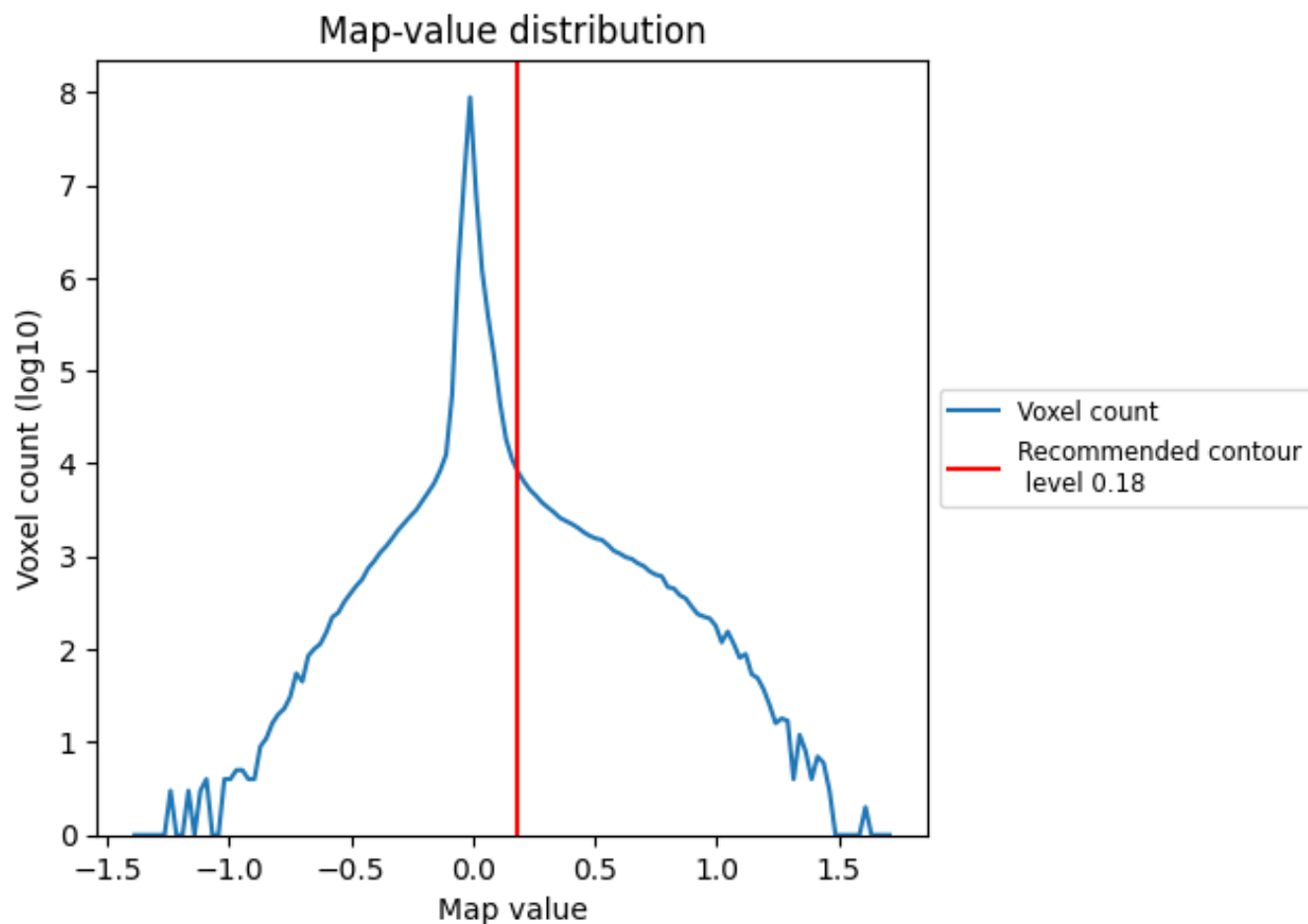
6.5 Mask visualisation

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

7 Map analysis [i](#)

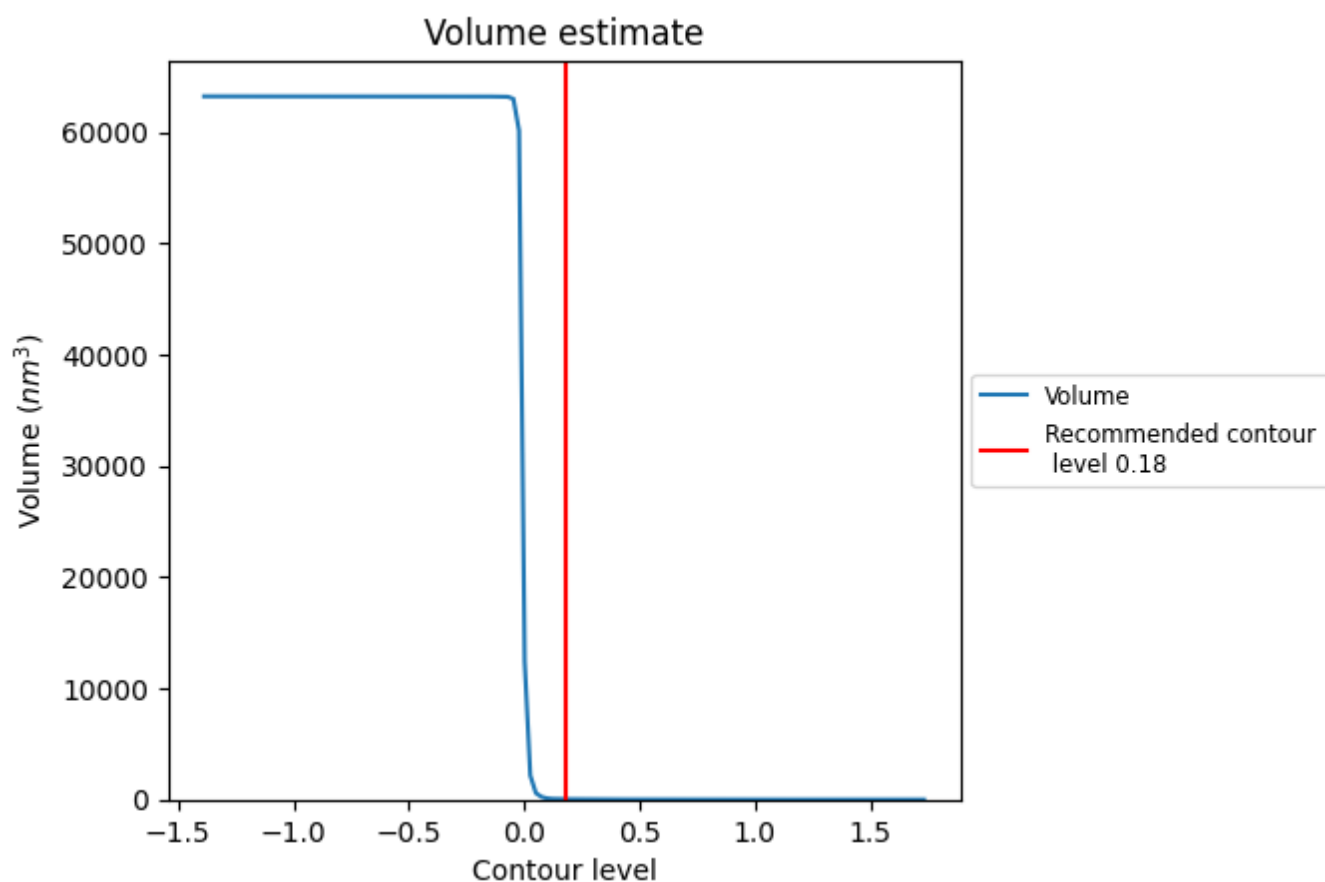
This section contains the results of statistical analysis of the map.

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.

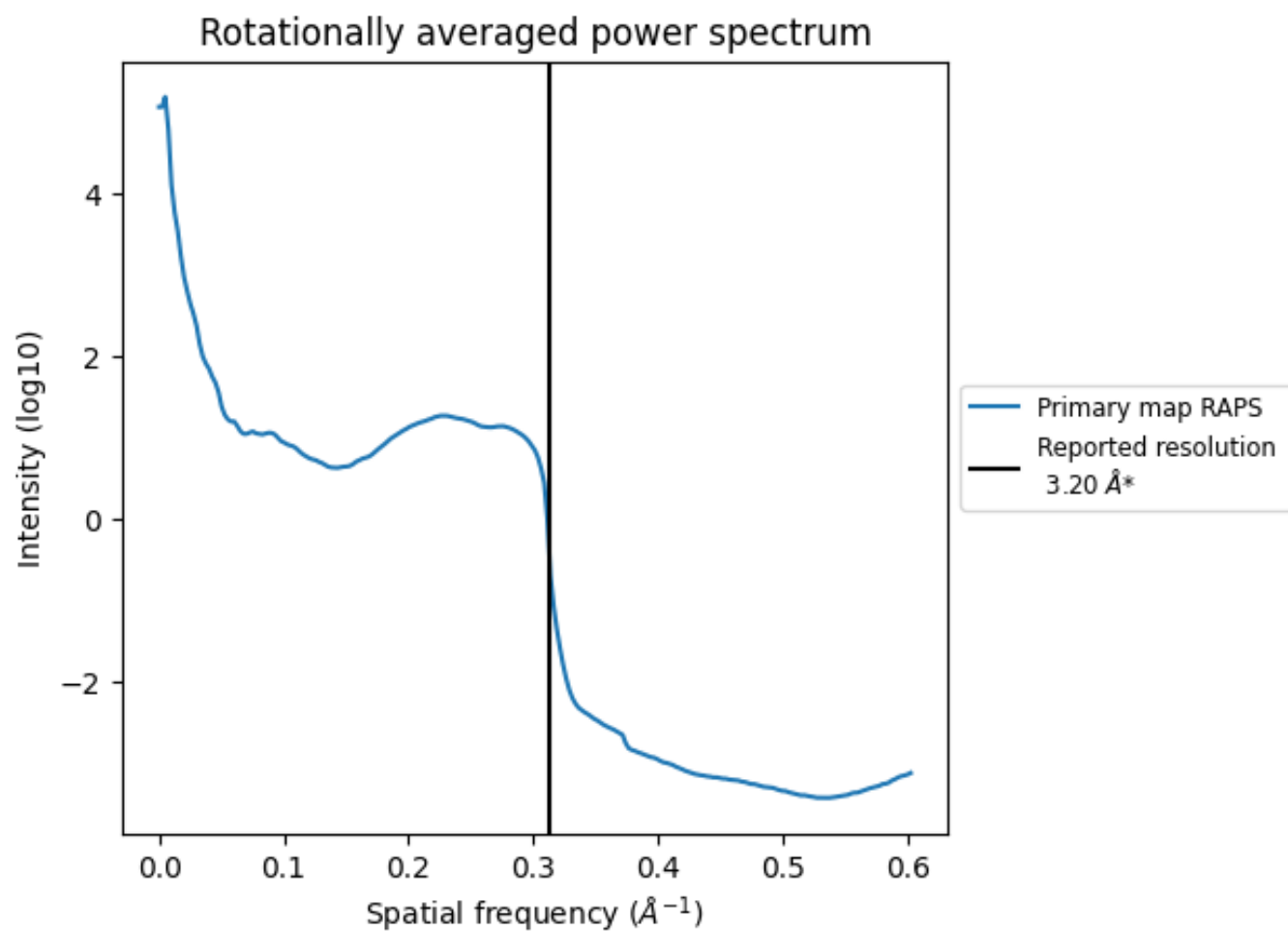
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 37 nm^3 ; this corresponds to an approximate mass of 34 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 0.312 Å⁻¹

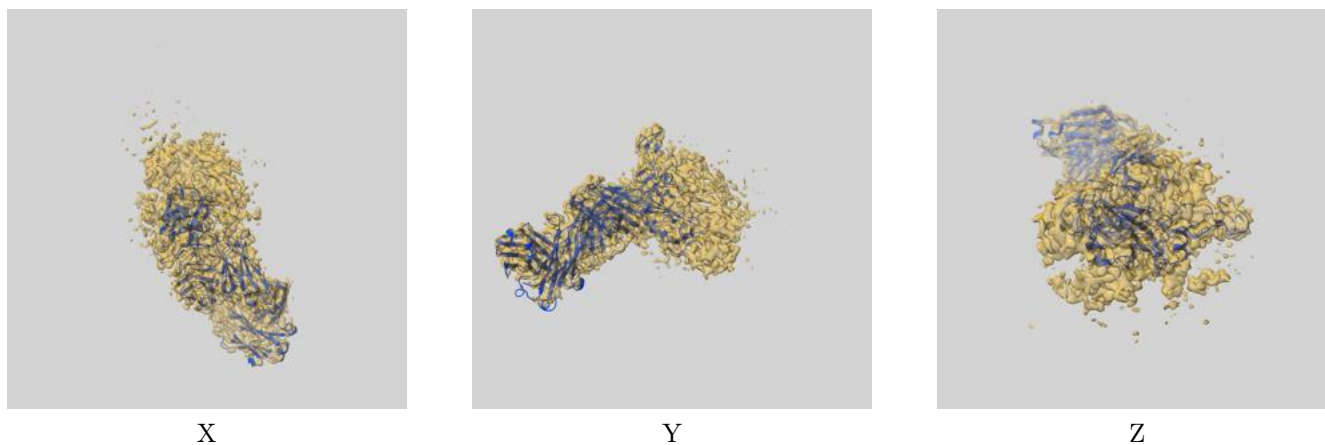
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

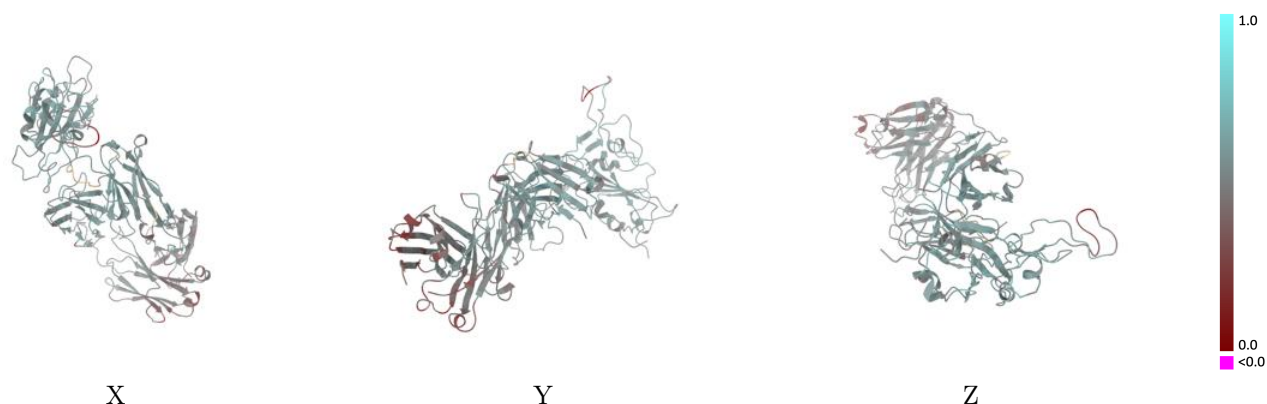
This section contains information regarding the fit between EMDB map EMD-26677 and PDB model 7UPX. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



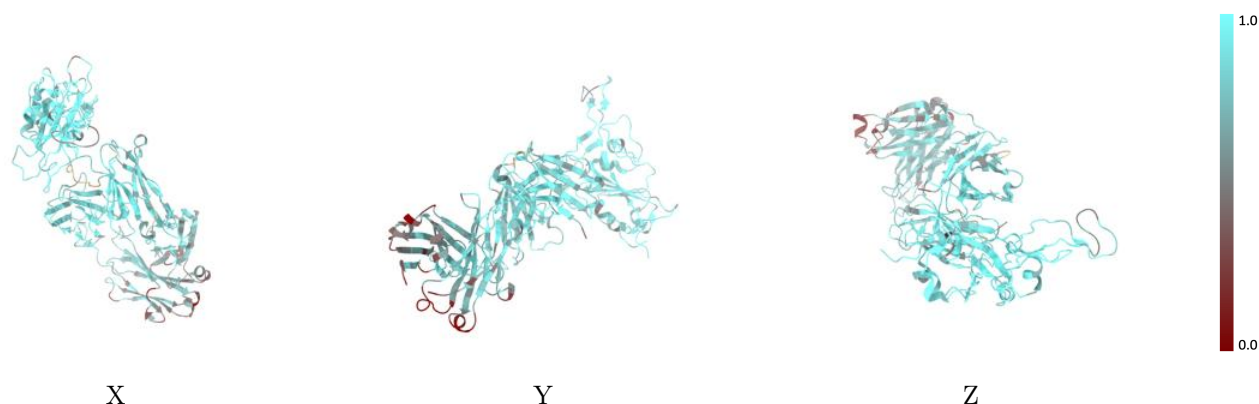
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



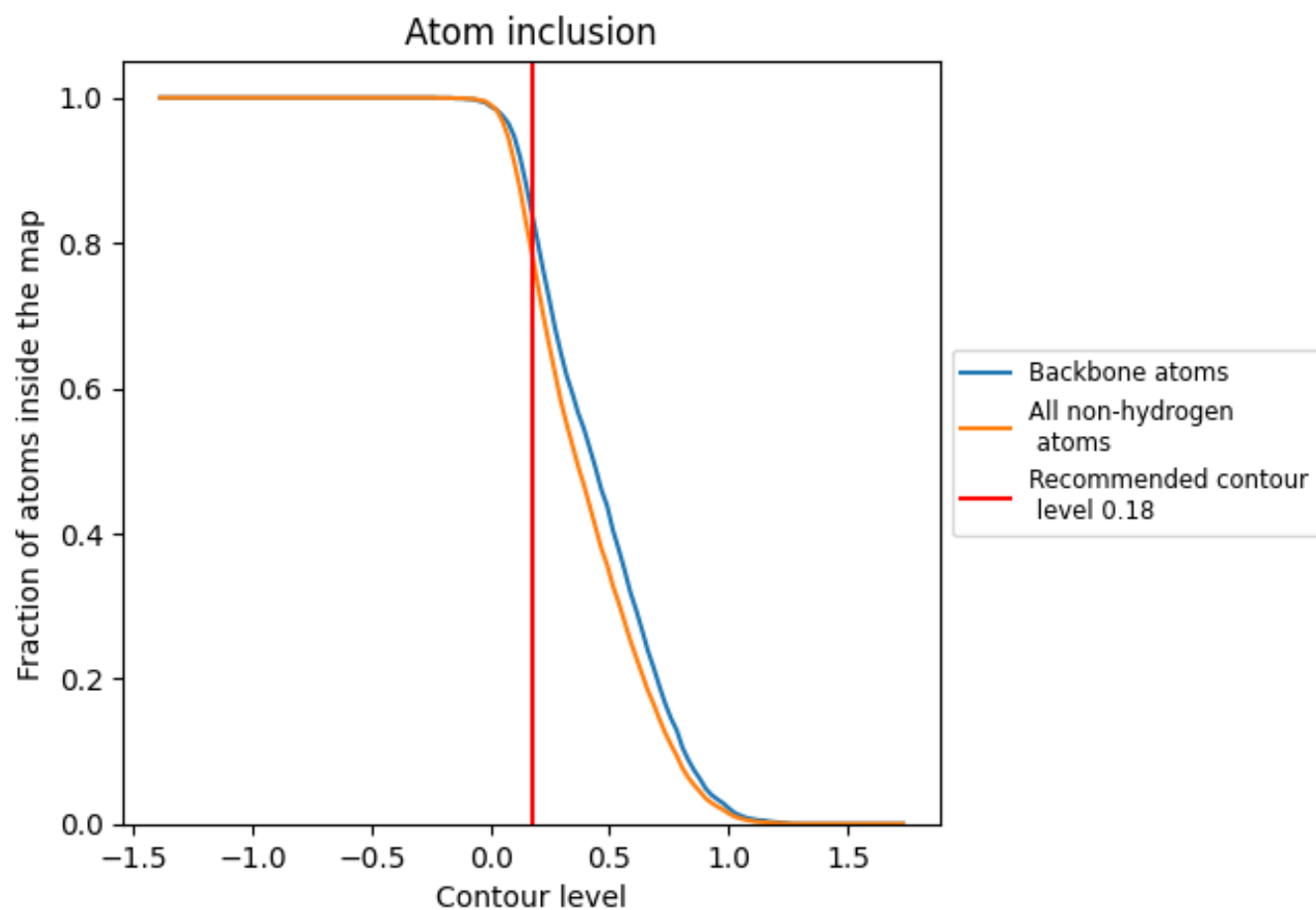
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7756	<div></div> 0.5130
A	<div></div> 0.8598	<div></div> 0.5420
B	<div></div> 0.7105	<div></div> 0.4890
H	<div></div> 0.7409	<div></div> 0.5090
L	<div></div> 0.7325	<div></div> 0.4900

