wwPDB EM Validation Summary Report

Oct 19, 2026 – 12:42 PM EDT

PDB ID	:	39JB / pdb_000039jb
EMDB ID	:	EMD-79526
Title	:	Structure of HCMV gH/gK bound to D11L, B1L, G2L Fabs
Authors	:	Ramamohan, A.R.; McLellan, J.S.
Deposited on	:	2026-10-12
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

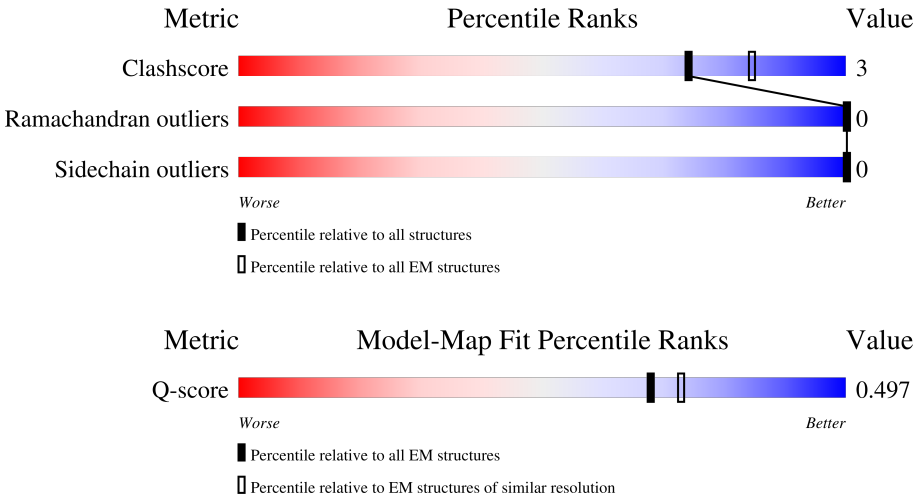
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.40 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.



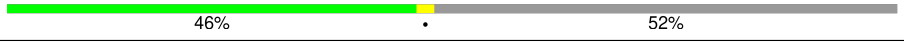
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	B	233	51% · 45%
2	C	217	45% 5% 50%
3	D	229	7% 45% 8% 47%
4	E	217	8% 45% · 53%

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Mol	Chain	Length	Quality of chain
5	G	221	
6	H	217	
7	U	347	
8	A	721	
9	F	2	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11132 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 B1L Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	128	980	626	164	185	5	0	0

- Molecule 2 is a protein called B1L Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	108	804	497	146	159	2	0	0

- Molecule 3 is a protein called D11L Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	122	938	596	160	177	5	0	0

- Molecule 4 is a protein called D11L Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	103	772	490	131	149	2	0	0

- Molecule 5 is a protein called G2L Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	117	911	580	152	177	2	0	0

- Molecule 6 is a protein called G2L Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	104	764	481	125	156	2	0	0

- Molecule 7 is a protein called HCMV gK.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	109	Total	C	N	O	S	0	0
			890	572	148	168	2		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	315	ALA	-	expression tag	UNP P16833
U	316	ALA	-	expression tag	UNP P16833
U	317	ALA	-	expression tag	UNP P16833
U	318	SER	-	expression tag	UNP P16833
U	319	TRP	-	expression tag	UNP P16833
U	320	SER	-	expression tag	UNP P16833
U	321	HIS	-	expression tag	UNP P16833
U	322	PRO	-	expression tag	UNP P16833
U	323	GLN	-	expression tag	UNP P16833
U	324	PHE	-	expression tag	UNP P16833
U	325	GLU	-	expression tag	UNP P16833
U	326	LYS	-	expression tag	UNP P16833
U	327	GLY	-	expression tag	UNP P16833
U	328	GLY	-	expression tag	UNP P16833
U	329	ALA	-	expression tag	UNP P16833
U	330	SER	-	expression tag	UNP P16833
U	331	GLY	-	expression tag	UNP P16833
U	332	GLY	-	expression tag	UNP P16833
U	333	GLY	-	expression tag	UNP P16833
U	334	GLY	-	expression tag	UNP P16833
U	335	SER	-	expression tag	UNP P16833
U	336	GLY	-	expression tag	UNP P16833
U	337	GLY	-	expression tag	UNP P16833
U	338	SER	-	expression tag	UNP P16833
U	339	ALA	-	expression tag	UNP P16833
U	340	TRP	-	expression tag	UNP P16833
U	341	SER	-	expression tag	UNP P16833
U	342	HIS	-	expression tag	UNP P16833
U	343	PRO	-	expression tag	UNP P16833
U	344	GLN	-	expression tag	UNP P16833
U	345	PHE	-	expression tag	UNP P16833
U	346	GLU	-	expression tag	UNP P16833
U	347	LYS	-	expression tag	UNP P16833

- Molecule 8 is a protein called Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	625	Total	C	N	O	S	0	0
			5045	3239	856	924	26		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P12824
A	5	SER	-	expression tag	UNP P12824
A	6	VAL	-	expression tag	UNP P12824
A	7	PRO	-	expression tag	UNP P12824
A	8	THR	-	expression tag	UNP P12824
A	9	GLN	-	expression tag	UNP P12824
A	10	VAL	-	expression tag	UNP P12824
A	11	LEU	-	expression tag	UNP P12824
A	12	GLY	-	expression tag	UNP P12824
A	13	LEU	-	expression tag	UNP P12824
A	14	LEU	-	expression tag	UNP P12824
A	15	LEU	-	expression tag	UNP P12824
A	16	LEU	-	expression tag	UNP P12824
A	17	TRP	-	expression tag	UNP P12824
A	18	LEU	-	expression tag	UNP P12824
A	19	THR	-	expression tag	UNP P12824
A	20	ASP	-	expression tag	UNP P12824
A	21	ALA	-	expression tag	UNP P12824
A	22	ARG	-	expression tag	UNP P12824
A	23	CYS	-	expression tag	UNP P12824
A	719	HIS	-	expression tag	UNP P12824
A	720	HIS	-	expression tag	UNP P12824
A	721	HIS	-	expression tag	UNP P12824
A	722	HIS	-	expression tag	UNP P12824
A	723	HIS	-	expression tag	UNP P12824
A	724	HIS	-	expression tag	UNP P12824

- Molecule 9 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
9	F	2	Total	C	N	O	0	0
			28	16	2	10		

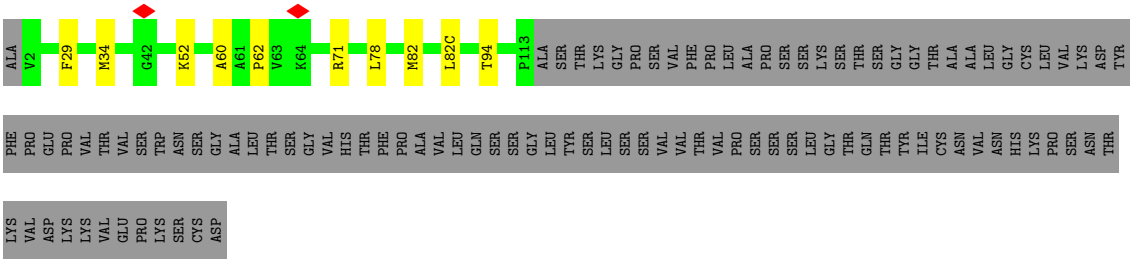
3 Residue-property plots (i)

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: B1L Fab Heavy Chain

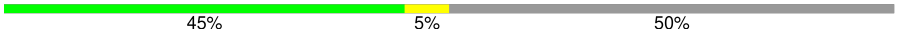
Chain B:

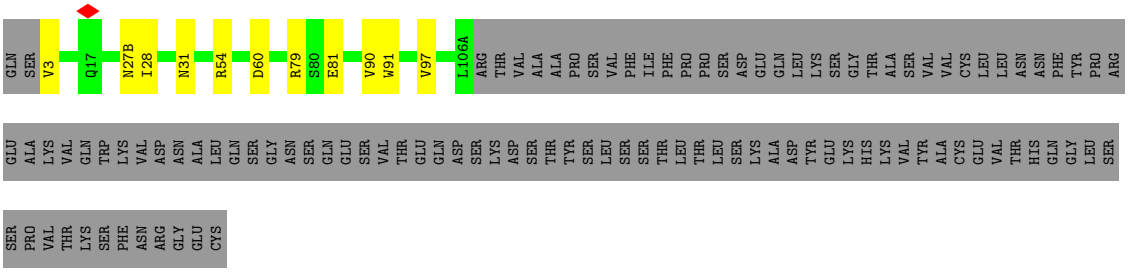




• Molecule 2: B1L Fab Light Chain

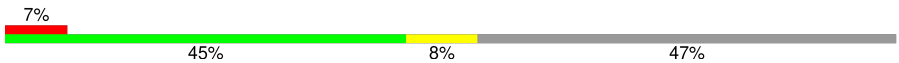
Chain C:

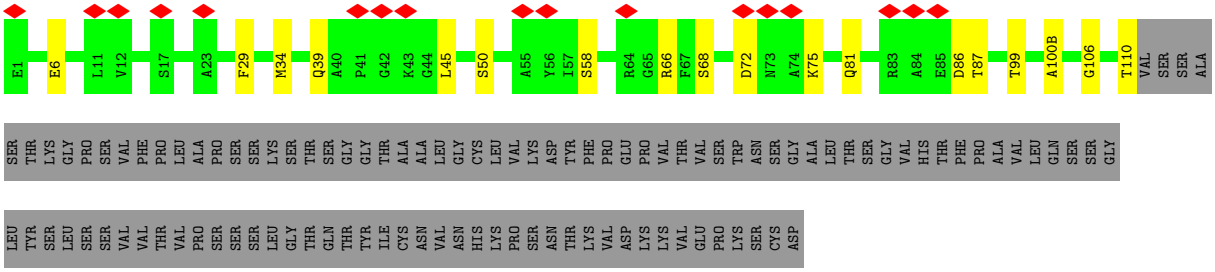




• Molecule 3: D11L Fab Heavy Chain

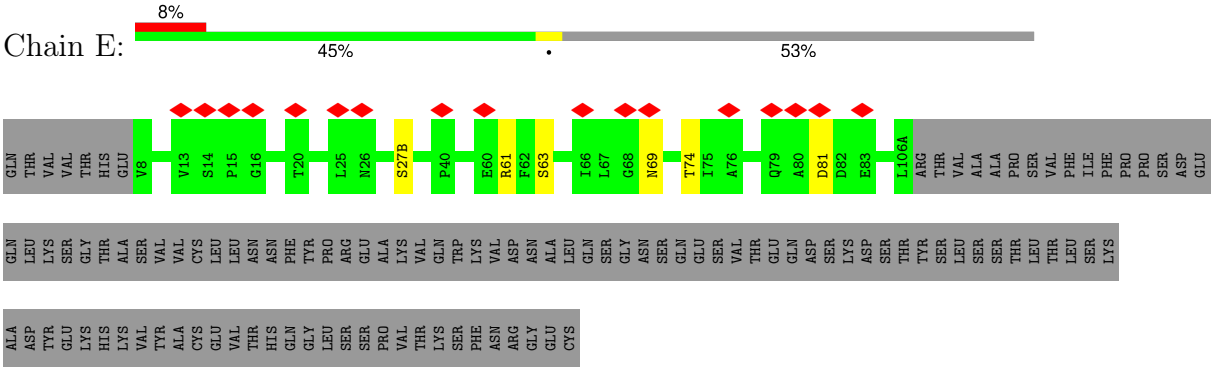
Chain D:





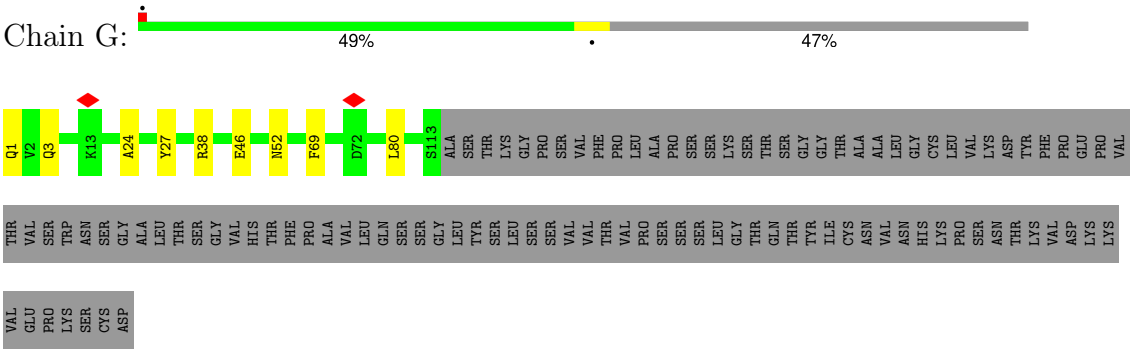
• Molecule 4: D11L Fab Light Chain

Chain E:



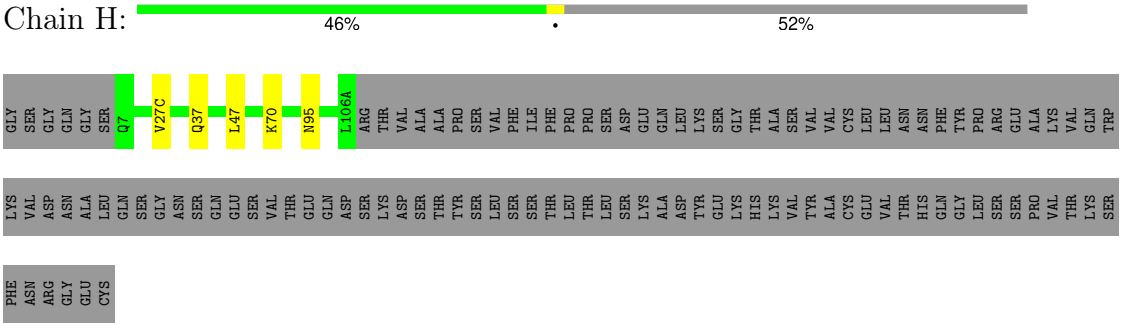
• Molecule 5: G2L Fab Heavy Chain

Chain G:



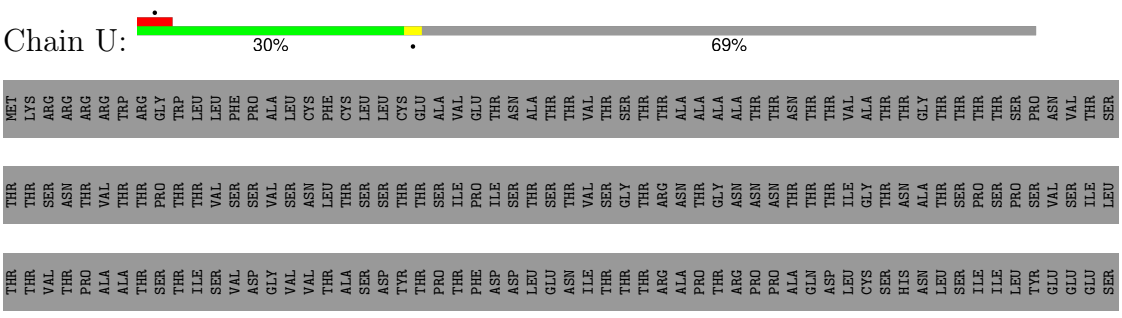
• Molecule 6: G2L Fab Light Chain

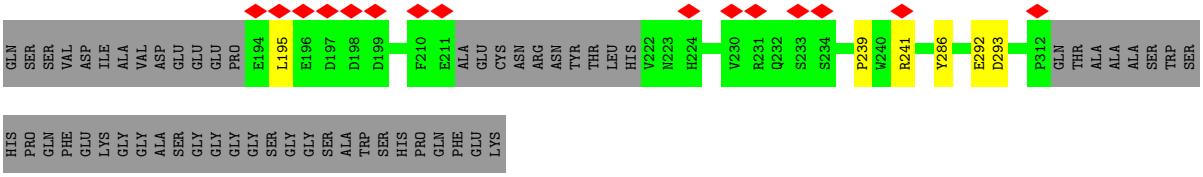
Chain H:



• Molecule 7: HCMV gK

Chain U:

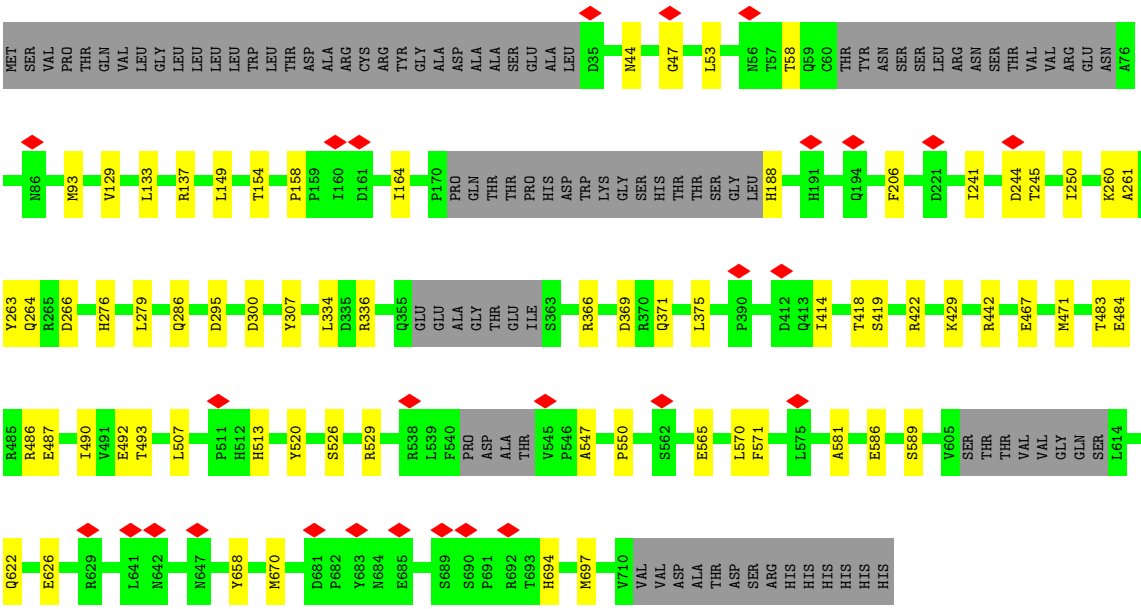




• Molecule 8: Envelope glycoprotein H

Chain A:





• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73502	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	74.3	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	62.074	Depositor
Minimum map value	-44.198	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.011	Depositor
Recommended contour level	8	Depositor
Map size (Å)	346.6112, 346.6112, 346.6112	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83320004, 0.83320004, 0.83320004	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	B	0.12	0/1007	0.31	0/1366
2	C	0.12	0/822	0.33	0/1118
3	D	0.08	0/961	0.30	0/1301
4	E	0.09	0/791	0.34	0/1079
5	G	0.11	0/936	0.28	0/1278
6	H	0.11	0/782	0.33	0/1068
7	U	0.10	0/917	0.29	0/1256
8	A	0.13	0/5164	0.36	0/7027
All	All	0.12	0/11380	0.33	0/15493

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	B	980	0	954	7	0
2	C	804	0	770	7	0
3	D	938	0	912	9	0
4	E	772	0	748	3	0
5	G	911	0	862	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	764	0	733	3	0
7	U	890	0	829	5	0
8	A	5045	0	5001	37	0
9	F	28	0	25	0	0
All	All	11132	0	10834	71	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 3.

The worst 5 of 71 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)
8:A:188:HIS:ND1	8:A:371:GLN:OE1	2.26	0.65
3:D:87:THR:HG23	3:D:110:THR:HA	1.78	0.64
2:C:31:ASN:ND2	2:C:91:TRP:O	2.30	0.64
5:G:52:ASN:OD1	8:A:622:GLN:NE2	2.31	0.63
8:A:264:GLN:NE2	8:A:266:ASP:OD1	2.31	0.61

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	B	126/233 (54%)	120 (95%)	6 (5%)	0	100	100
2	C	106/217 (49%)	101 (95%)	5 (5%)	0	100	100
3	D	120/229 (52%)	113 (94%)	7 (6%)	0	100	100
4	E	101/217 (46%)	97 (96%)	4 (4%)	0	100	100
5	G	115/221 (52%)	110 (96%)	5 (4%)	0	100	100
6	H	102/217 (47%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	105/347 (30%)	105 (100%)	0	0	100	100
8	A	613/721 (85%)	586 (96%)	27 (4%)	0	100	100
All	All	1388/2402 (58%)	1332 (96%)	56 (4%)	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	B	104/194 (54%)	104 (100%)	0	100	100
2	C	87/185 (47%)	87 (100%)	0	100	100
3	D	97/190 (51%)	97 (100%)	0	100	100
4	E	83/186 (45%)	83 (100%)	0	100	100
5	G	97/187 (52%)	97 (100%)	0	100	100
6	H	85/184 (46%)	85 (100%)	0	100	100
7	U	99/302 (33%)	99 (100%)	0	100	100
8	A	568/650 (87%)	568 (100%)	0	100	100
All	All	1220/2078 (59%)	1220 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
8	A	215	GLN
8	A	319	HIS
8	A	694	HIS
8	A	481	HIS
8	A	513	HIS

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)

2 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	$\#\|Z\| > 2$
9	NAG	F	1	9,8	14,14,15	0.75	0	17,19,21	0.94	1 (5%)
9	NAG	F	2	9	14,14,15	0.73	0	17,19,21	0.80	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
9	NAG	F	1	9,8	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	1	NAG	O5-C1-C2	-2.28	107.76	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

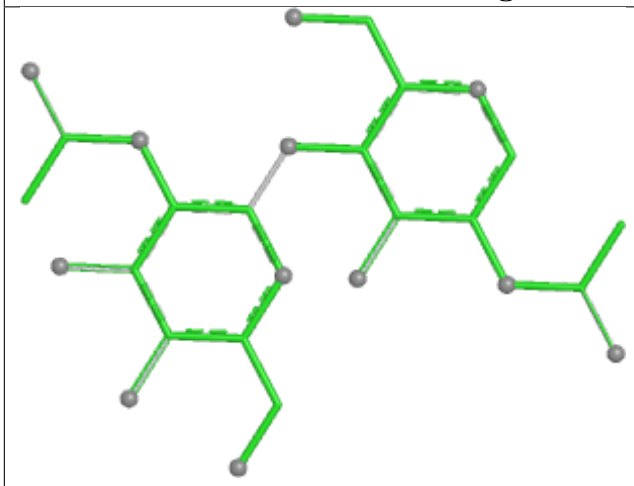
Mol	Chain	Res	Type	Atoms
9	F	2	NAG	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

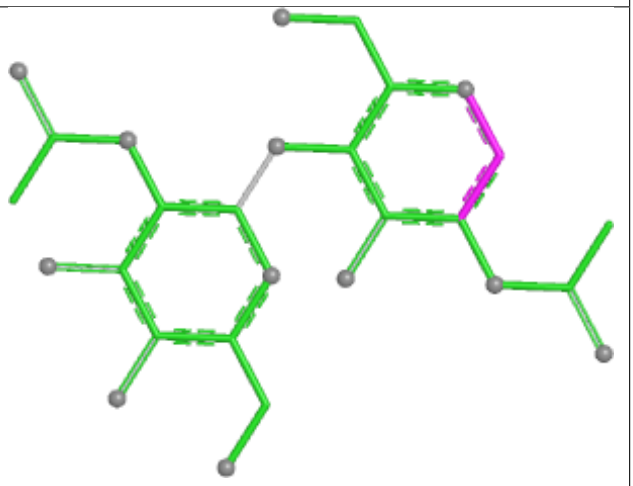
No monomer is involved in short contacts.

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

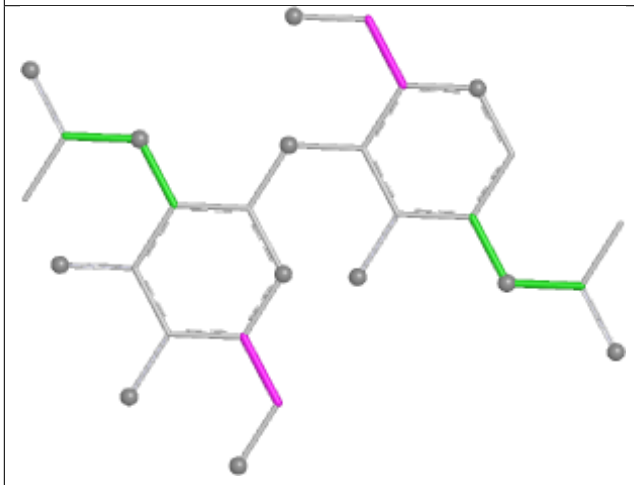
Oligosaccharide Chain F



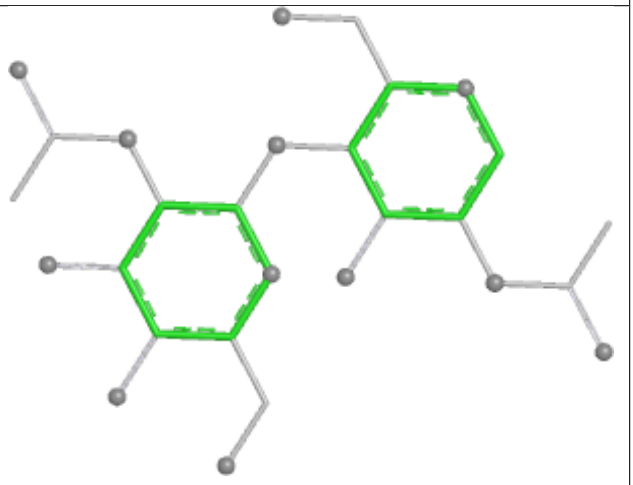
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

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.

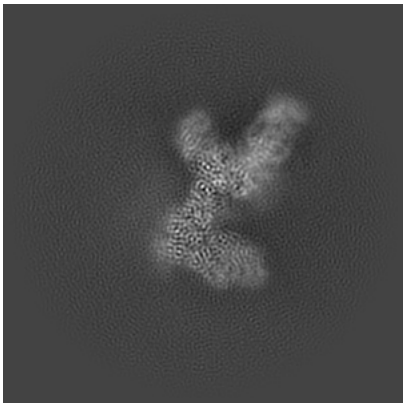
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-79526. These allow visual inspection of the internal detail of the map and identification of artifacts.

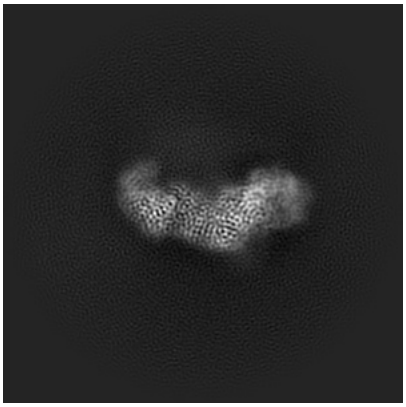
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

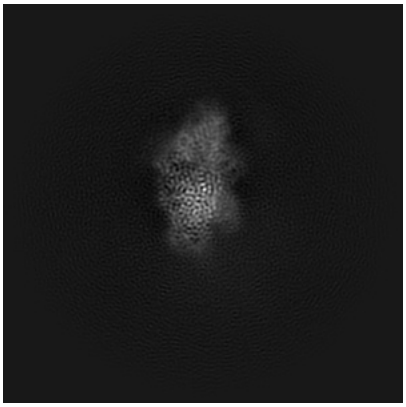
6.1.1 Primary map



X



Y

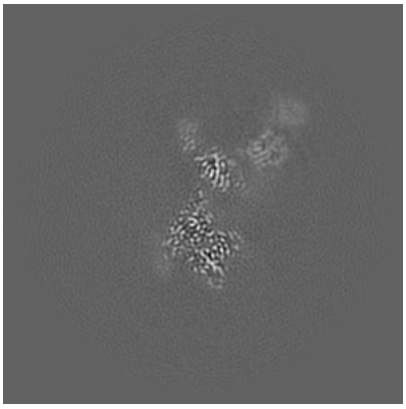


Z

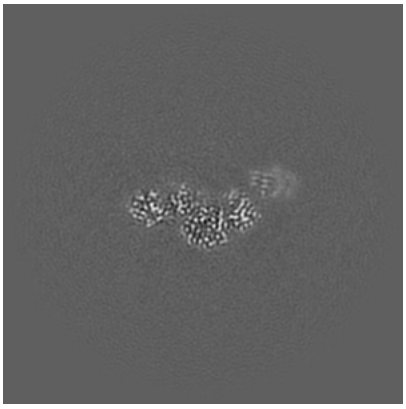
The images above show the map projected in three orthogonal directions.

6.2 Central slices

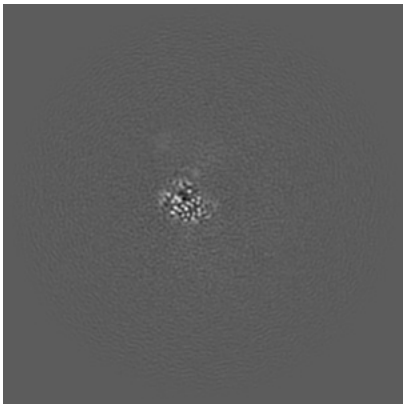
6.2.1 Primary map



X Index: 208



Y Index: 208

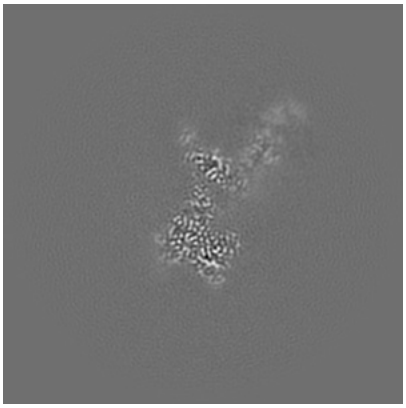


Z Index: 208

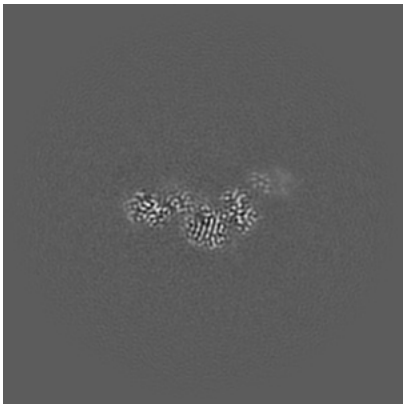
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

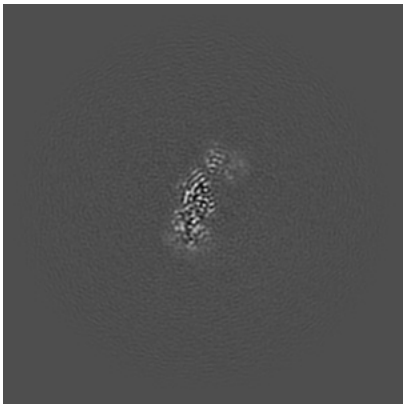
6.3.1 Primary map



X Index: 203



Y Index: 213

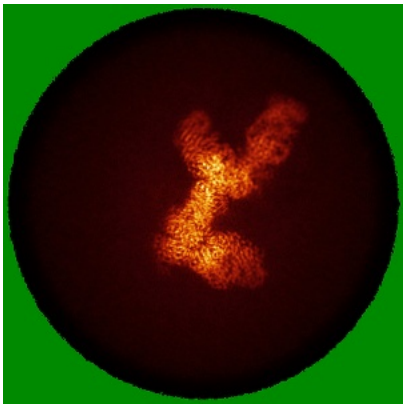


Z Index: 157

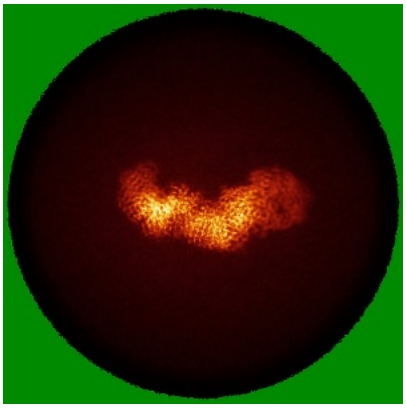
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

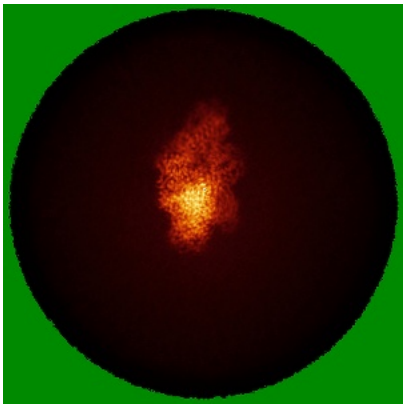
6.4.1 Primary map



X



Y

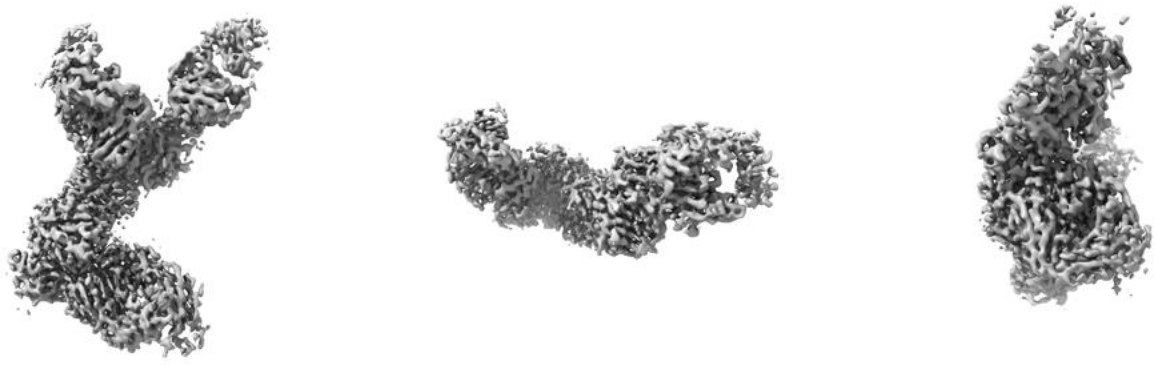


Z

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 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

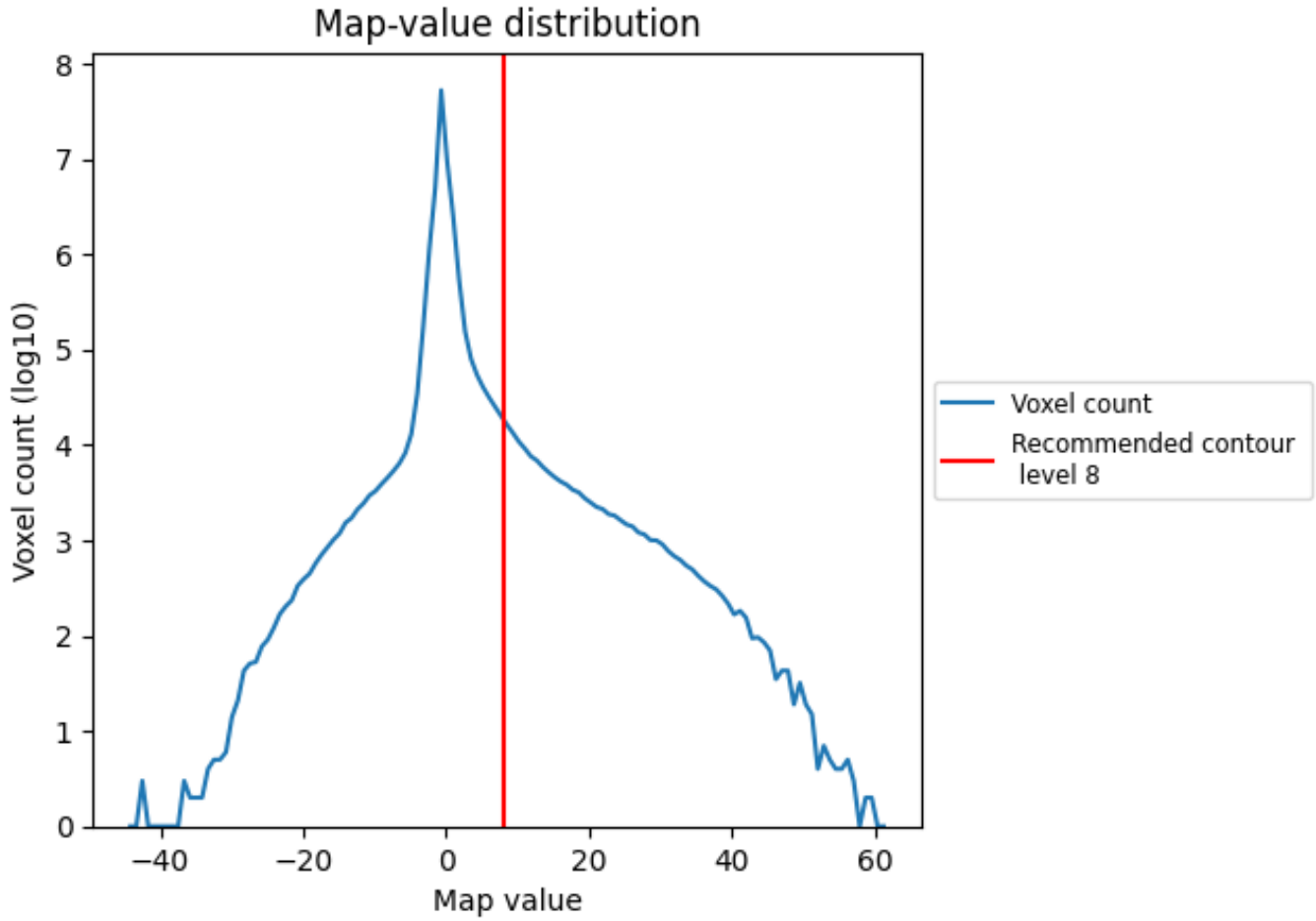
6.6 Mask visualisation (i)

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

7 Map analysis

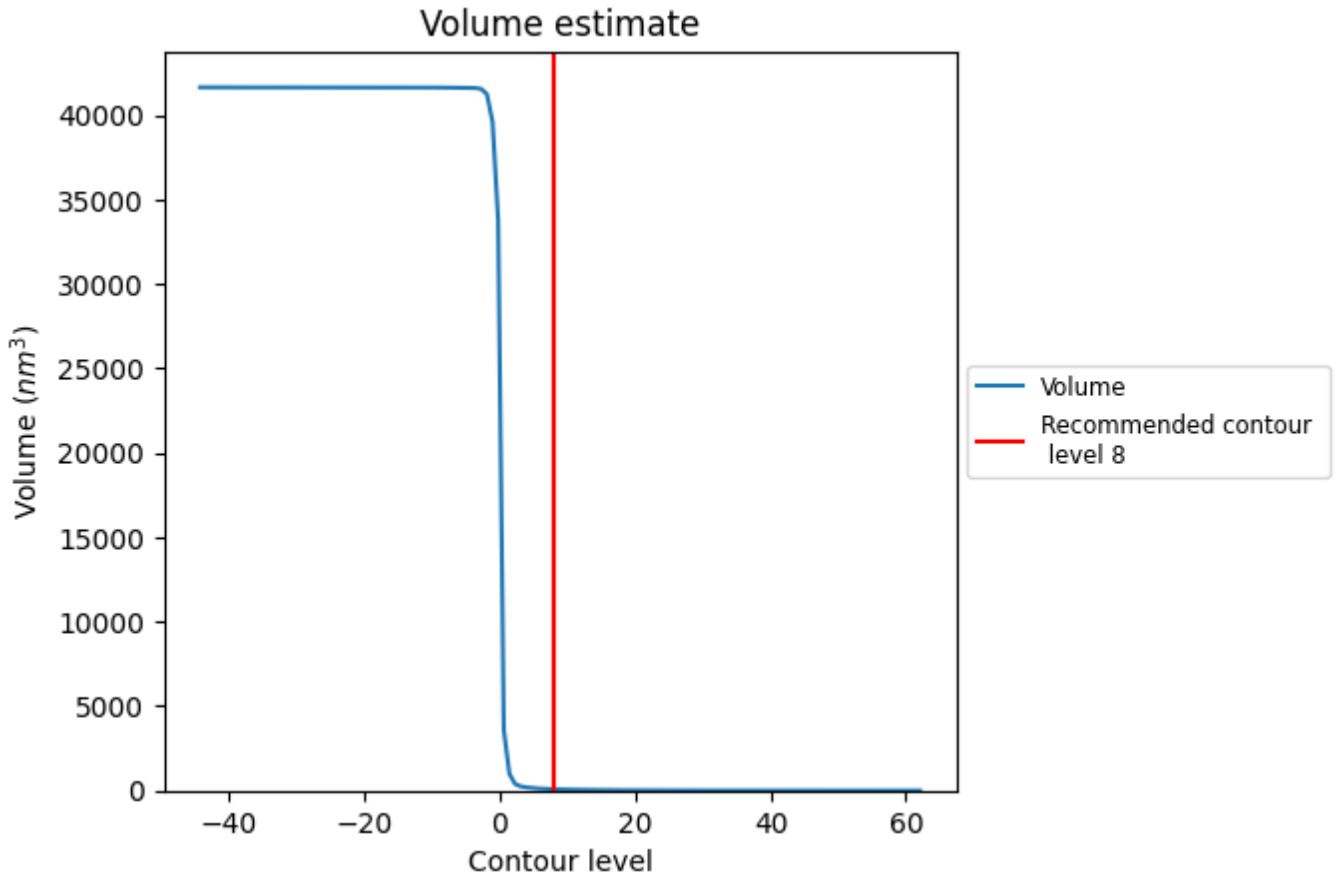
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

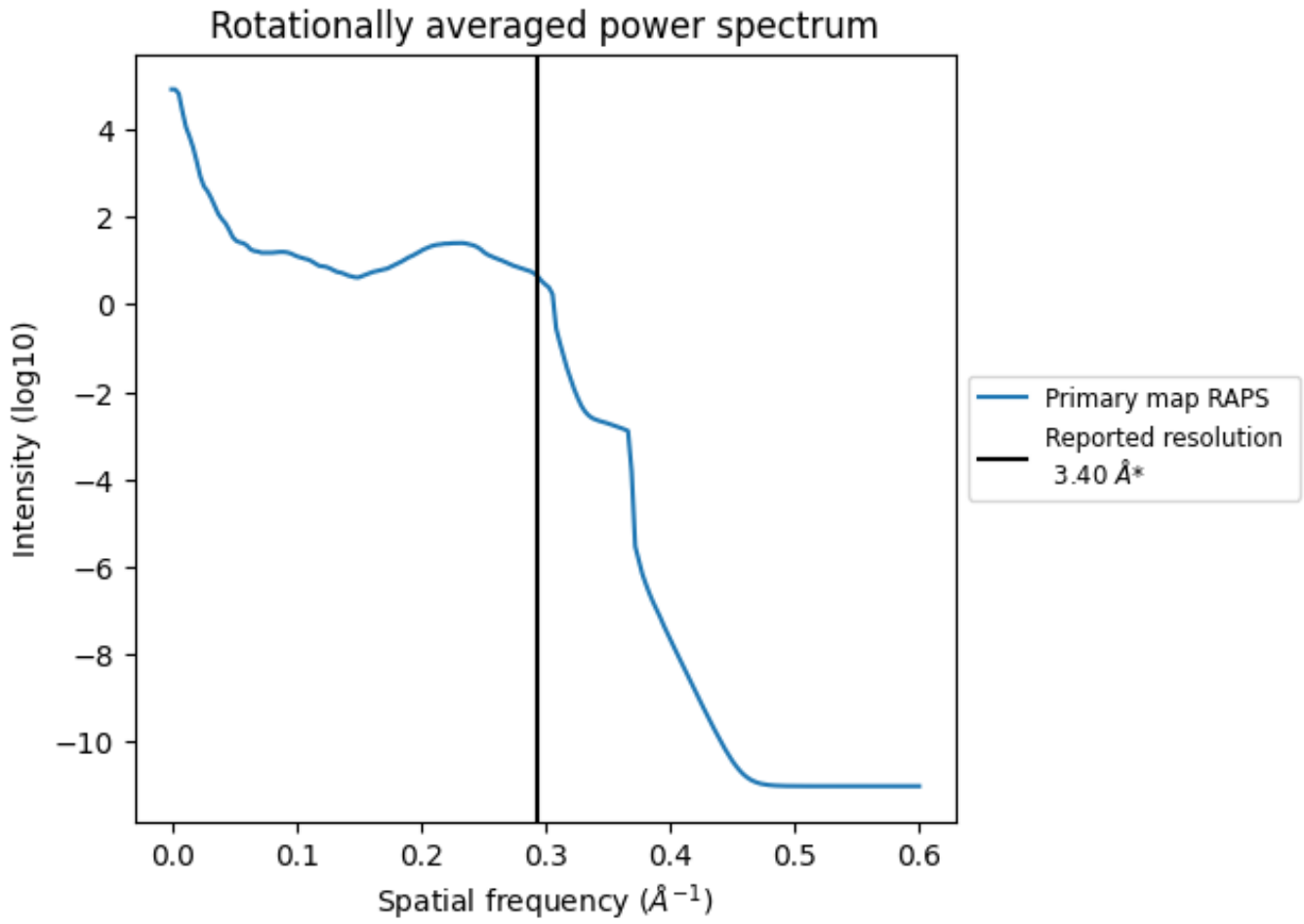
7.2 Volume estimate (i)



The volume at the recommended contour level is 79 nm^3; this corresponds to an approximate mass of 71 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 (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

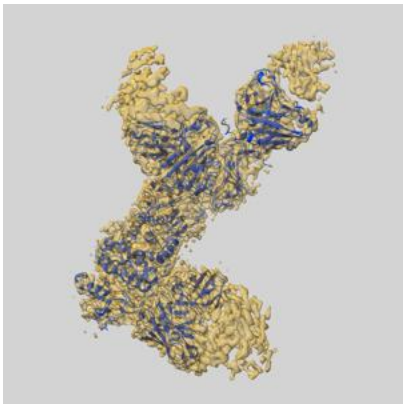
8 Fourier-Shell correlation

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

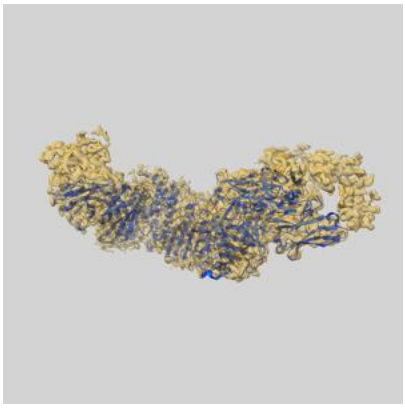
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-79526 and PDB model 39JB. Per-residue inclusion information can be found in section 3 on page 7.

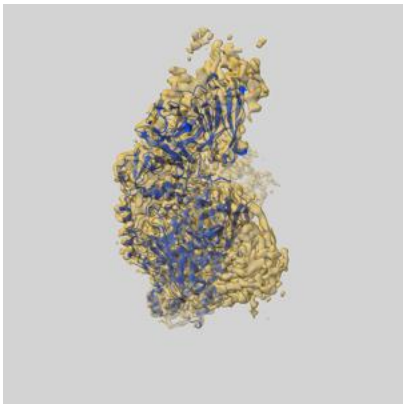
9.1 Map-model overlay



X



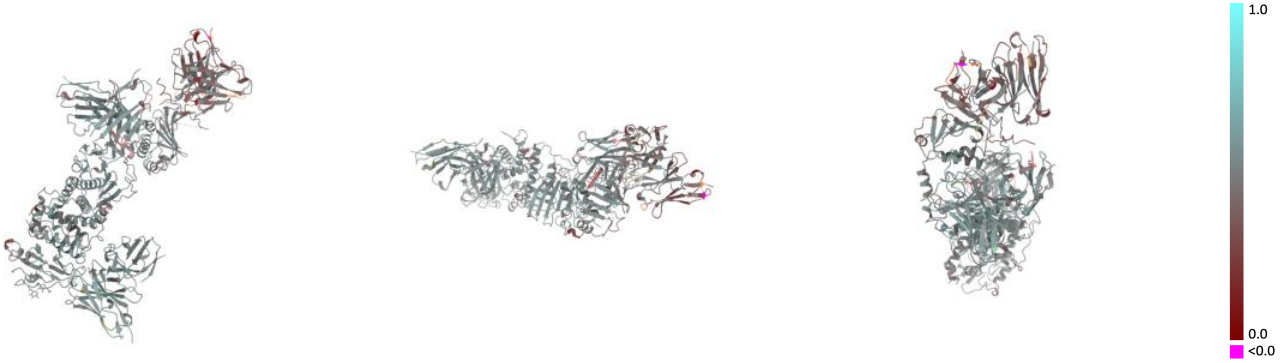
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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.

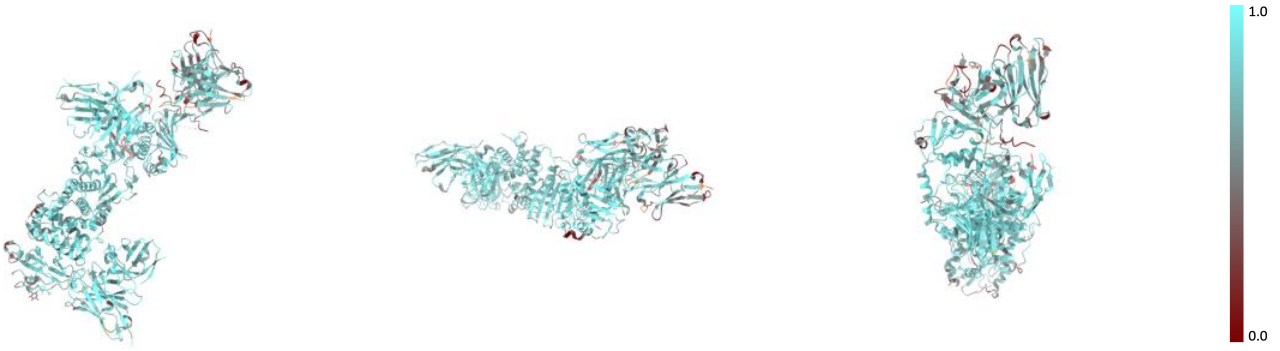
9.2 Q-score mapped to coordinate model (i)



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.

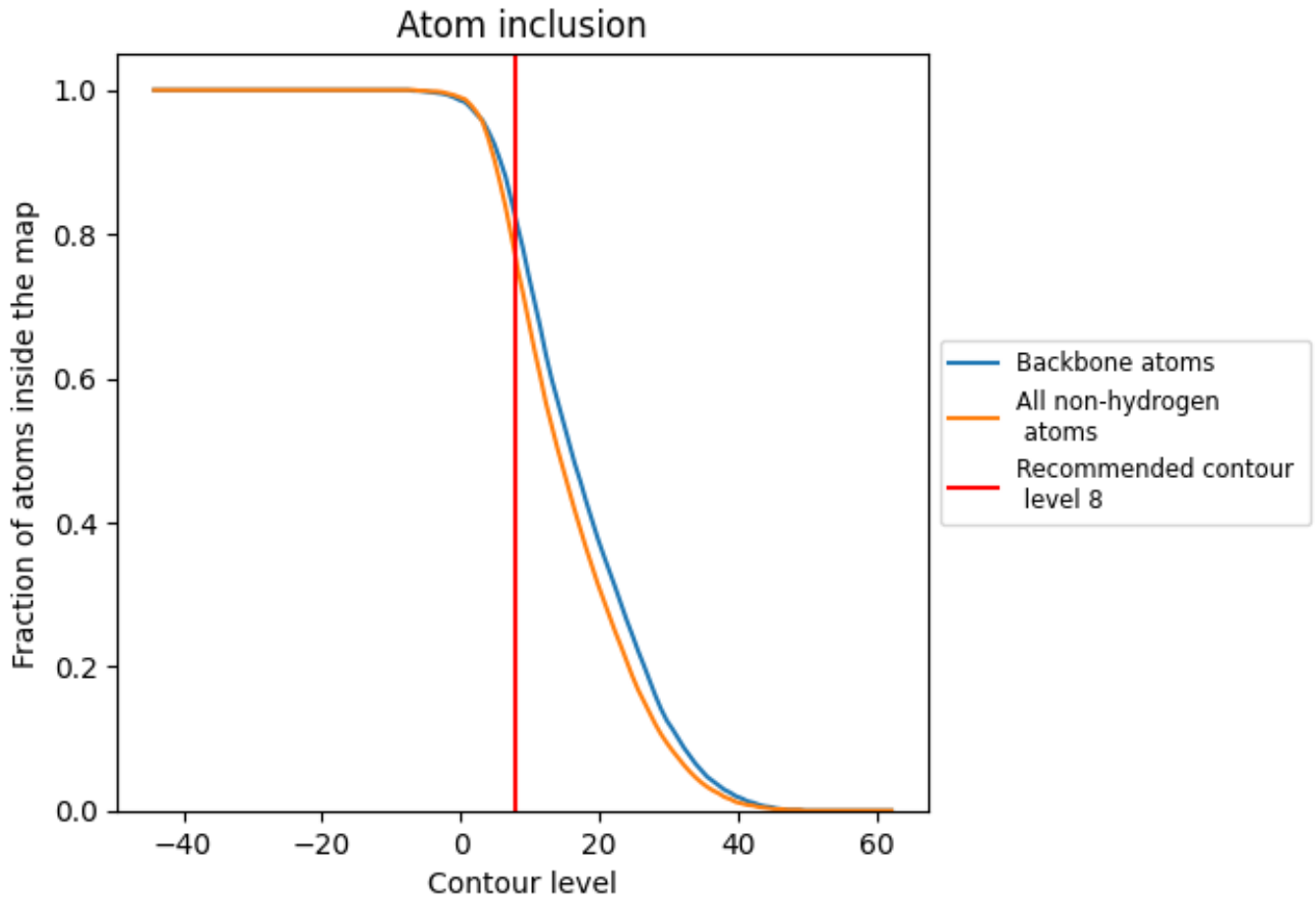
9.3 Atom inclusion mapped to coordinate model (i)



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 (8).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.4970
A	0.7820	0.5090
B	0.8300	0.5240
C	0.8340	0.5220
D	0.6460	0.4220
E	0.6150	0.3990
F	0.6070	0.5200
G	0.7930	0.5300
H	0.8100	0.5270
U	0.6990	0.4770

