wwPDB EM Validation Summary Report

Nov 9, 2026 – 07:26 PM JST

PDB ID	:	46DJ / pdb_000046dj
EMDB ID	:	EMD-83707
Title	:	Cryo-EM structure of a stabilized HCMV pentameric complex bound to antibodies 2C12, 7I13, and 13H11 (Composite Map)
Authors	:	Liu, P.; Yu, J.; Liu, T.; Liu, Y.; Wang, X.
Deposited on	:	2026-09-18
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:

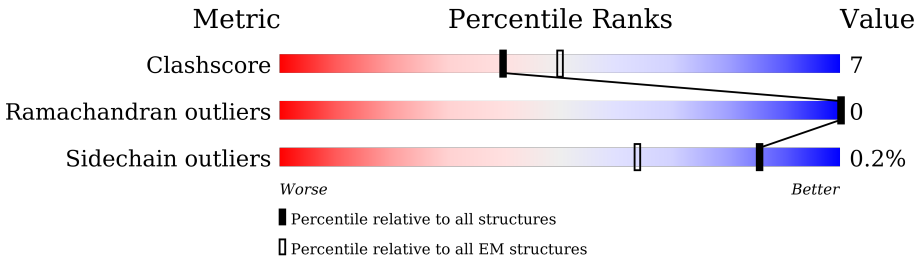
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

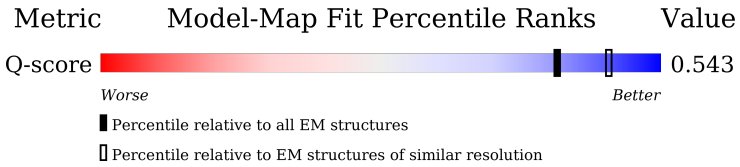
1 Overall quality at a glance (i)

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	A	728	15% 70% 15% 14%
2	B	278	72% 12% 16%
3	C	171	6% 60% 13% 27%
4	D	228	60% 12% 28%

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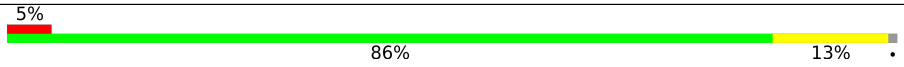
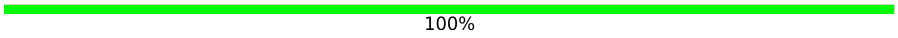
Mol	Chain	Length	Quality of chain
5	E	129	
6	H	124	
7	L	107	
8	P	125	
9	Q	113	
10	X	123	
11	Y	107	
12	F	2	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 15465 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	623	5017	3216	848	929	24	0	0

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P17176
A	1	ARG	-	expression tag	UNP P17176
A	2	PRO	-	expression tag	UNP P17176
A	3	GLY	-	expression tag	UNP P17176
A	4	LEU	-	expression tag	UNP P17176
A	5	PRO	-	expression tag	UNP P17176
A	6	SER	-	expression tag	UNP P17176
A	7	TYR	-	expression tag	UNP P17176
A	8	LEU	-	expression tag	UNP P17176
A	9	ILE	-	expression tag	UNP P17176
A	10	ILE	-	expression tag	UNP P17176
A	11	LEU	-	expression tag	UNP P17176
A	12	ALA	-	expression tag	UNP P17176
A	13	VAL	-	expression tag	UNP P17176
A	14	CYS	-	expression tag	UNP P17176
A	15	LEU	-	expression tag	UNP P17176
A	16	PHE	-	expression tag	UNP P17176
A	17	SER	-	expression tag	UNP P17176
A	18	HIS	-	expression tag	UNP P17176
A	19	LEU	-	expression tag	UNP P17176
A	20	LEU	-	expression tag	UNP P17176
A	21	SER	-	expression tag	UNP P17176
A	22	SER	-	expression tag	UNP P17176
A	23	GLN	-	expression tag	UNP P17176
A	24	TYR	-	expression tag	UNP P17176
A	25	GLY	-	expression tag	UNP P17176
A	26	ALA	-	expression tag	UNP P17176
A	27	ASP	-	expression tag	UNP P17176

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	-	expression tag	UNP P17176
A	29	ALA	-	expression tag	UNP P17176
A	30	SER	-	expression tag	UNP P17176
A	31	GLU	-	expression tag	UNP P17176
A	32	ALA	-	expression tag	UNP P17176
A	33	LEU	-	expression tag	UNP P17176
A	34	ASP	-	expression tag	UNP P17176
A	35	PRO	-	expression tag	UNP P17176
A	36	HIS	-	expression tag	UNP P17176
A	716	LEU	-	expression tag	UNP P17176
A	717	VAL	-	expression tag	UNP P17176
A	718	PRO	-	expression tag	UNP P17176
A	719	ARG	-	expression tag	UNP P17176
A	720	GLY	-	expression tag	UNP P17176
A	721	SER	-	expression tag	UNP P17176
A	722	HIS	-	expression tag	UNP P17176
A	723	HIS	-	expression tag	UNP P17176
A	724	HIS	-	expression tag	UNP P17176
A	725	HIS	-	expression tag	UNP P17176
A	726	HIS	-	expression tag	UNP P17176
A	727	HIS	-	expression tag	UNP P17176

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	233	Total	C	N	O	S	0	0
			1843	1173	323	339	8		

- Molecule 3 is a protein called UL128.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	124	Total	C	N	O	S	0	0
			999	626	182	182	9		

- Molecule 4 is a protein called Envelope glycoprotein UL130.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	164	Total	C	N	O	S	0	0
			1340	859	231	242	8		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	35	LYS	GLN	conflict	UNP F5HCP3
D	65	GLU	PRO	conflict	UNP F5HCP3
D	66	PHE	ARG	conflict	UNP F5HCP3
D	98	ILE	THR	conflict	UNP F5HCP3
D	215	LEU	-	expression tag	UNP F5HCP3
D	216	VAL	-	expression tag	UNP F5HCP3
D	217	PRO	-	expression tag	UNP F5HCP3
D	218	ARG	-	expression tag	UNP F5HCP3
D	219	GLY	-	expression tag	UNP F5HCP3
D	220	SER	-	expression tag	UNP F5HCP3
D	221	TRP	-	expression tag	UNP F5HCP3
D	222	SER	-	expression tag	UNP F5HCP3
D	223	HIS	-	expression tag	UNP F5HCP3
D	224	PRO	-	expression tag	UNP F5HCP3
D	225	GLN	-	expression tag	UNP F5HCP3
D	226	PHE	-	expression tag	UNP F5HCP3
D	227	GLU	-	expression tag	UNP F5HCP3
D	228	LYS	-	expression tag	UNP F5HCP3

- Molecule 5 is a protein called Protein UL131A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	111	Total	C	N	O	S	0	0
			917	571	173	171	2		

- Molecule 6 is a protein called 7I13 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	122	Total	C	N	O	S	0	0
			960	612	163	181	4		

- Molecule 7 is a protein called 7I13 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	106	Total	C	N	O	S	0	0
			804	506	138	158	2		

- Molecule 8 is a protein called 2C12 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	123	Total	C	N	O	S	0	0
			953	610	158	180	5		

- Molecule 9 is a protein called 2C12 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	112	Total	C	N	O	S	0	0
			828	519	140	165	4		

- Molecule 10 is a protein called 13H11 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	121	Total	C	N	O	S	0	0
			924	581	160	178	5		

- Molecule 11 is a protein called 13H11 Light chain.

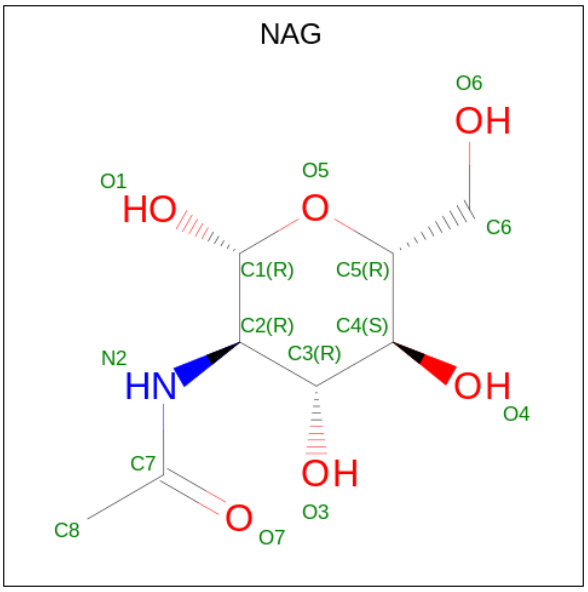
Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	104	Total	C	N	O	S	0	0
			782	496	130	153	3		

- Molecule 12 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
12	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	B	1	Total	C	N	O	0
			14	8	1	5	
13	D	1	Total	C	N	O	0
			14	8	1	5	
13	E	1	Total	C	N	O	0
			14	8	1	5	

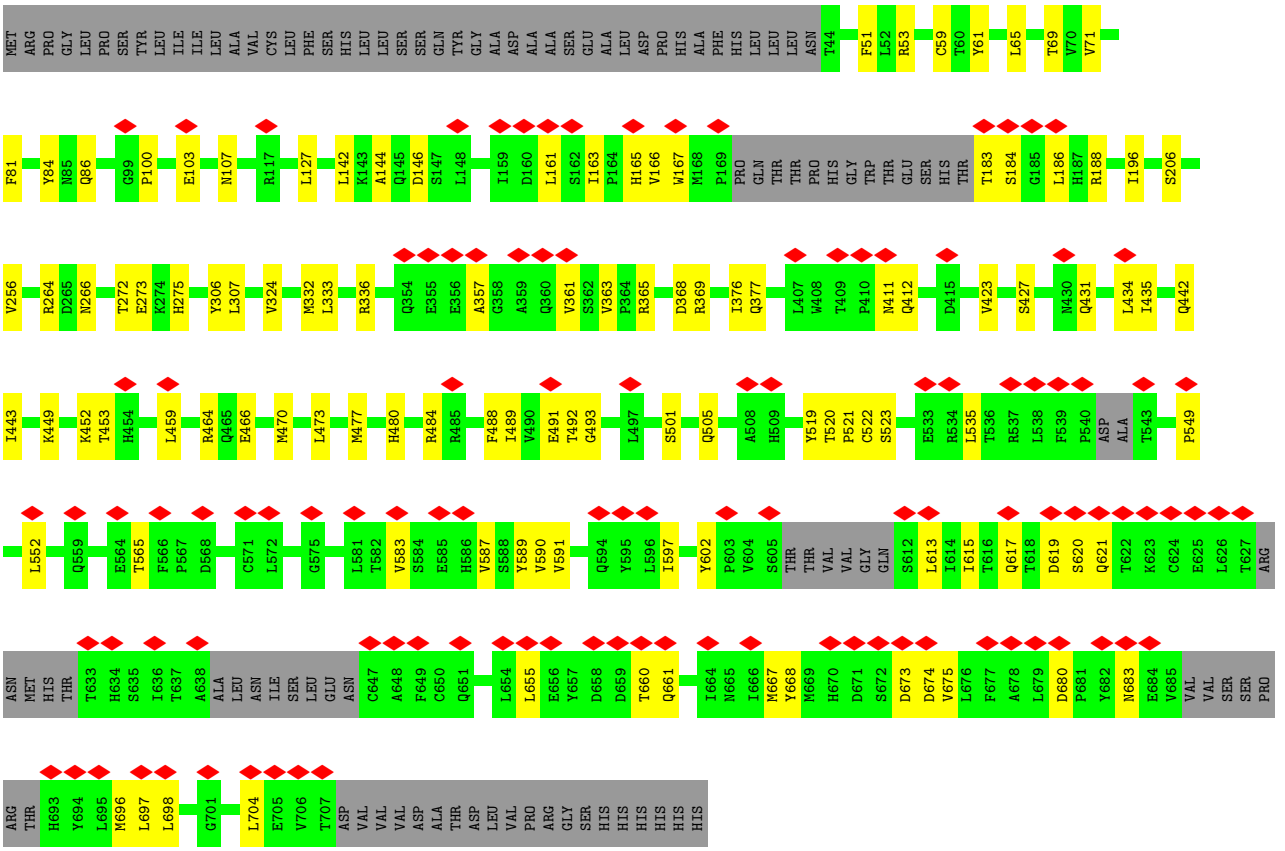
3 Residue-property plots (i)

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: Envelope glycoprotein H

Chain A:

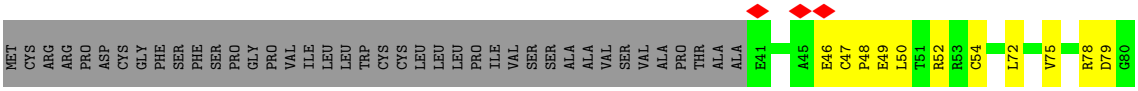




• Molecule 2: Envelope glycoprotein L

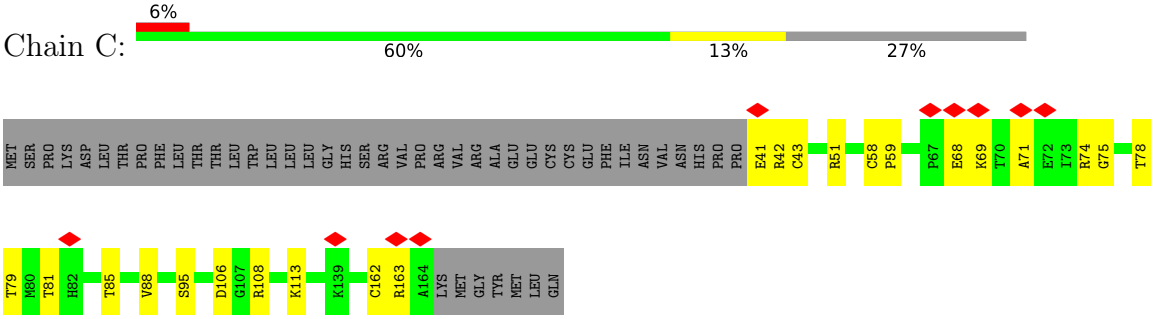
Chain B:



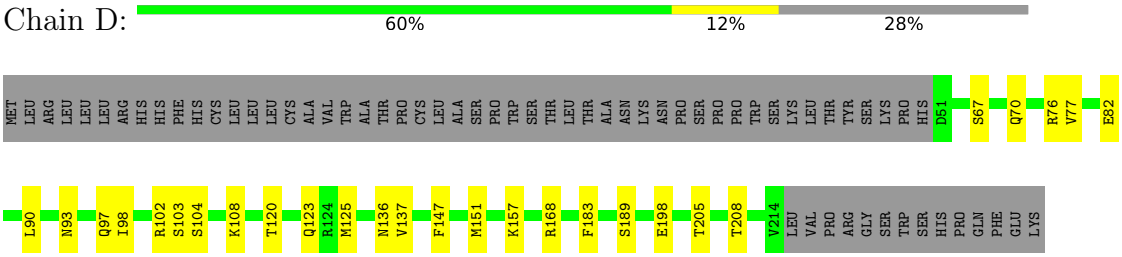




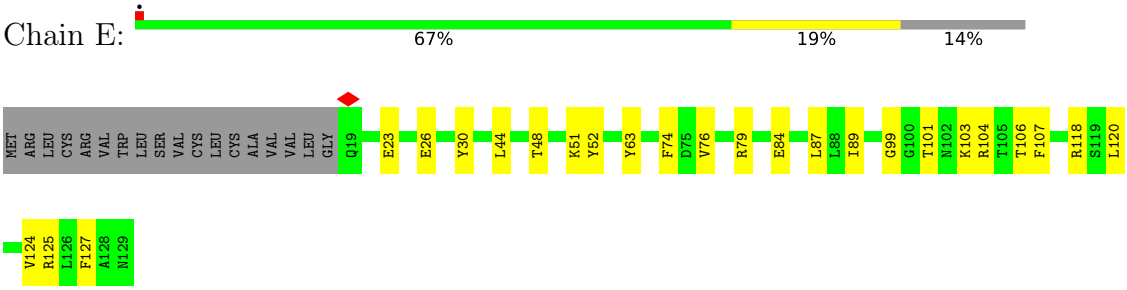
• Molecule 3: UL128



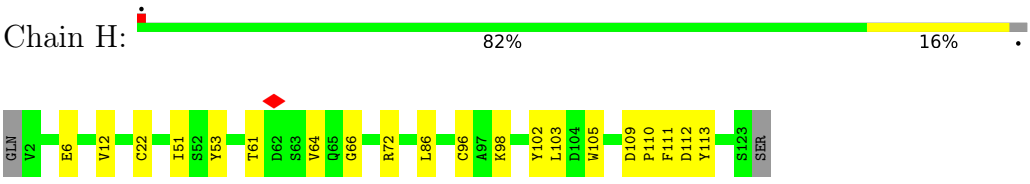
• Molecule 4: Envelope glycoprotein UL130



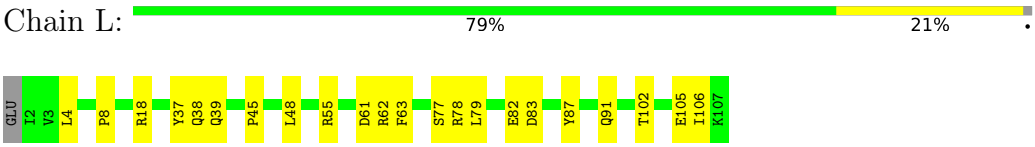
• Molecule 5: Protein UL131A



• Molecule 6: 7I13 Heavy chain



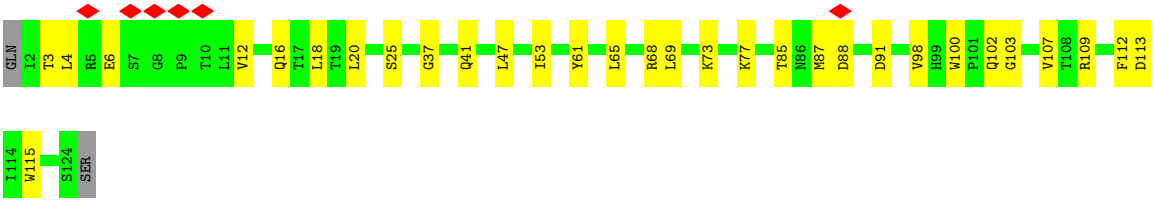
• Molecule 7: 7I13 Light chain



• Molecule 8: 2C12 Heavy chain

Chain P:





• Molecule 9: 2C12 Light chain

Chain Q:

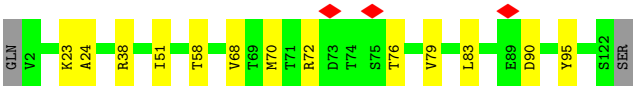




• Molecule 10: 13H11 Heavy chain

Chain X:





• Molecule 11: 13H11 Light chain

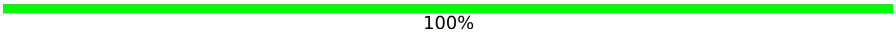
Chain Y:





• Molecule 12: 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	165404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.132	Depositor
Minimum map value	-2.765	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.12	0/5132	0.31	0/6982
2	B	0.18	0/1888	0.34	0/2577
3	C	0.17	0/1017	0.42	0/1372
4	D	0.18	0/1376	0.34	0/1868
5	E	0.15	0/937	0.34	0/1268
6	H	0.14	0/985	0.30	0/1336
7	L	0.14	0/823	0.28	0/1118
8	P	0.16	0/977	0.32	0/1339
9	Q	0.14	0/848	0.32	0/1151
10	X	0.13	0/944	0.31	0/1280
11	Y	0.13	0/800	0.33	0/1089
All	All	0.15	0/15727	0.33	0/21380

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	5017	0	4971	75	0
2	B	1843	0	1837	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	999	0	1001	17	0
4	D	1340	0	1312	18	0
5	E	917	0	878	23	0
6	H	960	0	915	13	0
7	L	804	0	782	14	0
8	P	953	0	951	21	0
9	Q	828	0	792	11	0
10	X	924	0	900	8	0
11	Y	782	0	773	11	0
12	F	28	0	25	0	0
13	A	28	0	26	1	0
13	B	14	0	13	0	0
13	D	14	0	13	0	0
13	E	14	0	13	0	0
All	All	15465	0	15202	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 218 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)
5:E:103:LYS:HZ2	5:E:104:ARG:HH21	1.25	0.84
1:A:196:ILE:HD11	1:A:206:SER:HB2	1.62	0.81
3:C:162:CYS:SG	3:C:163:ARG:N	2.61	0.73
1:A:256:VAL:O	1:A:264:ARG:NH2	2.24	0.69
1:A:183:THR:N	1:A:361:VAL:O	2.25	0.69

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	609/728 (84%)	586 (96%)	23 (4%)	0	100	100
2	B	231/278 (83%)	214 (93%)	17 (7%)	0	100	100
3	C	122/171 (71%)	115 (94%)	7 (6%)	0	100	100
4	D	162/228 (71%)	157 (97%)	5 (3%)	0	100	100
5	E	109/129 (84%)	107 (98%)	2 (2%)	0	100	100
6	H	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
7	L	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
8	P	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
9	Q	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
10	X	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
11	Y	102/107 (95%)	98 (96%)	4 (4%)	0	100	100
All	All	1909/2233 (86%)	1835 (96%)	74 (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	A	566/657 (86%)	565 (100%)	1 (0%)	87	85
2	B	202/238 (85%)	202 (100%)	0	100	100
3	C	110/154 (71%)	110 (100%)	0	100	100
4	D	150/209 (72%)	149 (99%)	1 (1%)	76	78
5	E	98/114 (86%)	98 (100%)	0	100	100
6	H	102/104 (98%)	102 (100%)	0	100	100
7	L	87/88 (99%)	87 (100%)	0	100	100
8	P	108/110 (98%)	108 (100%)	0	100	100
9	Q	92/93 (99%)	92 (100%)	0	100	100
10	X	101/103 (98%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	Y	87/90 (97%)	86 (99%)	1 (1%)	65 74
All	All	1703/1960 (87%)	1700 (100%)	3 (0%)	85 85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	675	VAL
4	D	137	VAL
11	Y	48	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
9	Q	81	GLN
10	X	35	HIS
1	A	377	GLN
1	A	661	GLN
4	D	138	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)

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	$\#\|Z\|>2$
12	NAG	F	1	12,1	14,14,15	0.29	0	17,19,21	0.55	0
12	NAG	F	2	12	14,14,15	0.52	0	17,19,21	0.59	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
12	NAG	F	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	F	2	12	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

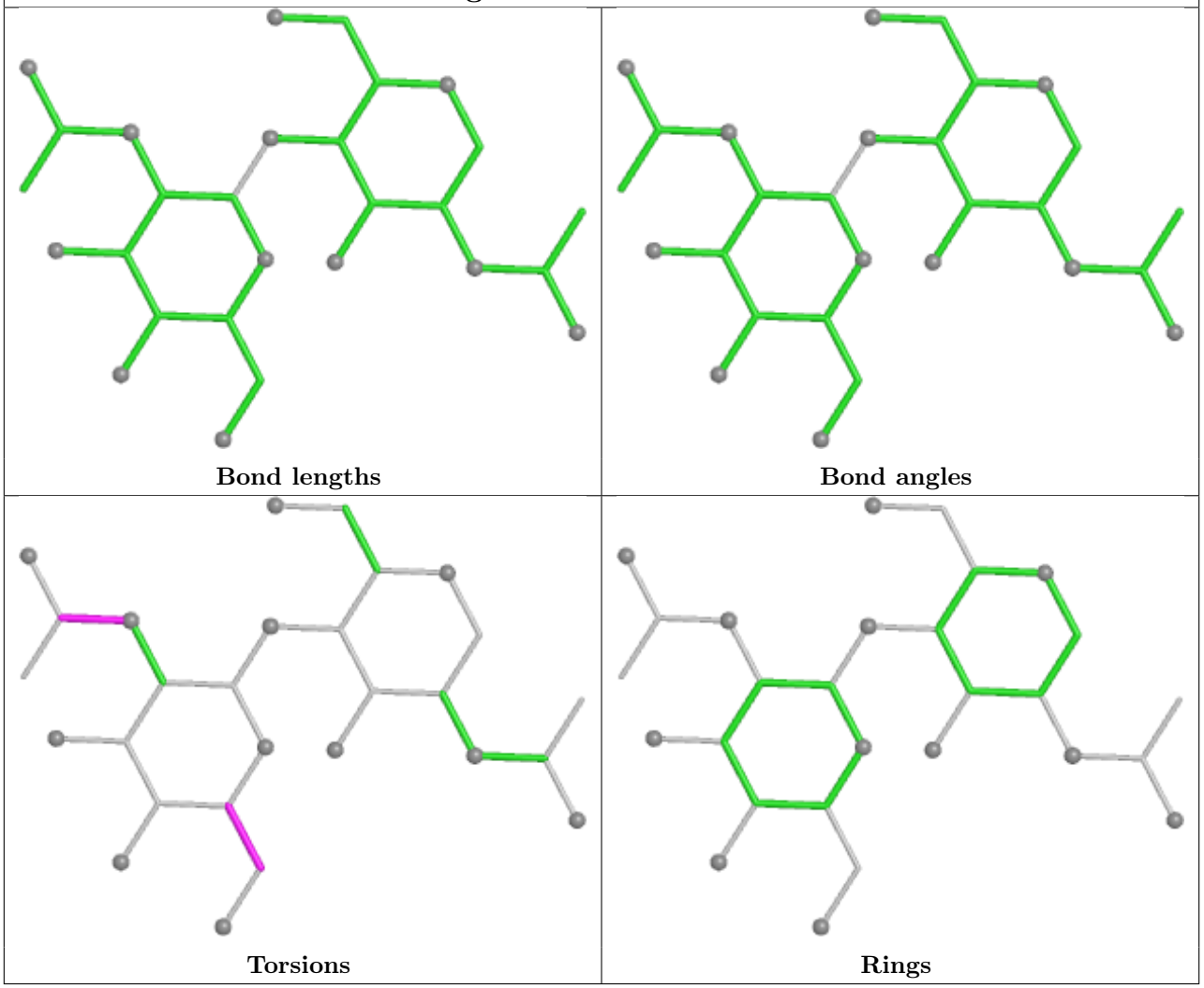
Mol	Chain	Res	Type	Atoms
12	F	2	NAG	C4-C5-C6-O6
12	F	2	NAG	O5-C5-C6-O6
12	F	2	NAG	C8-C7-N2-C2
12	F	2	NAG	O7-C7-N2-C2

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



5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
13	NAG	A	801	1	14,14,15	0.22	0	17,19,21	0.45	0
13	NAG	B	301	2	14,14,15	0.15	0	17,19,21	0.40	0
13	NAG	E	201	5	14,14,15	0.23	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	A	802	1	14,14,15	0.18	0	17,19,21	0.42	0
13	NAG	D	301	4	14,14,15	0.23	0	17,19,21	0.46	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
13	NAG	A	801	1	-	2/6/23/26	0/1/1/1
13	NAG	B	301	2	-	2/6/23/26	0/1/1/1
13	NAG	E	201	5	-	1/6/23/26	0/1/1/1
13	NAG	A	802	1	-	2/6/23/26	0/1/1/1
13	NAG	D	301	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	NAG	C4-C5-C6-O6
13	B	301	NAG	O5-C5-C6-O6
13	A	801	NAG	O5-C5-C6-O6
13	B	301	NAG	C4-C5-C6-O6
13	E	201	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
13	A	802	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

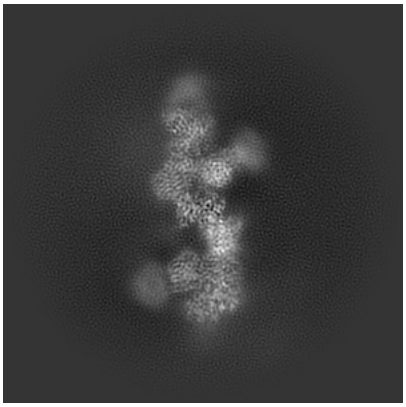
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-83707. These allow visual inspection of the internal detail of the map and identification of artifacts.

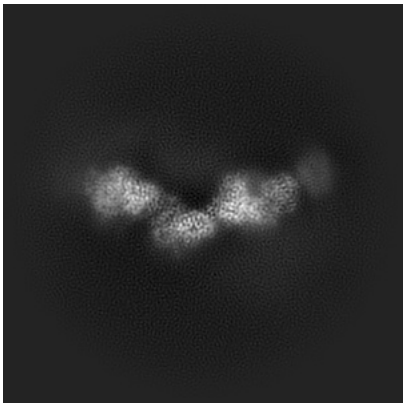
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

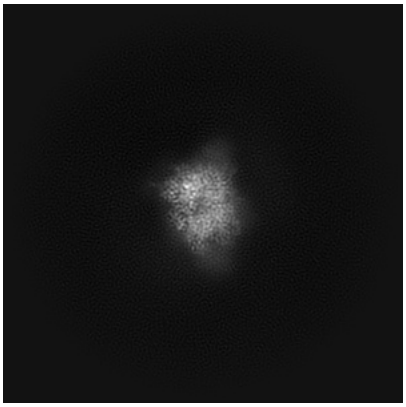
6.1.1 Primary map



X



Y

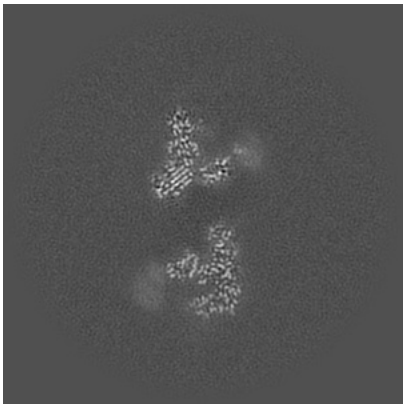


Z

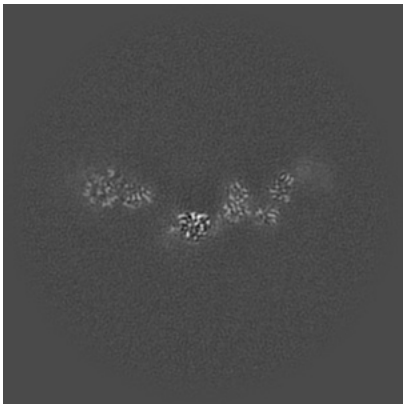
The images above show the map projected in three orthogonal directions.

6.2 Central slices

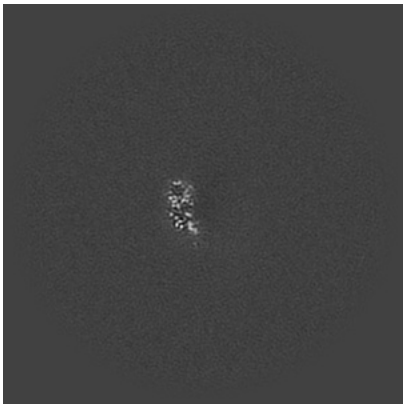
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

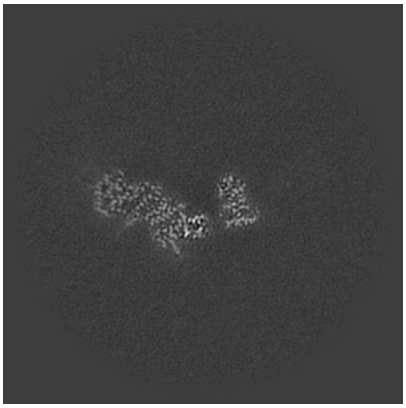
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

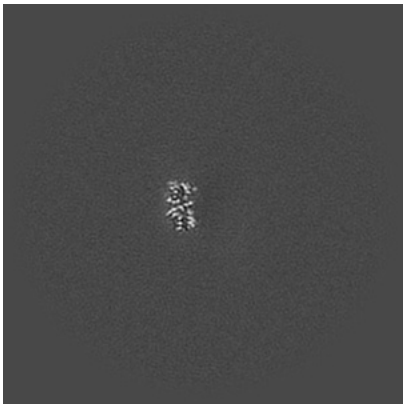
6.3.1 Primary map



X Index: 168



Y Index: 195

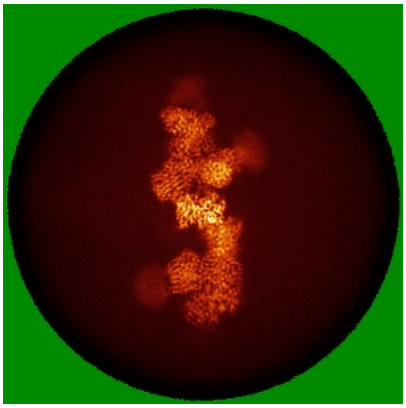


Z Index: 176

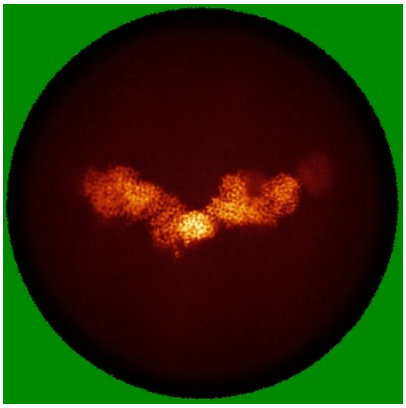
The images above show the largest variance slices of the map in three orthogonal directions.

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

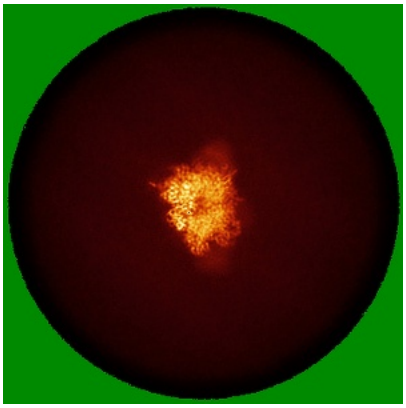
6.4.1 Primary map



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

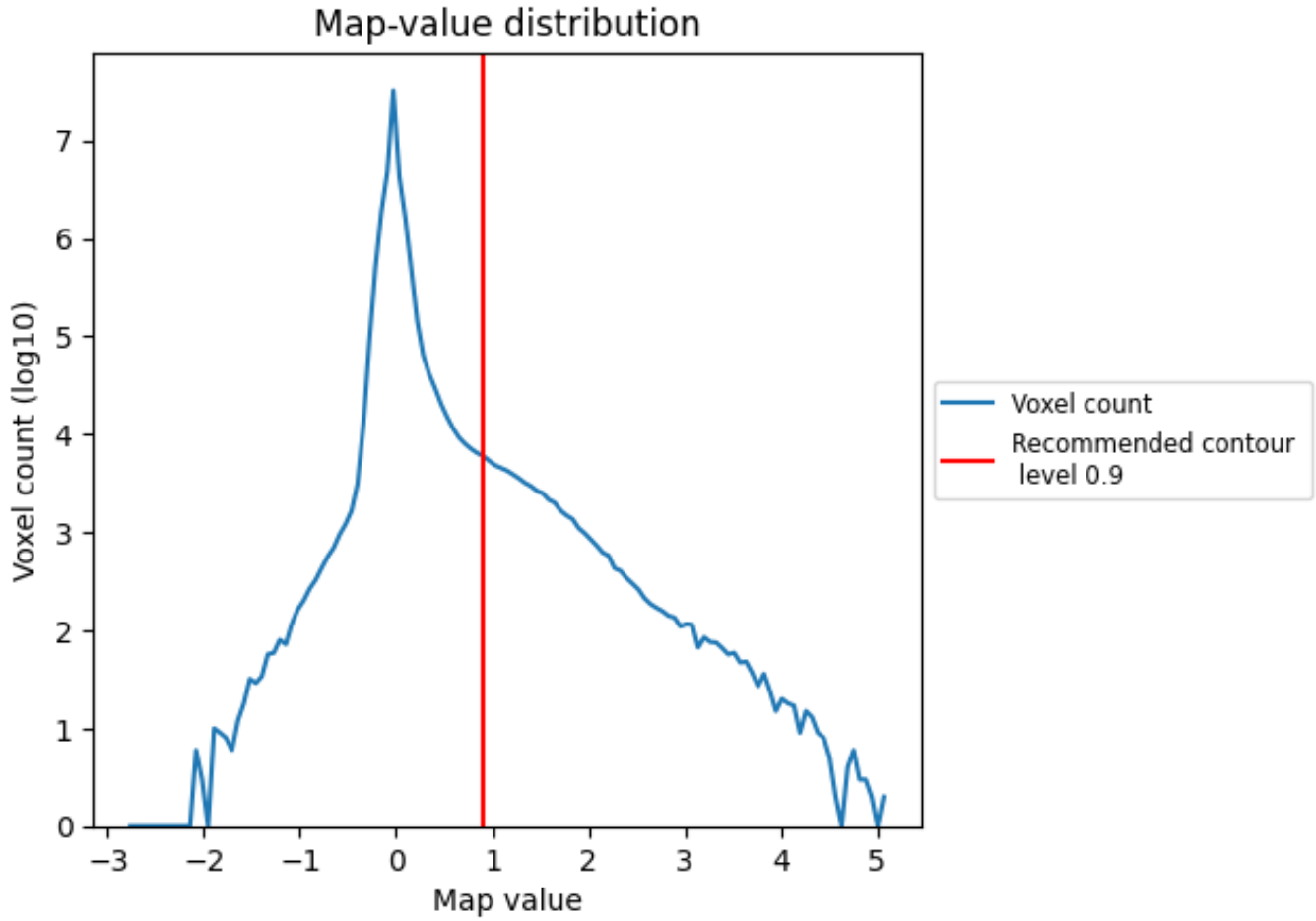
6.6 Mask visualisation (i)

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

7 Map analysis

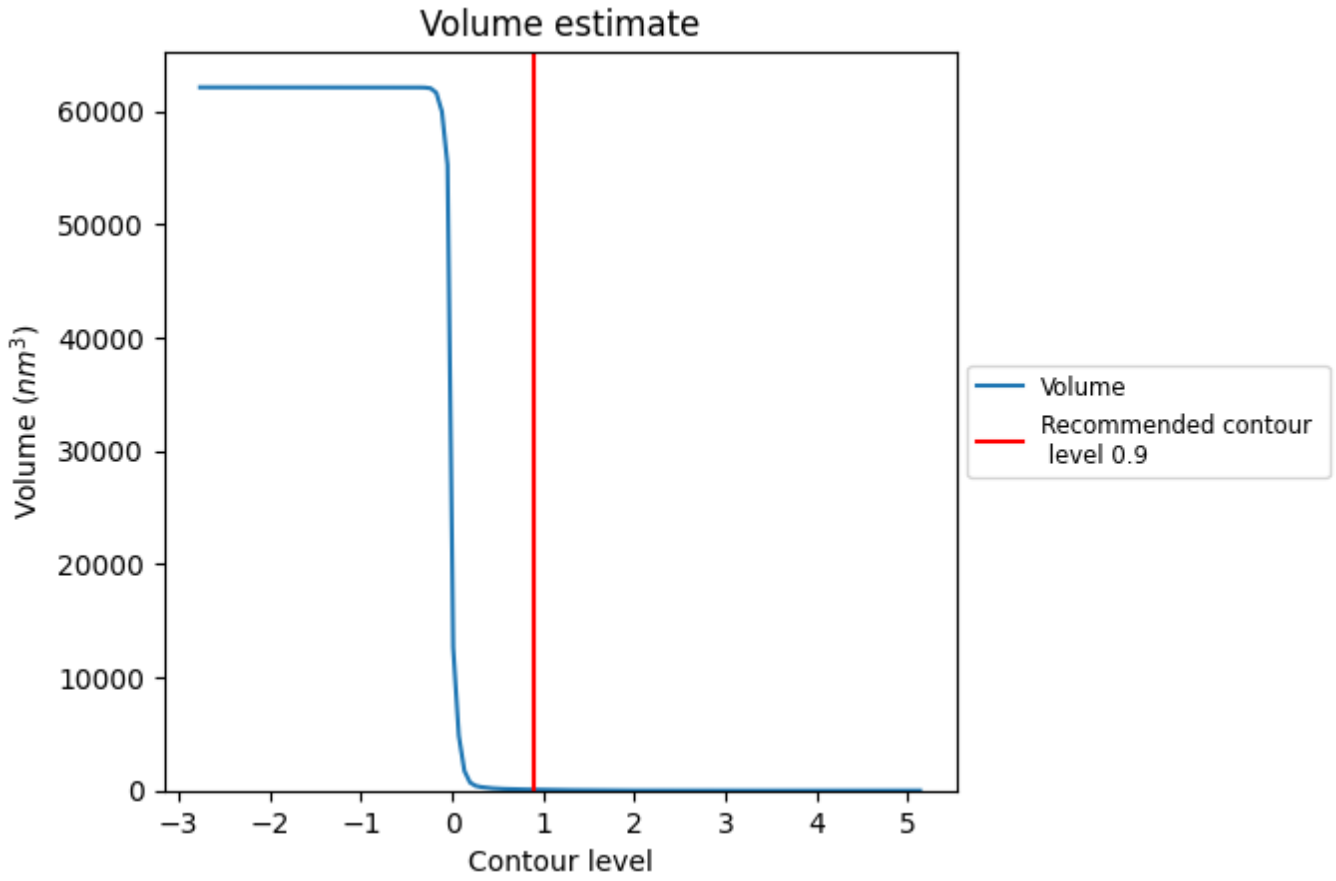
This section contains the results of statistical analysis of the map.

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.

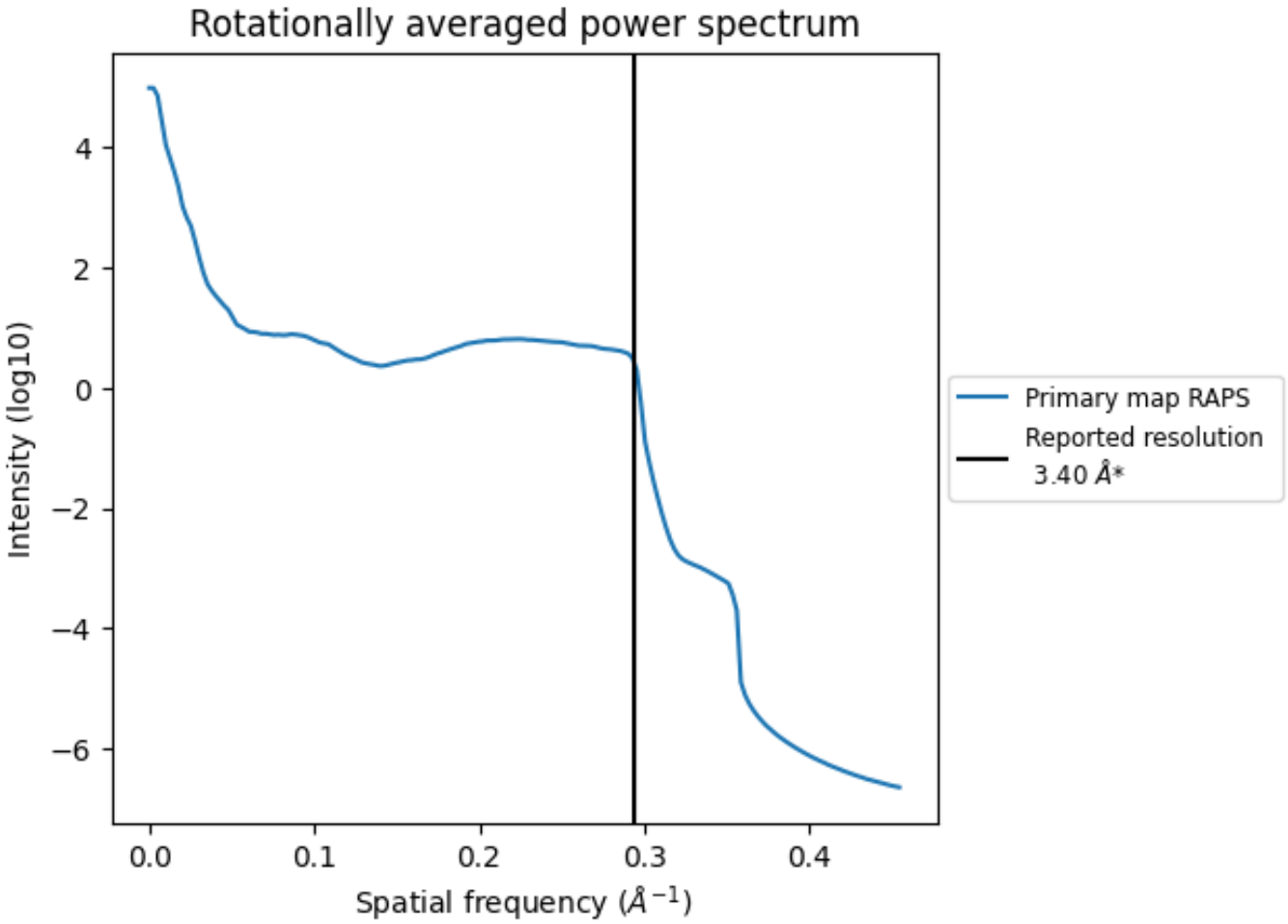
7.2 Volume estimate (i)



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 74 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}

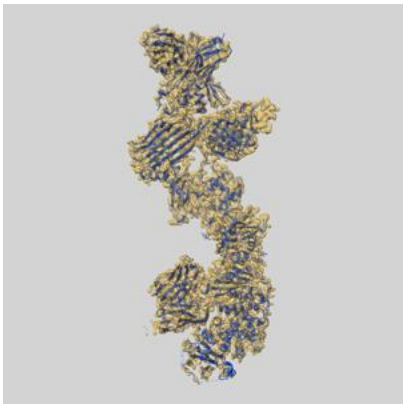
8 Fourier-Shell correlation

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

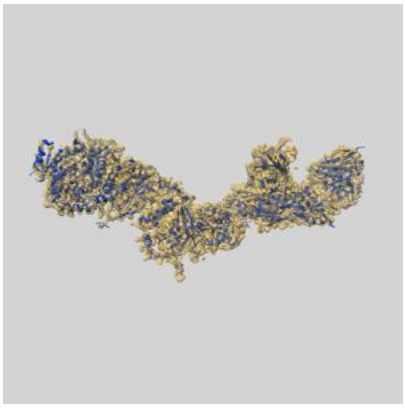
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-83707 and PDB model 46DJ. Per-residue inclusion information can be found in section 3 on page 9.

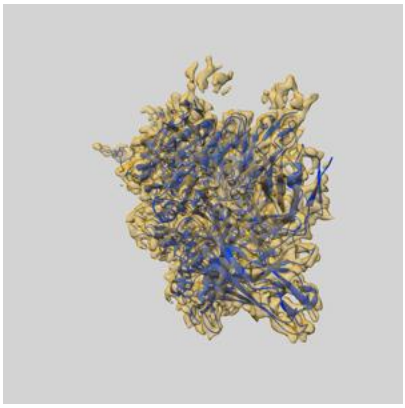
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



X Y Z

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

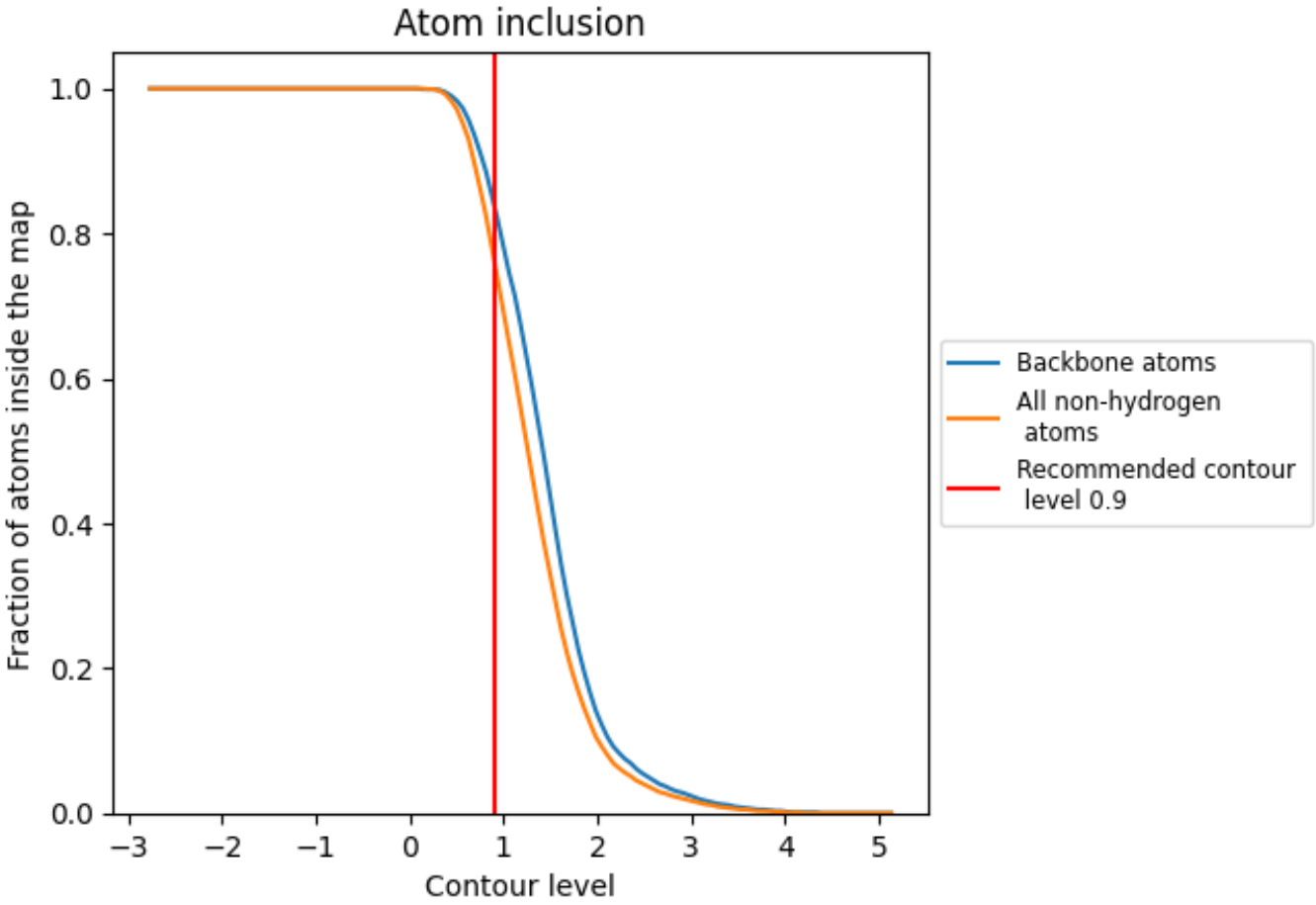
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 84% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.5430
A	0.6420	0.5290
B	0.8730	0.5450
C	0.7380	0.5390
D	0.9140	0.5520
E	0.8200	0.5530
F	0.8210	0.4490
H	0.8850	0.5620
L	0.8940	0.5580
P	0.7650	0.5450
Q	0.7470	0.5540
X	0.7530	0.5530
Y	0.7590	0.5490

