



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 07:18 AM EST

PDB ID : 6C5V  
EMDB ID : EMD-7344  
Title : An anti-gH/gL antibody that neutralizes dual-tropic infection defines a site of vulnerability on Epstein-Barr virus  
Authors : Snijder, J.; Ortego, M.S.; Weidle, C.; Stuart, A.B.; Gray, M.A.; McElrath, M.J.; Pancera, M.; Veesler, D.; McGuire, A.T.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2018-01-16  
Resolution : 4.80 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](mailto: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>.

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

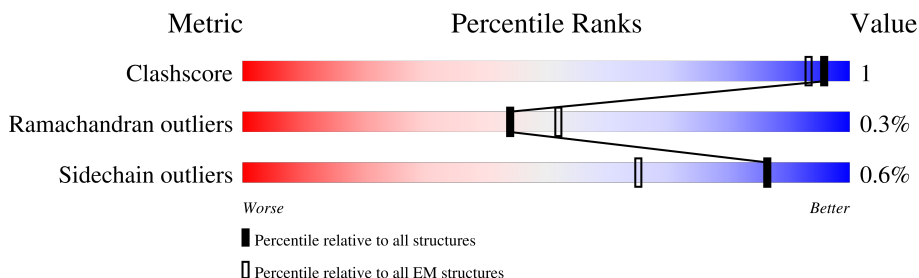
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 4.80 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  $\geq 3$ , 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	697	
2	B	139	
3	C	227	
4	H	226	
5	L	216	
6	D	6	

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 10649 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	655	5101	3273	841	956	31	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP K9US75
A	-5	ASP	-	expression tag	UNP K9US75
A	-4	ALA	-	expression tag	UNP K9US75
A	-3	MET	-	expression tag	UNP K9US75
A	-2	LYS	-	expression tag	UNP K9US75
A	-1	ARG	-	expression tag	UNP K9US75
A	0	GLY	-	expression tag	UNP K9US75
A	1	LEU	-	expression tag	UNP K9US75
A	2	CYS	-	expression tag	UNP K9US75
A	3	CYS	-	expression tag	UNP K9US75
A	4	VAL	-	expression tag	UNP K9US75
A	5	LEU	-	expression tag	UNP K9US75
A	6	LEU	-	expression tag	UNP K9US75
A	7	LEU	-	expression tag	UNP K9US75
A	8	CYS	-	expression tag	UNP K9US75
A	9	GLY	-	expression tag	UNP K9US75
A	10	ALA	-	expression tag	UNP K9US75
A	11	VAL	-	expression tag	UNP K9US75
A	12	PHE	-	expression tag	UNP K9US75
A	13	VAL	-	expression tag	UNP K9US75
A	14	SER	-	expression tag	UNP K9US75
A	15	PRO	-	expression tag	UNP K9US75
A	16	SER	-	expression tag	UNP K9US75
A	17	ALA	-	expression tag	UNP K9US75
A	18	SER	-	expression tag	UNP K9US75
A	680	GLY	-	expression tag	UNP K9US75
A	681	SER	-	expression tag	UNP K9US75
A	682	GLY	-	expression tag	UNP K9US75

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Chain	Residue	Modelled	Actual	Comment	Reference
A	683	SER	-	expression tag	UNP K9US75
A	684	GLY	-	expression tag	UNP K9US75
A	685	HIS	-	expression tag	UNP K9US75
A	686	HIS	-	expression tag	UNP K9US75
A	687	HIS	-	expression tag	UNP K9US75
A	688	HIS	-	expression tag	UNP K9US75
A	689	HIS	-	expression tag	UNP K9US75
A	690	HIS	-	expression tag	UNP K9US75

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
2	B	94	716	453	120	139	4	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP Q1HVF6
B	0	ASP	-	expression tag	UNP Q1HVF6
B	1	ALA	-	expression tag	UNP Q1HVF6
B	2	MET	-	expression tag	UNP Q1HVF6
B	3	LYS	-	expression tag	UNP Q1HVF6
B	4	ARG	-	expression tag	UNP Q1HVF6
B	5	GLY	-	expression tag	UNP Q1HVF6
B	6	LEU	-	expression tag	UNP Q1HVF6
B	7	CYS	-	expression tag	UNP Q1HVF6
B	8	CYS	-	expression tag	UNP Q1HVF6
B	9	VAL	-	expression tag	UNP Q1HVF6
B	10	LEU	-	expression tag	UNP Q1HVF6
B	11	LEU	-	expression tag	UNP Q1HVF6
B	12	LEU	-	expression tag	UNP Q1HVF6
B	13	CYS	-	expression tag	UNP Q1HVF6
B	14	GLY	-	expression tag	UNP Q1HVF6
B	15	ALA	-	expression tag	UNP Q1HVF6
B	16	VAL	-	expression tag	UNP Q1HVF6
B	17	PHE	-	expression tag	UNP Q1HVF6
B	18	VAL	-	expression tag	UNP Q1HVF6
B	19	SER	-	expression tag	UNP Q1HVF6
B	20	PRO	-	expression tag	UNP Q1HVF6
B	21	SER	-	expression tag	UNP Q1HVF6
B	22	ALA	-	expression tag	UNP Q1HVF6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	SER	-	expression tag	UNP Q1HVF6

- Molecule 3 is a protein called Glycoprotein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	177	1435	934	232	258	11	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	MET	-	expression tag	UNP P0C6Z5
C	9	ASP	-	expression tag	UNP P0C6Z5
C	10	ALA	-	expression tag	UNP P0C6Z5
C	11	MET	-	expression tag	UNP P0C6Z5
C	12	LYS	-	expression tag	UNP P0C6Z5
C	13	ARG	-	expression tag	UNP P0C6Z5
C	14	GLY	-	expression tag	UNP P0C6Z5
C	15	LEU	-	expression tag	UNP P0C6Z5
C	16	CYS	-	expression tag	UNP P0C6Z5
C	17	CYS	-	expression tag	UNP P0C6Z5
C	18	VAL	-	expression tag	UNP P0C6Z5
C	19	LEU	-	expression tag	UNP P0C6Z5
C	20	LEU	-	expression tag	UNP P0C6Z5
C	21	LEU	-	expression tag	UNP P0C6Z5
C	22	CYS	-	expression tag	UNP P0C6Z5
C	23	GLY	-	expression tag	UNP P0C6Z5
C	24	ALA	-	expression tag	UNP P0C6Z5
C	25	VAL	-	expression tag	UNP P0C6Z5
C	26	PHE	-	expression tag	UNP P0C6Z5
C	27	VAL	-	expression tag	UNP P0C6Z5
C	28	SER	-	expression tag	UNP P0C6Z5
C	29	PRO	-	expression tag	UNP P0C6Z5
C	30	SER	-	expression tag	UNP P0C6Z5
C	31	ALA	-	expression tag	UNP P0C6Z5
C	32	SER	-	expression tag	UNP P0C6Z5
C	224	GLY	-	expression tag	UNP P0C6Z5
C	225	SER	-	expression tag	UNP P0C6Z5
C	226	GLY	-	expression tag	UNP P0C6Z5
C	227	SER	-	expression tag	UNP P0C6Z5
C	228	GLY	-	expression tag	UNP P0C6Z5
C	229	HIS	-	expression tag	UNP P0C6Z5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	230	HIS	-	expression tag	UNP P0C6Z5
C	231	HIS	-	expression tag	UNP P0C6Z5
C	232	HIS	-	expression tag	UNP P0C6Z5
C	233	HIS	-	expression tag	UNP P0C6Z5
C	234	HIS	-	expression tag	UNP P0C6Z5

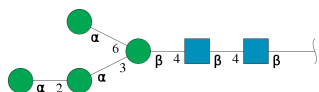
- Molecule 4 is a protein called Antibody Fab AMMO1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	215	1615	1022	272	313	8	0	0

- Molecule 5 is a protein called Antibody Fab AMMO1 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	212	1598	1001	274	319	4	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	D	6	72	40	2	30	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

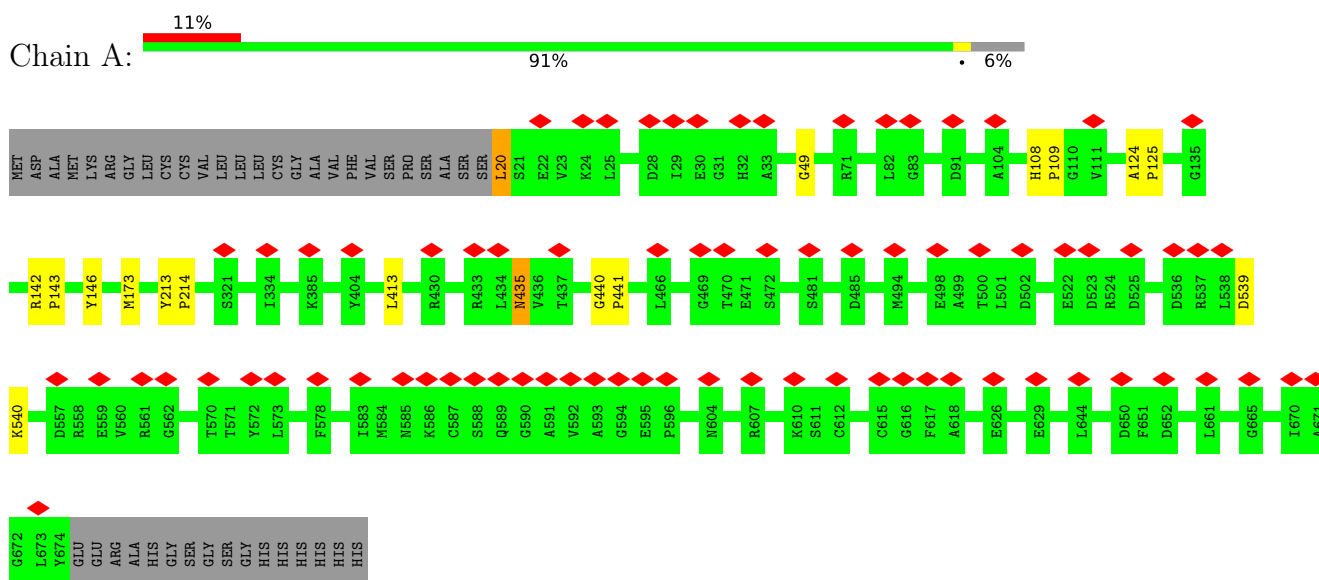


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total	C	N	O	0
			42	24	3	15	
7	A	1	Total	C	N	O	0
			42	24	3	15	
7	A	1	Total	C	N	O	0
			42	24	3	15	
7	B	1	Total	C	N	O	0
			28	16	2	10	
7	B	1	Total	C	N	O	0
			28	16	2	10	
7	C	1	Total	C	N	O	0
			42	24	3	15	
7	C	1	Total	C	N	O	0
			42	24	3	15	
7	C	1	Total	C	N	O	0
			42	24	3	15	

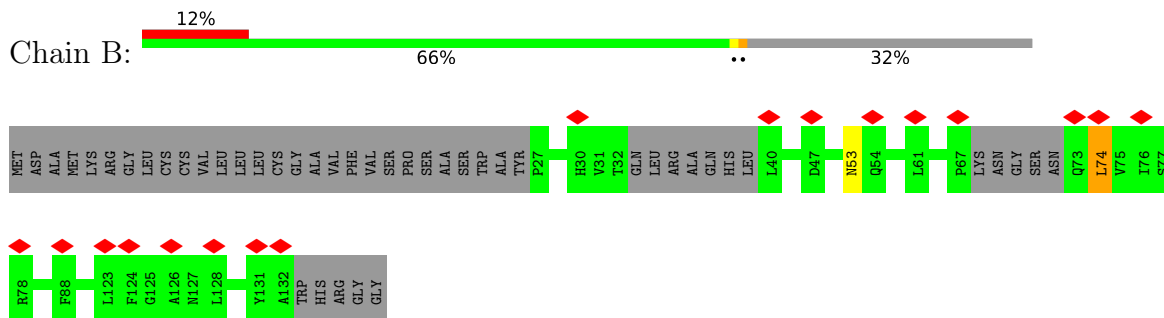
### 3 Residue-property plots [i](#)

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.

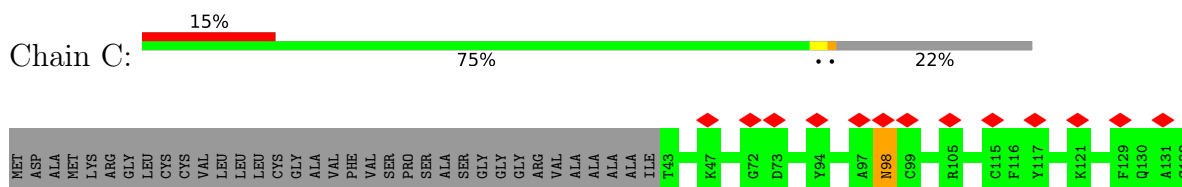
- Molecule 1: Envelope glycoprotein H



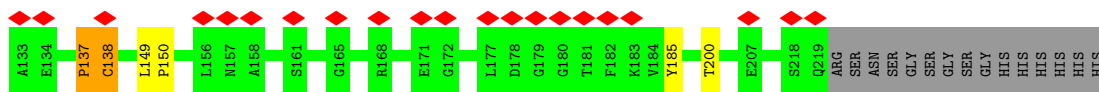
- Molecule 2: Envelope glycoprotein L



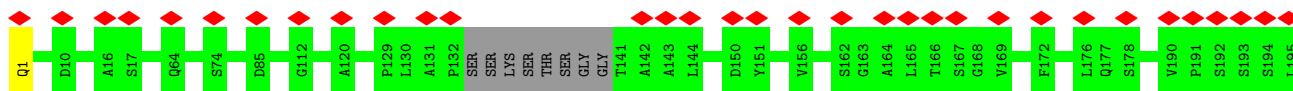
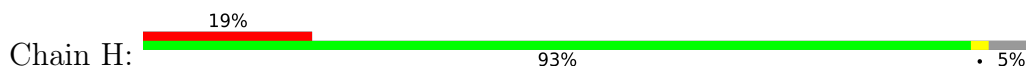
- Molecule 3: Glycoprotein 42



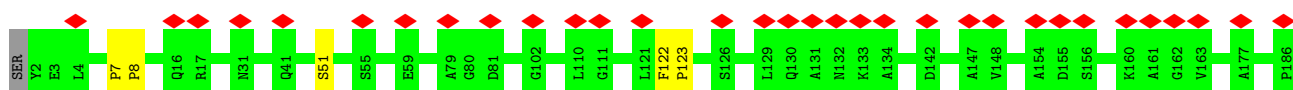




- Molecule 4: Antibody Fab AMMO1 heavy chain



- Molecule 5: Antibody Fab AMMO1 light chain



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72000	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 ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	304.64, 304.64, 304.64	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, PCA, MAN

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	0.79	0/5211	0.59	1/7073 (0.0%)
2	B	0.80	0/725	0.62	1/981 (0.1%)
3	C	0.75	0/1491	0.63	0/2044
4	H	0.72	0/1649	0.59	0/2253
5	L	0.74	0/1641	0.57	0/2245
All	All	0.77	0/10717	0.60	2/14596 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	LEU	CD1-CG-CD2	7.63	133.38	110.50
1	A	20	LEU	CD1-CG-CD2	6.66	130.49	110.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5101	0	5114	9	0
2	B	716	0	708	1	0
3	C	1435	0	1346	4	0
4	H	1615	0	1570	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	1598	0	1539	2	0
6	D	72	0	58	0	0
7	A	42	0	39	0	0
7	B	28	0	26	1	0
7	C	42	0	39	0	0
All	All	10649	0	10439	19	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 1.

The worst 5 of 19 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:C:137:PRO:O	3:C:138:CYS:C	2.45	0.55
4:H:207:LYS:N	4:H:208:PRO:CD	2.69	0.55
1:A:213:TYR:N	1:A:214:PRO:CD	2.73	0.51
1:A:108:HIS:HB2	1:A:109:PRO:CD	2.42	0.50
3:C:200:THR:OG1	4:H:1:PCA:OE	2.31	0.49

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	653/697 (94%)	636 (97%)	15 (2%)	2 (0%)	41	76
2	B	88/139 (63%)	88 (100%)	0	0	100	100
3	C	175/227 (77%)	169 (97%)	4 (2%)	2 (1%)	14	51
4	H	211/226 (93%)	206 (98%)	5 (2%)	0	100	100
5	L	210/216 (97%)	202 (96%)	8 (4%)	0	100	100
All	All	1337/1505 (89%)	1301 (97%)	32 (2%)	4 (0%)	44	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	GLY
1	A	413	LEU
3	C	138	CYS
3	C	137	PRO

### 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	561/594 (94%)	558 (100%)	3 (0%)	88	93
2	B	83/118 (70%)	82 (99%)	1 (1%)	71	84
3	C	162/197 (82%)	160 (99%)	2 (1%)	71	84
4	H	179/188 (95%)	179 (100%)	0	100	100
5	L	177/181 (98%)	176 (99%)	1 (1%)	86	92
All	All	1162/1278 (91%)	1155 (99%)	7 (1%)	86	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	74	LEU
3	C	98	ASN
5	L	51	SER
3	C	185	TYR
1	A	435	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	L	36	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](#)

1 non-standard protein/DNA/RNA residue is 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	PCA	H	1	4	7,8,9	0.55	0	9,10,12	1.10	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCA	H	1	4	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	PCA	1	0

## 5.5 Carbohydrates [i](#)

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
6	NAG	D	1	1,6	14,14,15	0.78	0	17,19,21	1.23	2 (11%)
6	NAG	D	2	6	14,14,15	1.11	1 (7%)	17,19,21	1.20	2 (11%)
6	BMA	D	3	6	11,11,12	1.88	3 (27%)	15,15,17	0.91	0
6	MAN	D	4	6	11,11,12	1.75	2 (18%)	15,15,17	0.87	0
6	MAN	D	5	6	11,11,12	1.75	3 (27%)	15,15,17	1.40	2 (13%)
6	MAN	D	6	6	11,11,12	1.89	2 (18%)	15,15,17	1.22	1 (6%)

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
6	NAG	D	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	1/6/23/26	0/1/1/1
6	BMA	D	3	6	-	2/2/19/22	0/1/1/1
6	MAN	D	4	6	-	2/2/19/22	0/1/1/1
6	MAN	D	5	6	-	1/2/19/22	0/1/1/1
6	MAN	D	6	6	-	2/2/19/22	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3	BMA	O2-C2	-4.31	1.34	1.43
6	D	5	MAN	O2-C2	-3.81	1.35	1.43
6	D	6	MAN	O2-C2	-3.66	1.35	1.43
6	D	6	MAN	C2-C3	-3.58	1.47	1.52
6	D	4	MAN	O2-C2	-3.16	1.36	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	D	1	NAG	C4-C3-C2	-3.24	106.27	111.02
6	D	5	MAN	C2-C3-C4	-3.07	105.58	110.89
6	D	5	MAN	C1-C2-C3	2.96	113.30	109.67
6	D	2	NAG	C3-C4-C5	-2.80	105.24	110.24
6	D	2	NAG	O5-C1-C2	-2.48	107.37	111.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

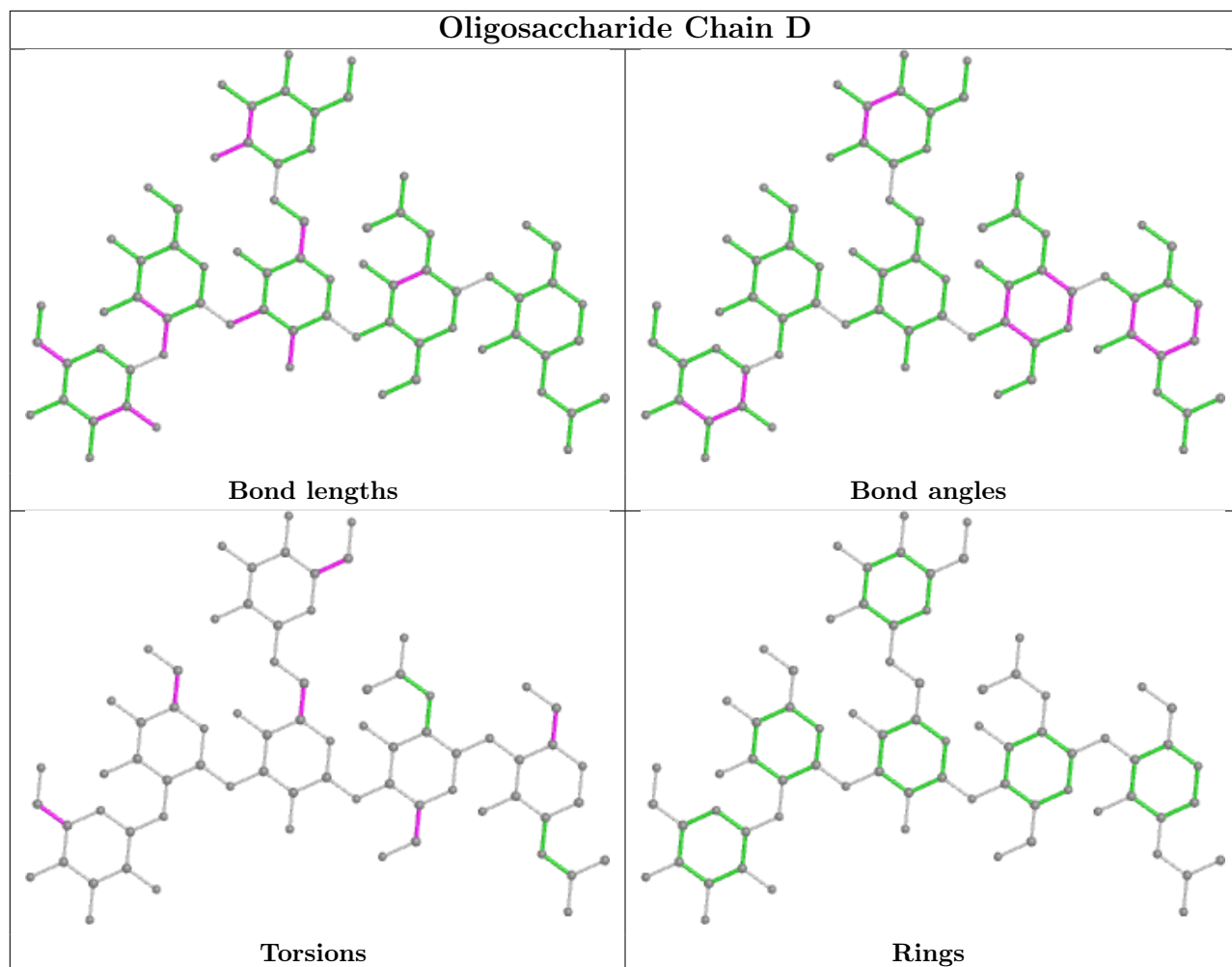
Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C4-C5-C6-O6
6	D	5	MAN	O5-C5-C6-O6
6	D	6	MAN	O5-C5-C6-O6
6	D	6	MAN	C4-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6

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.





## 5.6 Ligand geometry [i](#)

8 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
7	NAG	C	301	3	14,14,15	0.85	0	17,19,21	1.11	2 (11%)
7	NAG	A	708	1	14,14,15	0.72	0	17,19,21	1.22	1 (5%)
7	NAG	C	302	3	14,14,15	0.78	0	17,19,21	1.08	2 (11%)
7	NAG	A	709	1	14,14,15	0.73	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	202	2	14,14,15	1.25	1 (7%)	17,19,21	2.00	7 (41%)
7	NAG	B	201	2	14,14,15	0.82	0	17,19,21	1.46	2 (11%)
7	NAG	C	303	3	14,14,15	1.11	1 (7%)	17,19,21	2.60	3 (17%)
7	NAG	A	707	1	14,14,15	0.88	0	17,19,21	0.94	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
7	NAG	C	301	3	-	0/6/23/26	0/1/1/1
7	NAG	A	708	1	-	0/6/23/26	0/1/1/1
7	NAG	C	302	3	-	1/6/23/26	0/1/1/1
7	NAG	A	709	1	-	0/6/23/26	0/1/1/1
7	NAG	B	202	2	-	4/6/23/26	0/1/1/1
7	NAG	B	201	2	-	4/6/23/26	0/1/1/1
7	NAG	C	303	3	-	3/6/23/26	0/1/1/1
7	NAG	A	707	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	303	NAG	C2-N2	2.67	1.50	1.46
7	B	202	NAG	O5-C1	2.40	1.47	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	303	NAG	C4-C3-C2	-7.87	99.48	111.02
7	C	303	NAG	O5-C1-C2	-5.14	103.18	111.29
7	B	201	NAG	C4-C3-C2	-4.57	104.32	111.02
7	B	202	NAG	C4-C3-C2	-4.50	104.42	111.02
7	A	708	NAG	C4-C3-C2	-3.92	105.27	111.02

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	202	NAG	C1-C2-N2-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	C	303	NAG	O5-C5-C6-O6
7	B	202	NAG	C4-C5-C6-O6
7	B	202	NAG	O5-C5-C6-O6
7	C	303	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	202	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.

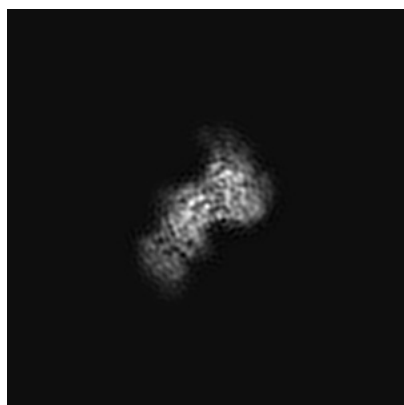
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7344. These allow visual inspection of the internal detail of the map and identification of artifacts.

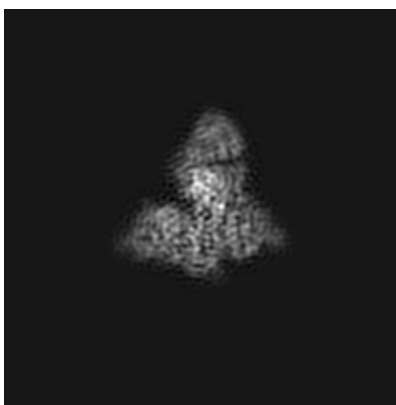
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

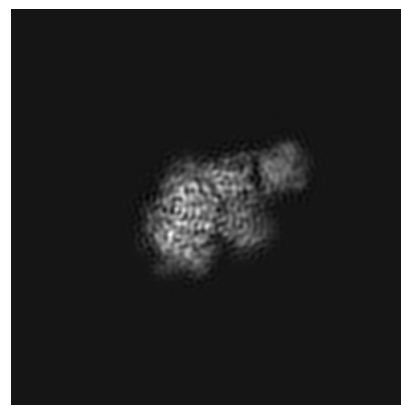
#### 6.1.1 Primary map



X



Y

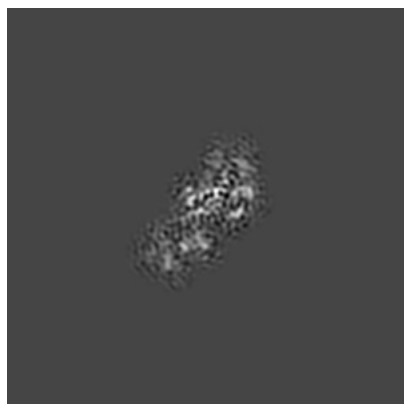


Z

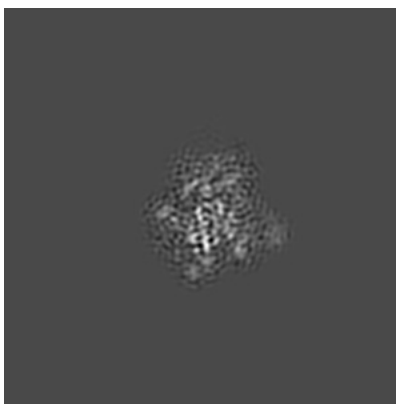
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

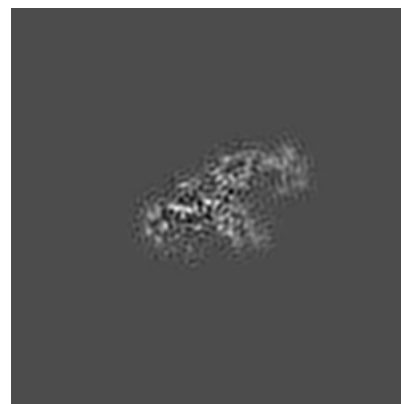
#### 6.2.1 Primary map



X Index: 112



Y Index: 112

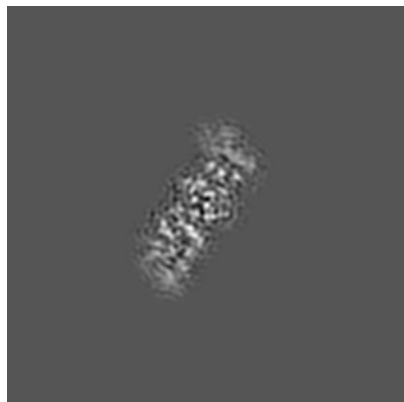


Z Index: 112

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

## 6.3 Largest variance slices [i](#)

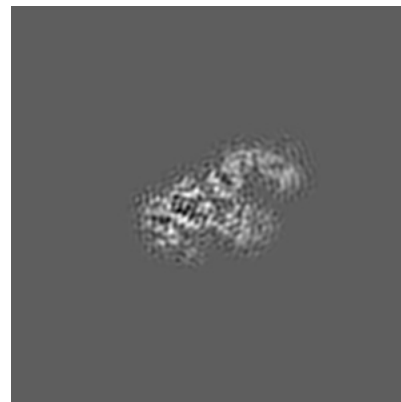
### 6.3.1 Primary map



X Index: 93



Y Index: 123

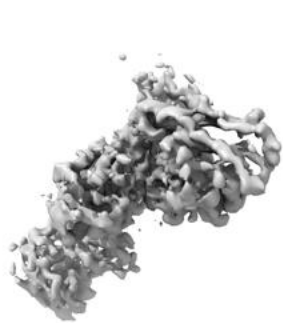


Z Index: 108

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

## 6.4 Orthogonal surface views [i](#)

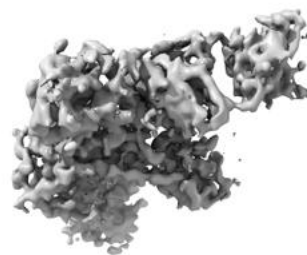
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

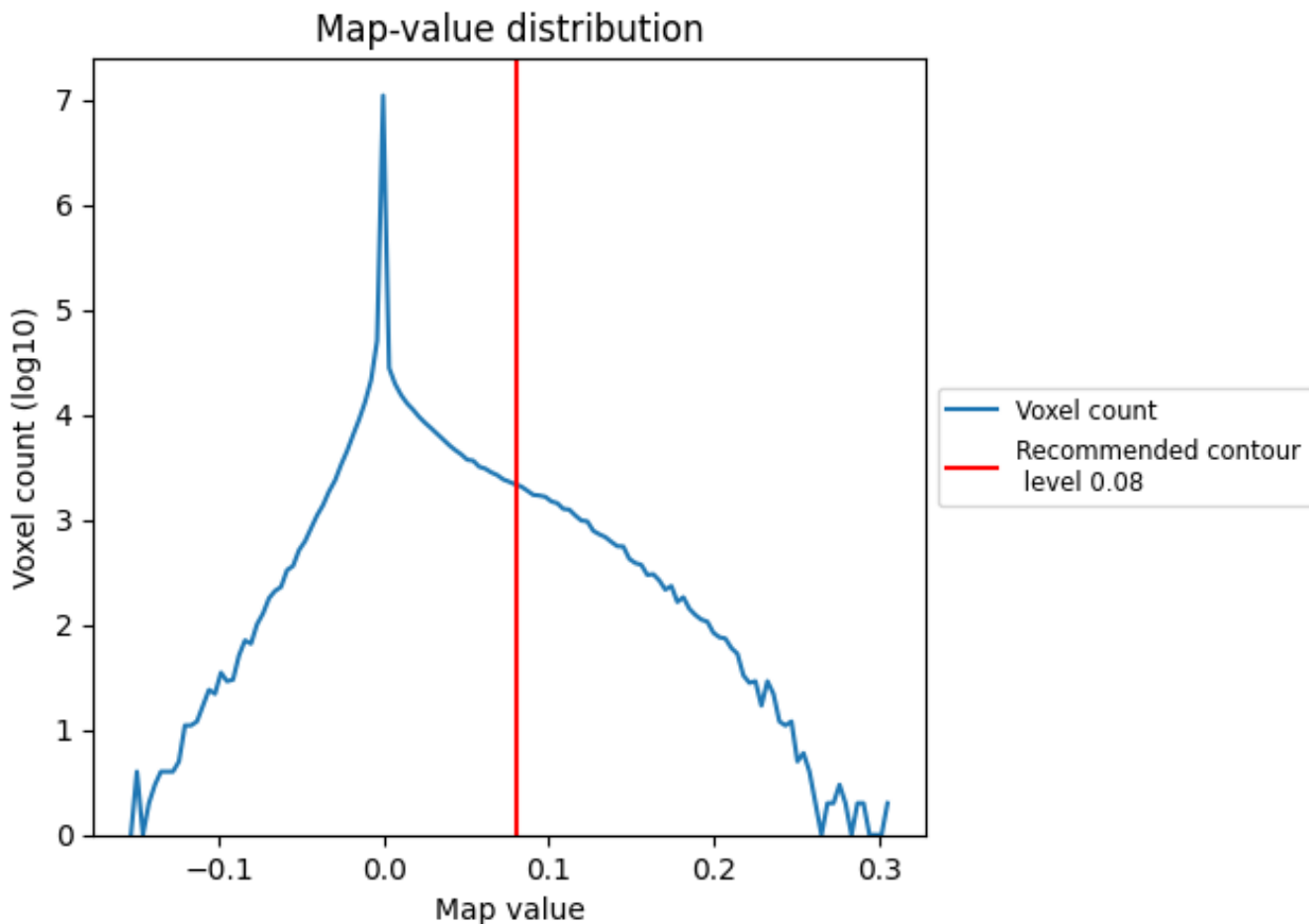
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

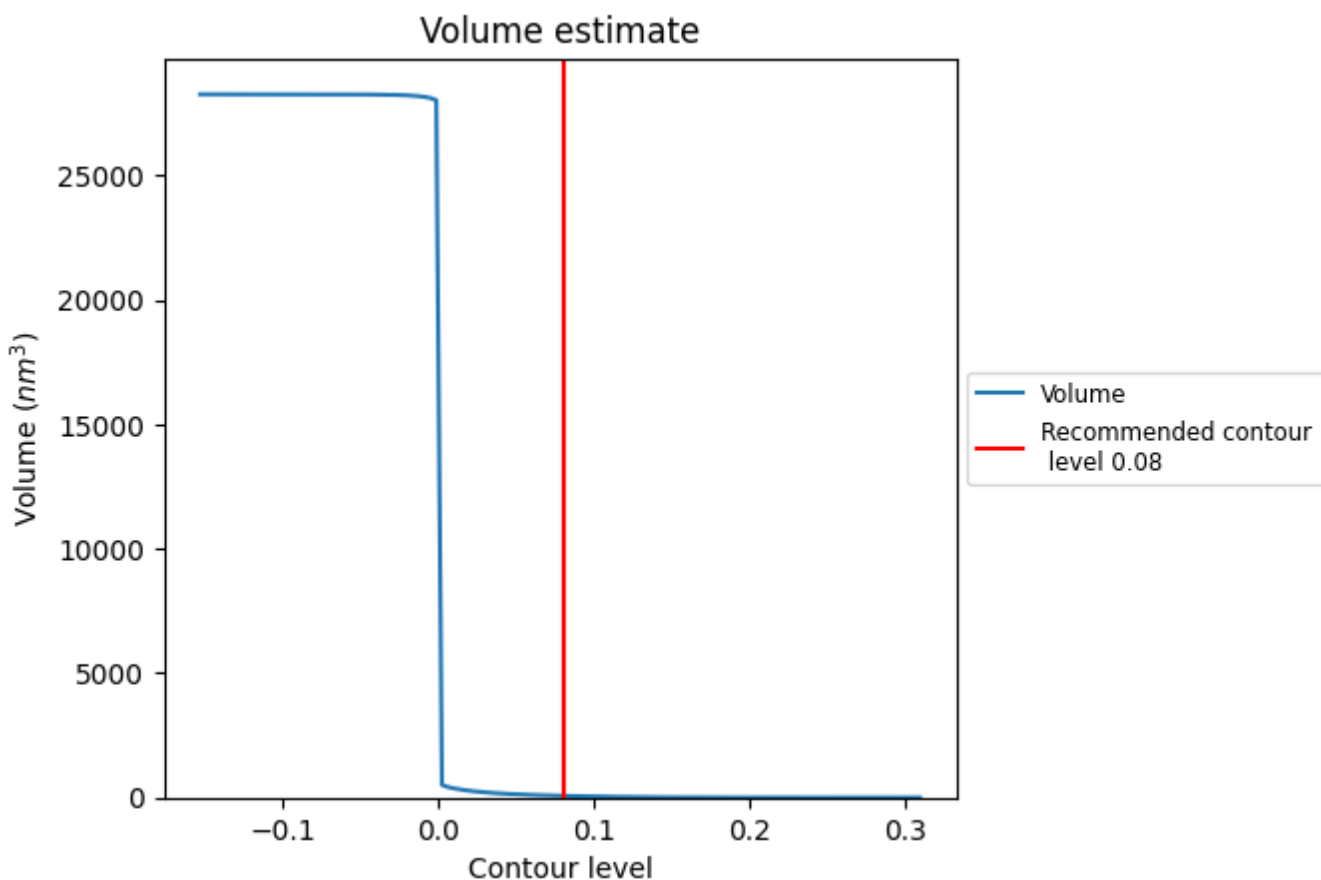
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

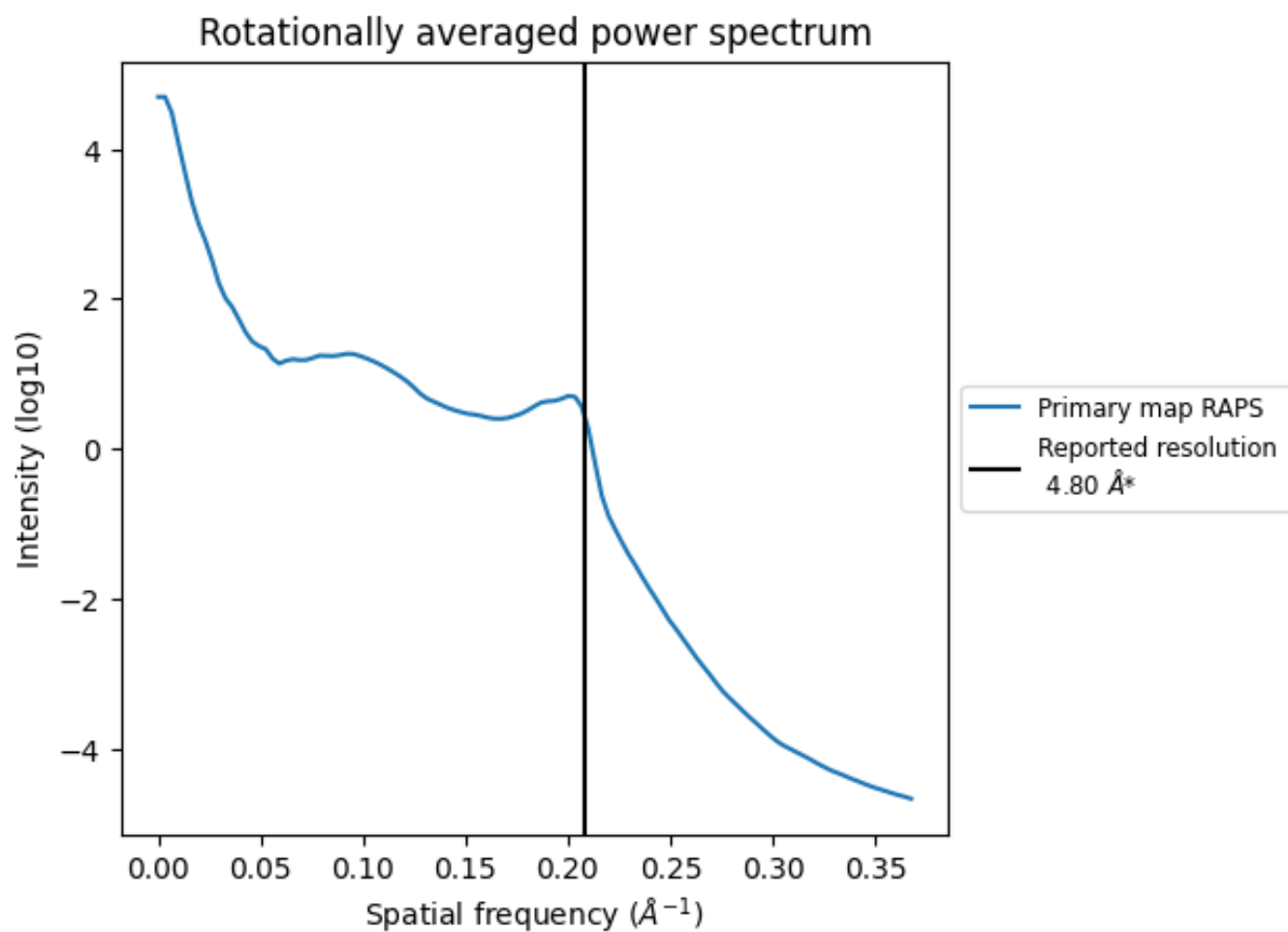


The volume at the recommended contour level is 69 nm<sup>3</sup>; this corresponds to an approximate mass of 62 kDa.

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  $0.208 \text{\AA}^{-1}$

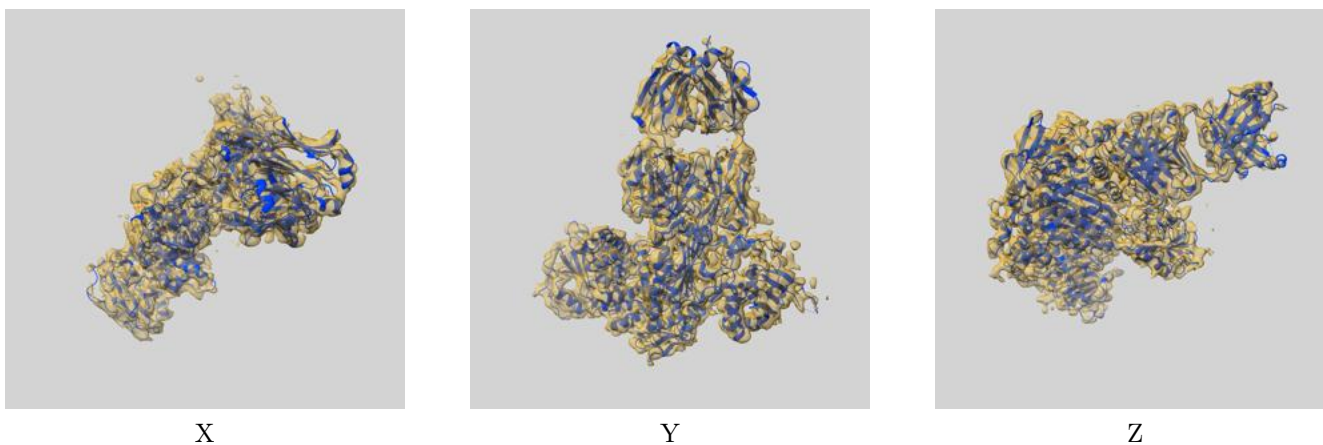
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

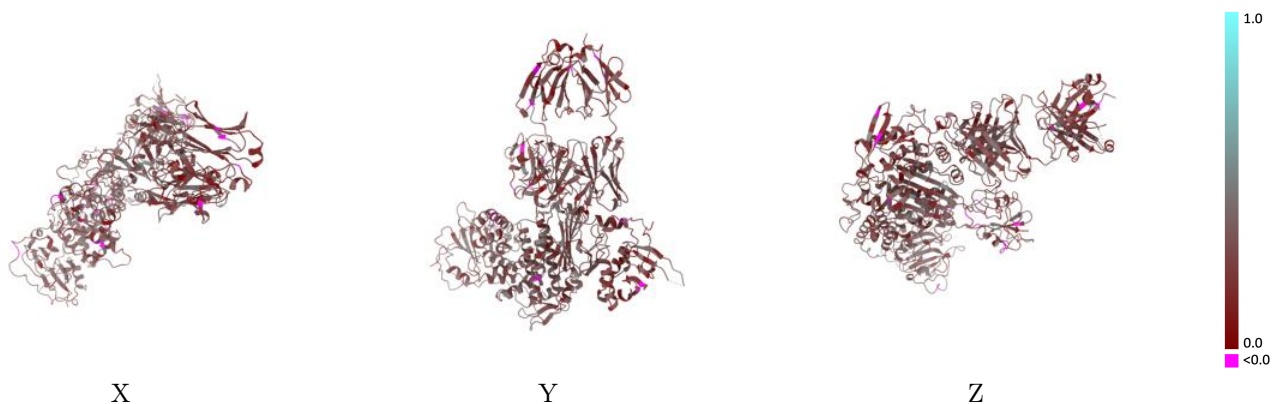
This section contains information regarding the fit between EMDB map EMD-7344 and PDB model 6C5V. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



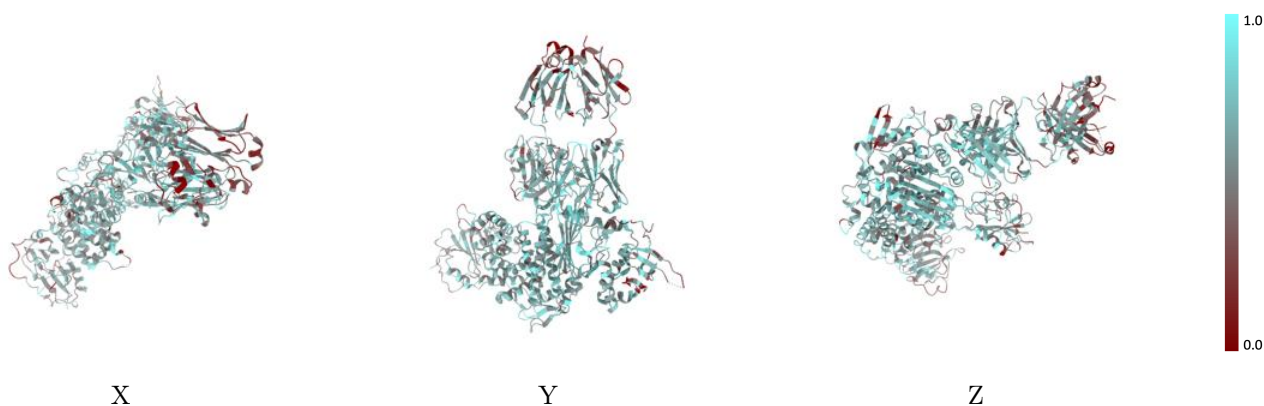
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



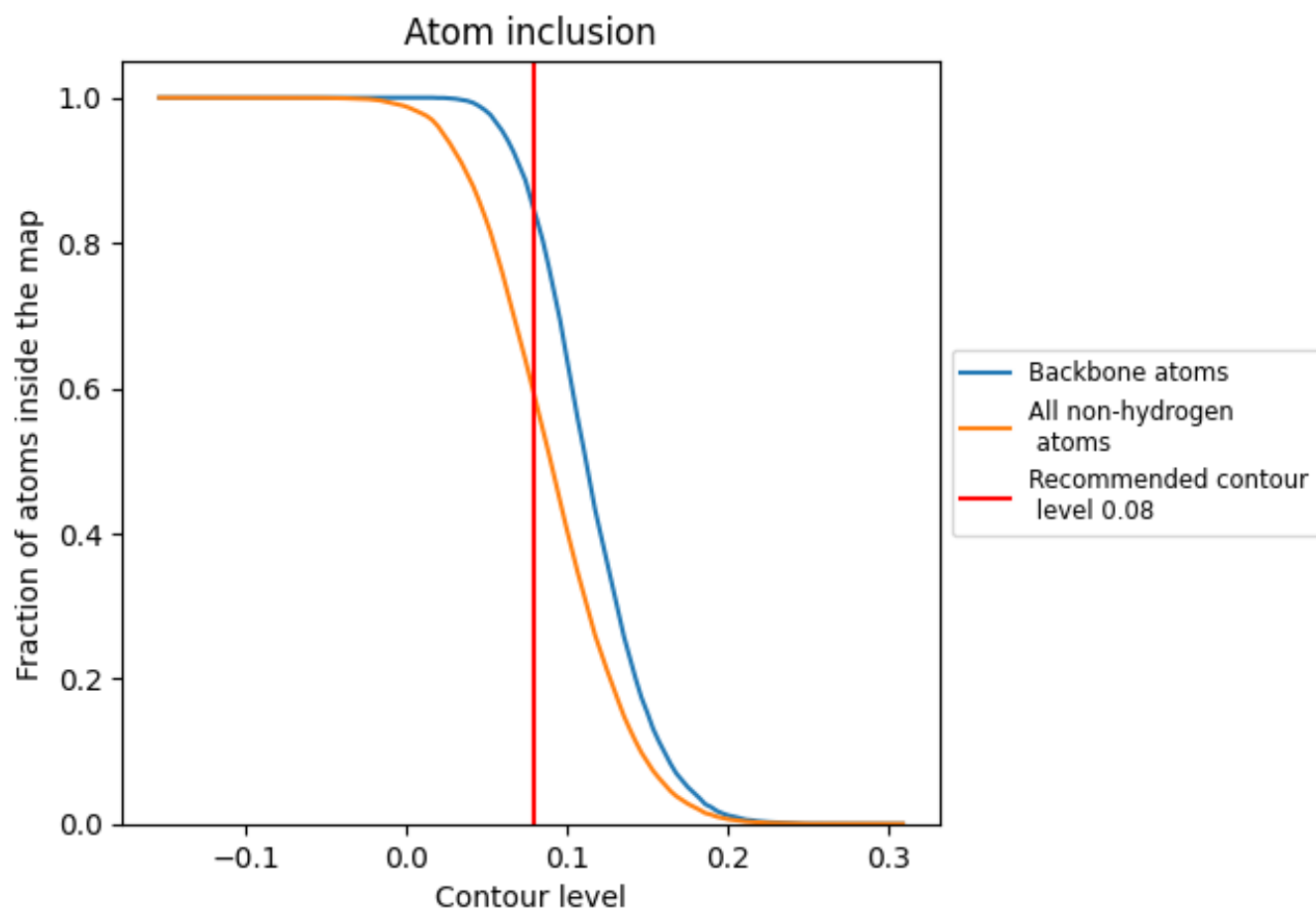
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 59% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5889	 0.2870
A	 0.6194	 0.2930
B	 0.5416	 0.2670
C	 0.5795	 0.2870
D	 0.3611	 0.3650
H	 0.5742	 0.2830
L	 0.5471	 0.2790

