



## wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 11:07 AM EST

PDB ID : 7USL  
EMDB ID : EMD-26738  
Title : Integrin alphaM/beta2 ectodomain in complex with adenylate cyclase toxin  
RTX751 and M1F5 Fab  
Authors : Goldsmith, J.A.; McLellan, J.S.  
Deposited on : 2022-04-25  
Resolution : 2.70 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) : 2.31.3

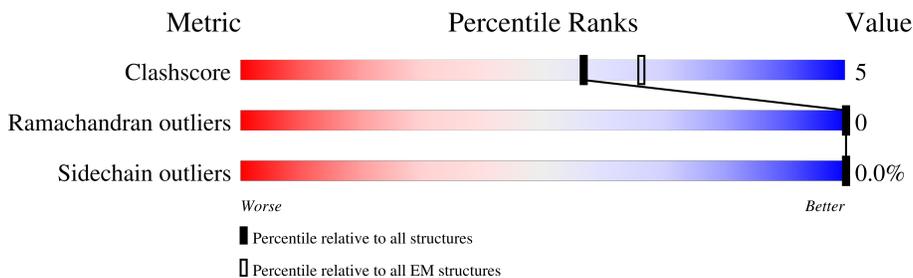
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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	1162	
2	B	730	
3	C	960	
4	H	228	
5	L	213	
6	D	2	
7	E	3	

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 19065 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 Integrin alpha-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	856	6627	4159	1163	1271	34	0	0

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	GLY	-	expression tag	UNP P11215
A	1090	CYS	-	expression tag	UNP P11215
A	1091	GLY	-	expression tag	UNP P11215
A	1092	GLY	-	expression tag	UNP P11215
A	1093	LEU	-	expression tag	UNP P11215
A	1094	GLU	-	expression tag	UNP P11215
A	1095	VAL	-	expression tag	UNP P11215
A	1096	LEU	-	expression tag	UNP P11215
A	1097	PHE	-	expression tag	UNP P11215
A	1098	GLN	-	expression tag	UNP P11215
A	1099	GLY	-	expression tag	UNP P11215
A	1100	PRO	-	expression tag	UNP P11215
A	1101	GLY	-	expression tag	UNP P11215
A	1102	GLU	-	expression tag	UNP P11215
A	1103	ASN	-	expression tag	UNP P11215
A	1104	ALA	-	expression tag	UNP P11215
A	1105	GLN	-	expression tag	UNP P11215
A	1106	CYS	-	expression tag	UNP P11215
A	1107	GLU	-	expression tag	UNP P11215
A	1108	LYS	-	expression tag	UNP P11215
A	1109	GLU	-	expression tag	UNP P11215
A	1110	LEU	-	expression tag	UNP P11215
A	1111	GLN	-	expression tag	UNP P11215
A	1112	ALA	-	expression tag	UNP P11215
A	1113	LEU	-	expression tag	UNP P11215
A	1114	GLU	-	expression tag	UNP P11215
A	1115	LYS	-	expression tag	UNP P11215
A	1116	GLU	-	expression tag	UNP P11215

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1117	ASN	-	expression tag	UNP P11215
A	1118	ALA	-	expression tag	UNP P11215
A	1119	GLN	-	expression tag	UNP P11215
A	1120	LEU	-	expression tag	UNP P11215
A	1121	GLU	-	expression tag	UNP P11215
A	1122	TRP	-	expression tag	UNP P11215
A	1123	GLU	-	expression tag	UNP P11215
A	1124	LEU	-	expression tag	UNP P11215
A	1125	GLN	-	expression tag	UNP P11215
A	1126	ALA	-	expression tag	UNP P11215
A	1127	LEU	-	expression tag	UNP P11215
A	1128	GLU	-	expression tag	UNP P11215
A	1129	LYS	-	expression tag	UNP P11215
A	1130	GLU	-	expression tag	UNP P11215
A	1131	LEU	-	expression tag	UNP P11215
A	1132	ALA	-	expression tag	UNP P11215
A	1133	GLN	-	expression tag	UNP P11215
A	1134	TRP	-	expression tag	UNP P11215
A	1135	SER	-	expression tag	UNP P11215
A	1136	HIS	-	expression tag	UNP P11215
A	1137	PRO	-	expression tag	UNP P11215
A	1138	GLN	-	expression tag	UNP P11215
A	1139	PHE	-	expression tag	UNP P11215
A	1140	GLU	-	expression tag	UNP P11215
A	1141	LYS	-	expression tag	UNP P11215
A	1142	GLY	-	expression tag	UNP P11215
A	1143	GLY	-	expression tag	UNP P11215
A	1144	GLY	-	expression tag	UNP P11215
A	1145	SER	-	expression tag	UNP P11215
A	1146	GLY	-	expression tag	UNP P11215
A	1147	GLY	-	expression tag	UNP P11215
A	1148	GLY	-	expression tag	UNP P11215
A	1149	GLY	-	expression tag	UNP P11215
A	1150	SER	-	expression tag	UNP P11215
A	1151	GLY	-	expression tag	UNP P11215
A	1152	GLY	-	expression tag	UNP P11215
A	1153	SER	-	expression tag	UNP P11215
A	1154	ALA	-	expression tag	UNP P11215
A	1155	TRP	-	expression tag	UNP P11215
A	1156	SER	-	expression tag	UNP P11215
A	1157	HIS	-	expression tag	UNP P11215
A	1158	PRO	-	expression tag	UNP P11215

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1159	GLN	-	expression tag	UNP P11215
A	1160	PHE	-	expression tag	UNP P11215
A	1161	GLU	-	expression tag	UNP P11215
A	1162	LYS	-	expression tag	UNP P11215

- Molecule 2 is a protein called Integrin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	673	5176	3182	929	1001	64	0	0

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	expression tag	UNP A0A494C0X7
B	679	GLY	-	expression tag	UNP A0A494C0X7
B	680	CYS	-	expression tag	UNP A0A494C0X7
B	681	GLY	-	expression tag	UNP A0A494C0X7
B	682	LEU	-	expression tag	UNP A0A494C0X7
B	683	GLU	-	expression tag	UNP A0A494C0X7
B	684	VAL	-	expression tag	UNP A0A494C0X7
B	685	LEU	-	expression tag	UNP A0A494C0X7
B	686	PHE	-	expression tag	UNP A0A494C0X7
B	687	GLN	-	expression tag	UNP A0A494C0X7
B	688	GLY	-	expression tag	UNP A0A494C0X7
B	689	PRO	-	expression tag	UNP A0A494C0X7
B	690	GLY	-	expression tag	UNP A0A494C0X7
B	691	LYS	-	expression tag	UNP A0A494C0X7
B	692	ASN	-	expression tag	UNP A0A494C0X7
B	693	ALA	-	expression tag	UNP A0A494C0X7
B	694	GLN	-	expression tag	UNP A0A494C0X7
B	695	CYS	-	expression tag	UNP A0A494C0X7
B	696	LYS	-	expression tag	UNP A0A494C0X7
B	697	LYS	-	expression tag	UNP A0A494C0X7
B	698	LYS	-	expression tag	UNP A0A494C0X7
B	699	LEU	-	expression tag	UNP A0A494C0X7
B	700	GLN	-	expression tag	UNP A0A494C0X7
B	701	ALA	-	expression tag	UNP A0A494C0X7
B	702	LEU	-	expression tag	UNP A0A494C0X7
B	703	LYS	-	expression tag	UNP A0A494C0X7
B	704	LYS	-	expression tag	UNP A0A494C0X7
B	705	LYS	-	expression tag	UNP A0A494C0X7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	706	ASN	-	expression tag	UNP A0A494C0X7
B	707	ALA	-	expression tag	UNP A0A494C0X7
B	708	GLN	-	expression tag	UNP A0A494C0X7
B	709	LEU	-	expression tag	UNP A0A494C0X7
B	710	LYS	-	expression tag	UNP A0A494C0X7
B	711	TRP	-	expression tag	UNP A0A494C0X7
B	712	LYS	-	expression tag	UNP A0A494C0X7
B	713	LEU	-	expression tag	UNP A0A494C0X7
B	714	GLN	-	expression tag	UNP A0A494C0X7
B	715	ALA	-	expression tag	UNP A0A494C0X7
B	716	LEU	-	expression tag	UNP A0A494C0X7
B	717	LYS	-	expression tag	UNP A0A494C0X7
B	718	LYS	-	expression tag	UNP A0A494C0X7
B	719	LYS	-	expression tag	UNP A0A494C0X7
B	720	LEU	-	expression tag	UNP A0A494C0X7
B	721	ALA	-	expression tag	UNP A0A494C0X7
B	722	GLN	-	expression tag	UNP A0A494C0X7
B	723	GLY	-	expression tag	UNP A0A494C0X7
B	724	GLY	-	expression tag	UNP A0A494C0X7
B	725	HIS	-	expression tag	UNP A0A494C0X7
B	726	HIS	-	expression tag	UNP A0A494C0X7
B	727	HIS	-	expression tag	UNP A0A494C0X7
B	728	HIS	-	expression tag	UNP A0A494C0X7
B	729	HIS	-	expression tag	UNP A0A494C0X7
B	730	HIS	-	expression tag	UNP A0A494C0X7

- Molecule 3 is a protein called Bifunctional hemolysin-adenylate cyclase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	715	5296	3222	952	1116	6	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	747	GLY	-	expression tag	UNP A5JW88
C	748	PRO	-	expression tag	UNP A5JW88
C	749	GLY	-	expression tag	UNP A5JW88
C	750	SER	-	expression tag	UNP A5JW88

- Molecule 4 is a protein called M1F5 fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	114	899	575	148	172	4	0	0

- Molecule 5 is a protein called M1F5 fab light chain.

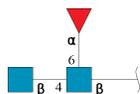
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	106	814	512	131	167	4	0	0

- Molecule 6 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
			Total	C	N	O		
6	D	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



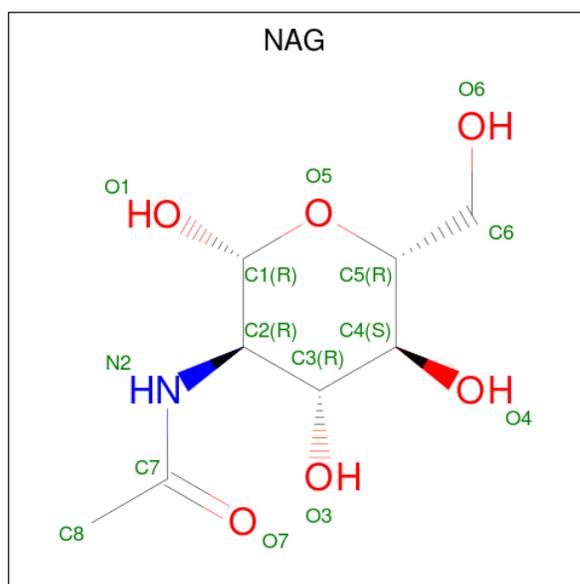
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	E	3	38	22	2	14	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	A	3	Total	Ca	0
			3	3	
8	B	1	Total	Ca	0
			1	1	
8	C	29	Total	Ca	0
			29	29	

- Molecule 9 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
9	A	1	Total	C	N	O	0
			126	72	9	45	
9	A	1	Total	C	N	O	0
			126	72	9	45	
9	A	1	Total	C	N	O	0
			126	72	9	45	
9	A	1	Total	C	N	O	0
			126	72	9	45	
9	A	1	Total	C	N	O	0
			126	72	9	45	
9	A	1	Total	C	N	O	0
			126	72	9	45	
9	A	1	Total	C	N	O	0
			126	72	9	45	
9	B	1	Total	C	N	O	0
			28	16	2	10	
9	B	1	Total	C	N	O	0
			28	16	2	10	







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	347508	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	271.230	Depositor
Minimum map value	-9.476	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.362	Depositor
Recommended contour level	7.0	Depositor
Map size ( $\text{\AA}$ )	362.67398, 362.67398, 362.67398	wwPDB
Map dimensions	338, 338, 338	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.073, 1.073, 1.073	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: FUC, NAG, CA

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	0.27	0/6757	0.53	0/9172
2	B	0.27	0/5273	0.55	0/7120
3	C	0.28	0/5362	0.55	0/7256
4	H	0.26	0/925	0.46	0/1252
5	L	0.27	0/832	0.49	0/1130
All	All	0.27	0/19149	0.53	0/25930

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 [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	6627	0	6505	76	0
2	B	5176	0	4962	54	0
3	C	5296	0	4987	62	0
4	H	899	0	856	5	0
5	L	814	0	781	4	0
6	D	28	0	25	0	0
7	E	38	0	34	0	0
8	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	0	0
8	C	29	0	0	0	0
9	A	126	0	117	5	0
9	B	28	0	26	0	0
All	All	19065	0	18293	192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 192 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)
1:A:50:CYS:HA	1:A:57:CYS:HB3	1.57	0.85
3:C:854:ARG:NH1	3:C:868:GLU:OE1	2.18	0.76
2:B:611:LYS:HD3	2:B:667:VAL:HB	1.69	0.74
1:A:815:VAL:HG22	1:A:865:ILE:HG12	1.71	0.73
2:B:554:GLU:OE1	2:B:577:ASN:ND2	2.23	0.72

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	848/1162 (73%)	824 (97%)	24 (3%)	0	100	100
2	B	671/730 (92%)	649 (97%)	22 (3%)	0	100	100
3	C	709/960 (74%)	680 (96%)	29 (4%)	0	100	100
4	H	112/228 (49%)	111 (99%)	1 (1%)	0	100	100
5	L	104/213 (49%)	101 (97%)	3 (3%)	0	100	100
All	All	2444/3293 (74%)	2365 (97%)	79 (3%)	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	741/1000 (74%)	741 (100%)	0	100	100
2	B	582/626 (93%)	582 (100%)	0	100	100
3	C	538/709 (76%)	537 (100%)	1 (0%)	93	98
4	H	97/197 (49%)	97 (100%)	0	100	100
5	L	93/189 (49%)	93 (100%)	0	100	100
All	All	2051/2721 (75%)	2050 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
3	C	854	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
2	B	577	ASN
3	C	963	GLN
3	C	977	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

5 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	0.29	0	17,19,21	0.39	0
6	NAG	D	2	6	14,14,15	0.25	0	17,19,21	0.48	0
7	NAG	E	1	1,7	14,14,15	0.26	0	17,19,21	0.41	0
7	NAG	E	2	7	14,14,15	0.23	0	17,19,21	0.43	0
7	FUC	E	3	7	10,10,11	0.59	0	14,14,16	0.82	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
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
7	NAG	E	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	1/6/23/26	0/1/1/1
7	FUC	E	3	7	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

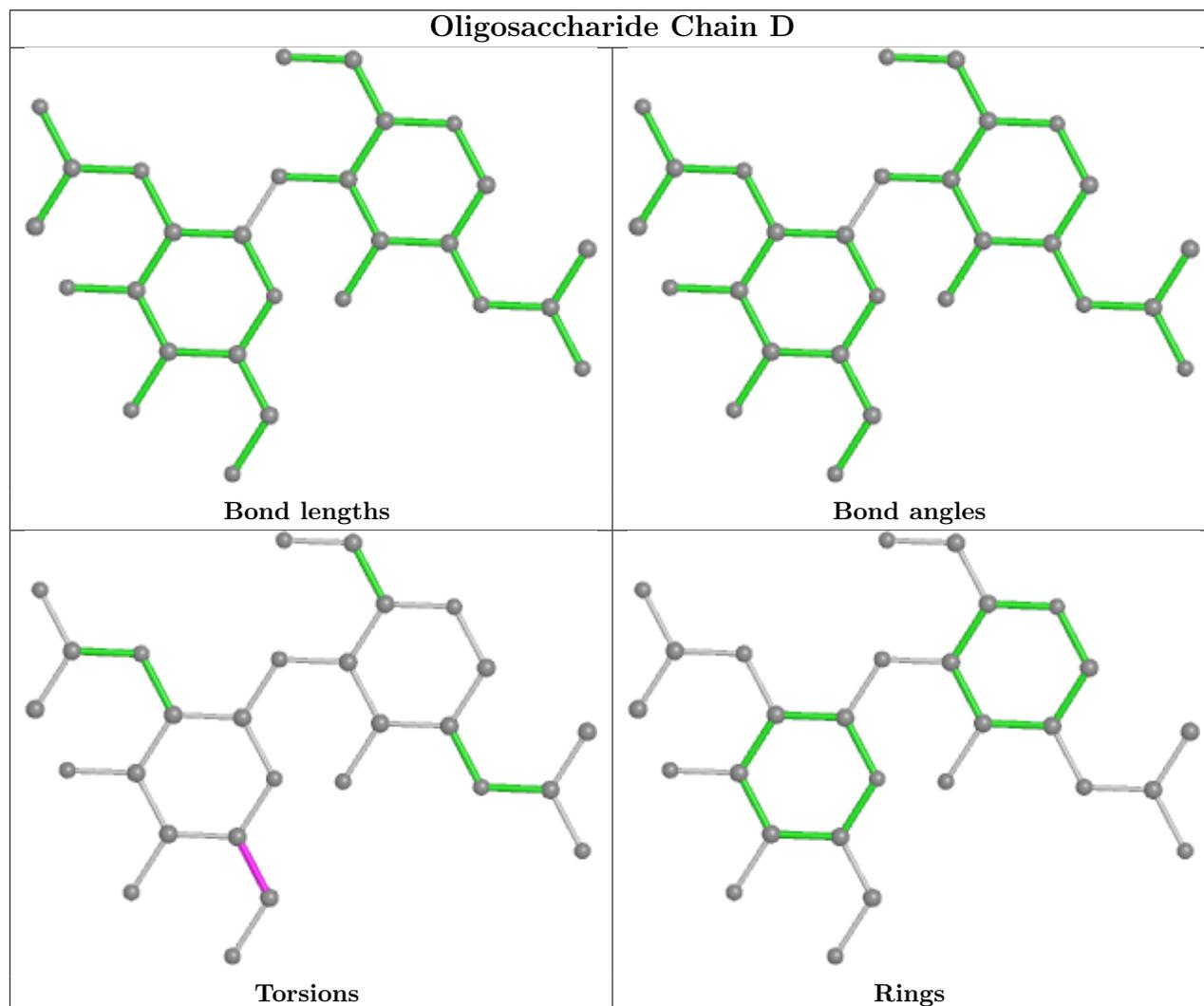
All (3) torsion outliers are listed below:

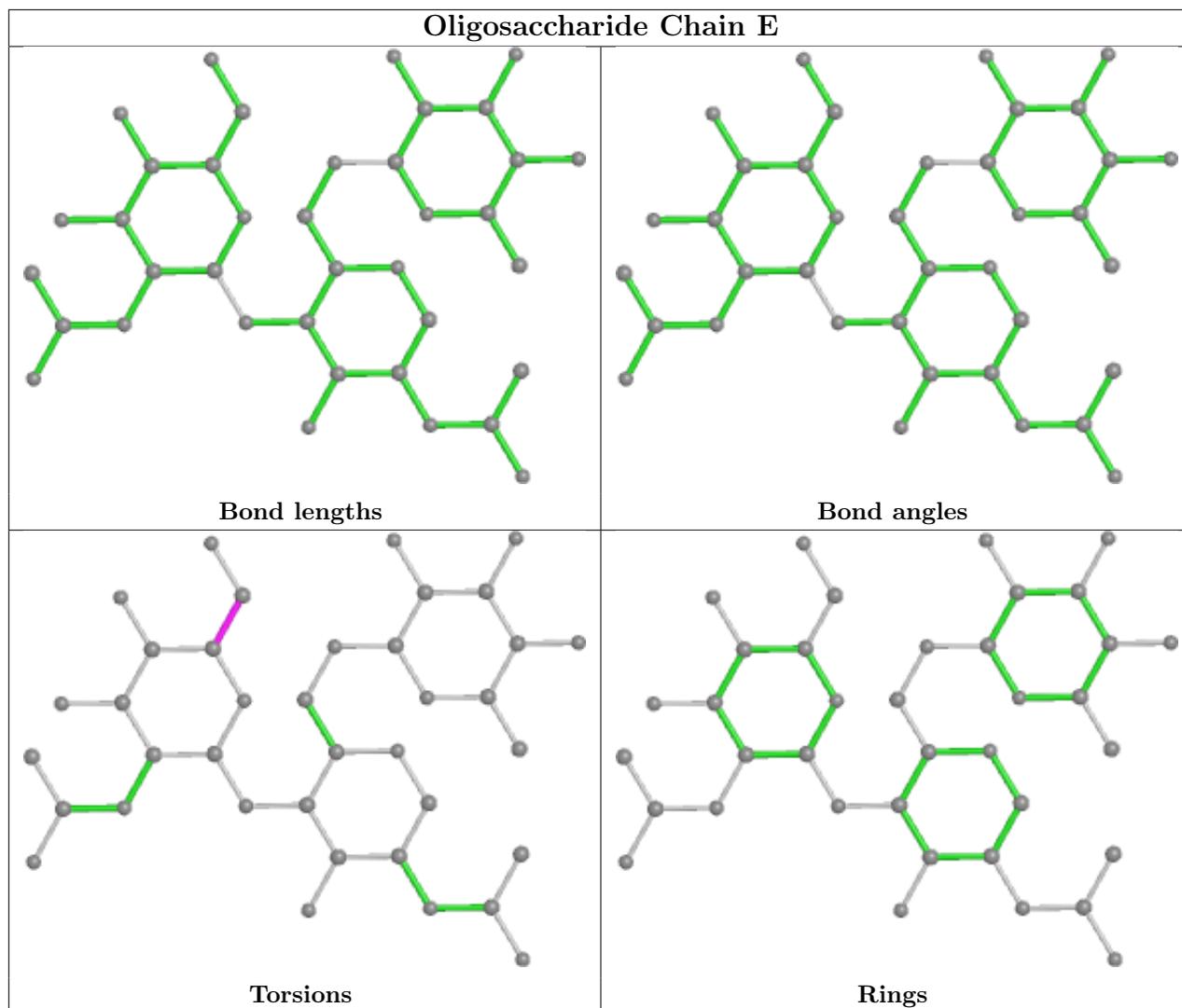
Mol	Chain	Res	Type	Atoms
6	D	2	NAG	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6

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.





## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 33 are monoatomic - leaving 11 for Mogul analysis.

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	A	1209	1	14,14,15	0.33	0	17,19,21	0.51	0
9	NAG	A	1204	1	14,14,15	0.23	0	17,19,21	0.50	0
9	NAG	A	1205	1	14,14,15	0.20	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	1207	1	14,14,15	0.29	0	17,19,21	0.44	0
9	NAG	B	802	2	14,14,15	0.21	0	17,19,21	0.39	0
9	NAG	A	1208	1	14,14,15	0.22	0	17,19,21	0.44	0
9	NAG	B	803	2	14,14,15	0.21	0	17,19,21	0.51	0
9	NAG	A	1211	1	14,14,15	0.26	0	17,19,21	0.46	0
9	NAG	A	1206	1	14,14,15	0.27	0	17,19,21	0.47	0
9	NAG	A	1212	1	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	A	1210	1	14,14,15	0.21	0	17,19,21	0.55	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	A	1209	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1204	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1207	1	-	2/6/23/26	0/1/1/1
9	NAG	B	802	2	-	2/6/23/26	0/1/1/1
9	NAG	A	1208	1	-	1/6/23/26	0/1/1/1
9	NAG	B	803	2	-	2/6/23/26	0/1/1/1
9	NAG	A	1211	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1212	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1210	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1209	NAG	C4-C5-C6-O6
9	B	802	NAG	C4-C5-C6-O6
9	A	1209	NAG	O5-C5-C6-O6
9	A	1207	NAG	C4-C5-C6-O6
9	A	1207	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1207	NAG	1	0
9	A	1211	NAG	1	0
9	A	1206	NAG	1	0
9	A	1210	NAG	2	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.

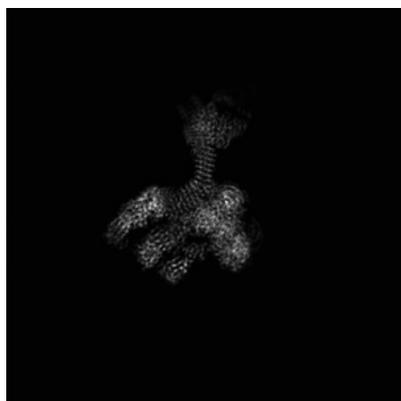
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26738. These allow visual inspection of the internal detail of the map and identification of artifacts.

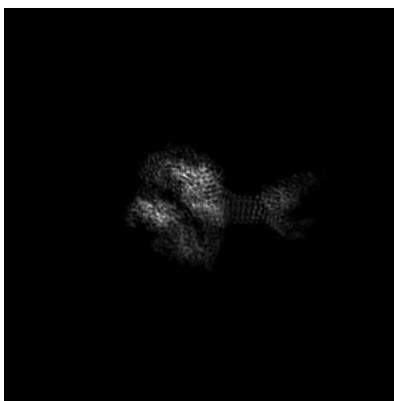
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

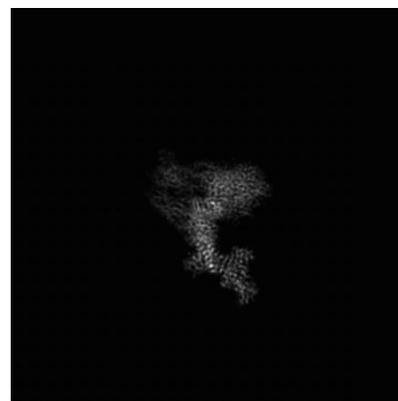
#### 6.1.1 Primary map



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: 169



Y Index: 169



Z Index: 169

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: 169



Y Index: 125



Z Index: 161

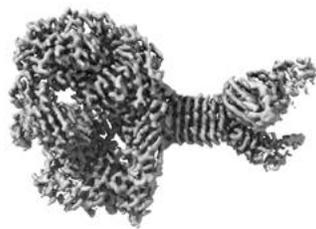
The images above show the largest variance slices of the map in three orthogonal directions.

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

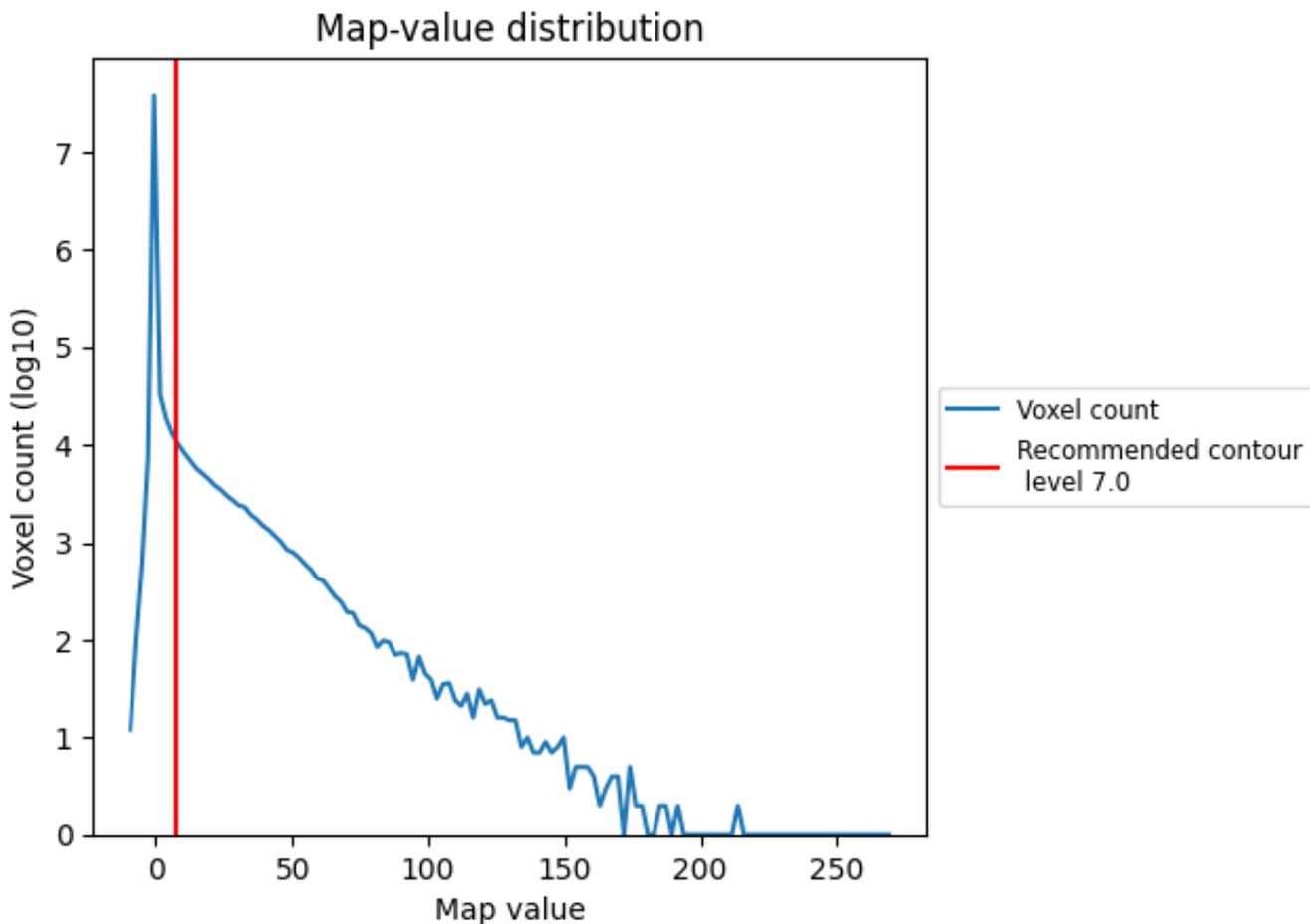
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

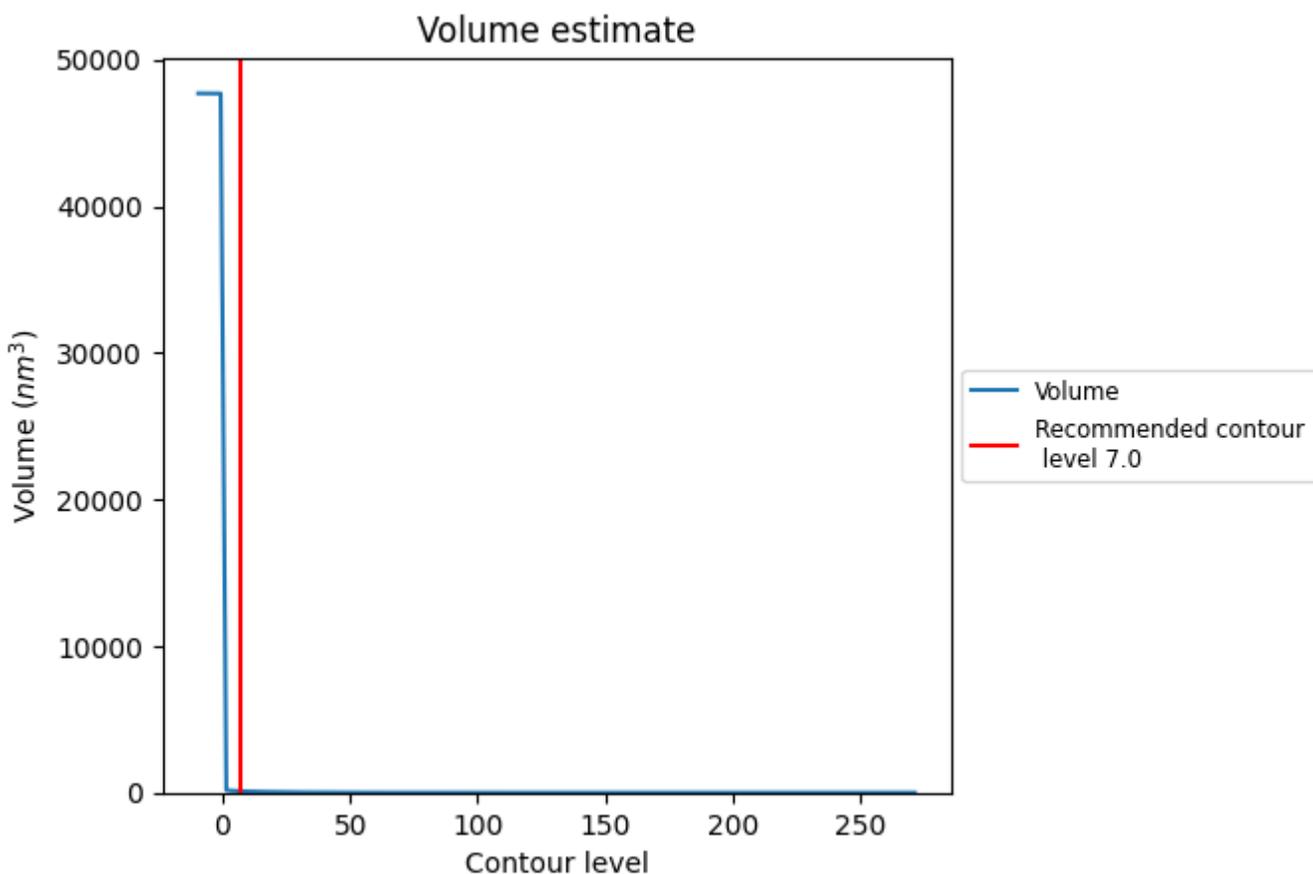
This section contains the results of statistical analysis of the map.

### 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.

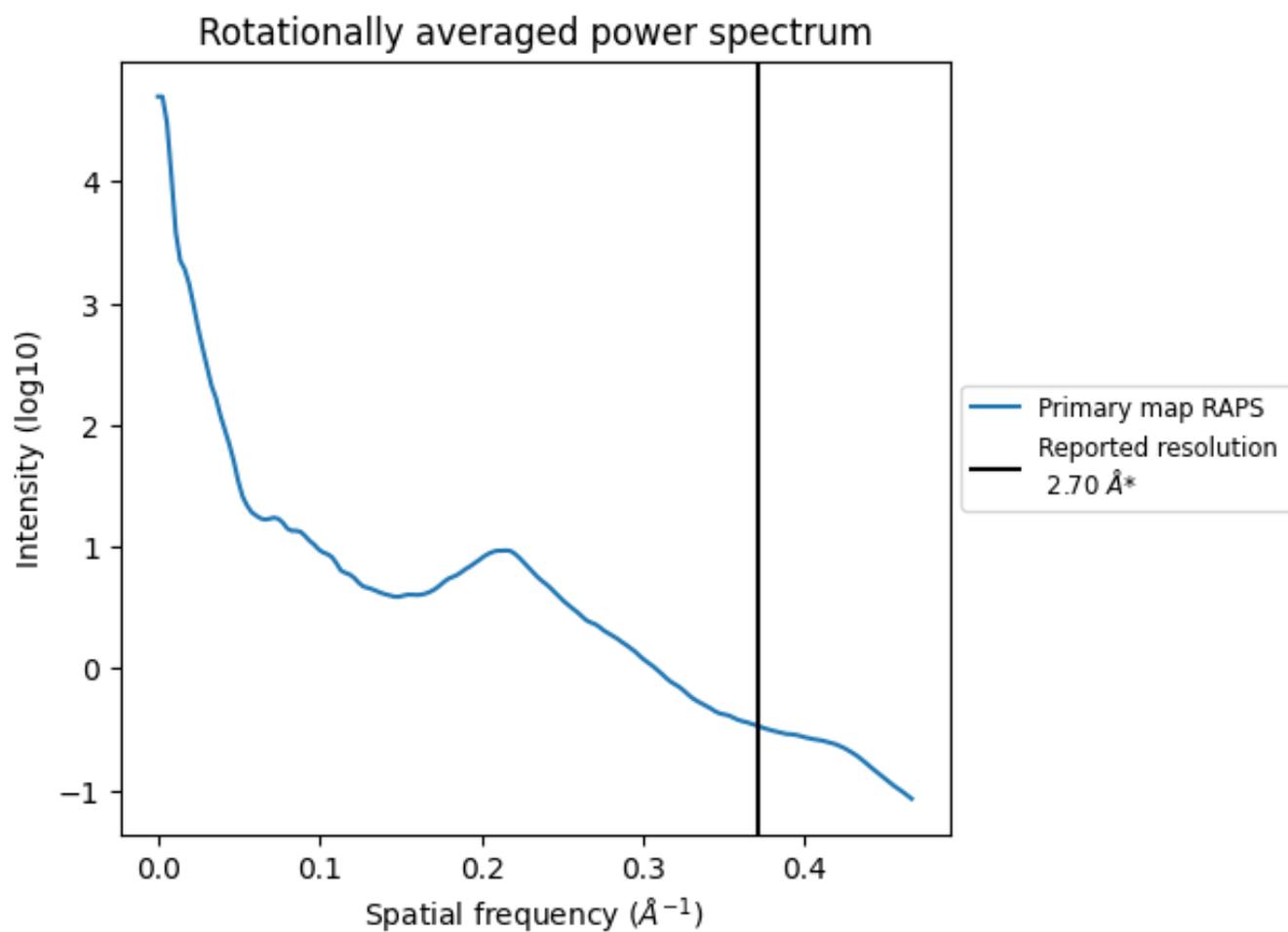
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm<sup>3</sup>; this corresponds to an approximate mass of 90 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 0.370 Å<sup>-1</sup>

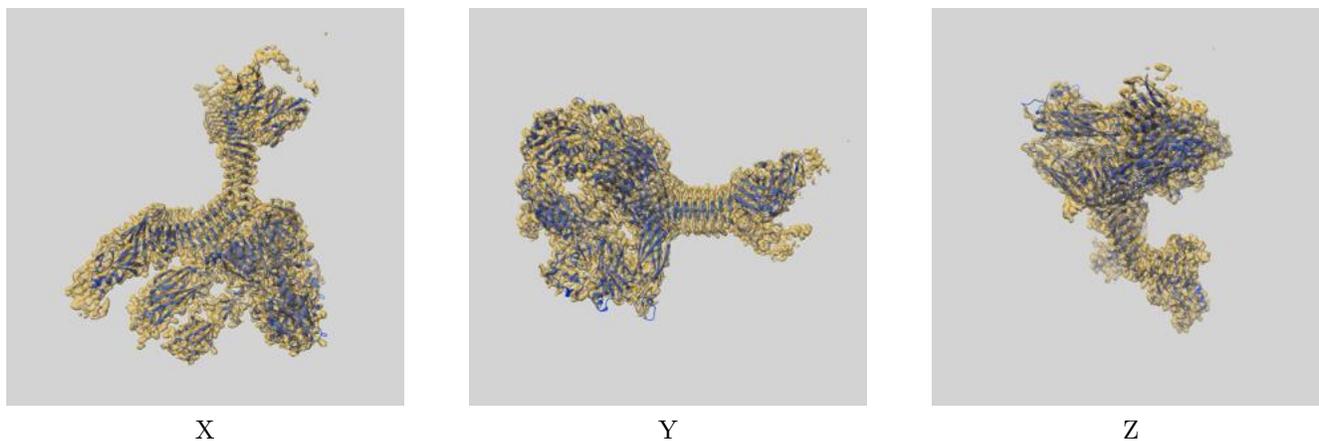
## 8 Fourier-Shell correlation

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

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

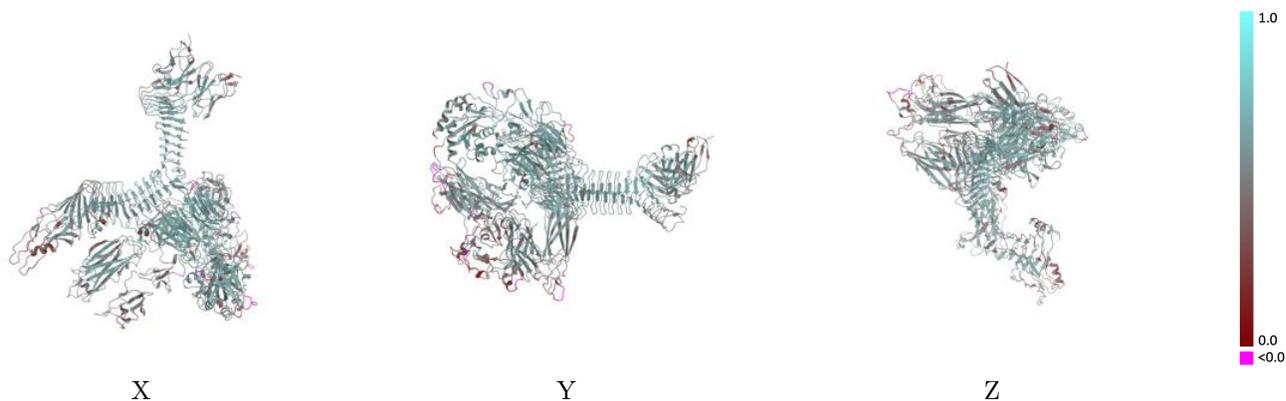
This section contains information regarding the fit between EMDB map EMD-26738 and PDB model 7USL. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



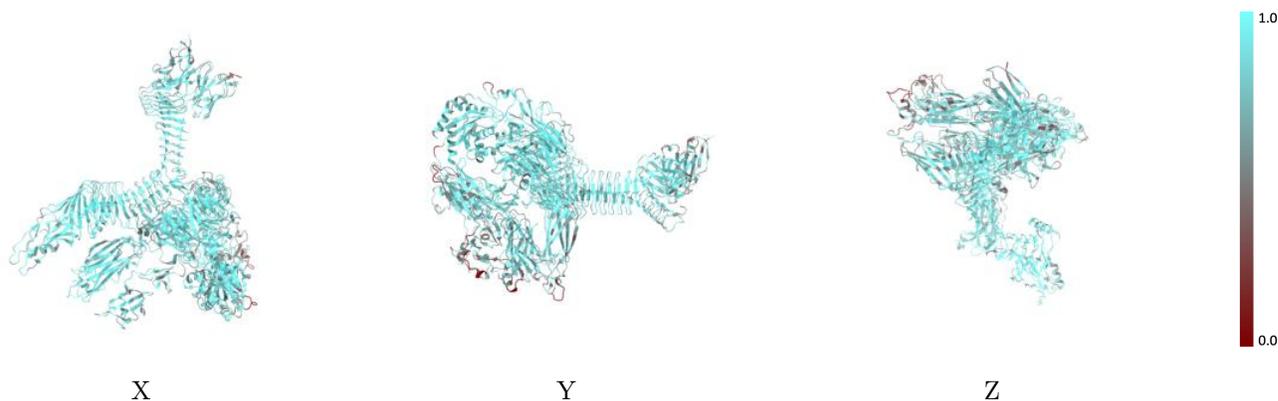
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



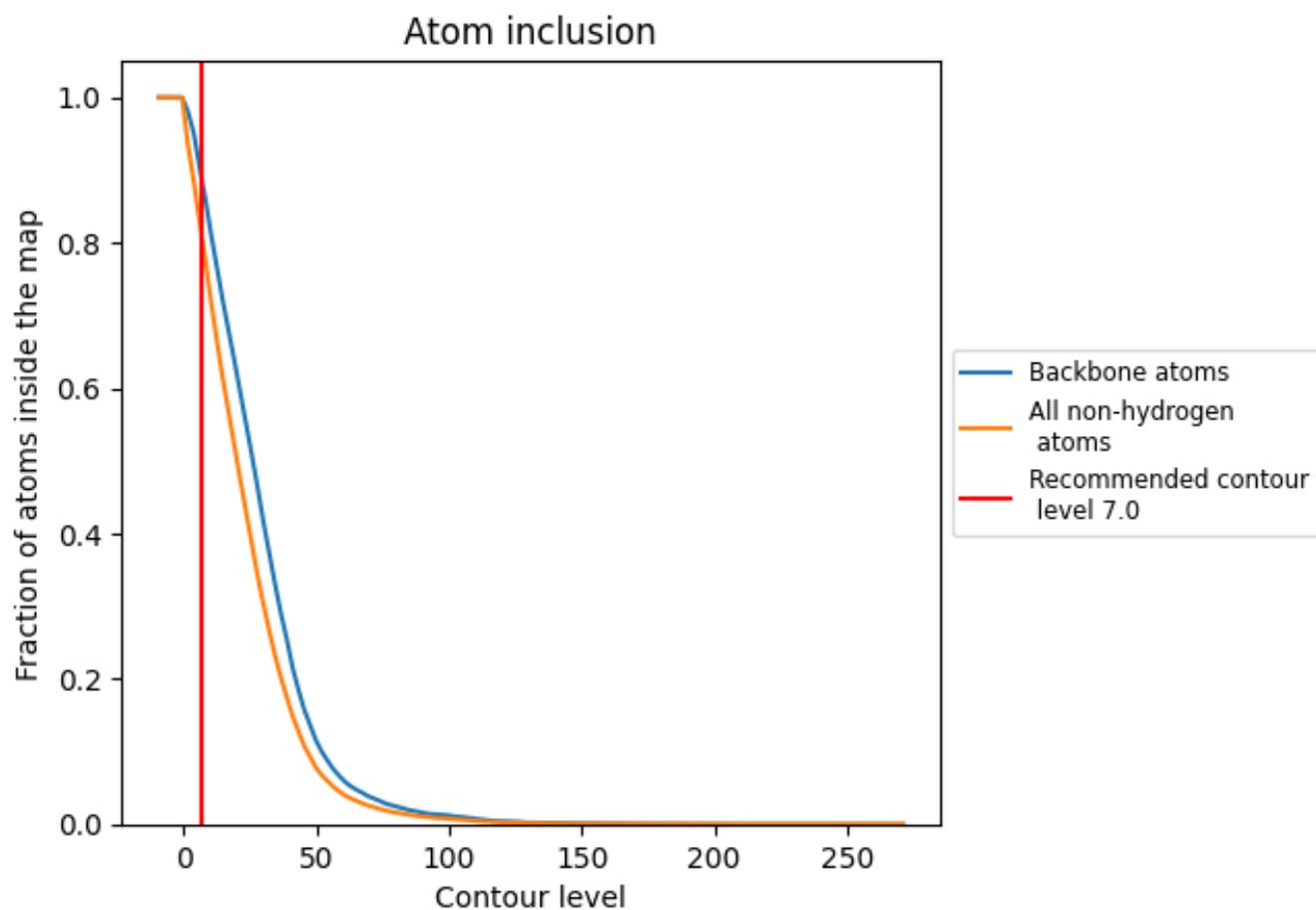
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (7.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7992	 0.5230
A	 0.8188	 0.5450
B	 0.7301	 0.4760
C	 0.8541	 0.5390
D	 0.8571	 0.6300
E	 0.8158	 0.5780
H	 0.7565	 0.5300
L	 0.7638	 0.5190

