WORLDWIDE PDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:54 AM EST

PDB ID	:	7M42
EMDB ID	:	EMD-23662
Title	:	Complex of SARS-CoV-2 receptor binding domain with the Fab fragments of neutralizing antibodies REGN10985 and REGN10989
Authors	:	Zhou, Y.; Romero Hernandez, A.; Saotome, K.; Franklin, M.C.
Deposited on	:	2021-03-19
Resolution	:	3.30 Å(reported)

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

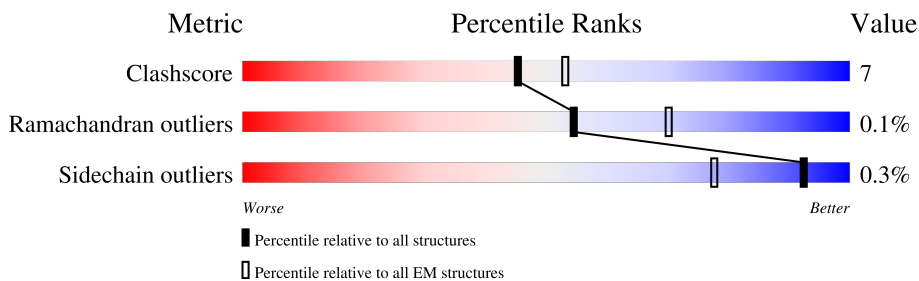|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et 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 3.30 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		0.3%

Worse   *Better*

▌Percentile relative to all structures

▯Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	216	• 79% 18% •
2	B	229	5% 83% 15% •
3	E	251	• 70% 8% 22%
4	C	218	30% 78% 20% •
5	D	234	33% 80% 17% •
6	F	3	33% 33% 67%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8115 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 REGN10989 antibody Fab fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	210	1551	968	256	322	5	0	0

- Molecule 2 is a protein called REGN10989 antibody Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1710	1084	292	327	7	0	0

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	195	1543	989	257	289	8	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	542	GLU	-	expression tag	UNP P0DTC2
E	543	GLN	-	expression tag	UNP P0DTC2
E	544	LYS	-	expression tag	UNP P0DTC2
E	545	LEU	-	expression tag	UNP P0DTC2
E	546	ILE	-	expression tag	UNP P0DTC2
E	547	SER	-	expression tag	UNP P0DTC2
E	548	GLU	-	expression tag	UNP P0DTC2
E	549	GLU	-	expression tag	UNP P0DTC2
E	550	ASP	-	expression tag	UNP P0DTC2
E	551	LEU	-	expression tag	UNP P0DTC2
E	552	GLY	-	expression tag	UNP P0DTC2
E	553	GLY	-	expression tag	UNP P0DTC2
E	554	GLU	-	expression tag	UNP P0DTC2
E	555	GLN	-	expression tag	UNP P0DTC2
E	556	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	557	LEU	-	expression tag	UNP P0DTC2
E	558	ILE	-	expression tag	UNP P0DTC2
E	559	SER	-	expression tag	UNP P0DTC2
E	560	GLU	-	expression tag	UNP P0DTC2
E	561	GLU	-	expression tag	UNP P0DTC2
E	562	ASP	-	expression tag	UNP P0DTC2
E	563	LEU	-	expression tag	UNP P0DTC2
E	564	HIS	-	expression tag	UNP P0DTC2
E	565	HIS	-	expression tag	UNP P0DTC2
E	566	HIS	-	expression tag	UNP P0DTC2
E	567	HIS	-	expression tag	UNP P0DTC2
E	568	HIS	-	expression tag	UNP P0DTC2
E	569	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is a protein called REGN10985 antibody Fab fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	213	Total	C	N	O	S	0	0
			1572	982	262	324	4		

- Molecule 5 is a protein called REGN10985 antibody Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	228	Total	C	N	O	S	0	0
			1700	1065	293	335	7		

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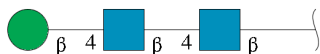

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	3	Total	C	N	O	0	0
			39	22	2	15		

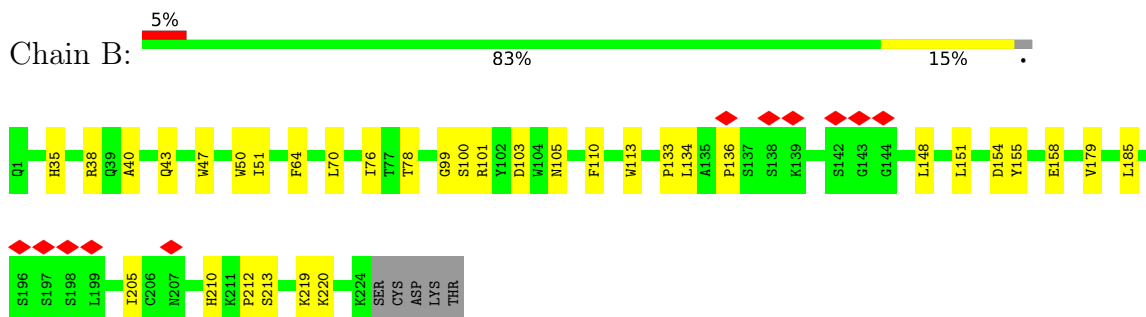# 3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: REGN10989 antibody Fab fragment light chain
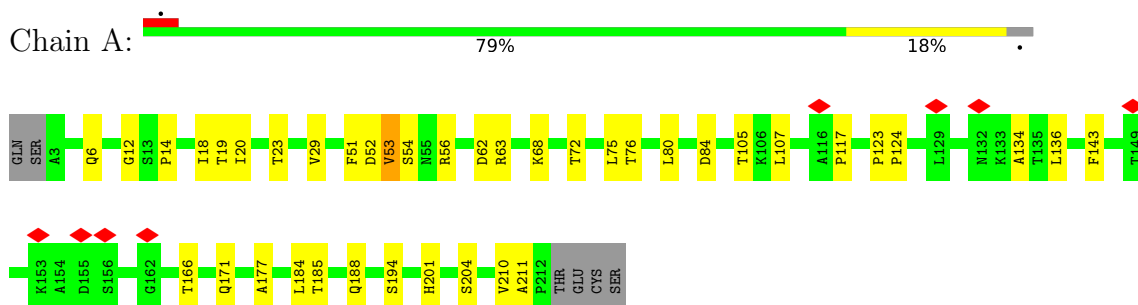
• Molecule 2: REGN10989 antibody Fab fragment heavy chain
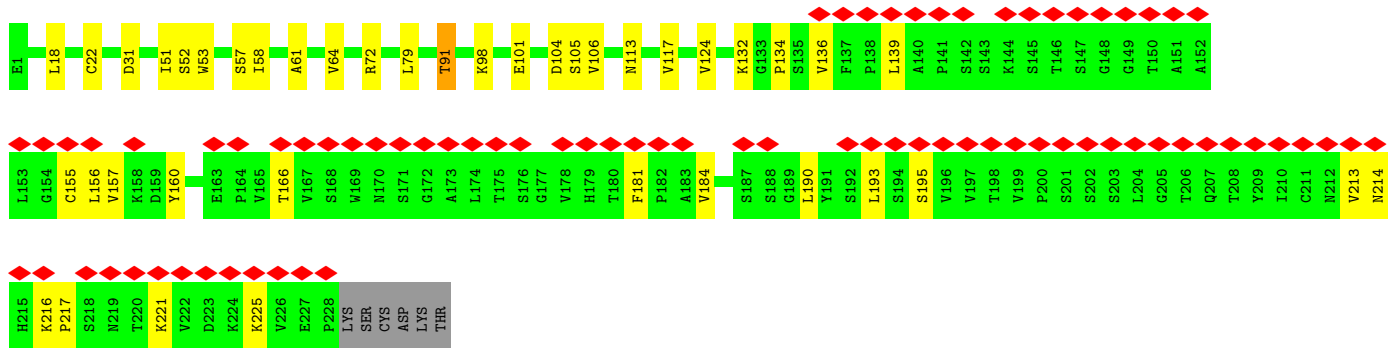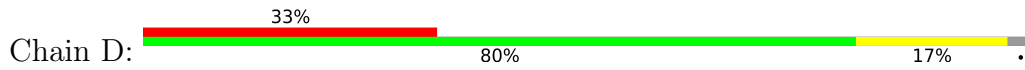

• Molecule 3: Spike protein S1
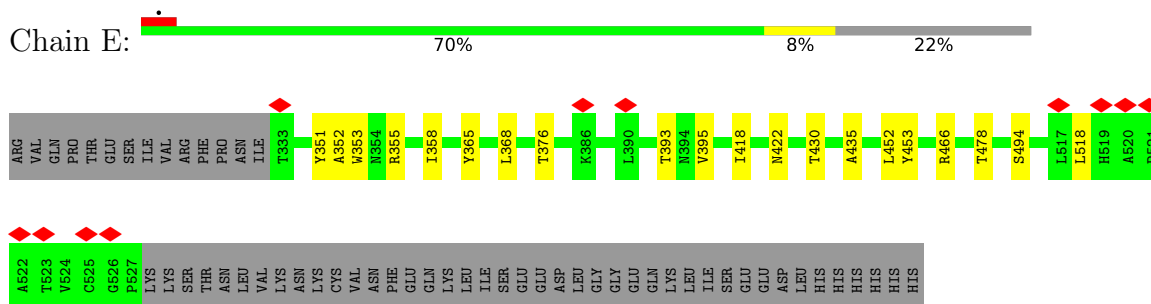
• Molecule 4: REGN10985 antibody Fab fragment light chain

GLN S2 Q6 A13 P14 G15 Q16 S25 S26 Q40 T44 A45 Y51 R63 G79 D84 E85 A86 C90 Q91 Y101 V109 A118 P119 S120 V121 T122 L123 F124 P125 P126 S127 S128 E129 E130 L131 Q132 A133 N134 K135 A136 T137 L138 V139 C140 L141 I142

S143 D144 F145 V150 T151 V152 A153 W154 K155 A156 D157 S158 S159 P160 V161 K162 A163 G164 V165 E166 T167 T168 S174 N175 N176 A180 S181 S182 Y183 L184 S185 L186 T187 P188 E189 Q190 W191 K192 S193 H194 R195 S196 Y197 S198 C199 Q200 V201 T202 H203 E204 G205 S206 T207 V208 E209 K210 T211

V212 A213 P214 THR GLU CYS SER

• Molecule 5: REGN10985 antibody Fab fragment heavy chain

Chain D:

33%

80% 17% •

E1 L18 C22 D31 I51 S52 W53 S57 I58 A61 V64 R72 L79 T91 K98 E101 D104 S105 V106 N113 V117 V124 K132 G133 P134 S135 V136 F137 P138 L139 A140 P141 S142 S143 K144 S145 T146 S147 G148 G149 T150 A151 A152

L153 G154 C155 L156 V157 K158 D159 Y160 E163 P164 V165 T166 V167 S168 W169 N170 S171 G172 A173 L174 T175 S176 G177 V178 H179 T180 F181 P182 A183 V184 S187 S188 S189 L190 Y191 S192 L193 S194 S195 V196 V197 T198 V199 P200 S201 S202 S203 L204 G205 T206 Q207 T208 Y209 I210 C211 N212 V213 N214

H215 K216 P217 S218 N219 T220 K221 V222 D223 K224 K225 V226 E227 P228 LYS SER CYS ASP LYS THR

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain F:

33%

33% 67%

NAG1 NAG2 BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146054	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 $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.320	Depositor
Minimum map value	-0.757	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	255.0, 255.0, 255.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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, BMA

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	0.24	0/1588	0.45	0/2168
2	B	0.24	0/1757	0.44	0/2396
3	E	0.25	0/1587	0.42	0/2161
4	C	0.25	0/1611	0.46	0/2202
5	D	0.24	0/1740	0.48	0/2369
All	All	0.24	0/8283	0.45	0/11296

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	1551	0	1497	24	0
2	B	1710	0	1666	18	0
3	E	1543	0	1459	9	0
4	C	1572	0	1517	29	0
5	D	1700	0	1660	28	0
6	F	39	0	34	2	0
All	All	8115	0	7833	106	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 106 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:19:THR:HG22	1:A:76:THR:HG22	1.63	0.81
1:A:52:ASP:O	1:A:54:SER:N	2.13	0.81
5:D:91:THR:HA	5:D:124:VAL:O	1.81	0.79
5:D:52:SER:HB3	5:D:106:VAL:HG23	1.68	0.76
5:D:136:VAL:HG21	5:D:213:VAL:HG21	1.74	0.68

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	208/216 (96%)	201 (97%)	6 (3%)	1 (0%)	29	61
2	B	222/229 (97%)	214 (96%)	8 (4%)	0	100	100
3	E	193/251 (77%)	186 (96%)	7 (4%)	0	100	100
4	C	211/218 (97%)	203 (96%)	8 (4%)	0	100	100
5	D	226/234 (97%)	218 (96%)	8 (4%)	0	100	100
All	All	1060/1148 (92%)	1022 (96%)	37 (4%)	1 (0%)	54	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL

5.3.2　Protein sidechains ⓘ

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	177/183 (97%)	177 (100%)	0	100	100
2	B	189/194 (97%)	189 (100%)	0	100	100
3	E	168/222 (76%)	166 (99%)	2 (1%)	71	83
4	C	177/182 (97%)	177 (100%)	0	100	100
5	D	189/195 (97%)	188 (100%)	1 (0%)	88	93
All	All	900/976 (92%)	897 (100%)	3 (0%)	92	96

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

Mol	Chain	Res	Type
3	E	430	THR
3	E	478	THR
5	D	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
4	C	81	GLN
4	C	194	HIS
5	D	186	GLN
5	D	170	ASN
1	A	198	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

5.4　Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

3 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
6	NAG	F	1	3,6	14,14,15	0.29	0	17,19,21	0.59	0
6	NAG	F	2	6	14,14,15	0.30	0	17,19,21	0.42	0
6	BMA	F	3	6	11,11,12	0.57	0	15,15,17	0.84	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
6	NAG	F	1	3,6	-	<mark>2/6/23/26</mark>	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	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	F	2	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	NAG	2	0

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

Oligosaccharide Chain F

Bond lengths — Bond angles — Torsions — Rings
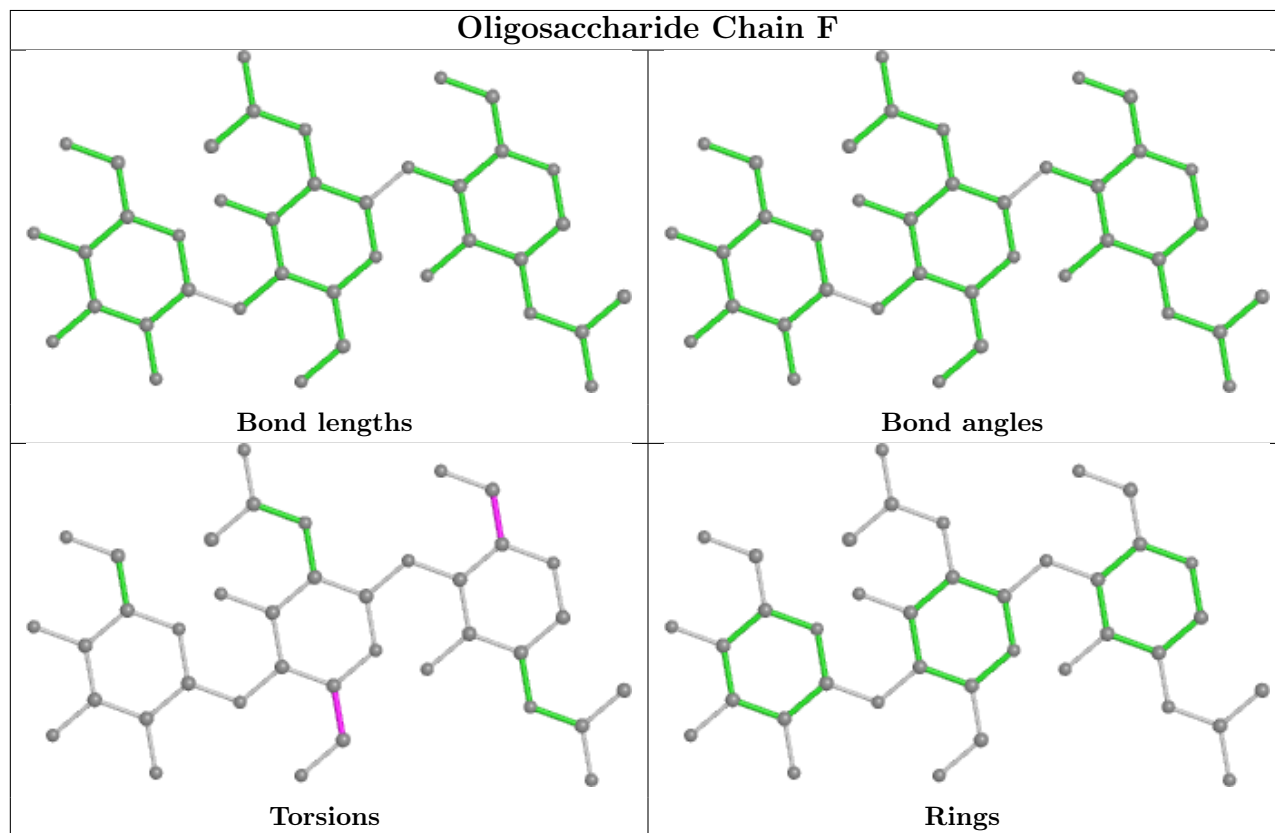
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-23662. 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 |
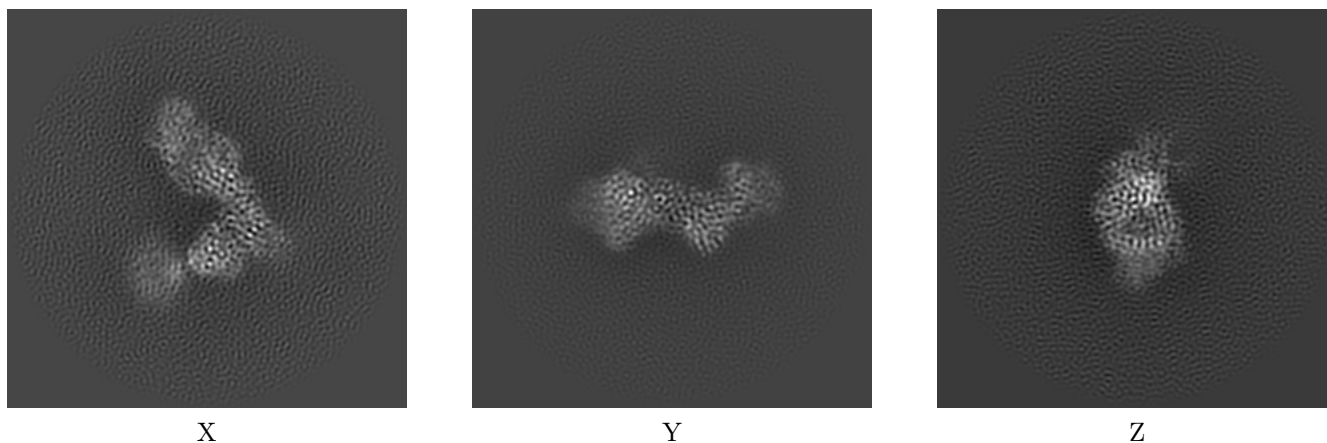
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 150 | Y Index: 150 | Z Index: 150 |
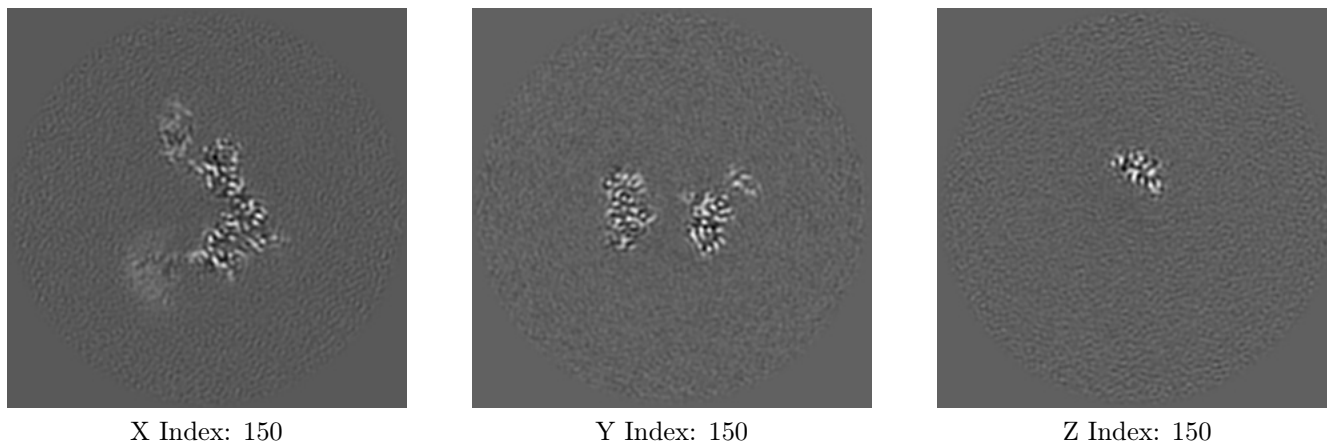
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
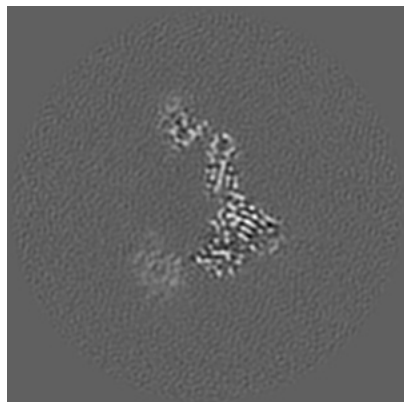
6.3.1 Primary map
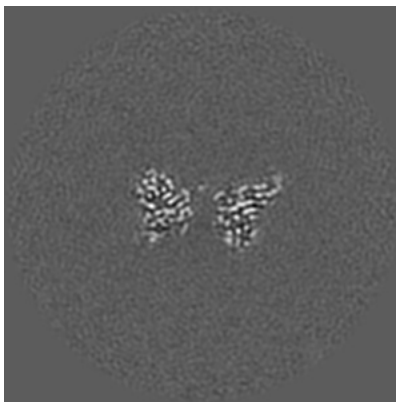
| X Index: 159 | Y Index: 156 | Z Index: 111 |
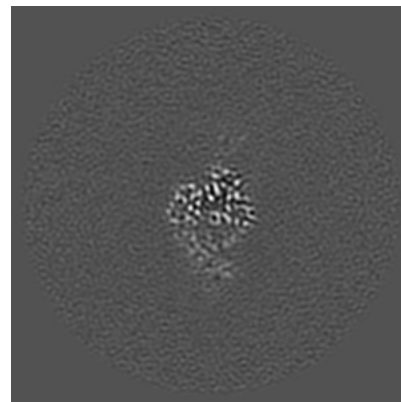
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
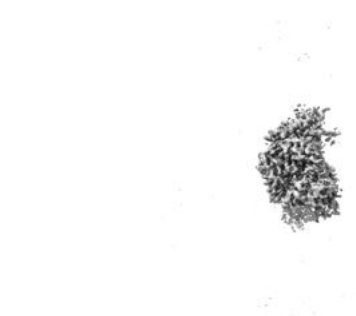
The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 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 ⓘ
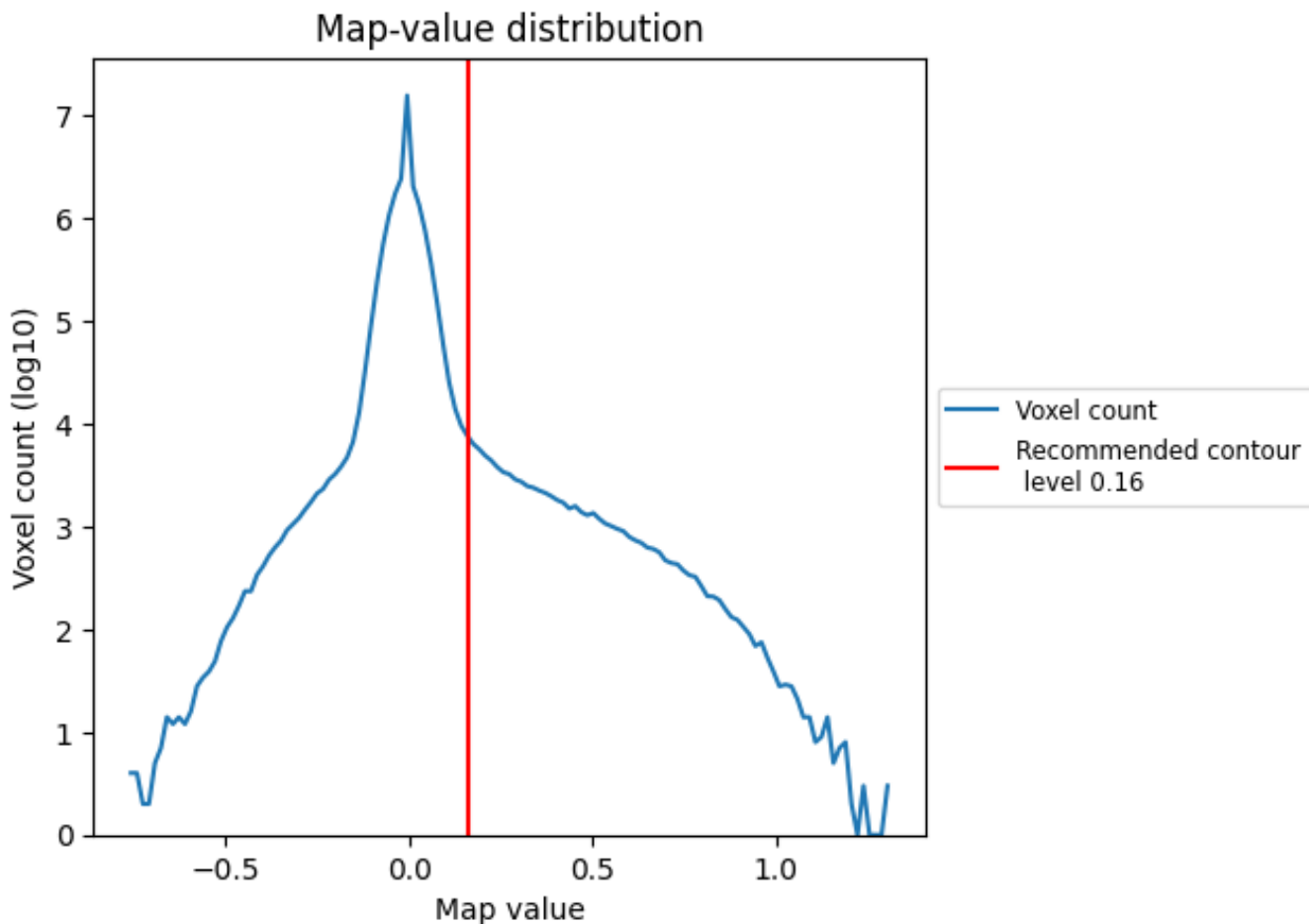
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
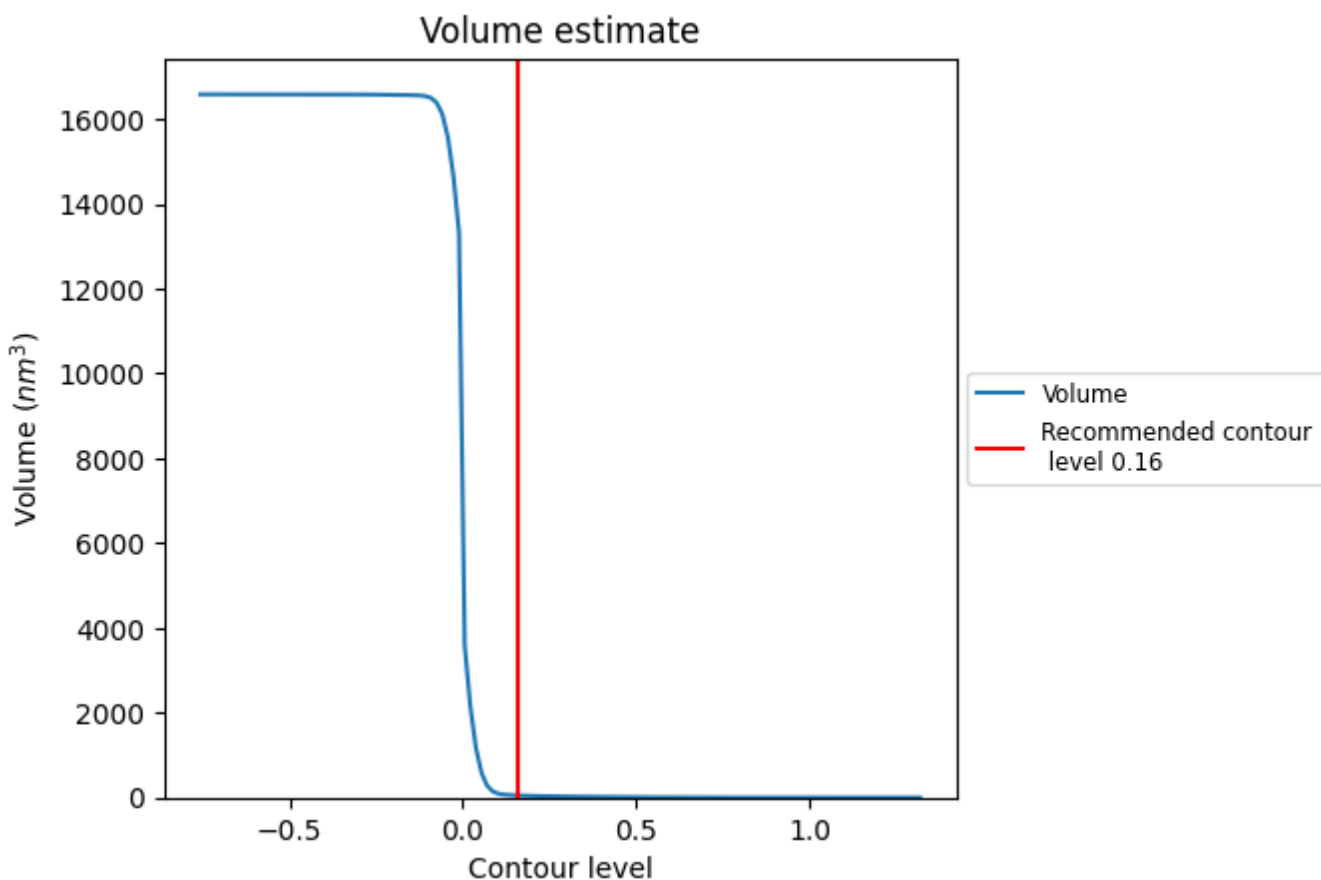
The volume at the recommended contour level is 49 nm^3; this corresponds to an approximate mass of 45 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ
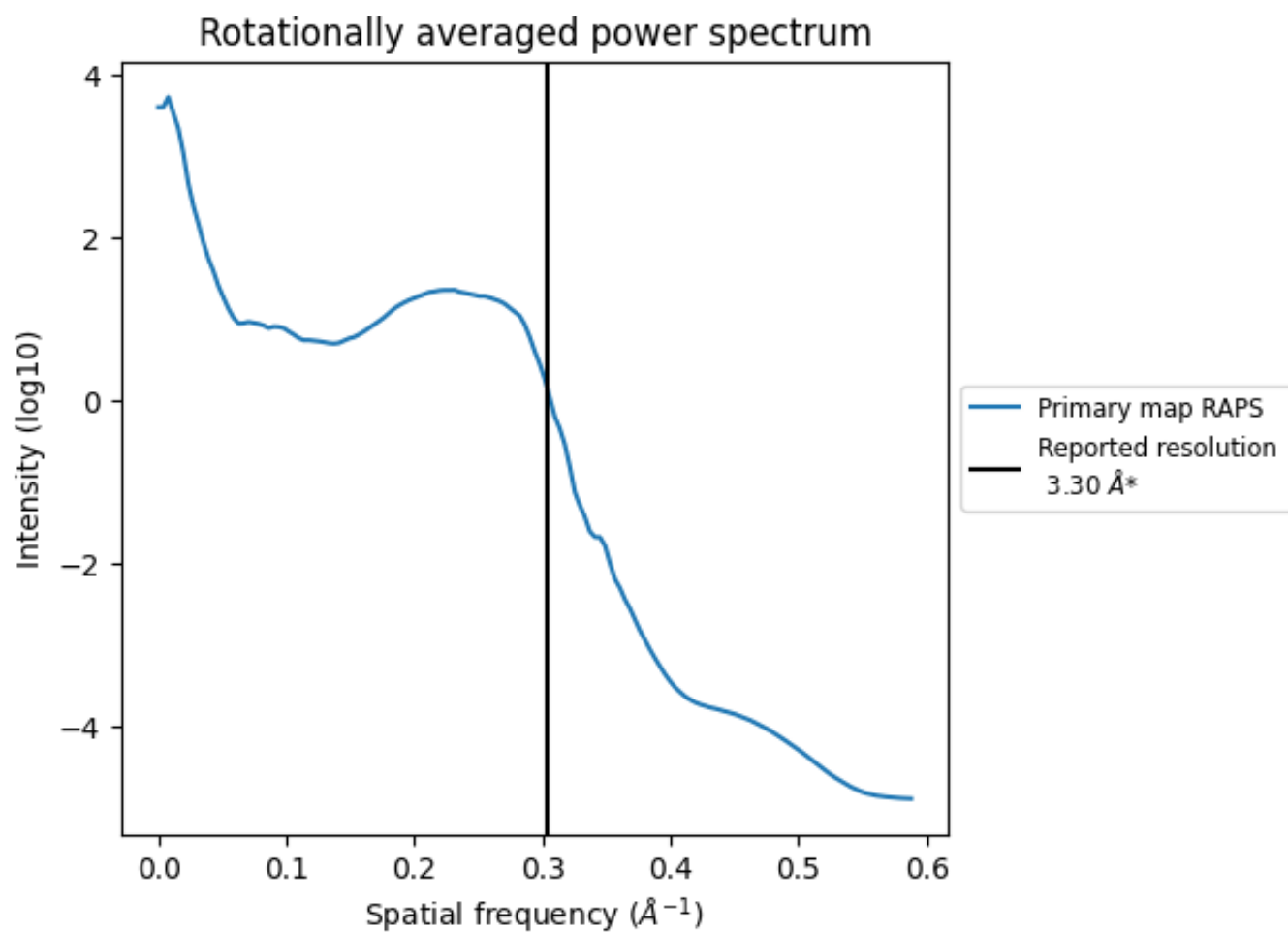
*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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-23662 and PDB model 7M42. Per-residue inclusion information can be found in section 3 on page 5.

9.1   Map-model overlay ⓘ

| X | Y | Z |
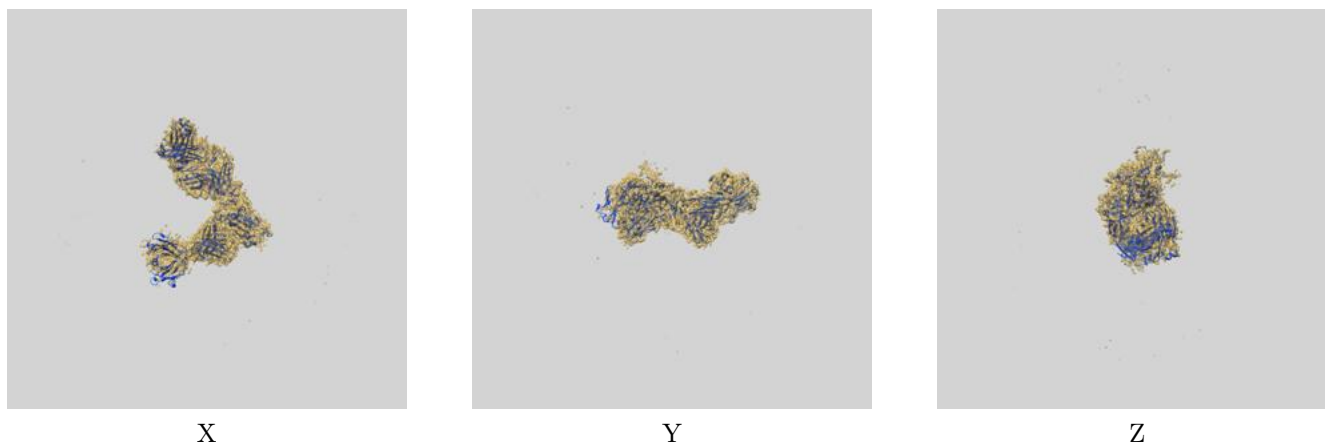
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ
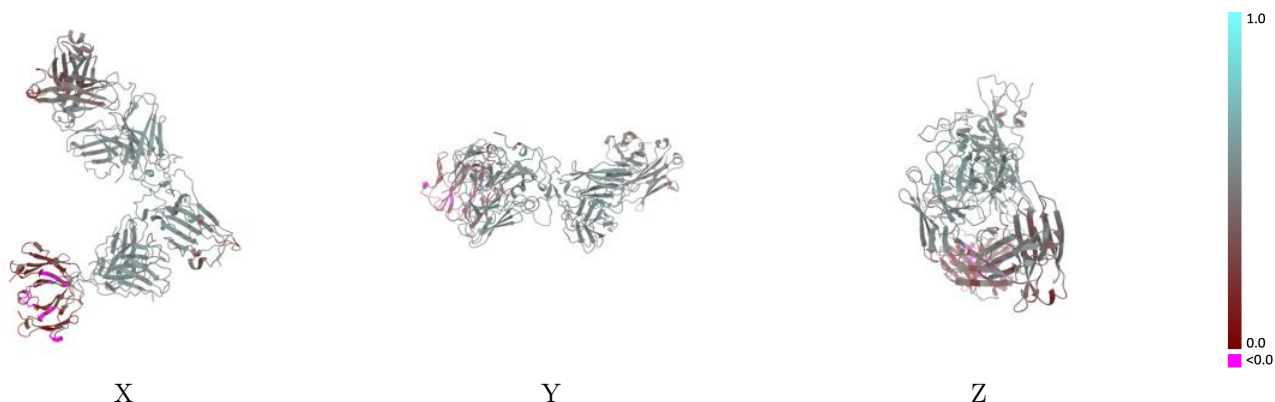
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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   ⓘ
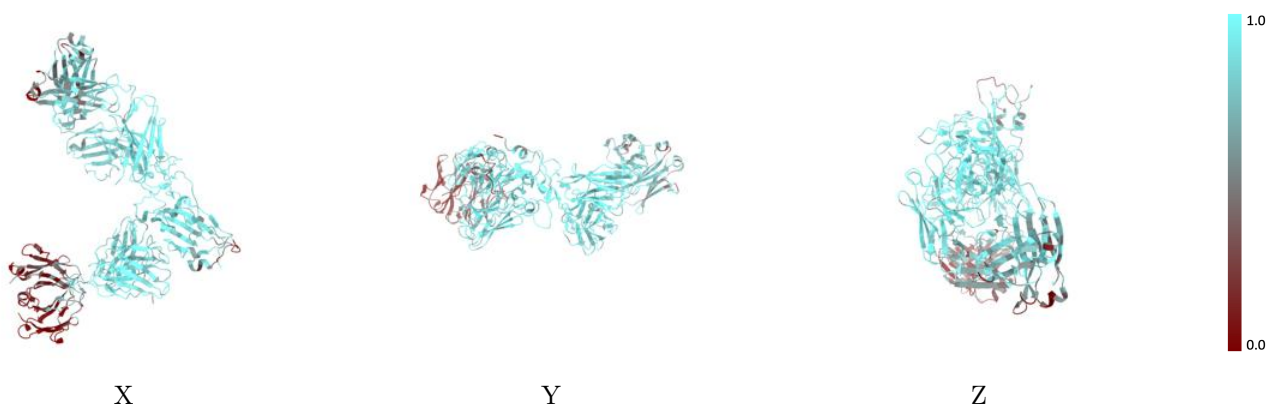
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion ⓘ
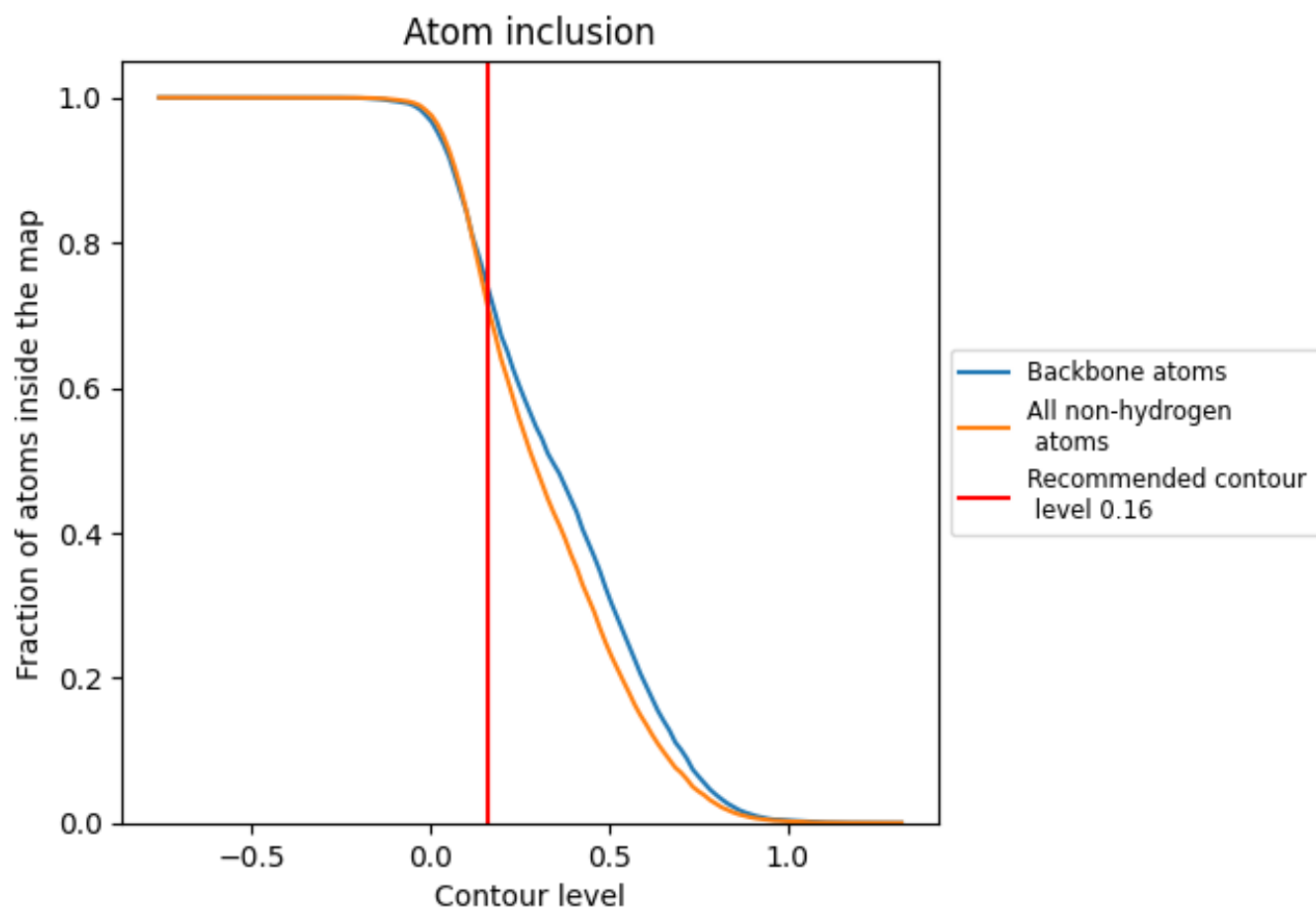
At the recommended contour level, 74% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7168	0.4490
A	0.7965	0.4770
B	0.8081	0.4950
C	0.5929	0.3850
D	0.5743	0.3840
E	0.8243	0.5090
F	0.5128	0.2980

1.0

0.0
<0.0