



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 07:37 PM EDT

PDB ID : 7RXD
EMDB ID : EMD-24729
Title : CryoEM structure of RBD domain of COVID-19 in complex with Legobody
Authors : Wu, X.D.; Rapoport, T.A.
Deposited on : 2021-08-22
Resolution : 3.60 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

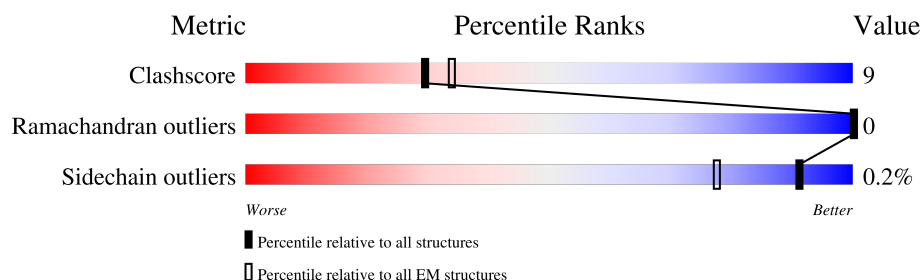
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	B	545	
2	H	234	
3	L	219	
4	N	129	
5	R	235	
6	A	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9007 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 Maltodextrin-binding protein, Immunoglobulin G-binding protein A, Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	439	Total	C	N	O	S	0	0
			3433	2210	556	660	7		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A0A4Z0THX4
B	361	ALA	GLN	conflict	UNP P99134
B	362	LEU	ASN	conflict	UNP P99134
B	365	ALA	TYR	conflict	UNP P99134
B	367	ILE	VAL	conflict	UNP P99134
B	369	ILE	ASN	conflict	UNP P99134
B	374	THR	ASN	conflict	UNP P99134
B	375	GLU	ALA	conflict	UNP P99134
B	376	GLU	ASP	conflict	UNP P99134
B	391	VAL	GLN	conflict	UNP P99134
B	393	LYS	ALA	conflict	UNP P99134
B	394	GLU	ASN	conflict	UNP P99134
B	395	ILE	VAL	conflict	UNP P99134
B	397	ALA	GLY	conflict	UNP P99134
B	400	LYS	GLN	conflict	UNP P99134
B	404	GLU	ASP	conflict	UNP P99134
B	405	HIS	SER	conflict	UNP P99134
B	?	-	ALA	deletion	UNP P99134
B	410	GLY	ASP	conflict	UNP P99134
B	411	GLY	ALA	conflict	UNP P99134
B	412	SER	GLN	conflict	UNP P99134
B	413	GLY	GLN	conflict	UNP P99134
B	414	GLY	ASN	conflict	UNP P99134
B	415	ALA	ASN	conflict	UNP P99134
B	416	GLY	PHE	conflict	UNP P99134
B	417	SER	ASN	conflict	UNP P99134
B	418	GLY	LYS	conflict	UNP P99134

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Chain	Residue	Modelled	Actual	Comment	Reference
B	468	GLY	-	linker	UNP P99134
B	469	GLY	-	linker	UNP P99134
B	470	GLY	-	linker	UNP P99134
B	471	SER	-	linker	UNP P99134
B	472	GLY	-	linker	UNP P99134
B	473	GLY	-	linker	UNP P99134
B	474	GLY	-	linker	UNP P99134
B	475	SER	-	linker	UNP P99134
B	476	GLY	-	linker	UNP P99134
B	477	GLY	-	linker	UNP P99134
B	478	SER	-	linker	UNP P99134
B	537	GLY	-	expression tag	UNP P06654
B	538	SER	-	expression tag	UNP P06654
B	539	GLY	-	expression tag	UNP P06654
B	540	HIS	-	expression tag	UNP P06654
B	541	HIS	-	expression tag	UNP P06654
B	542	HIS	-	expression tag	UNP P06654
B	543	HIS	-	expression tag	UNP P06654
B	544	HIS	-	expression tag	UNP P06654
B	545	HIS	-	expression tag	UNP P06654

- Molecule 2 is a protein called Fab_8D3_2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	207	Total	C	N	O	S	0	0
			1582	1006	262	305	9		

- Molecule 3 is a protein called Fab_8D3_2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	204	Total	C	N	O	S	0	0
			1588	1003	264	315	6		

- Molecule 4 is a protein called Nb_RBD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	125	Total	C	N	O	S	0	0
			990	621	177	188	4		

- Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	173	Total	C	N	O	S	0	0
			1391	897	231	258	5		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	307	GLY	-	expression tag	UNP P0DTC2
R	308	ASP	-	expression tag	UNP P0DTC2
R	309	TYR	-	expression tag	UNP P0DTC2
R	310	LYS	-	expression tag	UNP P0DTC2
R	311	ASP	-	expression tag	UNP P0DTC2
R	312	ASP	-	expression tag	UNP P0DTC2
R	313	ASP	-	expression tag	UNP P0DTC2
R	314	ASP	-	expression tag	UNP P0DTC2
R	315	LYS	-	expression tag	UNP P0DTC2
R	316	GLY	-	expression tag	UNP P0DTC2
R	317	GLY	-	expression tag	UNP P0DTC2
R	318	GLU	-	expression tag	UNP P0DTC2
R	319	ASN	-	expression tag	UNP P0DTC2
R	320	LEU	-	expression tag	UNP P0DTC2
R	321	TYR	-	expression tag	UNP P0DTC2
R	322	PHE	-	expression tag	UNP P0DTC2
R	323	GLN	-	expression tag	UNP P0DTC2
R	324	GLY	-	expression tag	UNP P0DTC2
R	325	GLY	-	expression tag	UNP P0DTC2
R	326	SER	-	expression tag	UNP P0DTC2
R	327	GLY	-	expression tag	UNP P0DTC2
R	328	ASP	-	expression tag	UNP P0DTC2
R	329	SER	-	expression tag	UNP P0DTC2
R	330	THR	-	expression tag	UNP P0DTC2
R	331	GLY	-	expression tag	UNP P0DTC2
R	332	SER	-	expression tag	UNP P0DTC2
R	333	SER	-	expression tag	UNP P0DTC2
R	527	GLY	-	expression tag	UNP P0DTC2
R	528	GLY	-	expression tag	UNP P0DTC2
R	529	GLY	-	expression tag	UNP P0DTC2
R	530	SER	-	expression tag	UNP P0DTC2
R	531	GLY	-	expression tag	UNP P0DTC2
R	532	SER	-	expression tag	UNP P0DTC2
R	533	GLY	-	expression tag	UNP P0DTC2
R	534	HIS	-	expression tag	UNP P0DTC2
R	535	HIS	-	expression tag	UNP P0DTC2
R	536	HIS	-	expression tag	UNP P0DTC2

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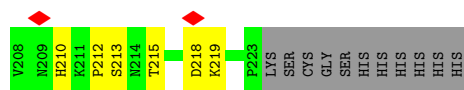
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Chain	Residue	Modelled	Actual	Comment	Reference
R	537	HIS	-	expression tag	UNP P0DTC2
R	538	HIS	-	expression tag	UNP P0DTC2
R	539	HIS	-	expression tag	UNP P0DTC2
R	540	HIS	-	expression tag	UNP P0DTC2
R	541	HIS	-	expression tag	UNP P0DTC2

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

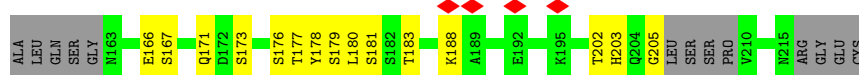
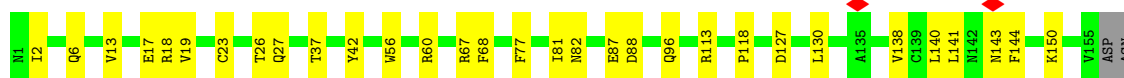


Mol	Chain	Residues	Atoms			AltConf	Trace
6	A	2	Total	C	O	0	0
			23	12	11		



- Molecule 3: Fab_8D3_2 light chain

Chain L: 72% 21% 7%



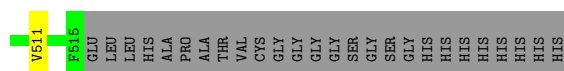
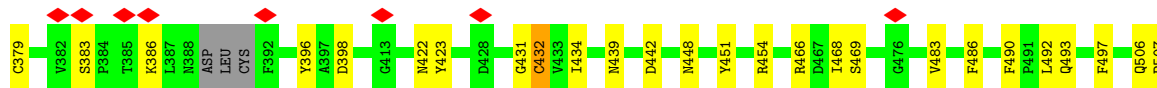
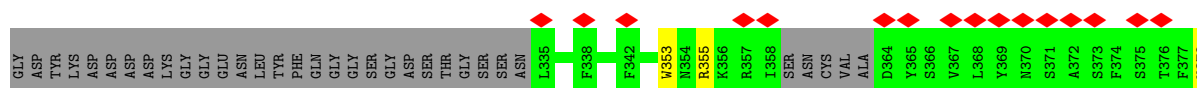
- Molecule 4: Nb_RBD

Chain N: 67% 30% 3%



- Molecule 5: Spike protein S1

Chain R: 10% 61% 12% 26%



- Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain A: 50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	282995	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 ($e^-/\text{\AA}^2$)	50.42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.233	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.024	Depositor
Map size (\AA)	243.79999, 243.79999, 243.79999	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.25	0/3511	0.43	0/4765
2	H	0.28	0/1624	0.50	0/2211
3	L	0.27	0/1623	0.49	0/2203
4	N	0.33	0/1015	0.54	0/1376
5	R	0.30	0/1430	0.51	1/1940 (0.1%)
All	All	0.28	0/9203	0.48	1/12495 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	432	CYS	CA-CB-SG	7.59	127.67	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	158	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3433	0	3391	53	0
2	H	1582	0	1532	35	0
3	L	1588	0	1549	34	0
4	N	990	0	933	27	0
5	R	1391	0	1316	24	0
6	A	23	0	21	1	0
All	All	9007	0	8742	160	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 9.

The worst 5 of 160 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:R:422:ASN:HD21	5:R:454:ARG:H	1.14	0.95
3:L:87:GLU:HA	3:L:173:SER:HB3	1.63	0.81
5:R:379:CYS:HA	5:R:432:CYS:HB3	1.63	0.81
2:H:207:ASN:ND2	2:H:218:ASP:OD1	2.14	0.80
5:R:379:CYS:HA	5:R:432:CYS:CB	2.16	0.75

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	B	429/545 (79%)	422 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	201/234 (86%)	196 (98%)	5 (2%)	0	100	100
3	L	198/219 (90%)	190 (96%)	8 (4%)	0	100	100
4	N	123/129 (95%)	120 (98%)	3 (2%)	0	100	100
5	R	167/235 (71%)	161 (96%)	6 (4%)	0	100	100
All	All	1118/1362 (82%)	1089 (97%)	29 (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	B	359/433 (83%)	357 (99%)	2 (1%)	84	92
2	H	176/199 (88%)	176 (100%)	0	100	100
3	L	180/192 (94%)	180 (100%)	0	100	100
4	N	101/106 (95%)	101 (100%)	0	100	100
5	R	150/196 (76%)	150 (100%)	0	100	100
All	All	966/1126 (86%)	964 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	HIS
1	B	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	242	ASN
1	B	324	ASN
1	B	356	GLN

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Mol	Chain	Res	Type
1	B	360	GLN
5	R	422	ASN

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 ⓘ

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	$\# Z > 2$
6	GLC	A	1	6	12,12,12	0.55	0	17,17,17	0.52	0
6	GLC	A	2	6	11,11,12	0.66	0	15,15,17	0.53	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	GLC	A	1	6	-	1/2/22/22	0/1/1/1
6	GLC	A	2	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

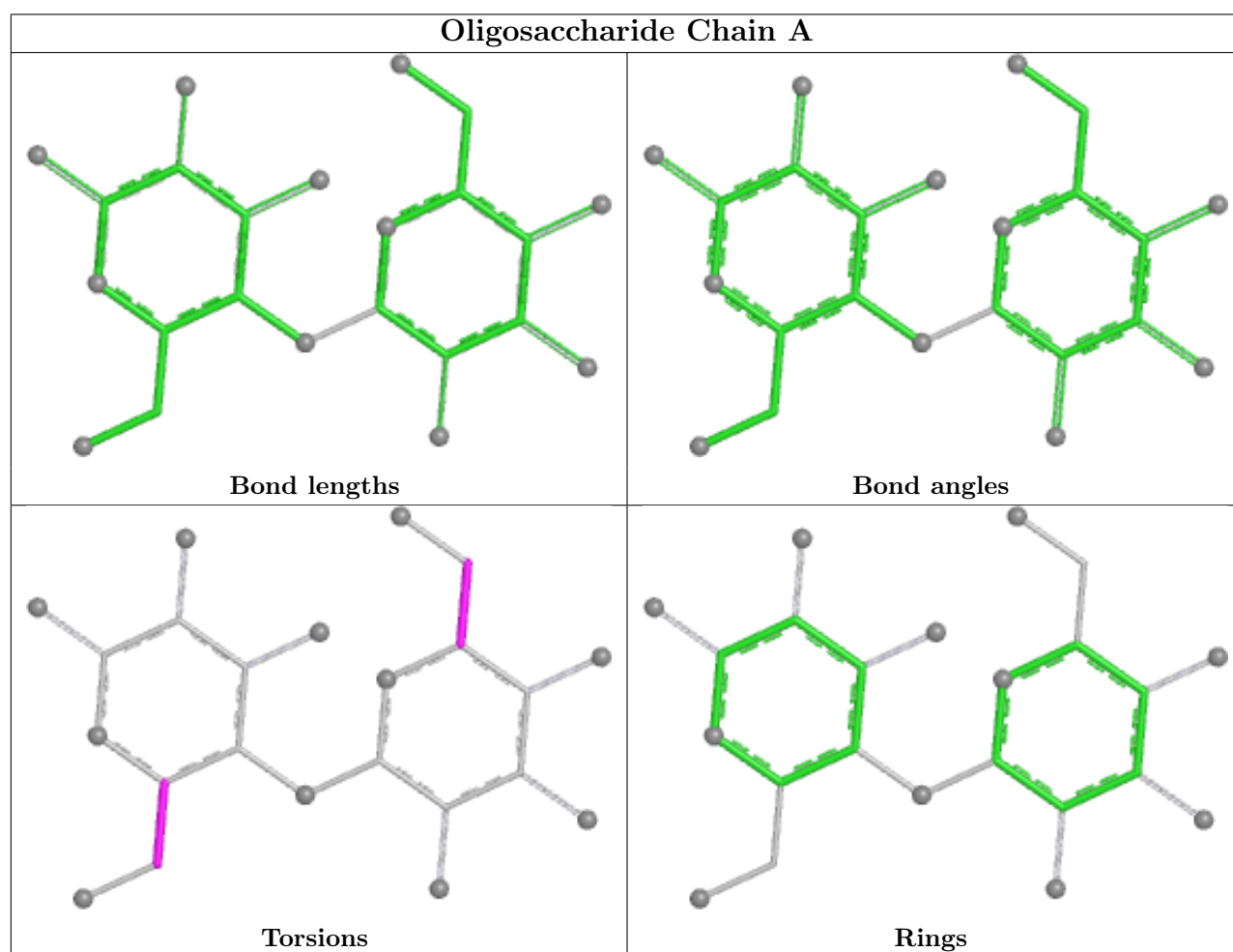
Mol	Chain	Res	Type	Atoms
6	A	2	GLC	O5-C5-C6-O6
6	A	1	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2	GLC	1	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.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

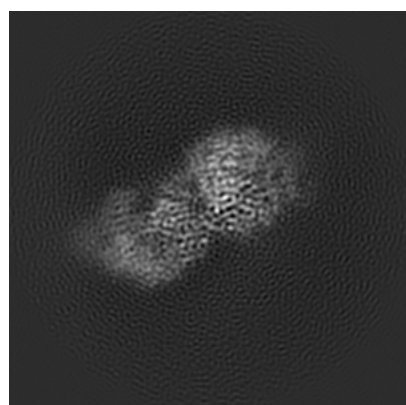
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24729. These allow visual inspection of the internal detail of the map and identification of artifacts.

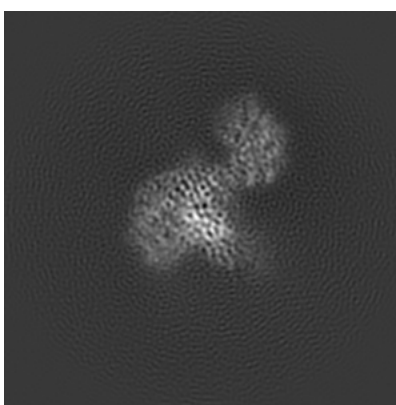
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

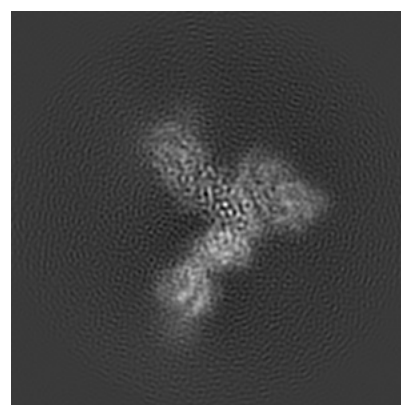
6.1.1 Primary map



X



Y

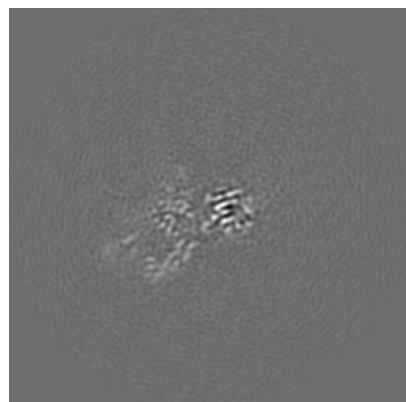


Z

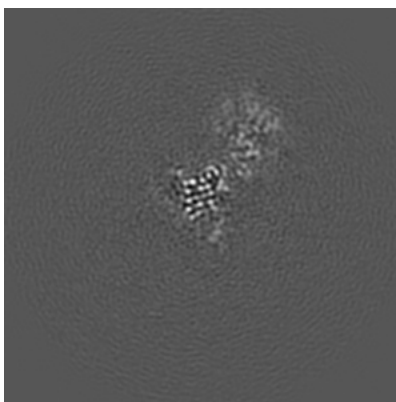
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

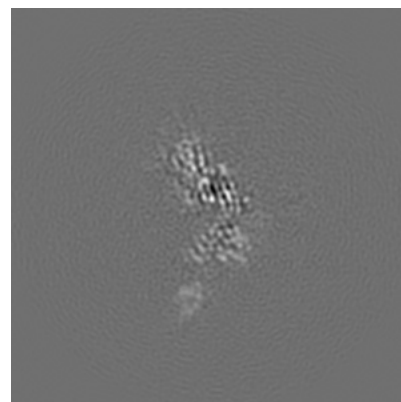
6.2.1 Primary map



X Index: 115



Y Index: 115

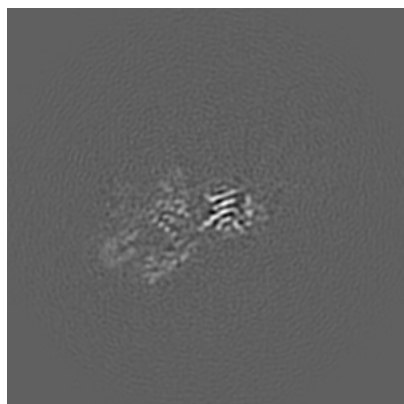


Z Index: 115

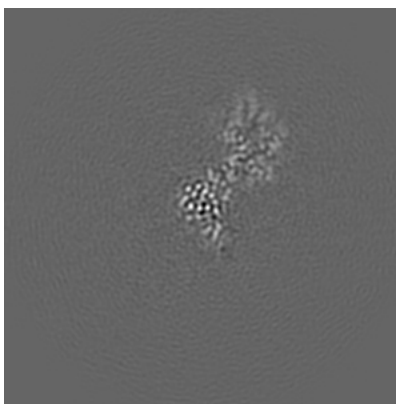
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

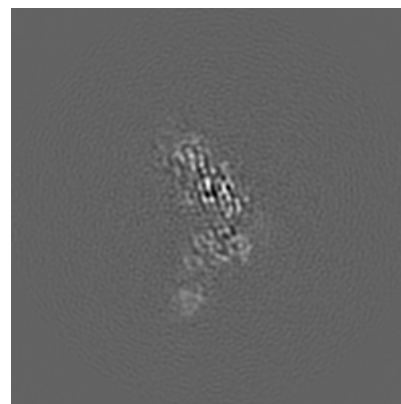
6.3.1 Primary map



X Index: 114



Y Index: 123

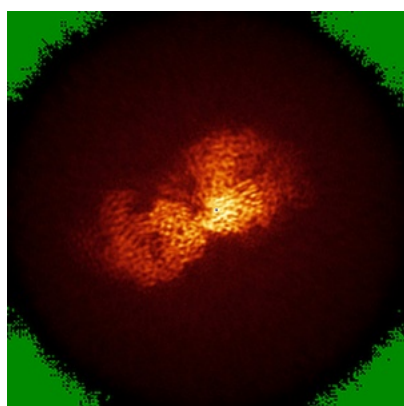


Z Index: 114

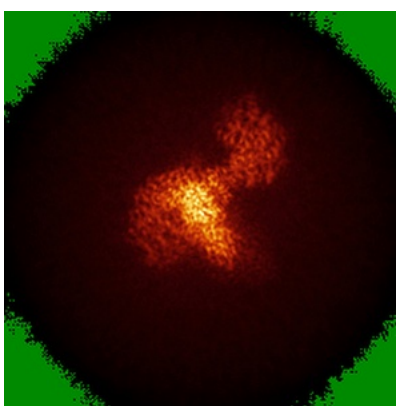
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

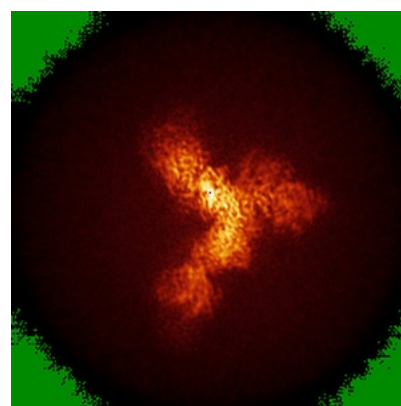
6.4.1 Primary map



X



Y

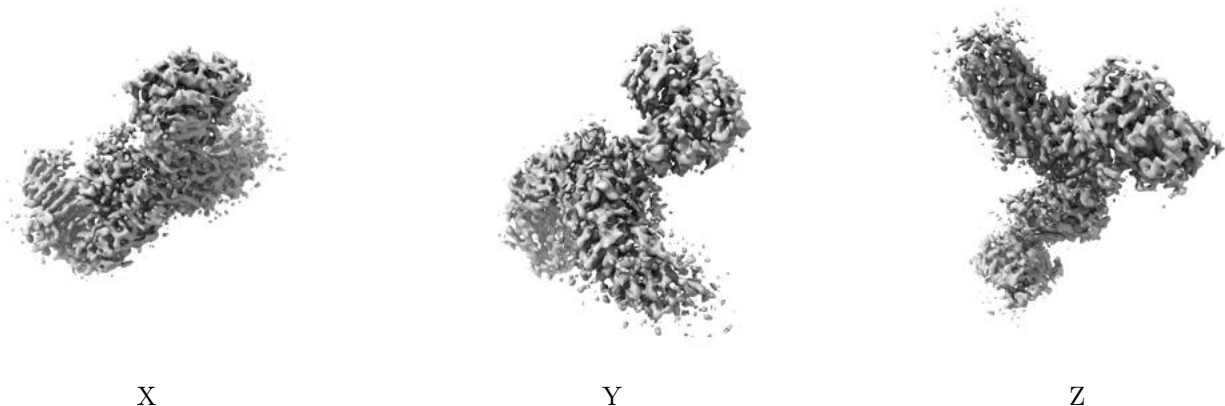


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

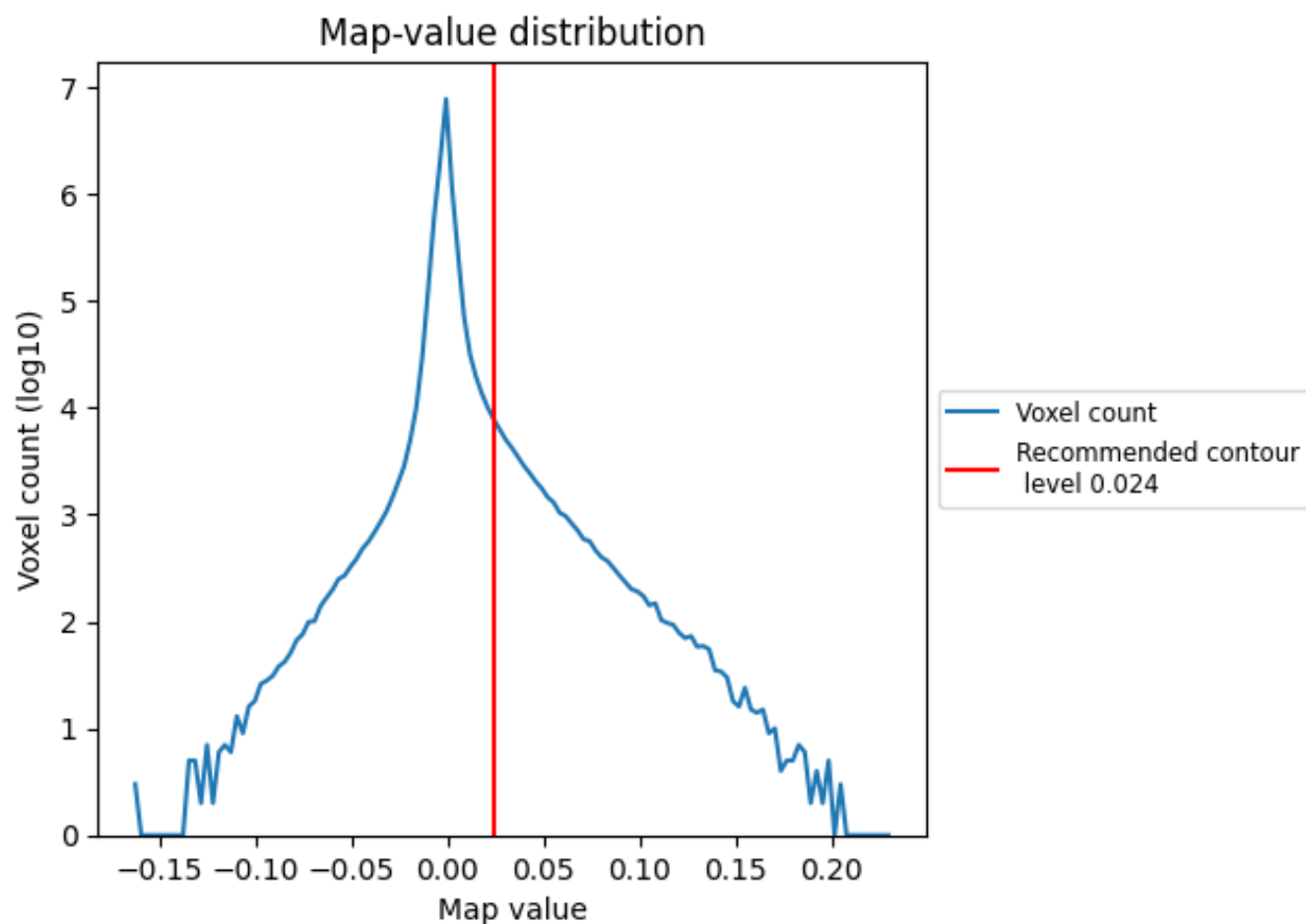
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

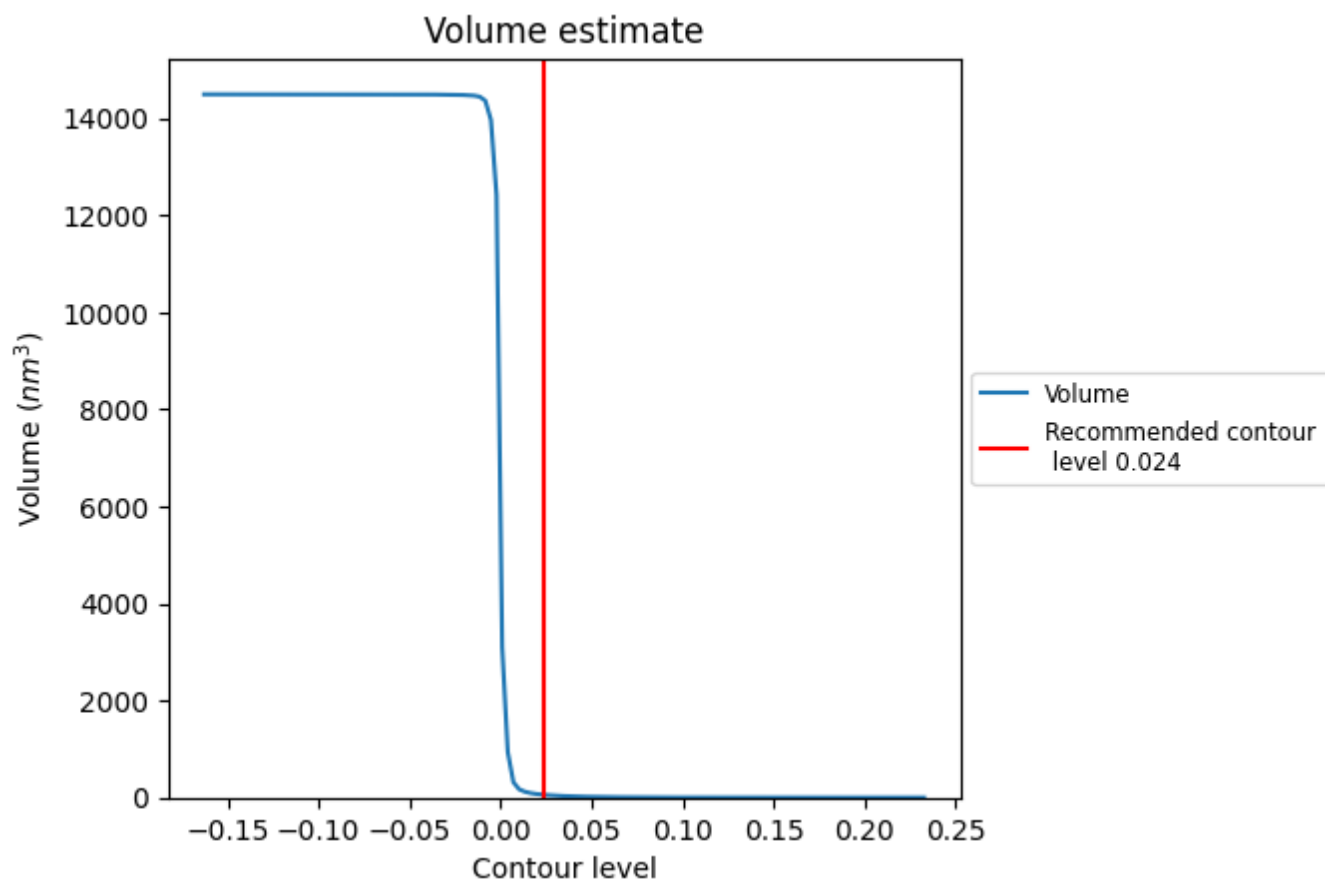
This section contains the results of statistical analysis of the map.

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.

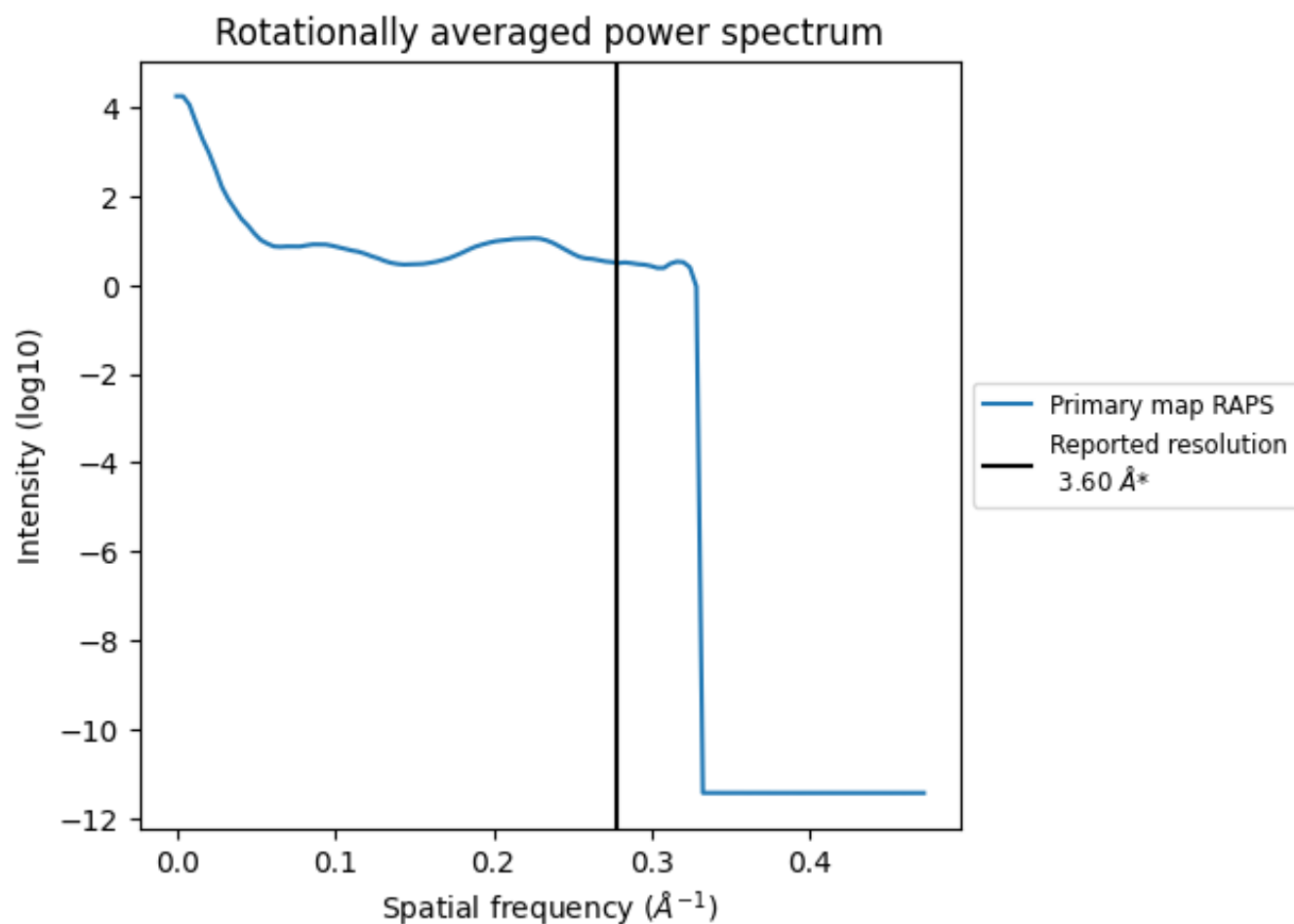
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57 nm³; this corresponds to an approximate mass of 51 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 0.278 Å⁻¹

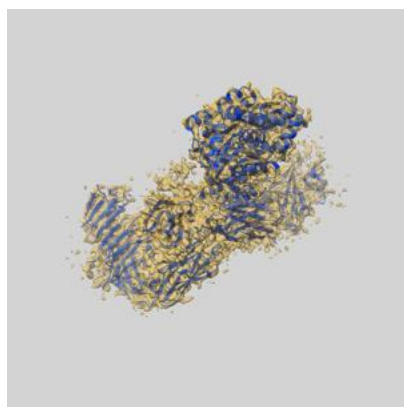
8 Fourier-Shell correlation

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

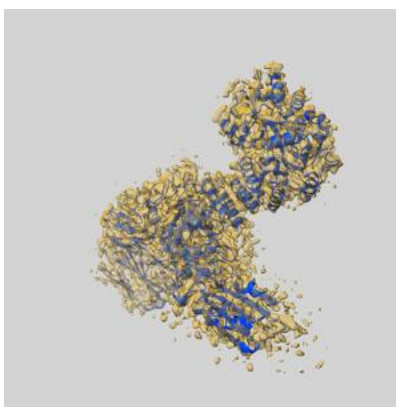
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24729 and PDB model 7RXD. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

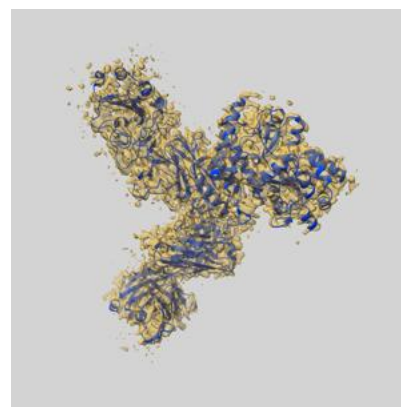
9.1 Map-model overlay [i](#)



X



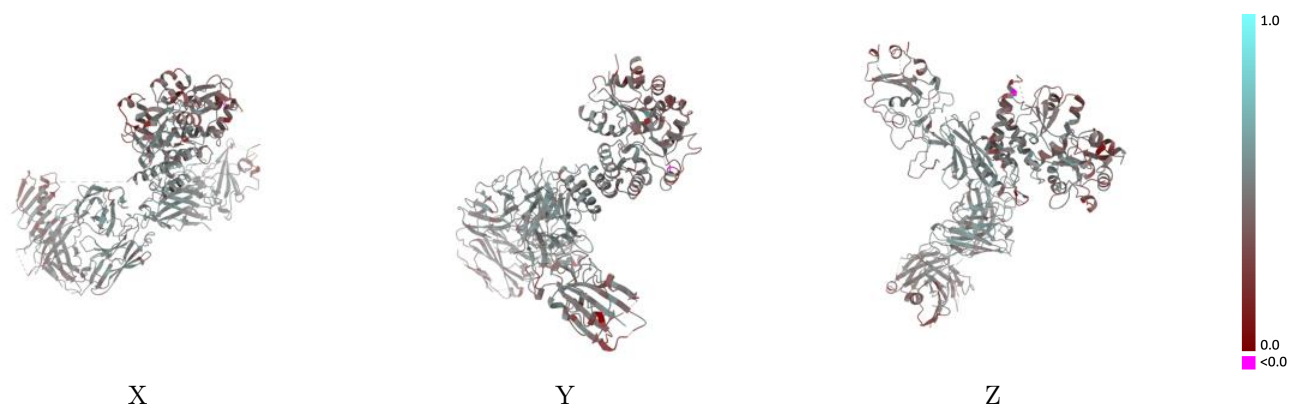
Y



Z

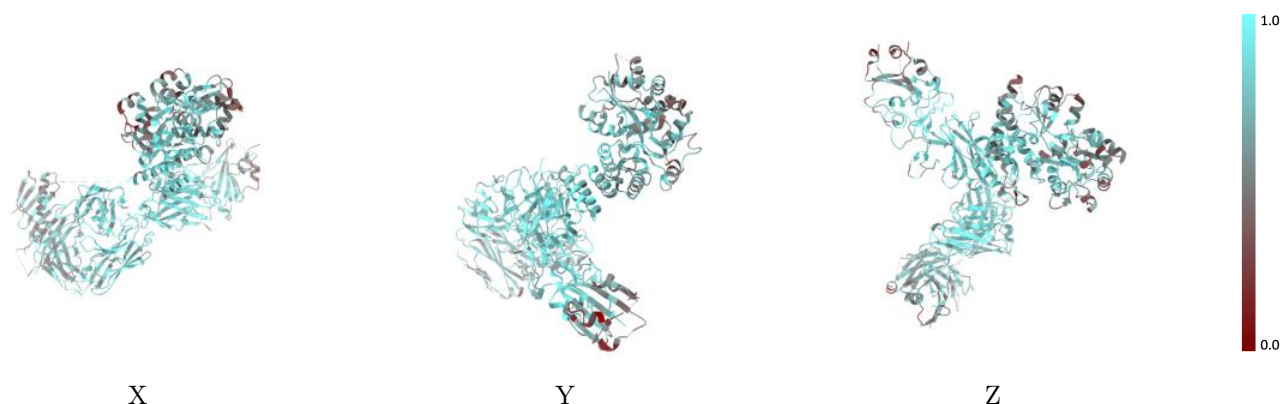
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



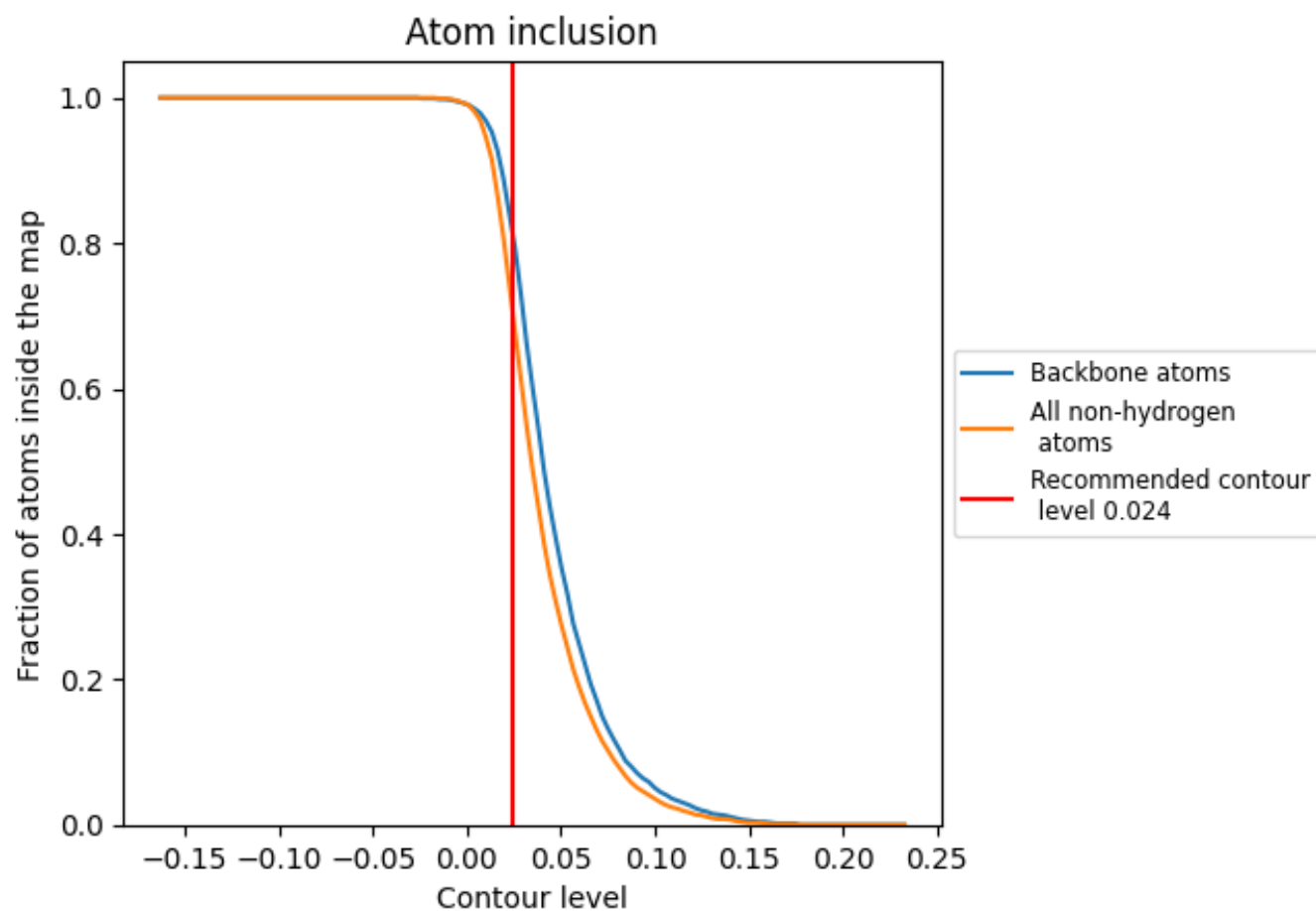
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 71% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7130	<div><div></div></div> 0.4570
A	<div><div></div></div> 0.8700	<div><div></div></div> 0.5250
B	<div><div></div></div> 0.6540	<div><div></div></div> 0.4330
H	<div><div></div></div> 0.7580	<div><div></div></div> 0.4840
L	<div><div></div></div> 0.7370	<div><div></div></div> 0.4630
N	<div><div></div></div> 0.8320	<div><div></div></div> 0.5050
R	<div><div></div></div> 0.6920	<div><div></div></div> 0.4470

1.0

0.0

<0.0