



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2024 – 03:19 pm GMT

PDB ID : 7NIU
EMDB ID : EMD-12365
Title : Nanodisc reconstituted human ABCB4 in complex with 4B1-Fab and QA2-Fab
(apo-inward-open conformation)
Authors : Nosol, K.; Locher, K.P.
Deposited on : 2021-02-14
Resolution : 4.20 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 : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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

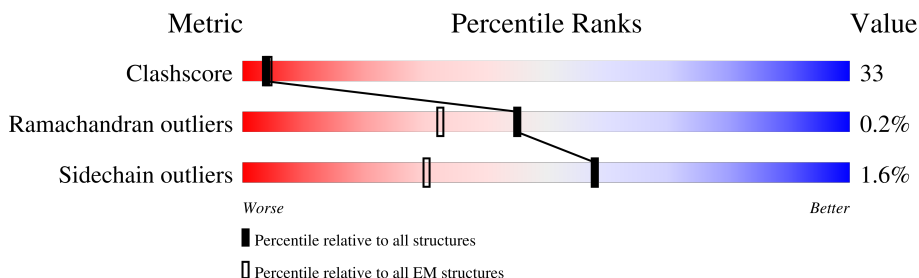
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	A	1279	
2	D	215	
3	E	234	
4	B	215	
5	C	241	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15495 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 Isoform 2 of Phosphatidylcholine translocator ABCB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1133	Total	C	N	O	S	0	0
			8780	5652	1487	1611	30		

- Molecule 2 is a protein called QA2 Fab-fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	208	Total	C	N	O	S	3	0
			1584	988	267	325	4		

- Molecule 3 is a protein called QA2 Fab-fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	229	Total	C	N	O	S	1	0
			1702	1069	286	339	8		

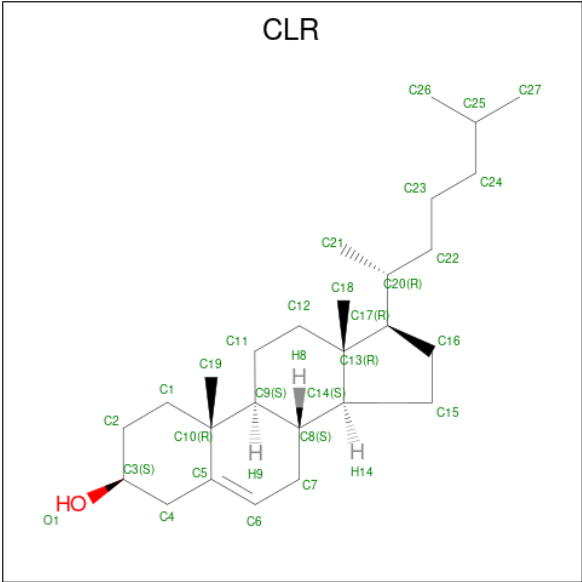
- Molecule 4 is a protein called 4B1 Fab-fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	211	Total	C	N	O	S	3	0
			1616	1012	272	327	5		

- Molecule 5 is a protein called 4B1 Fab-fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	234	Total	C	N	O	S	1	0
			1757	1114	289	348	6		

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).

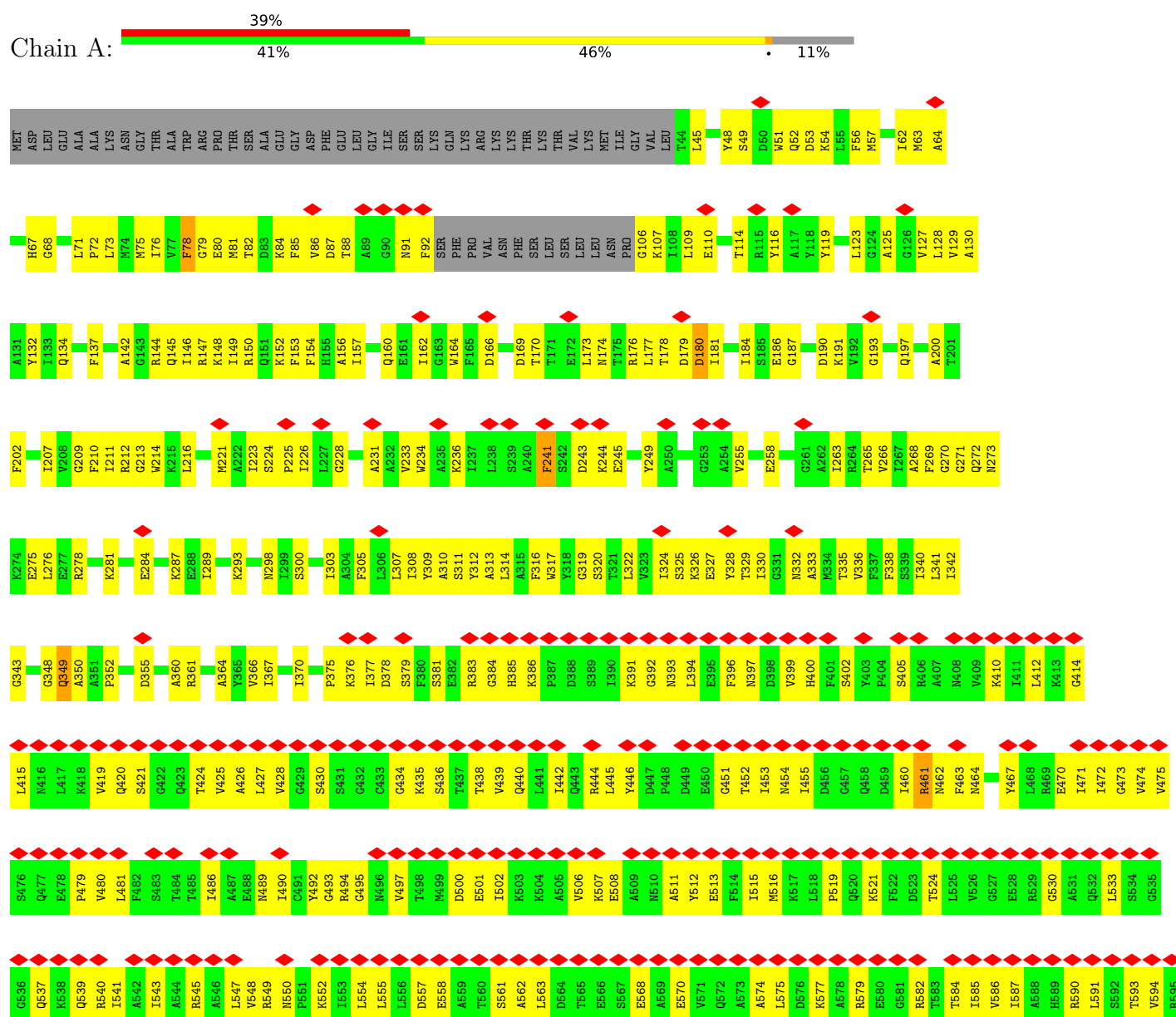


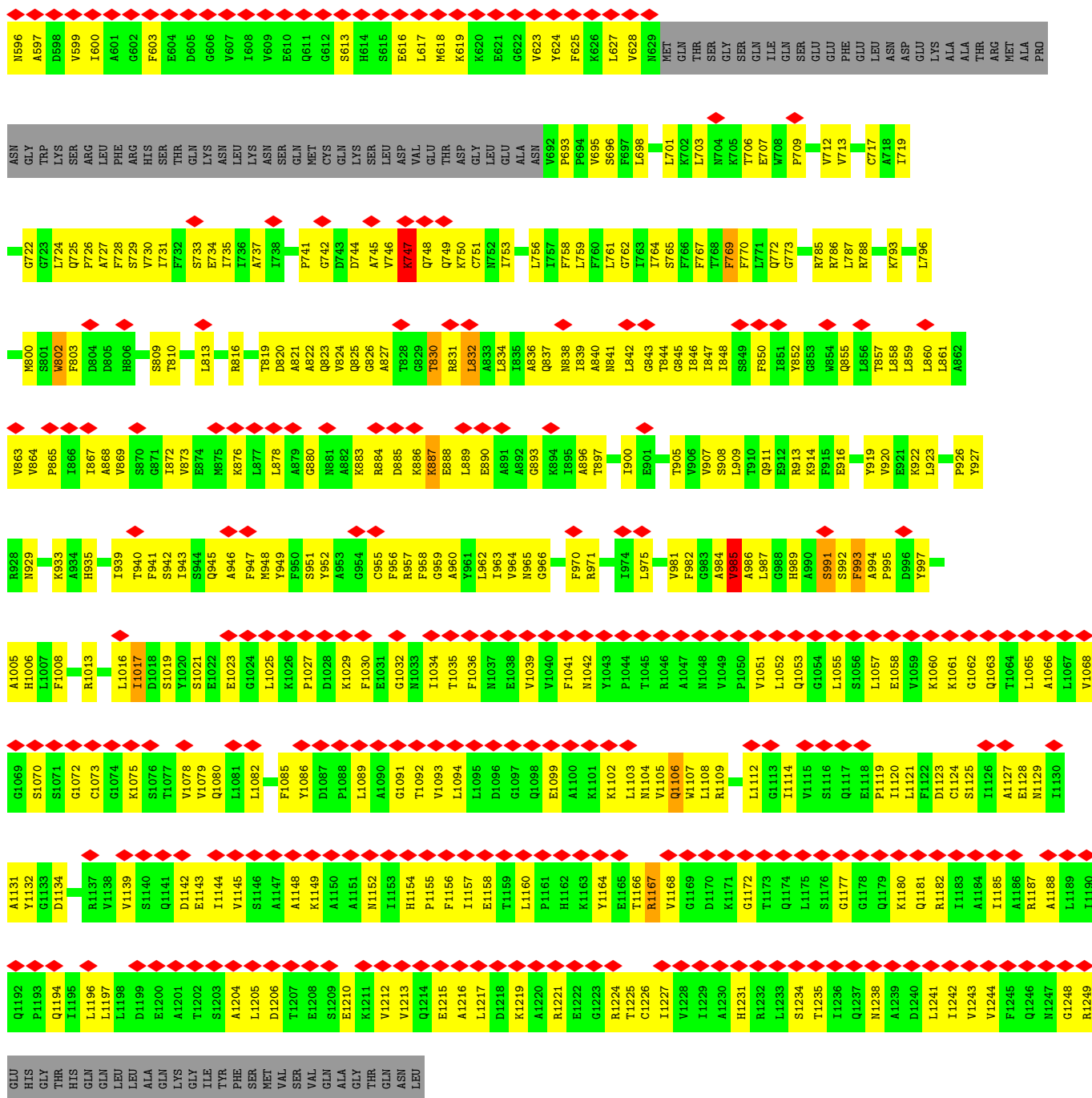
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	

3 Residue-property plots

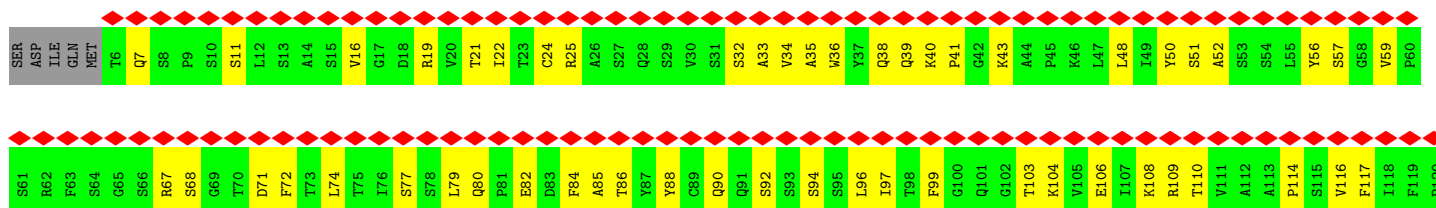
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

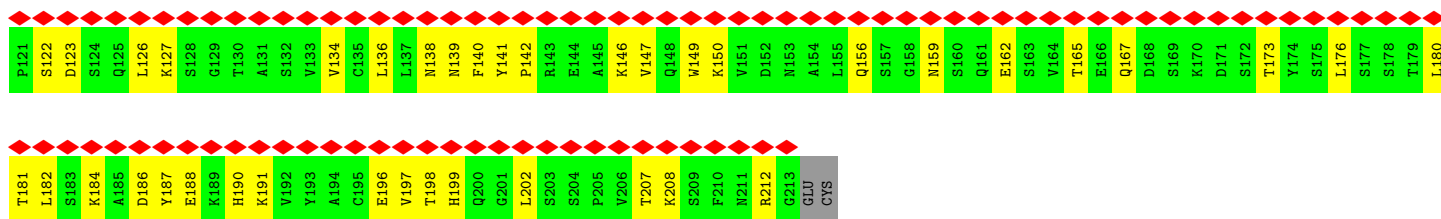
- Molecule 1: Isoform 2 of Phosphatidylcholine translocator ABCB4





• Molecule 2: QA2 Fab-fragment light chain





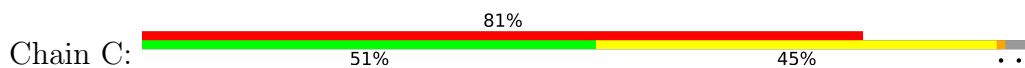
• Molecule 3: QA2 Fab-fragment heavy chain



• Molecule 4: 4B1 Fab-fragment light chain



• Molecule 5: 4B1 Fab-fragment heavy chain



P187	A188	V189	L190	Q191	S192	S193	G194	L195	Y196	S197	L198	S199	S200	V201	V202	T203	V204	P205	S206	S207	S208	L209	G210	T211	Q212	T213	Y214	I215	C216	N217	V218	N219	H220	K221	P222	S223	N224	T225	K226	V227	D228	K229	K230	V231	E232	P233	K234	S235	C236	ASP	LYS	THR	HIS	THR					
T127	L128	V129	T130	V131	S132	S133	A134	S135	T136	K137	G138	P139	S140	V141	F142	P143	L144	A145	P146	S147	S148	K149	S150	T151	S152	G153	G154	T155	A156	A157	L158	G159	C160	L161	V162	K163	D164	Y165	F166	P167	E168	P169	V170	T171	V172	S173	W174	N175	S176	G177	A178	L179	T180	S181	G182	V183	H184	T185	F186
D65	S66	V67	K68	G69	R70	F71	T72	A75	D76	K79	N80	T81	A82	Y83	L84	Q85	M86	N87	S88	L89	R90	A91	E92	D93	T94	A95	V96	Y97	Y98	C99	A100	R101	S102	F103	S104	I105	N106	G107	S108	Y109	S110	W111	W112	W113	D114	Q115	A116	A117	Y118	G119	L120	D121	Y122	W123	G124	Q125	G126		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34430	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 ($e^-/\text{\AA}^2$)	80.4	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	0.039	Depositor
Minimum map value	-0.027	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	295.68002, 295.68002, 295.68002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	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: CLR

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	0.50	0/8942	0.59	0/12083
2	D	0.31	0/1622	0.52	0/2202
3	E	0.33	0/1743	0.53	0/2374
4	B	0.29	0/1655	0.51	0/2245
5	C	0.33	0/1805	0.54	0/2464
All	All	0.43	0/15767	0.56	0/21368

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	8780	0	8929	634	0
2	D	1584	0	1555	88	0
3	E	1702	0	1658	118	0
4	B	1616	0	1593	122	0
5	C	1757	0	1687	116	0
6	A	56	0	92	18	0
All	All	15495	0	15514	1029	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 33.

The worst 5 of 1029 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:341:LEU:HD13	1:A:982:PHE:CE1	1.34	1.57
1:A:88:THR:HG23	1:A:92:PHE:CZ	1.59	1.35
1:A:341:LEU:HD13	1:A:982:PHE:CZ	1.73	1.24
5:C:40:VAL:HG11	5:C:123:TRP:CZ3	1.74	1.22
1:A:424:THR:HG21	1:A:579:ARG:NH2	1.53	1.21

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	1127/1279 (88%)	932 (83%)	190 (17%)	5 (0%)	30	67
2	D	208/215 (97%)	180 (86%)	28 (14%)	0	100	100
3	E	227/234 (97%)	200 (88%)	27 (12%)	0	100	100
4	B	211/215 (98%)	192 (91%)	19 (9%)	0	100	100
5	C	232/241 (96%)	201 (87%)	31 (13%)	0	100	100
All	All	2005/2184 (92%)	1705 (85%)	295 (15%)	5 (0%)	45	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	985	VAL
1	A	349	GLN
1	A	830	THR
1	A	747	LYS
1	A	1216	ALA

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	922/1048 (88%)	902 (98%)	20 (2%)	47	65
2	D	185/190 (97%)	185 (100%)	0	100	100
3	E	191/196 (97%)	188 (98%)	3 (2%)	58	73
4	B	187/189 (99%)	187 (100%)	0	100	100
5	C	194/201 (96%)	191 (98%)	3 (2%)	60	74
All	All	1679/1824 (92%)	1653 (98%)	26 (2%)	58	74

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	991	SER
1	A	1106	GLN
5	C	39	TRP
1	A	1017	ILE
1	A	1167	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1104	ASN
5	C	42	GLN
1	A	1231	HIS
5	C	87	ASN
4	B	161	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
6	CLR	A	1302	-	31,31,31	1.02	3 (9%)	48,48,48	2.62	19 (39%)
6	CLR	A	1301	-	31,31,31	1.07	2 (6%)	48,48,48	1.93	15 (31%)

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	CLR	A	1302	-	-	6/10/68/68	0/4/4/4
6	CLR	A	1301	-	-	9/10/68/68	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1302	CLR	C16-C17	2.92	1.60	1.54
6	A	1301	CLR	C16-C17	2.66	1.59	1.54
6	A	1301	CLR	C4-C3	2.50	1.56	1.52
6	A	1302	CLR	C8-C14	-2.22	1.49	1.53
6	A	1302	CLR	C13-C17	2.19	1.59	1.55

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1302	CLR	C1-C2-C3	8.61	121.51	110.47
6	A	1301	CLR	C3-C4-C5	6.02	122.23	112.03
6	A	1302	CLR	C12-C13-C14	-5.25	99.12	107.27
6	A	1302	CLR	C16-C17-C20	-5.22	104.06	112.15
6	A	1301	CLR	C19-C10-C5	4.39	115.44	108.34

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

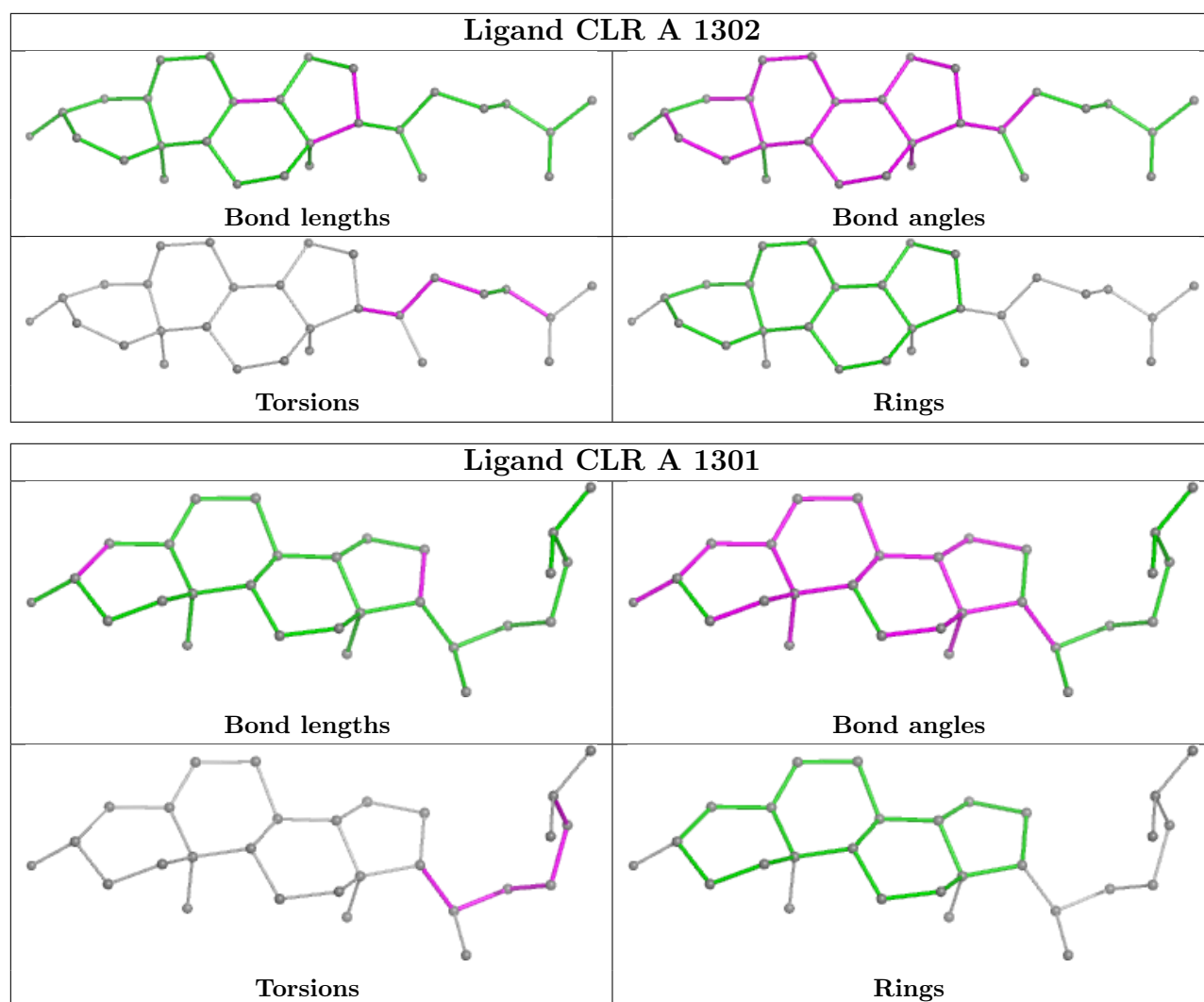
Mol	Chain	Res	Type	Atoms
6	A	1302	CLR	C21-C20-C22-C23
6	A	1301	CLR	C17-C20-C22-C23
6	A	1301	CLR	C20-C22-C23-C24
6	A	1301	CLR	C22-C23-C24-C25
6	A	1302	CLR	C17-C20-C22-C23

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1302	CLR	6	0
6	A	1301	CLR	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

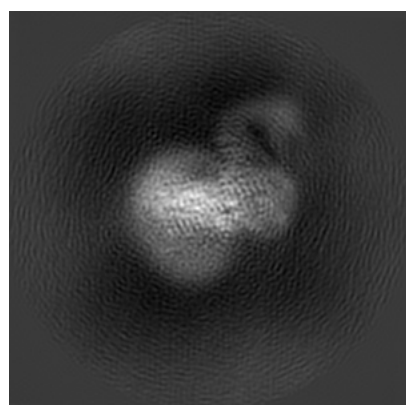
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12365. These allow visual inspection of the internal detail of the map and identification of artifacts.

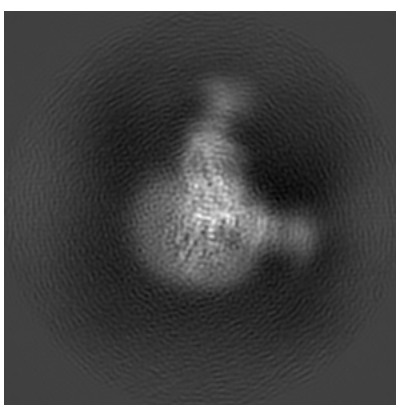
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

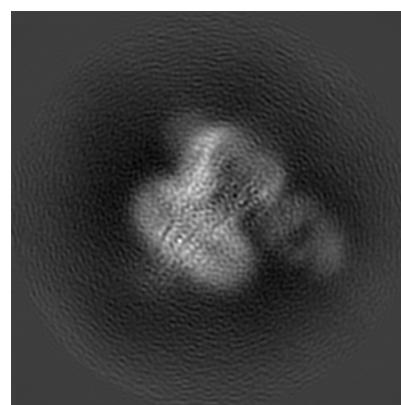
6.1.1 Primary map



X



Y

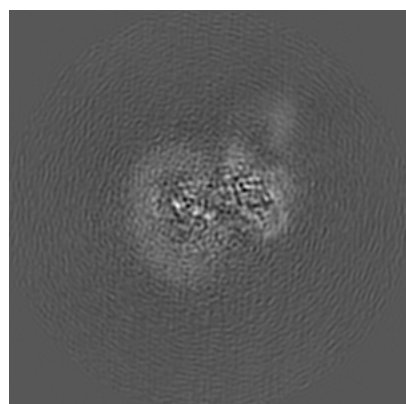


Z

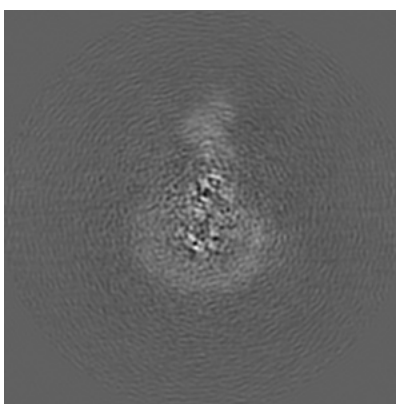
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

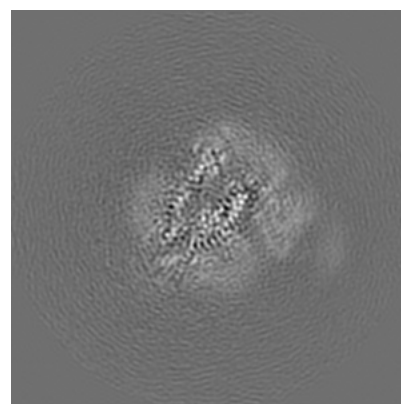
6.2.1 Primary map



X Index: 224



Y Index: 224

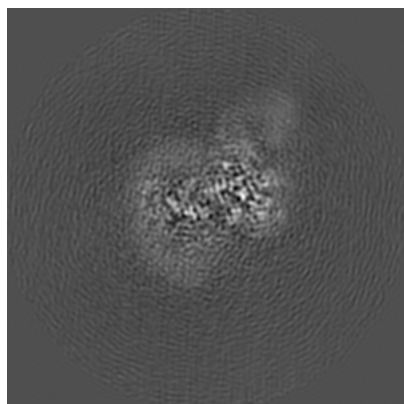


Z Index: 224

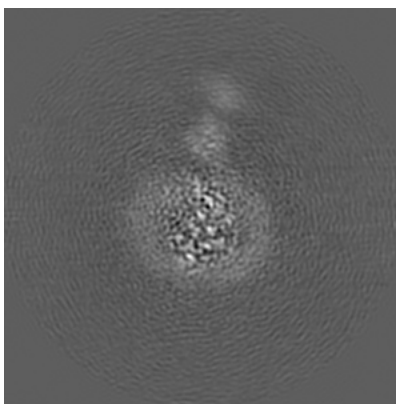
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

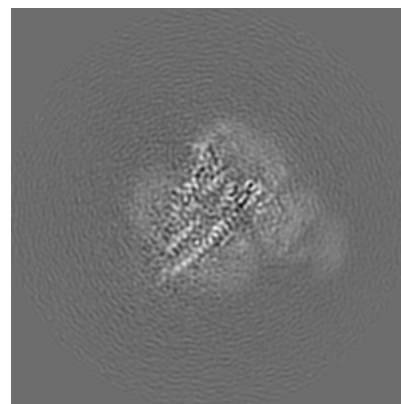
6.3.1 Primary map



X Index: 217



Y Index: 200

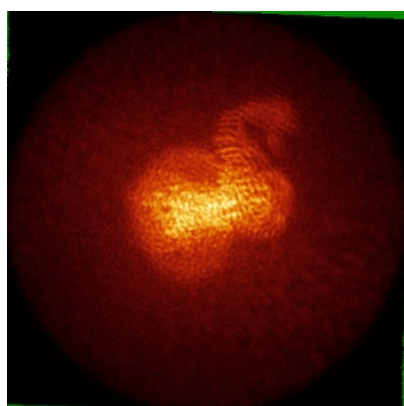


Z Index: 231

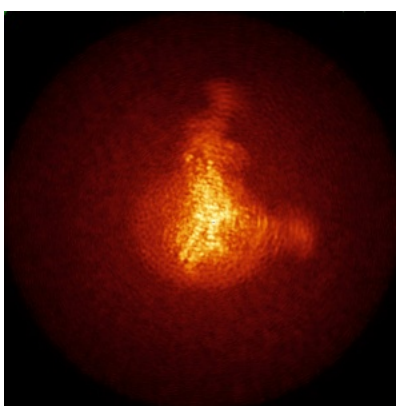
The images above show the largest variance slices of the map in three orthogonal directions.

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

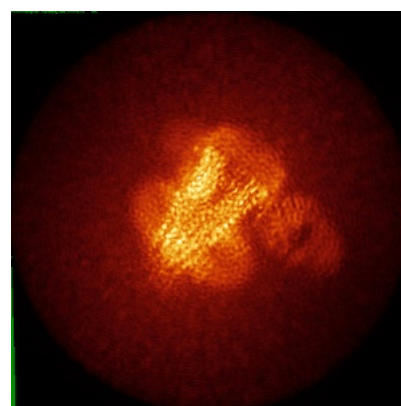
6.4.1 Primary map



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

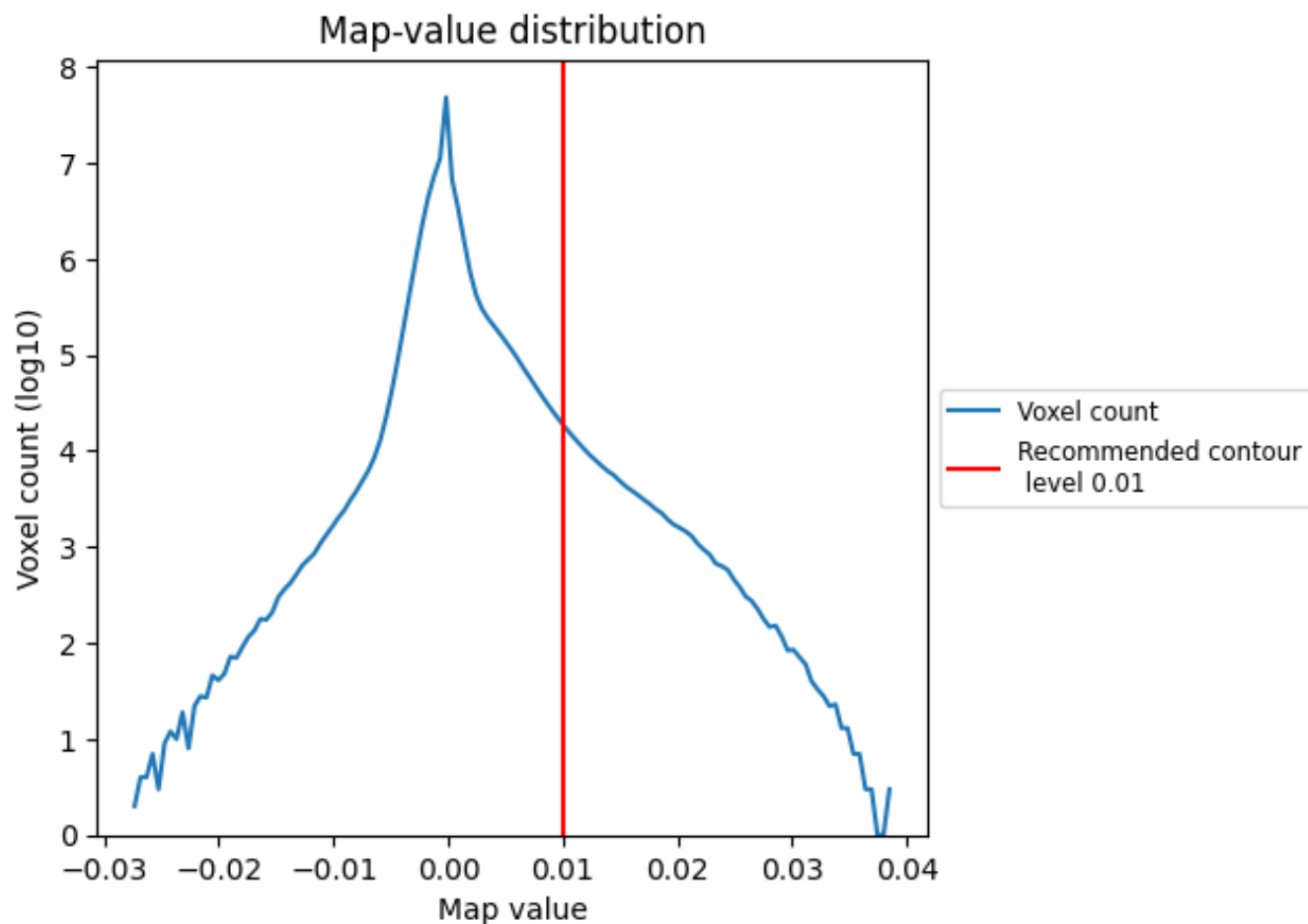
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

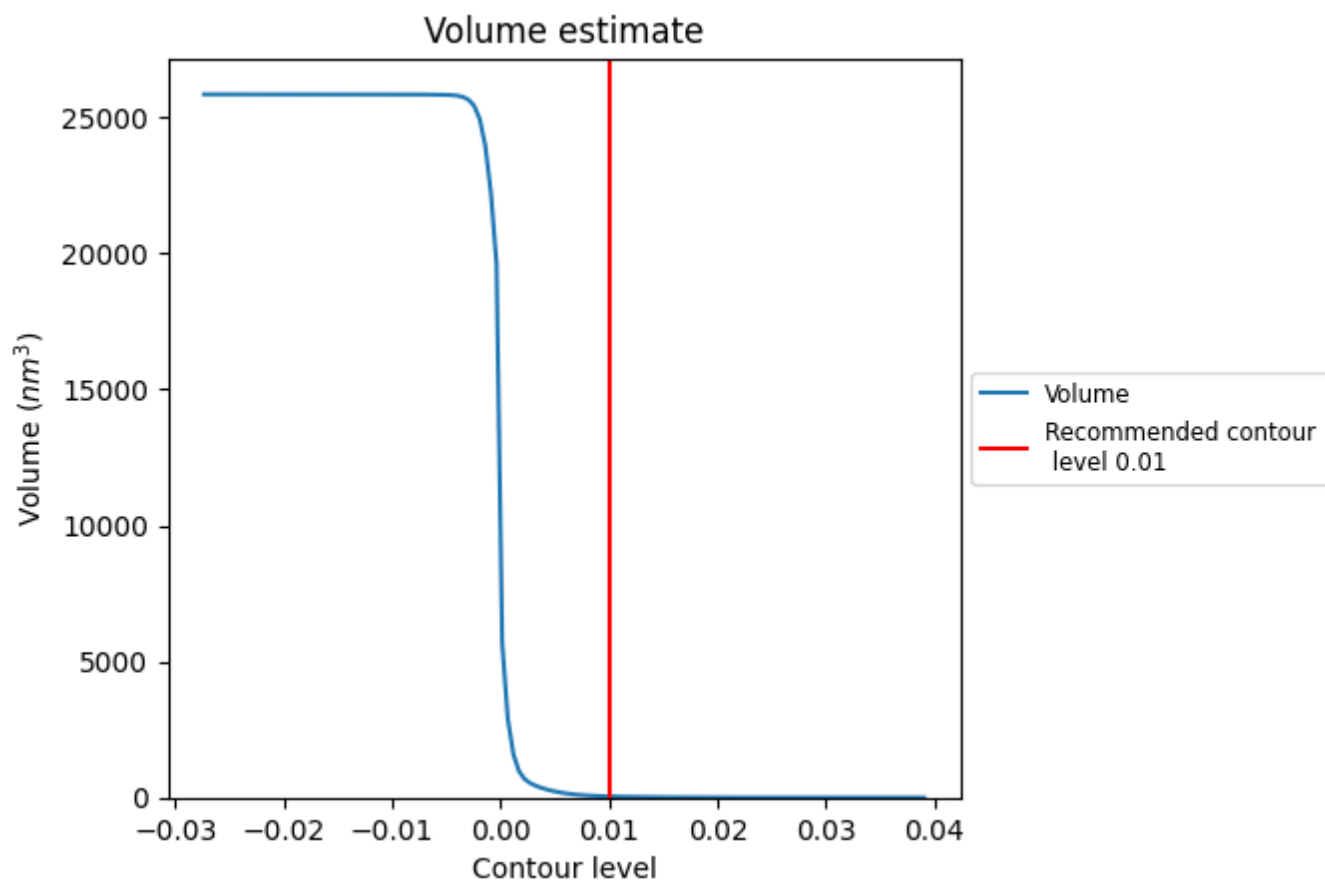
This section contains the results of statistical analysis of the map.

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.

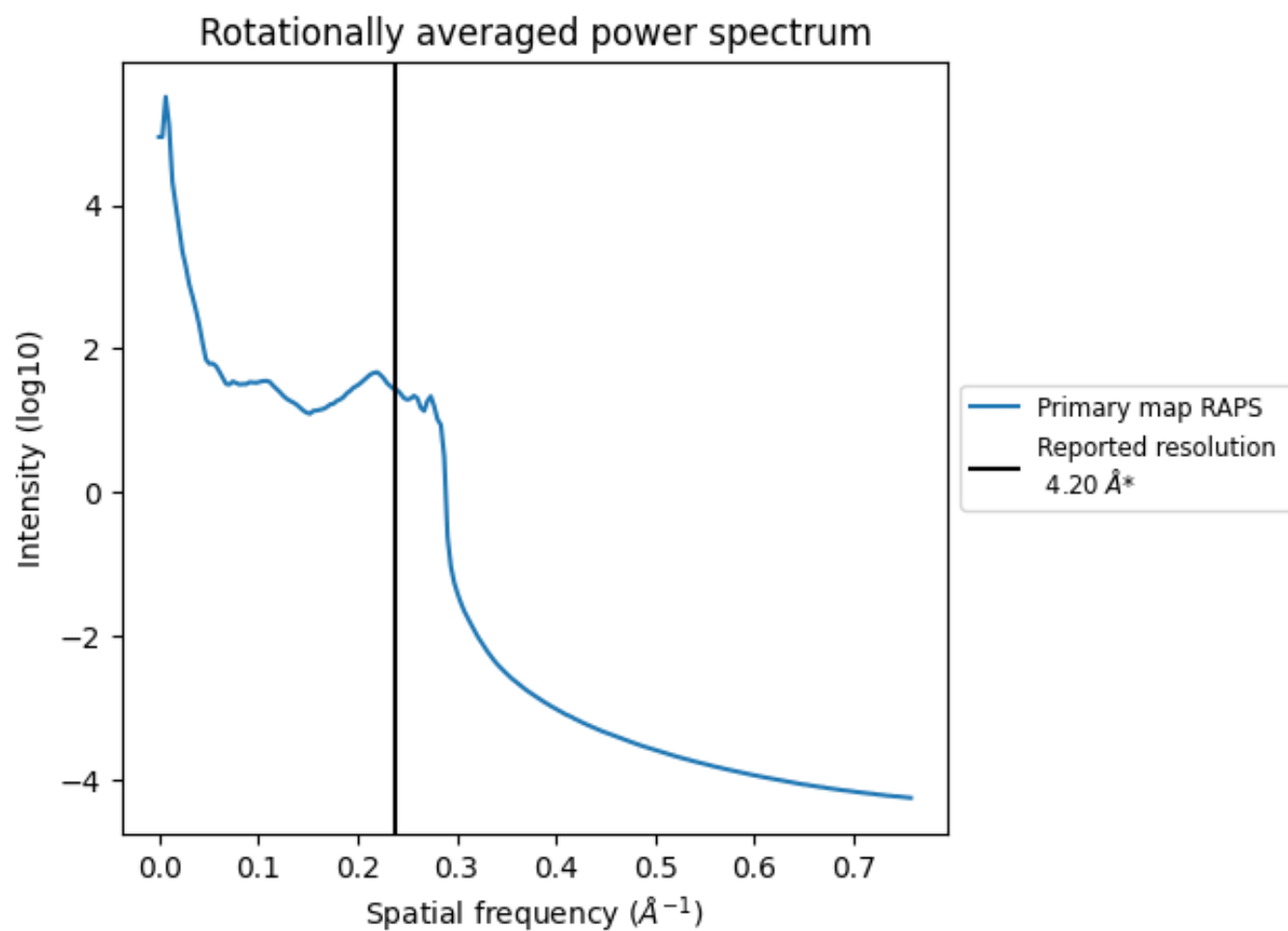
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm³; this corresponds to an approximate mass of 37 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 ⓘ

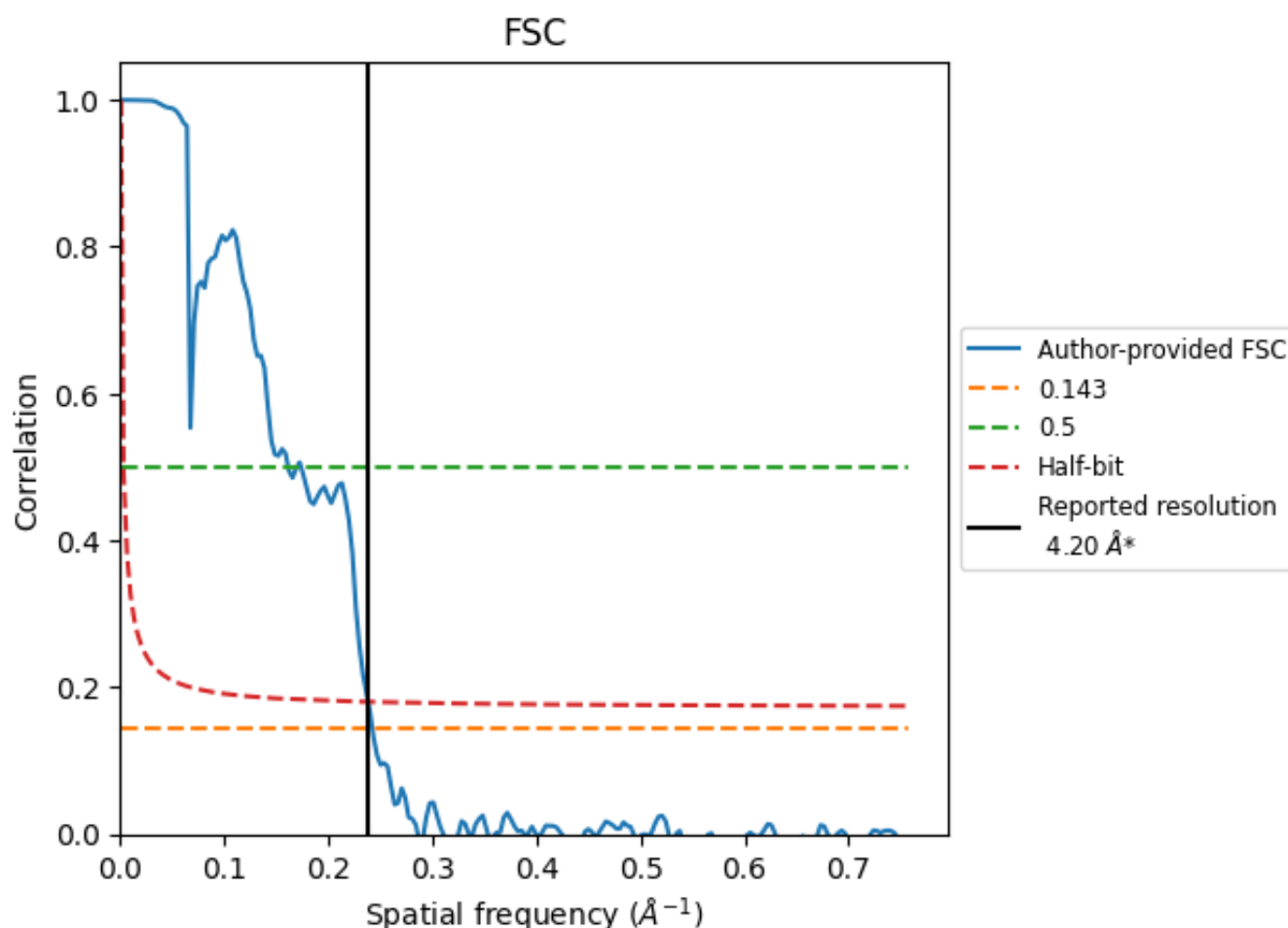


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

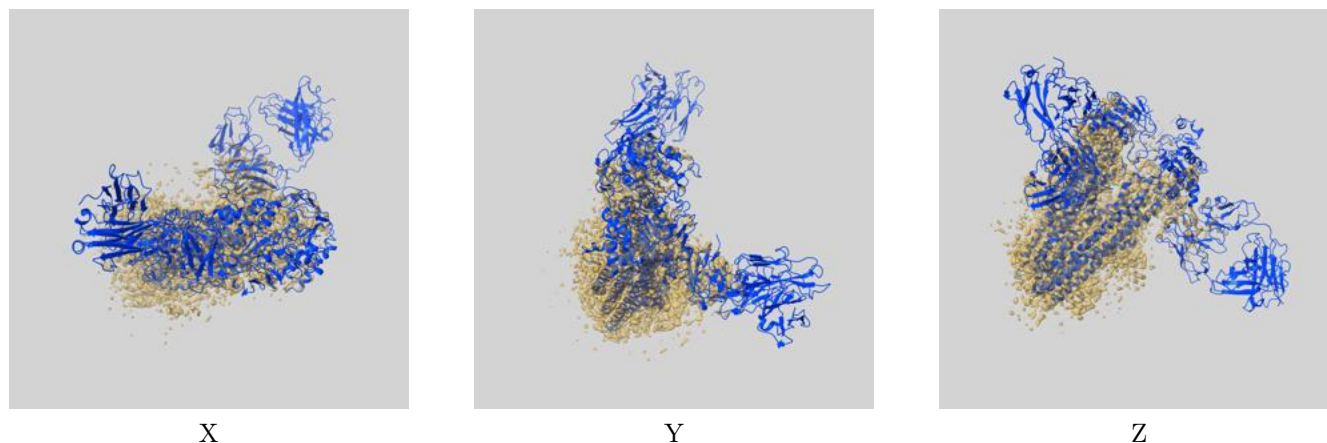
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.13	6.19	4.19
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12365 and PDB model 7NIU. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



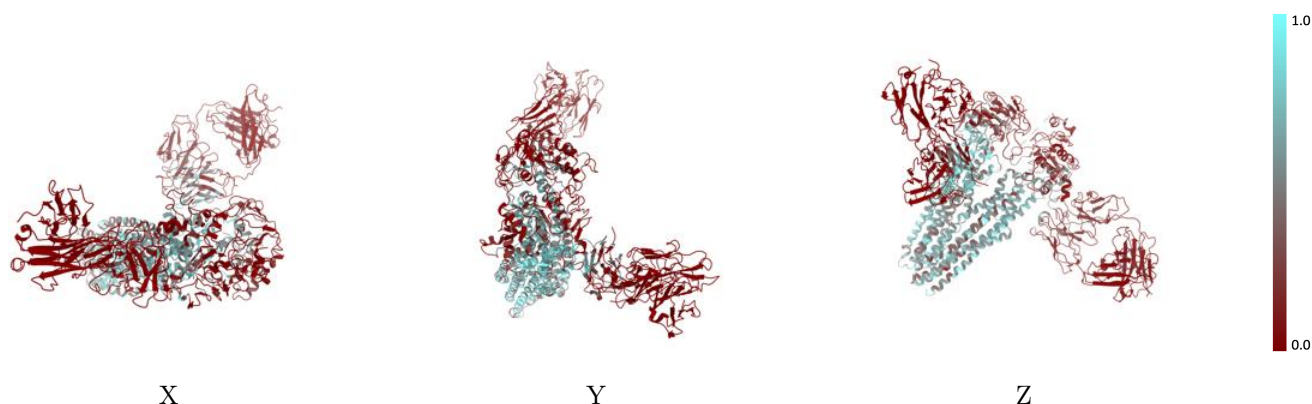
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



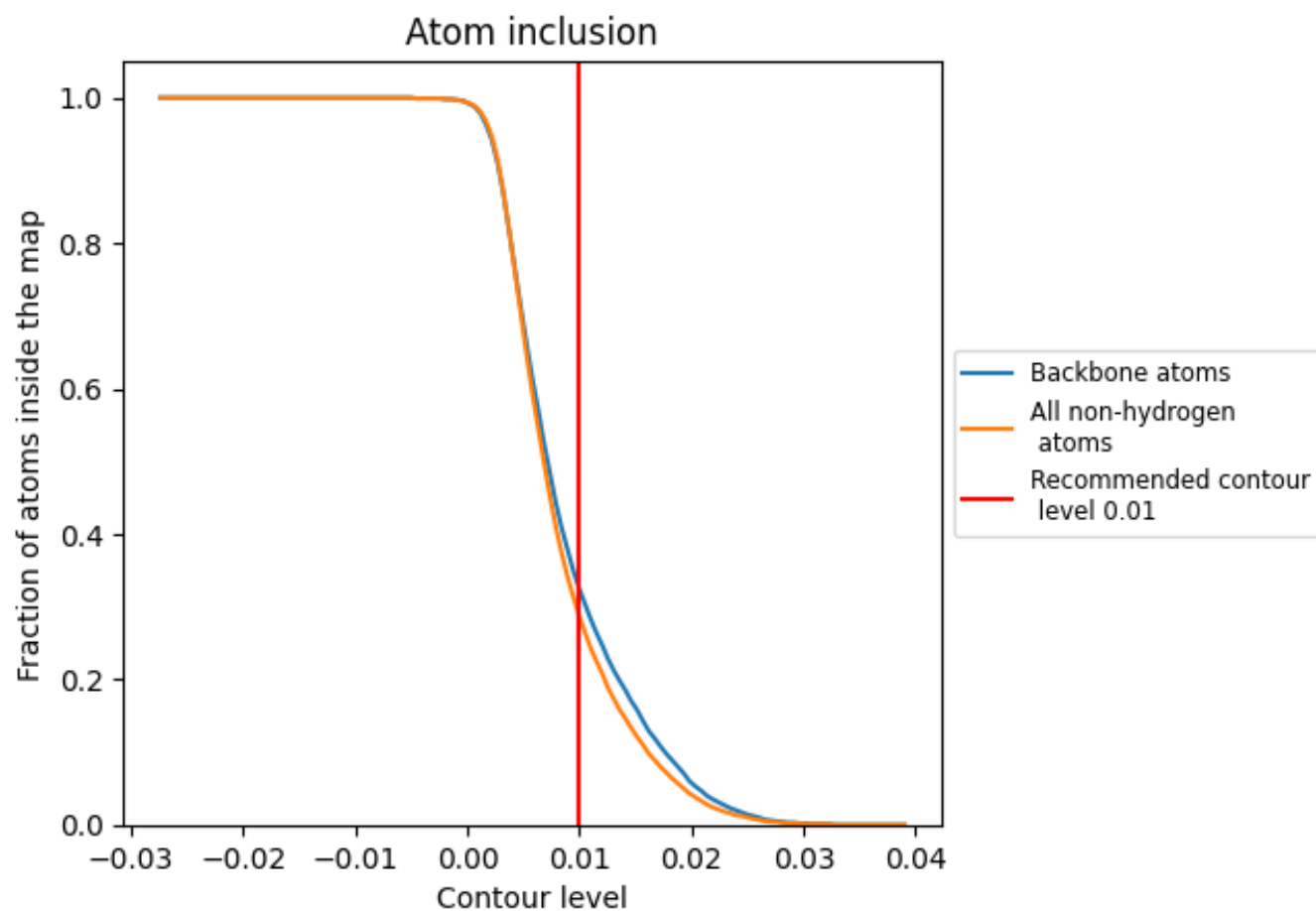
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 32% of all backbone atoms, 29% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2870	<div></div> 0.3330
A	<div></div> 0.4530	<div></div> 0.3870
B	<div></div> 0.0160	<div></div> 0.2400
C	<div></div> 0.1650	<div></div> 0.2890
D	<div></div> 0.0150	<div></div> 0.2480
E	<div></div> 0.0650	<div></div> 0.2700

