



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 03:51 PM UTC

PDB ID : 6VXJ / pdb_00006vxj
EMDB ID : EMD-21440
Title : Structure of ABCG2 bound to SN38
Authors : Orlando, B.J.; Liao, M.
Deposited on : 2020-02-22
Resolution : 4.10 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:

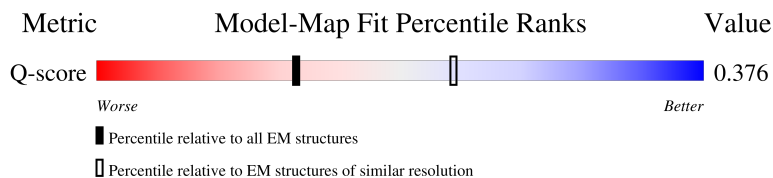
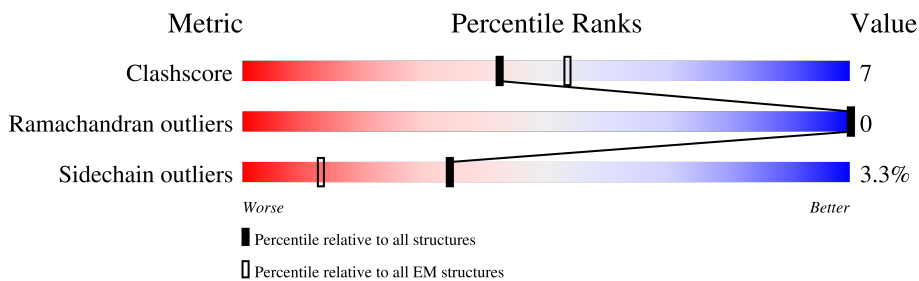
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	655	45% 68% 17% • 14%
1	B	655	47% 70% 15% • 14%

2 Entry composition [i](#)

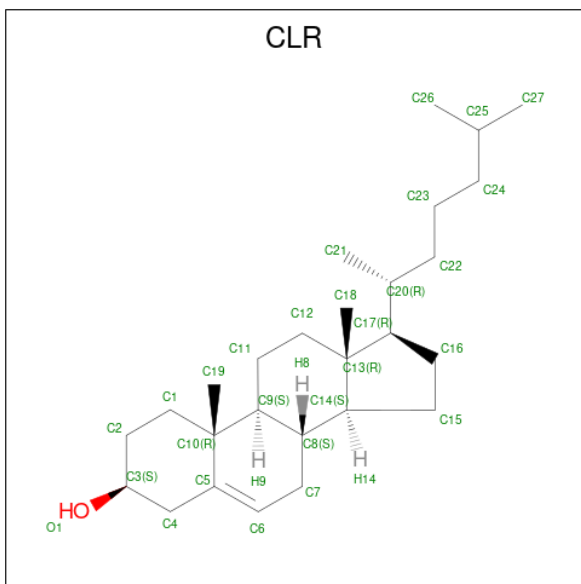
There are 3 unique types of molecules in this entry. The entry contains 8895 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Broad substrate specificity ATP-binding cassette transporter ABCG2.

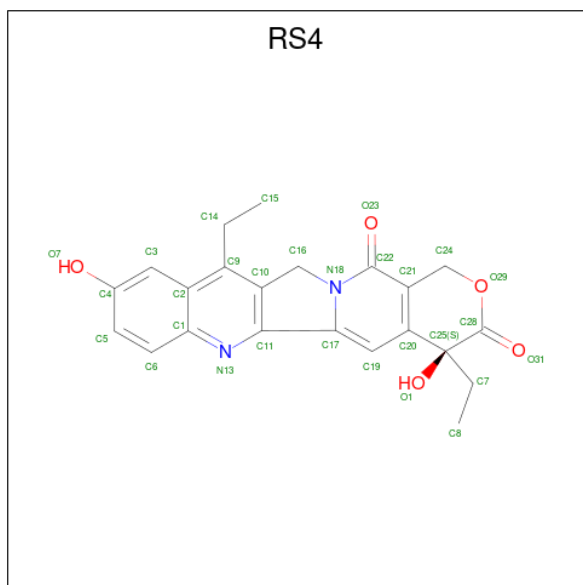
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	566	Total	C	N	O	S	0	0
			4405	2859	726	791	29		
1	B	566	Total	C	N	O	S	0	0
			4405	2859	726	791	29		

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 3 is 7-ethyl-10-hydroxycamptothecin (CCD ID: RS4) (formula: $C_{22}H_{20}N_2O_5$) (labeled as "Ligand of Interest" by depositor).

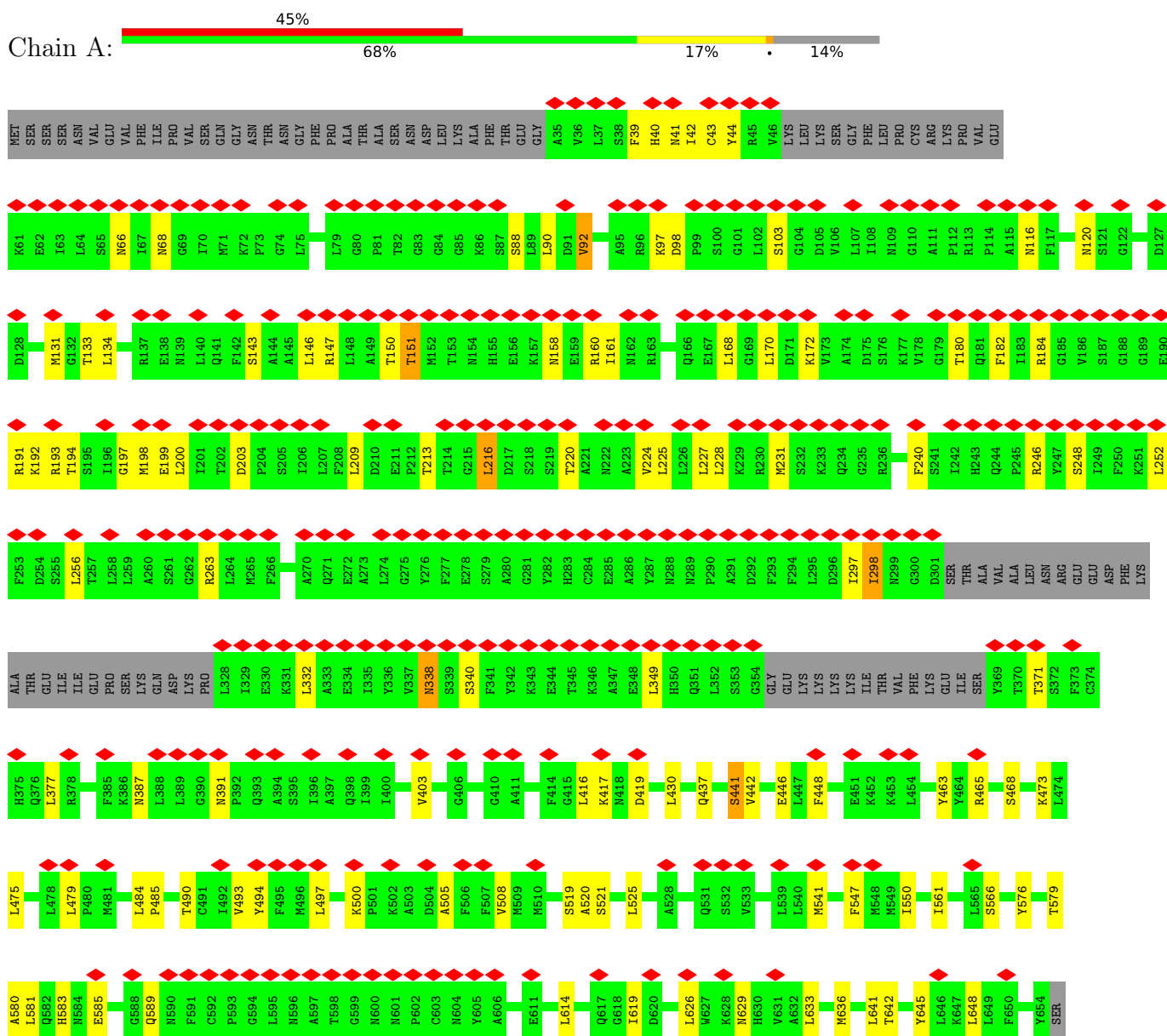


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	29	22	2	5	0

3 Residue-property plots i

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

- Molecule 1: Broad substrate specificity ATP-binding cassette transporter ABCG2



- Molecule 1: Broad substrate specificity ATP-binding cassette transporter ABCG2



MET	SER	SER	SER	ASN	VAL	GLU	VAL	PHE	ILE	PRO	VAL	SER	GLN	GLY	THR	ASN	ASN	GLY	PHE	PRO	ALA	THR	ALA	SER	ASN	ASP	LEU	LYS	ALA	PHE	THR	GLU	GLY	A35	V36	L37	S38	F39	H40	N41	I42	C43	Y44	R45	V46	LYS	LEU	LYS	SER	GLY	PHE	LEU	PRO	CYS	ARG	LYS	PRO	VAL	GLU
K61	E62	I63	L64	S65	N66	I67	N68	G69	I70	M71	K72	P73	G74	L75	L79	G80	P81	T82	G83	G84	G85	K86	S87	S88	L89	L90	D91	V92	L93	A94	A95	R96	K97	D98	P99	S100	G101	L102	S103	G104	D105	V106	L107	I108	N109	G110	A111	P112	R113	P114	A115	N116	F117	N120	S121	G122			
D127	D128	M131	G132	T133	L134	T135	V136	R137	E138	M139	L140	Q141	F142	S143	A144	A145	L146	R147	L148	A149	T150	T151	M152	T153	M154	H155	E156	K157	M158	E159	R160	I161	M162	R163	Q166	E167	L168	G169	L170	D171	K172	V173	A174	D175	S176	K177	G179	T180	Q181	F182	I183	R184	G185	V186	S187	G188			
G189	E190	R191	K192	R193	T194	S195	I196	G197	M198	E199	L200	T201	T202	D203	P204	S205	L206	L207	F208	L209	D210	E211	P212	T213	T214	G215	L216	D217	S218	S219	T220	A221	N222	A223	V224	L225	L226	L227	L228	K229	R230	M231	S232	K233	Q234	G235	R236	F240	S241	T242	H243	Q244	P245	R246	T247	S248	T249	F250	
K251	L252	F253	D254	S255	L256	T257	L258	L259	A260	S261	G262	R263	L264	M265	F266	A270	Q271	E272	A273	L274	G275	Y276	F277	E278	S279	G280	G281	T282	Y283	C284	E285	A286	N287	N288	M289	P290	A291	D292	F293	F294	L295	D296	T297	T298	N299	G300	D301	THR	ALA	VAL	ALA	LEU	ASN	ARG	GLU	ASP			
PHE	LYS	ALA	THR	GLU	ILE	ILE	PRO	GLU	SER	LYS	GLN	ASP	LYS	PRO	L328	I329	E330	K331	L332	A333	E334	I335	Y336	V337	N338	S339	S340	F341	Y342	K343	E344	T345	K346	E347	E348	L349	H350	Q351	L352	S353	G354	GLY	GLU	LYS	LYS	LYS	ILE	THR	VAL	PHE	LYS	GLU	ILE	SER	Y369	T370	T371		
H375	R376	F385	K386	N387	L388	L389	G390	N391	F392	Q393	A394	S395	I396	A397	I399	I400	V403	G410	A411	F414	G415	L416	K417	N418	D419	Q424	L430	Q437	C438	F439	S440	S441	V442	E446	E451	K452	K453	L454	Y463	Y464	R465	S468	L475	S476	D477														
L478	L479	P480	M481	L484	P485	T490	C491	F492	V493	Y494	F495	M496	L497	K500	P501	K502	A503	C603	D504	A505	F506	F507	V508	N509	M510	M514	S519	A520	S521	L525	A528	Q531	S532	L539	L540	M541	F547	M548	M549	I550	I561	S566	Y576	A580	L581	Q582													
H583	N584	E585	G588	Q589	N590	F591	C592	P593	G594	L595	N596	A597	T598	G599	N600	N601	P602	C603	N604	Y605	A606	E611	K616	O617	D620	L626	M627	K628	N629	M636	T642	Y645	L646	F650	L651	K652	K653	Y654	SER																				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	97737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.347	Depositor
Minimum map value	-0.214	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.085	Depositor
Map size (\AA)	236.16, 236.16, 236.16	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.23, 1.23, 1.23	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, RS4

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	0.30	0/4497	0.58	0/6085
1	B	0.30	0/4497	0.57	0/6085
All	All	0.30	0/8994	0.58	0/12170

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	484	LEU	Peptide
1	B	484	LEU	Peptide

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	4405	0	4482	64	0
1	B	4405	0	4482	56	0
2	A	28	0	46	1	0
2	B	28	0	46	2	0
3	B	29	0	0	0	0
All	All	8895	0	9056	121	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 121 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:41:ASN:H	1:A:68:ASN:HB3	1.60	0.67
1:A:338:ASN:OD1	1:A:338:ASN:N	2.27	0.67
1:A:430:LEU:HD22	1:A:581:LEU:HD23	1.77	0.67
1:B:41:ASN:H	1:B:68:ASN:HB3	1.60	0.67
1:B:338:ASN:N	1:B:338:ASN:OD1	2.27	0.65

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	558/655 (85%)	505 (90%)	53 (10%)	0	100	100
1	B	558/655 (85%)	505 (90%)	53 (10%)	0	100	100
All	All	1116/1310 (85%)	1010 (90%)	106 (10%)	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	482/560 (86%)	466 (97%)	16 (3%)	33	55
1	B	482/560 (86%)	466 (97%)	16 (3%)	33	55
All	All	964/1120 (86%)	932 (97%)	32 (3%)	34	55

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	340	SER
1	B	403	VAL
1	A	340	SER
1	A	338	ASN
1	B	441	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	ASN
1	B	222	ASN
1	B	457	HIS
1	B	162	ASN
1	B	244	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](#)

3 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
2	CLR	A	701	-	31,31,31	0.84	2 (6%)	48,48,48	1.61	7 (14%)
3	RS4	B	701	-	30,33,33	2.89	10 (33%)	32,52,52	2.11	9 (28%)
2	CLR	B	702	-	31,31,31	0.83	2 (6%)	48,48,48	1.59	7 (14%)

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
2	CLR	A	701	-	-	7/10/68/68	0/4/4/4
3	RS4	B	701	-	-	4/5/30/30	0/5/5/5
2	CLR	B	702	-	-	7/10/68/68	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	RS4	O29-C28	8.15	1.44	1.34
3	B	701	RS4	C21-C20	7.12	1.47	1.36
3	B	701	RS4	C10-C9	6.00	1.48	1.38
3	B	701	RS4	C2-C1	4.18	1.49	1.42
3	B	701	RS4	C22-N18	-4.07	1.33	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	RS4	C17-C11-N13	6.46	129.37	125.32
3	B	701	RS4	C10-C11-C17	-5.59	105.21	108.38
2	A	701	CLR	C13-C17-C20	-4.96	111.84	119.50
2	B	702	CLR	C13-C17-C20	-4.91	111.92	119.50
2	A	701	CLR	C13-C14-C8	-4.48	108.06	114.41

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

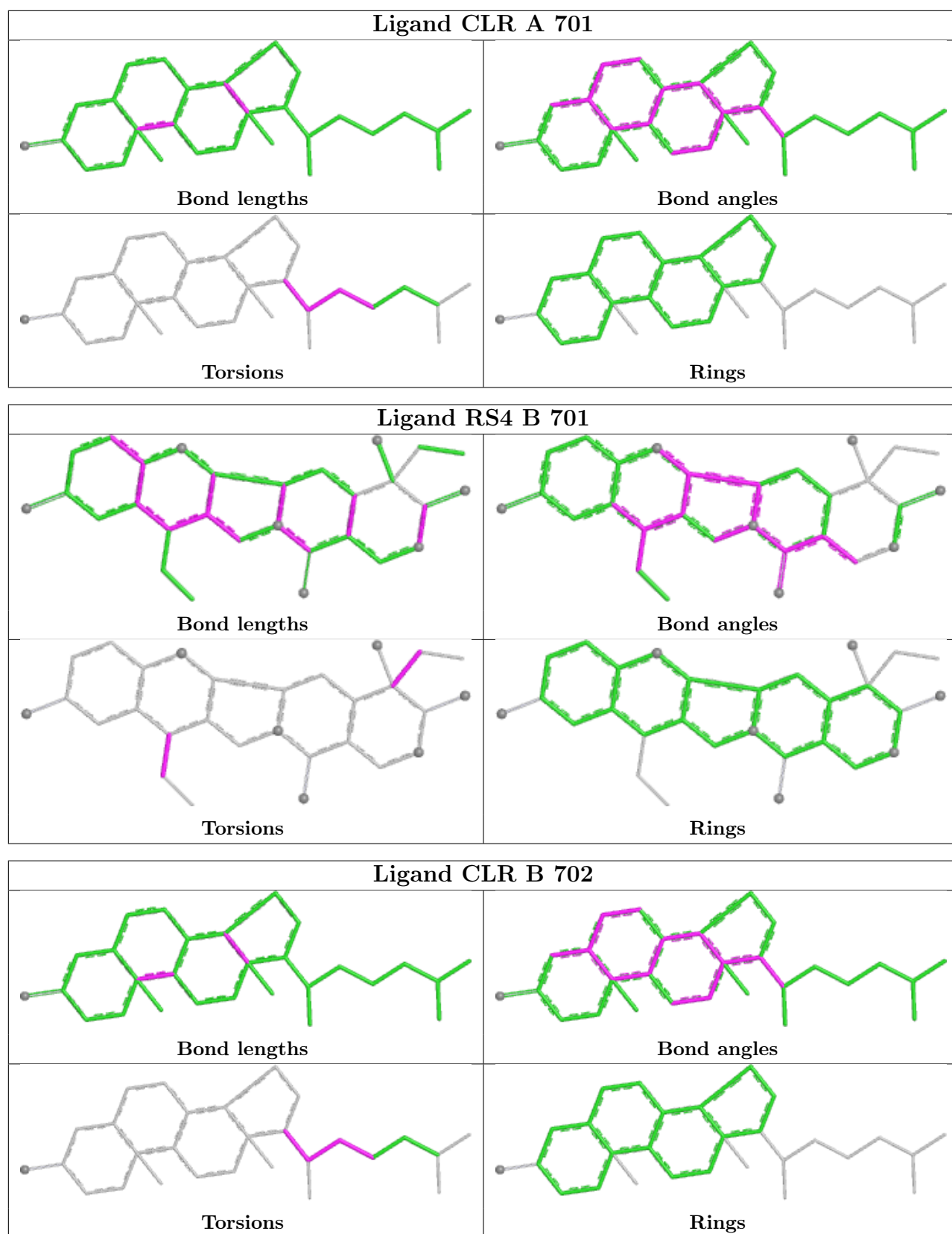
Mol	Chain	Res	Type	Atoms
3	B	701	RS4	C20-C25-C7-C8
3	B	701	RS4	C28-C25-C7-C8
3	B	701	RS4	O1-C25-C7-C8
2	A	701	CLR	C21-C20-C22-C23
2	B	702	CLR	C21-C20-C22-C23

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CLR	1	0
2	B	702	CLR	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 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.

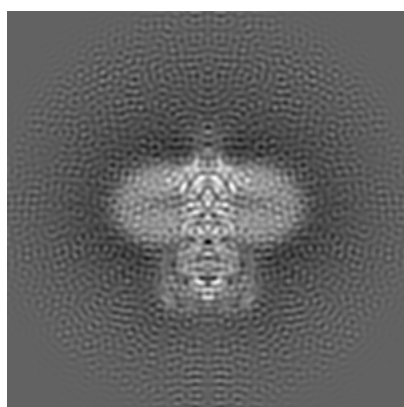
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21440. These allow visual inspection of the internal detail of the map and identification of artifacts.

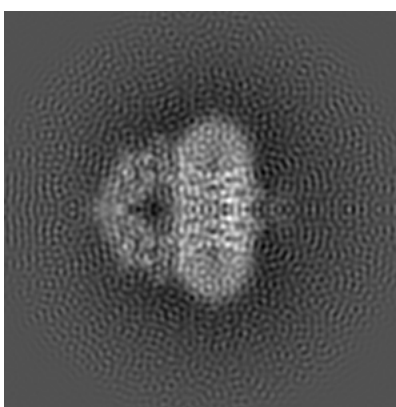
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

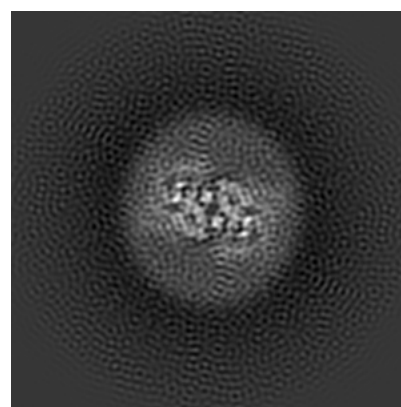
6.1.1 Primary map



X



Y

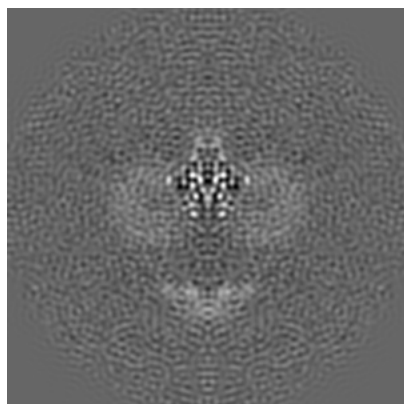


Z

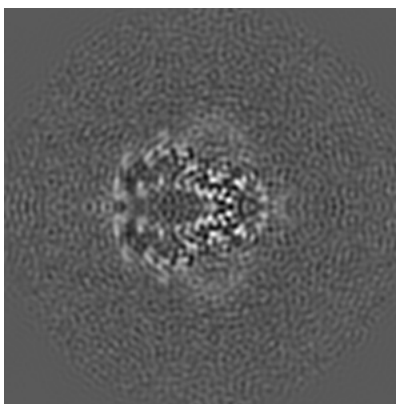
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

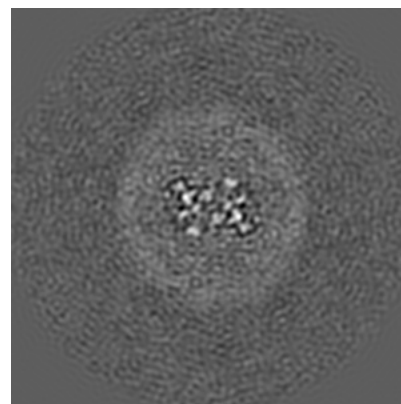
6.2.1 Primary map



X Index: 96



Y Index: 96

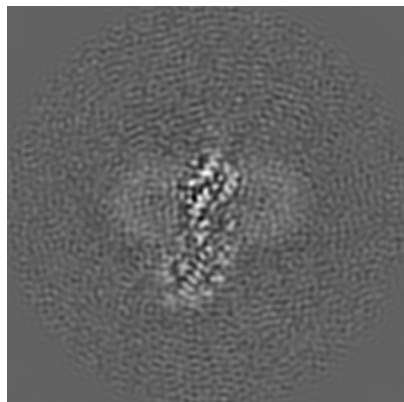


Z Index: 96

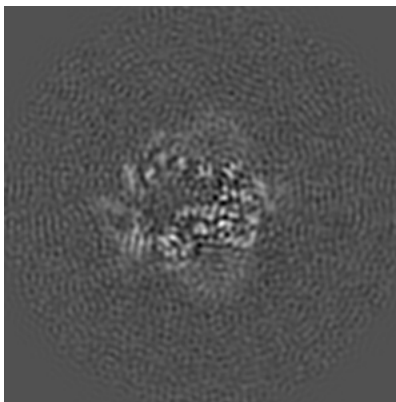
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

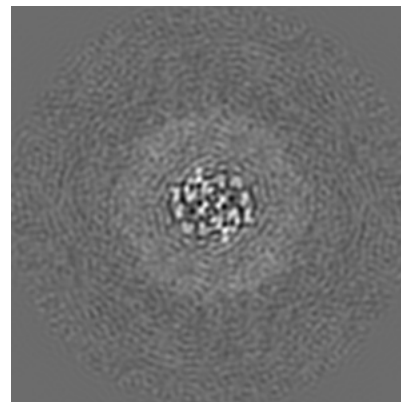
6.3.1 Primary map



X Index: 108



Y Index: 101

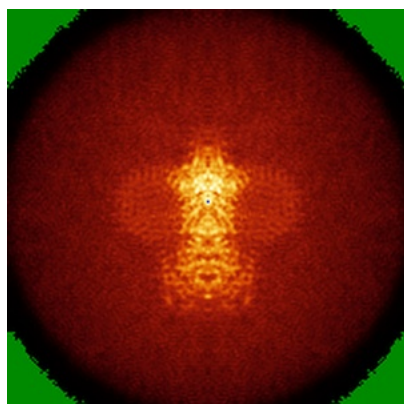


Z Index: 107

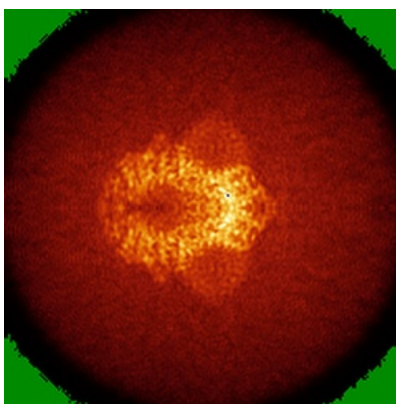
The images above show the largest variance slices of the map in three orthogonal directions.

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

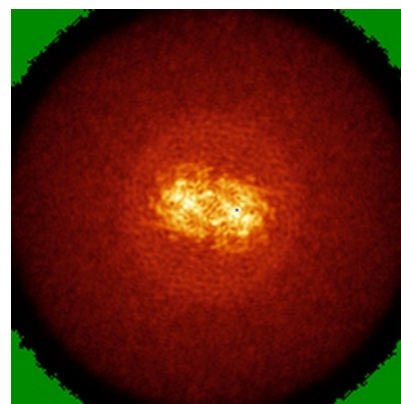
6.4.1 Primary map



X



Y

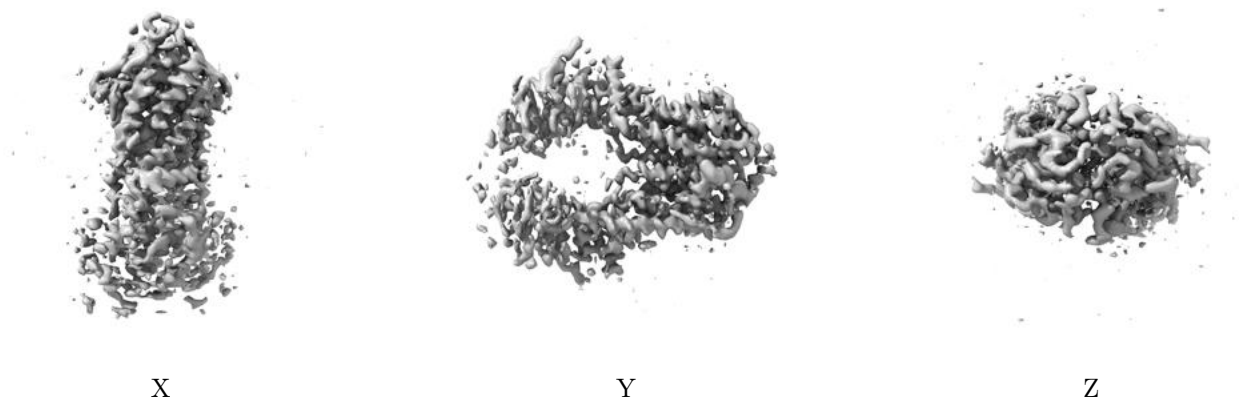


Z

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

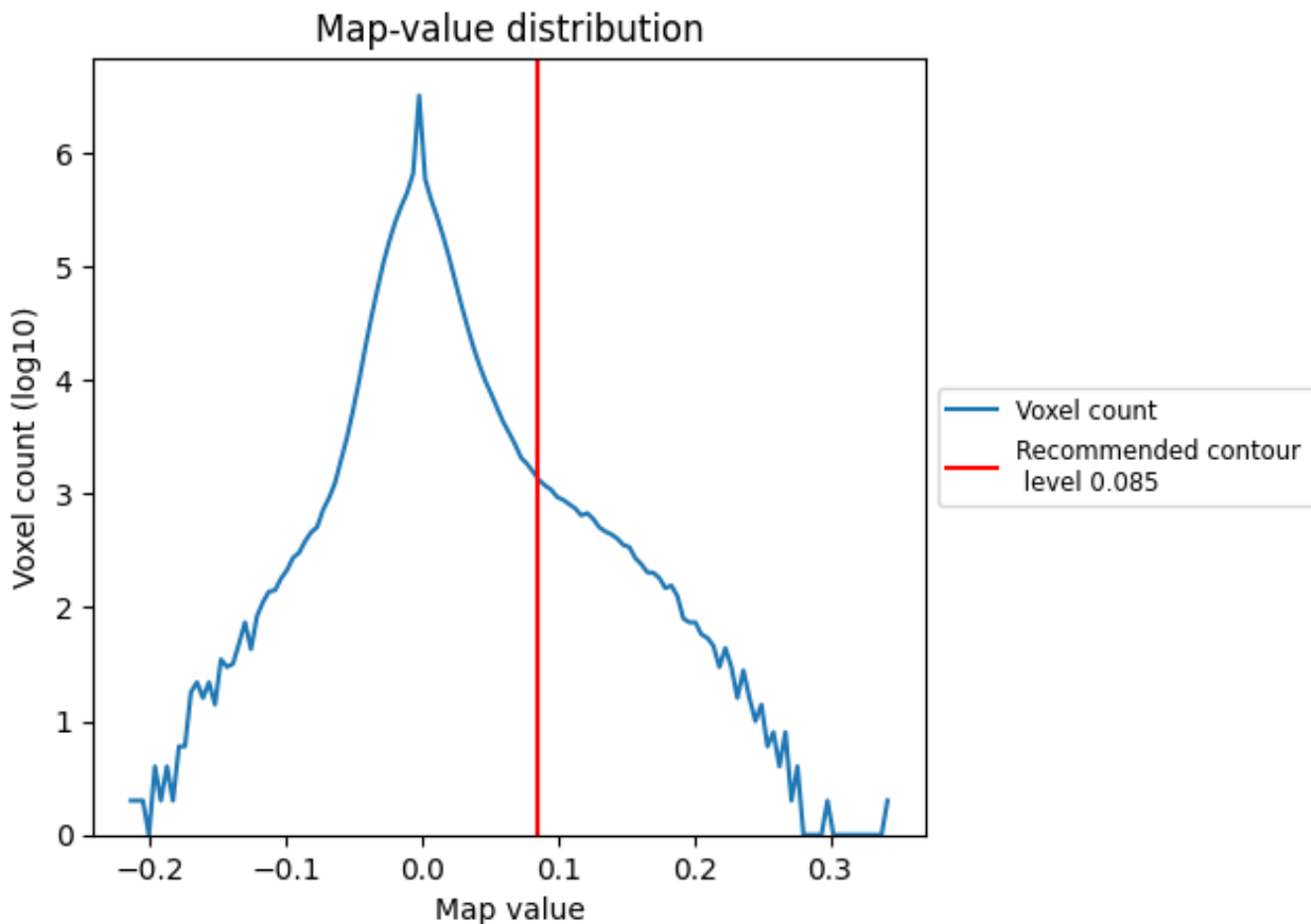
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

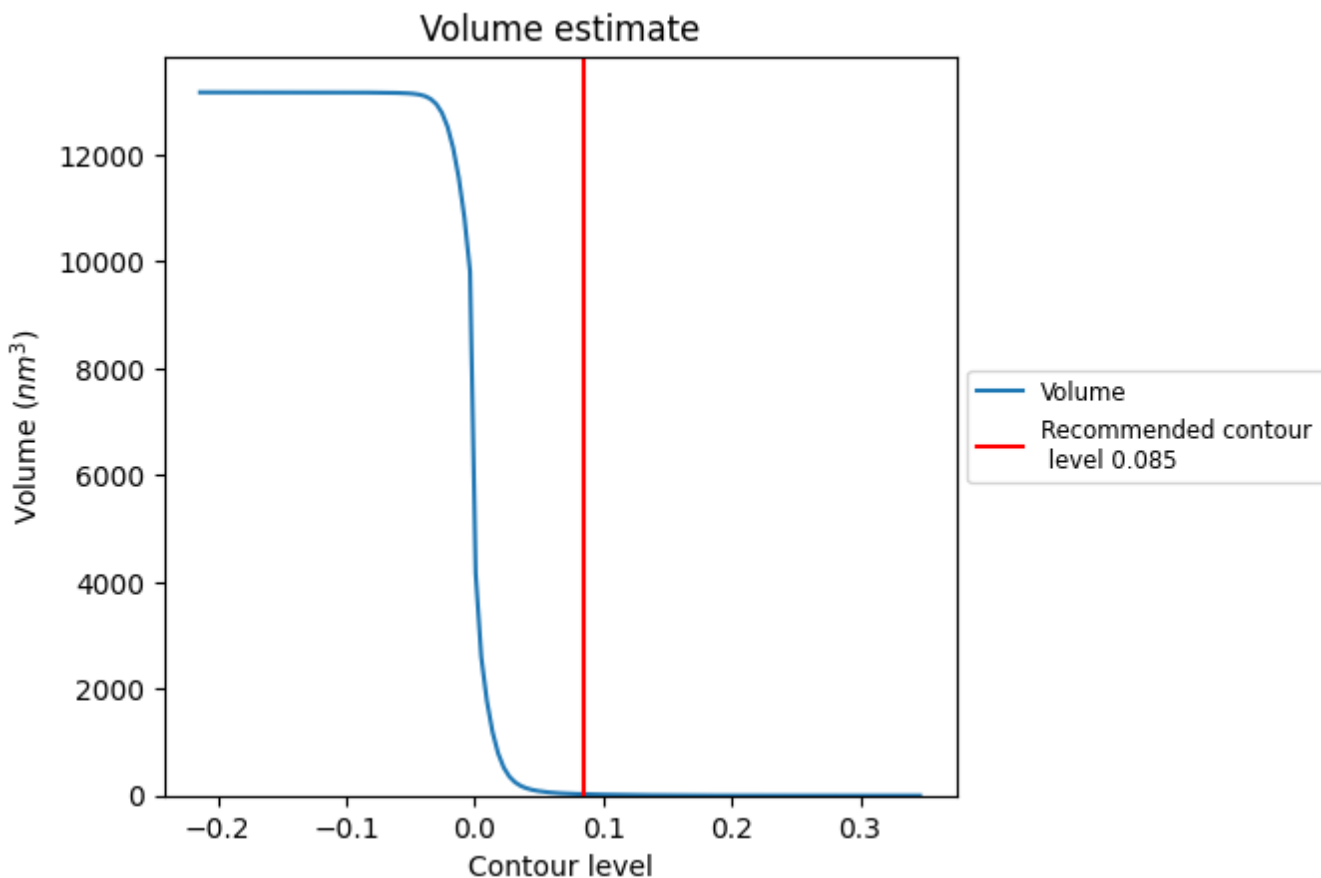
This section contains the results of statistical analysis of the map.

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.

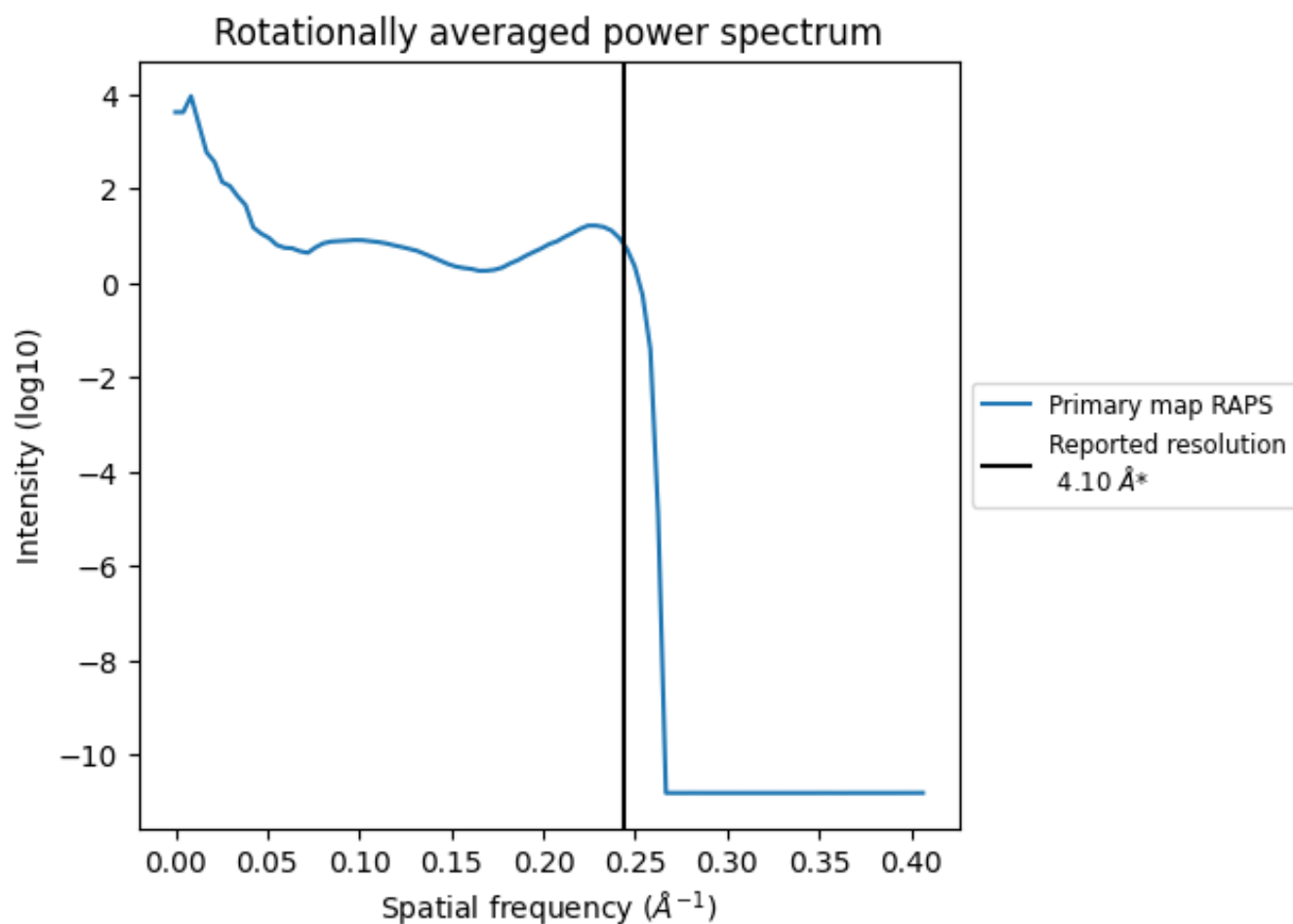
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26 nm³; this corresponds to an approximate mass of 23 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 [\(i\)](#)

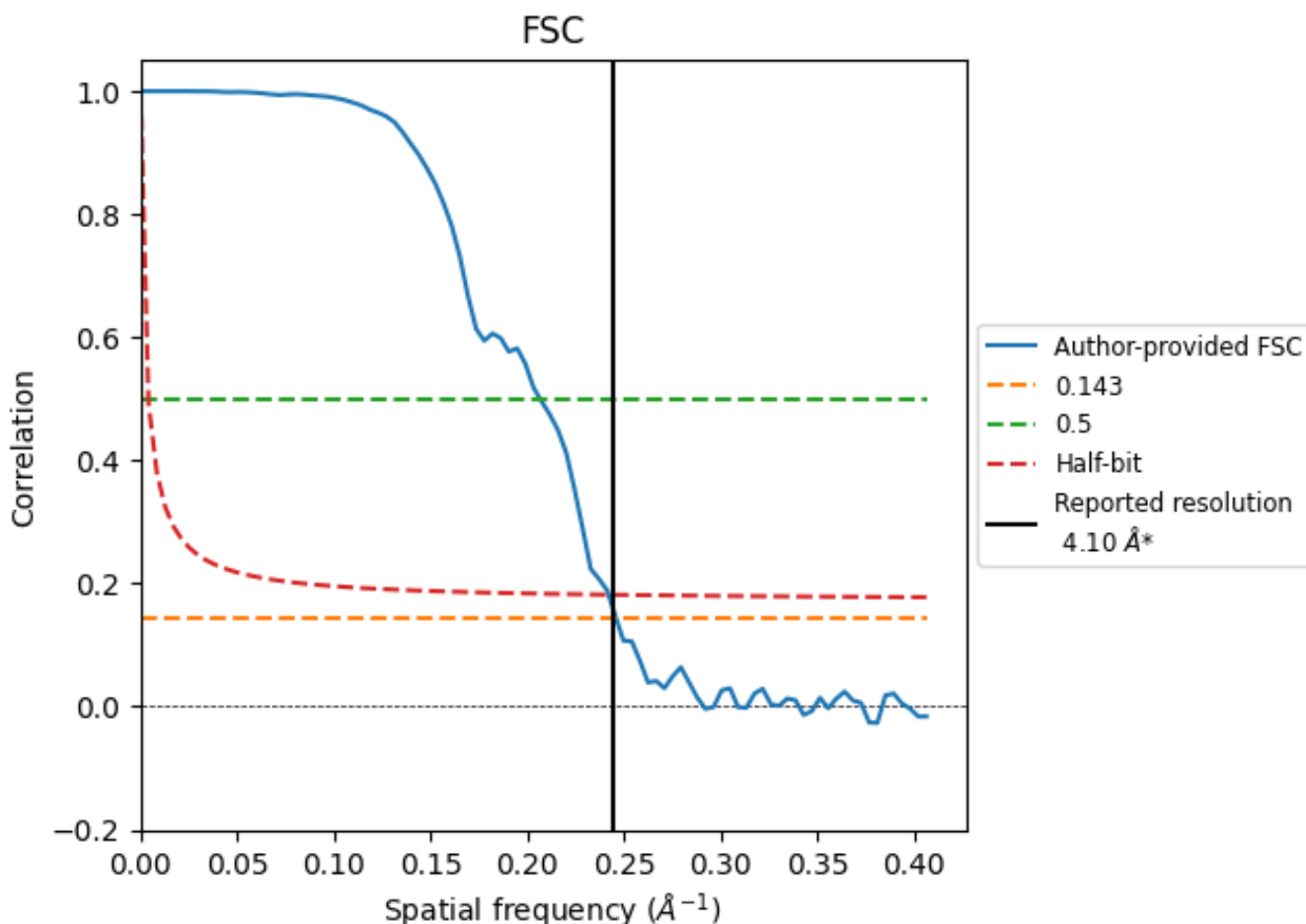


*Reported resolution corresponds to spatial frequency of 0.244\AA^{-1}

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

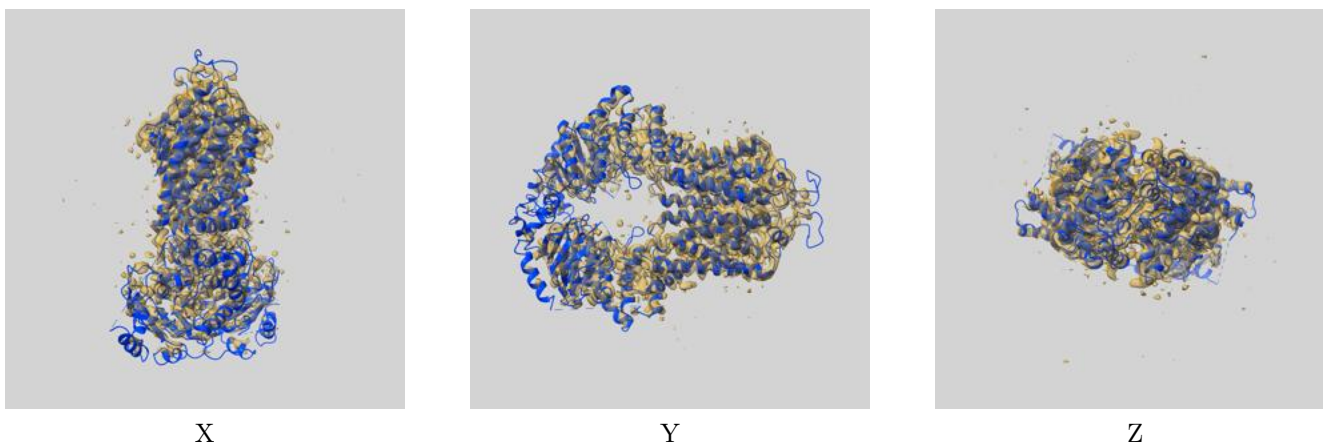
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.07	4.84	4.13
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

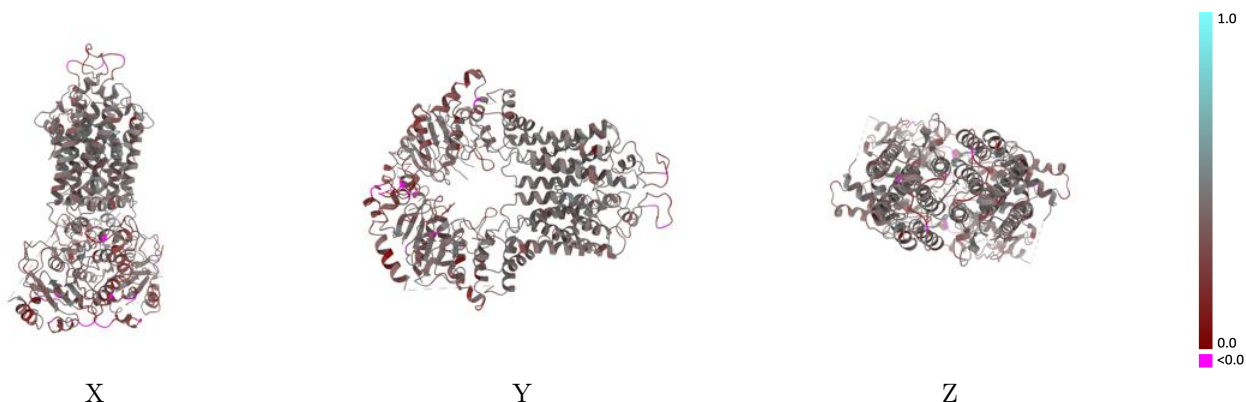
This section contains information regarding the fit between EMDB map EMD-21440 and PDB model 6VXJ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



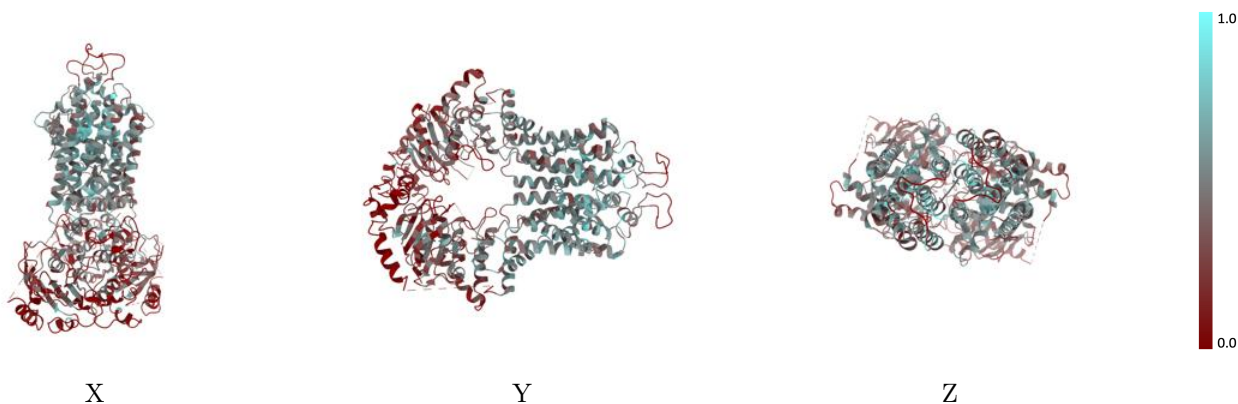
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



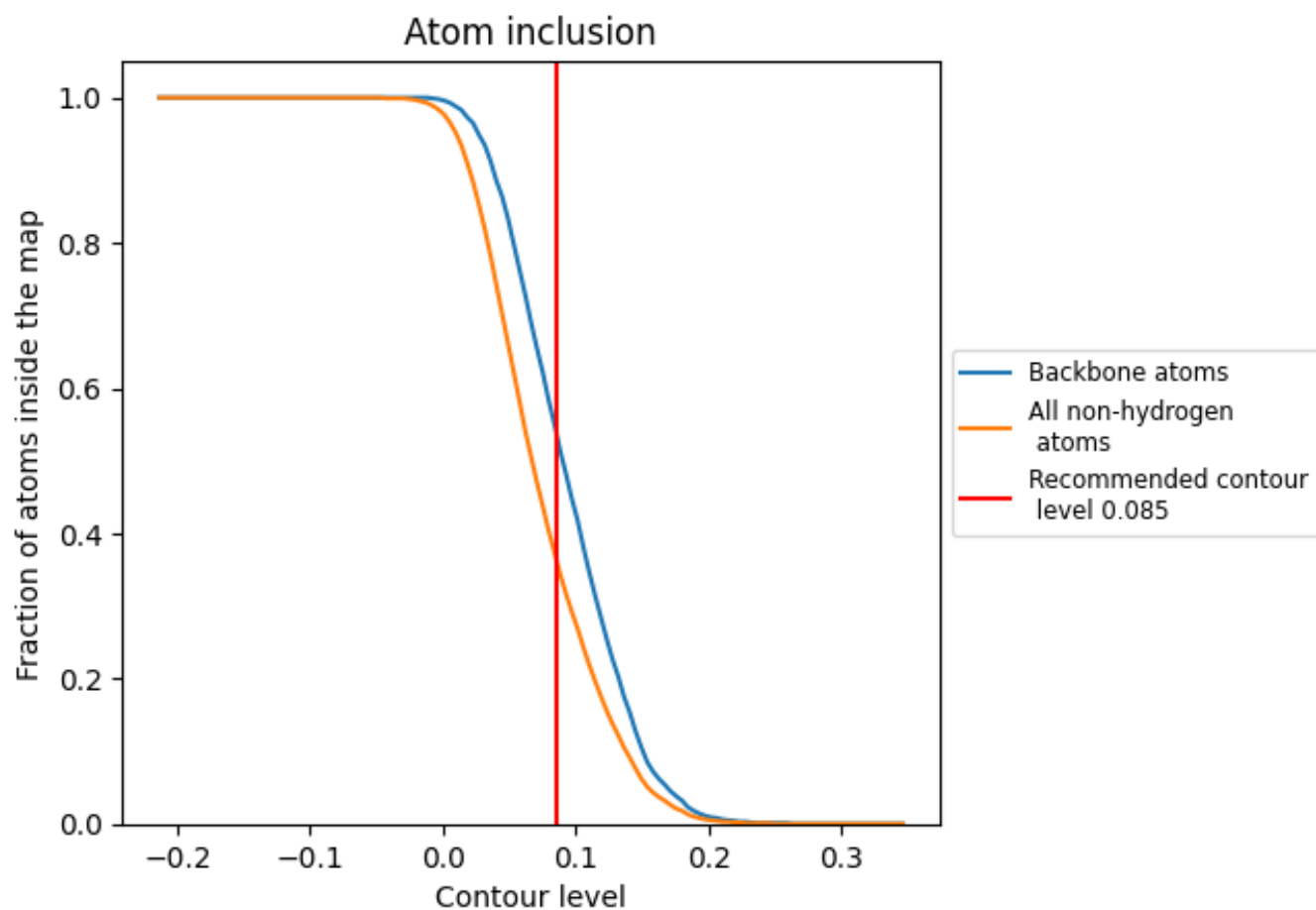
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).







9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 37% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3670	 0.3760
A	 0.3670	 0.3740
B	 0.3660	 0.3780

