



## wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 04:21 AM UTC

PDB ID : 8PEE / pdb\_00008pee  
EMDB ID : EMD-17630  
Title : ABCB1 L335C mutant (mABCB1) in the inward facing state bound to AAC  
Authors : Parey, K.; Janulienė, D.; Gewering, T.; Moeller, A.  
Deposited on : 2023-06-13  
Resolution : 3.80 Å (reported)  
Based on initial model : 6C0V

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

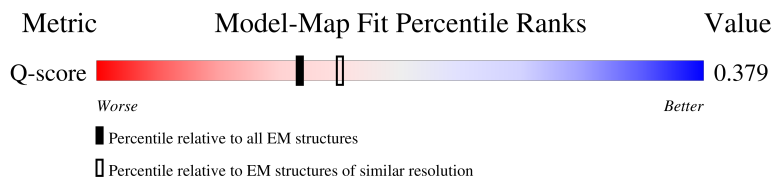
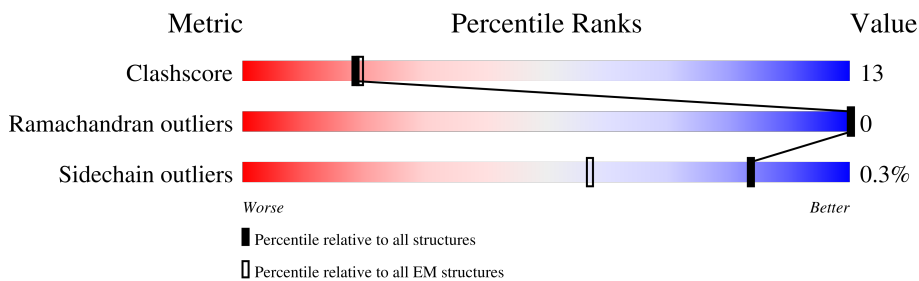
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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

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

The reported resolution of this entry is 3.80 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	10198 ( 3.30 - 4.30 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1328	<p>12% (red), 63% (green), 24% (yellow), 13% (grey)</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JIZ	A	1402	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9217 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 ATP-dependent translocase ABCB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1157	8967	5763	1527	1647	30	0	0

There are 65 discrepancies between the modelled and reference sequences:

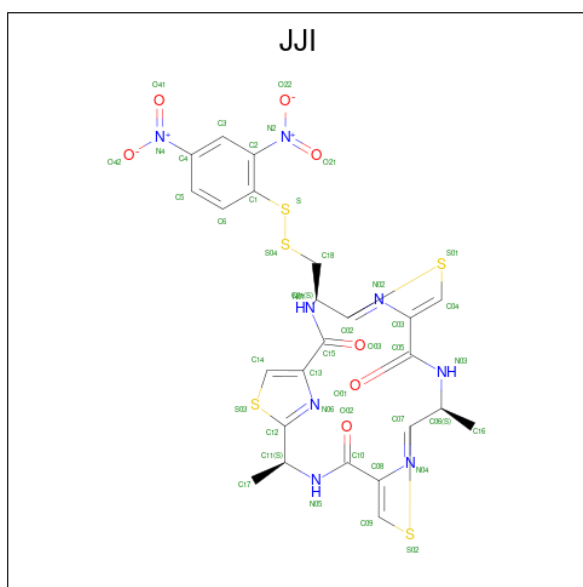
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	engineered mutation	UNP P21447
A	87	GLN	ASN	engineered mutation	UNP P21447
A	90	GLN	ASN	engineered mutation	UNP P21447
A	133	ALA	CYS	engineered mutation	UNP P21447
A	335	CYS	LEU	engineered mutation	UNP P21447
A	427	GLY	CYS	engineered mutation	UNP P21447
A	638	GLY	CYS	engineered mutation	UNP P21447
A	669	THR	CYS	engineered mutation	UNP P21447
A	713	ALA	CYS	engineered mutation	UNP P21447
A	952	ALA	CYS	engineered mutation	UNP P21447
A	1070	GLY	CYS	engineered mutation	UNP P21447
A	1121	ARG	CYS	engineered mutation	UNP P21447
A	1223	VAL	CYS	engineered mutation	UNP P21447
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	GLU	-	expression tag	UNP P21447
A	1280	ASN	-	expression tag	UNP P21447
A	1281	LEU	-	expression tag	UNP P21447
A	1282	TYR	-	expression tag	UNP P21447
A	1283	PHE	-	expression tag	UNP P21447
A	1284	GLN	-	expression tag	UNP P21447
A	1285	GLY	-	expression tag	UNP P21447
A	1286	GLY	-	expression tag	UNP P21447
A	1287	GLY	-	expression tag	UNP P21447
A	1288	ALA	-	expression tag	UNP P21447
A	1289	SER	-	expression tag	UNP P21447
A	1290	GLY	-	expression tag	UNP P21447
A	1291	GLY	-	expression tag	UNP P21447

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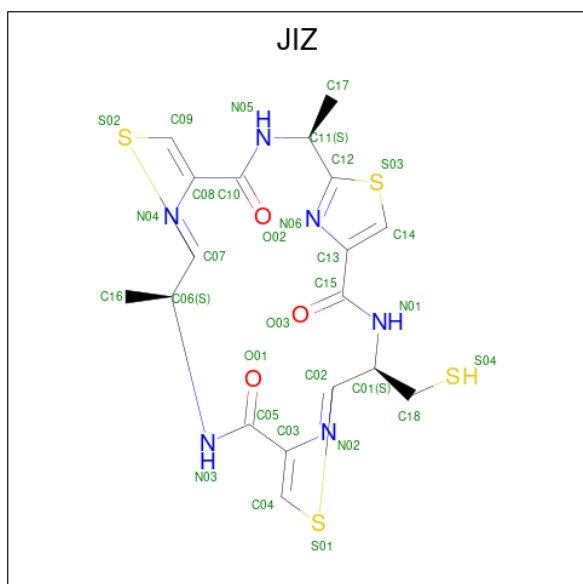
Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	SER	-	expression tag	UNP P21447
A	1293	TRP	-	expression tag	UNP P21447
A	1294	SER	-	expression tag	UNP P21447
A	1295	HIS	-	expression tag	UNP P21447
A	1296	PRO	-	expression tag	UNP P21447
A	1297	GLN	-	expression tag	UNP P21447
A	1298	PHE	-	expression tag	UNP P21447
A	1299	GLU	-	expression tag	UNP P21447
A	1300	LYS	-	expression tag	UNP P21447
A	1301	ALA	-	expression tag	UNP P21447
A	1302	ALA	-	expression tag	UNP P21447
A	1303	ALA	-	expression tag	UNP P21447
A	1304	GLY	-	expression tag	UNP P21447
A	1305	GLY	-	expression tag	UNP P21447
A	1306	GLY	-	expression tag	UNP P21447
A	1307	SER	-	expression tag	UNP P21447
A	1308	GLY	-	expression tag	UNP P21447
A	1309	GLY	-	expression tag	UNP P21447
A	1310	GLY	-	expression tag	UNP P21447
A	1311	SER	-	expression tag	UNP P21447
A	1312	TRP	-	expression tag	UNP P21447
A	1313	SER	-	expression tag	UNP P21447
A	1314	HIS	-	expression tag	UNP P21447
A	1315	PRO	-	expression tag	UNP P21447
A	1316	GLN	-	expression tag	UNP P21447
A	1317	PHE	-	expression tag	UNP P21447
A	1318	GLU	-	expression tag	UNP P21447
A	1319	LYS	-	expression tag	UNP P21447
A	1320	GLY	-	expression tag	UNP P21447
A	1321	SER	-	expression tag	UNP P21447
A	1322	GLY	-	expression tag	UNP P21447
A	1323	HIS	-	expression tag	UNP P21447
A	1324	HIS	-	expression tag	UNP P21447
A	1325	HIS	-	expression tag	UNP P21447
A	1326	HIS	-	expression tag	UNP P21447
A	1327	HIS	-	expression tag	UNP P21447
A	1328	HIS	-	expression tag	UNP P21447

- Molecule 2 is (4S,11S,18S)-4-[[[(2,4-dinitrophenyl)disulfanyl]methyl]-11,18-dimethyl-6,13,20-trithia-3,10,17,22,23,24-hexazatetracyclo[17.2.1.1<sup>5,8</sup>.1<sup>12,15</sup>]]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-trione (CCD ID: JJI) (formula: C<sub>24</sub>H<sub>20</sub>N<sub>8</sub>O<sub>7</sub>S<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	44	24	8	7	5	0

- Molecule 3 is (4 {S},11 {S},18 {S})-4,11-dimethyl-18-(sulfanylmethyl)-6,13,20-trithia-3,10,17,22,23,24-hexazatetracyclo[17.2.1.1<sup>^</sup>{5,8}.1<sup>^</sup>{12,15}]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-trione (CCD ID: JIZ) (formula: C<sub>18</sub>H<sub>18</sub>N<sub>6</sub>O<sub>3</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
3	A	1	31	18	6	3	4	0





TYR	A950	S1053	S1133	D1215	Q1259	HIS
PHE	F953	L1054	E1139	K1216	K1260	HIS
GLN	R954	E1055	E1139	A1217	GLY	HIS
GLY	A957	V1056	K1146	R1218	TYR	HIS
ALA	W958	K1057	E1147	R1219	PHE	HIS
SER	L959	G1058	E1147	G1220	SER	HIS
GLY	L964	Q1059	I1150	R1221	MET	HIS
GLY	M965	T1061	H1151	T1222	VAL	HIS
SER	E968	L1062	Q1152	V1223	VAL	HIS
PRO	M969	A1063	F1153	I1226	GLN	HIS
GLN	F974	L1064	I1154	A1227	ALA	HIS
GLU	I977	V1065	D1155	H1228	ALA	HIS
LYS	M978	G1066	P1158	R1229	ALA	HIS
ALA	F979	S1067	D1159	Q1234	ALA	HIS
ALA	A983	S1073	K1160	M1235	ALA	HIS
GLY	F996	T1074	Y1161	A1236	ALA	HIS
GLY	T998	V1075	M1162	D1237	ALA	HIS
SER	Y999	L1076	T1163	L1238	GLY	HIS
HIS	H1003	L1079	R1164	I1239	GLY	HIS
TRP	I1004	E1080	V1165	V1240	GLY	HIS
SER	I1005	R1081	G1166	V1241	SER	HIS
HIS	R1006	F1082	D1167	I1242	GLY	HIS
PRO	I1007	Y1083	K1168	GLY	GLY	HIS
GLN	E1013	D1084	G1169	K1246	GLY	HIS
GLN	I1014	P1085	T1170	V1247	GLY	HIS
GLU	D1015	M1086	S1173	K1248	TRP	HIS
LYS	S1016	A1087	Q1176	E1249	SER	HIS
GLY	Q1020	G1088	K1177	H1250	HIS	HIS
GLY	M1025	S1089	Q1178	G1251	GLN	HIS
HIS	M1026	D1089	R1178	T1252	PHE	HIS
HIS	L1027	G1094	R1179	H1253	GLU	HIS
HIS	E1028	K1095	I1180	Q1254	LYS	HIS
HIS	G1029	E1096	A1181	Q1255	GLY	HIS
	F1033	I1097	I1182	L1256	SER	HIS
	S1034	K1098	A1183	Q1259	HIS	HIS
	G1035	M1101	R1184	K1260	HIS	HIS
	V1036	W1104	V1187	GLY	HIS	HIS
	T1042	L1109	R1188	ILE	HIS	HIS
	R1043	G1110	Q1189	TYR	HIS	HIS
	P1044	L1114	P1190	PHE	HIS	HIS
	S1045	Q1114	H1191	SER	HIS	HIS
	L1049	E1115	I1192	SER	HIS	HIS
	L1052	P1116	L1193	MET	HIS	HIS
		I1117	L1194	VAL	HIS	HIS
		F1118	L1195	VAL	HIS	HIS
		L1118	S1200	GLN	HIS	HIS
		F1119	A1201	ALA	HIS	HIS
		D1120	ALA	ALA	HIS	HIS
		R1121	LYS	ALA	HIS	HIS
		T1127	L1202	ALA	HIS	HIS
		D1131	D1203	ALA	HIS	HIS
		N1132	T1204	ALA	HIS	HIS
			E1205	ALA	HIS	HIS
			K1208	ALA	HIS	HIS
			L1214	ALA	HIS	HIS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	75	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.763	Depositor
Minimum map value	-1.961	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	234.36, 234.36, 234.36	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: JIZ, Y01, JJI

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	0.31	0/9131	0.52	1/12342 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1234	GLN	N-CA-C	-5.57	104.43	111.11

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	8967	0	9148	224	0
2	A	44	0	0	3	0
3	A	31	0	0	5	0
4	A	175	0	239	20	0
All	All	9217	0	9387	241	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 13.

The worst 5 of 241 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)
4:A:1407:Y01:CAP	4:A:1407:Y01:CAQ	1.80	1.59
4:A:1407:Y01:CBI	4:A:1407:Y01:CBE	1.74	1.59
2:A:1401:JJI:N02	2:A:1401:JJI:C03	1.78	1.26
2:A:1401:JJI:N04	2:A:1401:JJI:C08	1.77	1.22
2:A:1401:JJI:N06	2:A:1401:JJI:C13	1.77	1.16

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	1153/1328 (87%)	1086 (94%)	67 (6%)	0	<b>100</b>   <b>100</b>

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	947/1086 (87%)	944 (100%)	3 (0%)	<b>86</b>   <b>84</b>

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

Mol	Chain	Res	Type
1	A	96	LYS
1	A	169	THR
1	A	999	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	805	ASN
1	A	1103	GLN
1	A	1259	GLN
1	A	1250	HIS
1	A	1254	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](#)

7 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	$\# Z  > 2$
4	Y01	A	1404	-	38,38,38	0.48	0	57,57,57	0.58	0
4	Y01	A	1405	-	38,38,38	0.46	0	57,57,57	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	Y01	A	1407	-	38,38,38	8.31	24 (63%)	57,57,57	2.00	18 (31%)
4	Y01	A	1403	-	38,38,38	0.46	0	57,57,57	0.81	1 (1%)
4	Y01	A	1406	-	38,38,38	0.49	0	57,57,57	0.80	2 (3%)
2	JJI	A	1401	-	47,48,48	5.25	21 (44%)	56,69,69	4.66	33 (58%)
3	JIZ	A	1402	1	34,34,34	5.41	24 (70%)	45,49,49	4.49	20 (44%)

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
4	Y01	A	1404	-	-	8/19/77/77	0/4/4/4
4	Y01	A	1405	-	-	12/19/77/77	0/4/4/4
4	Y01	A	1407	-	-	8/19/77/77	0/4/4/4
4	Y01	A	1403	-	-	10/19/77/77	0/4/4/4
4	Y01	A	1406	-	-	9/19/77/77	0/4/4/4
2	JJI	A	1401	-	-	8/46/50/50	0/5/5/5
3	JIZ	A	1402	1	-	7/38/38/38	0/4/4/4

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1407	Y01	CBD-CBG	-27.08	1.02	1.53
4	A	1407	Y01	CAU-CAS	-19.18	1.15	1.53
2	A	1401	JJI	C03-N02	18.75	1.78	1.38
2	A	1401	JJI	C08-N04	18.13	1.77	1.38
2	A	1401	JJI	C13-N06	18.09	1.77	1.38

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	JJI	C04-S01-C02	15.46	107.81	89.52
2	A	1401	JJI	C14-S03-C12	15.21	107.52	89.52
3	A	1402	JIZ	C09-S02-C07	15.04	107.31	89.52
2	A	1401	JJI	C09-S02-C07	14.85	107.09	89.52
3	A	1402	JIZ	C14-S03-C12	14.73	106.95	89.52

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

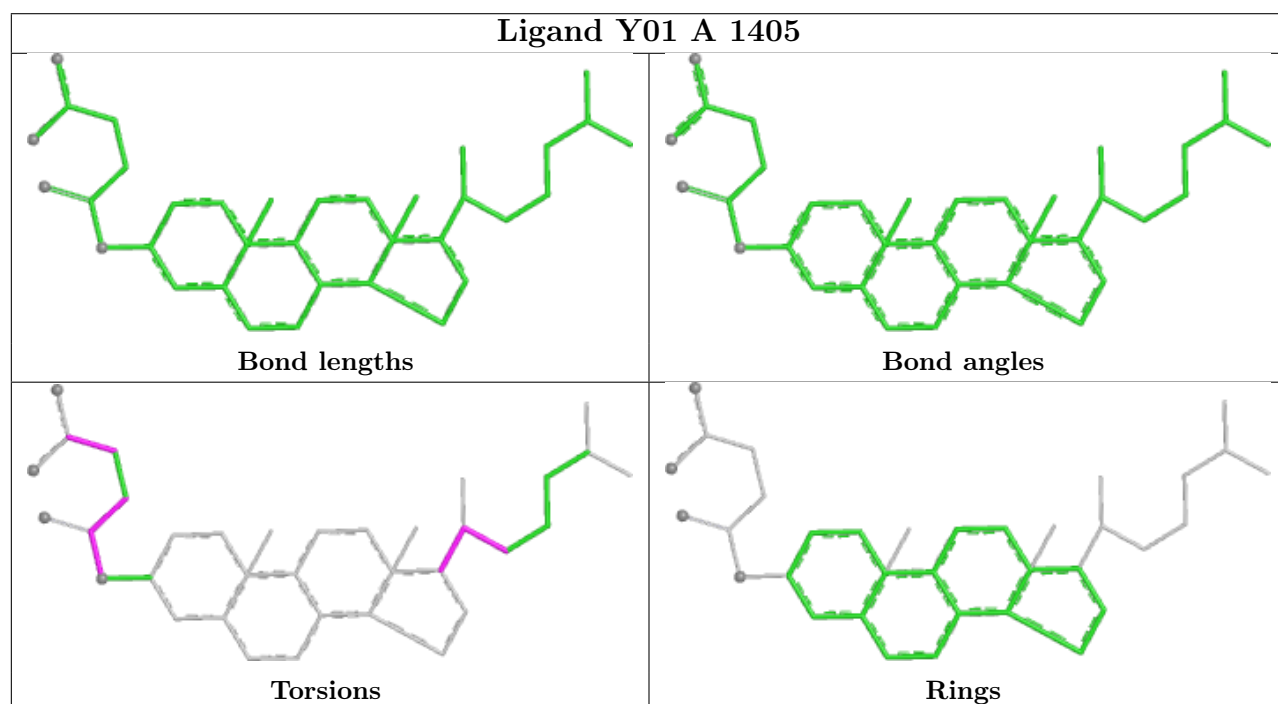
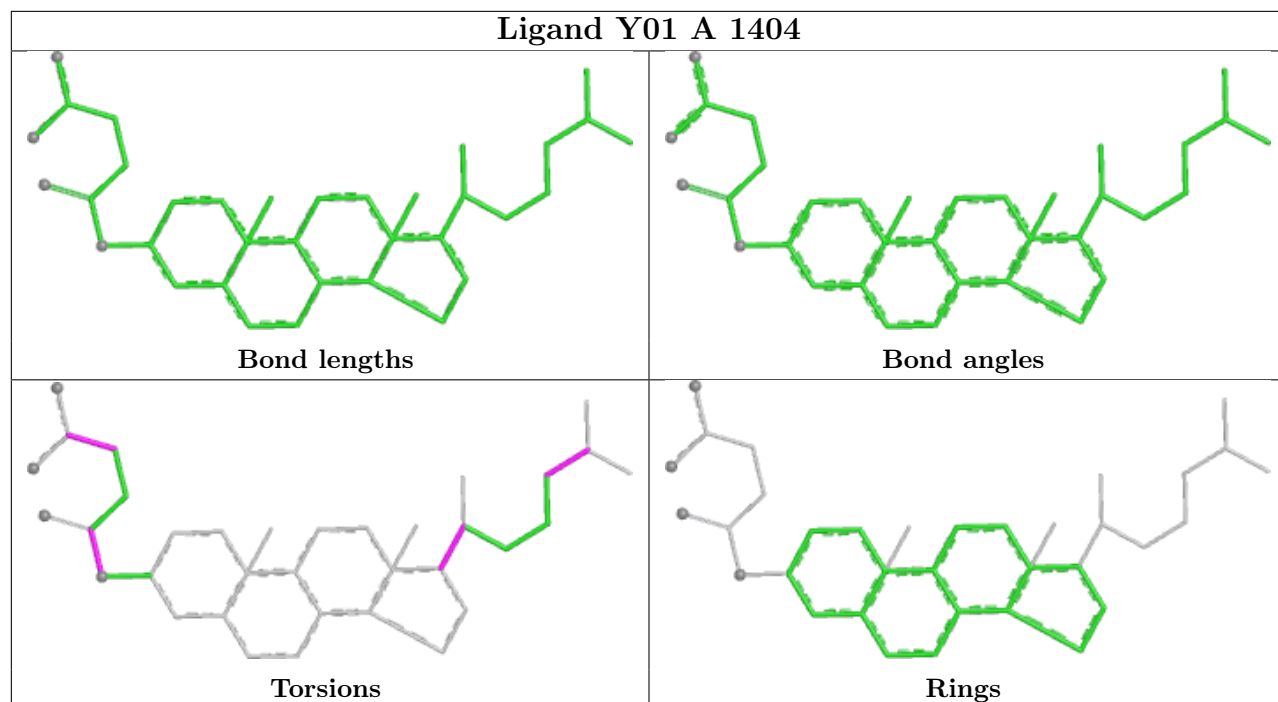
Mol	Chain	Res	Type	Atoms
2	A	1401	JJI	C04-C03-C05-N03
2	A	1401	JJI	C04-C03-C05-O01
2	A	1401	JJI	N02-C03-C05-N03
2	A	1401	JJI	N02-C03-C05-O01
3	A	1402	JIZ	C14-C13-C15-N01

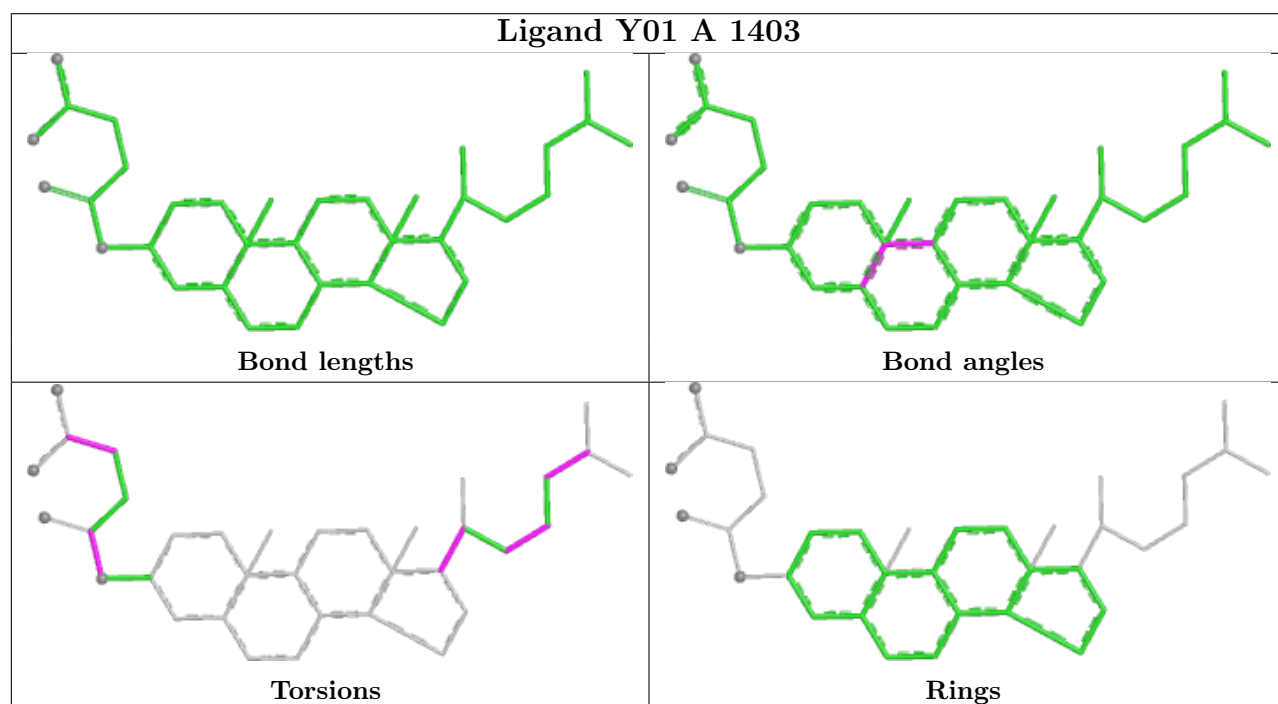
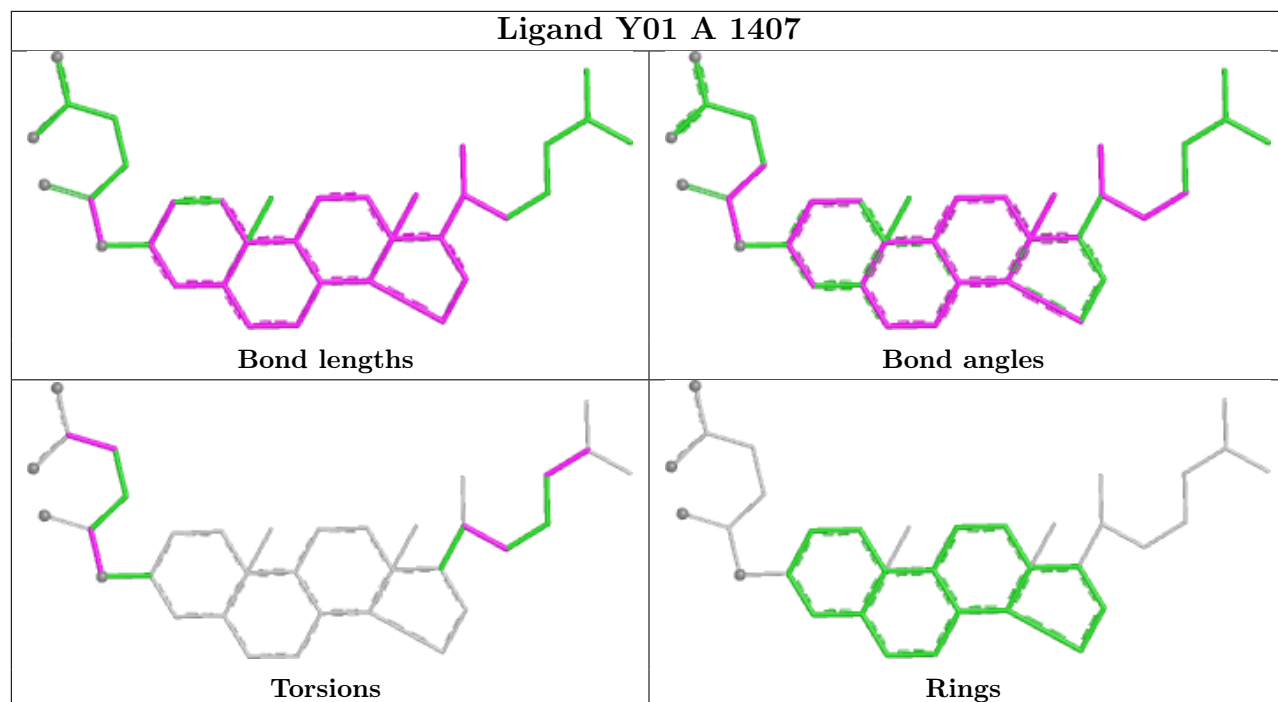
There are no ring outliers.

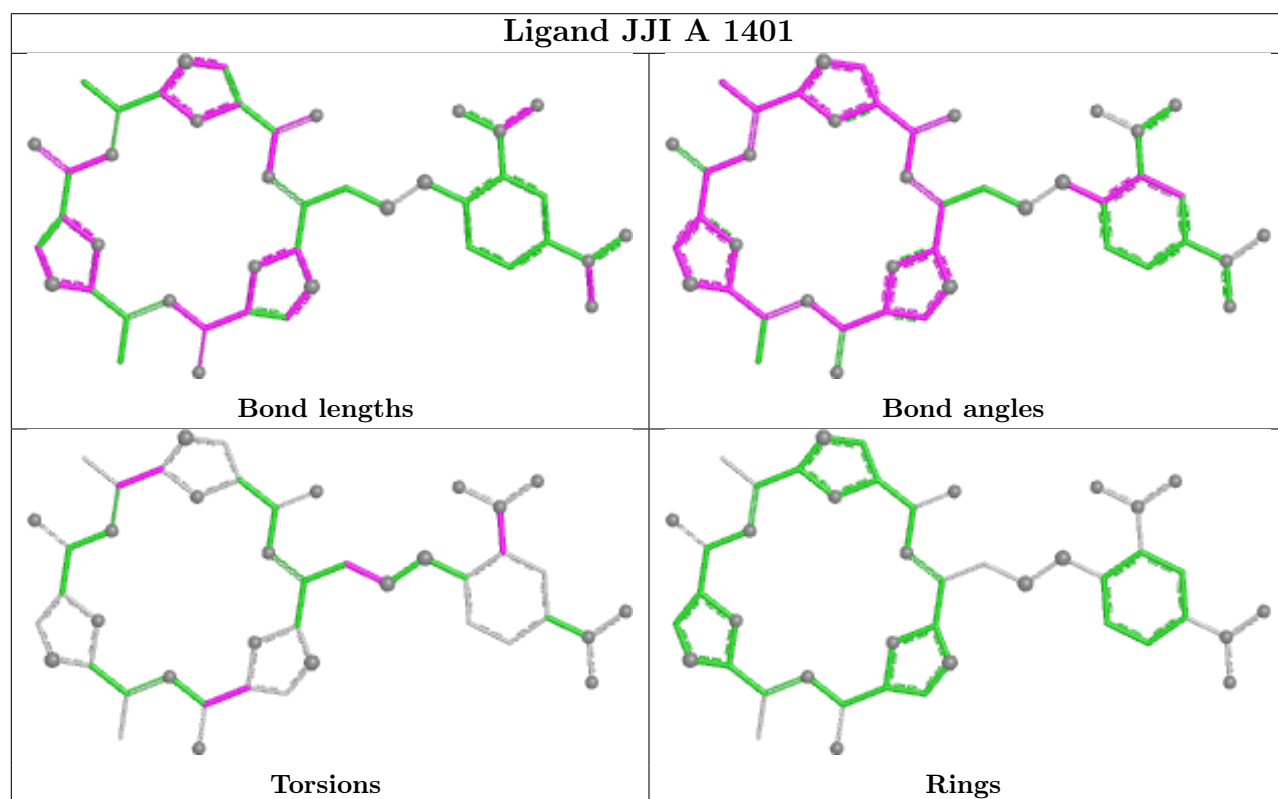
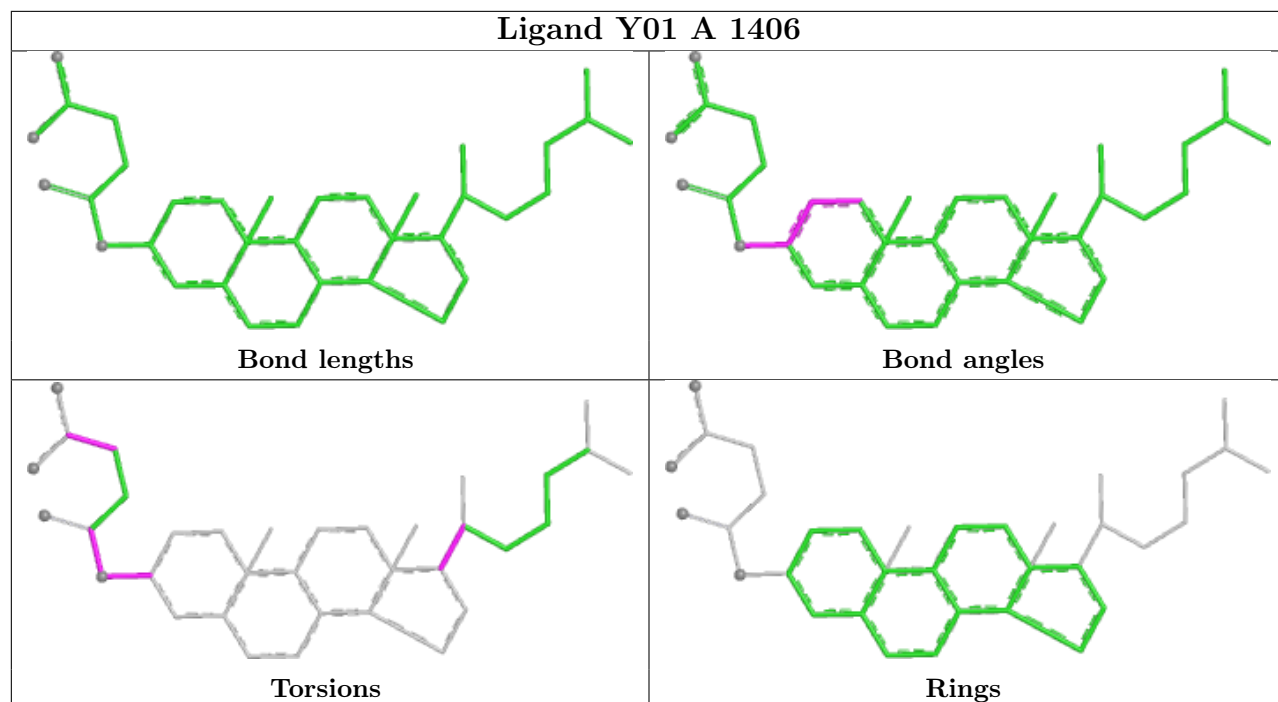
7 monomers are involved in 28 short contacts:

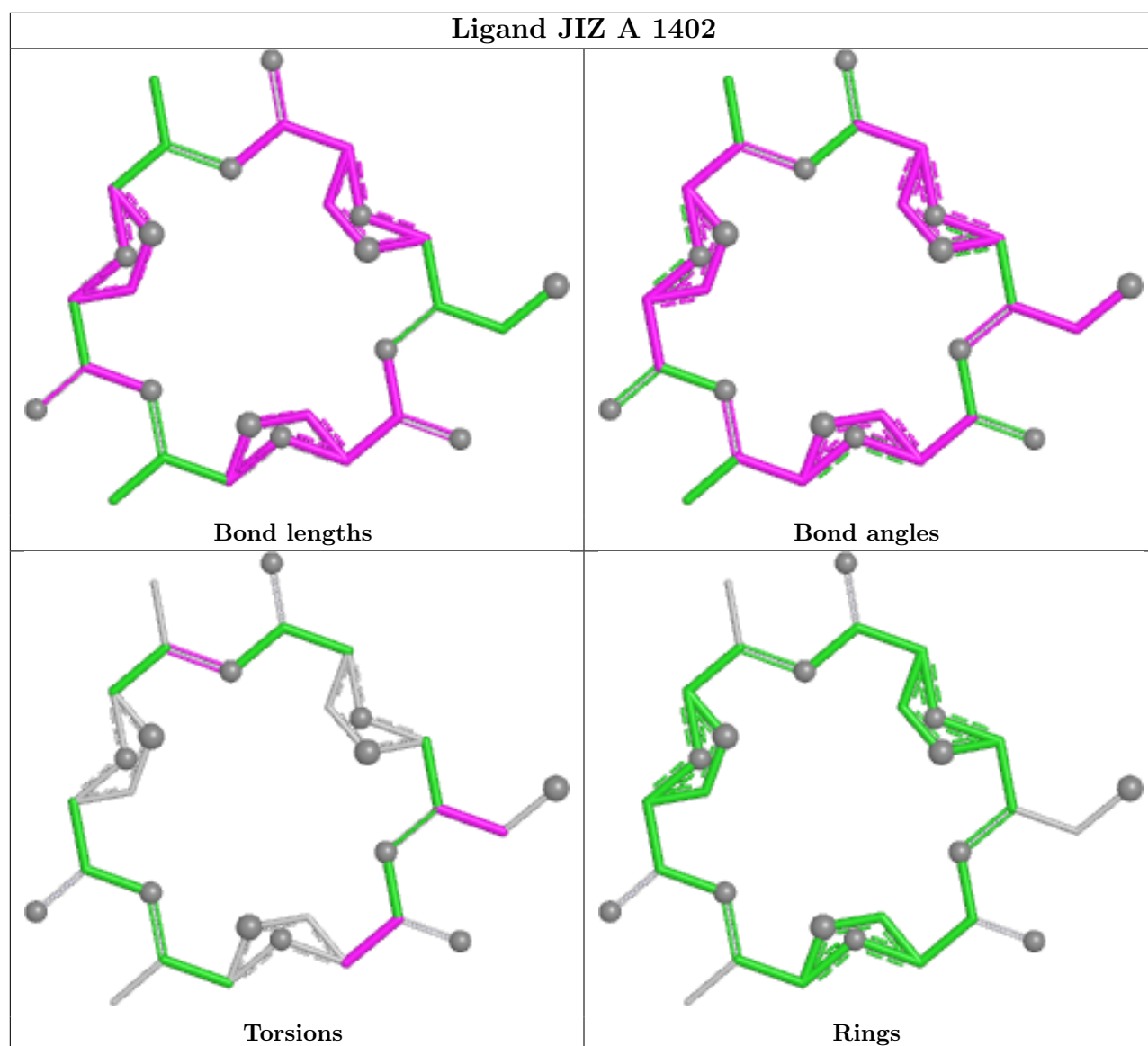
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1404	Y01	3	0
4	A	1405	Y01	4	0
4	A	1407	Y01	9	0
4	A	1403	Y01	3	0
4	A	1406	Y01	1	0
2	A	1401	JJI	3	0
3	A	1402	JIZ	5	0

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.

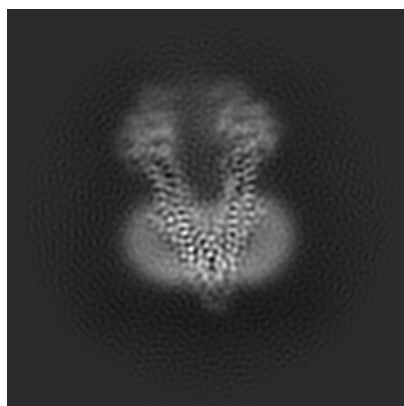
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17630. These allow visual inspection of the internal detail of the map and identification of artifacts.

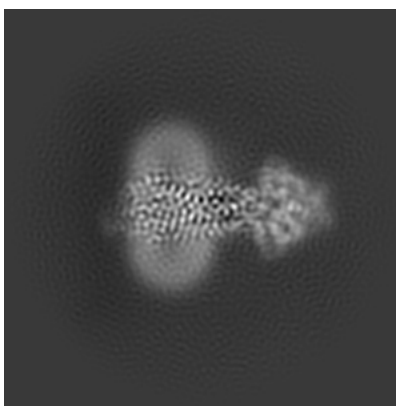
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

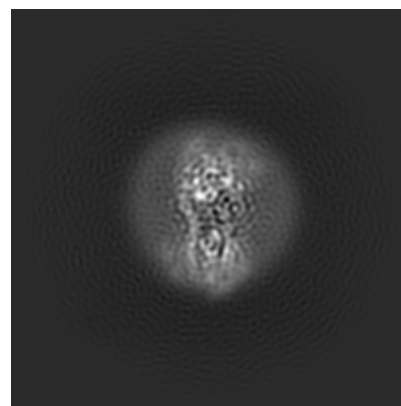
#### 6.1.1 Primary map



X

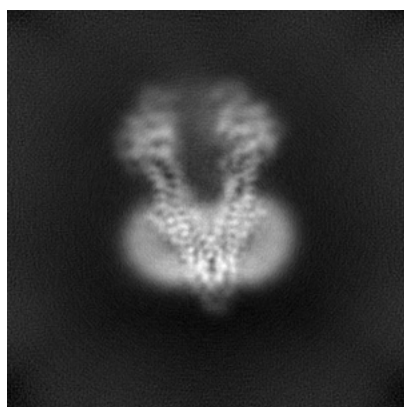


Y

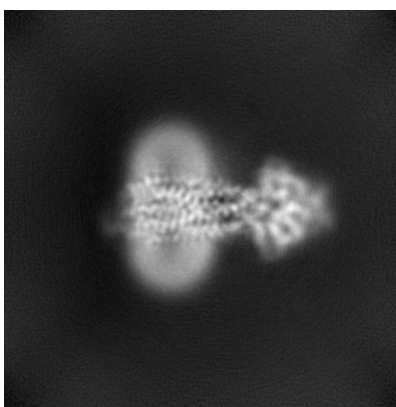


Z

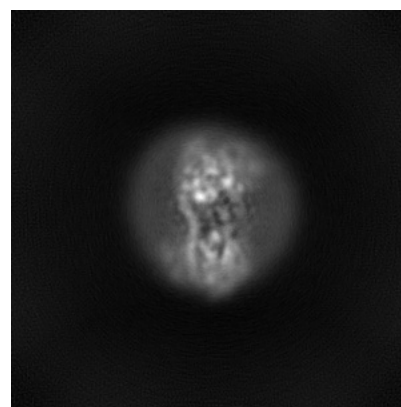
#### 6.1.2 Raw map



X



Y

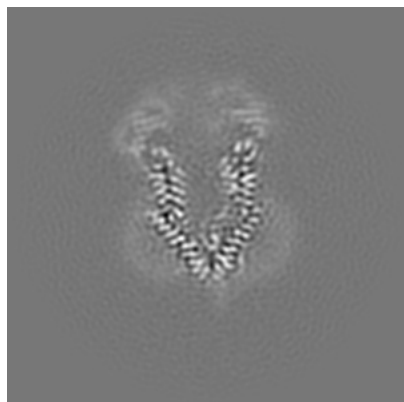


Z

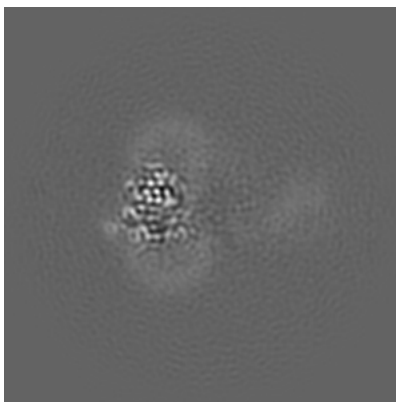
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

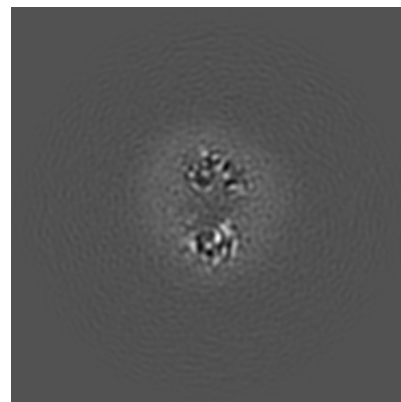
### 6.2.1 Primary map



X Index: 140

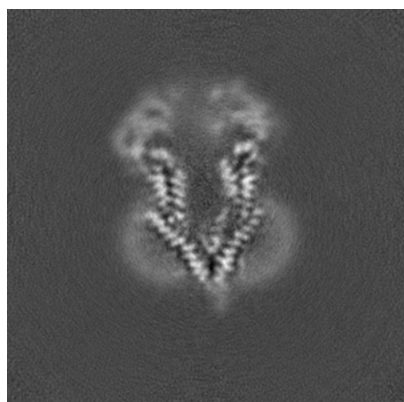


Y Index: 140

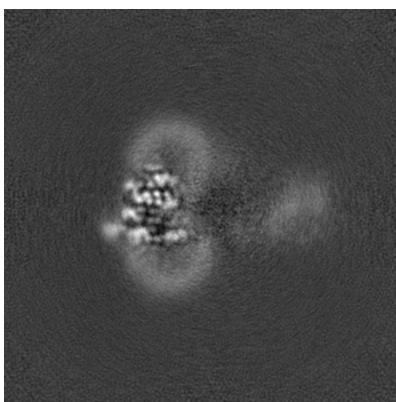


Z Index: 140

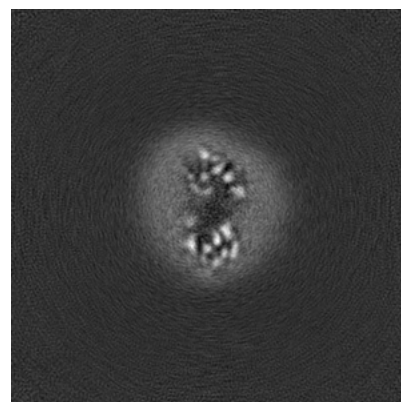
### 6.2.2 Raw map



X Index: 140



Y Index: 140

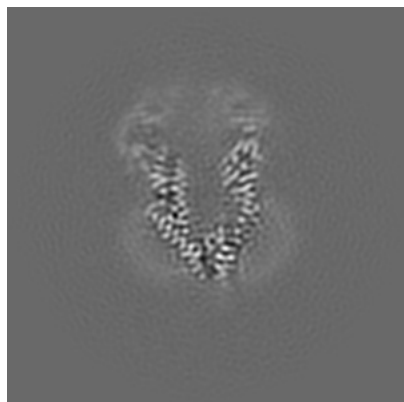


Z Index: 140

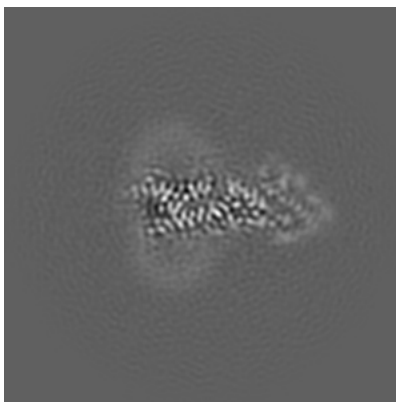
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

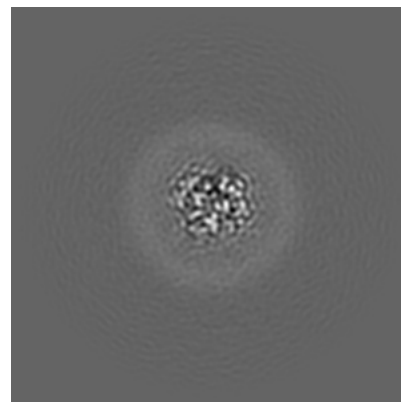
### 6.3.1 Primary map



X Index: 142

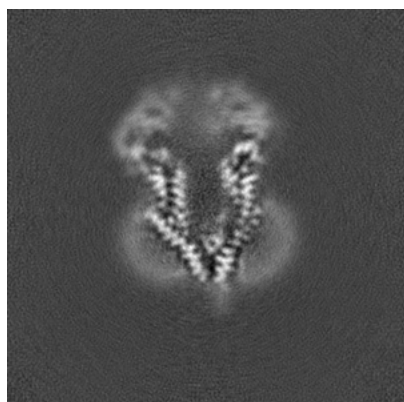


Y Index: 160

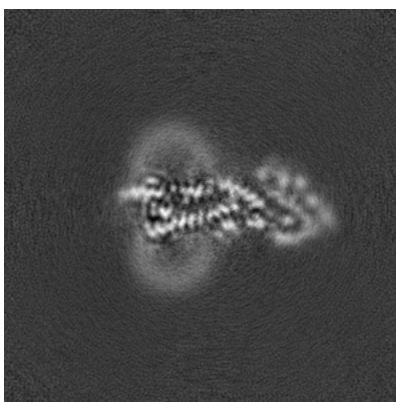


Z Index: 107

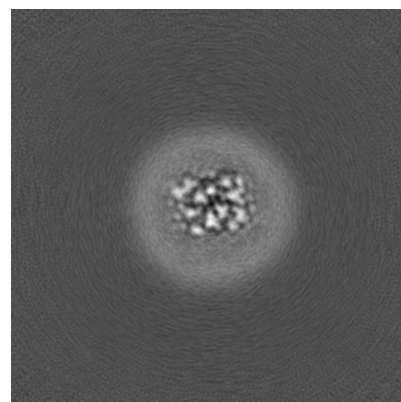
### 6.3.2 Raw map



X Index: 141



Y Index: 158

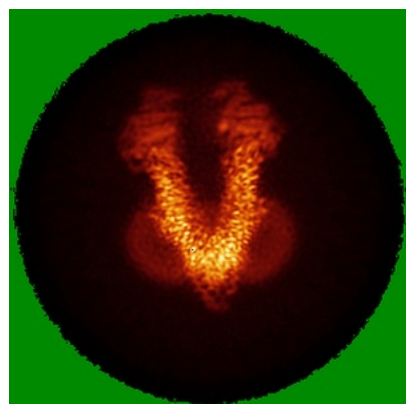


Z Index: 101

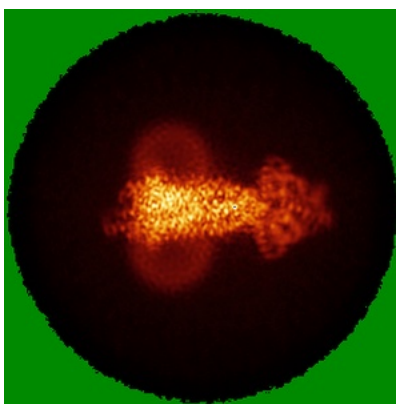
The images above show the largest variance slices of the map in three orthogonal directions.

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

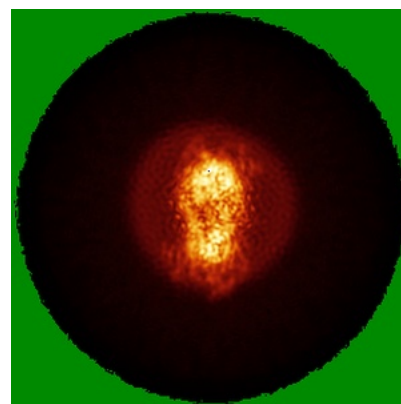
### 6.4.1 Primary map



X

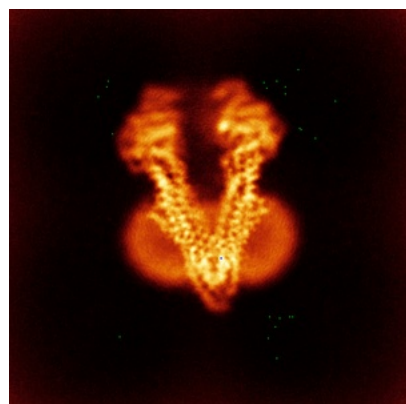


Y

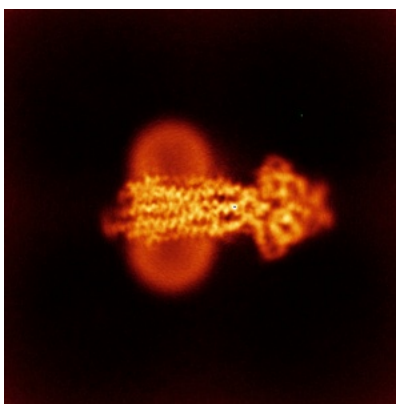


Z

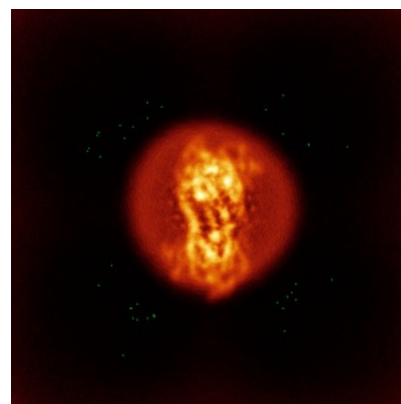
### 6.4.2 Raw map



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.

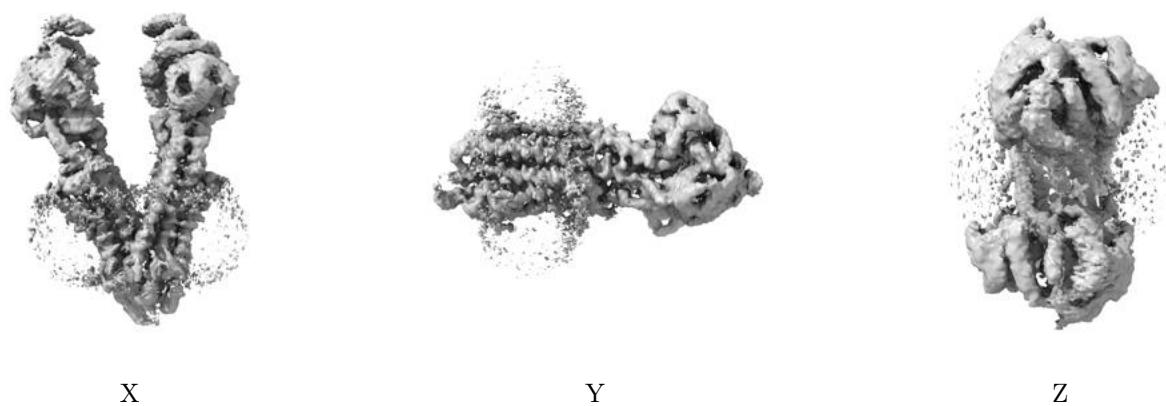
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

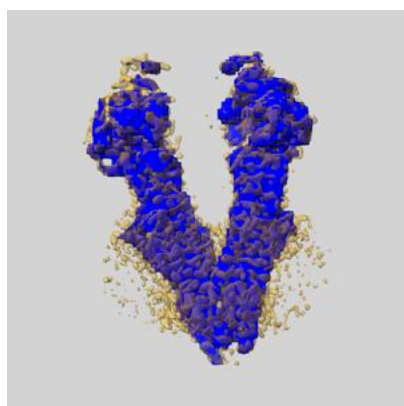
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

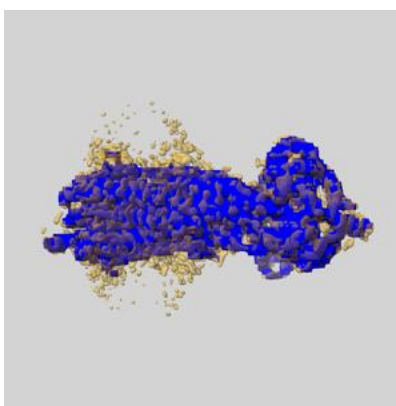
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

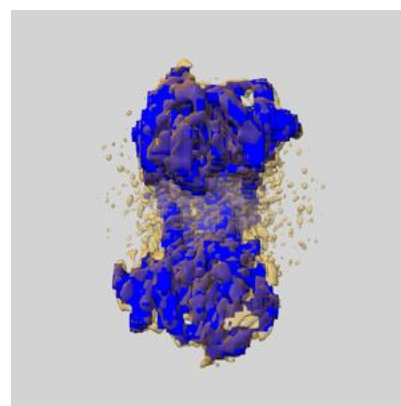
### 6.6.1 emd\_17630\_msk\_1.map [i](#)



X



Y

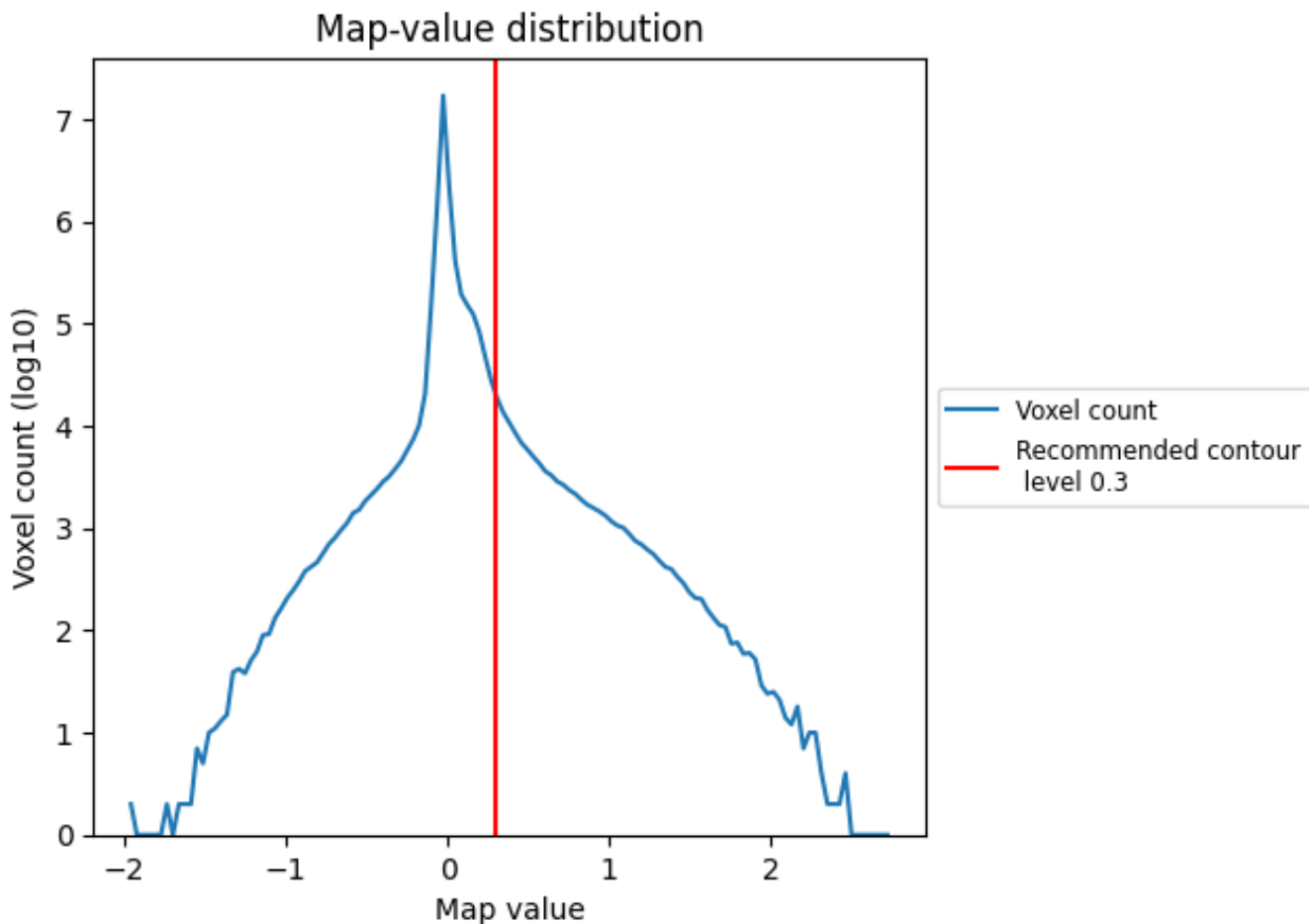


Z

## 7 Map analysis [i](#)

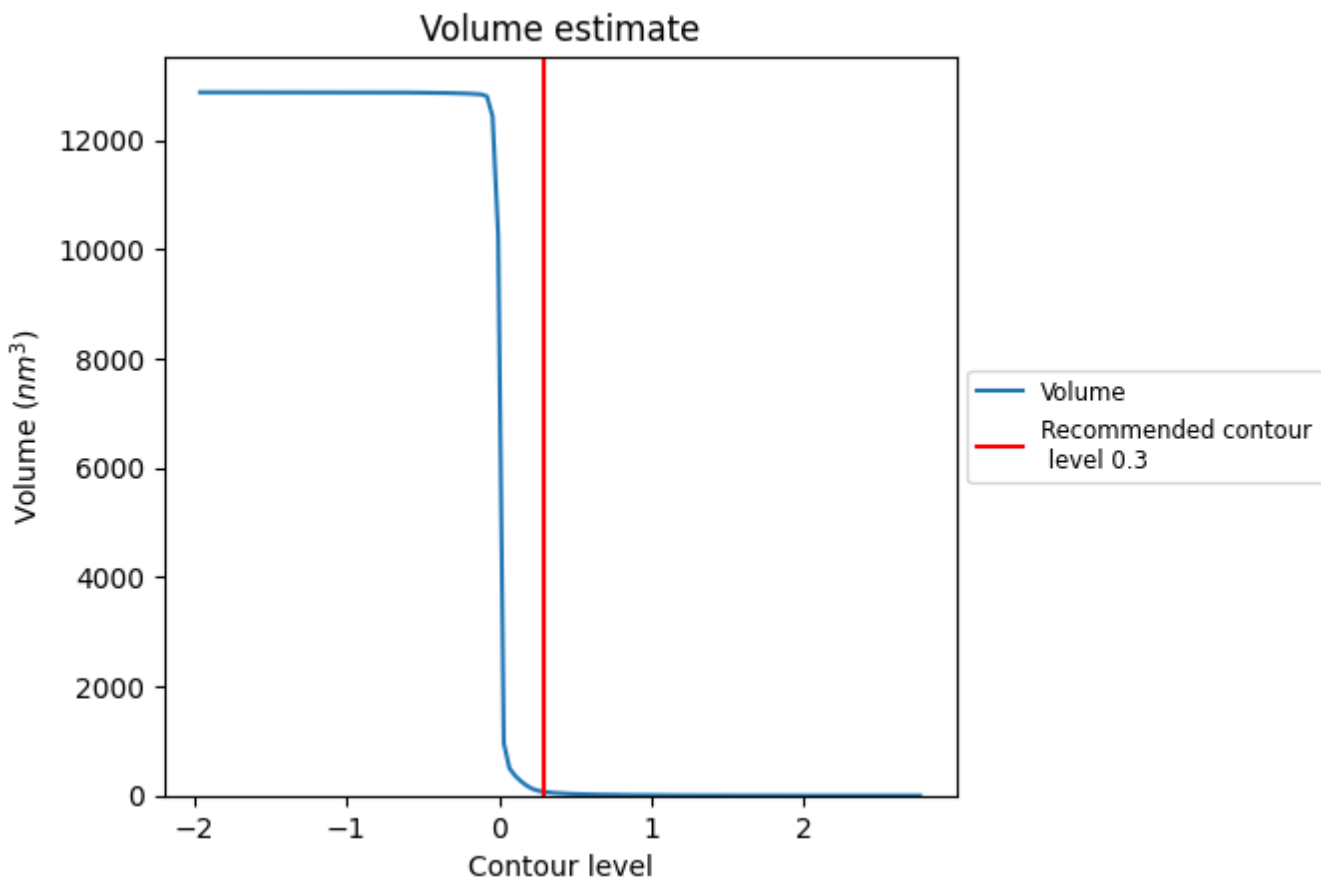
This section contains the results of statistical analysis of the map.

### 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.

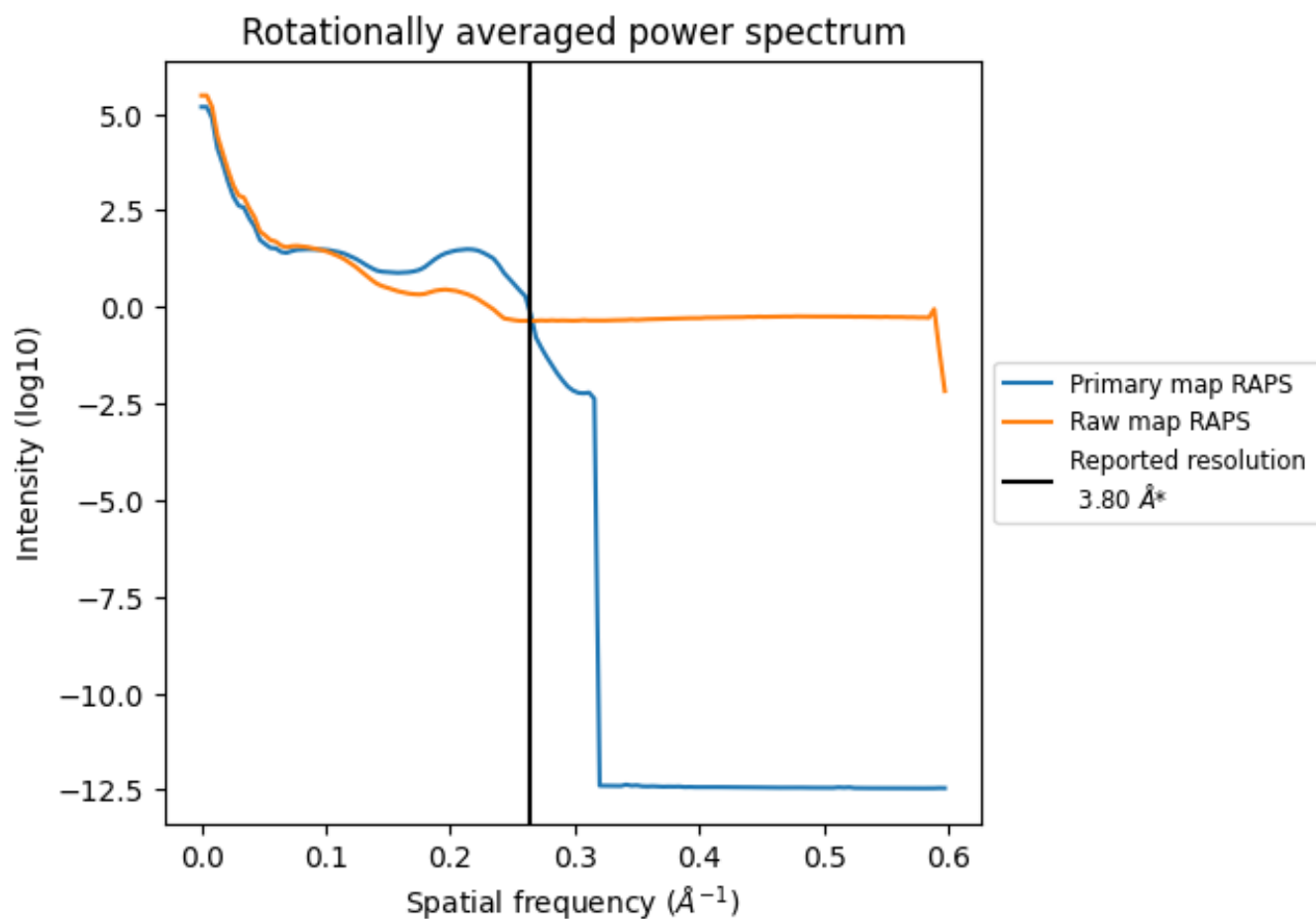
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 67 nm<sup>3</sup>; this corresponds to an approximate mass of 61 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](#)

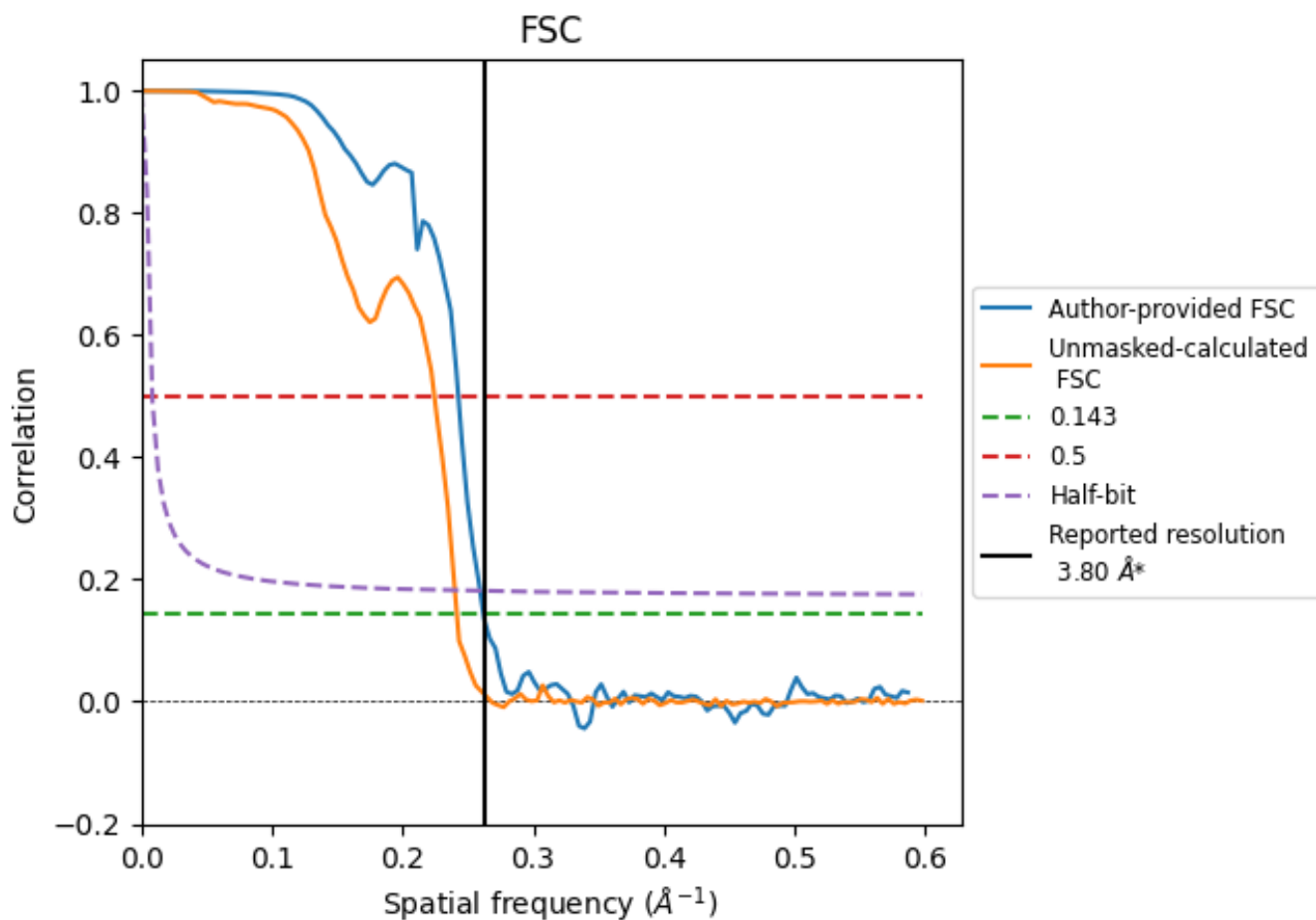


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

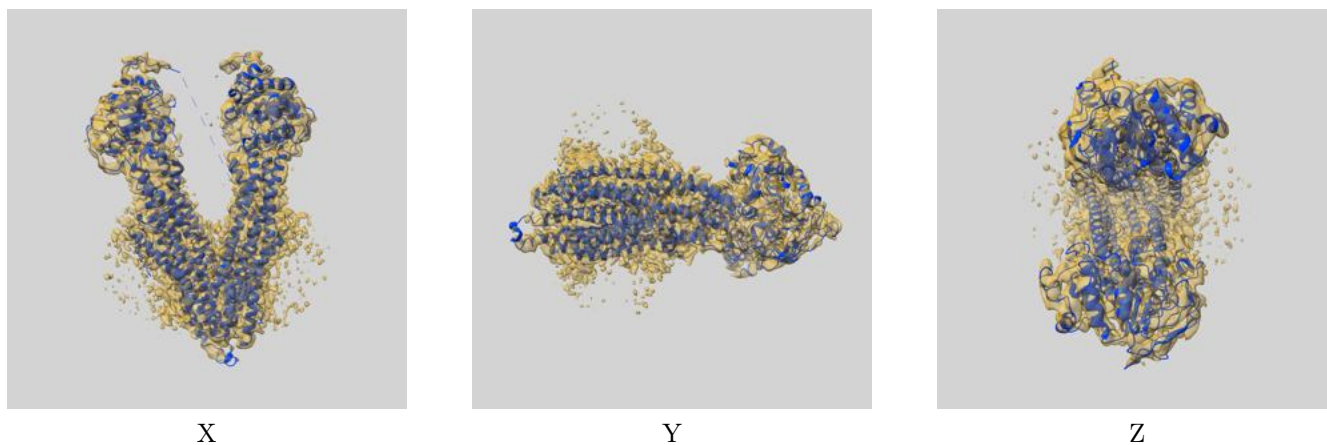
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.12	3.86
Unmasked-calculated*	4.14	4.46	4.17

\*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-17630 and PDB model 8PEE. Per-residue inclusion information can be found in section 3 on page 8.

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



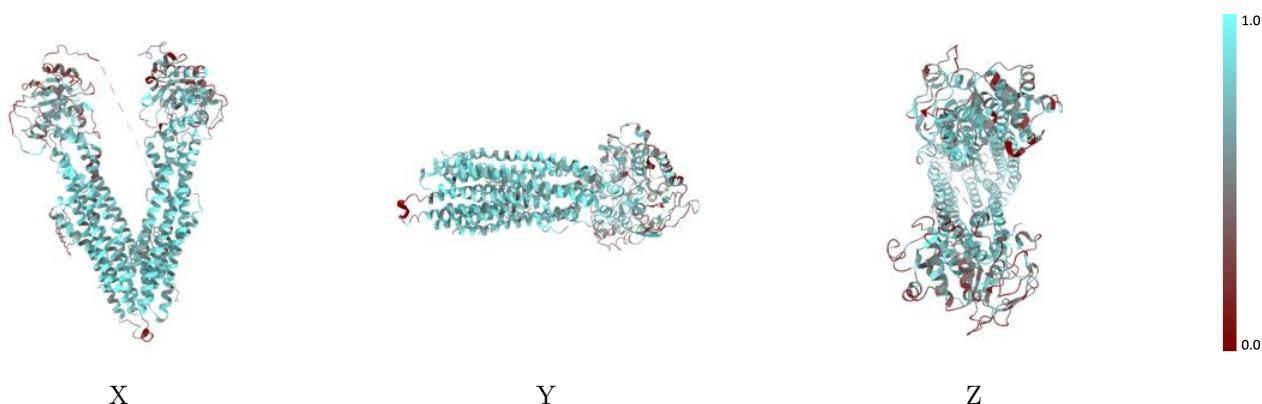
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



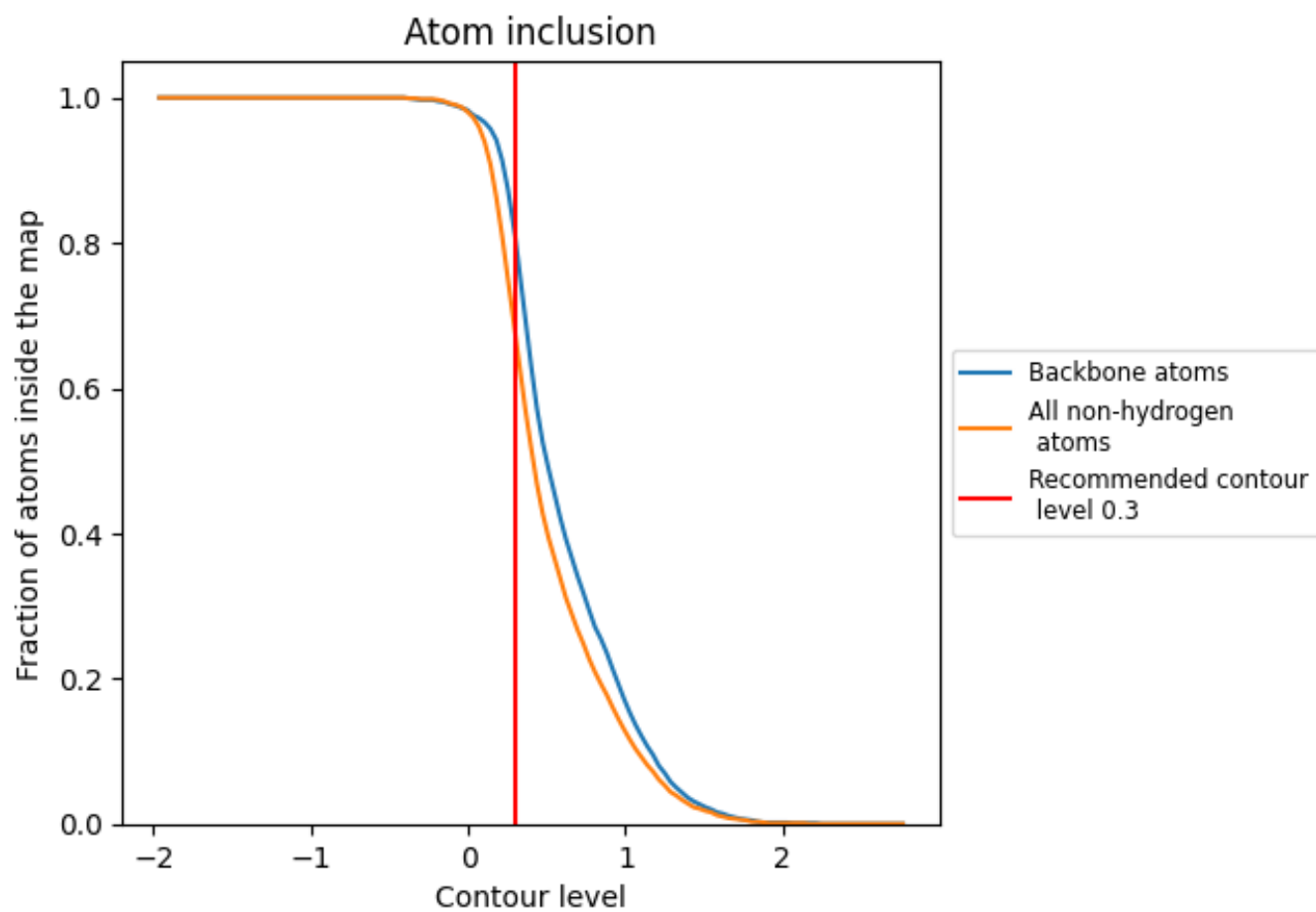
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6760	 0.3790
A	 0.6760	 0.3790

