



Full wwPDB EM Validation 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 Full wwPDB EM Validation 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:

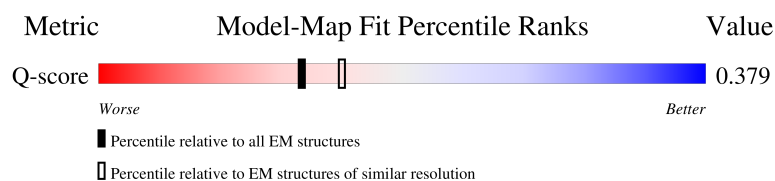
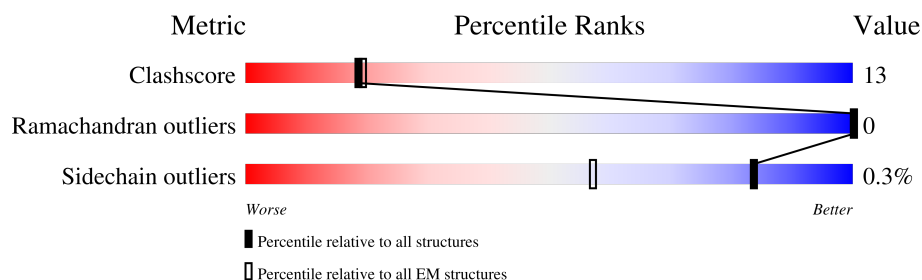
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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 ≥ 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	

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
1	A	1157	Total	C	N	O	S	0	0
			8967	5763	1527	1647	30		

There are 65 discrepancies between the modelled and reference sequences:

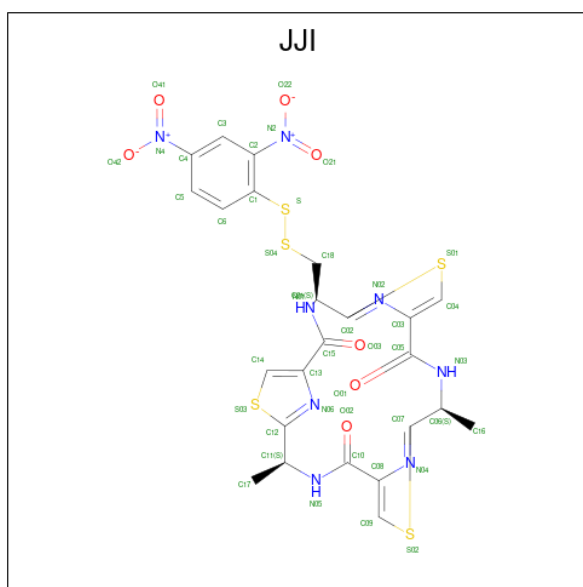
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	engineered mutation	UNP P21447
A	87	GLN	ASN	engineered mutation	UNP P21447
A	90	GLN	ASN	engineered mutation	UNP P21447
A	133	ALA	CYS	engineered mutation	UNP P21447
A	335	CYS	LEU	engineered mutation	UNP P21447
A	427	GLY	CYS	engineered mutation	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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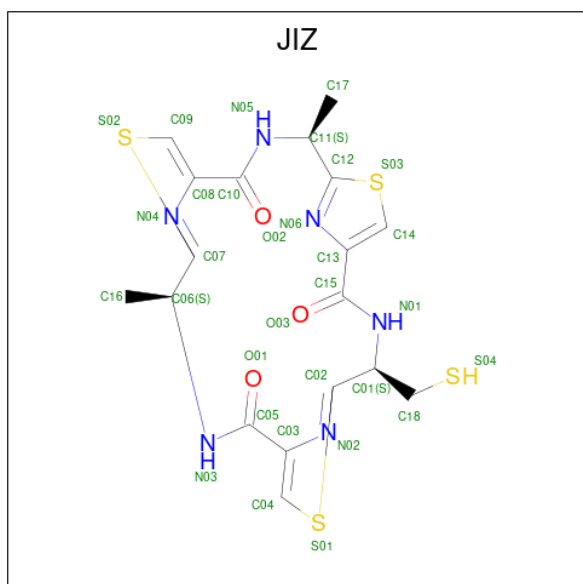
Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	SER	-	expression tag	UNP P21447
A	1293	TRP	-	expression tag	UNP P21447
A	1294	SER	-	expression tag	UNP P21447
A	1295	HIS	-	expression tag	UNP P21447
A	1296	PRO	-	expression tag	UNP P21447
A	1297	GLN	-	expression tag	UNP P21447
A	1298	PHE	-	expression 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[^]{5,8}.1[^]{12,15}}]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-trione (CCD ID: JJI) (formula: C₂₄H₂₀N₈O₇S₅) (labeled as "Ligand of Interest" by depositor).



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

- 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[17.2.1.1.1^{5,8}.1^{12,15}]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-trione (CCD ID: JIZ) (formula: C₁₈H₁₈N₆O₃S₄) (labeled as "Ligand of Interest" by depositor).



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

- Y01

Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 35	C 31	O 4	0
4	A	1	Total 35	C 31	O 4	0
4	A	1	Total 35	C 31	O 4	0
4	A	1	Total 35	C 31	O 4	0
4	A	1	Total 35	C 31	O 4	0

TYR	D1215	S1133	S1053	A950
PHE	K1216	E1139	L1054	F953
GLN	A1217	K1146	E1055	R954
GLY	R1218	E1147	V1056	A957
GLY	E1219	I1150	K1057	Y958
ALA	R1220	H1151	K1058	L959
SER	G1221	Q1152	Q1059	L964
GLY	T1222	H1152	T1060	M965
GLY	V1223	F1153	L1062	
SER	I1226	I1154	A1063	
TRP	A1227	T1155	L1064	E968
SER	H1228	D1155	V1065	M969
HIS	A1229	P1158	G1066	F974
PRO	R1229	D1159	S1067	
GLN		K1160		
PHE	Q1234	Y1161	S1073	I977
GLU	N1235	M1162	T1074	Y978
LYS	A1236	T1163	V1075	F979
ALA	D1237	L1164	Y1076	
ALA	L1238	R1165	L1079	A983
GLY	L1239	V1166	E1080	K996
GLY	V1240	G1166	R1081	A997
GLY	V1241	D1167	F1082	T998
SER	I1242	K1168	Y1083	V999
GLY	K1246	G1169	D1084	
GLY	V1247	T1170	P1085	H1003
SER	K1248	S1173	M1086	I1004
HIS	E1249	Q1176	A1087	I1005
PRO	H1250	Q1177	G1088	R1006
GLN	G1251	K1178	S1089	I1007
PHE	T1252	Q1179	D1093	
GLU	H1253	I1180	G1094	E1013
LYS	Q1254	A1181	K1095	I1014
GLY	Q1255	I1182	E1096	D1015
SER	L1256	A1183	I1097	S1016
GLY	Q1259	R1184	K1098	
HIS	K1260	V1187	N1101	Q1020
HIS	ILE	R1188	W1104	M1025
HIS	TYR	Q1189	L1109	M1026
HIS	PHE	P1190	G1110	L1027
HIS	SER	I1192	Q1114	E1028
	MET	L1193	E1115	G1029
	VAL	L1194	P1116	F1033
	VAL	L1195	I1117	G1035
	GLN		L1118	V1036
	ALA		F1119	
	GLY	S1200	R1121	T1042
	ALA	A1201	T1127	R1043
	LYS	L1202	D1131	P1044
	ARG	D1203	N1132	S1045
	SER	T1204		L1049
	LEU	E1205		L1052
	GLU	K1208		
	ASN	L1214		
	LEU			

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.

All (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
1:A:481:ALA:O	1:A:485:ARG:HG3	1.81	0.81
1:A:1064:LEU:HB2	1:A:1226:ILE:HG12	1.60	0.81
1:A:552:GLU:HB3	1:A:555:SER:HB2	1.64	0.78
1:A:1250:HIS:HB2	1:A:1253:HIS:ND1	1.98	0.78
4:A:1407:Y01:CBE	4:A:1407:Y01:CAU	2.60	0.76
1:A:265:GLY:HA3	1:A:1132:ASN:HD22	1.50	0.76
4:A:1407:Y01:CBE	4:A:1407:Y01:CAE	2.66	0.73
1:A:1118:LEU:HD21	1:A:1165:VAL:HG21	1.69	0.73
4:A:1407:Y01:CBE	4:A:1407:Y01:CBG	2.67	0.72
1:A:1036:VAL:HA	1:A:1088:GLY:HA3	1.72	0.72
1:A:266:GLN:HB3	1:A:793:LEU:HD23	1.73	0.70
1:A:1256:LEU:HD12	1:A:1259:GLN:HB2	1.72	0.69
1:A:263:PHE:HD1	1:A:1188:ARG:HH22	1.40	0.68
1:A:983:ALA:HB2	3:A:1402:JIZ:S02	2.34	0.68
4:A:1407:Y01:CAP	4:A:1407:Y01:CBI	2.66	0.66
1:A:1240:VAL:HG23	1:A:1242:ILE:CD1	2.25	0.66
1:A:498:LYS:HA	1:A:501:LYS:HD3	1.78	0.65
1:A:1240:VAL:HG23	1:A:1242:ILE:HD11	1.80	0.64
1:A:1118:LEU:HD13	1:A:1177:LYS:HZ1	1.62	0.64
1:A:608:HIS:HA	1:A:611:LEU:HD12	1.80	0.64
4:A:1407:Y01:CBI	4:A:1407:Y01:CBB	2.69	0.63
1:A:693:PHE:HE2	1:A:695:ARG:HE	1.47	0.63
1:A:550:LEU:HD11	1:A:569:LEU:HD22	1.81	0.62
4:A:1407:Y01:CAP	4:A:1407:Y01:CBG	2.78	0.62
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.82	0.61
1:A:1066:GLY:HA3	1:A:1073:SER:HB2	1.81	0.61
1:A:717:ASN:HB2	1:A:765:THR:HG21	1.82	0.61
1:A:821:VAL:HG21	1:A:1005:ILE:HD11	1.82	0.61
1:A:253:VAL:HG11	1:A:269:GLU:HG2	1.83	0.61
1:A:996:LYS:C	1:A:998:THR:H	2.09	0.61
1:A:900:PHE:HA	1:A:903:VAL:HG12	1.83	0.60
1:A:1067:SER:HA	1:A:1228:HIS:HE1	1.67	0.60
1:A:1154:ILE:HD12	1:A:1160:LYS:HD2	1.82	0.60
1:A:909:GLU:HA	1:A:909:GLU:OE1	2.00	0.60
1:A:727:ILE:HD13	1:A:754:LEU:HB3	1.82	0.60
1:A:1013:GLU:HG3	1:A:1016:SER:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ASP:OD1	1:A:508:PHE:N	2.36	0.59
1:A:1240:VAL:O	1:A:1242:ILE:HD12	2.03	0.59
1:A:121:VAL:HG21	1:A:946:TYR:HE2	1.66	0.58
1:A:573:ARG:HH22	1:A:591:ALA:HA	1.68	0.58
1:A:1033:PHE:HB3	1:A:1054:LEU:HB2	1.84	0.58
1:A:1193:LEU:HB2	1:A:1223:VAL:HG22	1.85	0.58
1:A:1195:LEU:HD13	1:A:1214:LEU:HD13	1.85	0.58
1:A:704:TRP:CG	1:A:705:PRO:HD3	2.39	0.58
1:A:974:PHE:O	1:A:978:VAL:HG22	2.03	0.57
1:A:217:ILE:HD11	4:A:1404:Y01:HAB3	1.85	0.57
1:A:1054:LEU:HD12	1:A:1062:LEU:HD21	1.87	0.57
1:A:844:ILE:O	1:A:848:ILE:HG13	2.04	0.57
1:A:178:ILE:O	1:A:182:ILE:HG12	2.05	0.57
1:A:870:VAL:O	1:A:874:MET:HG2	2.05	0.57
1:A:1228:HIS:HB2	1:A:1229:ARG:HH12	1.70	0.57
1:A:153:ASN:O	1:A:153:ASN:OD1	2.23	0.56
1:A:904:VAL:HA	1:A:909:GLU:OE2	2.05	0.56
1:A:35:VAL:HG12	1:A:36:LEU:HD23	1.86	0.56
1:A:122:LEU:HD12	1:A:939:SER:HB3	1.88	0.56
1:A:262:ALA:HB2	1:A:1082:PHE:HZ	1.69	0.56
1:A:401:LYS:O	1:A:404:GLN:NE2	2.37	0.55
1:A:1062:LEU:HD13	1:A:1240:VAL:HG22	1.87	0.55
1:A:1246:LYS:HG3	1:A:1247:VAL:HG23	1.89	0.55
1:A:510:MET:HG2	1:A:515:GLN:HG2	1.88	0.55
1:A:519:LEU:HG	1:A:519:LEU:O	2.07	0.55
1:A:232:LEU:HD11	1:A:287:LYS:HE2	1.89	0.54
1:A:1173:SER:HB3	1:A:1176:GLN:HE22	1.72	0.54
1:A:584:ARG:HE	1:A:585:LEU:H	1.55	0.54
1:A:464:GLU:HA	1:A:543:ARG:HH22	1.72	0.54
1:A:538:ALA:O	1:A:542:VAL:HG23	2.08	0.54
1:A:513:PRO:HB3	1:A:518:THR:OG1	2.07	0.53
1:A:314:THR:HG22	1:A:735:PHE:CE2	2.43	0.53
1:A:96:LYS:HG2	1:A:99:MET:SD	2.48	0.53
1:A:996:LYS:C	1:A:998:THR:N	2.66	0.53
1:A:1062:LEU:HD13	1:A:1240:VAL:CG2	2.38	0.53
1:A:533:GLN:NE2	1:A:553:ALA:O	2.41	0.53
1:A:107:MET:HE2	1:A:957:ALA:HB2	1.91	0.53
1:A:1178:GLN:O	1:A:1182:ILE:HD12	2.08	0.53
1:A:1151:HIS:HA	1:A:1154:ILE:HG12	1.91	0.53
1:A:246:ALA:HB2	1:A:276:ASN:HB3	1.90	0.52
1:A:1190:PRO:O	1:A:1221:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:PHE:HB3	1:A:603:VAL:HB	1.92	0.52
1:A:1240:VAL:HG23	1:A:1240:VAL:O	2.09	0.52
1:A:1116:PRO:HG2	1:A:1177:LYS:HG3	1.91	0.52
1:A:1127:ILE:O	1:A:1187:VAL:HG11	2.10	0.51
1:A:1150:ILE:HA	1:A:1179:ARG:HH21	1.75	0.51
1:A:1075:VAL:O	1:A:1079:LEU:HG	2.09	0.51
1:A:611:LEU:O	1:A:613:ARG:HG3	2.11	0.51
1:A:733:GLY:HA3	1:A:968:GLU:HG2	1.93	0.50
1:A:509:ILE:HA	1:A:513:PRO:HG2	1.94	0.50
1:A:210:LEU:O	1:A:214:ILE:HG13	2.11	0.50
1:A:612:MET:SD	1:A:612:MET:N	2.84	0.50
1:A:694:TRP:HA	1:A:697:LEU:HD13	1.92	0.50
1:A:575:GLY:C	1:A:576:ARG:HD3	2.37	0.50
1:A:1228:HIS:HB2	1:A:1229:ARG:NH1	2.26	0.50
1:A:70:ILE:HD13	1:A:113:TYR:HB3	1.93	0.50
1:A:1028:GLU:N	1:A:1093:ASP:OD2	2.43	0.50
1:A:1089:SER:OG	1:A:1096:GLU:OE2	2.30	0.50
1:A:1189:GLN:HG2	1:A:1221:ARG:HH22	1.77	0.49
1:A:706:TYR:O	1:A:772:THR:OG1	2.29	0.49
1:A:1169:GLY:O	1:A:1170:THR:C	2.55	0.49
1:A:716:ILE:O	1:A:720:LEU:HG	2.13	0.49
1:A:131:PHE:HE1	4:A:1405:Y01:HAS2	1.77	0.48
1:A:769:GLN:HG2	1:A:773:PHE:HD2	1.77	0.48
1:A:207:GLY:HA3	1:A:330:VAL:HG21	1.94	0.48
1:A:479:THR:HA	1:A:519:LEU:H	1.77	0.48
1:A:482:GLU:HA	1:A:485:ARG:HB2	1.95	0.48
1:A:285:ILE:O	1:A:289:ILE:HG12	2.13	0.48
1:A:496:ILE:O	1:A:500:VAL:HG23	2.14	0.48
1:A:792:MET:SD	1:A:810:LEU:HD21	2.54	0.48
1:A:1164:ARG:O	1:A:1170:THR:OG1	2.25	0.47
1:A:148:PHE:HA	1:A:151:ILE:HG22	1.96	0.47
1:A:391:LYS:HE3	1:A:391:LYS:HB2	1.72	0.47
1:A:1251:GLY:HA2	1:A:1254:GLN:NE2	2.29	0.47
1:A:421:LEU:HB3	1:A:581:ILE:HG13	1.96	0.47
1:A:332:PHE:CE1	3:A:1402:JIZ:S03	3.08	0.47
1:A:404:GLN:HB3	1:A:407:LYS:HE3	1.96	0.47
1:A:488:ARG:HG3	1:A:489:GLU:N	2.28	0.47
1:A:589:ARG:HA	1:A:589:ARG:HH11	1.80	0.47
1:A:954:ARG:HG2	4:A:1406:Y01:HAV2	1.97	0.47
1:A:1014:ILE:HG22	1:A:1015:ASP:OD1	2.15	0.47
4:A:1405:Y01:HAP1	4:A:1405:Y01:HBA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD22	1:A:336:ILE:HG12	1.96	0.47
1:A:140:ILE:HG13	1:A:179:ASN:HB2	1.96	0.47
1:A:696:ILE:HG23	1:A:697:LEU:HD12	1.96	0.47
1:A:1109:LEU:HD23	1:A:1192:ILE:HG23	1.97	0.47
1:A:1259:GLN:O	1:A:1260:LYS:C	2.57	0.47
1:A:411:LEU:HD12	1:A:602:ILE:HD11	1.97	0.47
1:A:156:ILE:HD13	1:A:439:LEU:HG	1.96	0.46
1:A:96:LYS:HD3	1:A:100:PHE:HE1	1.80	0.46
1:A:1034:SER:HA	1:A:1053:SER:HA	1.98	0.46
1:A:1054:LEU:HD11	1:A:1064:LEU:HD21	1.96	0.46
1:A:69:LEU:HA	1:A:329:THR:OG1	2.15	0.46
1:A:482:GLU:HG2	1:A:485:ARG:HD2	1.96	0.46
1:A:504:ASN:HB3	1:A:534:ARG:HG3	1.98	0.46
1:A:332:PHE:CZ	3:A:1402:JIZ:S03	3.09	0.46
1:A:69:LEU:HD12	1:A:202:ILE:HD12	1.98	0.46
1:A:197:PHE:O	1:A:201:ILE:HG12	2.16	0.46
1:A:379:HIS:CD2	1:A:381:PRO:HD3	2.51	0.46
1:A:594:ILE:H	1:A:606:GLY:H	1.64	0.46
1:A:949:TYR:CE1	1:A:953:PHE:HE2	2.33	0.46
4:A:1404:Y01:HAM1	4:A:1404:Y01:HBC	1.29	0.46
1:A:381:PRO:HD2	1:A:461:TYR:HE2	1.81	0.46
1:A:959:LEU:HD22	1:A:964:LEU:HD22	1.98	0.46
1:A:1150:ILE:HG22	1:A:1179:ARG:NE	2.31	0.46
4:A:1405:Y01:HAP1	4:A:1405:Y01:HAO2	1.42	0.46
1:A:58:ILE:HD13	1:A:194:ALA:HB2	1.98	0.46
1:A:1081:ARG:NH2	1:A:1097:ILE:O	2.49	0.46
1:A:78:PHE:HE1	1:A:103:LEU:HD21	1.81	0.45
1:A:208:TRP:O	1:A:212:LEU:HD23	2.16	0.45
1:A:1076:VAL:HG13	1:A:1226:ILE:HD12	1.98	0.45
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.98	0.45
1:A:833:PHE:HA	1:A:836:ILE:HG22	1.98	0.45
4:A:1407:Y01:CAQ	4:A:1407:Y01:CBE	2.74	0.45
1:A:210:LEU:HG	1:A:214:ILE:HD11	1.98	0.45
1:A:900:PHE:O	1:A:904:VAL:HG12	2.17	0.45
1:A:979:PHE:HB3	3:A:1402:JIZ:C10	2.47	0.45
4:A:1403:Y01:HAP1	4:A:1403:Y01:HAO1	1.61	0.45
1:A:86:LYS:HG3	1:A:89:THR:H	1.82	0.45
1:A:580:VAL:HG21	1:A:587:THR:HG21	1.98	0.45
1:A:1173:SER:HB3	1:A:1176:GLN:NE2	2.31	0.44
1:A:114:TYR:HB3	1:A:950:ALA:HB2	1.98	0.44
1:A:430:SER:O	1:A:434:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:LEU:HD12	1:A:839:LEU:HA	1.86	0.44
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.82	0.44
1:A:1150:ILE:HG22	1:A:1179:ARG:HE	1.82	0.44
1:A:121:VAL:HG21	1:A:946:TYR:CE2	2.50	0.44
1:A:1178:GLN:HA	1:A:1178:GLN:OE1	2.17	0.44
1:A:170:ARG:HG3	1:A:174:ASP:OD2	2.18	0.44
1:A:938:PHE:O	1:A:941:THR:HG22	2.18	0.44
1:A:438:ARG:NH1	1:A:455:ARG:HA	2.33	0.44
1:A:562:GLU:HG2	1:A:566:GLN:NE2	2.33	0.43
4:A:1403:Y01:HAM1	4:A:1403:Y01:HBC	1.68	0.43
1:A:469:VAL:HG21	1:A:550:LEU:HD13	1.99	0.43
1:A:704:TRP:CD2	1:A:705:PRO:HD3	2.53	0.43
1:A:1049:LEU:HD12	1:A:1052:LEU:HD11	2.00	0.43
1:A:1059:GLY:N	1:A:1222:THR:OG1	2.42	0.43
1:A:1067:SER:HA	1:A:1228:HIS:CE1	2.51	0.43
1:A:114:TYR:O	1:A:117:ILE:HG22	2.17	0.43
1:A:196:PHE:CD1	1:A:341:VAL:HB	2.53	0.43
1:A:493:MET:HA	1:A:496:ILE:HG12	1.99	0.43
1:A:1184:ARG:O	1:A:1187:VAL:HG12	2.17	0.43
1:A:480:ILE:HG12	1:A:518:THR:HB	1.99	0.43
1:A:715:ILE:HD11	1:A:833:PHE:HD1	1.83	0.43
1:A:505:ALA:HB2	1:A:534:ARG:NH2	2.34	0.43
1:A:1110:GLY:HA3	1:A:1193:LEU:HD22	2.01	0.43
1:A:109:THR:O	1:A:113:TYR:HD1	2.00	0.43
1:A:1118:LEU:HD13	1:A:1177:LYS:NZ	2.31	0.43
1:A:1242:ILE:HG13	1:A:1247:VAL:O	2.19	0.43
1:A:164:VAL:HG13	1:A:897:ILE:HG22	2.01	0.42
1:A:754:LEU:HD23	1:A:754:LEU:HA	1.87	0.42
1:A:563:ALA:N	1:A:566:GLN:OE1	2.44	0.42
1:A:281:LYS:HD3	1:A:782:LYS:HD2	2.01	0.42
1:A:314:THR:HG22	1:A:735:PHE:CZ	2.54	0.42
1:A:839:LEU:HD23	4:A:1403:Y01:HAK1	2.01	0.42
1:A:509:ILE:HD11	1:A:510:MET:HE3	2.01	0.42
1:A:593:VAL:HG13	1:A:605:GLN:HB2	2.02	0.42
1:A:1080:GLU:OE1	1:A:1080:GLU:N	2.50	0.42
1:A:388:LEU:O	1:A:413:VAL:HG22	2.20	0.42
1:A:1042:THR:HG23	1:A:1043:ARG:HG2	2.01	0.42
1:A:532:LYS:HA	1:A:535:ILE:HG22	2.02	0.42
1:A:1081:ARG:HH12	1:A:1098:LYS:HD3	1.85	0.42
1:A:296:GLY:HA2	1:A:766:PHE:HD2	1.84	0.41
1:A:1101:ASN:OD1	1:A:1104:TRP:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:HB2	1:A:736:THR:HG22	2.02	0.41
1:A:605:GLN:OE1	1:A:605:GLN:N	2.48	0.41
1:A:147:PHE:HE1	1:A:364:ILE:HG21	1.85	0.41
1:A:289:ILE:CD1	1:A:771:PHE:HA	2.51	0.41
1:A:584:ARG:HG3	1:A:586:SER:H	1.85	0.41
1:A:733:GLY:HA2	1:A:736:THR:OG1	2.20	0.41
1:A:1003:HIS:O	1:A:1007:ILE:HG13	2.20	0.41
1:A:813:ARG:O	1:A:817:ASP:HB2	2.20	0.41
1:A:39:PHE:HD1	1:A:50:MET:HE1	1.86	0.41
1:A:151:ILE:HD11	1:A:167:LEU:HD21	2.03	0.41
1:A:286:LYS:HA	1:A:286:LYS:HD3	1.83	0.41
1:A:857:LEU:HB3	1:A:977:ILE:HG21	2.01	0.41
1:A:217:ILE:HD13	1:A:305:SER:HA	2.02	0.41
1:A:478:THR:HG22	1:A:479:THR:H	1.86	0.41
1:A:272:ARG:HD2	1:A:1121:ARG:HH21	1.86	0.41
1:A:345:SER:OG	1:A:346:PRO:HD3	2.20	0.41
1:A:462:LEU:HA	1:A:465:ILE:HG12	2.03	0.41
1:A:1177:LYS:HD2	1:A:1180:ILE:HD11	2.02	0.41
1:A:249:VAL:O	1:A:253:VAL:HG22	2.21	0.41
1:A:543:ARG:HH21	1:A:907:THR:HG22	1.86	0.41
1:A:1060:GLN:HG3	1:A:1062:LEU:H	1.85	0.41
1:A:594:ILE:O	1:A:605:GLN:HA	2.21	0.41
1:A:756:LEU:HD22	4:A:1404:Y01:HAU2	2.02	0.40
1:A:1118:LEU:HB2	1:A:1177:LYS:HE2	2.02	0.40
1:A:50:MET:HG2	1:A:132:TRP:CZ3	2.56	0.40
1:A:64:LEU:HB3	1:A:65:PRO:HD3	2.02	0.40
1:A:127:ILE:HD11	4:A:1405:Y01:HBB	2.02	0.40
1:A:311:TRP:HE1	1:A:745:ARG:HH22	1.69	0.40
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.91	0.40
1:A:492:THR:HB	1:A:495:GLU:HB2	2.02	0.40
1:A:979:PHE:CZ	3:A:1402:JIZ:S03	3.14	0.40
1:A:1027:LEU:HD23	1:A:1191:HIS:CG	2.56	0.40
1:A:156:ILE:H	1:A:156:ILE:HD12	1.87	0.40
1:A:381:PRO:HD2	1:A:461:TYR:CE2	2.57	0.40
1:A:965:MET:HB2	1:A:969:ASN:HB2	2.04	0.40
1:A:1118:LEU:HD12	1:A:1119:PHE:H	1.86	0.40

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

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. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	153	ASN
1	A	191	GLN
1	A	241	HIS
1	A	514	HIS

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Mol	Chain	Res	Type
1	A	608	HIS
1	A	749	ASN
1	A	805	ASN
1	A	1103	GLN
1	A	1211	GLN
1	A	1235	ASN
1	A	1250	HIS
1	A	1254	GLN
1	A	1259	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
4	A	1407	Y01	CAU-CBI	-16.65	1.25	1.54
4	A	1407	Y01	CAK-CBD	-14.15	1.30	1.53
4	A	1407	Y01	CBH-CAZ	-13.28	1.27	1.52
3	A	1402	JIZ	C03-N02	11.98	1.64	1.38
3	A	1402	JIZ	C08-N04	10.98	1.62	1.38
4	A	1407	Y01	CBI-CBE	10.72	1.74	1.55
3	A	1402	JIZ	C13-N06	10.64	1.61	1.38
4	A	1407	Y01	CBH-CBF	10.09	1.72	1.56
4	A	1407	Y01	CAQ-CAP	9.50	1.80	1.54
4	A	1407	Y01	CBB-CBE	-9.09	1.38	1.54
4	A	1407	Y01	CAQ-CBG	9.03	1.72	1.54
3	A	1402	JIZ	C02-S01	-8.89	1.54	1.73
3	A	1402	JIZ	C04-C03	8.78	1.52	1.36
4	A	1407	Y01	CBD-CBF	-8.47	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1407	Y01	CAK-CAI	8.13	1.66	1.50
4	A	1407	Y01	CAT-CBH	7.32	1.67	1.54
3	A	1402	JIZ	C07-S02	-6.88	1.59	1.73
3	A	1402	JIZ	C12-S03	-6.87	1.59	1.73
4	A	1407	Y01	CBI-CBG	6.19	1.66	1.55
3	A	1402	JIZ	C09-S02	-6.14	1.56	1.71
3	A	1402	JIZ	C14-S03	-6.10	1.56	1.71
3	A	1402	JIZ	C07-N04	6.05	1.43	1.30
3	A	1402	JIZ	C12-N06	6.00	1.43	1.30
2	A	1401	JJI	C10-N05	5.98	1.46	1.34
3	A	1402	JIZ	C04-S01	-5.71	1.57	1.71
2	A	1401	JJI	C05-N03	5.60	1.45	1.34
3	A	1402	JIZ	C14-C13	5.51	1.46	1.36
3	A	1402	JIZ	C09-C08	5.41	1.46	1.36
3	A	1402	JIZ	C15-N01	5.32	1.45	1.34
3	A	1402	JIZ	C05-N03	5.29	1.45	1.34
2	A	1401	JJI	C15-N01	5.22	1.45	1.34
3	A	1402	JIZ	C10-N05	5.20	1.45	1.34
2	A	1401	JJI	C12-S03	-5.16	1.62	1.73
2	A	1401	JJI	C02-S01	-5.13	1.62	1.73
2	A	1401	JJI	C07-S02	-5.11	1.62	1.73
4	A	1407	Y01	CAR-CBC	-4.89	1.38	1.51
4	A	1407	Y01	CAP-CBE	4.76	1.64	1.54
4	A	1407	Y01	CAO-CBB	4.69	1.66	1.54
4	A	1407	Y01	CAV-CAZ	4.53	1.60	1.51
4	A	1407	Y01	CAE-CBI	3.93	1.60	1.54
4	A	1407	Y01	CAI-CAZ	3.78	1.40	1.33
2	A	1401	JJI	C02-N02	3.26	1.37	1.30
3	A	1402	JIZ	C02-N02	3.15	1.37	1.30
2	A	1401	JJI	C07-N04	3.12	1.37	1.30
2	A	1401	JJI	C04-S01	-3.06	1.64	1.71
2	A	1401	JJI	O41-N4	-3.04	1.17	1.22
2	A	1401	JJI	O21-N2	-3.00	1.17	1.22
4	A	1407	Y01	CAV-CBC	2.98	1.58	1.52
2	A	1401	JJI	C09-S02	-2.86	1.64	1.71
4	A	1407	Y01	OAW-CAY	2.83	1.42	1.34
2	A	1401	JJI	O02-C10	-2.83	1.18	1.23
2	A	1401	JJI	C14-S03	-2.82	1.65	1.71
2	A	1401	JJI	C12-N06	2.74	1.36	1.30
3	A	1402	JIZ	O02-C10	-2.63	1.18	1.23
4	A	1407	Y01	CAS-CBF	2.62	1.58	1.53
2	A	1401	JJI	O03-C15	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	JJI	O01-C05	-2.51	1.18	1.23
3	A	1402	JIZ	O01-C05	-2.49	1.18	1.23
3	A	1402	JIZ	O03-C15	-2.48	1.18	1.23
2	A	1401	JJI	C03-C05	2.12	1.52	1.48
4	A	1407	Y01	CAC-CBB	2.07	1.58	1.53
3	A	1402	JIZ	C03-C05	2.04	1.52	1.48
3	A	1402	JIZ	C13-C15	2.01	1.52	1.48
3	A	1402	JIZ	C08-C10	2.00	1.52	1.48

All (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
3	A	1402	JIZ	C04-S01-C02	13.61	105.62	89.52
2	A	1401	JJI	C06-N03-C05	-7.45	108.71	121.27
2	A	1401	JJI	C13-C15-N01	-6.80	105.57	115.22
2	A	1401	JJI	C07-C06-N03	-6.75	98.61	109.69
3	A	1402	JIZ	C04-C03-N02	-5.81	107.44	115.43
2	A	1401	JJI	C04-C03-N02	-5.41	107.98	115.43
2	A	1401	JJI	C01-C02-S01	5.26	128.79	121.79
2	A	1401	JJI	C09-C08-N04	-5.12	108.39	115.43
3	A	1402	JIZ	C09-C08-N04	-5.02	108.52	115.43
3	A	1402	JIZ	C14-C13-N06	-5.02	108.53	115.43
3	A	1402	JIZ	C01-C18-S04	-4.92	108.61	114.16
3	A	1402	JIZ	S02-C07-N04	-4.78	107.94	114.19
3	A	1402	JIZ	C12-C11-N05	-4.70	101.97	109.69
2	A	1401	JJI	S01-C02-N02	-4.68	108.07	114.19
3	A	1402	JIZ	S03-C12-N06	-4.65	108.11	114.19
2	A	1401	JJI	C14-C13-N06	-4.64	109.04	115.43
4	A	1407	Y01	CAS-CAU-CBI	4.49	120.31	112.74
2	A	1401	JJI	C17-C11-C12	-4.27	105.30	111.13
2	A	1401	JJI	C11-N05-C10	-4.26	114.09	121.27
4	A	1407	Y01	CAK-CBD-CBG	4.15	116.80	110.93
2	A	1401	JJI	C08-C10-N05	-4.12	109.37	115.22
2	A	1401	JJI	C14-C13-C15	4.12	130.77	123.92
3	A	1402	JIZ	C03-N02-C02	-4.07	106.44	110.65
2	A	1401	JJI	S03-C12-N06	-4.04	108.91	114.19
2	A	1401	JJI	S02-C07-N04	-4.00	108.97	114.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	JJI	C01-N01-C15	-3.92	115.40	122.00
2	A	1401	JJI	C02-C01-N01	-3.80	103.04	109.27
4	A	1407	Y01	CBF-CBD-CBG	3.78	114.03	109.09
4	A	1407	Y01	CAC-CBB-CAO	-3.77	104.51	110.34
4	A	1407	Y01	OAW-CAY-CAM	3.66	119.41	111.48
4	A	1407	Y01	CAE-CBI-CBE	-3.65	105.06	111.68
4	A	1407	Y01	CAT-CAR-CBC	3.54	116.10	110.33
3	A	1402	JIZ	C03-C04-S01	-3.51	106.19	110.24
4	A	1407	Y01	CAR-CBC-CAV	3.37	115.66	110.97
2	A	1401	JJI	C3-C2-C1	-3.29	119.54	122.97
2	A	1401	JJI	C09-C08-C10	3.22	129.28	123.92
2	A	1401	JJI	C13-C14-S03	-3.10	106.66	110.24
4	A	1407	Y01	CBG-CBI-CBE	2.91	103.44	100.10
2	A	1401	JJI	C17-C11-N05	-2.85	105.16	110.38
3	A	1402	JIZ	C14-C13-C15	2.83	128.62	123.92
4	A	1407	Y01	CBD-CAK-CAI	2.77	116.61	112.76
2	A	1401	JJI	C13-N06-C12	-2.69	107.86	110.65
4	A	1407	Y01	CBH-CAZ-CAI	-2.64	119.07	122.93
3	A	1402	JIZ	C07-C06-N03	-2.60	105.42	109.69
4	A	1407	Y01	CAK-CAI-CAZ	-2.58	120.66	125.02
4	A	1407	Y01	CAU-CBI-CBG	2.58	111.11	107.25
2	A	1401	JJI	C08-N04-C07	-2.54	108.02	110.65
2	A	1401	JJI	C2-C1-S	-2.52	119.36	121.87
2	A	1401	JJI	O03-C15-N01	2.50	127.49	123.09
4	A	1407	Y01	CAJ-CAO-CBB	-2.50	108.10	115.08
4	A	1407	Y01	CAQ-CBG-CBD	2.46	123.03	119.10
4	A	1407	Y01	CAU-CAS-CBF	2.43	117.26	113.14
4	A	1407	Y01	CAS-CBF-CBH	-2.39	110.13	113.08
4	A	1406	Y01	CAT-CAR-CBC	2.37	114.20	110.33
2	A	1401	JJI	C08-C09-S02	-2.35	107.53	110.24
3	A	1402	JIZ	C04-C03-C05	2.31	127.76	123.92
2	A	1401	JJI	O03-C15-C13	2.31	126.93	121.15
3	A	1402	JIZ	C08-C09-S02	-2.30	107.58	110.24
2	A	1401	JJI	C05-C03-N02	2.30	125.02	120.67
2	A	1401	JJI	C03-N02-C02	-2.27	108.31	110.65
3	A	1402	JIZ	C09-C08-C10	2.24	127.65	123.92
3	A	1402	JIZ	C13-C14-S03	-2.23	107.67	110.24
3	A	1402	JIZ	C05-C03-N02	2.18	124.79	120.67
4	A	1406	Y01	OAW-CBC-CAR	2.16	113.48	108.37
4	A	1403	Y01	CBF-CBH-CAZ	-2.11	106.57	109.65
2	A	1401	JJI	C03-C04-S01	-2.09	107.83	110.24
4	A	1407	Y01	CAU-CBI-CBE	2.07	119.64	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	JJI	C03-C05-N03	-2.05	112.31	115.22
3	A	1402	JIZ	C18-C01-N01	-2.01	108.42	111.28

There are no chirality outliers.

All (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
3	A	1402	JIZ	C14-C13-C15-O03
3	A	1402	JIZ	N06-C13-C15-N01
3	A	1402	JIZ	N06-C13-C15-O03
3	A	1402	JIZ	C02-C01-C18-S04
3	A	1402	JIZ	N01-C01-C18-S04
4	A	1403	Y01	OAG-CAY-OAW-CBC
4	A	1403	Y01	CAM-CAY-OAW-CBC
4	A	1404	Y01	OAG-CAY-OAW-CBC
4	A	1404	Y01	CAM-CAY-OAW-CBC
4	A	1407	Y01	CAM-CAY-OAW-CBC
4	A	1406	Y01	CAR-CBC-OAW-CAY
4	A	1403	Y01	CAC-CBB-CBE-CAP
4	A	1403	Y01	CAC-CBB-CBE-CBI
4	A	1407	Y01	OAG-CAY-OAW-CBC
4	A	1403	Y01	CAO-CBB-CBE-CBI
4	A	1405	Y01	CAJ-CAO-CBB-CAC
4	A	1403	Y01	CAO-CBB-CBE-CAP
4	A	1405	Y01	CAO-CBB-CBE-CBI
4	A	1405	Y01	CAJ-CAO-CBB-CBE
4	A	1405	Y01	CAC-CBB-CBE-CBI
4	A	1405	Y01	CAC-CBB-CBE-CAP
4	A	1405	Y01	CAO-CBB-CBE-CAP
4	A	1406	Y01	CAM-CAY-OAW-CBC
4	A	1406	Y01	OAG-CAY-OAW-CBC
4	A	1407	Y01	CAJ-CAN-CBA-CAB
4	A	1407	Y01	CAJ-CAN-CBA-CAA
4	A	1406	Y01	CAO-CBB-CBE-CBI
4	A	1406	Y01	CAC-CBB-CBE-CAP
4	A	1406	Y01	CAC-CBB-CBE-CBI
4	A	1405	Y01	CAL-CAM-CAY-OAW

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Mol	Chain	Res	Type	Atoms
4	A	1403	Y01	CAN-CAJ-CAO-CBB
4	A	1406	Y01	CAO-CBB-CBE-CAP
2	A	1401	JJI	N05-C11-C12-N06
4	A	1404	Y01	CAC-CBB-CBE-CBI
2	A	1401	JJI	C3-C2-N2-O21
4	A	1404	Y01	CAO-CBB-CBE-CBI
4	A	1407	Y01	CAJ-CAO-CBB-CBE
2	A	1401	JJI	C01-C18-S04-S
2	A	1401	JJI	C1-C2-N2-O21
4	A	1407	Y01	CAJ-CAO-CBB-CAC
4	A	1407	Y01	CAM-CAL-CAX-OAH
4	A	1404	Y01	CAM-CAL-CAX-OAF
4	A	1405	Y01	CAM-CAL-CAX-OAF
4	A	1405	Y01	CAL-CAM-CAY-OAG
4	A	1406	Y01	CAM-CAL-CAX-OAH
4	A	1404	Y01	CAO-CBB-CBE-CAP
4	A	1406	Y01	CAM-CAL-CAX-OAF
4	A	1407	Y01	CAM-CAL-CAX-OAF
4	A	1405	Y01	OAG-CAY-OAW-CBC
4	A	1403	Y01	CAM-CAL-CAX-OAH
4	A	1404	Y01	CAM-CAL-CAX-OAH
4	A	1405	Y01	CAM-CAL-CAX-OAH
4	A	1403	Y01	CAM-CAL-CAX-OAF
4	A	1405	Y01	CAM-CAY-OAW-CBC
3	A	1402	JIZ	C07-C06-N03-C05
4	A	1403	Y01	CAJ-CAN-CBA-CAA
4	A	1404	Y01	CAJ-CAN-CBA-CAB

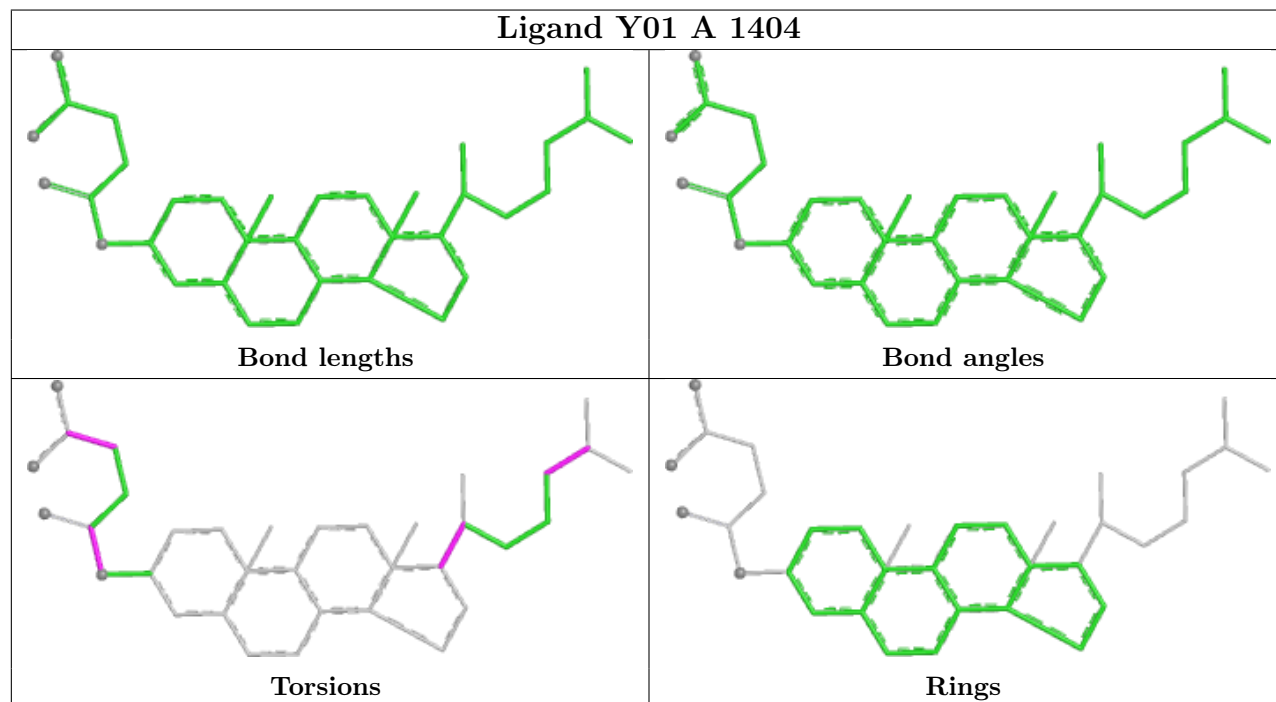
There are no ring outliers.

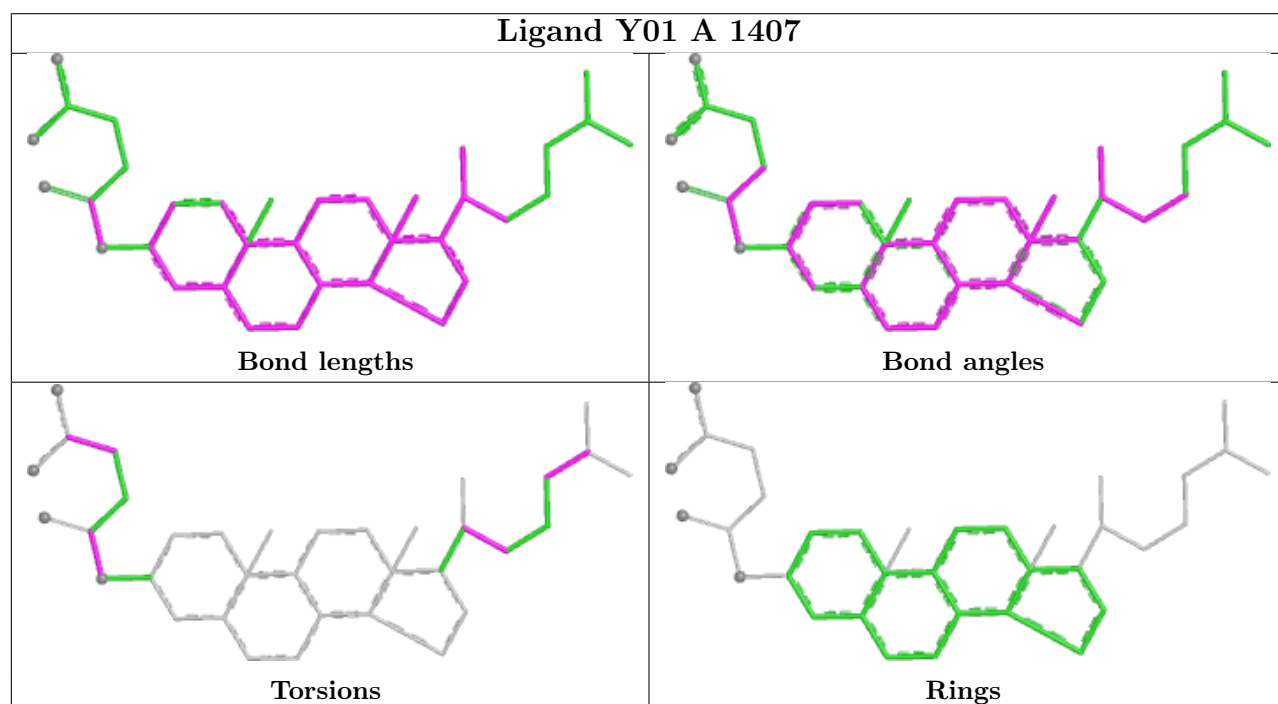
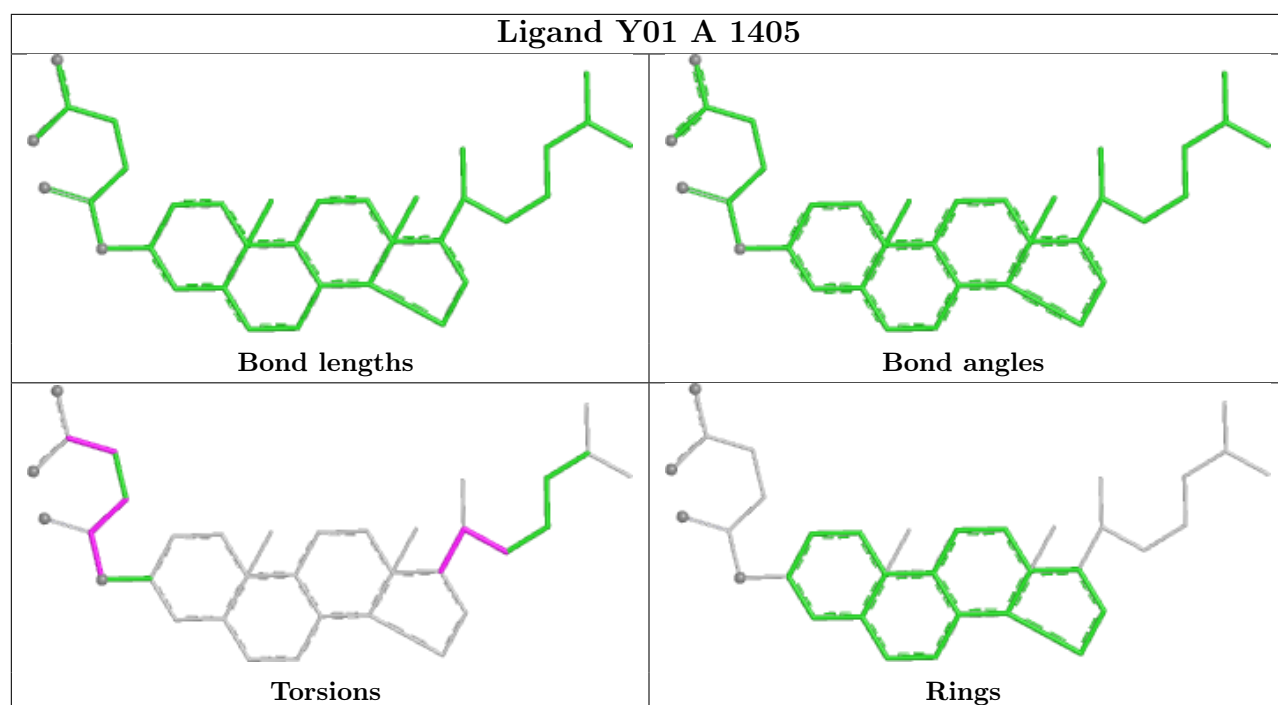
7 monomers are involved in 28 short contacts:

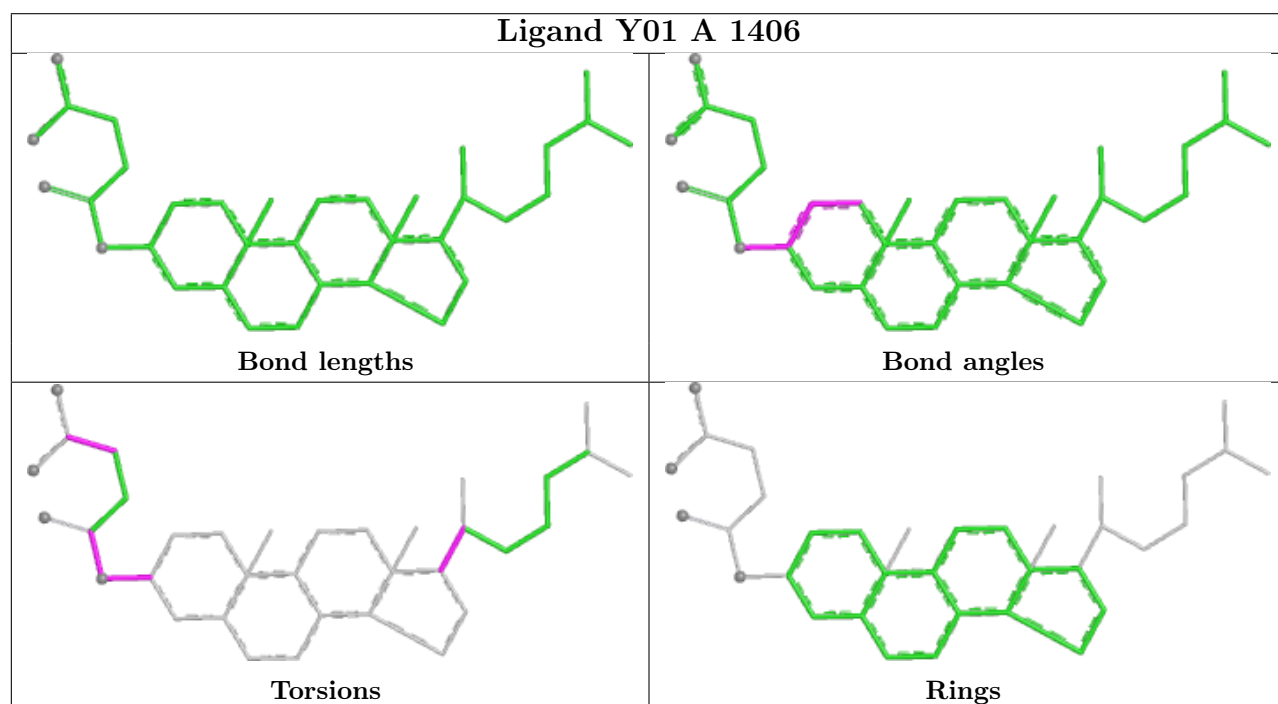
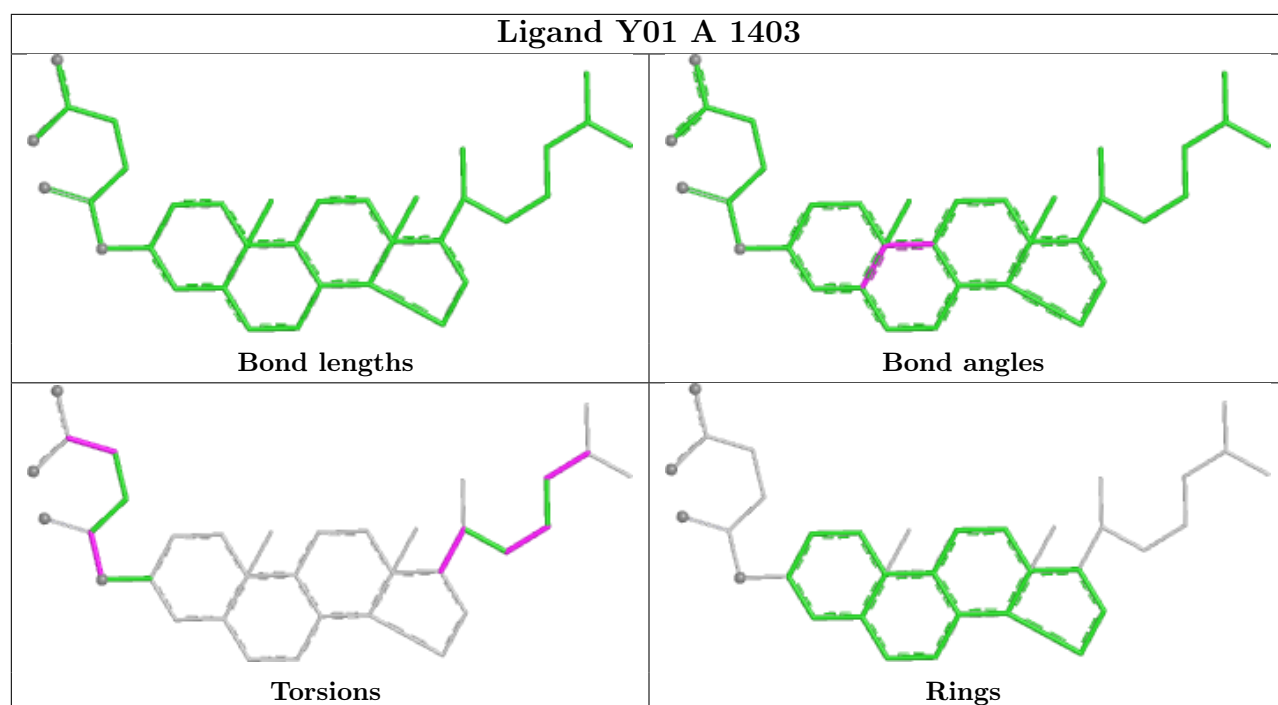
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1404	Y01	3	0
4	A	1405	Y01	4	0
4	A	1407	Y01	9	0
4	A	1403	Y01	3	0
4	A	1406	Y01	1	0
2	A	1401	JJI	3	0
3	A	1402	JIZ	5	0

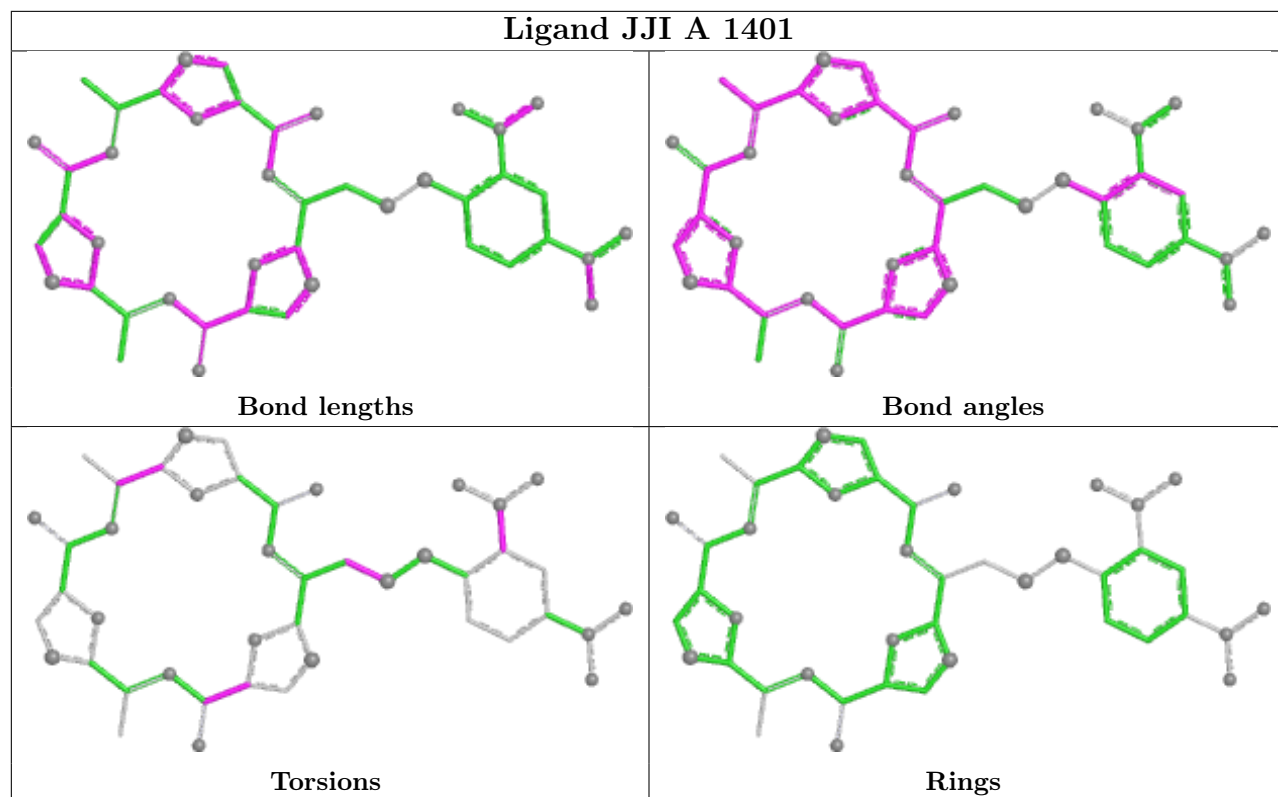
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

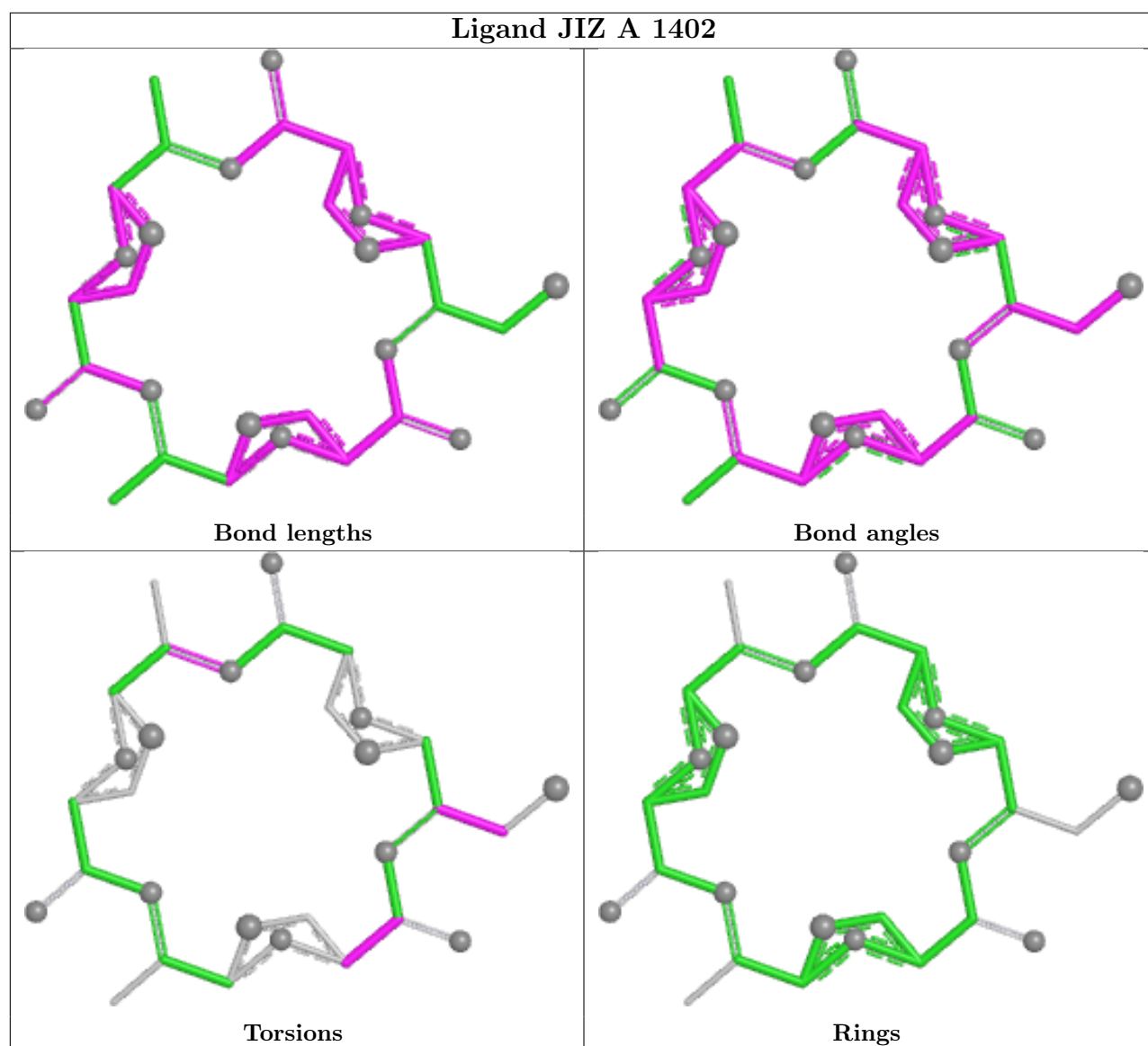
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

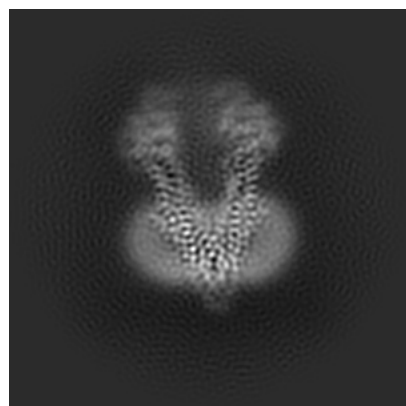
6 Map visualisation [i](#)

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.

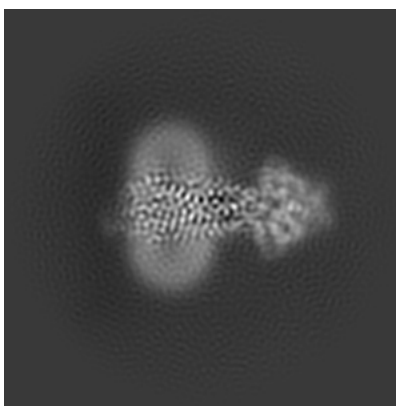
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

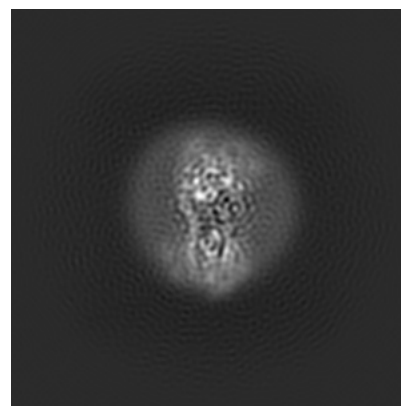
6.1.1 Primary map



X

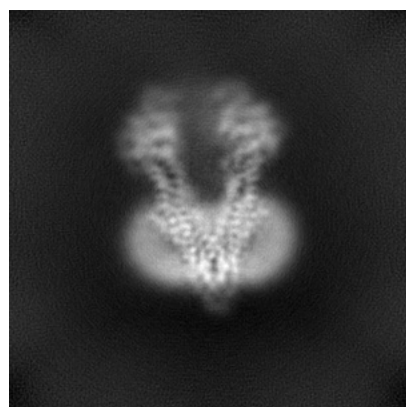


Y

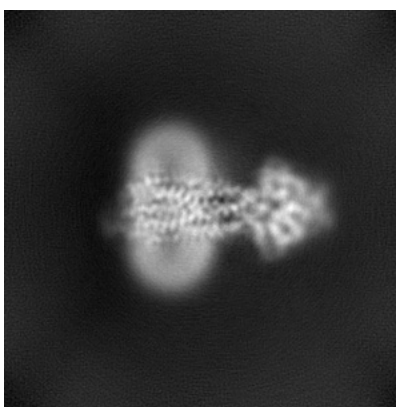


Z

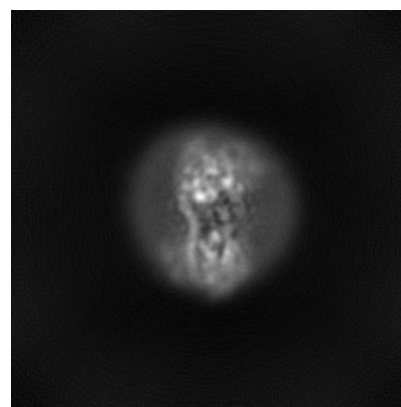
6.1.2 Raw map



X



Y

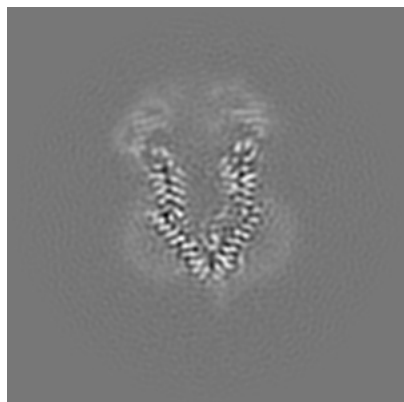


Z

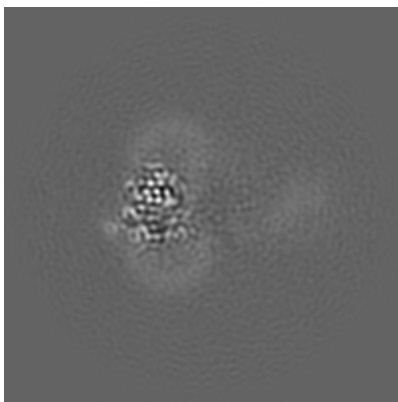
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

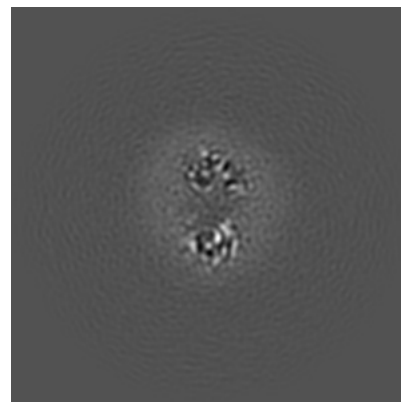
6.2.1 Primary map



X Index: 140

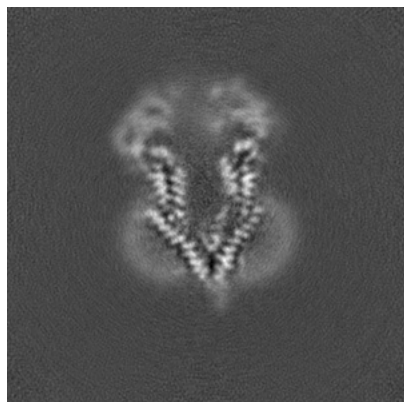


Y Index: 140

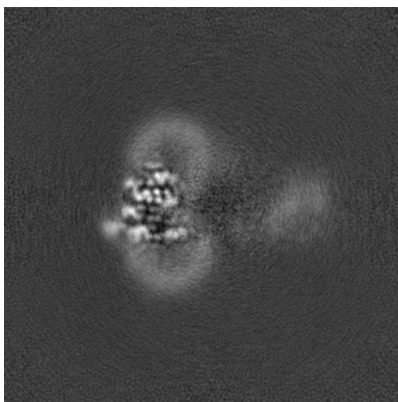


Z Index: 140

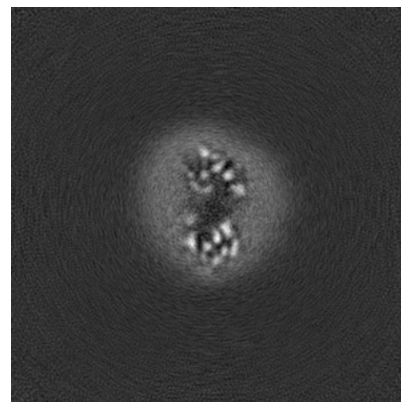
6.2.2 Raw map



X Index: 140



Y Index: 140

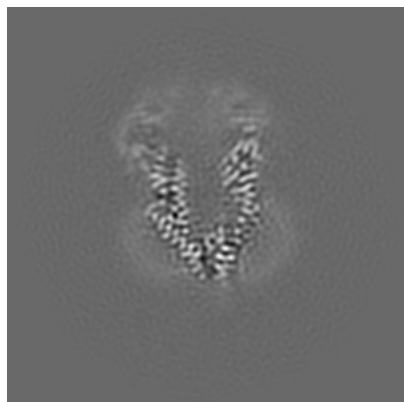


Z Index: 140

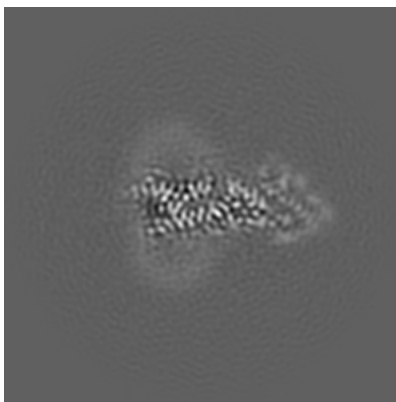
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

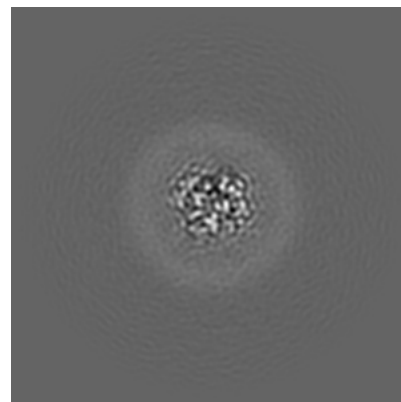
6.3.1 Primary map



X Index: 142

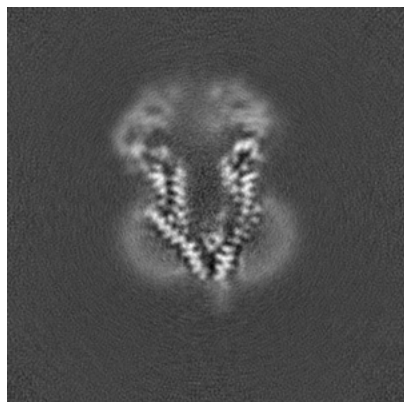


Y Index: 160

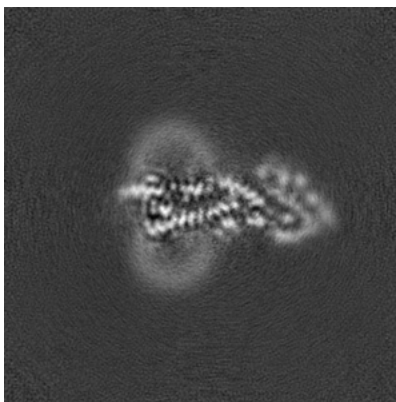


Z Index: 107

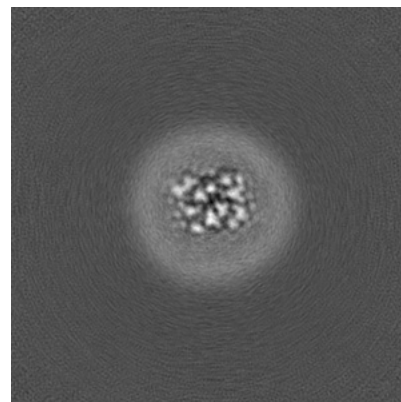
6.3.2 Raw map



X Index: 141



Y Index: 158

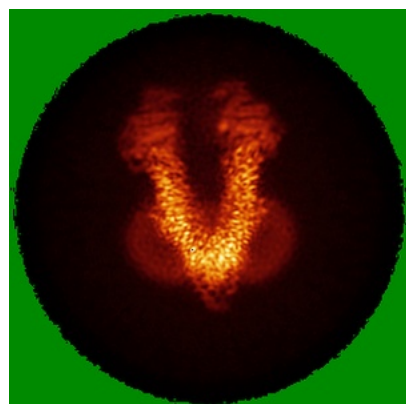


Z Index: 101

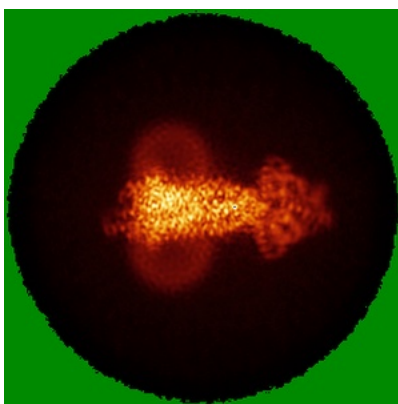
The images above show the largest variance slices of the map in three orthogonal directions.

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

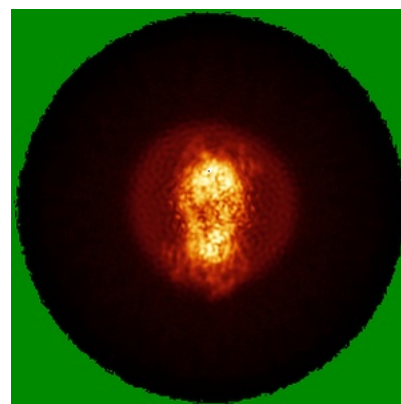
6.4.1 Primary map



X

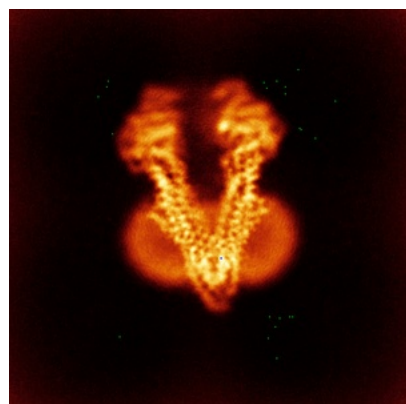


Y

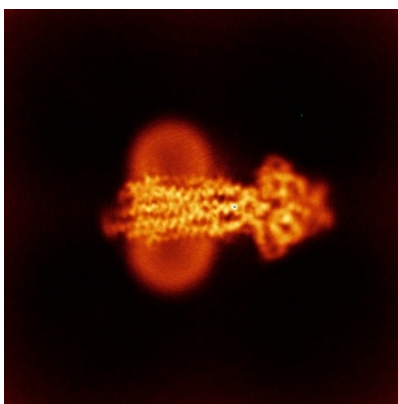


Z

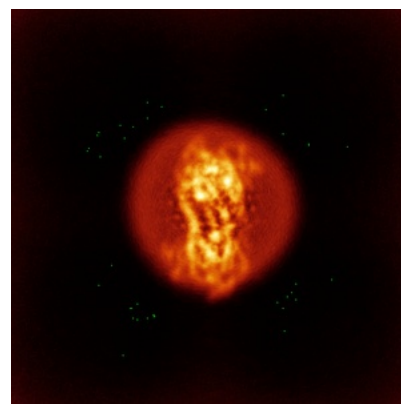
6.4.2 Raw map



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.

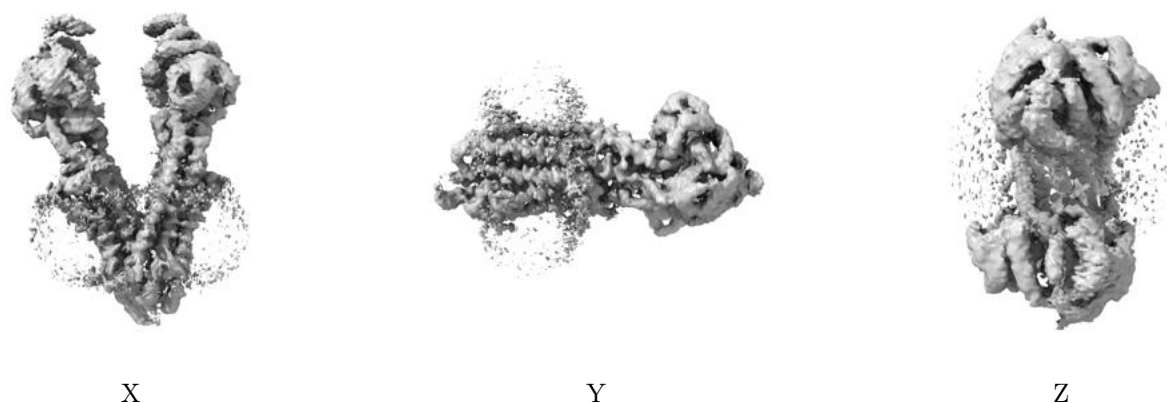
6.5 Orthogonal surface views [i](#)

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.

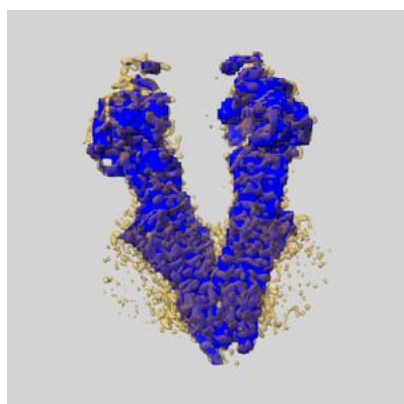
6.6 Mask visualisation [i](#)

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

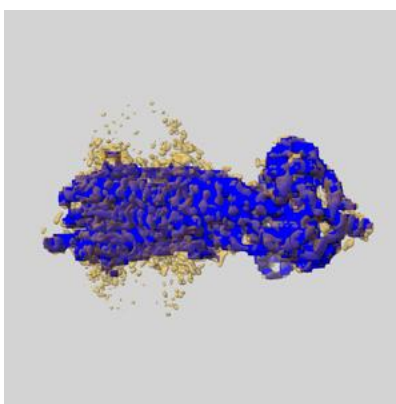
A mask typically either:

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

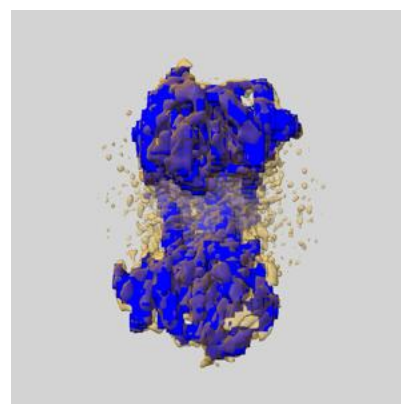
6.6.1 emd_17630_msk_1.map [i](#)



X



Y

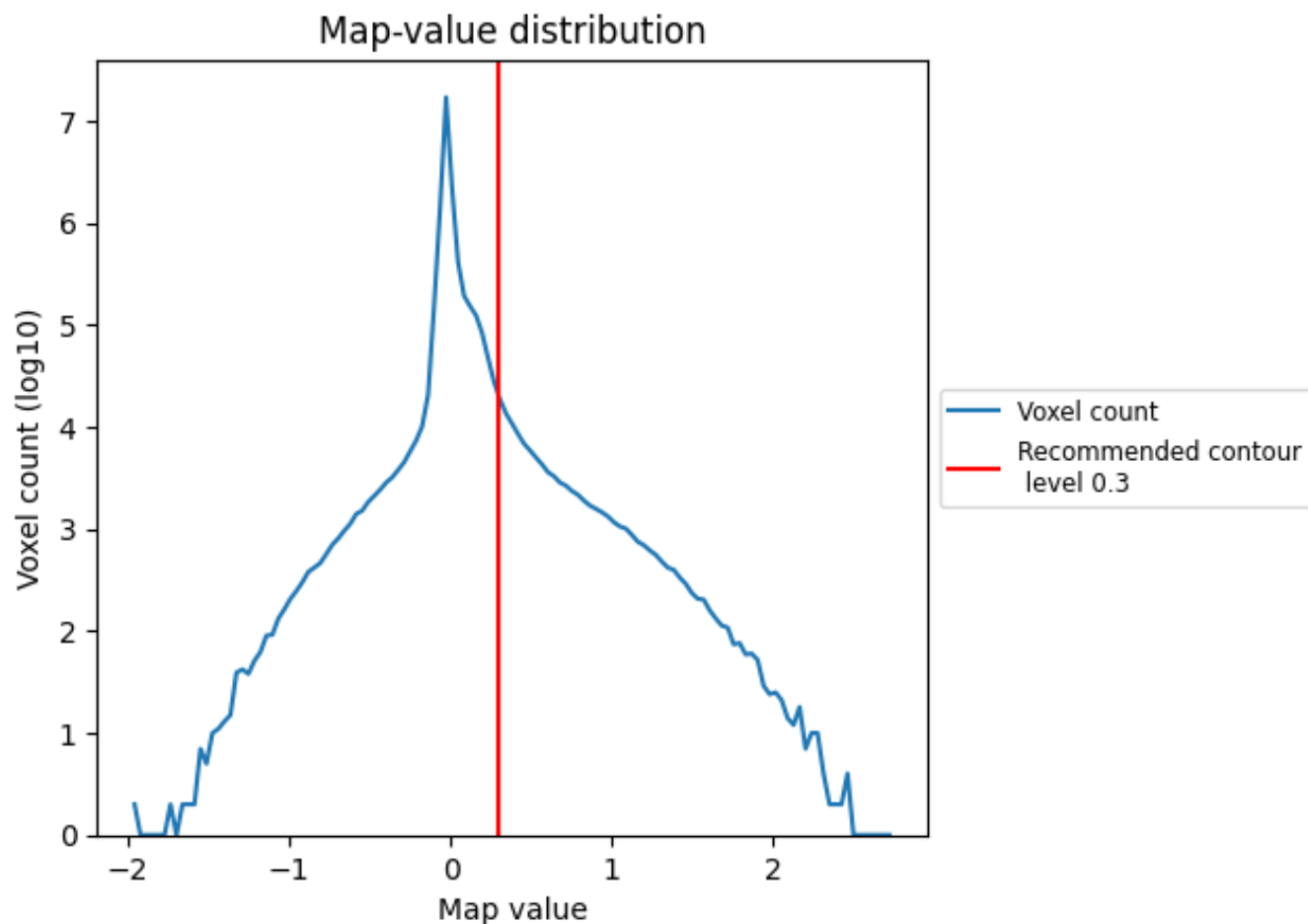


Z

7 Map analysis [i](#)

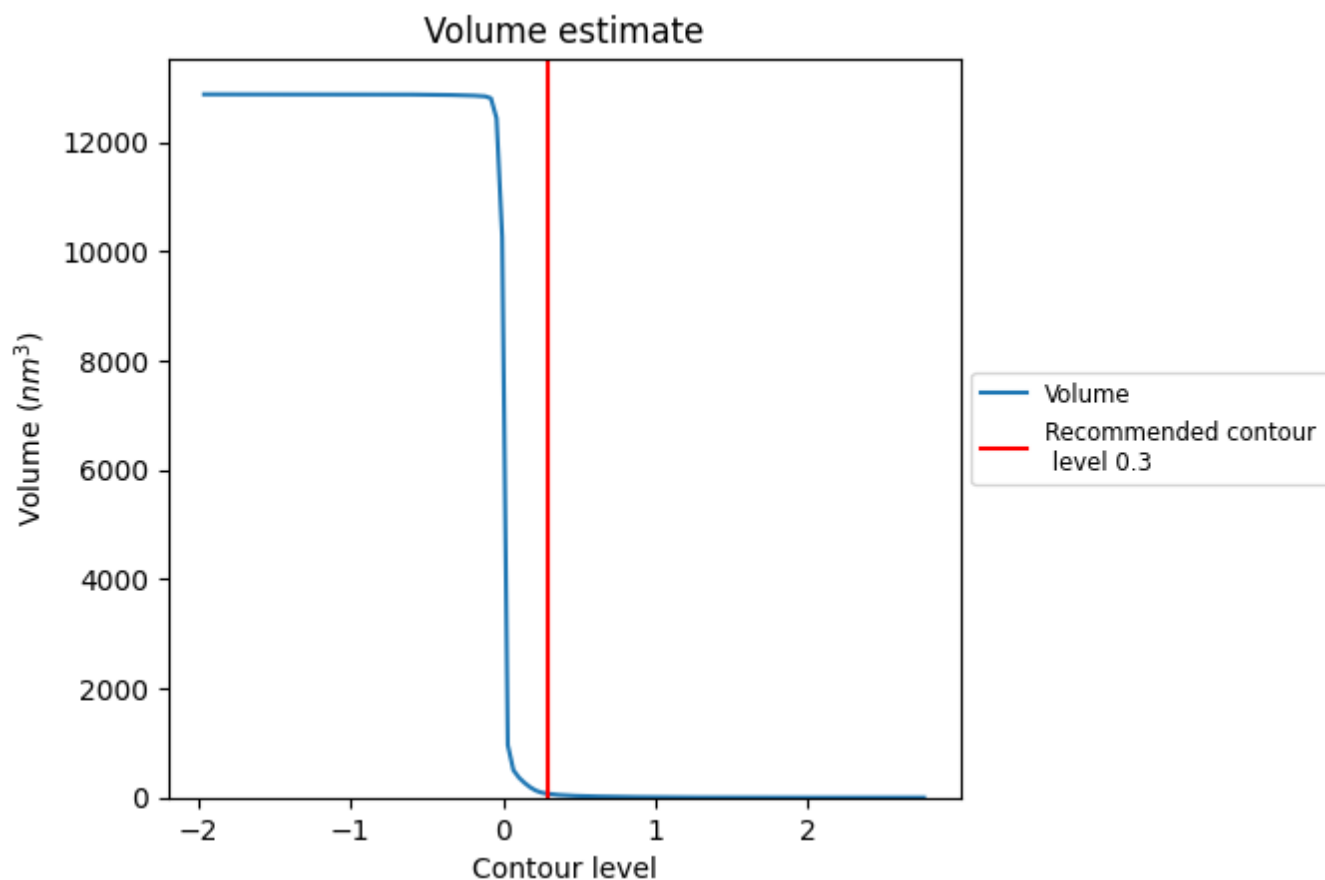
This section contains the results of statistical analysis of the map.

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.

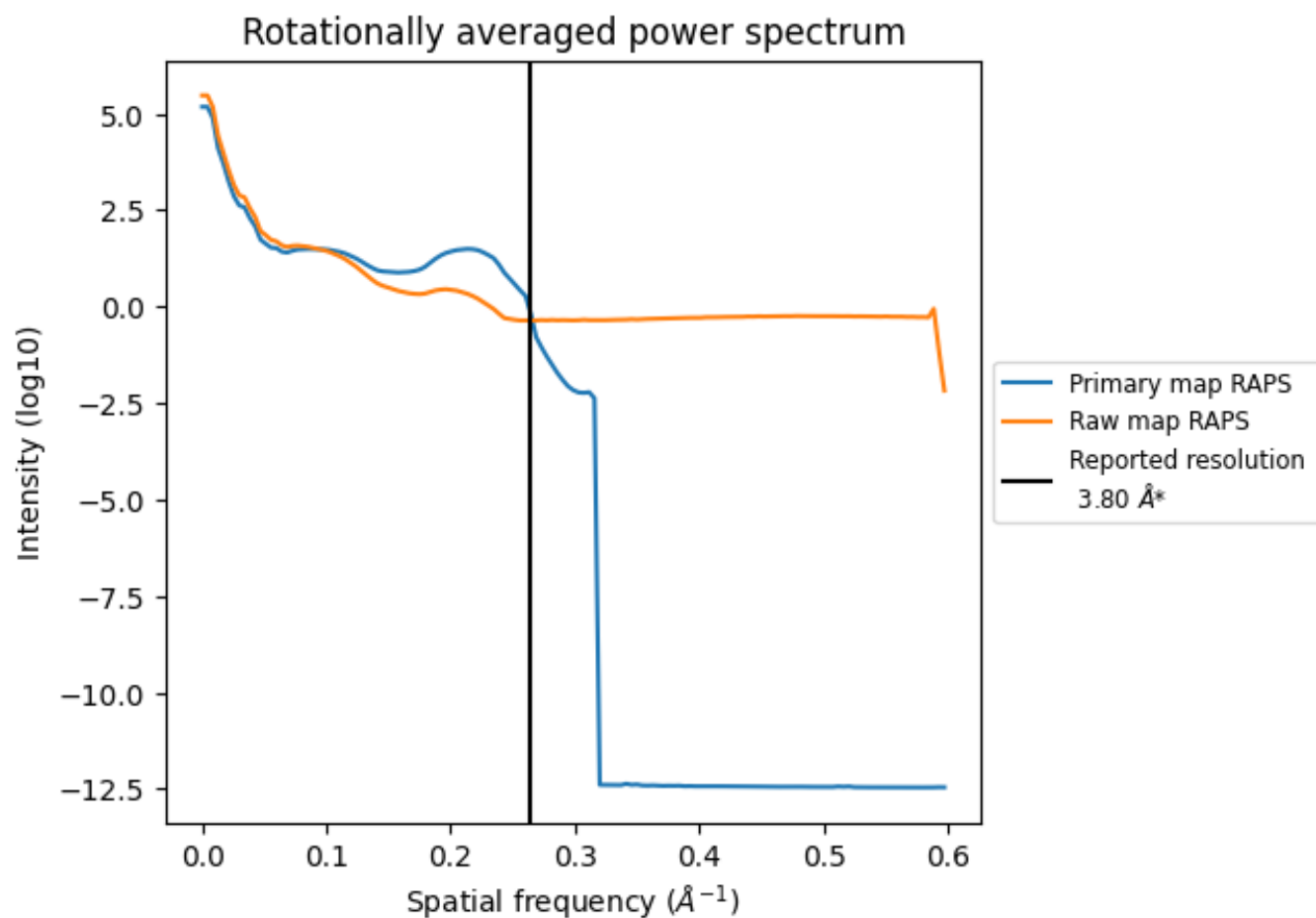
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm³; 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 ⓘ

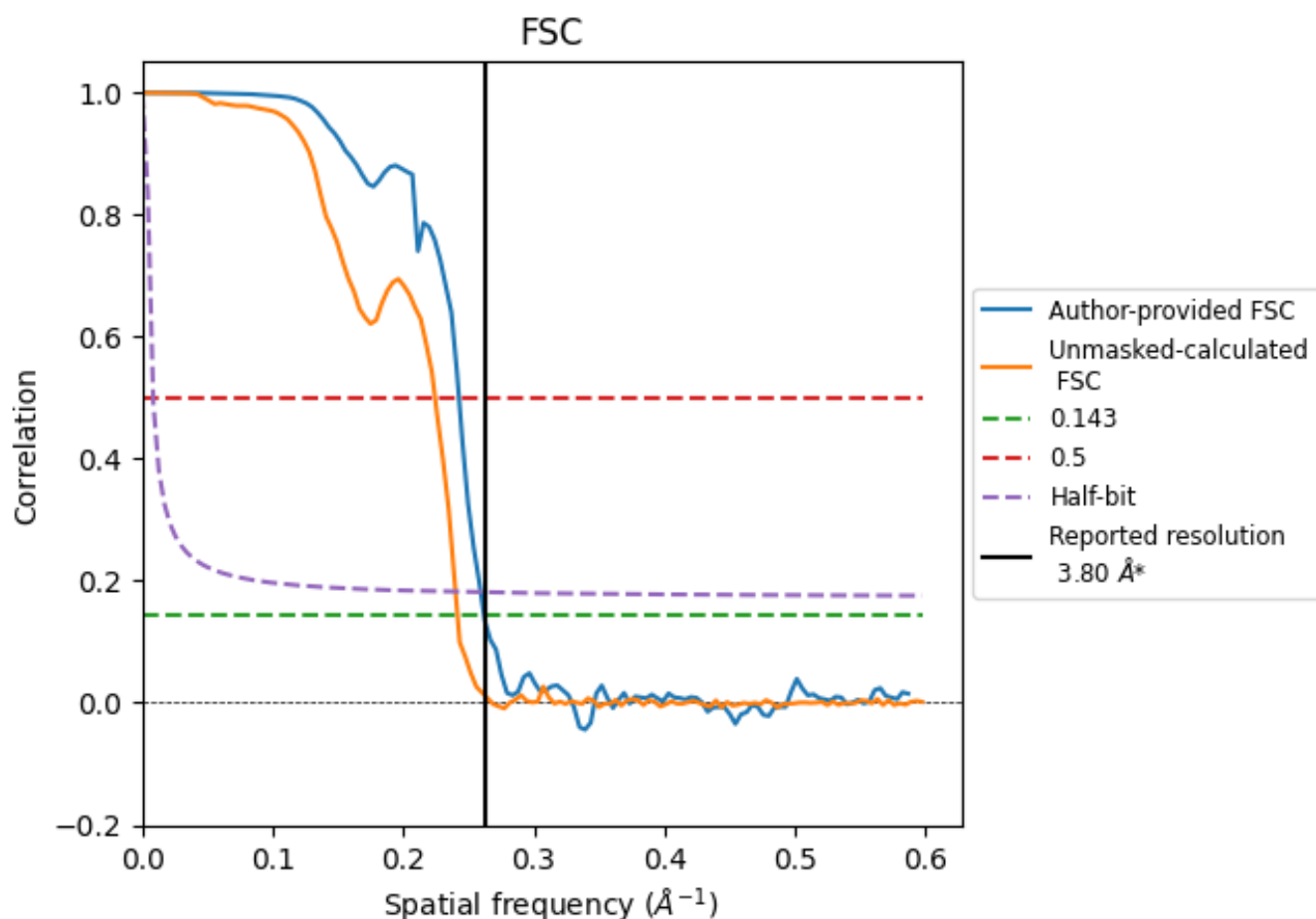


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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

8.2 Resolution estimates [i](#)

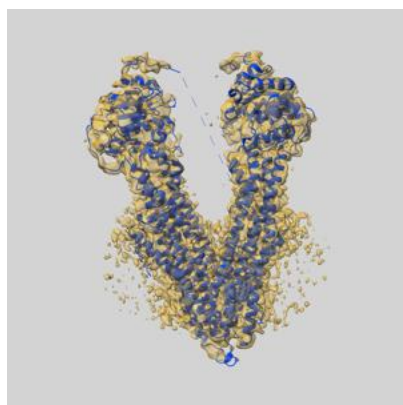
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.12	3.86
Unmasked-calculated*	4.14	4.46	4.17

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

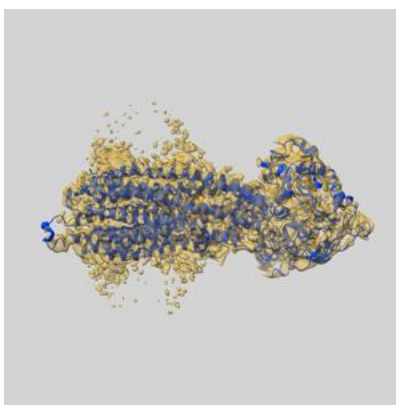
9 Map-model fit [i](#)

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.

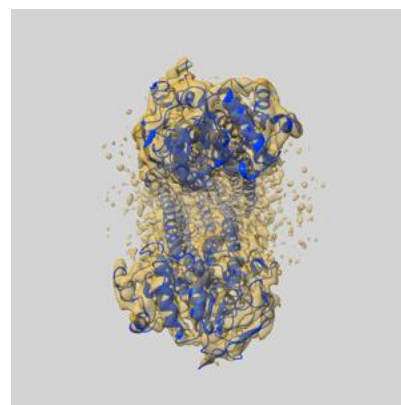
9.1 Map-model overlay [i](#)



X



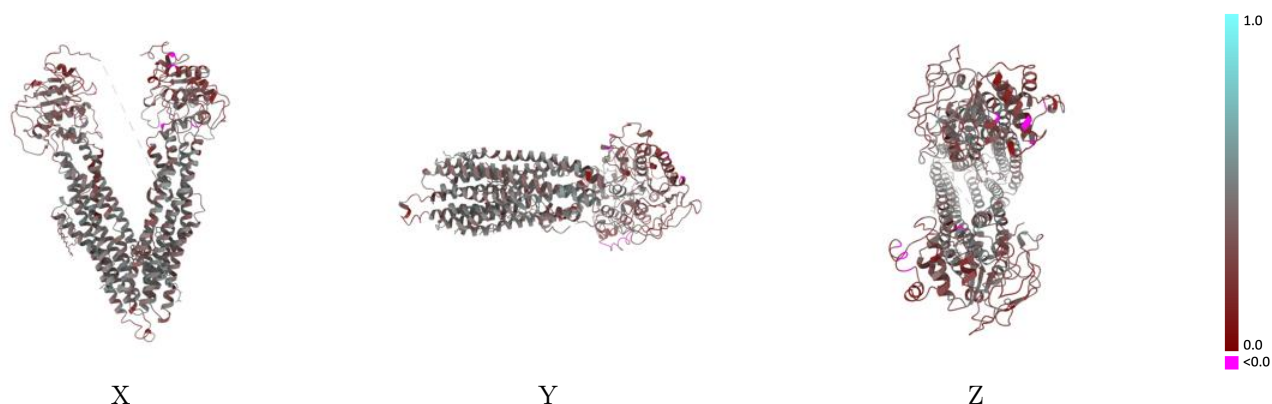
Y



Z

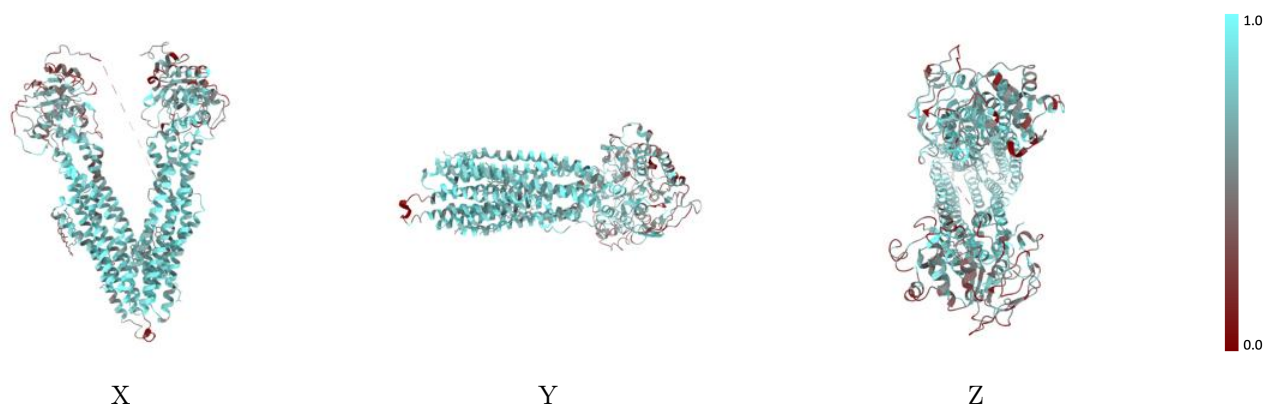
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



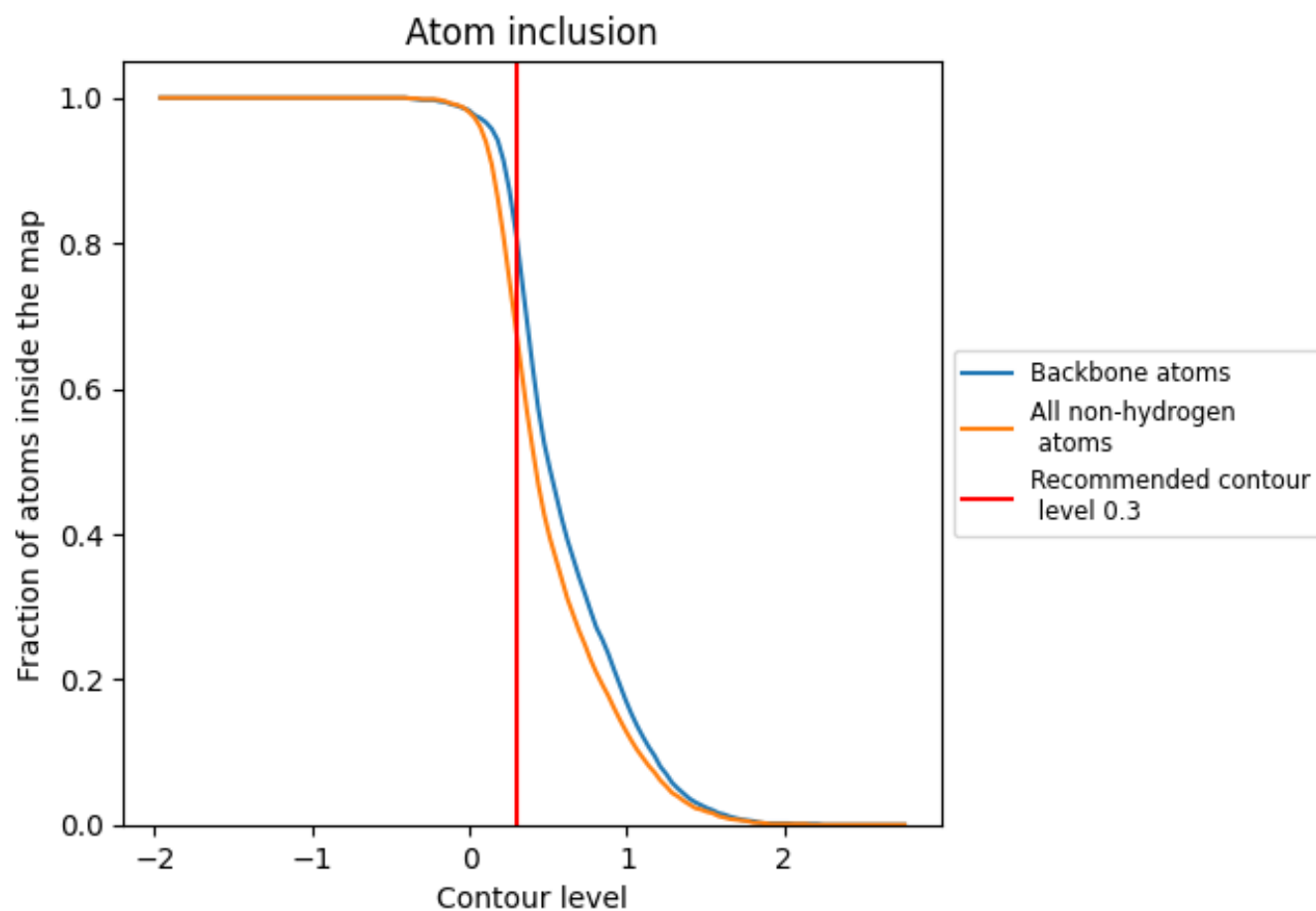
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

