



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:23 AM UTC

PDB ID : 7ZKA / pdb_00007zka
EMDB ID : EMD-14760
Title : ABCB1 V978C mutant (mABCB1) in the outward facing state bound to AAC
Authors : Parey, K.; Janulienė, D.; Gewering, T.; Urbatsch, I.; Zhang, Q.; Moeller, A.
Deposited on : 2022-04-12
Resolution : 2.90 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

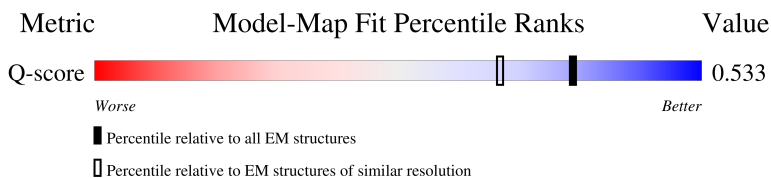
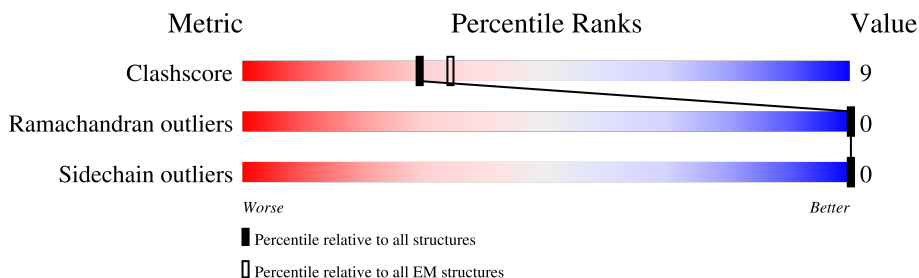
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9406 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	1177	Total	C	N	O	S	0	0
			9133	5875	1550	1676	32		

There are 65 discrepancies between the modelled and reference sequences:

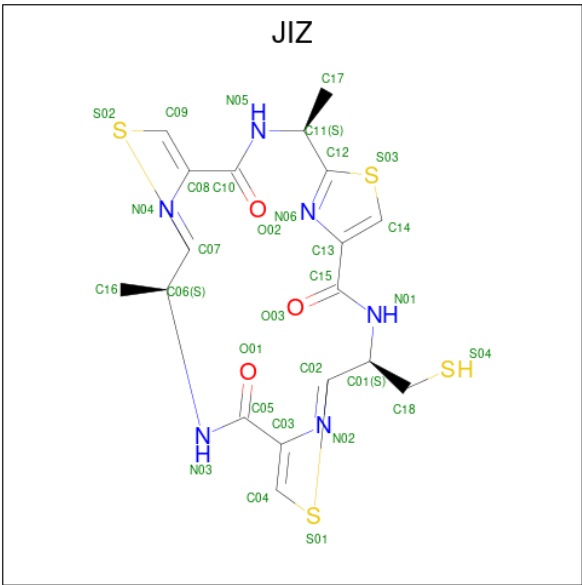
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	engineered mutation	UNP P21447
A	87	GLN	ASN	engineered mutation	UNP P21447
A	90	GLN	ASN	engineered mutation	UNP P21447
A	133	ALA	CYS	engineered mutation	UNP P21447
A	427	GLY	CYS	engineered mutation	UNP P21447
A	638	GLY	CYS	engineered mutation	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	978	CYS	VAL	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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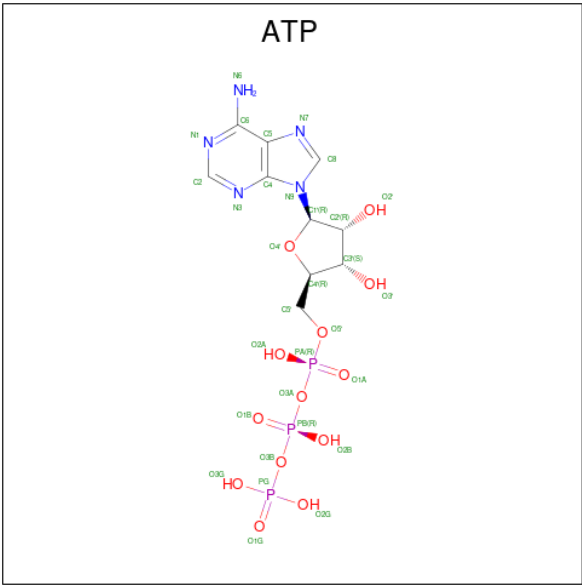
Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	SER	-	expression tag	UNP P21447
A	1293	TRP	-	expression tag	UNP P21447
A	1294	SER	-	expression tag	UNP P21447
A	1295	HIS	-	expression tag	UNP P21447
A	1296	PRO	-	expression tag	UNP P21447
A	1297	GLN	-	expression tag	UNP P21447
A	1298	PHE	-	expression 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 (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[^]{5,8}.1[^]{12,15}]tetracosa-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
2	A	1	Total	C	N	O	S	0
			31	18	6	3	4	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

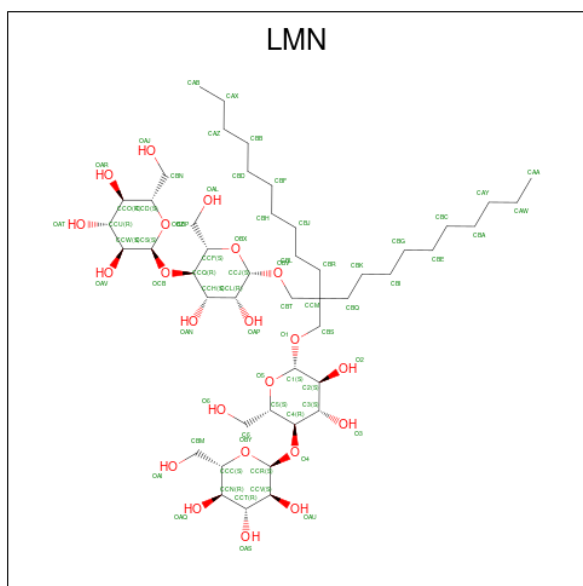


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

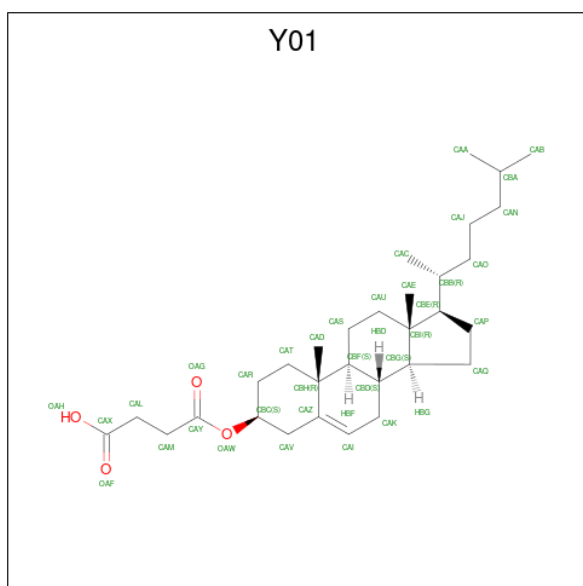
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	

- Molecule 5 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			69	47	22	

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total	O	0
			4	4	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	271467	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	0.740	Depositor
Minimum map value	-0.428	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	229.20001, 229.20001, 229.20001	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, LMN, ATP, MG, JIZ

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	0.27	0/9301	0.51	9/12572 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ILE	N-CA-C	-15.22	99.57	111.90
1	A	741	PRO	N-CA-C	12.45	131.27	113.47
1	A	746	GLN	N-CA-C	-7.59	103.00	111.28
1	A	740	PRO	N-CA-C	-6.88	102.31	110.70
1	A	86	LYS	N-CA-C	-6.69	105.01	112.57
1	A	519	LEU	CB-CA-C	5.45	118.53	109.53
1	A	517	ASP	N-CA-C	-5.32	106.02	112.88
1	A	472	GLU	CB-CA-C	5.26	117.17	110.34
1	A	749	ASN	N-CA-C	-5.14	106.10	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9133	0	9314	173	0
2	A	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	62	0	24	2	0
4	A	2	0	0	0	0
5	A	69	0	88	2	0
6	A	105	0	147	9	0
7	A	4	0	0	0	0
All	All	9406	0	9573	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (177) 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:39:PHE:HB2	6:A:1407:Y01:HAD2	1.55	0.89
1:A:1243:GLN:HB2	1:A:1248:LYS:HD2	1.66	0.77
1:A:1140:GLU:HA	1:A:1143:ARG:HG2	1.67	0.76
1:A:872:MET:HG2	1:A:995:ALA:HB2	1.67	0.76
1:A:880:LEU:HG	1:A:999:VAL:HG21	1.69	0.75
1:A:302:ILE:HD12	1:A:338:ALA:HB1	1.69	0.74
1:A:875:LEU:HD12	1:A:992:PRO:HB3	1.72	0.71
1:A:317:VAL:HG13	1:A:745:ARG:HH22	1.59	0.67
1:A:711:ILE:O	1:A:715:ILE:HG13	1.96	0.65
1:A:486:TYR:O	1:A:908:ARG:NH1	2.28	0.64
1:A:166:GLU:HB3	1:A:244:ALA:HB1	1.78	0.64
1:A:1123:ILE:HD13	1:A:1154:ILE:HD12	1.80	0.64
1:A:230:LYS:HA	6:A:1408:Y01:HAL2	1.80	0.64
1:A:1124:ALA:HB2	1:A:1161:TYR:HB3	1.78	0.63
1:A:874:MET:HE1	5:A:1406:LMN:HBD	1.80	0.63
1:A:193:MET:HE1	1:A:341:VAL:HG23	1.81	0.63
1:A:39:PHE:HD2	1:A:139:GLN:HE22	1.46	0.63
1:A:318:ILE:HG23	1:A:742:GLU:CD	2.24	0.63
1:A:1194:LEU:HD23	1:A:1224:ILE:HB	1.81	0.63
1:A:278:GLU:OE2	1:A:782:LYS:HE3	1.99	0.62
1:A:502:GLU:HG3	1:A:568:ALA:HB1	1.81	0.61
1:A:965:MET:HE1	1:A:970:VAL:HG12	1.82	0.61
1:A:703:GLU:HB2	1:A:706:TYR:HD2	1.65	0.61
1:A:828:ARG:O	1:A:831:VAL:HG22	2.01	0.61
1:A:607:ASN:HB3	1:A:610:GLU:HG3	1.82	0.60
1:A:1109:LEU:HG	1:A:1192:ILE:HB	1.83	0.60
1:A:232:LEU:HD21	1:A:349:GLU:HG3	1.85	0.58
1:A:421:LEU:HB3	1:A:429:LYS:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:TYR:CZ	1:A:335:LEU:HB3	2.38	0.58
1:A:1215:ASP:HA	1:A:1218:ARG:HG2	1.84	0.58
1:A:1079:LEU:HG	1:A:1109:LEU:HD21	1.86	0.57
1:A:1037:VAL:HB	1:A:1087:ALA:HB3	1.86	0.57
1:A:434:GLN:HG2	1:A:439:LEU:HD12	1.87	0.56
1:A:965:MET:SD	1:A:969:ASN:ND2	2.78	0.56
1:A:816:ASN:O	1:A:820:GLN:HG2	2.06	0.56
1:A:1199:THR:HG22	1:A:1202:LEU:HD22	1.87	0.56
1:A:1147:GLU:HG2	1:A:1213:ALA:HB1	1.86	0.56
1:A:1022:LEU:HB3	1:A:1100:LEU:HD23	1.88	0.55
1:A:1028:GLU:N	1:A:1093:ASP:OD2	2.39	0.54
1:A:433:VAL:HG13	1:A:549:LEU:HD13	1.89	0.54
1:A:570:ASP:OD1	1:A:573:ARG:NH1	2.41	0.54
1:A:716:ILE:HG21	1:A:765:THR:HG21	1.88	0.54
1:A:863:ILE:O	1:A:866:ILE:HG22	2.08	0.54
1:A:500:VAL:HG13	1:A:505:ALA:HB3	1.90	0.54
1:A:253:VAL:HG21	1:A:269:GLU:HB3	1.90	0.54
1:A:705:PRO:HA	1:A:708:VAL:HG22	1.90	0.54
1:A:1150:ILE:O	1:A:1154:ILE:HG12	2.09	0.53
1:A:411:LEU:HD13	1:A:602:ILE:HD13	1.90	0.53
1:A:721:GLN:HB3	1:A:722:PRO:HD3	1.90	0.53
1:A:554:THR:HG22	1:A:557:LEU:HD22	1.91	0.53
1:A:430:SER:OG	1:A:551:ASP:OD2	2.27	0.53
1:A:390:PHE:O	1:A:410:ASN:HA	2.09	0.53
1:A:128:GLN:HG3	1:A:129:VAL:N	2.25	0.52
1:A:1033:PHE:HB2	1:A:1054:LEU:HB3	1.90	0.52
1:A:713:ALA:O	1:A:717:ASN:ND2	2.42	0.52
1:A:1004:ILE:O	1:A:1008:ILE:HG12	2.10	0.52
1:A:1166:GLY:H	1:A:1171:GLN:HB2	1.74	0.52
1:A:135:ALA:O	1:A:139:GLN:HG3	2.10	0.51
1:A:784:LEU:HD22	1:A:1004:ILE:HG21	1.93	0.51
1:A:181:GLY:HA3	1:A:354:ALA:HB2	1.92	0.51
1:A:513:PRO:HD2	1:A:1046:ILE:HD11	1.92	0.51
1:A:1064:LEU:HD22	1:A:1242:ILE:HD11	1.93	0.51
1:A:289:ILE:O	1:A:293:ILE:HG12	2.10	0.51
1:A:704:TRP:N	1:A:705:PRO:HD2	2.25	0.51
1:A:713:ALA:HB3	1:A:769:GLN:HB2	1.93	0.51
1:A:144:ARG:HG3	1:A:175:VAL:HG11	1.93	0.51
1:A:265:GLY:O	1:A:269:GLU:HG2	2.11	0.50
1:A:816:ASN:OD1	1:A:820:GLN:NE2	2.38	0.50
1:A:832:ILE:HD11	1:A:990:PHE:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HA	6:A:1409:Y01:HAD3	1.94	0.49
1:A:155:GLU:OE2	1:A:371:ILE:N	2.35	0.49
1:A:381:PRO:HB2	1:A:384:ILE:HG12	1.94	0.49
1:A:224:SER:HG	1:A:228:TRP:CD1	2.30	0.49
1:A:156:ILE:HG13	1:A:439:LEU:HB3	1.94	0.49
1:A:604:GLU:HB3	1:A:611:LEU:HD22	1.94	0.49
1:A:966:THR:OG1	1:A:969:ASN:OD1	2.28	0.49
1:A:500:VAL:HG21	1:A:516:PHE:HE2	1.78	0.48
1:A:866:ILE:O	1:A:869:VAL:HB	2.13	0.48
6:A:1408:Y01:HAE2	6:A:1408:Y01:HAO2	1.95	0.48
1:A:207:GLY:HA3	1:A:330:VAL:HG21	1.96	0.48
1:A:159:PHE:CD2	1:A:164:VAL:HG11	2.48	0.48
1:A:703:GLU:HB2	1:A:706:TYR:CD2	2.46	0.48
1:A:1240:VAL:HG13	1:A:1247:VAL:HG23	1.94	0.48
1:A:828:ARG:O	1:A:832:ILE:HD12	2.13	0.48
1:A:306:TYR:CE1	1:A:335:LEU:HB3	2.48	0.48
1:A:1096:GLU:HG2	1:A:1098:LYS:H	1.79	0.48
1:A:174:ASP:OD1	1:A:240:LEU:HD13	2.14	0.48
1:A:1195:LEU:HD12	1:A:1225:VAL:HG22	1.97	0.47
1:A:54:THR:O	1:A:58:ILE:HG12	2.14	0.47
6:A:1408:Y01:HAC1	6:A:1408:Y01:HAP1	1.72	0.47
1:A:66:LEU:HD22	1:A:202:ILE:HD11	1.97	0.47
1:A:945:MET:HE3	1:A:978:CYS:SG	2.54	0.47
1:A:1030:ASN:OD1	1:A:1057:LYS:HD3	2.15	0.47
1:A:431:THR:OG1	3:A:1402:ATP:O2A	2.28	0.47
1:A:1064:LEU:HB2	1:A:1226:ILE:HG12	1.97	0.47
1:A:429:LYS:HB3	1:A:581:ILE:HD13	1.97	0.47
1:A:166:GLU:HG2	1:A:248:ALA:HB2	1.97	0.47
1:A:421:LEU:HD13	1:A:595:ALA:HB3	1.96	0.47
1:A:1036:VAL:HA	1:A:1088:GLY:HA3	1.96	0.47
1:A:791:SER:OG	1:A:1007:ILE:O	2.22	0.47
6:A:1408:Y01:HAC3	6:A:1408:Y01:HAA2	1.97	0.47
1:A:81:VAL:O	1:A:84:VAL:HG22	2.14	0.46
1:A:114:TYR:OH	2:A:1401:JIZ:O01	2.24	0.46
1:A:200:PHE:CE1	1:A:334:VAL:HG13	2.50	0.46
1:A:1026:MET:HB3	1:A:1026:MET:HE3	1.82	0.46
1:A:707:PHE:O	1:A:711:ILE:HG12	2.15	0.46
1:A:186:ILE:HD13	6:A:1407:Y01:HAC3	1.97	0.46
1:A:835:ASN:ND2	1:A:986:GLN:HB3	2.31	0.45
1:A:121:VAL:HA	1:A:124:VAL:HG22	1.97	0.45
1:A:292:ASN:ND2	1:A:770:GLY:HA3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:ARG:NH1	1:A:1097:ILE:O	2.49	0.45
1:A:1104:TRP:O	1:A:1108:GLN:HG2	2.16	0.45
1:A:505:ALA:O	1:A:509:ILE:HG13	2.16	0.45
1:A:68:MET:SD	1:A:336:ILE:HG13	2.55	0.45
1:A:274:ASN:O	1:A:278:GLU:HG2	2.17	0.45
1:A:406:LEU:HD22	1:A:409:LEU:HD22	1.99	0.45
1:A:821:VAL:O	1:A:825:THR:OG1	2.24	0.45
1:A:924:TYR:O	1:A:928:MET:HG2	2.16	0.45
1:A:1149:ASN:O	1:A:1179:ARG:NH1	2.49	0.45
1:A:1079:LEU:HD23	1:A:1194:LEU:HD11	1.99	0.45
1:A:324:ILE:HG13	1:A:328:LEU:HD13	1.98	0.44
1:A:857:LEU:HD13	1:A:977:ILE:HD13	1.99	0.44
1:A:864:ILE:HG23	1:A:941:THR:HG22	1.99	0.44
1:A:292:ASN:HB3	1:A:767:PHE:HA	2.00	0.44
1:A:1201:ALA:O	1:A:1202:LEU:HD12	2.18	0.44
1:A:235:PHE:HB3	1:A:287:LYS:HG3	2.00	0.44
1:A:66:LEU:O	1:A:70:ILE:HG12	2.18	0.43
1:A:688:VAL:HG12	1:A:688:VAL:O	2.17	0.43
1:A:64:LEU:HB3	1:A:65:PRO:HD3	2.00	0.43
1:A:832:ILE:HD11	1:A:990:PHE:CD1	2.53	0.43
1:A:125:ALA:HA	1:A:128:GLN:HG2	2.00	0.43
1:A:689:PRO:HA	1:A:690:PRO:HD3	1.95	0.43
1:A:835:ASN:HB3	1:A:983:ALA:HB1	2.00	0.43
1:A:156:ILE:HD12	1:A:901:ARG:HG3	2.00	0.43
1:A:210:LEU:HD21	1:A:331:PHE:CE1	2.53	0.43
1:A:414:LYS:HB2	1:A:417:GLN:OE1	2.19	0.43
1:A:232:LEU:HD12	1:A:287:LYS:HG2	2.00	0.43
1:A:306:TYR:CE2	1:A:335:LEU:HD13	2.54	0.42
1:A:298:ALA:O	1:A:302:ILE:HG12	2.19	0.42
1:A:326:GLN:O	1:A:330:VAL:HG23	2.19	0.42
1:A:546:LYS:HE3	1:A:546:LYS:HB3	1.82	0.42
1:A:1111:ILE:HG22	1:A:1194:LEU:HD12	2.01	0.42
1:A:1173:SER:OG	3:A:1402:ATP:O2G	2.37	0.42
1:A:1216:LYS:HE2	1:A:1216:LYS:HB3	1.85	0.42
1:A:603:VAL:HG23	1:A:604:GLU:HG2	2.01	0.42
1:A:758:LEU:HD23	1:A:758:LEU:HA	1.90	0.42
1:A:949:TYR:CE2	1:A:978:CYS:HB2	2.55	0.42
1:A:1040:TYR:HD2	1:A:1048:VAL:HG21	1.83	0.42
1:A:955:PHE:O	1:A:959:LEU:HG	2.19	0.42
1:A:210:LEU:HD21	1:A:331:PHE:HE1	1.85	0.42
1:A:240:LEU:HD12	1:A:357:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLN:HG3	1:A:439:LEU:HG	2.02	0.41
1:A:618:TYR:O	1:A:622:VAL:HG13	2.19	0.41
1:A:729:SER:OG	1:A:972:LEU:HD21	2.19	0.41
1:A:852:GLN:HG3	1:A:955:PHE:HE2	1.84	0.41
1:A:747:ASN:C	1:A:749:ASN:H	2.27	0.41
5:A:1406:LMN:HCR	5:A:1406:LMN:H3	1.92	0.41
1:A:113:TYR:O	1:A:117:ILE:HG12	2.20	0.41
1:A:696:ILE:HG13	1:A:1001:ALA:HB1	2.02	0.41
1:A:726:VAL:HG22	1:A:972:LEU:HD22	2.01	0.41
1:A:1151:HIS:NE2	1:A:1155:ASP:OD2	2.53	0.41
1:A:189:PHE:CD2	6:A:1407:Y01:HAB2	2.55	0.41
1:A:74:MET:HE2	1:A:74:MET:HB2	2.01	0.41
1:A:695:ARG:HE	1:A:695:ARG:HB3	1.72	0.41
1:A:867:ALA:O	1:A:870:VAL:HG22	2.21	0.41
1:A:1081:ARG:NH1	1:A:1098:LYS:HA	2.35	0.41
1:A:39:PHE:HB2	6:A:1407:Y01:CAD	2.37	0.41
1:A:506:TYR:CE1	1:A:510:MET:HE3	2.56	0.41
1:A:688:VAL:HG21	1:A:880:LEU:HD21	2.02	0.41
1:A:1264:PHE:HA	1:A:1267:VAL:HG12	2.02	0.41
1:A:134:LEU:O	1:A:138:ARG:HG3	2.22	0.40
1:A:967:PHE:O	1:A:970:VAL:HG22	2.22	0.40
1:A:96:LYS:HA	1:A:99:MET:HG3	2.04	0.40
1:A:192:ALA:CB	1:A:344:ALA:HB2	2.52	0.40
1:A:458:ASN:HB3	1:A:461:TYR:HB3	2.03	0.40
1:A:1054:LEU:HD11	1:A:1064:LEU:HD21	2.03	0.40
1:A:1249:GLU:HB3	1:A:1256:LEU:HD22	2.03	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	919/1328 (69%)	900 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	786/1086 (72%)	786 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	141	HIS
1	A	145	GLN
1	A	514	HIS
1	A	515	GLN
1	A	526	GLN
1	A	744	GLN
1	A	749	ASN
1	A	805	ASN
1	A	1255	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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$
5	LMN	A	1406	-	72,72,72	1.79	12 (16%)	92,98,98	1.22	13 (14%)
2	JIZ	A	1401	1	34,34,34	5.45	24 (70%)	45,49,49	4.45	20 (44%)
3	ATP	A	1402	4	32,33,33	0.29	0	48,52,52	0.29	0
6	Y01	A	1408	-	38,38,38	0.50	0	57,57,57	0.76	1 (1%)
6	Y01	A	1407	-	38,38,38	0.48	0	57,57,57	1.28	6 (10%)
3	ATP	A	1404	4	32,33,33	0.27	0	48,52,52	0.27	0
6	Y01	A	1409	-	38,38,38	0.44	0	57,57,57	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMN	A	1406	-	-	32/50/130/130	0/4/4/4
2	JIZ	A	1401	1	-	0/38/38/38	0/4/4/4
3	ATP	A	1402	4	-	7/22/38/38	0/3/3/3
6	Y01	A	1408	-	-	12/19/77/77	0/4/4/4
6	Y01	A	1407	-	-	7/19/77/77	0/4/4/4
3	ATP	A	1404	4	-	3/22/38/38	0/3/3/3
6	Y01	A	1409	-	-	8/19/77/77	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	JIZ	C03-N02	12.05	1.64	1.38
2	A	1401	JIZ	C08-N04	10.97	1.62	1.38
2	A	1401	JIZ	C13-N06	10.92	1.62	1.38
2	A	1401	JIZ	C04-C03	8.95	1.52	1.36
2	A	1401	JIZ	C02-S01	-8.75	1.55	1.73
2	A	1401	JIZ	C07-S02	-6.72	1.59	1.73
2	A	1401	JIZ	C12-S03	-6.70	1.59	1.73
2	A	1401	JIZ	C12-N06	6.17	1.43	1.30
2	A	1401	JIZ	C07-N04	6.13	1.43	1.30
2	A	1401	JIZ	C09-S02	-6.06	1.57	1.71
2	A	1401	JIZ	C14-S03	-6.01	1.57	1.71
2	A	1401	JIZ	C04-S01	-5.59	1.58	1.71
2	A	1401	JIZ	C14-C13	5.58	1.46	1.36
2	A	1401	JIZ	C05-N03	5.53	1.45	1.34
2	A	1401	JIZ	C15-N01	5.48	1.45	1.34
2	A	1401	JIZ	C09-C08	5.48	1.46	1.36
2	A	1401	JIZ	C10-N05	5.47	1.45	1.34
5	A	1406	LMN	O5-C1	5.40	1.55	1.41
5	A	1406	LMN	CBQ-CCM	5.20	1.63	1.54
5	A	1406	LMN	O1-C1	-5.07	1.31	1.40
5	A	1406	LMN	CBS-CCM	3.82	1.62	1.53
5	A	1406	LMN	CBR-CCM	3.73	1.60	1.54
2	A	1401	JIZ	C02-N02	3.26	1.37	1.30
5	A	1406	LMN	OAN-CCH	2.50	1.49	1.43
5	A	1406	LMN	CBT-CCM	2.50	1.59	1.53
2	A	1401	JIZ	O01-C05	-2.50	1.18	1.23
2	A	1401	JIZ	O02-C10	-2.46	1.18	1.23
2	A	1401	JIZ	O03-C15	-2.45	1.18	1.23
5	A	1406	LMN	OBY-CCR	2.44	1.48	1.41
5	A	1406	LMN	O4-C4	2.33	1.49	1.43
2	A	1401	JIZ	C03-C05	2.32	1.53	1.48
5	A	1406	LMN	OBZ-CCS	2.31	1.47	1.41
2	A	1401	JIZ	C13-C15	2.21	1.53	1.48
2	A	1401	JIZ	C08-C10	2.20	1.52	1.48
5	A	1406	LMN	OAT-CCU	2.08	1.48	1.43
5	A	1406	LMN	OAS-CCT	2.03	1.48	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	JIZ	C09-S02-C07	15.01	107.27	89.52
2	A	1401	JIZ	C14-S03-C12	14.87	107.12	89.52
2	A	1401	JIZ	C04-S01-C02	13.39	105.36	89.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	JIZ	C04-C03-N02	-6.06	107.10	115.43
2	A	1401	JIZ	C14-C13-N06	-5.16	108.33	115.43
2	A	1401	JIZ	C09-C08-N04	-5.07	108.45	115.43
2	A	1401	JIZ	S02-C07-N04	-4.91	107.77	114.19
2	A	1401	JIZ	S03-C12-N06	-4.85	107.85	114.19
2	A	1401	JIZ	C01-C18-S04	-4.18	109.45	114.16
2	A	1401	JIZ	C03-N02-C02	-3.84	106.69	110.65
5	A	1406	LMN	CCR-O4-C4	-3.37	109.99	117.98
2	A	1401	JIZ	C03-C04-S01	-3.20	106.55	110.24
6	A	1407	Y01	CAK-CBD-CBG	2.93	115.09	110.93
6	A	1407	Y01	CBH-CBF-CBD	-2.90	108.47	112.71
6	A	1407	Y01	CBG-CBI-CBE	2.89	103.41	100.10
5	A	1406	LMN	CCL-CCH-CCQ	2.80	116.04	109.68
2	A	1401	JIZ	C12-C11-N05	-2.73	105.20	109.69
5	A	1406	LMN	CCS-OCB-CCQ	-2.73	111.51	117.98
5	A	1406	LMN	CCT-CCN-CCC	2.69	115.10	110.23
6	A	1407	Y01	CBF-CBD-CBG	2.66	112.56	109.09
6	A	1407	Y01	CAL-CAM-CAY	2.53	120.96	113.44
2	A	1401	JIZ	C04-C03-C05	2.41	127.93	123.92
5	A	1406	LMN	C2-C3-C4	2.41	115.15	109.68
2	A	1401	JIZ	C14-C13-C15	2.37	127.85	123.92
2	A	1401	JIZ	C09-C08-C10	2.34	127.81	123.92
5	A	1406	LMN	OBX-CCF-CCQ	2.33	114.54	109.72
6	A	1408	Y01	CBI-CBE-CBB	2.32	123.08	119.50
5	A	1406	LMN	CCH-CCQ-CCF	2.32	116.07	110.93
5	A	1406	LMN	CBL-CBR-CCM	-2.29	110.23	117.19
5	A	1406	LMN	CBK-CBQ-CCM	-2.28	110.28	117.19
2	A	1401	JIZ	C05-C03-N02	2.27	124.97	120.67
2	A	1401	JIZ	C07-C06-N03	-2.25	105.99	109.69
2	A	1401	JIZ	C08-C09-S02	-2.25	107.65	110.24
5	A	1406	LMN	OBY-CCC-CCN	2.24	113.74	109.70
6	A	1407	Y01	CBI-CBG-CBD	-2.22	111.26	114.41
2	A	1401	JIZ	C13-C14-S03	-2.13	107.78	110.24
2	A	1401	JIZ	C01-C02-S01	2.06	124.53	121.79
5	A	1406	LMN	OAN-CCH-CCL	-2.03	105.59	110.38
5	A	1406	LMN	C1-C2-C3	2.02	114.27	110.01
5	A	1406	LMN	OBZ-CCD-CCO	2.00	113.31	109.70

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1402	ATP	C5'-O5'-PA-O2A
3	A	1402	ATP	C5'-O5'-PA-O3A
5	A	1406	LMN	C2-C1-O1-CBS
5	A	1406	LMN	O5-C1-O1-CBS
5	A	1406	LMN	CCM-CBS-O1-C1
5	A	1406	LMN	CBK-CBQ-CCM-CBT
5	A	1406	LMN	O1-CBS-CCM-CBQ
5	A	1406	LMN	O1-CBS-CCM-CBR
5	A	1406	LMN	OBX-CCJ-OBV-CBT
6	A	1408	Y01	CAO-CBB-CBE-CBI
6	A	1408	Y01	OAG-CAY-OAW-CBC
6	A	1408	Y01	CAR-CBC-OAW-CAY
5	A	1406	LMN	OBZ-CCS-OCB-CCQ
6	A	1408	Y01	CAM-CAY-OAW-CBC
5	A	1406	LMN	OAL-CBP-CCF-OBX
5	A	1406	LMN	OBY-CCR-O4-C4
5	A	1406	LMN	OAL-CBP-CCF-CCQ
5	A	1406	LMN	CCL-CCJ-OBV-CBT
5	A	1406	LMN	O5-C5-C6-O6
6	A	1408	Y01	CAC-CBB-CBE-CAP
5	A	1406	LMN	O1-CBS-CCM-CBT
6	A	1407	Y01	CAN-CAJ-CAO-CBB
5	A	1406	LMN	CBB-CBD-CBF-CBH
6	A	1407	Y01	CAR-CBC-OAW-CAY
5	A	1406	LMN	CBA-CBC-CBE-CBG
6	A	1409	Y01	CAM-CAY-OAW-CBC
6	A	1407	Y01	CAM-CAY-OAW-CBC
5	A	1406	LMN	OAI-CBM-CCC-OBY
5	A	1406	LMN	CBJ-CBL-CBR-CCM
6	A	1407	Y01	CAV-CBC-OAW-CAY
5	A	1406	LMN	OAJ-CBN-CCD-OBZ
6	A	1409	Y01	OAG-CAY-OAW-CBC
6	A	1408	Y01	CAO-CBB-CBE-CAP
6	A	1407	Y01	OAG-CAY-OAW-CBC
5	A	1406	LMN	CBK-CBQ-CCM-CBS
5	A	1406	LMN	CAY-CBA-CBC-CBE
5	A	1406	LMN	CBH-CBJ-CBL-CBR
5	A	1406	LMN	C3-C4-O4-CCR
6	A	1408	Y01	CAC-CBB-CBE-CBI
5	A	1406	LMN	CCH-CCQ-OCB-CCS
5	A	1406	LMN	CBK-CBQ-CCM-CBR
5	A	1406	LMN	CBG-CBI-CBK-CBQ
5	A	1406	LMN	C5-C4-O4-CCR

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Mol	Chain	Res	Type	Atoms
5	A	1406	LMN	C4-C5-C6-O6
3	A	1402	ATP	O4'-C4'-C5'-O5'
5	A	1406	LMN	CAZ-CBB-CBD-CBF
5	A	1406	LMN	CBC-CBE-CBG-CBI
5	A	1406	LMN	CCF-CCQ-OCB-CCS
6	A	1408	Y01	CAO-CAJ-CAN-CBA
6	A	1409	Y01	CAC-CBB-CBE-CBI
3	A	1404	ATP	PA-O3A-PB-O2B
3	A	1402	ATP	C3'-C4'-C5'-O5'
5	A	1406	LMN	CAX-CAZ-CBB-CBD
3	A	1402	ATP	C5'-O5'-PA-O1A
6	A	1408	Y01	CAV-CBC-OAW-CAY
6	A	1409	Y01	CAO-CBB-CBE-CBI
3	A	1402	ATP	PA-O3A-PB-O2B
6	A	1409	Y01	CAC-CBB-CBE-CAP
6	A	1409	Y01	CAO-CBB-CBE-CAP
6	A	1407	Y01	CAM-CAL-CAX-OAF
6	A	1407	Y01	CAM-CAL-CAX-OAH
3	A	1404	ATP	O4'-C4'-C5'-O5'
3	A	1404	ATP	PA-O3A-PB-O1B
6	A	1408	Y01	CAM-CAL-CAX-OAH
6	A	1409	Y01	CAJ-CAN-CBA-CAB
6	A	1409	Y01	CAN-CAJ-CAO-CBB
6	A	1408	Y01	CAX-CAL-CAM-CAY
6	A	1408	Y01	CAM-CAL-CAX-OAF
3	A	1402	ATP	PA-O3A-PB-O1B

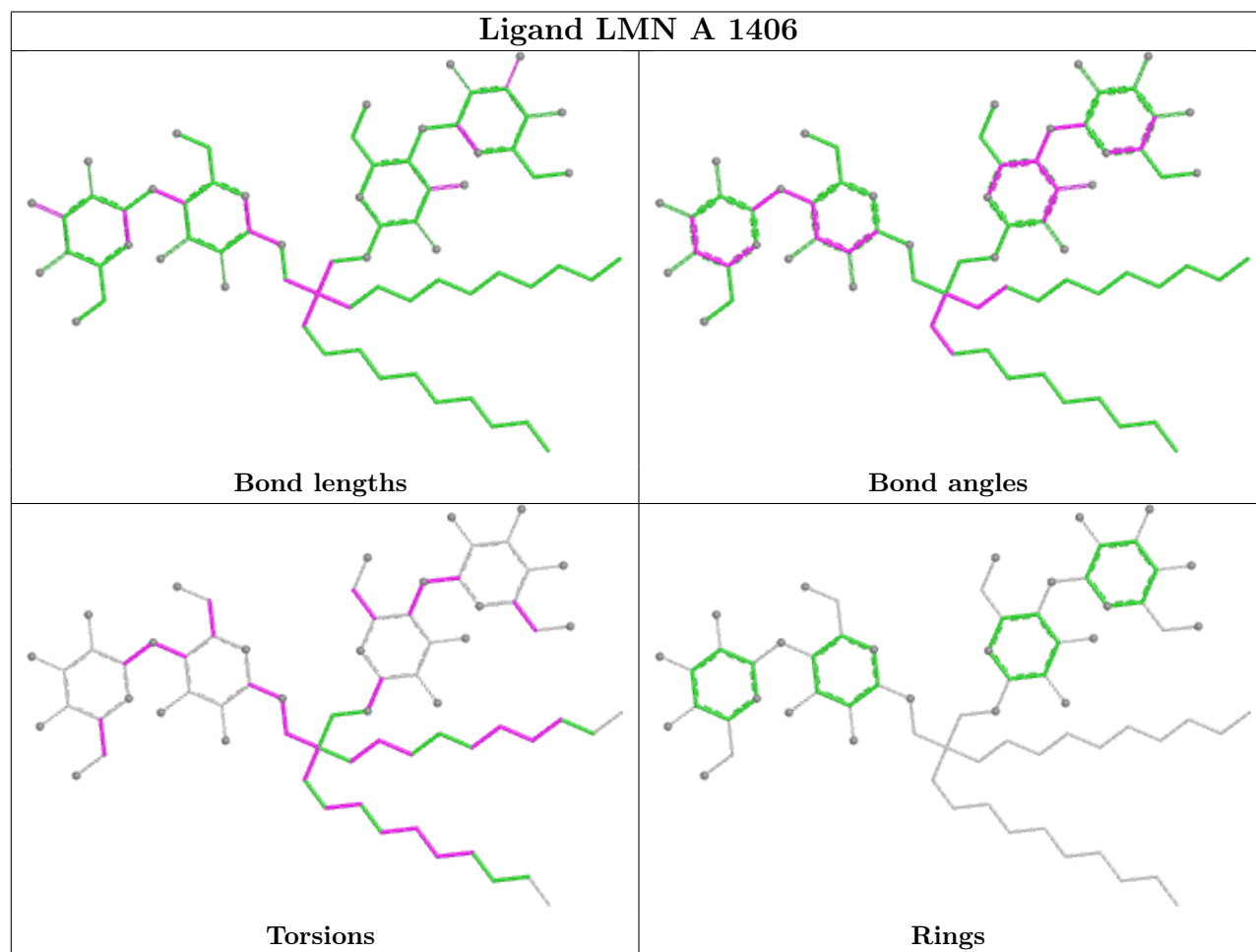
There are no ring outliers.

6 monomers are involved in 14 short contacts:

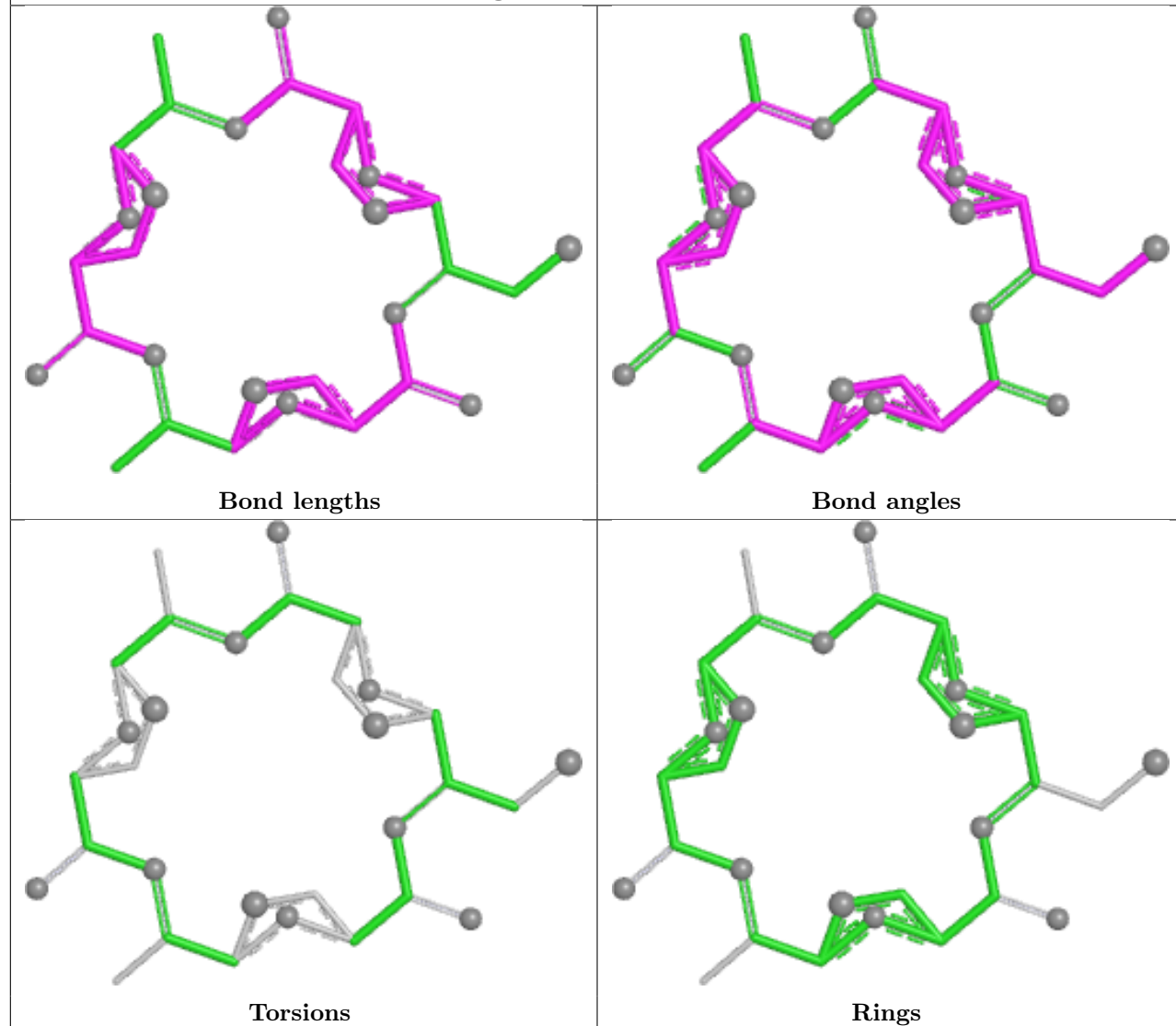
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1406	LMN	2	0
2	A	1401	JIZ	1	0
3	A	1402	ATP	2	0
6	A	1408	Y01	4	0
6	A	1407	Y01	4	0
6	A	1409	Y01	1	0

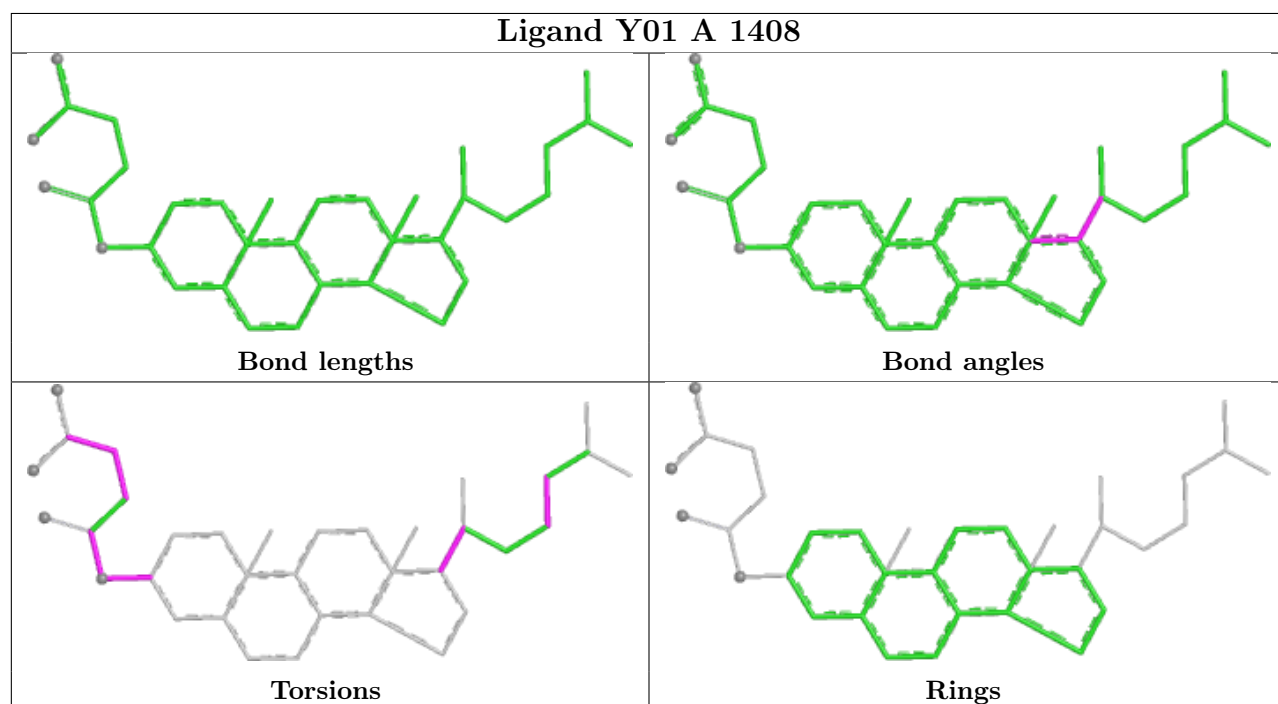
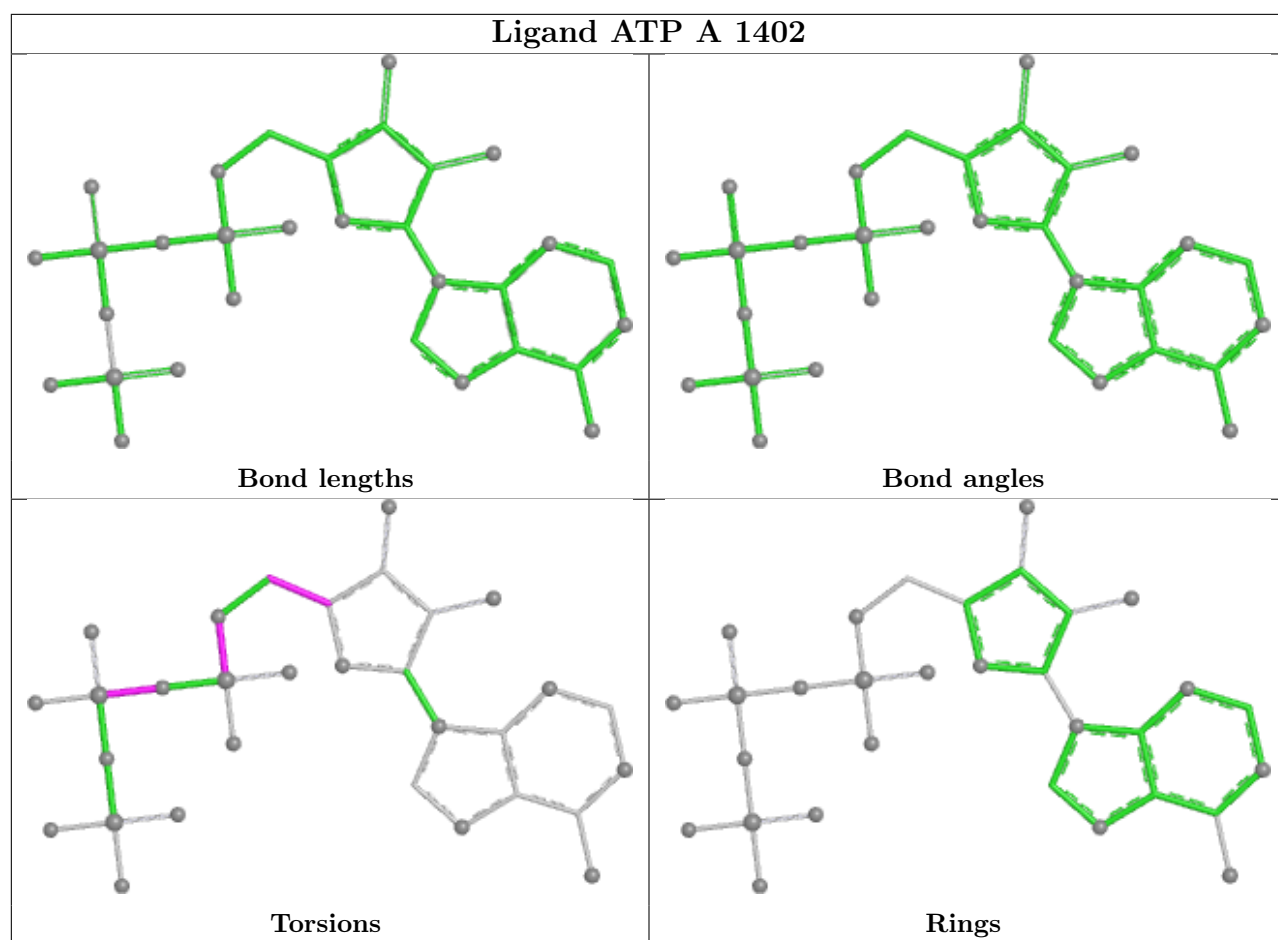
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

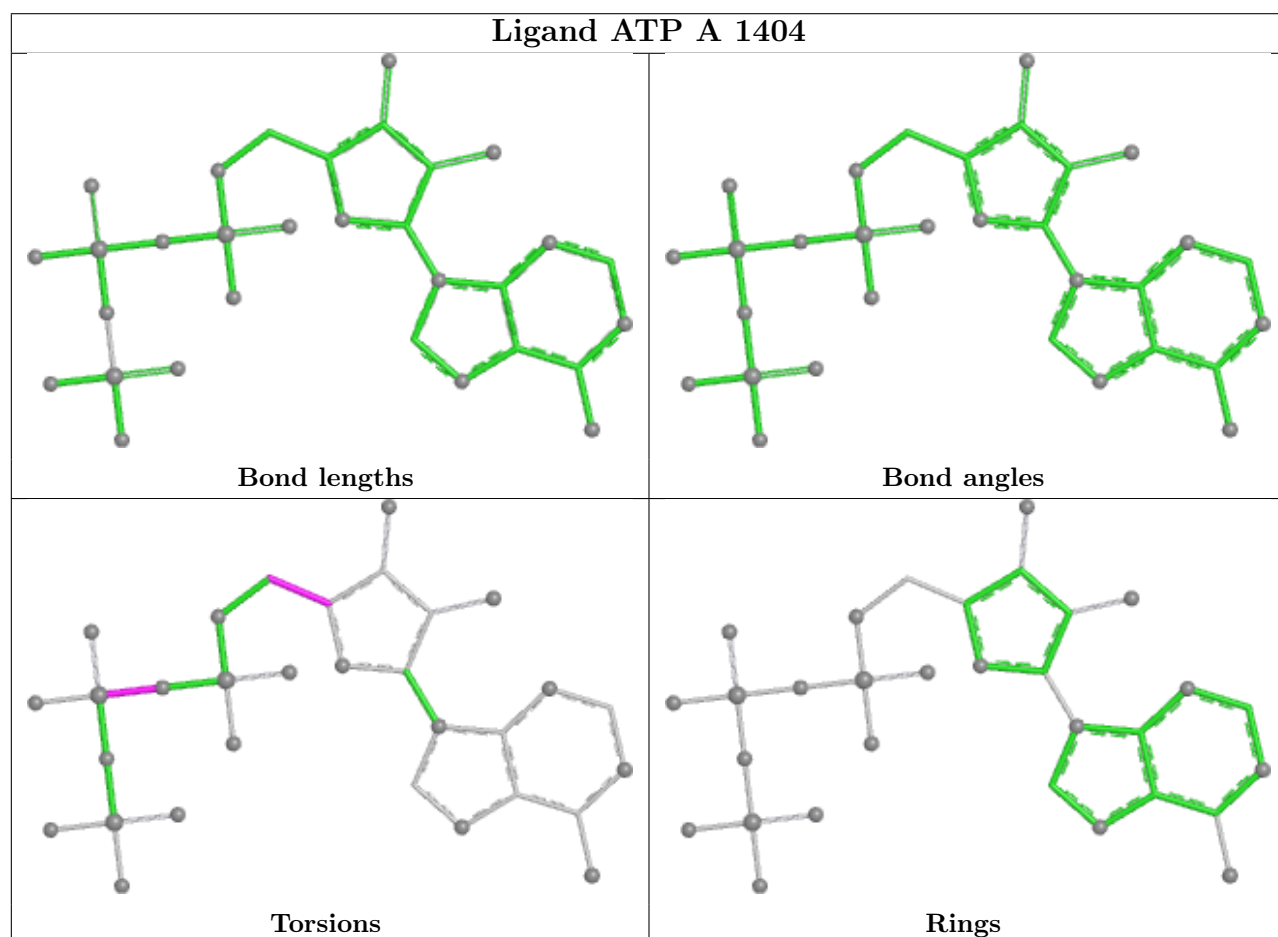
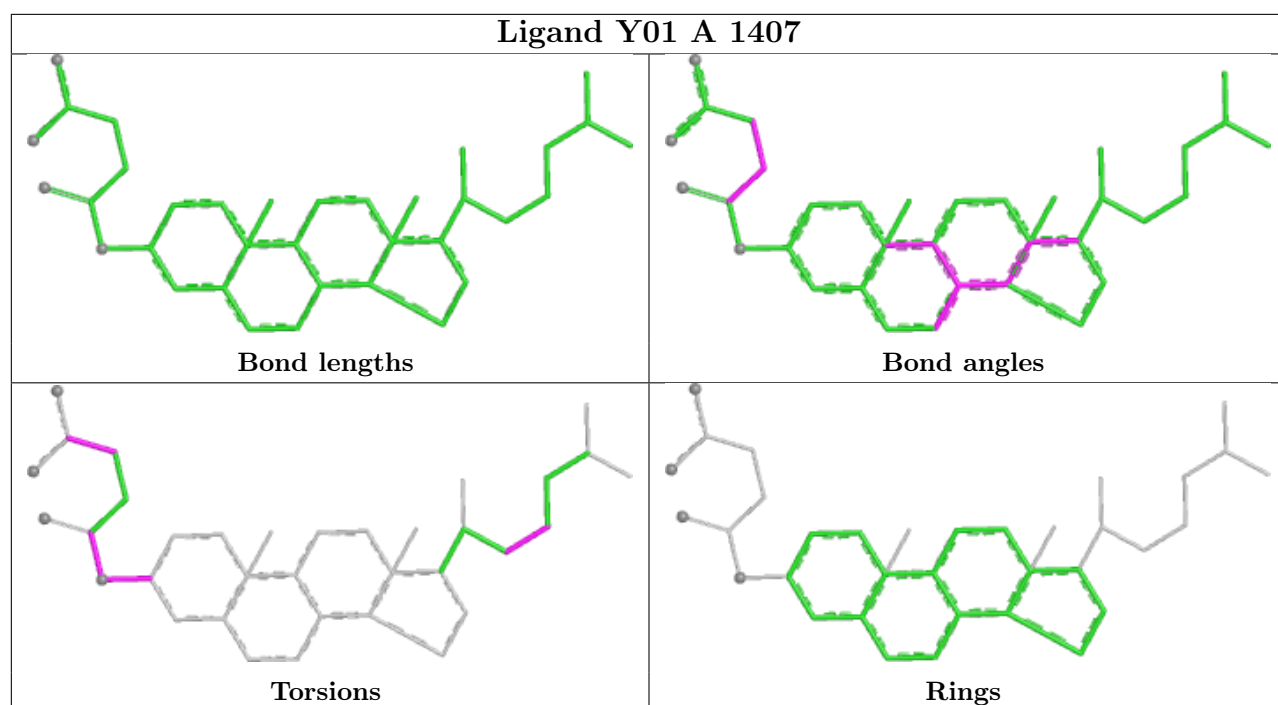
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

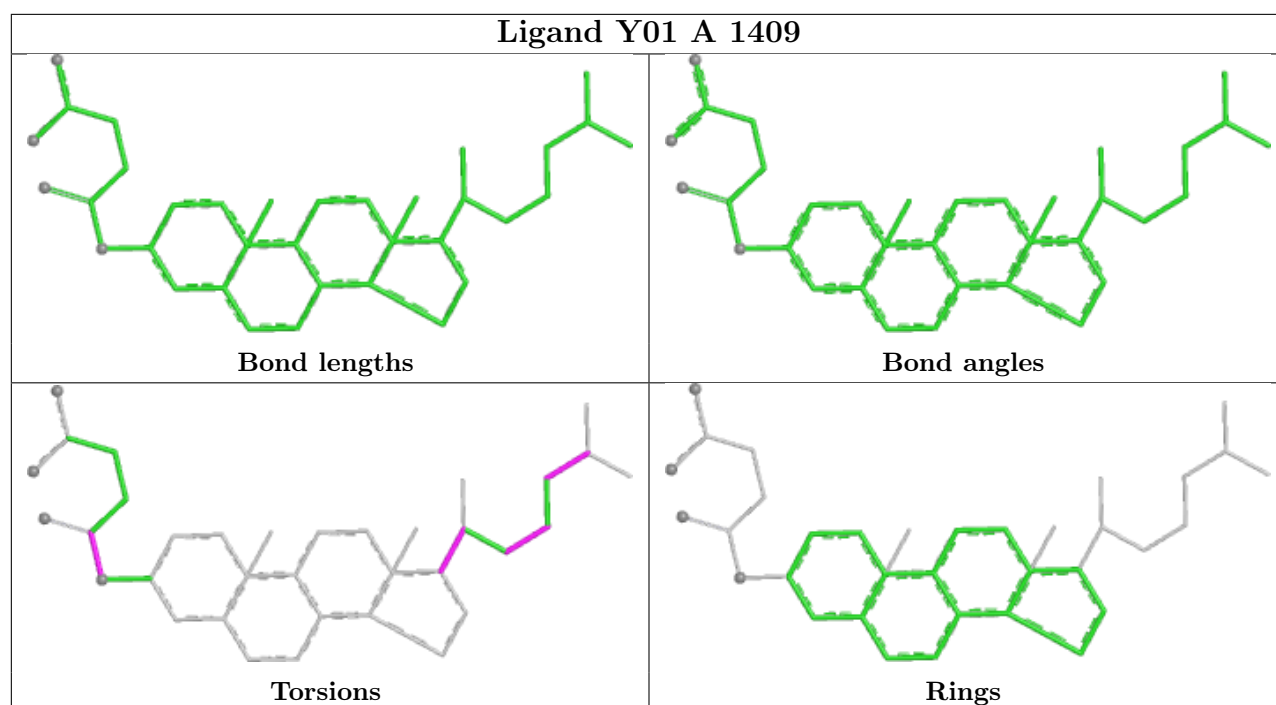


Ligand JIZ A 1401









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.

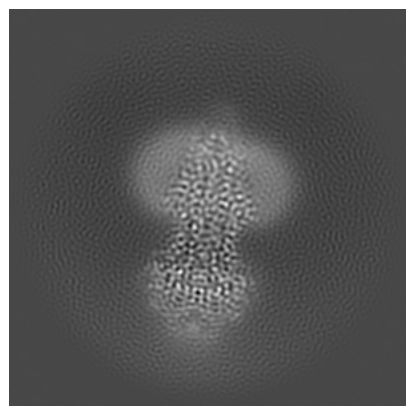
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14760. These allow visual inspection of the internal detail of the map and identification of artifacts.

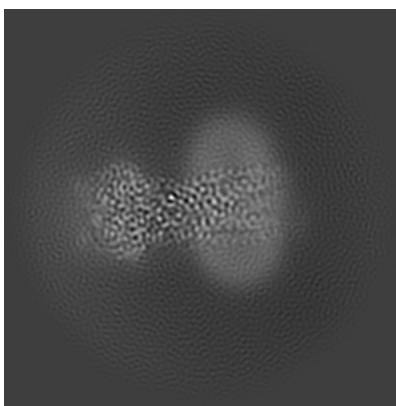
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

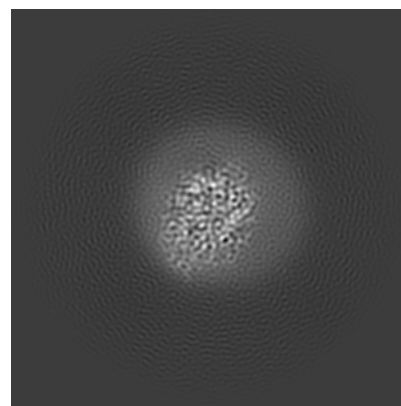
6.1.1 Primary map



X

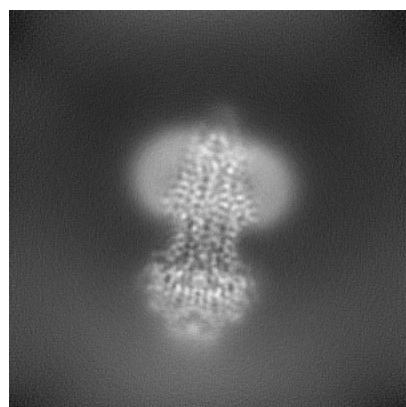


Y

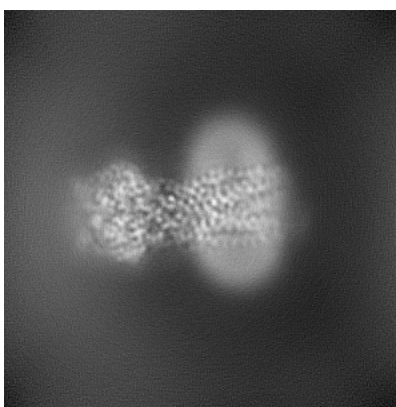


Z

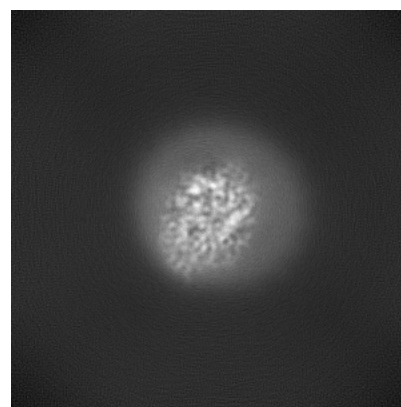
6.1.2 Raw map



X



Y

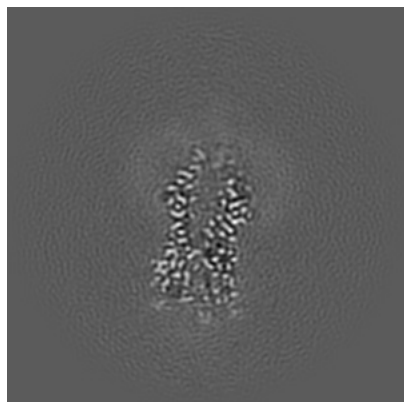


Z

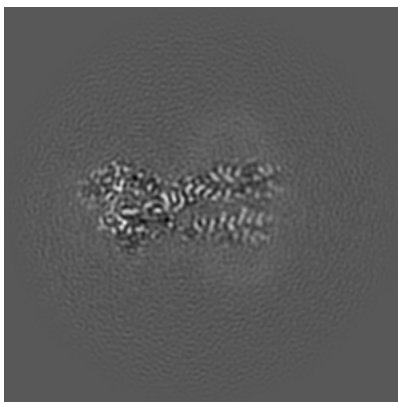
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

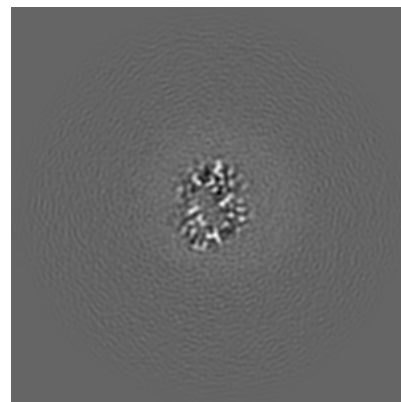
6.2.1 Primary map



X Index: 200

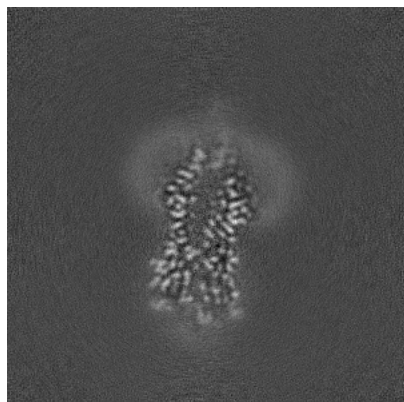


Y Index: 200

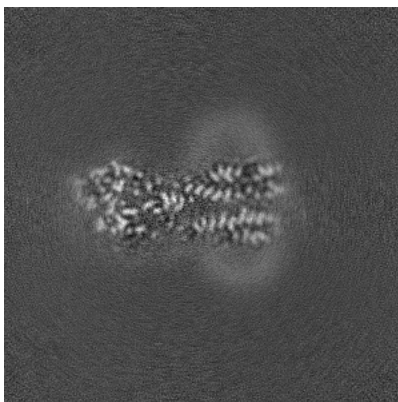


Z Index: 200

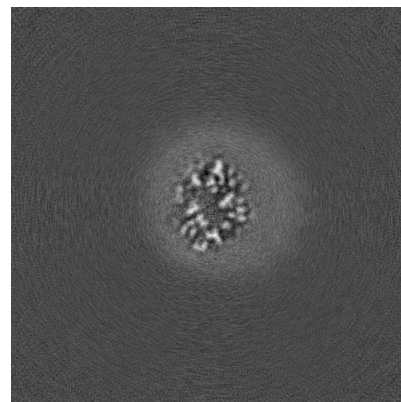
6.2.2 Raw map



X Index: 200



Y Index: 200

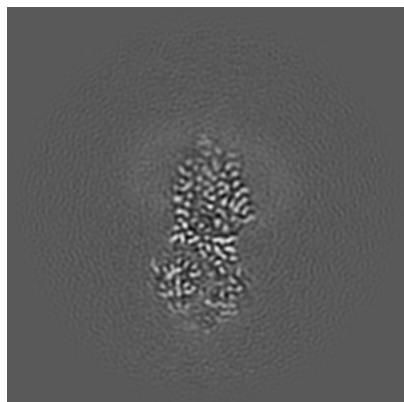


Z Index: 200

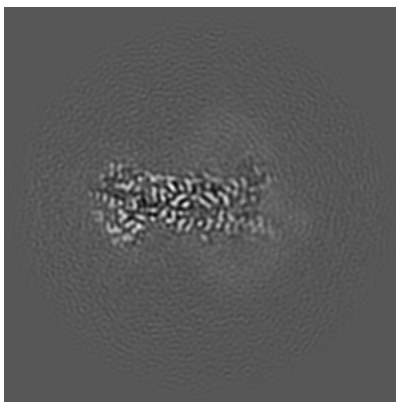
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

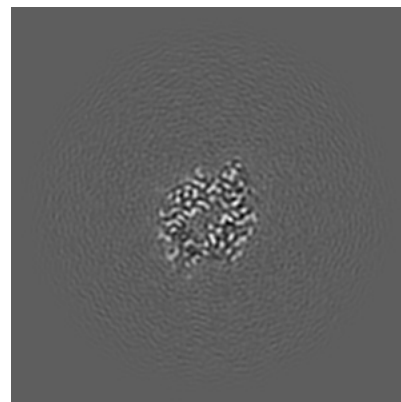
6.3.1 Primary map



X Index: 211

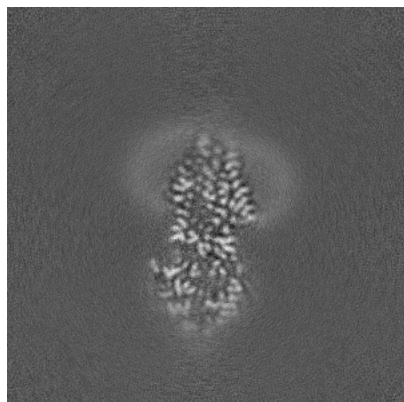


Y Index: 218

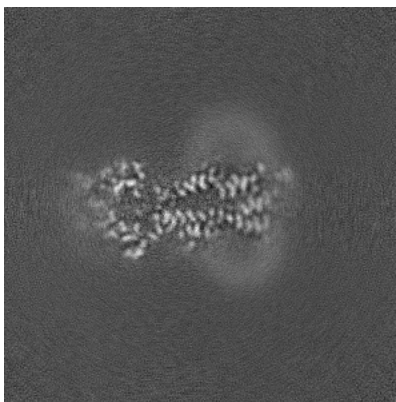


Z Index: 131

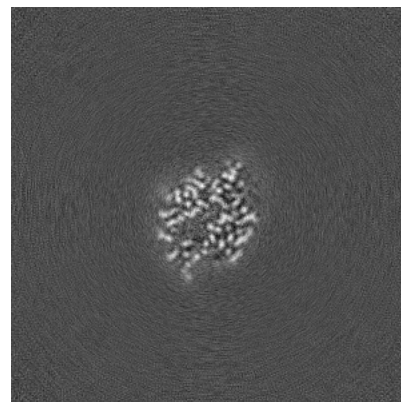
6.3.2 Raw map



X Index: 210



Y Index: 191

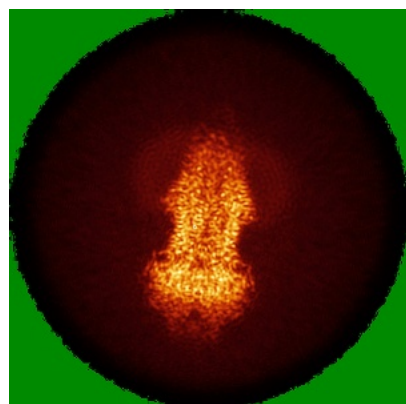


Z Index: 132

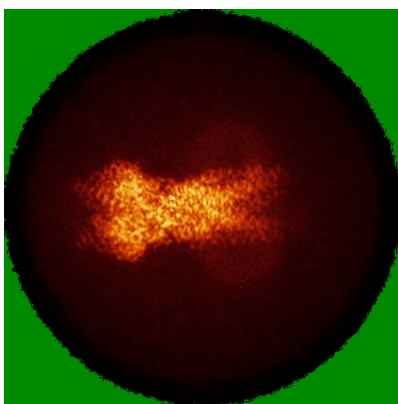
The images above show the largest variance slices of the map in three orthogonal directions.

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

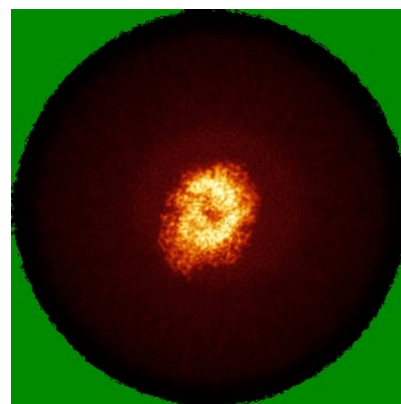
6.4.1 Primary map



X

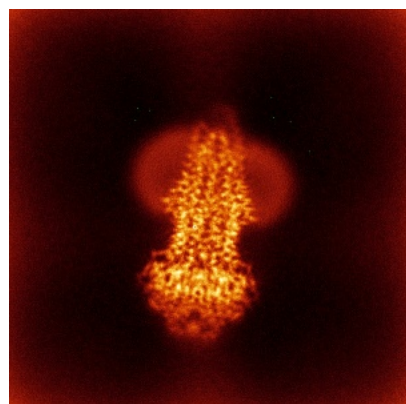


Y

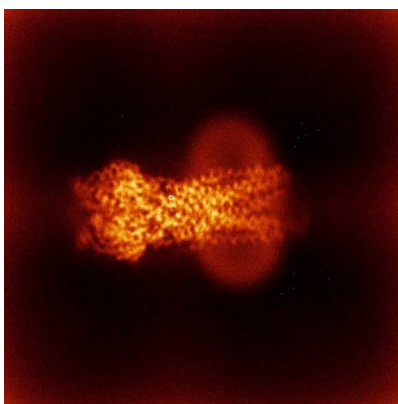


Z

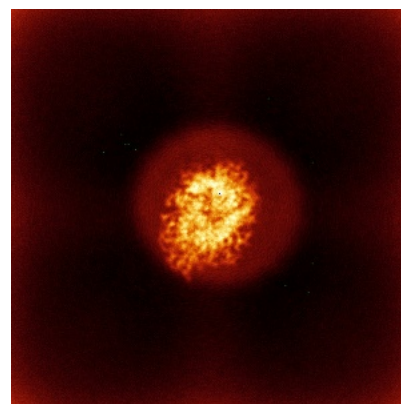
6.4.2 Raw map



X



Y

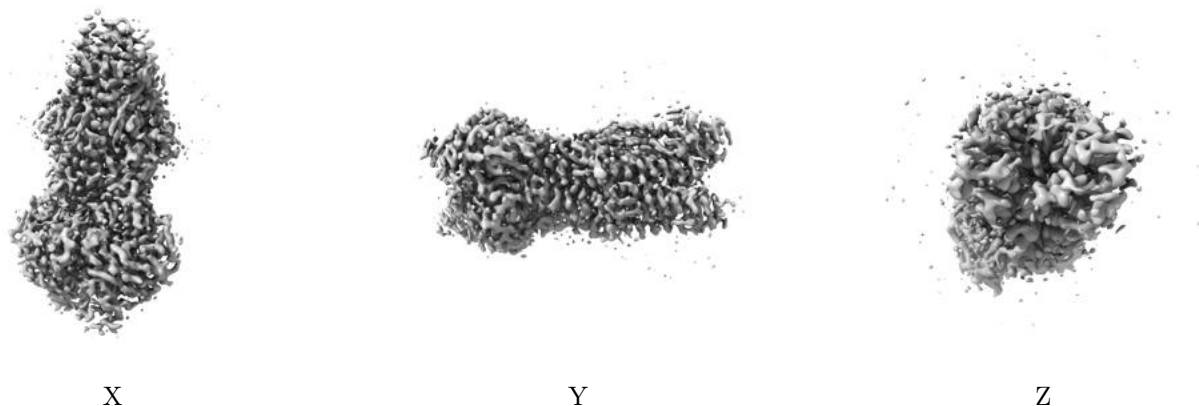


Z

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.

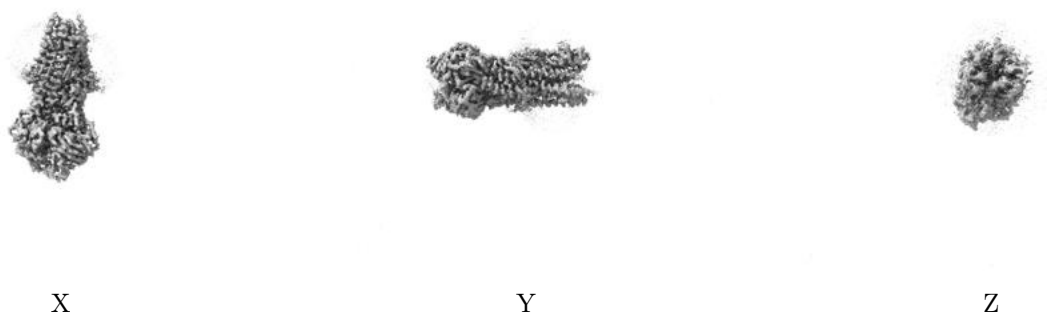
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

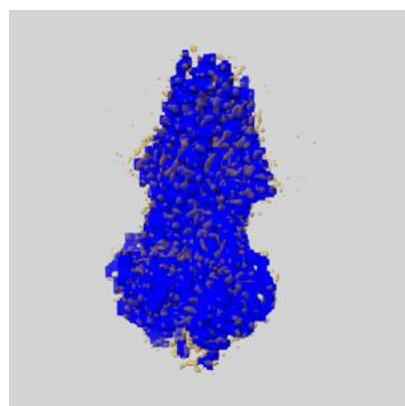
6.6 Mask visualisation [i](#)

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

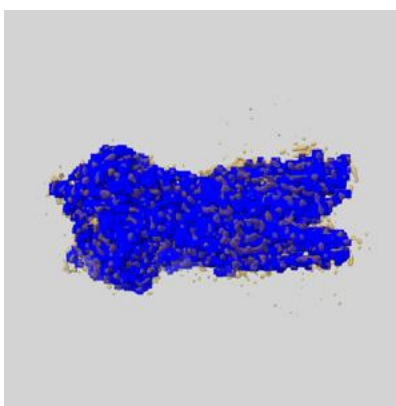
A mask typically either:

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

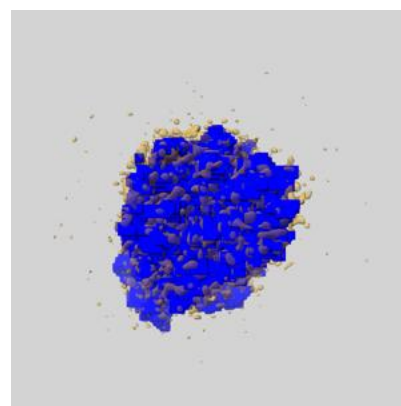
6.6.1 emd_14760_msk_1.map [i](#)



X



Y

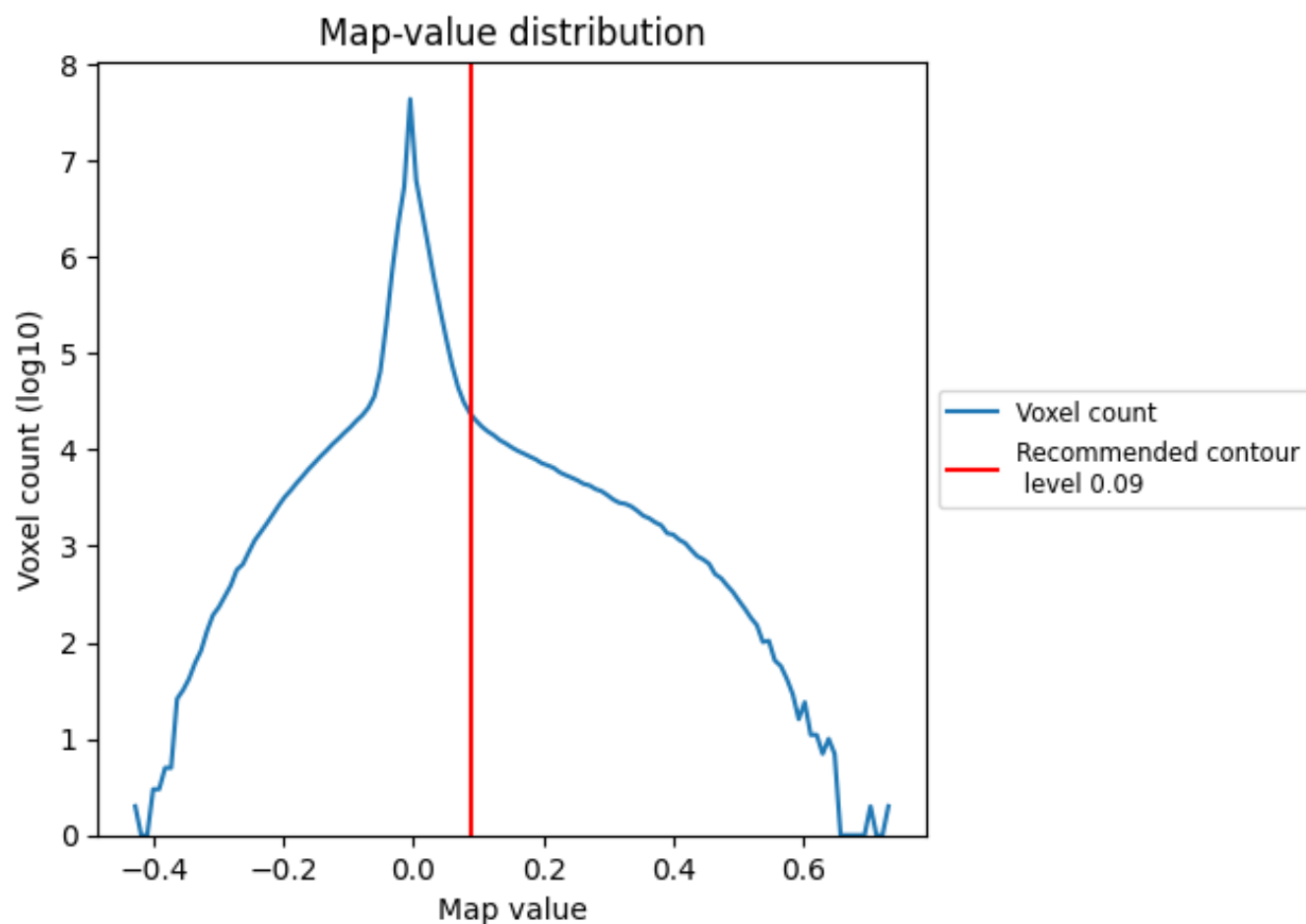


Z

7 Map analysis [i](#)

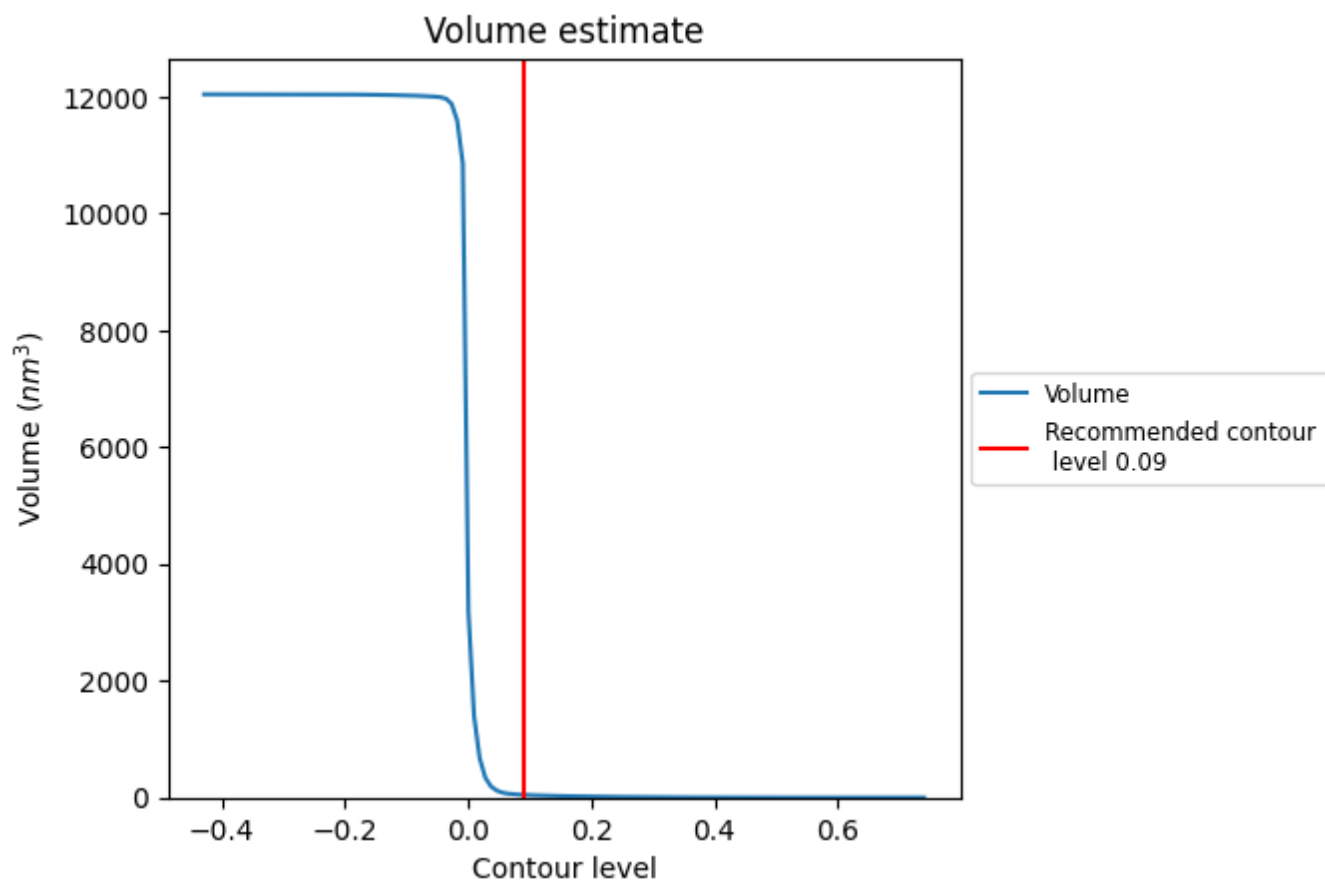
This section contains the results of statistical analysis of the map.

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.

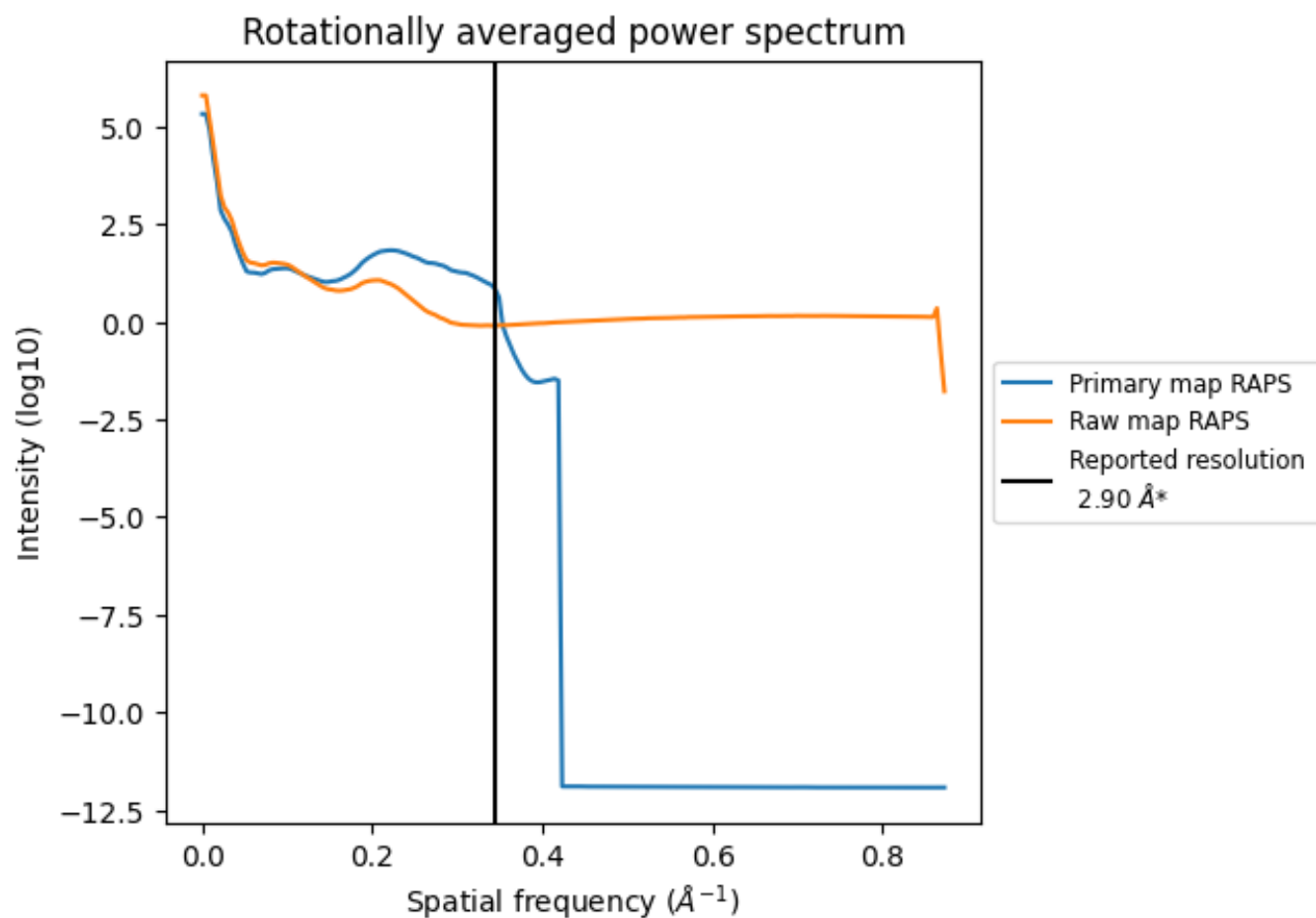
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 42 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 ⓘ

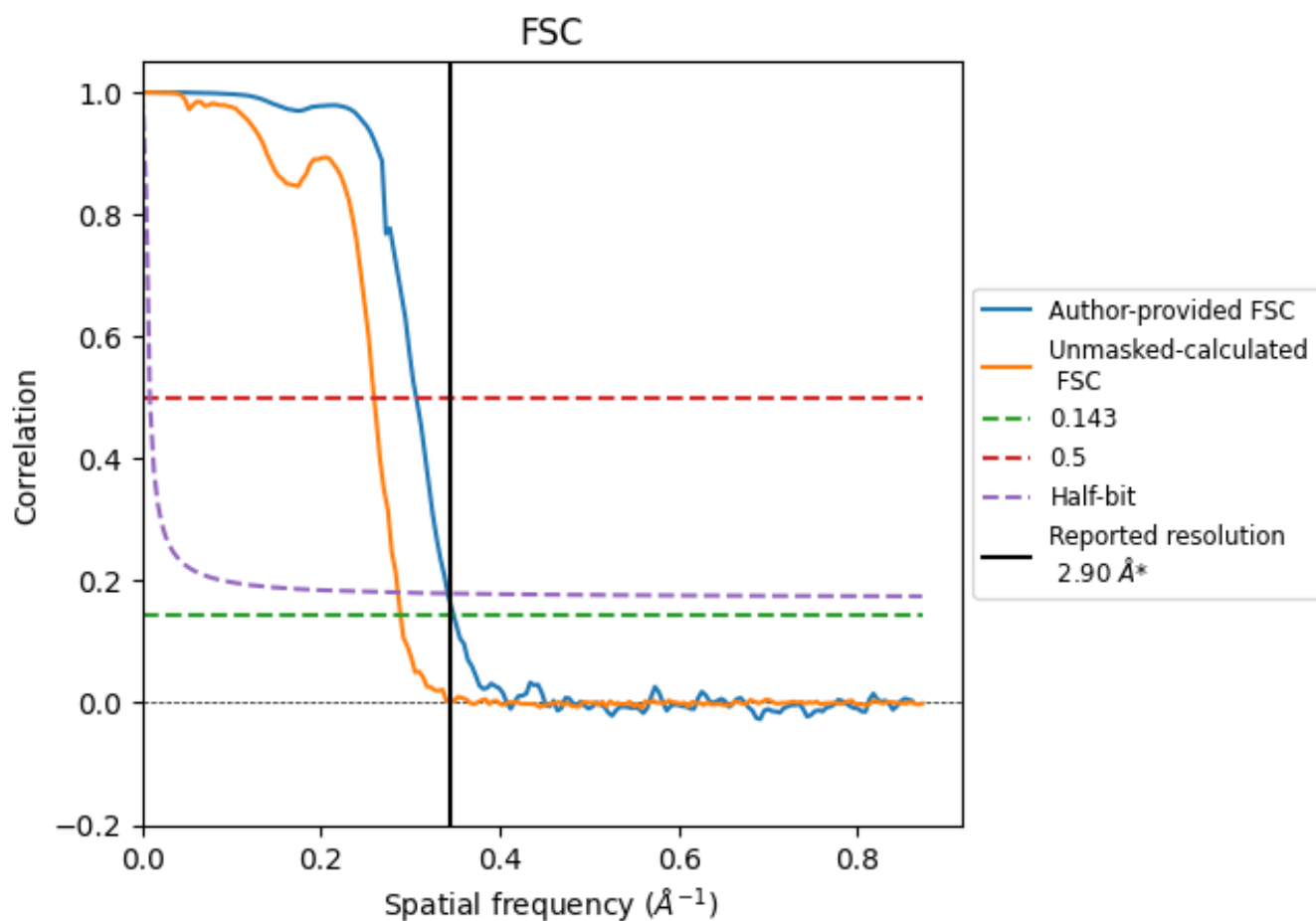


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

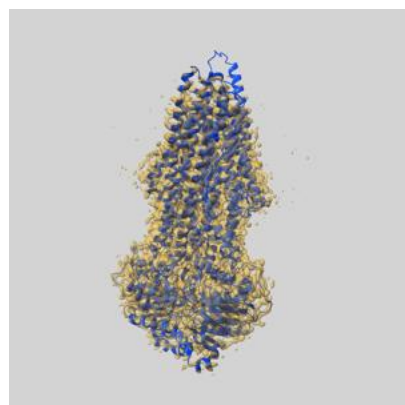
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.26	2.92
Unmasked-calculated*	3.46	3.85	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.9 by more than 10 %

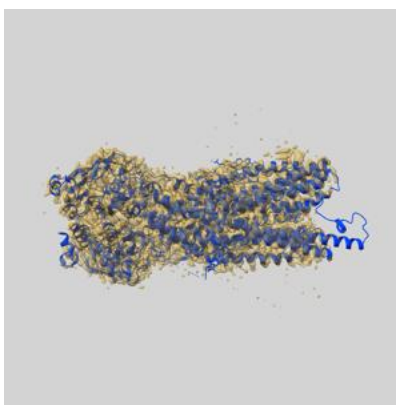
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14760 and PDB model 7ZKA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

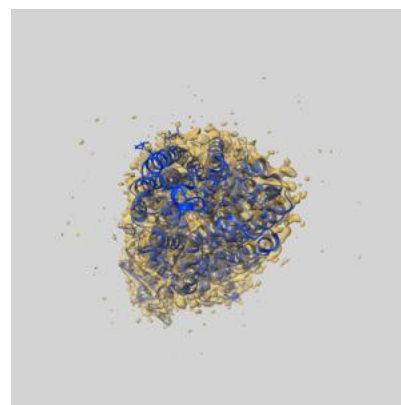
9.1 Map-model overlay [i](#)



X



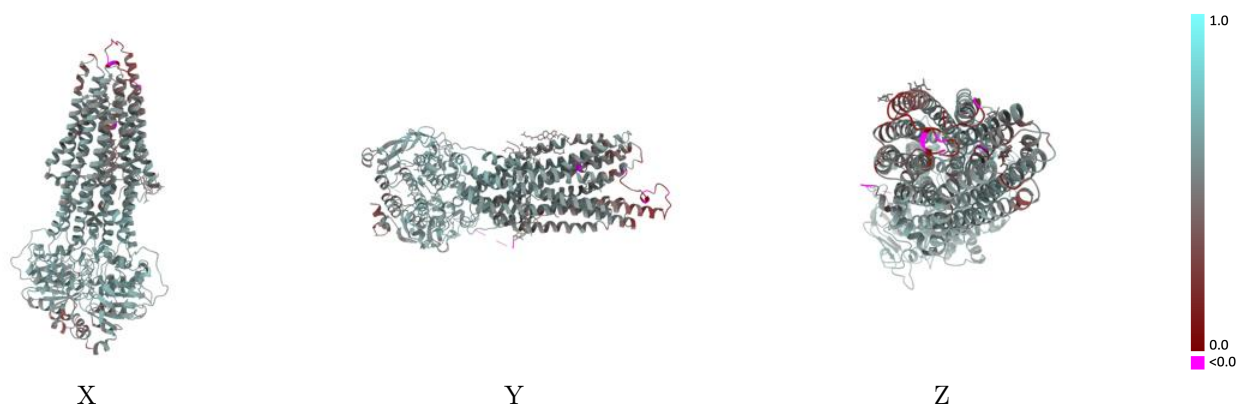
Y



Z

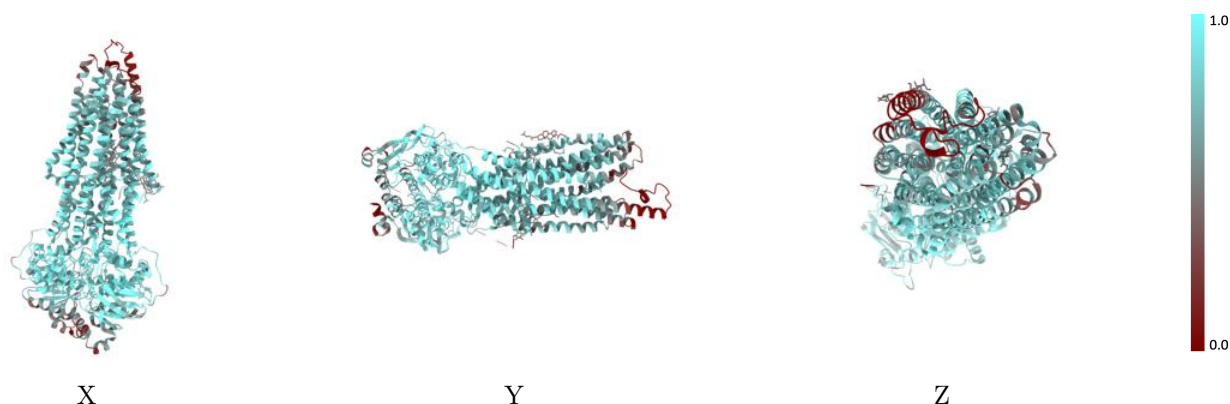
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



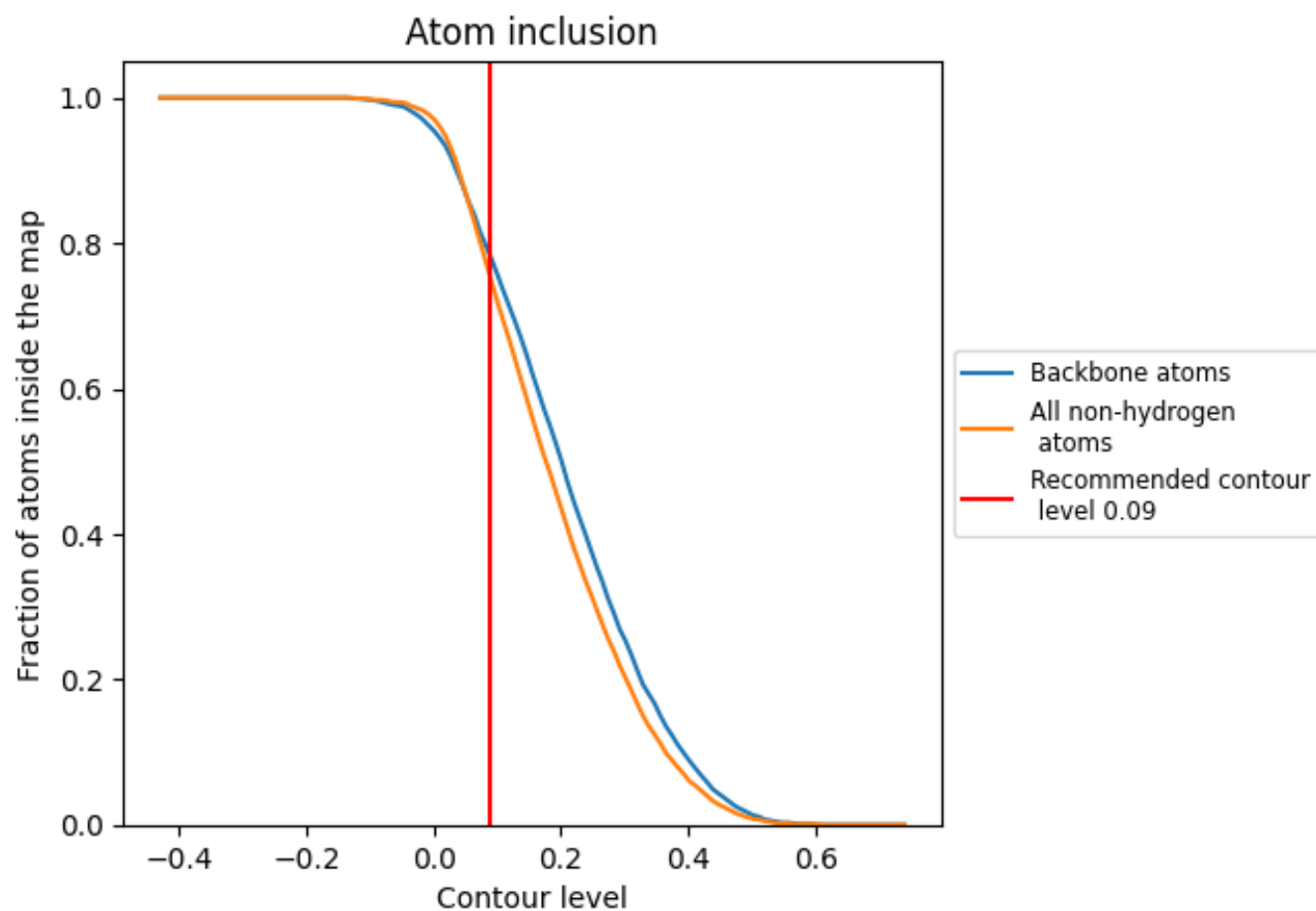
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 75% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.5330
A	0.7520	0.5330

