



Full wwPDB EM Validation Report ⓘ

Nov 16, 2024 – 01:16 PM EST

PDB ID : 8TO8
EMDB ID : EMD-41439
Title : Escherichia coli RNA polymerase unwinding intermediate (I1b) at the lambda PR promoter
Authors : Darst, S.A.; Saecker, R.M.; Mueller, A.U.
Deposited on : 2023-08-03
Resolution : 2.90 Å(reported)

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

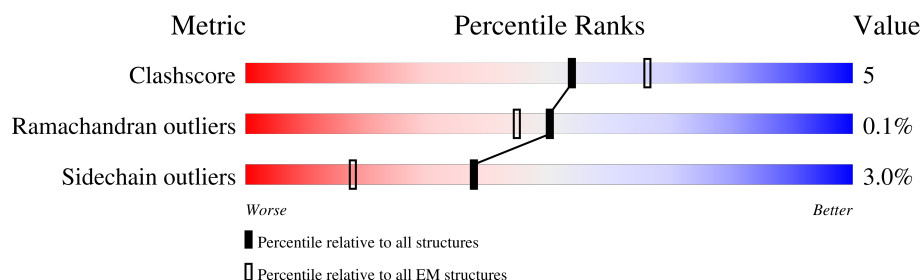
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	G	329	
1	H	329	
1	M	329	
2	I	1342	
3	J	1407	
4	K	91	
5	L	613	
6	O	105	

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Mol	Chain	Length	Quality of chain
7	P	105	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 31131 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	232	Total	C	N	O	S	0	0
			1772	1107	315	344	6		
1	H	219	Total	C	N	O	S	0	0
			1684	1052	298	328	6		
1	M	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1337	Total	C	N	O	S	0	0
			10513	6602	1831	2037	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1336	Total	C	N	O	S	0	0
			10382	6523	1851	1959	49		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	75	Total	C	N	O	S	0	0
			600	365	114	120	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	513	Total	C	N	O	S	0	0
			3999	2501	722	753	23		

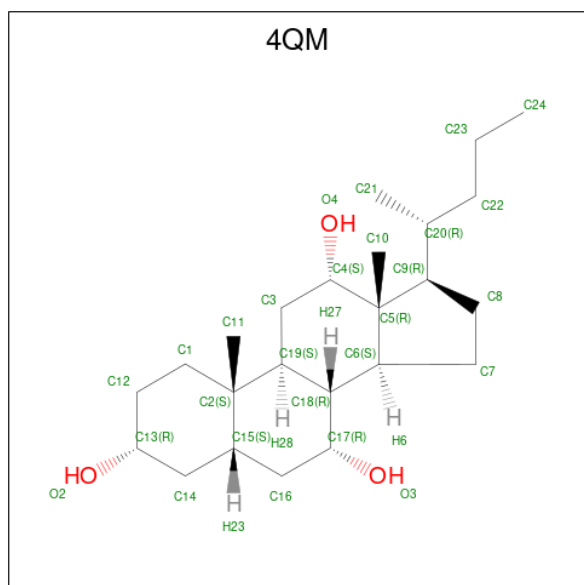
- Molecule 6 is a DNA chain called Nontemplate strand of lambda PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	39	Total	C	N	O	P	0	0
			798	381	135	243	39		

- Molecule 7 is a DNA chain called Template strand of lamdba PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	34	Total	C	N	O	P	0	0
			701	331	140	196	34		

- Molecule 8 is (3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-10,13-dimethyl-17-[(2R)-pentan-2-yl]-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol (three-letter code: 4QM) (formula: C₂₄H₄₂O₃).



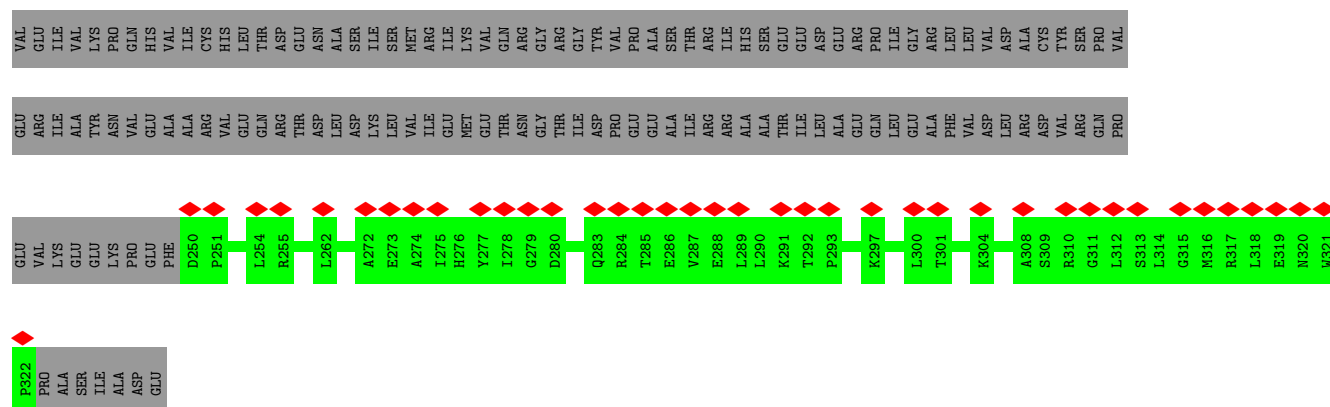
Mol	Chain	Residues	Atoms			AltConf
8	I	1	Total	C	O	0
			27	24	3	
8	I	1	Total	C	O	0
			26	23	3	
8	J	1	Total	C	O	0
			27	24	3	
8	L	1	Total	C	O	0
			27	24	3	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

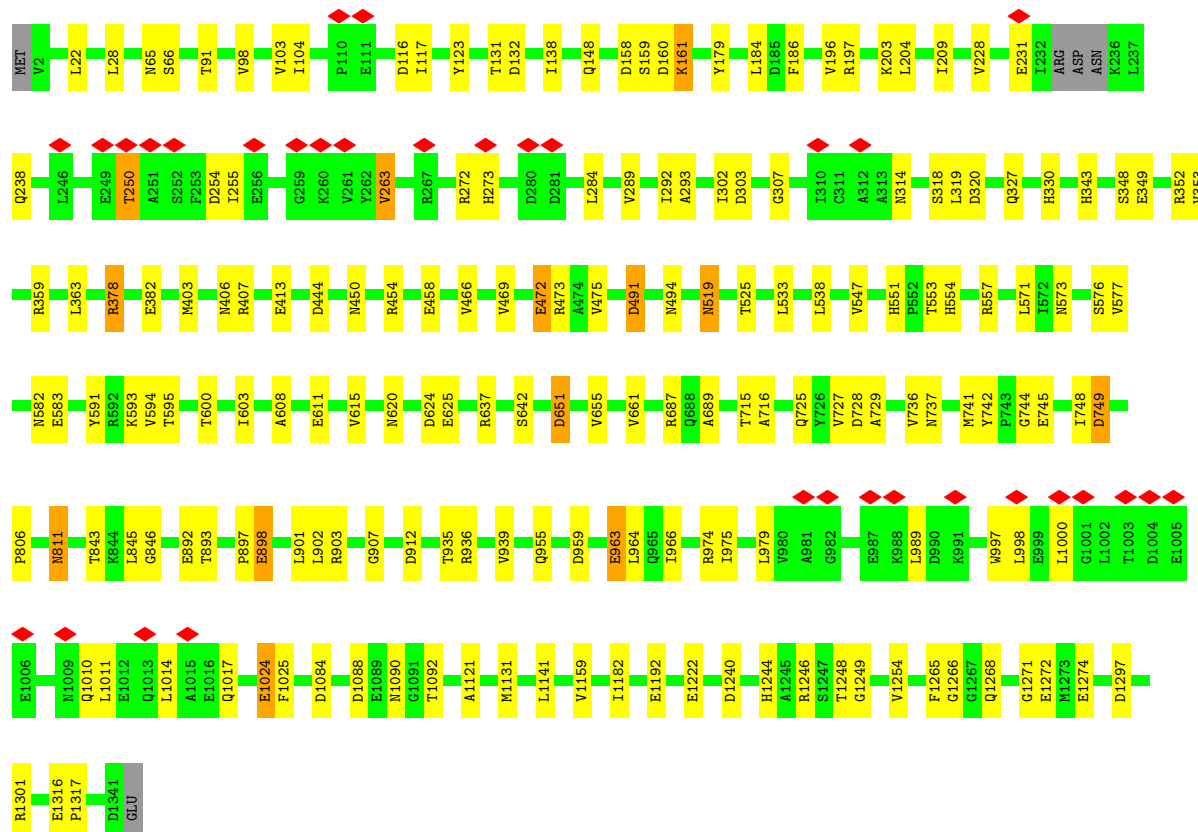
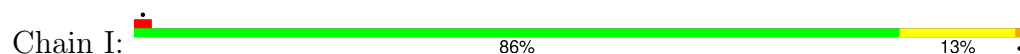
Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

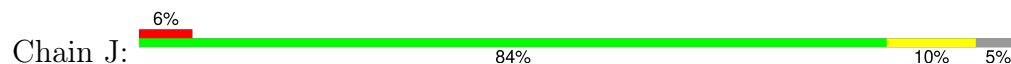
Mol	Chain	Residues	Atoms		AltConf
10	J	2	Total	Zn	0
			2	2	

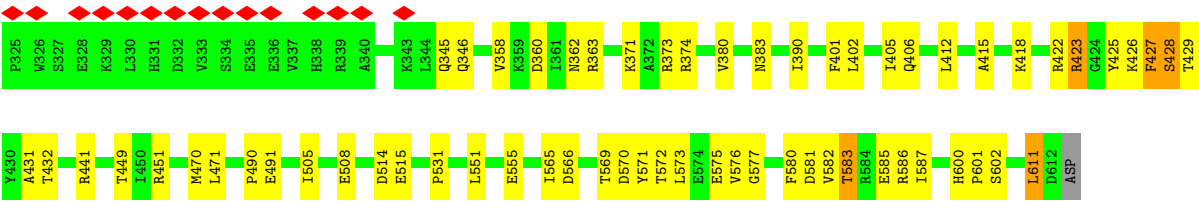


• Molecule 2: DNA-directed RNA polymerase subunit beta

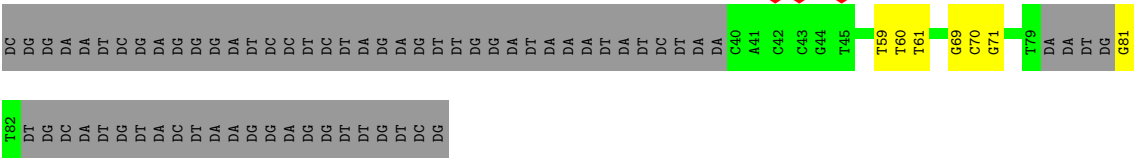


• Molecule 3: DNA-directed RNA polymerase subunit beta'

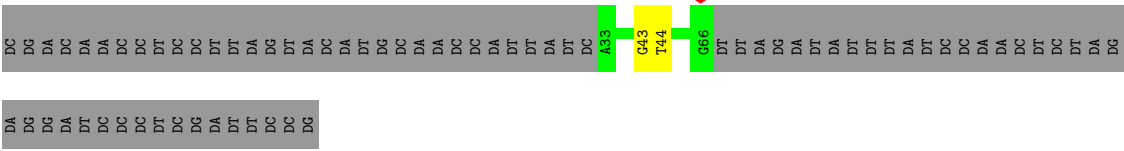




• Molecule 6: Nontemplate strand of lamdba PR promoter DNA



• Molecule 7: Template strand of lamdba PR promoter DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153655	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.373	Depositor
Minimum map value	-2.733	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	324.096, 324.096, 324.096	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84400004, 0.84400004, 0.84400004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 4QM, ZN

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	G	0.28	0/1794	0.53	0/2435
1	H	0.26	0/1703	0.52	0/2308
1	M	0.23	0/579	0.47	0/784
2	I	0.29	0/10680	0.51	0/14413
3	J	0.28	0/10539	0.52	0/14231
4	K	0.25	0/602	0.52	0/810
5	L	0.28	0/4047	0.49	0/5449
6	O	0.52	0/889	0.95	0/1366
7	P	0.51	0/789	0.80	0/1215
All	All	0.30	0/31622	0.54	0/43011

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	L	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	373	ARG	Sidechain
5	L	422	ARG	Sidechain

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	G	1772	0	1791	14	0
1	H	1684	0	1717	27	0
1	M	572	0	602	0	0
2	I	10513	0	10525	106	0
3	J	10382	0	10599	87	0
4	K	600	0	607	4	0
5	L	3999	0	3954	67	0
6	O	798	0	446	7	0
7	P	701	0	379	2	0
8	I	53	0	0	8	0
8	J	27	0	0	5	0
8	L	27	0	0	5	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	31131	0	30620	308	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 5.

All (308) 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)
8:I:1402:4QM:C19	8:I:1402:4QM:C3	1.82	1.57
8:L:701:4QM:C3	8:L:701:4QM:C19	1.83	1.52
8:I:1401:4QM:C3	8:I:1401:4QM:C19	1.82	1.52
8:J:1504:4QM:C19	8:J:1504:4QM:C3	1.82	1.51
2:I:91:THR:OG1	2:I:138:ILE:O	1.94	0.84
1:H:41:ASN:OD1	1:H:44:ARG:NH2	2.15	0.80
5:L:441:ARG:NH2	6:O:71:DG:OP2	2.14	0.79
2:I:349:GLU:N	2:I:349:GLU:OE1	2.16	0.77
5:L:360:ASP:OD1	5:L:363:ARG:NH2	2.18	0.76
1:H:95:LYS:NZ	1:H:120:ASP:OD2	2.13	0.76
2:I:749:ASP:N	2:I:749:ASP:OD1	2.20	0.75
2:I:348:SER:OG	2:I:349:GLU:OE1	2.04	0.74
1:G:45:ARG:NH2	2:I:1084:ASP:OD1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ARG:NH1	1:H:233:ASP:OD1	2.21	0.74
8:L:701:4QM:C3	8:L:701:4QM:C2	2.66	0.73
3:J:1186:TYR:OH	3:J:1188:GLU:OE1	2.06	0.73
5:L:576:VAL:HG13	5:L:587:ILE:HD13	1.71	0.72
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.23	0.72
5:L:570:ASP:OD1	5:L:571:TYR:N	2.22	0.71
8:J:1504:4QM:C3	8:J:1504:4QM:C2	2.66	0.71
3:J:500:ILE:O	3:J:500:ILE:HG22	1.92	0.70
5:L:555:GLU:OE1	5:L:555:GLU:N	2.25	0.70
4:K:42:GLU:N	4:K:42:GLU:OE1	2.25	0.70
5:L:94:THR:O	5:L:95:THR:OG1	2.10	0.70
5:L:161:LEU:O	5:L:265:GLN:NE2	2.24	0.70
3:J:161:THR:OG1	3:J:162:GLU:OE1	2.10	0.70
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.74	0.70
2:I:1316:GLU:N	2:I:1316:GLU:OE1	2.25	0.69
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.09	0.69
8:I:1402:4QM:C3	8:I:1402:4QM:C2	2.65	0.69
3:J:572:THR:HG21	3:J:589:TYR:OH	1.93	0.69
5:L:125:ASP:OD2	5:L:129:GLN:NE2	2.26	0.69
8:I:1401:4QM:C3	8:I:1401:4QM:C2	2.66	0.68
2:I:148:GLN:OE1	2:I:454:ARG:NH1	2.26	0.68
5:L:313:ASP:OD1	5:L:345:GLN:NE2	2.26	0.68
1:H:77:ASP:OD1	1:H:78:ILE:N	2.27	0.67
5:L:575:GLU:N	5:L:575:GLU:OE1	2.28	0.67
2:I:314:ASN:OD1	2:I:352:ARG:NH1	2.27	0.66
5:L:247:GLU:OE1	5:L:247:GLU:N	2.29	0.66
1:G:58:GLU:HG2	1:G:172:LEU:HD23	1.78	0.66
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.12	0.65
3:J:199:GLU:OE1	3:J:200:GLN:N	2.30	0.65
3:J:1233:ILE:O	3:J:1237:VAL:HG12	1.96	0.65
2:I:444:ASP:O	2:I:450:ASN:ND2	2.30	0.64
1:H:93:GLN:OE1	1:H:94:GLY:N	2.30	0.64
2:I:728:ASP:OD1	2:I:729:ALA:N	2.30	0.64
8:J:1504:4QM:C3	8:J:1504:4QM:C18	2.70	0.64
2:I:254:ASP:OD1	2:I:255:ILE:N	2.30	0.63
2:I:1271:GLY:N	2:I:1274:GLU:OE1	2.31	0.63
2:I:318:SER:OG	2:I:320:ASP:OD1	2.07	0.63
3:J:833:GLU:OE1	3:J:1242:ARG:NH1	2.32	0.63
2:I:378:ARG:NH2	2:I:382:GLU:OE1	2.31	0.63
3:J:1276:GLU:OE1	3:J:1276:GLU:N	2.32	0.63
5:L:16:GLY:O	5:L:20:GLY:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.18	0.62
1:H:192:VAL:HG23	1:H:198:LEU:HD12	1.82	0.61
8:I:1402:4QM:C3	8:I:1402:4QM:C18	2.70	0.61
5:L:292:VAL:O	5:L:296:LYS:N	2.34	0.61
3:J:707:ILE:HA	3:J:708:ASN:HB2	1.83	0.61
3:J:1057:SER:OG	3:J:1110:GLU:OE2	2.20	0.60
2:I:403:MET:SD	2:I:407:ARG:NH2	2.74	0.60
1:H:61:ILE:HB	1:H:64:VAL:HG22	1.84	0.60
2:I:65:ASN:OD1	2:I:66:SER:N	2.35	0.60
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.84	0.60
5:L:582:VAL:HG11	5:L:586:ARG:HB3	1.83	0.60
3:J:661:VAL:HG23	3:J:682:VAL:HG22	1.83	0.59
3:J:256:ASP:OD1	8:J:1504:4QM:O2	2.20	0.59
2:I:472:GLU:OE1	2:I:473:ARG:N	2.36	0.59
5:L:380:VAL:HG13	5:L:412:LEU:HD23	1.84	0.59
5:L:138:PRO:O	5:L:141:ILE:HG22	2.02	0.59
5:L:145:LEU:HD21	5:L:224:LEU:HG	1.83	0.59
3:J:495:ASN:N	3:J:495:ASN:OD1	2.36	0.58
5:L:577:GLY:HA2	5:L:587:ILE:HD11	1.84	0.58
1:G:182:ARG:NH1	2:I:1090:ASN:O	2.36	0.58
2:I:935:THR:HB	2:I:939:VAL:HG21	1.86	0.58
3:J:137:ARG:HH22	3:J:159:ILE:HD13	1.68	0.58
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.22	0.58
3:J:147:ILE:HG22	3:J:188:LEU:CD1	2.34	0.58
5:L:293:GLU:OE1	5:L:293:GLU:N	2.37	0.58
5:L:415:ALA:O	5:L:418:LYS:N	2.35	0.58
3:J:162:GLU:OE1	3:J:162:GLU:N	2.34	0.57
3:J:1329:THR:O	3:J:1333:THR:OG1	2.13	0.57
2:I:406:ASN:ND2	2:I:413:GLU:O	2.38	0.57
3:J:137:ARG:NH2	3:J:159:ILE:HD13	2.20	0.57
1:H:127:GLN:N	1:H:127:GLN:OE1	2.36	0.57
3:J:1164:SER:N	3:J:1176:VAL:O	2.38	0.57
5:L:401:PHE:CZ	5:L:405:ILE:HD11	2.39	0.57
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.37	0.57
8:L:701:4QM:C3	8:L:701:4QM:C18	2.72	0.57
3:J:450:HIS:O	3:J:453:VAL:HG22	2.05	0.56
2:I:651:ASP:OD1	2:I:651:ASP:N	2.38	0.56
8:I:1401:4QM:C3	8:I:1401:4QM:C18	2.69	0.56
1:G:77:ASP:OD1	1:G:77:ASP:N	2.35	0.56
2:I:1024:GLU:OE1	2:I:1025:PHE:N	2.39	0.56
5:L:427:PHE:C	5:L:429:THR:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:148:GLU:OE2	3:J:156:ARG:NE	2.39	0.56
3:J:733:SER:OG	3:J:736:GLN:OE1	2.24	0.56
3:J:572:THR:HG21	3:J:589:TYR:CE2	2.41	0.56
3:J:825:VAL:HG12	3:J:833:GLU:HB3	1.88	0.56
2:I:158:ASP:OD1	2:I:159:SER:N	2.37	0.55
3:J:155:GLU:OE1	3:J:155:GLU:N	2.38	0.55
3:J:1226:VAL:HG13	3:J:1261:LEU:HD11	1.88	0.55
2:I:902:LEU:HD21	5:L:611:LEU:HG	1.88	0.55
2:I:1268:GLN:OE1	3:J:352:ARG:NH1	2.39	0.55
5:L:427:PHE:O	5:L:429:THR:N	2.40	0.55
2:I:936:ARG:O	2:I:939:VAL:HG22	2.07	0.55
5:L:358:VAL:O	5:L:362:ASN:ND2	2.39	0.55
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.35	0.54
3:J:70:CYS:SG	3:J:71:LEU:N	2.81	0.54
5:L:127:ILE:O	5:L:130:VAL:HG22	2.08	0.54
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.40	0.54
3:J:1361:THR:HG22	4:K:21:LEU:HD21	1.90	0.54
2:I:519:ASN:ND2	2:I:689:ALA:O	2.41	0.54
2:I:196:VAL:HG21	2:I:209:ILE:HD12	1.88	0.54
5:L:426:LYS:O	5:L:427:PHE:C	2.47	0.54
3:J:24:LEU:HD21	3:J:116:PHE:CZ	2.44	0.54
3:J:298:MET:HG2	5:L:402:LEU:HD23	1.90	0.54
2:I:1244:HIS:NE2	2:I:1266:GLY:O	2.38	0.53
2:I:1246:ARG:NH1	2:I:1265:PHE:O	2.40	0.53
3:J:1051:ASP:O	3:J:1055:GLY:N	2.40	0.52
1:G:159:ILE:HG23	1:G:159:ILE:O	2.10	0.52
2:I:624:ASP:OD1	2:I:625:GLU:N	2.38	0.52
7:P:43:DG:H2'	7:P:44:DT:H72	1.91	0.52
2:I:620:ASN:ND2	2:I:620:ASN:O	2.42	0.52
2:I:353:VAL:HG12	2:I:353:VAL:O	2.09	0.52
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.92	0.52
1:H:197:ASP:N	1:H:197:ASP:OD1	2.43	0.52
2:I:577:VAL:HG23	2:I:661:VAL:O	2.10	0.51
2:I:892:GLU:O	2:I:893:THR:OG1	2.28	0.51
1:H:54:CYS:SG	1:H:92:VAL:HG12	2.50	0.51
1:H:202:VAL:HG12	1:H:202:VAL:O	2.11	0.51
3:J:1344:LEU:H	3:J:1344:LEU:HD22	1.75	0.51
6:O:69:DG:H4'	6:O:70:DC:OP1	2.11	0.51
3:J:393:THR:OG1	3:J:394:ILE:N	2.44	0.50
2:I:104:ILE:HD11	2:I:116:ASP:HB3	1.92	0.50
2:I:843:THR:OG1	2:I:846:GLY:O	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:427:PHE:HD1	5:L:431:ALA:HB2	1.76	0.50
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.94	0.50
2:I:1248:THR:HG21	5:L:531:PRO:HG2	1.93	0.50
1:H:172:LEU:HD23	1:H:172:LEU:H	1.76	0.50
2:I:203:LYS:O	2:I:204:LEU:HD12	2.11	0.49
2:I:897:PRO:O	2:I:898:GLU:HB2	2.12	0.49
2:I:303:ASP:O	2:I:307:GLY:N	2.45	0.49
3:J:1164:SER:OG	3:J:1176:VAL:O	2.25	0.49
5:L:371:LYS:O	5:L:374:ARG:HG3	2.12	0.49
2:I:231:GLU:O	2:I:238:GLN:N	2.43	0.49
2:I:963:GLU:OE1	2:I:964:LEU:N	2.45	0.49
5:L:601:PRO:O	5:L:602:SER:OG	2.29	0.49
3:J:891:ASP:OD1	3:J:1286:LYS:NZ	2.42	0.48
5:L:309:ASN:OD1	5:L:311:THR:OG1	2.31	0.48
3:J:202:ARG:NH2	3:J:225:GLU:OE2	2.43	0.48
5:L:143:TYR:CD2	5:L:269:LEU:HD21	2.49	0.48
1:H:118:ASP:HB3	1:H:121:VAL:HG22	1.96	0.48
2:I:748:ILE:HD12	2:I:966:ILE:HG22	1.94	0.48
2:I:897:PRO:O	2:I:898:GLU:CB	2.62	0.48
3:J:134:ASP:OD2	3:J:159:ILE:HD11	2.13	0.48
1:G:224:LEU:HD23	1:H:228:LEU:HD11	1.96	0.48
2:I:292:ILE:O	2:I:292:ILE:HG22	2.14	0.48
1:H:207:THR:HG22	1:H:208:ASN:H	1.79	0.48
3:J:500:ILE:O	3:J:500:ILE:CG2	2.61	0.48
5:L:234:THR:OG1	5:L:248:GLU:OE1	2.24	0.48
3:J:963:VAL:HG23	3:J:975:ILE:HG23	1.96	0.48
6:O:59:DT:H4'	6:O:60:DT:OP1	2.12	0.48
2:I:1272:GLU:OE1	3:J:798:ARG:NH1	2.44	0.47
2:I:955:GLN:NE2	2:I:959:ASP:OD1	2.47	0.47
2:I:491:ASP:N	2:I:491:ASP:OD1	2.47	0.47
1:G:13:LEU:HD21	1:G:26:VAL:HG23	1.97	0.47
3:J:528:THR:O	3:J:528:THR:HG22	2.15	0.47
3:J:572:THR:HG21	3:J:589:TYR:CZ	2.49	0.47
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.97	0.47
2:I:1131:MET:HE3	2:I:1141:LEU:HD12	1.97	0.47
5:L:600:HIS:ND1	5:L:601:PRO:O	2.44	0.47
1:H:196:THR:HG22	1:H:196:THR:O	2.15	0.47
3:J:294:ASN:OD1	5:L:406:GLN:NE2	2.45	0.47
5:L:572:THR:OG1	5:L:573:LEU:N	2.47	0.47
8:L:701:4QM:C3	8:L:701:4QM:C1	2.93	0.47
5:L:451:ARG:NH2	6:O:70:DC:OP2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:VAL:HG13	1:G:233:ASP:N	2.30	0.46
3:J:961:SER:OG	3:J:983:LYS:NZ	2.48	0.46
3:J:1158:GLU:OE1	3:J:1222:ARG:NH1	2.48	0.46
1:G:14:VAL:HG11	1:G:29:GLU:HB2	1.98	0.46
2:I:302:ILE:O	2:I:330:HIS:NE2	2.39	0.46
2:I:582:ASN:OD1	2:I:583:GLU:N	2.46	0.46
2:I:741:MET:O	2:I:742:TYR:HB2	2.15	0.46
2:I:901:LEU:HD22	5:L:565:ILE:HD11	1.97	0.46
3:J:111:THR:O	3:J:239:LEU:N	2.46	0.46
3:J:492:SER:O	3:J:495:ASN:O	2.34	0.46
5:L:244:THR:HG22	5:L:244:THR:O	2.16	0.46
2:I:553:THR:CG2	2:I:608:ALA:HB1	2.46	0.46
2:I:1010:GLN:O	2:I:1014:LEU:HD13	2.16	0.46
2:I:132:ASP:OD1	2:I:132:ASP:N	2.49	0.46
3:J:146:VAL:CG2	3:J:160:LEU:HD11	2.45	0.46
3:J:827:GLU:OE1	3:J:827:GLU:N	2.49	0.46
2:I:184:LEU:HD21	2:I:186:PHE:CZ	2.51	0.45
2:I:466:VAL:O	2:I:469:VAL:HG12	2.16	0.45
2:I:576:SER:OG	2:I:577:VAL:N	2.47	0.45
3:J:220:ARG:O	3:J:224:LEU:HD23	2.16	0.45
1:H:5:VAL:O	1:H:5:VAL:HG22	2.16	0.45
2:I:594:VAL:HG12	2:I:595:THR:O	2.17	0.45
2:I:184:LEU:C	2:I:184:LEU:HD23	2.36	0.45
3:J:706:VAL:HG11	3:J:716:GLN:NE2	2.30	0.45
8:J:1504:4QM:C3	8:J:1504:4QM:C1	2.94	0.45
2:I:845:LEU:HD12	2:I:845:LEU:H	1.81	0.45
3:J:1072:LYS:O	3:J:1075:ARG:NH1	2.50	0.45
2:I:131:THR:HG22	2:I:132:ASP:N	2.32	0.45
3:J:489:ASN:OD1	3:J:489:ASN:N	2.48	0.45
5:L:569:THR:HG22	5:L:570:ASP:N	2.32	0.45
5:L:163:THR:HG23	5:L:262:VAL:HG22	1.97	0.45
2:I:557:ARG:NH2	2:I:611:GLU:OE1	2.39	0.45
3:J:120:LEU:HB2	3:J:121:PRO:HD3	1.99	0.45
5:L:390:ILE:HD12	5:L:432:THR:HG23	1.99	0.45
5:L:427:PHE:CD1	5:L:431:ALA:HB2	2.52	0.45
1:H:192:VAL:HG23	1:H:198:LEU:CD1	2.45	0.45
2:I:637:ARG:HA	2:I:642:SER:HA	1.98	0.44
2:I:806:PRO:O	2:I:811:ASN:ND2	2.47	0.44
2:I:975:ILE:HG23	2:I:1011:LEU:HD22	1.98	0.44
2:I:615:VAL:HG23	2:I:615:VAL:O	2.16	0.44
2:I:901:LEU:HD22	5:L:565:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:510:LEU:HD11	3:J:624:ILE:HG23	1.98	0.44
2:I:715:THR:HG22	2:I:716:ALA:H	1.83	0.44
4:K:15:ASN:OD1	4:K:16:ARG:N	2.51	0.44
1:H:78:ILE:HD13	1:H:81:ILE:HD12	1.99	0.44
5:L:427:PHE:C	5:L:429:THR:N	2.71	0.44
5:L:577:GLY:CA	5:L:587:ILE:HD11	2.47	0.44
2:I:22:LEU:HD13	2:I:603:ILE:HD13	2.00	0.44
2:I:748:ILE:HD12	2:I:966:ILE:CG2	2.48	0.44
2:I:1297:ASP:OD2	2:I:1317:PRO:O	2.36	0.44
5:L:228:TYR:OH	5:L:232:ARG:NH1	2.51	0.44
1:H:83:LEU:HD11	3:J:526:VAL:HG12	2.00	0.43
2:I:1121:ALA:HB2	2:I:1182:ILE:HD12	2.00	0.43
5:L:147:GLN:NE2	5:L:265:GLN:OE1	2.52	0.43
1:G:16:ILE:N	1:G:16:ILE:HD12	2.33	0.43
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.51	0.43
2:I:1088:ASP:OD1	2:I:1092:THR:OG1	2.32	0.43
3:J:127:LEU:O	3:J:220:ARG:NH2	2.51	0.43
2:I:903:ARG:O	2:I:907:GLY:N	2.52	0.43
8:I:1402:4QM:C3	8:I:1402:4QM:C1	2.96	0.43
5:L:98:VAL:HG11	6:O:81:DG:H22	1.84	0.43
5:L:514:ASP:OD1	5:L:515:GLU:N	2.52	0.43
2:I:997:TRP:HE3	2:I:1000:LEU:HD11	1.84	0.43
8:I:1401:4QM:C3	8:I:1401:4QM:C1	2.96	0.43
5:L:235:ILE:O	5:L:235:ILE:HG22	2.19	0.43
2:I:715:THR:HG22	2:I:716:ALA:N	2.33	0.42
1:H:133:LEU:O	1:H:134:THR:HG22	2.18	0.42
5:L:145:LEU:HD22	5:L:225:ARG:HG2	1.99	0.42
2:I:745:GLU:O	2:I:974:ARG:NH1	2.44	0.42
5:L:505:ILE:HD11	8:L:701:4QM:C16	2.48	0.42
2:I:250:THR:HG23	2:I:250:THR:O	2.18	0.42
3:J:349:TYR:HB3	3:J:470:VAL:HG13	2.00	0.42
1:G:224:LEU:CD2	1:H:228:LEU:HD11	2.48	0.42
3:J:572:THR:HG21	3:J:589:TYR:HE2	1.84	0.42
2:I:359:ARG:O	2:I:363:LEU:HD13	2.20	0.42
3:J:880:VAL:HG12	3:J:881:LYS:N	2.35	0.42
2:I:160:ASP:O	2:I:161:LYS:HG2	2.20	0.42
3:J:147:ILE:O	3:J:147:ILE:CG1	2.67	0.42
4:K:8:ASP:O	4:K:12:LYS:HG2	2.20	0.42
5:L:577:GLY:O	5:L:581:ASP:N	2.53	0.42
6:O:69:DG:H2''	6:O:70:DC:O5'	2.20	0.42
2:I:494:ASN:OD1	2:I:494:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1211:SER:OG	3:J:1212:ASP:N	2.51	0.42
1:H:64:VAL:HG11	1:H:78:ILE:HG13	2.02	0.42
3:J:325:LYS:HD3	5:L:508:GLU:HG2	2.01	0.42
3:J:161:THR:HG1	3:J:162:GLU:H	1.68	0.41
3:J:1038:THR:OG1	3:J:1077:ALA:O	2.26	0.41
2:I:289:VAL:HG22	2:I:319:LEU:HD22	2.02	0.41
2:I:547:VAL:O	2:I:547:VAL:HG22	2.20	0.41
3:J:279:LEU:HD23	3:J:279:LEU:O	2.19	0.41
2:I:744:GLY:O	2:I:1017:GLN:NE2	2.50	0.41
3:J:857:LEU:HD11	3:J:871:LEU:HD21	2.02	0.41
5:L:426:LYS:O	5:L:429:THR:N	2.52	0.41
2:I:103:VAL:HG12	2:I:117:ILE:HG22	2.01	0.41
2:I:736:VAL:HG12	2:I:737:ASN:N	2.36	0.41
2:I:998:LEU:HD12	2:I:998:LEU:N	2.36	0.41
3:J:912:GLY:O	3:J:1359:ALA:O	2.39	0.41
1:H:19:VAL:O	1:H:19:VAL:HG12	2.21	0.41
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.55	0.41
3:J:726:ALA:HB2	3:J:737:ILE:HD11	2.01	0.41
2:I:593:LYS:O	2:I:600:THR:OG1	2.35	0.41
2:I:979:LEU:HD13	2:I:989:LEU:HD11	2.03	0.41
5:L:118:ASP:O	5:L:121:LYS:HG2	2.20	0.41
5:L:124:GLU:OE1	5:L:128:ASN:ND2	2.54	0.41
5:L:490:PRO:O	5:L:491:GLU:HB3	2.21	0.41
1:H:5:VAL:HG13	1:H:6:THR:HG23	2.03	0.41
3:J:138:VAL:HG21	3:J:145:VAL:CG2	2.51	0.41
3:J:342:LEU:HD13	3:J:1352:ILE:HG23	2.02	0.41
5:L:583:THR:O	5:L:585:GLU:N	2.54	0.41
2:I:131:THR:HG22	2:I:132:ASP:OD1	2.21	0.41
2:I:525:THR:HG21	2:I:687:ARG:CD	2.51	0.41
2:I:811:ASN:ND2	2:I:811:ASN:O	2.47	0.41
7:P:43:DG:H2'	7:P:44:DT:C7	2.51	0.41
2:I:551:HIS:CE1	2:I:553:THR:HG1	2.38	0.40
3:J:357:VAL:O	3:J:449:LEU:O	2.40	0.40
5:L:426:LYS:O	5:L:428:SER:N	2.53	0.40
2:I:284:LEU:HD23	2:I:284:LEU:N	2.36	0.40
2:I:1248:THR:HG22	2:I:1249:GLY:N	2.37	0.40
3:J:333:GLY:O	3:J:339:ARG:NH1	2.49	0.40
3:J:382:TYR:HE1	3:J:401:VAL:HG21	1.86	0.40
5:L:118:ASP:OD1	5:L:118:ASP:N	2.54	0.40
1:G:98:VAL:HG22	1:G:99:ILE:N	2.36	0.40
1:H:78:ILE:O	1:H:79:LEU:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:263:VAL:HG21	2:I:273:HIS:CE1	2.57	0.40
2:I:293:ALA:HB2	2:I:319:LEU:HD21	2.02	0.40
3:J:1109:LEU:N	3:J:1109:LEU:HD12	2.36	0.40
3:J:1273:ASP:OD1	3:J:1273:ASP:N	2.54	0.40
3:J:1287:ILE:HG22	3:J:1290:ARG:NH2	2.36	0.40
5:L:423:ARG:HD3	5:L:425:TYR:CD2	2.57	0.40
5:L:426:LYS:HG3	5:L:429:THR:OG1	2.21	0.40
6:O:60:DT:H2'	6:O:61:DT:H72	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	G	230/329 (70%)	219 (95%)	11 (5%)	0	100	100
1	H	215/329 (65%)	199 (93%)	15 (7%)	1 (0%)	25	56
1	M	71/329 (22%)	69 (97%)	2 (3%)	0	100	100
2	I	1333/1342 (99%)	1244 (93%)	88 (7%)	1 (0%)	48	77
3	J	1330/1407 (94%)	1268 (95%)	62 (5%)	0	100	100
4	K	73/91 (80%)	70 (96%)	3 (4%)	0	100	100
5	L	503/613 (82%)	477 (95%)	25 (5%)	1 (0%)	44	73
All	All	3755/4440 (85%)	3546 (94%)	206 (6%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	898	GLU
1	H	69	SER
5	L	428	SER

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	G	193/286 (68%)	185 (96%)	8 (4%)	26	60
1	H	186/286 (65%)	176 (95%)	10 (5%)	18	49
1	M	65/286 (23%)	65 (100%)	0	100	100
2	I	1145/1157 (99%)	1114 (97%)	31 (3%)	40	73
3	J	1118/1168 (96%)	1088 (97%)	30 (3%)	40	73
4	K	65/75 (87%)	64 (98%)	1 (2%)	60	85
5	L	408/540 (76%)	393 (96%)	15 (4%)	29	64
All	All	3180/3798 (84%)	3085 (97%)	95 (3%)	37	71

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	56	VAL
1	G	62	ASP
1	G	77	ASP
1	G	96	ASP
1	G	100	LEU
1	G	177	TYR
1	G	210	THR
1	G	231	PHE
1	H	13	LEU
1	H	14	VAL
1	H	15	ASP
1	H	27	THR
1	H	70	THR
1	H	111	THR
1	H	134	THR
1	H	146	VAL
1	H	170	ARG
1	H	204	GLU
2	I	28	LEU
2	I	98	VAL

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Mol	Chain	Res	Type
2	I	123	TYR
2	I	161	LYS
2	I	197	ARG
2	I	228	VAL
2	I	250	THR
2	I	263	VAL
2	I	272	ARG
2	I	327	GLN
2	I	343	HIS
2	I	378	ARG
2	I	472	GLU
2	I	475	VAL
2	I	491	ASP
2	I	519	ASN
2	I	538	LEU
2	I	554	HIS
2	I	573	ASN
2	I	651	ASP
2	I	655	VAL
2	I	725	GLN
2	I	727	VAL
2	I	749	ASP
2	I	811	ASN
2	I	912	ASP
2	I	963	GLU
2	I	1024	GLU
2	I	1159	VAL
2	I	1240	ASP
2	I	1301	ARG
3	J	18	ASP
3	J	60	ARG
3	J	79	LYS
3	J	80	HIS
3	J	98	ARG
3	J	134	ASP
3	J	199	GLU
3	J	201	LEU
3	J	282	LEU
3	J	293	ARG
3	J	299	LEU
3	J	359	PRO
3	J	393	THR

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Mol	Chain	Res	Type
3	J	430	HIS
3	J	470	VAL
3	J	489	ASN
3	J	495	ASN
3	J	527	LEU
3	J	545	HIS
3	J	603	LYS
3	J	642	ASP
3	J	666	GLU
3	J	800	LEU
3	J	807	LEU
3	J	897	HIS
3	J	1135	THR
3	J	1143	ASP
3	J	1261	LEU
3	J	1305	ASP
3	J	1343	GLU
4	K	11	GLU
5	L	124	GLU
5	L	139	GLU
5	L	264	LYS
5	L	289	LYS
5	L	346	GLN
5	L	423	ARG
5	L	427	PHE
5	L	449	THR
5	L	470	MET
5	L	471	LEU
5	L	551	LEU
5	L	566	ASP
5	L	580	PHE
5	L	583	THR
5	L	611	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	L	345	GLN
5	L	437	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 ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
8	4QM	I	1402	-	29,29,30	5.35	15 (51%)	47,47,48	2.43	14 (29%)
8	4QM	J	1504	-	30,30,30	5.29	15 (50%)	47,48,48	2.59	19 (40%)
8	4QM	L	701	-	30,30,30	5.28	16 (53%)	47,48,48	2.52	17 (36%)
8	4QM	I	1401	-	30,30,30	5.25	15 (50%)	47,48,48	2.50	16 (34%)

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
8	4QM	I	1402	-	-	2/6/71/72	0/4/4/4
8	4QM	J	1504	-	-	5/7/72/72	0/4/4/4
8	4QM	L	701	-	-	5/7/72/72	0/4/4/4
8	4QM	I	1401	-	-	7/7/72/72	0/4/4/4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	701	4QM	C3-C19	18.11	1.83	1.53
8	J	1504	4QM	C3-C19	18.04	1.82	1.53
8	I	1402	4QM	C3-C19	17.98	1.82	1.53
8	I	1401	4QM	C3-C19	17.95	1.82	1.53
8	J	1504	4QM	C3-C4	12.65	1.73	1.53
8	I	1402	4QM	C3-C4	12.43	1.73	1.53
8	I	1401	4QM	C3-C4	12.41	1.73	1.53
8	L	701	4QM	C3-C4	12.34	1.73	1.53
8	I	1402	4QM	C5-C4	-9.50	1.40	1.54
8	L	701	4QM	C5-C4	-9.50	1.40	1.54
8	J	1504	4QM	C2-C19	-9.40	1.39	1.56
8	I	1401	4QM	C5-C4	-9.37	1.40	1.54
8	I	1402	4QM	C2-C19	-9.31	1.39	1.56
8	J	1504	4QM	C5-C4	-9.30	1.40	1.54
8	I	1401	4QM	C2-C19	-9.21	1.40	1.56
8	L	701	4QM	C2-C19	-9.20	1.40	1.56
8	L	701	4QM	C8-C7	6.30	1.71	1.54
8	I	1402	4QM	C8-C7	6.27	1.71	1.54
8	J	1504	4QM	C8-C7	6.25	1.71	1.54
8	I	1401	4QM	C8-C7	6.24	1.71	1.54
8	J	1504	4QM	C5-C6	-5.01	1.47	1.55
8	I	1401	4QM	C5-C6	-4.99	1.47	1.55
8	J	1504	4QM	C18-C6	-4.95	1.44	1.53
8	L	701	4QM	C5-C6	-4.92	1.47	1.55
8	I	1402	4QM	C5-C6	-4.80	1.47	1.55
8	I	1401	4QM	C18-C6	-4.68	1.44	1.53
8	L	701	4QM	C18-C6	-4.66	1.45	1.53
8	I	1402	4QM	C18-C6	-4.54	1.45	1.53
8	L	701	4QM	O4-C4	-4.20	1.36	1.43
8	I	1401	4QM	O4-C4	-4.19	1.36	1.43
8	I	1402	4QM	O4-C4	-4.13	1.36	1.43
8	J	1504	4QM	O4-C4	-4.10	1.36	1.43
8	L	701	4QM	C7-C6	3.34	1.61	1.54
8	I	1402	4QM	C7-C6	3.33	1.61	1.54
8	I	1401	4QM	C14-C15	-3.29	1.48	1.53
8	I	1401	4QM	C7-C6	3.29	1.61	1.54
8	I	1402	4QM	C14-C15	-3.28	1.48	1.53
8	J	1504	4QM	C7-C6	3.26	1.61	1.54
8	J	1504	4QM	C14-C15	-3.22	1.48	1.53
8	L	701	4QM	C14-C15	-3.19	1.48	1.53
8	L	701	4QM	C2-C15	3.01	1.60	1.55
8	I	1401	4QM	C20-C9	-2.92	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	4QM	C20-C9	-2.83	1.49	1.54
8	L	701	4QM	C20-C9	-2.78	1.49	1.54
8	I	1402	4QM	C20-C9	-2.75	1.49	1.54
8	I	1401	4QM	C2-C15	2.71	1.59	1.55
8	J	1504	4QM	C2-C15	2.65	1.59	1.55
8	I	1402	4QM	C2-C15	2.58	1.59	1.55
8	I	1401	4QM	C5-C9	2.55	1.59	1.55
8	I	1402	4QM	C14-C13	2.55	1.56	1.52
8	I	1402	4QM	C5-C9	2.52	1.59	1.55
8	L	701	4QM	C5-C9	2.49	1.59	1.55
8	J	1504	4QM	C5-C9	2.47	1.59	1.55
8	J	1504	4QM	C14-C13	2.43	1.56	1.52
8	I	1401	4QM	C14-C13	2.40	1.56	1.52
8	L	701	4QM	C14-C13	2.40	1.56	1.52
8	J	1504	4QM	O2-C13	-2.26	1.36	1.43
8	I	1401	4QM	O2-C13	-2.25	1.36	1.43
8	L	701	4QM	O2-C13	-2.23	1.36	1.43
8	I	1402	4QM	O2-C13	-2.20	1.37	1.43
8	L	701	4QM	C16-C15	2.00	1.57	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	1504	4QM	C9-C5-C4	-8.60	109.92	117.67
8	I	1401	4QM	C9-C5-C4	-8.49	110.03	117.67
8	L	701	4QM	C9-C5-C4	-8.21	110.28	117.67
8	I	1402	4QM	C9-C5-C4	-7.97	110.50	117.67
8	L	701	4QM	C5-C9-C20	-6.62	111.47	119.48
8	J	1504	4QM	C5-C9-C20	-6.16	112.02	119.48
8	I	1401	4QM	C5-C9-C20	-5.88	112.36	119.48
8	L	701	4QM	C7-C6-C18	-5.73	110.50	118.36
8	I	1402	4QM	C7-C6-C18	-5.66	110.60	118.36
8	J	1504	4QM	C7-C6-C18	-5.65	110.60	118.36
8	I	1402	4QM	C5-C9-C20	-5.62	112.67	119.48
8	I	1401	4QM	C7-C6-C18	-5.43	110.90	118.36
8	I	1401	4QM	C6-C5-C4	5.29	112.25	107.42
8	J	1504	4QM	C6-C5-C4	4.92	111.92	107.42
8	L	701	4QM	C9-C5-C6	4.63	104.76	100.11
8	I	1402	4QM	C6-C5-C4	4.49	111.52	107.42
8	L	701	4QM	C6-C5-C4	4.23	111.28	107.42
8	J	1504	4QM	C9-C5-C6	4.15	104.28	100.11
8	I	1402	4QM	C9-C5-C6	4.10	104.23	100.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1402	4QM	C19-C3-C4	-3.76	109.38	114.29
8	I	1401	4QM	C19-C3-C4	-3.70	109.46	114.29
8	I	1402	4QM	C14-C15-C2	-3.68	108.74	112.66
8	L	701	4QM	C19-C3-C4	-3.58	109.61	114.29
8	I	1401	4QM	C9-C5-C6	3.52	103.65	100.11
8	J	1504	4QM	C7-C6-C5	3.45	106.89	103.54
8	I	1402	4QM	C3-C19-C2	-3.44	110.21	113.70
8	J	1504	4QM	C8-C9-C5	3.43	106.87	103.54
8	I	1401	4QM	C8-C9-C5	3.42	106.85	103.54
8	J	1504	4QM	C16-C15-C2	-3.30	109.15	112.66
8	L	701	4QM	C7-C6-C5	3.16	106.61	103.54
8	I	1401	4QM	C16-C15-C2	-3.14	109.32	112.66
8	J	1504	4QM	C14-C15-C2	-3.04	109.42	112.66
8	I	1402	4QM	C8-C9-C5	2.94	106.40	103.54
8	J	1504	4QM	C19-C3-C4	-2.93	110.46	114.29
8	L	701	4QM	C3-C19-C2	-2.92	110.74	113.70
8	L	701	4QM	C8-C9-C5	2.90	106.35	103.54
8	I	1401	4QM	C3-C19-C2	-2.89	110.77	113.70
8	I	1401	4QM	C14-C15-C2	-2.88	109.59	112.66
8	I	1402	4QM	C7-C6-C5	2.73	106.19	103.54
8	J	1504	4QM	C3-C19-C2	-2.72	110.95	113.70
8	L	701	4QM	C16-C15-C2	-2.64	109.85	112.66
8	L	701	4QM	C2-C19-C18	-2.63	108.90	111.84
8	I	1401	4QM	C7-C6-C5	2.60	106.07	103.54
8	L	701	4QM	C19-C18-C17	-2.58	108.61	111.86
8	J	1504	4QM	C5-C6-C18	-2.58	111.45	114.72
8	L	701	4QM	C21-C20-C9	-2.57	109.02	112.88
8	J	1504	4QM	C19-C18-C6	-2.57	106.16	109.75
8	J	1504	4QM	C21-C20-C9	-2.47	109.17	112.88
8	I	1401	4QM	C3-C19-C18	-2.43	107.31	110.89
8	I	1402	4QM	C16-C15-C2	-2.41	110.09	112.66
8	J	1504	4QM	C15-C16-C17	-2.37	111.58	114.40
8	I	1401	4QM	C21-C20-C9	-2.36	109.33	112.88
8	L	701	4QM	C5-C6-C18	-2.36	111.72	114.72
8	I	1401	4QM	C19-C18-C6	-2.30	106.54	109.75
8	I	1401	4QM	C15-C16-C17	-2.27	111.70	114.40
8	I	1401	4QM	C6-C18-C17	-2.19	108.95	111.85
8	J	1504	4QM	C12-C1-C2	-2.17	109.08	112.74
8	J	1504	4QM	C6-C18-C17	-2.14	109.01	111.85
8	L	701	4QM	C14-C15-C2	-2.09	110.44	112.66
8	L	701	4QM	C6-C18-C17	-2.09	109.08	111.85
8	I	1402	4QM	C3-C19-C18	-2.08	107.81	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	1504	4QM	C3-C19-C18	-2.04	107.87	110.89
8	I	1402	4QM	C19-C18-C17	-2.03	109.30	111.86
8	L	701	4QM	C16-C15-C14	-2.02	108.92	111.23
8	J	1504	4QM	C2-C19-C18	-2.02	109.59	111.84
8	I	1402	4QM	C15-C14-C13	-2.01	109.68	112.71

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1504	4QM	C21-C20-C9-C8
8	J	1504	4QM	C21-C20-C9-C5
8	I	1401	4QM	C21-C20-C22-C23
8	J	1504	4QM	C22-C20-C9-C5
8	J	1504	4QM	C22-C20-C9-C8
8	I	1401	4QM	C9-C20-C22-C23
8	L	701	4QM	C21-C20-C9-C5
8	J	1504	4QM	C20-C22-C23-C24
8	L	701	4QM	C21-C20-C9-C8
8	I	1401	4QM	C21-C20-C9-C5
8	L	701	4QM	C21-C20-C22-C23
8	I	1401	4QM	C20-C22-C23-C24
8	I	1401	4QM	C21-C20-C9-C8
8	I	1402	4QM	C21-C20-C22-C23
8	L	701	4QM	C22-C20-C9-C5
8	I	1401	4QM	C22-C20-C9-C5
8	L	701	4QM	C22-C20-C9-C8
8	I	1401	4QM	C22-C20-C9-C8
8	I	1402	4QM	C21-C20-C9-C5

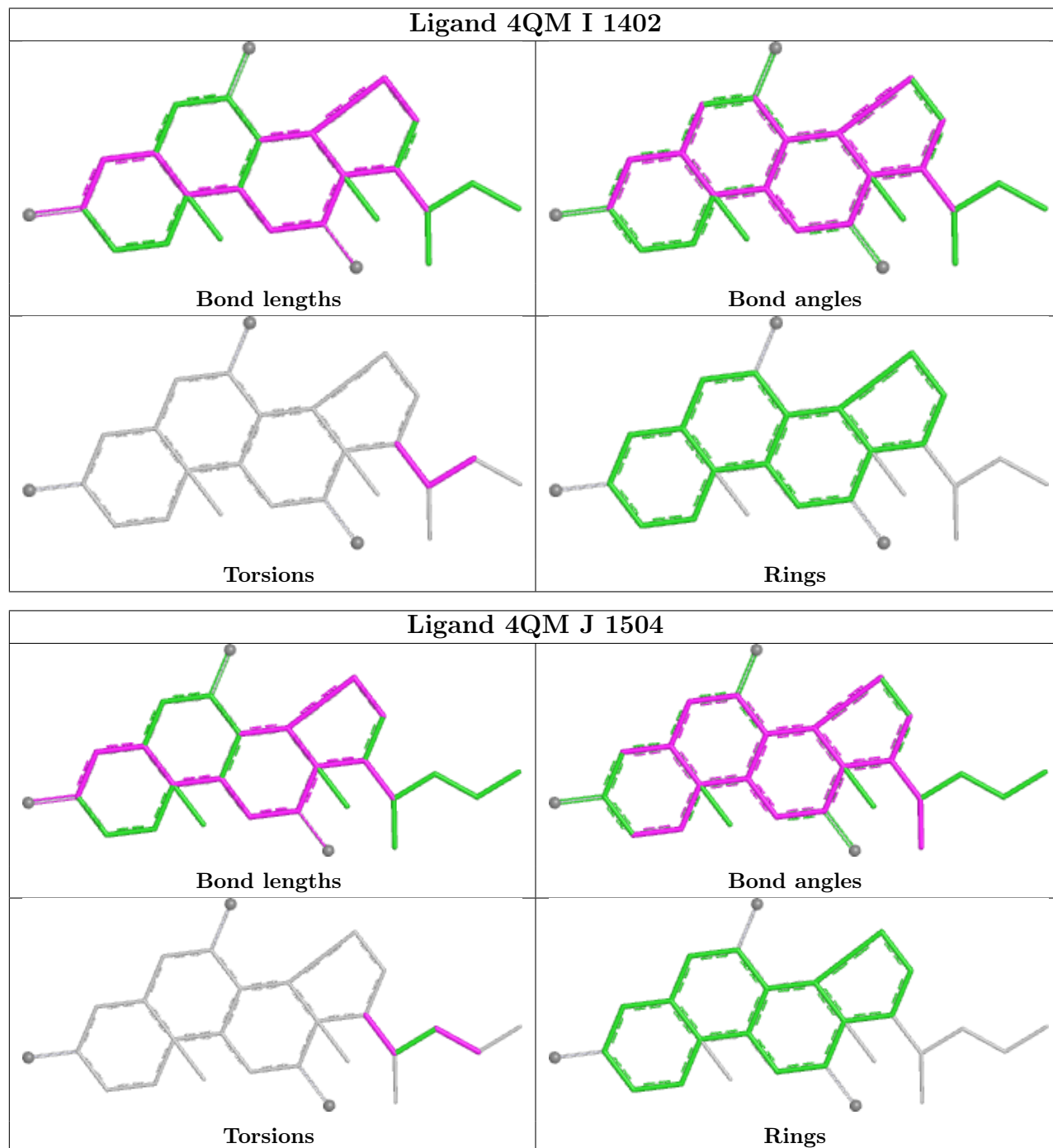
There are no ring outliers.

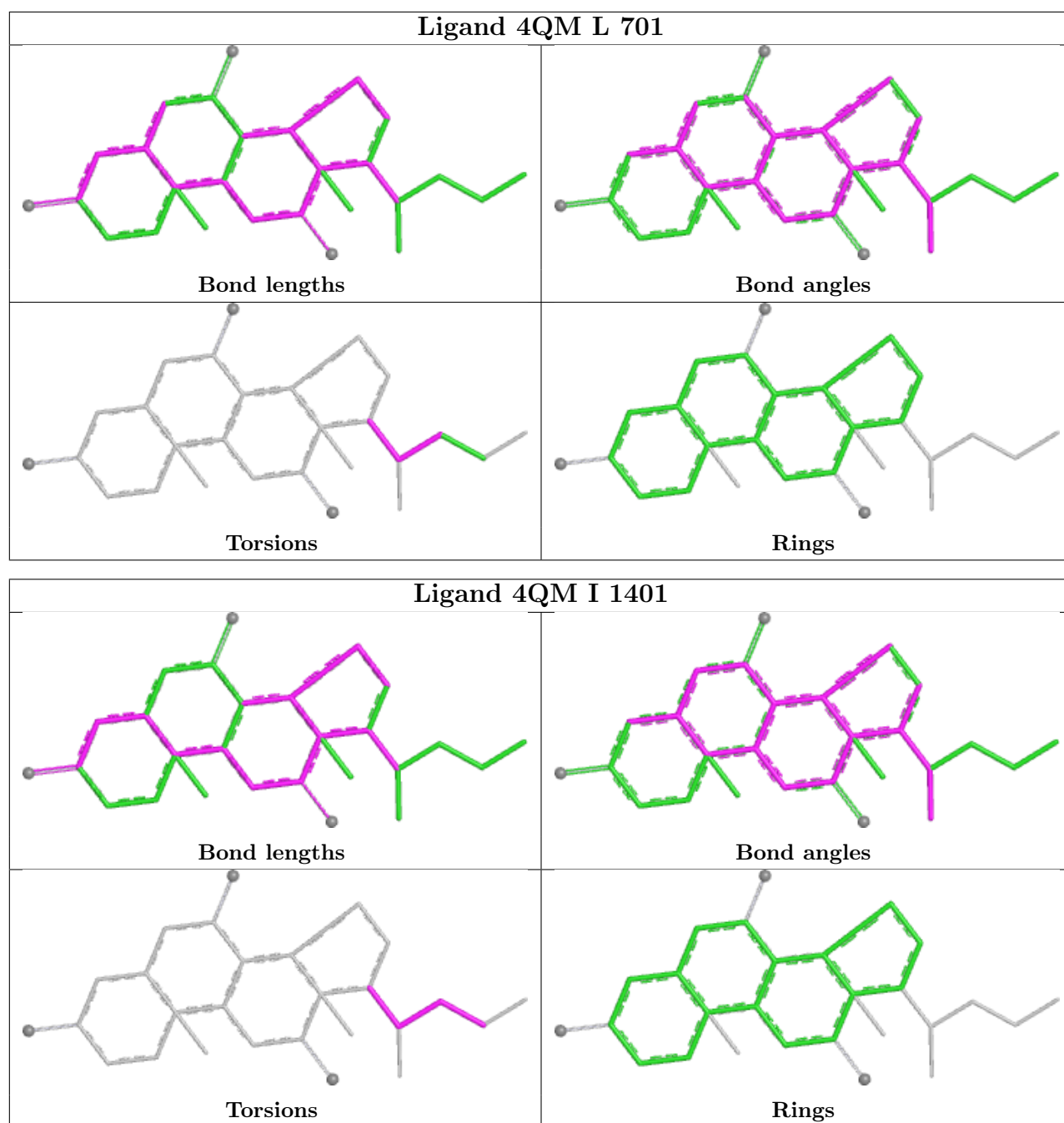
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1402	4QM	4	0
8	J	1504	4QM	5	0
8	L	701	4QM	5	0
8	I	1401	4QM	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	O	1
5	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	75:DA	O3'	79:DT	P	14.92
1	L	52:ASP	C	77:ALA	N	10.24

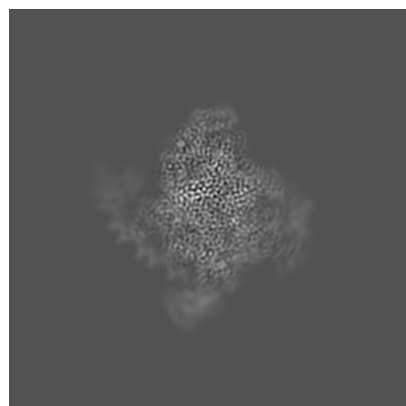
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41439. These allow visual inspection of the internal detail of the map and identification of artifacts.

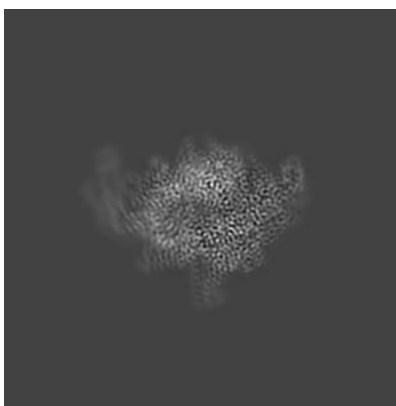
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

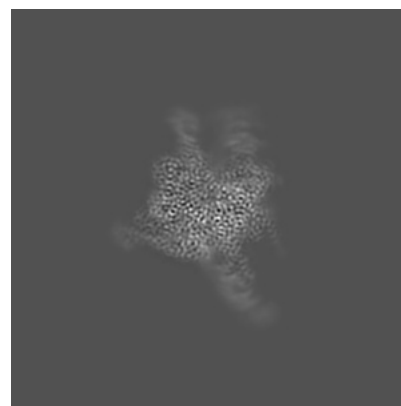
6.1.1 Primary map



X

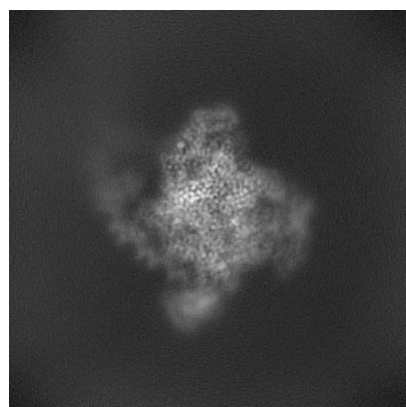


Y

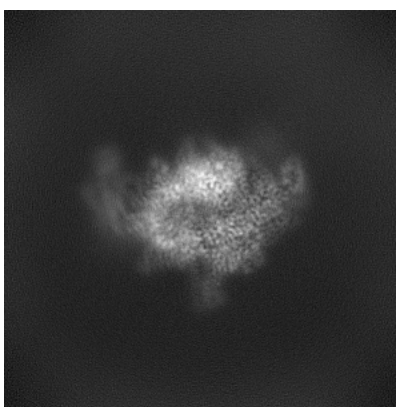


Z

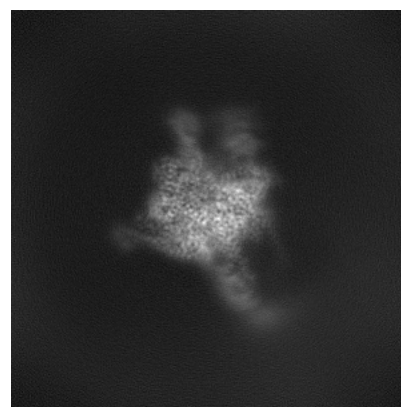
6.1.2 Raw map



X



Y

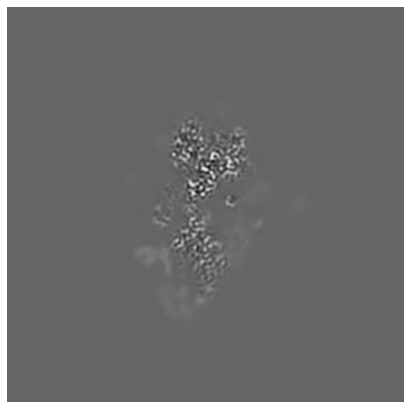


Z

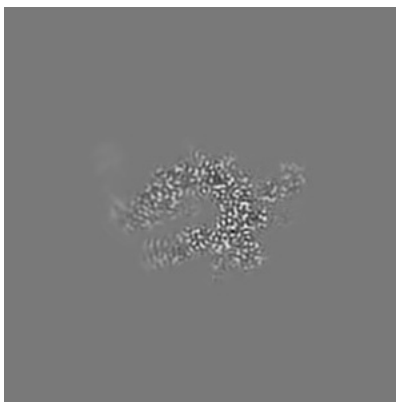
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

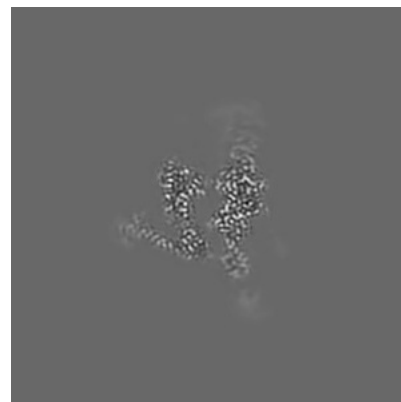
6.2.1 Primary map



X Index: 192

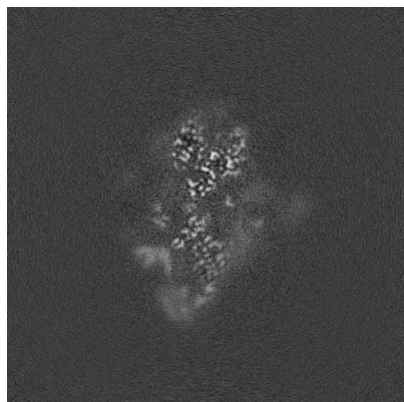


Y Index: 192

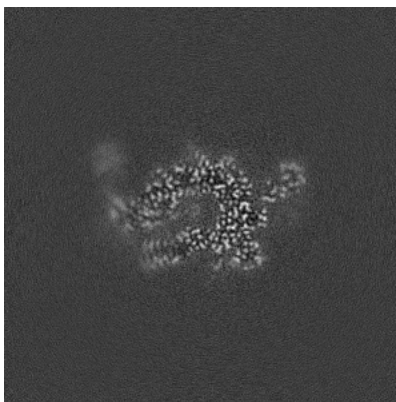


Z Index: 192

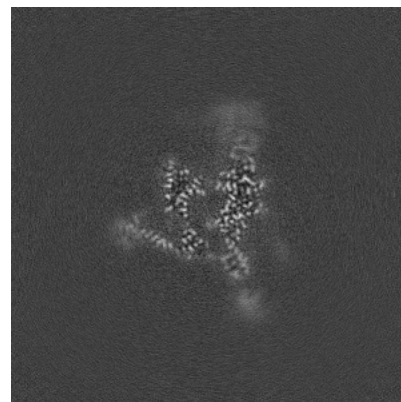
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

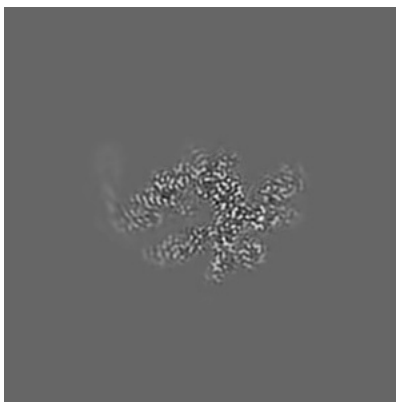
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

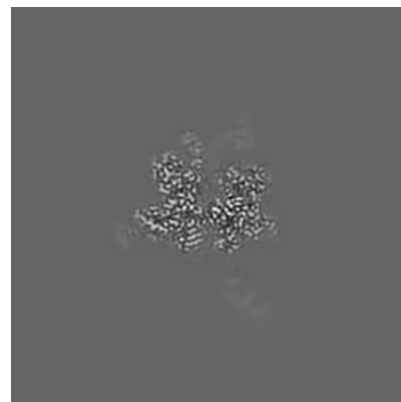
6.3.1 Primary map



X Index: 209

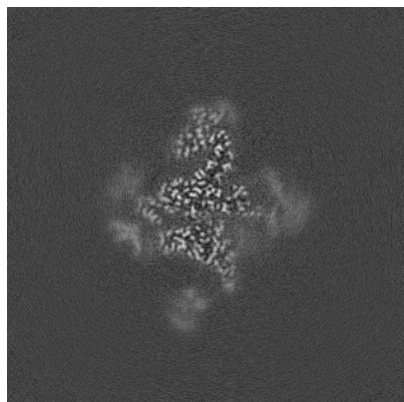


Y Index: 186

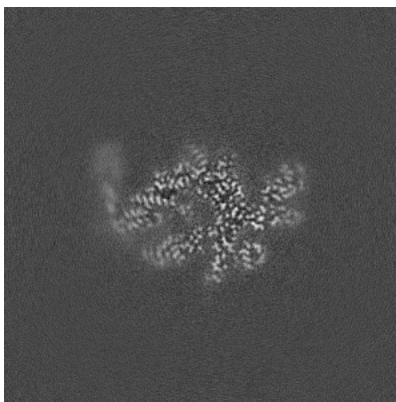


Z Index: 206

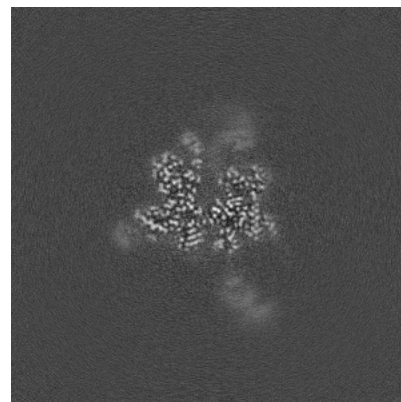
6.3.2 Raw map



X Index: 210



Y Index: 186

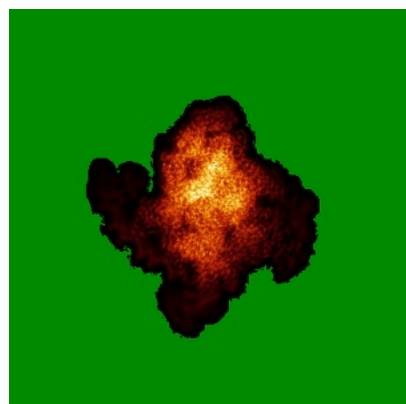


Z Index: 206

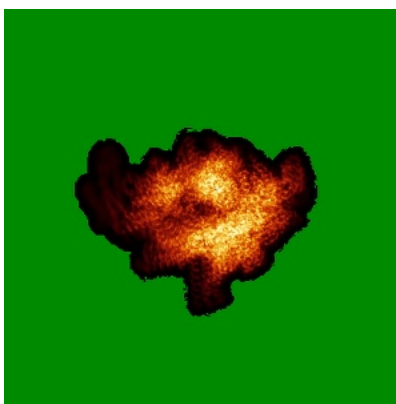
The images above show the largest variance slices of the map in three orthogonal directions.

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

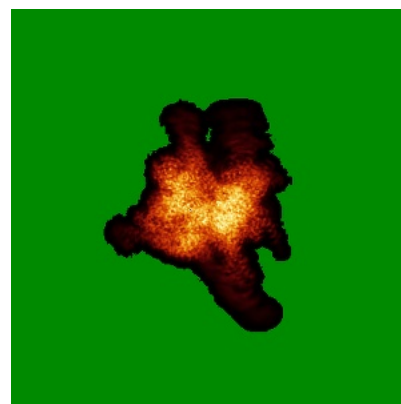
6.4.1 Primary map



X

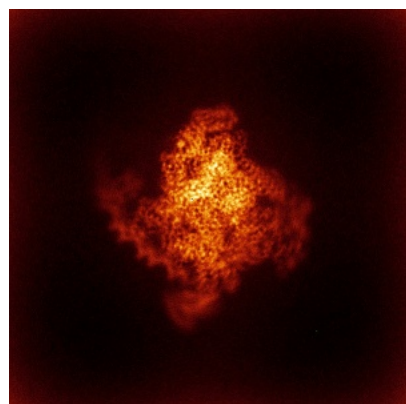


Y

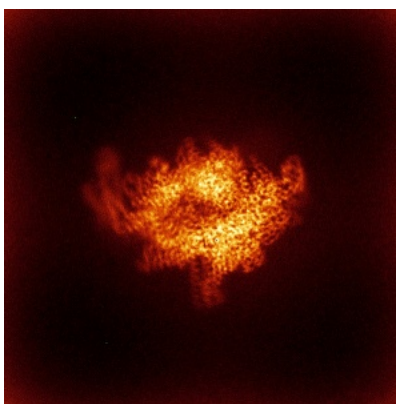


Z

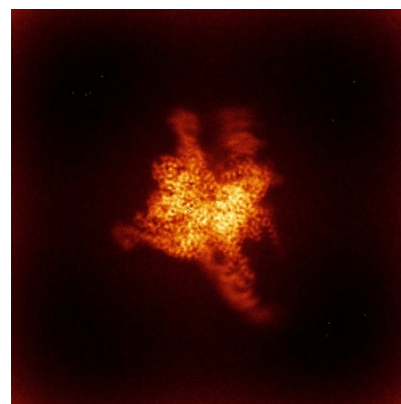
6.4.2 Raw map



X



Y

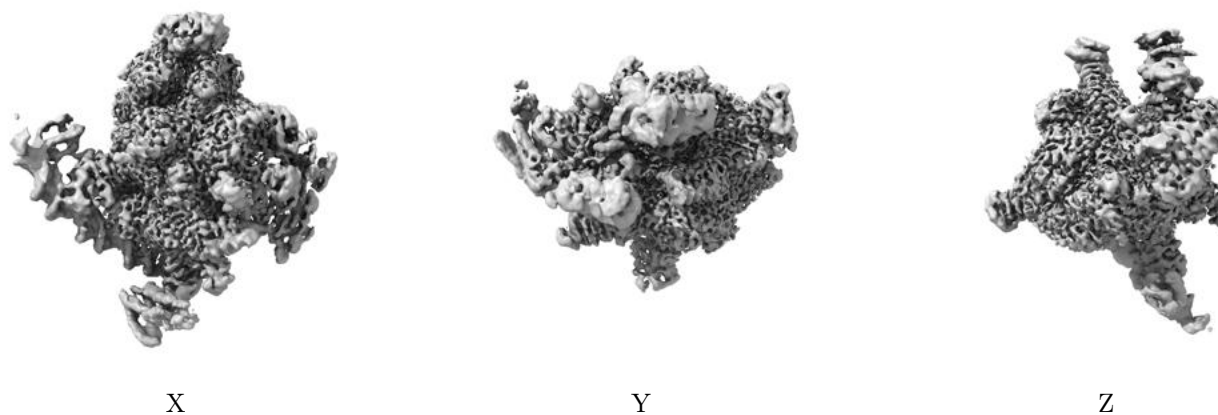


Z

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.

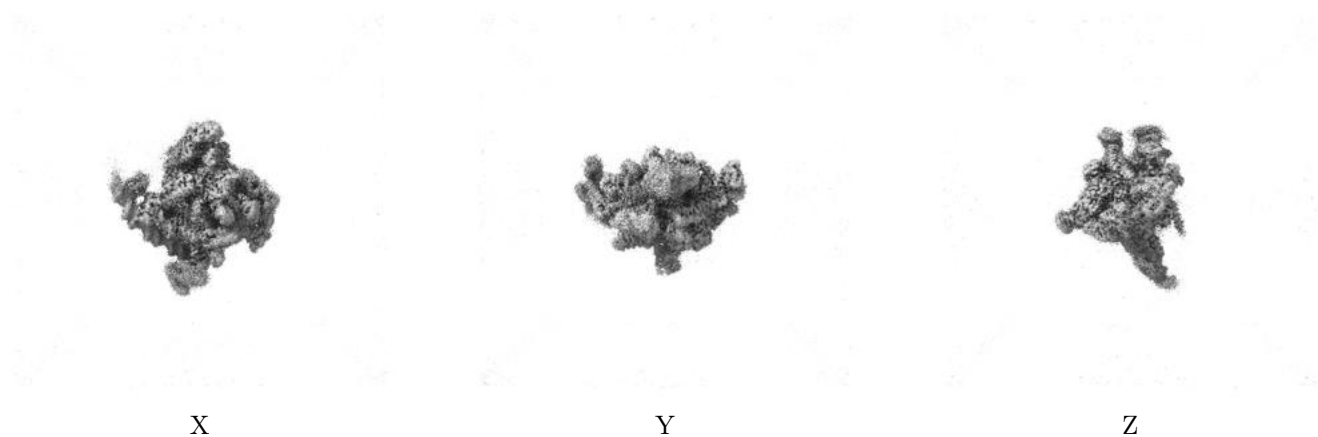
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

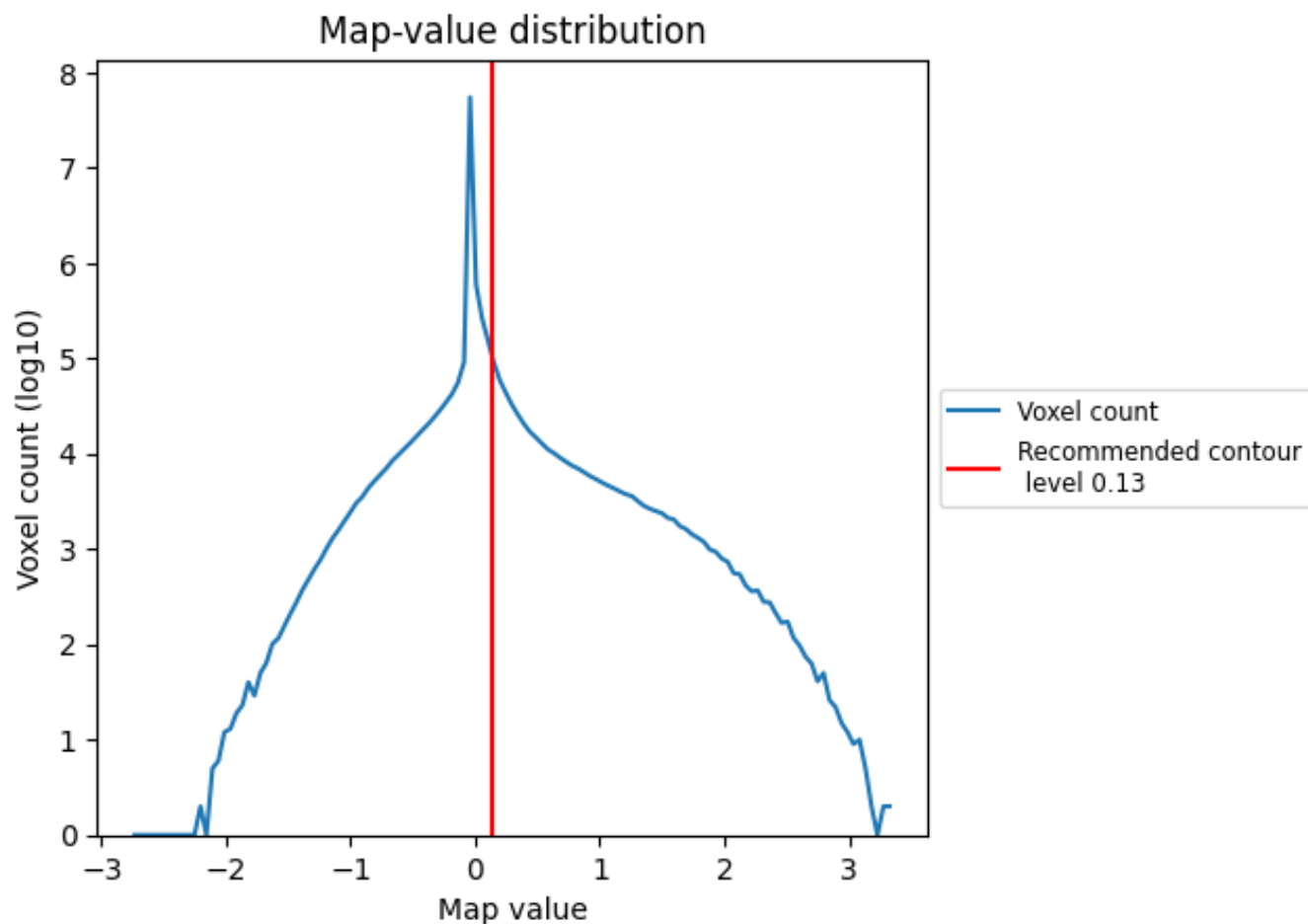
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

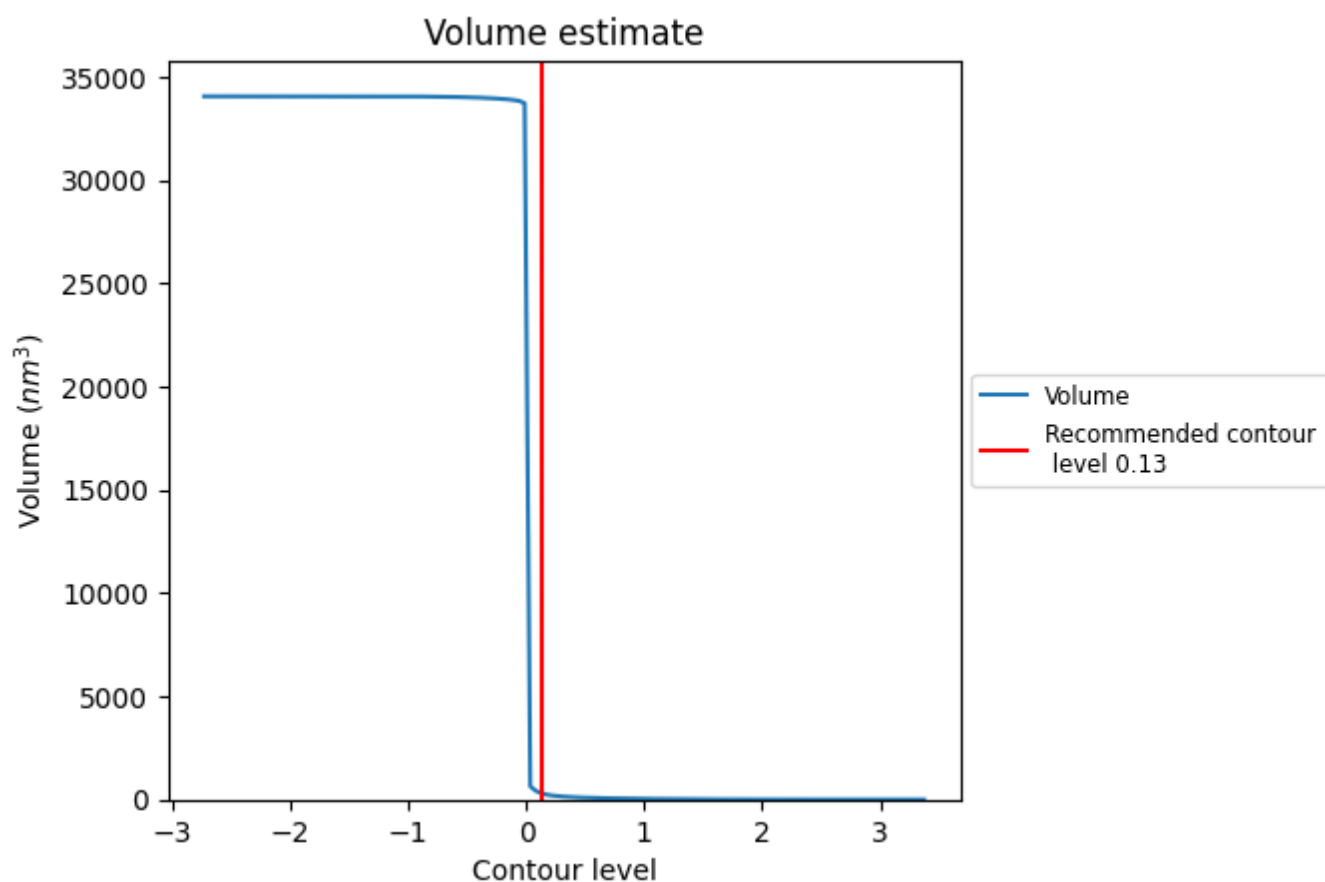
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

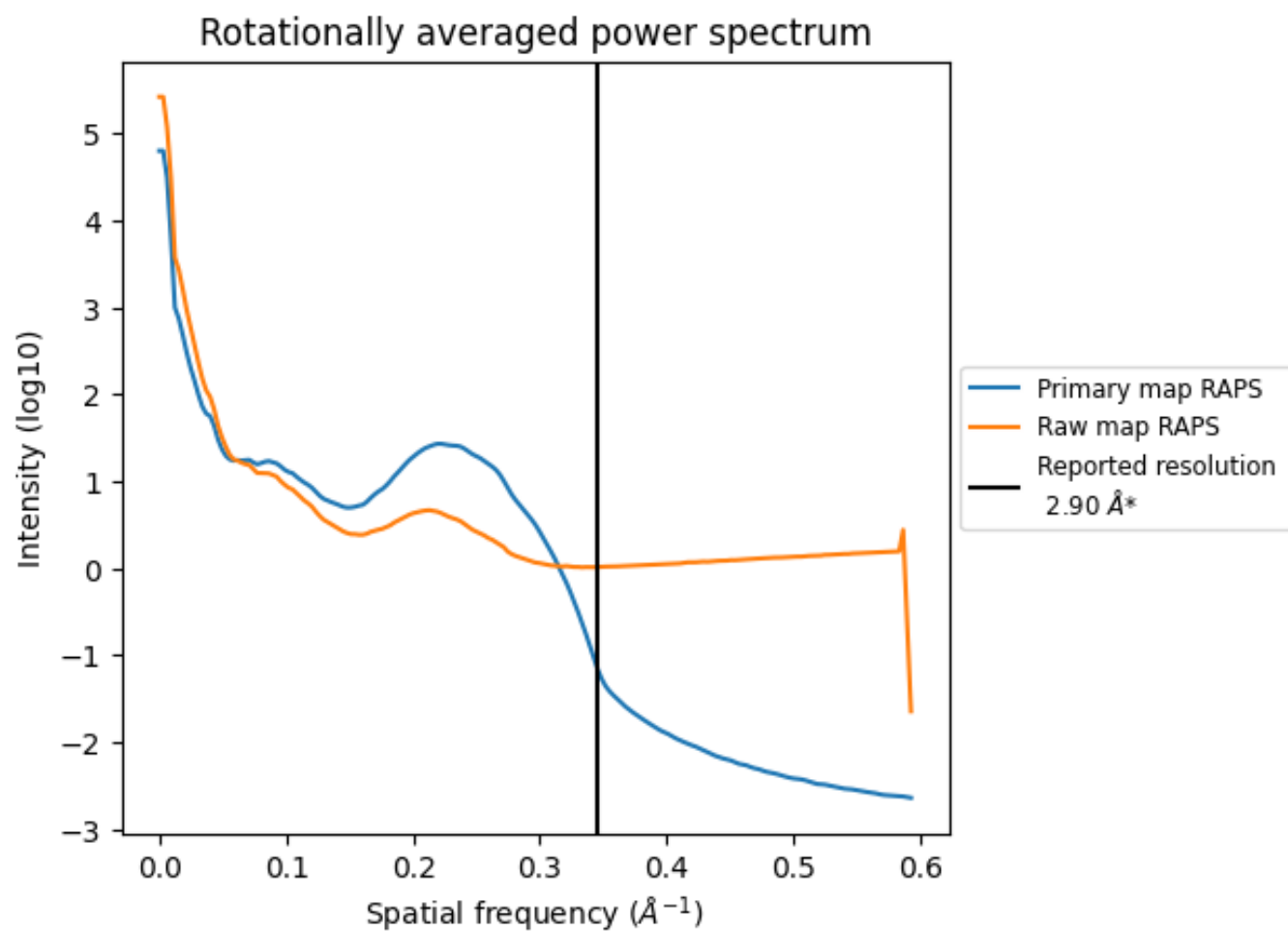
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 301 nm³; this corresponds to an approximate mass of 272 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 ⓘ

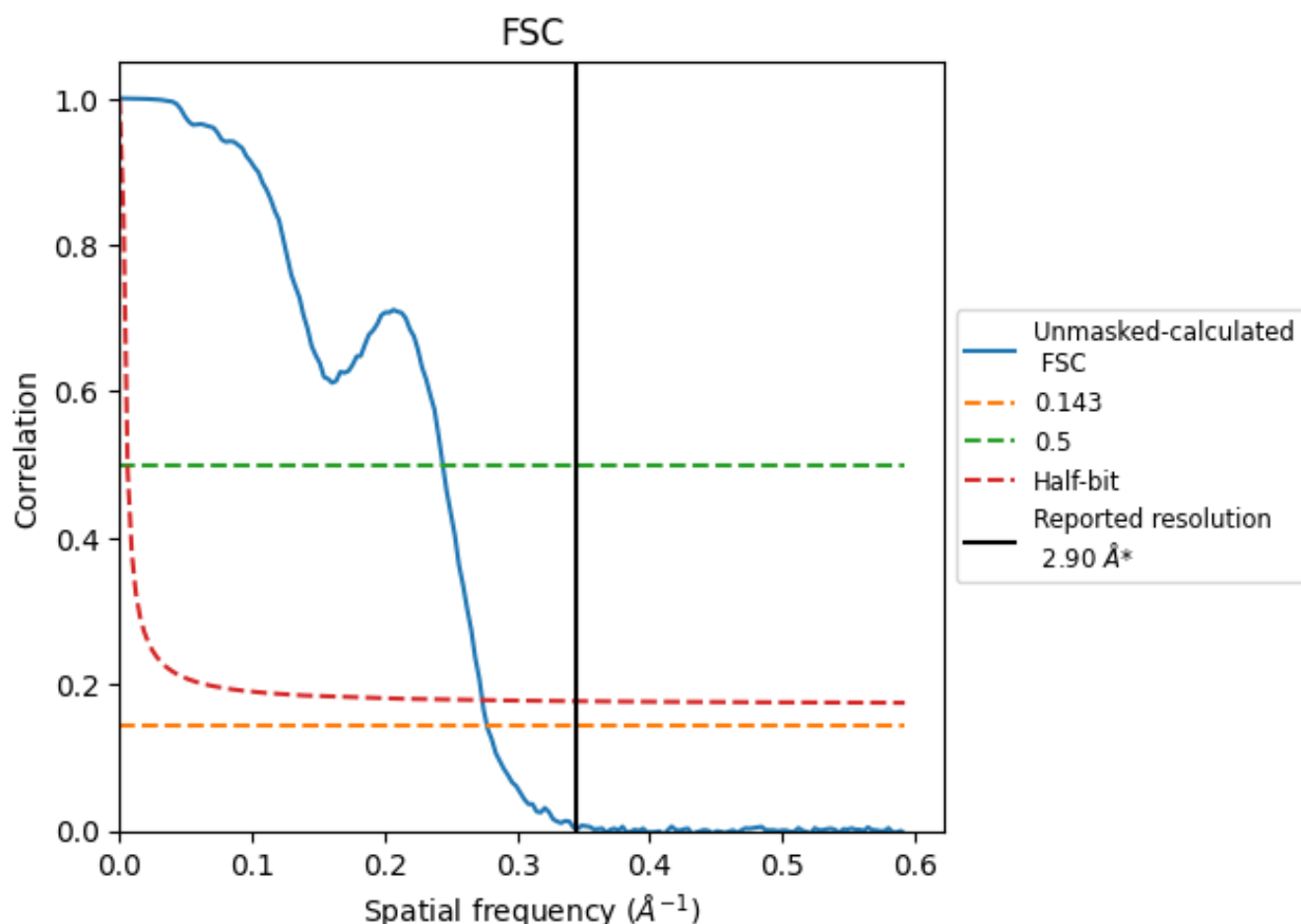


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

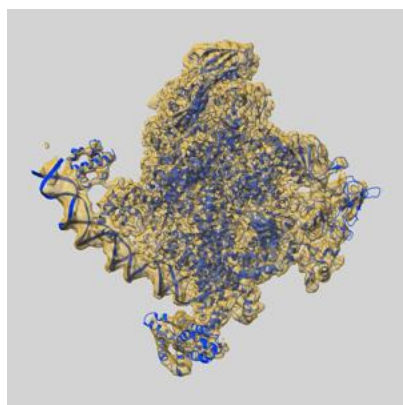
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	4.10	3.65

*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 3.61 differs from the reported value 2.9 by more than 10 %

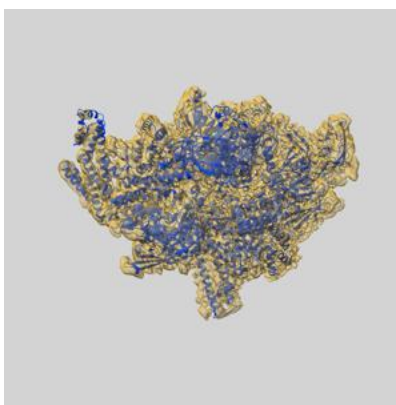
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41439 and PDB model 8TO8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

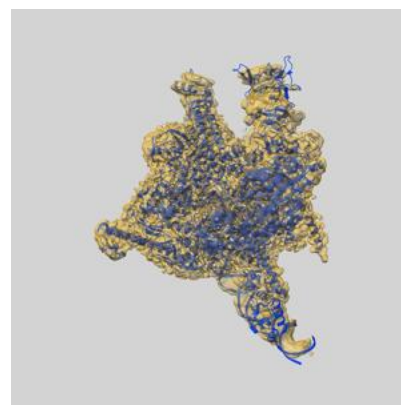
9.1 Map-model overlay [i](#)



X



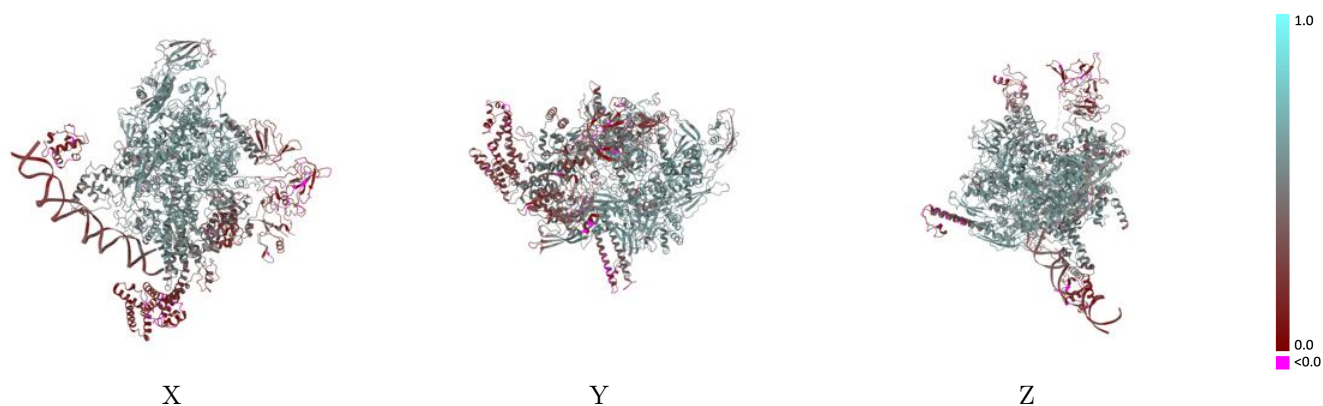
Y



Z

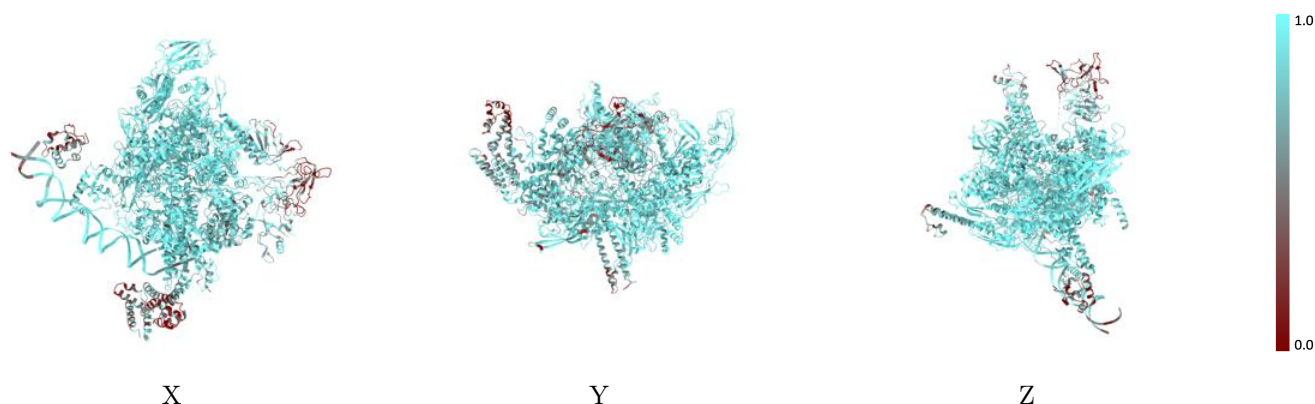
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



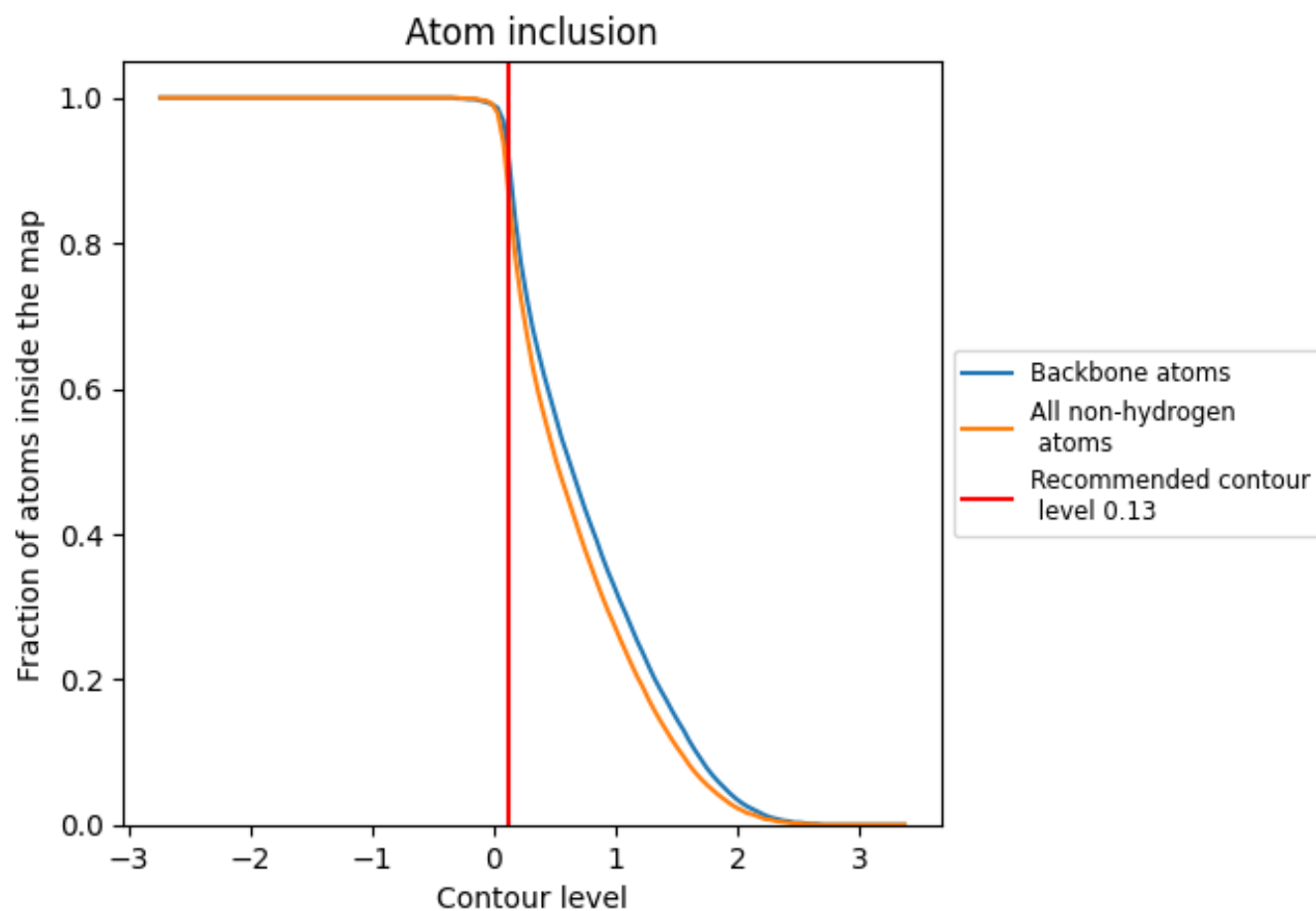
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8580	<div></div> 0.4610
G	<div></div> 0.9590	<div></div> 0.5600
H	<div></div> 0.9380	<div></div> 0.5120
I	<div></div> 0.9050	<div></div> 0.5020
J	<div></div> 0.8650	<div></div> 0.4860
K	<div></div> 0.9060	<div></div> 0.5330
L	<div></div> 0.7100	<div></div> 0.3270
M	<div></div> 0.3660	<div></div> 0.1540
O	<div></div> 0.8200	<div></div> 0.2850
P	<div></div> 0.8630	<div></div> 0.2620

1.0

0.0

<0.0