



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:32 AM UTC

PDB ID : 7PW9 / pdb_00007pw9
EMDB ID : EMD-13679
Title : Human SMG1-9 kinase complex bound to AMPPNP
Authors : Langer, L.M.; Conti, E.
Deposited on : 2021-10-06
Resolution : 3.12 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

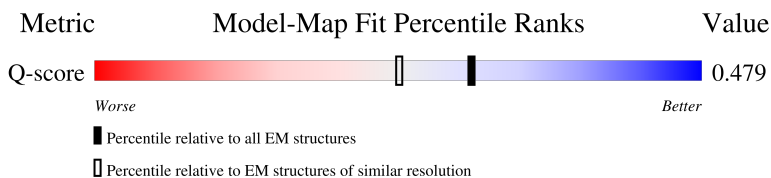
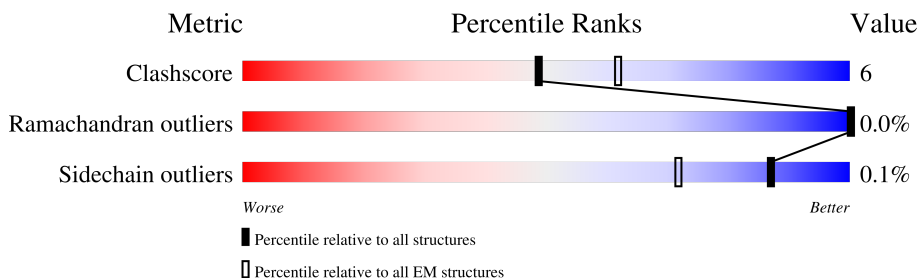
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.12 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	14478 (2.62 - 3.62)

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	3657	
2	C	352	

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 Serine/threonine-protein kinase SMG1,Serine/threonine-prote
in kinase SMG1,Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SM
G1,Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1,Serine/th
reonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1952	Total	C	N	O	S	0	0
			13831	8884	2456	2428	63		

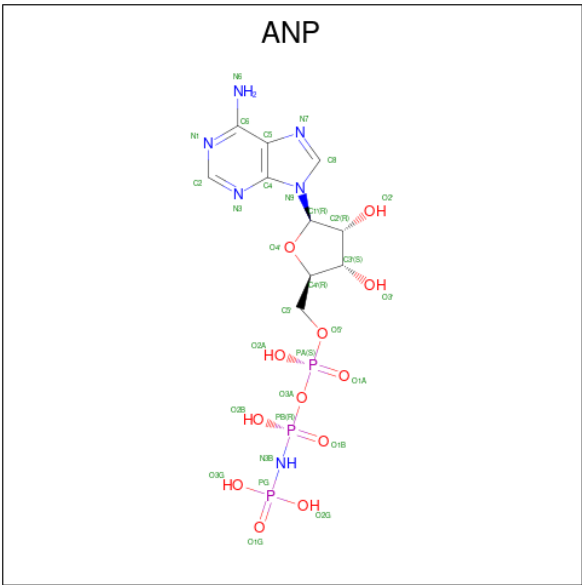
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	743	ARG	LYS	conflict	UNP Q96Q15
A	1209	SER	ALA	conflict	UNP Q96Q15

- Molecule 2 is a protein called Protein SMG9.

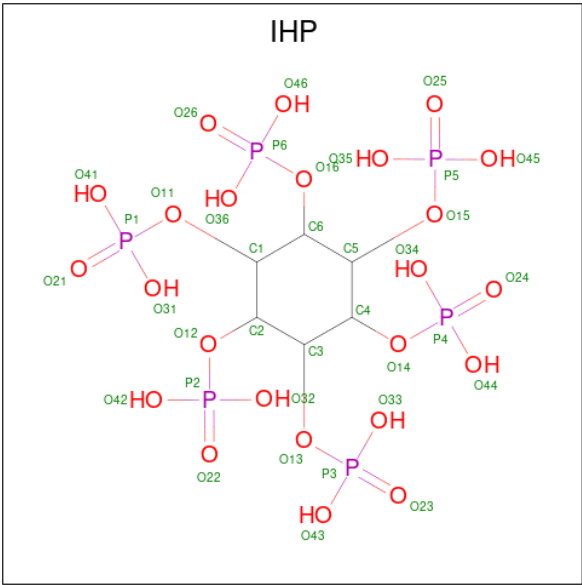
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	309	Total	C	N	O	S	0	0
			2409	1562	415	415	17		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

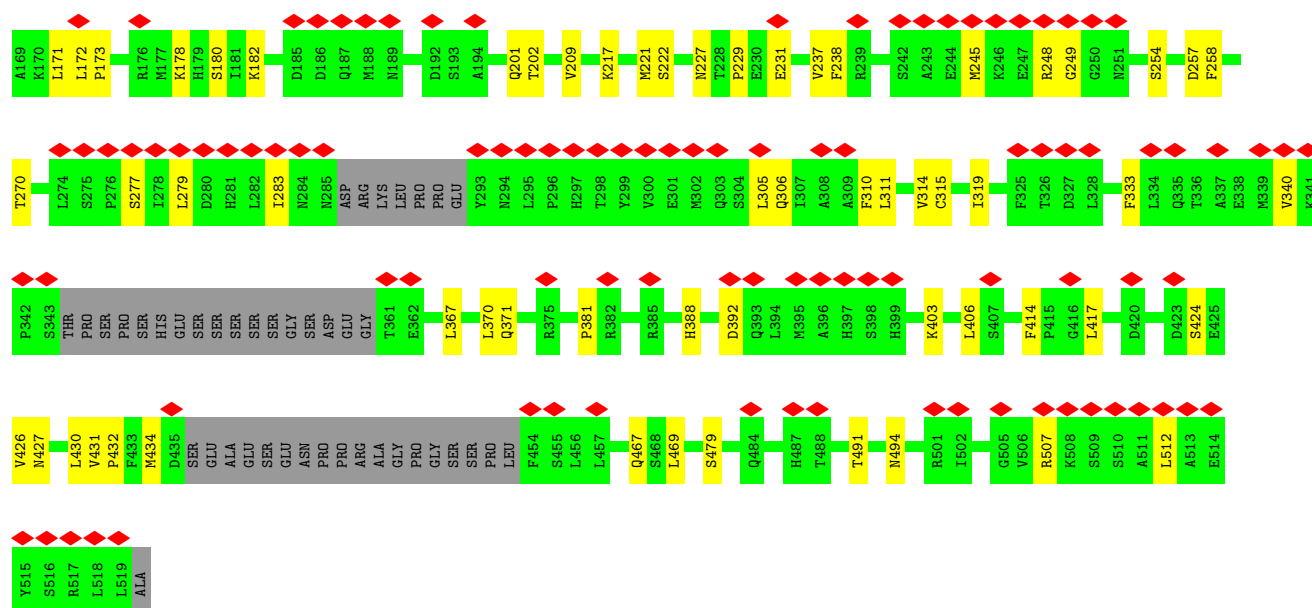
Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total Mg 1 1	0





SER	VAL	ALA	CYS	SER	PRO	LYS	LYS	ALA	VAL	ARG	ASP	PRO	LYS	THR	GLY	LYS	ALA	VAL	GLN	GLU	ARG	ASN	S3507	R3615	R3623	D3624	V3625	D3626	P3627	N3628	R3629	R3630	Q3636	V3661
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

Chain C:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168050	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 ($e^-/\text{\AA}^2$)	60.99	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.596	Depositor
Minimum map value	-2.477	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.818	Depositor
Map size (Å)	292.8128, 292.8128, 292.8128	wwPDB
Map dimensions	344, 344, 344	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85120004, 0.85120004, 0.85120004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ANP, IHP

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	0.16	1/13105 (0.0%)	0.34	0/17900
2	C	0.10	0/2465	0.34	0/3346
All	All	0.16	1/15570 (0.0%)	0.34	0/21246

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	LEU	CA-C	-5.92	1.44	1.52

There are no bond angle outliers.

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	13831	0	12513	141	0
2	C	2409	0	2356	45	0
3	A	31	0	13	2	0
4	A	36	0	6	0	0
5	C	31	0	12	1	0
6	C	1	0	0	0	0
All	All	16339	0	14900	181	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 6.

All (181) 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:742:MET:HE1	1:A:757:PHE:CD1	2.01	0.94
1:A:679:ILE:HG21	1:A:741:LEU:HD21	1.59	0.84
1:A:732:MET:SD	1:A:767:ASN:ND2	2.52	0.82
1:A:742:MET:HE1	1:A:757:PHE:CE1	2.20	0.76
1:A:558:ILE:HG13	1:A:559:PRO:HD3	1.68	0.75
1:A:585:LEU:HD12	1:A:586:PRO:HD2	1.69	0.74
2:C:367:LEU:O	2:C:427:ASN:ND2	2.23	0.70
1:A:2186:PRO:HB2	1:A:2319:ARG:HD2	1.75	0.69
1:A:1422:MET:HE2	1:A:1479:TRP:HB2	1.74	0.69
2:C:403:LYS:HG2	2:C:426:VAL:HG12	1.73	0.69
2:C:227:ASN:ND2	2:C:231:GLU:OE1	2.29	0.65
1:A:679:ILE:HD13	1:A:741:LEU:CD2	2.29	0.62
1:A:2160:LEU:HD22	1:A:2203:GLY:HA3	1.81	0.62
1:A:991:GLU:OE1	1:A:1049:ARG:NH2	2.33	0.62
1:A:2404:ARG:NH2	1:A:3636:GLN:OE1	2.33	0.62
1:A:524:PHE:HZ	1:A:552:VAL:HG11	1.65	0.61
1:A:679:ILE:CD1	1:A:741:LEU:HD23	2.30	0.61
1:A:1501:MET:HE2	1:A:1561:LEU:HD21	1.81	0.61
2:C:270:THR:HG21	2:C:311:LEU:HD11	1.81	0.61
1:A:2248:ARG:HG3	1:A:2249:PRO:HD2	1.82	0.60
1:A:1352:LEU:HD11	1:A:1392:PRO:HB3	1.84	0.59
2:C:182:LYS:NZ	2:C:254:SER:O	2.34	0.59
2:C:305:LEU:HD12	2:C:340:VAL:HG21	1.84	0.59
1:A:2133:THR:HG21	3:A:3701:ANP:H5'2	1.84	0.59
1:A:536:HIS:HB3	1:A:541:VAL:HG11	1.85	0.59
1:A:1300:LEU:HD22	1:A:1364:VAL:HG22	1.84	0.59
2:C:491:THR:H	2:C:494:ASN:HB2	1.67	0.59
2:C:414:PHE:HB3	2:C:417:LEU:HD23	1.83	0.59
1:A:2336:ARG:NH2	1:A:2354:ASP:O	2.35	0.59
1:A:858:HIS:HB3	2:C:201:GLN:NE2	2.18	0.58
1:A:741:LEU:HG	1:A:741:LEU:O	2.03	0.58
2:C:392:ASP:OD2	2:C:424:SER:OG	2.20	0.58
1:A:742:MET:CE	1:A:757:PHE:CE1	2.87	0.58
1:A:2105:THR:HG22	1:A:2107:ILE:H	1.68	0.58
1:A:637:THR:HG23	1:A:640:ALA:H	1.67	0.57
1:A:503:LEU:O	1:A:507:ILE:HD12	2.03	0.57
2:C:249:GLY:O	2:C:277:SER:OG	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1857:LEU:HD12	1:A:1861:ILE:HD12	1.86	0.57
1:A:888:TYR:O	2:C:479:SER:OG	2.18	0.56
1:A:1467:LYS:HD2	1:A:1499:HIS:HB3	1.88	0.56
1:A:464:LEU:HG	1:A:510:GLN:HG2	1.86	0.56
1:A:1834:GLU:O	1:A:1838:ARG:NH1	2.38	0.56
1:A:1623:ALA:HB1	1:A:1751:TYR:CE1	2.42	0.55
1:A:1811:LEU:O	1:A:1847:ARG:NH2	2.37	0.55
1:A:1031:ARG:O	1:A:1035:MET:HG3	2.07	0.55
1:A:1313:TRP:O	1:A:1314:GLN:NE2	2.38	0.55
1:A:2254:TYR:HA	1:A:2257:ILE:HG22	1.90	0.55
2:C:381:PRO:HB3	2:C:417:LEU:HD11	1.88	0.55
1:A:2257:ILE:HD12	1:A:2283:VAL:HG21	1.89	0.54
1:A:2193:TYR:OH	1:A:2353:ILE:O	2.25	0.54
1:A:2358:CYS:SG	1:A:2359:PHE:N	2.80	0.54
2:C:209:VAL:HG22	2:C:319:ILE:HB	1.89	0.54
2:C:229:PRO:HG2	2:C:467:GLN:HG3	1.88	0.54
1:A:2166:ILE:HD12	1:A:2331:ILE:HD11	1.90	0.54
1:A:364:PHE:O	1:A:368:MET:HG2	2.08	0.53
1:A:1738:ASP:O	1:A:1745:LYS:NZ	2.40	0.53
2:C:222:SER:O	2:C:227:ASN:HB2	2.08	0.53
1:A:2266:LEU:HD23	1:A:2270:VAL:HG21	1.90	0.53
1:A:1233:SER:HB2	1:A:1249:LEU:HD12	1.90	0.53
2:C:202:THR:HG22	2:C:491:THR:HG22	1.91	0.53
1:A:836:THR:O	1:A:840:GLU:HG2	2.10	0.52
1:A:748:TYR:HB3	1:A:751:LEU:HD12	1.91	0.52
1:A:656:HIS:HA	2:C:381:PRO:HG2	1.92	0.52
2:C:305:LEU:HD22	2:C:333:PHE:HE1	1.75	0.52
1:A:679:ILE:HD12	1:A:741:LEU:HD23	1.91	0.51
1:A:1857:LEU:HD11	1:A:1948:VAL:HG11	1.91	0.51
1:A:743:ARG:HD2	1:A:786:LEU:HA	1.92	0.51
1:A:2360:GLU:OE2	1:A:3615:ARG:NH2	2.41	0.51
1:A:978:LEU:O	1:A:982:LEU:HG	2.10	0.51
1:A:2324:MET:SD	1:A:2352:HIS:HD2	2.34	0.51
1:A:3625:VAL:HG13	1:A:3625:VAL:O	2.11	0.51
1:A:1444:LEU:O	1:A:1447:GLN:HG3	2.11	0.51
1:A:679:ILE:HD13	1:A:741:LEU:HD21	1.92	0.51
1:A:550:GLN:HB2	1:A:620:THR:HG21	1.92	0.50
1:A:1325:LYS:NZ	1:A:1361:GLU:OE2	2.45	0.50
2:C:217:LYS:NZ	5:C:601:ATP:O3G	2.40	0.50
1:A:1463:VAL:HG21	1:A:1496:GLN:HG2	1.94	0.50
1:A:875:HIS:HB3	2:C:173:PRO:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:ASN:OD1	1:A:1188:ASN:ND2	2.45	0.49
1:A:2122:HIS:C	1:A:2122:HIS:HD1	2.19	0.49
1:A:1481:PRO:O	1:A:1485:ILE:HG12	2.12	0.49
1:A:679:ILE:HD13	1:A:741:LEU:HD23	1.91	0.49
2:C:245:MET:HG2	2:C:248:ARG:HH11	1.78	0.49
1:A:679:ILE:CD1	1:A:741:LEU:CD2	2.89	0.49
1:A:719:LYS:NZ	1:A:759:LYS:HG3	2.28	0.49
1:A:1445:LEU:HD12	1:A:1490:LEU:HD22	1.95	0.49
2:C:279:LEU:O	2:C:283:ILE:HG12	2.13	0.48
1:A:1115:GLU:O	1:A:1435:ARG:NE	2.29	0.48
2:C:388:HIS:CD2	2:C:426:VAL:HG22	2.48	0.48
1:A:1630:GLY:HA2	1:A:1633:VAL:HG12	1.95	0.48
1:A:947:ILE:HG22	1:A:1033:SER:HB3	1.96	0.48
1:A:2172:ILE:HD12	1:A:2413:LEU:HD22	1.96	0.48
1:A:540:GLU:O	1:A:544:VAL:HG22	2.13	0.47
1:A:497:ILE:HG23	1:A:533:LEU:HD11	1.96	0.47
1:A:2092:LEU:HB2	1:A:2126:GLY:HA2	1.95	0.47
1:A:2190:ALA:HB1	1:A:2324:MET:HE3	1.97	0.47
3:A:3701:ANP:O2A	3:A:3701:ANP:O1B	2.32	0.47
2:C:180:SER:HB2	2:C:257:ASP:OD1	2.15	0.47
1:A:1070:GLU:O	1:A:1074:MET:HG3	2.14	0.46
1:A:1035:MET:HE2	1:A:1075:MET:HE3	1.98	0.46
1:A:1442:THR:HG22	1:A:1490:LEU:HD21	1.97	0.46
1:A:1541:GLY:O	1:A:1545:GLN:HG3	2.15	0.46
1:A:1297:SER:O	1:A:1402:TYR:OH	2.27	0.46
1:A:1328:SER:OG	1:A:1357:SER:OG	2.28	0.46
1:A:2331:ILE:HG12	1:A:2358:CYS:SG	2.56	0.46
1:A:1605:TYR:HB3	1:A:1622:LEU:HB2	1.97	0.46
2:C:371:GLN:HB2	2:C:430:LEU:HD23	1.98	0.46
2:C:381:PRO:HG3	2:C:417:LEU:HD21	1.98	0.45
1:A:547:ALA:O	1:A:550:GLN:HG2	2.17	0.45
2:C:388:HIS:HD2	2:C:426:VAL:HG22	1.80	0.45
1:A:742:MET:HE2	1:A:752:PHE:CE1	2.52	0.45
1:A:863:SER:HB3	2:C:171:LEU:HD12	1.98	0.45
1:A:742:MET:CE	1:A:757:PHE:CD1	2.88	0.45
1:A:1559:SER:C	1:A:1563:LYS:HZ2	2.25	0.45
2:C:403:LYS:HB2	2:C:403:LYS:HE2	1.75	0.44
2:C:237:VAL:HG23	2:C:238:PHE:CD2	2.52	0.44
1:A:975:ASN:O	1:A:979:ARG:HG3	2.17	0.44
1:A:580:LEU:HD21	1:A:653:LEU:HD11	1.98	0.44
1:A:991:GLU:HA	1:A:994:MET:HE2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:VAL:HG23	1:A:908:THR:HG23	2.00	0.44
1:A:2215:PHE:HB2	1:A:2338:LEU:HB3	1.99	0.44
1:A:1360:LEU:O	1:A:1363:THR:HG22	2.18	0.44
1:A:838:ILE:HG22	1:A:1342:VAL:HG13	2.00	0.43
2:C:311:LEU:O	2:C:315:CYS:HB2	2.18	0.43
1:A:2324:MET:HE2	1:A:2324:MET:HA	1.99	0.43
1:A:747:THR:O	1:A:750:PRO:HD2	2.18	0.43
2:C:257:ASP:OD1	2:C:258:PHE:N	2.51	0.43
1:A:2165:ARG:HD2	1:A:2417:PHE:CE1	2.53	0.43
2:C:370:LEU:HD11	2:C:431:VAL:HG23	1.99	0.43
1:A:994:MET:HG2	1:A:1016:PHE:CE1	2.54	0.43
1:A:719:LYS:HZ1	1:A:759:LYS:HG3	1.84	0.43
1:A:1382:LEU:HD12	1:A:1431:PHE:CE1	2.54	0.43
1:A:2131:LEU:HB2	1:A:2137:PRO:HD2	2.00	0.43
1:A:1430:LYS:NZ	1:A:1486:GLU:OE2	2.38	0.43
2:C:432:PRO:HD3	2:C:469:LEU:HD12	2.01	0.43
1:A:2293:PRO:HB3	1:A:2377:GLN:HG2	2.01	0.42
1:A:1249:LEU:HD23	1:A:1295:ARG:HG2	2.00	0.42
1:A:1944:MET:O	1:A:1948:VAL:HG12	2.20	0.42
1:A:765:LEU:O	1:A:768:THR:HG22	2.20	0.42
1:A:1504:LEU:HD21	1:A:1527:THR:OG1	2.19	0.42
1:A:1293:LEU:HD22	1:A:1360:LEU:HD12	2.01	0.42
1:A:1945:VAL:HG12	1:A:1949:GLN:OE1	2.19	0.42
2:C:178:LYS:HD3	2:C:178:LYS:HA	1.84	0.42
1:A:1955:LEU:HA	1:A:1958:VAL:HG12	2.02	0.42
1:A:859:PRO:HD2	2:C:201:GLN:NE2	2.35	0.42
1:A:1623:ALA:HB2	1:A:1750:ALA:HB1	2.02	0.42
1:A:1324:LEU:HD13	1:A:1361:GLU:HA	2.01	0.42
1:A:1623:ALA:HB1	1:A:1751:TYR:CD1	2.54	0.42
1:A:1623:ALA:HB2	1:A:1750:ALA:CB	2.50	0.42
1:A:790:LEU:HD12	1:A:791:PRO:HD2	2.01	0.41
1:A:870:LEU:HD22	1:A:946:ILE:HD13	2.01	0.41
1:A:1054:LEU:HG	1:A:1058:MET:HE2	2.01	0.41
1:A:1463:VAL:O	1:A:1467:LYS:HB2	2.19	0.41
1:A:2195:VAL:HG12	1:A:2205:ILE:HG12	2.02	0.41
1:A:1401:MET:SD	1:A:1421:LEU:HD21	2.60	0.41
1:A:1631:ARG:HA	1:A:1744:TYR:OH	2.21	0.41
2:C:171:LEU:HD23	2:C:171:LEU:H	1.84	0.41
2:C:172:LEU:HD13	2:C:173:PRO:HD2	2.02	0.41
2:C:306:GLN:HG2	2:C:512:LEU:HD13	2.01	0.41
1:A:502:ASN:O	1:A:506:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ILE:HG22	1:A:634:LEU:HD12	2.02	0.41
1:A:1544:LYS:HE2	1:A:1597:PRO:HD3	2.03	0.41
1:A:558:ILE:HG13	1:A:559:PRO:CD	2.45	0.41
1:A:544:VAL:O	1:A:548:VAL:HG23	2.20	0.41
1:A:2035:PRO:HB2	1:A:2094:GLU:HA	2.02	0.41
1:A:606:ASN:O	1:A:610:VAL:HG23	2.21	0.41
1:A:2337:HIS:CE1	1:A:2339:ASP:HB2	2.56	0.41
2:C:209:VAL:CG2	2:C:221:MET:HE2	2.51	0.41
2:C:306:GLN:OE1	2:C:507:ARG:NH1	2.54	0.41
2:C:406:LEU:HD23	2:C:406:LEU:O	2.21	0.41
1:A:1230:TYR:CZ	1:A:1234:LEU:HD11	2.56	0.41
2:C:310:PHE:O	2:C:314:VAL:HG22	2.21	0.41
1:A:2151:PRO:HG2	1:A:2207:TRP:HB3	2.03	0.40
1:A:2195:VAL:HG12	1:A:2205:ILE:HG23	2.03	0.40
1:A:797:ARG:O	1:A:801:VAL:HG23	2.21	0.40
1:A:3623:ARG:NH1	1:A:3630:ARG:HB2	2.36	0.40
1:A:917:ILE:HD11	1:A:982:LEU:HB3	2.04	0.40
1:A:1445:LEU:HD23	1:A:1445:LEU:HA	1.93	0.40
1:A:2278:HIS:CE1	1:A:2279:VAL:HG23	2.56	0.40
1:A:1237:PHE:HB2	1:A:1245:CYS:SG	2.62	0.40
2:C:434:MET:HE2	2:C:434:MET:HB3	1.94	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	1707/3657 (47%)	1653 (97%)	53 (3%)	1 (0%)	48	77
2	C	301/352 (86%)	287 (95%)	14 (5%)	0	100	100
All	All	2008/4009 (50%)	1940 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	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	A	1226/2797 (44%)	1225 (100%)	1 (0%)	88	90
2	C	251/318 (79%)	251 (100%)	0	100	100
All	All	1477/3115 (47%)	1476 (100%)	1 (0%)	87	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	741	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	577	ASN
1	A	623	ASN
1	A	645	ASN
1	A	956	ASN
1	A	1112	GLN
1	A	1344	GLN
1	A	1353	GLN
1	A	1388	HIS
1	A	1542	GLN
1	A	1758	ASN
1	A	1832	HIS
1	A	2168	GLN
1	A	2222	GLN
1	A	3628	ASN
2	C	179	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	187	GLN
2	C	201	GLN
2	C	294	ASN
2	C	316	HIS
2	C	322	GLN
2	C	366	HIS
2	C	463	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	ATP	C	601	6	32,33,33	0.32	0	48,52,52	0.27	0
3	ANP	A	3701	-	33,33,33	0.93	4 (12%)	45,52,52	0.58	0
4	IHP	A	3702	-	36,36,36	1.57	6 (16%)	60,60,60	0.98	2 (3%)

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	ATP	C	601	6	-	3/22/38/38	0/3/3/3
3	ANP	A	3701	-	-	7/18/38/38	0/3/3/3
4	IHP	A	3702	-	-	9/30/54/54	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3702	IHP	P3-O13	3.74	1.66	1.59
4	A	3702	IHP	P4-O14	3.41	1.65	1.59
4	A	3702	IHP	P5-O15	3.28	1.65	1.59
4	A	3702	IHP	P6-O16	3.27	1.65	1.59
4	A	3702	IHP	P1-O11	3.21	1.65	1.59
4	A	3702	IHP	P2-O12	3.16	1.65	1.59
3	A	3701	ANP	PG-O1G	2.56	1.50	1.46
3	A	3701	ANP	PG-N3B	2.46	1.69	1.63
3	A	3701	ANP	PB-O1B	2.40	1.49	1.46
3	A	3701	ANP	PB-O3A	-2.24	1.56	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3702	IHP	P1-O11-C1	-2.12	117.77	123.43
4	A	3702	IHP	P4-O14-C4	-2.05	117.96	123.43

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3701	ANP	PB-N3B-PG-O1G
3	A	3701	ANP	PA-O3A-PB-O2B
3	A	3701	ANP	C5'-O5'-PA-O1A
3	A	3701	ANP	C5'-O5'-PA-O3A
4	A	3702	IHP	C2-C3-O13-P3
4	A	3702	IHP	C4-C3-O13-P3
3	A	3701	ANP	O4'-C4'-C5'-O5'
3	A	3701	ANP	C3'-C4'-C5'-O5'
5	C	601	ATP	PG-O3B-PB-O1B
4	A	3702	IHP	C6-C5-O15-P5
5	C	601	ATP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

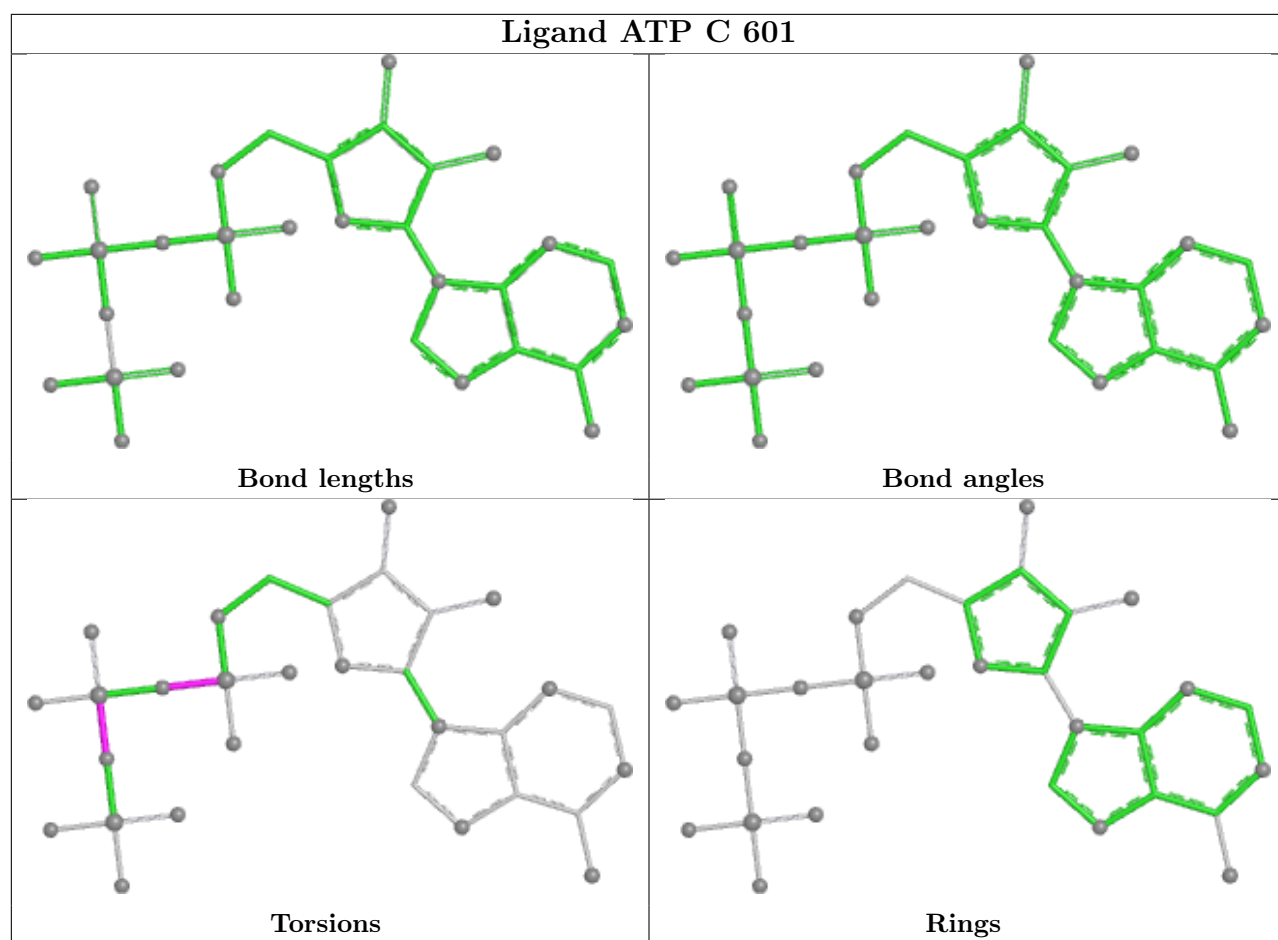
Mol	Chain	Res	Type	Atoms
4	A	3702	IHP	C5-C6-O16-P6
4	A	3702	IHP	C1-O11-P1-O31
4	A	3702	IHP	C4-C5-O15-P5
4	A	3702	IHP	C5-O15-P5-O25
4	A	3702	IHP	C6-O16-P6-O26
5	C	601	ATP	PG-O3B-PB-O2B
4	A	3702	IHP	C6-C1-O11-P1
3	A	3701	ANP	PA-O3A-PB-O1B

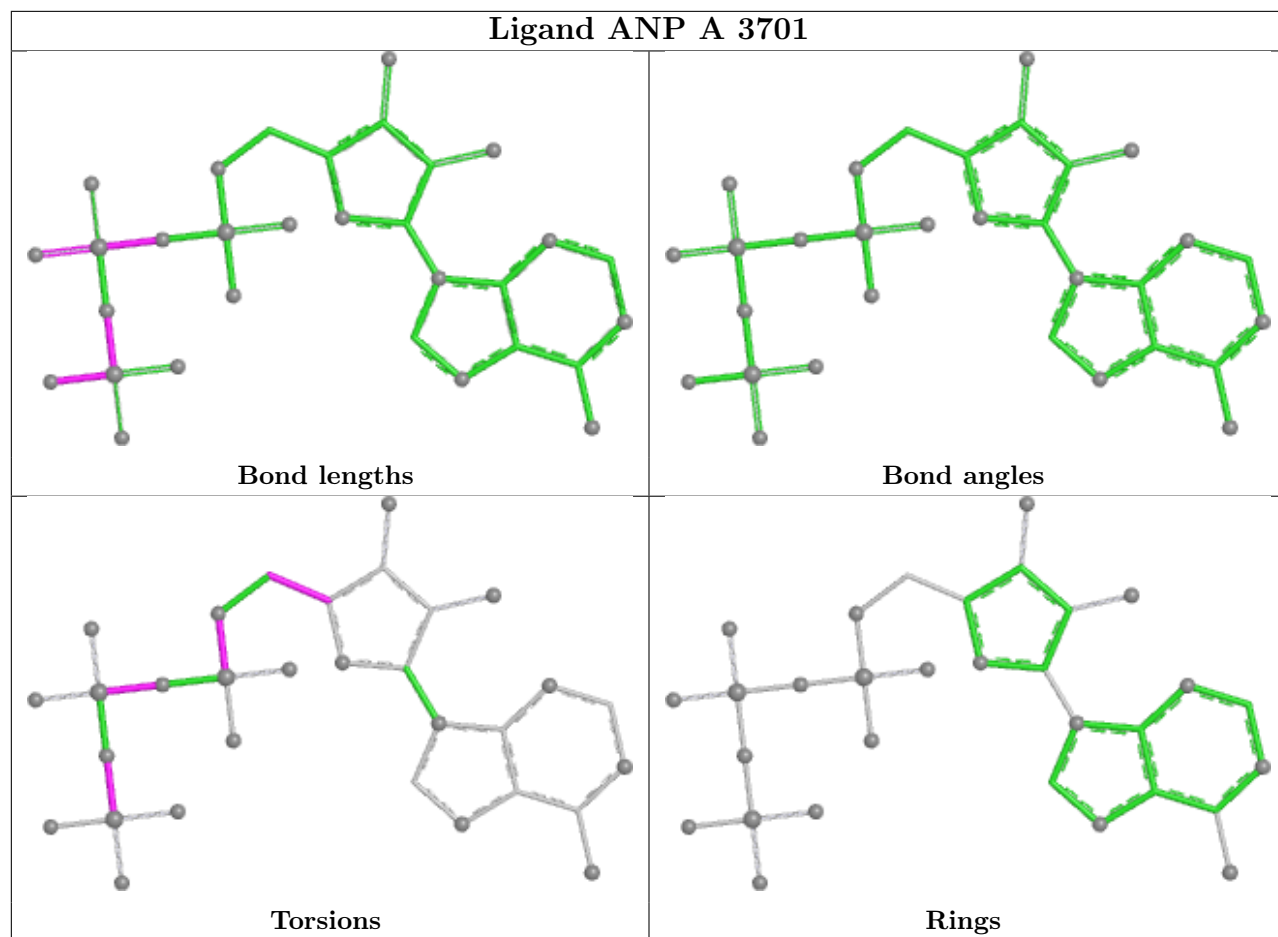
There are no ring outliers.

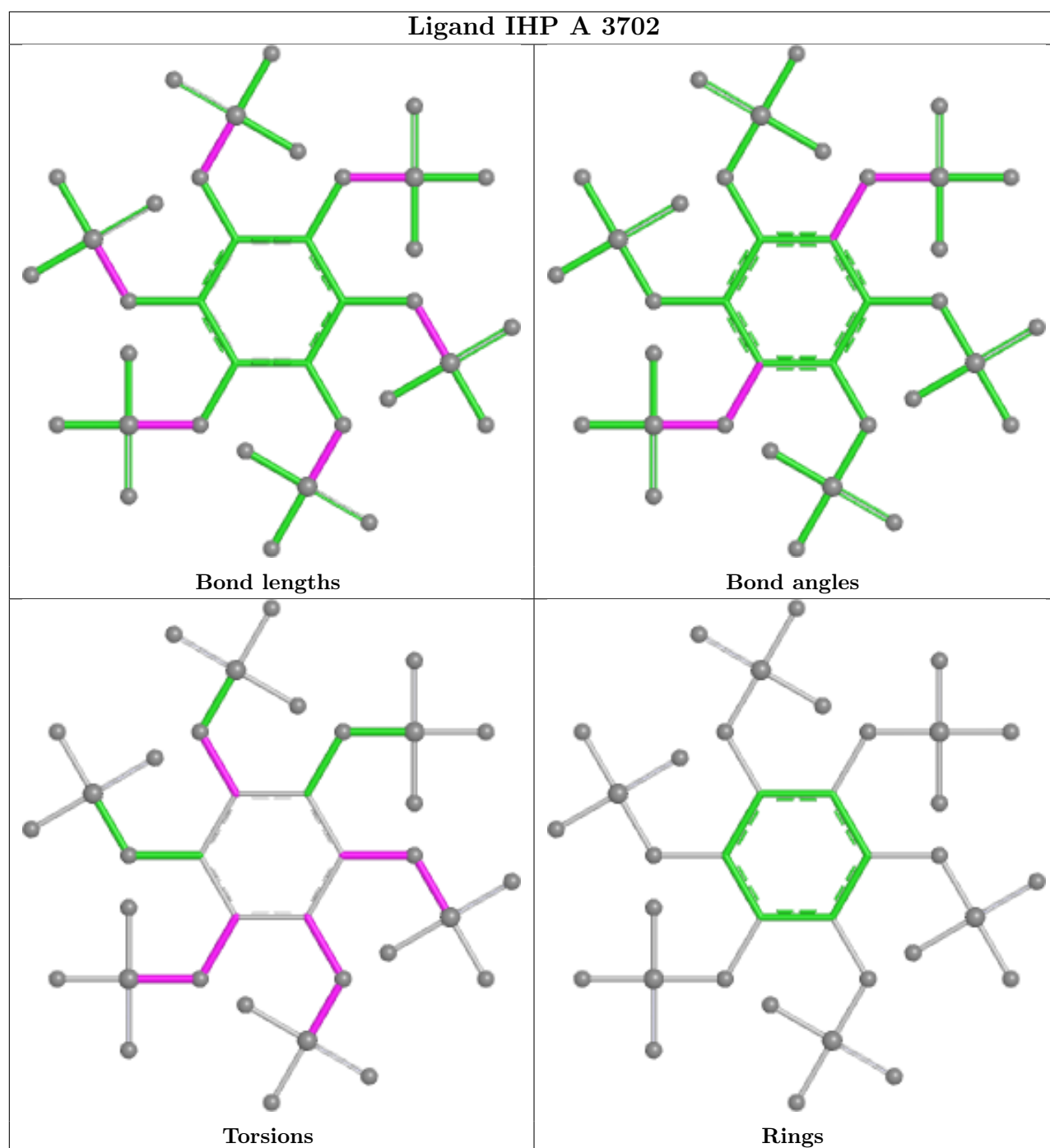
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	ATP	1	0
3	A	3701	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

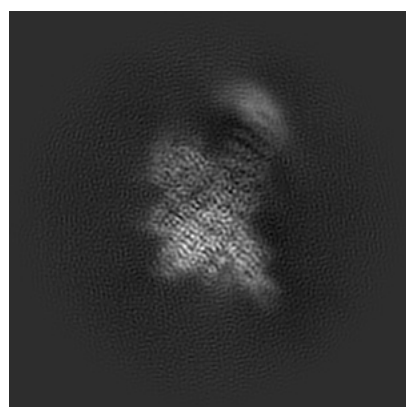
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13679. These allow visual inspection of the internal detail of the map and identification of artifacts.

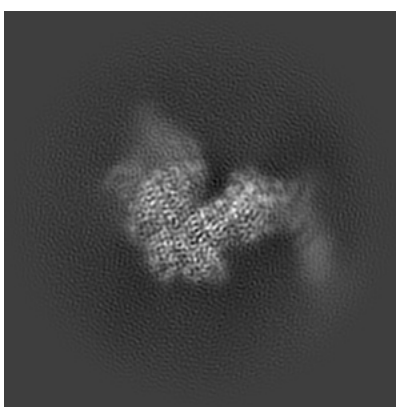
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

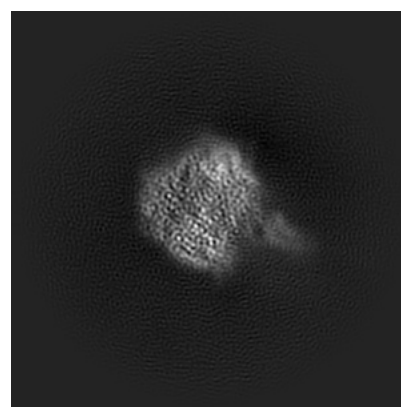
6.1.1 Primary map



X



Y

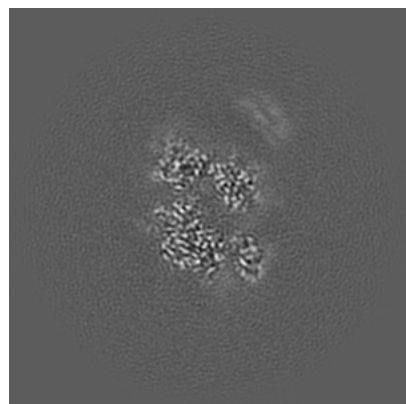


Z

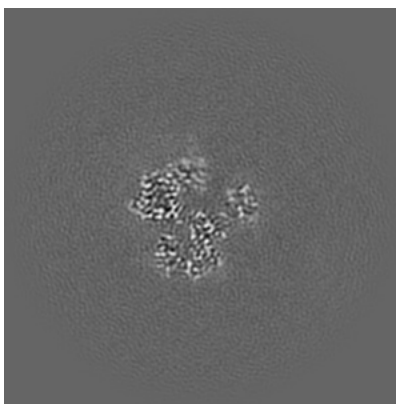
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

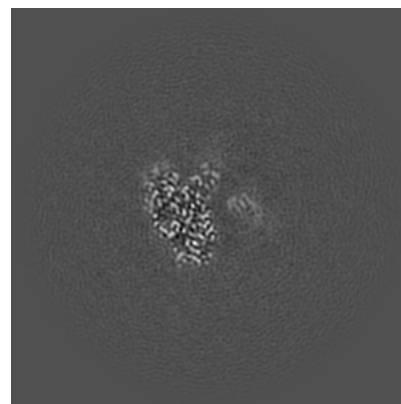
6.2.1 Primary map



X Index: 172



Y Index: 172

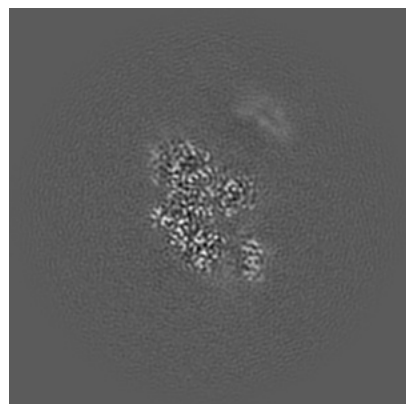


Z Index: 172

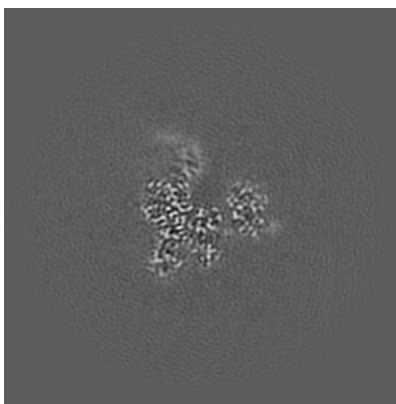
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

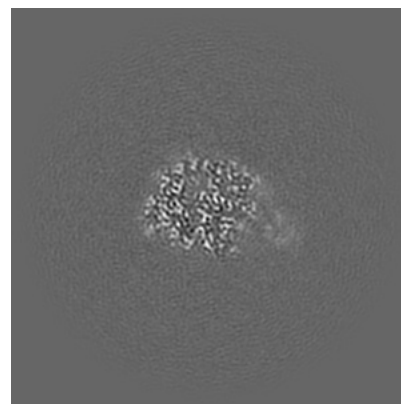
6.3.1 Primary map



X Index: 166



Y Index: 161

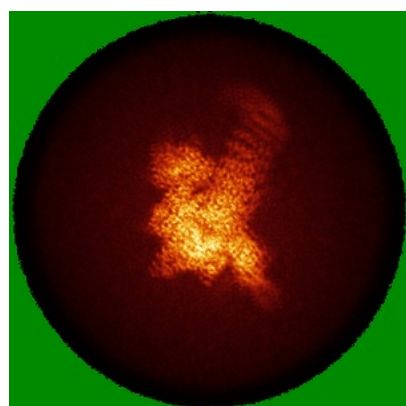


Z Index: 143

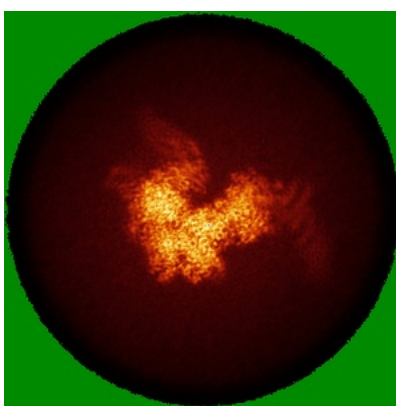
The images above show the largest variance slices of the map in three orthogonal directions.

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

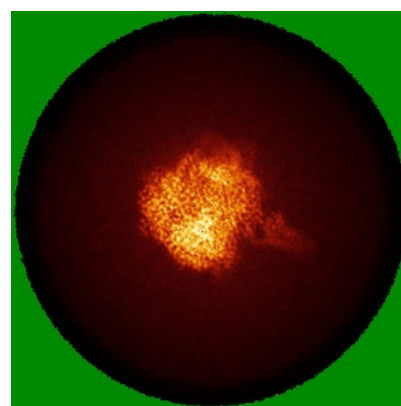
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.818. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

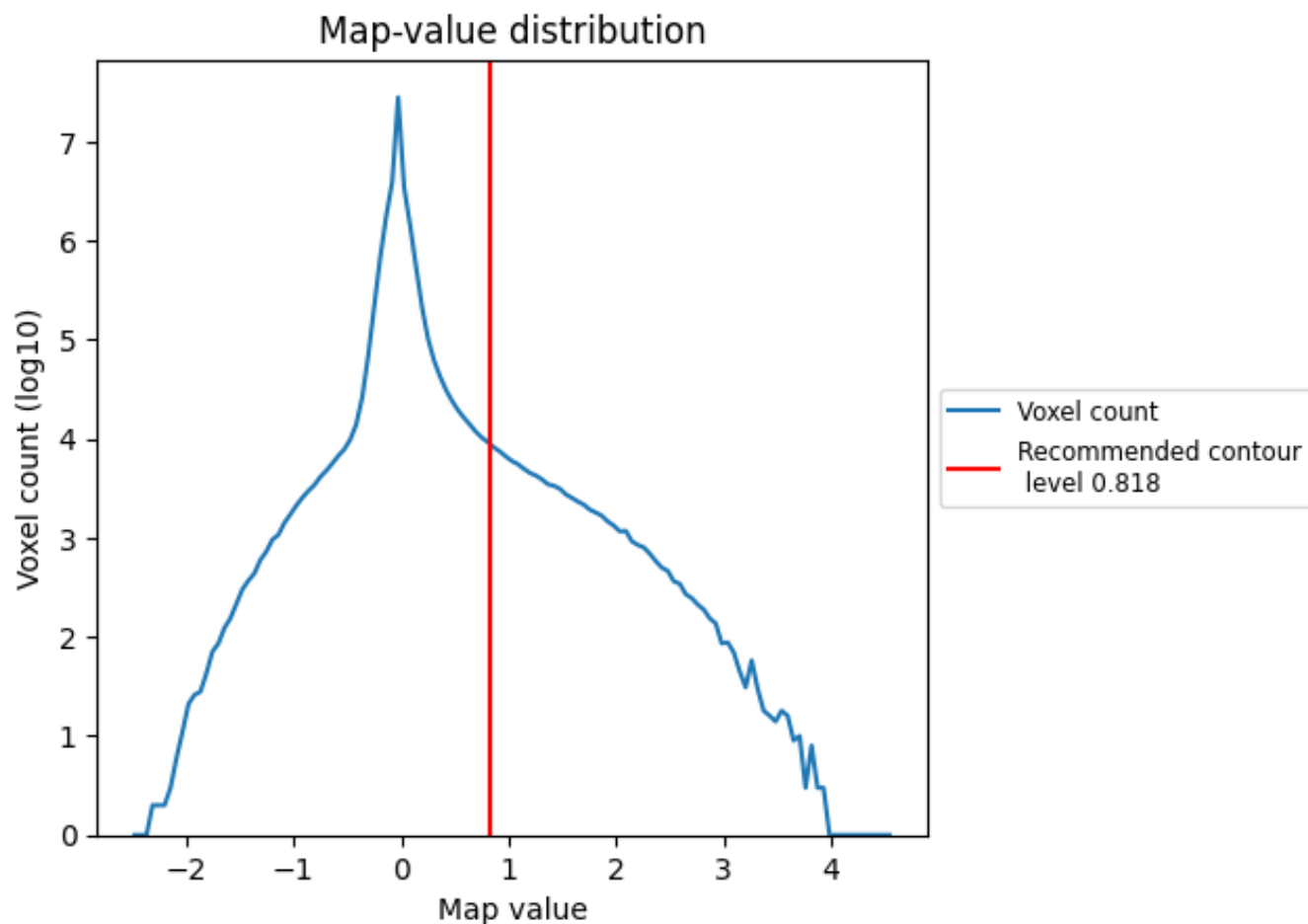
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

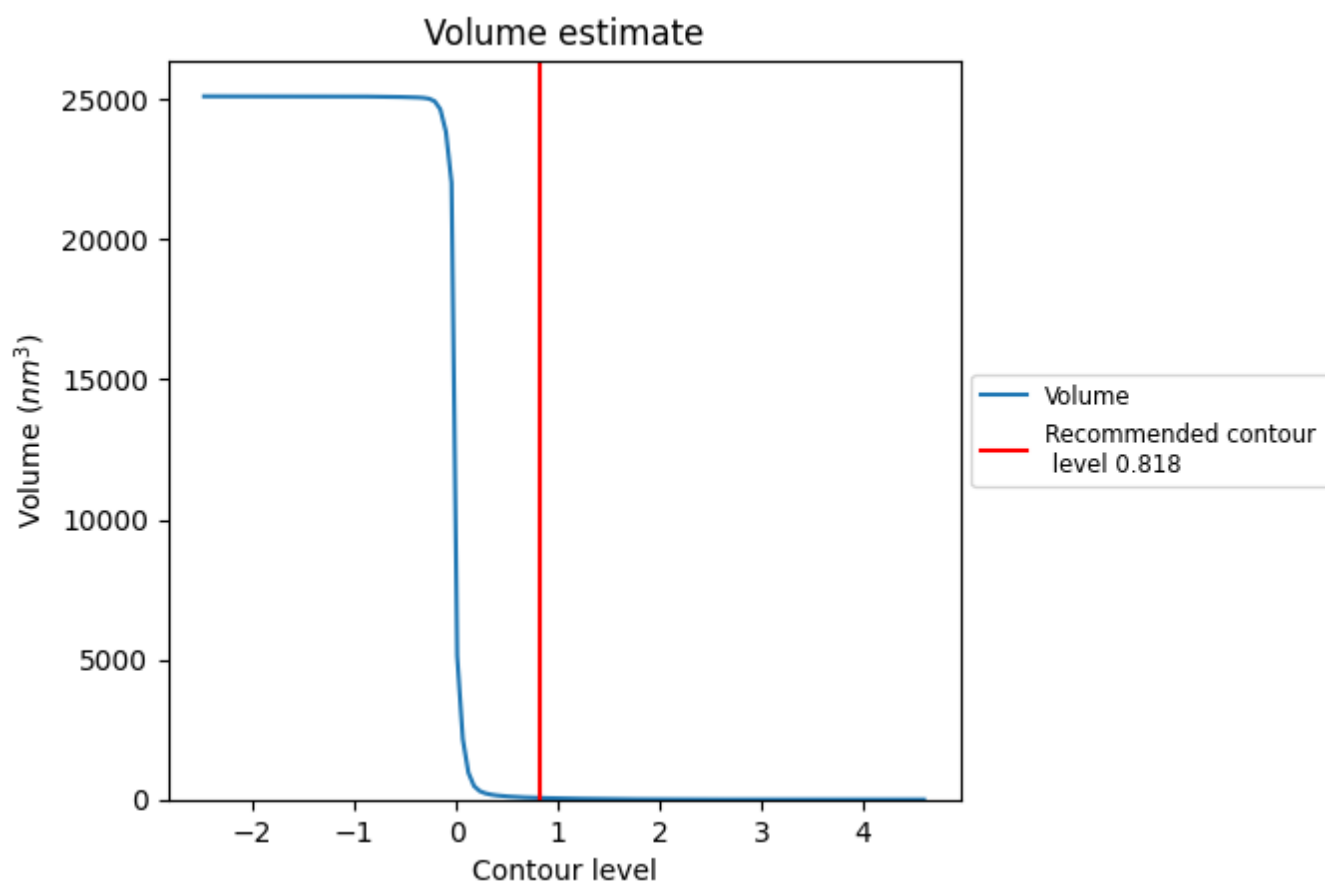
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

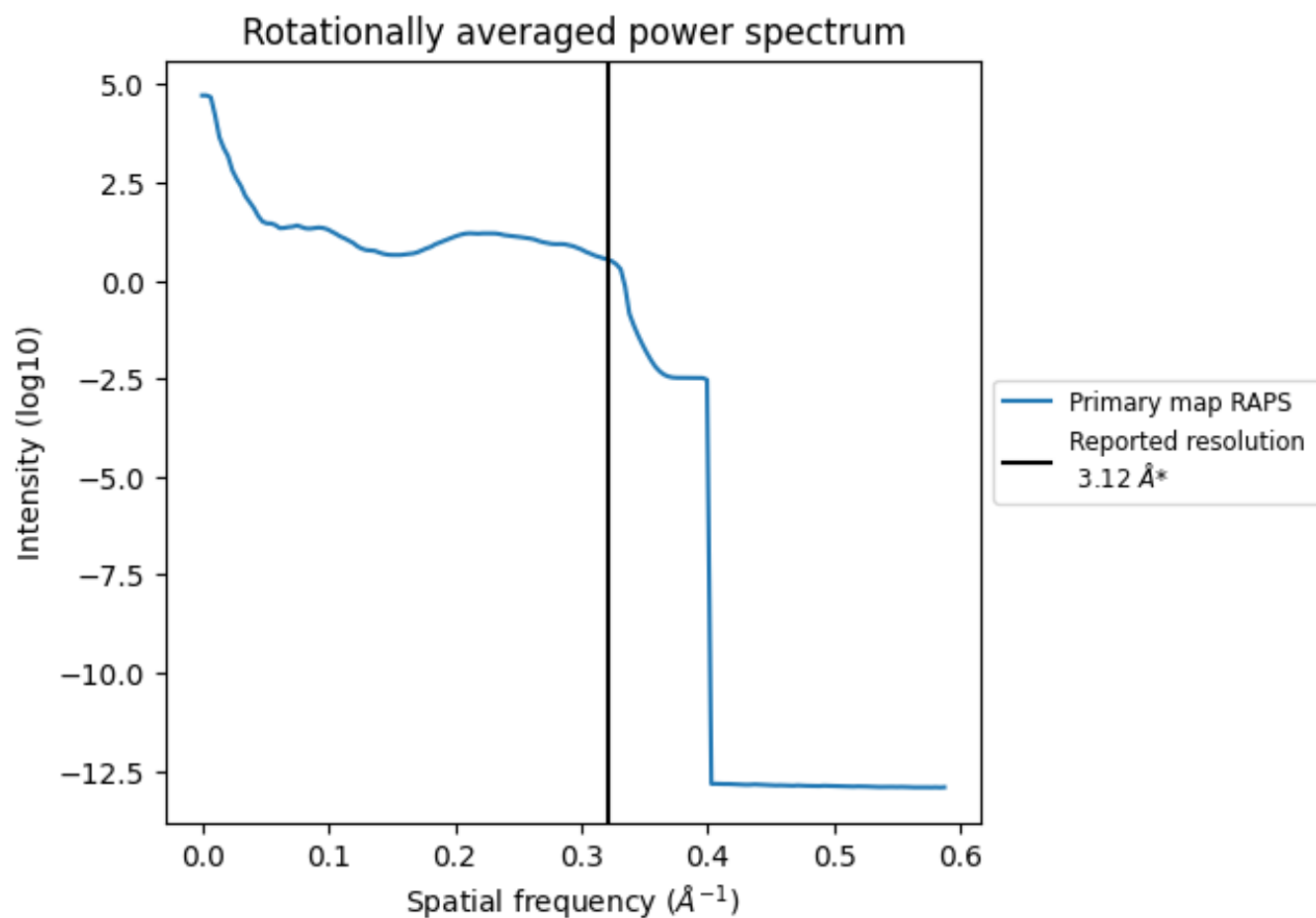
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 54 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 0.321 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

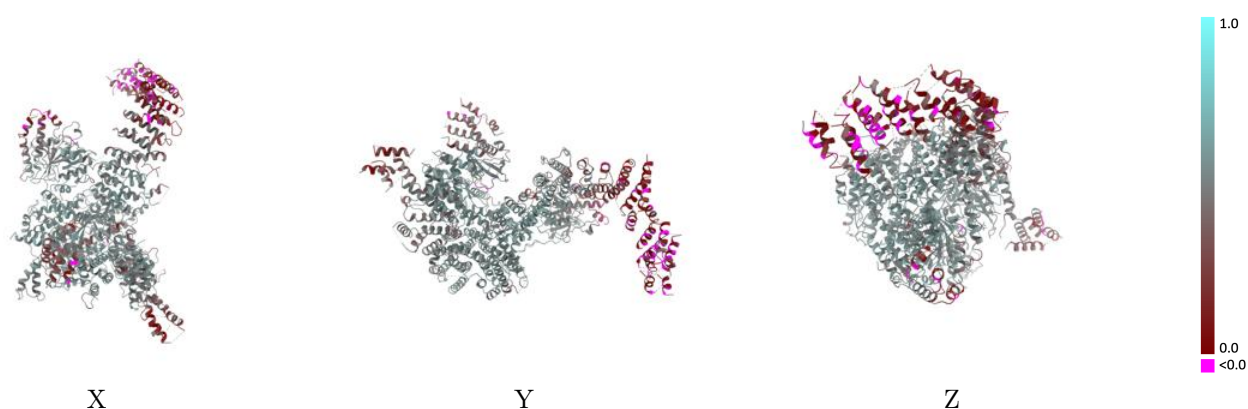
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-13679 and PDB model 7PW9. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

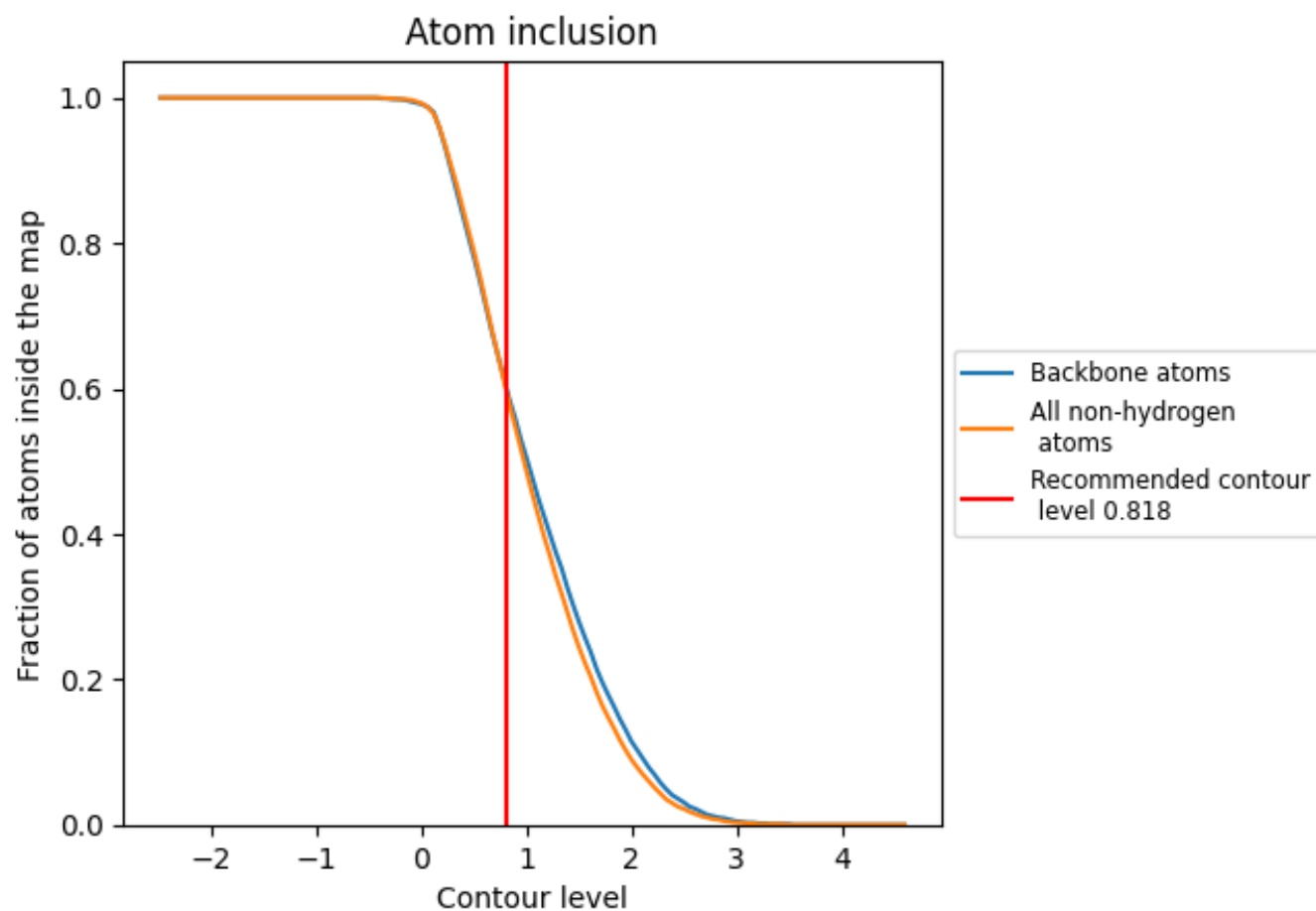


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 59% 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 (0.818) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.4790
A	0.5960	0.4810
C	0.5610	0.4690

