



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:37 AM EST

PDB ID : 7M74
EMDB ID : EMD-23708
Title : ATP-bound AMP-activated protein kinase
Authors : Yan, Y.; Mukherjee, S.; Harikumar, K.G.; Strutzenberg, T.; Zhou, X.E.; Powell, S.K.; Xu, T.; Sheldon, R.; Lamp, J.; Brunzelle, J.S.; Radziwon, K.; Ellis, A.; Novick, S.J.; Vega, I.E.; Jones, R.; Miller, L.J.; Xu, H.E.; Griffin, P.R.; Kossiakoff, A.A.; Melcher, K.
Deposited on : 2021-03-26
Resolution : 3.93 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

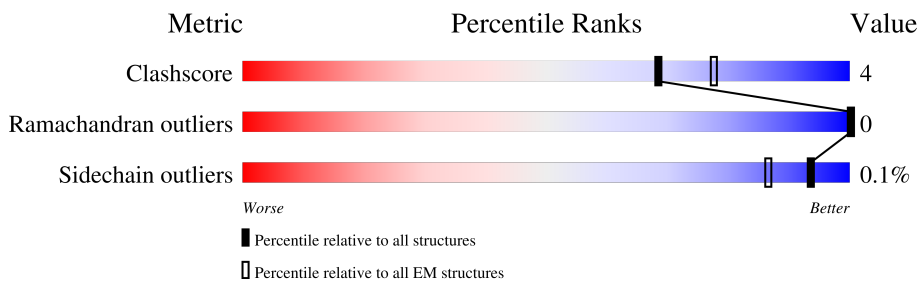
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	484	
2	B	198	
3	G	306	
4	M	373	
5	L	211	
6	H	228	
7	N	120	
8	D	2	

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 13457 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	380	3083	1977	541	547	18	0	0

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	93	736	479	123	130	4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	75	MET	-	initiating methionine	UNP O43741
B	199	ALA	GLU	conflict	UNP O43741
B	200	ALA	GLU	conflict	UNP O43741

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	300	2421	1572	403	439	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	22	MET	-	expression tag	UNP P54619
G	23	GLY	-	expression tag	UNP P54619

- Molecule 4 is a protein called Maltose/maltodextrin ABC transporter substrate-binding protein MalE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	367	2834	1826	460	542	6	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	MET	-	initiating methionine	UNP A0A6D0N546
M	82	ALA	ASP	conflict	UNP A0A6D0N546
M	83	ALA	LYS	conflict	UNP A0A6D0N546
M	239	ALA	LYS	conflict	UNP A0A6D0N546
M	367	ASN	-	expression tag	UNP A0A6D0N546
M	368	ALA	-	expression tag	UNP A0A6D0N546
M	369	ALA	-	expression tag	UNP A0A6D0N546
M	370	GLU	-	expression tag	UNP A0A6D0N546
M	371	PHE	-	expression tag	UNP A0A6D0N546

- Molecule 5 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	211	1601	997	271	328	5	0	0

- Molecule 6 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	228	1723	1098	279	339	7	0	0

- Molecule 7 is a protein called Nanobody.

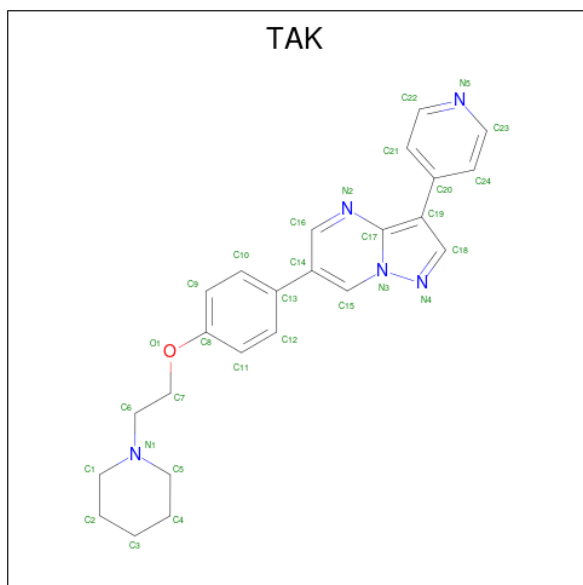
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	120	925	574	163	184	4	0	0

- Molecule 8 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



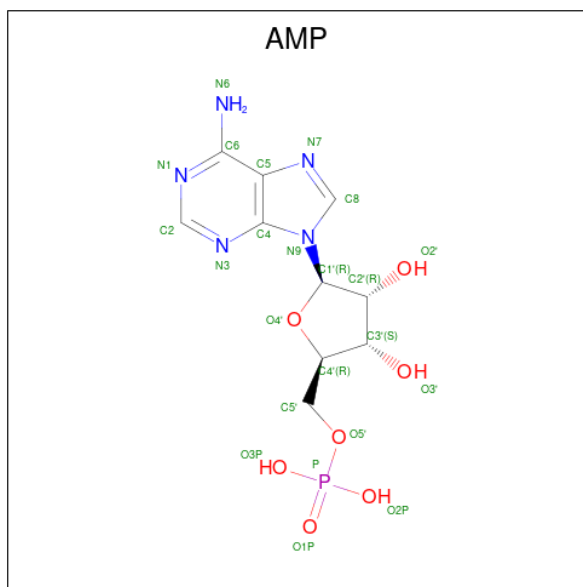
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
8	D	2	23	12	11	0	0

- Molecule 9 is 6-[4-(2-piperidin-1-ylethoxy)phenyl]-3-pyridin-4-ylpyrazolo[1,5-a]pyrimidine (three-letter code: TAK) (formula: C₂₄H₂₅N₅O) (labeled as "Ligand of Interest" by depositor).

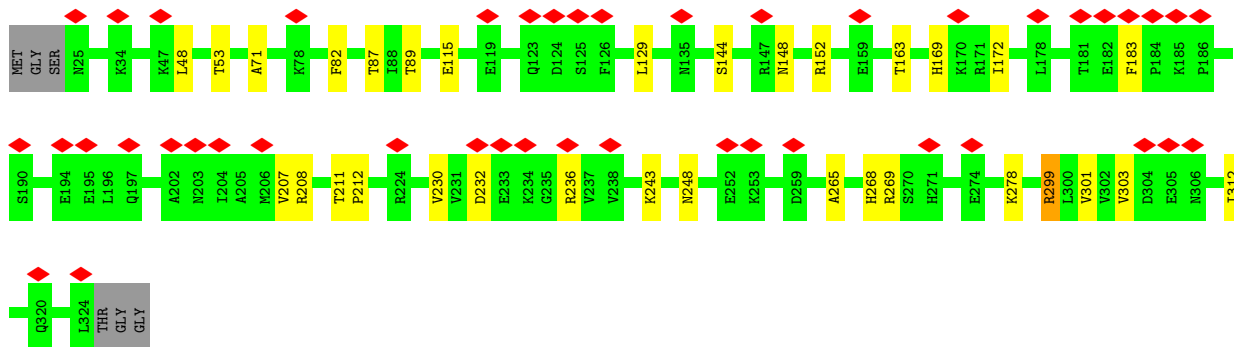


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	A	1	30	24	5	1	0

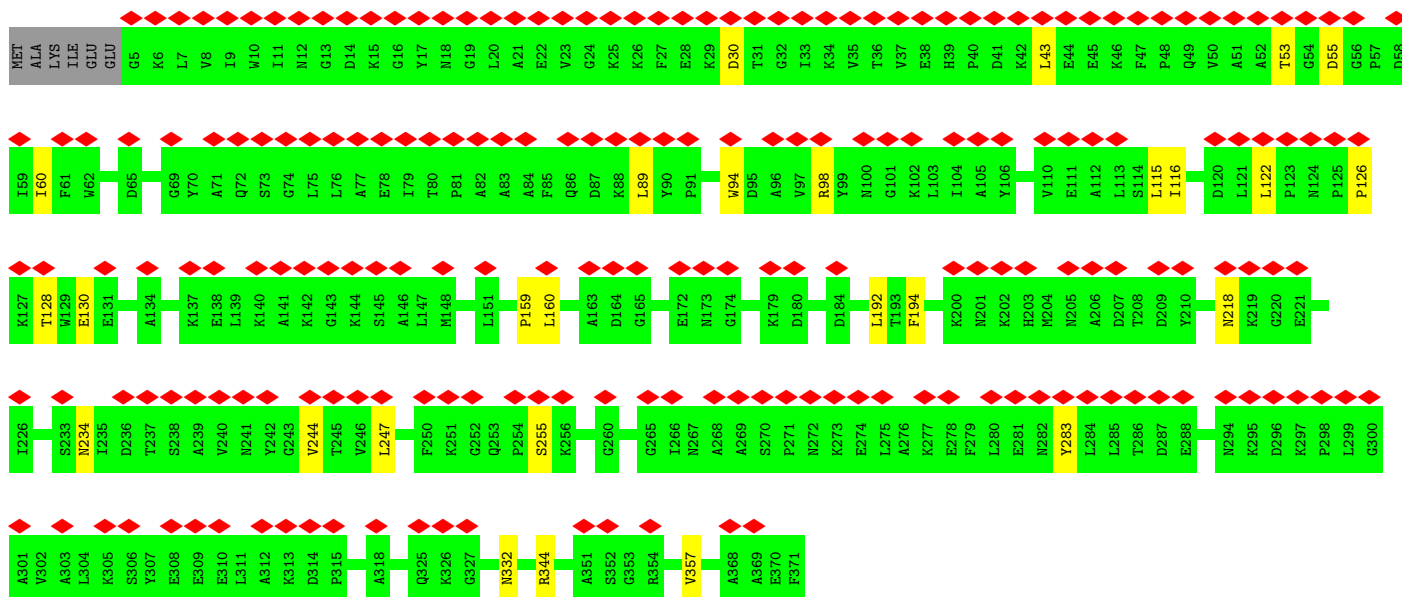
- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



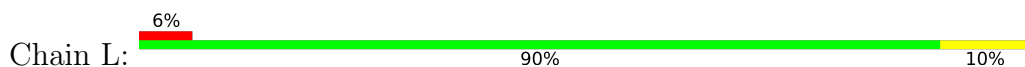
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	G	1	23	10	5	7	1	0



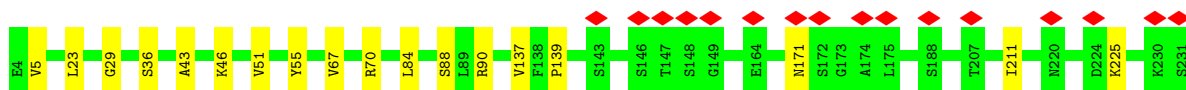
• Molecule 4: Maltose/maltodextrin ABC transporter substrate-binding protein MalE



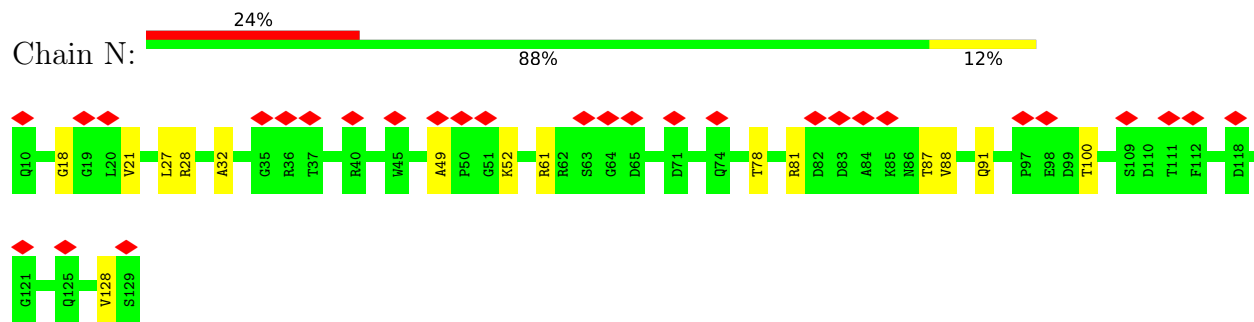
• Molecule 5: Fab light chain



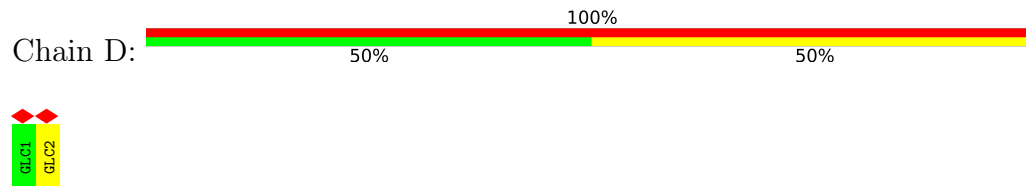
• Molecule 6: Fab heavy chain



• Molecule 7: Nanobody



- Molecule 8: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	569379	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 ($e^-/\text{\AA}^2$)	66	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	0.031	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	231.84, 231.84, 231.84	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, ADP, ATP, AMP, TAK

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	0.25	0/3155	0.45	0/4259
2	B	0.25	0/758	0.52	0/1034
3	G	0.28	1/2472 (0.0%)	0.48	0/3356
4	M	0.26	0/2904	0.45	0/3947
5	L	0.26	0/1634	0.49	0/2217
6	H	0.26	0/1770	0.51	0/2414
7	N	0.25	0/944	0.47	0/1276
All	All	0.26	1/13637 (0.0%)	0.47	0/18503

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	183	PHE	C-N	5.23	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3083	0	3125	37	0
2	B	736	0	758	9	0
3	G	2421	0	2488	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	2834	0	2792	14	0
5	L	1601	0	1562	11	0
6	H	1723	0	1670	10	0
7	N	925	0	870	9	0
8	D	23	0	21	1	0
9	A	30	0	25	0	0
10	G	31	0	12	2	0
11	G	27	0	12	1	0
12	G	23	0	12	0	0
All	All	13457	0	13347	103	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 4.

All (103) 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:218:ASP:H	1:A:224:LEU:HD12	1.63	0.64
1:A:79:ILE:HG23	1:A:96:GLU:HG2	1.81	0.62
3:G:301:VAL:HG12	3:G:312:ILE:HG12	1.83	0.60
5:L:7:GLN:NE2	5:L:24:CYS:SG	2.75	0.59
1:A:79:ILE:HD12	1:A:158:ALA:HA	1.84	0.58
7:N:18:GLY:HA2	7:N:27:LEU:HD21	1.87	0.56
1:A:239:LEU:HD12	1:A:243:VAL:HG13	1.88	0.56
5:L:22:ILE:HG12	5:L:103:THR:HG21	1.88	0.56
1:A:438:ARG:NH2	1:A:440:ASN:OD1	2.40	0.55
1:A:260:THR:H	1:A:263:ASP:HB2	1.72	0.54
1:A:71:LYS:HE2	1:A:83:GLN:HA	1.89	0.54
1:A:87:THR:HG22	1:A:89:SER:H	1.73	0.54
3:G:278:LYS:HD3	3:G:303:VAL:HG21	1.90	0.54
1:A:435:ARG:NH2	2:B:180:ASP:OD2	2.41	0.53
7:N:100:THR:HB	7:N:128:VAL:HG22	1.89	0.53
4:M:98:ARG:O	4:M:332:ASN:ND2	2.42	0.53
6:H:70:ARG:NH2	6:H:88:SER:O	2.42	0.52
1:A:241:PRO:HA	1:A:244:ILE:HG22	1.91	0.52
3:G:48:LEU:HD21	3:G:163:THR:HG23	1.90	0.52
3:G:269:ARG:NH2	10:G:401:ATP:O2'	2.43	0.52
1:A:398:TRP:HD1	2:B:244:LEU:HD13	1.74	0.52
7:N:61:ARG:O	7:N:81:ARG:NH1	2.43	0.51
2:B:215:VAL:HG21	2:B:237:MET:HG2	1.92	0.51
6:H:36:SER:HB3	6:H:55:TYR:HD1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:43:ALA:HB3	6:H:46:LYS:HB2	1.93	0.51
6:H:70:ARG:HH22	6:H:90:ARG:HG3	1.76	0.51
1:A:193:ALA:HB1	1:A:197:VAL:HG21	1.93	0.50
1:A:76:PRO:O	1:A:156:LYS:NZ	2.44	0.50
3:G:82:PHE:HB3	3:G:129:LEU:HD13	1.92	0.50
7:N:49:ALA:HB3	7:N:52:LYS:HB2	1.93	0.50
1:A:414:GLU:OE2	1:A:417:ARG:NH2	2.44	0.50
6:H:137:VAL:O	6:H:225:LYS:NZ	2.44	0.50
4:M:115:LEU:HB2	4:M:247:LEU:HD23	1.94	0.50
1:A:119:ARG:NH1	1:A:272:GLN:OE1	2.41	0.49
5:L:90:GLN:HE22	5:L:92:SER:HB2	1.76	0.49
4:M:192:LEU:HD23	4:M:357:VAL:HG13	1.95	0.49
1:A:49:LEU:HB2	1:A:91:ILE:HB	1.93	0.49
4:M:116:ILE:HG12	4:M:244:VAL:HG22	1.94	0.49
6:H:171:ASN:HD22	6:H:211:ILE:HD13	1.78	0.48
3:G:208:ARG:HB2	3:G:211:THR:HG23	1.95	0.48
7:N:32:ALA:HB2	7:N:87:THR:HG22	1.95	0.48
5:L:5:MET:HB2	5:L:27:SER:HB3	1.96	0.48
4:M:43:LEU:HD13	4:M:60:ILE:HD11	1.96	0.48
5:L:117:PHE:HB2	5:L:136:LEU:HB3	1.96	0.48
1:A:216:PHE:HD1	1:A:227:LYS:HG2	1.78	0.48
1:A:438:ARG:HD3	1:A:540:MET:HG2	1.96	0.47
5:L:139:ASN:HA	5:L:173:THR:HB	1.95	0.47
7:N:28:ARG:NH1	7:N:91:GLN:OE1	2.47	0.47
1:A:13:VAL:HA	1:A:20:LEU:HD12	1.95	0.47
1:A:50:ASN:HD22	1:A:53:LYS:HE3	1.78	0.47
1:A:445:THR:HG21	1:A:529:ARG:HB2	1.97	0.47
1:A:51:ARG:HD3	1:A:55:ARG:HH11	1.81	0.46
5:L:91:GLN:NE2	5:L:93:SER:OG	2.47	0.46
1:A:84:VAL:HG22	1:A:93:MET:HG2	1.98	0.46
1:A:529:ARG:NH2	1:A:536:GLU:OE1	2.49	0.46
3:G:299:ARG:NH2	10:G:401:ATP:O1A	2.49	0.46
1:A:447:SER:HA	1:A:529:ARG:HH12	1.81	0.46
7:N:78:THR:HB	7:N:91:GLN:HB3	1.97	0.45
3:G:152:ARG:NH2	11:G:402:ADP:O3B	2.49	0.45
5:L:64:SER:HG	5:L:75:THR:HG1	1.63	0.45
1:A:447:SER:HB3	1:A:529:ARG:HH22	1.81	0.45
3:G:248:ASN:HD22	3:G:268:HIS:CD2	2.35	0.45
4:M:159:PRO:HB3	4:M:255:SER:HB3	1.98	0.45
1:A:82:TYR:HB2	1:A:94:VAL:HG23	1.99	0.45
1:A:134:ARG:NH1	1:A:281:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:122:LEU:HD21	4:M:126:PRO:HD3	1.99	0.45
1:A:239:LEU:HD11	1:A:244:ILE:HD13	1.98	0.45
1:A:455:GLN:HB2	2:B:205:PRO:HG2	1.99	0.45
3:G:232:ASP:OD1	3:G:236:ARG:N	2.48	0.45
4:M:344:ARG:HH21	8:D:2:GLC:H61	1.82	0.45
2:B:244:LEU:HB3	2:B:252:VAL:HB	1.98	0.44
1:A:425:GLU:OE1	1:A:437:ARG:NH2	2.50	0.44
4:M:160:LEU:HD11	4:M:194:PHE:HD2	1.82	0.44
3:G:207:VAL:HG23	3:G:230:VAL:HG12	1.98	0.44
1:A:170:GLU:HG3	1:A:173:ARG:H	1.82	0.44
3:G:89:THR:OG1	3:G:243:LYS:NZ	2.42	0.44
3:G:169:HIS:HA	3:G:172:ILE:HD12	2.00	0.44
4:M:30:ASP:OD2	4:M:283:TYR:OH	2.36	0.44
2:B:241:LEU:HD11	2:B:253:LEU:HD12	1.99	0.43
2:B:254:SER:HB3	2:B:267:LEU:HD23	2.00	0.43
3:G:53:THR:HG22	3:G:115:GLU:HB2	2.00	0.43
4:M:53:THR:OG1	4:M:55:ASP:OD1	2.34	0.43
4:M:218:ASN:ND2	4:M:234:ASN:O	2.52	0.43
5:L:66:SER:HG	5:L:73:THR:HG1	1.62	0.42
1:A:159:ASP:OD1	1:A:159:ASP:N	2.52	0.42
1:A:217:ASP:N	1:A:217:ASP:OD1	2.52	0.42
7:N:81:ARG:HA	7:N:88:VAL:HA	2.01	0.42
6:H:23:LEU:HD21	6:H:84:LEU:HD23	2.01	0.42
1:A:59:VAL:HG12	1:A:61:GLY:H	1.85	0.42
3:G:265:ALA:O	3:G:268:HIS:ND1	2.46	0.42
2:B:209:PRO:HD2	2:B:212:LEU:HD12	2.01	0.42
6:H:51:VAL:HG23	6:H:67:VAL:HG21	2.01	0.42
5:L:17:GLY:H	5:L:79:LEU:HB3	1.85	0.41
5:L:199:HIS:CD2	5:L:201:GLY:H	2.39	0.41
1:A:467:SER:H	2:B:239:ASN:HB3	1.84	0.41
3:G:144:SER:OG	3:G:148:ASN:ND2	2.53	0.41
3:G:71:ALA:HA	3:G:87:THR:HG22	2.03	0.41
6:H:139:PRO:HD3	6:H:225:LYS:HZ2	1.86	0.41
7:N:21:VAL:HG11	7:N:27:LEU:HD13	2.02	0.41
4:M:128:THR:HG22	4:M:130:GLU:H	1.86	0.41
1:A:39:LEU:HD11	3:G:212:PRO:HG2	2.03	0.40
4:M:89:LEU:HB2	4:M:94:TRP:HE1	1.85	0.40
6:H:5:VAL:HG22	6:H:29:GLY:HA3	2.02	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	376/484 (78%)	368 (98%)	8 (2%)	0	100	100
2	B	91/198 (46%)	82 (90%)	9 (10%)	0	100	100
3	G	298/306 (97%)	288 (97%)	10 (3%)	0	100	100
4	M	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
5	L	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
6	H	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
7	N	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
All	All	1683/1920 (88%)	1632 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/440 (78%)	343 (100%)	0	100	100
2	B	85/181 (47%)	84 (99%)	1 (1%)	71	83
3	G	276/279 (99%)	275 (100%)	1 (0%)	91	94
4	M	289/294 (98%)	289 (100%)	0	100	100
5	L	185/185 (100%)	185 (100%)	0	100	100
6	H	191/191 (100%)	191 (100%)	0	100	100
7	N	96/96 (100%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1465/1666 (88%)	1463 (100%)	2 (0%)	93 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	237	MET
3	G	299	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	220	HIS
1	A	249	HIS
3	G	148	ASN
3	G	169	HIS
4	M	335	GLN
5	L	90	GLN
5	L	91	GLN
5	L	139	ASN
5	L	199	HIS
6	H	171	ASN

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](#)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GLC	D	1	8	12,12,12	0.62	0	17,17,17	0.65	0
8	GLC	D	2	8	11,11,12	0.53	0	15,15,17	0.70	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
8	GLC	D	1	8	-	0/2/22/22	0/1/1/1
8	GLC	D	2	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

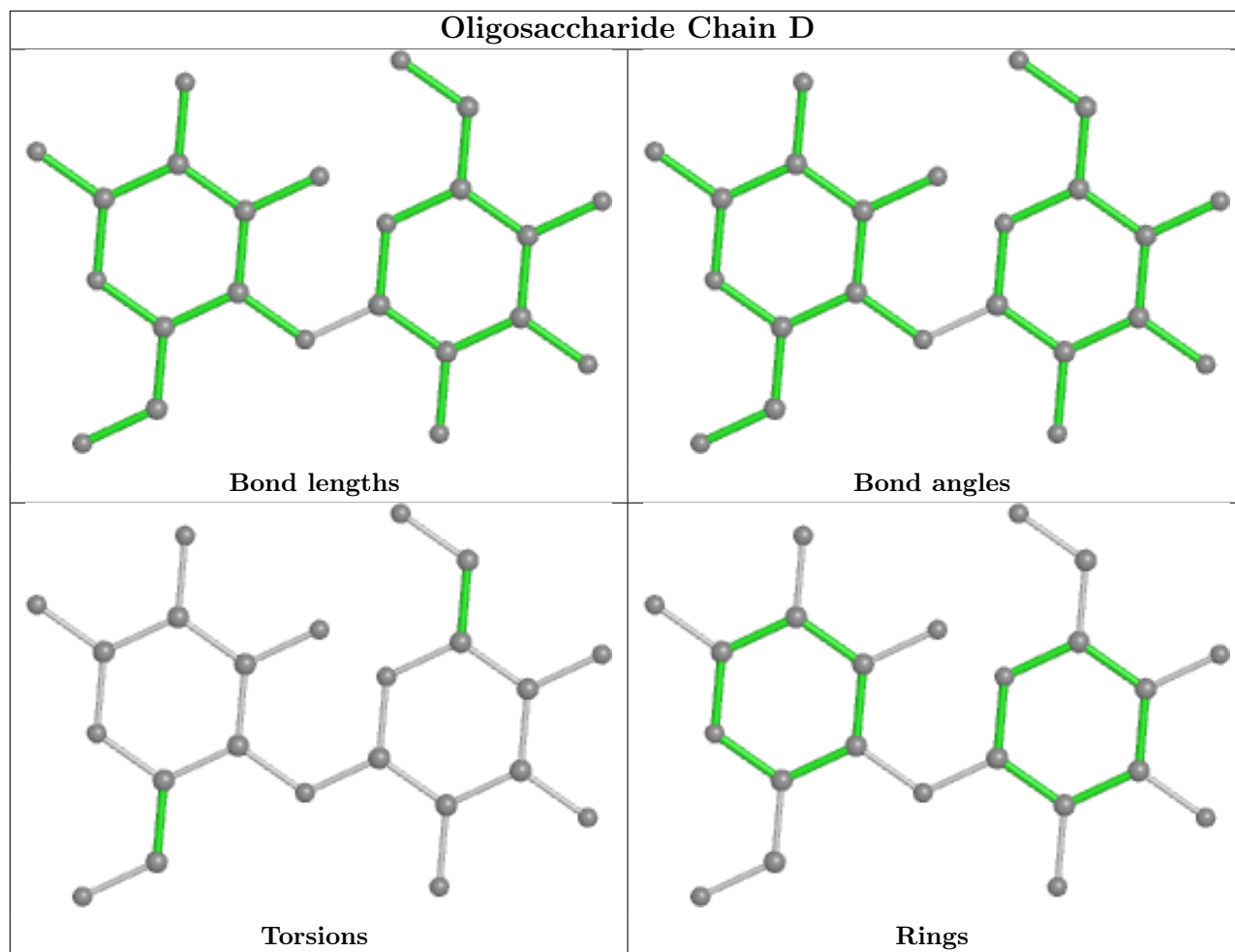
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2	GLC	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 oligosaccharide.



5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	AMP	G	403	-	22,25,25	0.89	1 (4%)	25,38,38	1.21	2 (8%)
11	ADP	G	402	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
10	ATP	G	401	-	26,33,33	0.94	1 (3%)	31,52,52	1.51	5 (16%)
9	TAK	A	601	-	28,34,34	0.71	0	30,46,46	2.00	7 (23%)

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
12	AMP	G	403	-	-	0/6/26/26	0/3/3/3
11	ADP	G	402	-	-	2/12/32/32	0/3/3/3
10	ATP	G	401	-	-	3/18/38/38	0/3/3/3
9	TAK	A	601	-	-	2/6/22/22	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	401	ATP	C5-C4	2.50	1.47	1.40
12	G	403	AMP	C5-C4	2.48	1.47	1.40
11	G	402	ADP	C5-C4	2.47	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	601	TAK	C18-N4-N3	7.48	109.14	103.70
9	A	601	TAK	C14-C16-N2	-3.68	120.04	125.05
9	A	601	TAK	C16-N2-C17	3.57	121.28	116.73
11	G	402	ADP	PA-O3A-PB	-3.46	120.94	132.83
11	G	402	ADP	N3-C2-N1	-3.29	123.53	128.68
10	G	401	ATP	PB-O3B-PG	-3.28	121.56	132.83
10	G	401	ATP	N3-C2-N1	-3.24	123.61	128.68
11	G	402	ADP	C3'-C2'-C1'	3.22	105.82	100.98
12	G	403	AMP	N3-C2-N1	-3.21	123.67	128.68
10	G	401	ATP	PA-O3A-PB	-3.06	122.34	132.83
10	G	401	ATP	C3'-C2'-C1'	2.97	105.44	100.98
10	G	401	ATP	C4-C5-N7	-2.75	106.53	109.40
9	A	601	TAK	C5-N1-C1	2.68	114.86	108.83
12	G	403	AMP	C4-C5-N7	-2.67	106.61	109.40
11	G	402	ADP	C4-C5-N7	-2.63	106.66	109.40
9	A	601	TAK	C24-C23-N5	-2.49	120.57	123.81
9	A	601	TAK	C23-N5-C22	2.44	122.59	116.85
9	A	601	TAK	C21-C22-N5	-2.42	120.66	123.81

There are no chirality outliers.

All (7) torsion outliers are listed below:

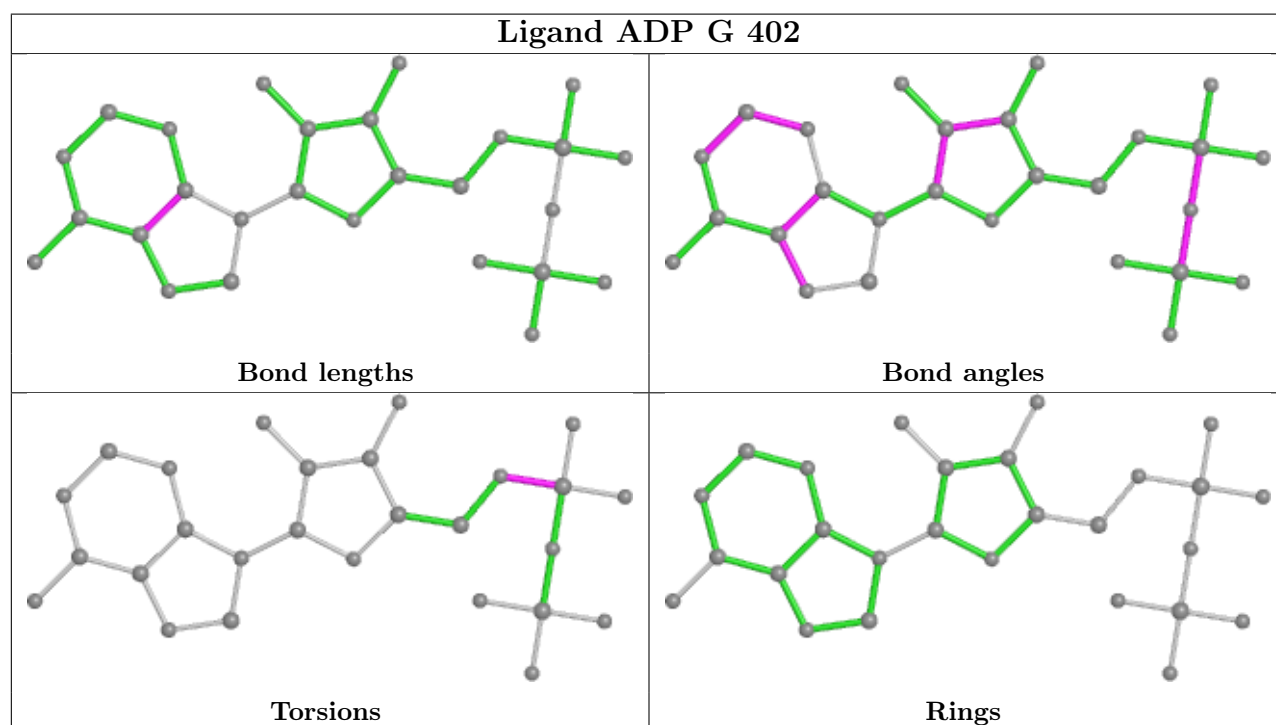
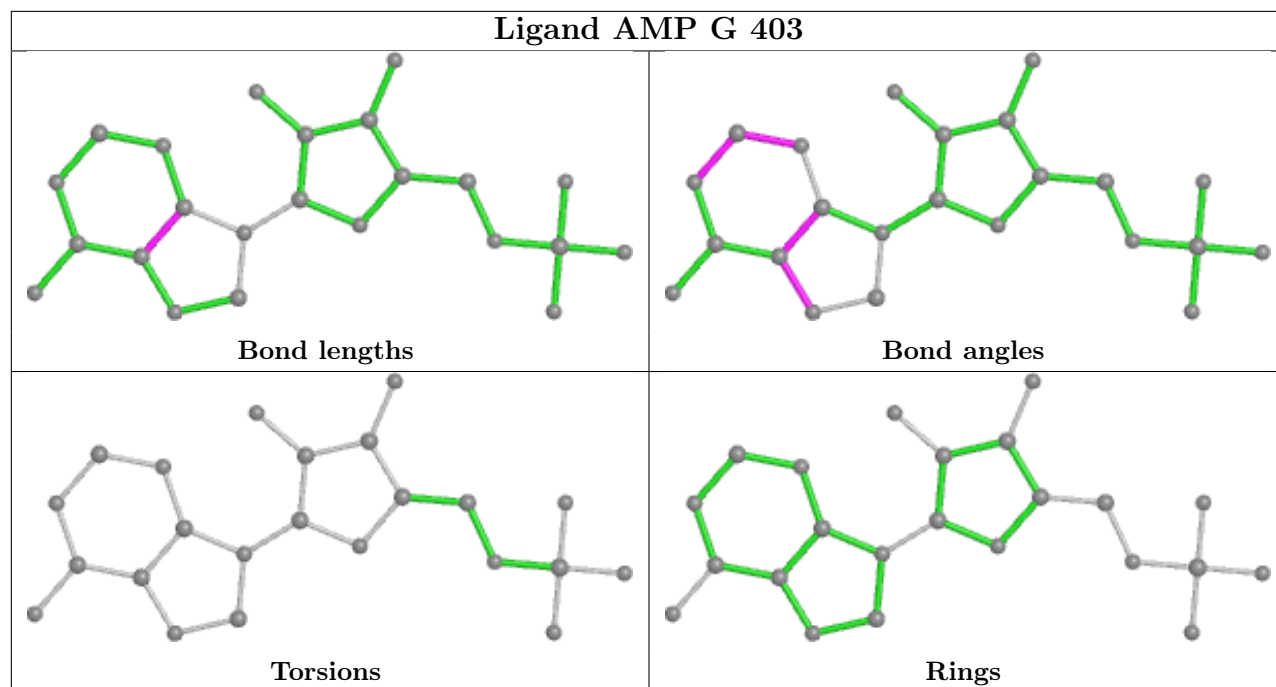
Mol	Chain	Res	Type	Atoms
10	G	401	ATP	PB-O3A-PA-O5'
11	G	402	ADP	C5'-O5'-PA-O3A
10	G	401	ATP	O4'-C4'-C5'-O5'
9	A	601	TAK	C11-C8-O1-C7
9	A	601	TAK	C9-C8-O1-C7
10	G	401	ATP	C3'-C4'-C5'-O5'
11	G	402	ADP	C5'-O5'-PA-O2A

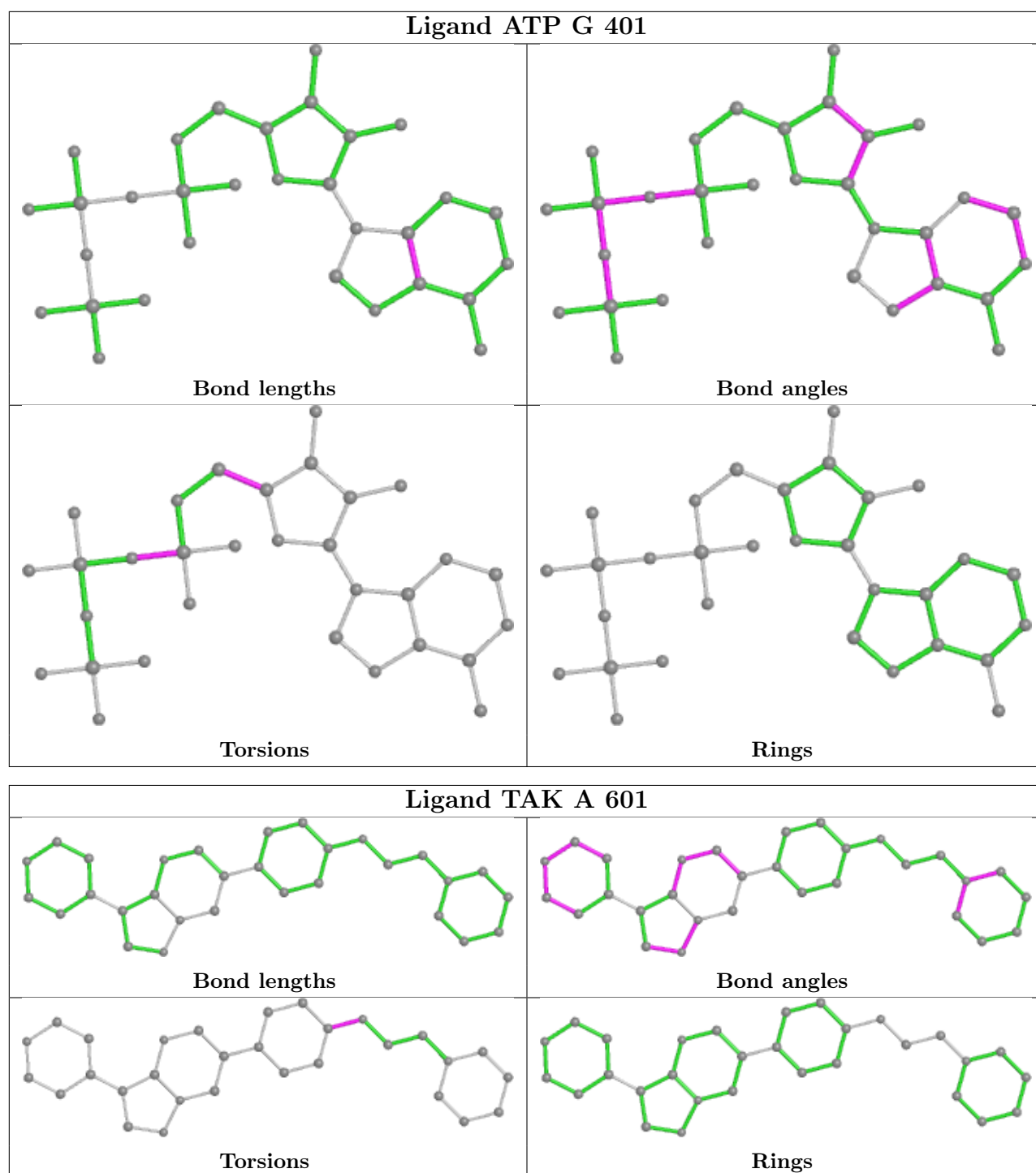
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	402	ADP	1	0
10	G	401	ATP	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.

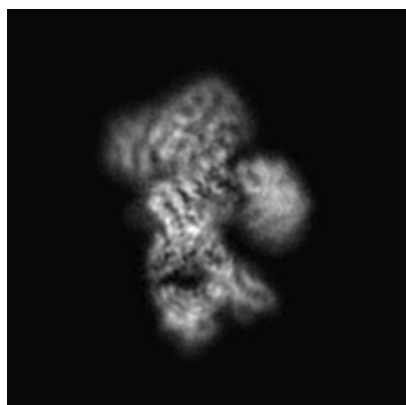
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23708. These allow visual inspection of the internal detail of the map and identification of artifacts.

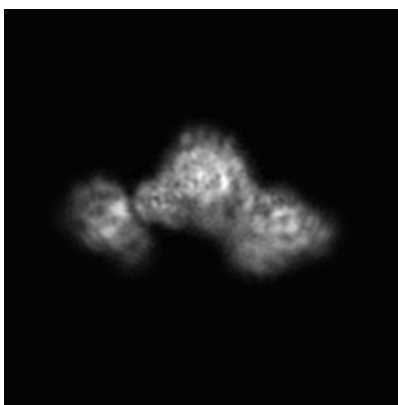
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

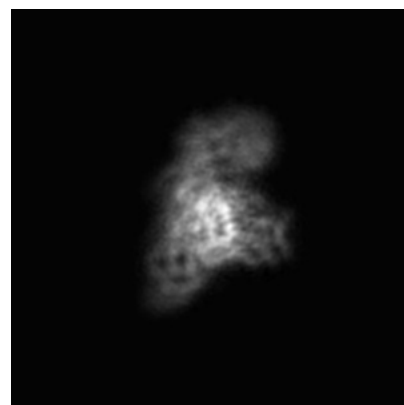
6.1.1 Primary map



X



Y

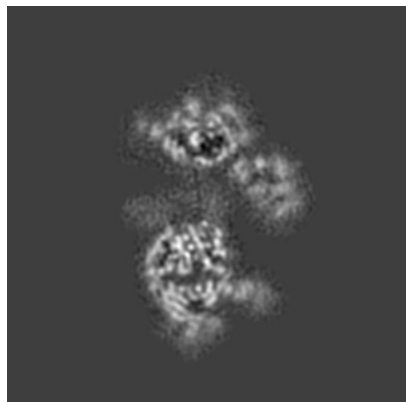


Z

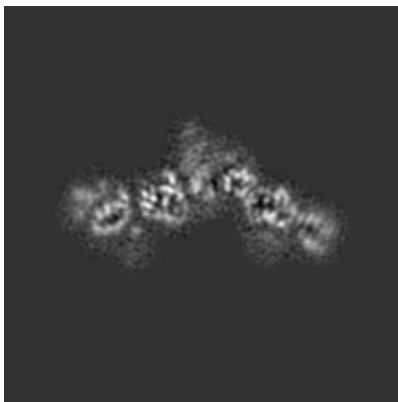
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

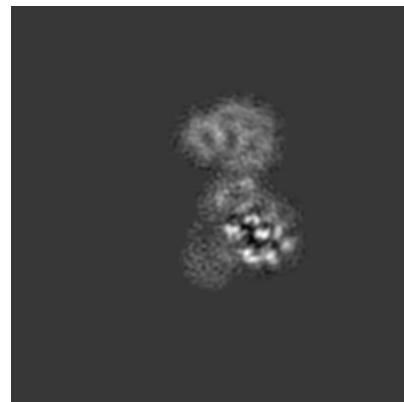
6.2.1 Primary map



X Index: 140



Y Index: 140

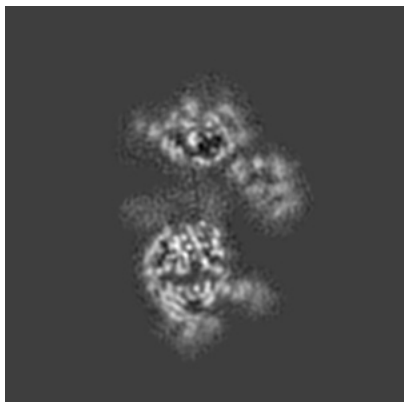


Z Index: 140

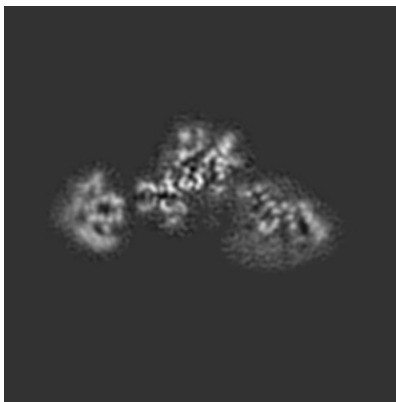
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

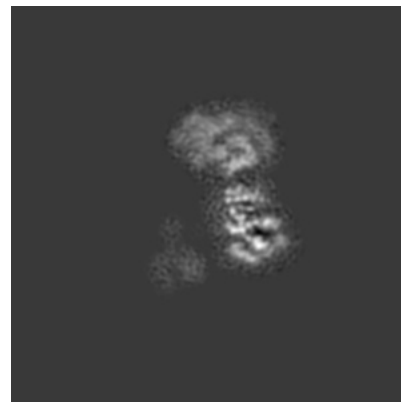
6.3.1 Primary map



X Index: 140



Y Index: 128



Z Index: 153

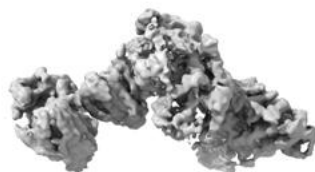
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

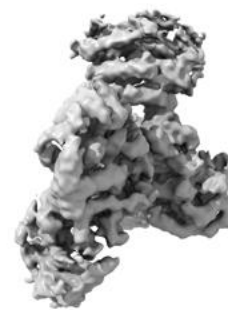
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

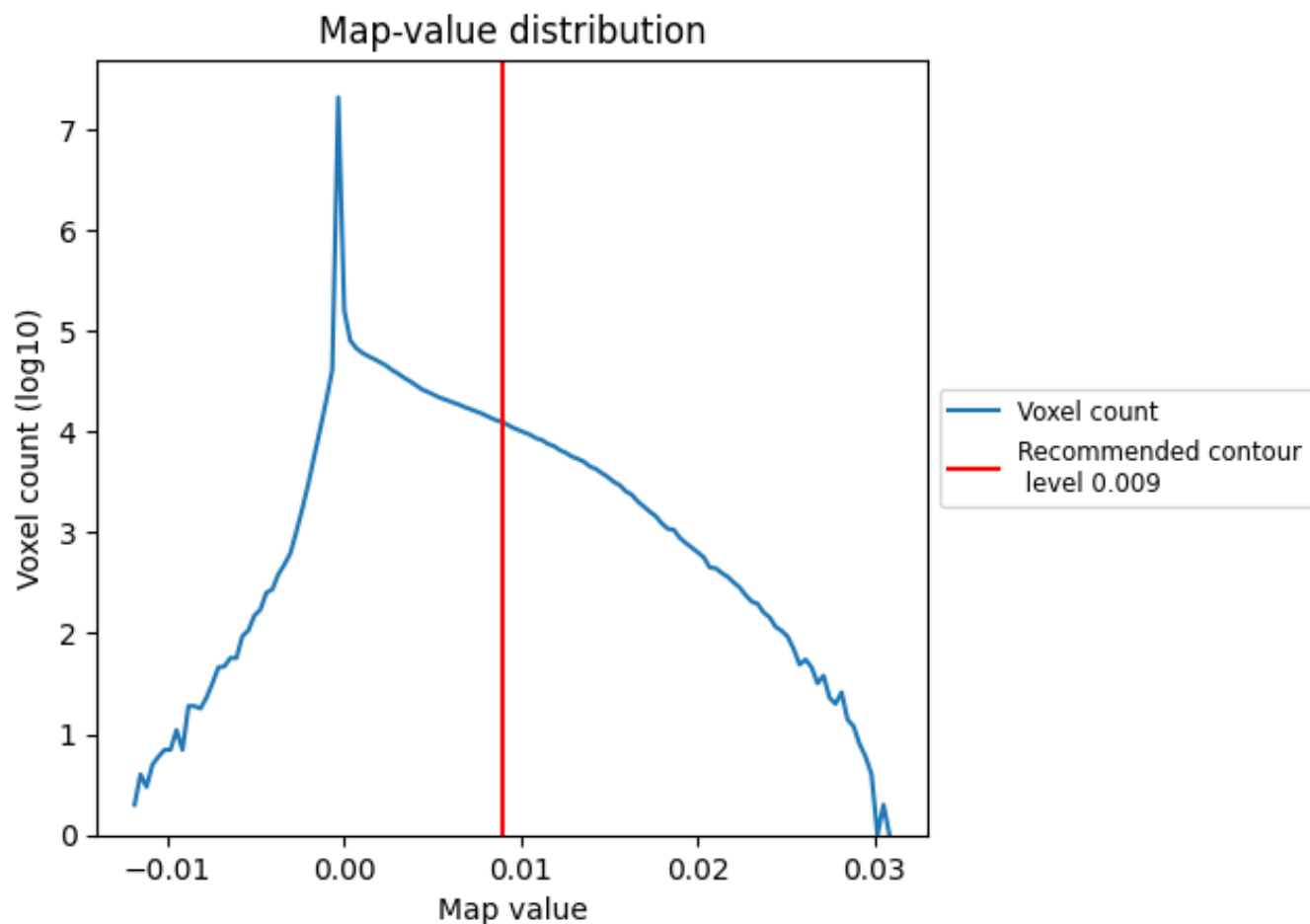
6.5 Mask visualisation

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

7 Map analysis [i](#)

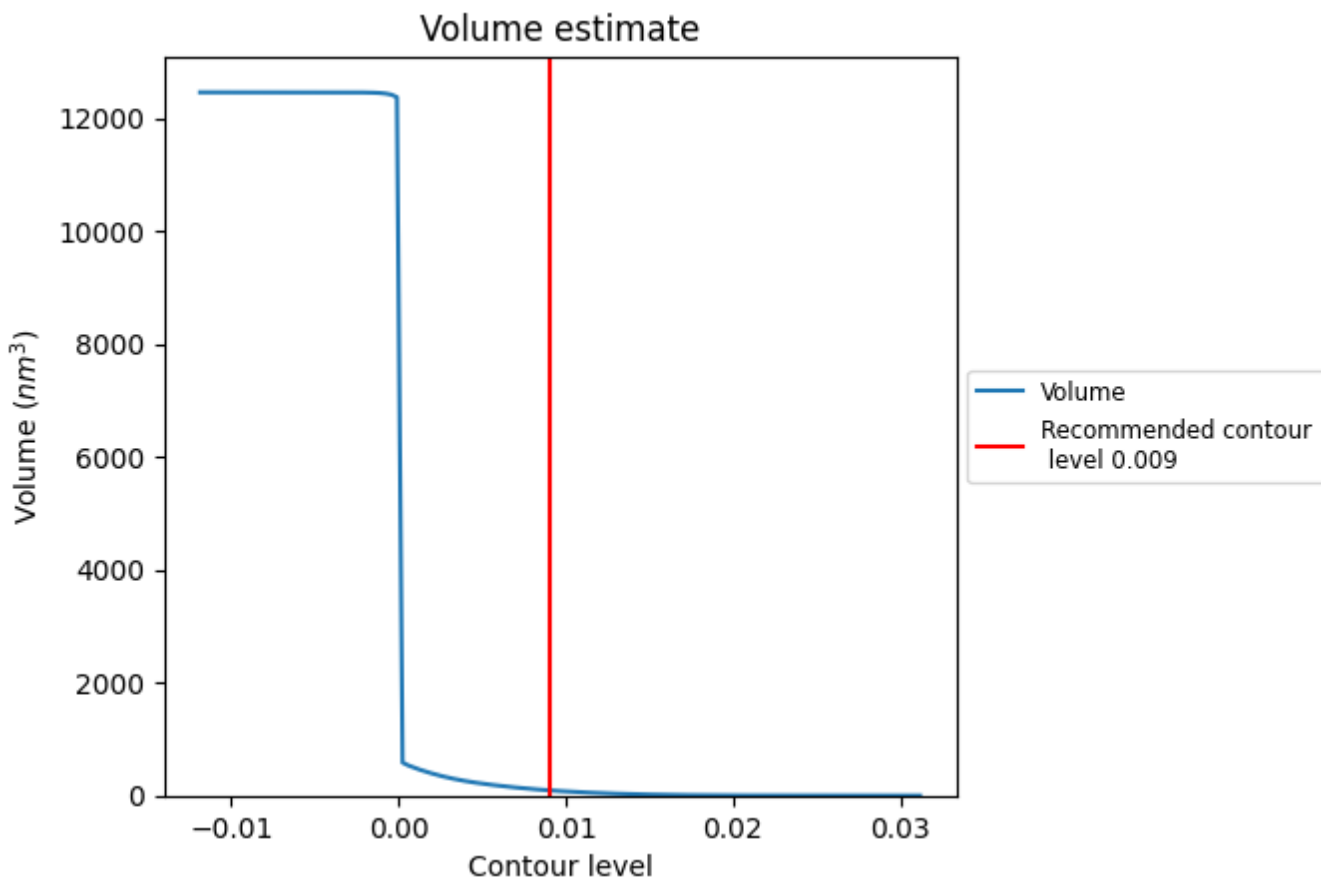
This section contains the results of statistical analysis of the map.

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.

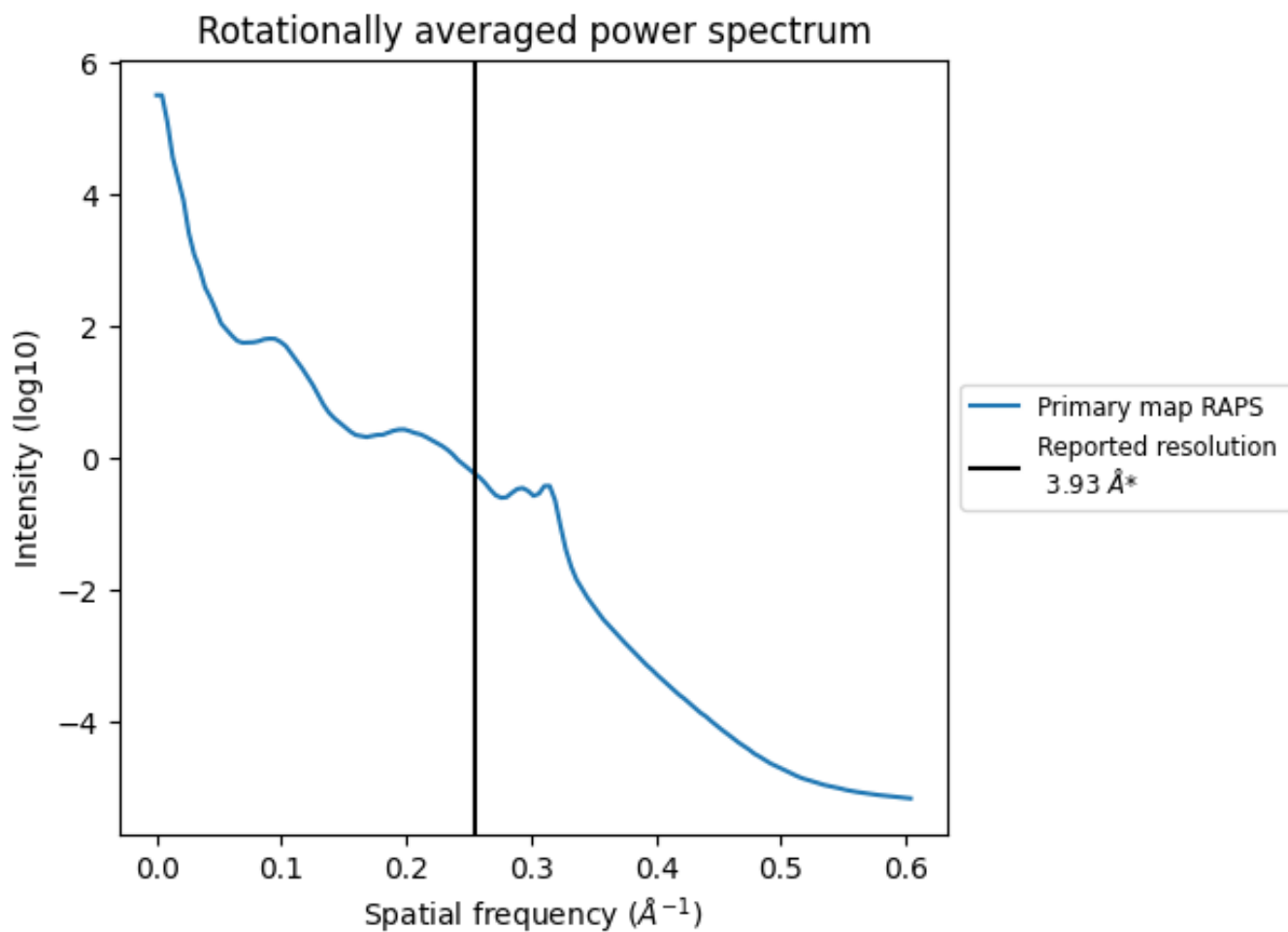
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.254 \AA^{-1}

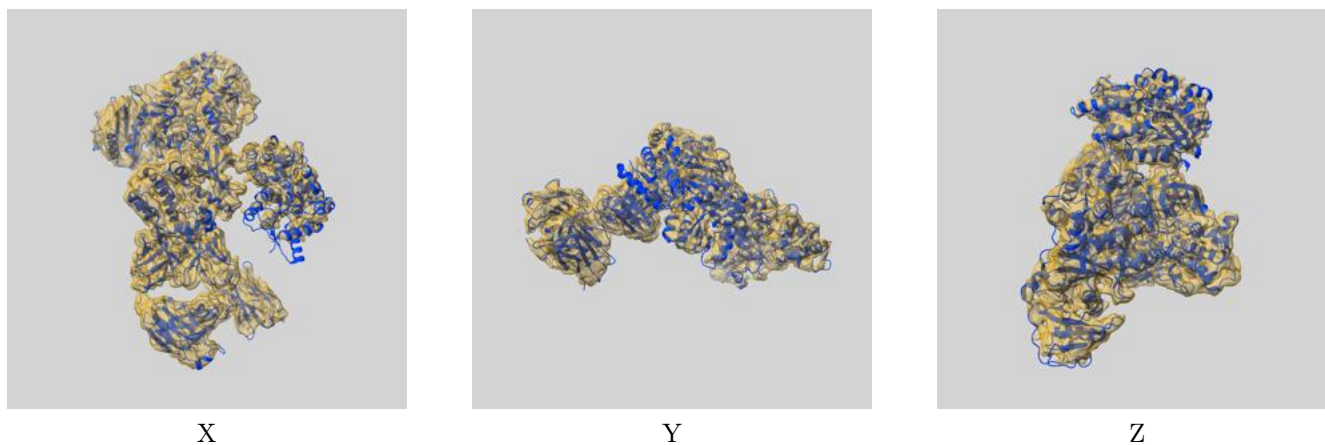
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

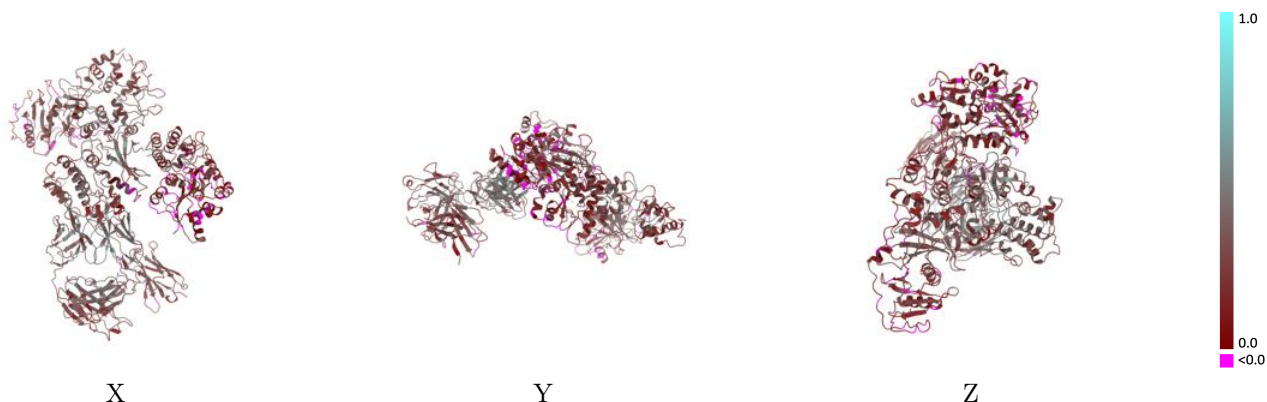
This section contains information regarding the fit between EMDB map EMD-23708 and PDB model 7M74. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



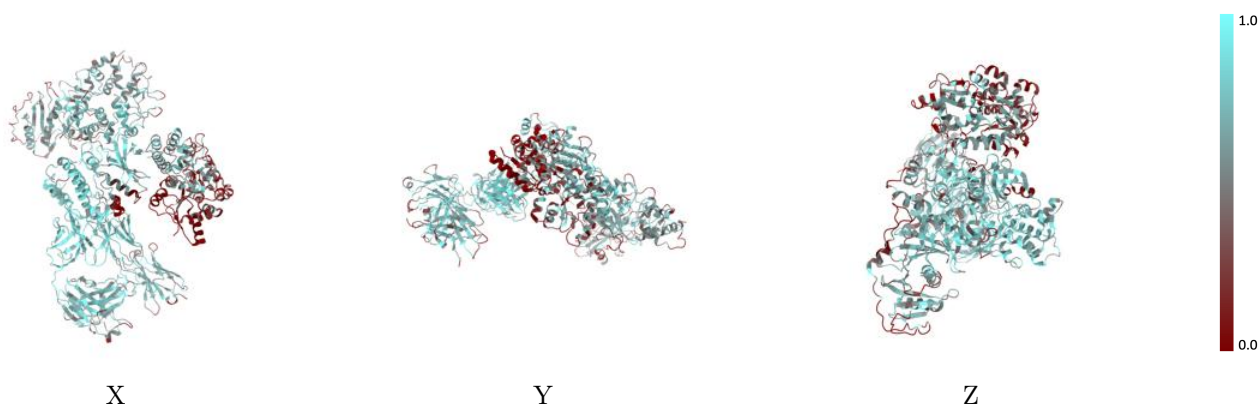
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



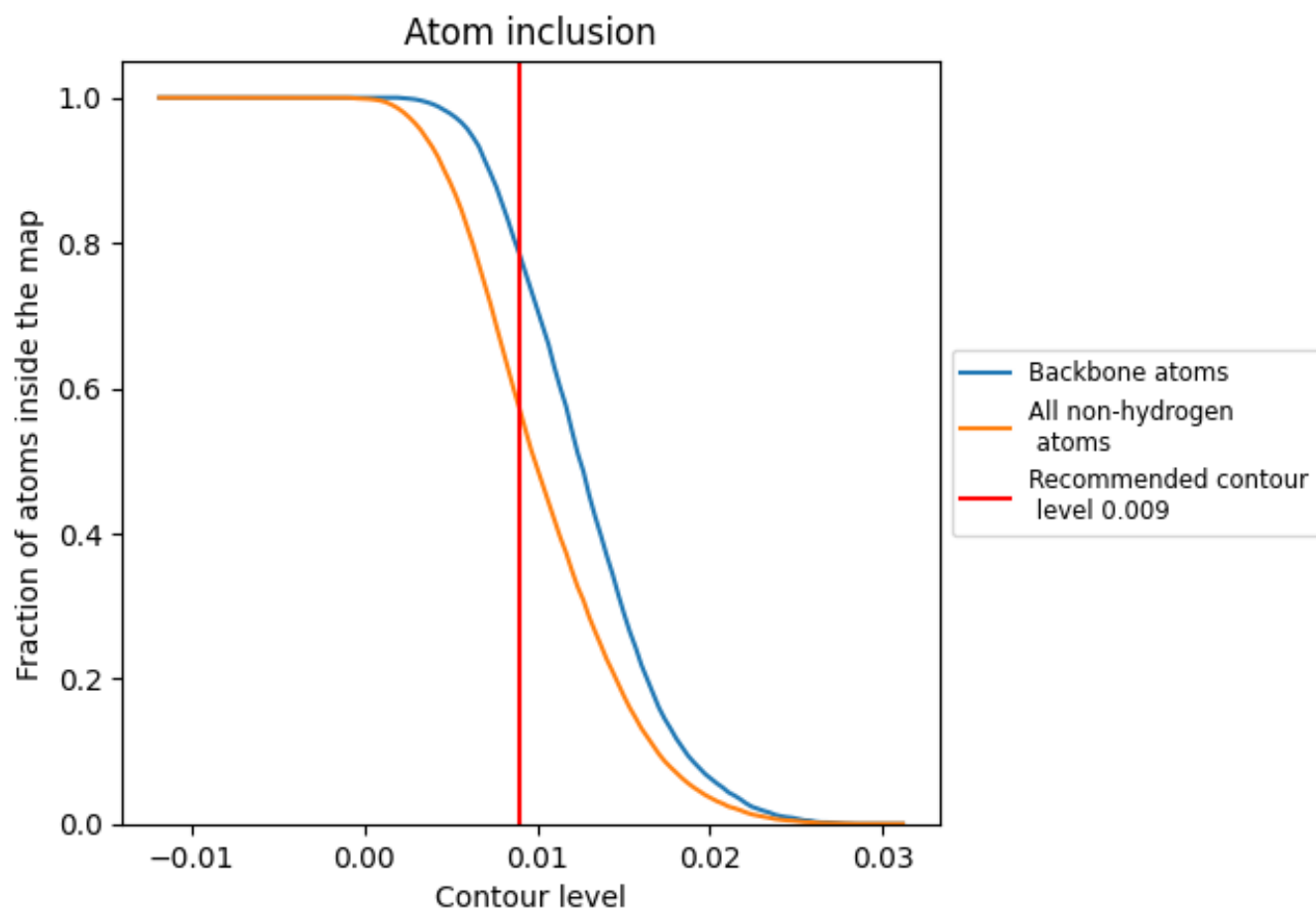
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 57% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5705	 0.2700
A	 0.6245	 0.2850
B	 0.3715	 0.1930
D	 0.1739	 0.2870
G	 0.6168	 0.3000
H	 0.7221	 0.3500
L	 0.7189	 0.3540
M	 0.3588	 0.1630
N	 0.5452	 0.2340

