



Full wwPDB EM Validation Report ⓘ

Jul 27, 2023 – 04:17 PM EDT

PDB ID : 7T5Q
EMDB ID : EMD-25707
Title : Cryo-EM Structure of a Transition State of Arp2/3 Complex Activation
Authors : Rebowksi, G.; van Eeuwen, T.; Boczkowska, M.; Dominguez, R.
Deposited on : 2021-12-13
Resolution : 3.40 Å (reported)
Based on initial model : 4JD2

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.dev50
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) : 2.34

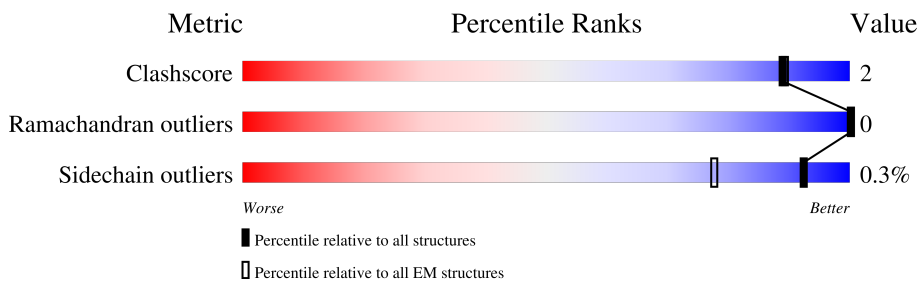
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



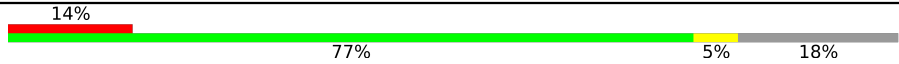

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	418	
2	B	394	
3	C	370	
4	D	300	
5	E	178	
6	F	168	
7	G	151	
8	H	375	

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Mol	Chain	Length	Quality of chain
9	I	346	
10	J	333	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 21671 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	384	3080	1978	515	574	13	0	0

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	372	2972	1903	507	546	16	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	328	2578	1641	448	475	14	0	0

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	283	2287	1453	396	430	8	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	174	1414	908	236	261	9	0	0

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	166	1364	871	238	246	9	0	0

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	63	482	313	81	87	1	0	0

- Molecule 8 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	359	2812	1785	470	538	19	0	0

- Molecule 9 is a protein called F-actin-capping protein subunit alpha-1/Actin nucleation-promoting factor WASL chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	283	2295	1446	402	440	7	0	0

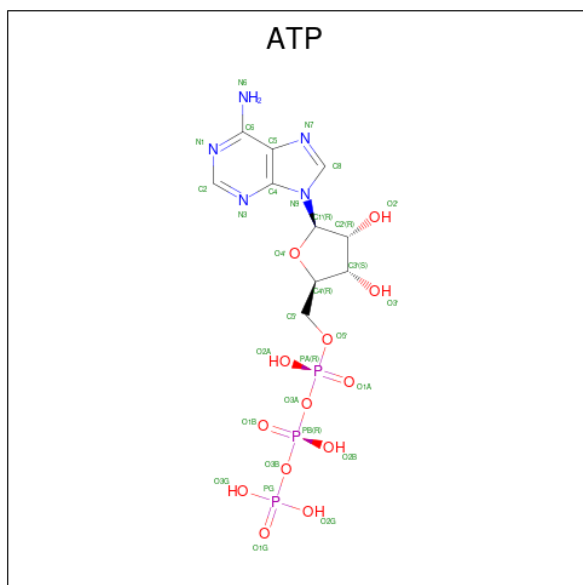
- Molecule 10 is a protein called F-actin-capping protein subunit beta/Actin nucleation-promoting factor WASL chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	291	2295	1432	397	454	12	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

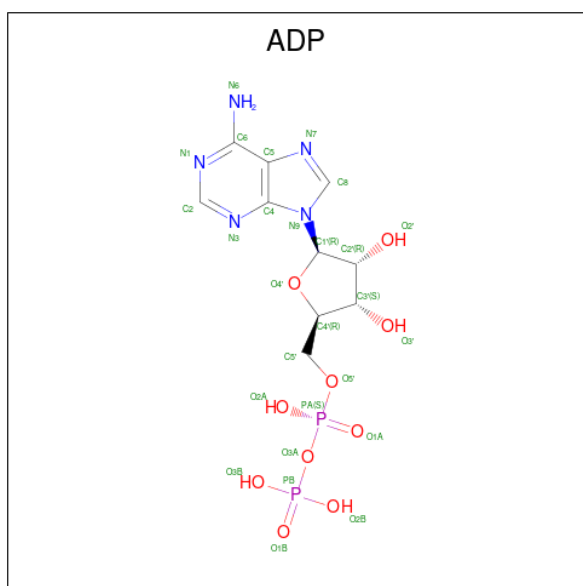
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	H	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

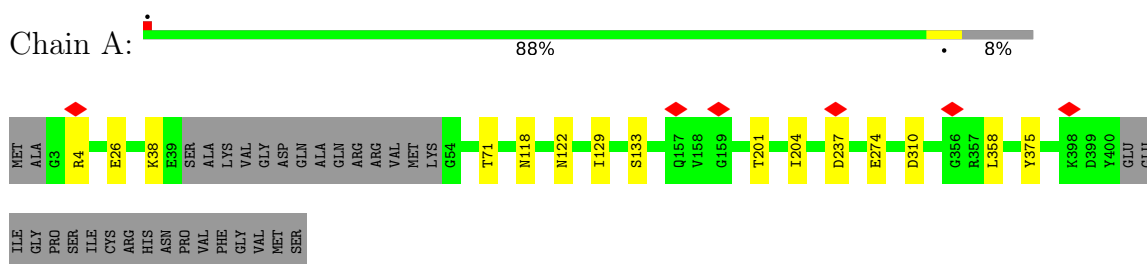


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

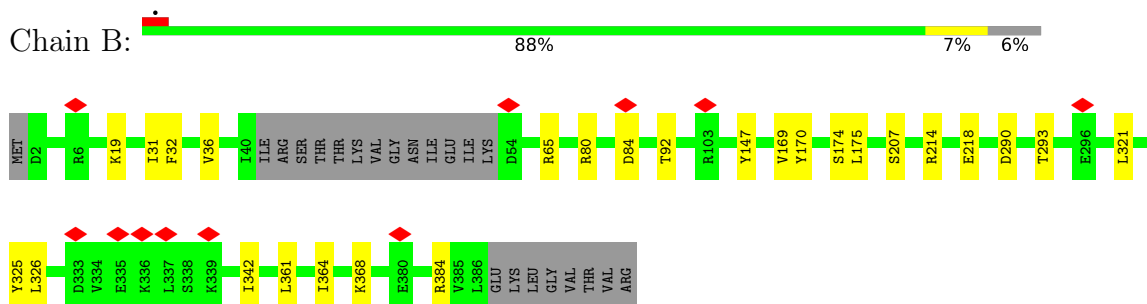
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

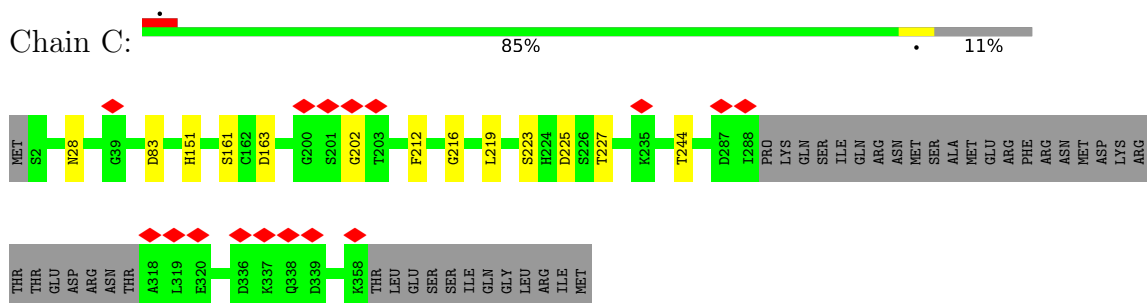
- Molecule 1: Actin-related protein 3



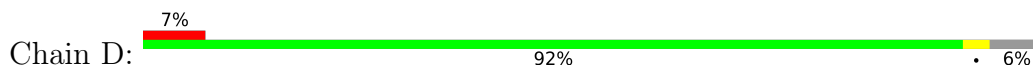
- Molecule 2: Actin-related protein 2

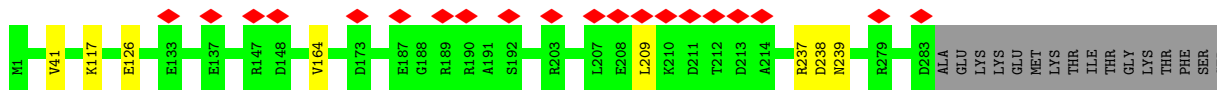


- Molecule 3: Actin-related protein 2/3 complex subunit 1A



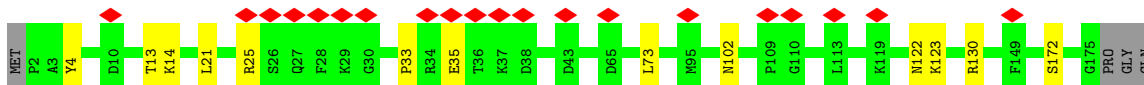
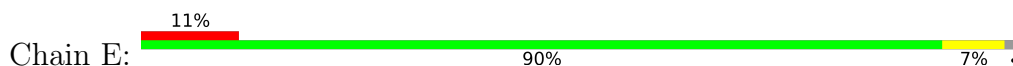
- Molecule 4: Actin-related protein 2/3 complex subunit 2



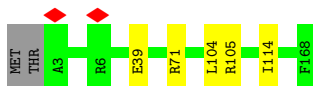


ARG

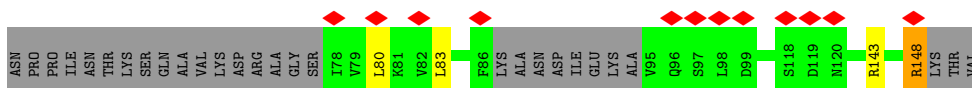
- Molecule 5: Actin-related protein 2/3 complex subunit 3



- Molecule 6: Actin-related protein 2/3 complex subunit 4



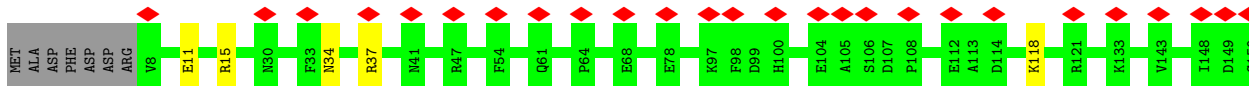
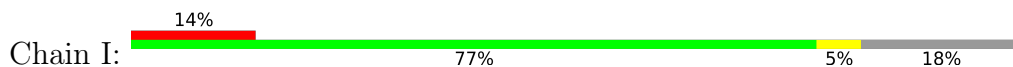
- Molecule 7: Actin-related protein 2/3 complex subunit 5

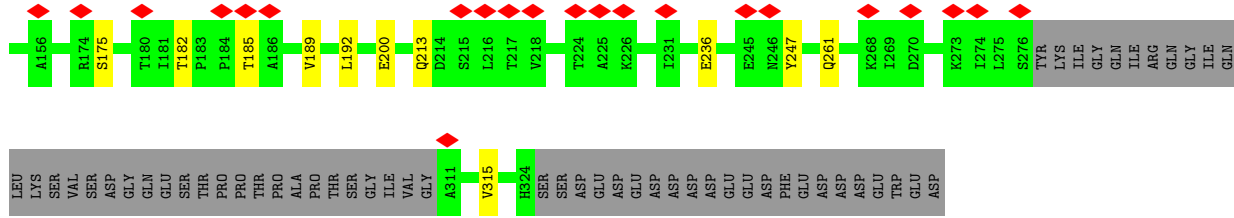


- Molecule 8: Actin, alpha skeletal muscle

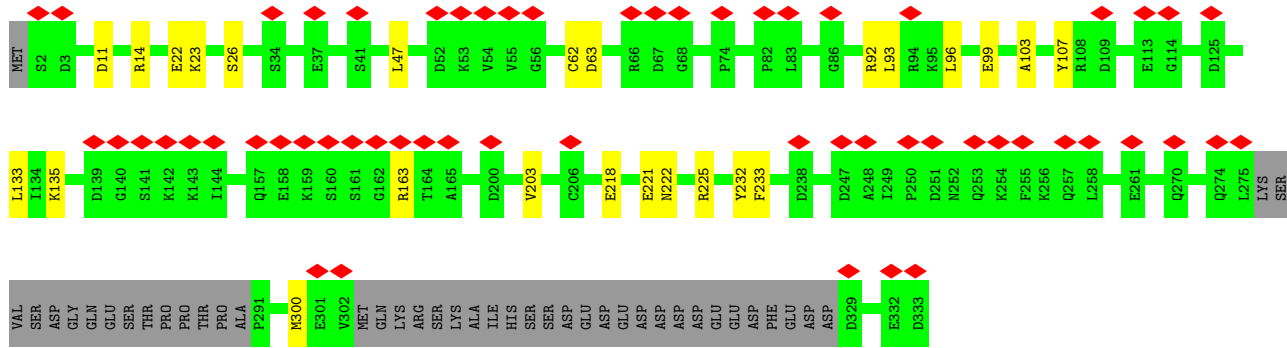
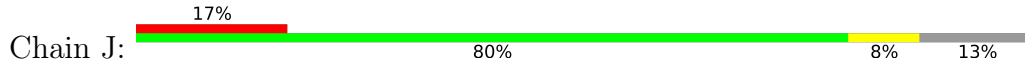


- Molecule 9: F-actin-capping protein subunit alpha-1/Actin nucleation-promoting factor WASL chimera





• Molecule 10: F-actin-capping protein subunit beta/Actin nucleation-promoting factor WASL chimera



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was done in cryoSPARC for initial 2D classification and then repeated in CTFFIND4 (Relion) for classification and final reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.890	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.066	Depositor
Map size (Å)	302.72, 302.72, 302.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: MG, HIC, ATP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/3158	0.62	0/4285
2	B	0.30	0/3033	0.64	0/4100
3	C	0.29	0/2648	0.61	0/3596
4	D	0.31	0/2336	0.63	0/3154
5	E	0.31	0/1448	0.59	0/1953
6	F	0.30	0/1386	0.61	0/1858
7	G	0.32	0/488	0.62	0/657
8	H	0.28	0/2860	0.61	0/3873
9	I	0.31	0/2345	0.63	0/3172
10	J	0.31	0/2331	0.63	0/3144
All	All	0.30	0/22033	0.62	0/29792

There are no bond length outliers.

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	3080	0	3032	9	0
2	B	2972	0	2989	15	0
3	C	2578	0	2511	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2287	0	2252	4	0
5	E	1414	0	1416	8	0
6	F	1364	0	1403	3	0
7	G	482	0	507	3	0
8	H	2812	0	2783	10	0
9	I	2295	0	2226	12	0
10	J	2295	0	2273	15	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	H	1	0	0	0	0
12	A	31	0	12	0	0
12	B	31	0	12	0	0
13	H	27	0	12	0	0
All	All	21671	0	21428	76	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 2.

All (76) 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:H:222:ASP:HB3	8:H:225:ASN:HB3	1.72	0.72
1:A:129:ILE:O	1:A:133:SER:OG	2.08	0.71
2:B:326:LEU:O	2:B:326:LEU:HD23	1.91	0.70
10:J:218:GLU:OE2	10:J:222:ASN:ND2	2.25	0.69
9:I:11:GLU:OE1	9:I:15:ARG:NH1	2.26	0.68
3:C:161:SER:OG	3:C:163:ASP:OD1	2.12	0.67
9:I:247:TYR:OH	10:J:233:PHE:O	2.13	0.65
9:I:34:ASN:OD1	9:I:37:ARG:NH2	2.31	0.62
5:E:102:ASN:OD1	5:E:130:ARG:NH1	2.32	0.62
9:I:200:GLU:O	10:J:232:TYR:OH	2.11	0.62
3:C:223:SER:OG	3:C:227:THR:OG1	2.18	0.61
9:I:192:LEU:HD21	9:I:236:GLU:OE2	2.01	0.60
9:I:182:THR:OG1	9:I:185:THR:O	2.17	0.59
8:H:149:THR:O	8:H:296:ASN:ND2	2.36	0.58
1:A:26:GLU:OE2	1:A:375:TYR:OH	2.21	0.58
3:C:244:THR:O	7:G:143:ARG:NH2	2.37	0.57
4:D:126:GLU:OE1	4:D:237:ARG:NE	2.38	0.57
4:D:41:VAL:HG21	4:D:117:LYS:HD2	1.86	0.57
1:A:358:LEU:HD21	8:H:241:GLU:HG3	1.87	0.56
2:B:19:LYS:HG2	2:B:31:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ASP:OD1	2:B:293:THR:OG1	2.25	0.54
2:B:65:ARG:NH1	2:B:207:SER:O	2.41	0.54
2:B:214:ARG:NH1	2:B:218:GLU:OE1	2.40	0.53
5:E:14:LYS:HD3	5:E:21:LEU:HD23	1.90	0.53
10:J:22:GLU:OE1	10:J:22:GLU:N	2.43	0.52
3:C:223:SER:OG	3:C:225:ASP:OD1	2.26	0.52
5:E:25:ARG:N	5:E:35:GLU:OE1	2.43	0.51
10:J:62:CYS:SG	10:J:63:ASP:N	2.84	0.51
1:A:38:LYS:NZ	1:A:71:THR:OG1	2.44	0.49
9:I:261:GLN:OE1	10:J:225:ARG:NH1	2.45	0.49
8:H:250:ILE:HD11	8:H:253:GLU:OE2	2.13	0.49
10:J:99:GLU:O	10:J:103:ALA:N	2.44	0.48
6:F:39:GLU:OE2	6:F:71:ARG:NH1	2.47	0.48
8:H:222:ASP:CB	8:H:225:ASN:HB3	2.42	0.47
8:H:149:THR:HG23	8:H:296:ASN:HD21	1.78	0.47
2:B:32:PHE:CZ	2:B:92:THR:HG22	2.50	0.47
3:C:83:ASP:N	3:C:83:ASP:OD1	2.48	0.47
4:D:238:ASP:OD1	4:D:239:ASN:N	2.48	0.47
2:B:36:VAL:HG11	2:B:84:ASP:HB3	1.98	0.46
5:E:21:LEU:HD21	5:E:33:PRO:HD2	1.97	0.46
10:J:23:LYS:O	10:J:26:SER:OG	2.24	0.46
6:F:104:LEU:HD11	6:F:114:ILE:HD11	1.98	0.46
1:A:201:THR:HA	1:A:204:ILE:HG22	1.97	0.46
10:J:47:LEU:O	10:J:135:LYS:NZ	2.49	0.45
1:A:274:GLU:OE2	1:A:274:GLU:N	2.45	0.45
7:G:80:LEU:HD12	7:G:83:LEU:HD12	1.98	0.45
10:J:11:ASP:OD1	10:J:14:ARG:NH1	2.50	0.45
1:A:310:ASP:OD2	8:H:62:ARG:NH1	2.50	0.45
2:B:364:ILE:CD1	9:I:315:VAL:HG11	2.47	0.45
8:H:331:ALA:HB1	8:H:335:ARG:HD3	1.98	0.45
6:F:39:GLU:OE1	6:F:105:ARG:NH1	2.50	0.44
10:J:107:TYR:OH	10:J:221:GLU:OE1	2.27	0.44
10:J:300:MET:SD	10:J:300:MET:N	2.90	0.44
3:C:151:HIS:NE2	3:C:216:GLY:O	2.47	0.44
9:I:175:SER:HB3	9:I:192:LEU:HD23	1.99	0.44
1:A:118:ASN:OD1	1:A:122:ASN:ND2	2.49	0.44
2:B:325:TYR:CG	2:B:325:TYR:O	2.71	0.44
2:B:364:ILE:HD11	9:I:315:VAL:HG11	1.99	0.44
5:E:73:LEU:HD11	5:E:172:SER:HA	1.98	0.44
2:B:321:LEU:HD13	2:B:342:ILE:HD11	2.00	0.44
3:C:202:GLY:O	7:G:148:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:163:ARG:O	10:J:203:VAL:N	2.49	0.43
2:B:80:ARG:NH1	8:H:194:THR:O	2.52	0.42
5:E:13:THR:OG1	5:E:14:LYS:N	2.51	0.42
8:H:304:THR:O	8:H:304:THR:HG22	2.20	0.41
10:J:62:CYS:HB2	10:J:133:LEU:HD21	2.03	0.41
10:J:93:LEU:HD12	10:J:96:LEU:HD12	2.03	0.41
2:B:147:TYR:CE2	2:B:361:LEU:HD13	2.56	0.41
9:I:189:VAL:HG13	9:I:213:GLN:OE1	2.20	0.41
3:C:212:PHE:CE1	3:C:219:LEU:HD13	2.56	0.41
5:E:122:ASN:OD1	5:E:123:LYS:N	2.53	0.41
4:D:164:VAL:HG11	4:D:209:LEU:HD11	2.03	0.41
2:B:174:SER:OG	2:B:175:LEU:N	2.54	0.40
9:I:175:SER:CB	9:I:192:LEU:HD23	2.51	0.40
1:A:237:ASP:OD1	5:E:4:TYR:OH	2.34	0.40
2:B:169:VAL:HG22	2:B:170:TYR:O	2.22	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	380/418 (91%)	367 (97%)	13 (3%)	0	100	100
2	B	368/394 (93%)	335 (91%)	33 (9%)	0	100	100
3	C	324/370 (88%)	301 (93%)	23 (7%)	0	100	100
4	D	281/300 (94%)	265 (94%)	16 (6%)	0	100	100
5	E	172/178 (97%)	165 (96%)	7 (4%)	0	100	100
6	F	164/168 (98%)	159 (97%)	5 (3%)	0	100	100
7	G	59/151 (39%)	56 (95%)	3 (5%)	0	100	100
8	H	354/375 (94%)	336 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	279/346 (81%)	261 (94%)	18 (6%)	0	100	100
10	J	285/333 (86%)	277 (97%)	8 (3%)	0	100	100
All	All	2666/3033 (88%)	2522 (95%)	144 (5%)	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	335/363 (92%)	334 (100%)	1 (0%)	92	97
2	B	324/345 (94%)	322 (99%)	2 (1%)	86	94
3	C	284/323 (88%)	283 (100%)	1 (0%)	91	95
4	D	249/264 (94%)	249 (100%)	0	100	100
5	E	156/159 (98%)	156 (100%)	0	100	100
6	F	153/155 (99%)	153 (100%)	0	100	100
7	G	53/123 (43%)	52 (98%)	1 (2%)	57	78
8	H	304/317 (96%)	303 (100%)	1 (0%)	92	97
9	I	250/306 (82%)	249 (100%)	1 (0%)	91	95
10	J	258/297 (87%)	257 (100%)	1 (0%)	91	95
All	All	2366/2652 (89%)	2358 (100%)	8 (0%)	92	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
2	B	368	LYS
2	B	384	ARG
3	C	28	ASN
7	G	148	ARG
8	H	147	ARG

Continued on next page...

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Mol	Chain	Res	Type
9	I	118	LYS
10	J	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	149	GLN
8	H	296	ASN
8	H	371	HIS
10	J	209	HIS
10	J	212	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](#)

1 non-standard protein/DNA/RNA residue is 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	HIC	H	73	8	8,11,12	1.62	2 (25%)	6,14,16	1.40	1 (16%)

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	HIC	H	73	8	-	0/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	73	HIC	CD2-CG	3.49	1.41	1.36
8	H	73	HIC	CZ-NE2	-2.05	1.42	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	73	HIC	CB-CA-C	-2.80	106.23	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are 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
12	ATP	B	502	11	26,33,33	0.63	0	31,52,52	1.08	2 (6%)
12	ATP	A	502	11	26,33,33	0.63	0	31,52,52	1.17	4 (12%)
13	ADP	H	401	11	24,29,29	0.86	1 (4%)	29,45,45	1.45	4 (13%)

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	ATP	B	502	11	-	4/18/38/38	0/3/3/3
12	ATP	A	502	11	-	4/18/38/38	0/3/3/3
13	ADP	H	401	11	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	401	ADP	C5-C4	2.09	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	401	ADP	PA-O3A-PB	-3.78	119.85	132.83
13	H	401	ADP	N3-C2-N1	-3.45	123.29	128.68
13	H	401	ADP	C4-C5-N7	-2.72	106.57	109.40
12	A	502	ATP	O4'-C1'-C2'	-2.67	103.03	106.93
13	H	401	ADP	C3'-C2'-C1'	2.60	104.90	100.98
12	B	502	ATP	C5-C6-N6	2.30	123.85	120.35
12	A	502	ATP	C5-C6-N6	2.27	123.80	120.35
12	A	502	ATP	PB-O3B-PG	2.04	139.84	132.83
12	B	502	ATP	PB-O3B-PG	2.01	139.74	132.83
12	A	502	ATP	O3'-C3'-C2'	-2.01	105.33	111.82

There are no chirality outliers.

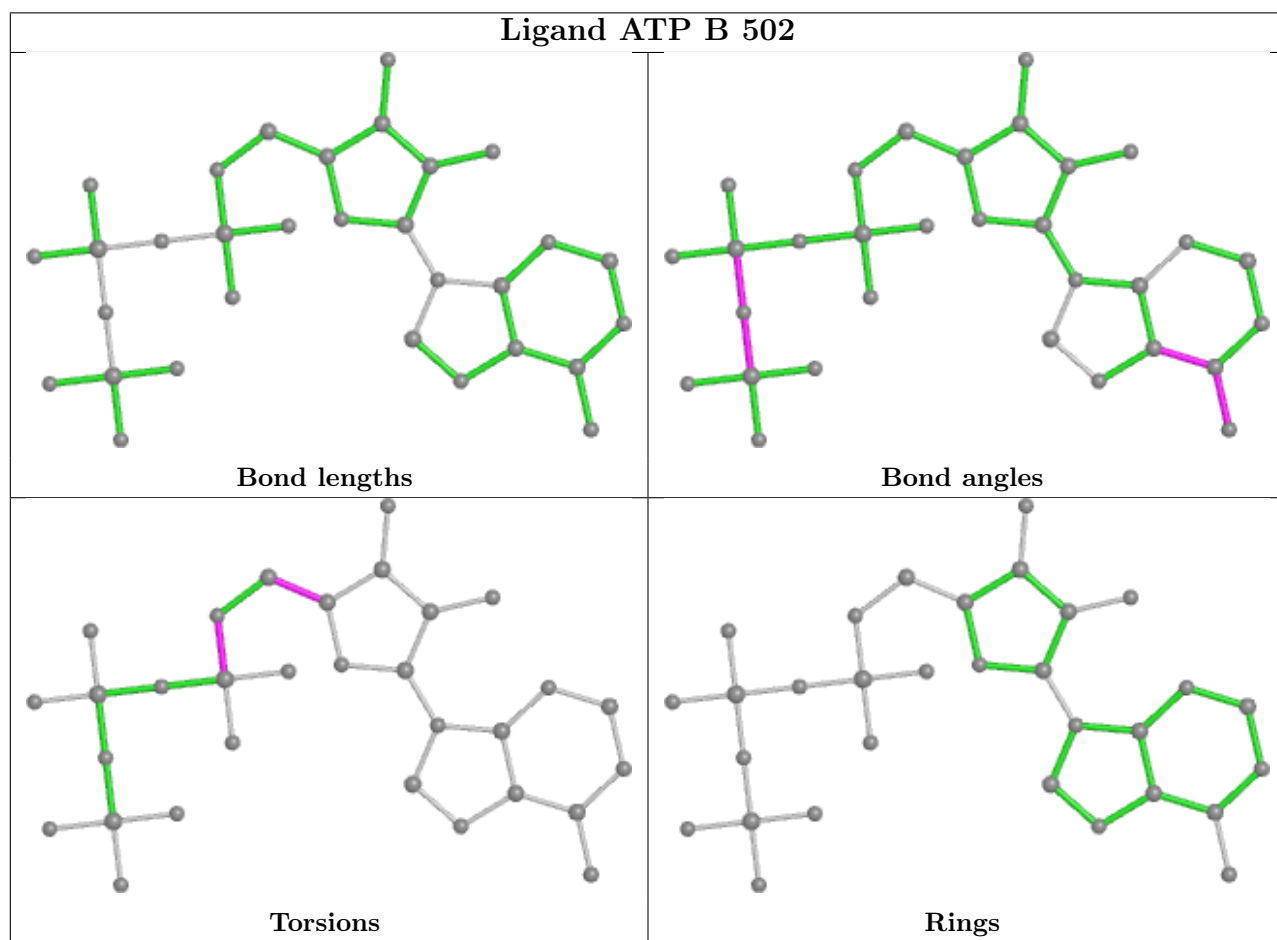
All (12) torsion outliers are listed below:

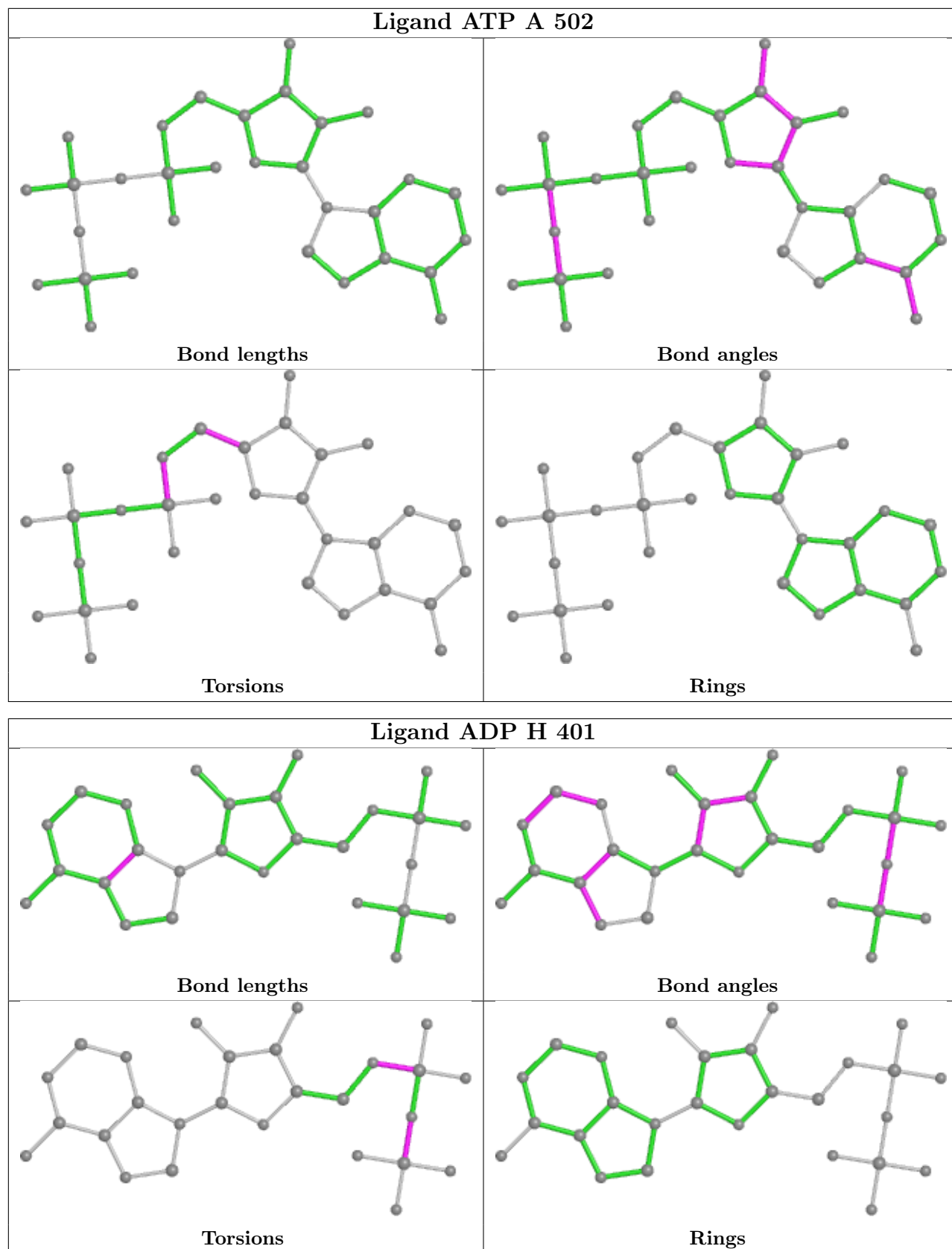
Mol	Chain	Res	Type	Atoms
12	A	502	ATP	C5'-O5'-PA-O2A
12	A	502	ATP	C5'-O5'-PA-O3A
12	A	502	ATP	O4'-C4'-C5'-O5'
12	B	502	ATP	C5'-O5'-PA-O3A
12	B	502	ATP	C3'-C4'-C5'-O5'
13	H	401	ADP	C5'-O5'-PA-O1A
12	A	502	ATP	C3'-C4'-C5'-O5'
12	B	502	ATP	O4'-C4'-C5'-O5'
13	H	401	ADP	PA-O3A-PB-O1B
13	H	401	ADP	C5'-O5'-PA-O3A
12	B	502	ATP	C5'-O5'-PA-O1A
13	H	401	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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.

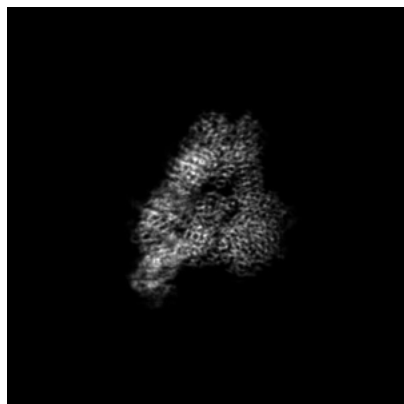
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25707. These allow visual inspection of the internal detail of the map and identification of artifacts.

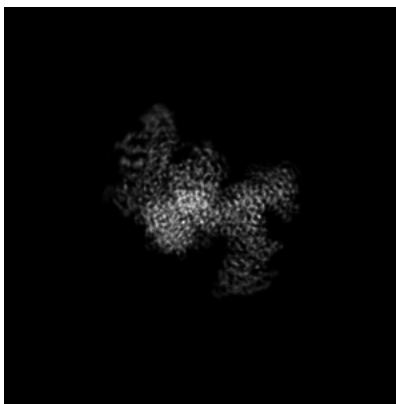
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

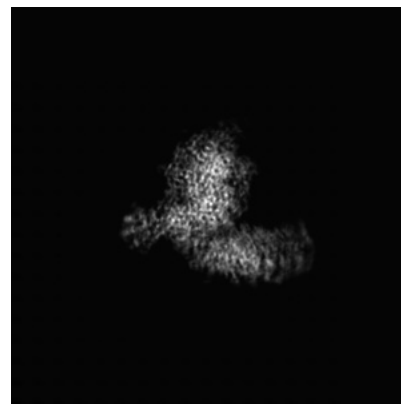
6.1.1 Primary map



X

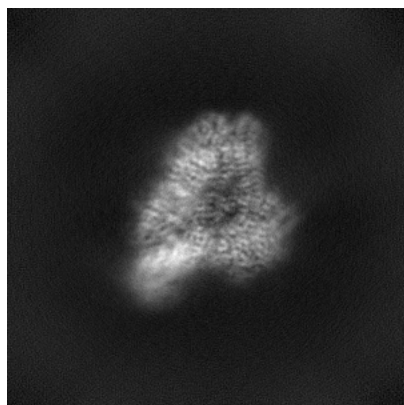


Y

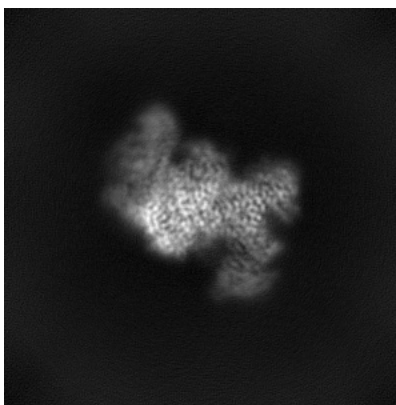


Z

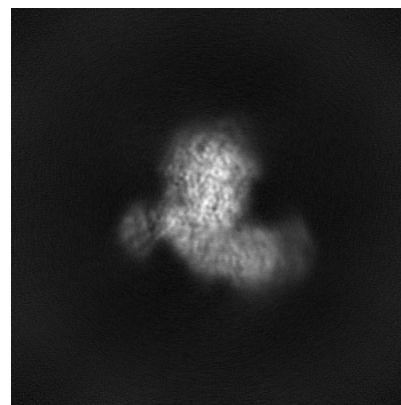
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

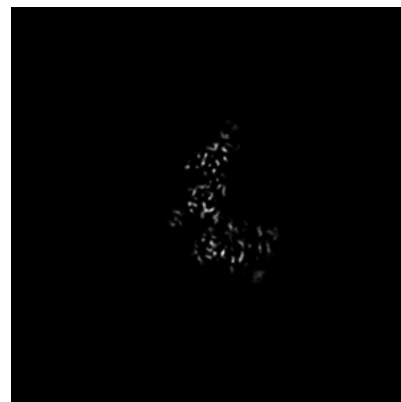
6.2.1 Primary map



X Index: 176

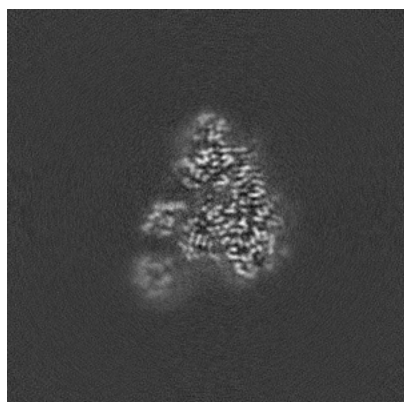


Y Index: 176

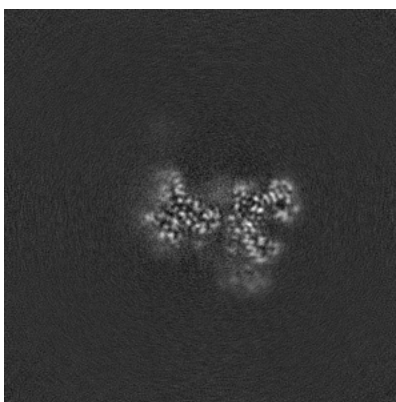


Z Index: 176

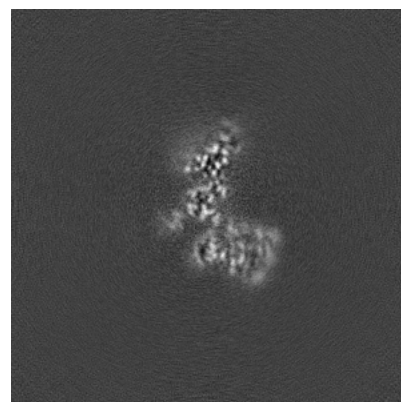
6.2.2 Raw map



X Index: 176



Y Index: 176



Z Index: 176

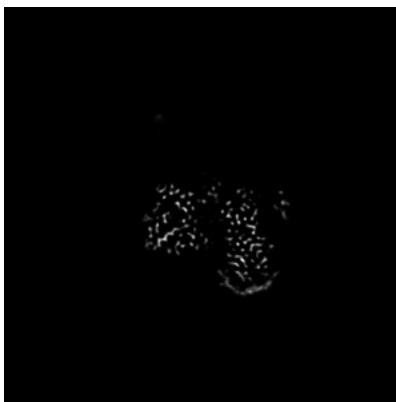
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 176

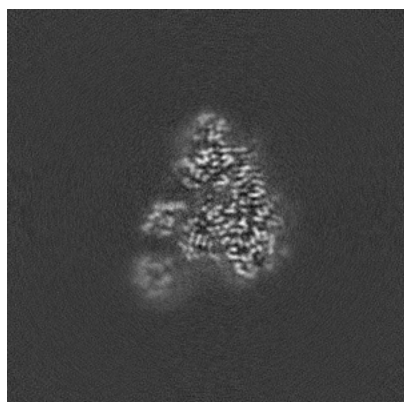


Y Index: 164

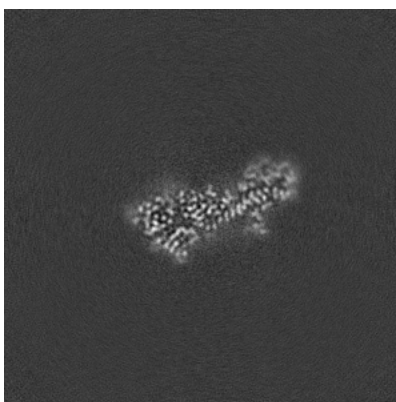


Z Index: 154

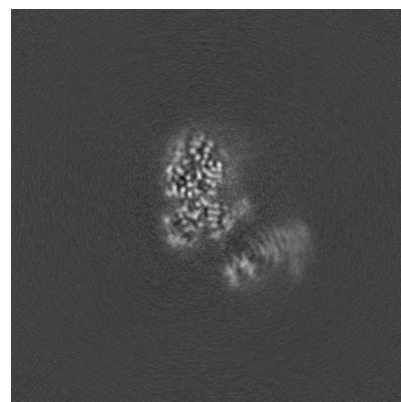
6.3.2 Raw map



X Index: 176



Y Index: 207

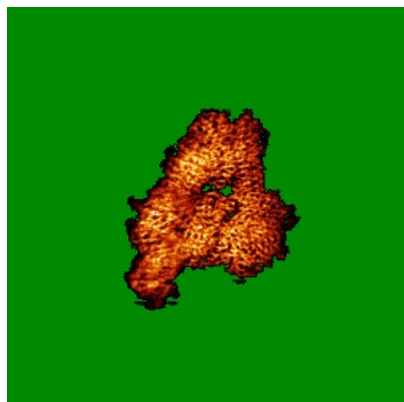


Z Index: 146

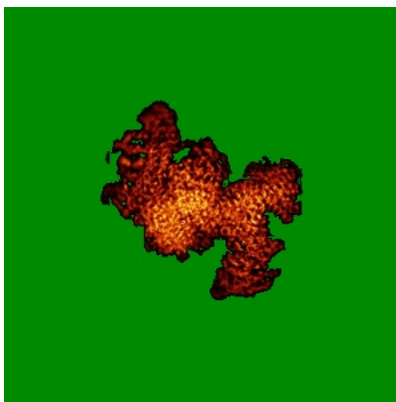
The images above show the largest variance slices of the map in three orthogonal directions.

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

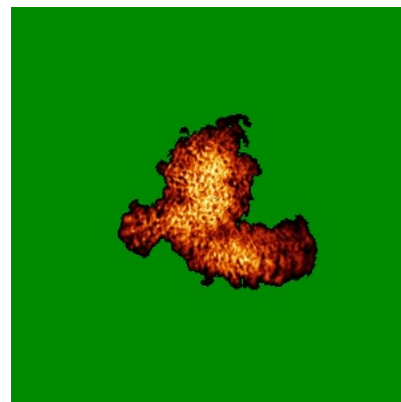
6.4.1 Primary map



X

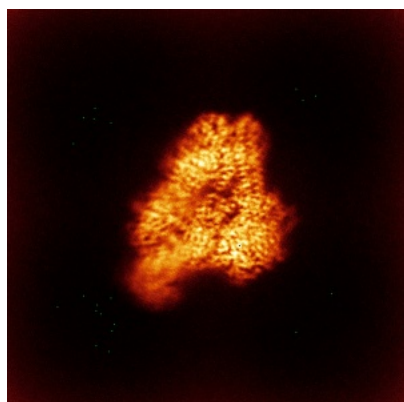


Y

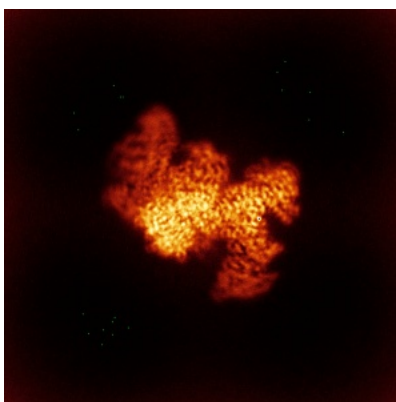


Z

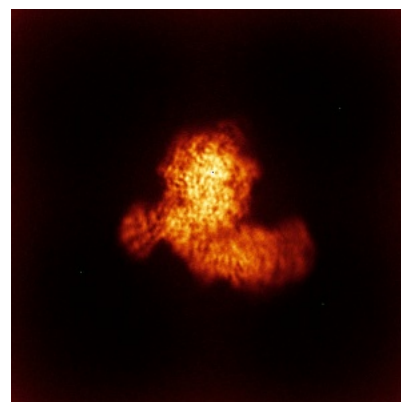
6.4.2 Raw map



X



Y

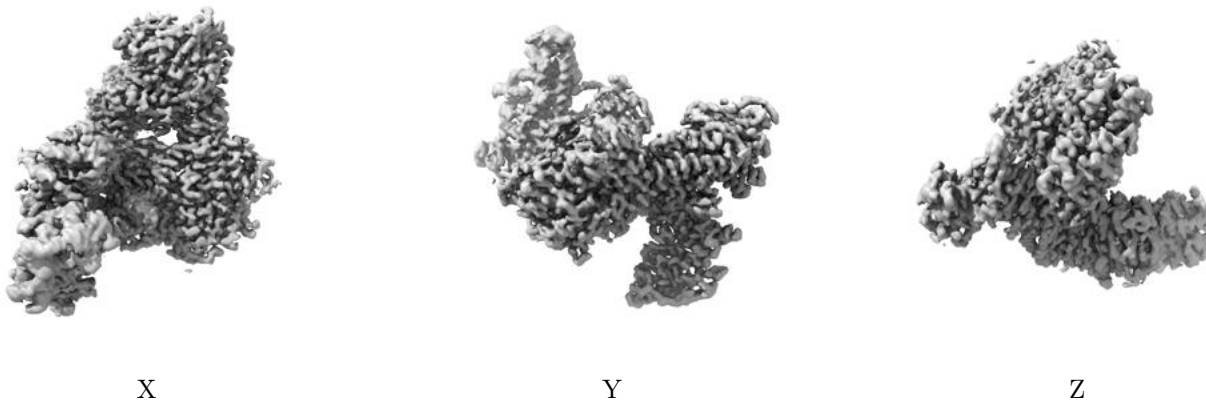


Z

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.

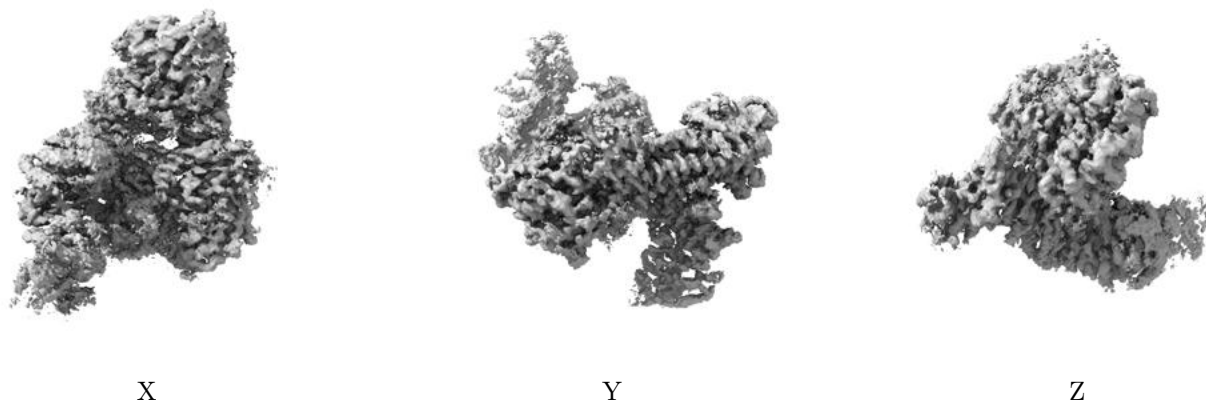
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.066. 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.

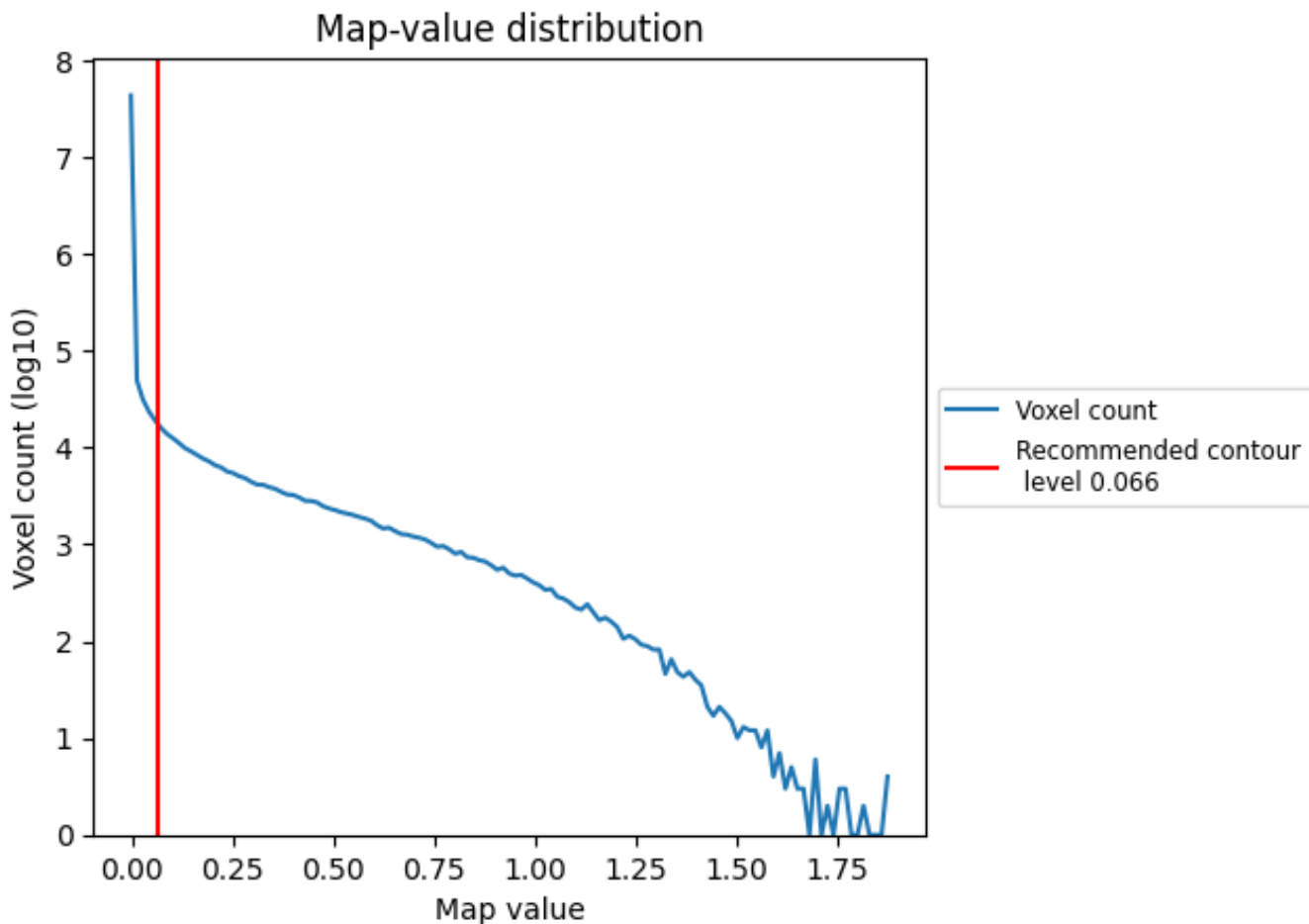
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

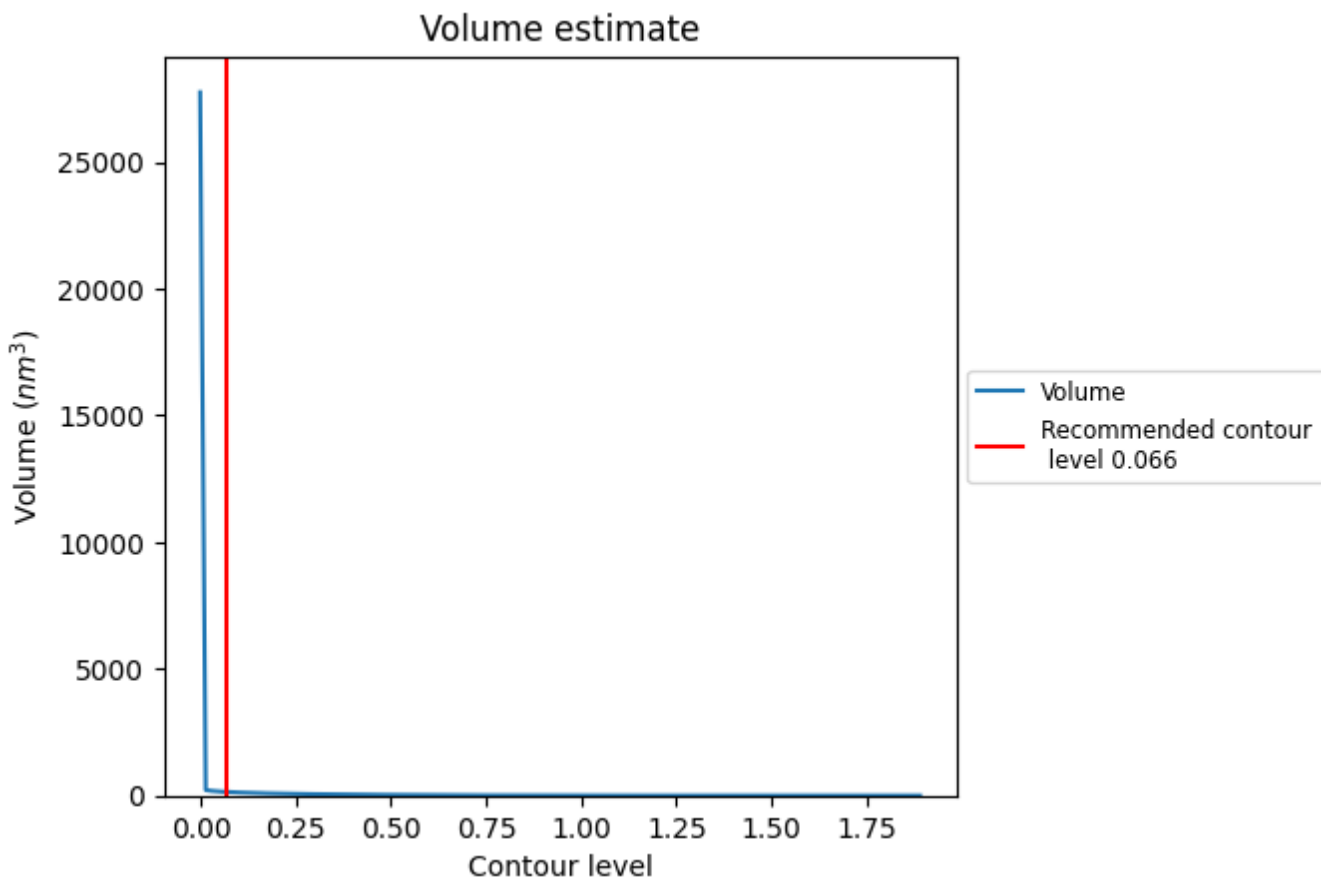
This section contains the results of statistical analysis of the map.

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.

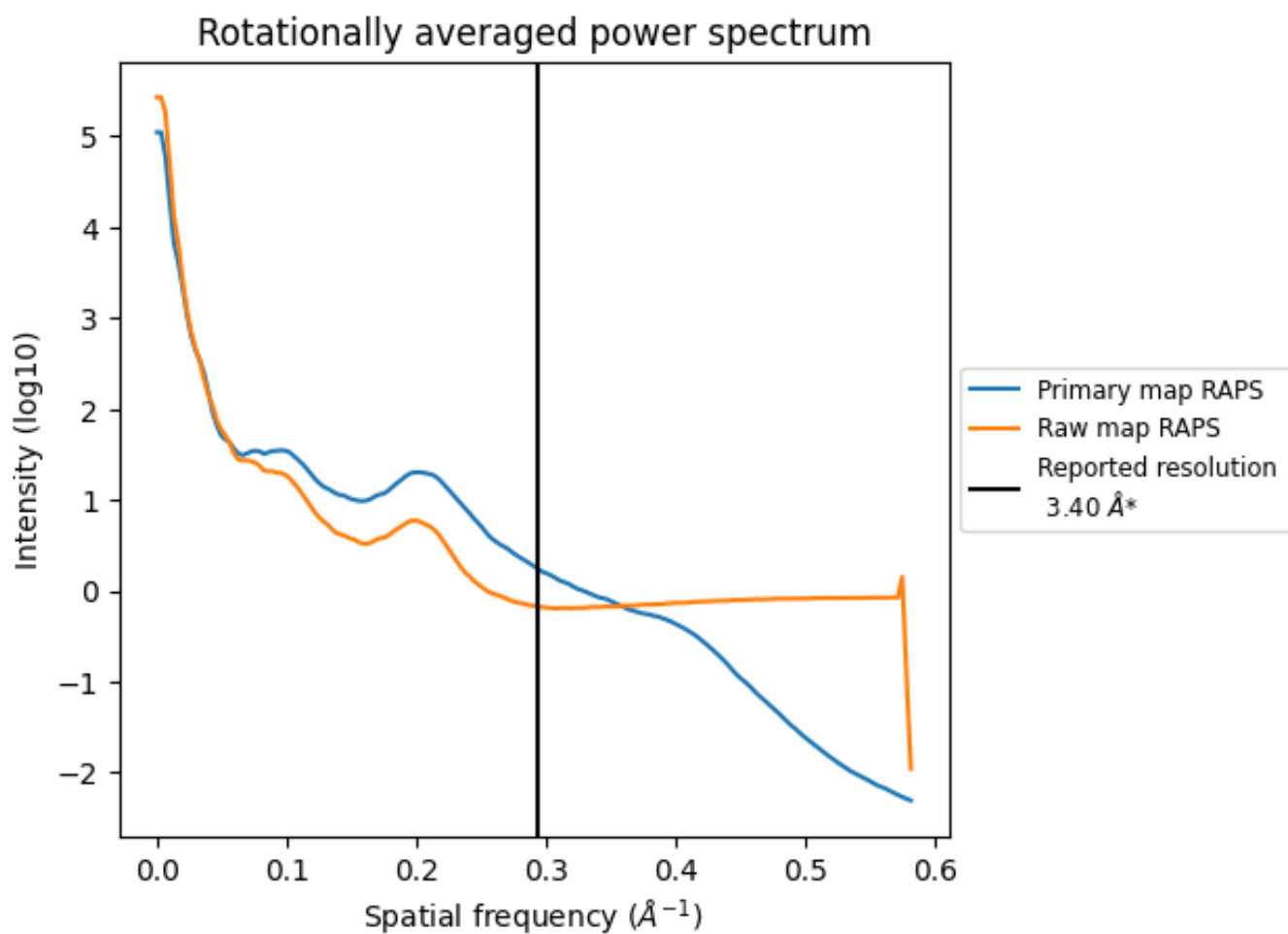
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145 nm³; this corresponds to an approximate mass of 131 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](#)

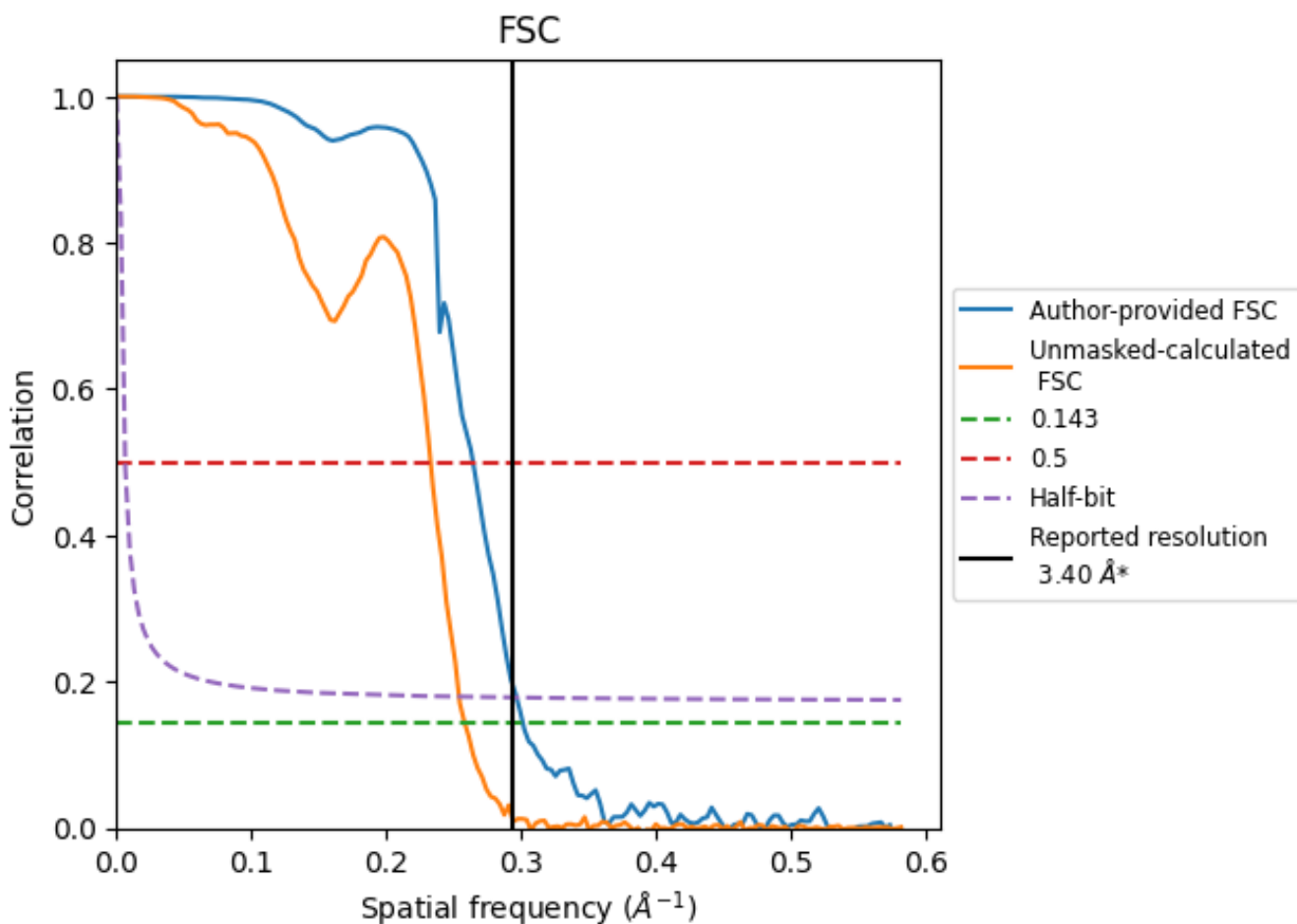


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

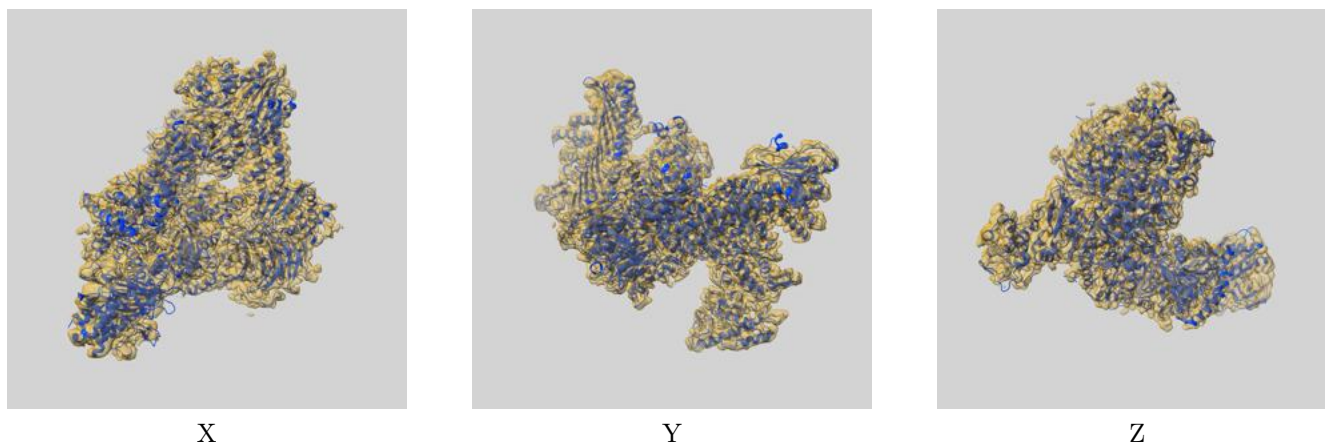
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.32	3.79	3.37
Unmasked-calculated*	3.87	4.30	3.94

*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 3.87 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

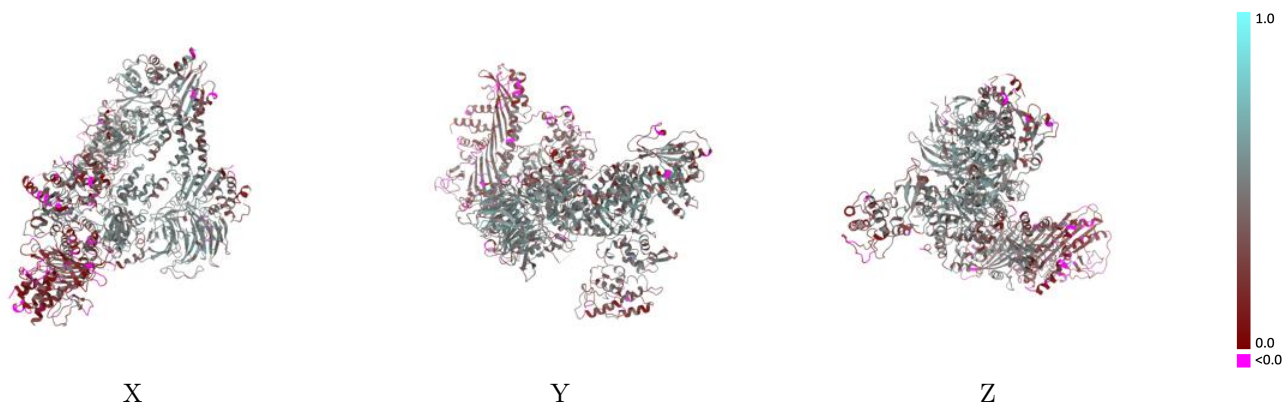
This section contains information regarding the fit between EMDB map EMD-25707 and PDB model 7T5Q. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



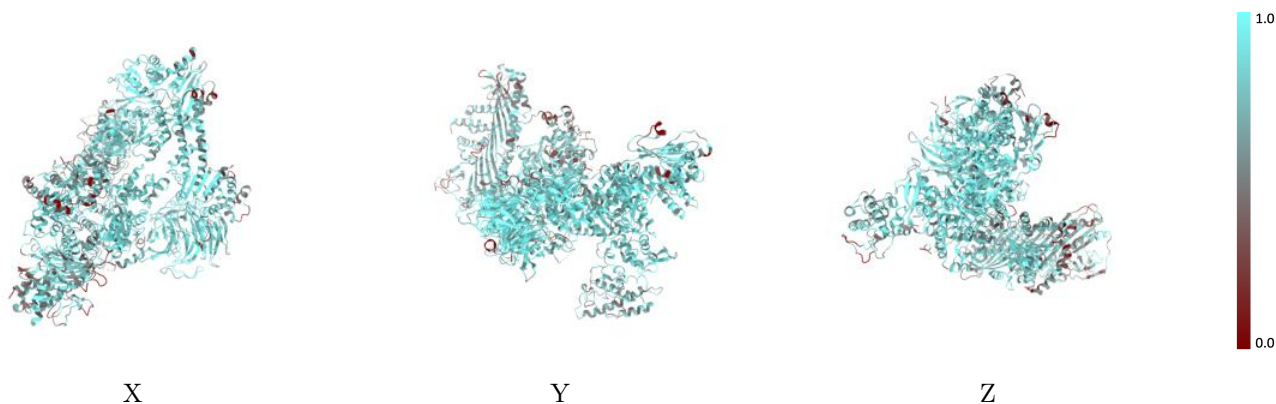
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



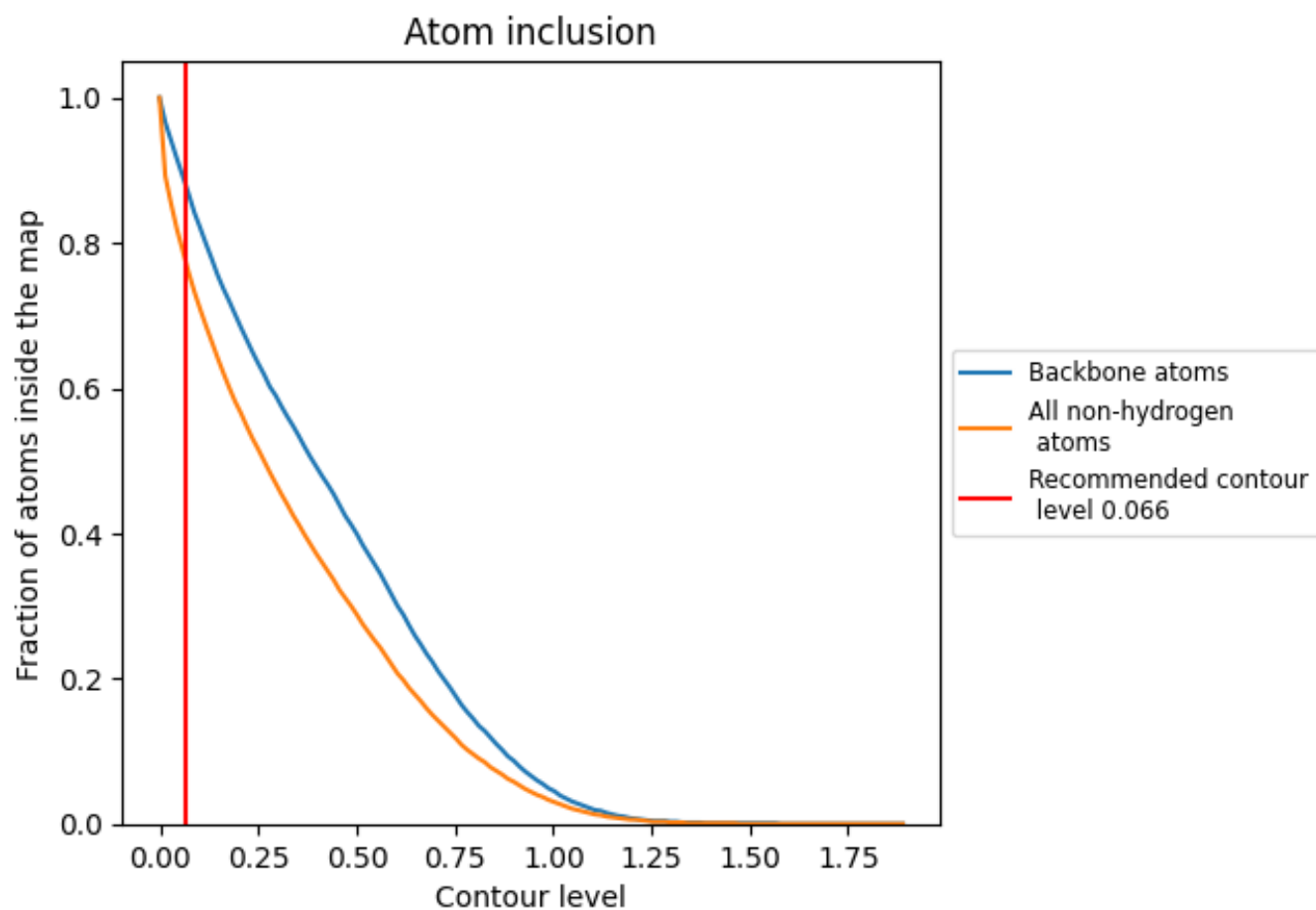
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.066).























9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 77% 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 (0.066) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.3850
A	 0.8500	 0.4730
B	 0.8460	 0.4580
C	 0.8460	 0.4770
D	 0.7760	 0.4220
E	 0.6760	 0.2840
F	 0.8720	 0.4920
G	 0.6400	 0.3280
H	 0.7640	 0.3660
I	 0.6600	 0.2050
J	 0.6340	 0.2400

