



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 01:12 pm BST

PDB ID : 8OOP
EMDB ID : EMD-17025
Title : CryoEM Structure INO80core Hexasome complex composite model state2
Authors : Zhang, M.; Jungblut, A.; Hoffmann, T.; Eustermann, S.
Deposited on : 2023-04-05
Resolution : 2.70 Å(reported)
Based on initial models : 8A5Q, 6FML, 7OHC

This is a wwPDB EM Validation Summary 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.dev92
Mogul : 1.8.4, 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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

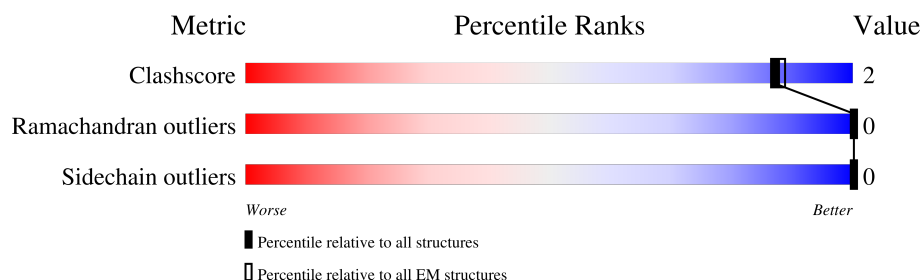
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.






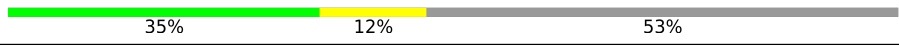


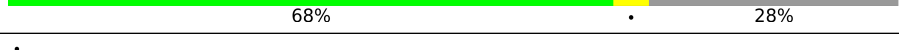
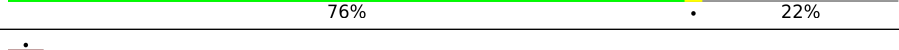
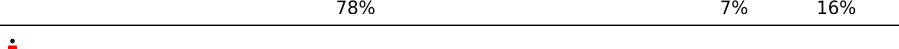
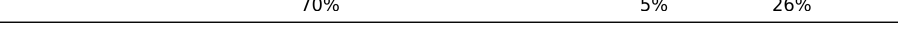
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	462	 95%
1	B	462	 91% 5%
1	C	462	 98%
2	D	488	 87% 10%
2	E	488	 89% 9%
2	F	488	 87% 10%
3	G	1134	 59% 38%
4	H	492	 8% 92%

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Mol	Chain	Length	Quality of chain
5	I	219	 49%50%
6	J	769	 80%18%
7	K	226	 32%17%51%
8	L	226	 35%12%53%
9	M	135	 53%45%
9	Q	135	 70%27%
10	N	102	 68%28%
10	R	102	 76%22%
11	O	129	 78%7%16%
12	P	125	 70%5%26%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 40747 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 RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3432	2154	610	653	15		
1	B	438	Total	C	N	O	S	0	0
			3352	2103	597	637	15		
1	C	459	Total	C	N	O	S	0	0
			3511	2199	627	670	15		

- Molecule 2 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	441	Total	C	N	O	S	0	0
			3401	2129	597	660	15		
2	E	443	Total	C	N	O	S	0	0
			3414	2136	600	663	15		
2	F	439	Total	C	N	O	S	0	0
			3394	2125	596	658	15		

- Molecule 3 is a protein called Chromatin-remodeling ATPase Ino80.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	704	Total	C	N	O	S	0	0
			5736	3657	1020	1024	35		

- Molecule 4 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	38	Total	C	N	O	S	0	0
			283	181	51	48	3		

- Molecule 5 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	109	Total	C	N	O	S	0	0
			873	546	167	156	4		

- Molecule 6 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	630	Total	C	N	O	S	0	0
			4472	2820	806	830	16		

- Molecule 7 is a DNA chain called DNA strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	110	Total	C	N	O	P	0	0
			2243	1063	410	660	110		

- Molecule 8 is a DNA chain called DNA Strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	107	Total	C	N	O	P	0	0
			2201	1041	411	642	107		

- Molecule 9 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	74	Total	C	N	O	S	0	0
			602	381	113	104	4		
9	Q	98	Total	C	N	O	S	0	0
			810	511	157	138	4		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	73	Total	C	N	O	S	0	0
			587	370	115	101	1		
10	R	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

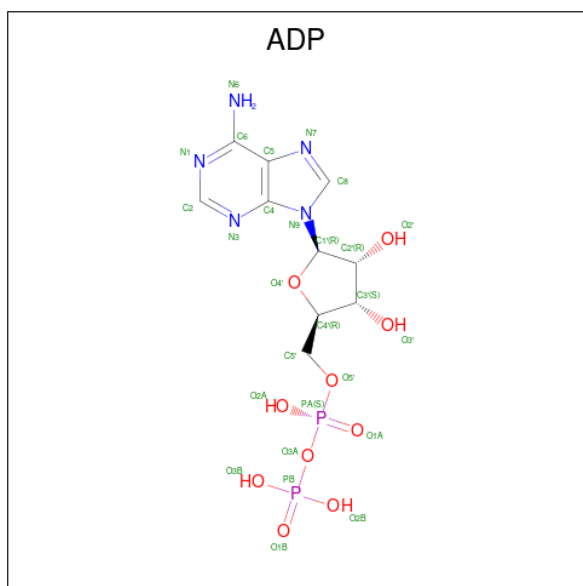
- Molecule 11 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	109	Total	C	N	O	0	0
			842	531	167	144		

- Molecule 12 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	93	Total	C	N	O	S	0	0
			729	458	131	138	2		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

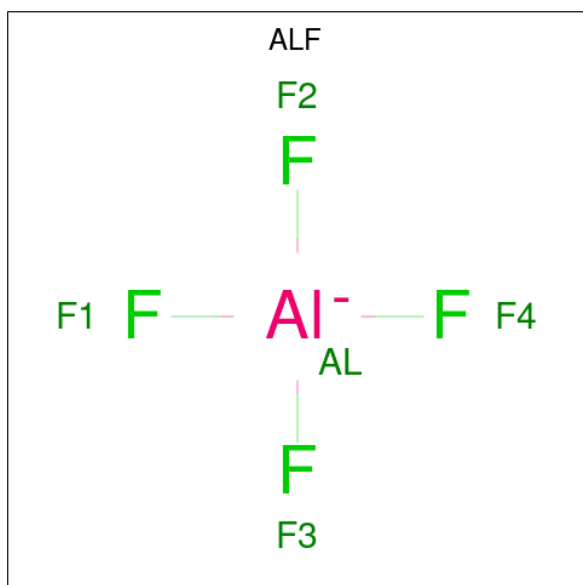


Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

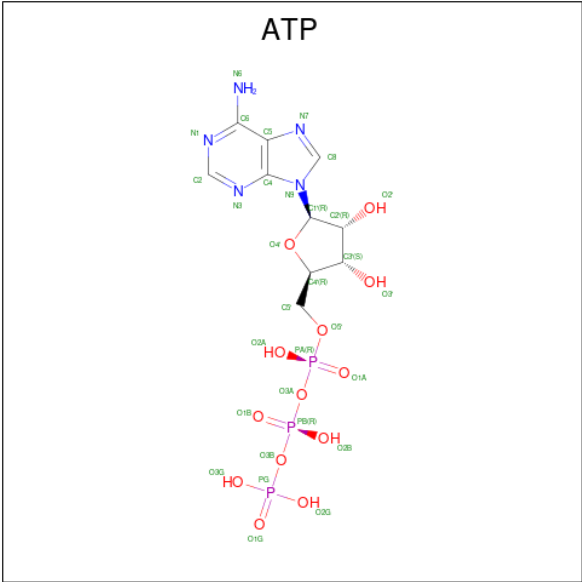
Mol	Chain	Residues	Atoms		AltConf
14	G	1	Total	Mg	0
			1	1	
14	J	1	Total	Mg	0
			1	1	

- Molecule 15 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
15	G	1	Total	Al	F	0
			5	1	4	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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.

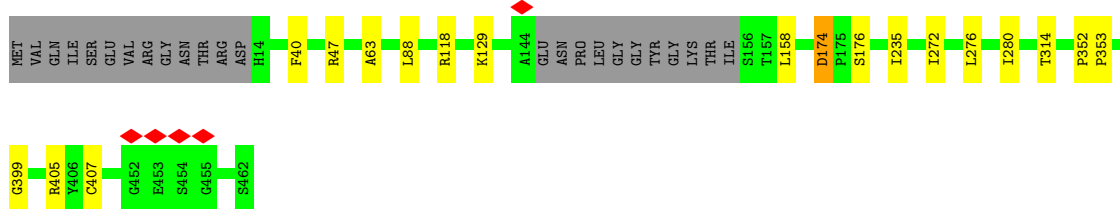
- Molecule 1: RuvB-like protein 1

Chain A:  95%



- Molecule 1: RuvB-like protein 1

Chain B:  91% 5%




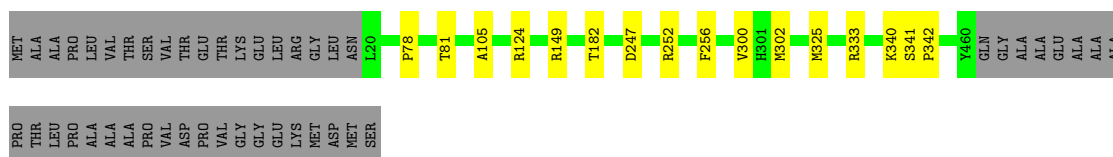
- Molecule 1: RuvB-like protein 1

Chain C:  98%




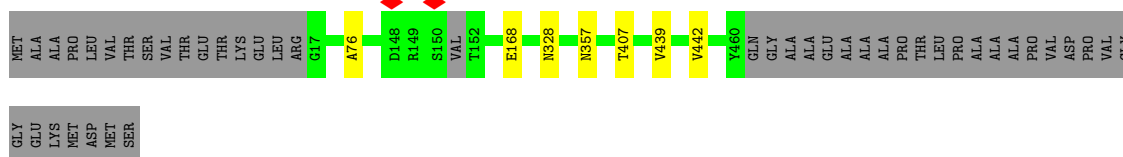
- Molecule 2: RuvB-like protein 2

Chain D:  87% 10%




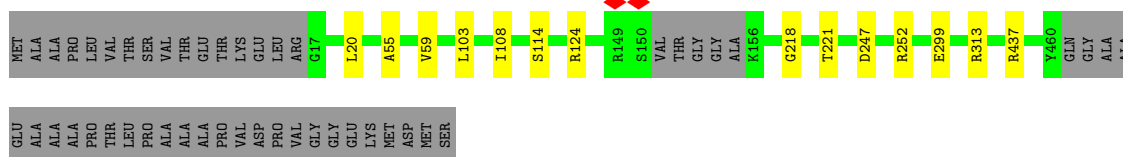
- Molecule 2: RuvB-like protein 2

Chain E:  89% 9%



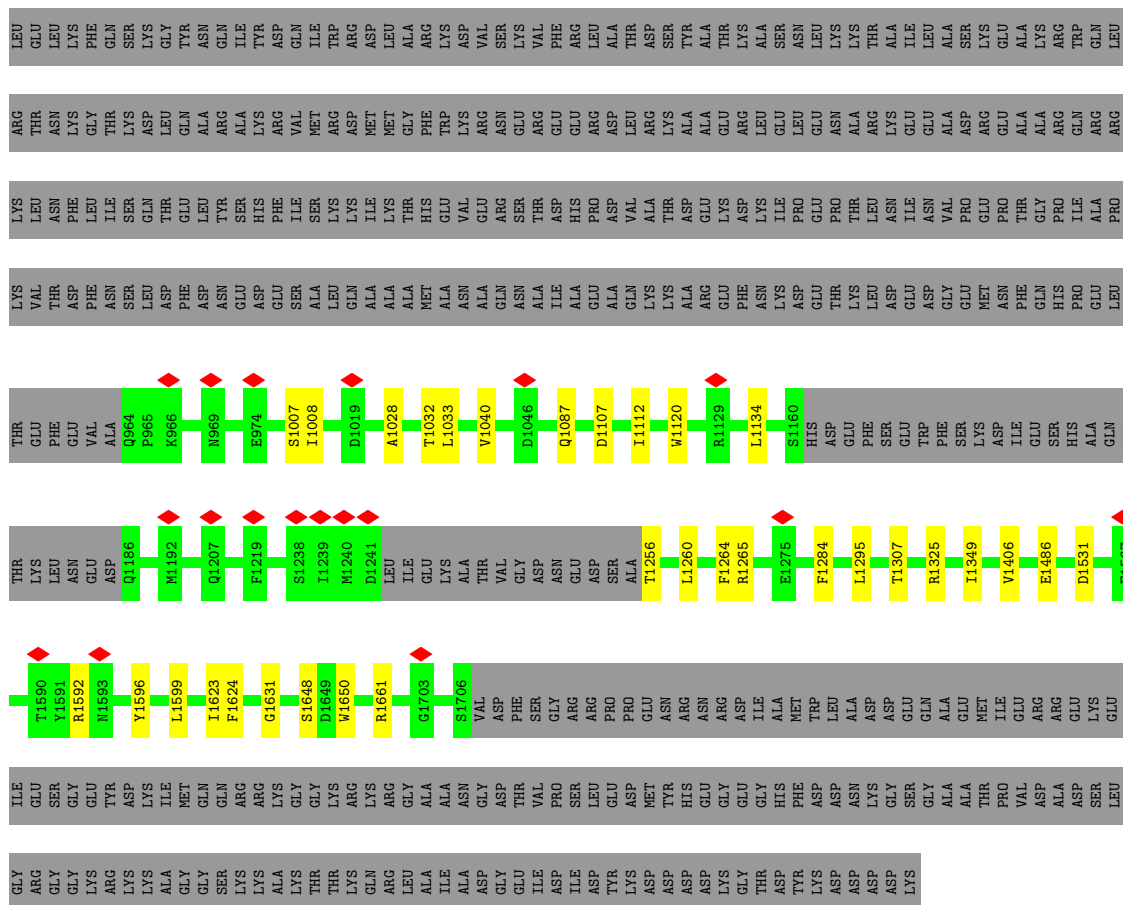
- Molecule 2: RuvB-like protein 2

Chain F:  87% 10%

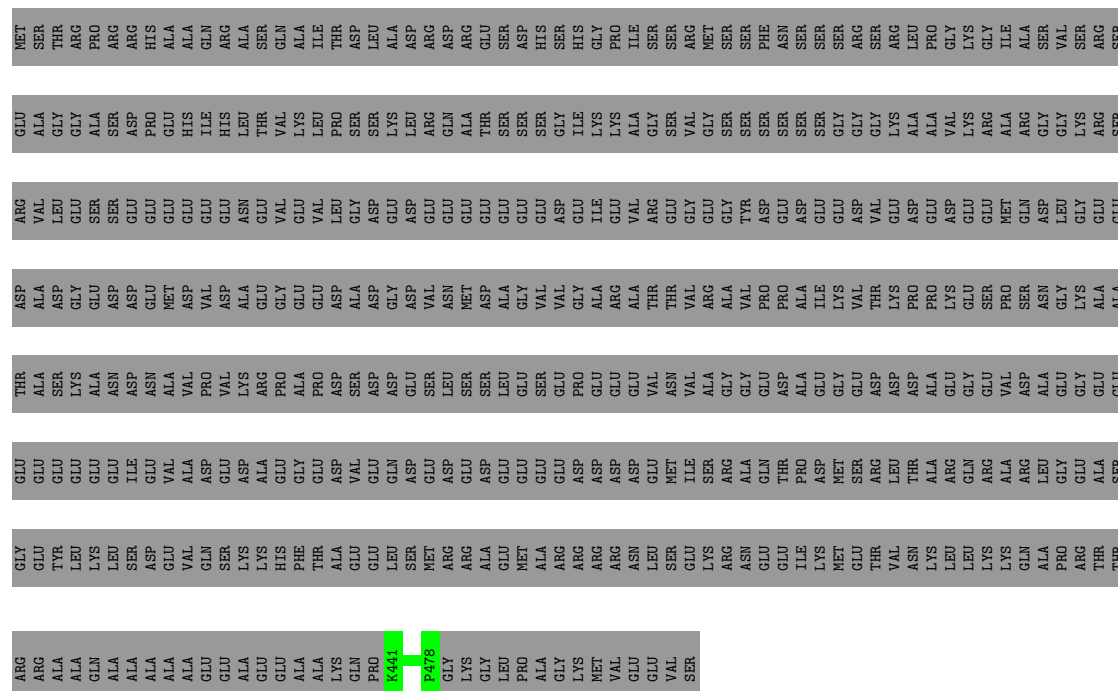


- Molecule 3: Chromatin-remodeling ATPase Ino80

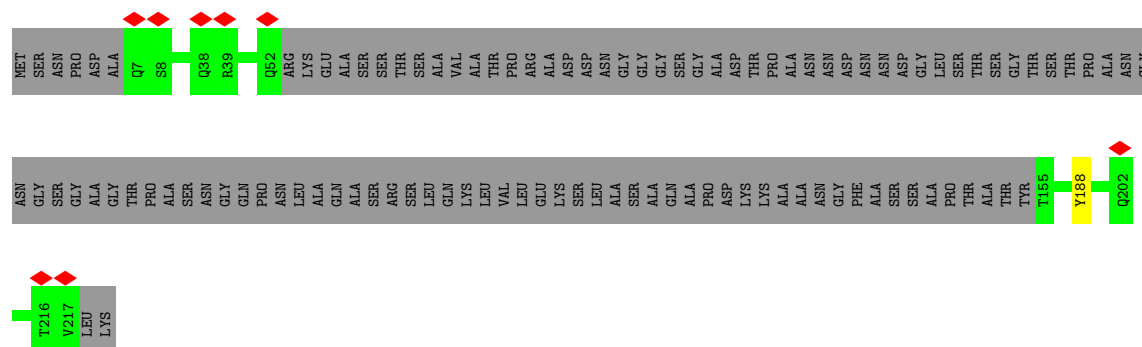
Chain G:  59% 38%



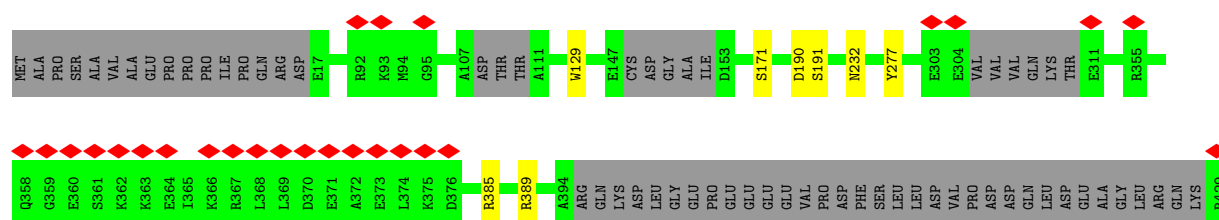
- Molecule 4: Ino eighty subunit 2

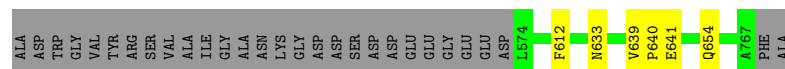


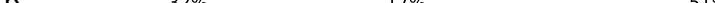
- Molecule 5: Chromatin-remodeling complex subunit IES6

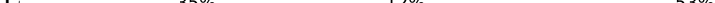


- Molecule 6: Actin-related protein 5





Chain K:  32% 17% 51%

Chain L:  35% 12% 53%



Chain M: 53% . 45%

Chain Q: 70% 27%

Chain N:  68% 28%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98967	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.515	Depositor
Minimum map value	-5.442	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.324	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	295.92, 295.92, 295.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/3481	0.59	0/4703
1	B	0.29	0/3398	0.62	3/4589 (0.1%)
1	C	0.26	0/3560	0.57	0/4809
2	D	0.27	0/3445	0.58	0/4640
2	E	0.28	0/3457	0.58	0/4654
2	F	0.27	0/3437	0.56	0/4627
3	G	0.29	0/5866	0.61	0/7926
4	H	0.26	0/290	0.55	0/393
5	I	0.26	0/893	0.59	0/1207
6	J	0.26	0/4564	0.52	0/6225
7	K	0.79	0/2513	0.61	0/3873
8	L	0.78	0/2470	0.60	0/3812
9	M	0.28	0/609	0.64	0/816
9	Q	0.29	0/822	0.67	0/1102
10	N	0.28	0/592	0.65	0/794
10	R	0.28	0/645	0.65	0/862
11	O	0.26	0/852	0.61	0/1147
12	P	0.27	0/740	0.56	0/993
All	All	0.38	0/41634	0.59	3/57172 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
2	D	0	1
2	F	0	2
3	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	LEU	CA-CB-CG	6.08	129.27	115.30
1	B	158	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	174	ASP	CB-CG-OD1	5.57	123.31	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	118	ARG	Sidechain
1	B	405	ARG	Sidechain
1	C	8	ARG	Sidechain
2	D	252	ARG	Sidechain
2	F	252	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3432	0	3518	5	0
1	B	3352	0	3438	10	0
1	C	3511	0	3595	5	0
2	D	3401	0	3472	8	0
2	E	3414	0	3482	5	0
2	F	3394	0	3464	9	0
3	G	5736	0	5776	24	0
4	H	283	0	289	0	0
5	I	873	0	868	1	0
6	J	4472	0	3904	10	0
7	K	2243	0	1233	50	0
8	L	2201	0	1200	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	602	0	632	2	0
9	Q	810	0	851	2	0
10	N	587	0	635	3	0
10	R	638	0	676	1	0
11	O	842	0	908	7	0
12	P	729	0	751	5	0
13	A	27	0	12	0	0
13	B	27	0	12	0	0
13	C	27	0	12	0	0
13	D	27	0	12	0	0
13	E	27	0	12	0	0
13	F	27	0	12	0	0
13	G	27	0	12	0	0
14	G	1	0	0	0	0
14	J	1	0	0	0	0
15	G	5	0	0	0	0
16	J	31	0	12	0	0
All	All	40747	0	38788	150	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.

The worst 5 of 150 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)
7:K:24:DA:H2''	7:K:25:DG:C8	2.19	0.78
7:K:-68:DG:N2	8:L:69:DT:O2	2.19	0.74
8:L:-16:DT:H2''	8:L:-15:DA:C8	2.27	0.70
7:K:-35:DA:H2''	7:K:-34:DG:C8	2.31	0.66
8:L:63:DG:H8	8:L:63:DG:OP2	1.80	0.65

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	447/462 (97%)	433 (97%)	14 (3%)	0	100	100
1	B	434/462 (94%)	420 (97%)	14 (3%)	0	100	100
1	C	457/462 (99%)	449 (98%)	8 (2%)	0	100	100
2	D	439/488 (90%)	436 (99%)	3 (1%)	0	100	100
2	E	439/488 (90%)	430 (98%)	9 (2%)	0	100	100
2	F	435/488 (89%)	430 (99%)	5 (1%)	0	100	100
3	G	698/1134 (62%)	671 (96%)	27 (4%)	0	100	100
4	H	36/492 (7%)	35 (97%)	1 (3%)	0	100	100
5	I	105/219 (48%)	103 (98%)	2 (2%)	0	100	100
6	J	618/769 (80%)	598 (97%)	20 (3%)	0	100	100
9	M	72/135 (53%)	71 (99%)	1 (1%)	0	100	100
9	Q	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
10	N	71/102 (70%)	70 (99%)	1 (1%)	0	100	100
10	R	78/102 (76%)	75 (96%)	3 (4%)	0	100	100
11	O	107/129 (83%)	105 (98%)	2 (2%)	0	100	100
12	P	91/125 (73%)	90 (99%)	1 (1%)	0	100	100
All	All	4623/6192 (75%)	4511 (98%)	112 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/377 (97%)	365 (100%)	0	100	100
1	B	357/377 (95%)	357 (100%)	0	100	100
1	C	374/377 (99%)	374 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	369/402 (92%)	369 (100%)	0	100	100
2	E	370/402 (92%)	370 (100%)	0	100	100
2	F	369/402 (92%)	369 (100%)	0	100	100
3	G	625/989 (63%)	625 (100%)	0	100	100
4	H	30/398 (8%)	30 (100%)	0	100	100
5	I	93/171 (54%)	93 (100%)	0	100	100
6	J	371/644 (58%)	371 (100%)	0	100	100
9	M	64/110 (58%)	64 (100%)	0	100	100
9	Q	86/110 (78%)	86 (100%)	0	100	100
10	N	62/78 (80%)	62 (100%)	0	100	100
10	R	65/78 (83%)	65 (100%)	0	100	100
11	O	85/98 (87%)	85 (100%)	0	100	100
12	P	80/105 (76%)	80 (100%)	0	100	100
All	All	3765/5118 (74%)	3765 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	1447	ASN
6	J	654	GLN
12	P	81	ASN
2	D	357	ASN
2	E	24	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
13	ADP	A	501	-	24,29,29	1.00	1 (4%)	29,45,45	1.34	3 (10%)
13	ADP	D	501	-	24,29,29	0.99	1 (4%)	29,45,45	1.34	4 (13%)
13	ADP	F	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.19	2 (6%)
13	ADP	G	2001	14	24,29,29	0.99	1 (4%)	29,45,45	1.55	3 (10%)
13	ADP	B	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.27	4 (13%)
15	ALF	G	2003	-	0,4,4	-	-	-	-	-
13	ADP	E	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.26	3 (10%)
16	ATP	J	801	14	26,33,33	0.65	0	31,52,52	0.76	2 (6%)
13	ADP	C	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.23	3 (10%)

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
13	ADP	A	501	-	-	2/12/32/32	0/3/3/3
13	ADP	D	501	-	-	6/12/32/32	0/3/3/3
13	ADP	F	501	-	-	0/12/32/32	0/3/3/3
13	ADP	G	2001	14	-	3/12/32/32	0/3/3/3
13	ADP	B	501	-	-	4/12/32/32	0/3/3/3
13	ADP	E	501	-	-	1/12/32/32	0/3/3/3
16	ATP	J	801	14	-	9/18/38/38	0/3/3/3
13	ADP	C	501	-	-	3/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	ADP	C5-C4	2.44	1.47	1.40
13	G	2001	ADP	C5-C4	2.42	1.47	1.40
13	A	501	ADP	C5-C4	2.41	1.47	1.40
13	F	501	ADP	C5-C4	2.40	1.47	1.40
13	E	501	ADP	C5-C4	2.35	1.47	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	2001	ADP	PA-O3A-PB	-4.90	116.00	132.83
13	E	501	ADP	N3-C2-N1	-3.62	123.03	128.68
13	B	501	ADP	N3-C2-N1	-3.61	123.04	128.68
13	A	501	ADP	N3-C2-N1	-3.57	123.09	128.68
13	F	501	ADP	N3-C2-N1	-3.54	123.14	128.68

There are no chirality outliers.

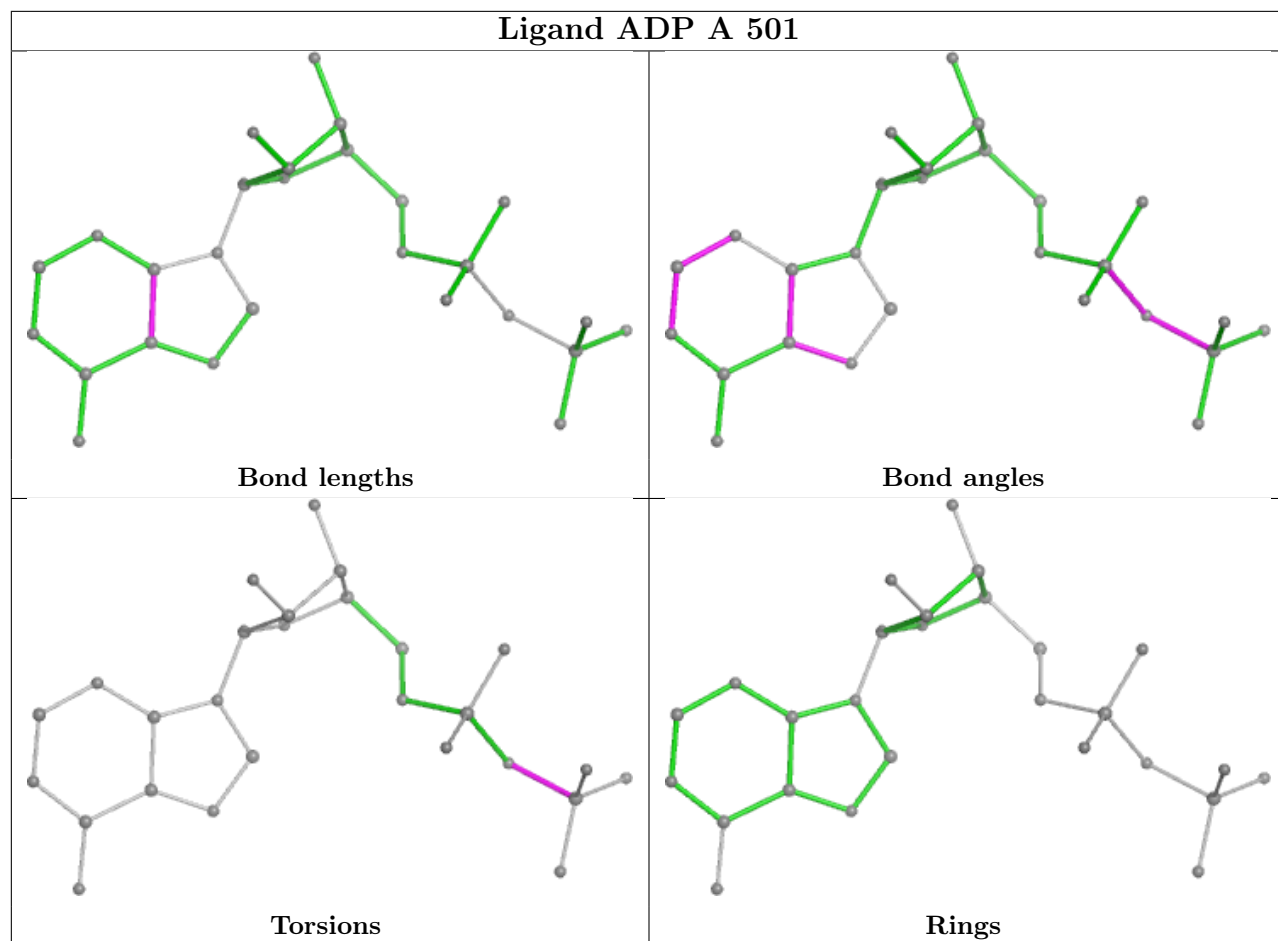
5 of 28 torsion outliers are listed below:

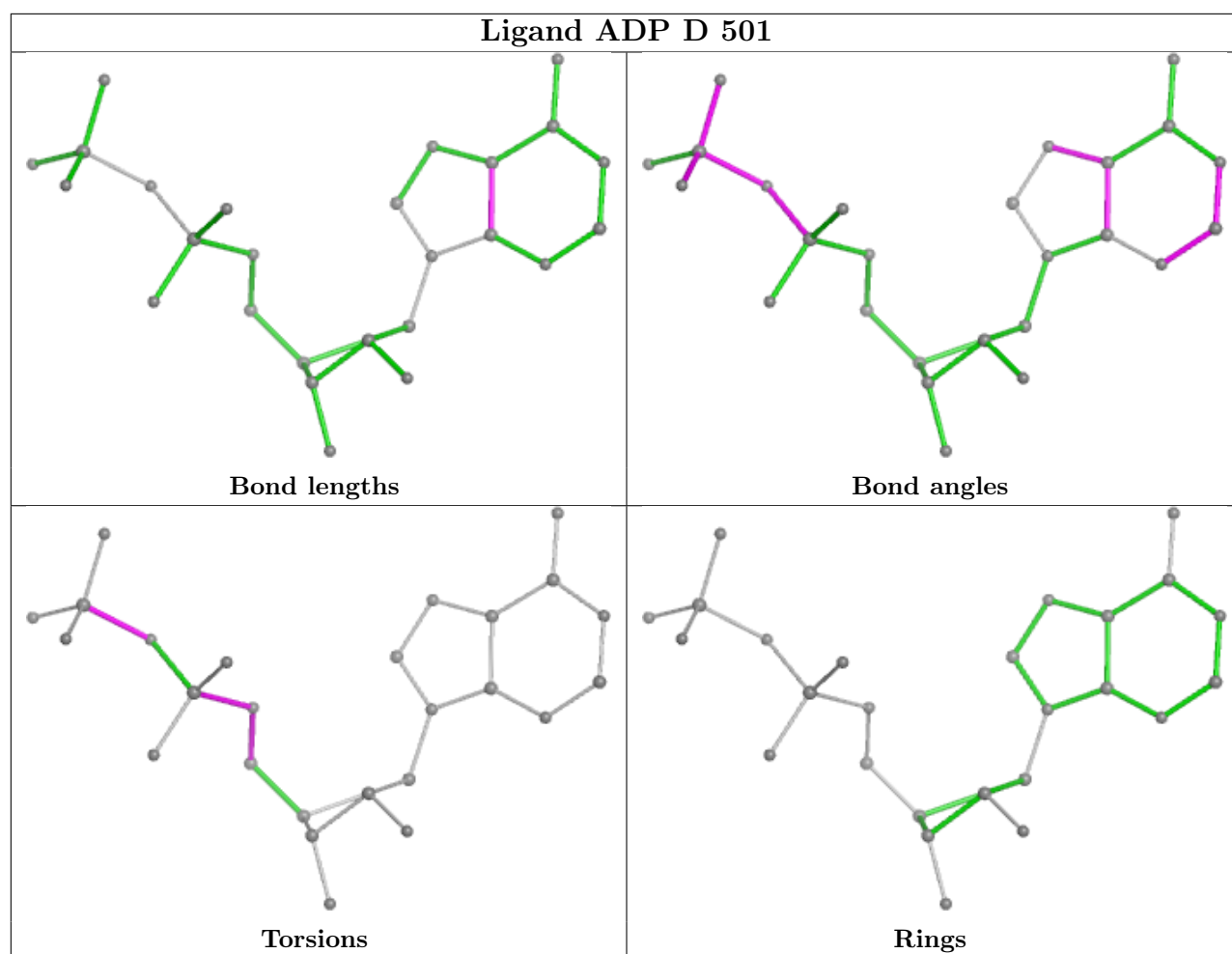
Mol	Chain	Res	Type	Atoms
13	A	501	ADP	PA-O3A-PB-O2B
13	B	501	ADP	PA-O3A-PB-O2B
13	B	501	ADP	PA-O3A-PB-O3B
13	C	501	ADP	PA-O3A-PB-O2B
13	D	501	ADP	PA-O3A-PB-O3B

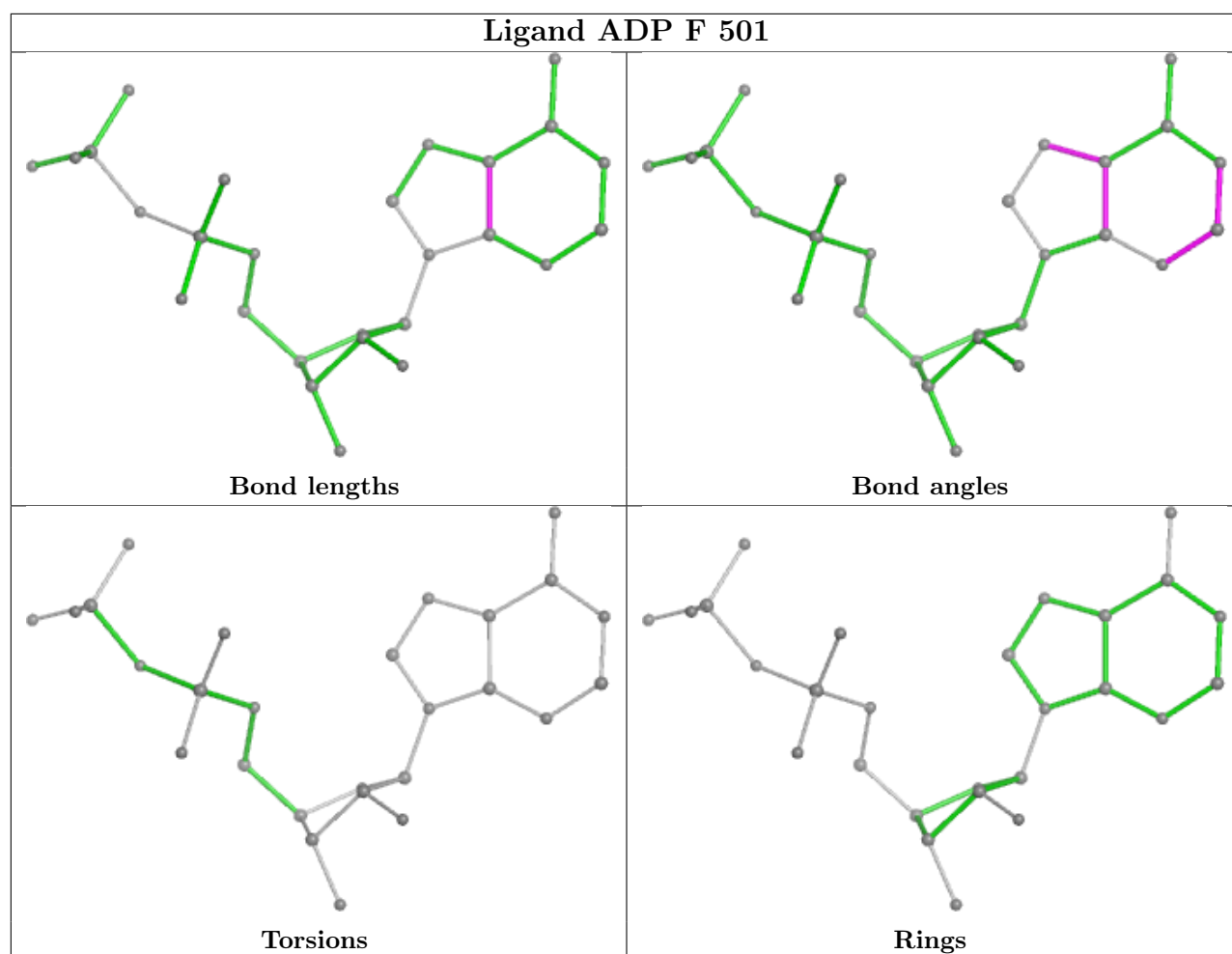
There are no ring outliers.

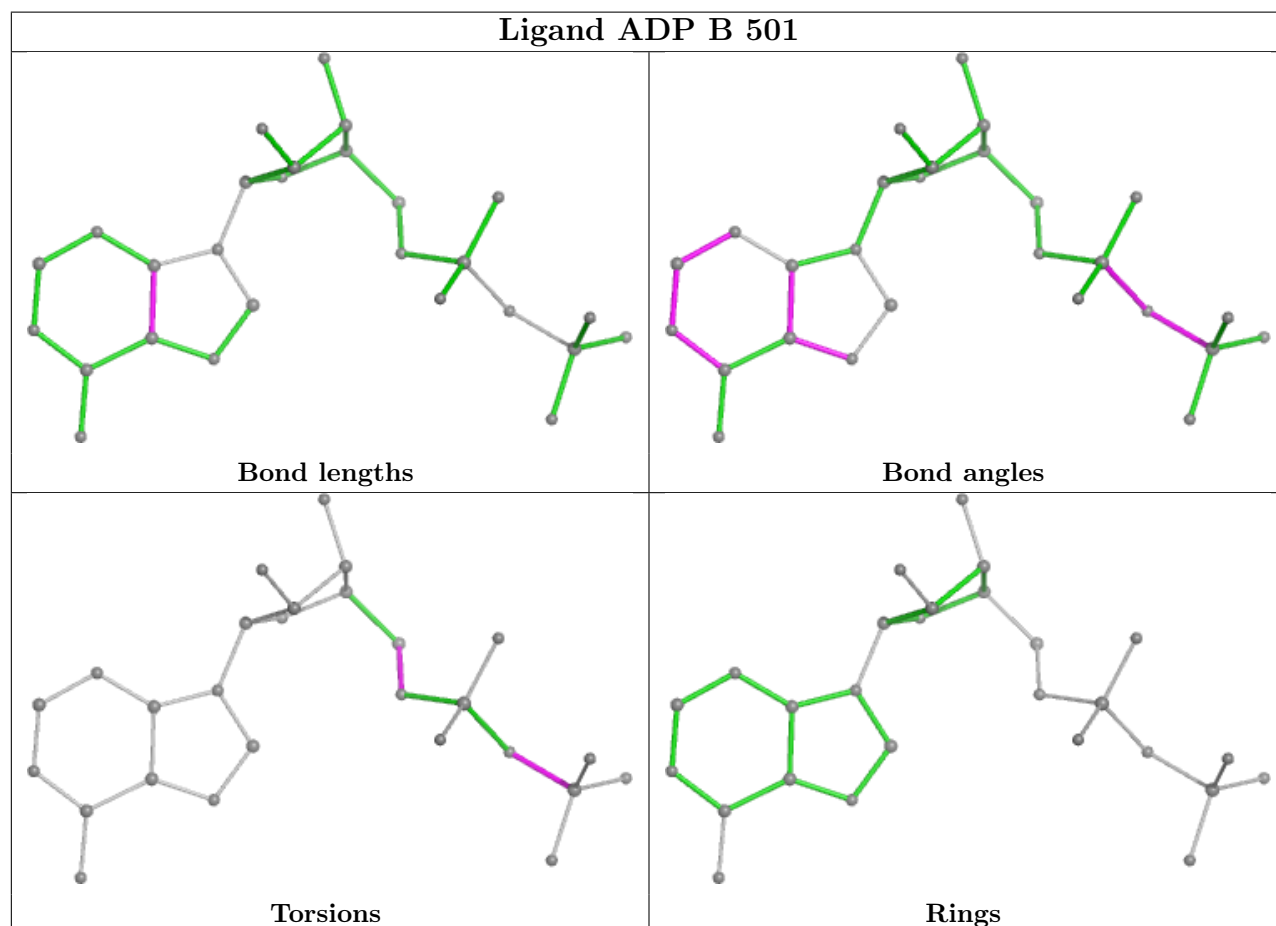
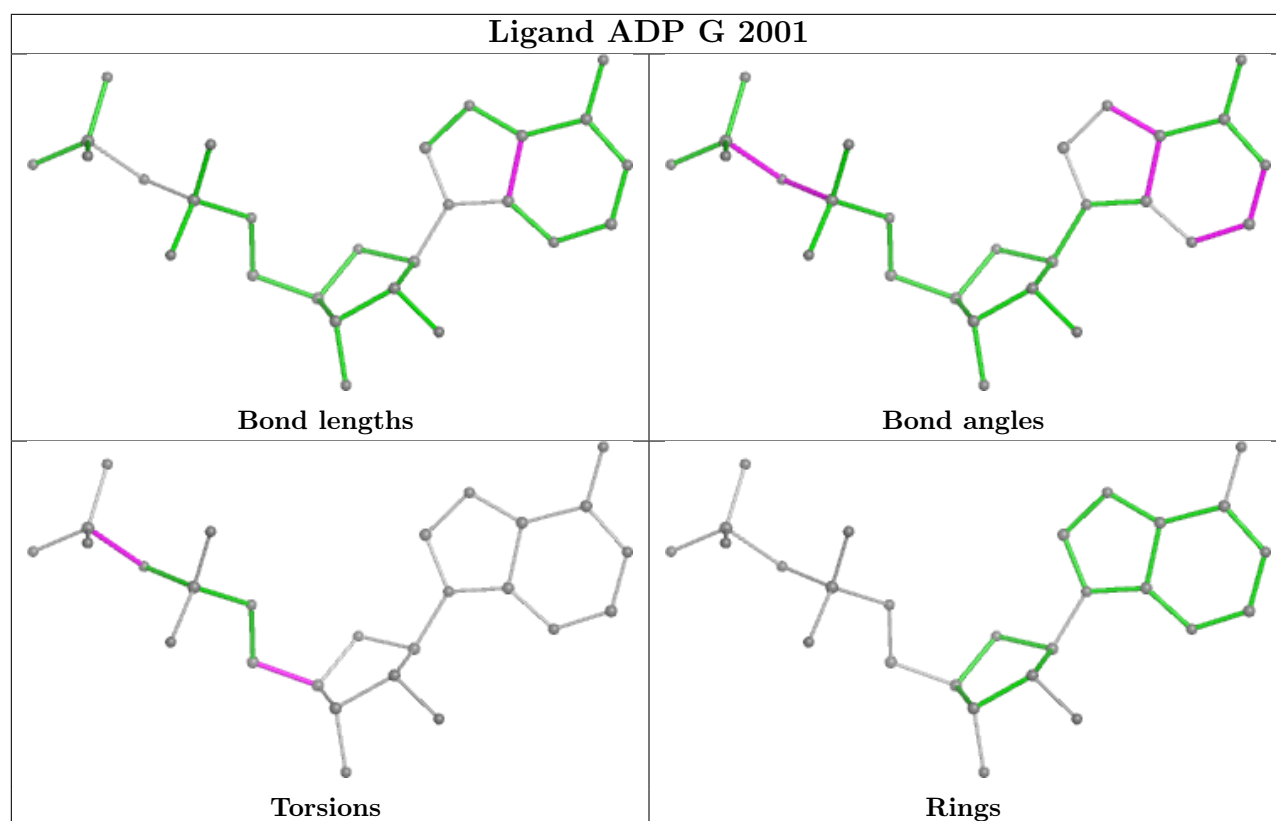
No monomer is involved in short contacts.

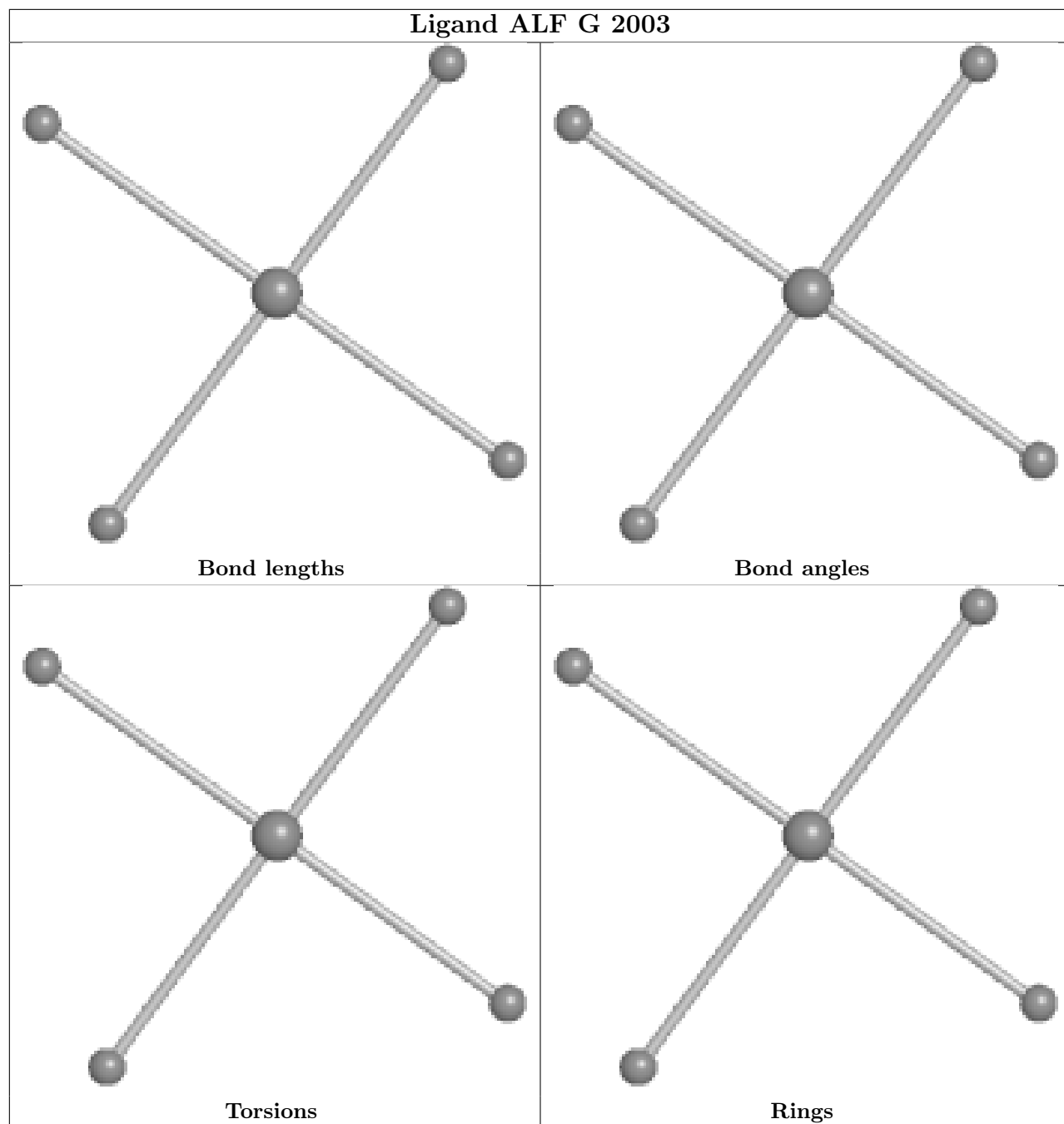
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

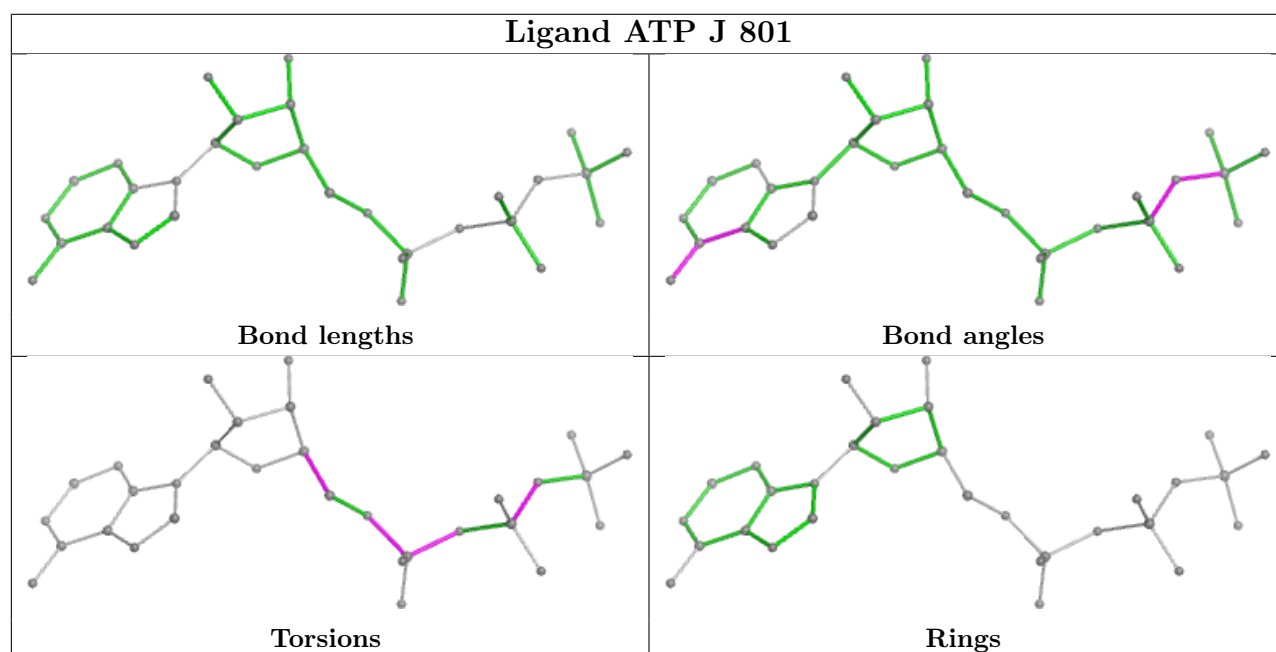
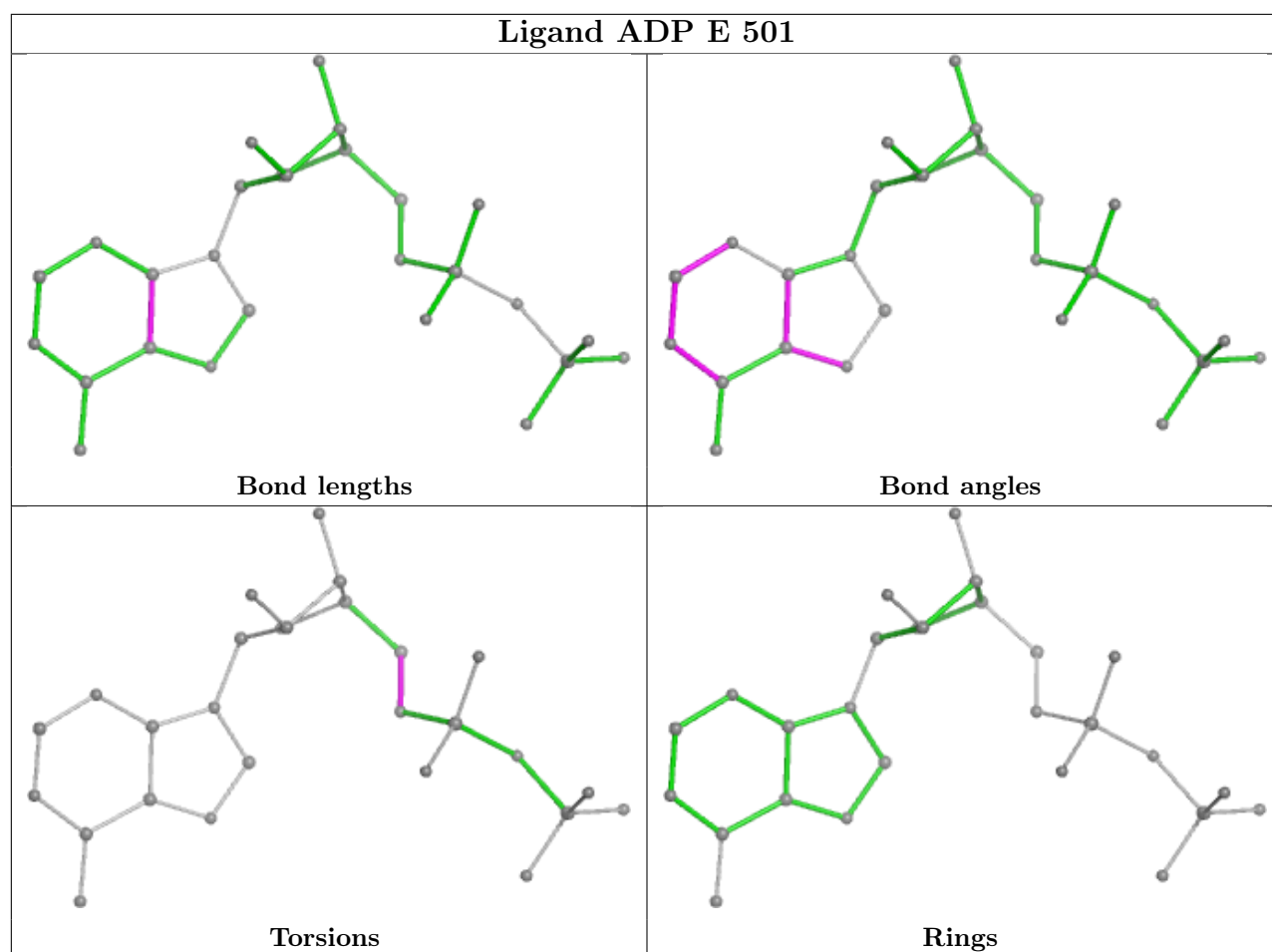


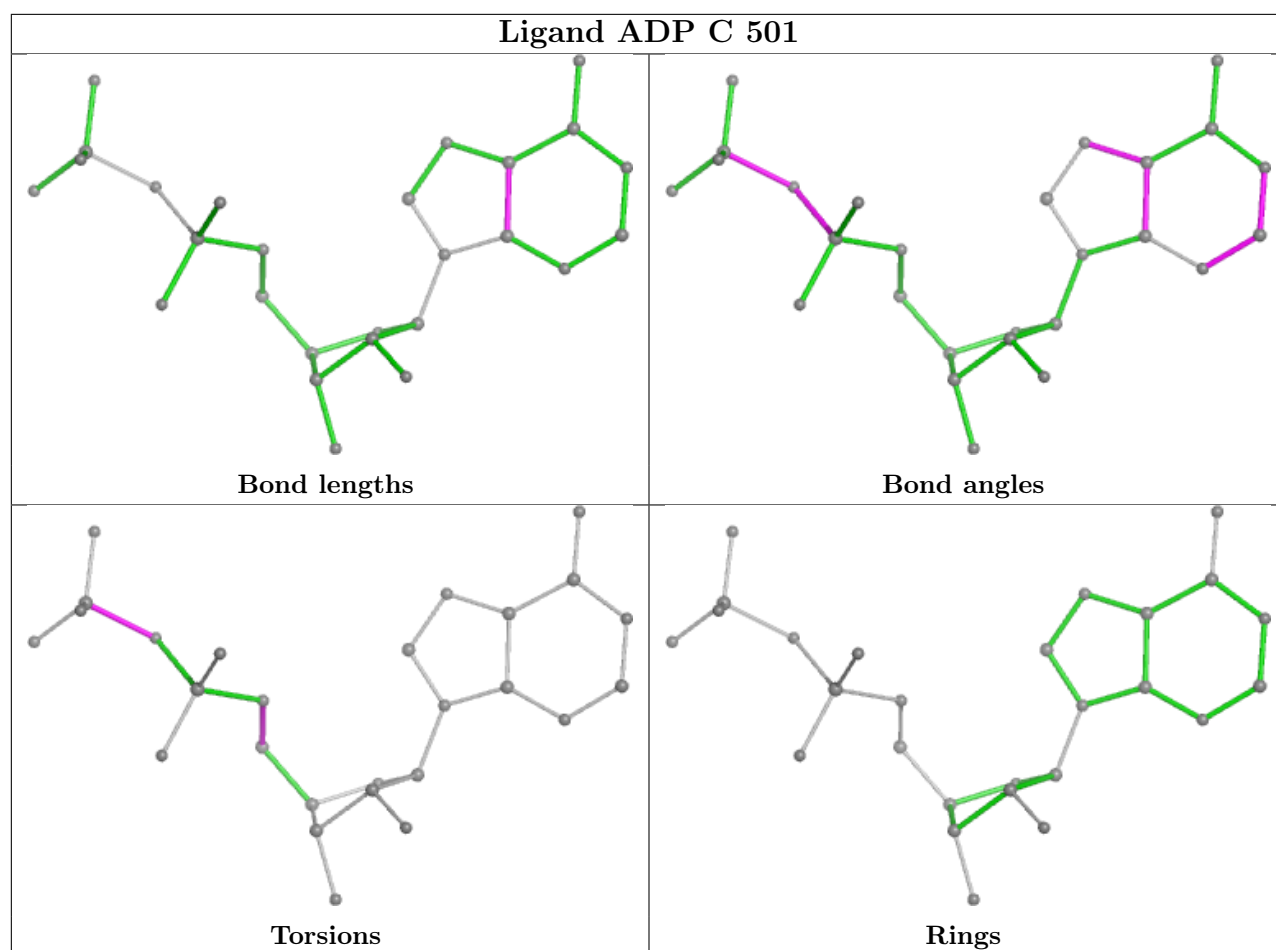












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

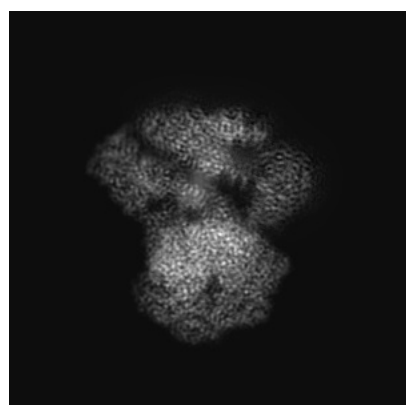
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17025. These allow visual inspection of the internal detail of the map and identification of artifacts.

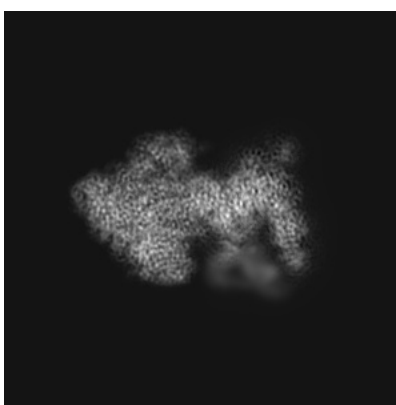
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

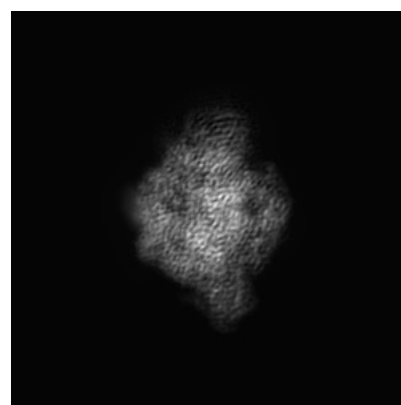
6.1.1 Primary map



X



Y

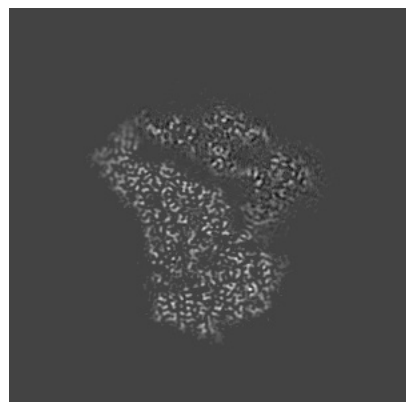


Z

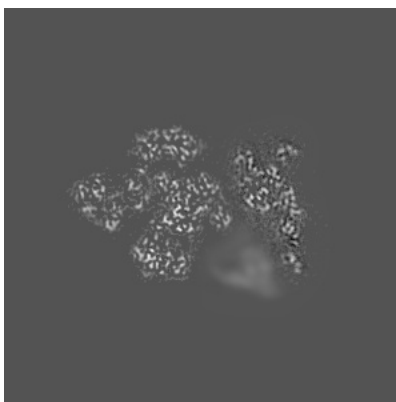
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

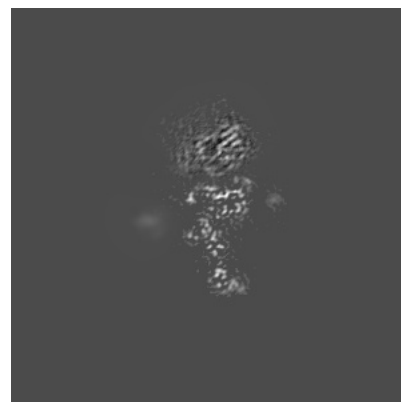
6.2.1 Primary map



X Index: 180



Y Index: 180

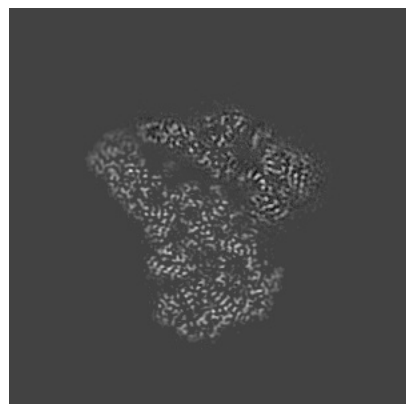


Z Index: 180

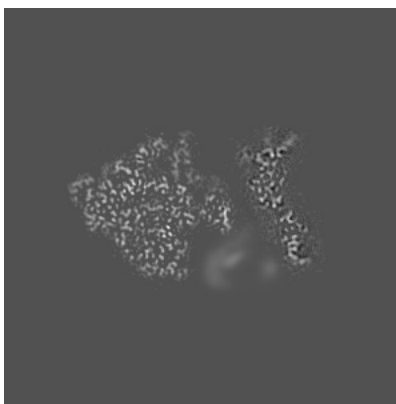
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 187



Y Index: 164

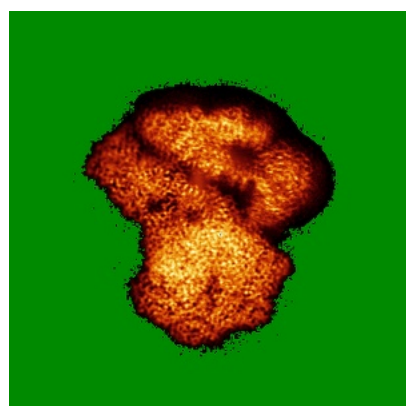


Z Index: 131

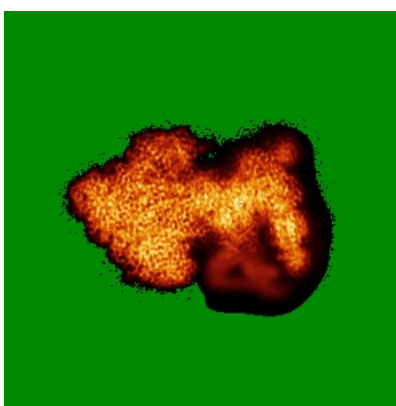
The images above show the largest variance slices of the map in three orthogonal directions.

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

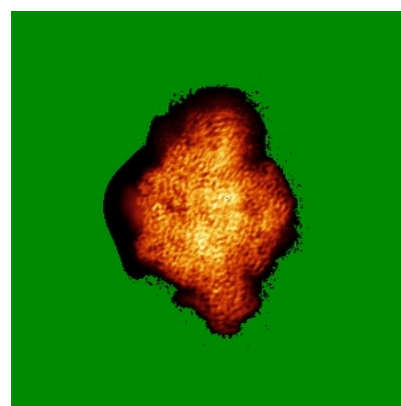
6.4.1 Primary map



X



Y

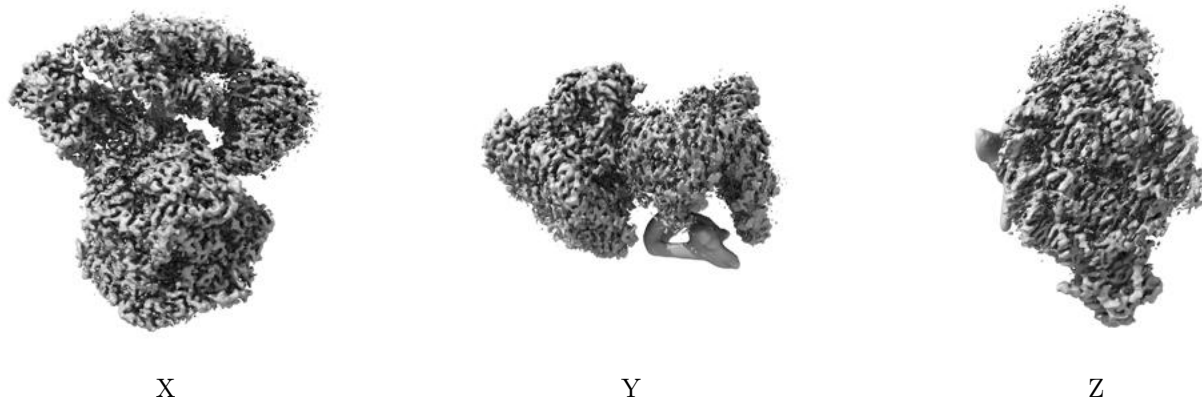


Z

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 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

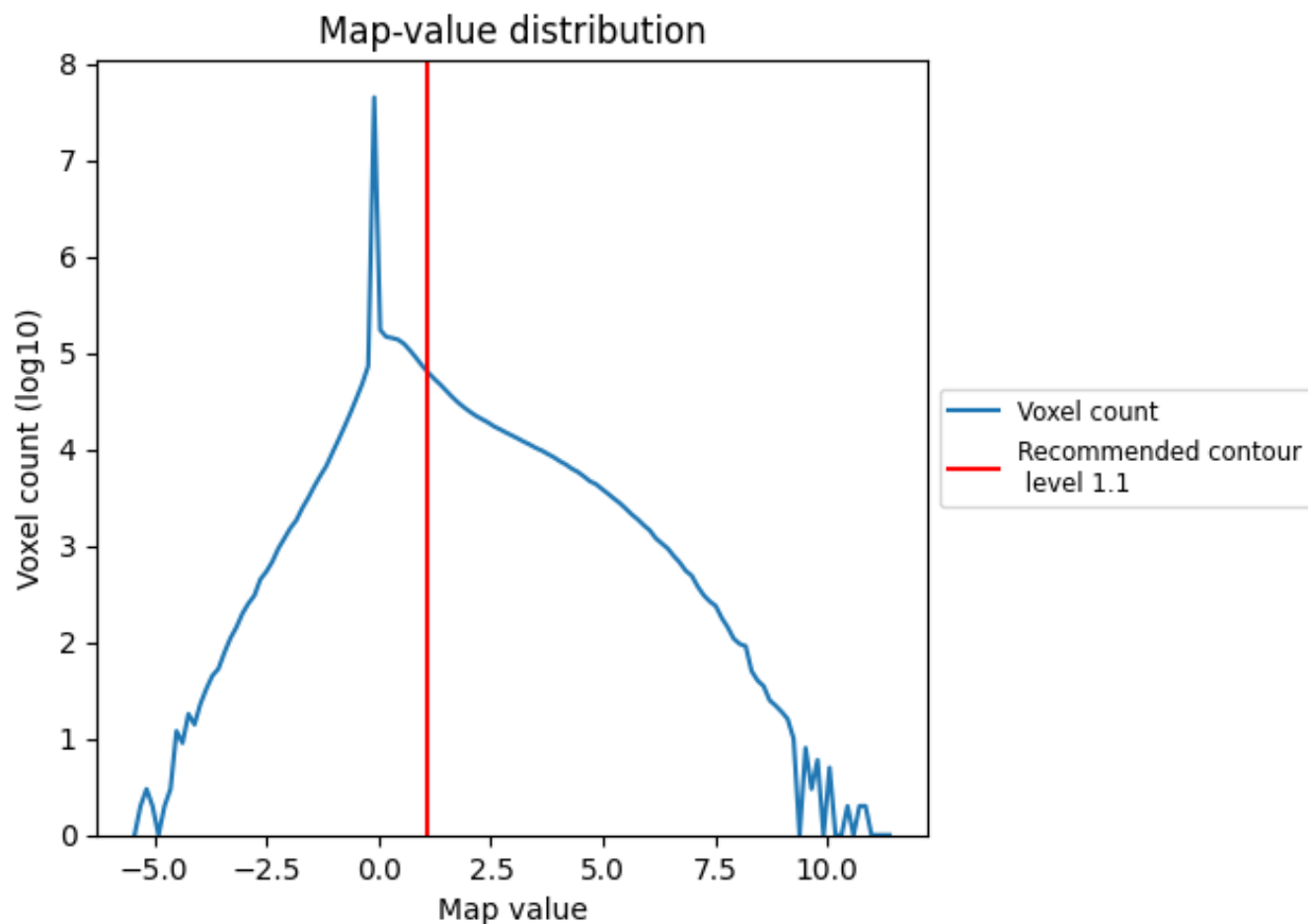
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

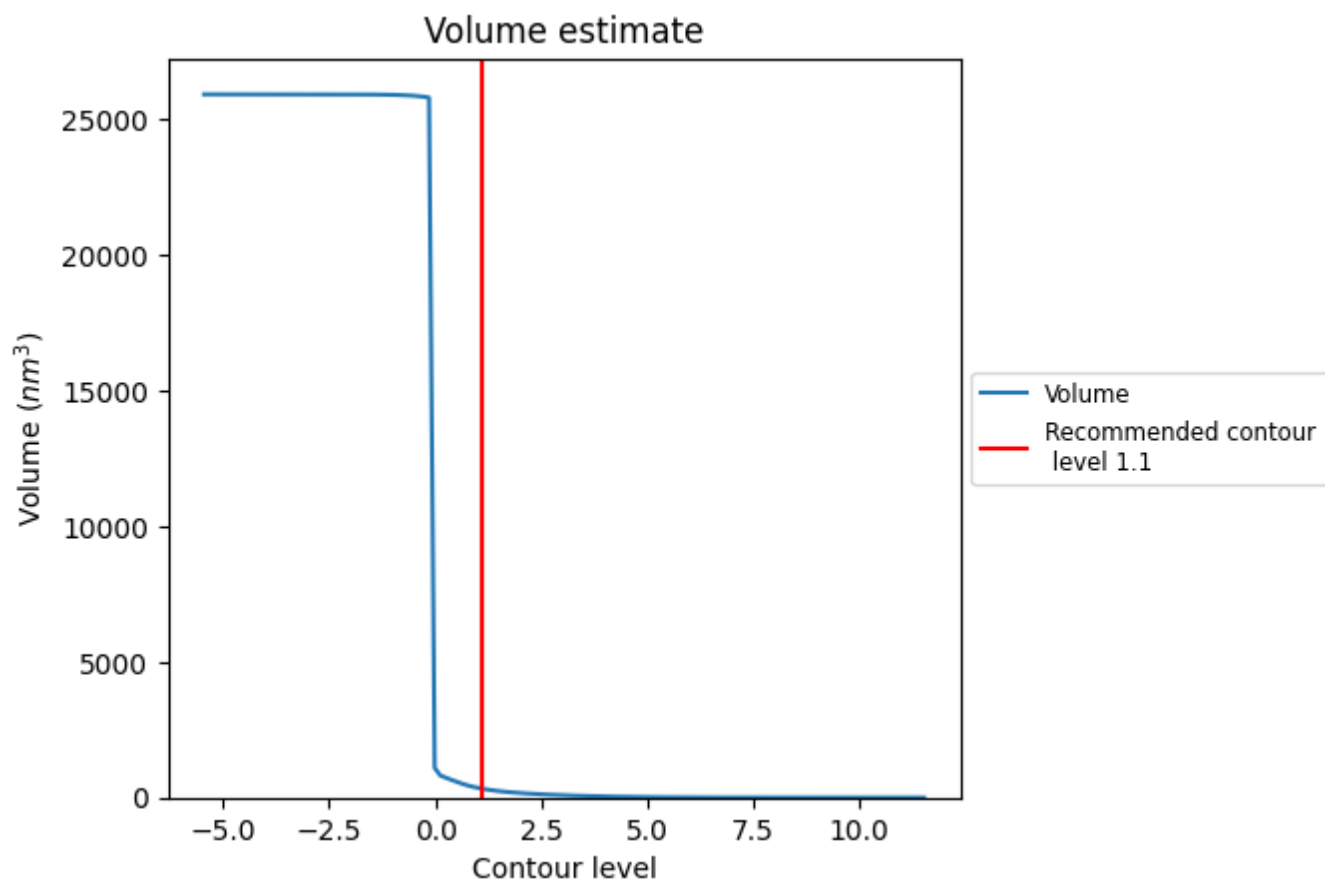
This section contains the results of statistical analysis of the map.

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.

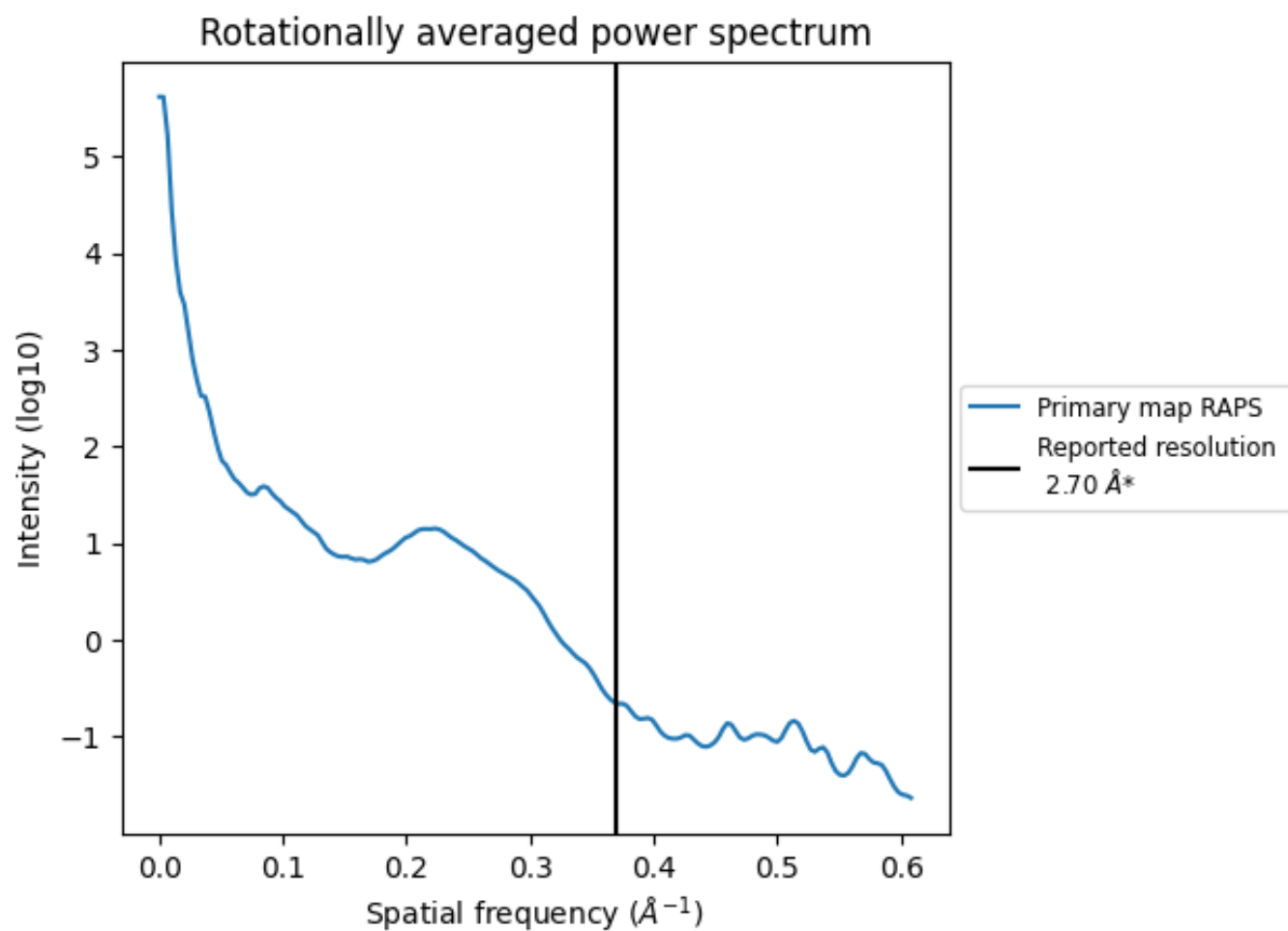
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm^3 ; this corresponds to an approximate mass of 297 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 0.370 Å⁻¹

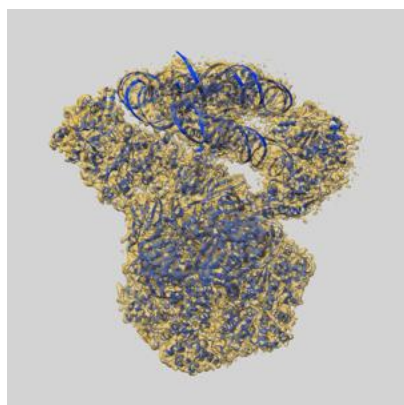
8 Fourier-Shell correlation

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

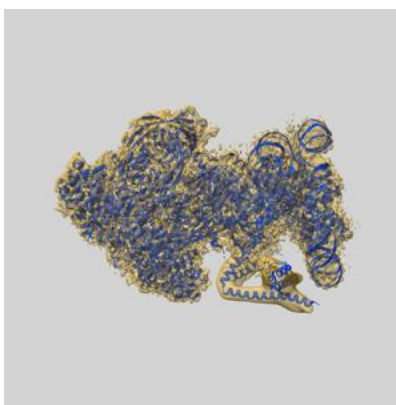
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17025 and PDB model 8OOP. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

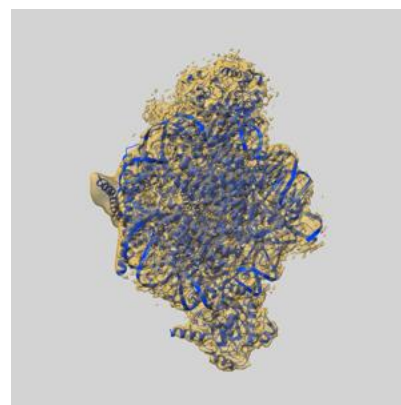
9.1 Map-model overlay [i](#)



X



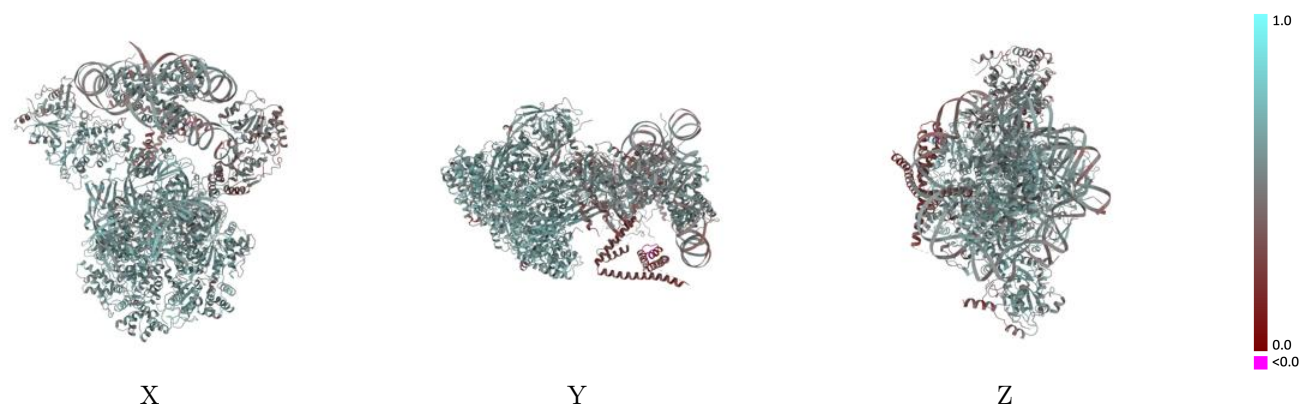
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.1 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](#)



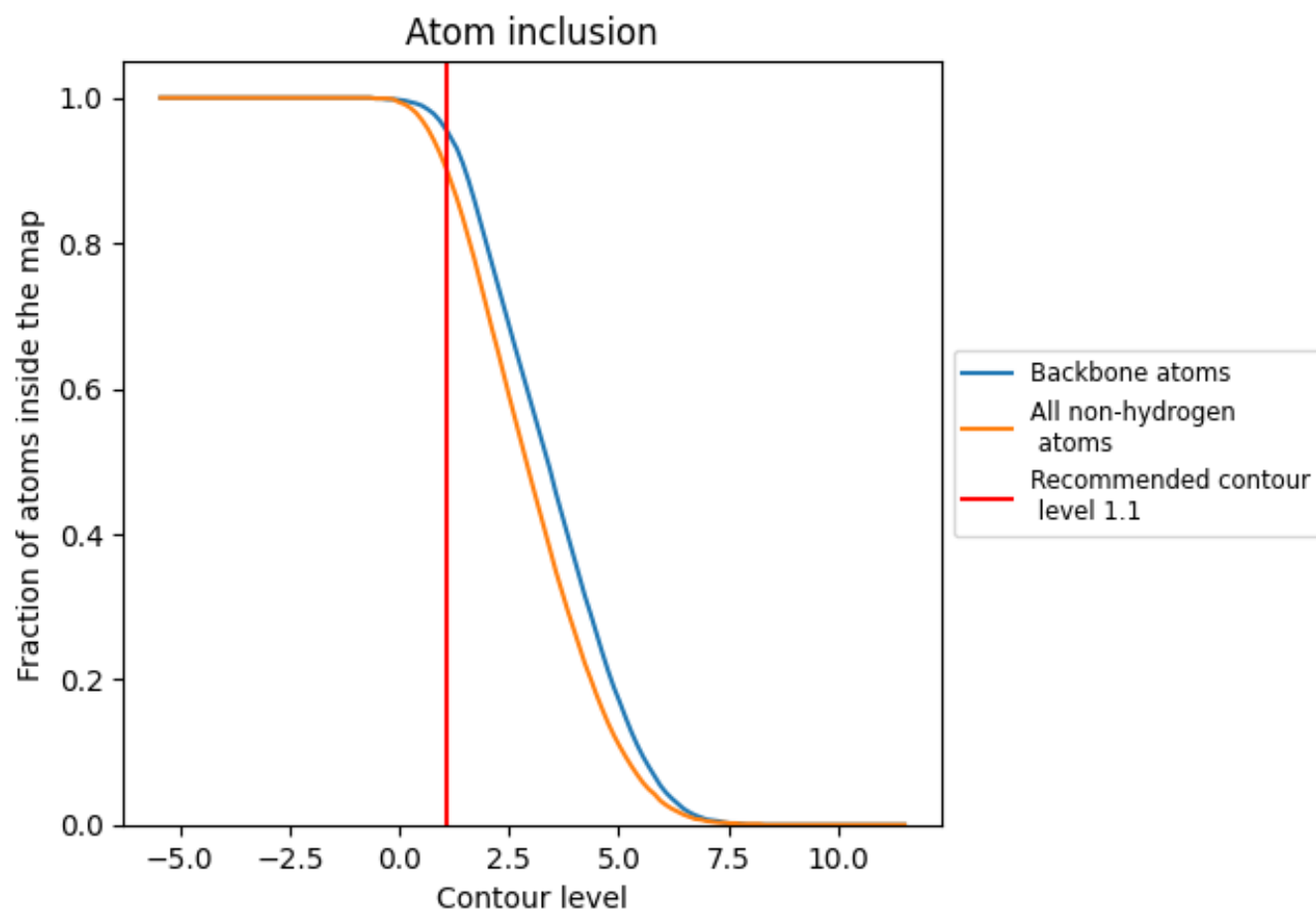
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.5540
A	 0.9260	 0.6050
B	 0.9330	 0.6020
C	 0.9190	 0.5880
D	 0.9190	 0.5840
E	 0.9300	 0.6070
F	 0.9260	 0.5990
G	 0.8450	 0.5120
H	 0.9280	 0.5690
I	 0.8150	 0.5190
J	 0.8920	 0.4970
K	 0.8700	 0.4840
L	 0.8820	 0.4890
M	 0.8970	 0.5410
N	 0.8560	 0.5240
O	 0.8710	 0.5450
P	 0.8820	 0.5420
Q	 0.8750	 0.5450
R	 0.8870	 0.5360

