



wwPDB EM Validation Summary Report ⓘ

Apr 7, 2025 – 04:51 PM EDT

PDB ID : 9B7J / pdb_00009b7j
EMDB ID : EMD-44306
Title : Cryo-EM structure of human dynactin complex bound to Chlamydia effector Dre1
Authors : Pawar, K.I.; Verba, K.A.
Deposited on : 2024-03-27
Resolution : 3.49 Å(reported)

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:

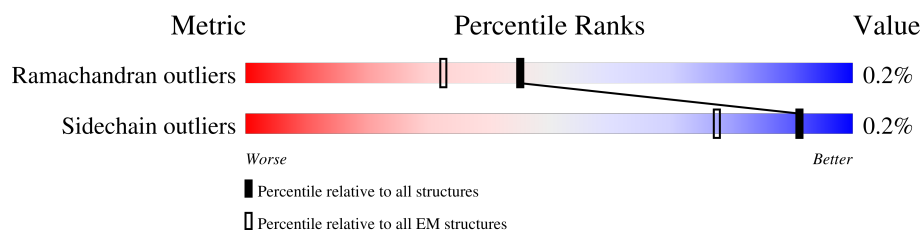
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 3.49 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	376	 10% 95% ..
1	B	376	 96% ..
1	C	376	 98% .
1	D	376	 97% ..
1	E	376	 96% ..
1	F	376	 96% ..
1	G	376	 96% ..
1	I	376	 7% 97% ..
2	H	375	 97% ..

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Mol	Chain	Length	Quality of chain
3	J	417	
4	K	460	
5	L	182	
6	M	190	
7	N	286	
8	O	272	
9	P	401	
9	Q	401	
9	p	401	
9	q	401	
10	R	186	
10	r	186	
11	S	1278	
12	T	83	
13	U	87	
14	s	1278	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 113042 atoms, of which 56723 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 Alpha-centractin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	B	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	C	375	Total	C	H	N	O	S	0	0
			5982	1918	2984	514	556	10		
1	D	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	E	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	F	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	G	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	I	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	370	Total	C	H	N	O	S	0	0
			5742	1827	2857	486	550	22		

- Molecule 3 is a protein called Actin-related protein 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	J	387	Total	C	H	N	O	S	0	0
			6140	1944	3113	514	552	17		

- Molecule 4 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	K	361	Total	C	H	N	O	S	0	0
			5895	1848	2982	517	525	23		

- Molecule 5 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	182	Total	C	H	N	O	S	0	0
			2846	897	1438	241	257	13		

- Molecule 6 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	M	156	Total	C	H	N	O	S	0	0
			2408	753	1217	206	222	10		

- Molecule 7 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	N	284	Total	C	H	N	O	S	0	0
			4532	1454	2221	402	449	6		

- Molecule 8 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	O	269	Total	C	H	N	O	S	0	0
			4236	1323	2114	370	418	11		

- Molecule 9 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	P	339	Total	C	H	N	O	S	0	0
			5411	1672	2739	462	533	5		
9	Q	278	Total	C	H	N	O	S	0	0
			4436	1373	2248	375	434	6		
9	p	326	Total	C	H	N	O	S	0	0
			5107	1581	2573	432	513	8		
9	q	337	Total	C	H	N	O	S	0	0
			5312	1651	2669	448	538	6		

- Molecule 10 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	179	Total	C	H	N	O	S	0	0
			2905	908	1475	249	269	4		
10	r	170	Total	C	H	N	O	S	0	0
			2786	872	1417	238	255	4		

- Molecule 11 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	S	154	Total	C	H	N	O	S	0	0
			2444	760	1234	218	229	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1282	ASP	SER	conflict	UNP Q14203

- Molecule 12 is a protein called Dynactin subunit 1, p150-glued.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	83	Total	C	H	N	O	0	0
			1079	332	581	83	83		

- Molecule 13 is a protein called Dynactin subunit 2, p50 dynamitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	87	Total	C	H	N	O	0	0
			1131	348	609	87	87		

- Molecule 14 is a protein called Dynactin subunit 1.

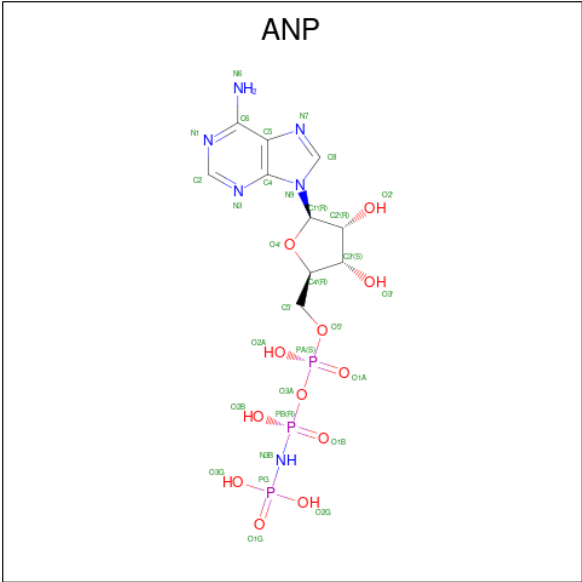
Mol	Chain	Residues	Atoms						AltConf	Trace
14	s	189	Total	C	H	N	O	S	0	0
			2940	910	1484	261	280	5		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						AltConf
15	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
15	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
15	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
15	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
15	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
15	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
15	G	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
15	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

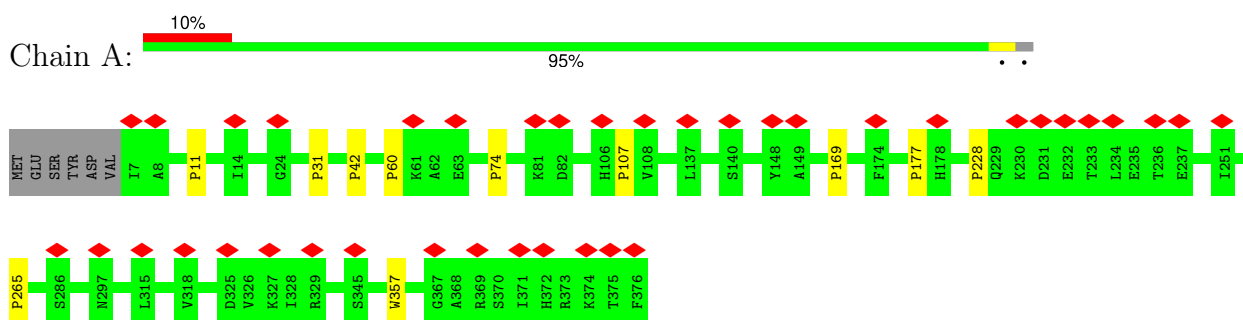
- Molecule 16 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



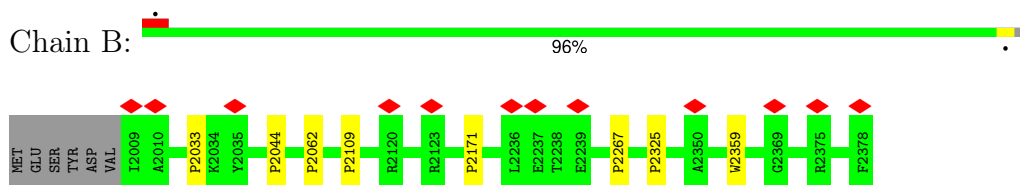
3 Residue-property plots [i](#)

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.

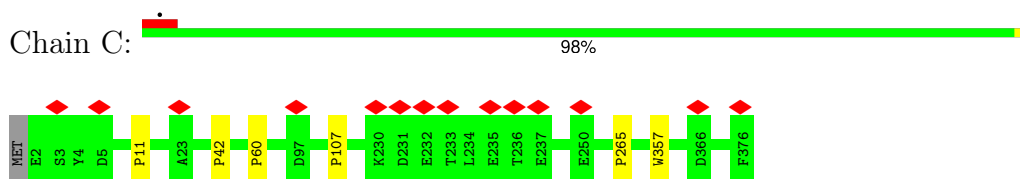
- Molecule 1: Alpha-centractin



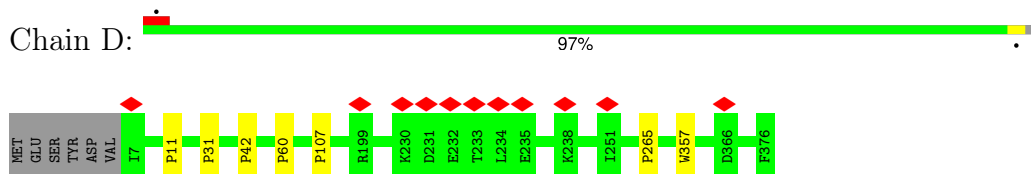
- Molecule 1: Alpha-centractin



- Molecule 1: Alpha-centractin

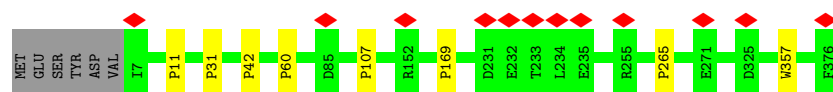


- Molecule 1: Alpha-centractin



- Molecule 1: Alpha-centractin

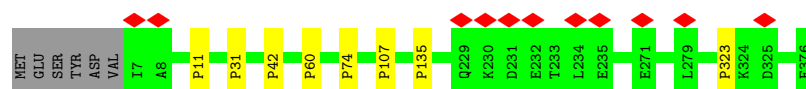




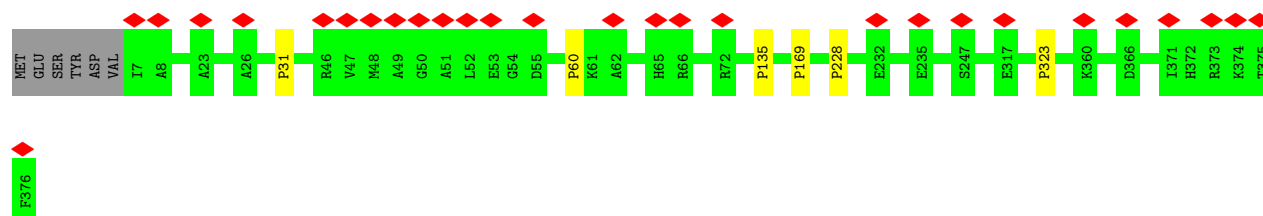
- Molecule 1: Alpha-centractin



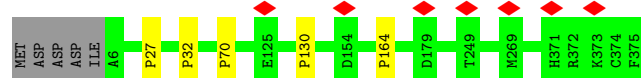
- Molecule 1: Alpha-centractin



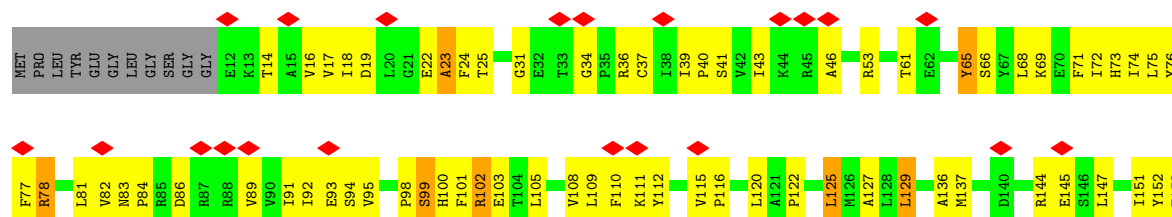
- Molecule 1: Alpha-centractin

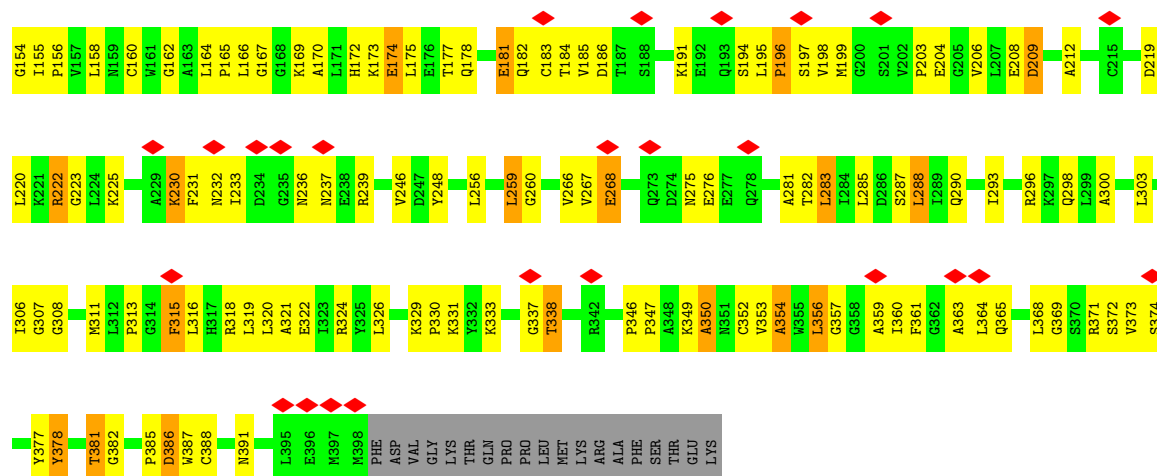


- Molecule 2: Actin, cytoplasmic 1

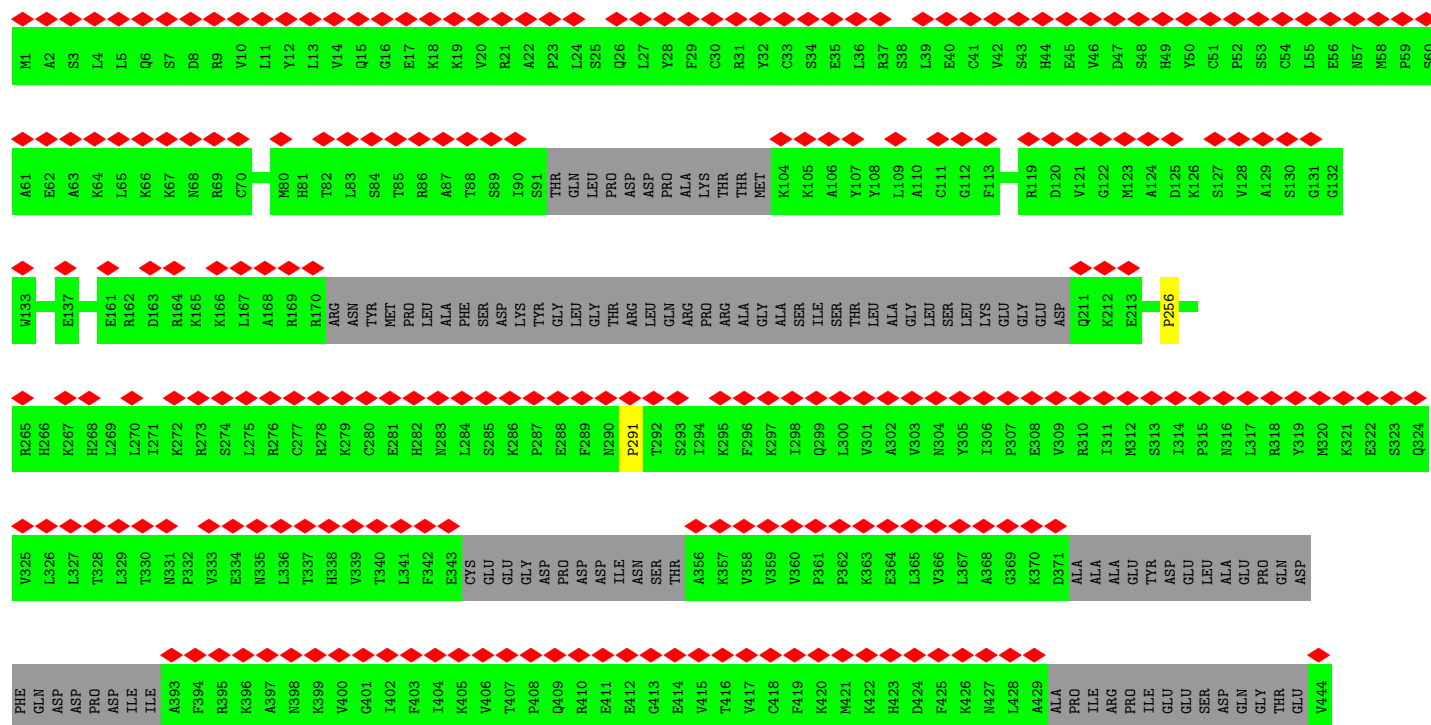
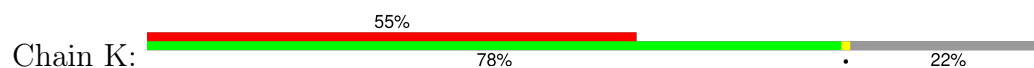


- Molecule 3: Actin-related protein 10

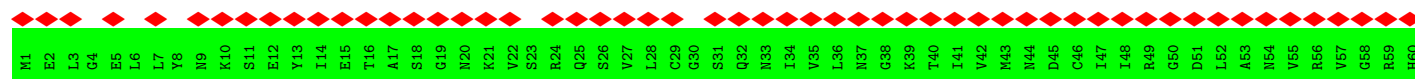
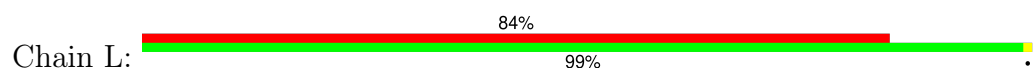


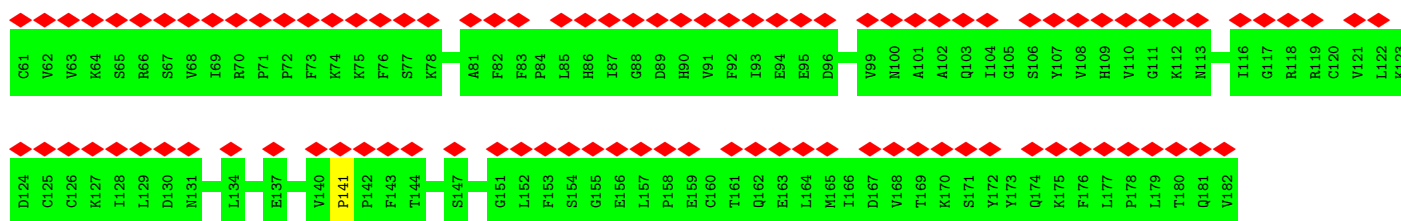


• Molecule 4: Dynactin subunit 4

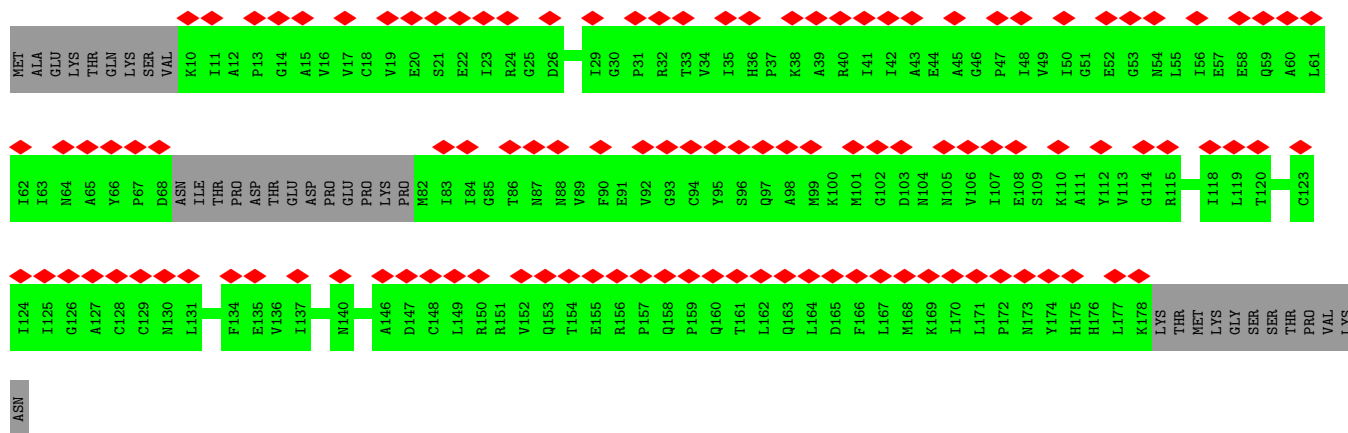
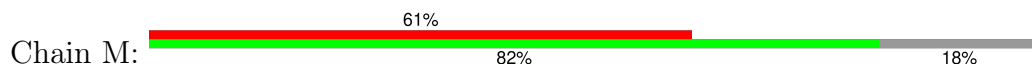


• Molecule 5: Dynactin subunit 5

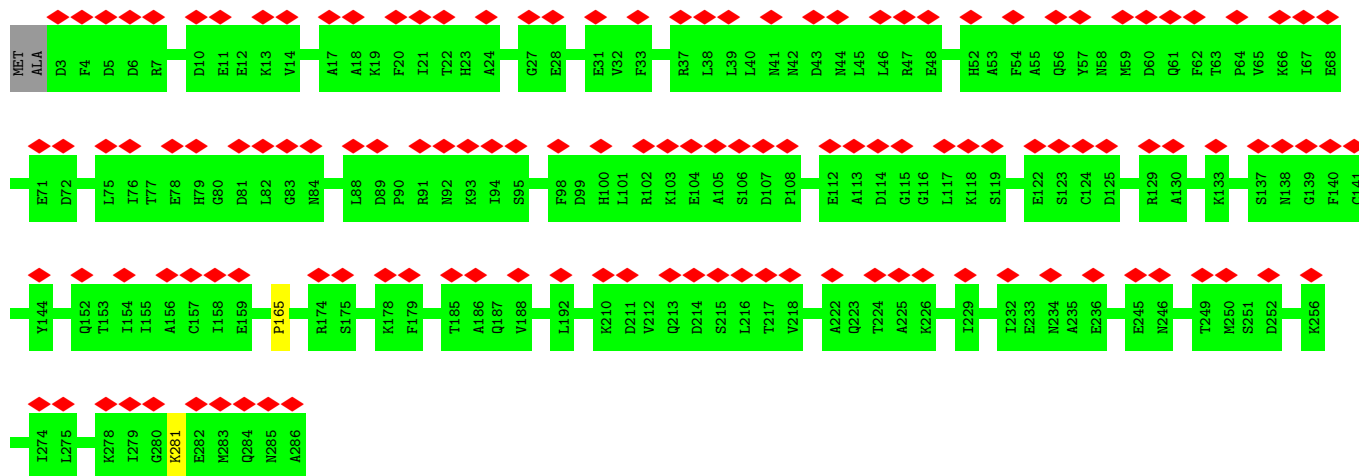




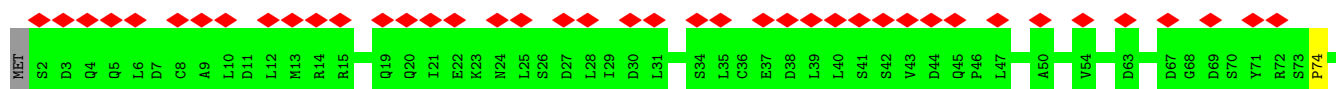
• Molecule 6: Dynactin subunit 6

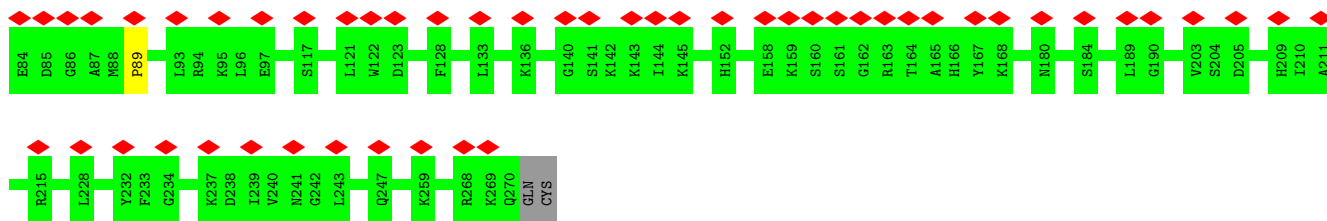


• Molecule 7: F-actin-capping protein subunit alpha-1

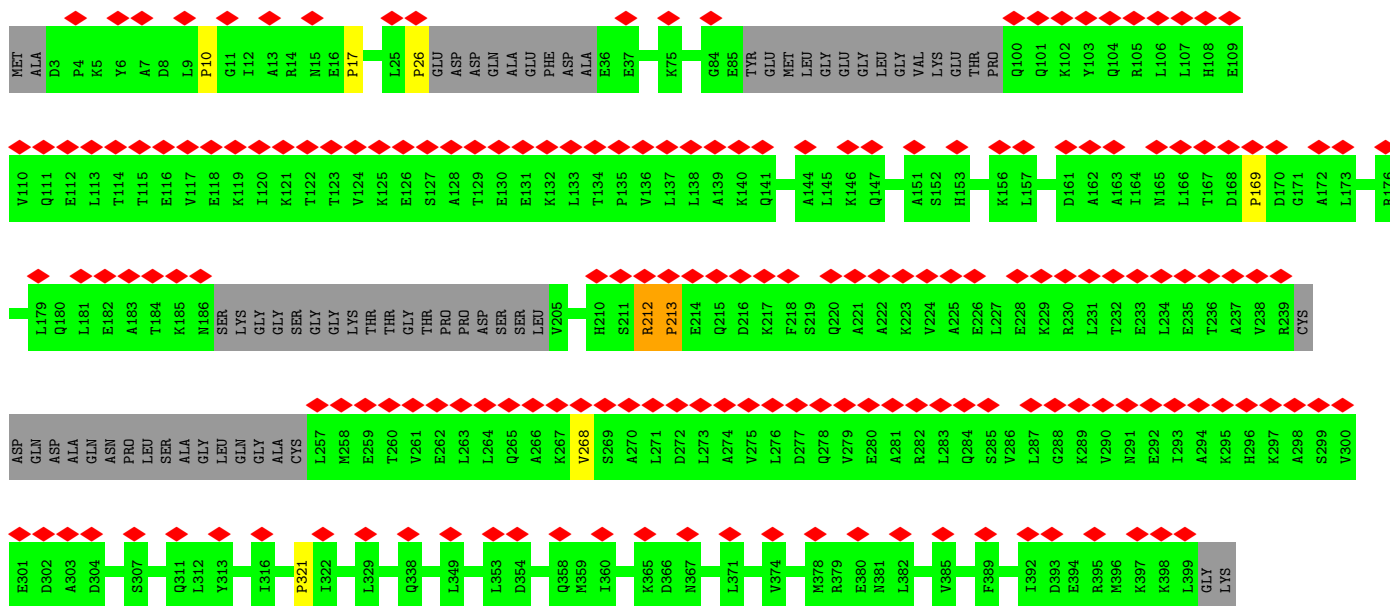
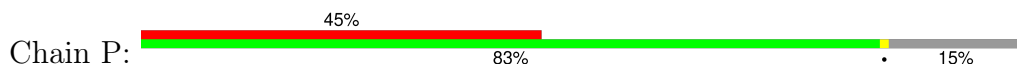


• Molecule 8: F-actin-capping protein subunit beta

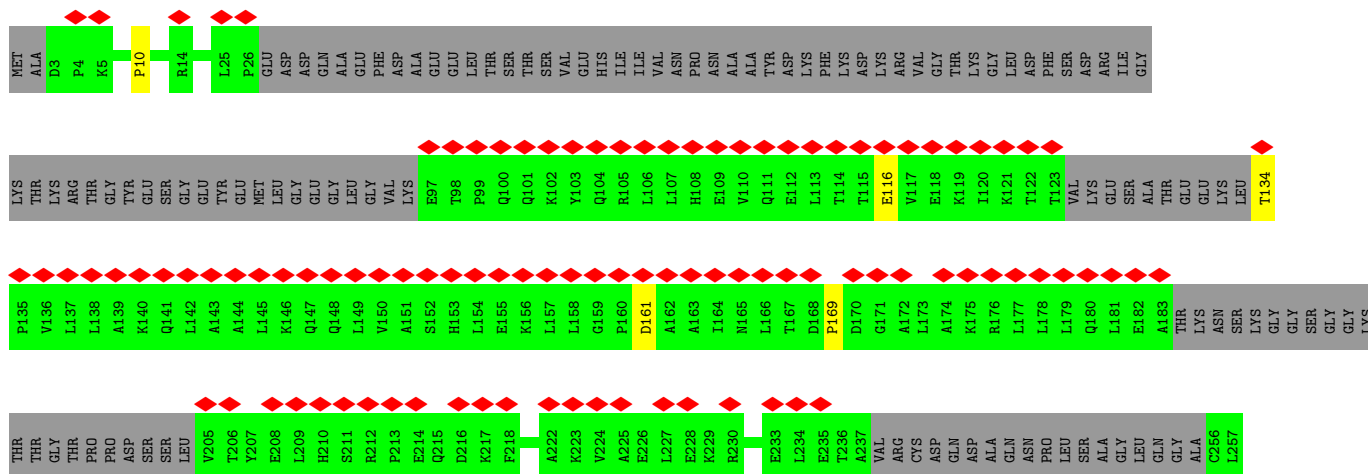




- Molecule 9: Dynactin subunit 2

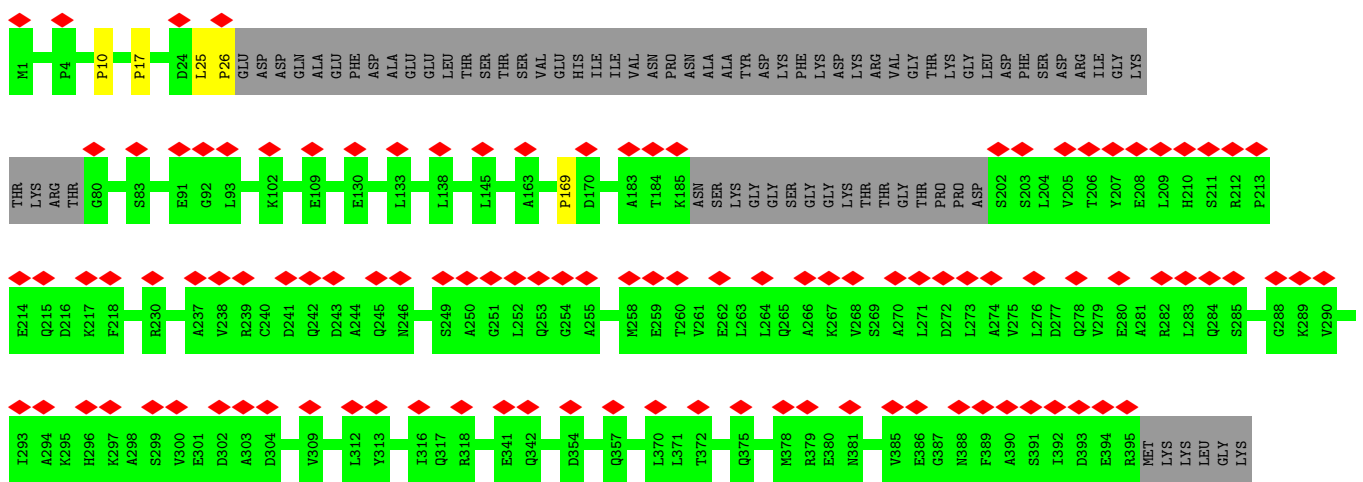
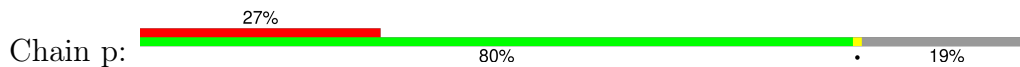


- Molecule 9: Dynactin subunit 2

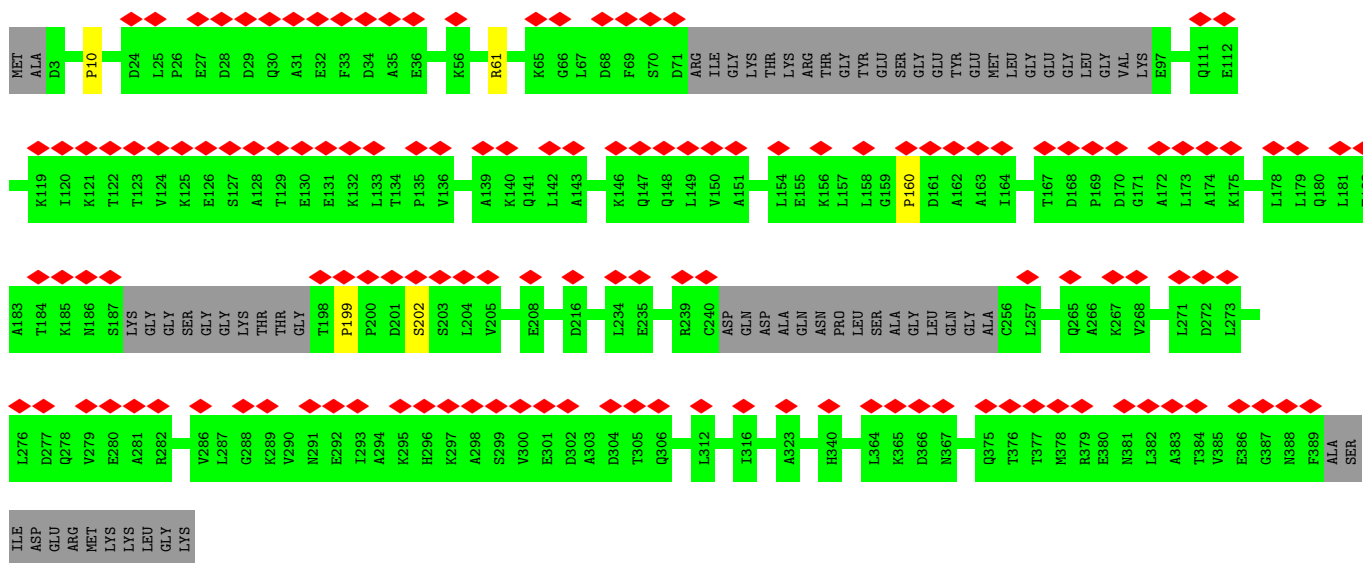
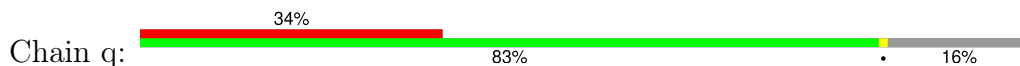




• Molecule 9: Dynactin subunit 2

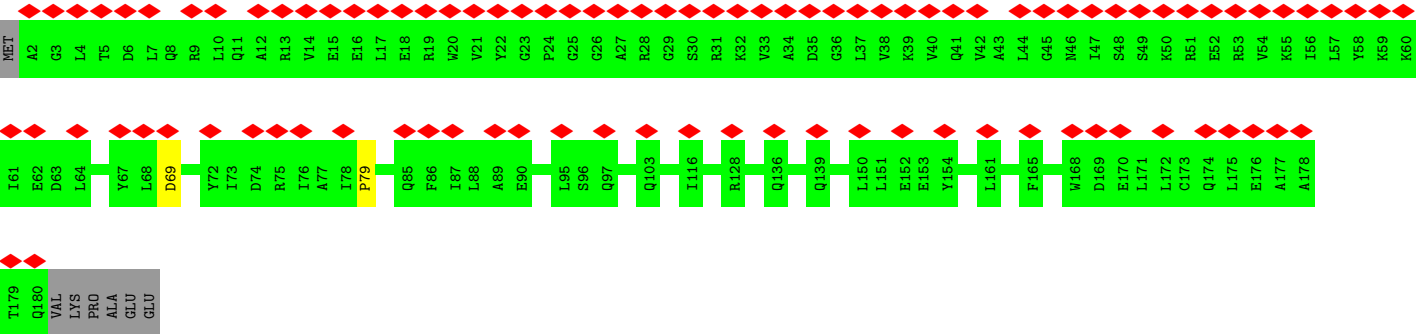


• Molecule 9: Dynactin subunit 2

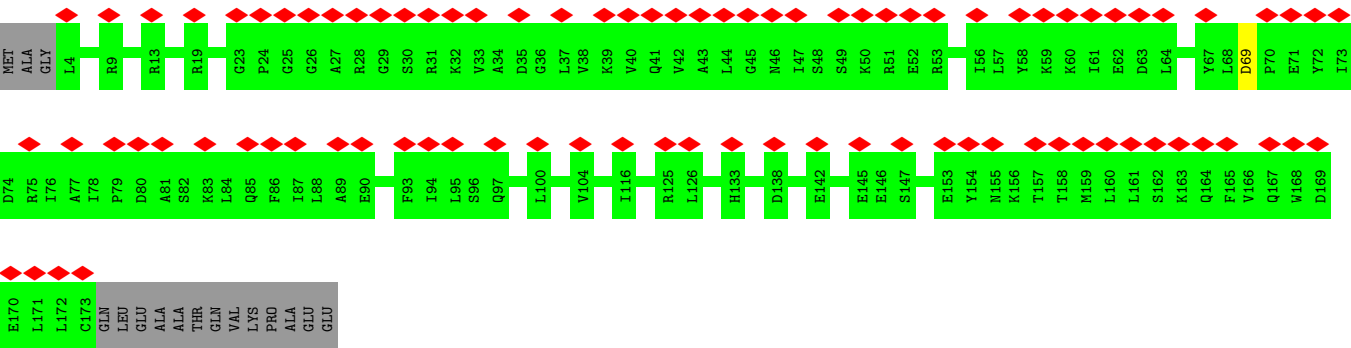
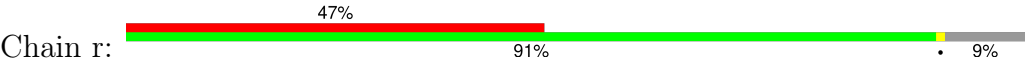


• Molecule 10: Dynactin subunit 3

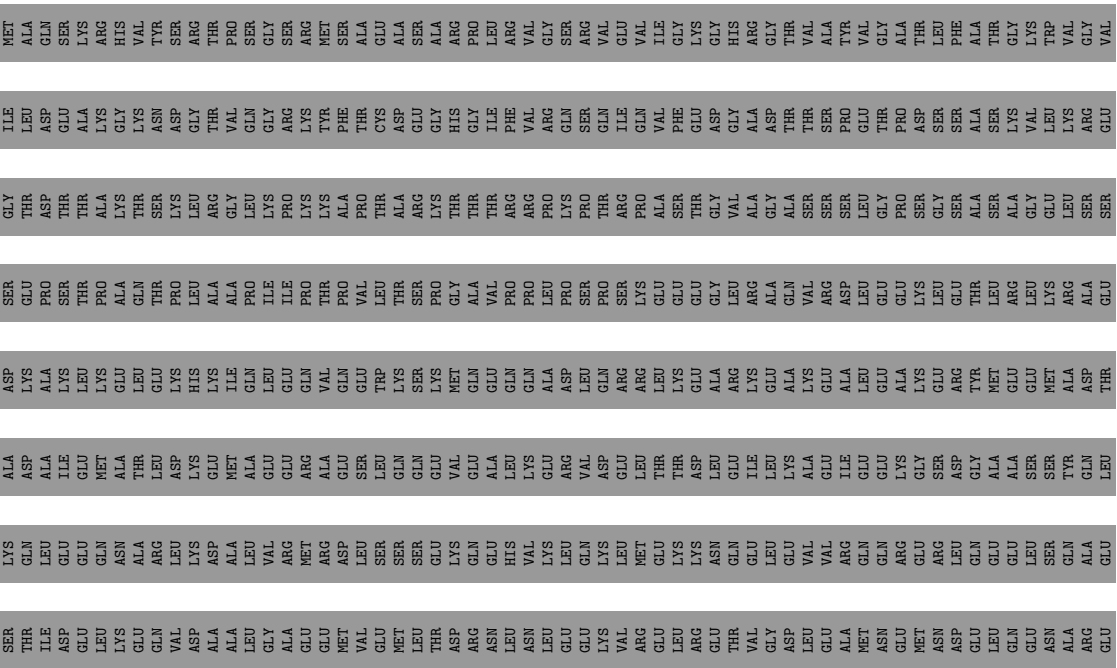


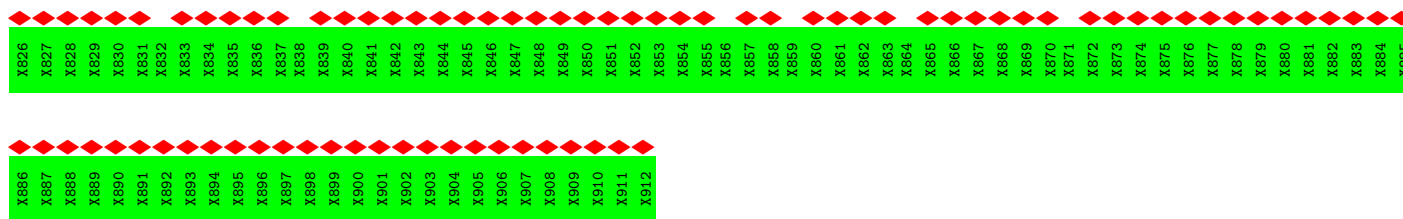


• Molecule 10: Dynactin subunit 3



• Molecule 11: Dynactin subunit 1





- Molecule 14: Dynactin subunit 1

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45091	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 ($e^-/\text{\AA}^2$)	57.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.993	Depositor
Minimum map value	-14.456	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.573	Depositor
Recommended contour level	6	Depositor
Map size (Å)	721.44, 721.44, 721.44	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, ADP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.01	10/3025 (0.3%)	0.74	0/4085
1	B	0.99	7/3025 (0.2%)	0.74	0/4085
1	C	1.00	5/3068 (0.2%)	0.74	0/4144
1	D	0.99	6/3025 (0.2%)	0.74	0/4085
1	E	0.99	7/3025 (0.2%)	0.74	0/4085
1	F	1.00	8/3025 (0.3%)	0.74	0/4085
1	G	1.01	8/3025 (0.3%)	0.74	0/4085
1	I	1.00	6/3025 (0.2%)	0.74	0/4085
2	H	0.98	5/2948 (0.2%)	0.75	0/3991
3	J	2.01	106/3088 (3.4%)	2.22	203/4188 (4.8%)
4	K	0.76	4/2970 (0.1%)	0.59	0/4005
5	L	0.71	1/1435 (0.1%)	0.60	0/1941
6	M	0.71	0/1209	0.64	0/1641
7	N	0.75	1/2363 (0.0%)	0.57	0/3197
8	O	0.95	2/2156 (0.1%)	0.75	0/2906
9	P	0.86	5/2700 (0.2%)	0.76	1/3646 (0.0%)
9	Q	0.85	2/2211 (0.1%)	0.80	5/2993 (0.2%)
9	p	0.85	4/2562 (0.2%)	0.74	0/3469
9	q	0.84	2/2675 (0.1%)	0.77	0/3626
10	R	0.84	1/1449 (0.1%)	0.83	0/1957
10	r	0.80	0/1388	0.75	0/1874
11	S	0.86	3/1229 (0.2%)	0.83	1/1660 (0.1%)
14	s	0.76	1/1481 (0.1%)	0.72	0/2005
All	All	1.01	194/56107 (0.3%)	0.88	210/75838 (0.3%)

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
3	J	0	29

The worst 5 of 194 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	102	ARG	N-CA	-11.59	1.23	1.46
3	J	330	PRO	N-CA	-10.70	1.29	1.47
3	J	206	VAL	CA-C	-9.83	1.27	1.52
3	J	318	ARG	CA-C	-9.20	1.29	1.52
9	P	213	PRO	N-CD	-9.09	1.35	1.47

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	144	ARG	O-C-N	27.02	165.94	122.70
3	J	196	PRO	C-N-CA	-23.71	62.42	121.70
3	J	144	ARG	CA-C-N	-20.73	71.60	117.20
3	J	308	GLY	C-N-CA	-13.14	88.85	121.70
3	J	356	LEU	C-N-CA	-12.52	96.00	122.30

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	53	ARG	Mainchain
3	J	65	TYR	Mainchain
3	J	78	ARG	Peptide,Mainchain
3	J	92	ILE	Mainchain
3	J	99	SER	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	B	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	C	373/376 (99%)	364 (98%)	9 (2%)	0	100	100
1	D	368/376 (98%)	358 (97%)	10 (3%)	0	100	100
1	E	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	F	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	G	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	I	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
2	H	368/375 (98%)	356 (97%)	12 (3%)	0	100	100
3	J	379/417 (91%)	358 (94%)	18 (5%)	3 (1%)	16	51
4	K	349/460 (76%)	343 (98%)	6 (2%)	0	100	100
5	L	180/182 (99%)	176 (98%)	4 (2%)	0	100	100
6	M	152/190 (80%)	144 (95%)	8 (5%)	0	100	100
7	N	282/286 (99%)	278 (99%)	4 (1%)	0	100	100
8	O	267/272 (98%)	260 (97%)	7 (3%)	0	100	100
9	P	329/401 (82%)	312 (95%)	13 (4%)	4 (1%)	11	43
9	Q	268/401 (67%)	261 (97%)	6 (2%)	1 (0%)	30	64
9	p	320/401 (80%)	309 (97%)	10 (3%)	1 (0%)	37	68
9	q	329/401 (82%)	309 (94%)	18 (6%)	2 (1%)	22	56
10	R	177/186 (95%)	167 (94%)	9 (5%)	1 (1%)	22	56
10	r	168/186 (90%)	163 (97%)	4 (2%)	1 (1%)	22	56
11	S	146/1278 (11%)	140 (96%)	6 (4%)	0	100	100
14	s	187/1278 (15%)	180 (96%)	6 (3%)	1 (0%)	25	59
All	All	6850/9722 (70%)	6617 (97%)	219 (3%)	14 (0%)	45	75

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	283	LEU
9	P	213	PRO
9	p	25	LEU
9	q	202	SER

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Mol	Chain	Res	Type
9	Q	161	ASP

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	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	B	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	C	323/324 (100%)	322 (100%)	1 (0%)	91	96
1	D	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	E	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	F	318/324 (98%)	317 (100%)	1 (0%)	91	96
1	G	318/324 (98%)	318 (100%)	0	100	100
1	I	318/324 (98%)	318 (100%)	0	100	100
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	339/363 (93%)	338 (100%)	1 (0%)	91	96
4	K	330/412 (80%)	330 (100%)	0	100	100
5	L	163/163 (100%)	163 (100%)	0	100	100
6	M	132/164 (80%)	132 (100%)	0	100	100
7	N	251/252 (100%)	250 (100%)	1 (0%)	89	95
8	O	238/241 (99%)	238 (100%)	0	100	100
9	P	298/343 (87%)	298 (100%)	0	100	100
9	Q	245/343 (71%)	244 (100%)	1 (0%)	89	95
9	p	281/343 (82%)	281 (100%)	0	100	100
9	q	298/343 (87%)	297 (100%)	1 (0%)	91	96
10	R	154/160 (96%)	154 (100%)	0	100	100
10	r	149/160 (93%)	149 (100%)	0	100	100
11	S	137/1080 (13%)	137 (100%)	0	100	100
14	s	164/1080 (15%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6041/8357 (72%)	6031 (100%)	10 (0%)	91	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	N	281	LYS
9	Q	318	ARG
9	q	61	ARG
1	D	357	TRP
1	E	357	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
9	P	375	GLN
9	Q	278	GLN
14	s	1184	GLN
11	S	1161	GLN
7	N	203	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 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	$\# Z > 2$
15	ADP	D	800	-	24,29,29	0.74	0	29,45,45	0.71	1 (3%)
15	ADP	E	800	-	24,29,29	0.73	0	29,45,45	0.69	1 (3%)
15	ADP	F	800	-	24,29,29	0.72	0	29,45,45	0.70	1 (3%)
15	ADP	B	2401	-	24,29,29	0.74	0	29,45,45	0.70	1 (3%)
16	ANP	H	401	-	29,33,33	1.74	6 (20%)	31,52,52	1.57	7 (22%)
15	ADP	C	800	-	24,29,29	0.76	0	29,45,45	0.71	1 (3%)
15	ADP	G	800	-	24,29,29	0.71	0	29,45,45	0.70	1 (3%)
15	ADP	A	800	-	24,29,29	0.73	0	29,45,45	0.71	1 (3%)
15	ADP	I	800	-	24,29,29	0.71	0	29,45,45	0.73	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	D	800	-	-	4/12/32/32	0/3/3/3
15	ADP	E	800	-	-	4/12/32/32	0/3/3/3
15	ADP	F	800	-	-	4/12/32/32	0/3/3/3
15	ADP	B	2401	-	-	3/12/32/32	0/3/3/3
16	ANP	H	401	-	-	6/14/38/38	0/3/3/3
15	ADP	C	800	-	-	4/12/32/32	0/3/3/3
15	ADP	G	800	-	-	4/12/32/32	0/3/3/3
15	ADP	A	800	-	-	7/12/32/32	0/3/3/3
15	ADP	I	800	-	-	4/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	401	ANP	PG-N3B	4.37	1.74	1.63
16	H	401	ANP	PG-O1G	3.96	1.52	1.46
16	H	401	ANP	PB-N3B	3.56	1.72	1.63
16	H	401	ANP	PB-O1B	3.39	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	401	ANP	PB-O2B	-2.38	1.50	1.56

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	401	ANP	N3-C2-N1	-4.09	123.12	128.67
16	H	401	ANP	O1B-PB-N3B	-3.47	106.67	111.77
16	H	401	ANP	O1G-PG-N3B	-2.76	107.71	111.77
16	H	401	ANP	O2B-PB-O1B	2.65	115.55	109.87
16	H	401	ANP	O2A-PA-O1A	2.64	124.73	112.44

There are no chirality outliers.

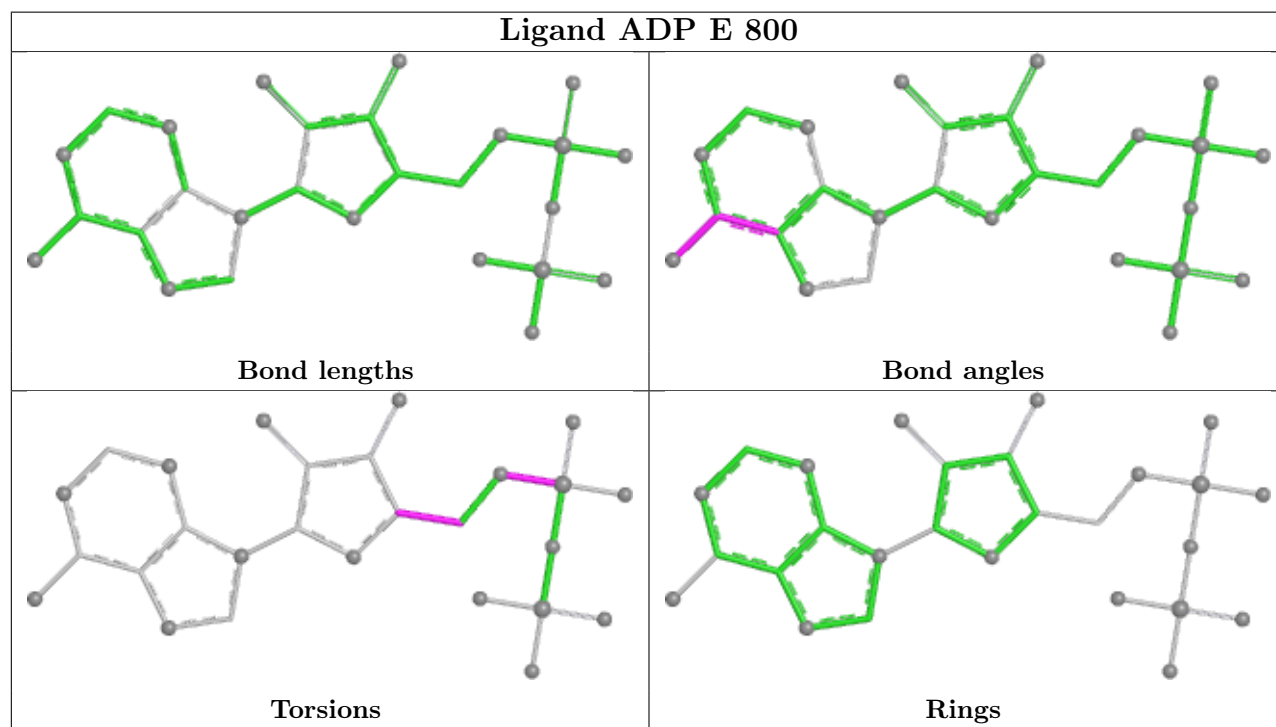
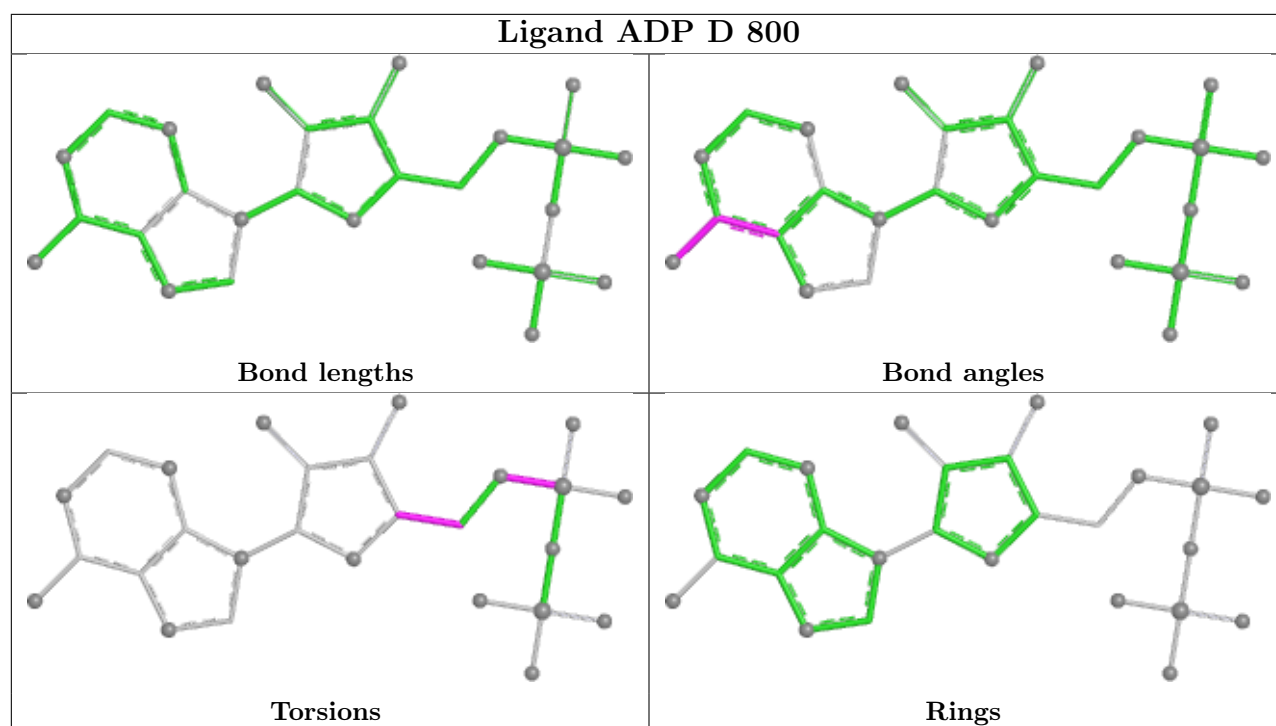
5 of 40 torsion outliers are listed below:

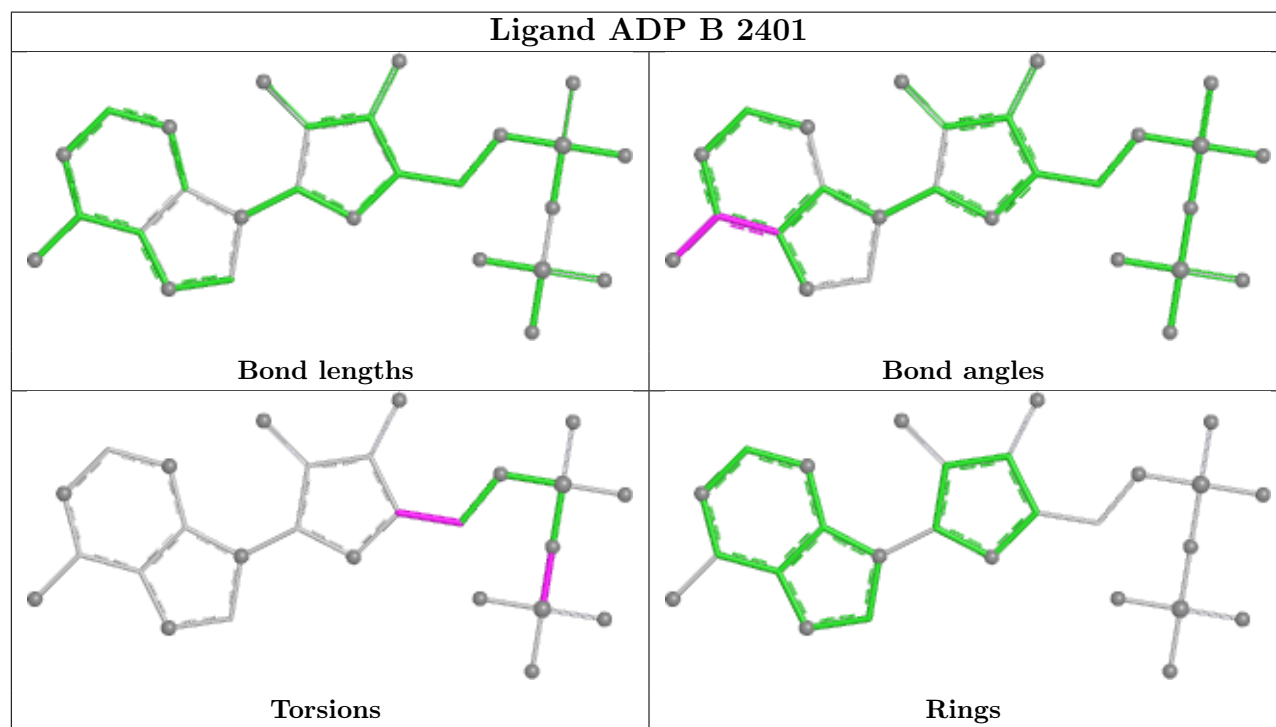
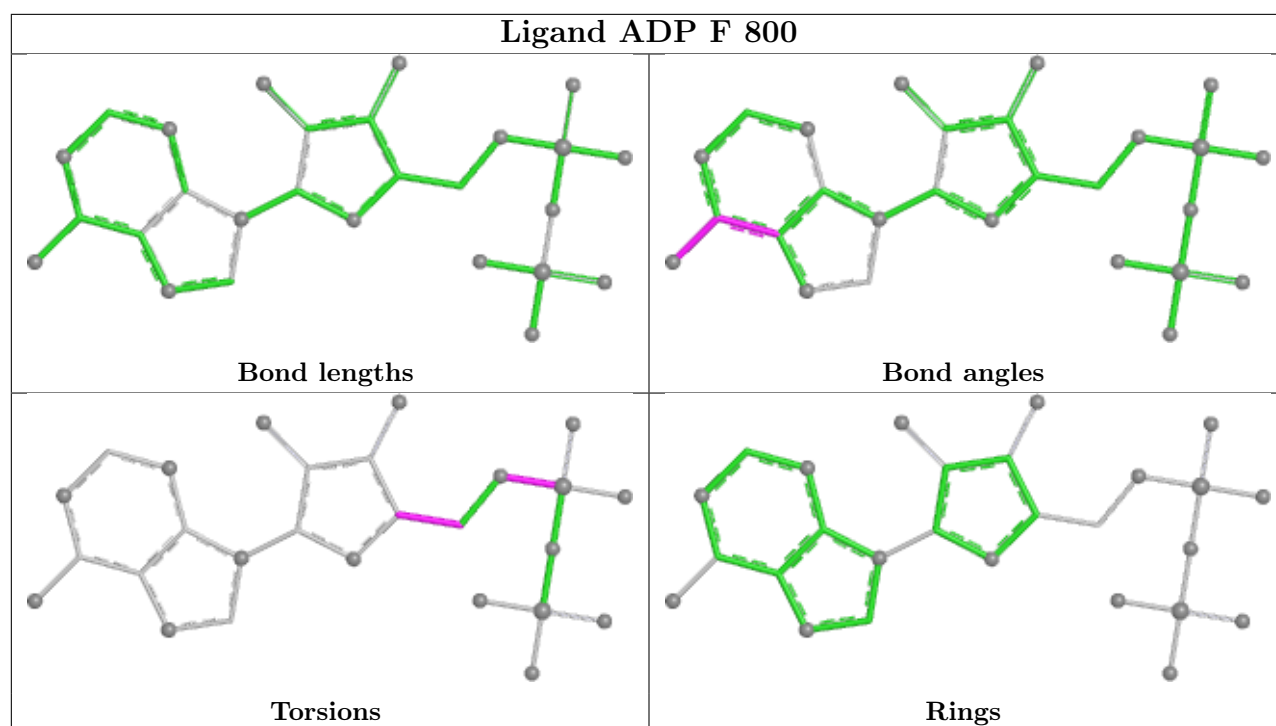
Mol	Chain	Res	Type	Atoms
15	A	800	ADP	PA-O3A-PB-O2B
15	A	800	ADP	PA-O3A-PB-O3B
15	A	800	ADP	C5'-O5'-PA-O1A
15	C	800	ADP	C5'-O5'-PA-O1A
15	C	800	ADP	C5'-O5'-PA-O3A

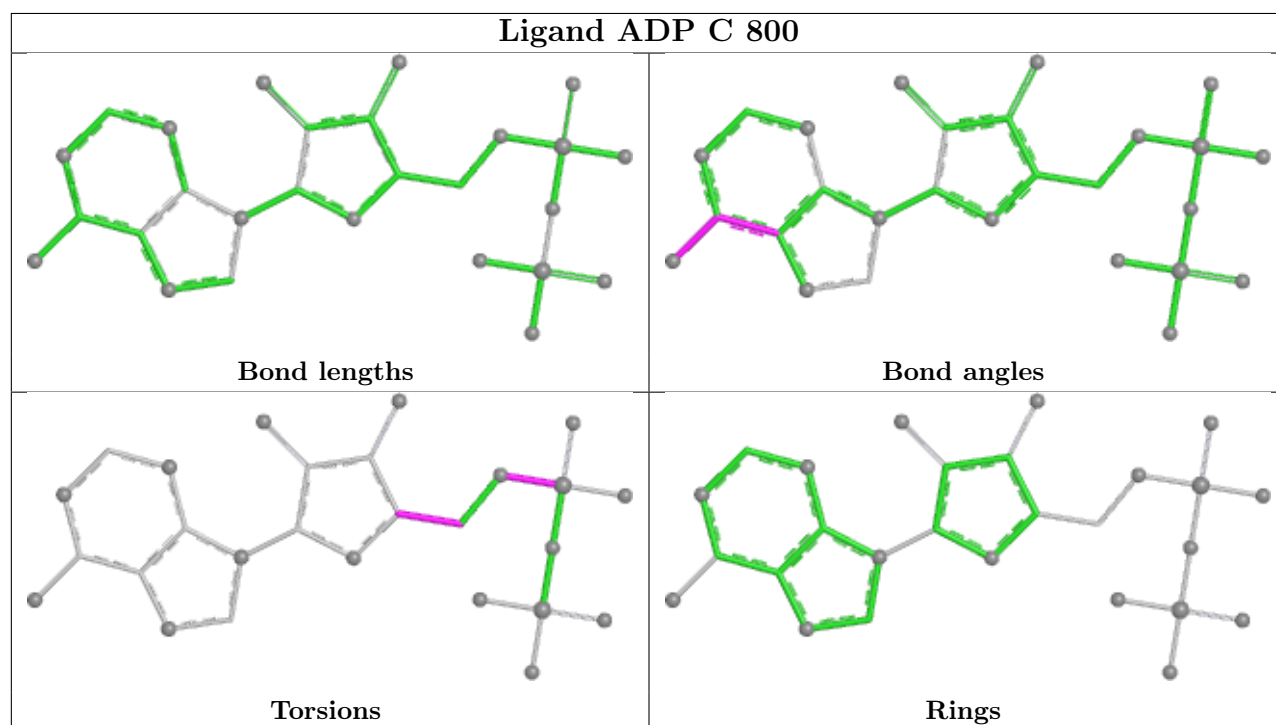
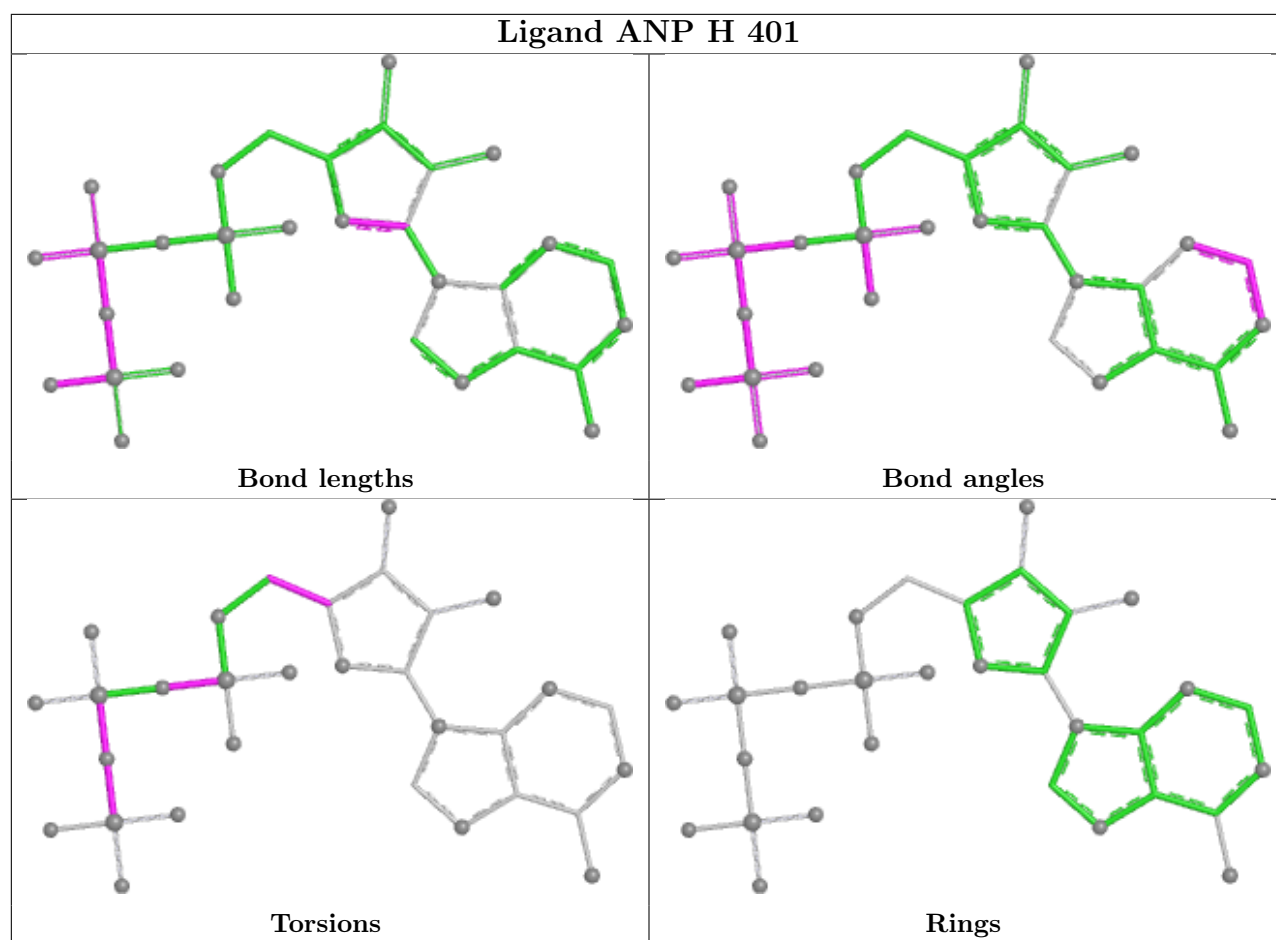
There are no ring outliers.

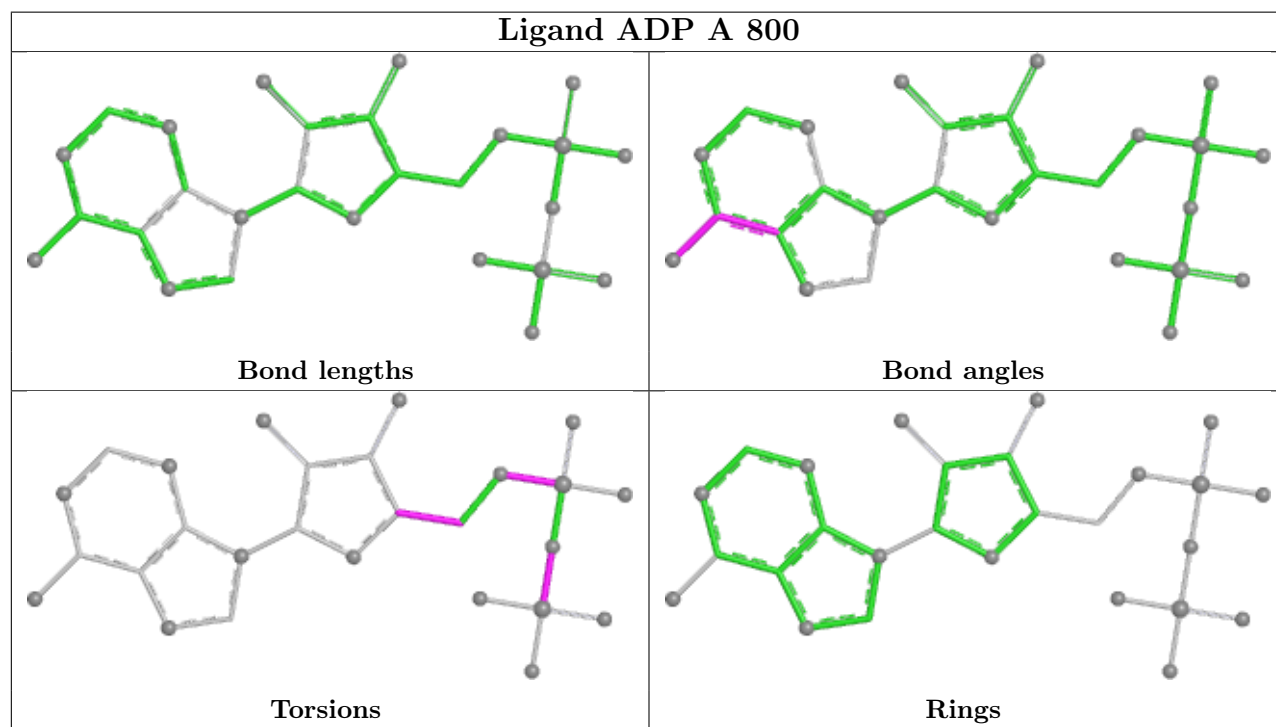
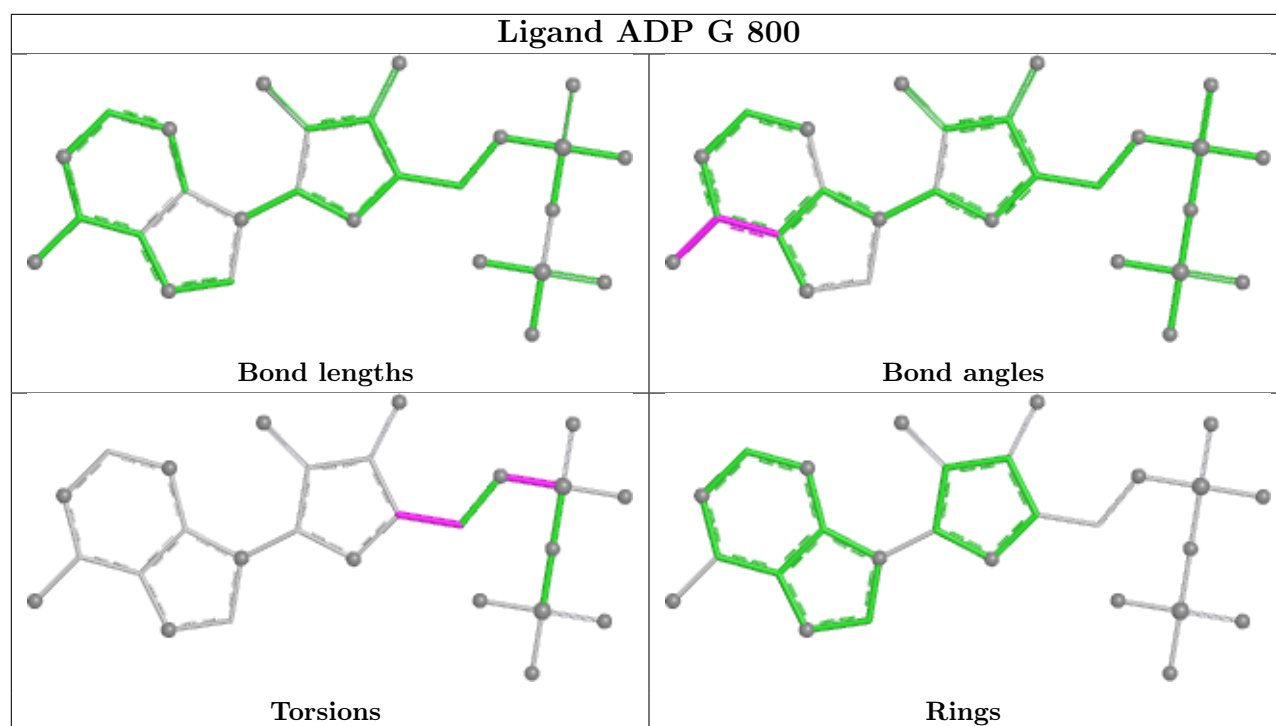
No monomer is involved in short contacts.

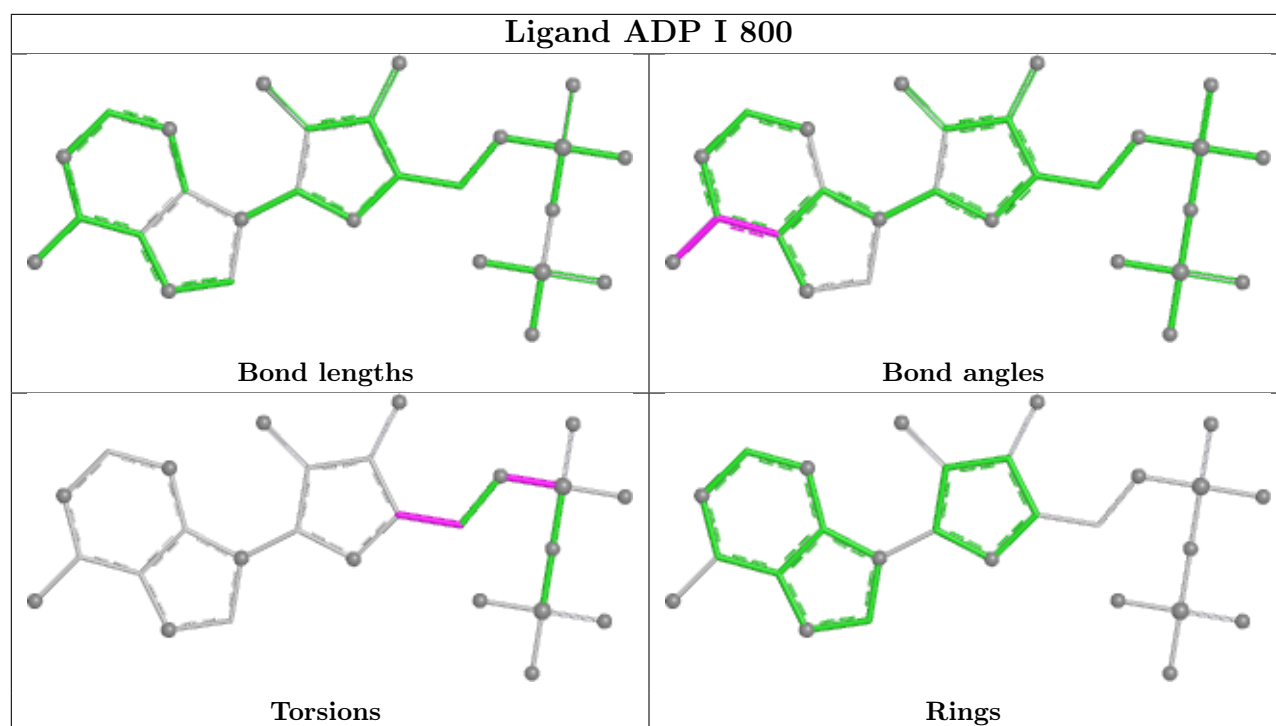
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	9
11	S	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	1243:VAL	C	1252:TYR	N	35.42
1	J	94:SER	C	95:VAL	N	3.81
1	J	116:PRO	C	117:SER	N	2.93
1	J	55:VAL	C	56:GLN	N	2.79
1	J	89:VAL	C	90:VAL	N	1.20

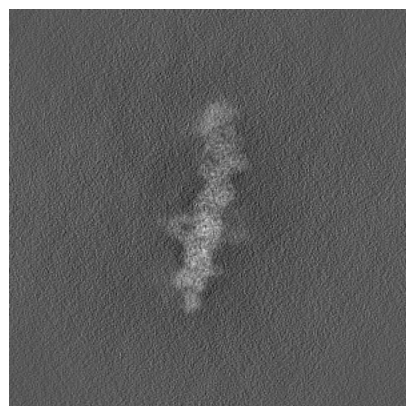
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44306. These allow visual inspection of the internal detail of the map and identification of artifacts.

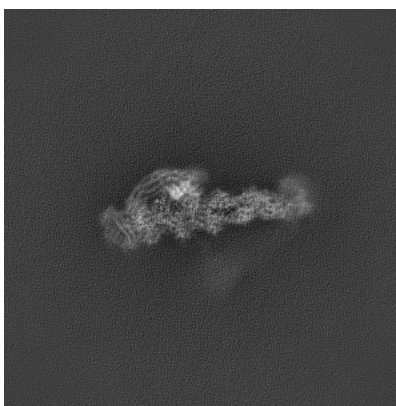
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

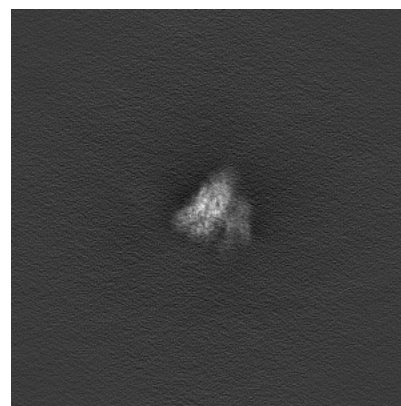
6.1.1 Primary map



X

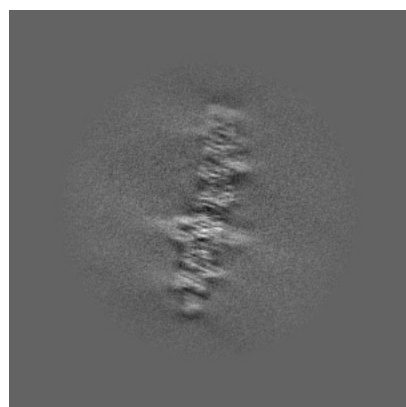


Y

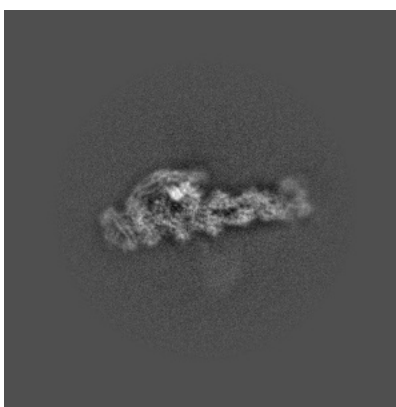


Z

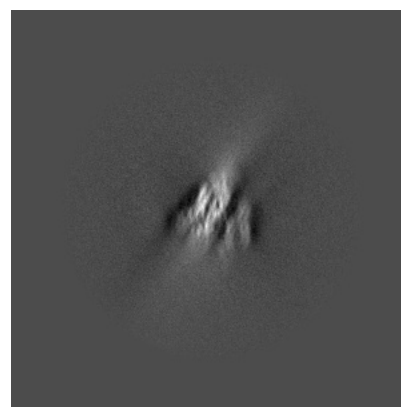
6.1.2 Raw map



X



Y

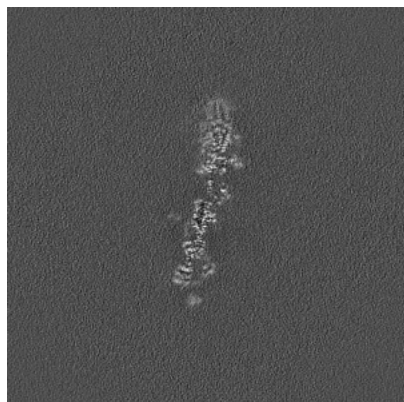


Z

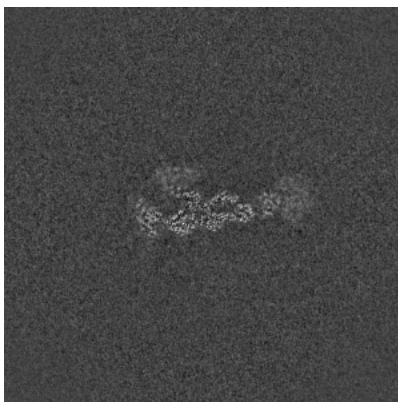
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 432

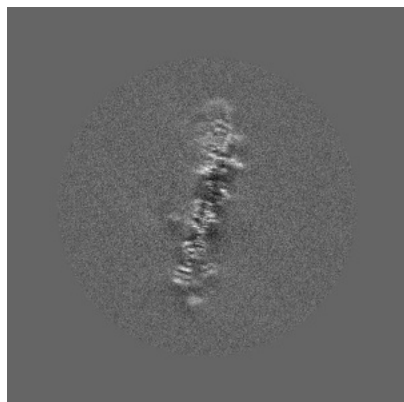


Y Index: 432

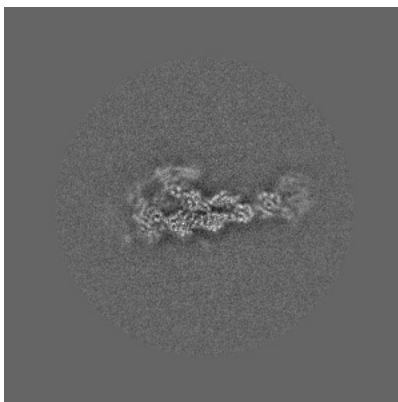


Z Index: 432

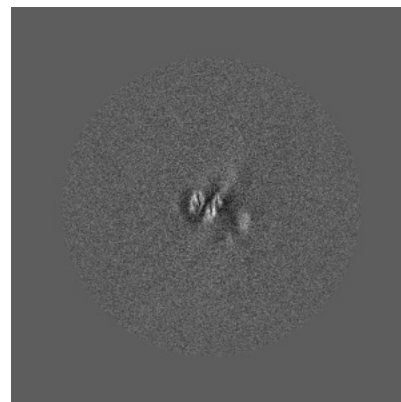
6.2.2 Raw map



X Index: 432



Y Index: 432

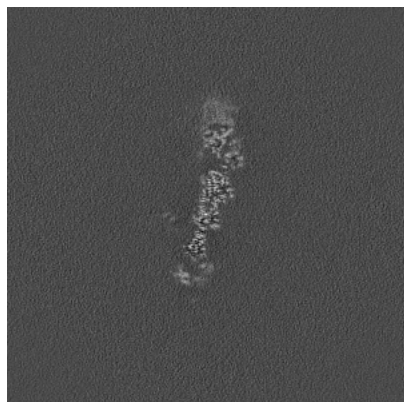


Z Index: 432

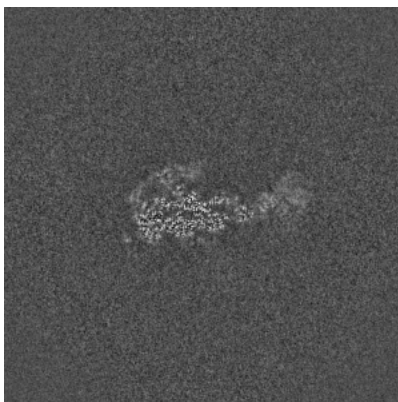
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

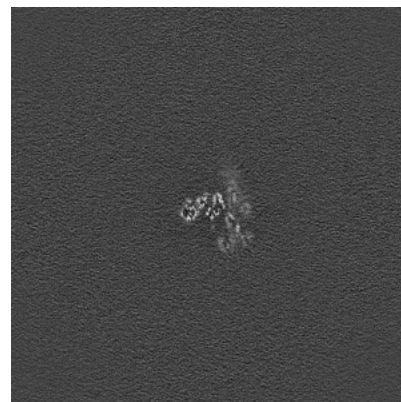
6.3.1 Primary map



X Index: 441

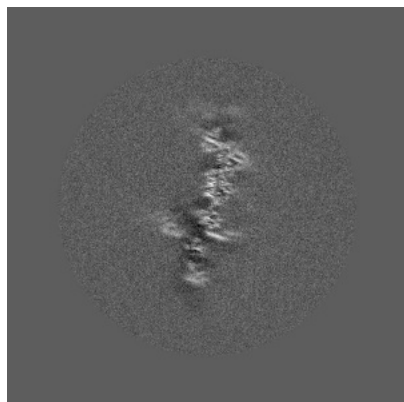


Y Index: 426

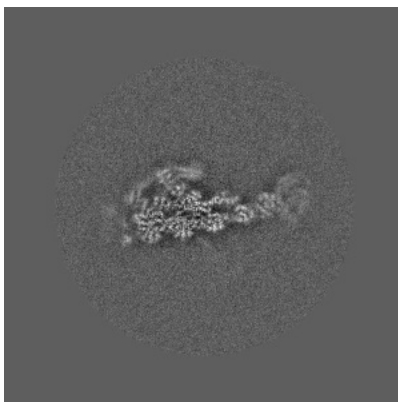


Z Index: 392

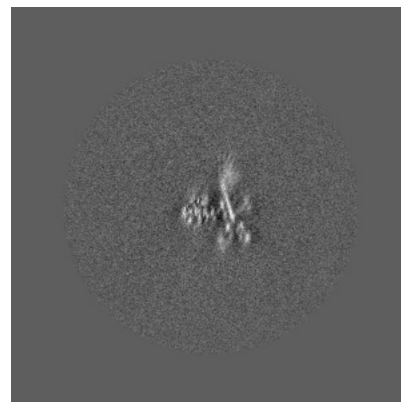
6.3.2 Raw map



X Index: 454



Y Index: 426

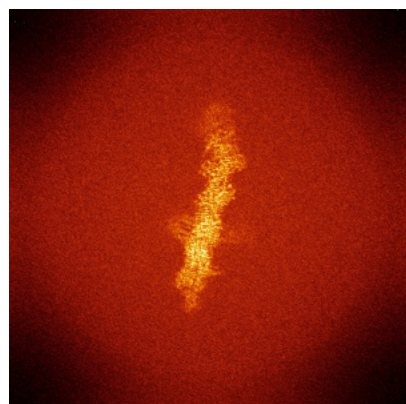


Z Index: 376

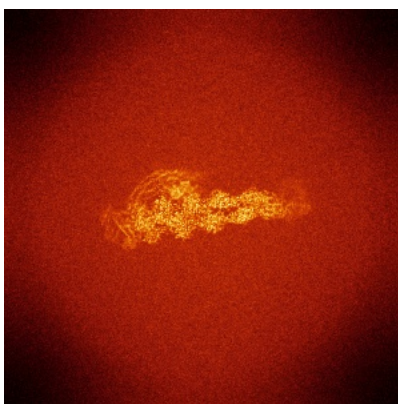
The images above show the largest variance slices of the map in three orthogonal directions.

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

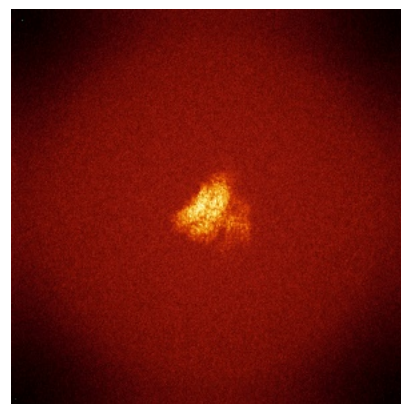
6.4.1 Primary map



X

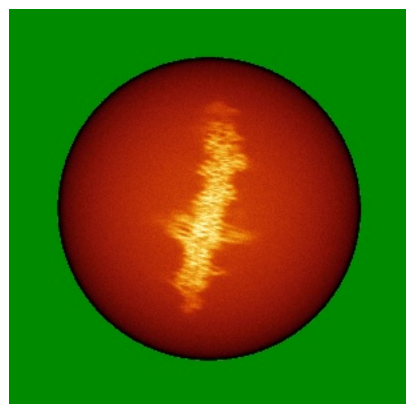


Y

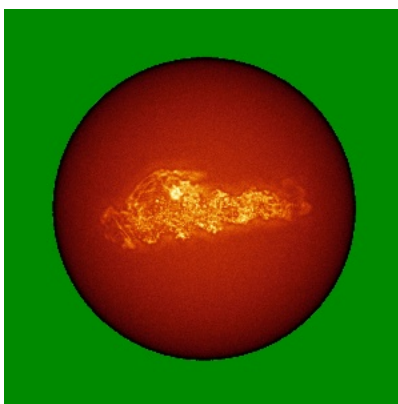


Z

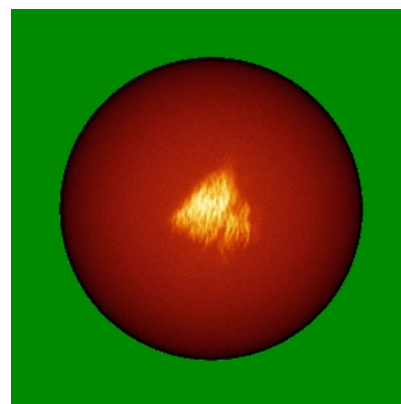
6.4.2 Raw map



X



Y

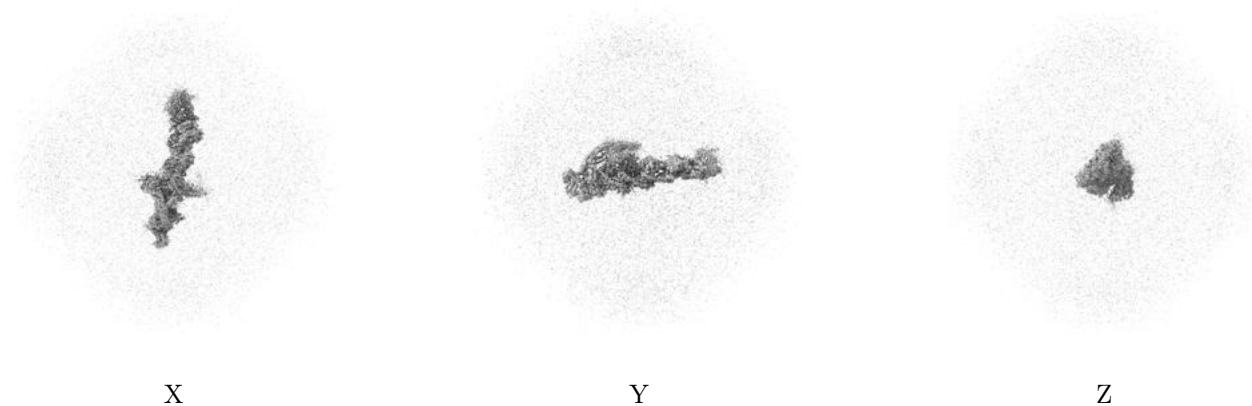


Z

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 6.0. 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.

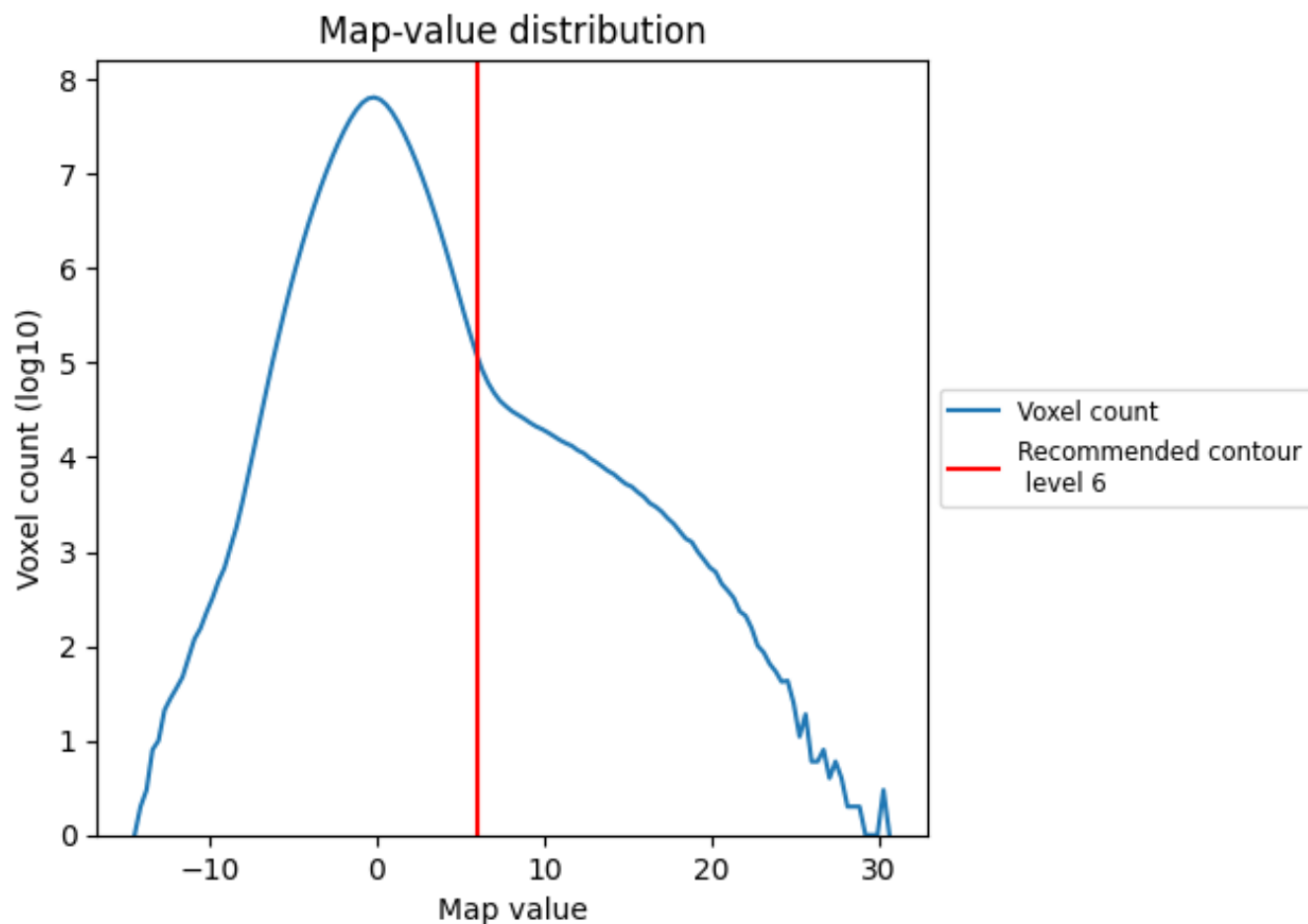
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

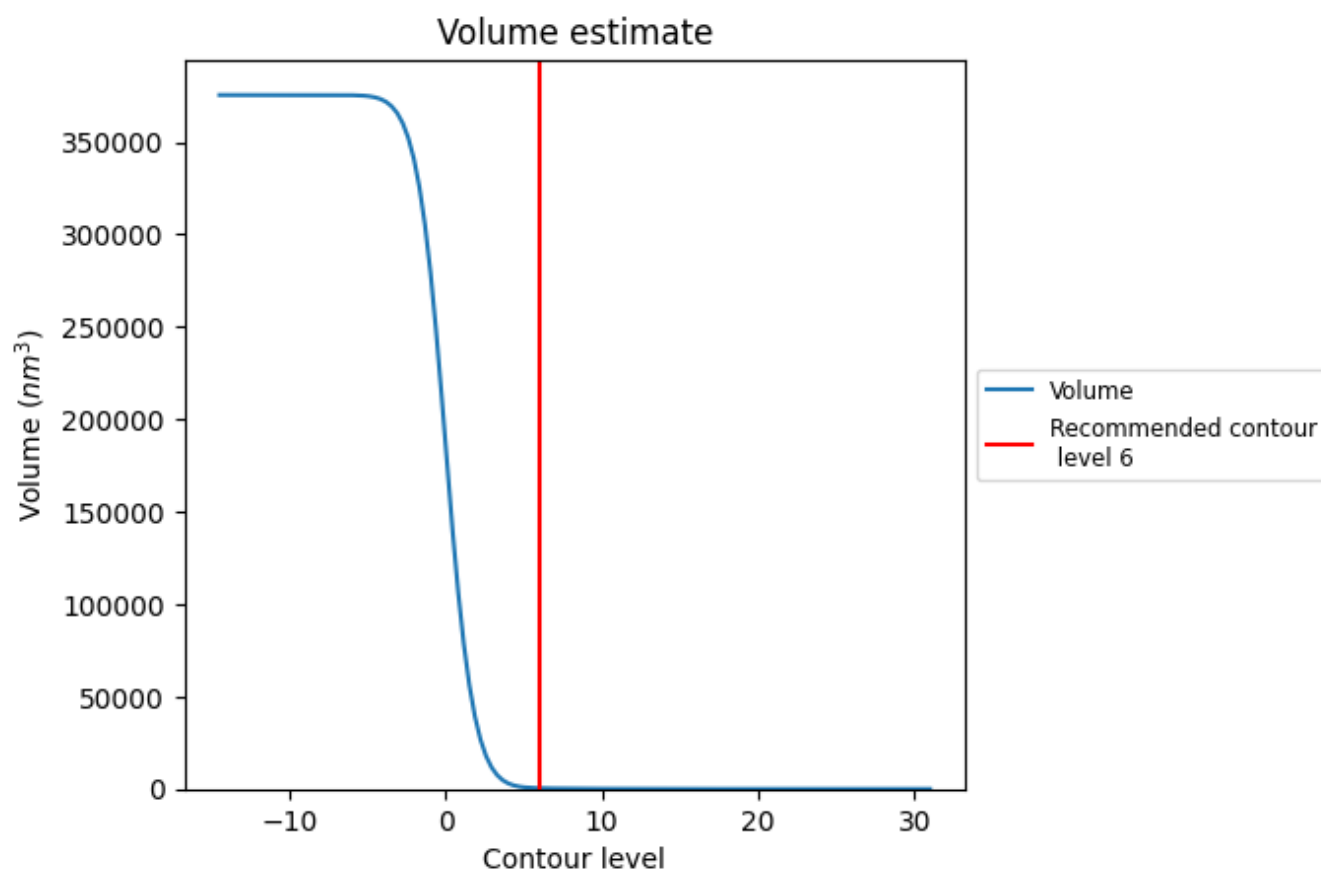
This section contains the results of statistical analysis of the map.

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.

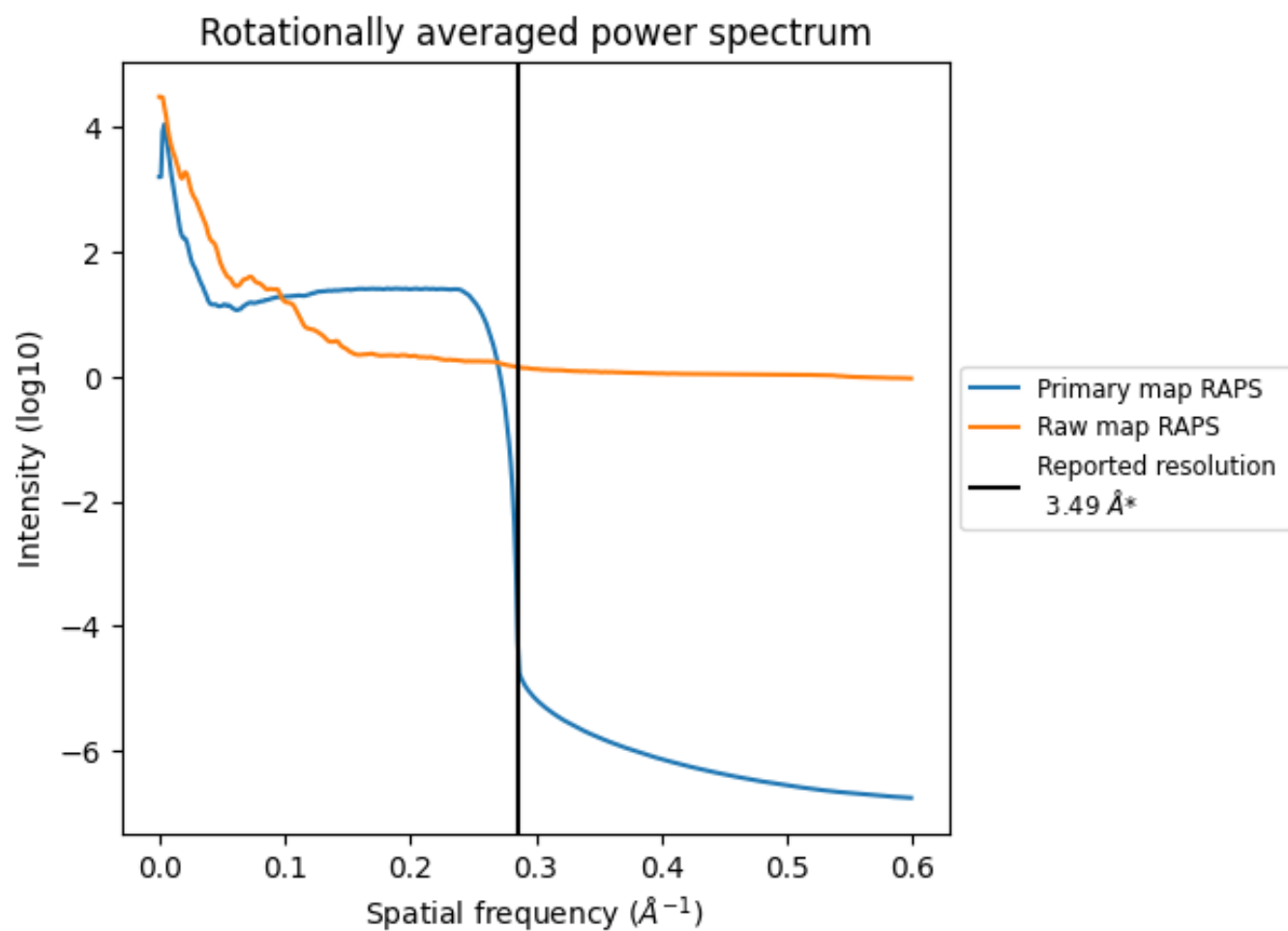
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 417 nm³; this corresponds to an approximate mass of 376 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 ⓘ

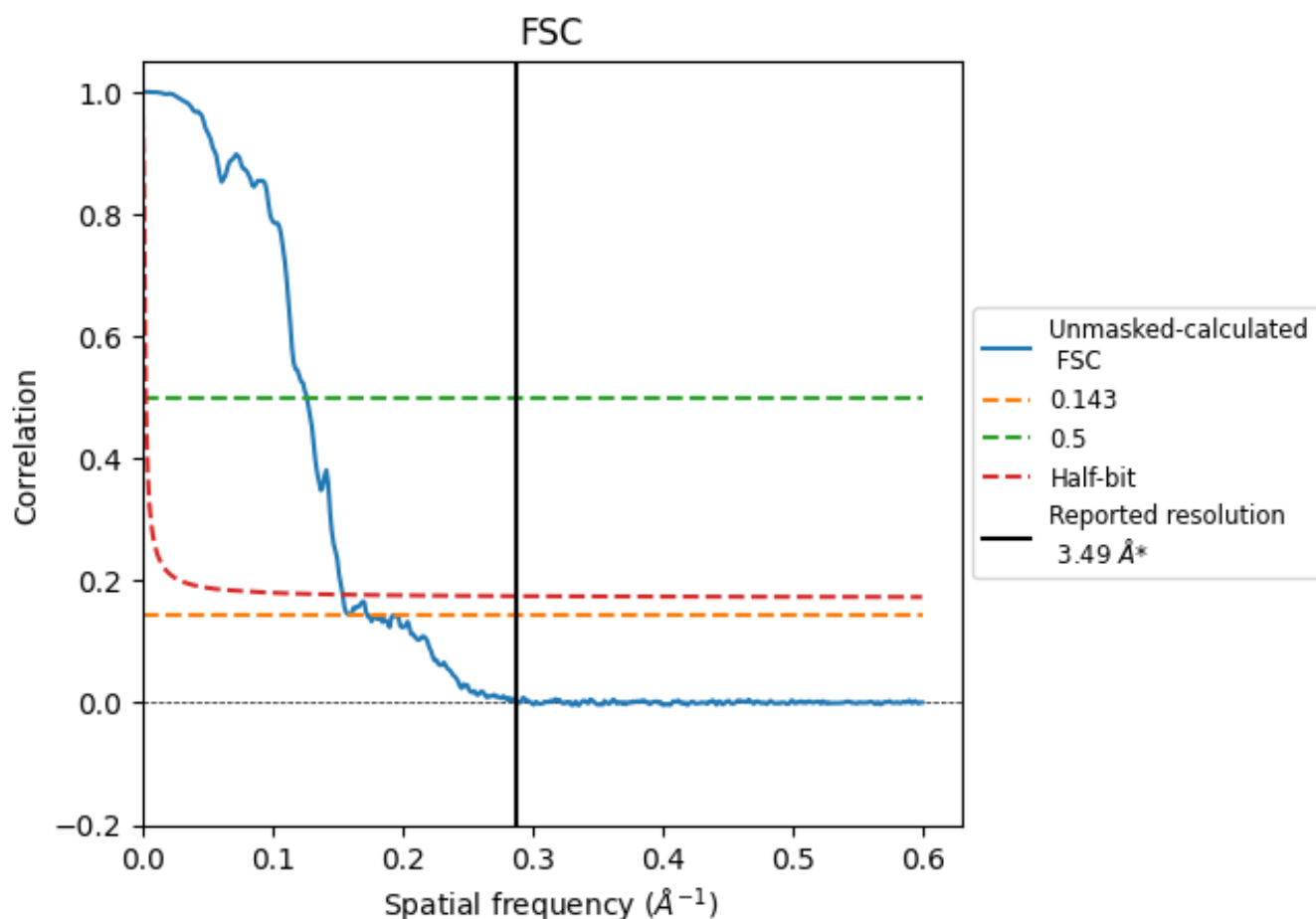


*Reported resolution corresponds to spatial frequency of 0.287 \AA^{-1}

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 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

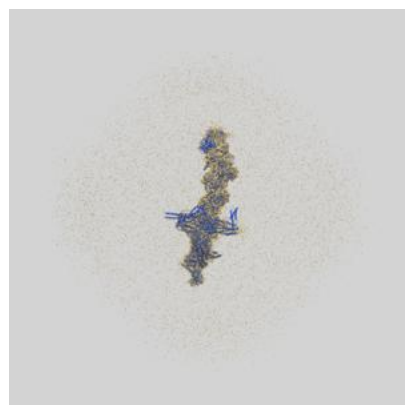
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.79	7.91	6.50

*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 5.79 differs from the reported value 3.49 by more than 10 %

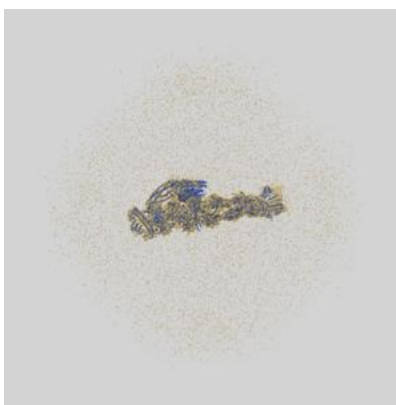
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44306 and PDB model 9B7J. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

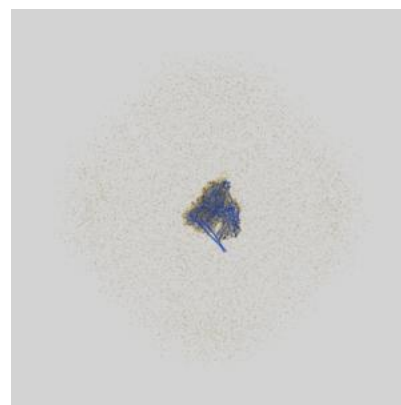
9.1 Map-model overlay [i](#)



X



Y



Z

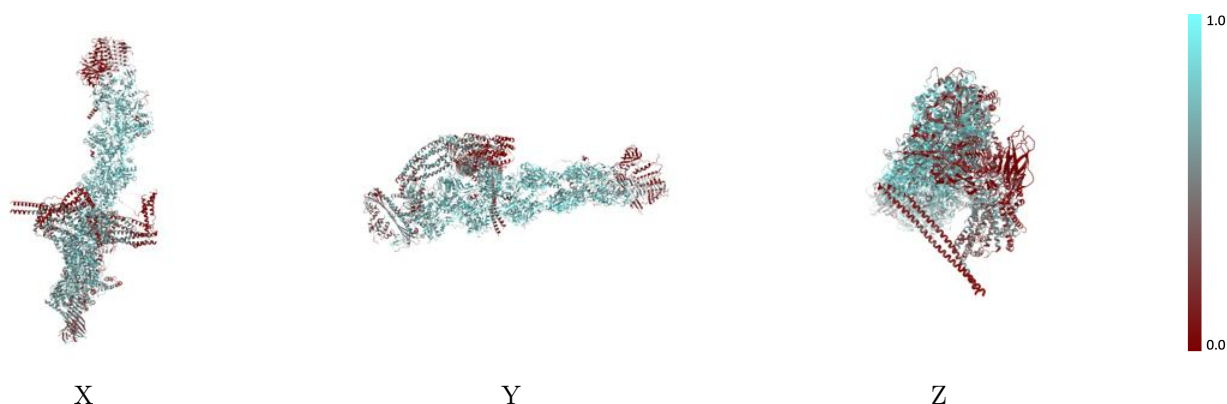
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



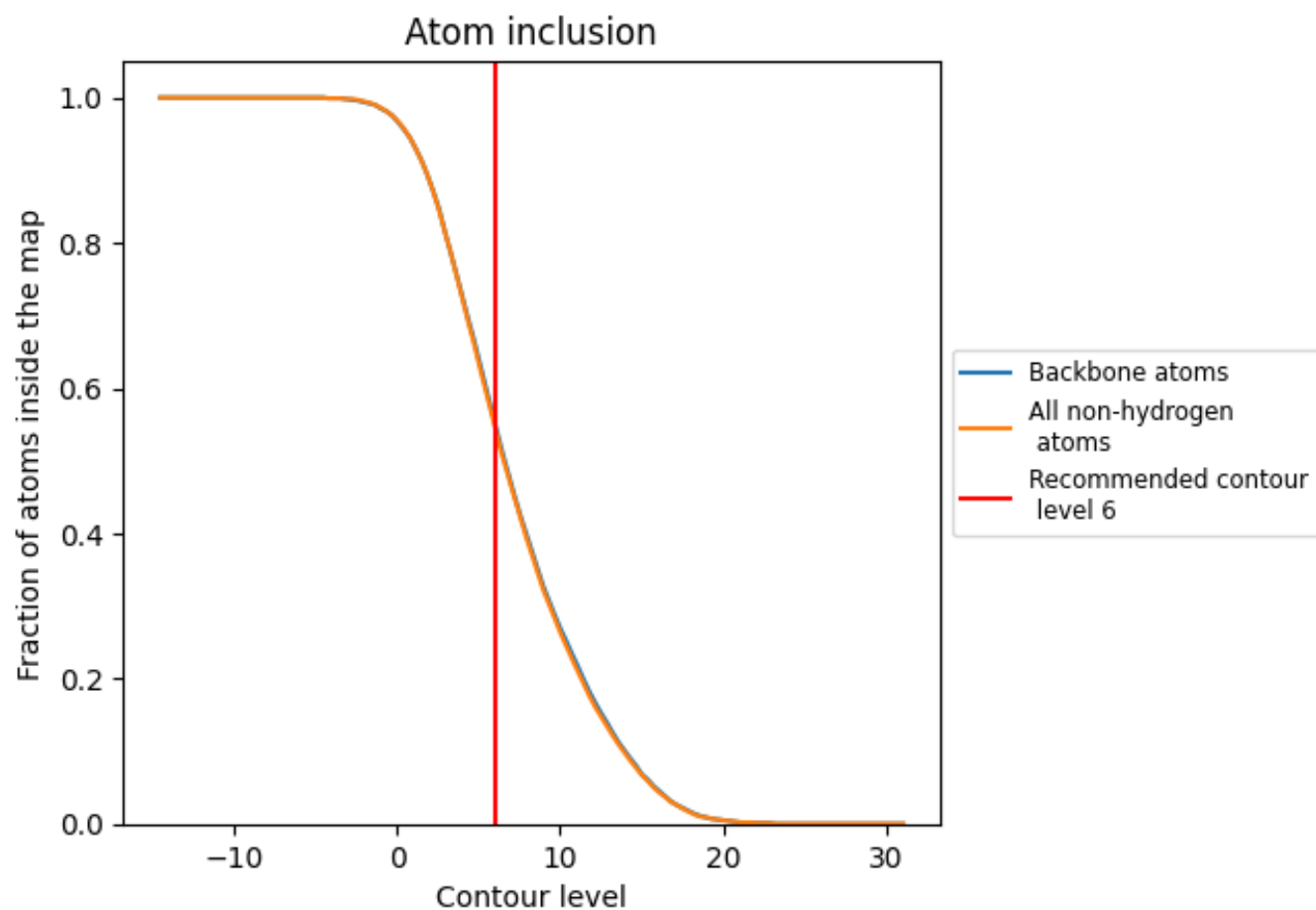
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 55% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5480	 0.2800
A	 0.6440	 0.3200
B	 0.7130	 0.3640
C	 0.7460	 0.4090
D	 0.7500	 0.3870
E	 0.7460	 0.3880
F	 0.7650	 0.3890
G	 0.7540	 0.3930
H	 0.7480	 0.3770
I	 0.6800	 0.3300
J	 0.6380	 0.2850
K	 0.2430	 0.1450
L	 0.1820	 0.1210
M	 0.2770	 0.1510
N	 0.4240	 0.1870
O	 0.5190	 0.2220
P	 0.3840	 0.1820
Q	 0.3310	 0.1580
R	 0.3610	 0.1770
S	 0.3390	 0.1490
T	 0.0980	 0.1550
U	 0.0900	 0.1450
p	 0.4950	 0.2340
q	 0.4520	 0.2180
r	 0.3930	 0.1830
s	 0.5030	 0.2650

