



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 10:56 pm GMT

PDB ID : 6F3A
EMDB ID : EMD-2860
Title : Cryo-EM structure of a single dynein tail domain bound to dynactin and BICD2N
Authors : Urnavicius, L.; Lau, C.K.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.; Yildiz, A.; Carter, A.P.
Deposited on : 2017-11-28
Resolution : 8.20 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:

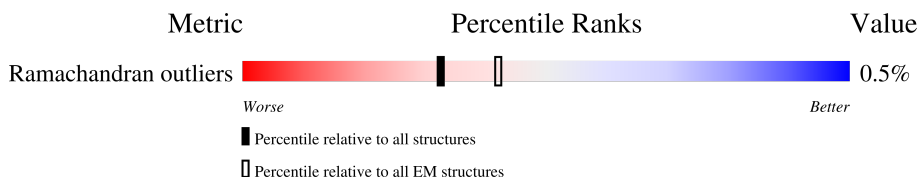
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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	154571	4023

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	97%
1	B	376	98%
1	C	376	97%
1	D	376	97%
1	E	376	98%
1	F	376	98%
1	G	376	97%
1	I	376	97%
2	H	375	99%
3	J	390	95%
4	K	286	96%

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Mol	Chain	Length	Quality of chain
5	L	272	99%
6	M	587	100%
7	N	616	100%
8	O	65	100%
8	P	65	100%
9	Q	87	55% 100%
9	R	87	100%
10	U	190	5% 89% 9%
11	V	182	90% 9%
12	Y	264	100%
13	Z	52	100%
14	a	68	76% 24%
15	b	89	84% 16%
15	c	89	39% 61%
15	d	89	27% 73%
16	e	1455	5% 54% 46%
16	f	1455	7% 57% 43%
17	g	612	14% 65% 35%
17	h	612	9% 65% 34%
18	j	492	97%
19	k	96	85% 97%
19	l	96	39% 97%
20	z	53	8% 100%
21	5	275	18% 100%
21	6	275	16% 100%

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 48864 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	370	1822	1082	370	370	0	0
1	B	370	1822	1082	370	370	0	0
1	C	370	1822	1082	370	370	0	0
1	D	370	1822	1082	370	370	0	0
1	E	370	1822	1082	370	370	0	0
1	F	370	1822	1082	370	370	0	0
1	G	370	1822	1082	370	370	0	0
1	I	370	1822	1082	370	370	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	H	370	1822	1082	370	370	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	J	369	1819	1081	369	369	0	0

- Molecule 4 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	K	278	1378	822	278	278	0	0

- Molecule 5 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	L	269	1327	789	269	269	0	0

- Molecule 6 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	M	587	2935	1761	587	587	0	0

- Molecule 7 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	N	616	3080	1848	616	616	0	0

- Molecule 8 is a protein called Dynactin Subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	O	65	323	193	65	65	0	0
8	P	65	323	193	65	65	0	0

- Molecule 9 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Q	87	435	261	87	87	0	0
9	R	87	435	261	87	87	0	0

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	U	172	843	500	171	172	0	1

- Molecule 11 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	V	165	812	482	165	165	0	0

- Molecule 12 is a protein called Dynactin Subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	Y	264	1320	792	264	264	0	0

- Molecule 13 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Z	52	260	156	52	52	0	0

- Molecule 14 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	a	52	259	155	52	52	0	0

- Molecule 15 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	b	75	369	219	75	75	0	0
15	c	35	174	104	35	35	0	0
15	d	24	119	71	24	24	0	0

- Molecule 16 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	e	785	3898	2328	785	785	0	0
16	f	832	4128	2470	832	826	0	0

- Molecule 17 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	397	Total	C	N	O	0	0
			1961	1167	397	397		
17	h	401	Total	C	N	O	0	0
			1980	1178	401	401		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	484	SER	THR	conflict	UNP Q13409
g	499	GLY	ASP	conflict	UNP Q13409
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409

- Molecule 18 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	j	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 19 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	k	93	Total	C	N	O	0	0
			462	276	93	93		
19	l	93	Total	C	N	O	0	0
			462	276	93	93		

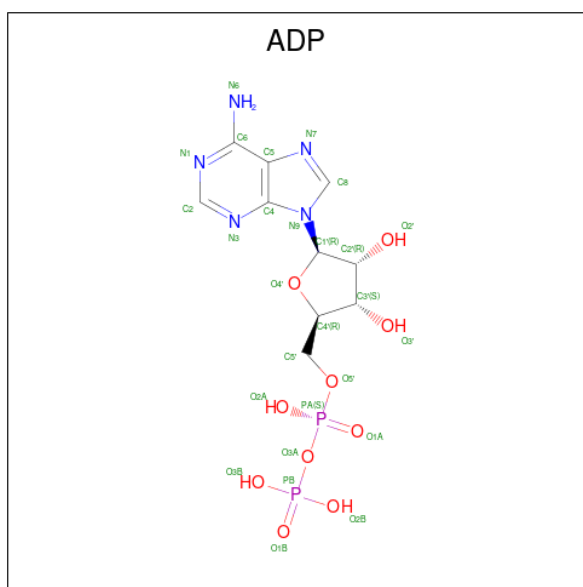
- Molecule 20 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 21 is a protein called BICD2N.

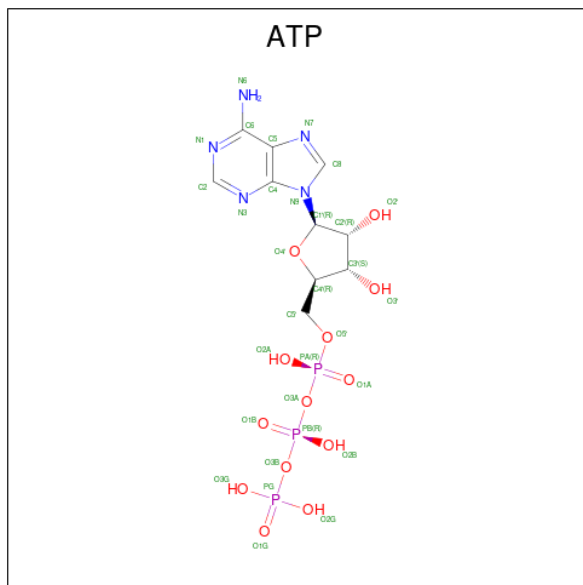
Mol	Chain	Residues	Atoms				AltConf	Trace
21	5	275	Total	C	N	O	0	0
			1375	825	275	275		
21	6	275	Total	C	N	O	0	0
			1375	825	275	275		

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 23 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



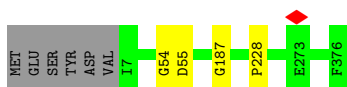
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	H	1	31	10	5	13	3	0

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.

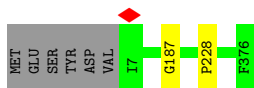
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain A:  97%



- Molecule 1: ARP1 actin related protein 1 homolog A

Chain B:  98%



- Molecule 1: ARP1 actin related protein 1 homolog A

Chain C:  97%



- Molecule 1: ARP1 actin related protein 1 homolog A

Chain D:  97%



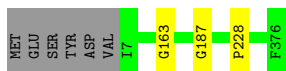
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain E:  98%



- Molecule 1: ARP1 actin related protein 1 homolog A

Chain F:  98%



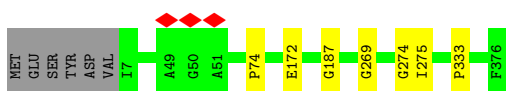
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain G:  97%



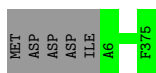
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain I:  97%



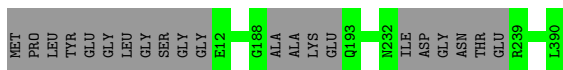
- Molecule 2: Actin, cytoplasmic 1

Chain H:  99%



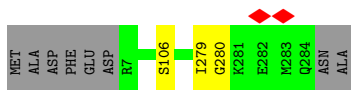
- Molecule 3: Actin related protein 10 homolog

Chain J:  95% 5%



- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:  96%



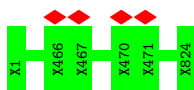
- Molecule 5: F-actin capping protein beta subunit

Chain L:  99%



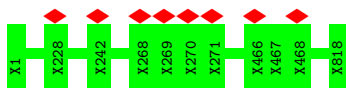
- Molecule 6: Dynactin Subunit 2

Chain M:  100%



- Molecule 7: Dynactin Subunit 2

Chain N:  100%



- Molecule 8: Dynactin Subunit 3

Chain O:  100%

There are no outlier residues recorded for this chain.

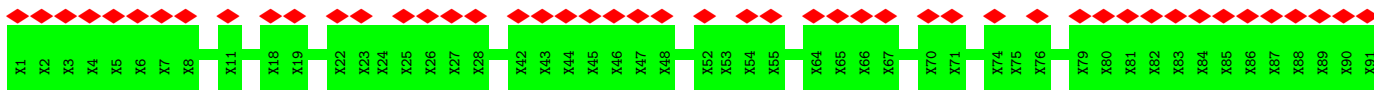
- Molecule 8: Dynactin Subunit 3

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Dynactin Subunit 2

Chain Q:  55%
100%




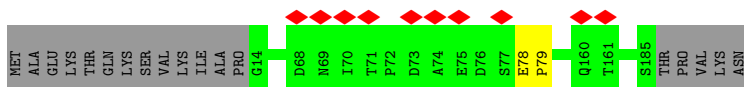
- Molecule 9: Dynactin Subunit 2

Chain R:  100%


There are no outlier residues recorded for this chain.

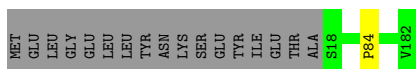
- Molecule 10: Dynactin 6

Chain U:  5%
89% 9%

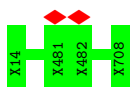


- Molecule 11: Dynactin subunit 5

Chain V:  90% 9%



• Molecule 12: Dynactin Subunit 4

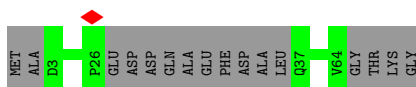
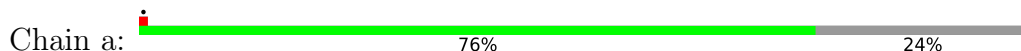


• Molecule 13: Dynactin Subunit 1

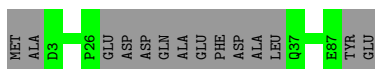
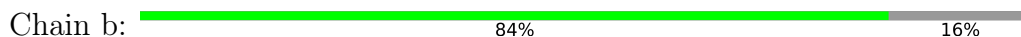


There are no outlier residues recorded for this chain.

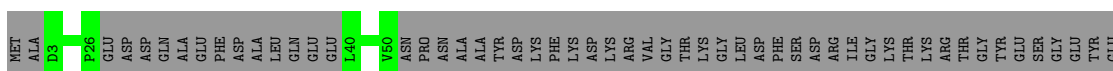
• Molecule 14: Dynactin subunit 2



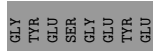
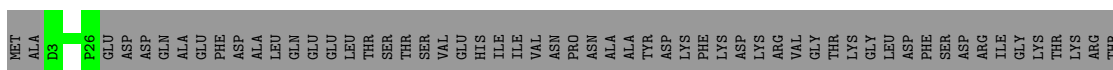
• Molecule 15: Dynactin subunit 2



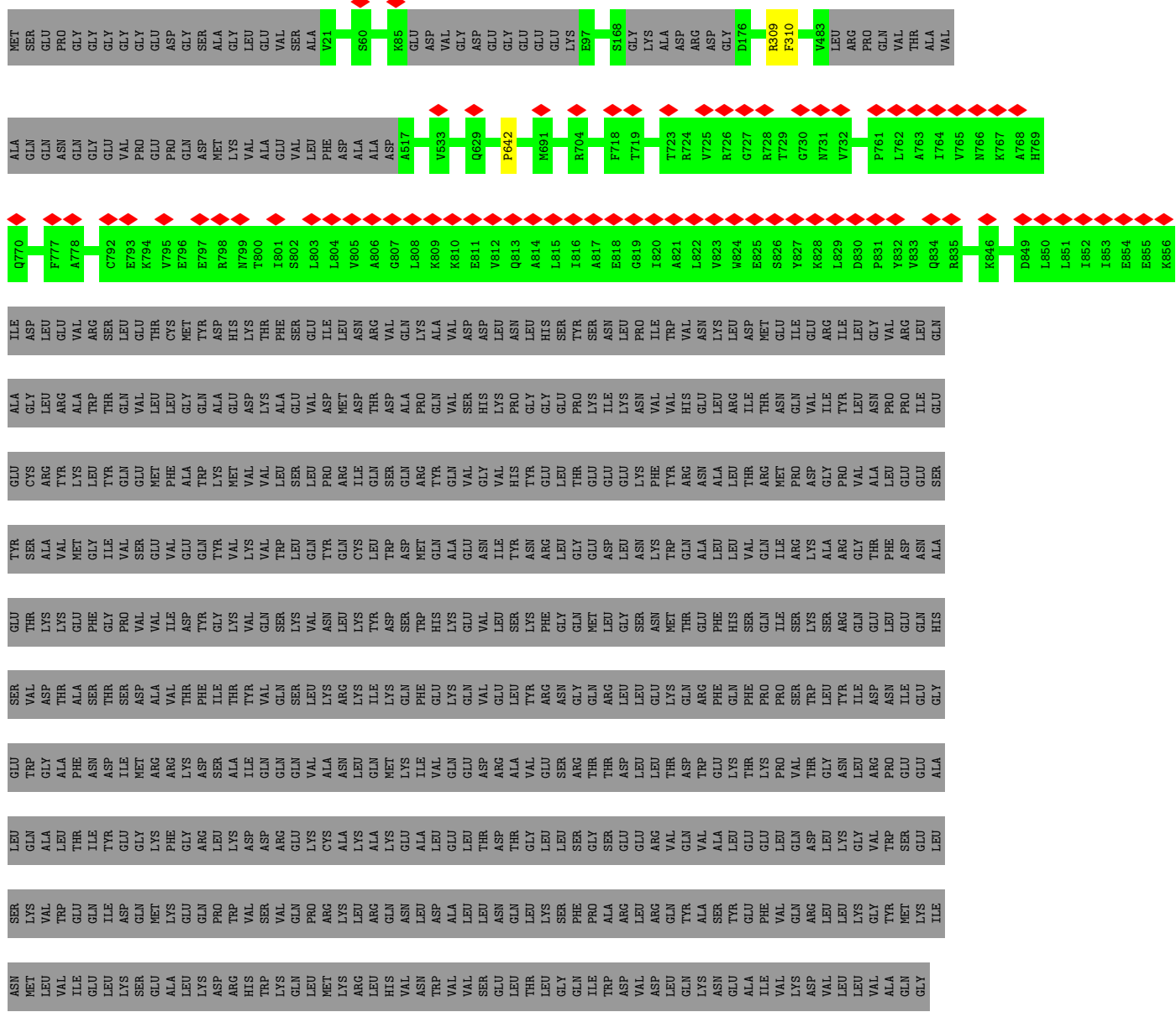
• Molecule 15: Dynactin subunit 2



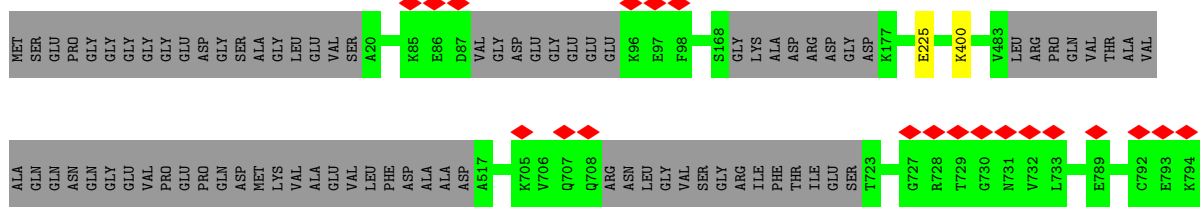
• Molecule 15: Dynactin subunit 2

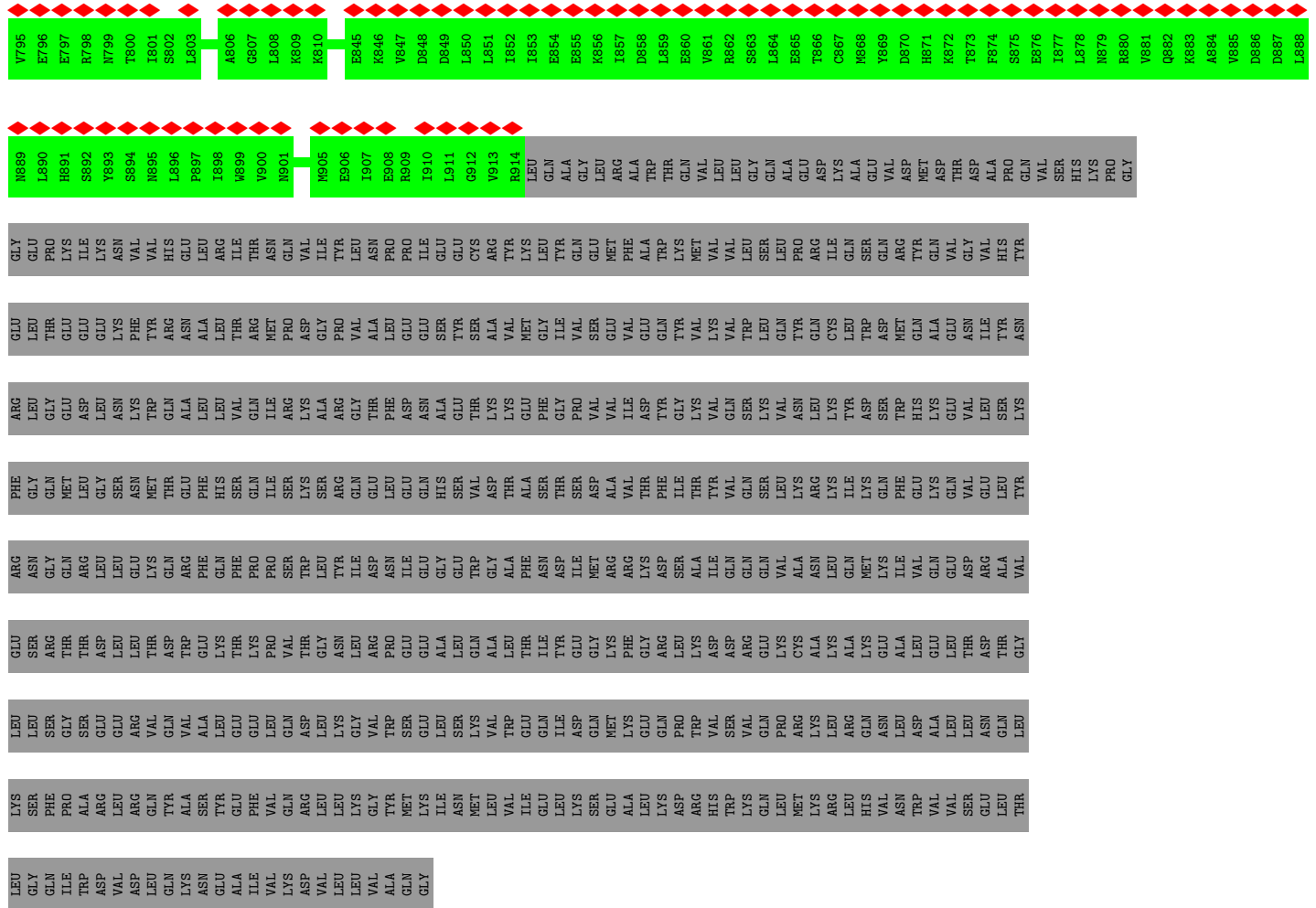


• Molecule 16: Cytoplasmic dynein 1 heavy chain 1

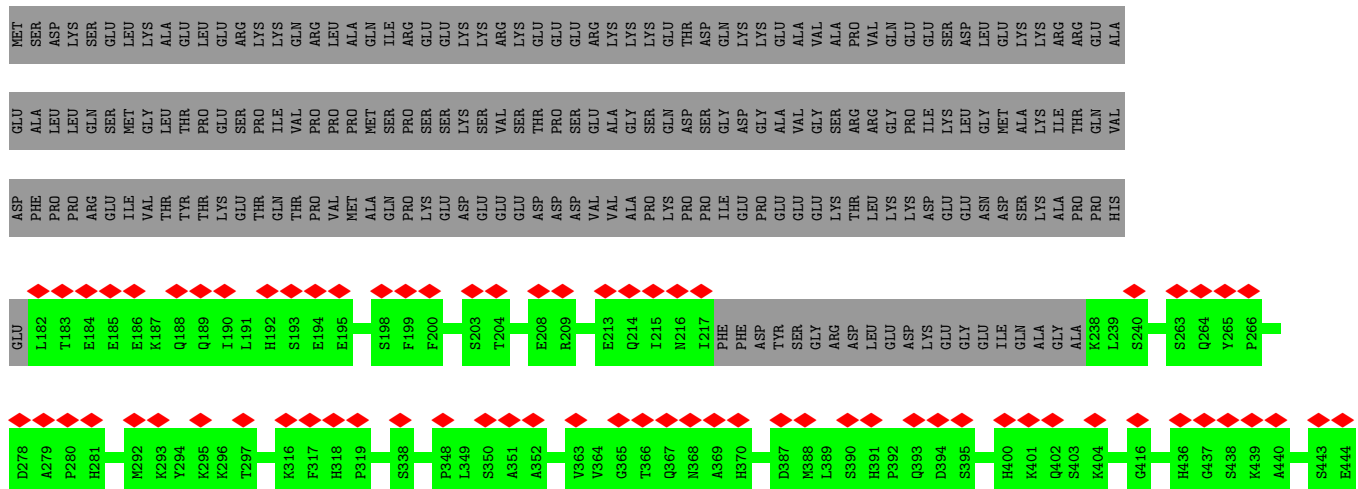


● Molecule 16: Cytoplasmic dynein 1 heavy chain 1

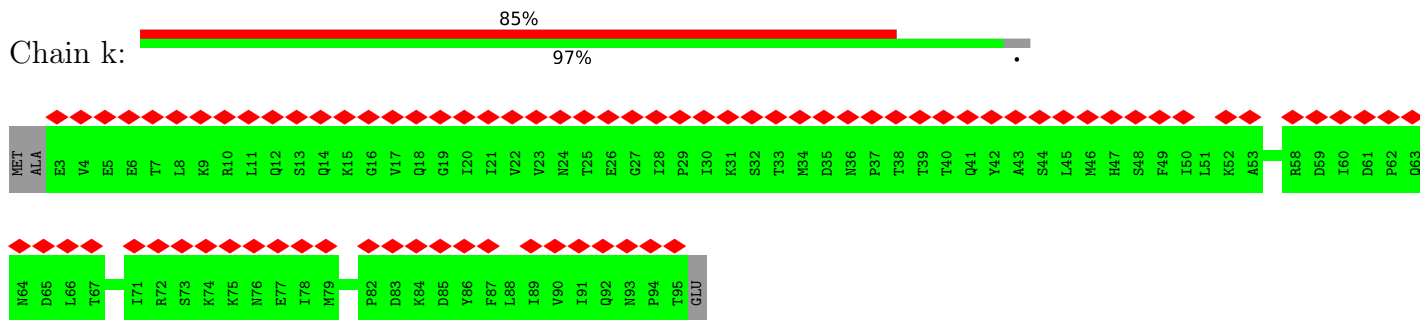




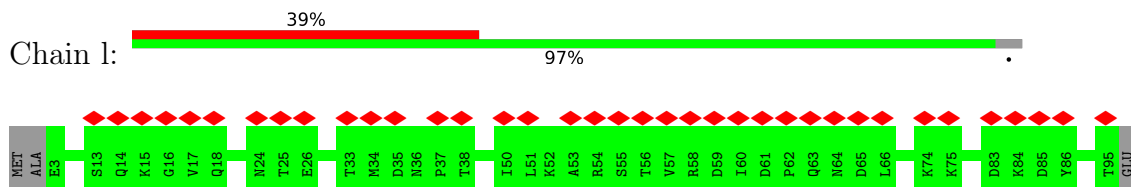
● Molecule 17: Cytoplasmic dynein 1 intermediate chain 2



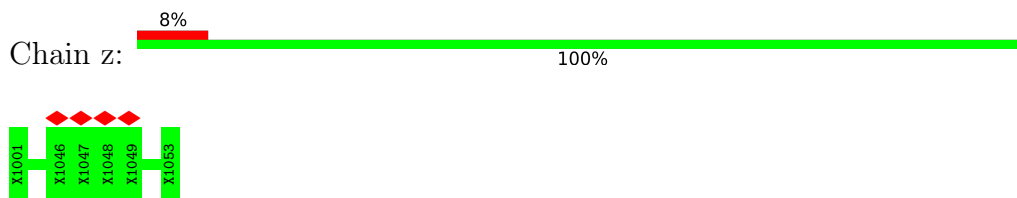
• Molecule 19: Dynein light chain roadblock-type 1



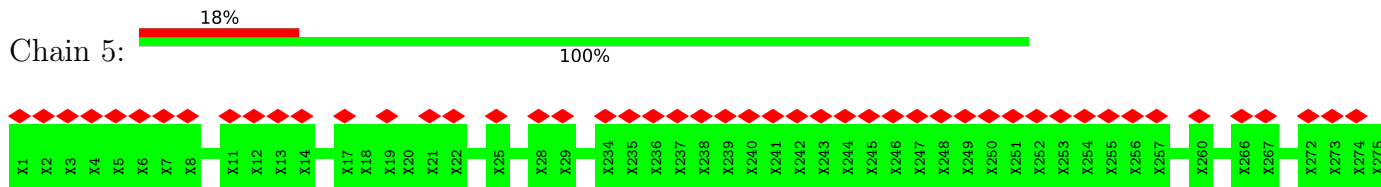
• Molecule 19: Dynein light chain roadblock-type 1



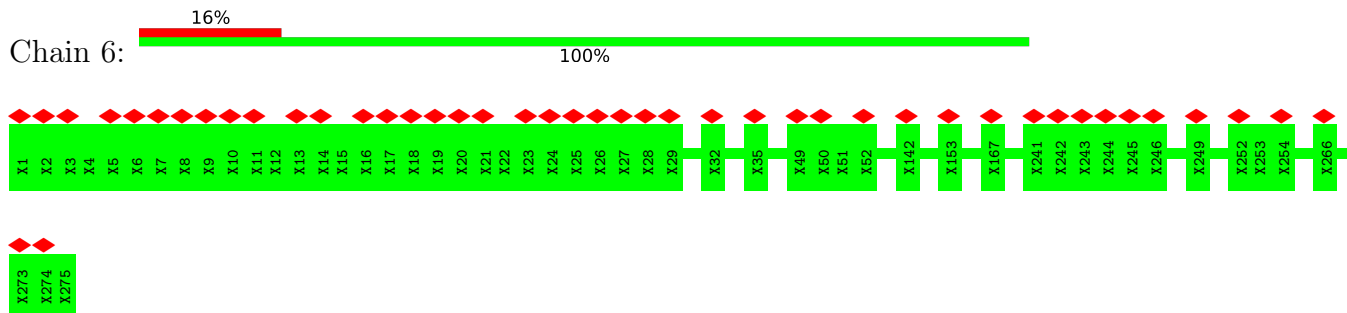
• Molecule 20: Dynactin Subunit 1



• Molecule 21: BICD2N



• Molecule 21: BICD2N



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85744	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	578.88, 578.88, 578.88	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: ADP, ATP

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	0.41	0/1821	0.76	1/2531 (0.0%)
1	B	0.43	0/1821	0.74	0/2531
1	C	0.47	1/1821 (0.1%)	0.82	2/2531 (0.1%)
1	D	0.47	0/1821	0.78	1/2531 (0.0%)
1	E	0.46	0/1821	0.80	1/2531 (0.0%)
1	F	0.48	0/1821	0.78	1/2531 (0.0%)
1	G	0.46	0/1821	0.84	1/2531 (0.0%)
1	I	0.43	0/1821	0.76	2/2531 (0.1%)
2	H	0.42	0/1821	0.76	0/2531
3	J	0.41	0/1816	0.73	0/2522
4	K	0.35	0/1377	0.74	1/1919 (0.1%)
5	L	0.40	0/1326	0.71	1/1844 (0.1%)
10	U	0.38	0/841	0.65	0/1168
11	V	0.29	0/811	0.63	0/1126
14	a	0.39	0/257	0.82	0/356
15	b	0.42	0/367	0.88	0/507
15	c	0.39	0/172	0.82	0/237
15	d	0.36	0/118	0.76	0/163
16	e	0.29	0/3894	0.52	1/5429 (0.0%)
16	f	0.33	0/4123	0.62	1/5745 (0.0%)
17	g	0.33	0/1959	0.73	0/2725
17	h	0.35	0/1978	0.81	0/2751
18	j	0.26	0/74	0.55	0/102
19	k	0.31	0/461	0.61	0/642
19	l	0.28	0/461	0.57	0/642
All	All	0.39	1/36424 (0.0%)	0.72	13/50657 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	335	GLU	CA-CB	-6.00	1.40	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	GLY	N-CA-C	-10.65	86.47	113.10
1	I	274	GLY	N-CA-C	-9.15	90.23	113.10
1	C	274	GLY	N-CA-C	-8.38	92.16	113.10
1	G	274	GLY	N-CA-C	-7.54	94.24	113.10
1	E	274	GLY	N-CA-C	-7.18	95.16	113.10

There are no chirality outliers.

There are no planarity outliers.

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%)	319 (87%)	46 (12%)	3 (1%)	19	60
1	B	368/376 (98%)	321 (87%)	45 (12%)	2 (0%)	29	69
1	C	368/376 (98%)	325 (88%)	40 (11%)	3 (1%)	19	60
1	D	368/376 (98%)	316 (86%)	49 (13%)	3 (1%)	19	60
1	E	368/376 (98%)	321 (87%)	45 (12%)	2 (0%)	29	69
1	F	368/376 (98%)	316 (86%)	50 (14%)	2 (0%)	29	69
1	G	368/376 (98%)	325 (88%)	40 (11%)	3 (1%)	19	60
1	I	368/376 (98%)	333 (90%)	30 (8%)	5 (1%)	11	46
2	H	368/375 (98%)	326 (89%)	42 (11%)	0	100	100
3	J	363/390 (93%)	310 (85%)	53 (15%)	0	100	100
4	K	276/286 (96%)	236 (86%)	38 (14%)	2 (1%)	22	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	267/272 (98%)	237 (89%)	30 (11%)	0	100	100
10	U	169/190 (89%)	126 (75%)	41 (24%)	2 (1%)	13	50
11	V	163/182 (90%)	126 (77%)	36 (22%)	1 (1%)	25	66
14	a	48/68 (71%)	39 (81%)	9 (19%)	0	100	100
15	b	71/89 (80%)	55 (78%)	16 (22%)	0	100	100
15	c	31/89 (35%)	22 (71%)	9 (29%)	0	100	100
15	d	22/89 (25%)	18 (82%)	4 (18%)	0	100	100
16	e	777/1455 (53%)	694 (89%)	81 (10%)	2 (0%)	41	77
16	f	822/1455 (56%)	750 (91%)	71 (9%)	1 (0%)	51	86
17	g	393/612 (64%)	341 (87%)	52 (13%)	0	100	100
17	h	397/612 (65%)	328 (83%)	67 (17%)	2 (0%)	29	69
18	j	13/492 (3%)	11 (85%)	2 (15%)	0	100	100
19	k	91/96 (95%)	75 (82%)	16 (18%)	0	100	100
19	l	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
All	All	7306/9856 (74%)	6355 (87%)	918 (13%)	33 (0%)	32	69

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	279	ILE
10	U	79	PRO
17	h	491	LEU
1	A	187	GLY
1	B	187	GLY

5.3.2 Protein sidechains [i](#)

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	ADP	F	800	-	24,29,29	0.99	1 (4%)	29,45,45	1.52	5 (17%)
22	ADP	I	800	-	24,29,29	0.95	1 (4%)	29,45,45	1.54	6 (20%)
22	ADP	A	800	-	24,29,29	0.93	1 (4%)	29,45,45	1.53	5 (17%)
22	ADP	J	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.67	7 (24%)
22	ADP	G	800	-	24,29,29	0.94	1 (4%)	29,45,45	1.68	4 (13%)
22	ADP	B	800	-	24,29,29	0.96	1 (4%)	29,45,45	1.66	8 (27%)
22	ADP	D	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.68	6 (20%)
23	ATP	H	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.59	5 (16%)
22	ADP	E	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.75	10 (34%)
22	ADP	C	800	-	24,29,29	0.99	2 (8%)	29,45,45	1.60	7 (24%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ADP	F	800	-	-	1/12/32/32	0/3/3/3
22	ADP	I	800	-	-	1/12/32/32	0/3/3/3
22	ADP	A	800	-	-	3/12/32/32	0/3/3/3
22	ADP	J	800	-	-	5/12/32/32	0/3/3/3
22	ADP	G	800	-	-	1/12/32/32	0/3/3/3
22	ADP	B	800	-	-	3/12/32/32	0/3/3/3
22	ADP	D	800	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	ATP	H	401	-	-	2/18/38/38	0/3/3/3
22	ADP	E	800	-	-	3/12/32/32	0/3/3/3
22	ADP	C	800	-	-	5/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	800	ADP	C5-C4	2.35	1.47	1.40
22	J	800	ADP	C2'-C1'	-2.35	1.50	1.53
22	D	800	ADP	C2'-C1'	-2.25	1.50	1.53
22	F	800	ADP	C5-C4	2.25	1.46	1.40
23	H	401	ATP	C5-C4	2.24	1.46	1.40

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	800	ADP	PA-O3A-PB	-4.97	115.75	132.83
22	A	800	ADP	PA-O3A-PB	-4.79	116.40	132.83
22	D	800	ADP	PA-O3A-PB	-4.29	118.11	132.83
23	H	401	ATP	PB-O3B-PG	-3.98	119.16	132.83
22	C	800	ADP	PA-O3A-PB	-3.88	119.52	132.83

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

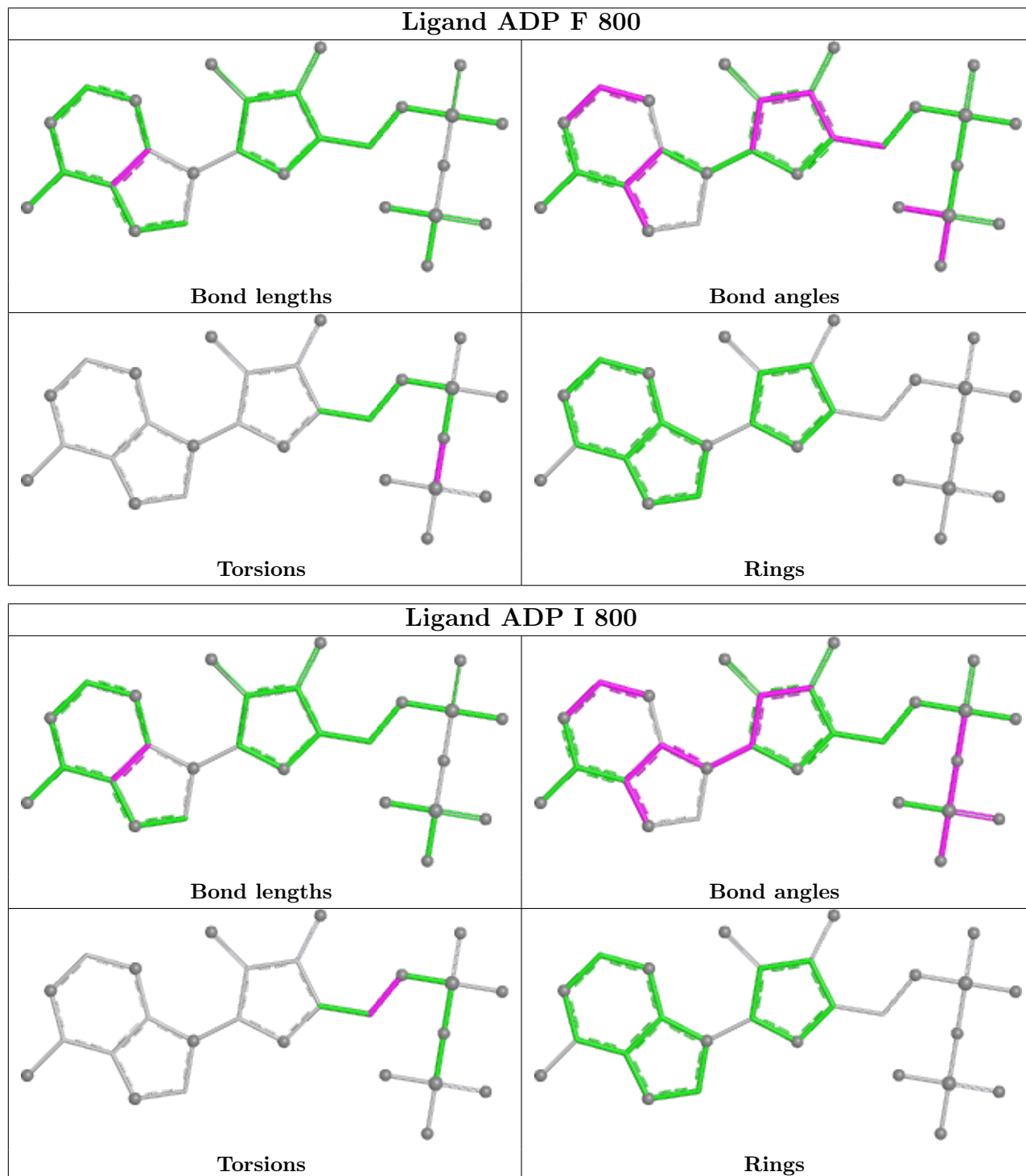
Mol	Chain	Res	Type	Atoms
22	A	800	ADP	O4'-C4'-C5'-O5'
22	A	800	ADP	C3'-C4'-C5'-O5'
22	C	800	ADP	C5'-O5'-PA-O3A
22	C	800	ADP	C3'-C4'-C5'-O5'
22	D	800	ADP	O4'-C4'-C5'-O5'

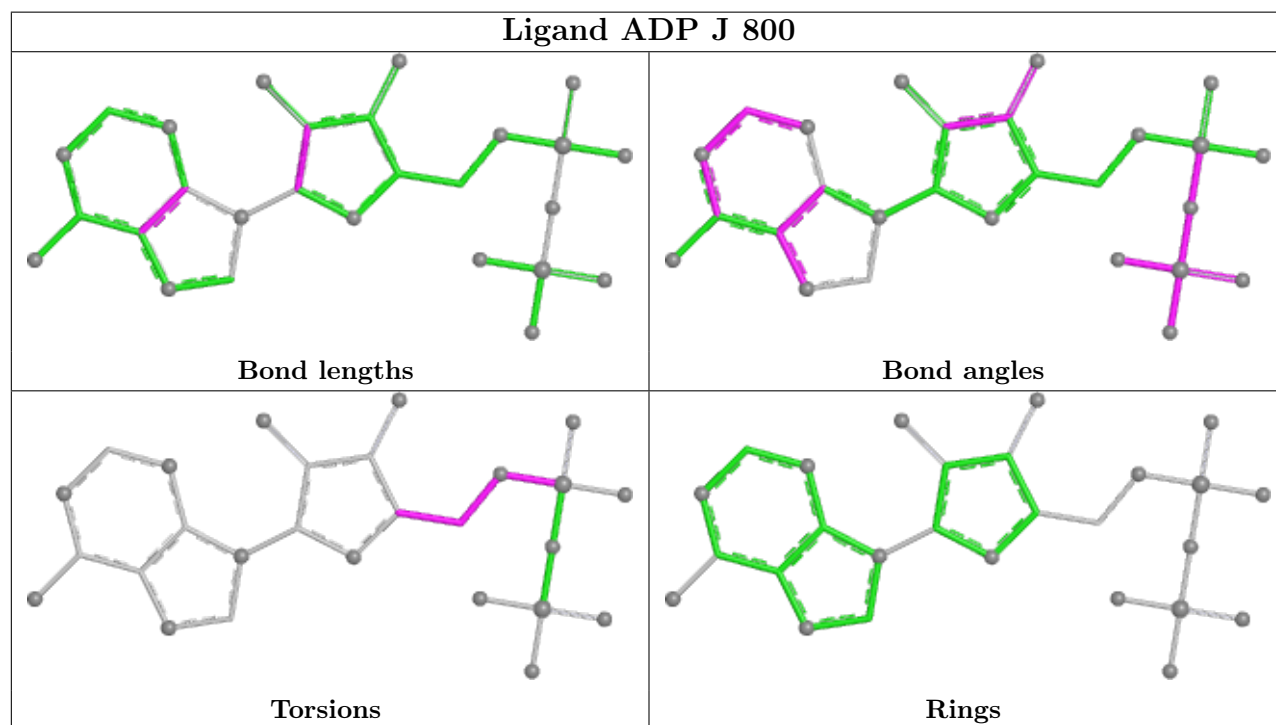
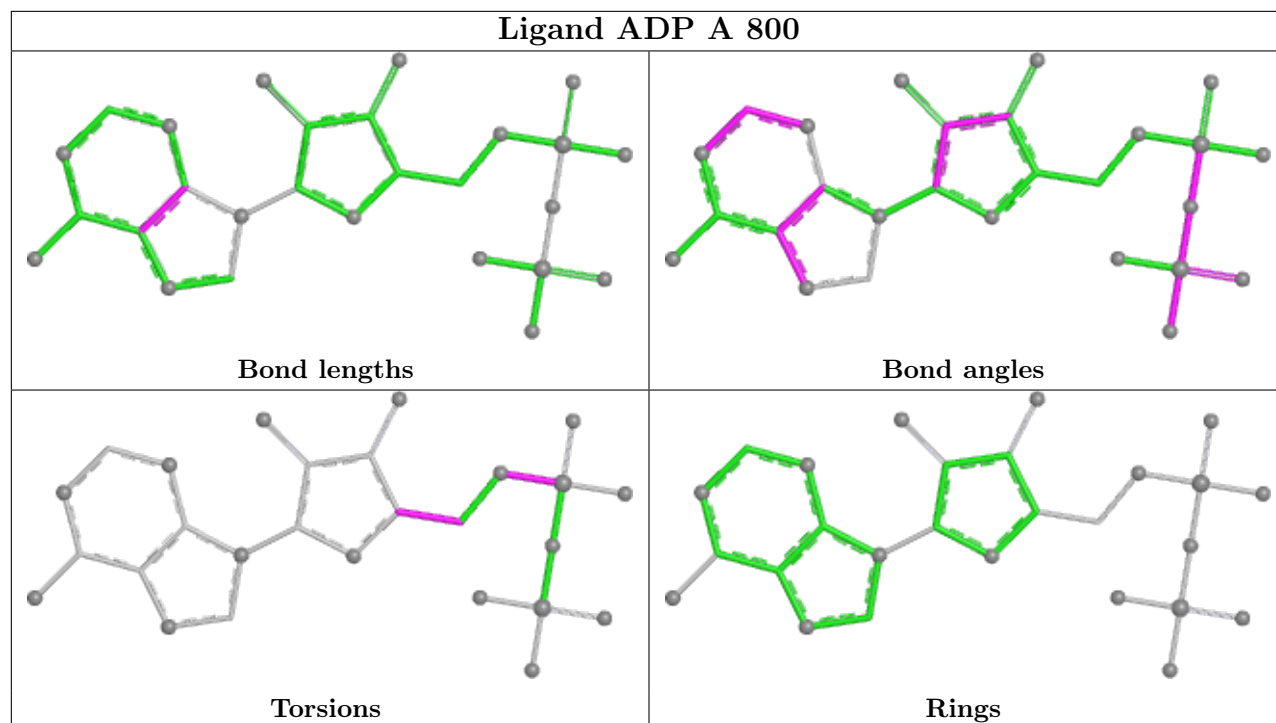
There are no ring outliers.

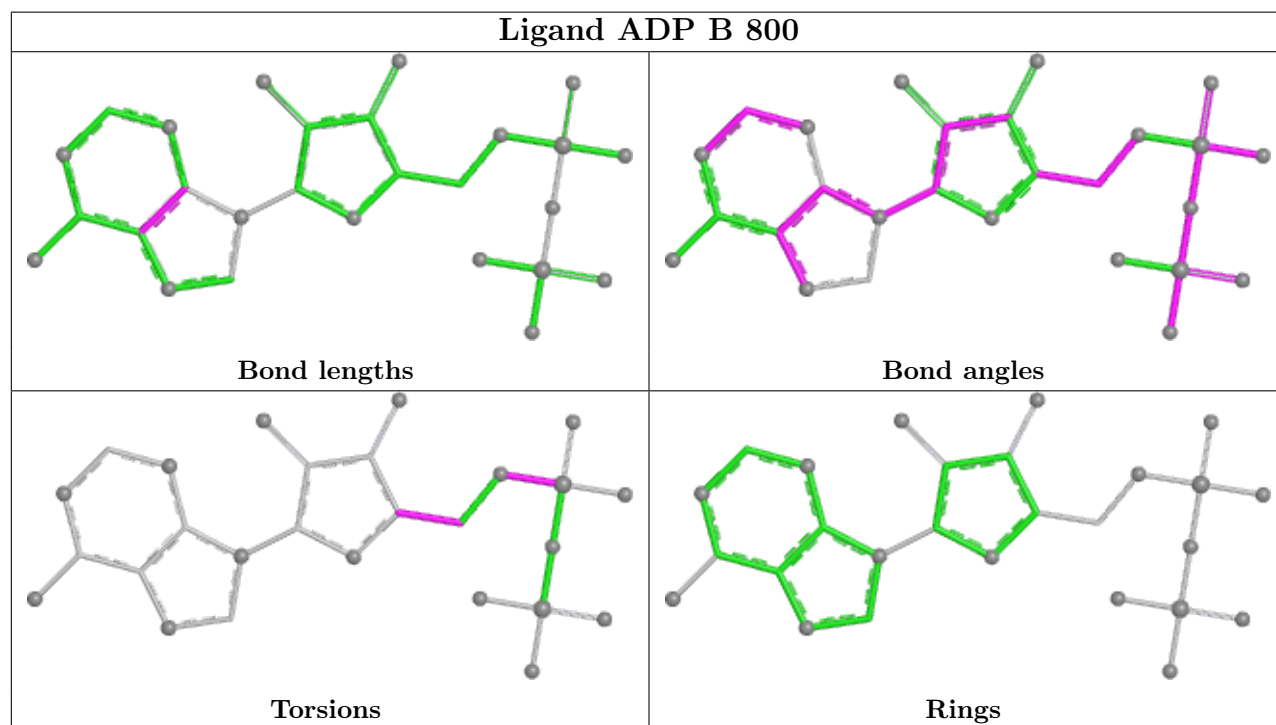
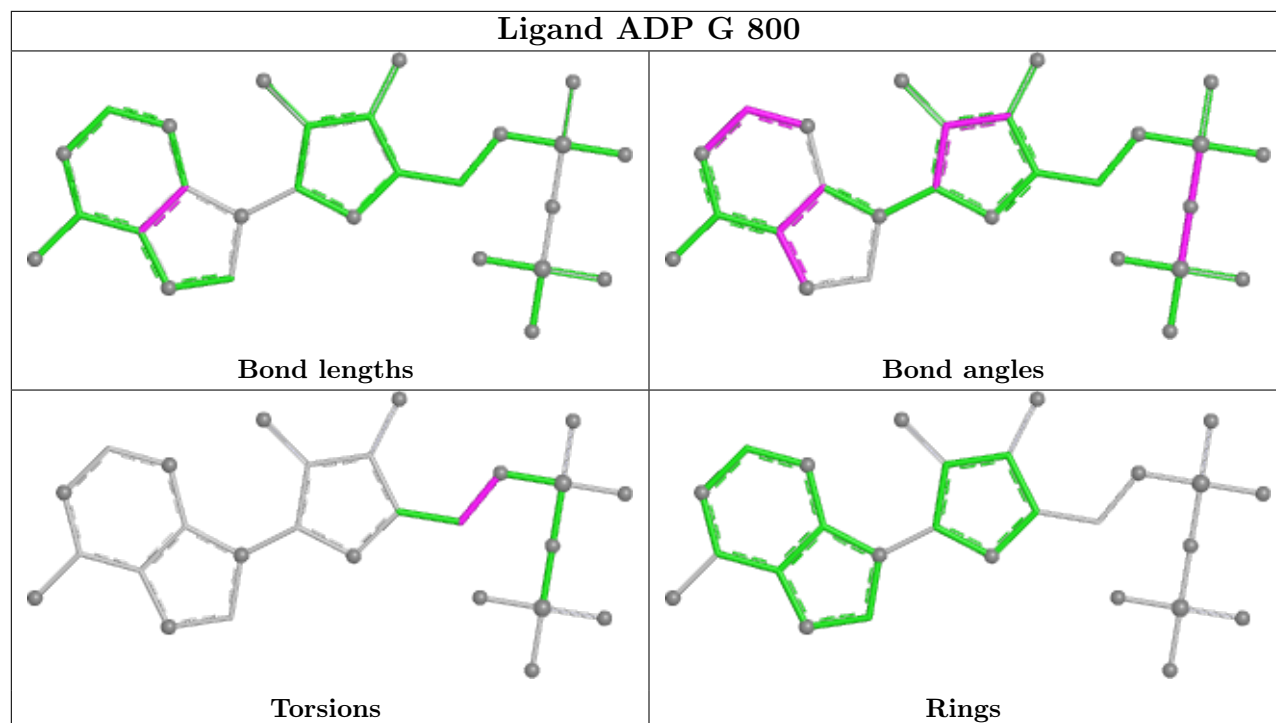
No monomer is involved in short contacts.

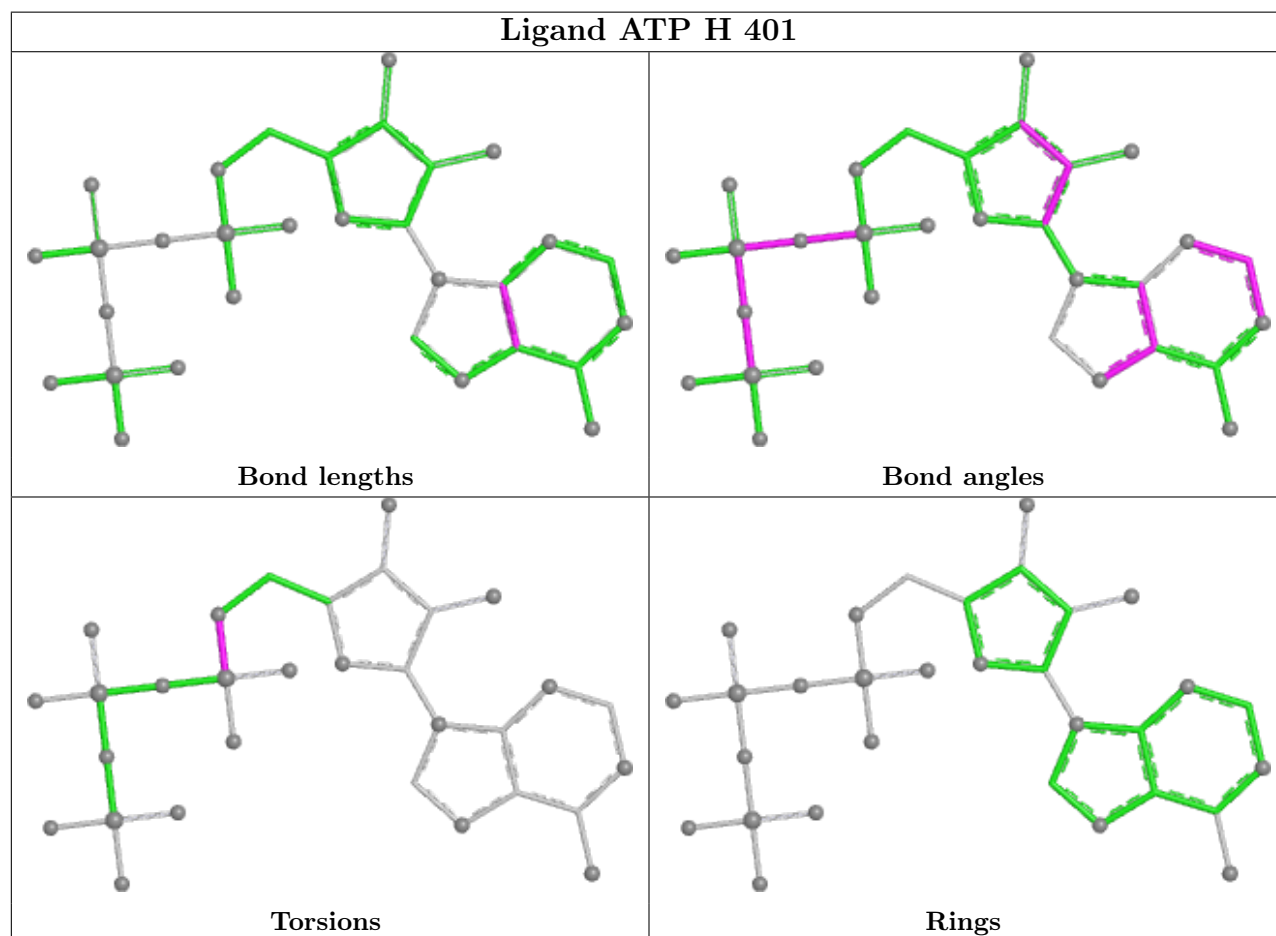
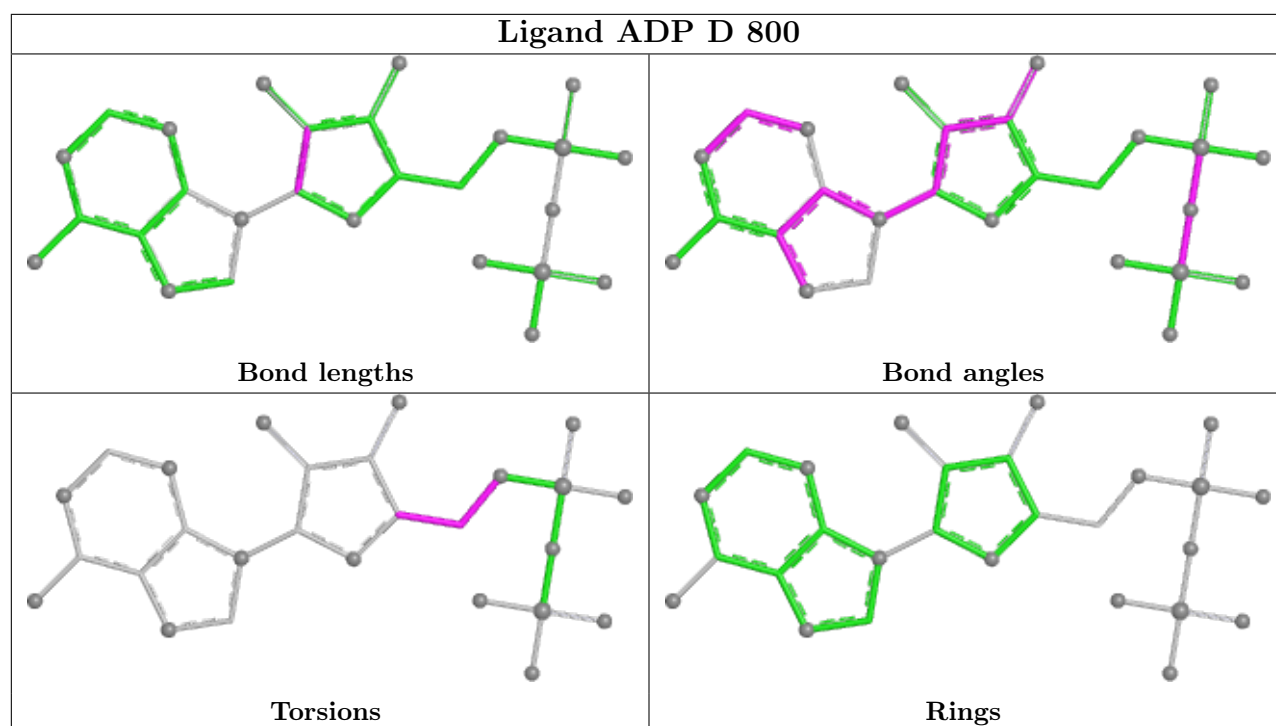
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

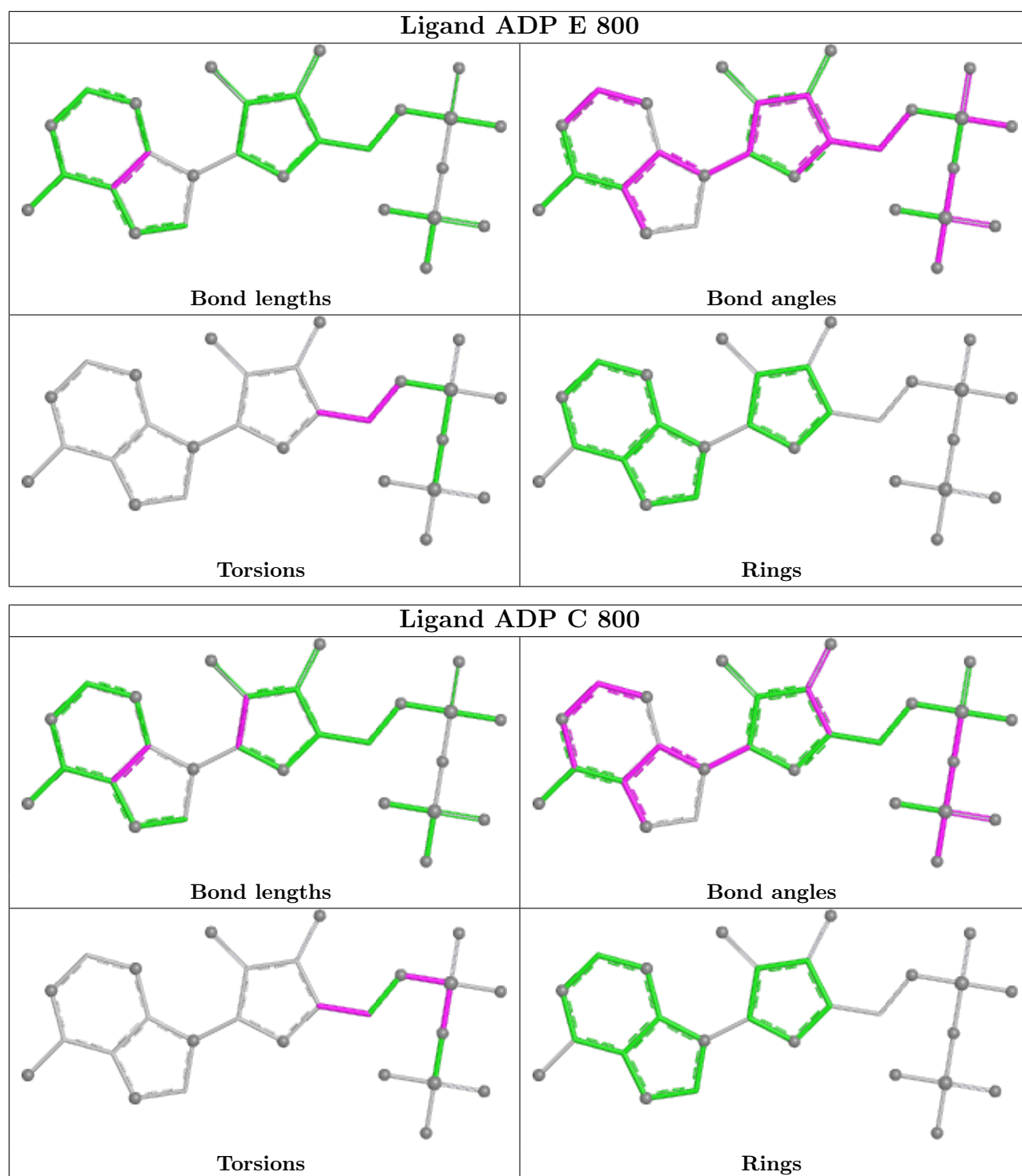
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	Y	12
7	N	5
6	M	5
8	O	3
8	P	3
9	R	2
9	Q	2

The worst 5 of 32 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	171:UNK	C	201:UNK	N	103.17
1	N	367:UNK	C	401:UNK	N	94.98
1	M	171:UNK	C	201:UNK	N	93.67
1	M	367:UNK	C	401:UNK	N	83.48
1	N	634:UNK	C	701:UNK	N	69.69

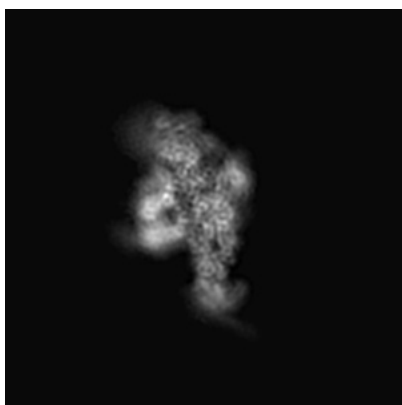
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2860. These allow visual inspection of the internal detail of the map and identification of artifacts.

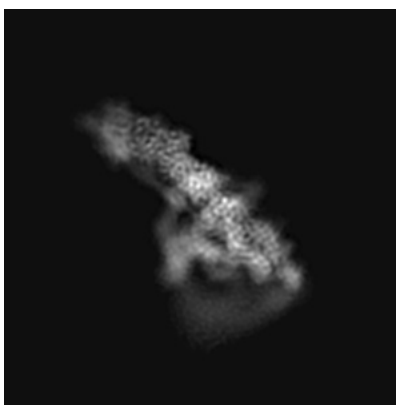
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

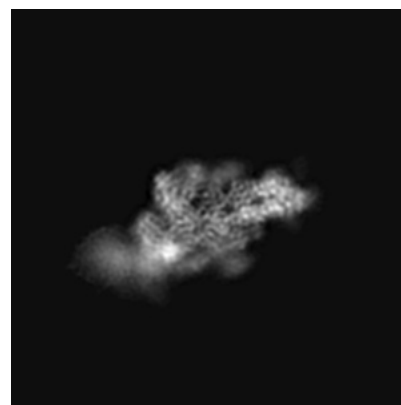
6.1.1 Primary map



X



Y

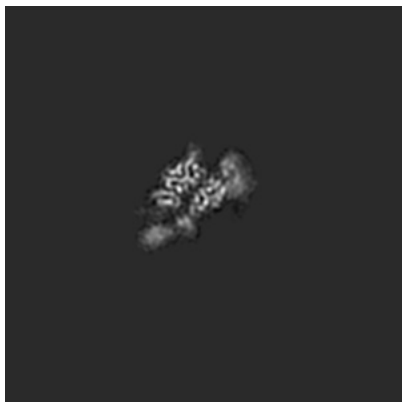


Z

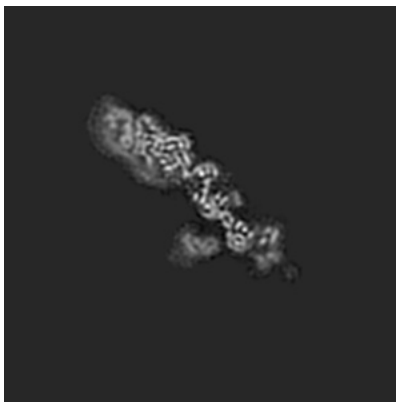
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

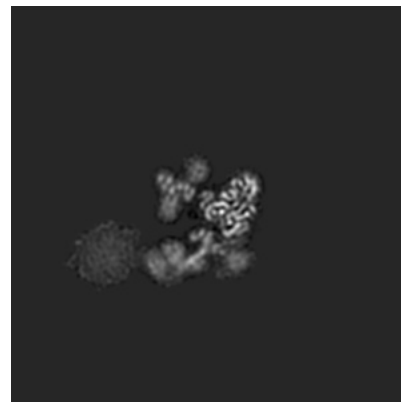
6.2.1 Primary map



X Index: 216



Y Index: 216

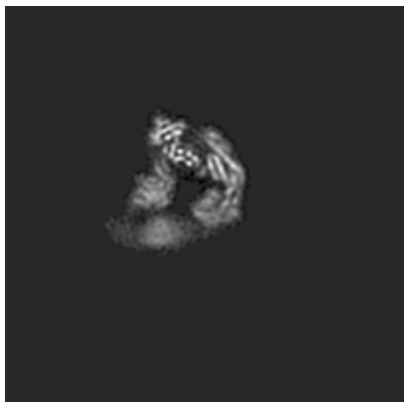


Z Index: 216

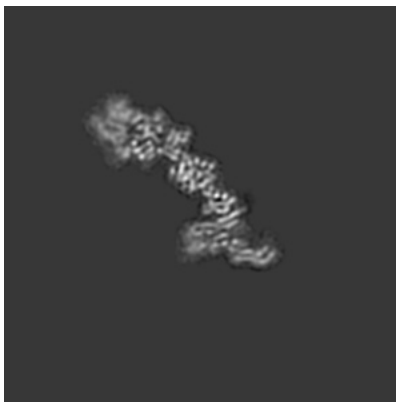
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

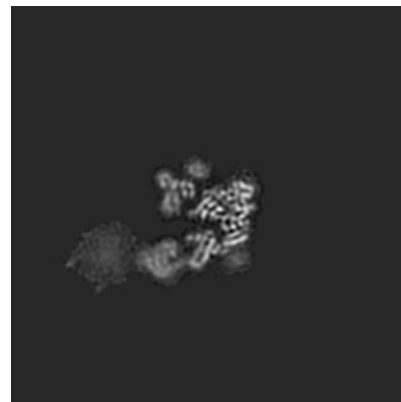
6.3.1 Primary map



X Index: 166



Y Index: 230



Z Index: 221

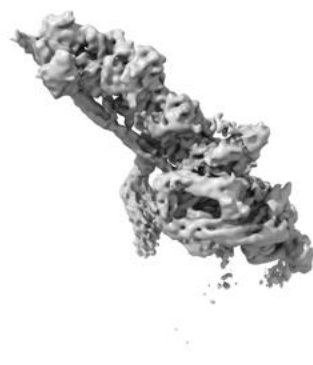
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

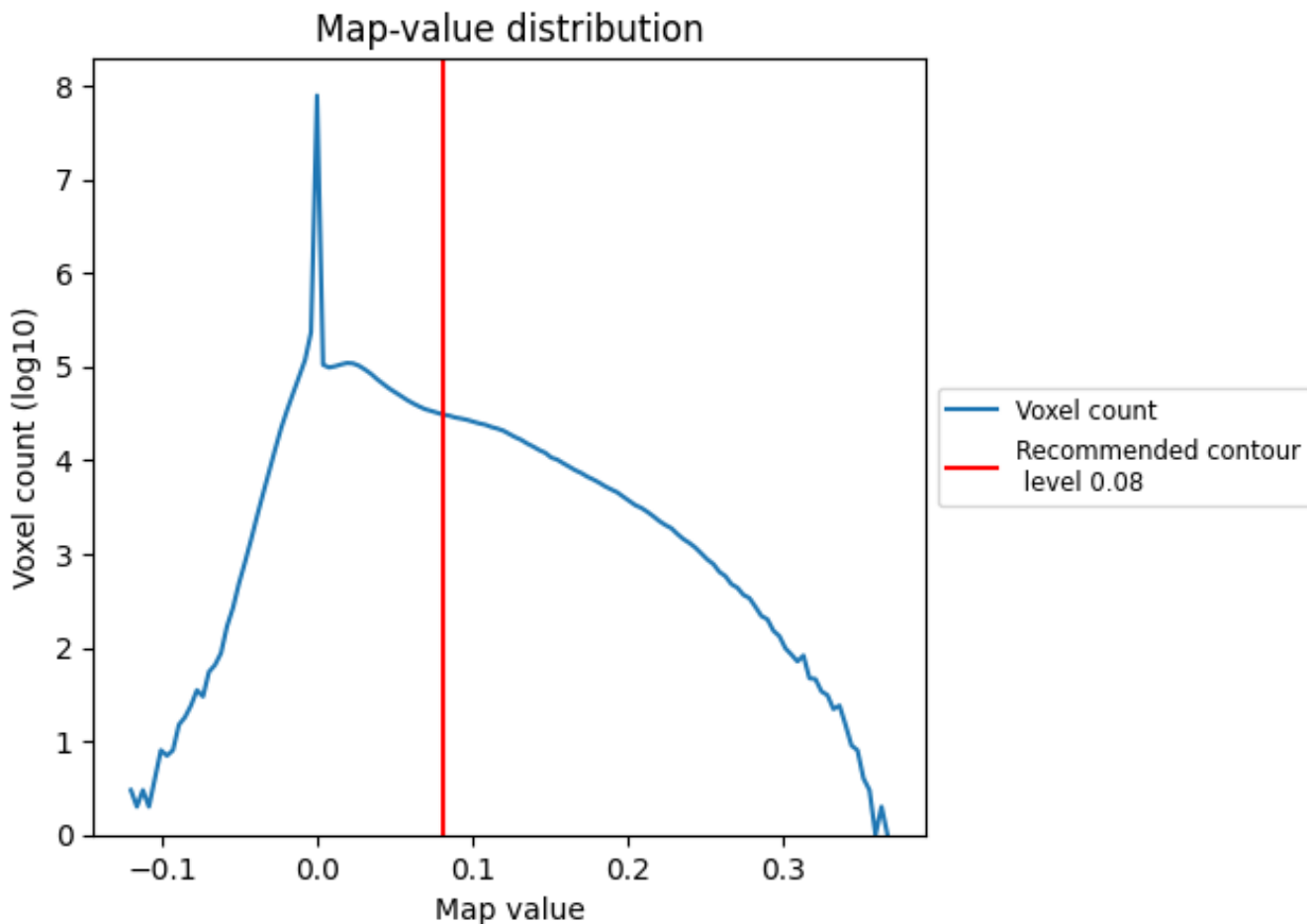
6.5 Mask visualisation

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

7 Map analysis [i](#)

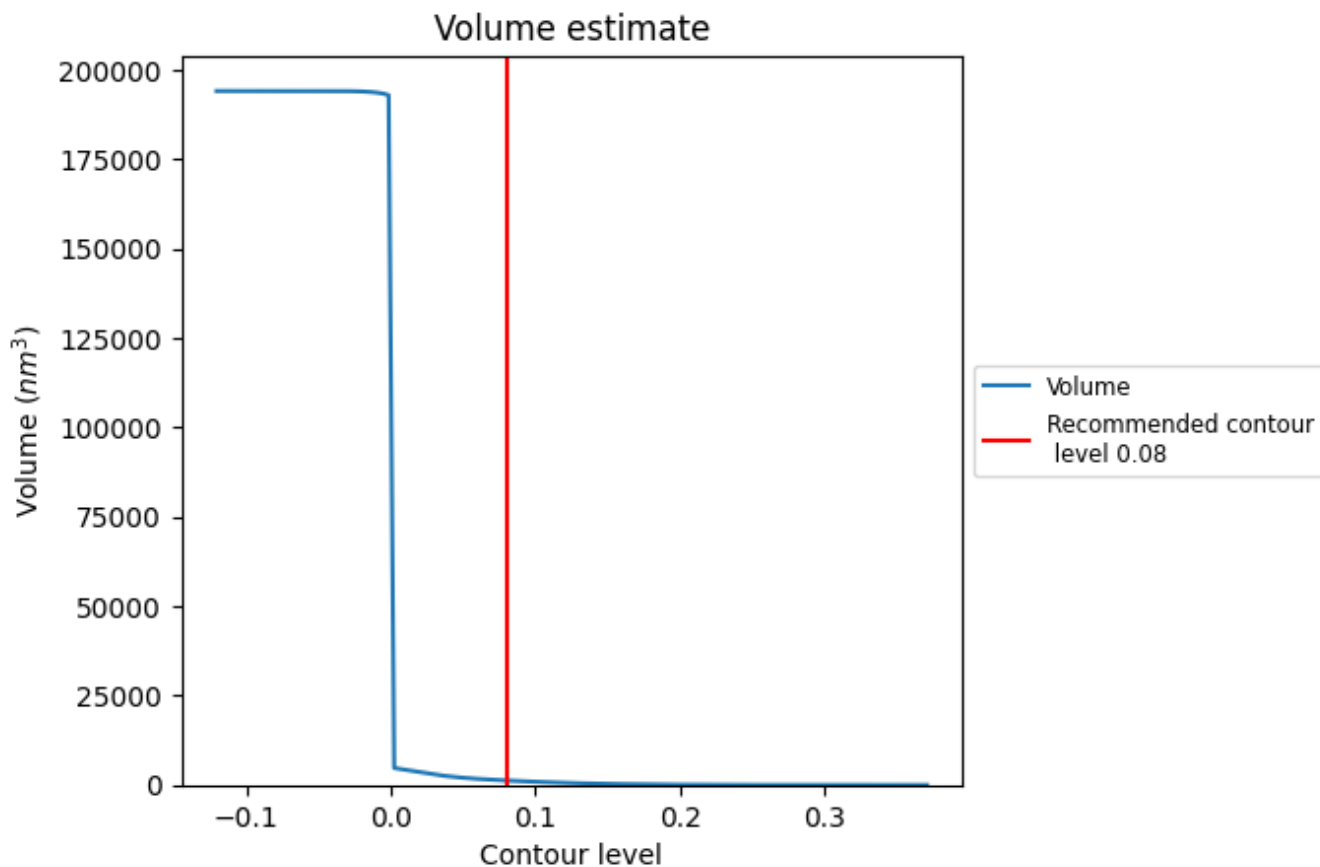
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

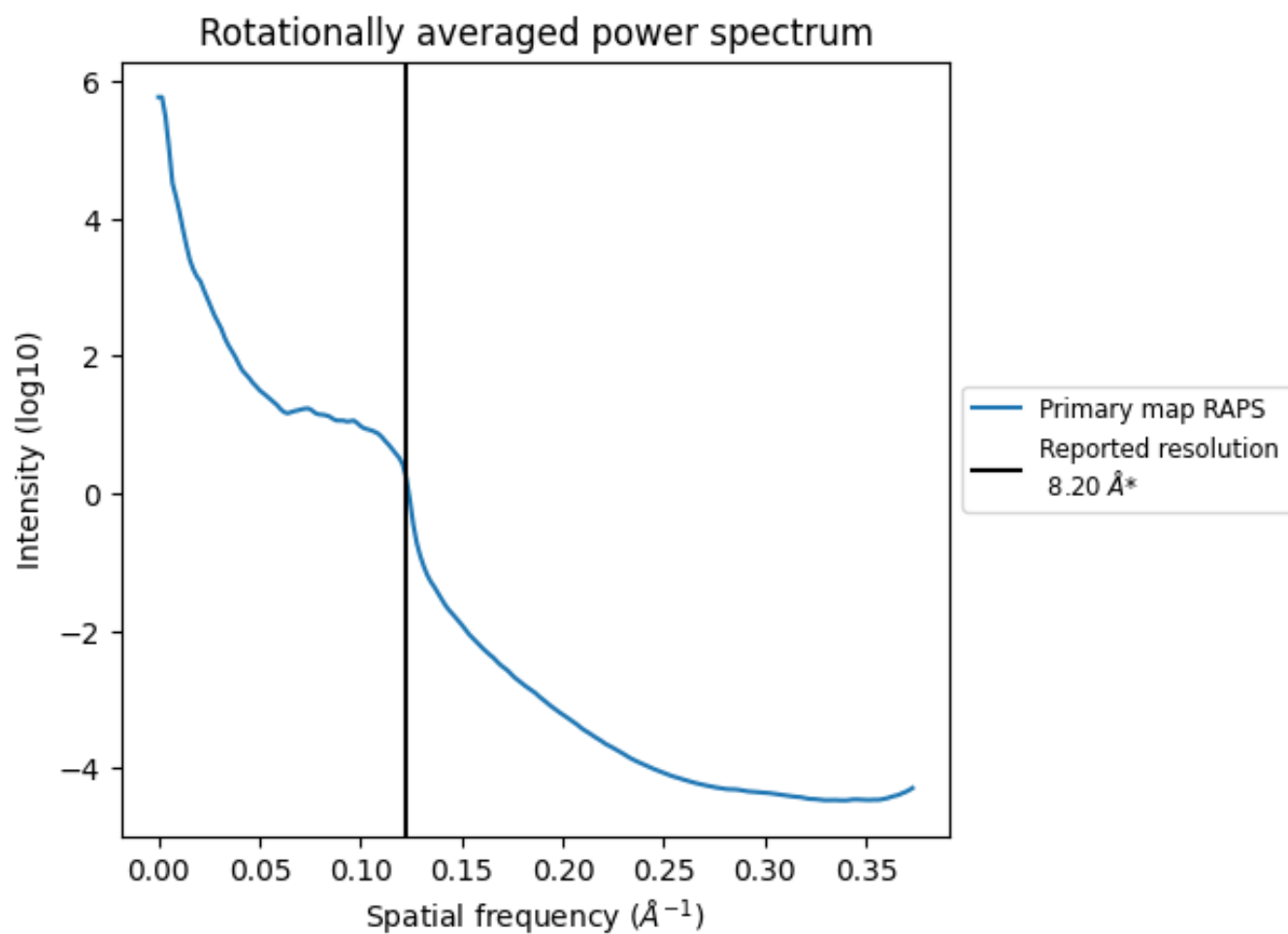
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1254 nm³; this corresponds to an approximate mass of 1133 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 0.122 Å⁻¹

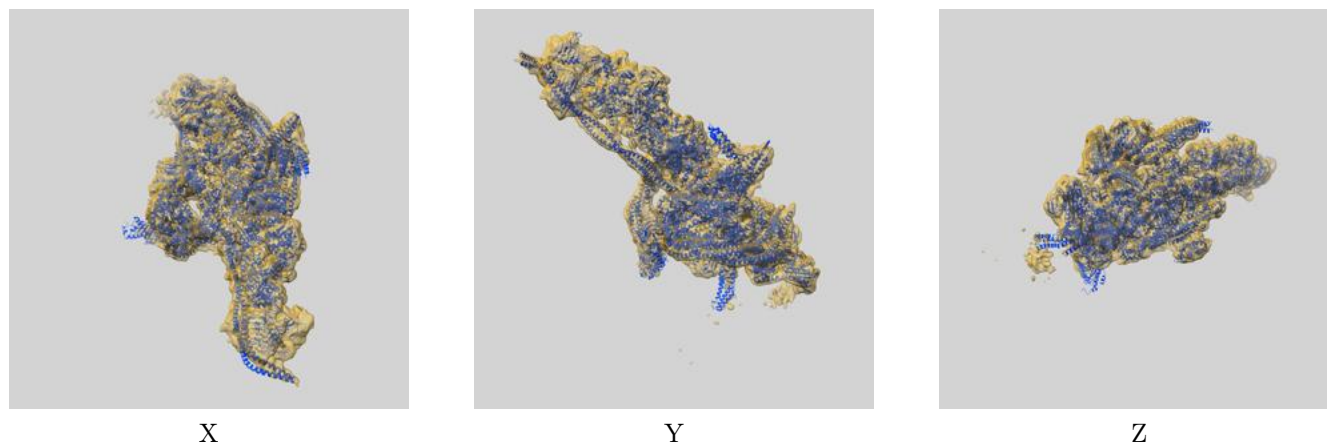
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

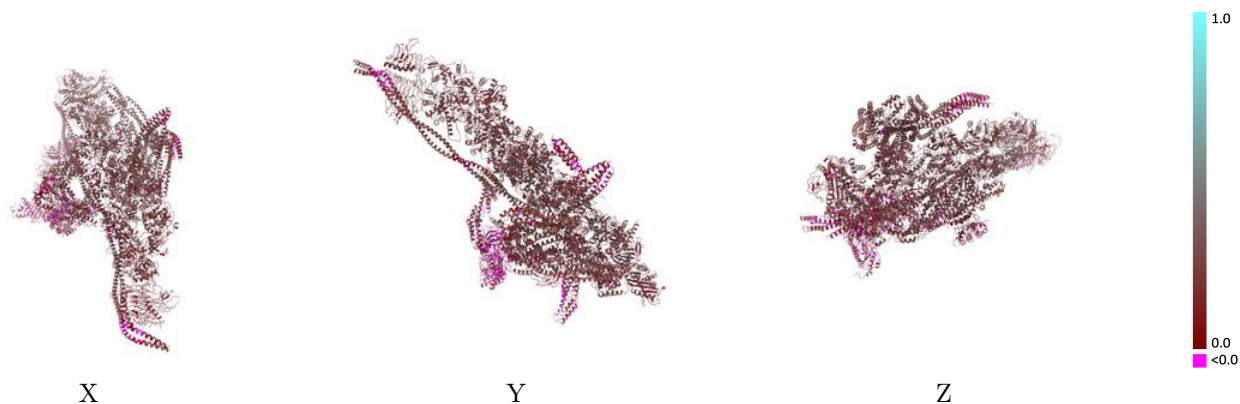
This section contains information regarding the fit between EMDB map EMD-2860 and PDB model 6F3A. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



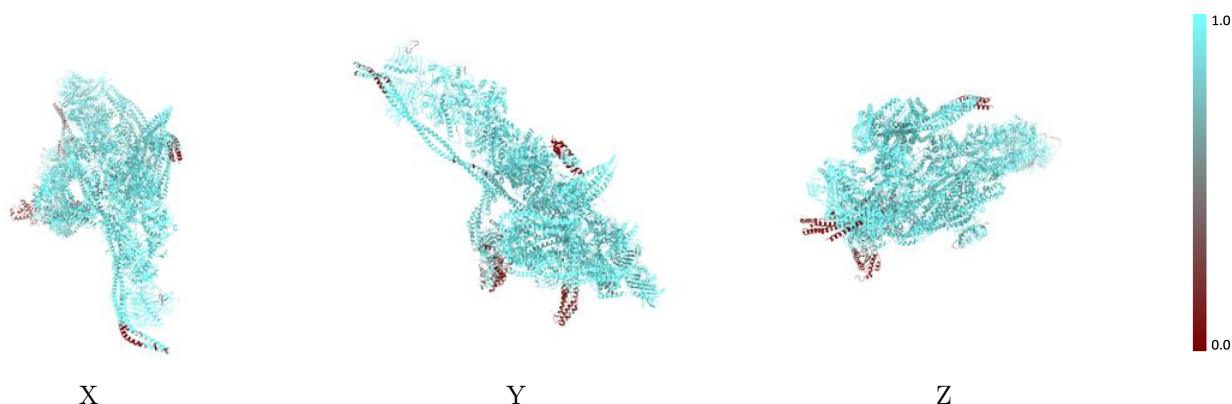
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



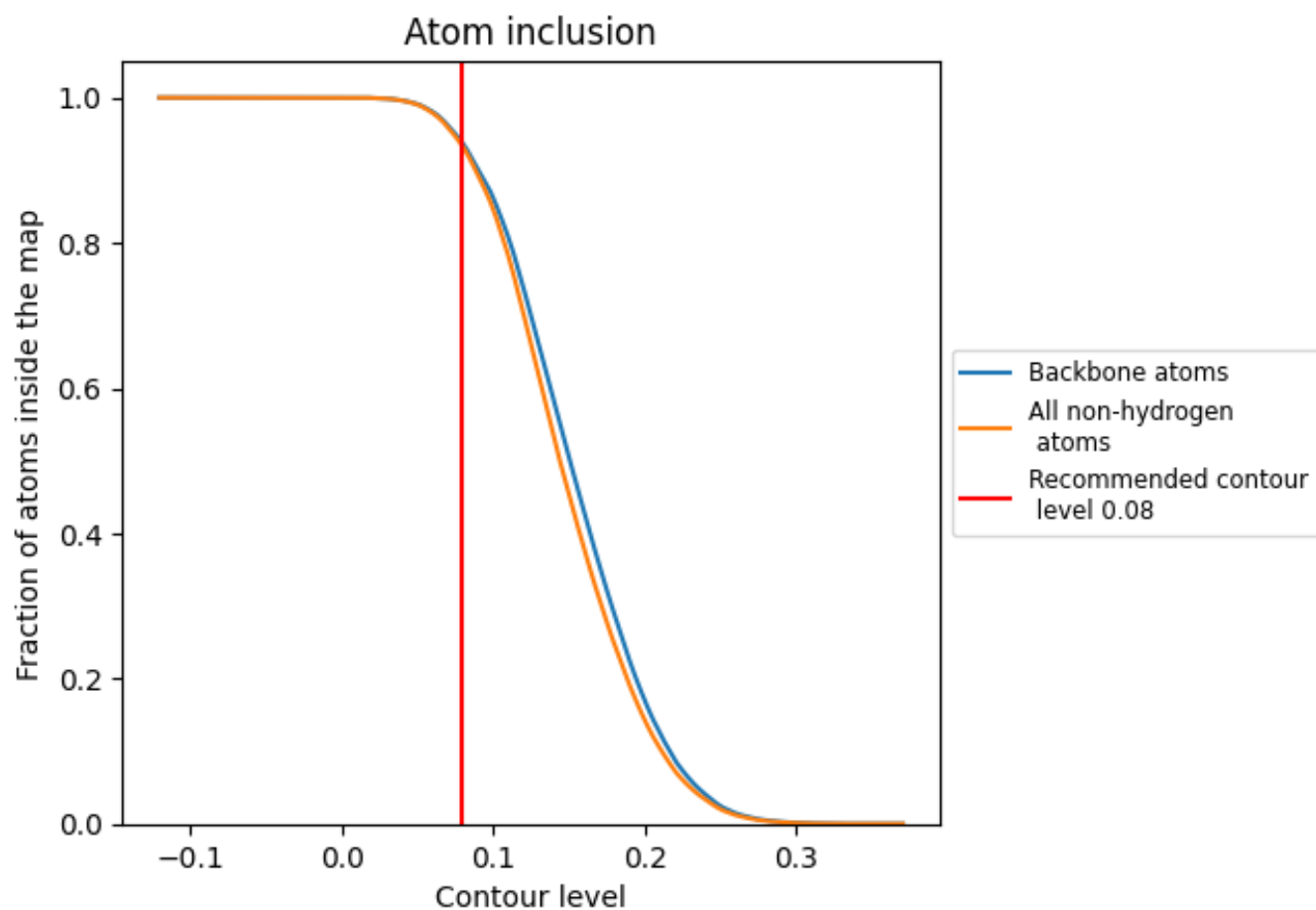
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9327	 0.2280
5	 0.8182	 0.2340
6	 0.8182	 0.2130
A	 0.9973	 0.2510
B	 0.9973	 0.2640
C	 0.9941	 0.2690
D	 0.9968	 0.2650
E	 0.9957	 0.2720
F	 0.9941	 0.2680
G	 0.9984	 0.2650
H	 0.9962	 0.2690
I	 0.9892	 0.2510
J	 0.9978	 0.2680
K	 0.9913	 0.2460
L	 0.9985	 0.2550
M	 0.9881	 0.2430
N	 0.9821	 0.2570
O	 1.0000	 0.2620
P	 1.0000	 0.2870
Q	 0.4414	 0.1280
R	 1.0000	 0.2840
U	 0.9371	 0.1700
V	 1.0000	 0.2350
Y	 0.9909	 0.2810
Z	 1.0000	 0.2800
a	 0.9768	 0.3170
b	 0.9973	 0.3000
c	 0.9828	 0.2780
d	 0.9832	 0.2960
e	 0.8974	 0.1650
f	 0.8743	 0.2210
g	 0.7787	 0.0560
h	 0.8556	 0.1380
j	 0.5333	 0.1620
k	 0.1385	 0.0480



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Chain	Atom inclusion	Q-score
l	 0.5887	 0.0700
z	 0.9208	 0.2330