



Full wwPDB EM Validation Report ⓘ

Dec 28, 2024 – 12:24 PM EST

PDB ID : 6ZNL
EMDB ID : EMD-11313
Title : Cryo-EM structure of the dynactin complex
Authors : Lau, C.K.; Lacey, S.E.; Carter, A.P.
Deposited on : 2020-07-06
Resolution : 3.80 Å(reported)

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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:

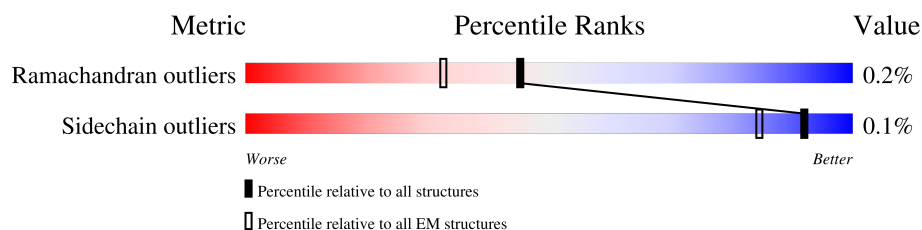
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.80 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.




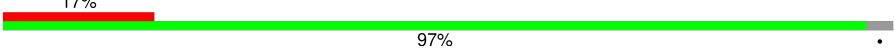
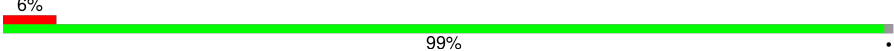


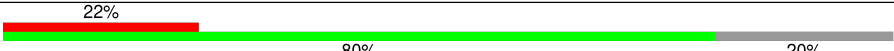
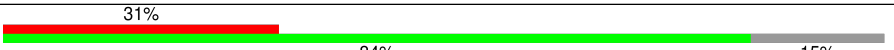
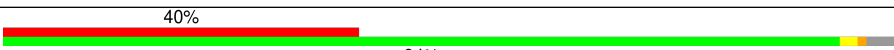
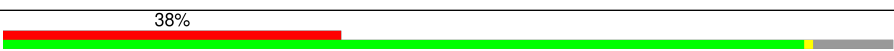

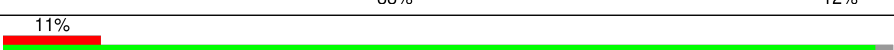


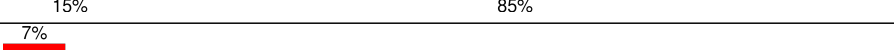
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	B	376	
1	C	376	
1	D	376	
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	

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Mol	Chain	Length	Quality of chain
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	m	405	
6	n	405	
7	O	186	
7	o	186	
8	U	190	
9	V	182	
10	Y	467	
11	Z	1286	
11	z	1286	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 52864 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
1	A	370	Total	C	N	O	S	0	0
			2944	1886	509	539	10		
1	B	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	C	375	Total	C	N	O	S	0	0
			2998	1918	514	556	10		
1	D	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	E	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	F	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	G	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	I	370	Total	C	N	O	S	0	0
			2941	1885	509	537	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	370	Total	C	N	O	S	0	0
			2885	1827	486	550	22		

- Molecule 3 is a protein called Arp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	379	Total	C	N	O	S	0	0
			2932	1888	496	532	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	278	Total	C	N	O	S	0	0
			2264	1428	396	434	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	269	Total	C	N	O	S	0	0
			2122	1323	370	418	11		

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	340	Total	C	N	O	S	0	0
			2238	1382	408	443	5		
6	N	280	Total	C	N	O	S	0	0
			1767	1089	327	346	5		
6	m	325	Total	C	N	O	S	0	0
			2262	1413	397	446	6		
6	n	343	Total	C	N	O	S	0	0
			2349	1471	423	451	4		

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	179	Total	C	N	O	S	0	0
			1183	736	210	233	4		
7	o	170	Total	C	N	O	S	0	0
			1082	679	208	194	1		

- Molecule 8 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	167	Total	C	N	O	S	0	0
			1224	771	212	231	10		

- Molecule 9 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	179	Total	C	N	O	S	0	0
			1260	818	222	211	9		

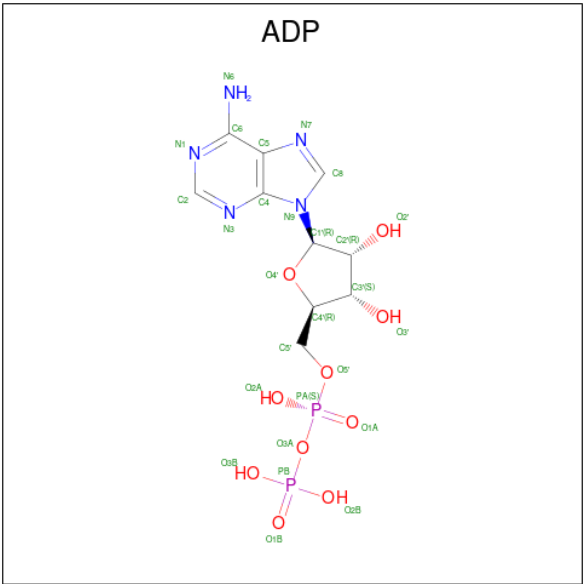
- Molecule 10 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	410	Total	C	N	O	S	0	0
			2960	1868	543	529	20		

- Molecule 11 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	192	Total	C	N	O	S	0	0
			1444	904	262	275	3		
11	z	155	Total	C	N	O	S	0	0
			952	583	189	177	3		

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



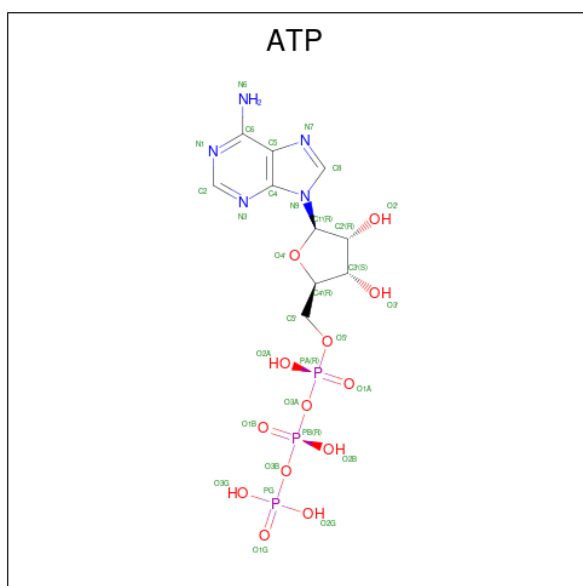
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



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

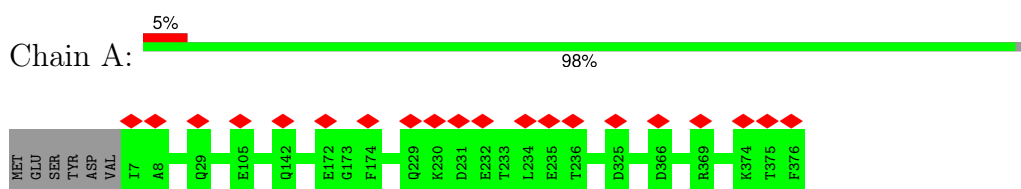
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	Y	3	Total	Zn	0
			3	3	

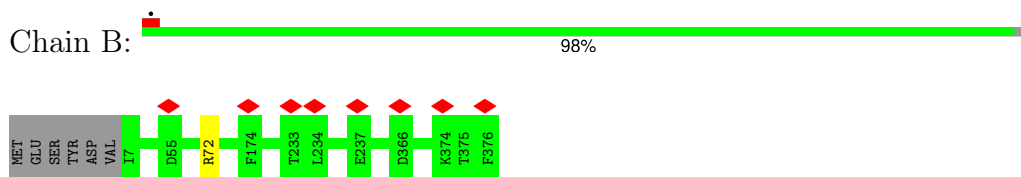
3 Residue-property plots [i](#)

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.

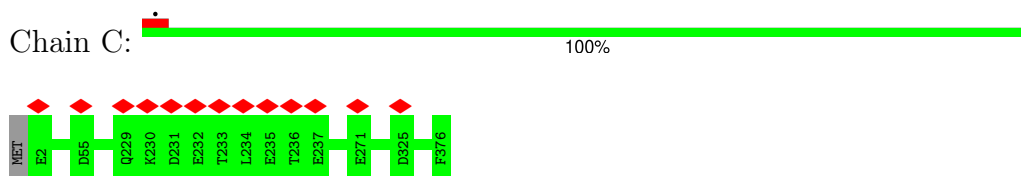
- Molecule 1: ARP1 actin related protein 1 homolog A



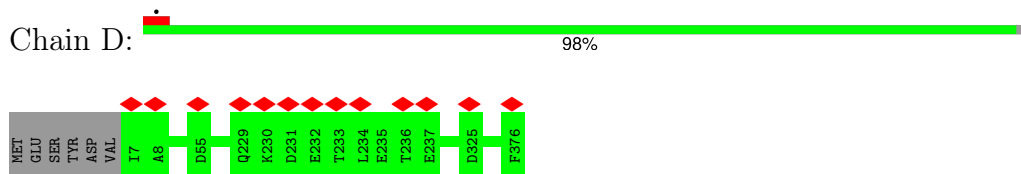
- Molecule 1: ARP1 actin related protein 1 homolog A



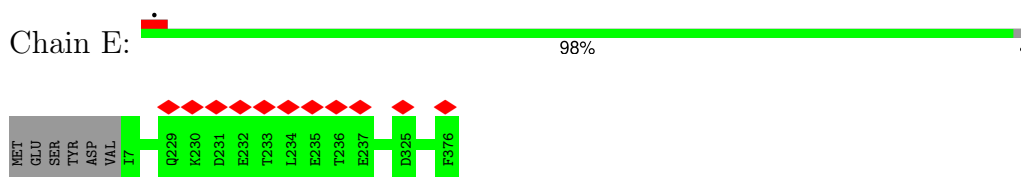
- Molecule 1: ARP1 actin related protein 1 homolog A



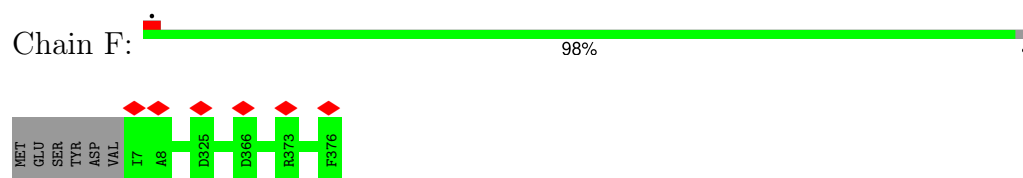
- Molecule 1: ARP1 actin related protein 1 homolog A



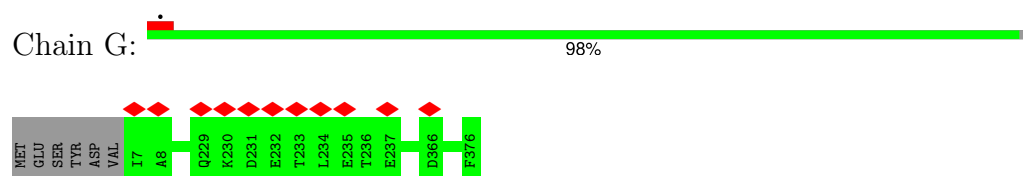
- Molecule 1: ARP1 actin related protein 1 homolog A



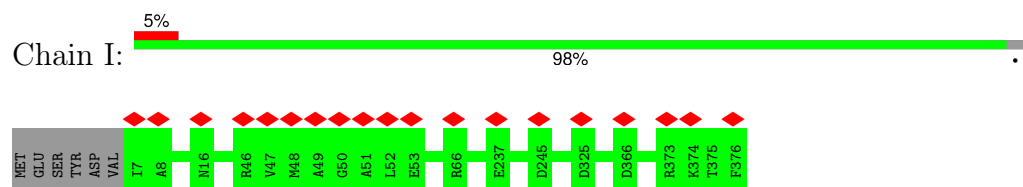
- Molecule 1: ARP1 actin related protein 1 homolog A



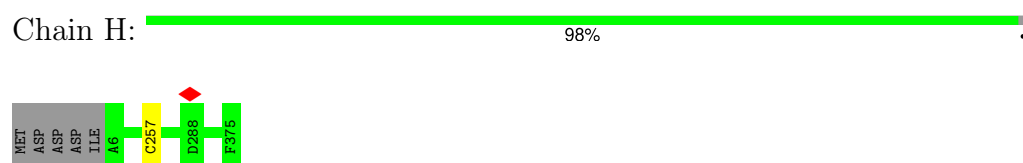
- Molecule 1: ARP1 actin related protein 1 homolog A



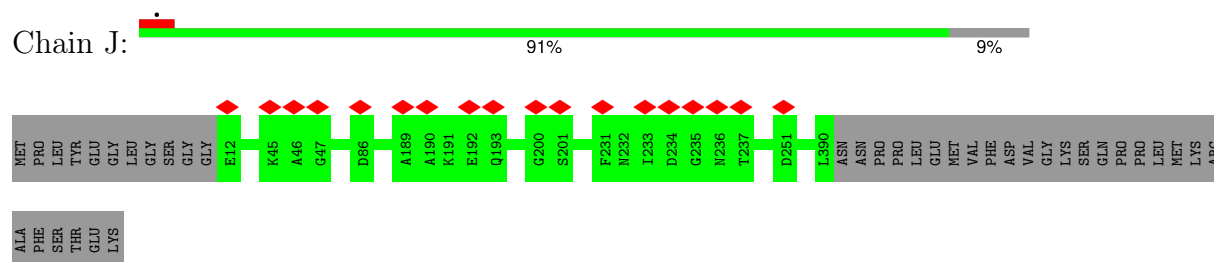
- Molecule 1: ARP1 actin related protein 1 homolog A



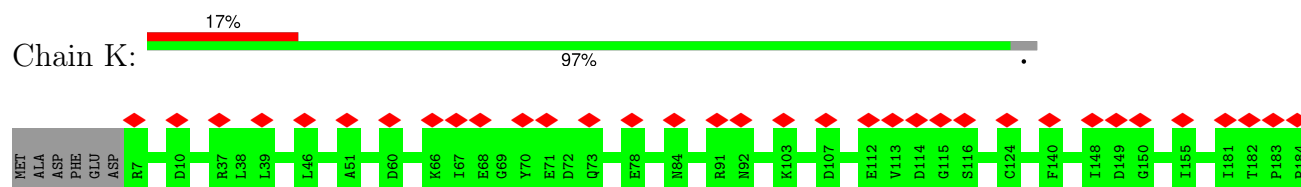
- Molecule 2: Actin, cytoplasmic 1

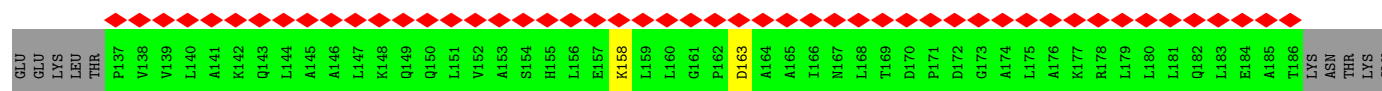


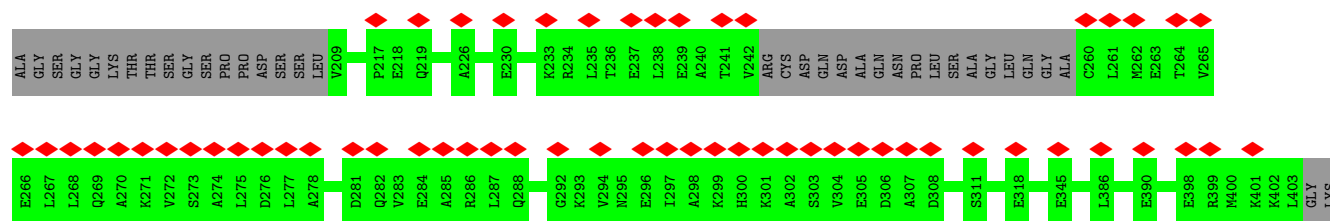
- Molecule 3: Arp11



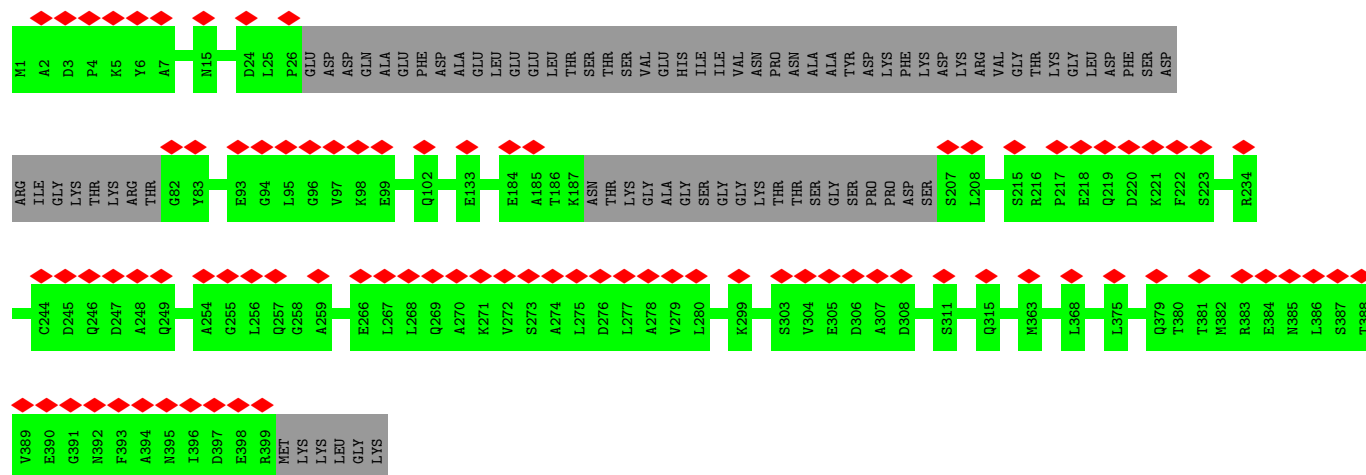
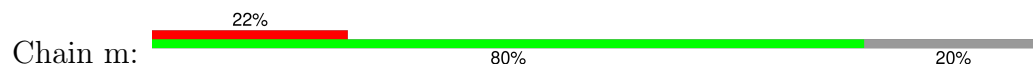
- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1



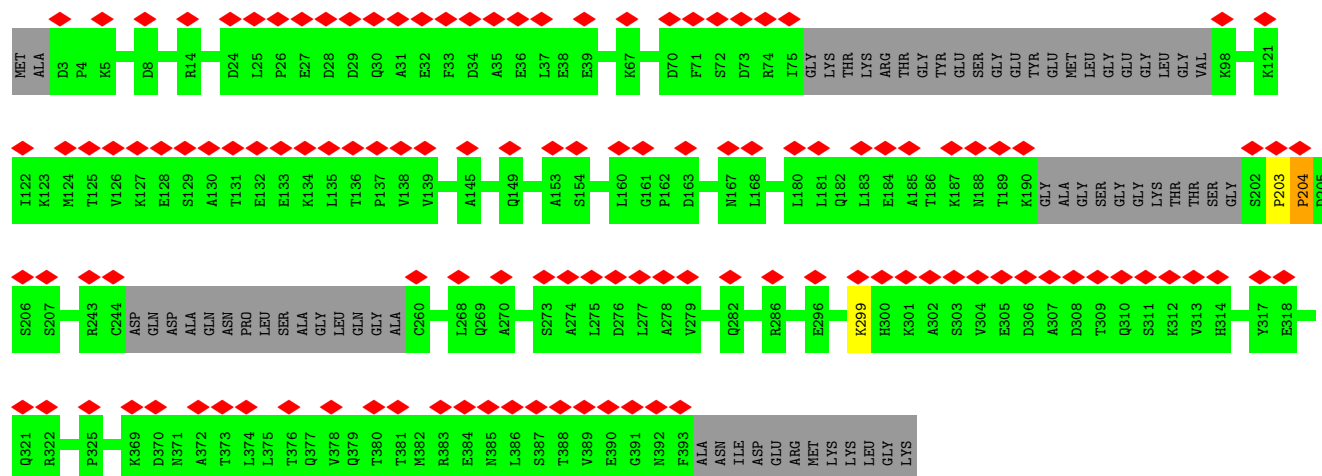
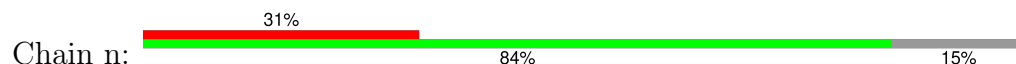




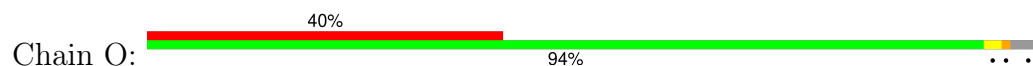
• Molecule 6: Dynactin subunit 2

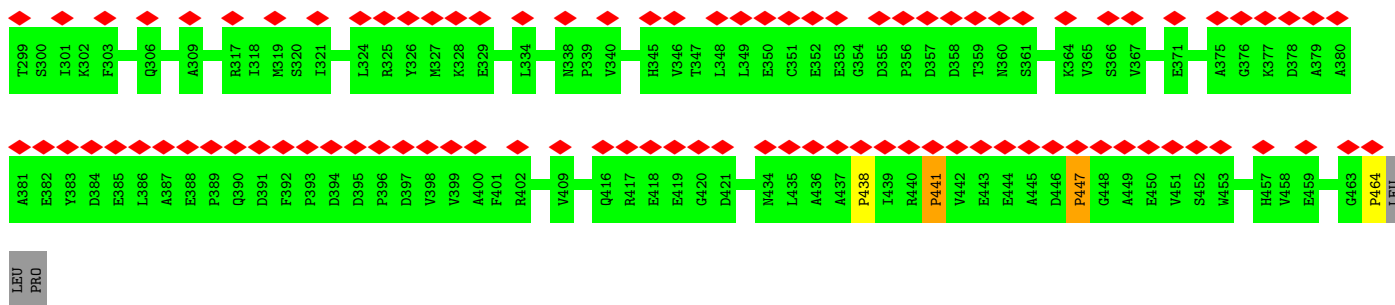


• Molecule 6: Dynactin subunit 2



• Molecule 7: Dynactin subunit 3

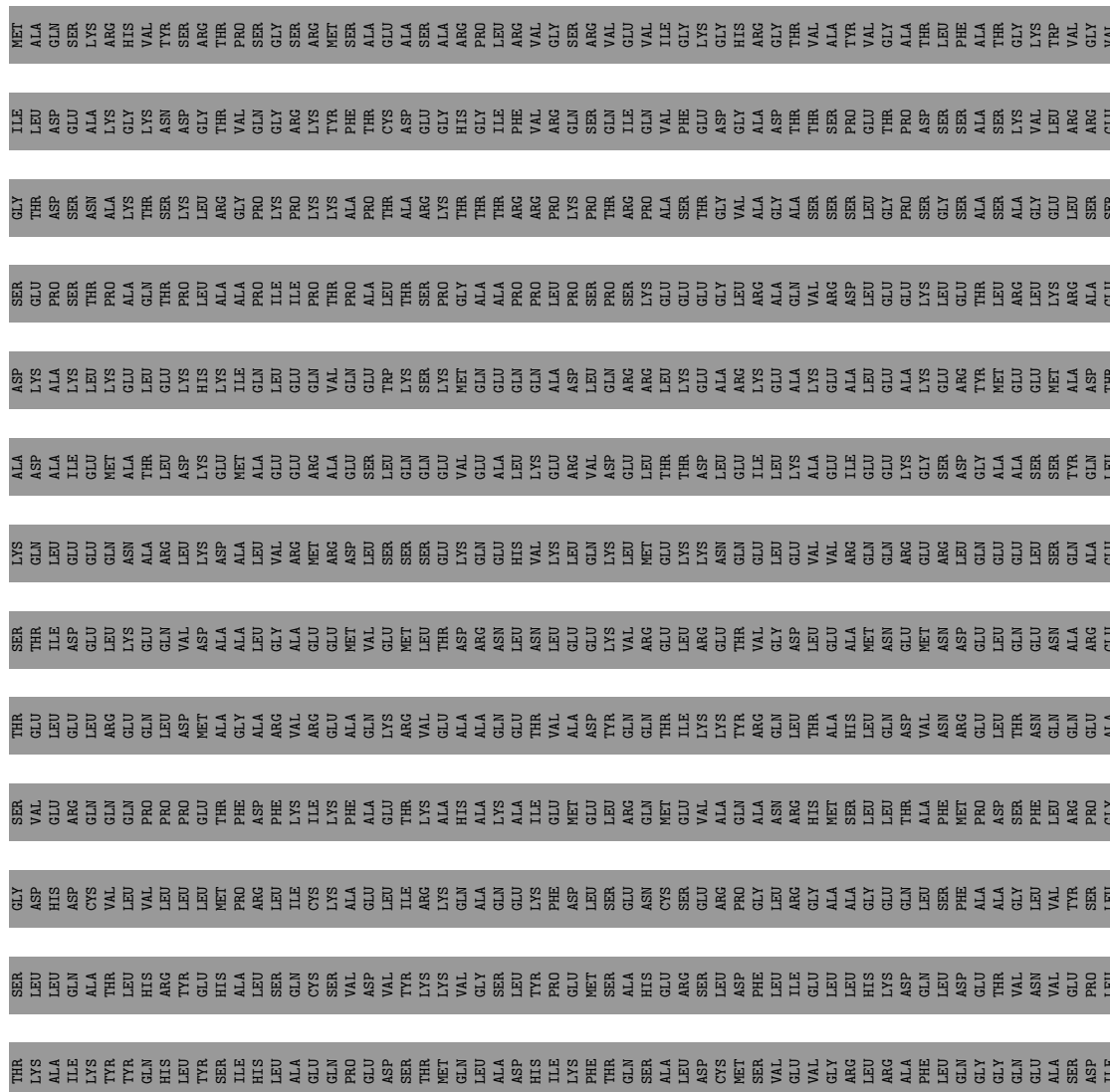




- Molecule 11: Dynactin subunit 1

[illegible]

- Molecule 11: Dynactin subunit 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	336972	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 ($e^-/\text{\AA}^2$)	52	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	0.258	Depositor
Minimum map value	-0.184	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.053	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/3013	0.77	0/4070
1	B	0.67	0/3025	0.79	0/4085
1	C	0.67	0/3068	0.78	0/4144
1	D	0.66	0/3025	0.78	0/4085
1	E	0.67	0/3025	0.78	0/4085
1	F	0.68	0/3025	0.78	0/4085
1	G	0.67	0/3025	0.77	0/4085
1	I	0.67	0/3010	0.75	0/4066
2	H	0.68	0/2948	0.73	0/3991
3	J	0.68	0/2994	0.75	0/4066
4	K	0.68	0/2316	0.75	0/3135
5	L	0.69	0/2156	0.76	0/2906
6	M	0.77	0/2259	0.81	1/3090 (0.0%)
6	N	0.79	0/1783	0.82	0/2451
6	m	0.73	0/2287	0.77	0/3119
6	n	0.74	0/2375	0.80	2/3246 (0.1%)
7	O	0.77	0/1194	0.81	2/1631 (0.1%)
7	o	0.79	0/1093	0.81	1/1498 (0.1%)
8	U	0.71	0/1241	0.79	0/1691
9	V	0.71	0/1286	0.78	0/1757
10	Y	0.71	0/3020	0.81	5/4119 (0.1%)
11	Z	0.70	0/1467	0.77	1/1992 (0.1%)
11	z	0.80	0/955	0.95	8/1302 (0.6%)
All	All	0.70	0/53590	0.78	20/72699 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	z	1133	PRO	N-CA-CB	6.13	110.65	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	1147	PRO	N-CA-CB	6.06	110.58	103.30
11	z	1197	PRO	N-CA-CB	6.01	110.51	103.30
11	z	1132	PRO	N-CA-CB	6.00	110.50	103.30
11	z	1147	PRO	N-CA-CB	5.85	110.32	103.30
11	z	1143	PRO	N-CA-CB	5.82	110.29	103.30
6	n	204	PRO	N-CA-CB	5.77	110.22	103.30
7	O	70	PRO	N-CA-CB	5.76	110.21	103.30
11	z	1192	PRO	N-CA-CB	5.71	110.15	103.30
10	Y	447	PRO	N-CA-CB	5.70	110.14	103.30
10	Y	438	PRO	N-CA-CB	5.65	110.08	103.30
10	Y	441	PRO	N-CA-CB	5.65	110.08	103.30
10	Y	464	PRO	N-CA-CB	5.62	110.04	103.30
11	z	1204	PRO	N-CA-CB	5.60	110.02	103.30
7	O	24	PRO	N-CA-CB	5.47	109.87	103.30
6	M	217	PRO	N-CA-CB	5.46	109.85	103.30
7	o	70	PRO	N-CA-CB	5.41	109.79	103.30
11	z	1142	PRO	N-CA-CB	5.33	109.69	103.30
10	Y	175	PRO	N-CA-CB	5.29	109.65	103.30
6	n	203	PRO	N-CA-CB	5.21	109.56	103.30

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%)	353 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	355 (96%)	13 (4%)	0	100	100
1	E	368/376 (98%)	358 (97%)	10 (3%)	0	100	100
1	F	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
1	G	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
1	I	368/376 (98%)	347 (94%)	21 (6%)	0	100	100
2	H	368/375 (98%)	352 (96%)	16 (4%)	0	100	100
3	J	377/417 (90%)	347 (92%)	30 (8%)	0	100	100
4	K	276/286 (96%)	259 (94%)	17 (6%)	0	100	100
5	L	267/272 (98%)	258 (97%)	9 (3%)	0	100	100
6	M	330/405 (82%)	299 (91%)	29 (9%)	2 (1%)	22	55
6	N	270/405 (67%)	258 (96%)	10 (4%)	2 (1%)	19	52
6	m	319/405 (79%)	301 (94%)	18 (6%)	0	100	100
6	n	335/405 (83%)	305 (91%)	28 (8%)	2 (1%)	22	55
7	O	177/186 (95%)	159 (90%)	15 (8%)	3 (2%)	7	34
7	o	168/186 (90%)	154 (92%)	13 (8%)	1 (1%)	22	55
8	U	165/190 (87%)	141 (86%)	24 (14%)	0	100	100
9	V	177/182 (97%)	161 (91%)	16 (9%)	0	100	100
10	Y	404/467 (86%)	355 (88%)	46 (11%)	3 (1%)	19	52
11	Z	190/1286 (15%)	176 (93%)	13 (7%)	1 (0%)	25	58
11	z	147/1286 (11%)	139 (95%)	7 (5%)	1 (1%)	19	52
All	All	6919/9761 (71%)	6504 (94%)	400 (6%)	15 (0%)	45	74

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
7	O	24	PRO
10	Y	175	PRO
10	Y	441	PRO
6	n	204	PRO
11	z	1142	PRO
6	n	299	LYS

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Mol	Chain	Res	Type
6	N	158	LYS
6	N	163	ASP
7	O	61	ILE
7	O	69	ASP
7	o	69	ASP
10	Y	447	PRO
6	M	166	ILE
11	Z	1147	PRO

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	315/324 (97%)	315 (100%)	0	100	100
1	B	318/324 (98%)	317 (100%)	1 (0%)	91	92
1	C	323/324 (100%)	323 (100%)	0	100	100
1	D	318/324 (98%)	318 (100%)	0	100	100
1	E	318/324 (98%)	318 (100%)	0	100	100
1	F	318/324 (98%)	318 (100%)	0	100	100
1	G	318/324 (98%)	318 (100%)	0	100	100
1	I	314/324 (97%)	314 (100%)	0	100	100
2	H	313/318 (98%)	312 (100%)	1 (0%)	91	92
3	J	323/363 (89%)	323 (100%)	0	100	100
4	K	247/254 (97%)	247 (100%)	0	100	100
5	L	238/241 (99%)	237 (100%)	1 (0%)	89	91
6	M	164/346 (47%)	164 (100%)	0	100	100
6	N	112/346 (32%)	112 (100%)	0	100	100
6	m	197/346 (57%)	197 (100%)	0	100	100
6	n	192/346 (56%)	192 (100%)	0	100	100
7	O	87/160 (54%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	o	67/160 (42%)	67 (100%)	0	100	100
8	U	129/163 (79%)	129 (100%)	0	100	100
9	V	121/163 (74%)	121 (100%)	0	100	100
10	Y	274/416 (66%)	274 (100%)	0	100	100
11	Z	154/1074 (14%)	154 (100%)	0	100	100
11	z	53/1074 (5%)	52 (98%)	1 (2%)	52	69
All	All	5213/8362 (62%)	5209 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	ARG
2	H	257	CYS
5	L	84	GLU
11	z	1274	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	ATP	H	401	-	28,33,33	0.70	0	34,52,52	0.76	1 (2%)
12	ADP	G	800	-	24,29,29	0.71	0	29,45,45	0.70	1 (3%)
12	ADP	F	800	-	24,29,29	0.72	0	29,45,45	0.72	1 (3%)
12	ADP	C	800	-	24,29,29	0.73	0	29,45,45	0.72	1 (3%)
12	ADP	D	800	-	24,29,29	0.73	0	29,45,45	0.72	1 (3%)
12	ADP	J	800	-	24,29,29	0.76	0	29,45,45	0.79	1 (3%)
12	ADP	B	800	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
12	ADP	I	800	-	24,29,29	0.72	0	29,45,45	0.73	1 (3%)
12	ADP	E	800	-	24,29,29	0.72	0	29,45,45	0.72	1 (3%)
12	ADP	A	800	-	24,29,29	0.73	0	29,45,45	0.71	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
13	ATP	H	401	-	-	6/18/38/38	0/3/3/3
12	ADP	G	800	-	-	4/12/32/32	0/3/3/3
12	ADP	F	800	-	-	2/12/32/32	0/3/3/3
12	ADP	C	800	-	-	3/12/32/32	0/3/3/3
12	ADP	D	800	-	-	4/12/32/32	0/3/3/3
12	ADP	J	800	-	-	3/12/32/32	0/3/3/3
12	ADP	B	800	-	-	3/12/32/32	0/3/3/3
12	ADP	I	800	-	-	4/12/32/32	0/3/3/3
12	ADP	E	800	-	-	4/12/32/32	0/3/3/3
12	ADP	A	800	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	401	ATP	C5-C6-N6	2.29	123.79	120.31
12	A	800	ADP	C5-C6-N6	2.27	123.77	120.31
12	I	800	ADP	C5-C6-N6	2.27	123.77	120.31
12	D	800	ADP	C5-C6-N6	2.26	123.75	120.31
12	F	800	ADP	C5-C6-N6	2.23	123.70	120.31
12	E	800	ADP	C5-C6-N6	2.20	123.66	120.31
12	G	800	ADP	C5-C6-N6	2.19	123.65	120.31
12	B	800	ADP	C5-C6-N6	2.19	123.65	120.31
12	C	800	ADP	C5-C6-N6	2.17	123.62	120.31
12	J	800	ADP	C5-C6-N6	2.16	123.61	120.31

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	800	ADP	PA-O3A-PB-O3B
12	B	800	ADP	C5'-O5'-PA-O1A
12	C	800	ADP	C5'-O5'-PA-O1A
12	D	800	ADP	C5'-O5'-PA-O2A
12	D	800	ADP	C5'-O5'-PA-O3A
12	E	800	ADP	C5'-O5'-PA-O2A
12	E	800	ADP	C5'-O5'-PA-O3A
12	G	800	ADP	C5'-O5'-PA-O2A
12	G	800	ADP	C5'-O5'-PA-O3A
12	I	800	ADP	C5'-O5'-PA-O2A
12	I	800	ADP	C5'-O5'-PA-O3A
13	H	401	ATP	PB-O3A-PA-O5'
13	H	401	ATP	C5'-O5'-PA-O1A
13	H	401	ATP	C5'-O5'-PA-O3A
12	D	800	ADP	C3'-C4'-C5'-O5'
12	E	800	ADP	C3'-C4'-C5'-O5'
12	F	800	ADP	C3'-C4'-C5'-O5'
12	C	800	ADP	C3'-C4'-C5'-O5'
12	G	800	ADP	C3'-C4'-C5'-O5'
12	A	800	ADP	C3'-C4'-C5'-O5'
12	B	800	ADP	C3'-C4'-C5'-O5'
12	D	800	ADP	O4'-C4'-C5'-O5'
12	I	800	ADP	C3'-C4'-C5'-O5'
12	E	800	ADP	O4'-C4'-C5'-O5'
12	G	800	ADP	O4'-C4'-C5'-O5'
12	F	800	ADP	O4'-C4'-C5'-O5'
12	C	800	ADP	O4'-C4'-C5'-O5'
12	B	800	ADP	O4'-C4'-C5'-O5'

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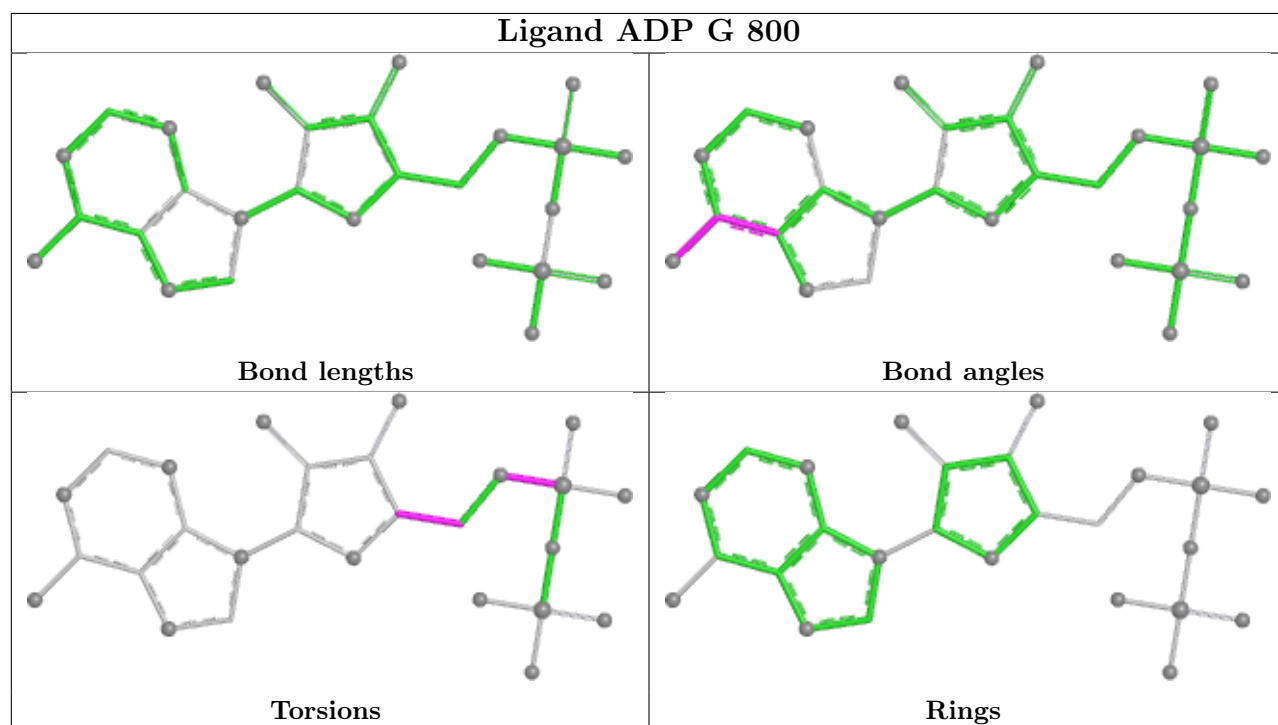
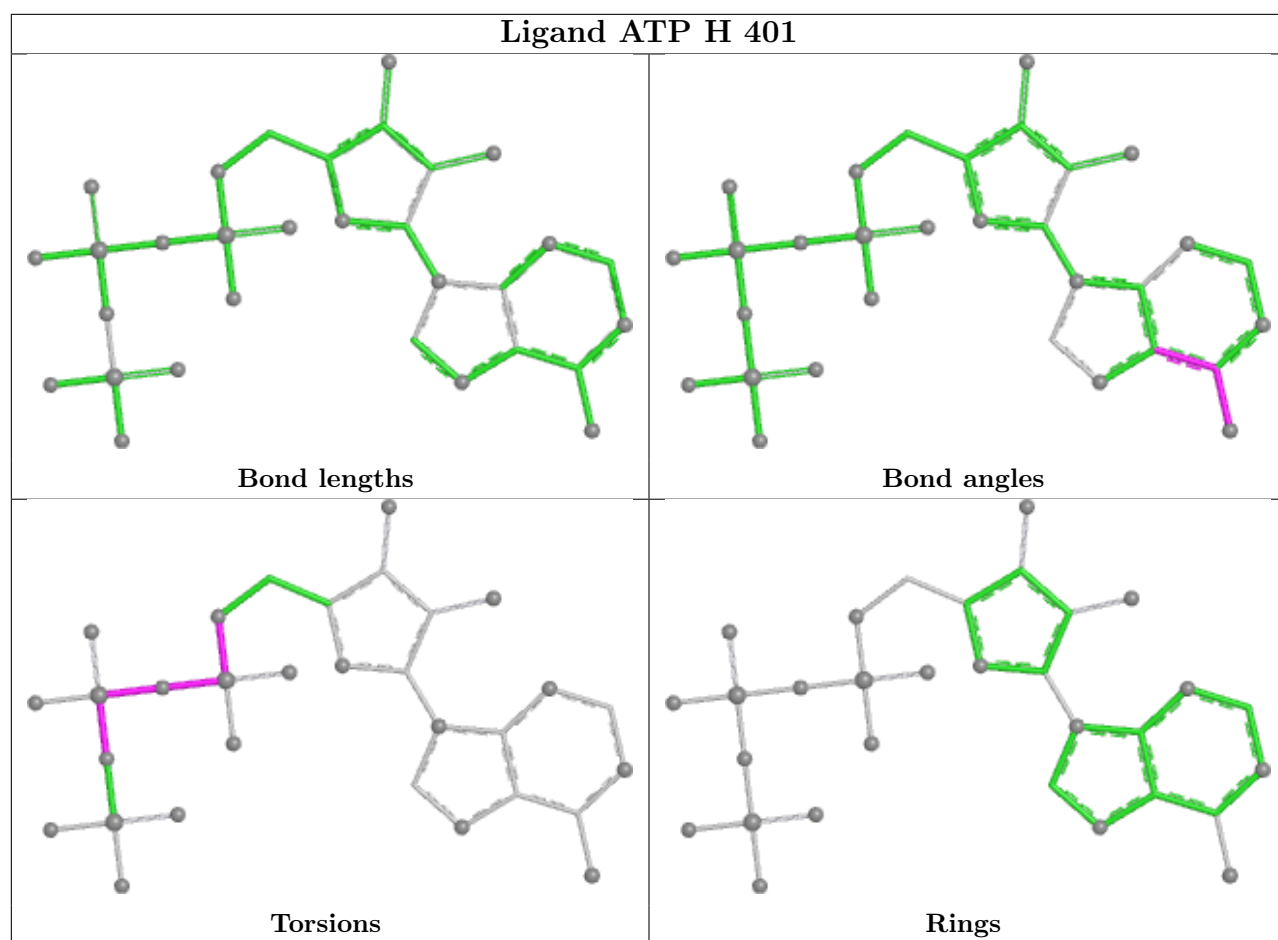
Continued from previous page...

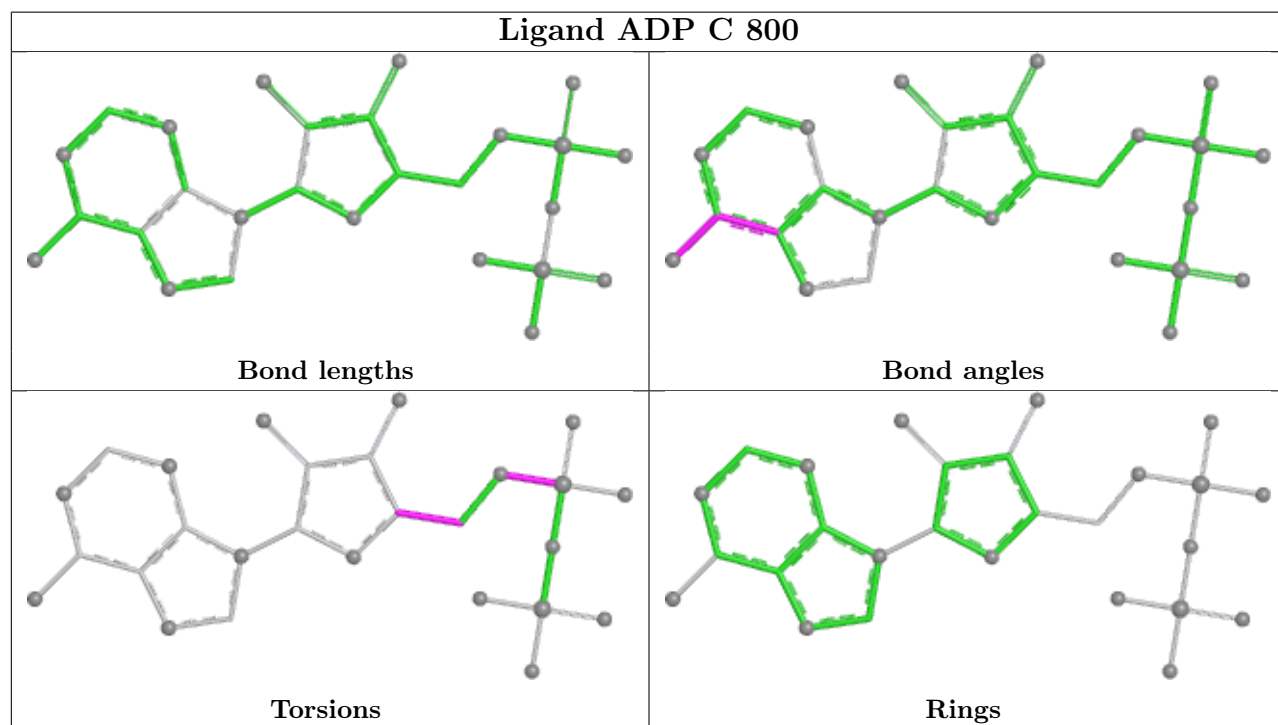
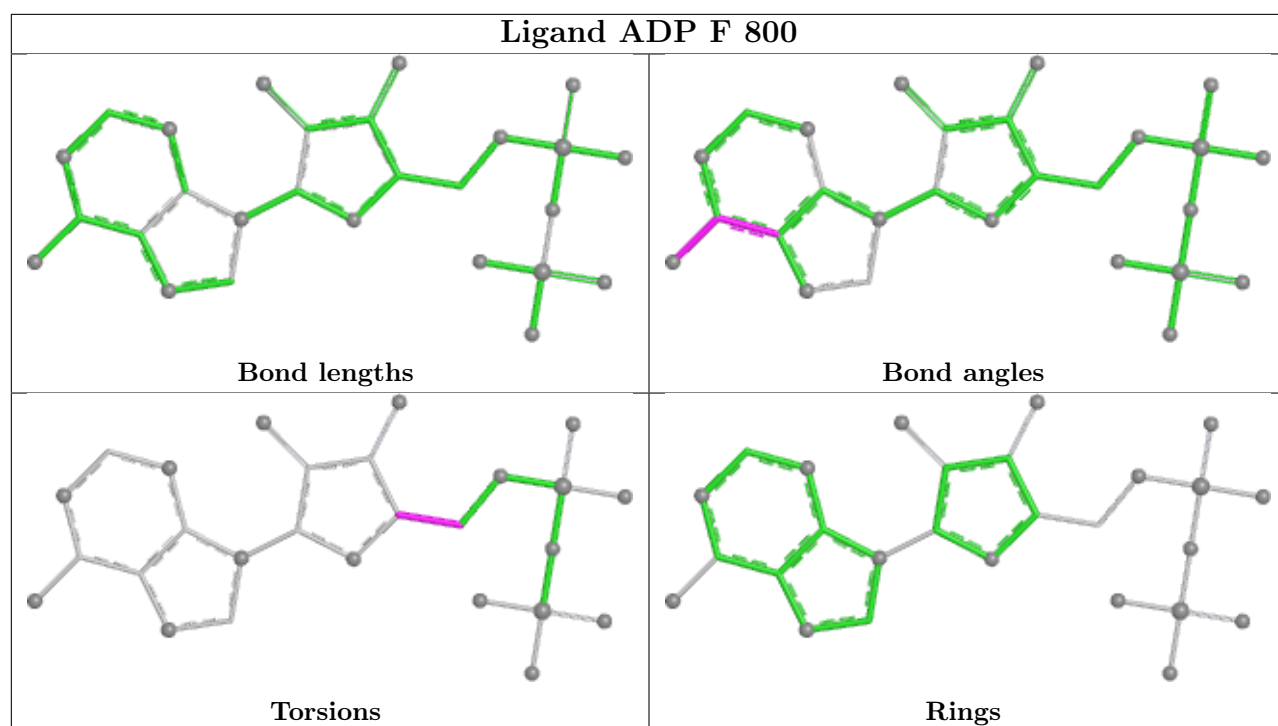
Mol	Chain	Res	Type	Atoms
12	A	800	ADP	O4'-C4'-C5'-O5'
12	J	800	ADP	PB-O3A-PA-O2A
13	H	401	ATP	PA-O3A-PB-O2B
12	A	800	ADP	C5'-O5'-PA-O2A
12	A	800	ADP	C5'-O5'-PA-O3A
12	J	800	ADP	C5'-O5'-PA-O1A
12	I	800	ADP	O4'-C4'-C5'-O5'
13	H	401	ATP	PG-O3B-PB-O2B
12	J	800	ADP	PB-O3A-PA-O1A
13	H	401	ATP	PA-O3A-PB-O1B

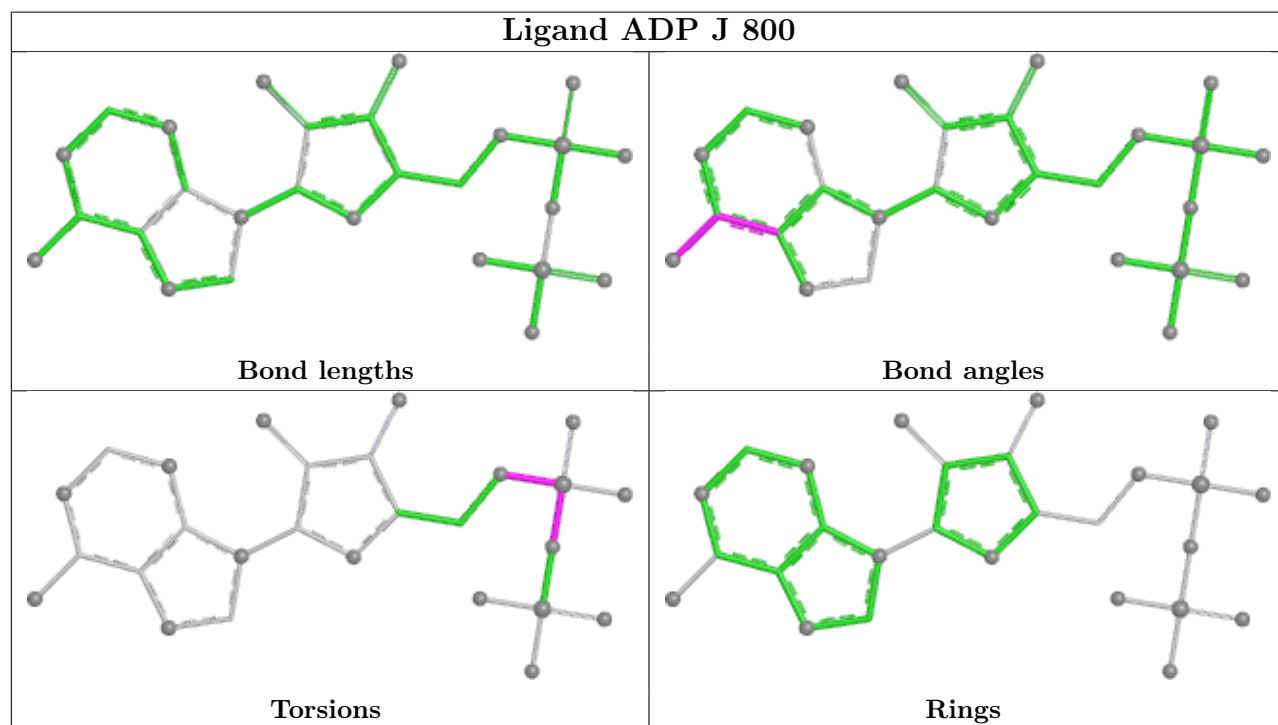
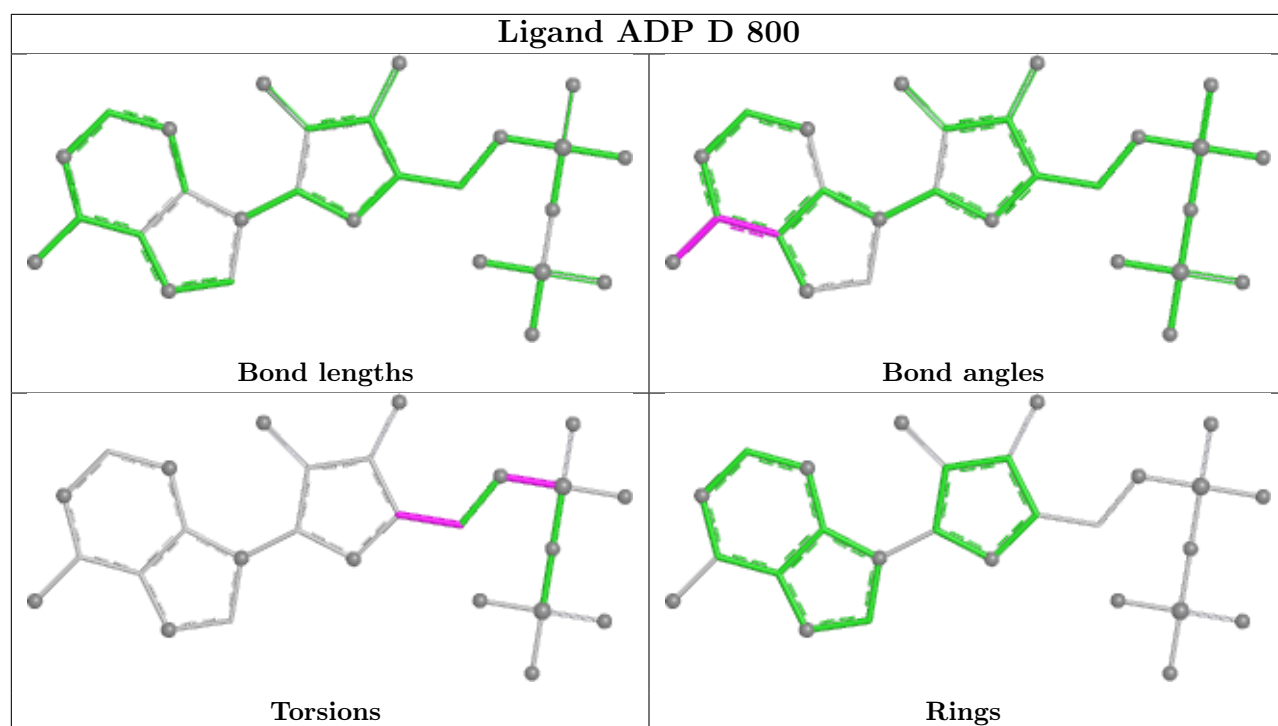
There are no ring outliers.

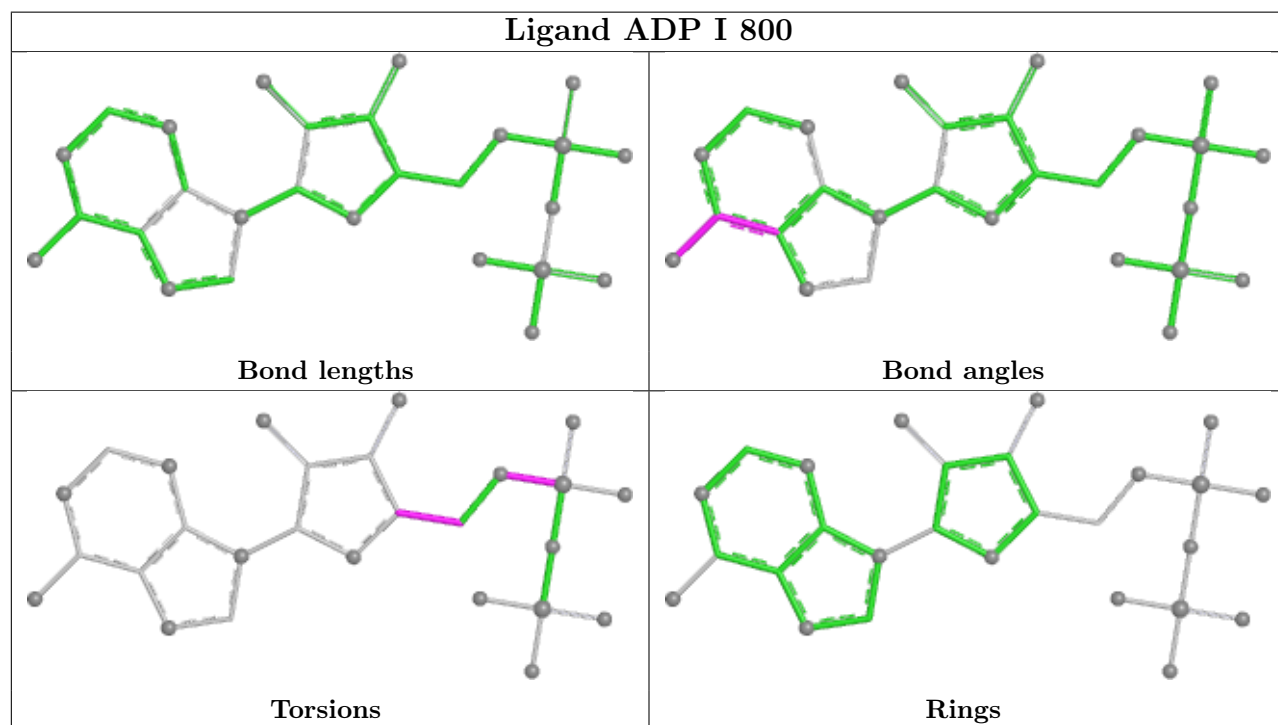
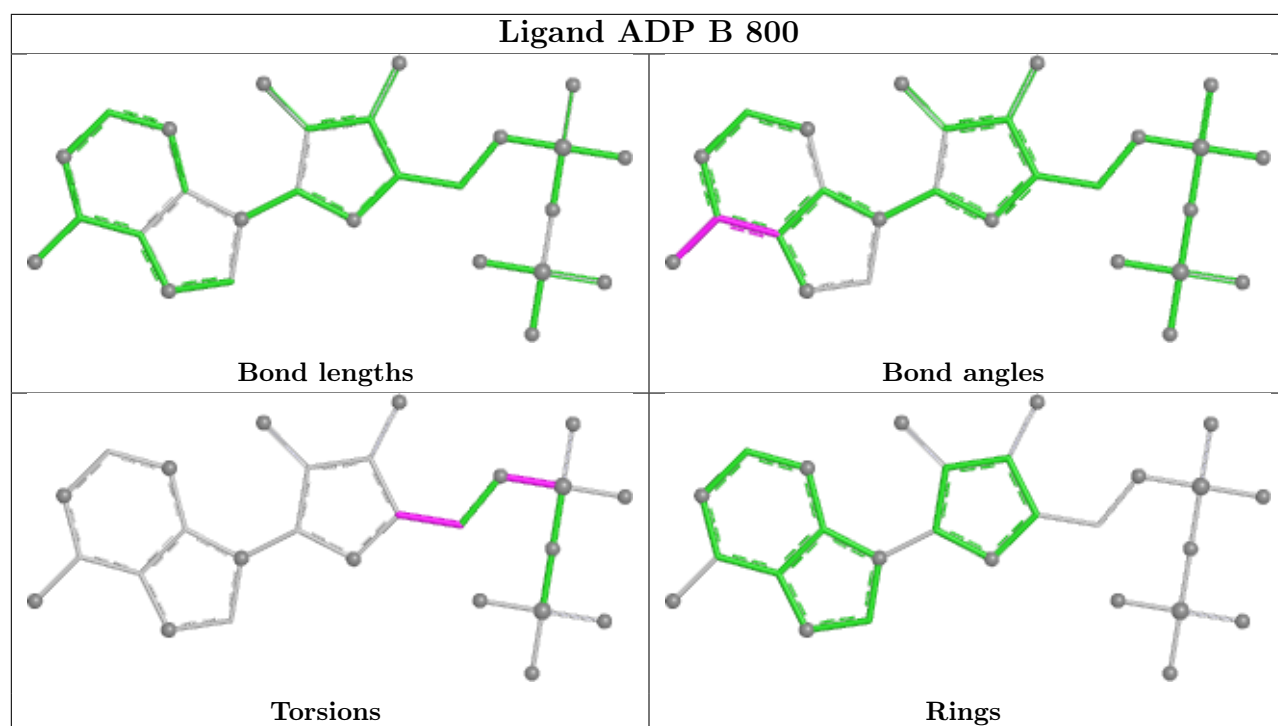
No monomer is involved in short contacts.

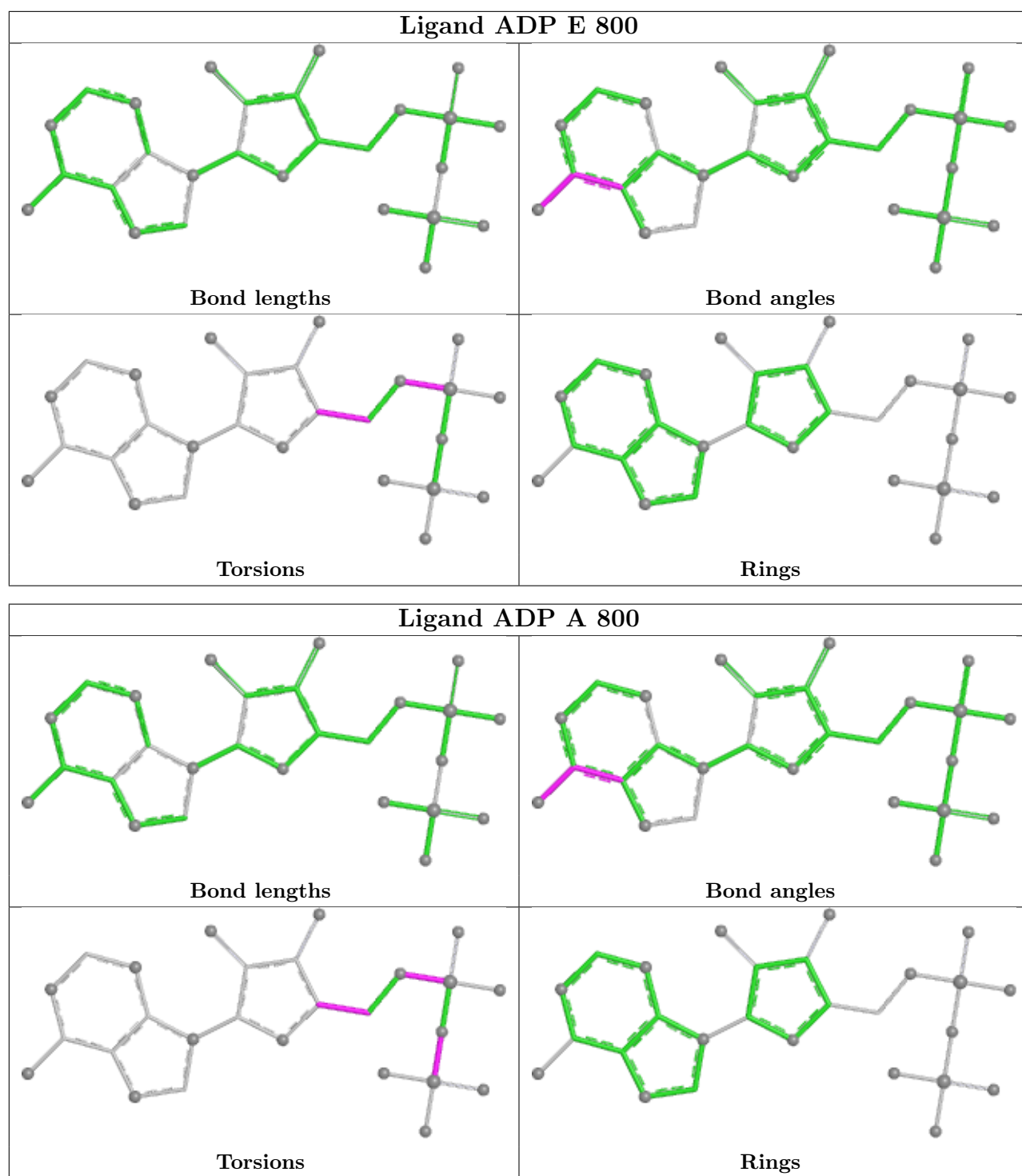
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	1220:VAL	C	1252:TYR	N	34.09

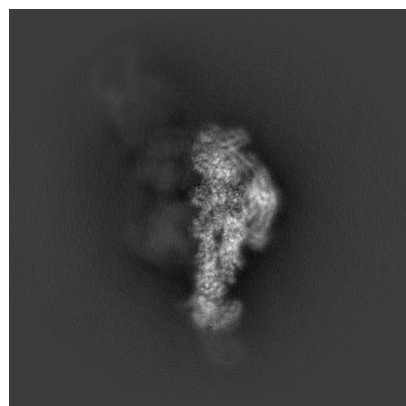
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11313. These allow visual inspection of the internal detail of the map and identification of artifacts.

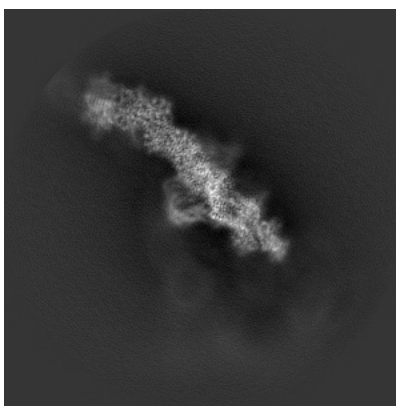
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

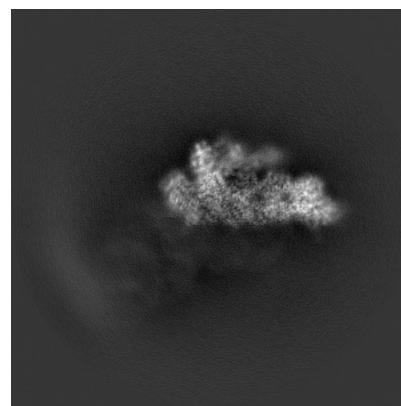
6.1.1 Primary map



X

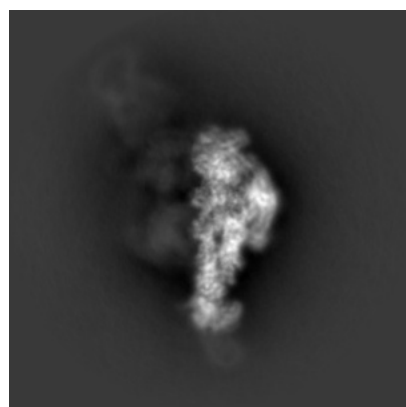


Y

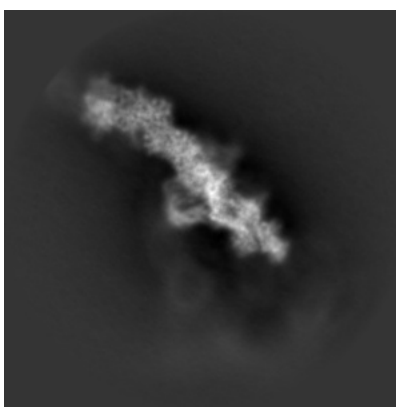


Z

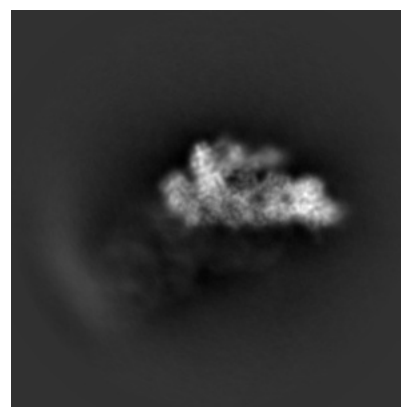
6.1.2 Raw map



X



Y

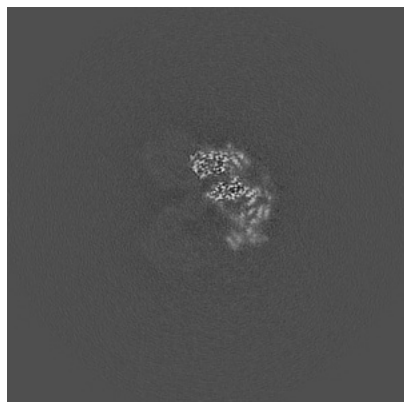


Z

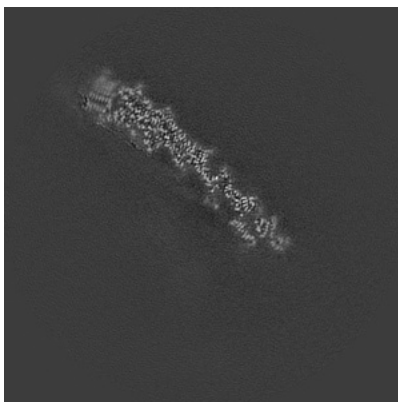
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

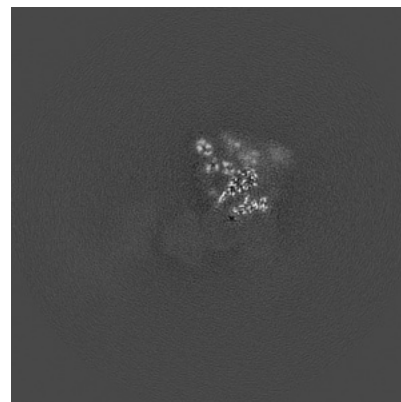
6.2.1 Primary map



X Index: 216

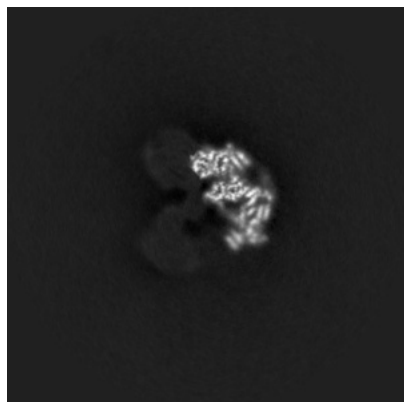


Y Index: 216

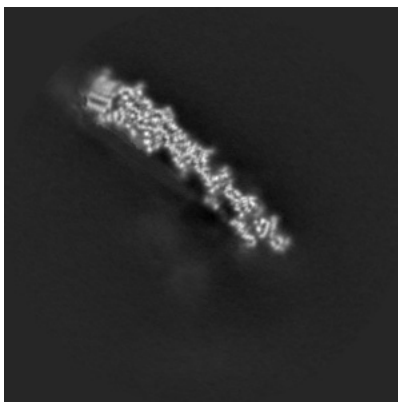


Z Index: 216

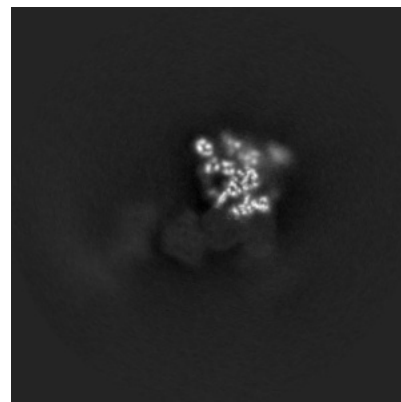
6.2.2 Raw map



X Index: 216



Y Index: 216

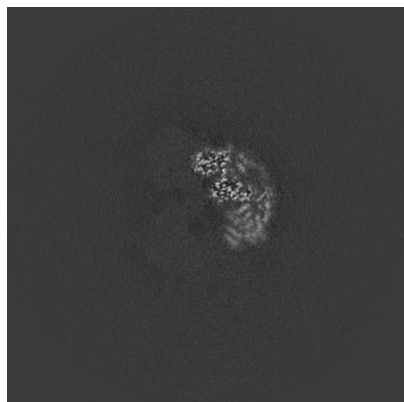


Z Index: 216

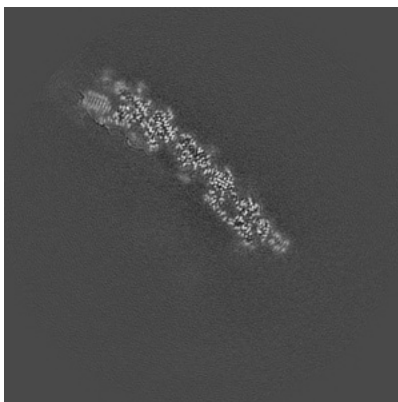
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

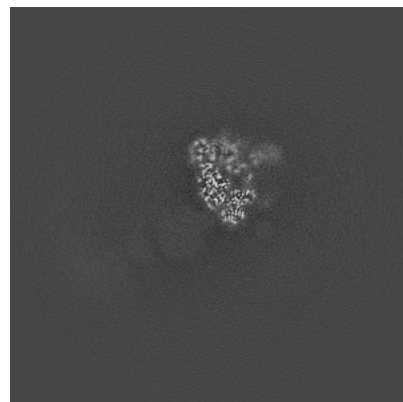
6.3.1 Primary map



X Index: 212

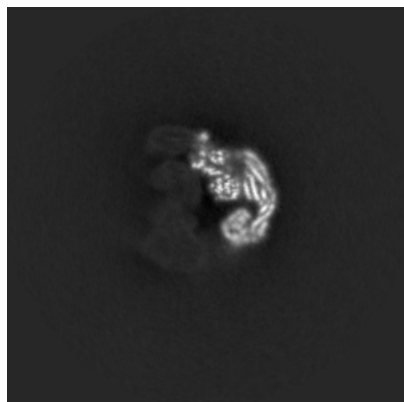


Y Index: 220

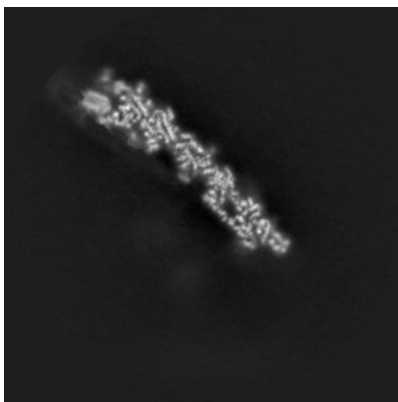


Z Index: 228

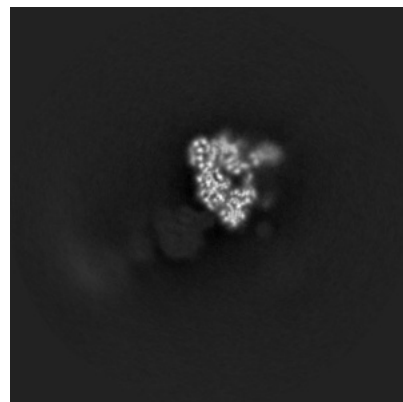
6.3.2 Raw map



X Index: 205



Y Index: 220

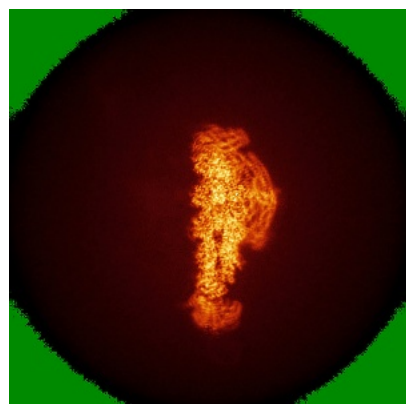


Z Index: 229

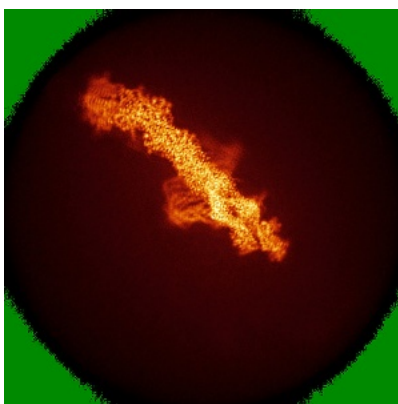
The images above show the largest variance slices of the map in three orthogonal directions.

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

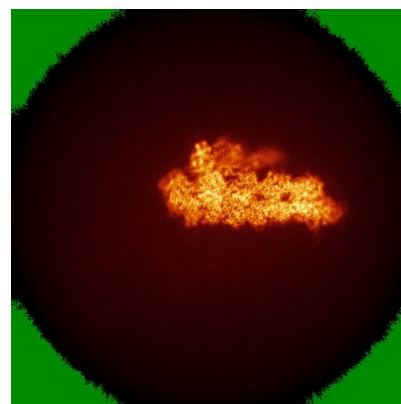
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

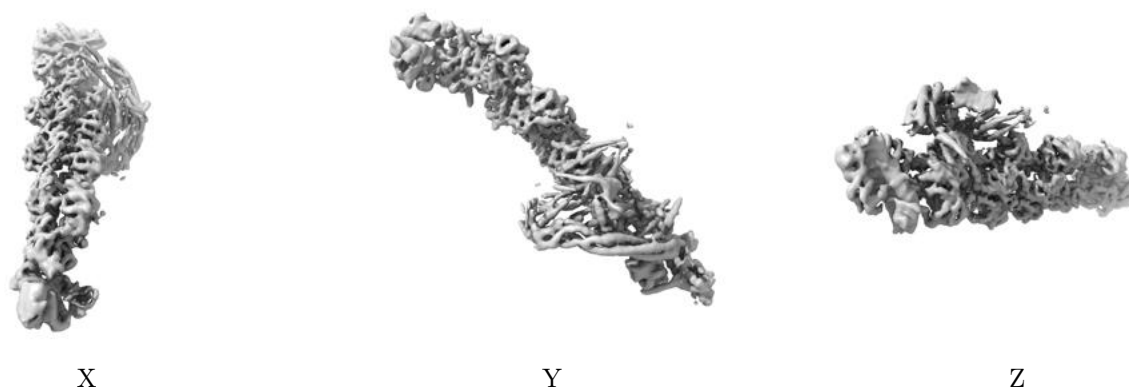
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.053. 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.

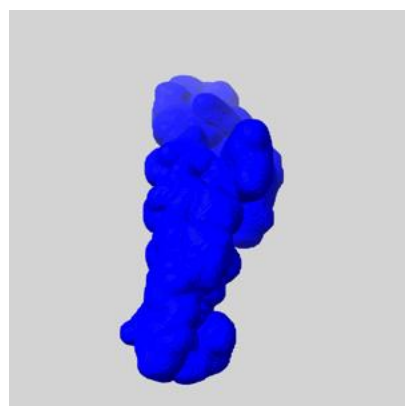
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

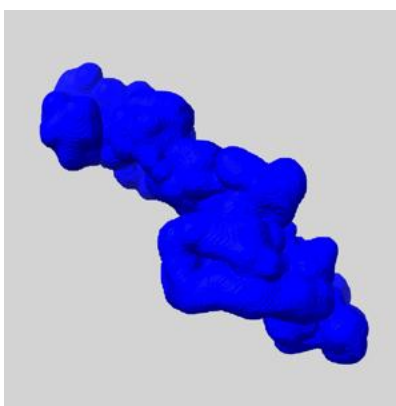
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

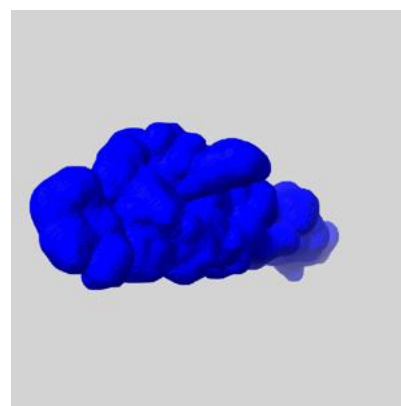
6.6.1 emd_11313_msk_1.map [i](#)



X



Y

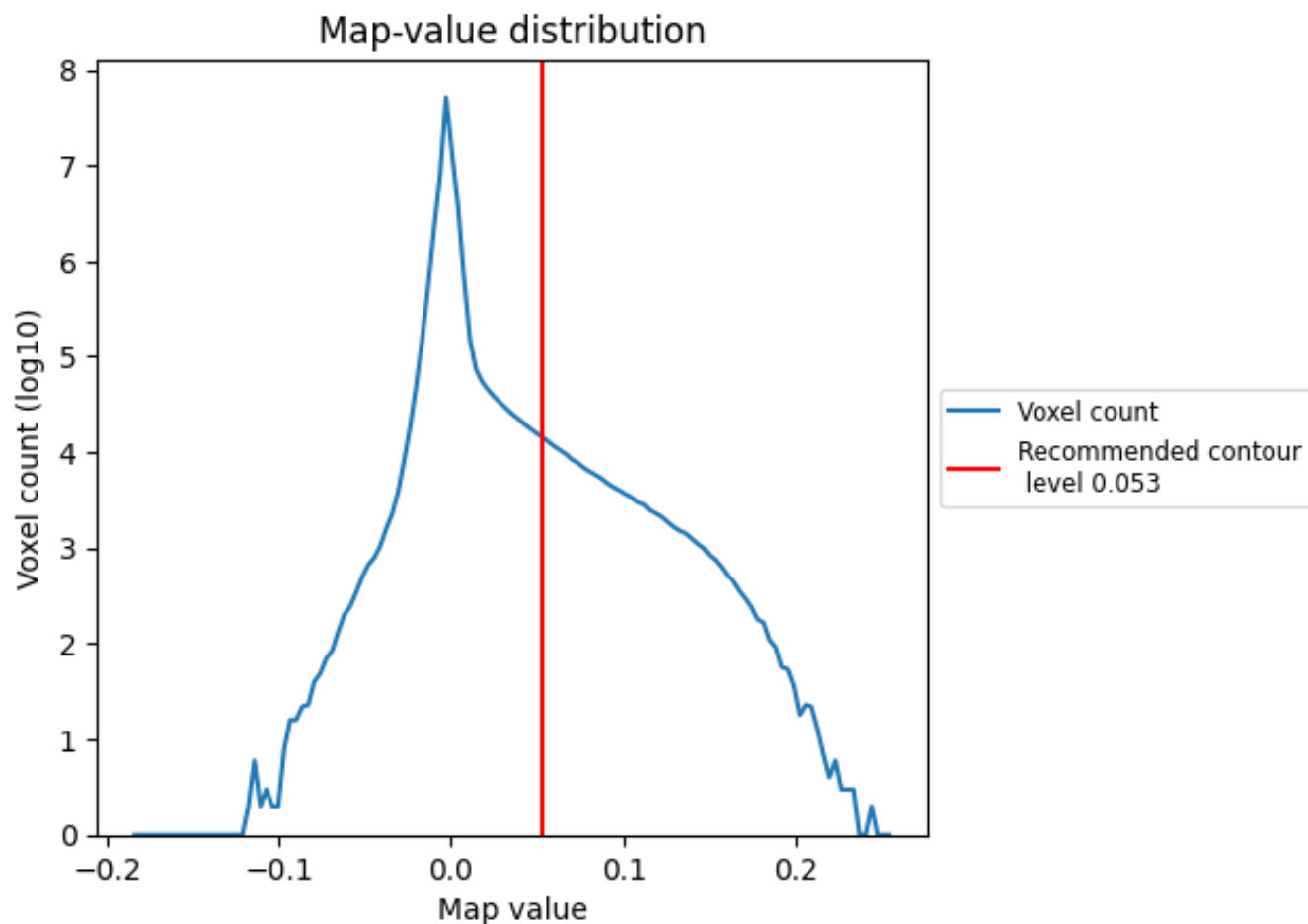


Z

7 Map analysis [i](#)

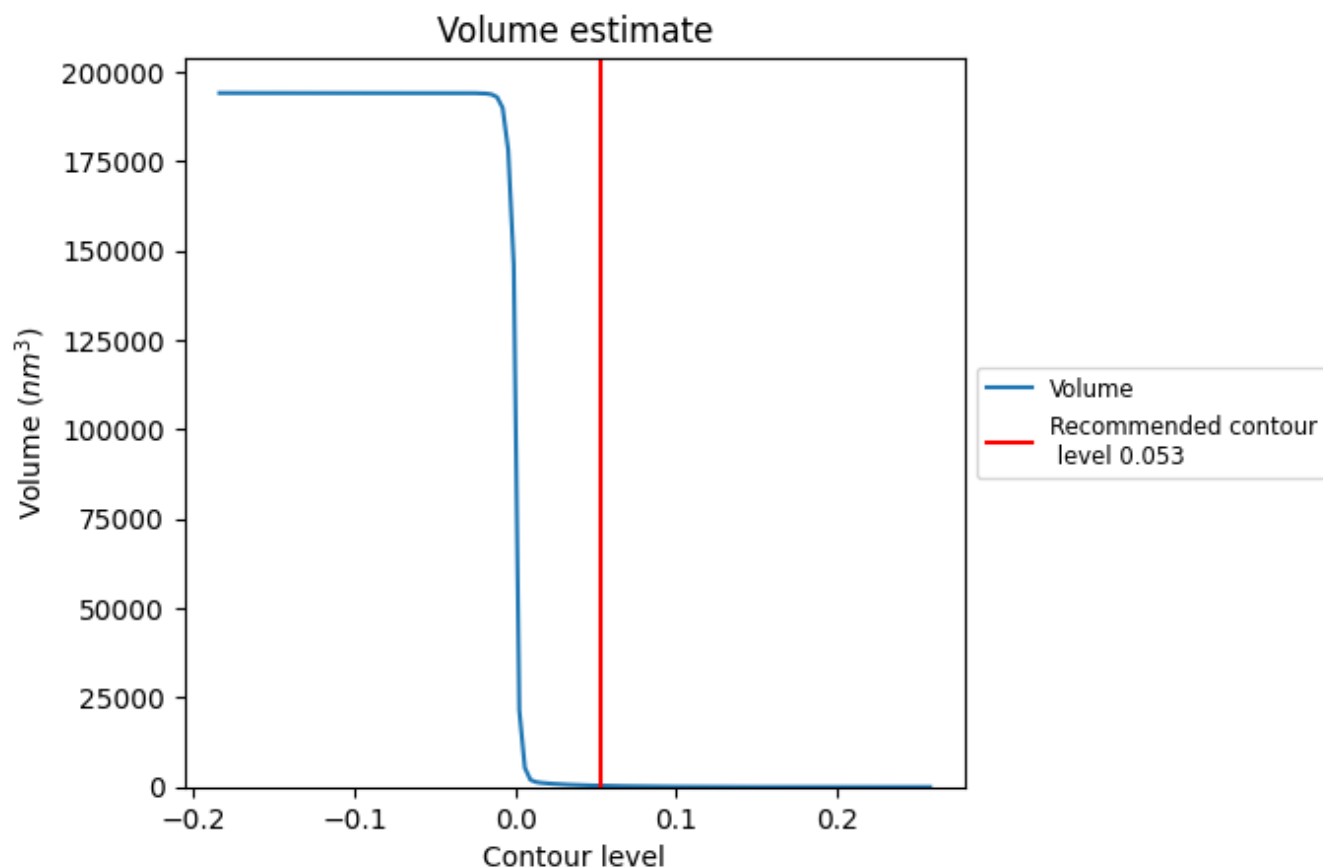
This section contains the results of statistical analysis of the map.

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.

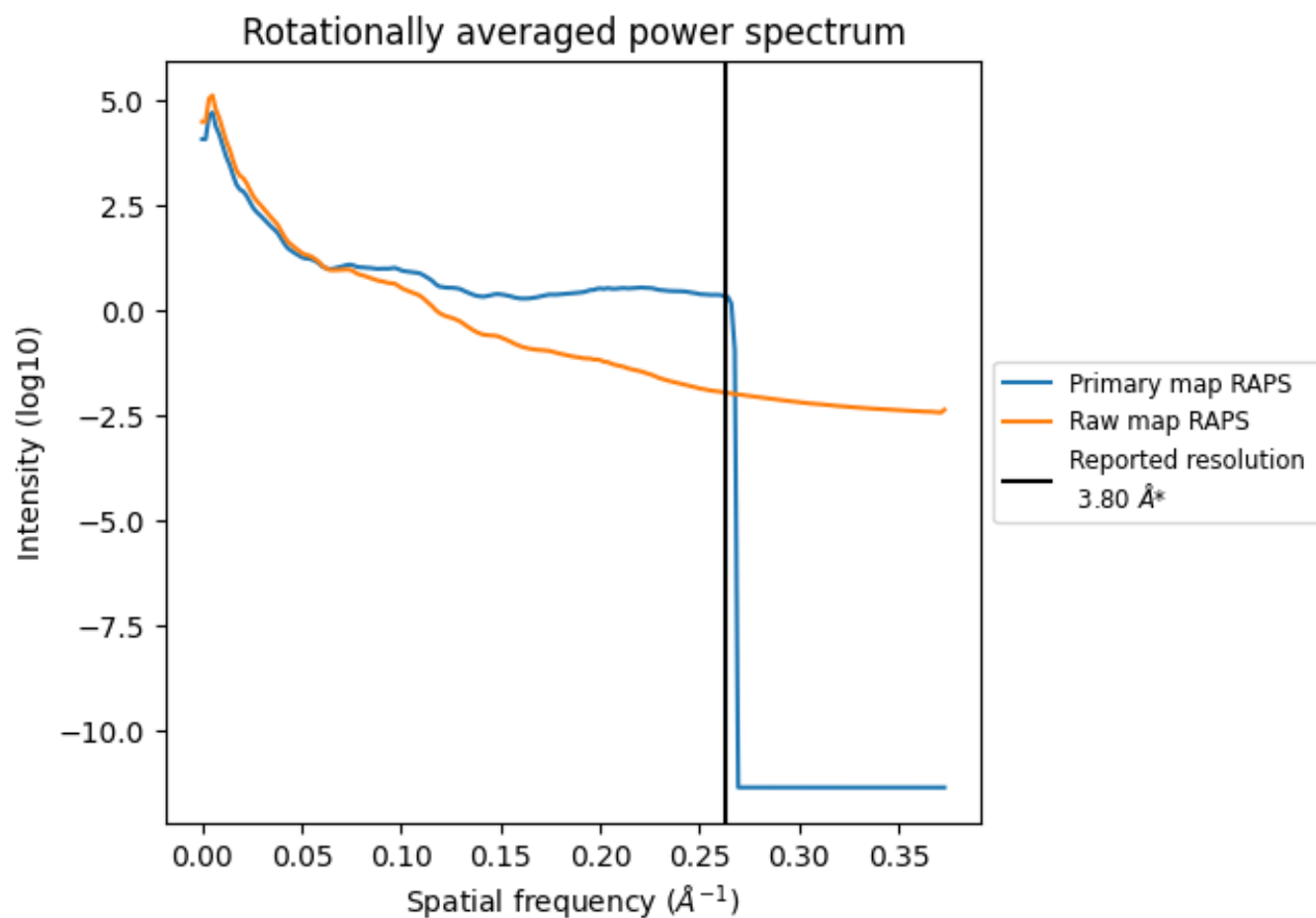
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 353 nm^3 ; this corresponds to an approximate mass of 318 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 ⓘ

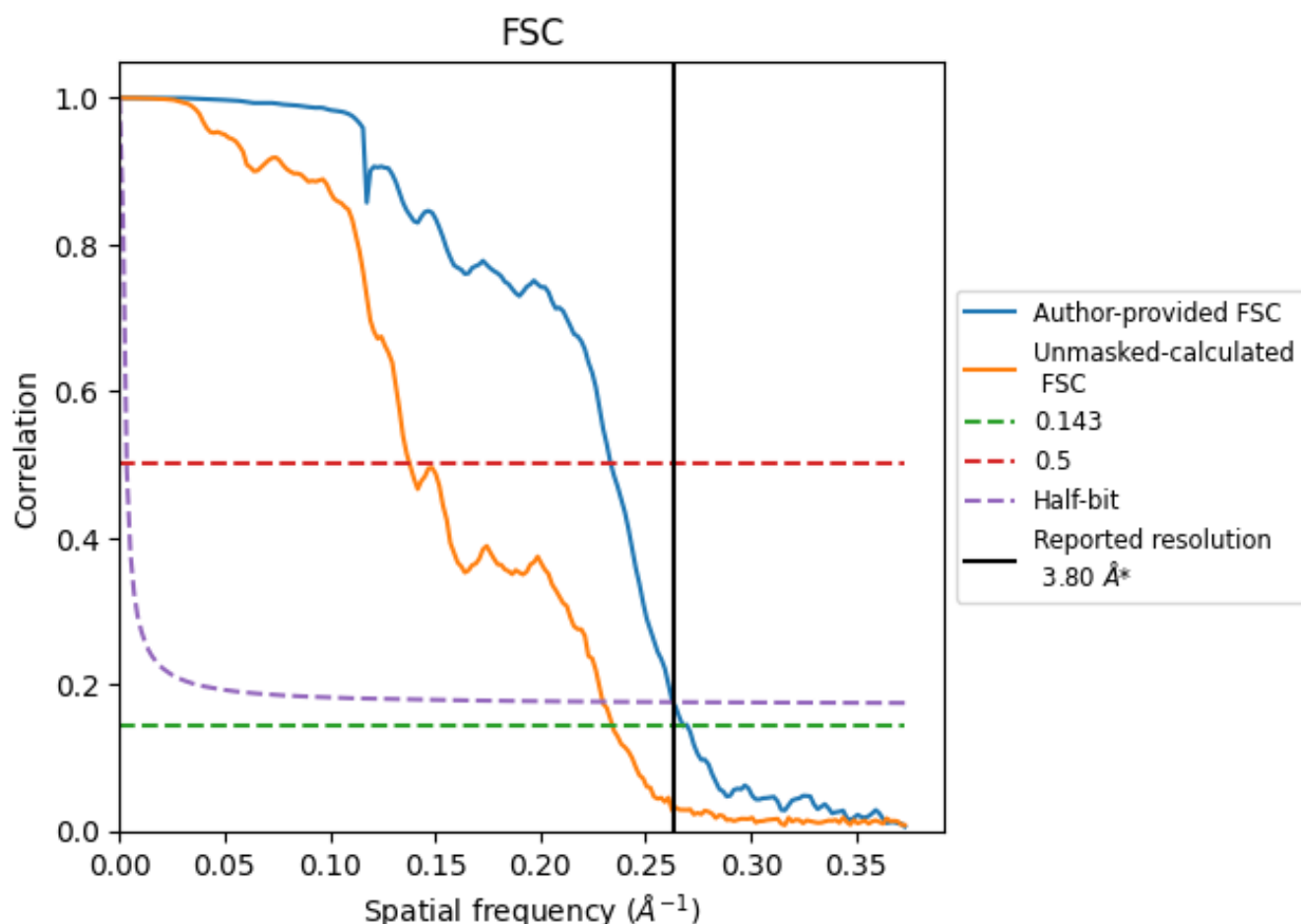


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

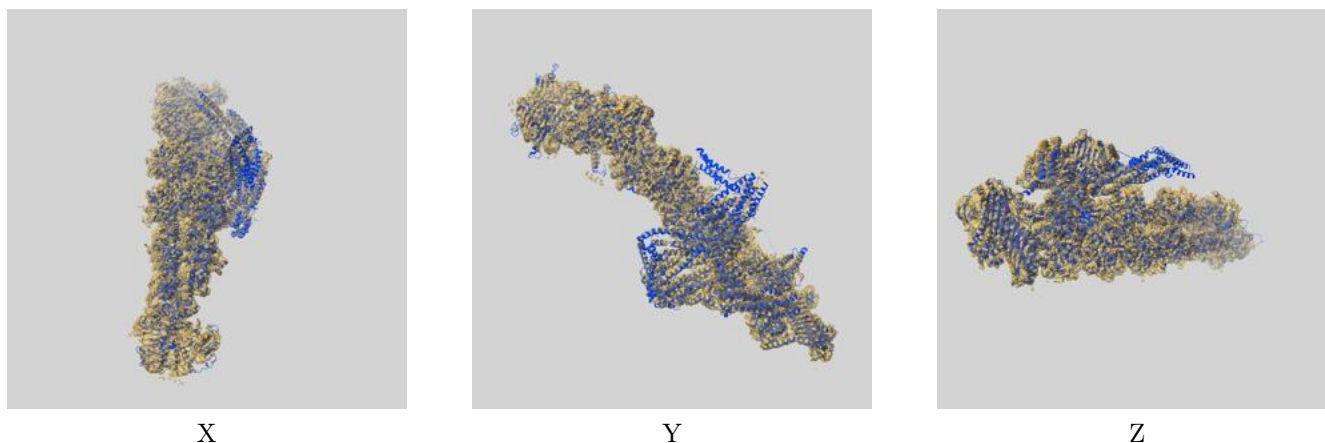
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.74	4.28	3.80
Unmasked-calculated*	4.27	7.25	4.36

*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 4.27 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

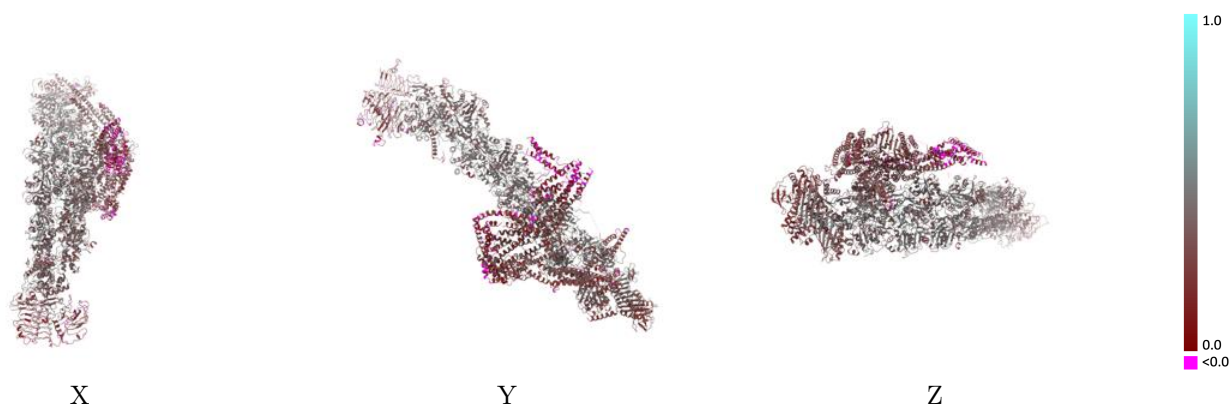
This section contains information regarding the fit between EMDB map EMD-11313 and PDB model 6ZNL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



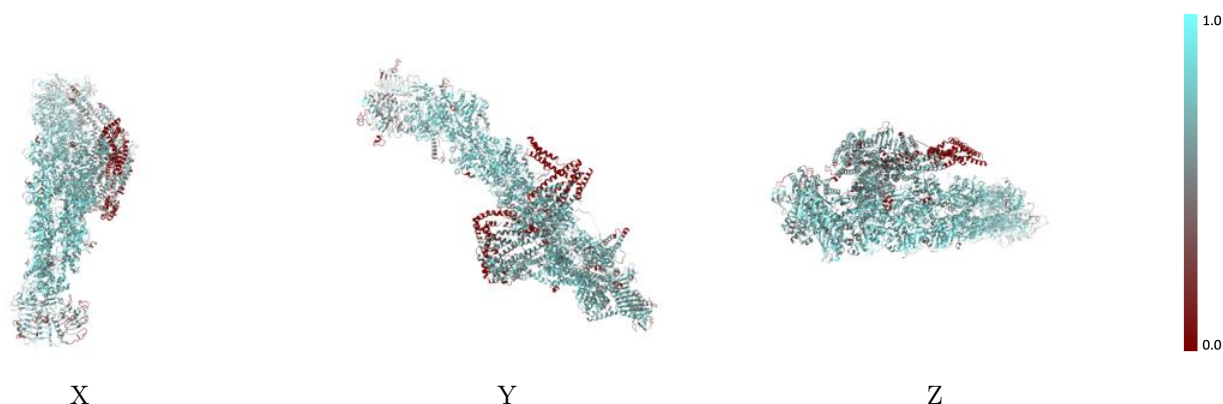
The images above show the 3D surface view of the map at the recommended contour level 0.053 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



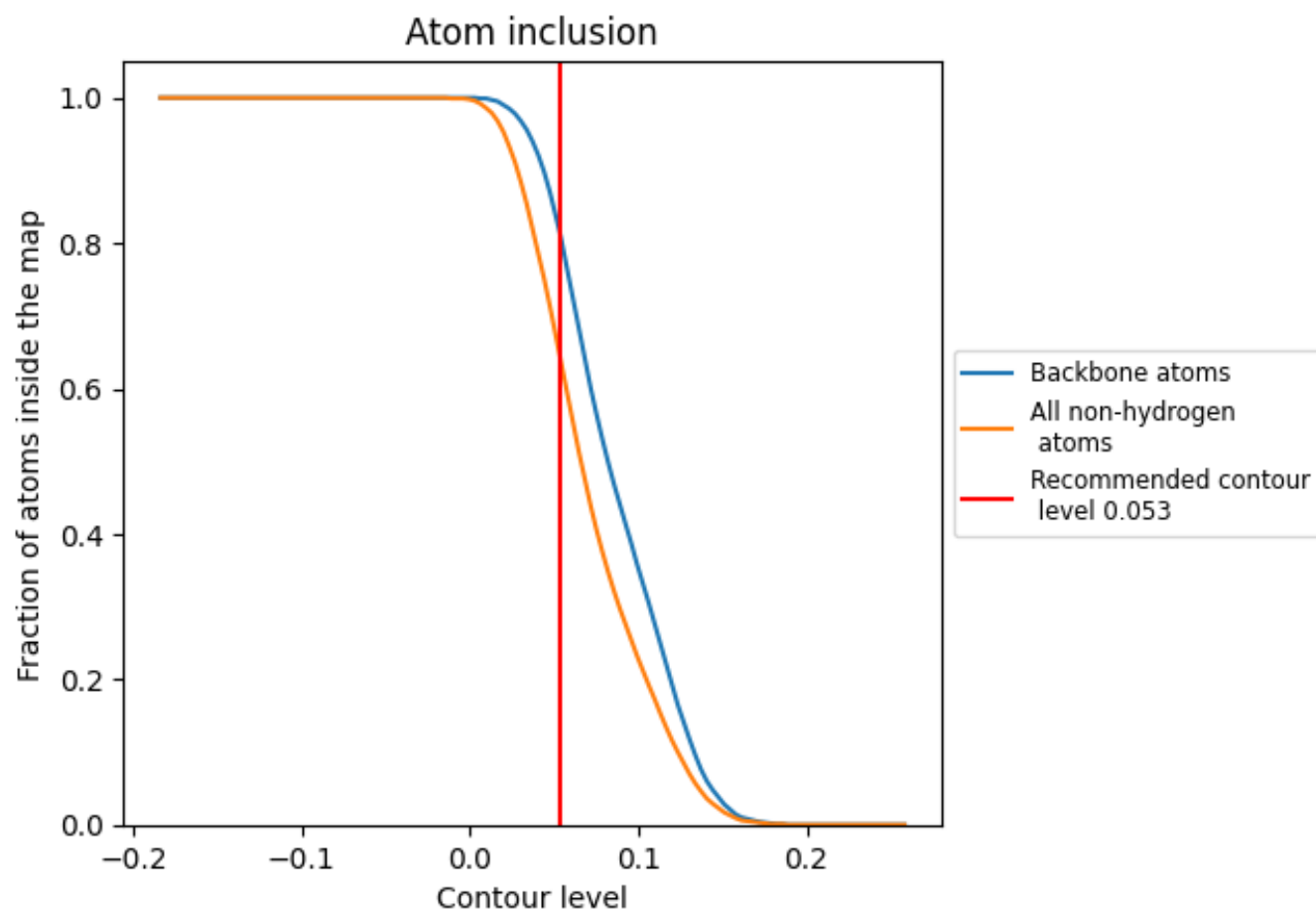
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.053).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 65% 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 (0.053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6490	 0.3520
A	 0.6960	 0.3760
B	 0.7530	 0.4130
C	 0.7400	 0.4330
D	 0.7520	 0.4250
E	 0.7370	 0.4250
F	 0.7580	 0.4170
G	 0.7530	 0.4200
H	 0.7760	 0.4280
I	 0.7300	 0.3930
J	 0.7340	 0.3990
K	 0.5980	 0.2980
L	 0.6680	 0.3360
M	 0.4820	 0.2560
N	 0.4180	 0.2070
O	 0.4680	 0.2370
U	 0.4700	 0.2040
V	 0.6290	 0.3070
Y	 0.5320	 0.2750
Z	 0.5920	 0.3100
m	 0.5460	 0.2950
n	 0.5010	 0.2860
o	 0.4950	 0.2540
z	 0.3750	 0.1970

