



# wwPDB EM Validation Summary Report ⓘ

Oct 20, 2025 – 01:04 PM EDT

PDB ID : 9DGS / pdb\_00009dgs  
EMDB ID : EMD-46846  
Title : Dynactin and dynein tail region of dynein-dynactin complex on microtubules  
Authors : Rao, Q.; Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
Resolution : 3.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

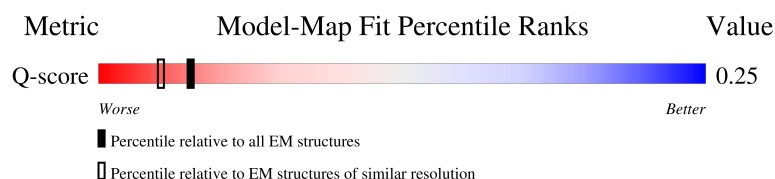
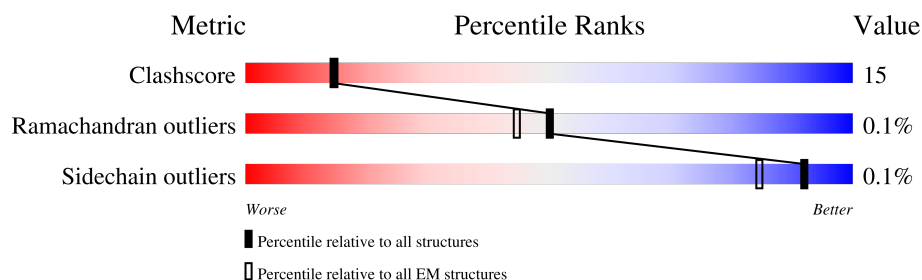
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.









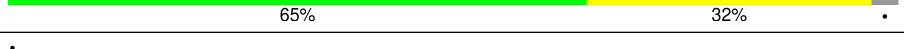
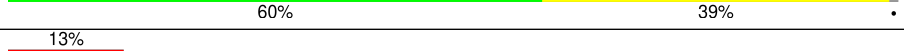
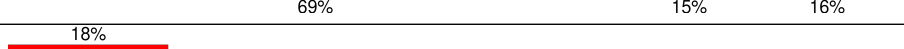
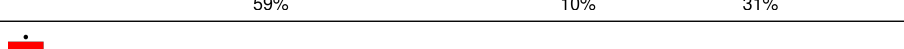
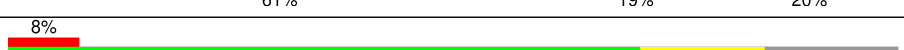

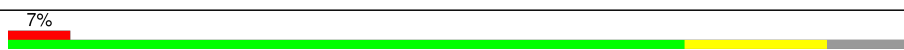

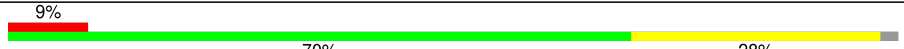








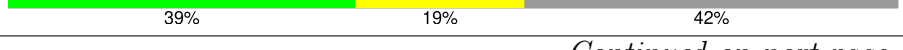

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8855 ( 3.40 - 4.40 )

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  $\geq 3$ , 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	

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Mol	Chain	Length	Quality of chain
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	P	405	
6	Q	405	
7	O	186	
7	R	186	
8	U	190	
9	V	182	
10	W	1281	
10	Z	1281	
11	Y	467	
12	e	4646	
12	f	4646	
12	m	4646	
12	n	4646	
13	g	612	
13	h	612	

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Mol	Chain	Length	Quality of chain
13	o	612	<p>41% 17% 42%</p>
13	p	612	<p>37% 42% 16%</p>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 85480 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 Alpha-centractin.

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 Actin-related protein 10.

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 F-actin-capping protein subunit 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 subunit beta.

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	P	325	Total	C	N	O	S	0	0
			2262	1413	397	446	6		
6	Q	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	R	170	Total	C	N	O	S	0	0
			1082	679	208	194	1		

- Molecule 8 is a protein called Dynactin subunit 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	152	Total	C	N	O	S	0	0
			937	574	186	174	3		
10	Z	192	Total	C	N	O	S	0	0
			1444	904	262	275	3		

- Molecule 11 is a protein called Dynactin subunit 4.

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

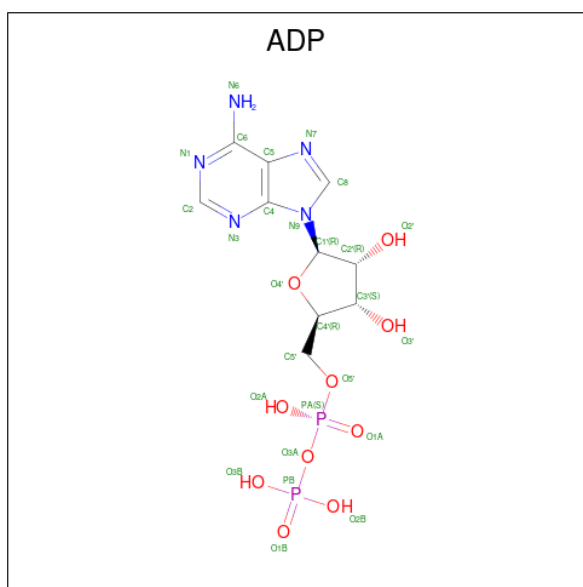
- Molecule 12 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	e	798	Total	C	N	O	S	0	0
			4724	2897	879	944	4		
12	f	808	Total	C	N	O	S	0	0
			6570	4162	1175	1216	17		
12	m	792	Total	C	N	O	S	0	0
			5722	3529	1090	1089	14		
12	n	755	Total	C	N	O	S	0	0
			5424	3342	1034	1036	12		

- Molecule 13 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	g	358	Total	C	N	O		0	0
			1767	1051	358	358			
13	h	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		
13	o	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		
13	p	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		

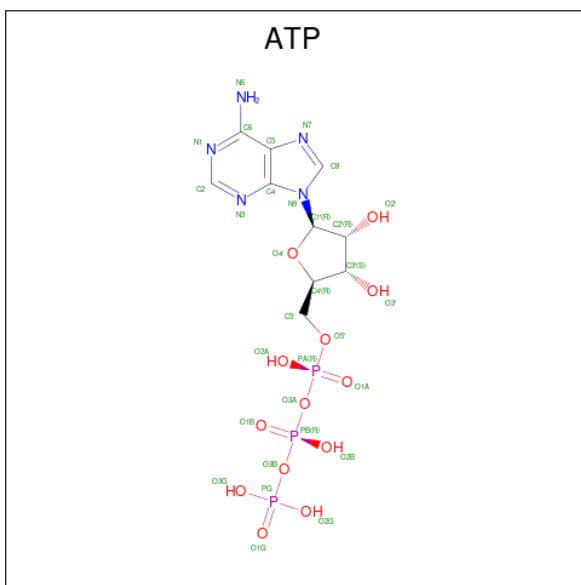
- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





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

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

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

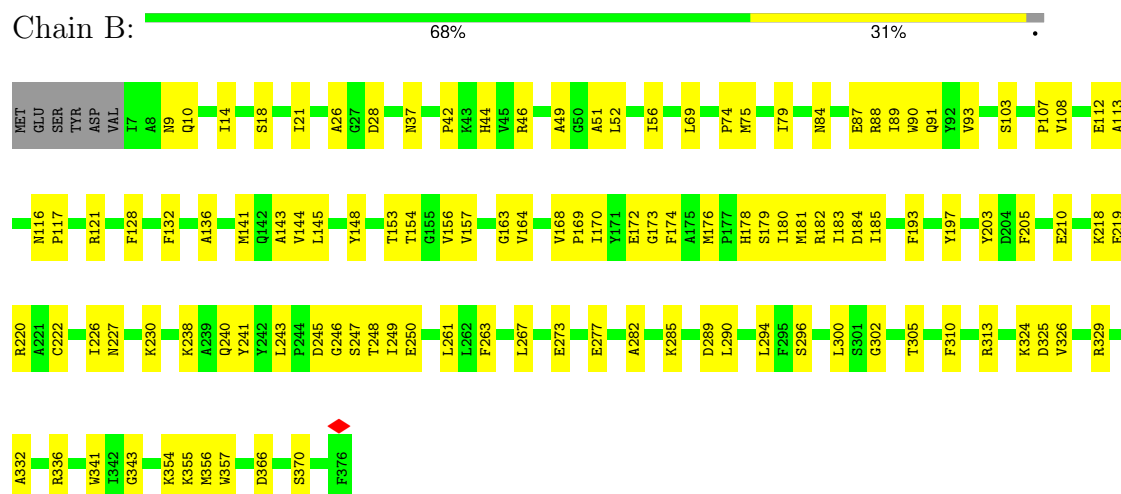
### 3 Residue-property plots

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

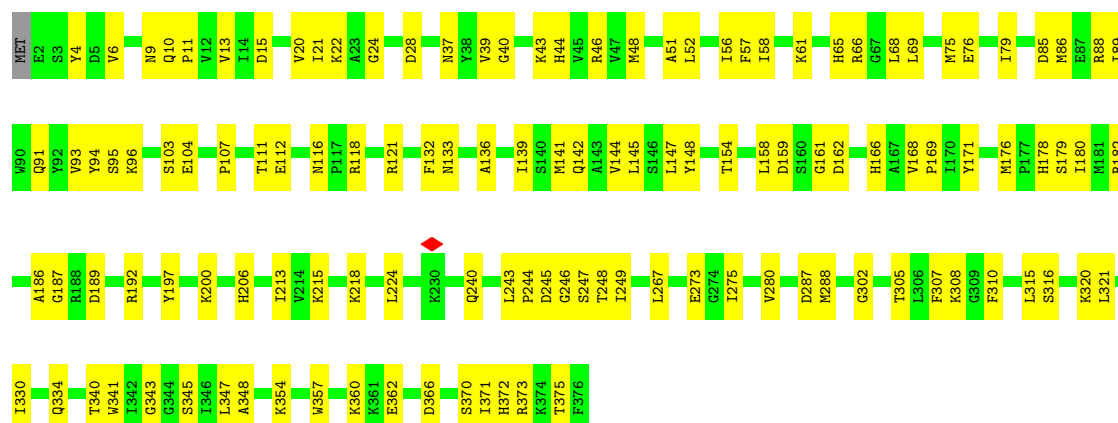


#### • Molecule 1: Alpha-centractin



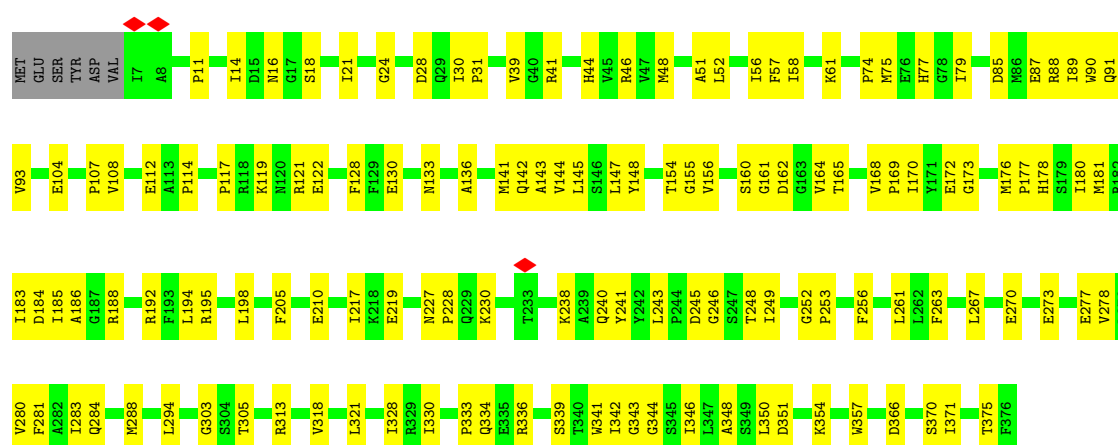
#### • Molecule 1: Alpha-centractin

Chain C:  66% 33%



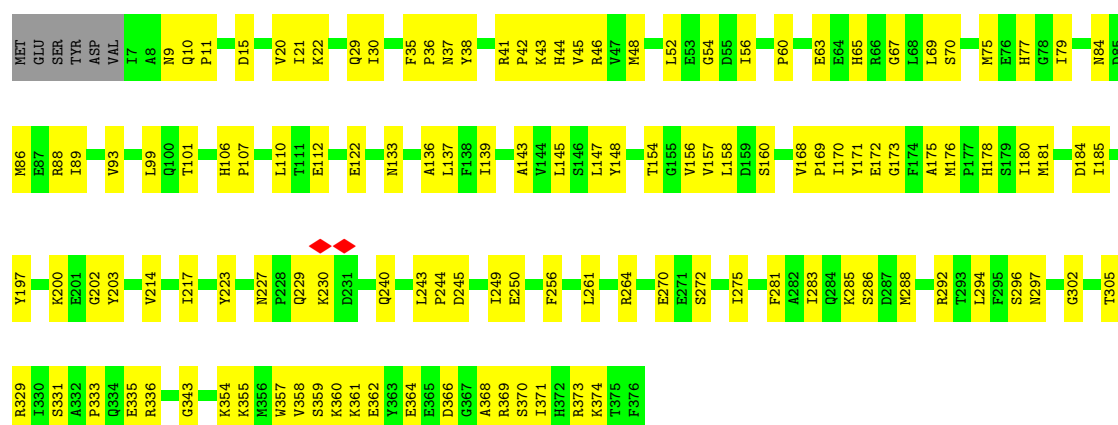
• Molecule 1: Alpha-centractin

Chain D:  63% 36%

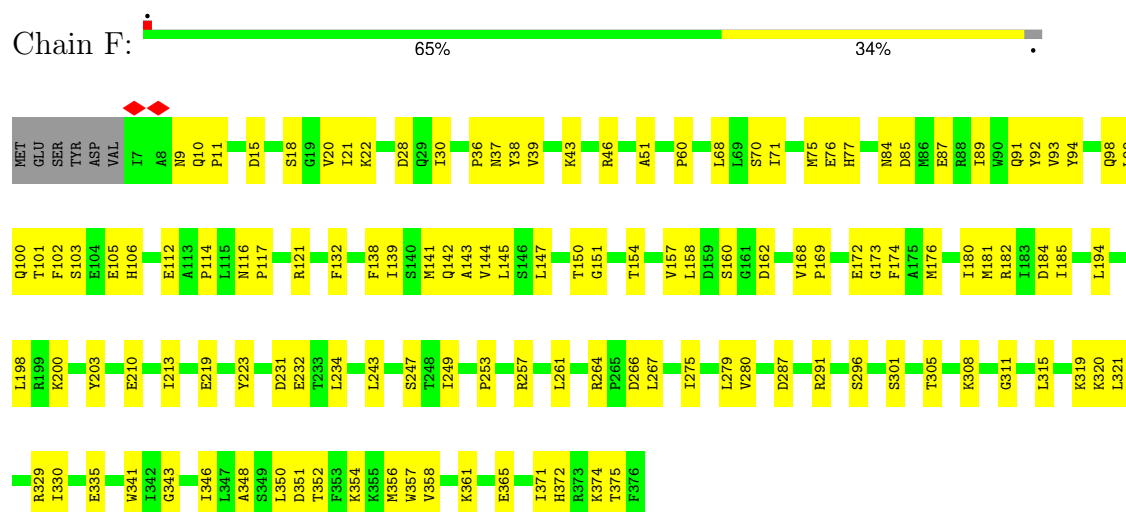


• Molecule 1: Alpha-centractin

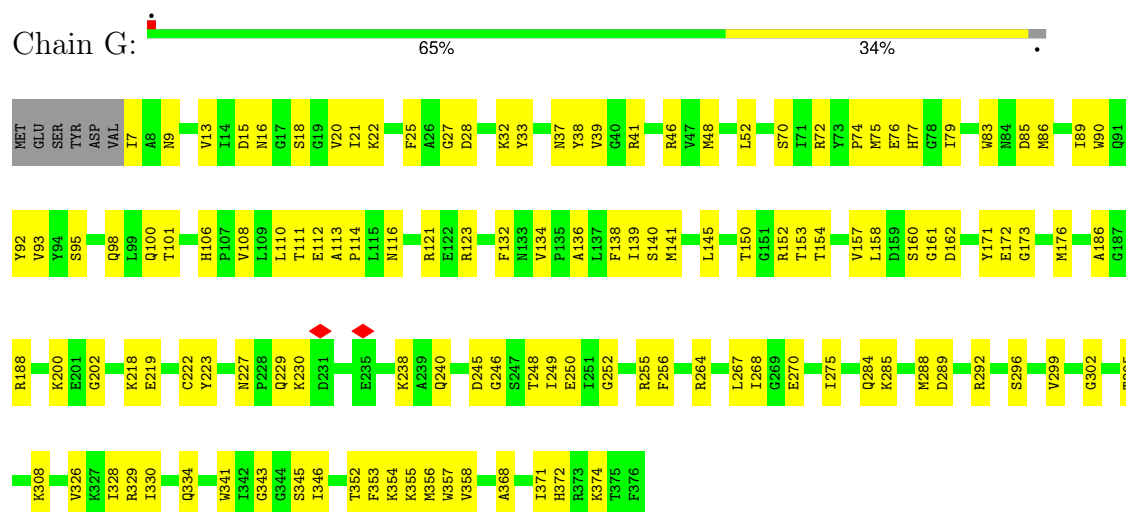
Chain E:  65% 33%



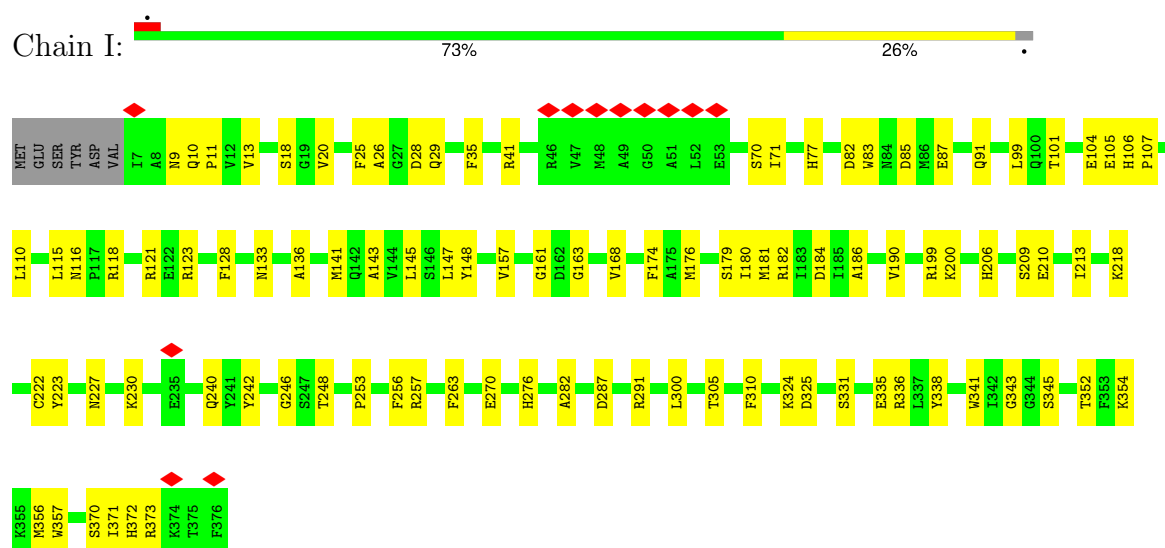
• Molecule 1: Alpha-centractin



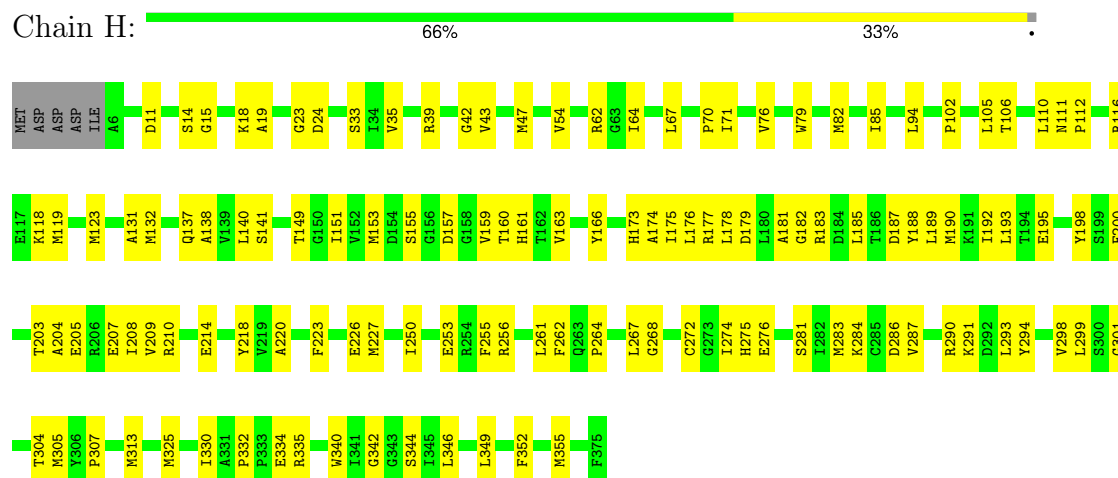
• Molecule 1: Alpha-centractin



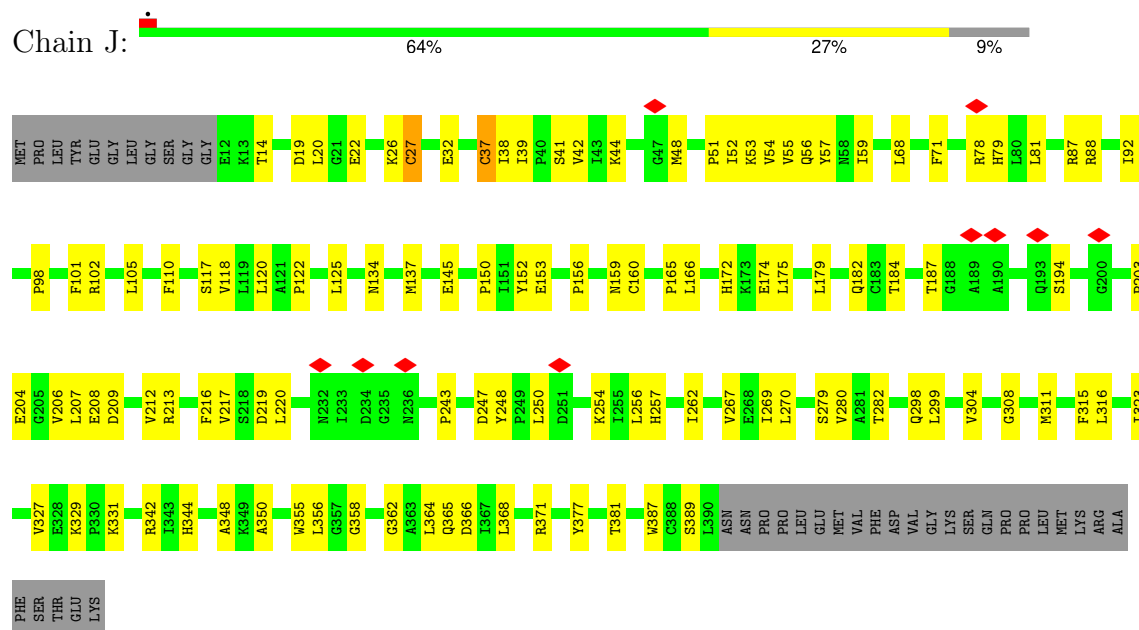
• Molecule 1: Alpha-centractin



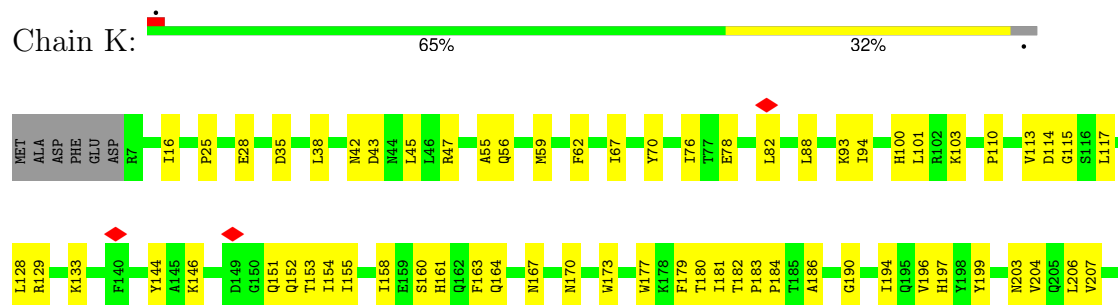
• Molecule 2: Actin, cytoplasmic 1



• Molecule 3: Actin-related protein 10

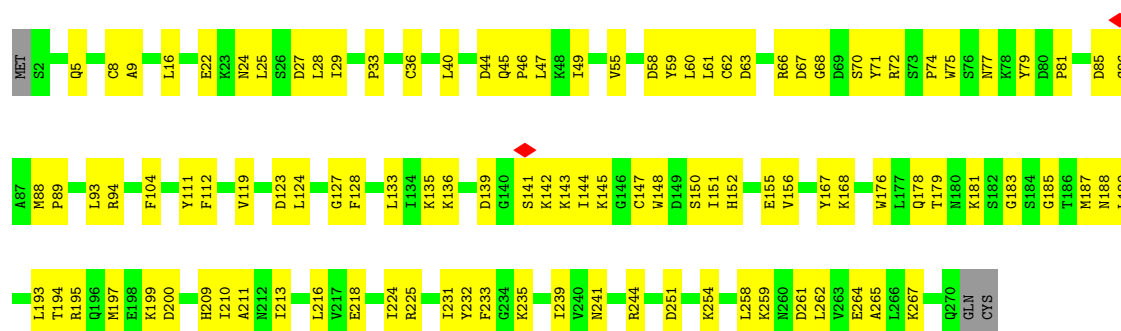


• Molecule 4: F-actin-capping protein subunit alpha-1

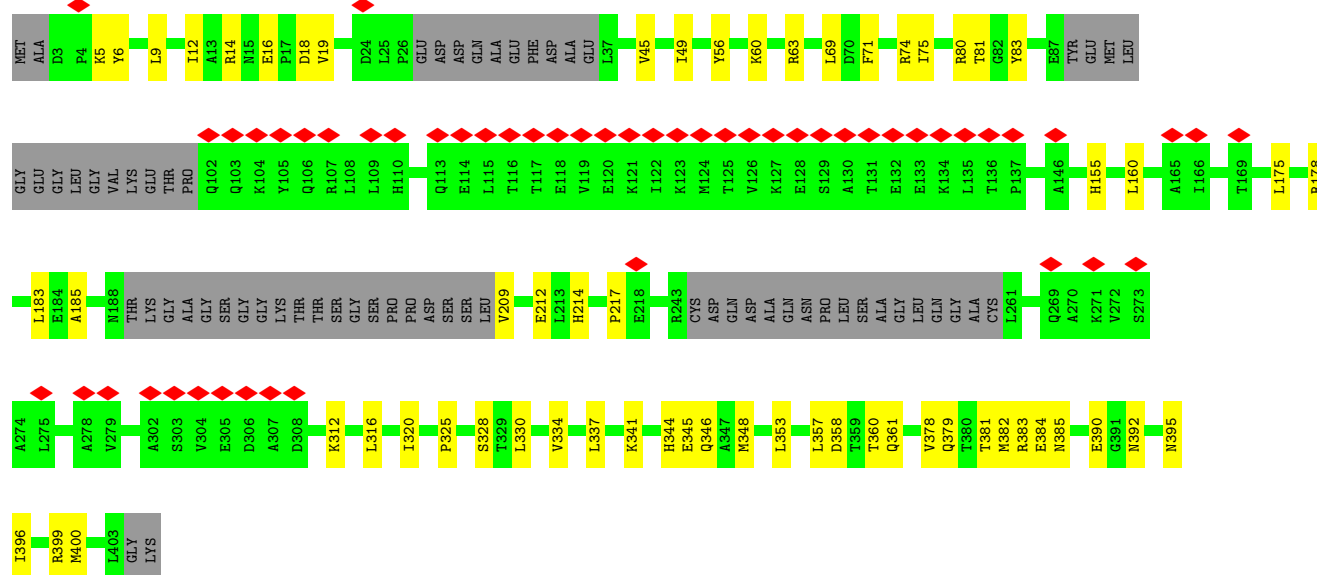




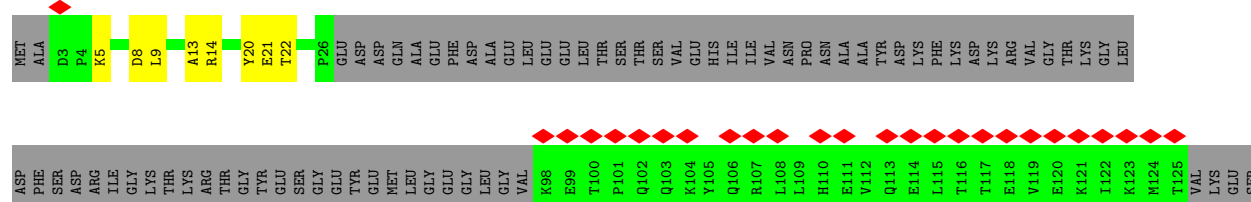
• Molecule 5: F-actin-capping protein subunit beta



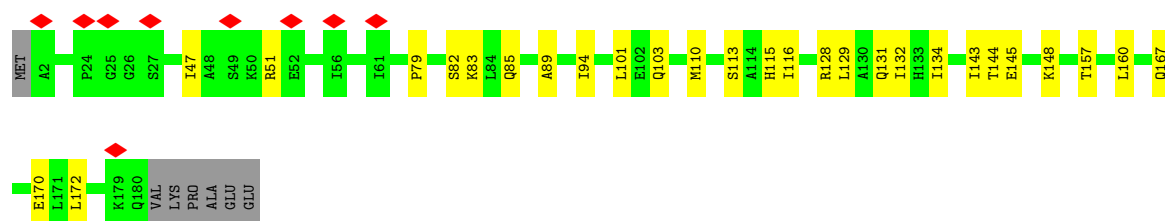
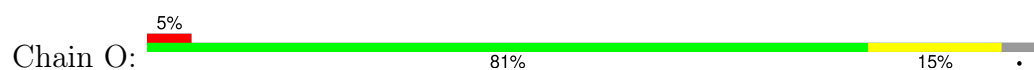
• Molecule 6: Dynactin subunit 2



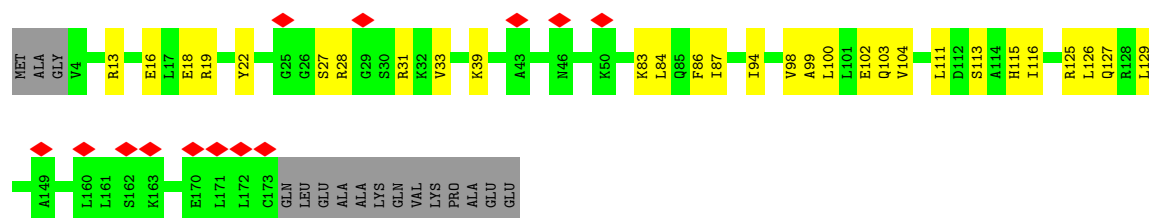
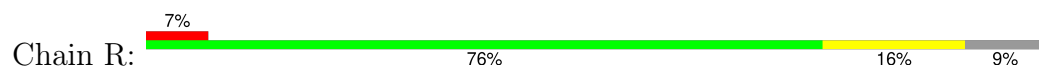
• Molecule 6: Dynactin subunit 2



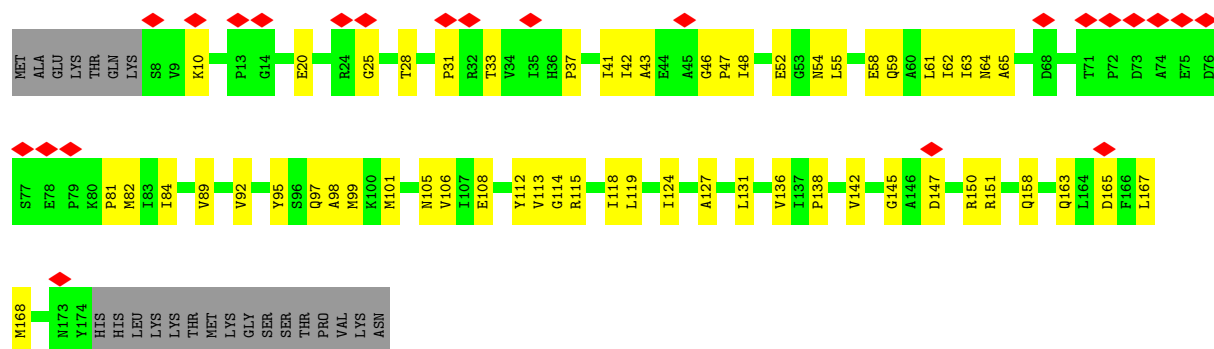
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



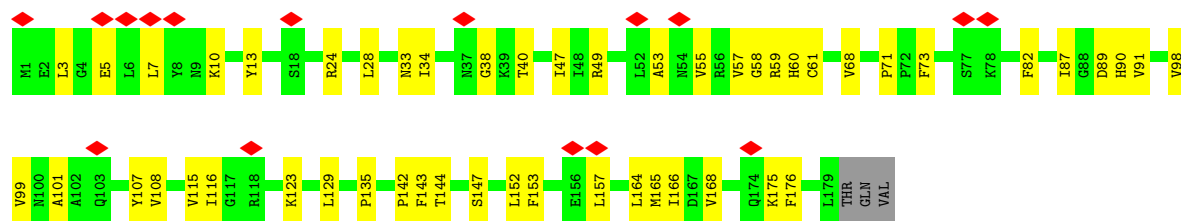
• Molecule 7: Dynactin subunit 3



• Molecule 8: Dynactin subunit 6



• Molecule 9: Dynactin subunit 5



• Molecule 10: Dynactin subunit 1



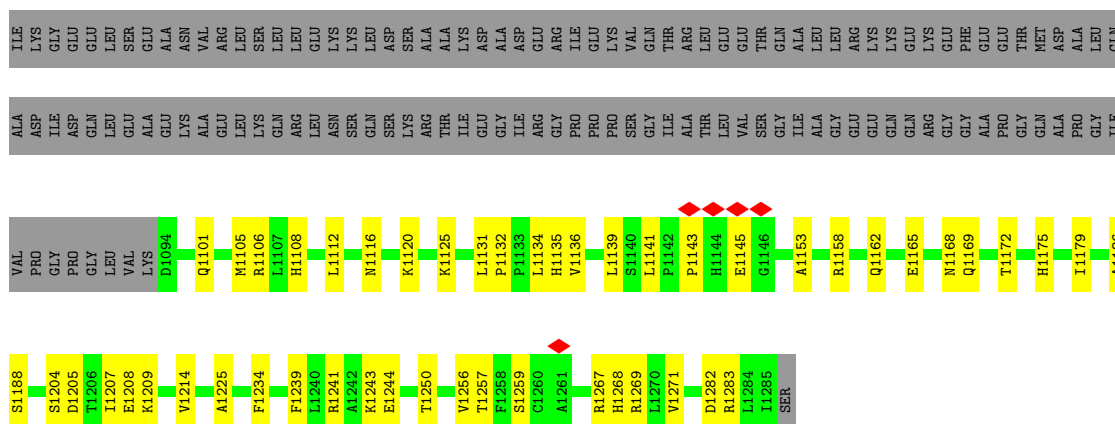




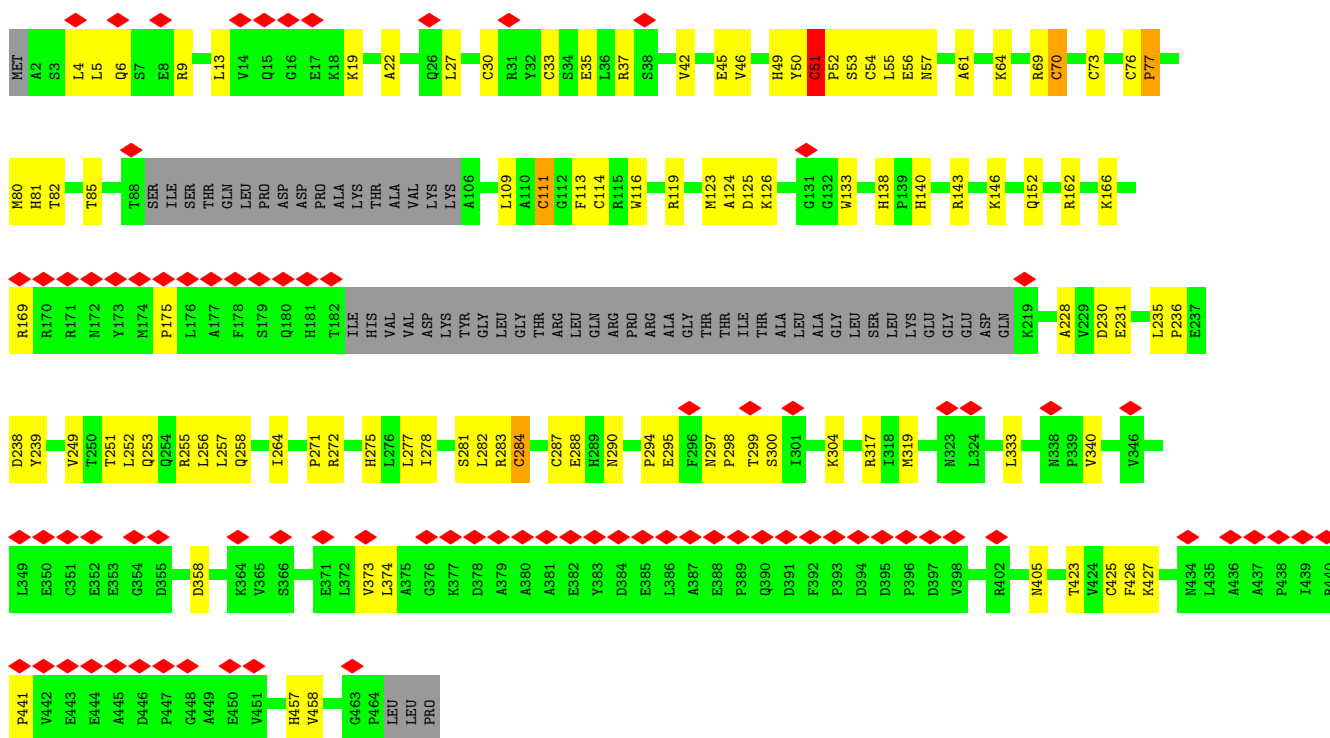


Chain Z:  11% 85%

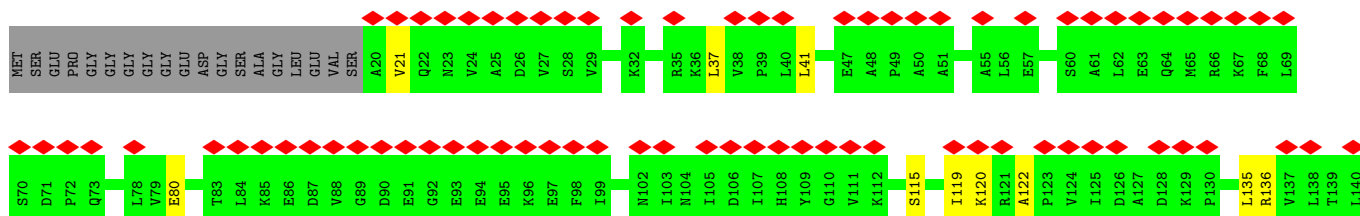




• Molecule 11: Dynactin subunit 4



• Molecule 12: Cytoplasmic dynein 1 heavy chain 1







WORLDWIDE  
PDB  
PROTEIN DATA BANK



















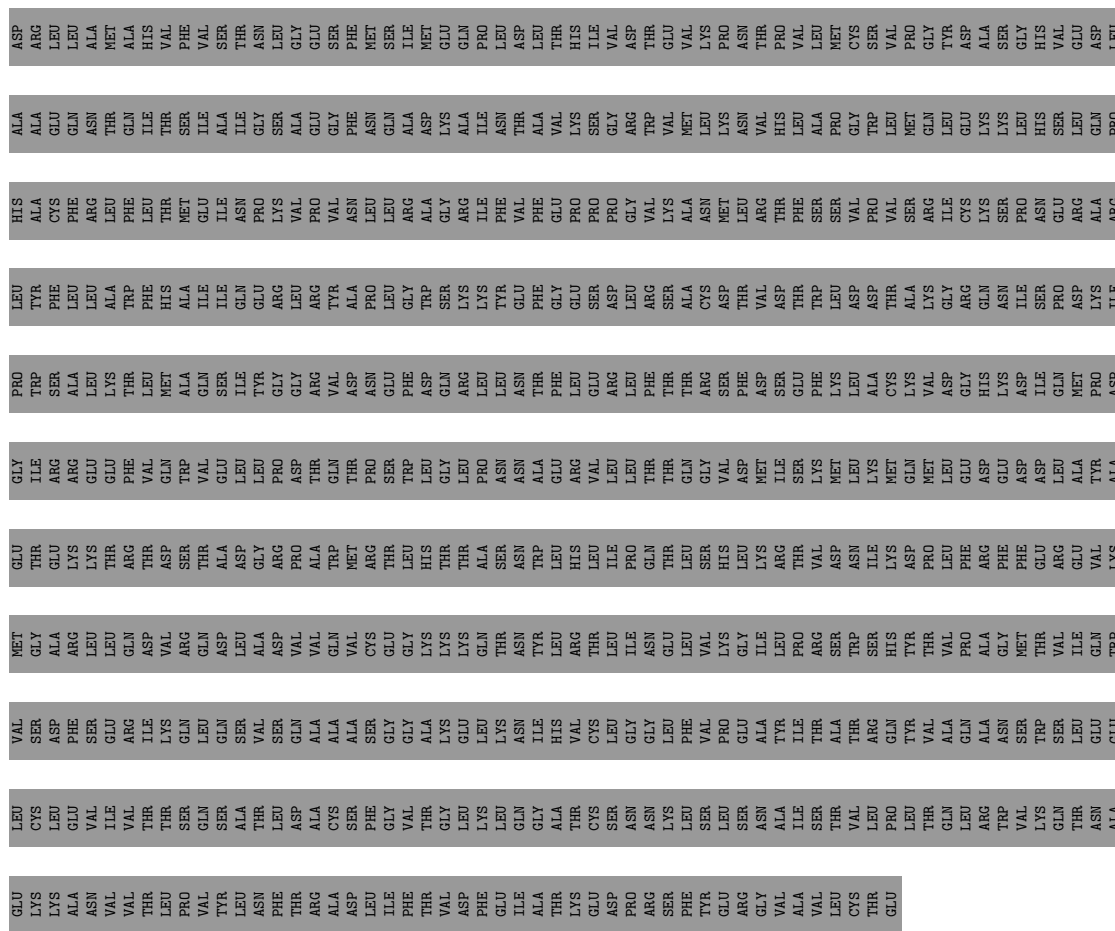




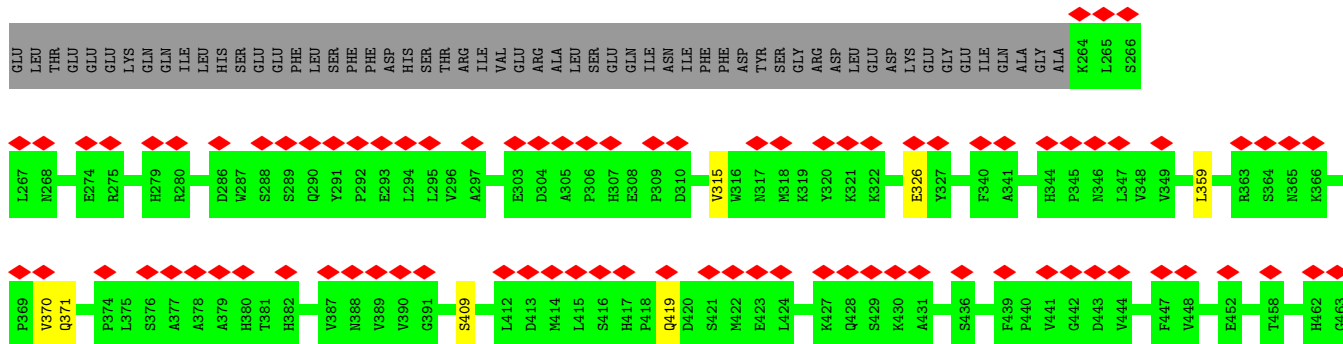
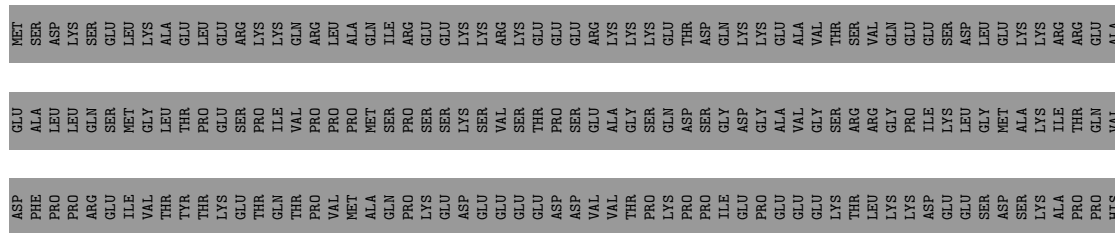


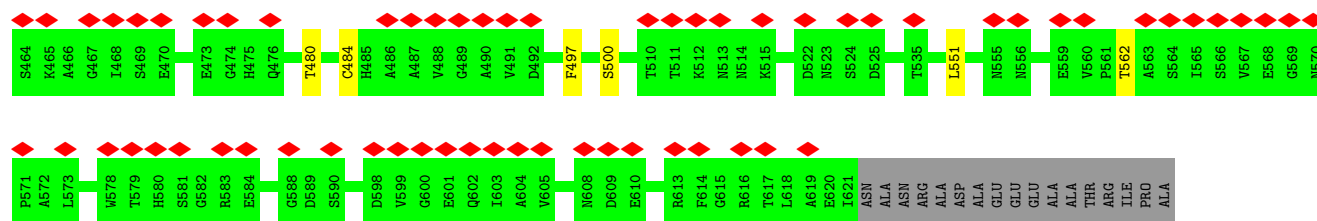






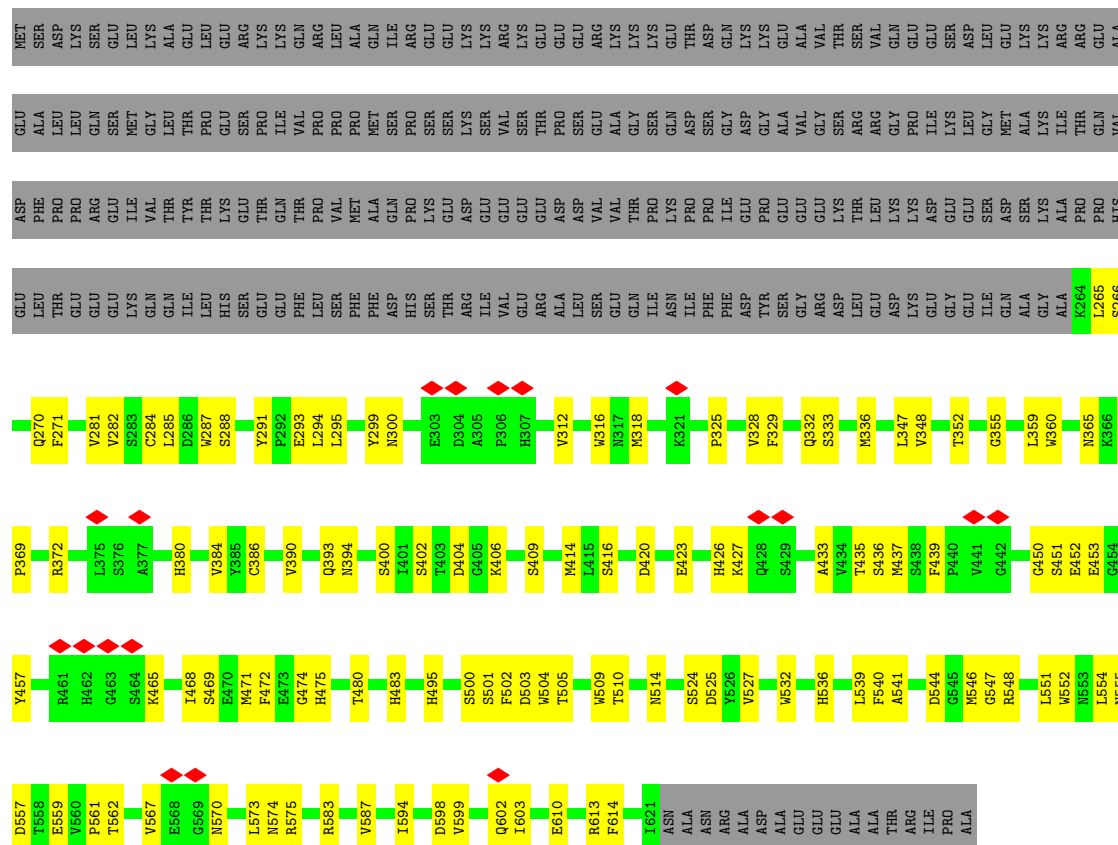
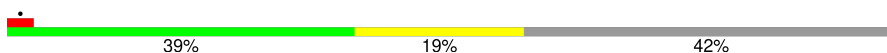
- Molecule 13: Cytoplasmic dynein 1 intermediate chain 2





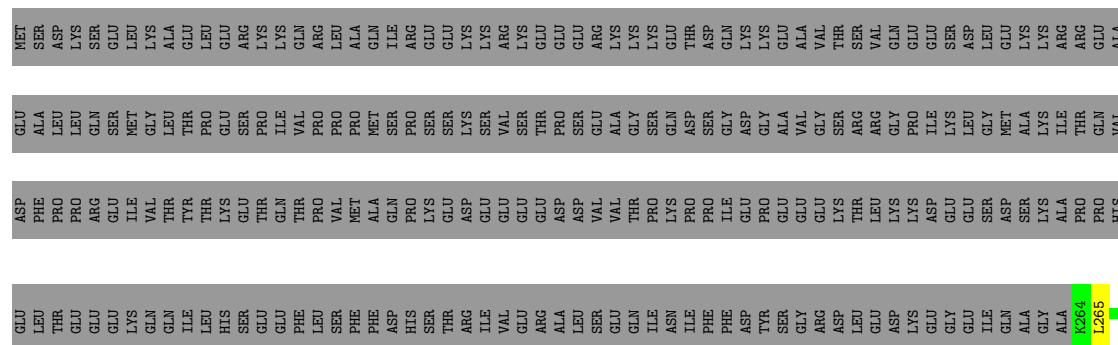
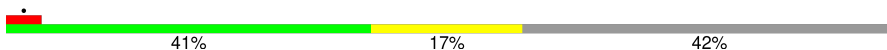
• Molecule 13: Cytoplasmic dynein 1 intermediate chain 2

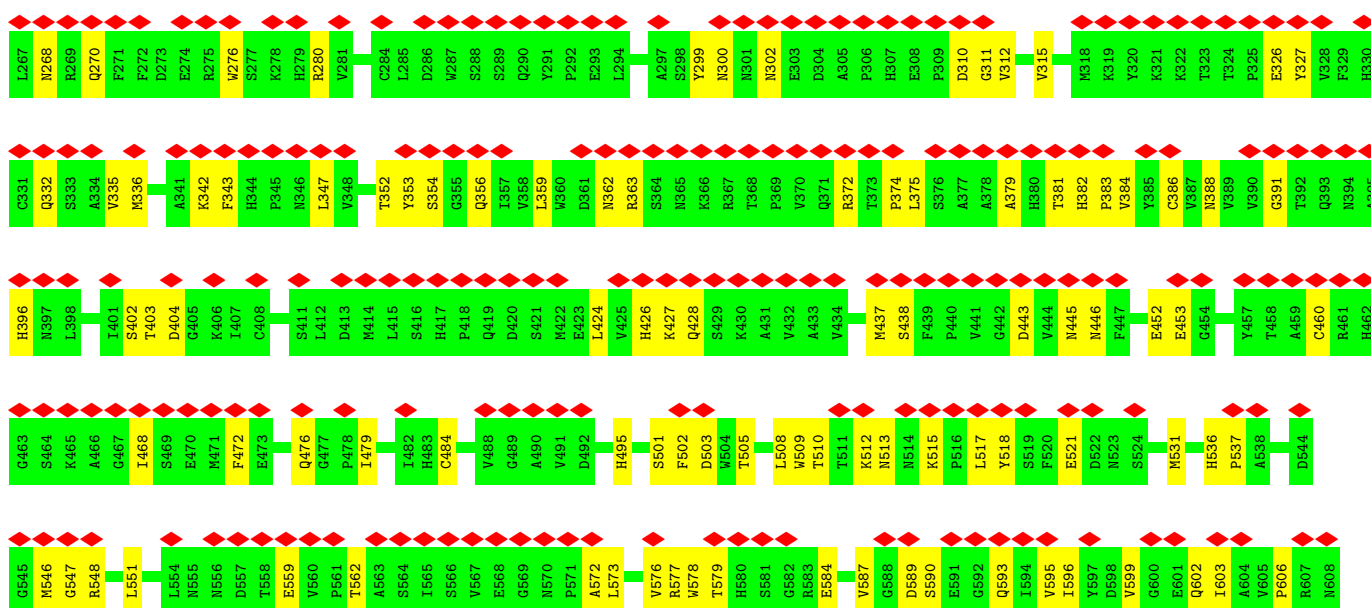
Chain h:



• Molecule 13: Cytoplasmic dynein 1 intermediate chain 2

Chain o:





D609	E610	W611	A612	R613	F614	G615	R616	T617	L618	A619	E620	I621	ASN	ALA	ASN	ASN	ARG	ALA	ASP	ALA	GLU	GLU	GLU	ALA	ALA	THR	ARG	ILE	PRO	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.582	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	633.6, 633.6, 633.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.14	0/3013	0.35	0/4070
1	B	0.16	0/3025	0.42	0/4085
1	C	0.17	0/3068	0.40	0/4144
1	D	0.15	0/3025	0.37	0/4085
1	E	0.16	0/3025	0.41	0/4085
1	F	0.17	0/3025	0.41	0/4085
1	G	0.17	0/3025	0.39	0/4085
1	I	0.13	0/3010	0.36	0/4066
2	H	0.16	0/2948	0.36	0/3991
3	J	0.23	0/2994	0.44	0/4066
4	K	0.14	0/2316	0.34	0/3135
5	L	0.14	0/2156	0.32	0/2906
6	M	0.16	0/2259	0.43	0/3090
6	N	0.16	0/1783	0.40	0/2451
6	P	0.16	0/2287	0.39	0/3119
6	Q	0.16	0/2375	0.38	0/3246
7	O	0.14	0/1194	0.42	0/1631
7	R	0.18	0/1093	0.49	0/1498
8	U	0.19	0/1241	0.48	0/1691
9	V	0.14	0/1286	0.38	0/1757
10	W	0.15	0/940	0.43	0/1281
10	Z	0.16	0/1467	0.44	0/1992
11	Y	0.34	0/3020	0.51	1/4119 (0.0%)
12	e	0.27	0/4754	0.47	0/6541
12	f	0.23	0/6683	0.46	2/9015 (0.0%)
12	m	0.17	0/5807	0.35	0/7751
12	n	0.27	0/5501	0.45	0/7337
13	g	0.11	0/1766	0.28	0/2457
13	h	0.13	0/2887	0.35	0/3938
13	o	0.12	0/2887	0.32	1/3938 (0.0%)
13	p	0.12	0/2887	0.32	1/3938 (0.0%)
All	All	0.19	0/86747	0.40	5/117593 (0.0%)



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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	Y	0	1
12	n	0	2
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	428	GLN	CB-CA-C	-5.17	110.59	116.54
13	p	428	GLN	CB-CA-C	-5.17	110.59	116.54
11	Y	51	CYS	CB-CA-C	5.05	116.40	108.63
12	f	37	LEU	CA-C-N	5.03	131.44	122.13
12	f	37	LEU	C-N-CA	5.03	131.44	122.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	Y	37	ARG	Sidechain
12	n	704	ARG	Sidechain
12	n	709	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2944	0	2938	87	0
1	B	2956	0	2950	114	0
1	C	2998	0	2983	98	0
1	D	2956	0	2950	105	0
1	E	2956	0	2950	103	0
1	F	2956	0	2950	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2956	0	2950	96	0
1	I	2941	0	2936	70	0
2	H	2885	0	2856	98	0
3	J	2932	0	3001	83	0
4	K	2264	0	2186	78	0
5	L	2122	0	2113	77	0
6	M	2238	0	1829	65	0
6	N	1767	0	1356	42	0
6	P	2262	0	2060	82	0
6	Q	2349	0	2069	58	0
7	O	1183	0	981	35	0
7	R	1082	0	881	33	0
8	U	1224	0	1215	39	0
9	V	1260	0	1213	37	0
10	W	937	0	707	34	0
10	Z	1444	0	1446	54	0
11	Y	2960	0	2711	79	0
12	e	4724	0	3273	56	0
12	f	6570	0	6693	307	0
12	m	5722	0	5269	216	0
12	n	5424	0	4963	264	0
13	g	1767	0	796	7	0
13	h	2808	0	2670	93	0
13	o	2808	0	2670	80	0
13	p	2808	0	2670	148	0
14	A	27	0	12	2	0
14	B	27	0	12	1	0
14	C	27	0	12	2	0
14	D	27	0	12	3	0
14	E	27	0	12	0	0
14	F	27	0	12	1	0
14	G	27	0	12	1	0
14	I	27	0	12	0	0
14	J	27	0	12	1	0
15	H	31	0	12	8	0
16	Y	3	0	0	0	0
All	All	85480	0	79355	2432	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 2432 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:755:TRP:CZ2	13:p:453:GLU:HA	1.19	1.63
12:n:755:TRP:CZ2	13:p:453:GLU:CA	1.80	1.62
12:n:779:ILE:CG2	13:p:375:LEU:HD22	1.33	1.55
12:e:717:ILE:HA	12:e:824:TRP:CE2	1.39	1.54
12:n:779:ILE:HG21	13:p:375:LEU:CD2	1.33	1.52

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	B	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	C	373/376 (99%)	361 (97%)	12 (3%)	0	100	100
1	D	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	E	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	F	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	I	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
3	J	377/417 (90%)	365 (97%)	12 (3%)	0	100	100
4	K	276/286 (96%)	268 (97%)	8 (3%)	0	100	100
5	L	267/272 (98%)	261 (98%)	6 (2%)	0	100	100
6	M	330/405 (82%)	311 (94%)	18 (6%)	1 (0%)	37	70
6	N	270/405 (67%)	262 (97%)	7 (3%)	1 (0%)	30	65
6	P	319/405 (79%)	312 (98%)	7 (2%)	0	100	100
6	Q	335/405 (83%)	318 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	O	177/186 (95%)	165 (93%)	12 (7%)	0	100	100
7	R	168/186 (90%)	160 (95%)	8 (5%)	0	100	100
8	U	165/190 (87%)	157 (95%)	8 (5%)	0	100	100
9	V	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
10	W	144/1281 (11%)	138 (96%)	5 (4%)	1 (1%)	19	54
10	Z	190/1281 (15%)	184 (97%)	6 (3%)	0	100	100
11	Y	404/467 (86%)	377 (93%)	24 (6%)	3 (1%)	19	54
12	e	792/4646 (17%)	745 (94%)	45 (6%)	2 (0%)	37	70
12	f	804/4646 (17%)	763 (95%)	39 (5%)	2 (0%)	44	75
12	m	786/4646 (17%)	758 (96%)	27 (3%)	1 (0%)	48	80
12	n	747/4646 (16%)	720 (96%)	26 (4%)	1 (0%)	48	80
13	g	356/612 (58%)	353 (99%)	3 (1%)	0	100	100
13	h	356/612 (58%)	346 (97%)	10 (3%)	0	100	100
13	o	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
13	p	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
All	All	11469/30783 (37%)	11047 (96%)	410 (4%)	12 (0%)	50	80

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
10	W	1142	PRO
11	Y	175	PRO
11	Y	441	PRO
12	f	38	VAL

### 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	318/324 (98%)	318 (100%)	0	100	100
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%)	313 (100%)	0	100	100
3	J	323/363 (89%)	321 (99%)	2 (1%)	84	88
4	K	247/254 (97%)	247 (100%)	0	100	100
5	L	238/241 (99%)	238 (100%)	0	100	100
6	M	164/346 (47%)	164 (100%)	0	100	100
6	N	112/346 (32%)	112 (100%)	0	100	100
6	P	197/346 (57%)	197 (100%)	0	100	100
6	Q	192/346 (56%)	192 (100%)	0	100	100
7	O	87/160 (54%)	87 (100%)	0	100	100
7	R	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	W	53/1078 (5%)	53 (100%)	0	100	100
10	Z	154/1078 (14%)	154 (100%)	0	100	100
11	Y	274/416 (66%)	269 (98%)	5 (2%)	54	71
12	e	230/4122 (6%)	230 (100%)	0	100	100
12	f	718/4122 (17%)	717 (100%)	1 (0%)	92	95
12	m	538/4122 (13%)	538 (100%)	0	100	100
12	n	504/4122 (12%)	502 (100%)	2 (0%)	89	91
13	h	309/535 (58%)	308 (100%)	1 (0%)	91	92
13	o	309/535 (58%)	309 (100%)	0	100	100
13	p	309/535 (58%)	309 (100%)	0	100	100
All	All	8130/26463 (31%)	8119 (100%)	11 (0%)	92	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	f	213	ILE
13	h	393	GLN
12	n	704	ARG
12	n	685	ASP
11	Y	111	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
12	f	799	ASN
12	n	473	HIS
13	h	397	ASN
12	m	589	ASN
12	n	676	HIS

### 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
14	ADP	G	800	-	24,29,29	0.88	0	29,45,45	1.18	2 (6%)
14	ADP	C	800	-	24,29,29	0.85	0	29,45,45	1.09	2 (6%)
15	ATP	H	401	-	28,33,33	0.70	0	34,52,52	0.61	1 (2%)
14	ADP	E	800	-	24,29,29	0.88	0	29,45,45	1.13	2 (6%)
14	ADP	D	800	-	24,29,29	0.90	0	29,45,45	1.19	2 (6%)
14	ADP	J	800	-	24,29,29	0.95	1 (4%)	29,45,45	1.24	3 (10%)
14	ADP	B	800	-	24,29,29	0.87	0	29,45,45	1.13	2 (6%)
14	ADP	I	800	-	24,29,29	0.88	0	29,45,45	1.19	2 (6%)
14	ADP	F	800	-	24,29,29	0.86	0	29,45,45	1.12	2 (6%)
14	ADP	A	800	-	24,29,29	0.89	0	29,45,45	1.11	2 (6%)

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
14	ADP	G	800	-	-	0/12/32/32	0/3/3/3
14	ADP	C	800	-	-	3/12/32/32	0/3/3/3
15	ATP	H	401	-	-	10/18/38/38	0/3/3/3
14	ADP	E	800	-	-	2/12/32/32	0/3/3/3
14	ADP	D	800	-	-	5/12/32/32	0/3/3/3
14	ADP	J	800	-	-	7/12/32/32	0/3/3/3
14	ADP	B	800	-	-	0/12/32/32	0/3/3/3
14	ADP	I	800	-	-	3/12/32/32	0/3/3/3
14	ADP	F	800	-	-	8/12/32/32	0/3/3/3
14	ADP	A	800	-	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	800	ADP	PA-O3A	2.18	1.61	1.59

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	800	ADP	N3-C2-N1	-3.62	123.76	128.67
14	G	800	ADP	N3-C2-N1	-3.58	123.81	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	I	800	ADP	N3-C2-N1	-3.53	123.88	128.67
14	A	800	ADP	N3-C2-N1	-3.50	123.92	128.67
14	E	800	ADP	N3-C2-N1	-3.46	123.97	128.67

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	800	ADP	C5'-O5'-PA-O3A
14	D	800	ADP	C5'-O5'-PA-O2A
14	D	800	ADP	C5'-O5'-PA-O3A
14	D	800	ADP	C3'-C4'-C5'-O5'
14	F	800	ADP	C5'-O5'-PA-O1A

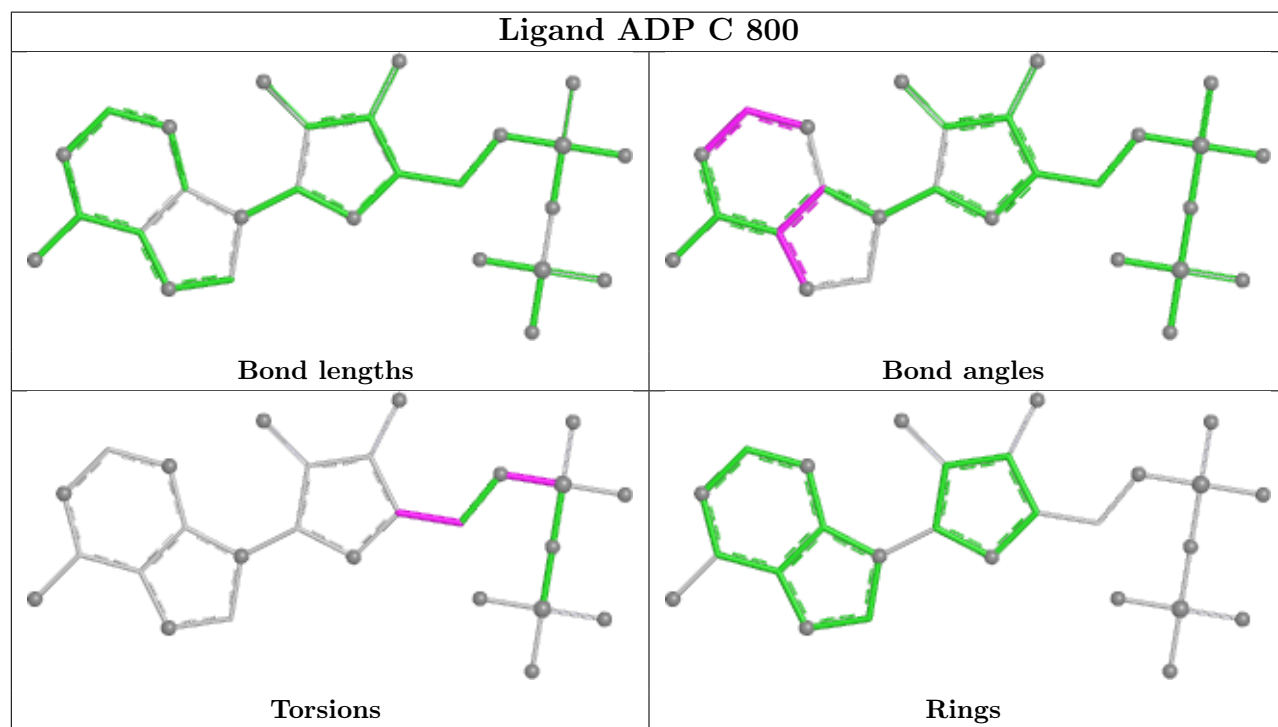
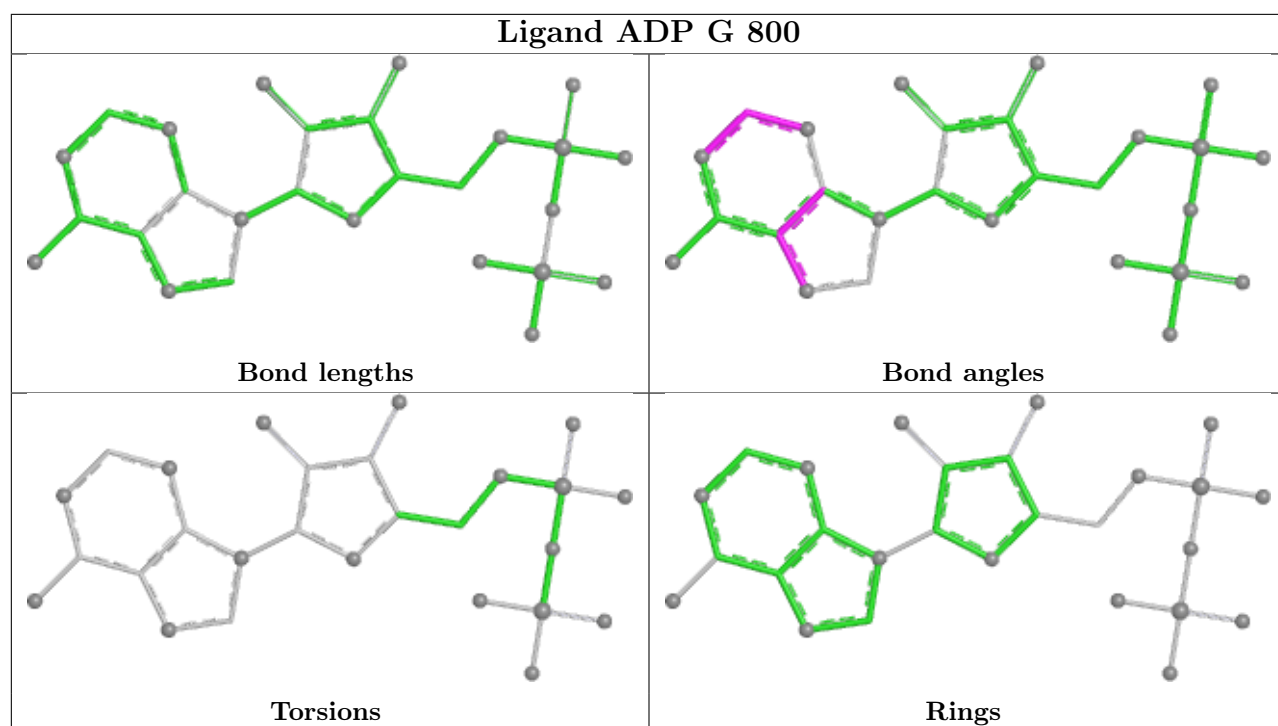
There are no ring outliers.

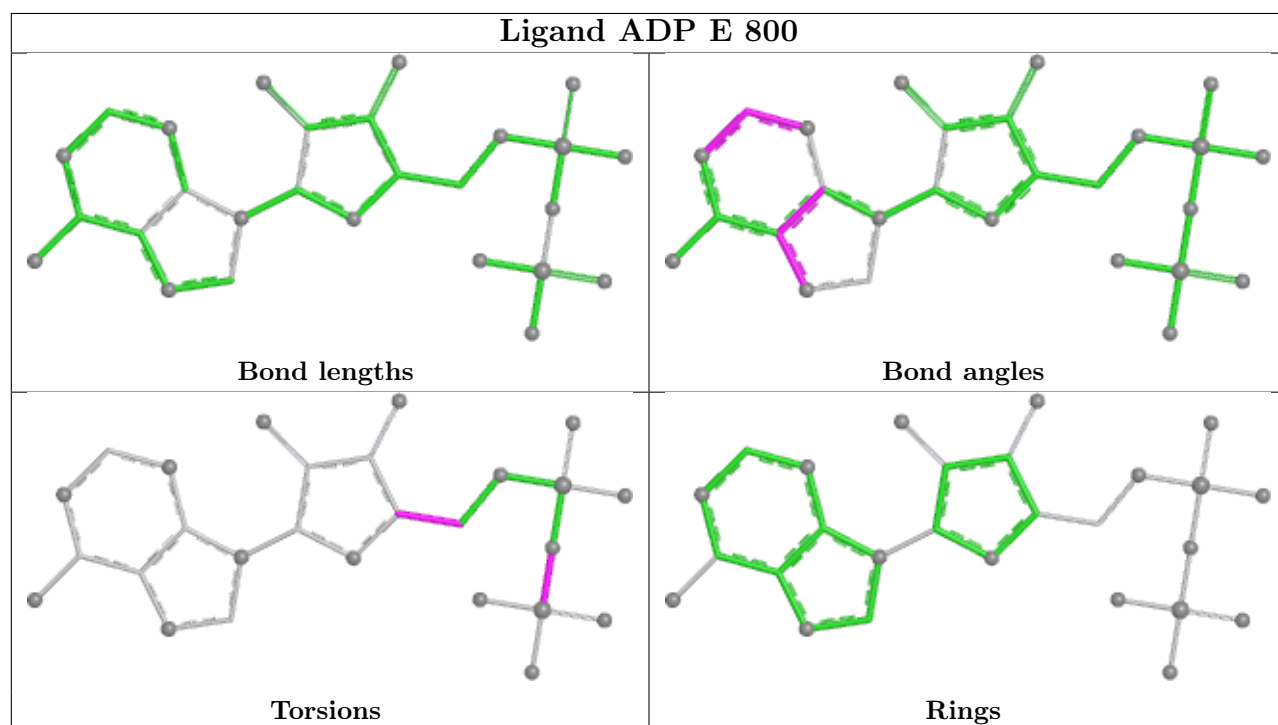
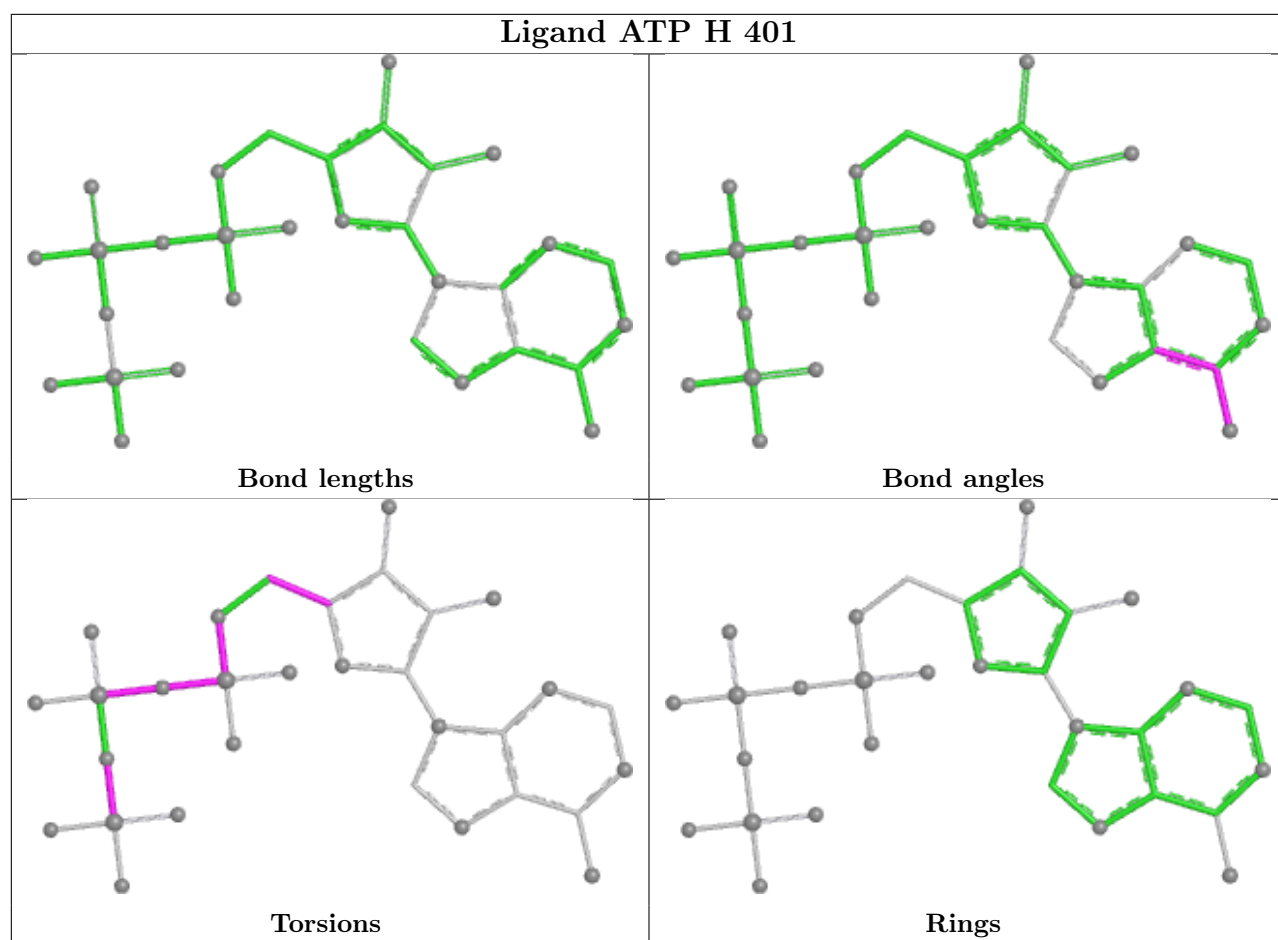
8 monomers are involved in 19 short contacts:

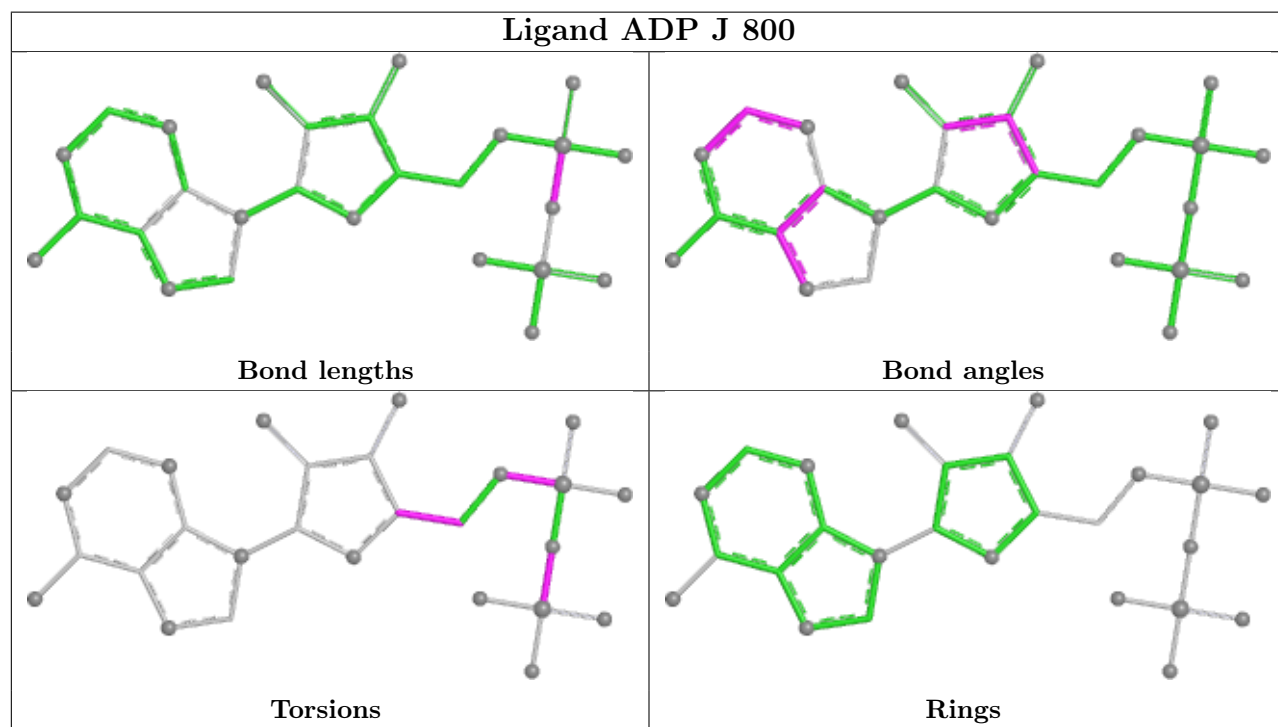
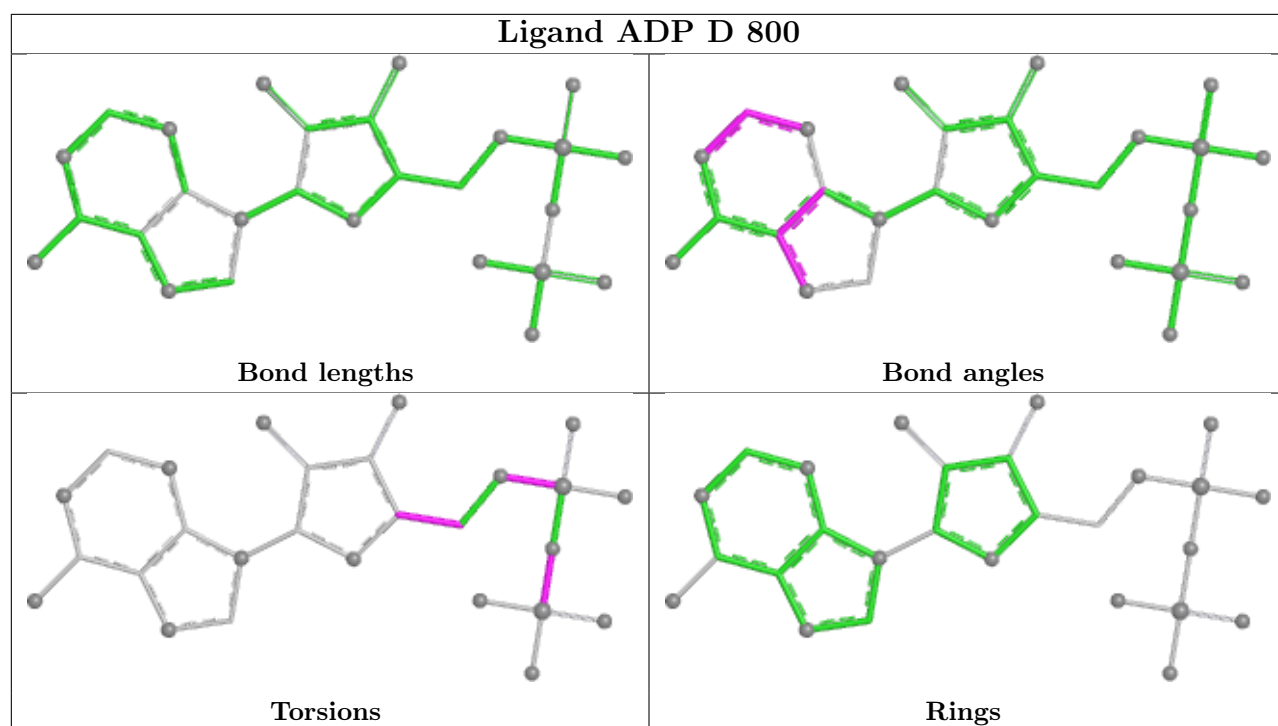
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	800	ADP	1	0
14	C	800	ADP	2	0
15	H	401	ATP	8	0
14	D	800	ADP	3	0
14	J	800	ADP	1	0
14	B	800	ADP	1	0
14	F	800	ADP	1	0
14	A	800	ADP	2	0

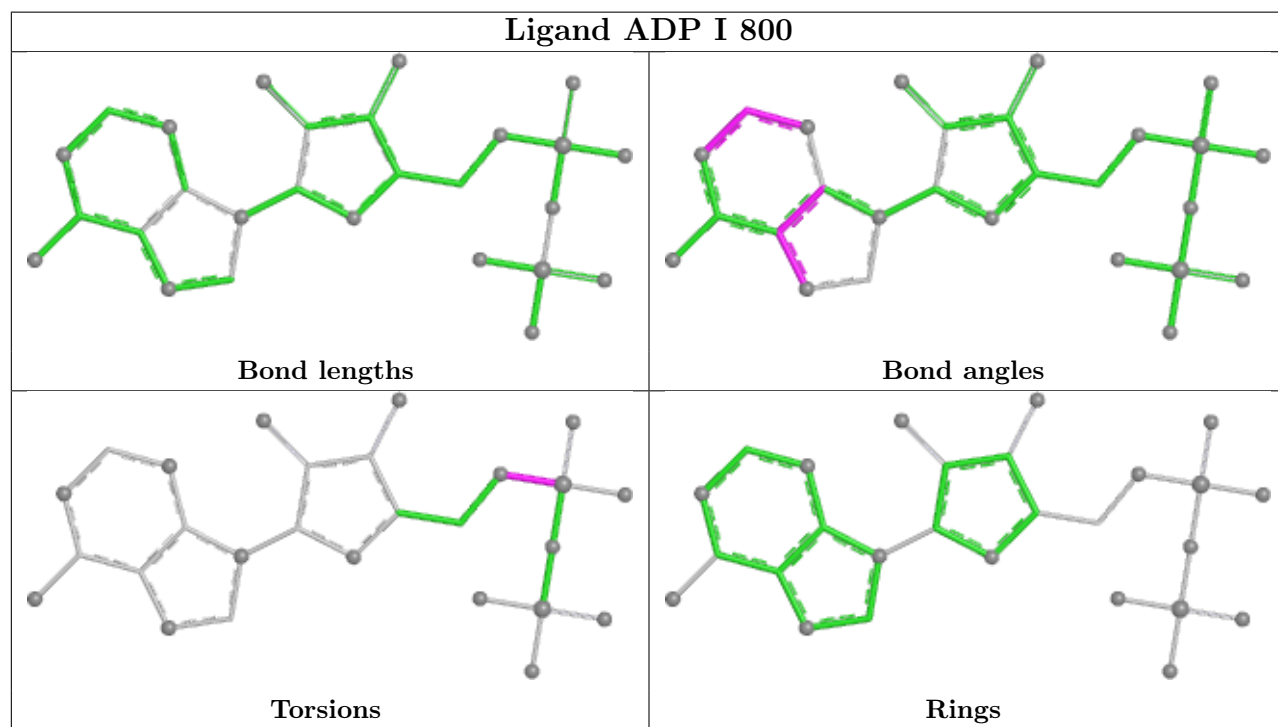
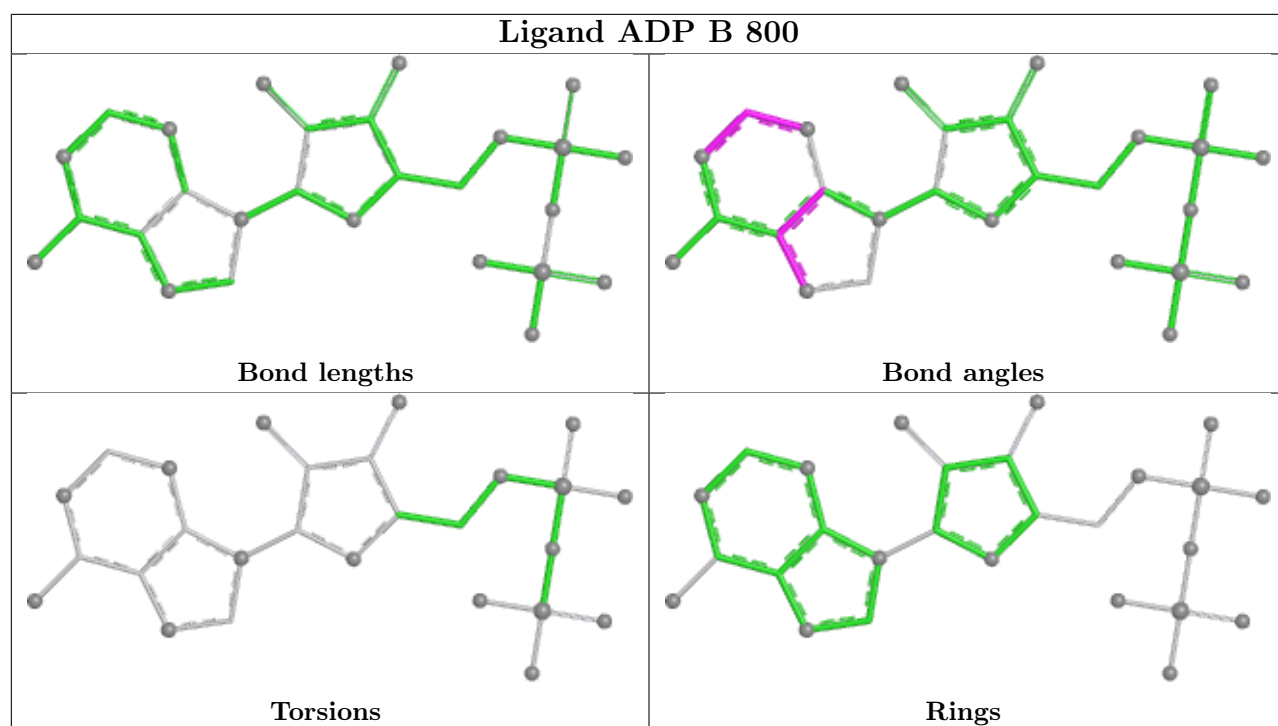
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

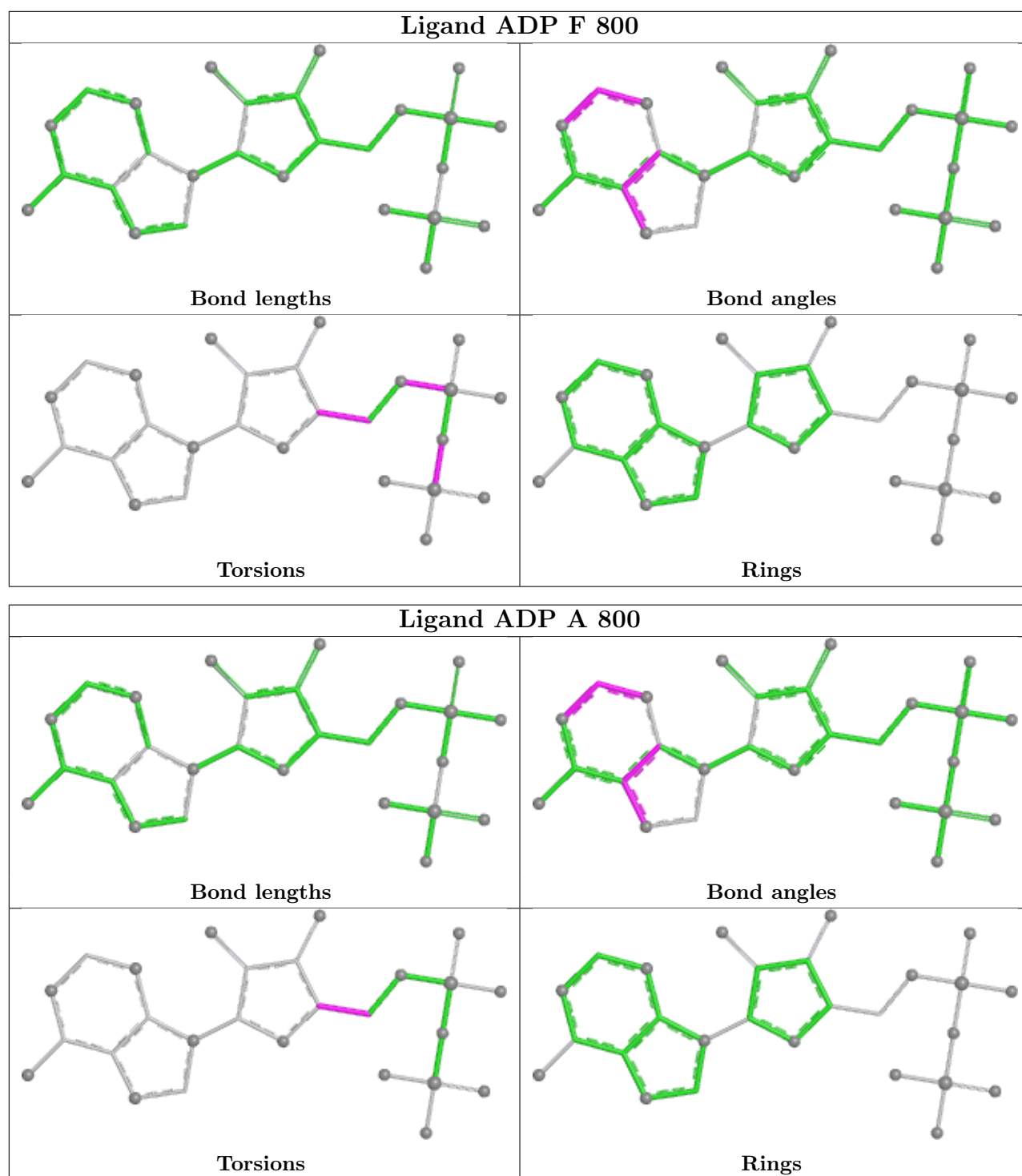












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

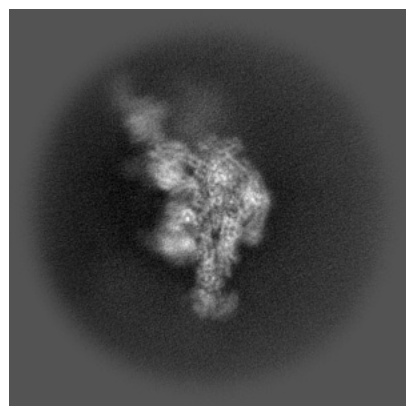
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46846. These allow visual inspection of the internal detail of the map and identification of artifacts.

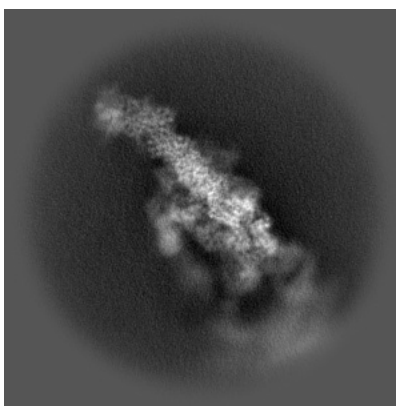
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

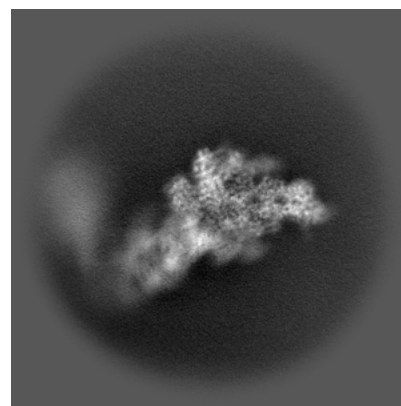
#### 6.1.1 Primary map



X

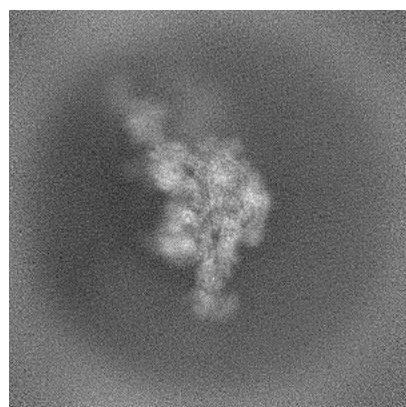


Y

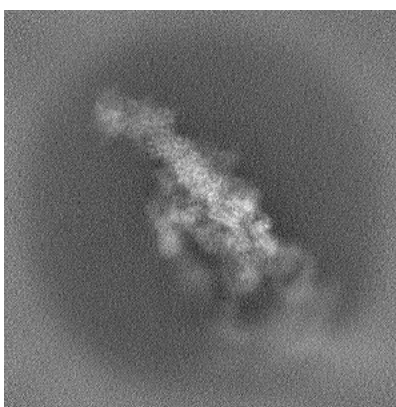


Z

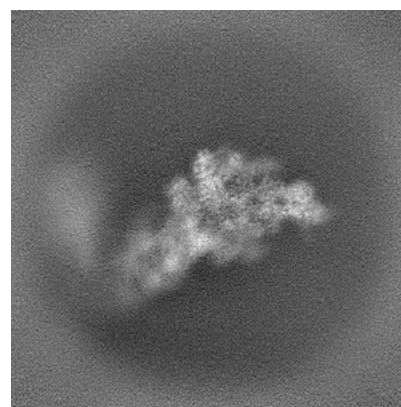
#### 6.1.2 Raw map



X



Y



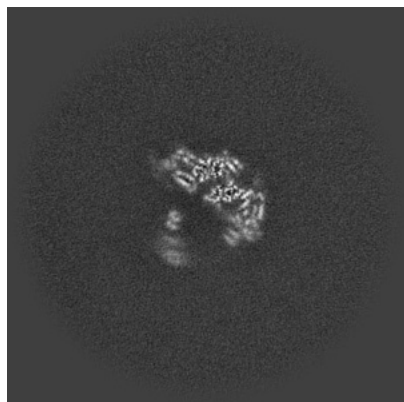
Z

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

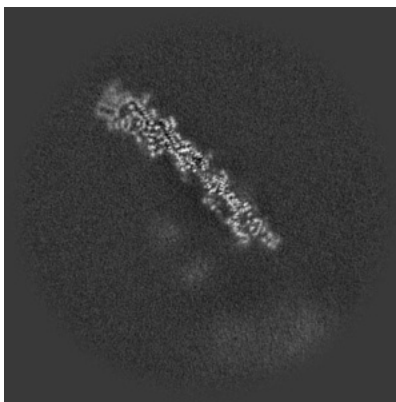


## 6.2 Central slices [i](#)

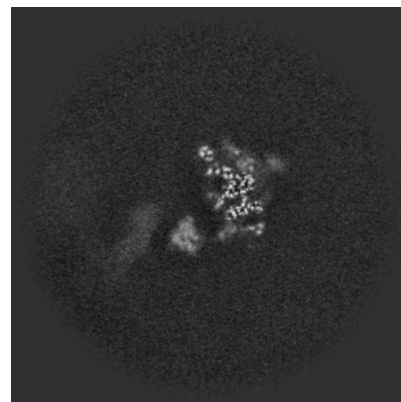
### 6.2.1 Primary map



X Index: 256



Y Index: 256

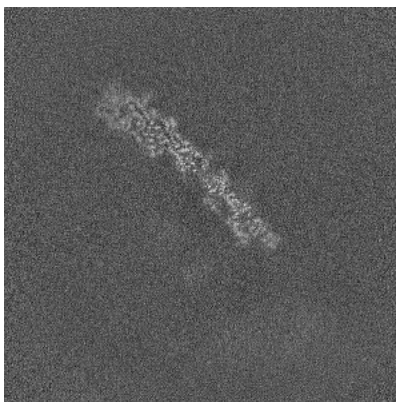


Z Index: 256

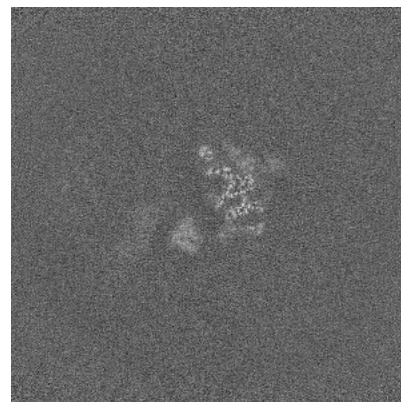
### 6.2.2 Raw map



X Index: 256



Y Index: 256



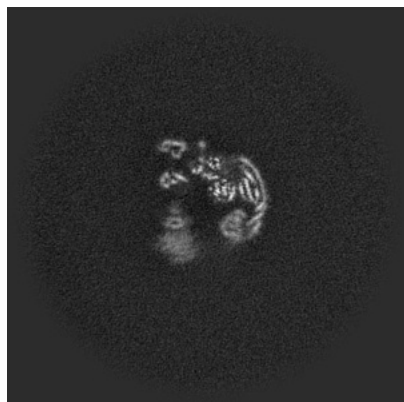
Z Index: 256

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

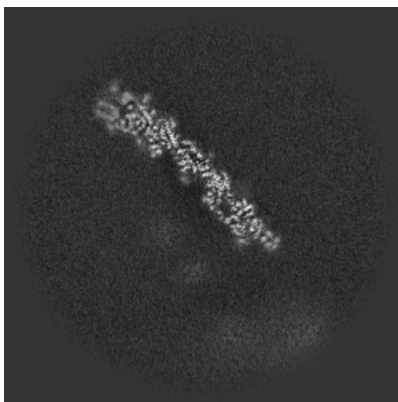


## 6.3 Largest variance slices [i](#)

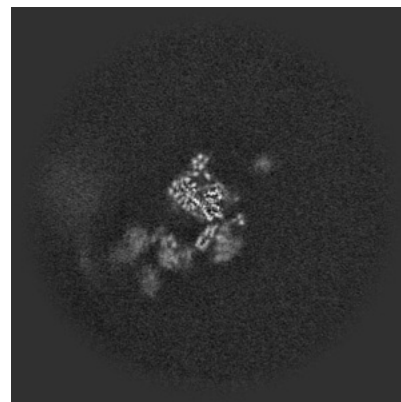
### 6.3.1 Primary map



X Index: 244

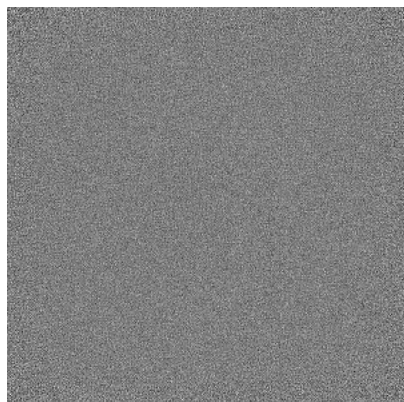


Y Index: 258

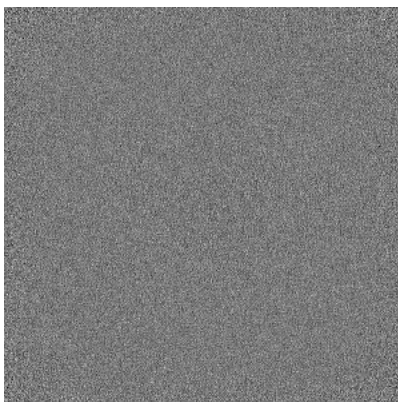


Z Index: 298

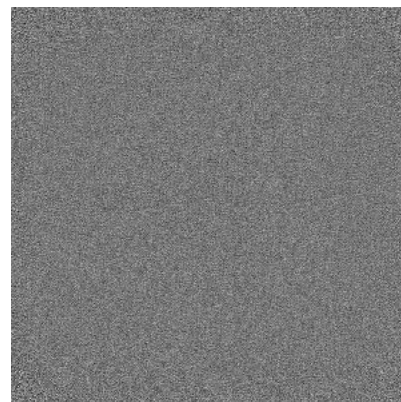
### 6.3.2 Raw map



X Index: 0



Y Index: 0

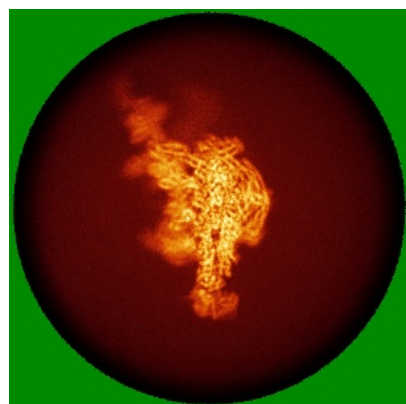


Z Index: 0

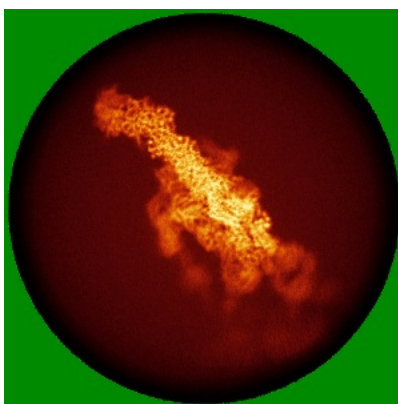
The images above show the largest variance slices of the map in three orthogonal directions.

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

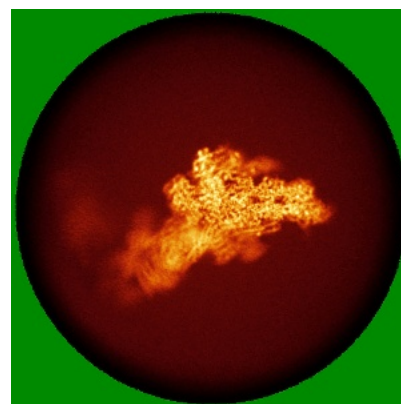
### 6.4.1 Primary map



X

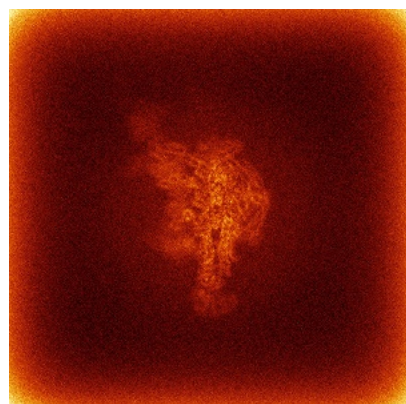


Y

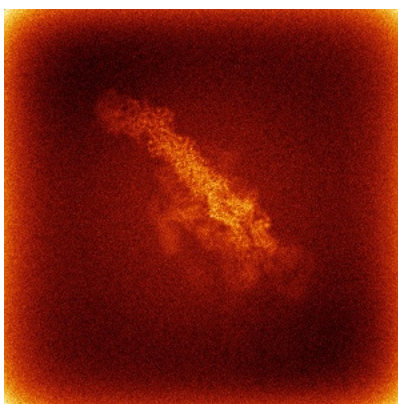


Z

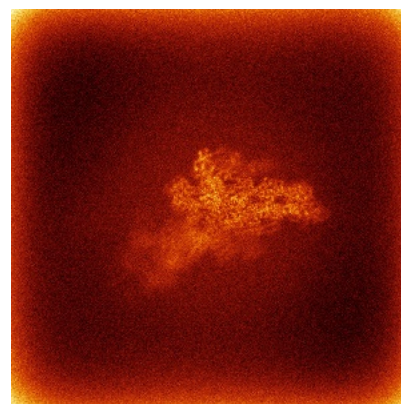
### 6.4.2 Raw map



X



Y

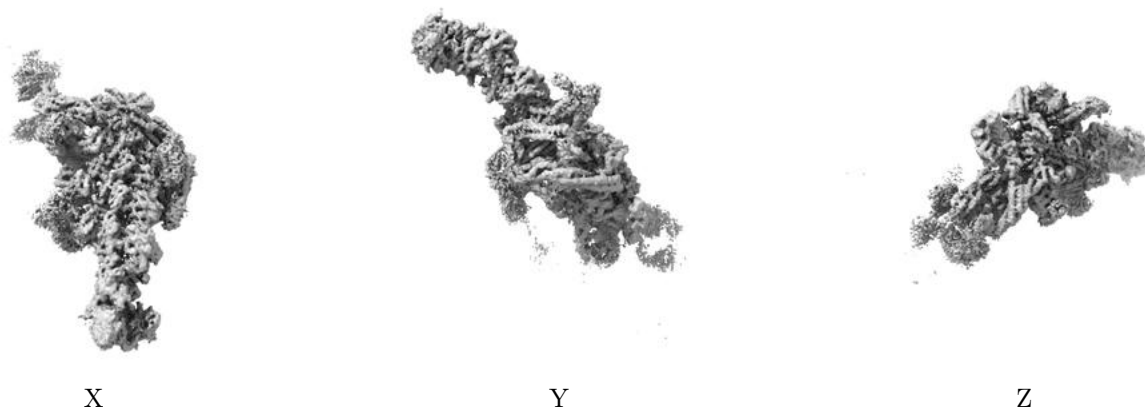


Z

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.

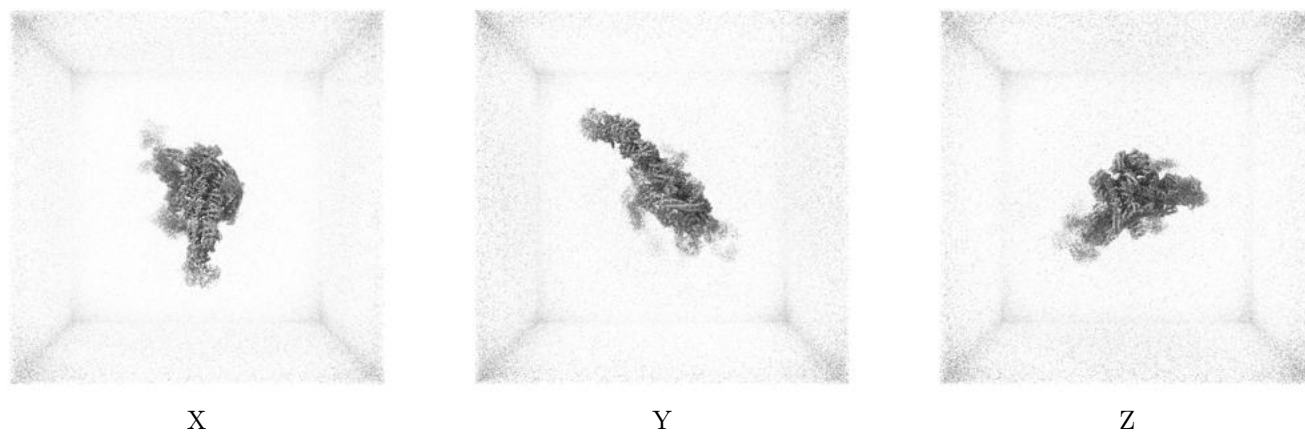
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

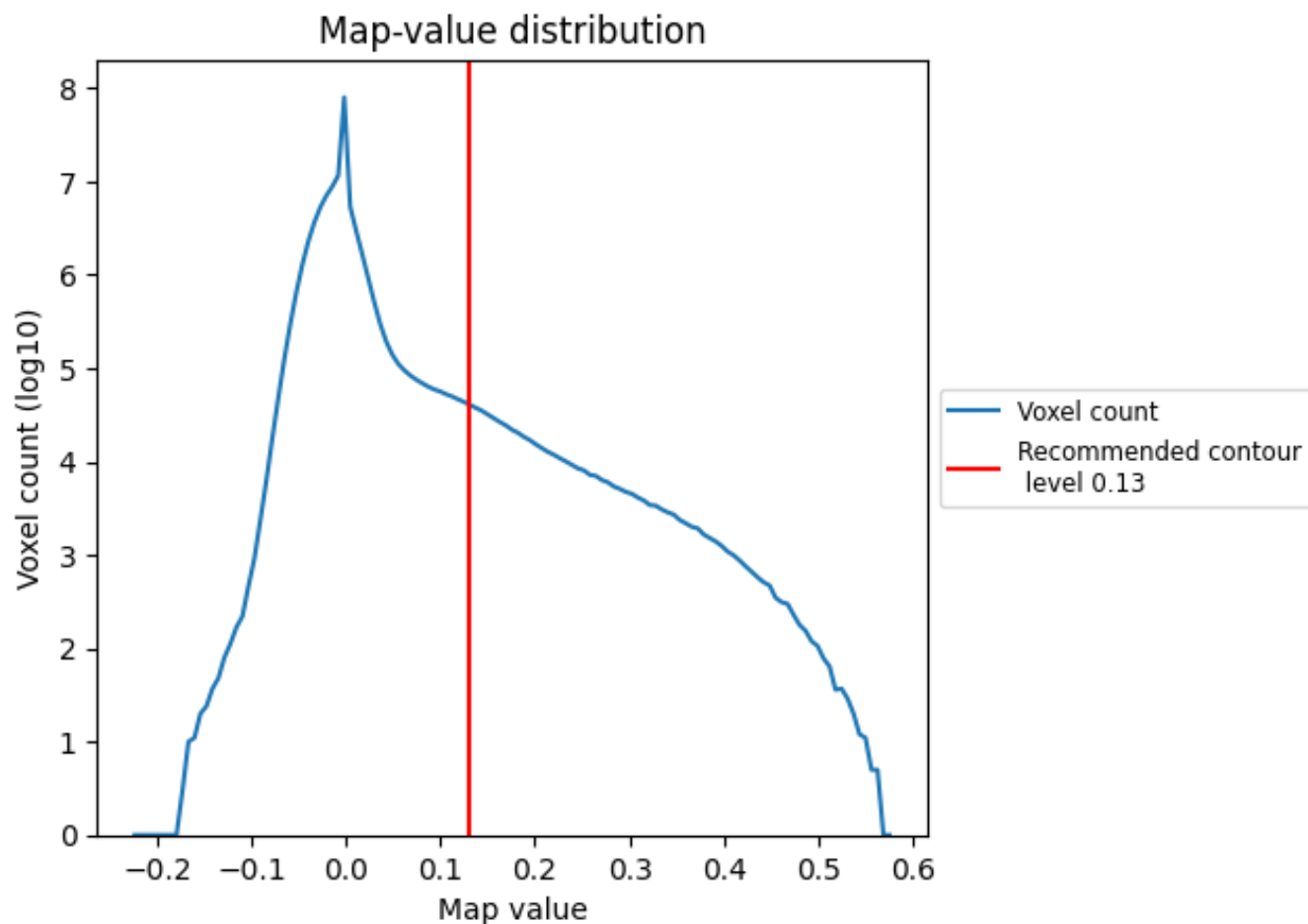
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

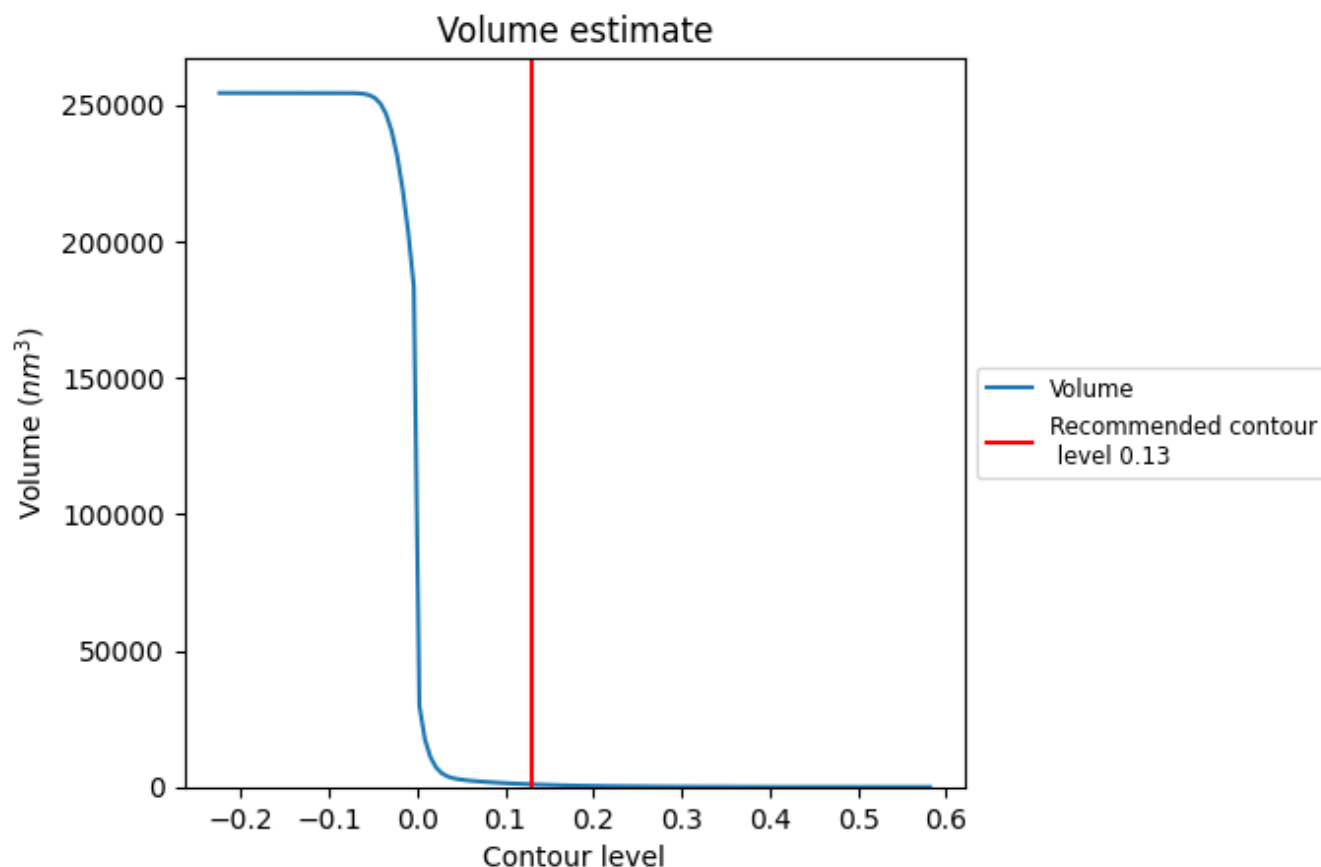
This section contains the results of statistical analysis of the map.

### 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.

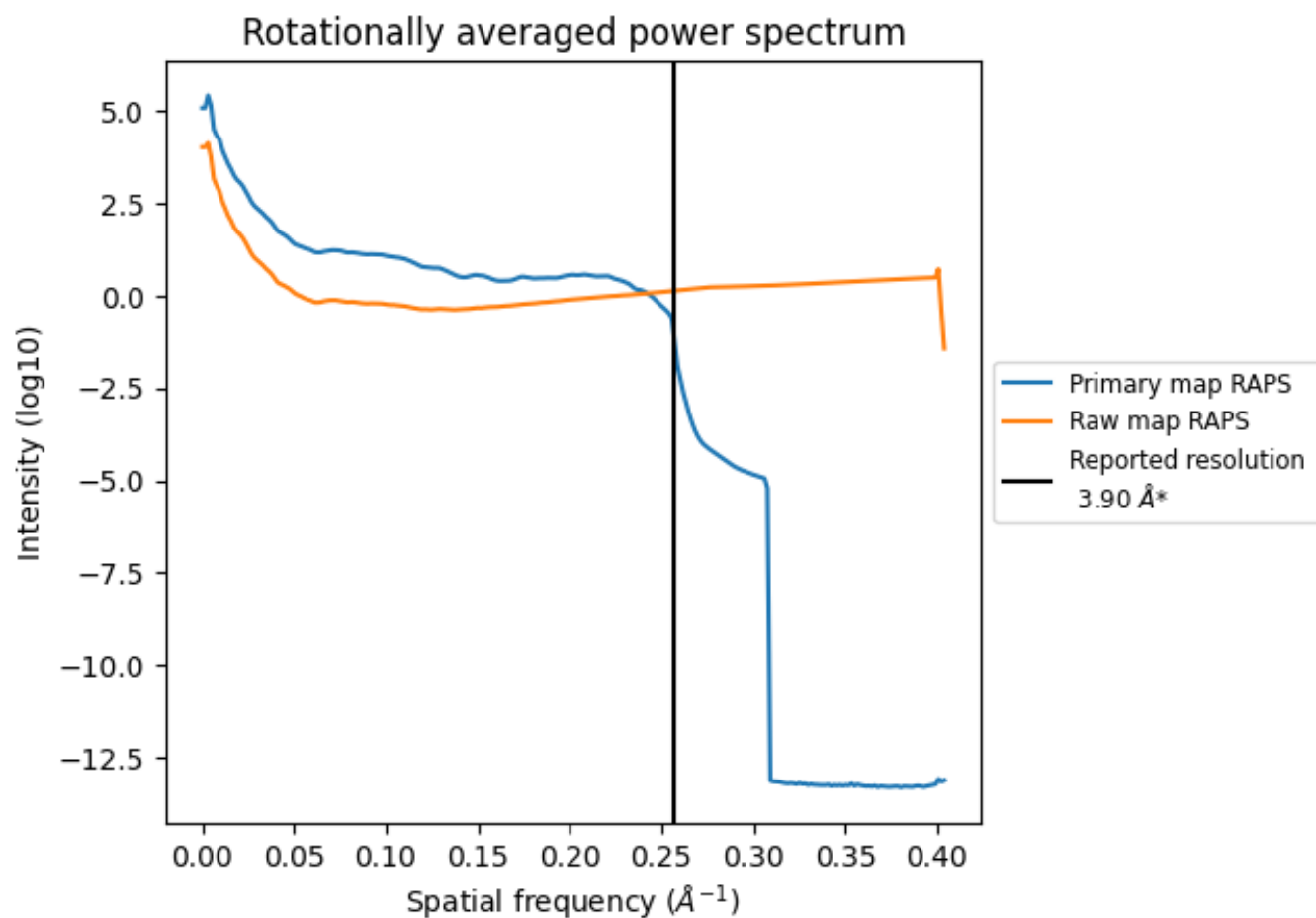
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 955  $\text{nm}^3$ ; this corresponds to an approximate mass of 863 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 ⓘ



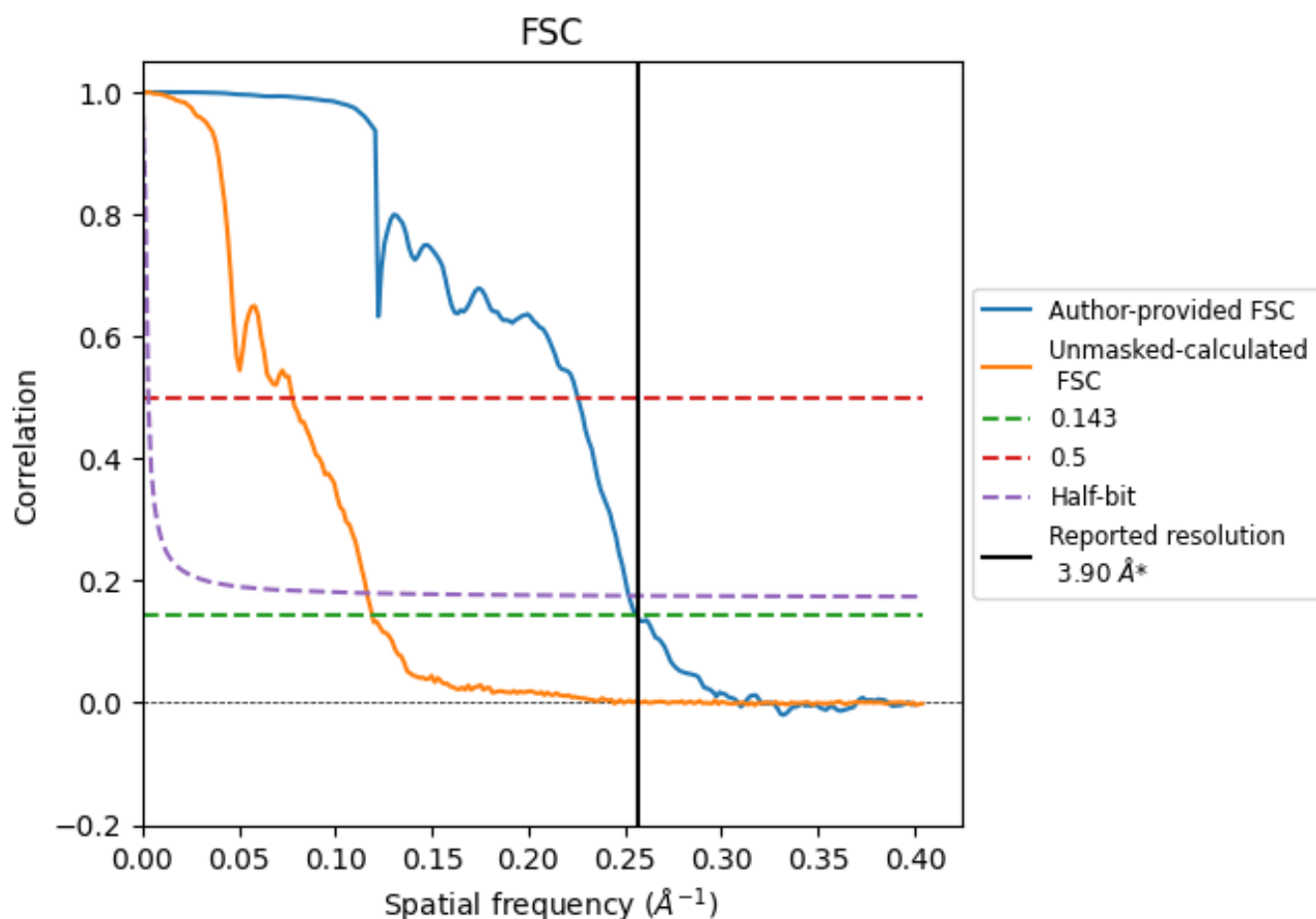
\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>



## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.43	3.97
Unmasked-calculated*	8.40	12.84	8.59

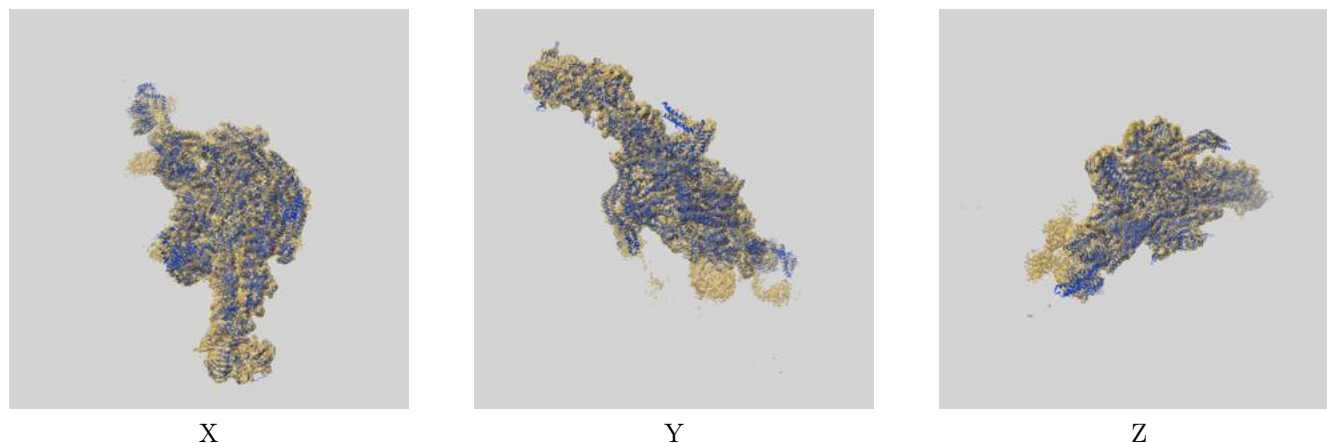
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.40 differs from the reported value 3.9 by more than 10 %



## 9 Map-model fit [i](#)

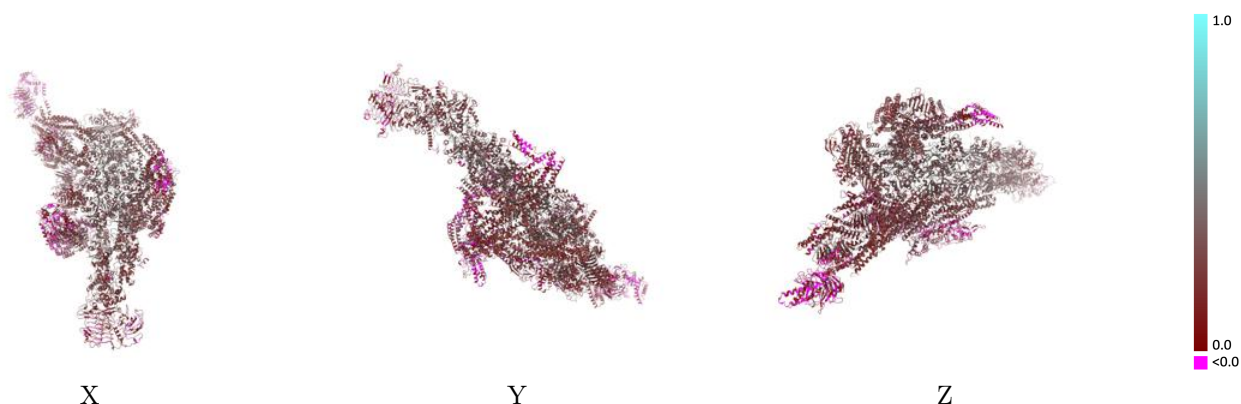
This section contains information regarding the fit between EMDB map EMD-46846 and PDB model 9DGS. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



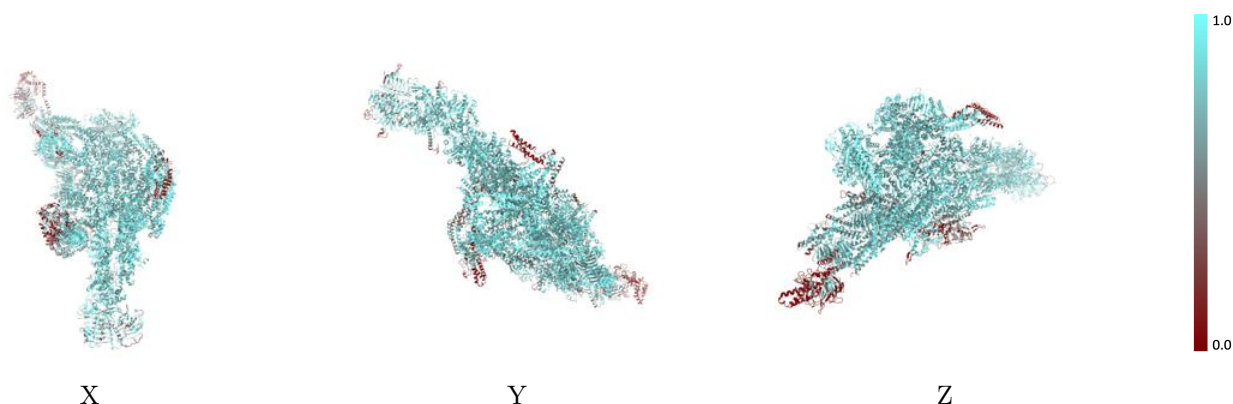
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



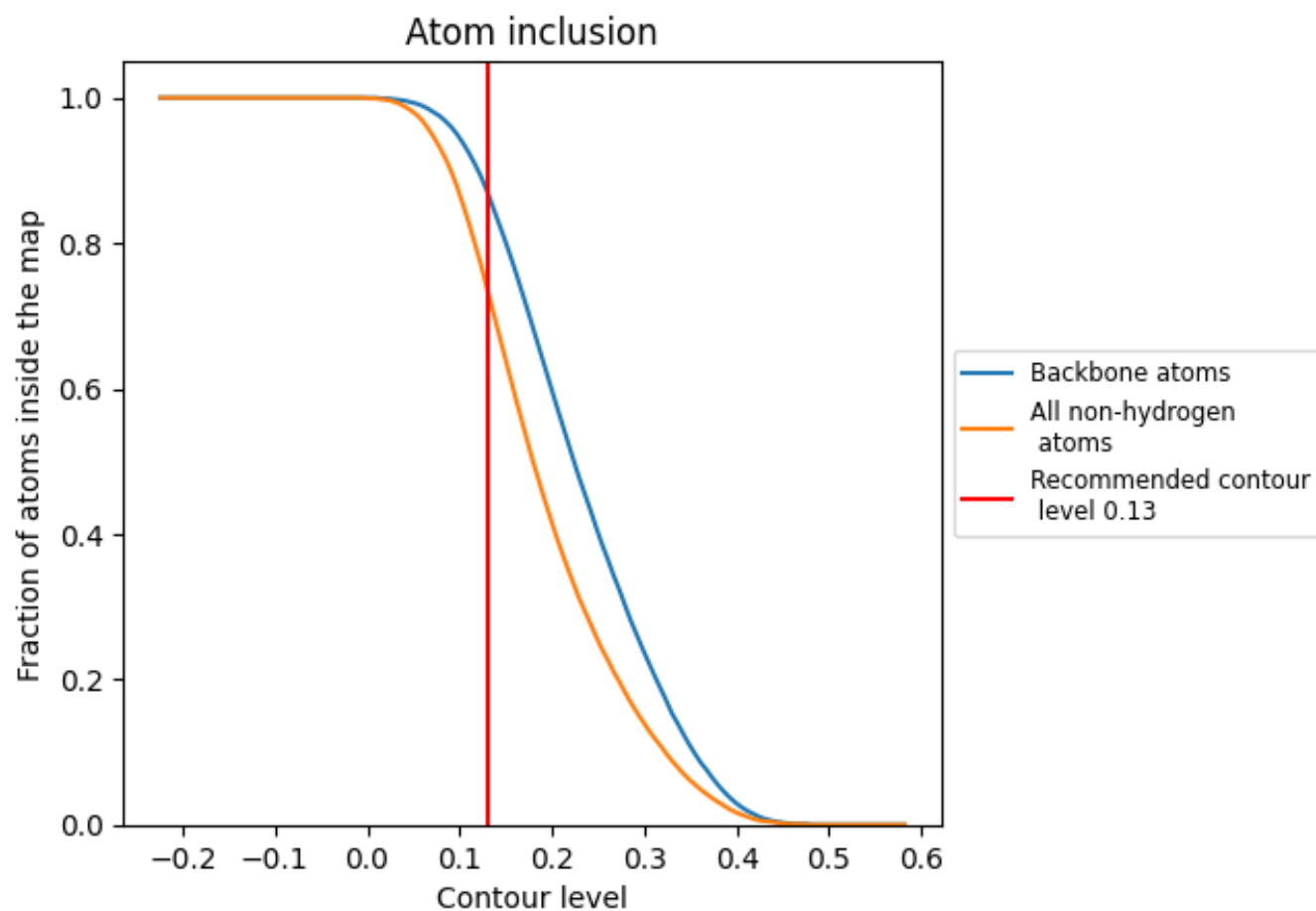
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.2500
A	 0.8350	 0.3150
B	 0.8510	 0.3500
C	 0.8500	 0.3670
D	 0.8590	 0.3650
E	 0.8420	 0.3610
F	 0.8570	 0.3590
G	 0.8420	 0.3440
H	 0.8420	 0.3470
I	 0.8150	 0.2910
J	 0.7850	 0.2860
K	 0.8150	 0.2520
L	 0.8190	 0.2630
M	 0.7450	 0.2350
N	 0.6990	 0.2060
O	 0.8200	 0.2050
P	 0.8050	 0.2670
Q	 0.7700	 0.2570
R	 0.8270	 0.2240
U	 0.6650	 0.1530
V	 0.7160	 0.1860
W	 0.7700	 0.2050
Y	 0.6720	 0.2130
Z	 0.8170	 0.2780
e	 0.5260	 0.1590
f	 0.6400	 0.1700
g	 0.5720	 0.1210
h	 0.8050	 0.1880
m	 0.7460	 0.2430
n	 0.6100	 0.1950
o	 0.7350	 0.2260
p	 0.3350	 0.0830

