



wwPDB EM Validation Summary Report ⓘ

May 2, 2026 – 03:47 PM EDT

PDB ID : 9DGT / pdb_00009dgt
EMDB ID : EMD-46847
Title : structure of dynactin, dynein tail with one BICDR from dynein-dynactin-BI
CDR on microtubules
Authors : Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 7.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

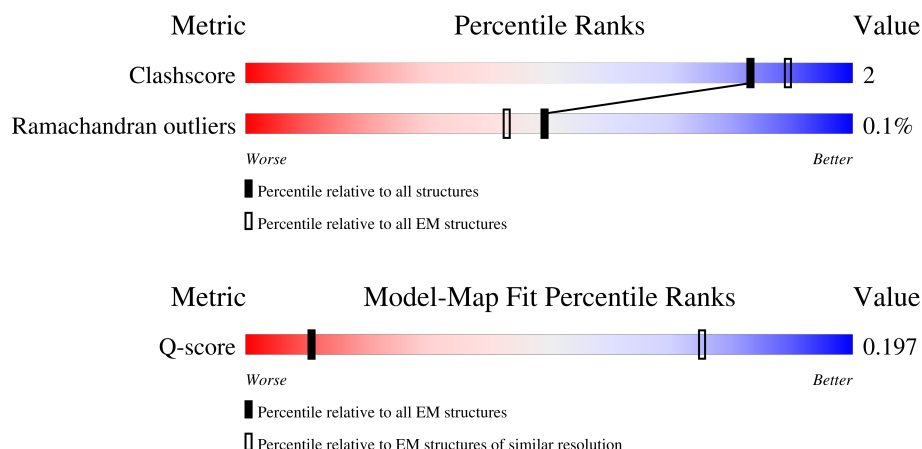
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 7.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



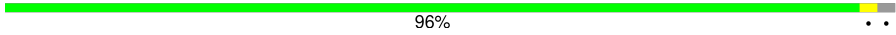
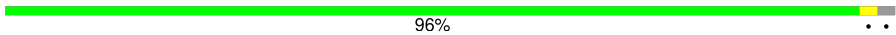
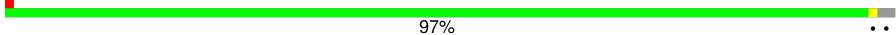
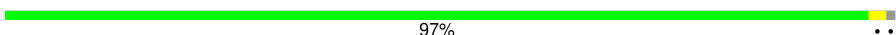


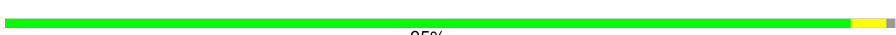




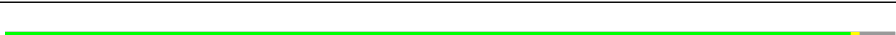

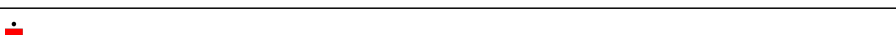
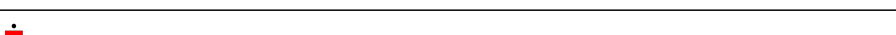
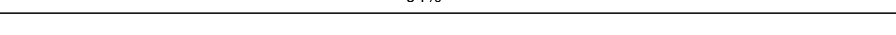

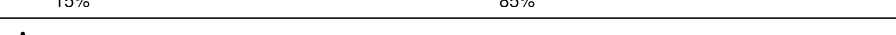







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	444 (6.70 - 7.70)

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	 94%
1	B	376	 96%
1	C	376	 98%
1	D	376	 94%
1	E	376	 95%

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Mol	Chain	Length	Quality of chain
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	c	577	
12	d	577	
13	e	4646	
13	f	4646	
13	m	4646	
13	n	4646	
14	g	612	

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Mol	Chain	Length	Quality of chain
14	h	612	<div><div></div><div>55%</div><div></div><div>42%</div></div>
14	o	612	<div><div></div><div>56%</div><div></div><div>42%</div></div>
14	p	612	<div><div></div><div>56%</div><div></div><div>42%</div></div>
15	j	492	<div><div></div><div>97%</div><div></div></div>
15	q	492	<div><div></div><div>97%</div><div></div></div>

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 59534 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	0	0
			1822	1082	370	370		
1	B	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	C	375	Total	C	N	O	0	0
			1847	1097	375	375		
1	D	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	E	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	F	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	G	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	I	370	Total	C	N	O	0	0
			1822	1082	370	370		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	379	Total	C	N	O	0	0
			1868	1110	379	379		

- 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	0	0
			1378	822	278	278		

- 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	0	0
			1327	789	269	269		

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	340	Total	C	N	O	0	0
			1689	1009	340	340		
6	N	280	Total	C	N	O	0	0
			1394	834	280	280		
6	P	325	Total	C	N	O	0	0
			1612	962	325	325		
6	Q	343	Total	C	N	O	0	0
			1707	1021	343	343		

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	179	Total	C	N	O	0	0
			888	530	179	179		
7	R	170	Total	C	N	O	0	0
			844	504	170	170		

- Molecule 8 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	167	Total	C	N	O	0	0
			822	488	167	167		

- Molecule 9 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	179	Total	C	N	O	0	0
			881	523	179	179		

- Molecule 10 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	152	Total	C	N	O	0	0
			754	450	152	152		
10	Z	192	Total	C	N	O	0	0
			952	568	192	192		

- Molecule 11 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	410	Total	C	N	O	0	0
			2038	1218	410	410		

- Molecule 12 is a protein called BICD family-like cargo adapter 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	c	220	Total	C	N	O	0	0
			1095	655	220	220		
12	d	220	Total	C	N	O	0	0
			1095	655	220	220		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	798	Total	C	N	O	0	0
			3959	2363	798	798		
13	f	808	Total	C	N	O	0	0
			4009	2393	808	808		
13	m	792	Total	C	N	O	0	0
			3750	2166	792	792		
13	n	755	Total	C	N	O	0	0
			3566	2056	755	755		

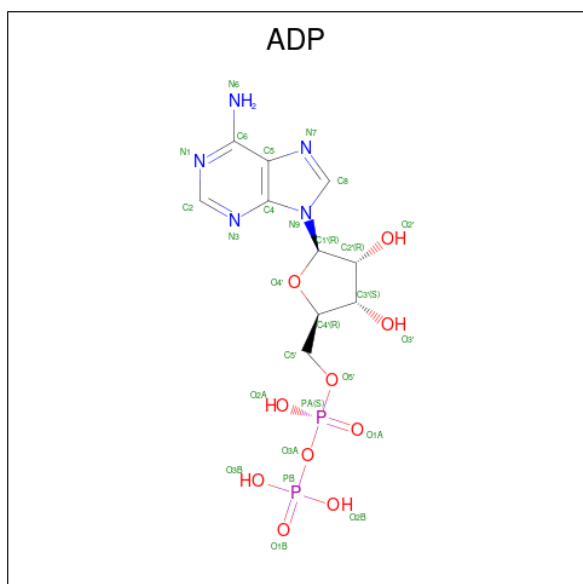
- Molecule 14 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	g	358	Total	C	N	O	0	0
			1767	1051	358	358		
14	h	358	Total	C	N	O	0	0
			1767	1051	358	358		
14	o	358	Total	C	N	O	0	0
			1767	1051	358	358		
14	p	358	Total	C	N	O	0	0
			1767	1051	358	358		

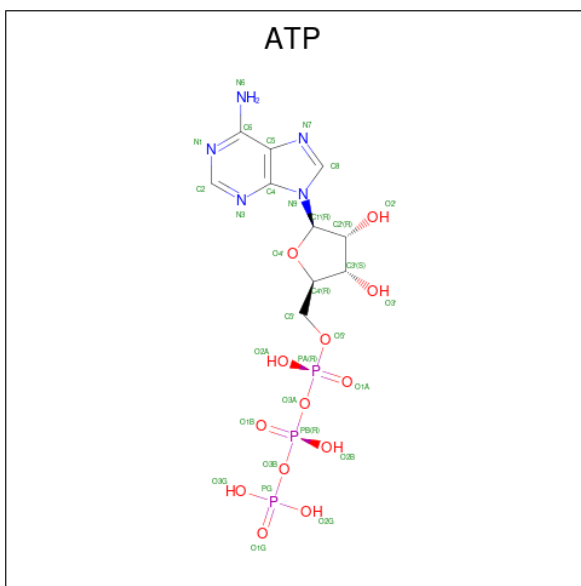
- Molecule 15 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	j	14	Total	C	N	O	0	0
			69	41	14	14		
15	q	14	Total	C	N	O	0	0
			69	41	14	14		

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

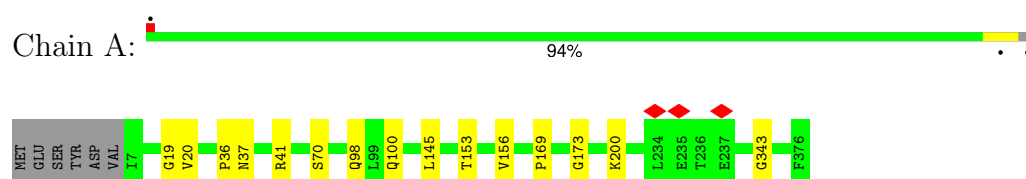
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

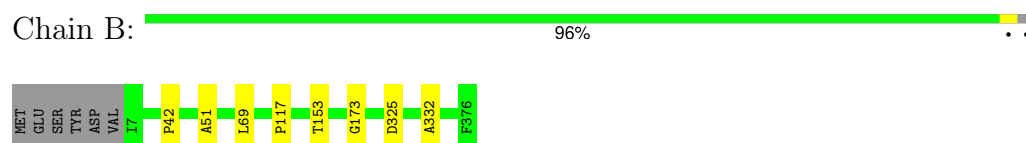
3 Residue-property plots [i](#)

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.

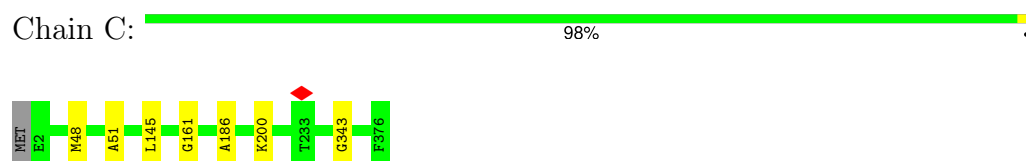
- Molecule 1: Alpha-centractin



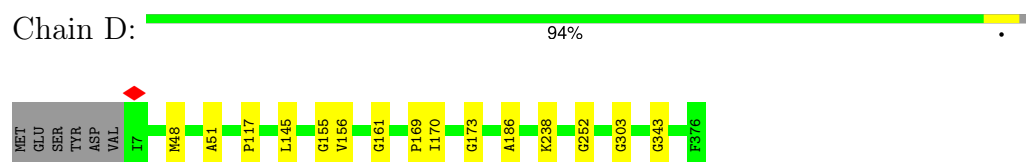
- Molecule 1: Alpha-centractin



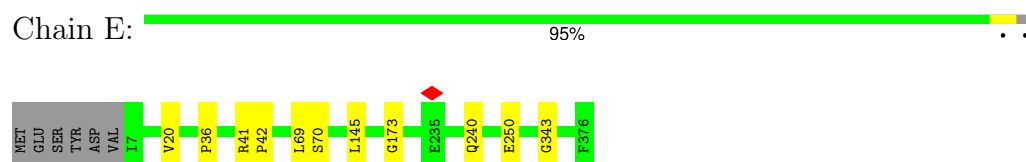
- Molecule 1: Alpha-centractin



- Molecule 1: Alpha-centractin

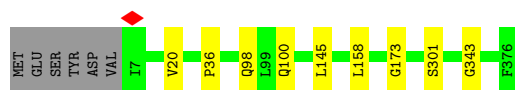


- Molecule 1: Alpha-centractin



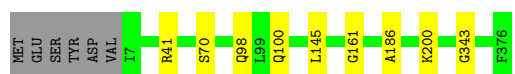
- Molecule 1: Alpha-centractin

Chain F:  96% 



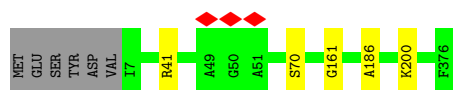
- Molecule 1: Alpha-centractin

Chain G:  96% 



- Molecule 1: Alpha-centractin

Chain I:  97% 





- Molecule 2: Actin, cytoplasmic 1

Chain H:  97% 



- Molecule 3: Actin-related protein 10

Chain J:  89% 



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

Chain K:  93% 



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

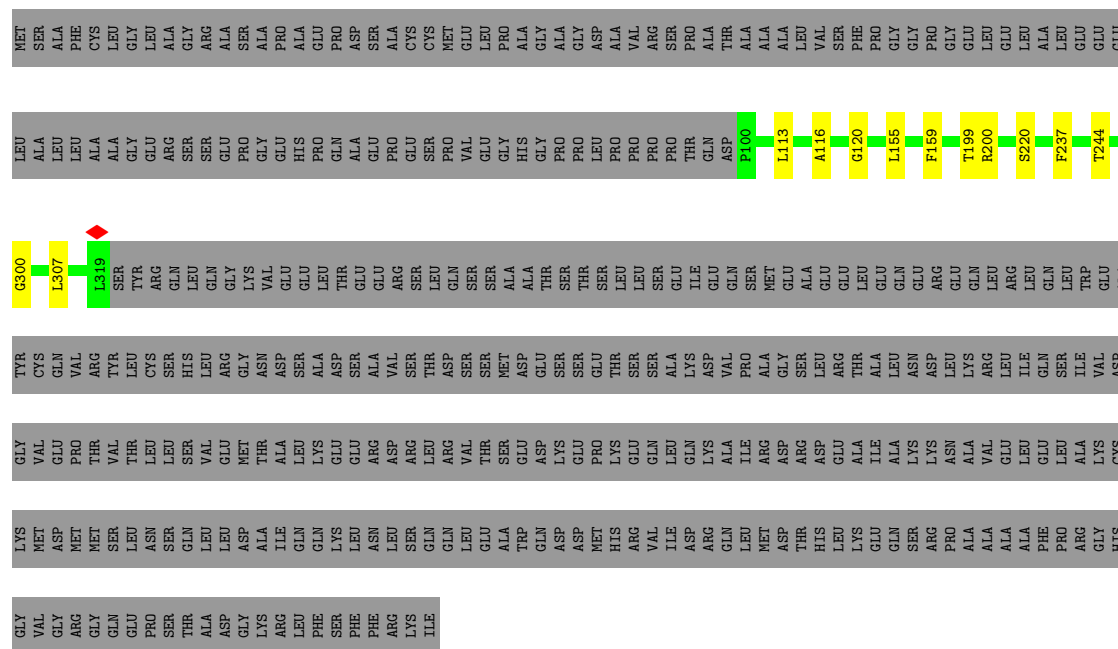
Chain L:  95% 



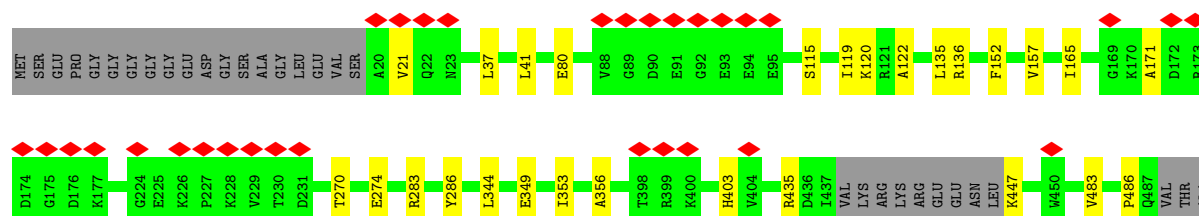
[illegible]



- Molecule 12: BICD family-like cargo adapter 1



- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

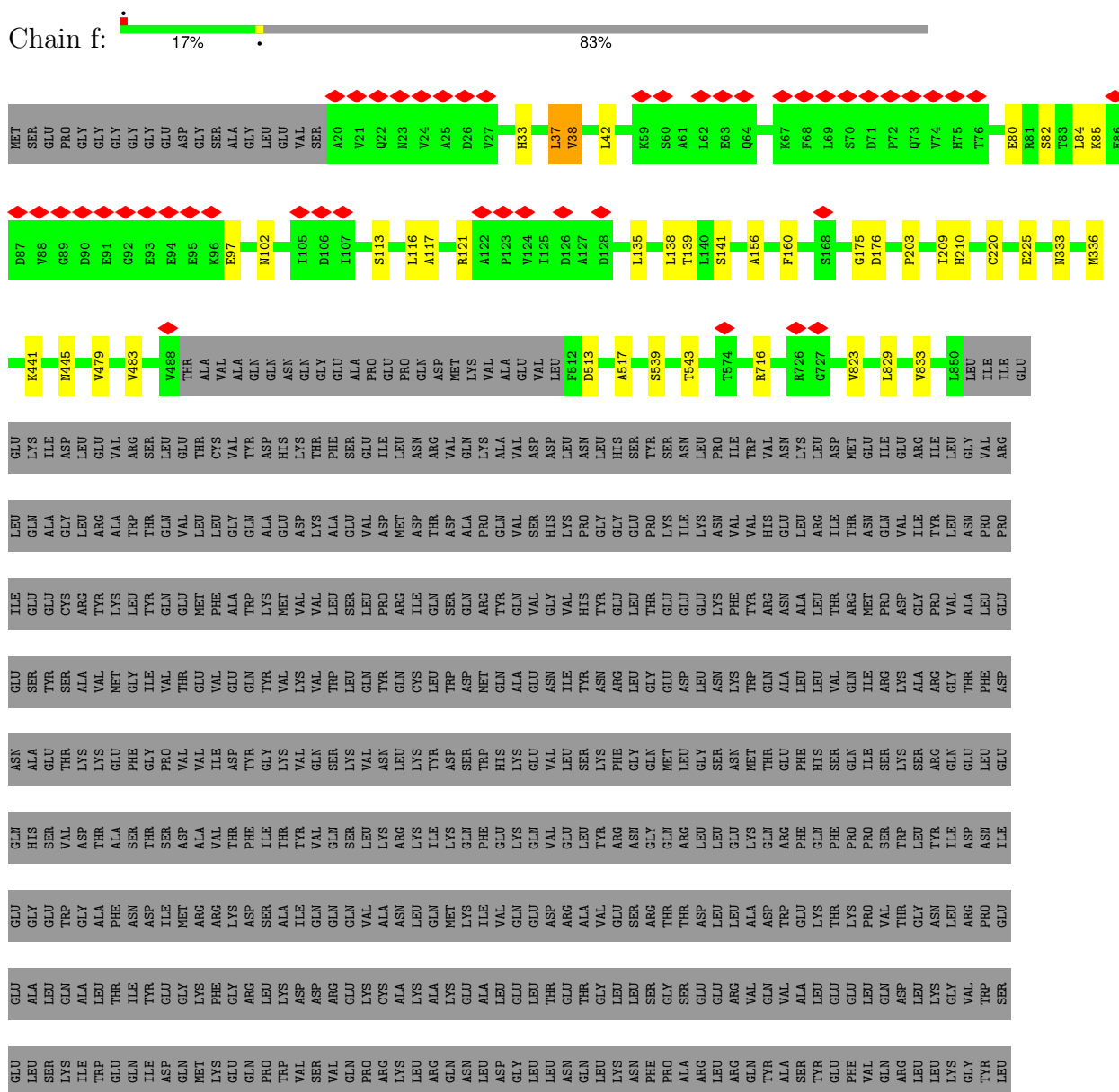








- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

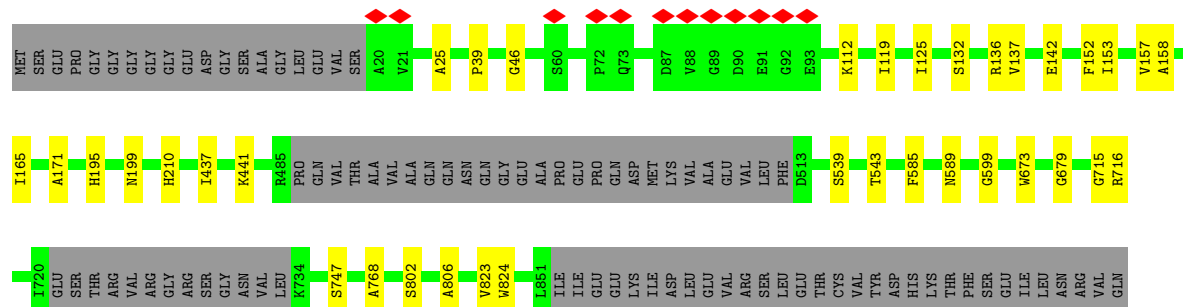






- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

Chain m:  16% 83%









- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

[illegible]

WORLDWIDE
PDB
PROTEIN DATA BANK



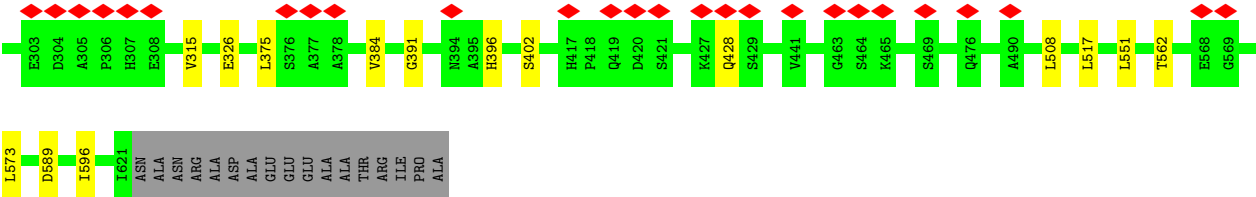
[illegible]

- Molecule 14: Cytoplasmic dynein 1 intermediate chain 2



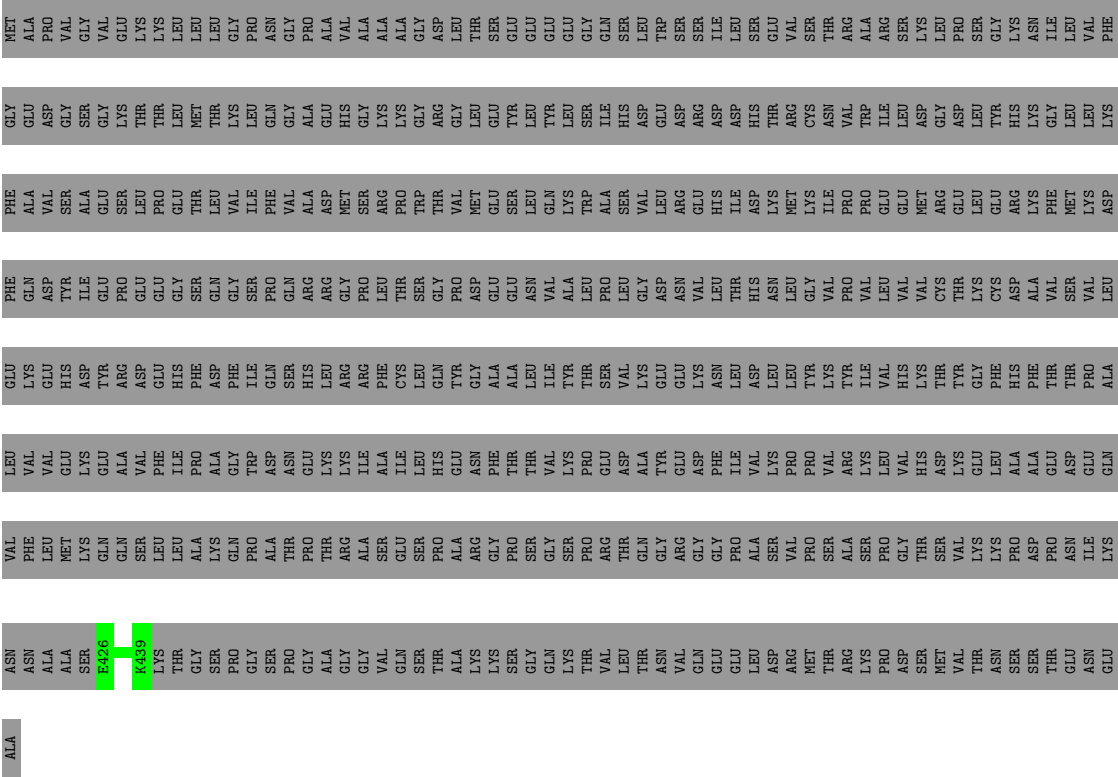
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	Y291	LEU	PHE	ALA	SER
	P292	THR	PRO	LEU	ASP
	E293	GLU	ARG	LEU	LYS
	V315	GLU	GLU	GLN	SER
	E326	LYS	ILE	MET	GLU
	L359	GLN	VAL	GLY	LEU
	V370	GLN	THR	THR	ALA
	Q371	ILE	TYR	LEU	GLU
	S409	THR	THR	PRO	ARG
B	D413	LEU	VAL	PRO	ARG
	M414	SER	MET	PRO	ALA
	Q419	PHE	GLN	MET	GLN
	V441	ASP	GLN	SER	ILE
	T480	HIS	PRO	PRO	ARG
	C484	SER	LYS	SER	GLU
	G489	THR	GLU	SER	GLU
	A490	ARG	ASP	LYS	LYS
	V491	ALA	VAL	ALA	ARG
	D492	GLU	VAL	GLY	LYS
C	F497	GLN	LYS	SER	LYS
	S500	ASN	PRO	ASP	GLU
	L551	ILE	ILE	GLY	THR
	T562	PHE	ILE	GLY	GLN
	E568	ASP	GLU	ASP	VAL
	G569	LEU	THR	ARG	THR
	H580	GLU	LEU	ARG	VAL
	S581	ASP	LYS	GLY	GLN
	G582	LYS	LYS	PRO	GLU
	R583	GLU	ASP	ILE	GLU
D	E601	ILE	SER	GLY	LEU
	Q602	GLN	ASP	MET	GLU
	M608	ALA	SER	ALA	LYS
	D609	GLY	LYS	LYS	ARG
		ALA	ILE	ILE	ARG
		THR	THR	THR	ARG
		GLN	GLN	GLN	ALA
		VAL	THR	VAL	GLU
		ILE	THR	VAL	ALA
		GLU	THR	VAL	GLU

ASP
ALA
GLU
GLU
GLU
ALA
ALA
THR
ARG
ILE
PRO
ALA



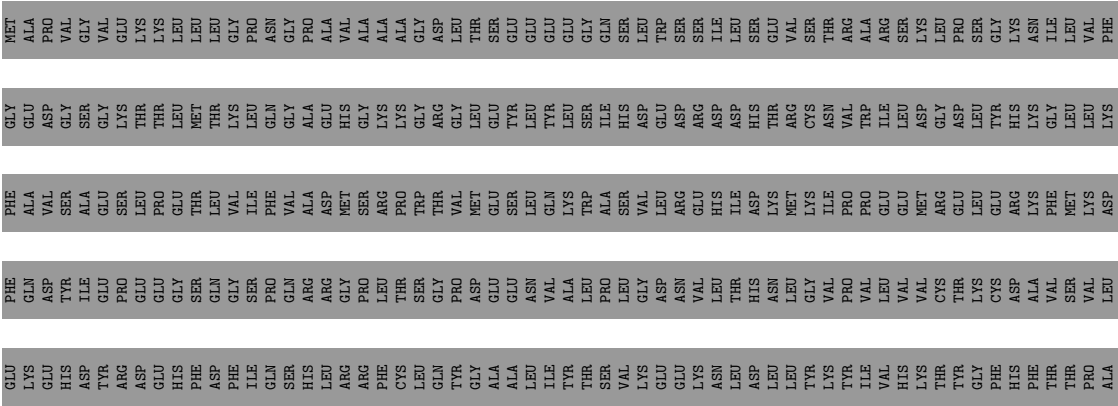
• Molecule 15: Dynein light intermediate chain

Chain j: . 97%



• Molecule 15: Dynein light intermediate chain

Chain q: . 97%



ALA	ASN	VAL	LEU
	ASN	PHE	LEU
	ALA	ALA	VAL
	ALA	MET	GLU
	SER	LYS	LYS
	E426	GLN	GLU
		GLN	ALA
		SER	VAL
	E439	LEU	PHE
	LYS	LEU	ILE
	THR	GLY	PRO
	GLY	ALA	LYS
	SER	LYS	ALA
	PRO	GLN	GLY
	GLY	PRO	THR
	SER	ALA	ASP
	PRO	THR	ASN
	GLY	PRO	GLU
	ALA	THR	LYS
	GLY	ARG	LYS
	GLY	ALA	LYS
	VAL	SER	ILE
	GLN	GLU	ILE
	SER	SER	LEU
	THR	PRO	HTS
	ALA	ALA	GLU
	LYS	ARG	ASN
	LYS	GLY	PHE
	SER	PRO	THR
	GLY	SER	THR
	GLN	GLY	VAL
	LYS	SER	LYS
	THR	PRO	PRO
	VAL	ARG	GLU
	LEU	THR	ASP
	THR	GLN	ALA
	ASN	GLY	TYR
	VAL	ARG	GLU
	GLN	GLY	ASP
	GLU	GLY	PHE
	GLU	PRO	ILE
	LEU	ALA	VAL
	ASP	SER	LYS
	ARG	VAL	PRO
	MET	PRO	PRO
	THR	SER	VAL
	ARG	ALA	ARG
	LYS	SER	LYS
	PRO	PRO	LEU
	ASP	GLY	VAL
	SER	THR	HIS
	MET	SER	ASP
	VAL	VAL	LYS
	THR	LYS	GLU
	ASN	LYS	LEU
	SER	PRO	ALA
	SER	ASP	ALA
	THR	PRO	GLU
	GLU	ASN	ASP
	ASN	ILE	GLN
	GLU	TYR	GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	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	0.461	Depositor
Minimum map value	-0.198	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	666.62396, 666.62396, 666.62396	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.736, 1.736, 1.736	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, ADP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/1821	0.40	0/2531
1	B	0.18	0/1821	0.48	0/2531
1	C	0.18	0/1846	0.46	0/2566
1	D	0.17	0/1821	0.42	0/2531
1	E	0.17	0/1821	0.46	0/2531
1	F	0.18	0/1821	0.46	0/2531
1	G	0.18	0/1821	0.44	0/2531
1	I	0.15	0/1821	0.43	0/2531
2	H	0.17	0/1821	0.40	0/2531
3	J	0.28	0/1867	0.50	0/2596
4	K	0.16	0/1377	0.40	0/1919
5	L	0.16	0/1326	0.37	0/1844
6	M	0.17	0/1684	0.45	0/2343
6	N	0.15	0/1389	0.40	0/1933
6	P	0.16	0/1609	0.41	0/2240
6	Q	0.16	0/1703	0.39	0/2373
7	O	0.15	0/887	0.44	0/1236
7	R	0.17	0/843	0.49	0/1175
8	U	0.21	0/821	0.54	0/1140
9	V	0.15	0/880	0.42	0/1222
10	W	0.16	0/750	0.45	0/1040
10	Z	0.17	0/951	0.48	0/1325
11	Y	0.40	0/2035	0.58	1/2837 (0.0%)
12	c	0.38	0/1094	0.67	0/1527
12	d	0.37	0/1094	0.66	0/1527
13	e	0.29	0/3956	0.48	0/5515
13	f	0.26	0/4007	0.51	2/5588 (0.0%)
13	m	0.19	0/3747	0.39	0/5115
13	n	0.32	0/3562	0.49	0/4855
14	g	0.11	0/1766	0.29	0/2457
14	h	0.14	0/1766	0.40	0/2457
14	o	0.13	0/1766	0.37	1/2457 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	p	0.14	0/1766	0.37	1/2457 (0.0%)
15	j	0.24	0/68	0.50	0/93
15	q	0.27	0/68	0.44	0/93
All	All	0.22	0/59196	0.46	5/82178 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	o	428	GLN	CB-CA-C	-5.18	110.58	116.54
14	p	428	GLN	CB-CA-C	-5.15	110.61	116.54
11	Y	51	CYS	CB-CA-C	5.04	116.40	108.63
13	f	37	LEU	CA-C-N	5.04	131.45	122.13
13	f	37	LEU	C-N-CA	5.04	131.45	122.13

There are no chirality outliers.

There are no planarity outliers.

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	1822	0	820	8	0
1	B	1822	0	820	7	0
1	C	1847	0	830	5	0
1	D	1822	0	820	10	0
1	E	1822	0	820	7	0
1	F	1822	0	820	6	0
1	G	1822	0	820	5	0
1	I	1822	0	820	3	0
2	H	1822	0	835	6	0
3	J	1868	0	823	5	0
4	K	1378	0	611	6	0
5	L	1327	0	585	13	0
6	M	1689	0	765	2	0
6	N	1394	0	632	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	1612	0	747	5	0
6	Q	1707	0	769	1	0
7	O	888	0	413	1	0
7	R	844	0	385	1	0
8	U	822	0	370	2	0
9	V	881	0	379	4	0
10	W	754	0	336	2	0
10	Z	952	0	434	2	0
11	Y	2038	0	886	4	0
12	c	1095	0	471	18	0
12	d	1095	0	471	10	0
13	e	3959	0	1773	26	0
13	f	4009	0	1794	24	0
13	m	3750	0	1534	19	0
13	n	3566	0	1454	10	0
14	g	1767	0	796	7	0
14	h	1767	0	796	11	0
14	o	1767	0	796	8	0
14	p	1767	0	796	10	0
15	j	69	0	31	0	0
15	q	69	0	31	0	0
16	A	27	0	12	0	0
16	B	27	0	12	0	0
16	C	27	0	12	0	0
16	D	27	0	12	1	0
16	E	27	0	12	0	0
16	F	27	0	12	0	0
16	G	27	0	12	0	0
16	I	27	0	12	0	0
16	J	27	0	12	1	0
17	H	31	0	12	3	0
18	Y	3	0	0	0	0
All	All	59534	0	26403	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 207 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)
13:n:776:PRO:CB	14:p:375:LEU:O	1.81	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:161:SER:CB	12:c:132:ARG:HA	1.75	1.15
5:L:161:SER:CB	12:c:131:SER:C	2.27	1.08
5:L:160:SER:CB	12:c:128:GLN:HA	1.86	1.05
5:L:161:SER:CB	12:c:132:ARG:CA	2.38	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	36	72
6	N	270/405 (67%)	262 (97%)	7 (3%)	1 (0%)	30	67
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%)	18	56
10	Z	190/1281 (15%)	185 (97%)	5 (3%)	0	100	100
11	Y	404/467 (86%)	377 (93%)	24 (6%)	3 (1%)	18	56
12	c	218/577 (38%)	206 (94%)	12 (6%)	0	100	100
12	d	218/577 (38%)	207 (95%)	11 (5%)	0	100	100
13	e	792/4646 (17%)	745 (94%)	45 (6%)	2 (0%)	36	72
13	f	804/4646 (17%)	763 (95%)	39 (5%)	2 (0%)	43	78
13	m	786/4646 (17%)	758 (96%)	27 (3%)	1 (0%)	48	83
13	n	747/4646 (16%)	721 (96%)	25 (3%)	1 (0%)	48	83
14	g	356/612 (58%)	353 (99%)	3 (1%)	0	100	100
14	h	356/612 (58%)	346 (97%)	10 (3%)	0	100	100
14	o	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
14	p	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
15	j	12/492 (2%)	11 (92%)	1 (8%)	0	100	100
15	q	12/492 (2%)	12 (100%)	0	0	100	100
All	All	11929/32921 (36%)	11485 (96%)	432 (4%)	12 (0%)	49	83

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
13	f	38	VAL

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
16	ADP	J	800	-	28,29,29	1.44	5 (17%)	43,45,45	1.84	9 (20%)
16	ADP	F	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.81	9 (20%)
16	ADP	I	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.87	9 (20%)
16	ADP	G	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.84	8 (18%)
16	ADP	A	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	8 (18%)
16	ADP	D	800	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	9 (20%)
16	ADP	B	800	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
16	ADP	C	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.79	8 (18%)
17	ATP	H	401	-	32,33,33	0.36	0	48,52,52	0.31	0
16	ADP	E	800	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)

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
16	ADP	J	800	-	-	7/16/32/32	0/3/3/3
16	ADP	F	800	-	-	8/16/32/32	0/3/3/3
16	ADP	I	800	-	-	3/16/32/32	0/3/3/3
16	ADP	G	800	-	-	0/16/32/32	0/3/3/3
16	ADP	A	800	-	-	1/16/32/32	0/3/3/3
16	ADP	D	800	-	-	5/16/32/32	0/3/3/3
16	ADP	B	800	-	-	0/16/32/32	0/3/3/3
16	ADP	C	800	-	-	3/16/32/32	0/3/3/3
17	ATP	H	401	-	-	10/22/38/38	0/3/3/3
16	ADP	E	800	-	-	2/16/32/32	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	800	ADP	C5-C4	4.70	1.47	1.39
16	I	800	ADP	C5-C4	4.68	1.47	1.39
16	E	800	ADP	C5-C4	4.65	1.47	1.39
16	A	800	ADP	C5-C4	4.64	1.47	1.39
16	B	800	ADP	C5-C4	4.64	1.47	1.39

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	800	ADP	C5-C4-N3	-5.93	118.55	126.72
16	A	800	ADP	C5-C4-N3	-5.93	118.55	126.72
16	E	800	ADP	C5-C4-N3	-5.91	118.58	126.72
16	I	800	ADP	C5-C4-N3	-5.91	118.58	126.72
16	B	800	ADP	C5-C4-N3	-5.89	118.60	126.72

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

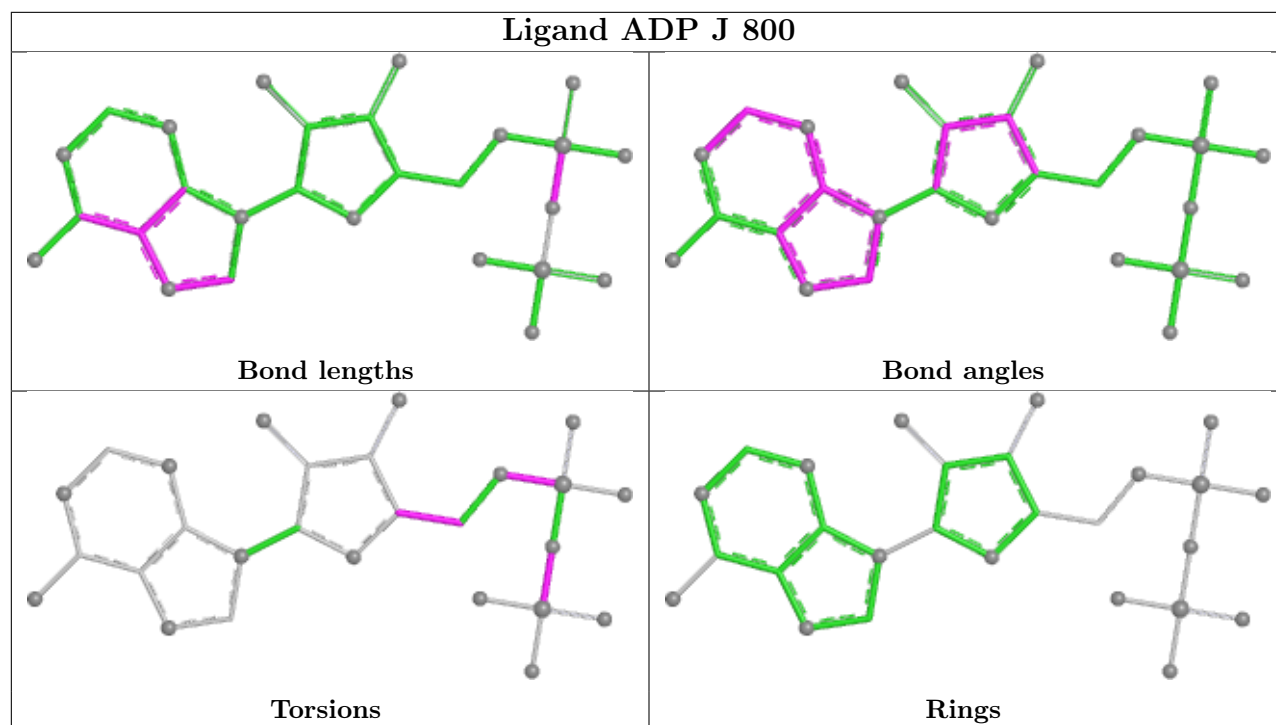
Mol	Chain	Res	Type	Atoms
16	C	800	ADP	C5'-O5'-PA-O3A
16	D	800	ADP	C5'-O5'-PA-O2A
16	D	800	ADP	C5'-O5'-PA-O3A
16	D	800	ADP	C3'-C4'-C5'-O5'
16	F	800	ADP	C5'-O5'-PA-O1A

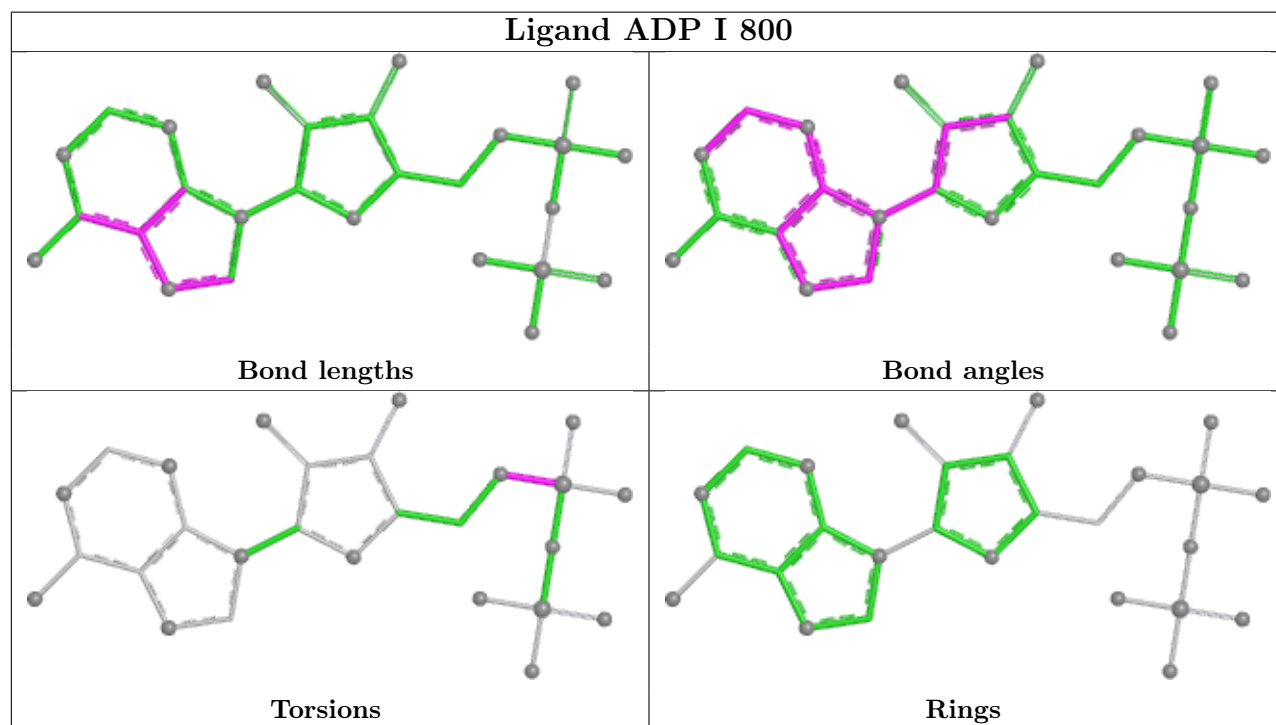
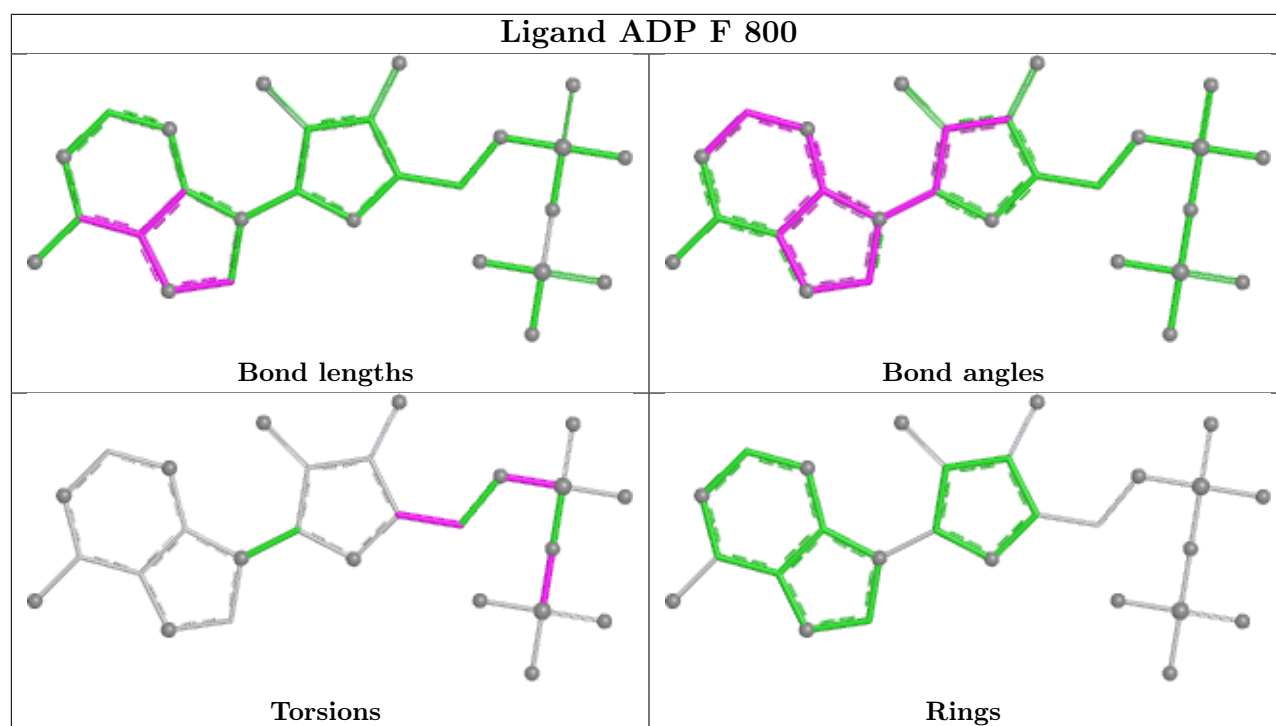
There are no ring outliers.

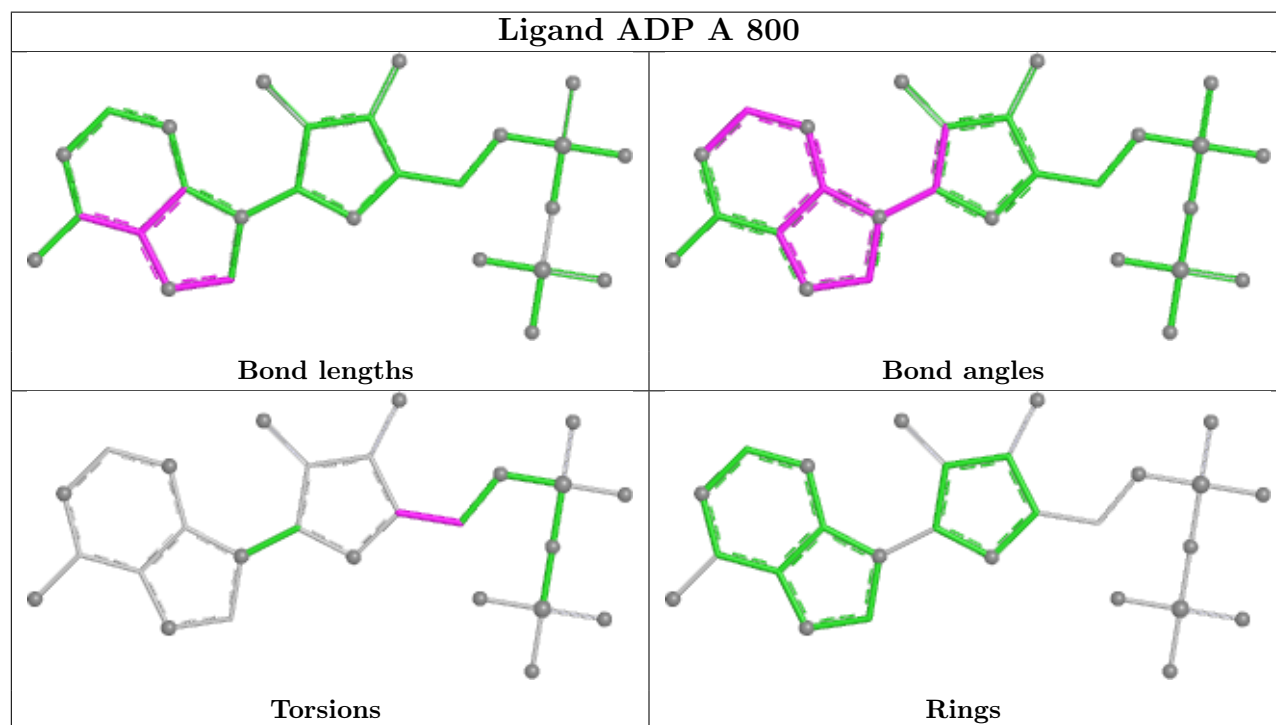
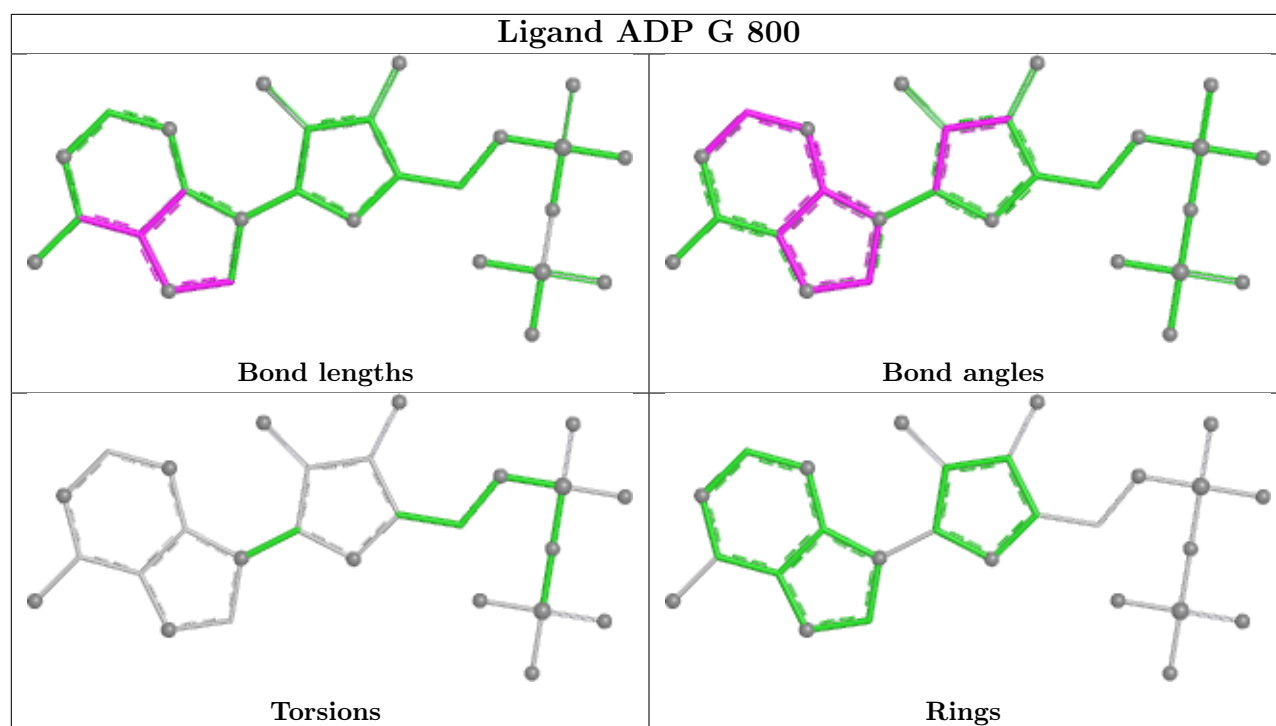
3 monomers are involved in 5 short contacts:

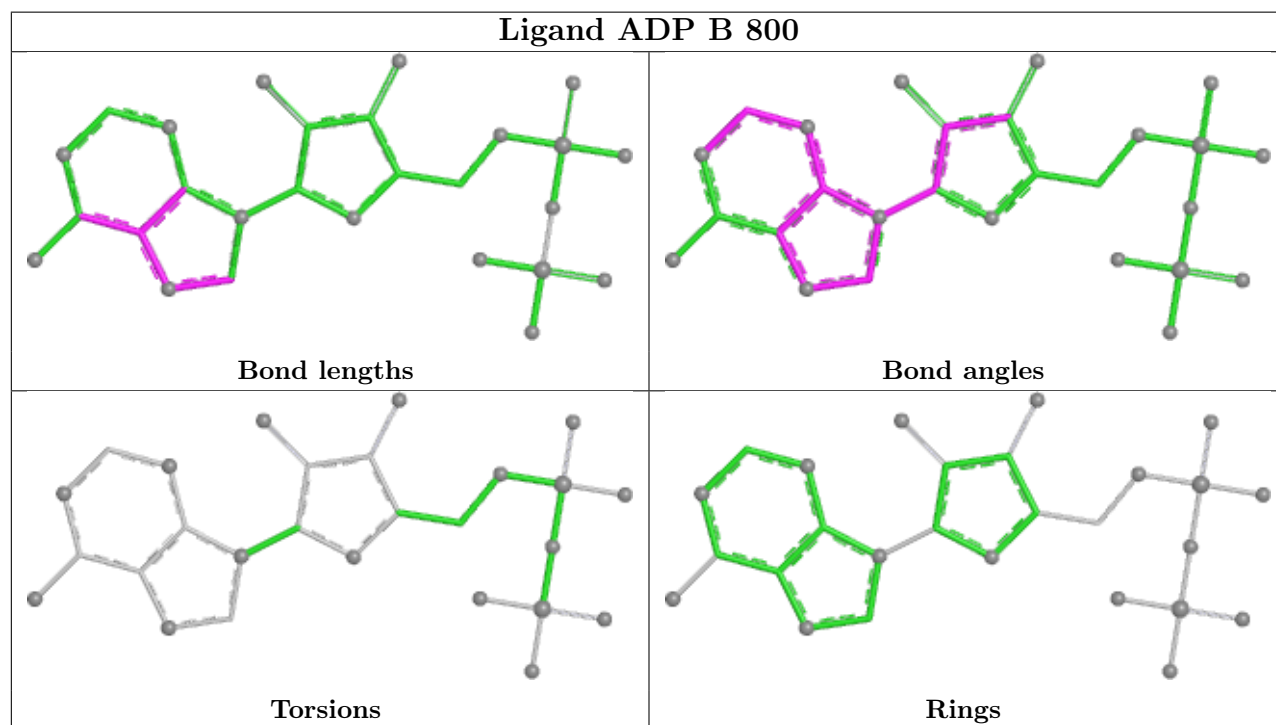
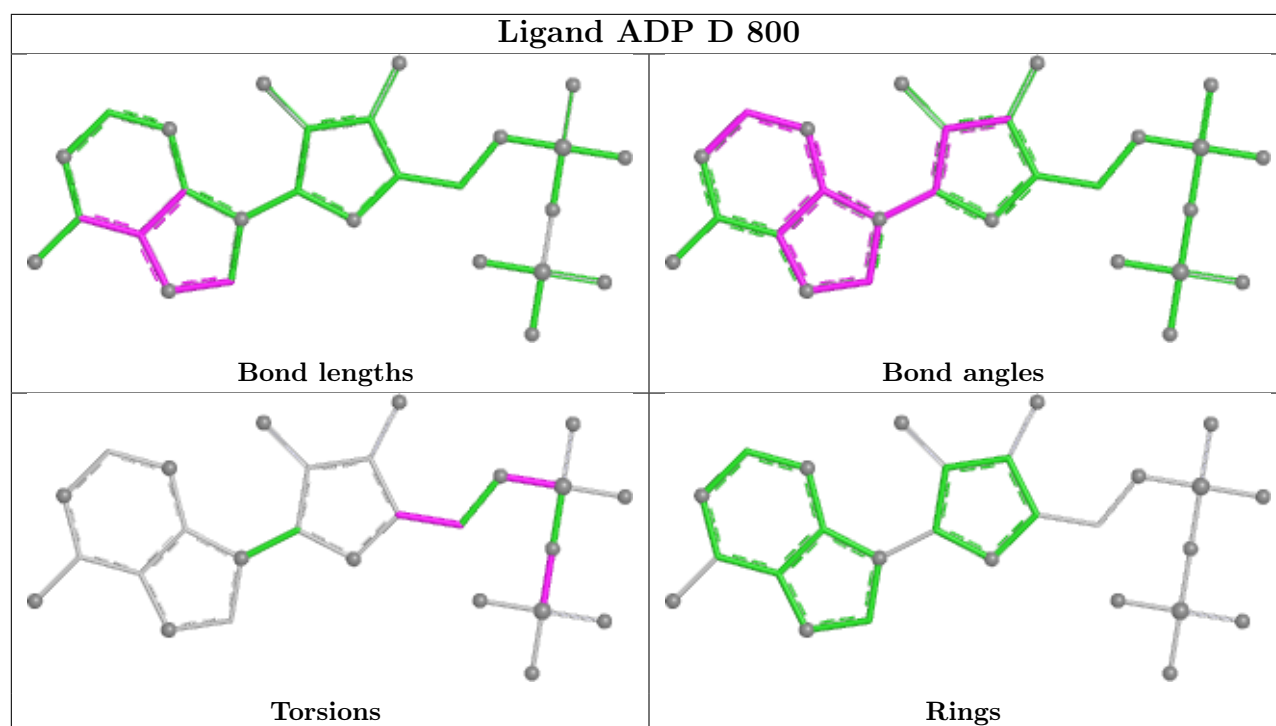
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	J	800	ADP	1	0
16	D	800	ADP	1	0
17	H	401	ATP	3	0

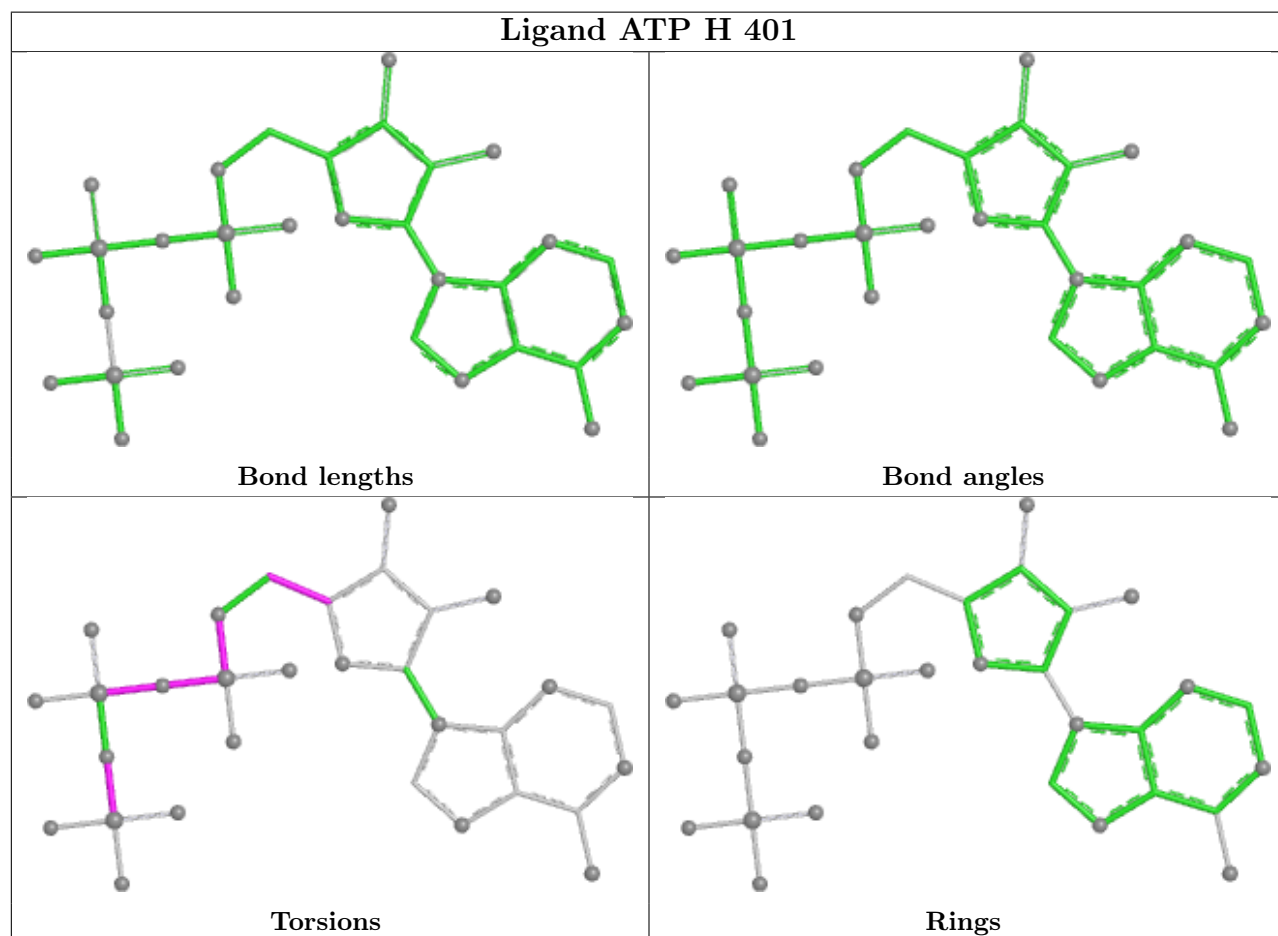
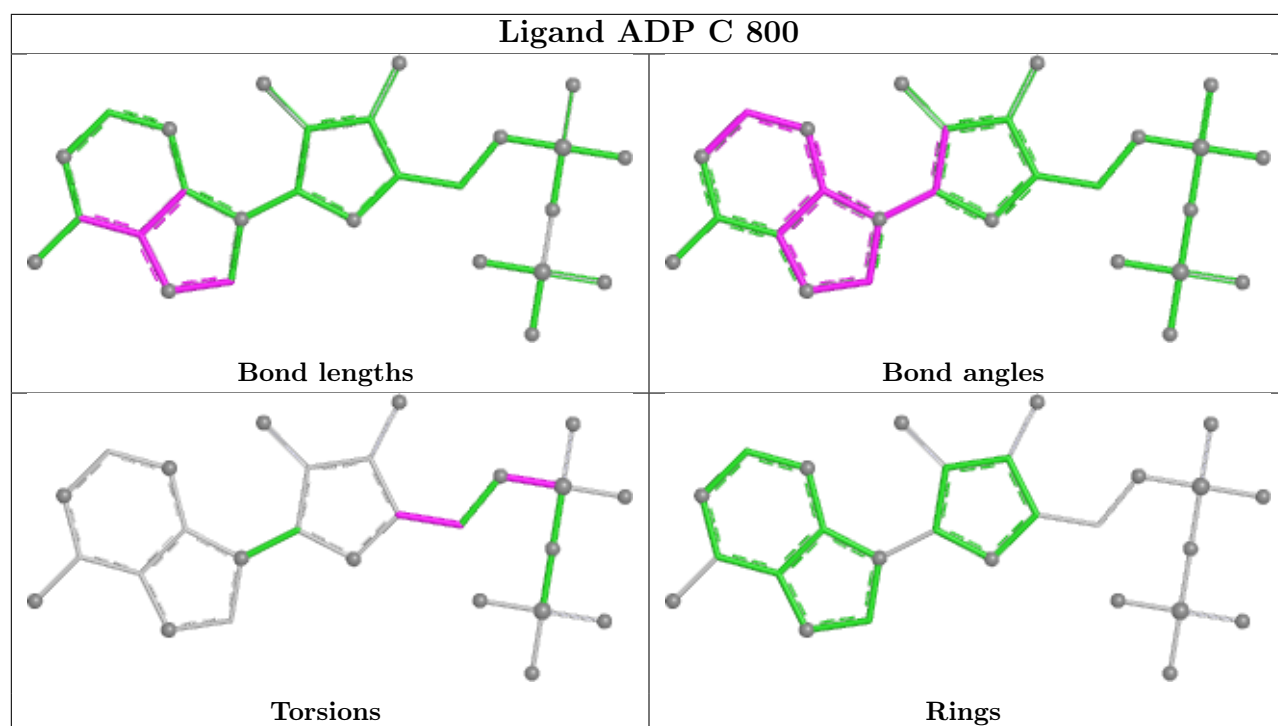
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

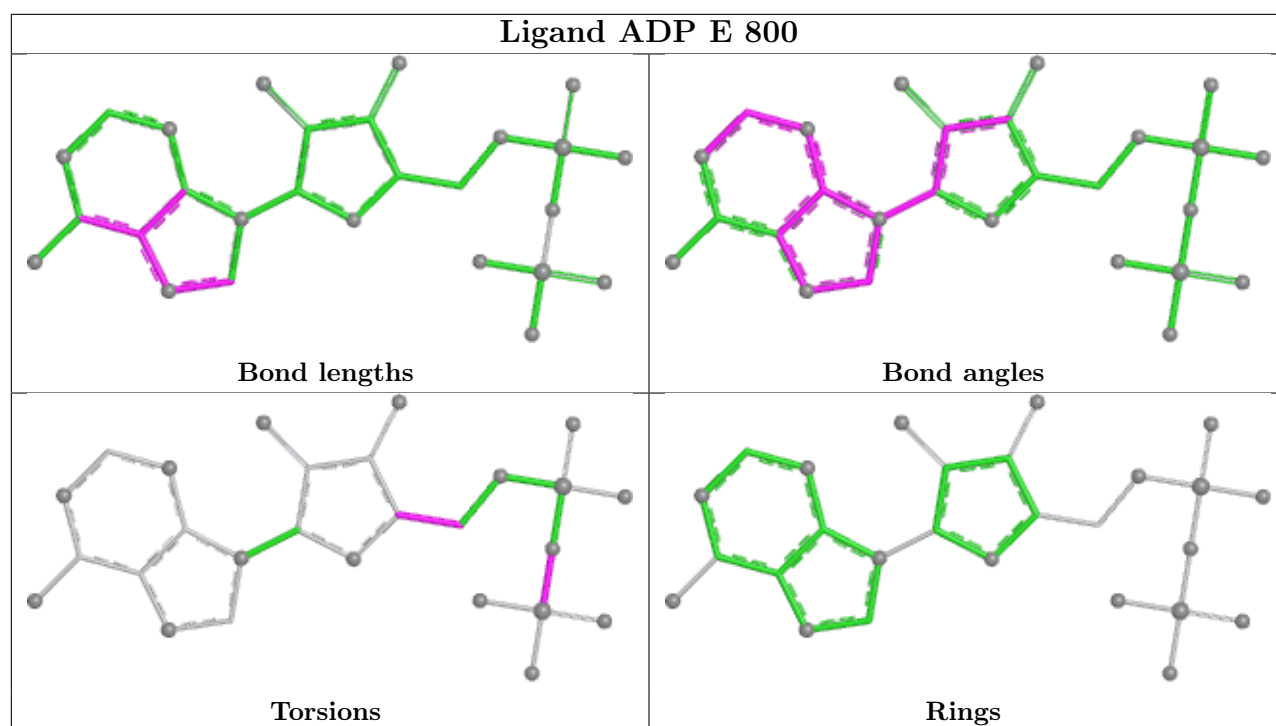












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

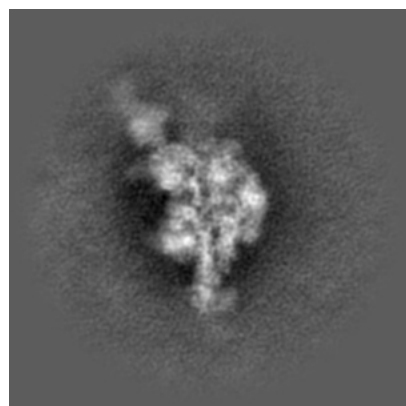
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46847. These allow visual inspection of the internal detail of the map and identification of artifacts.

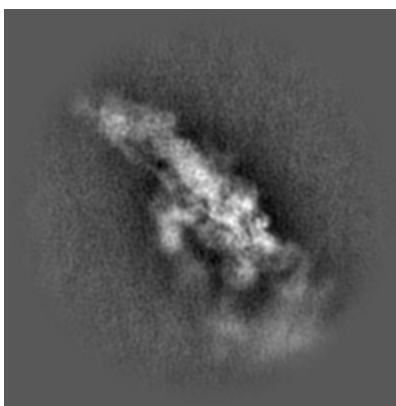
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

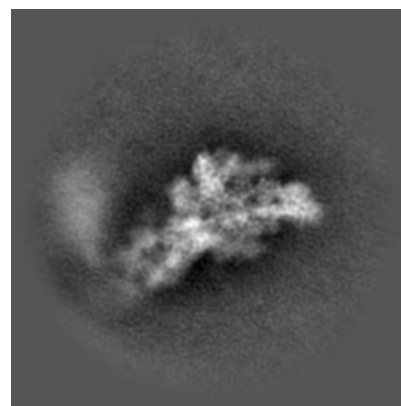
6.1.1 Primary map



X

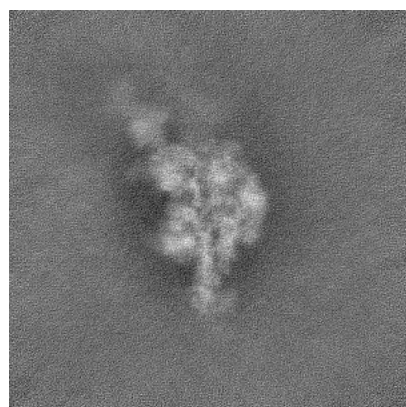


Y

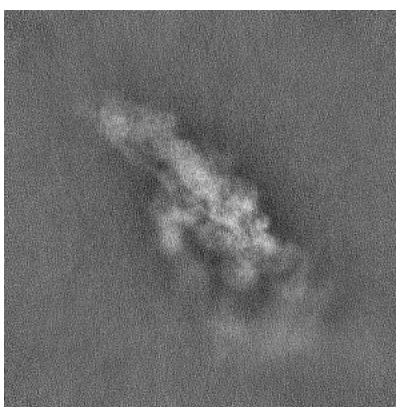


Z

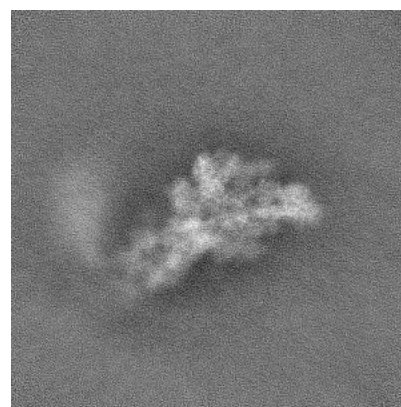
6.1.2 Raw map



X



Y

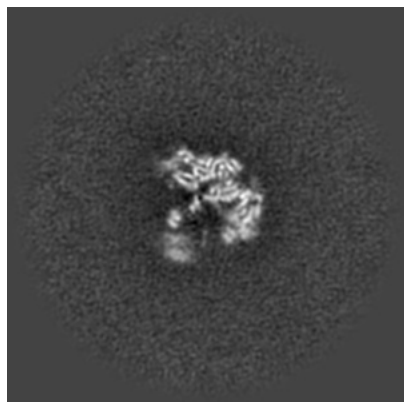


Z

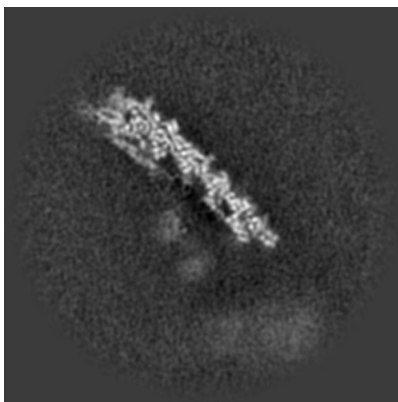
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

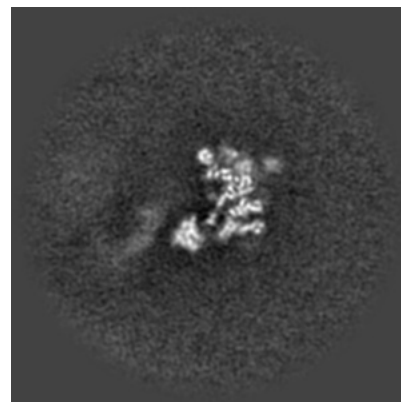
6.2.1 Primary map



X Index: 192

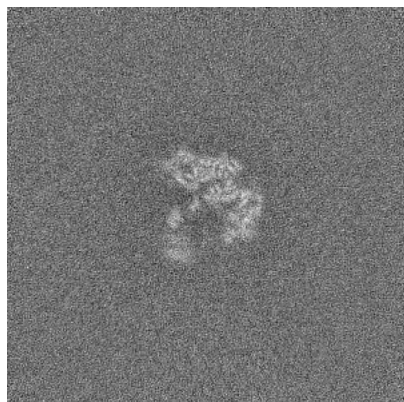


Y Index: 192

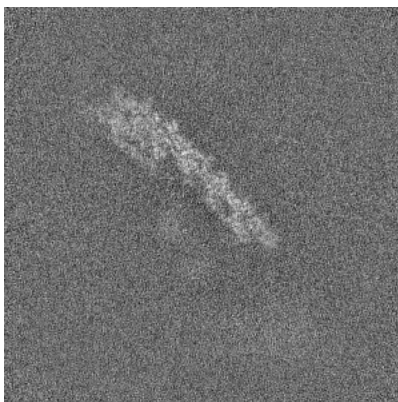


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

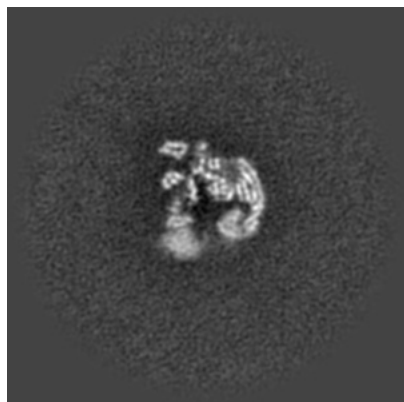


Z Index: 192

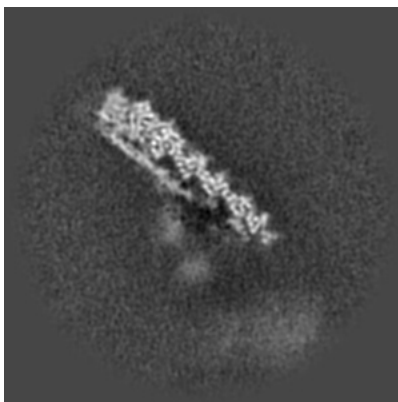
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

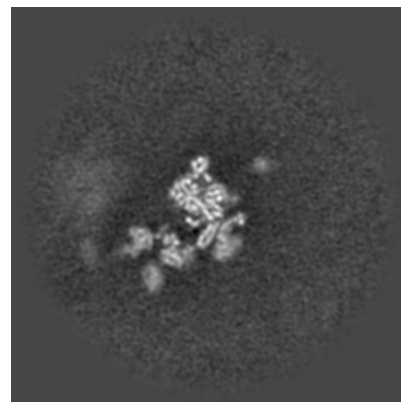
6.3.1 Primary map



X Index: 183

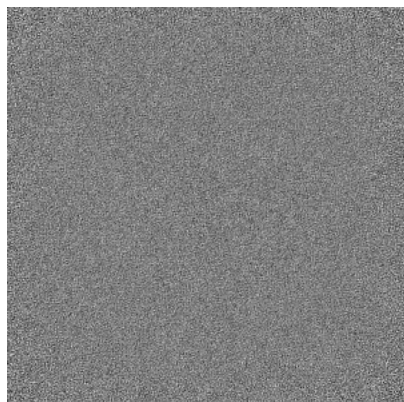


Y Index: 188

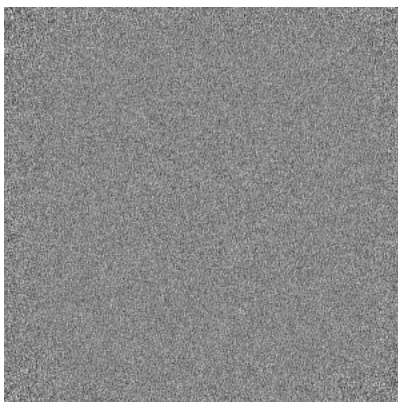


Z Index: 223

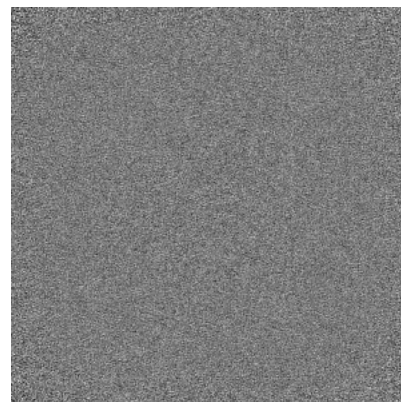
6.3.2 Raw map



X Index: 0



Y Index: 0

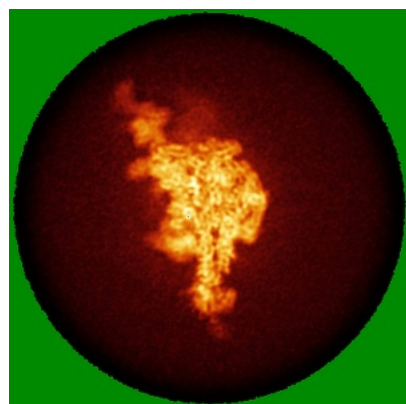


Z Index: 0

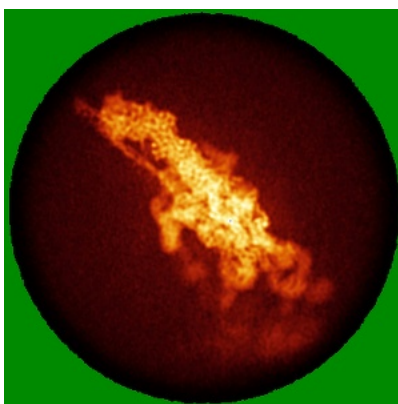
The images above show the largest variance slices of the map in three orthogonal directions.

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

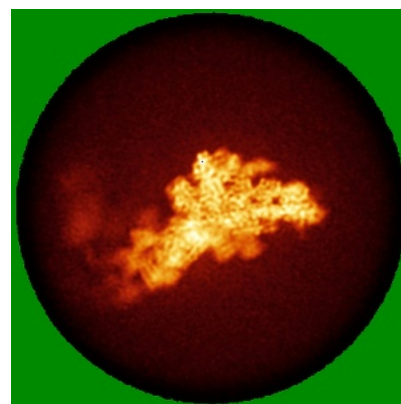
6.4.1 Primary map



X

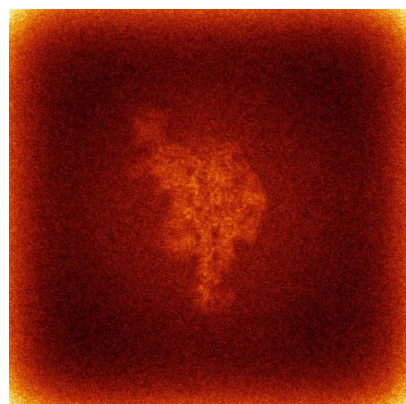


Y

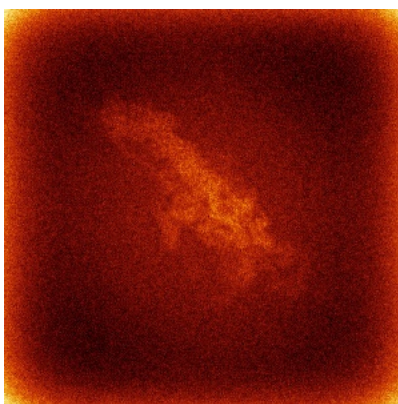


Z

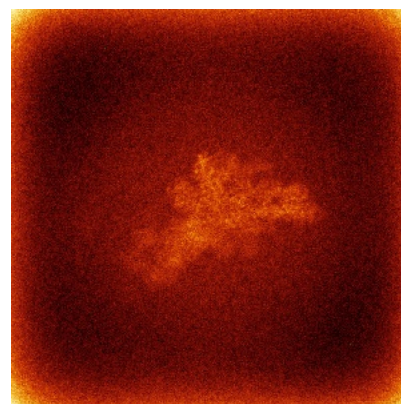
6.4.2 Raw map



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.

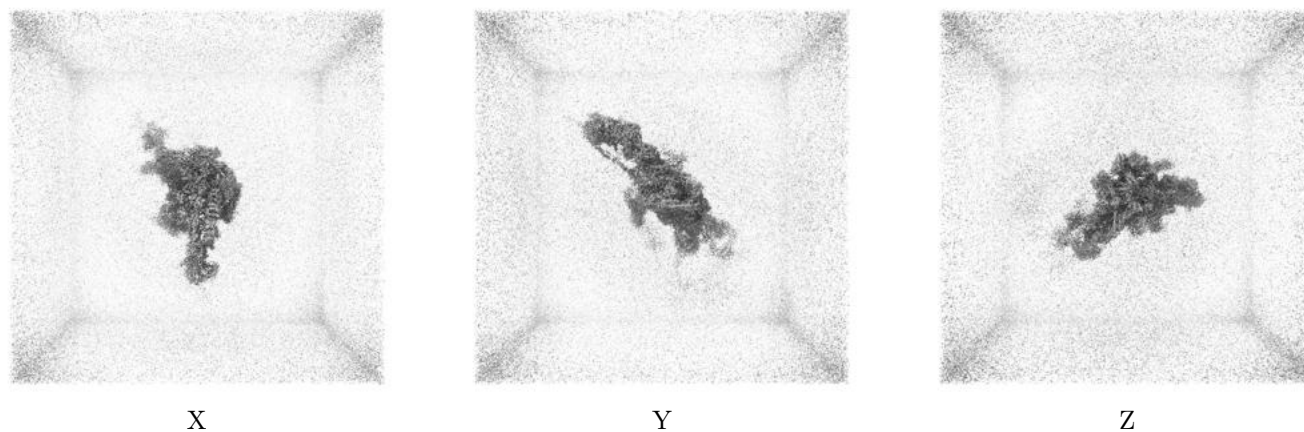
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

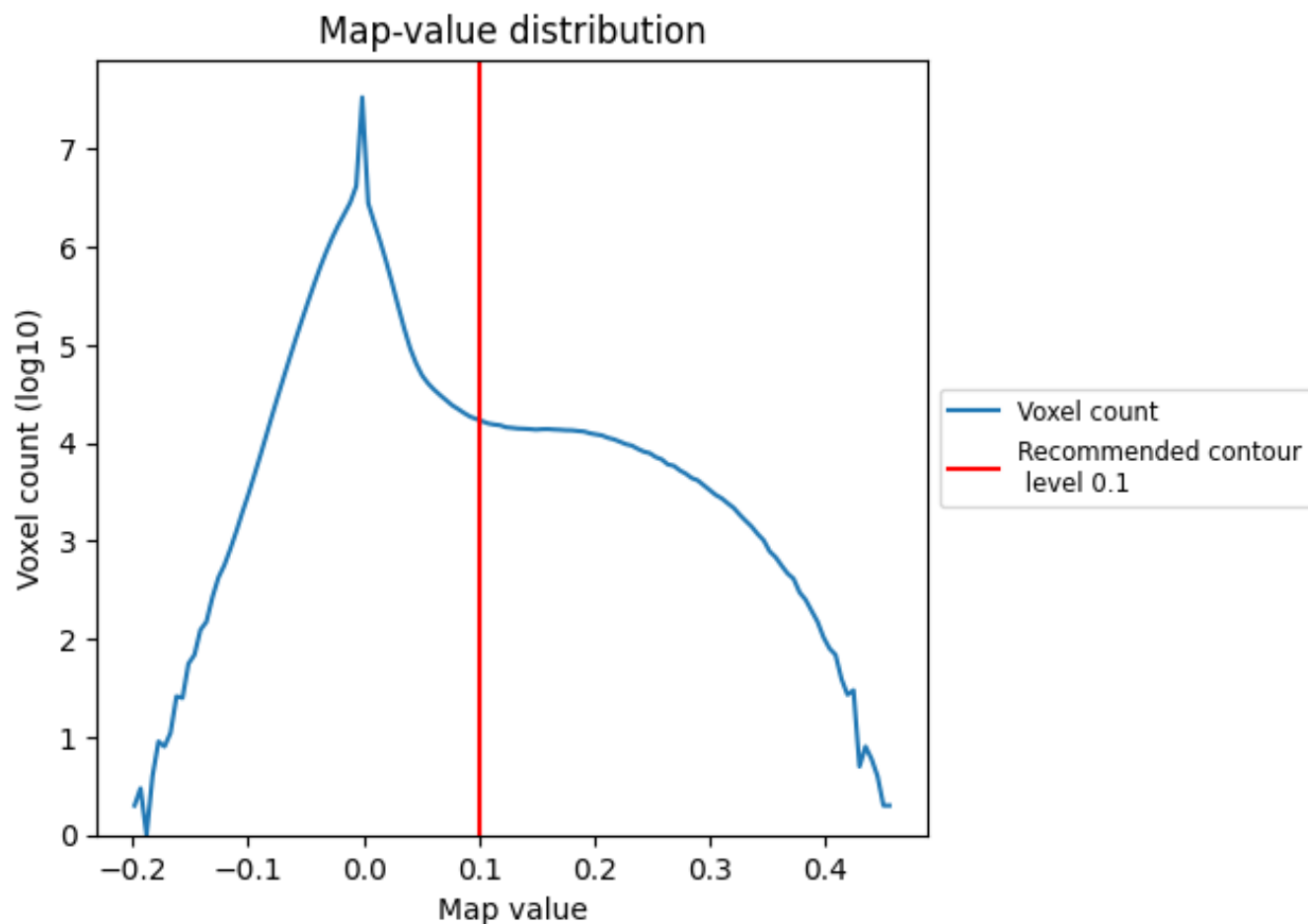
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

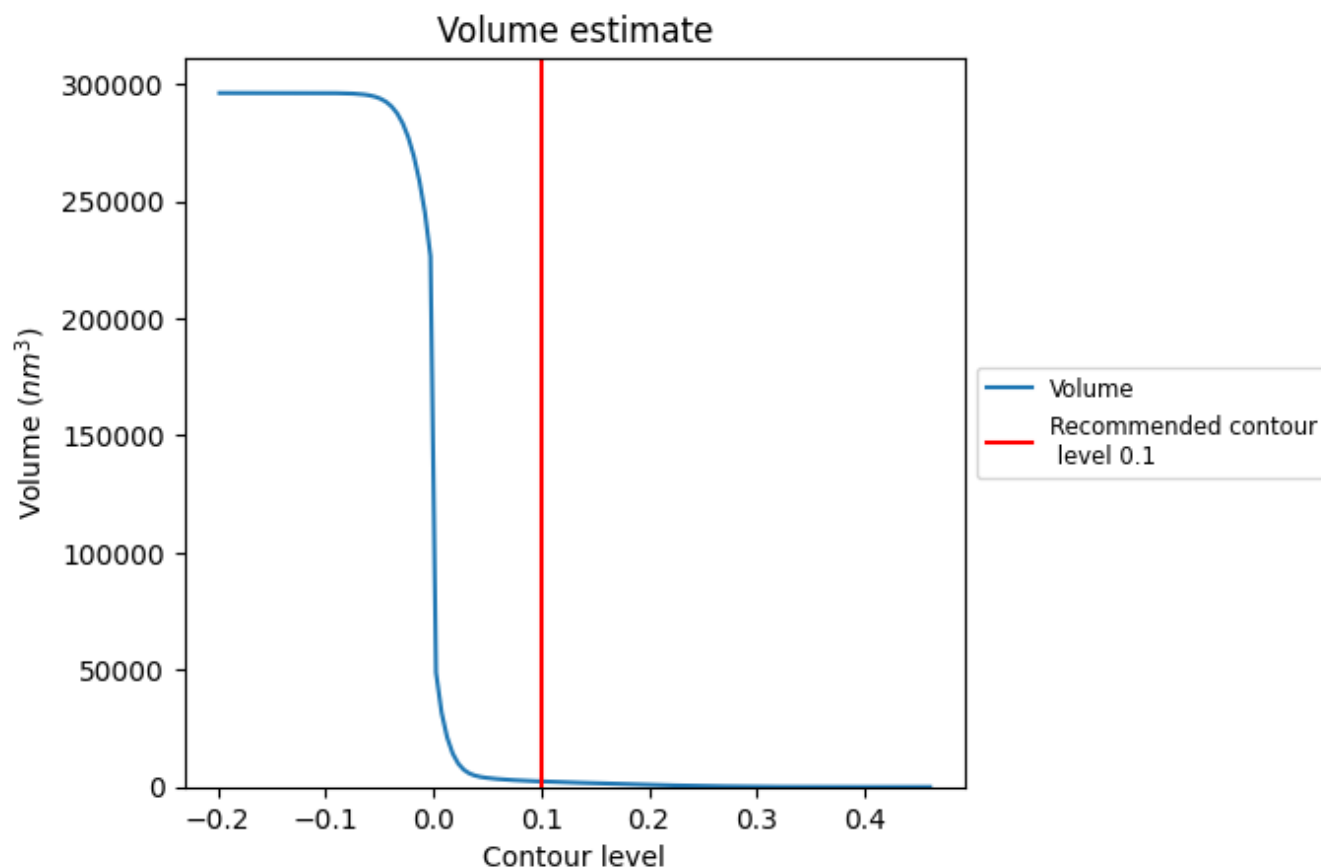
This section contains the results of statistical analysis of the map.

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.

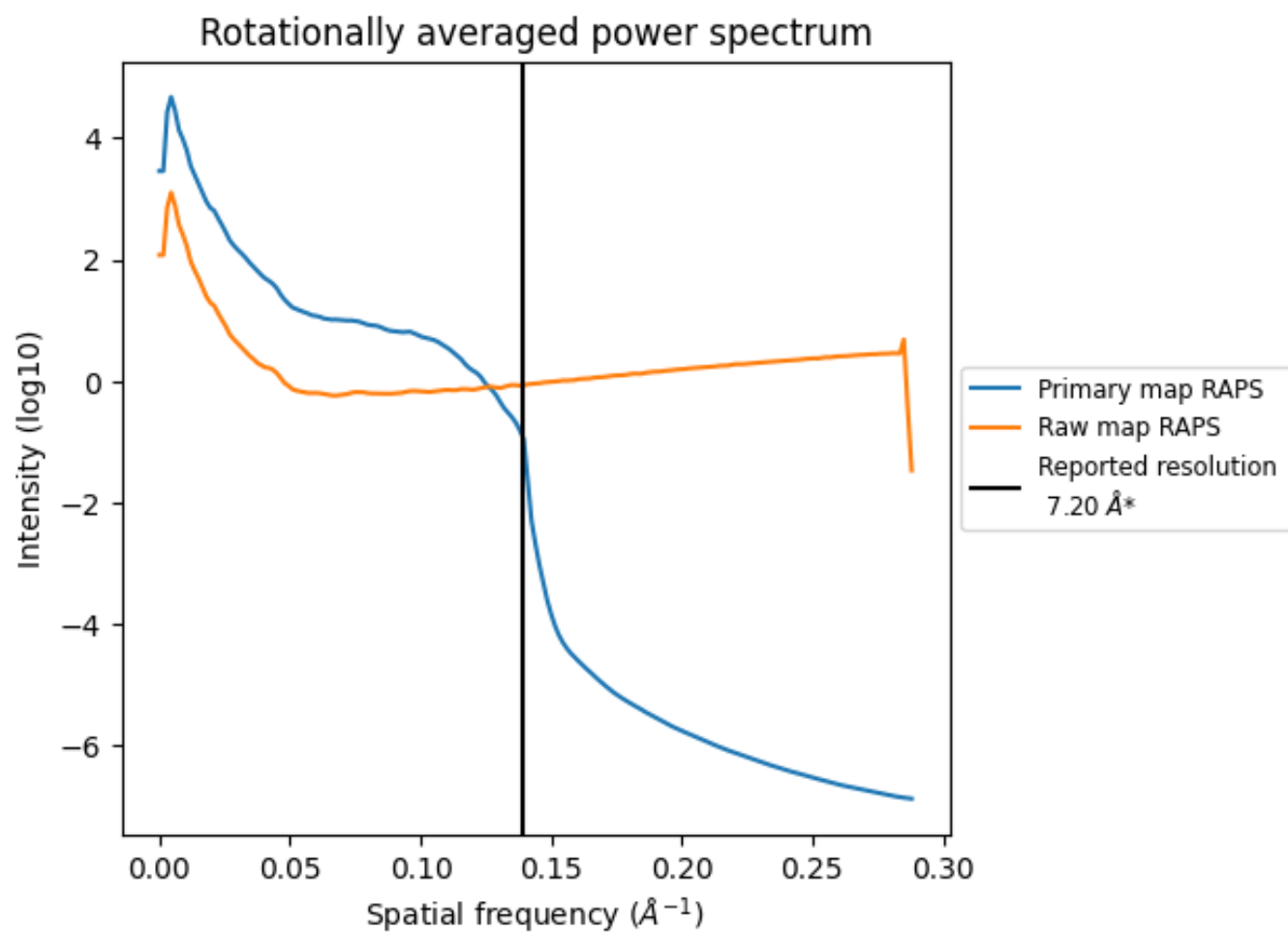
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2360 nm³; this corresponds to an approximate mass of 2132 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 ⓘ

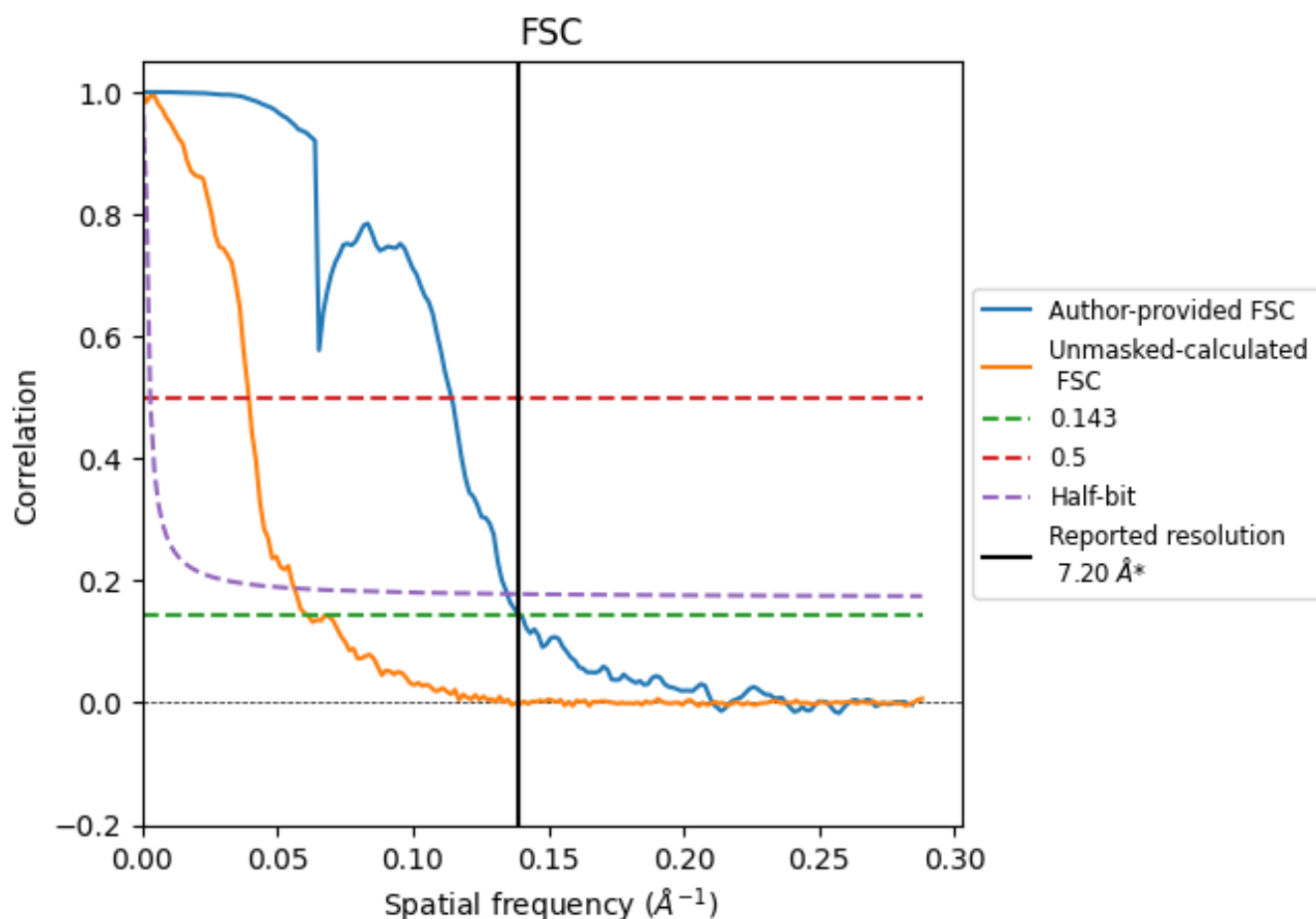


*Reported resolution corresponds to spatial frequency of 0.139 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.139 Å⁻¹

8.2 Resolution estimates [i](#)

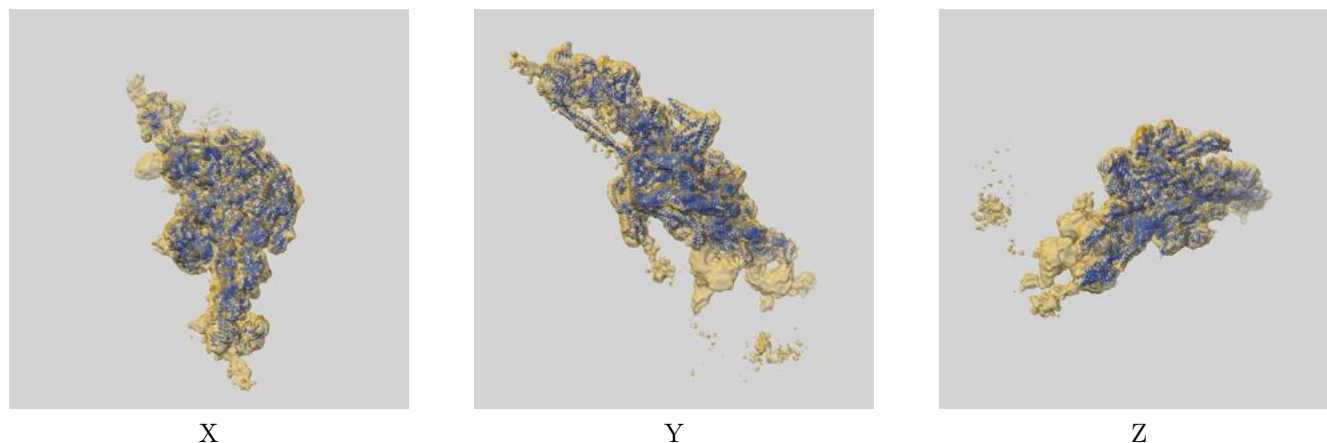
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.16	8.76	7.42
Unmasked-calculated*	16.39	25.45	17.79

*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 16.39 differs from the reported value 7.2 by more than 10 %

9 Map-model fit [i](#)

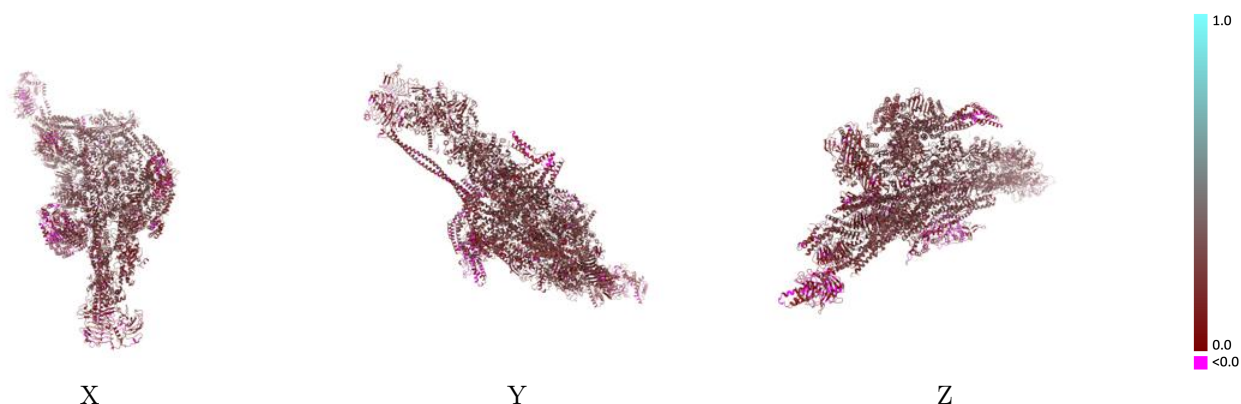
This section contains information regarding the fit between EMDB map EMD-46847 and PDB model 9DGT. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



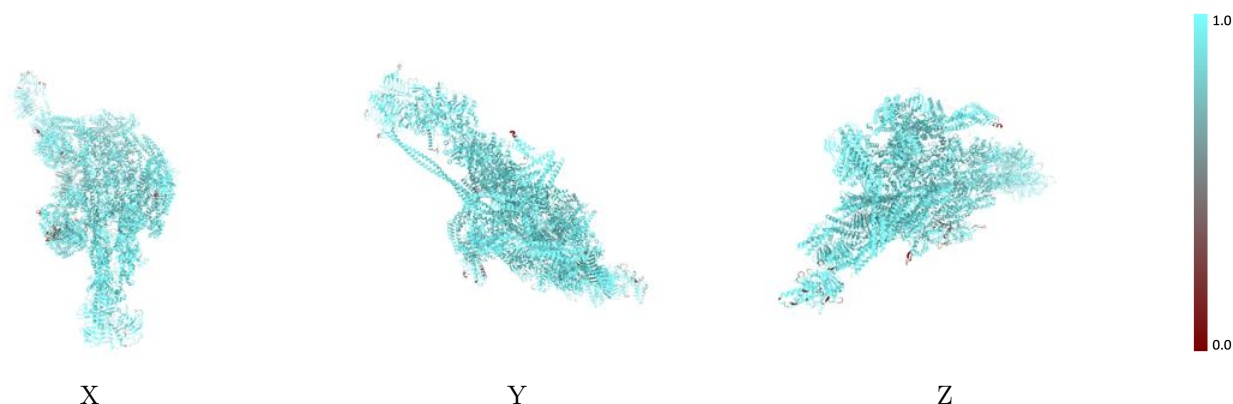
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



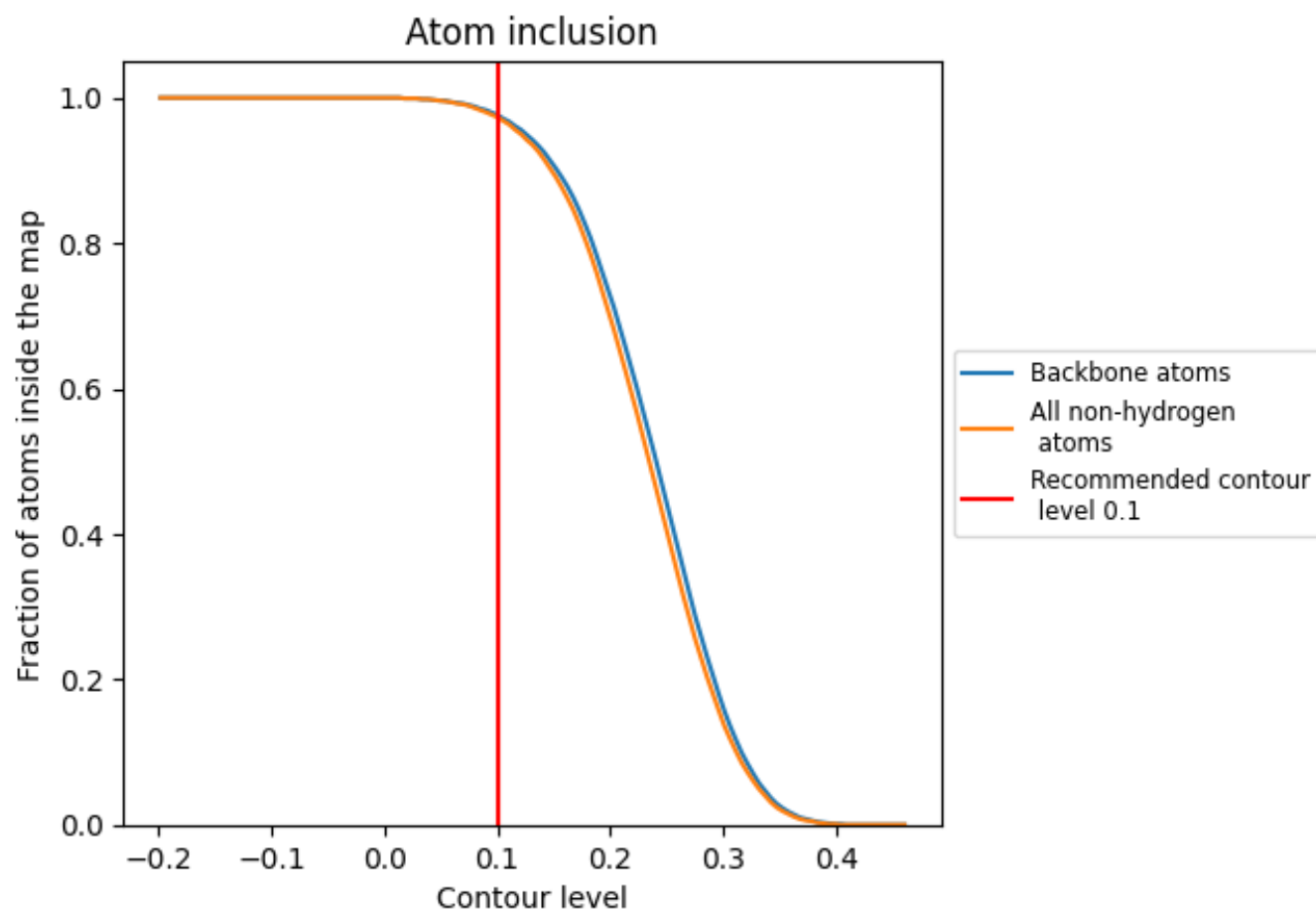
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9730	 0.1970
A	 0.9920	 0.2270
B	 0.9970	 0.2240
C	 0.9960	 0.2360
D	 0.9950	 0.2330
E	 0.9970	 0.2390
F	 0.9960	 0.2340
G	 0.9980	 0.2420
H	 0.9970	 0.2410
I	 0.9890	 0.2170
J	 0.9910	 0.2180
K	 0.9980	 0.2190
L	 0.9920	 0.2050
M	 0.9860	 0.2060
N	 0.9510	 0.2000
O	 0.9990	 0.2240
P	 0.9940	 0.2360
Q	 0.9400	 0.2300
R	 0.9920	 0.2040
U	 0.9720	 0.1450
V	 0.9640	 0.1120
W	 0.9680	 0.1930
Y	 0.9470	 0.1620
Z	 0.9970	 0.2230
c	 0.9970	 0.2380
d	 0.9910	 0.2050
e	 0.9290	 0.1320
f	 0.9360	 0.1830
g	 0.9330	 0.0820
h	 0.9880	 0.1620
j	 0.9710	 0.2030
m	 0.9790	 0.2220
n	 0.9490	 0.2020
o	 0.9860	 0.1740
p	 0.9290	 0.0870
q	 0.9860	 0.2010

