



# wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:37 PM UTC

PDB ID : 9B85 / pdb\_00009b85  
EMDB ID : EMD-44333  
Title : Cryo-EM structure of human dynactin complex bound to Chlamydia effector Dre1  
Authors : Pawar, K.I.; Verba, K.A.  
Deposited on : 2024-03-28  
Resolution : 3.47 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:

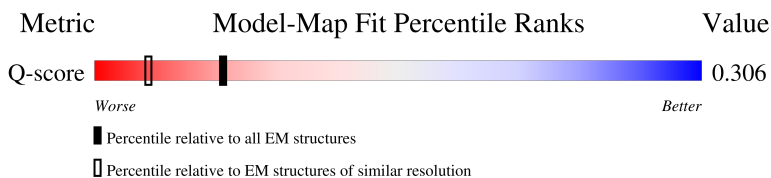
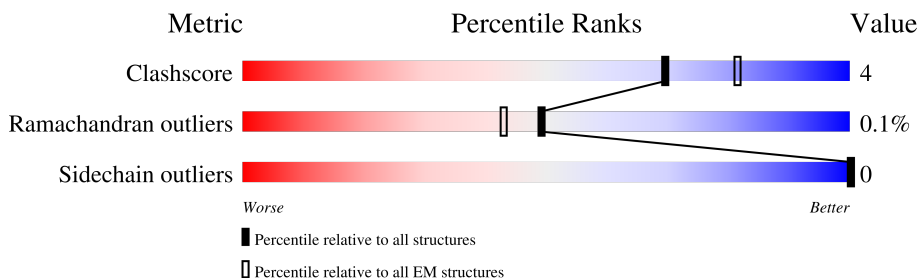
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

The reported resolution of this entry is 3.47 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 ( 2.97 - 3.97 )

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	90% 8% .
1	B	376	91% 8% .
1	C	376	90% 10%
1	D	376	89% 10% .

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Mol	Chain	Length	Quality of chain
1	E	376	 90% 8%
1	F	376	 88% 11%
1	G	376	 92% 6%
1	I	376	 89% 9%
2	H	375	 93% 6%
3	J	417	 12% 43% 32% 5% 7%
4	K	460	 43% 76% 22%
5	L	182	 66% 96%
6	M	190	 33% 75% 7% 18%
7	N	286	 17% 94% 6%
8	O	272	 8% 96%
9	P	401	 16% 82%
9	Q	401	 6% 94%
9	p	401	 8% 91%
9	q	401	 5% 11% 88%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 82296 atoms, of which 41052 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
			Total	C	H	N	O	S		
1	A	370	5907	1892	2951	509	545	10	0	0
1	B	370	5907	1892	2951	509	545	10	0	0
1	C	375	5982	1918	2984	514	556	10	0	0
1	D	370	5907	1892	2951	509	545	10	0	0
1	E	370	5907	1892	2951	509	545	10	0	0
1	F	370	5907	1892	2951	509	545	10	0	0
1	G	370	5907	1892	2951	509	545	10	0	0
1	I	370	5907	1892	2951	509	545	10	0	0

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

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

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

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

- Molecule 4 is a protein called Dynactin subunit 4.

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

- Molecule 5 is a protein called Dynactin subunit 5.

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

- Molecule 6 is a protein called Dynactin subunit 6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	N	286	4559	1462	2235	404	451	7	0	0

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

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

- Molecule 9 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			
9	P	74	1141	361	560	98	122	0	0	
9	Q	24	361	118	173	29	41	0	0	
9	p	37	543	179	257	42	63	2	0	0
9	q	48	733	238	354	59	82	0	0	

- Molecule 10 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>).

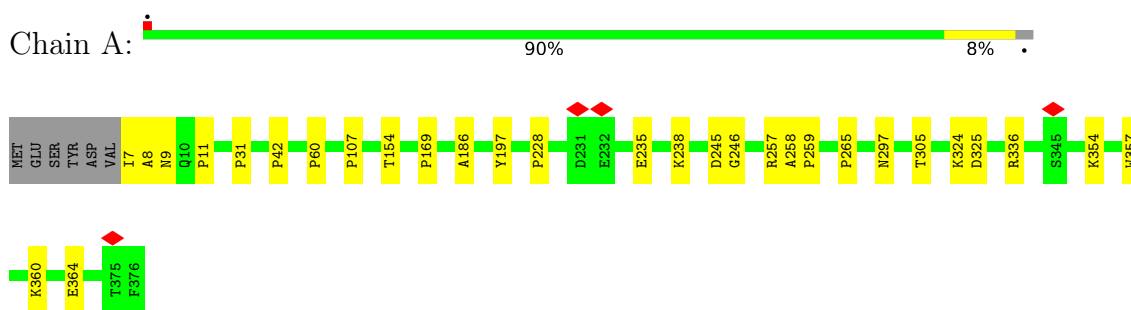




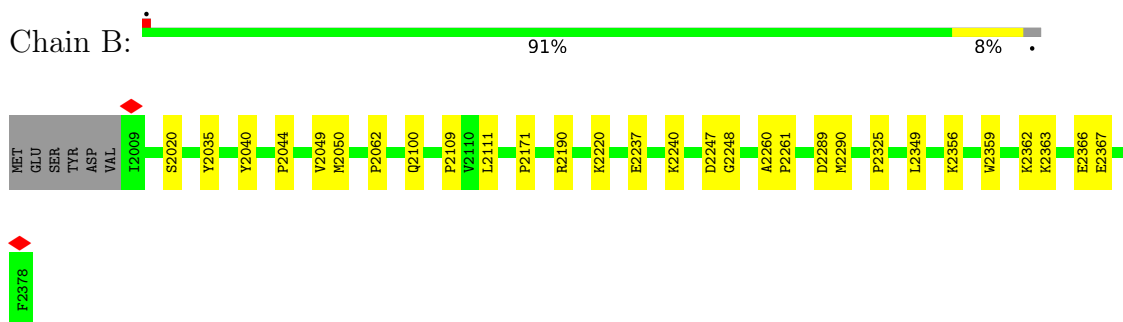
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

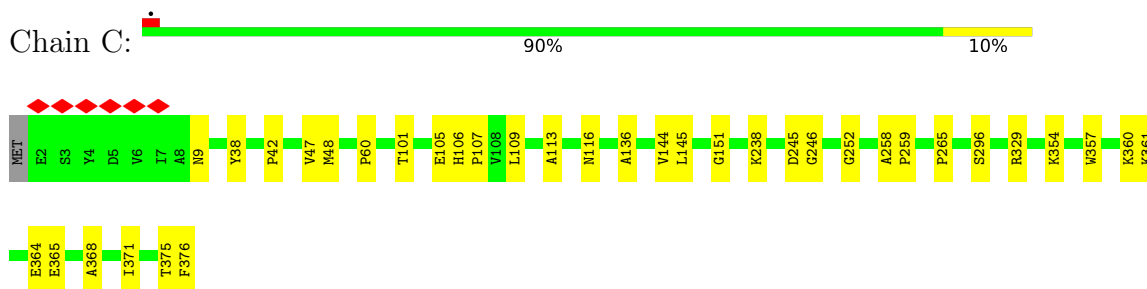
- Molecule 1: Alpha-centractin



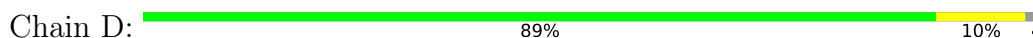
- Molecule 1: Alpha-centractin

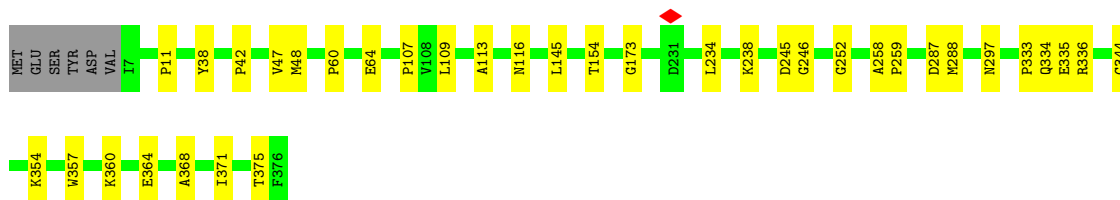


- Molecule 1: Alpha-centractin

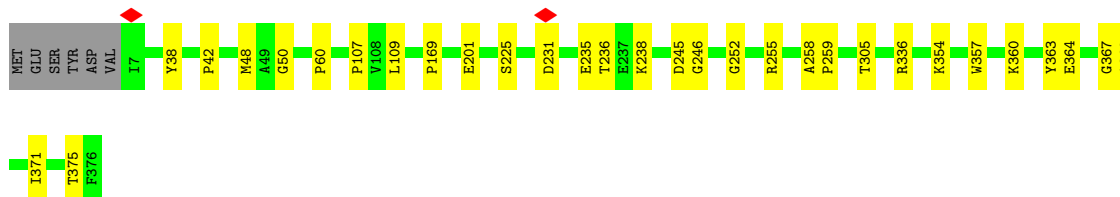
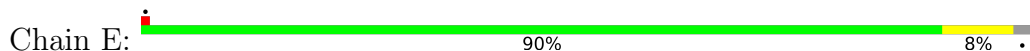


- Molecule 1: Alpha-centractin

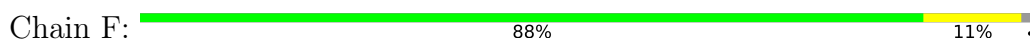




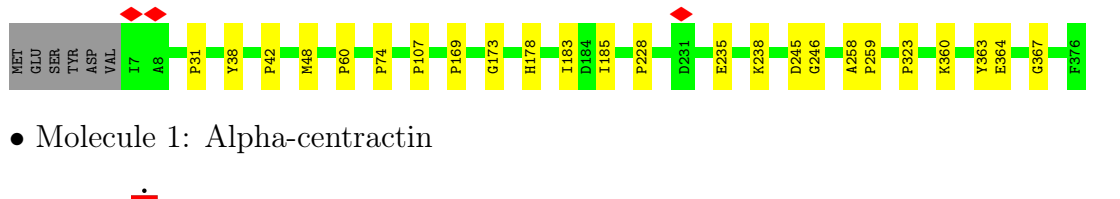
• Molecule 1: Alpha-centractin



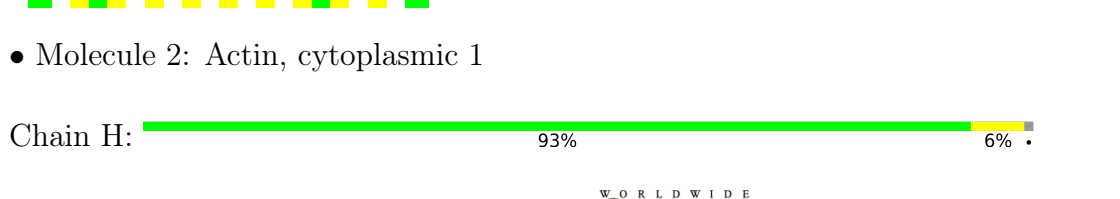
• Molecule 1: Alpha-centractin



• Molecule 1: Alpha-centractin



• Molecule 1: Alpha-centractin

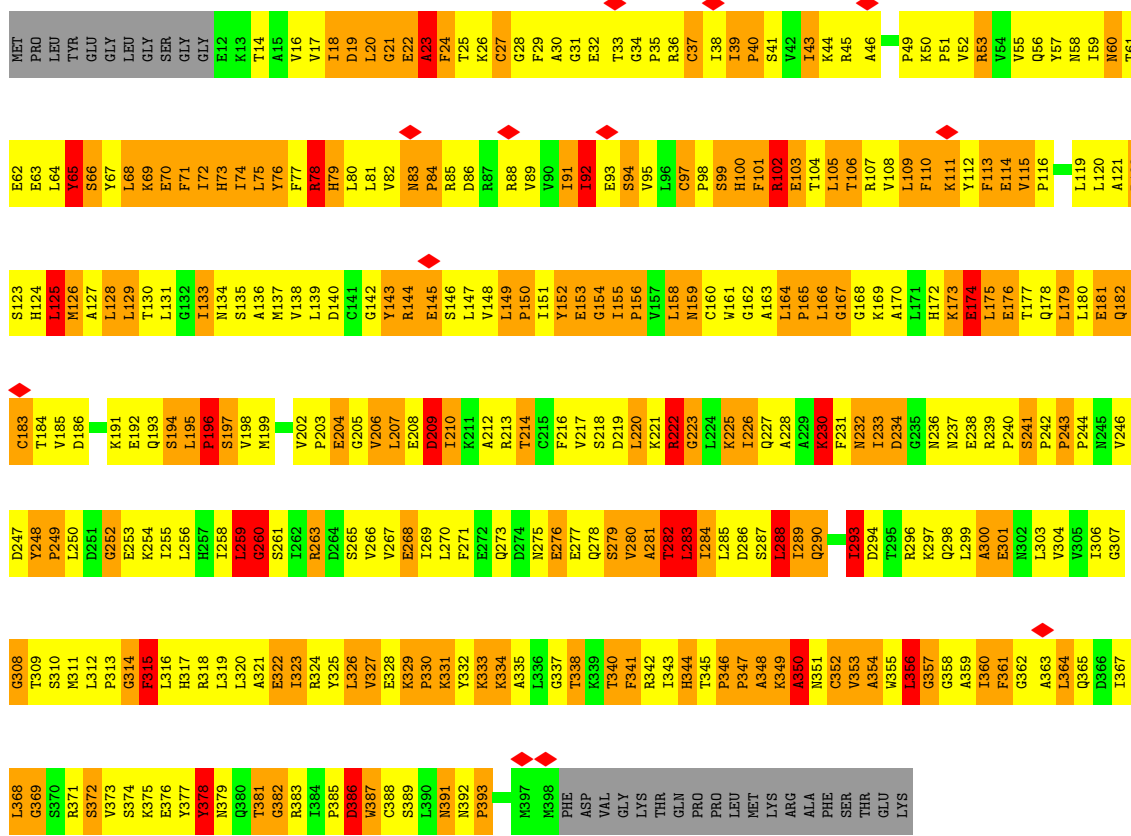


• Molecule 2: Actin, cytoplasmic 1





• Molecule 3: Actin-related protein 10









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	57.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	26.658	Depositor
Minimum map value	-12.272	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	1.217	Depositor
Recommended contour level	4	Depositor
Map size ( $\text{\AA}$ )	721.44, 721.44, 721.44	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.835, 0.835, 0.835	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.18	8/3025 (0.3%)	1.48	4/4085 (0.1%)
1	B	1.16	5/3025 (0.2%)	1.47	0/4085
1	C	1.16	4/3068 (0.1%)	1.47	0/4144
1	D	1.15	4/3025 (0.1%)	1.46	2/4085 (0.0%)
1	E	1.15	4/3025 (0.1%)	1.45	0/4085
1	F	1.18	7/3025 (0.2%)	1.49	0/4085
1	G	1.18	8/3025 (0.3%)	1.50	0/4085
1	I	1.17	6/3025 (0.2%)	1.47	0/4085
2	H	1.16	4/2948 (0.1%)	1.53	2/3991 (0.1%)
3	J	3.17	354/3088 (11.5%)	3.91	608/4188 (14.5%)
4	K	0.72	4/2970 (0.1%)	0.85	0/4005
5	L	0.70	2/1435 (0.1%)	0.86	0/1941
6	M	0.68	0/1209	0.89	0/1641
7	N	0.72	2/2376 (0.1%)	0.90	0/3214
8	O	1.18	2/2156 (0.1%)	1.54	0/2906
9	P	0.93	1/591 (0.2%)	1.22	2/797 (0.3%)
9	Q	1.03	1/193 (0.5%)	1.24	0/265
9	p	1.13	2/292 (0.7%)	1.23	3/395 (0.8%)
9	q	0.93	1/387 (0.3%)	1.26	0/528
All	All	1.35	419/41888 (1.0%)	1.69	621/56610 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	29

The worst 5 of 419 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	83	ASN	CA-C	-20.17	1.38	1.53
3	J	206	VAL	CA-C	-18.29	1.27	1.52
3	J	102	ARG	N-CA	-17.75	1.23	1.46
3	J	318	ARG	CA-C	-17.66	1.28	1.52
3	J	346	PRO	CA-C	-14.87	1.38	1.52

The worst 5 of 621 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	196	PRO	CA-C-N	-39.51	62.40	123.24
3	J	196	PRO	C-N-CA	-39.51	62.40	123.24
3	J	144	ARG	O-C-N	35.76	166.03	123.12
3	J	195	LEU	CA-C-N	-26.55	86.66	119.84
3	J	195	LEU	C-N-CA	-26.55	86.66	119.84

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	50	LYS	Peptide
3	J	53	ARG	Mainchain
3	J	65	TYR	Mainchain
3	J	78	ARG	Mainchain
3	J	92	ILE	Mainchain

## 5.2 Too-close contacts [i](#)

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	2956	2951	2950	11	0
1	B	2956	2951	2950	16	0
1	C	2998	2984	2983	20	0
1	D	2956	2951	2950	19	0
1	E	2956	2951	2950	19	0
1	F	2956	2951	2950	23	0
1	G	2956	2951	2950	10	0
1	I	2956	2951	2950	18	0
2	H	2885	2857	2856	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	3027	3113	3108	124	0
4	K	2913	2982	2975	4	0
5	L	1408	1438	1440	3	0
6	M	1191	1217	1215	8	0
7	N	2324	2235	2237	12	0
8	O	2122	2114	2113	5	0
9	P	581	560	558	6	0
9	Q	188	173	172	0	0
9	p	286	257	258	6	0
9	q	379	354	352	2	0
10	A	27	12	12	0	0
10	B	27	12	12	1	0
10	C	27	12	12	0	0
10	D	27	12	12	0	0
10	E	27	12	12	0	0
10	F	27	12	12	0	0
10	G	27	12	12	0	0
10	I	27	12	12	0	0
11	H	31	15	13	0	0
12	K	3	0	0	0	0
All	All	41244	41052	41026	298	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 4.

The worst 5 of 298 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)
3:J:109:LEU:O	3:J:110:PHE:C	1.82	1.08
3:J:109:LEU:O	3:J:111:LYS:N	2.06	0.89
3:J:109:LEU:O	3:J:110:PHE:HB3	1.77	0.83
3:J:166:LEU:HB2	3:J:167:GLY:HA2	1.61	0.82
3:J:233:ILE:O	3:J:234:ASP:C	2.16	0.79

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%)	357 (97%)	11 (3%)	0	100	100
1	B	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	C	373/376 (99%)	365 (98%)	8 (2%)	0	100	100
1	D	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	E	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	F	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	I	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
3	J	379/417 (91%)	357 (94%)	19 (5%)	3 (1%)	16	49
4	K	349/460 (76%)	342 (98%)	7 (2%)	0	100	100
5	L	180/182 (99%)	176 (98%)	3 (2%)	1 (1%)	21	53
6	M	152/190 (80%)	145 (95%)	7 (5%)	0	100	100
7	N	284/286 (99%)	279 (98%)	5 (2%)	0	100	100
8	O	267/272 (98%)	261 (98%)	6 (2%)	0	100	100
9	P	70/401 (18%)	65 (93%)	4 (6%)	1 (1%)	9	38
9	Q	22/401 (6%)	21 (96%)	1 (4%)	0	100	100
9	p	33/401 (8%)	28 (85%)	4 (12%)	1 (3%)	3	25
9	q	44/401 (11%)	42 (96%)	2 (4%)	0	100	100
All	All	5097/6794 (75%)	4935 (97%)	156 (3%)	6 (0%)	49	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	283	LEU
9	p	25	LEU

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Mol	Chain	Res	Type
3	J	23	ALA
3	J	145	GLU
5	L	179	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/324 (98%)	318 (100%)	0	100	100
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	318/324 (98%)	318 (100%)	0	100	100
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	339/363 (93%)	339 (100%)	0	100	100
4	K	330/412 (80%)	330 (100%)	0	100	100
5	L	163/163 (100%)	163 (100%)	0	100	100
6	M	132/164 (80%)	132 (100%)	0	100	100
7	N	252/252 (100%)	252 (100%)	0	100	100
8	O	238/241 (99%)	238 (100%)	0	100	100
9	P	64/343 (19%)	64 (100%)	0	100	100
9	Q	21/343 (6%)	21 (100%)	0	100	100
9	p	30/343 (9%)	30 (100%)	0	100	100
9	q	43/343 (12%)	43 (100%)	0	100	100
All	All	4474/5877 (76%)	4474 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	81	HIS
5	L	103	GLN
5	L	60	HIS
7	N	246	ASN
1	F	133	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	ADP	A	800	-	28,29,29	0.44	0	43,45,45	0.43	0
10	ADP	I	800	-	28,29,29	0.47	0	43,45,45	0.44	0
10	ADP	G	800	-	28,29,29	0.43	0	43,45,45	0.43	0
11	ANP	H	401	-	33,33,33	1.94	9 (27%)	45,52,52	1.99	15 (33%)
10	ADP	C	800	-	28,29,29	0.47	0	43,45,45	0.44	0
10	ADP	B	2401	-	28,29,29	0.45	0	43,45,45	0.43	0
10	ADP	F	800	-	28,29,29	0.46	0	43,45,45	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	ADP	D	800	-	28,29,29	0.44	0	43,45,45	0.45	0
10	ADP	E	800	-	28,29,29	0.43	0	43,45,45	0.44	0

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
10	ADP	A	800	-	-	7/16/32/32	0/3/3/3
10	ADP	I	800	-	-	4/16/32/32	0/3/3/3
10	ADP	G	800	-	-	4/16/32/32	0/3/3/3
11	ANP	H	401	-	-	7/18/38/38	0/3/3/3
10	ADP	C	800	-	-	4/16/32/32	0/3/3/3
10	ADP	B	2401	-	-	3/16/32/32	0/3/3/3
10	ADP	F	800	-	-	4/16/32/32	0/3/3/3
10	ADP	D	800	-	-	4/16/32/32	0/3/3/3
10	ADP	E	800	-	-	4/16/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	401	ANP	C5-C4	5.01	1.48	1.39
11	H	401	ANP	PG-N3B	4.34	1.74	1.63
11	H	401	ANP	PG-O1G	3.93	1.52	1.46
11	H	401	ANP	PB-N3B	3.58	1.72	1.63
11	H	401	ANP	PB-O1B	3.43	1.51	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	401	ANP	C5-C4-N3	-5.14	119.64	126.72
11	H	401	ANP	N3-C4-N9	4.53	134.88	127.17
11	H	401	ANP	C4-N9-C8	3.94	109.88	105.74
11	H	401	ANP	C2-N3-C4	3.74	120.95	111.83
11	H	401	ANP	N3-C2-N1	-3.60	123.13	128.58

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

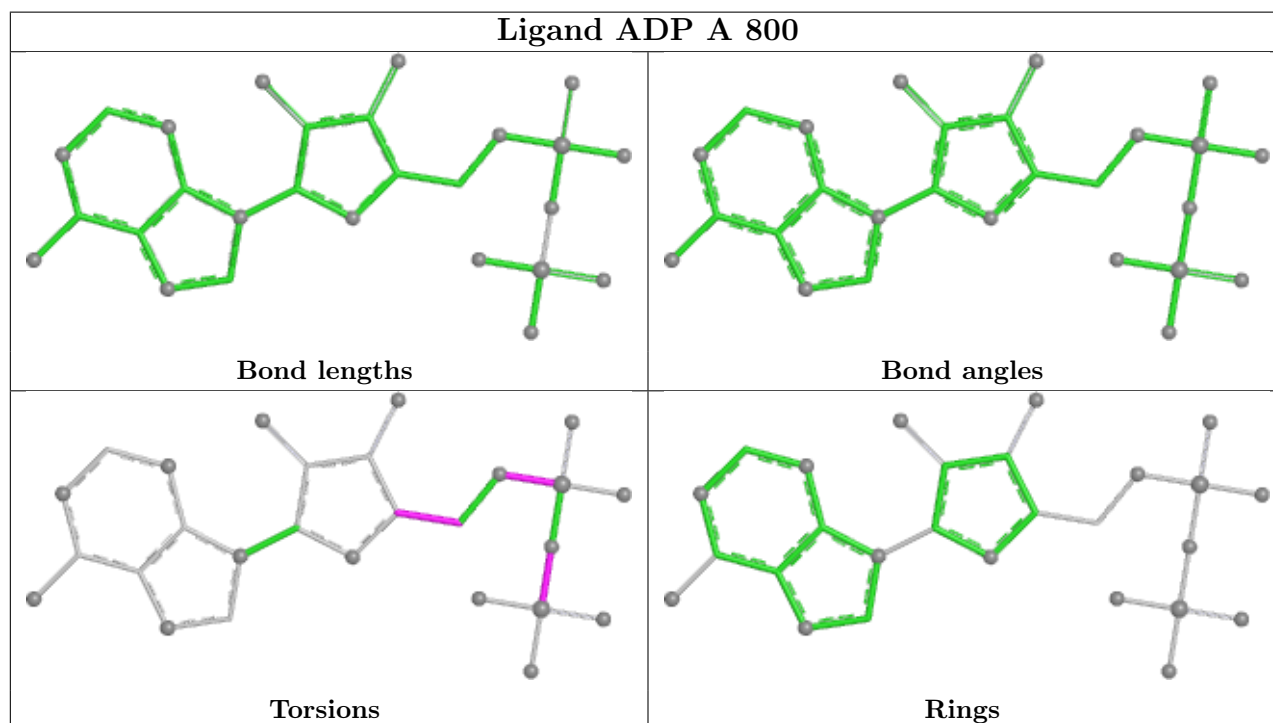
Mol	Chain	Res	Type	Atoms
10	A	800	ADP	PA-O3A-PB-O2B
10	A	800	ADP	PA-O3A-PB-O3B
10	A	800	ADP	C5'-O5'-PA-O1A
10	A	800	ADP	C5'-O5'-PA-O3A
10	C	800	ADP	C5'-O5'-PA-O1A

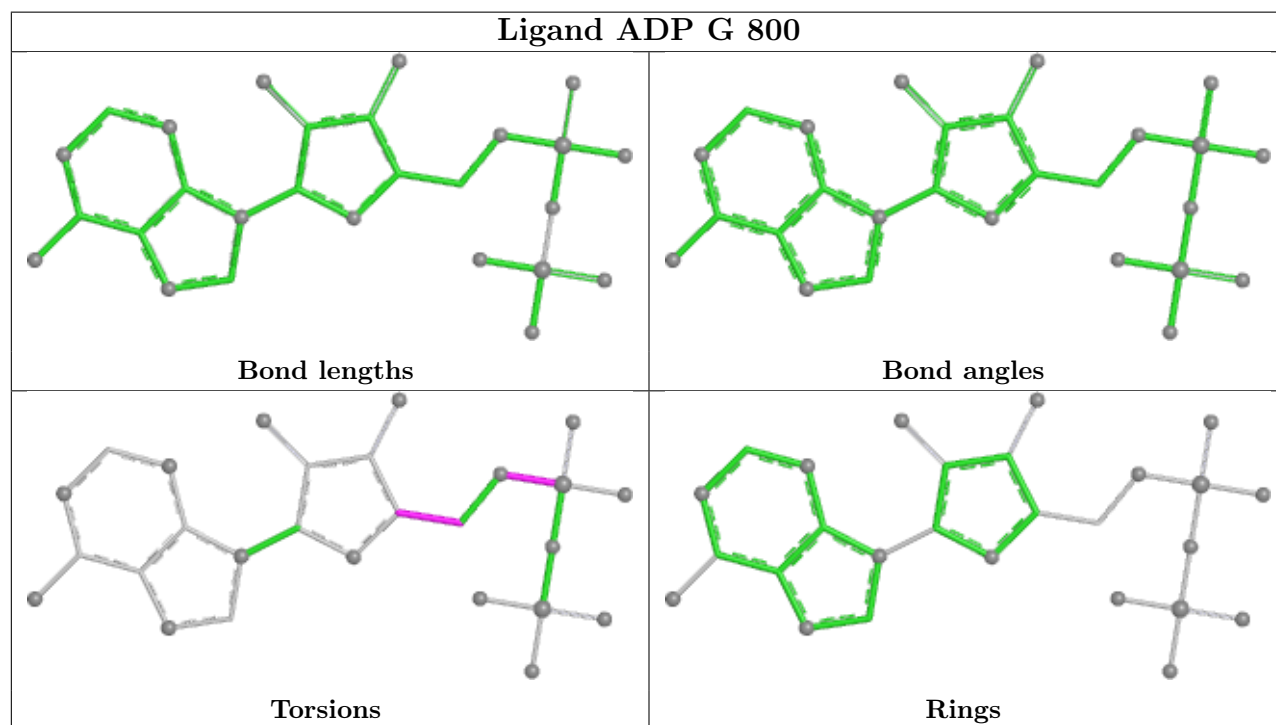
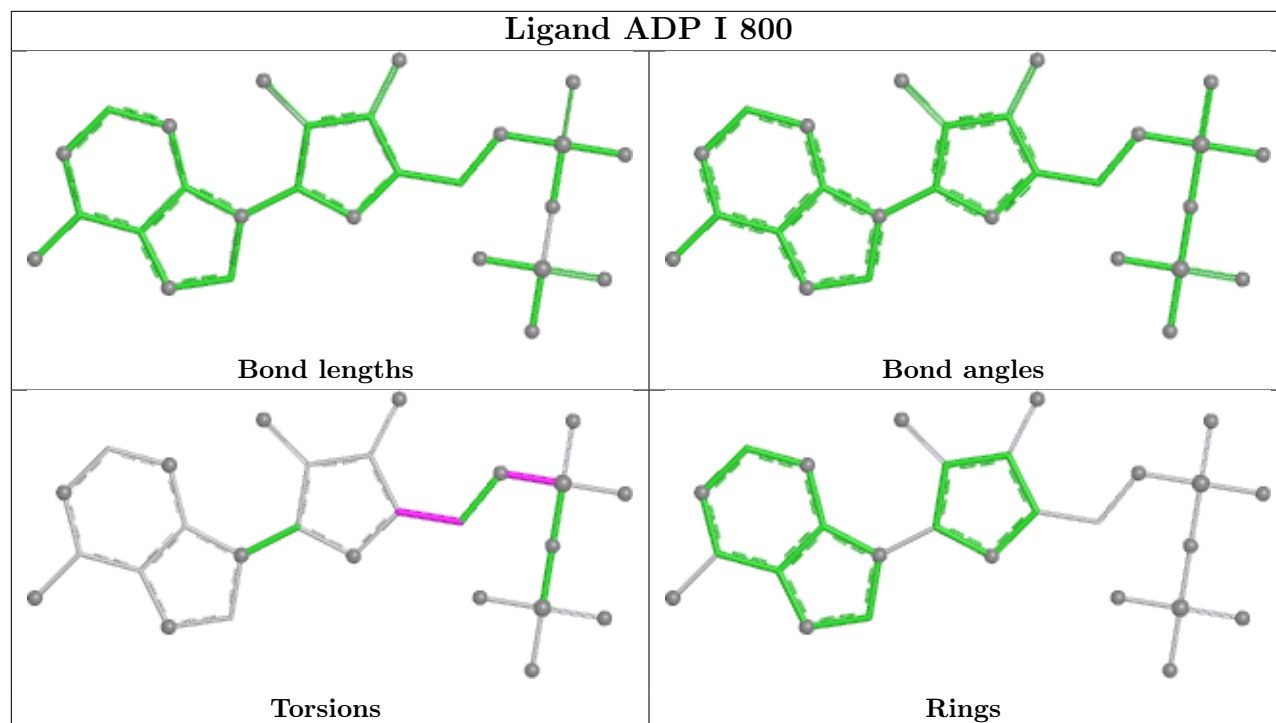
There are no ring outliers.

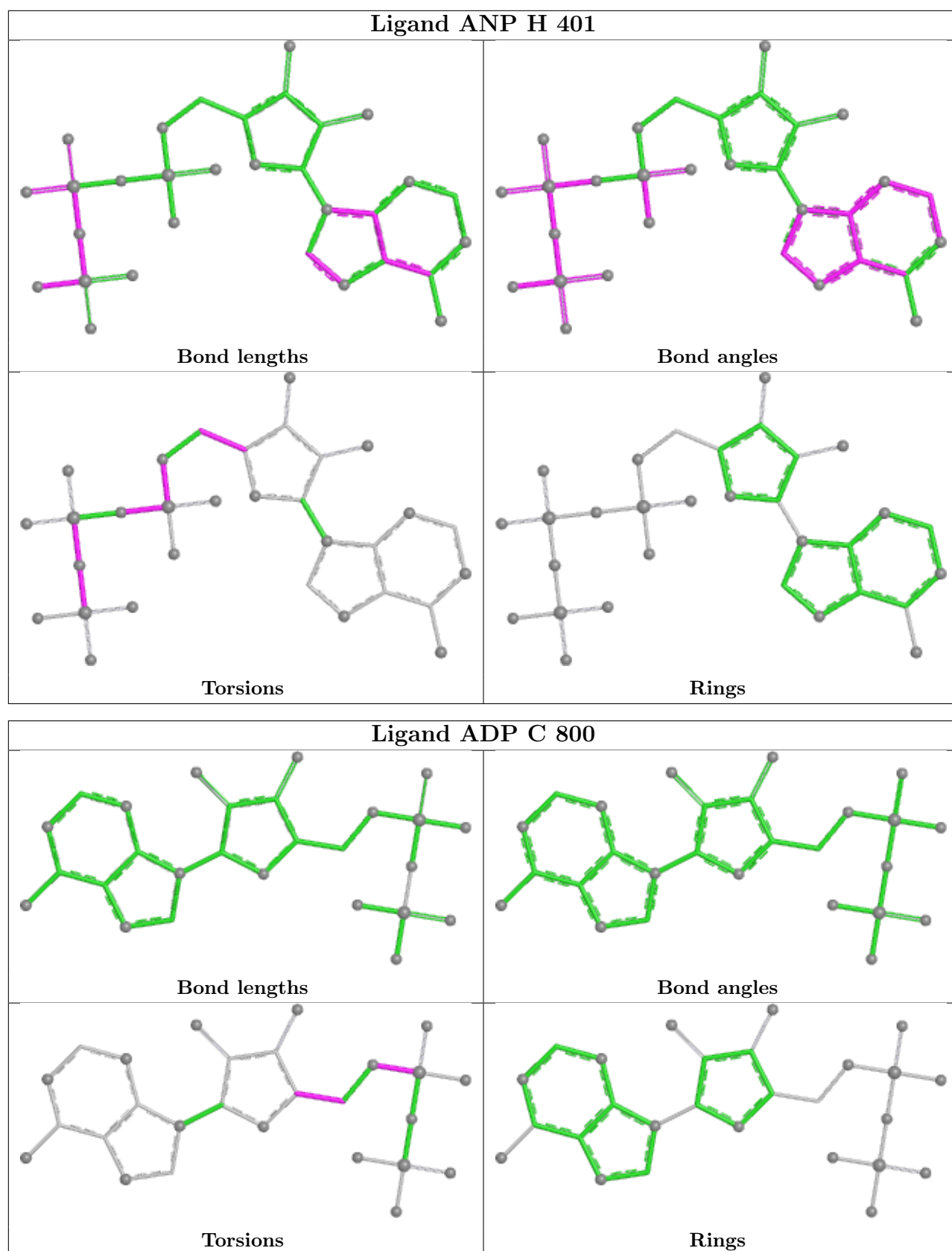
1 monomer is involved in 1 short contact:

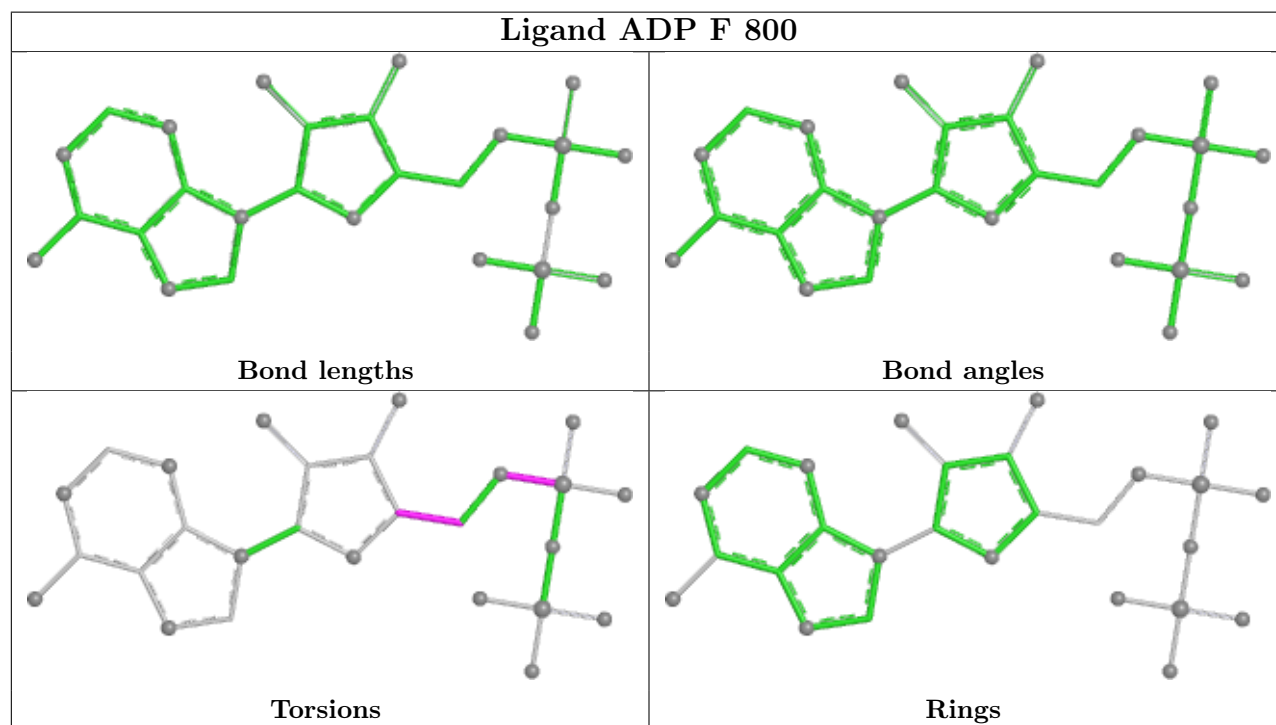
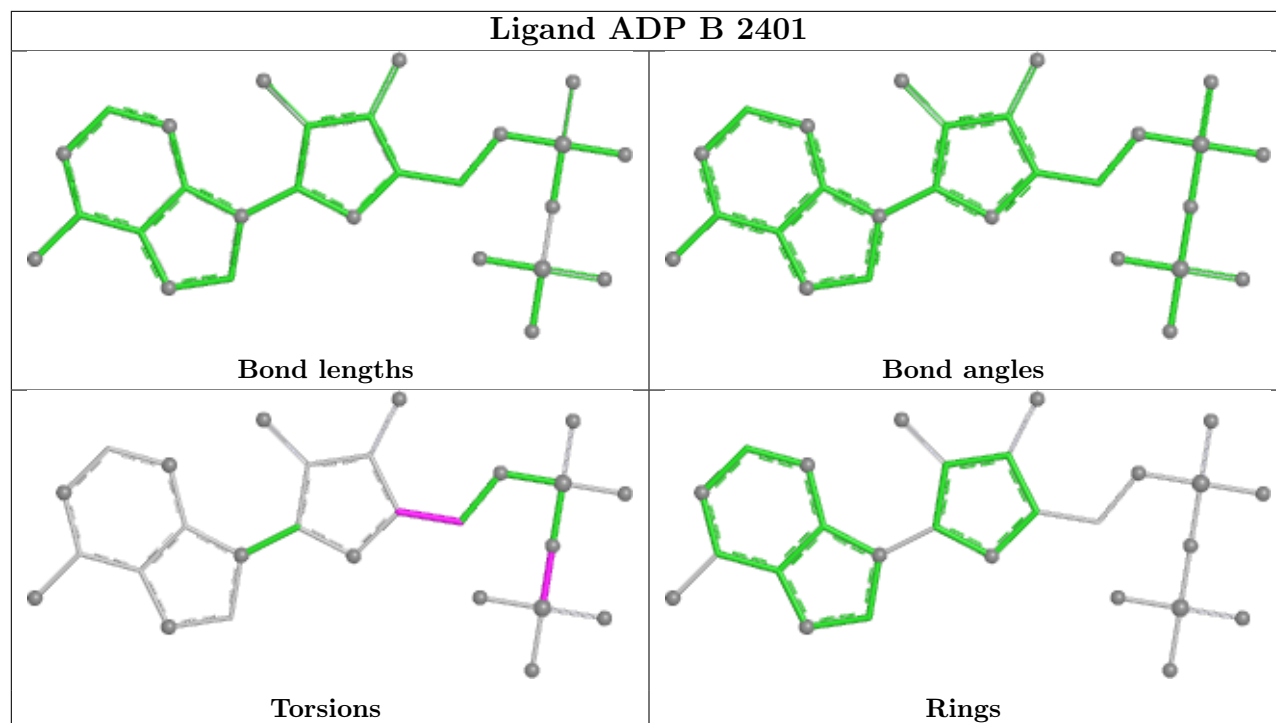
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	2401	ADP	1	0

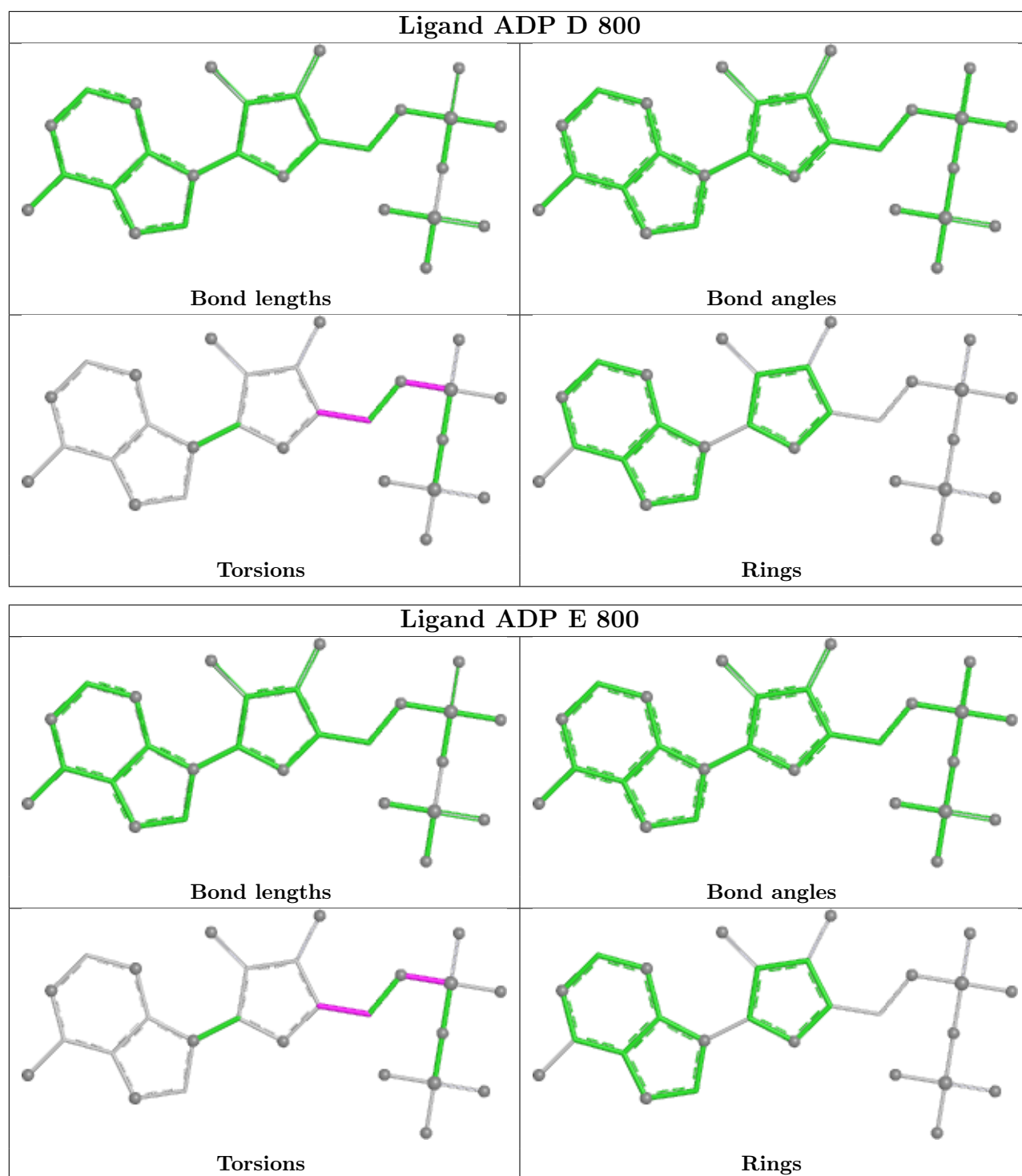
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	9

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	94:SER	C	95:VAL	N	3.80
1	J	116:PRO	C	117:SER	N	2.93
1	J	55:VAL	C	56:GLN	N	2.80
1	J	329:LYS	C	330:PRO	N	1.20
1	J	89:VAL	C	90:VAL	N	1.19

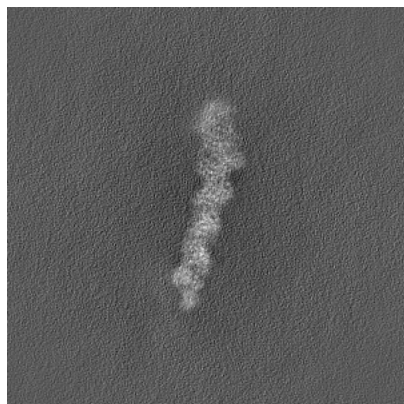
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44333. These allow visual inspection of the internal detail of the map and identification of artifacts.

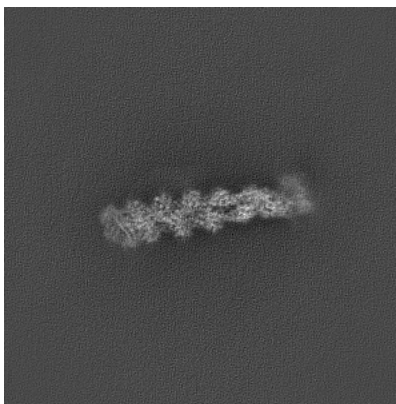
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

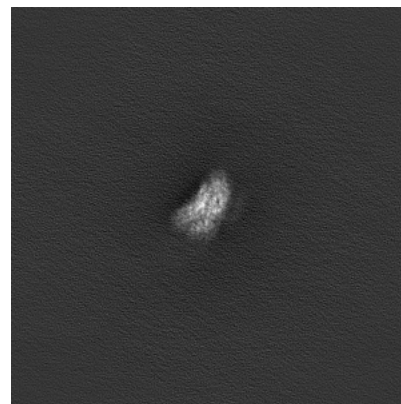
#### 6.1.1 Primary map



X

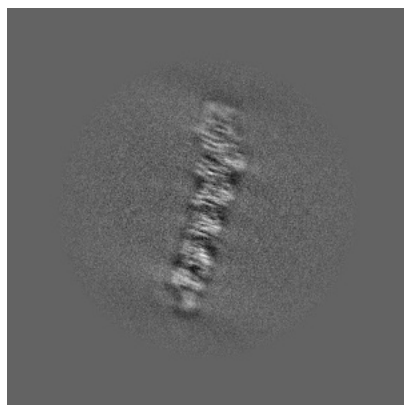


Y

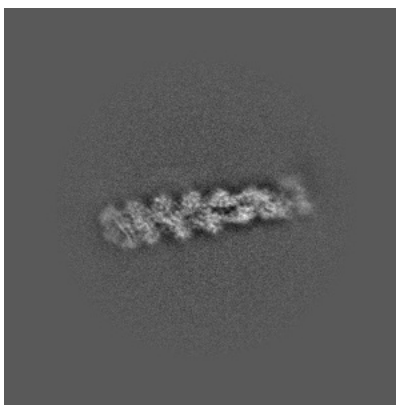


Z

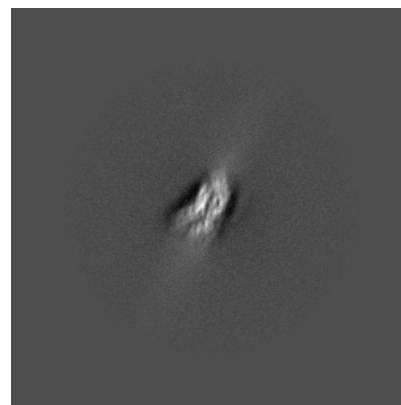
#### 6.1.2 Raw map



X



Y



Z

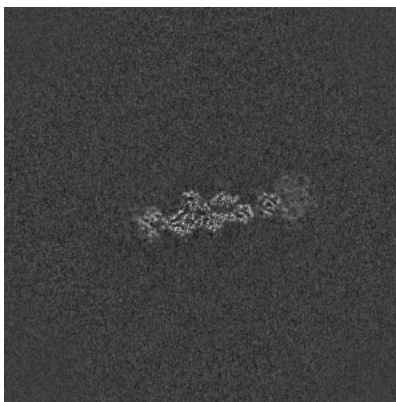
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

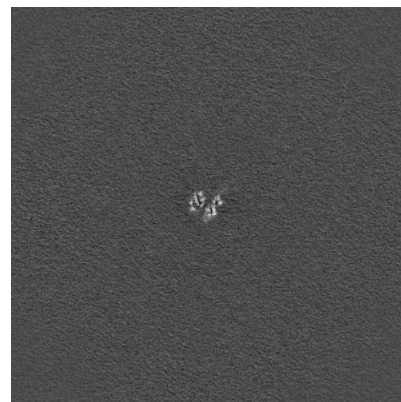
### 6.2.1 Primary map



X Index: 432

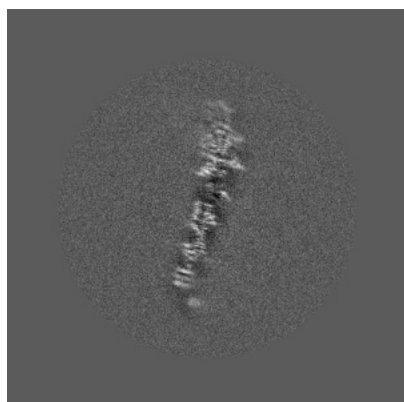


Y Index: 432

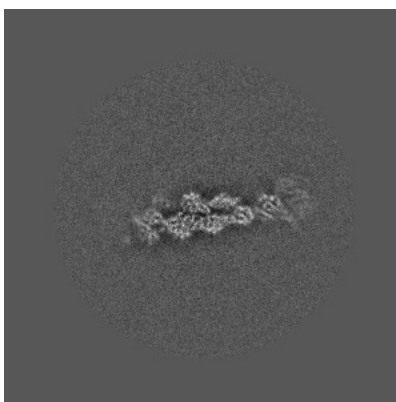


Z Index: 432

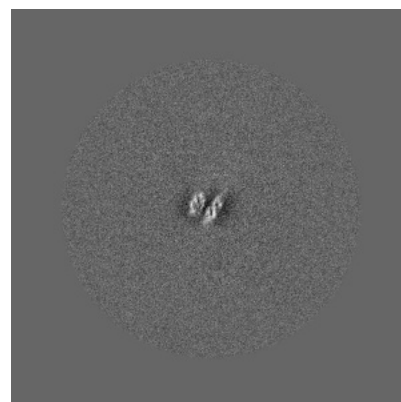
### 6.2.2 Raw map



X Index: 432



Y Index: 432

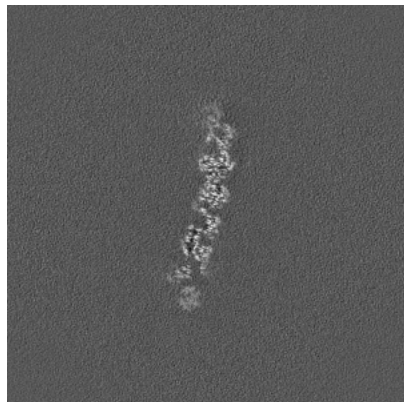


Z Index: 432

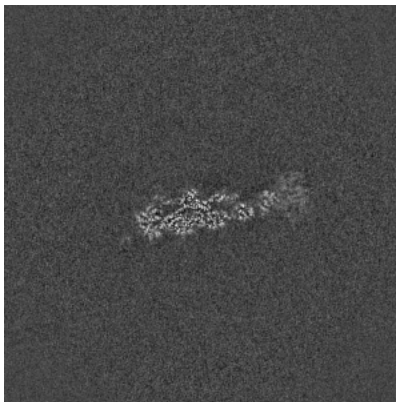
The images above show central slices of the map in three orthogonal directions.

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

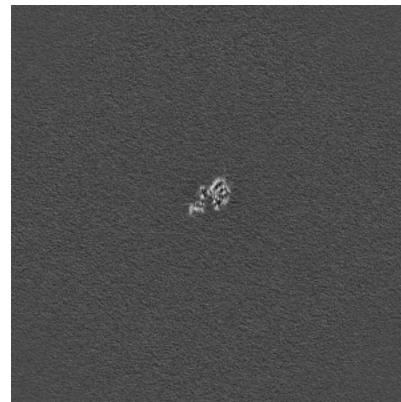
### 6.3.1 Primary map



X Index: 416

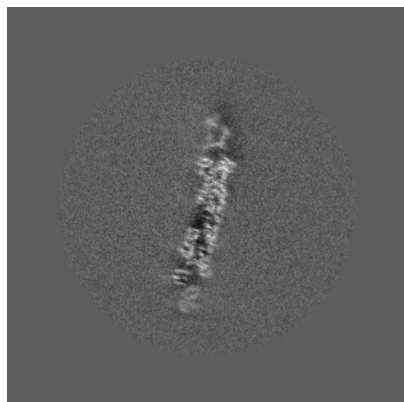


Y Index: 428

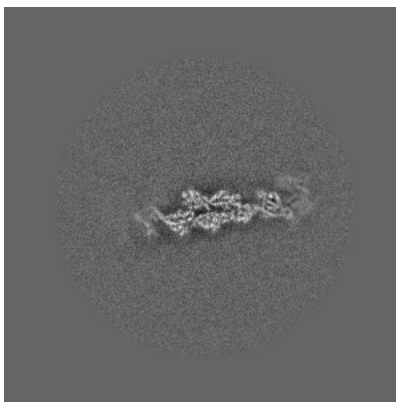


Z Index: 467

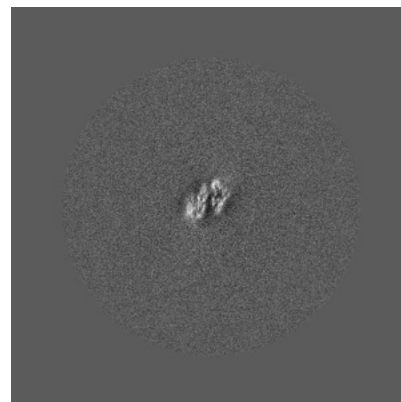
### 6.3.2 Raw map



X Index: 411



Y Index: 438

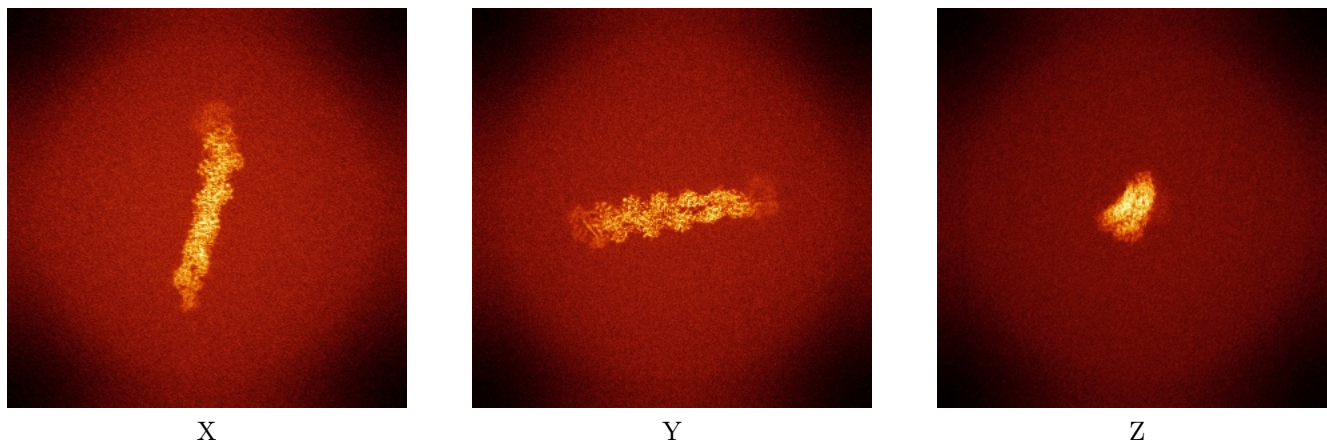


Z Index: 455

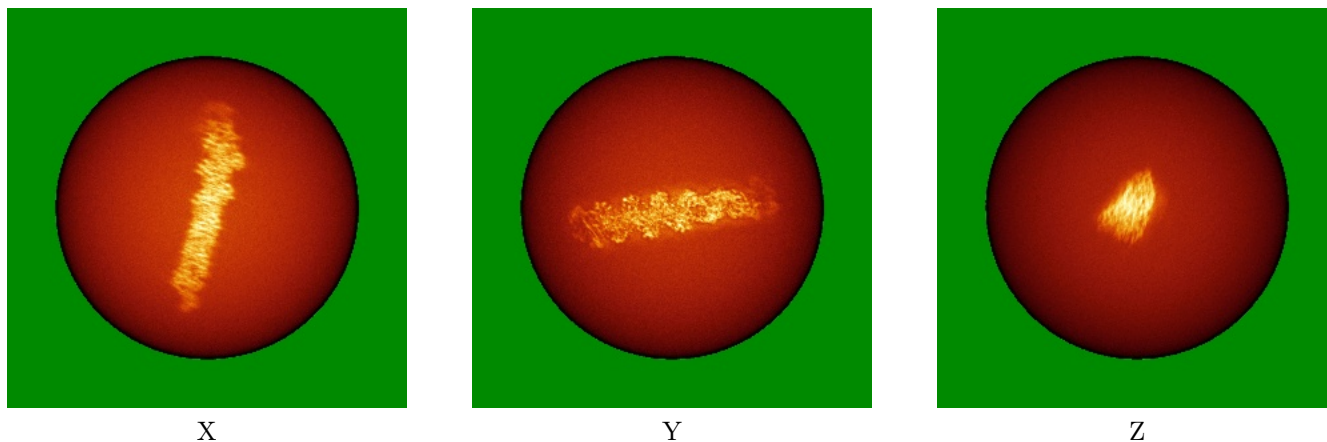
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

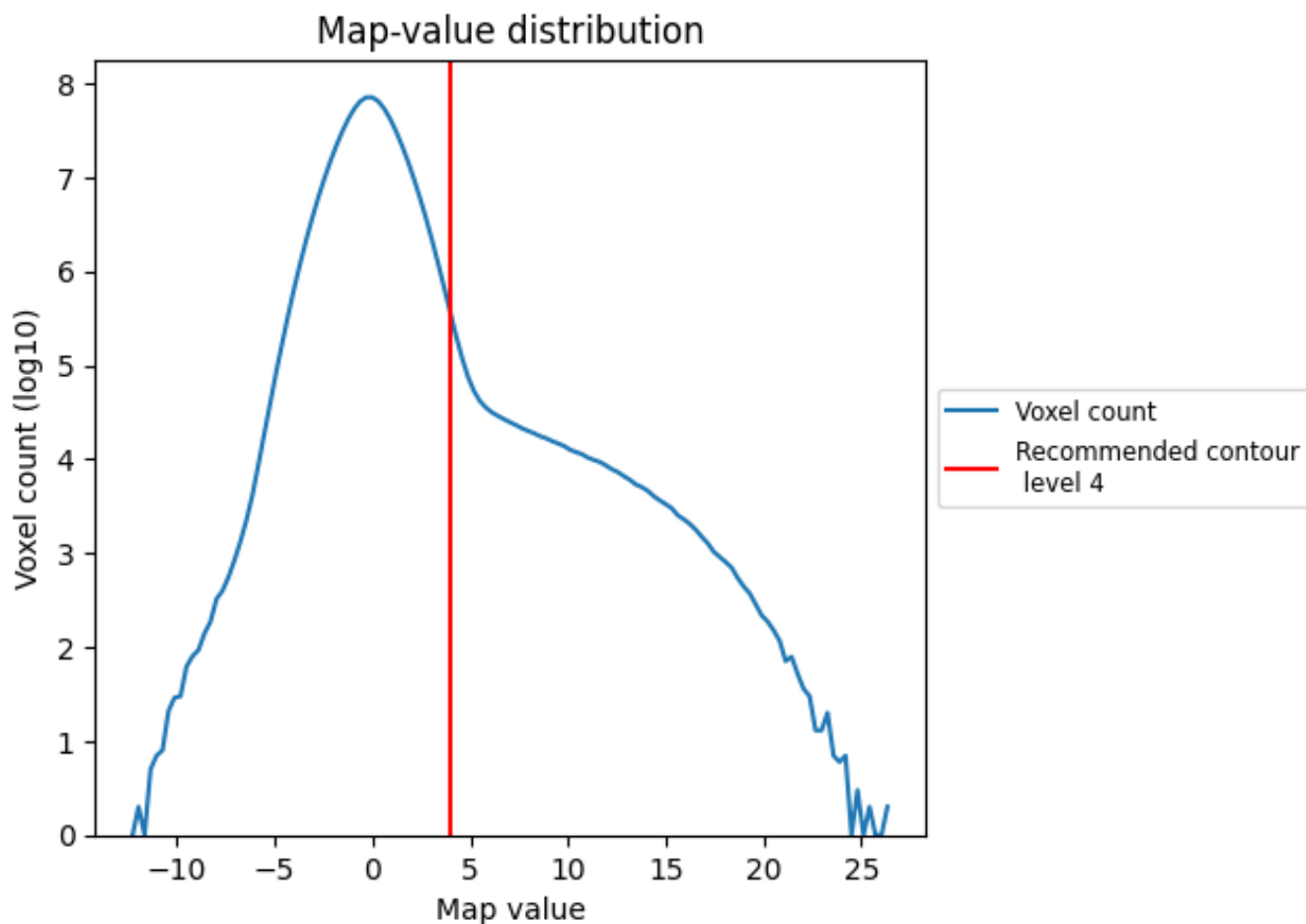
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

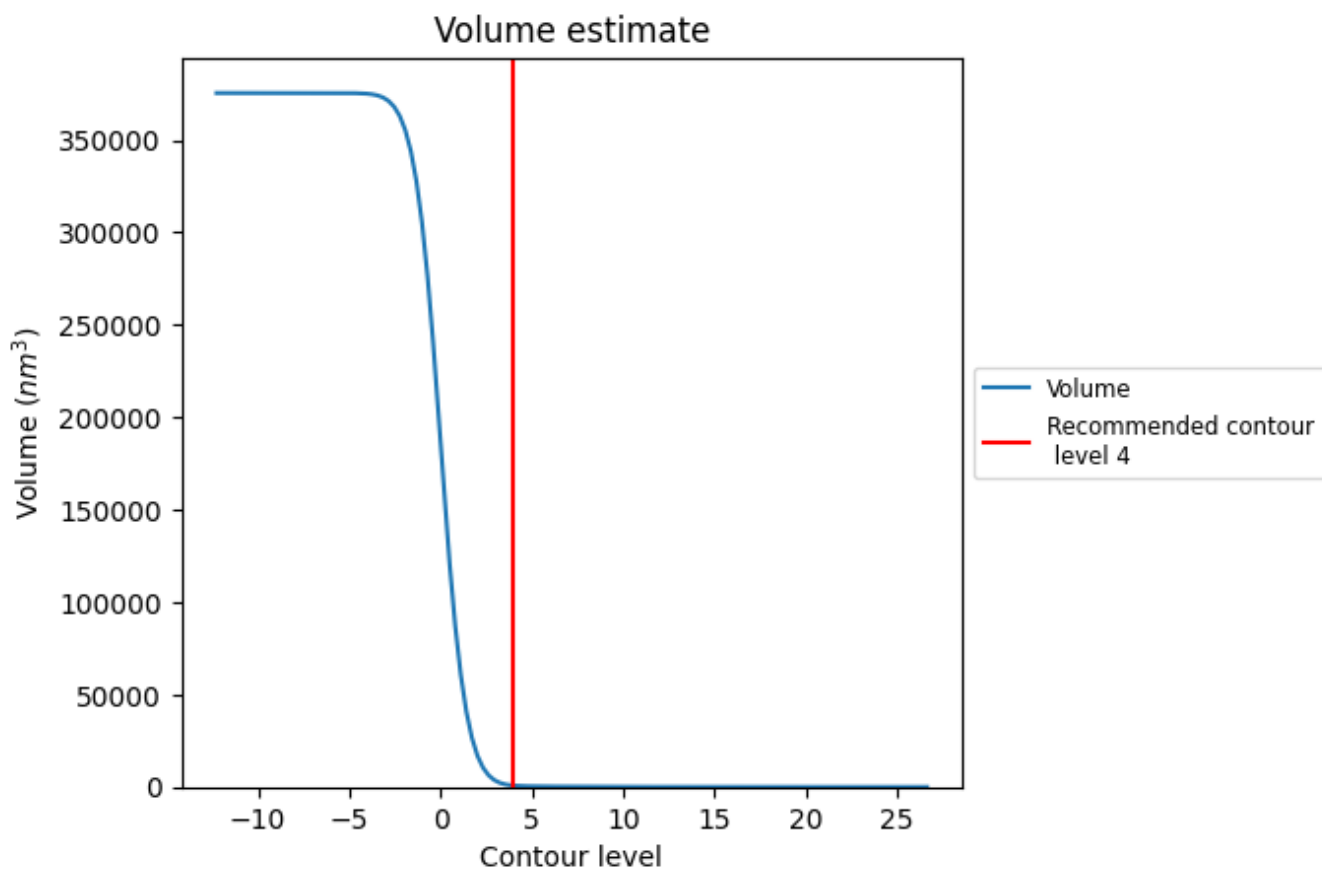
This section contains the results of statistical analysis of the map.

### 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.

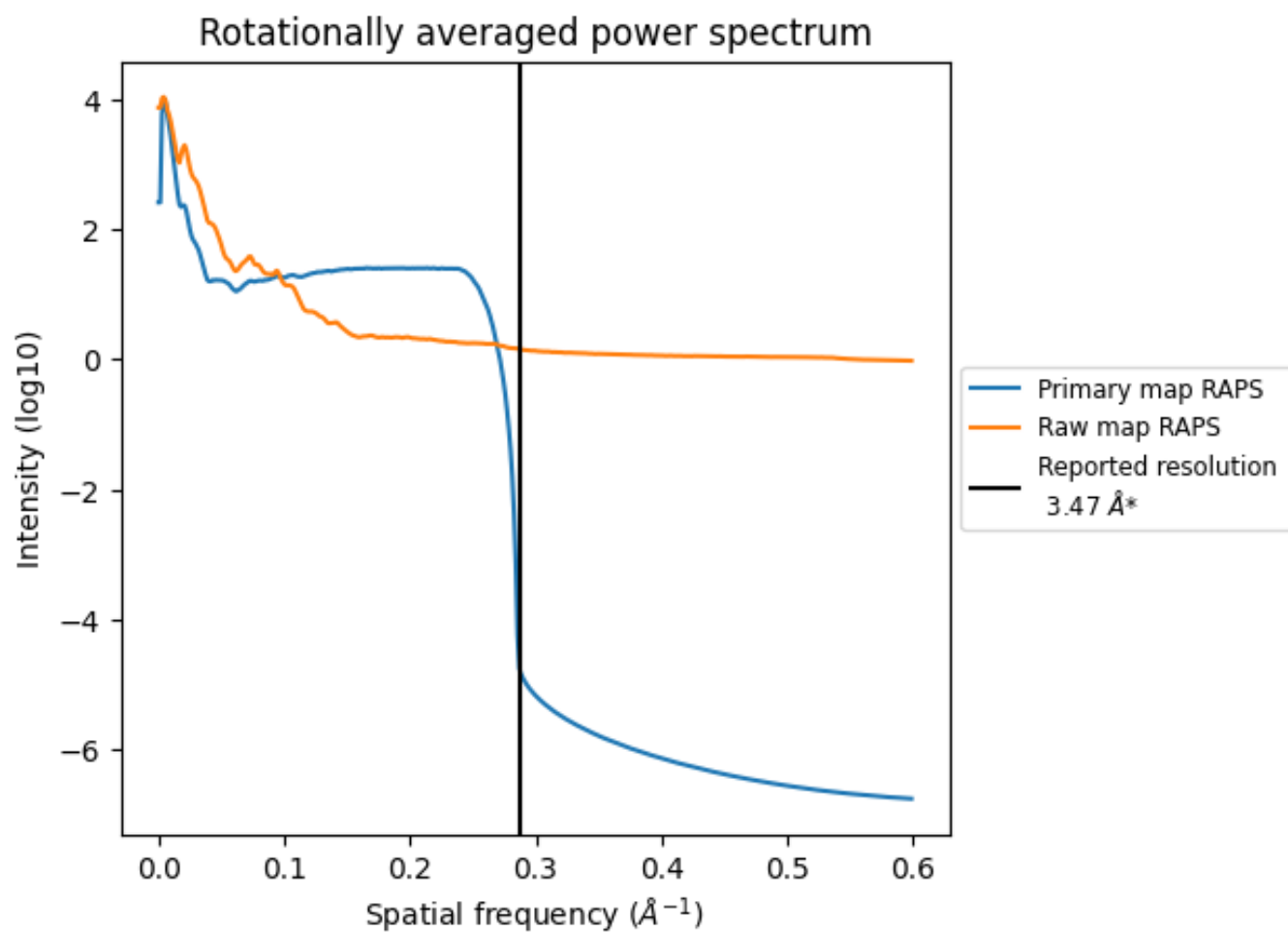
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 765  $\text{nm}^3$ ; this corresponds to an approximate mass of 691 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

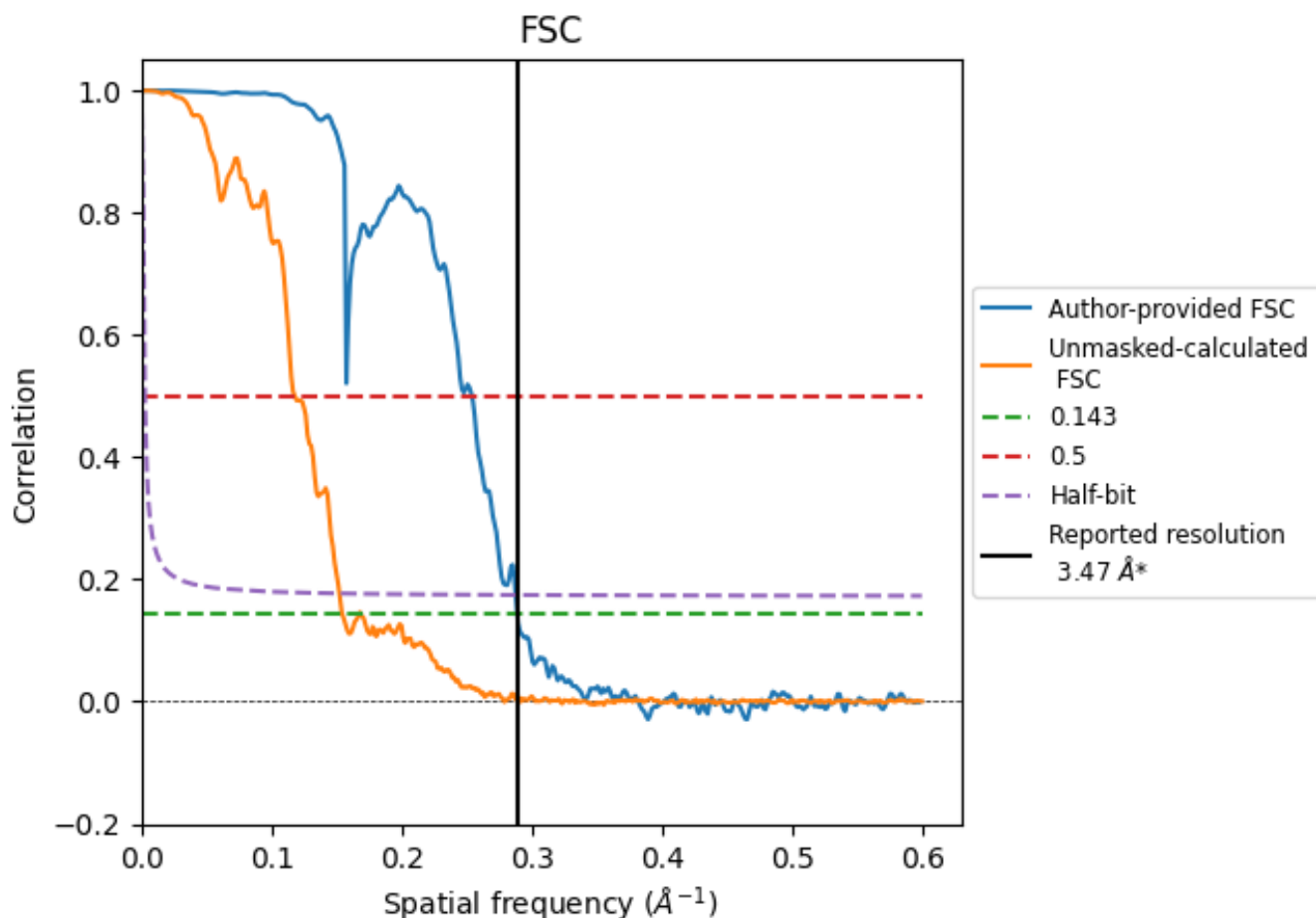


\*Reported resolution corresponds to spatial frequency of 0.288 Å<sup>-1</sup>

## 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 0.288 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

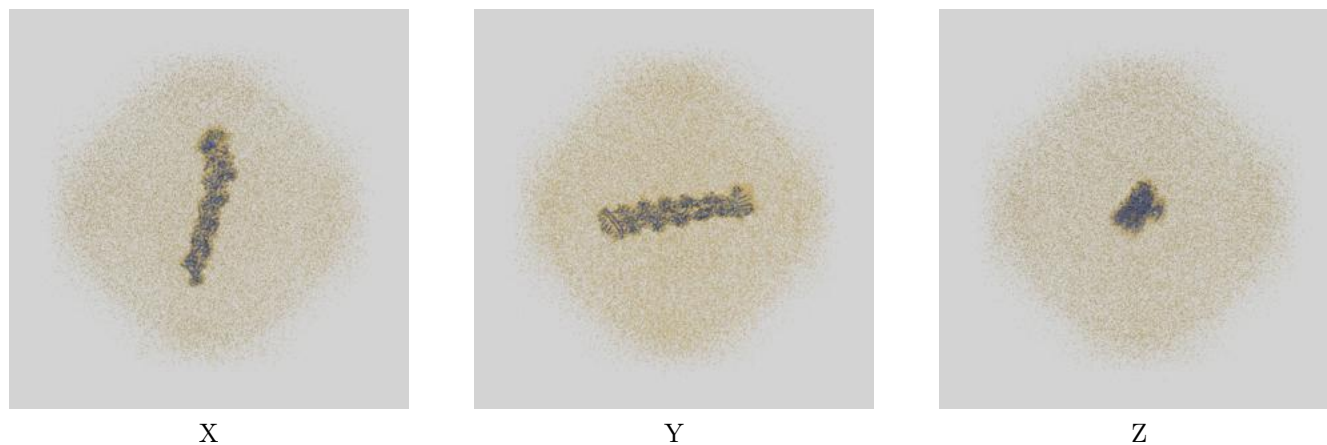
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.47	3.94	3.48
Unmasked-calculated*	6.49	8.50	6.58

\*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 6.49 differs from the reported value 3.47 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-44333 and PDB model 9B85. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



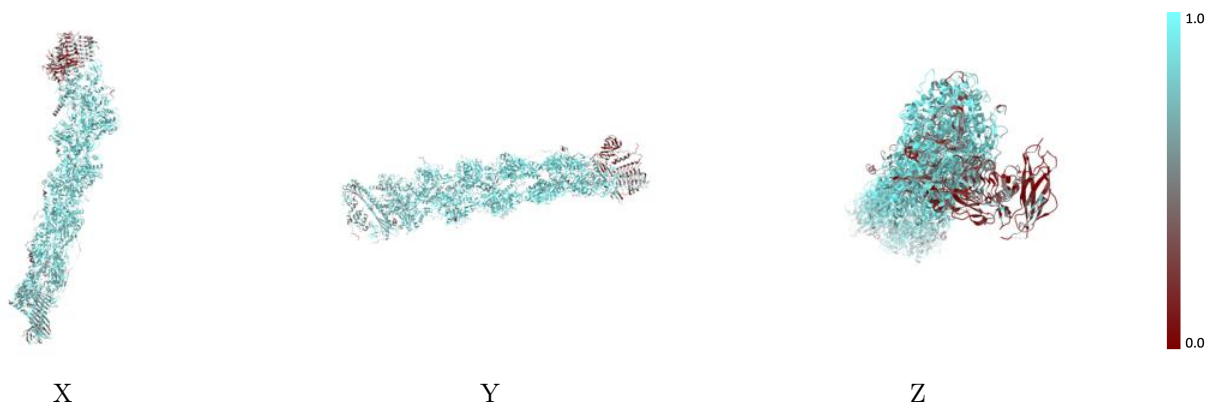
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



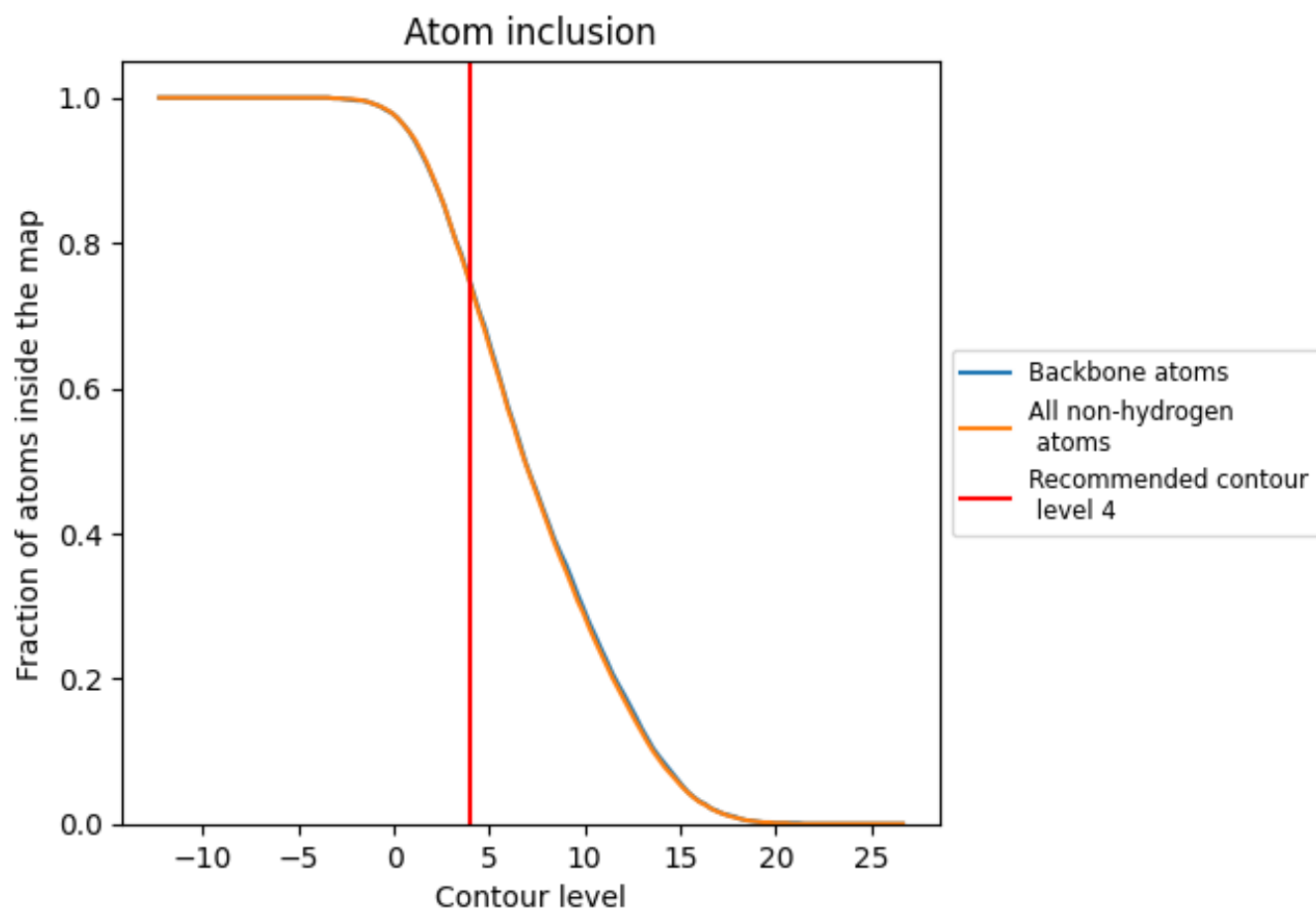
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.3060
A	 0.7800	 0.3070
B	 0.8140	 0.3470
C	 0.8420	 0.3770
D	 0.8680	 0.3910
E	 0.8560	 0.3800
F	 0.8700	 0.3870
G	 0.8630	 0.3920
H	 0.8650	 0.3760
I	 0.8220	 0.3250
J	 0.7910	 0.2870
K	 0.3990	 0.1340
L	 0.3250	 0.1000
M	 0.4630	 0.1350
N	 0.6200	 0.1810
O	 0.7150	 0.2340
P	 0.6710	 0.3050
Q	 0.4950	 0.2500
p	 0.4890	 0.2020
q	 0.4440	 0.2400

