



wwPDB EM Validation Summary Report ⓘ

May 20, 2024 – 03:19 pm BST

PDB ID : 8P94
EMDB ID : EMD-17558
Title : Cryo-EM structure of cortactin stabilized Arp2/3-complex nucleated actin branches
Authors : Liu, T.; Moores, C.A.
Deposited on : 2023-06-05
Resolution : 3.30 Å(reported)
Based on initial model : .

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:

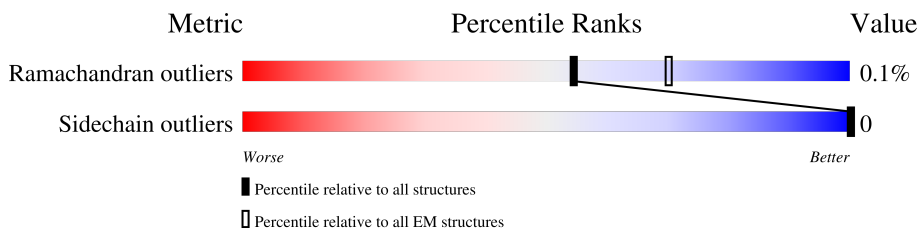
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	418	99%
2	B	394	100%
3	C	372	98%
4	D	300	100%
5	E	178	100%
6	F	168	99%
7	G	153	6% 99%
8	H	375	8% 99%
8	J	375	99%

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Mol	Chain	Length	Quality of chain
8	K	375	99%
8	N	375	99%
8	O	375	99%
8	P	375	99%
8	Q	375	99%
8	R	375	99%
8	S	375	99%
8	W	375	47% 99%
9	I	546	7% 18% 82%
10	U	286	96% 97%
11	V	272	98% 99%
12	a	7	57% 43%
12	b	7	57% 43%
12	c	7	57% 43%
12	d	7	29% 71% 29%
12	h	7	57% 43%
12	i	7	57% 43%
12	j	7	57% 43%
12	k	7	57% 43%
12	l	7	57% 43%
12	m	7	57% 43%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 100470 atoms, of which 49812 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	414	6577	2119	3267	561	615	15	0	0

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	394	6336	2012	3188	539	580	17	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	363	5594	1783	2778	497	515	21	0	0

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	300	4817	1536	2397	420	455	9	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	178	2887	925	1443	241	268	10	0	0

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	167	2781	875	1410	239	248	9	0	0

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	152	2356	734	1178	212	230	2	0	0

- Molecule 8 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	372	5718	1828	2835	479	554	22	0	0
8	J	372	5772	1837	2871	488	554	22	0	0
8	K	372	5762	1835	2864	488	554	21	0	0
8	N	372	5772	1837	2871	488	554	22	0	0
8	O	372	5772	1837	2871	488	554	22	0	0
8	P	372	5772	1837	2871	488	554	22	0	0
8	Q	372	5772	1837	2871	488	554	22	0	0
8	R	372	5767	1836	2869	488	552	22	0	0
8	S	372	5772	1837	2871	488	554	22	0	0
8	W	372	5728	1829	2842	482	554	21	0	0

- Molecule 9 is a protein called Src substrate cortactin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	96	1497	475	720	144	156	2	0	0

- Molecule 10 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	U	276	4336	1400	2117	378	435	6	0	0

- Molecule 11 is a protein called Isoform 2 of F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	V	270	4220	1322	2102	365	419	12	0	0

- Molecule 12 is a protein called Phalloidin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	a	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	b	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	c	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	d	7	Total 55	C 35	H 8	N 11	O 1	S	0	0
12	h	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	i	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	j	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	k	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	l	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0
12	m	7	Total 103	C 35	H 48	N 8	O 11	S 1	0	0

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

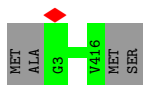
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total 1	Mg 1	0
14	B	1	Total 1	Mg 1	0
14	H	1	Total 1	Mg 1	0
14	J	1	Total 1	Mg 1	0
14	K	1	Total 1	Mg 1	0
14	N	1	Total 1	Mg 1	0
14	O	1	Total 1	Mg 1	0
14	P	1	Total 1	Mg 1	0
14	Q	1	Total 1	Mg 1	0
14	R	1	Total 1	Mg 1	0
14	S	1	Total 1	Mg 1	0
14	W	1	Total 1	Mg 1	0

3 Residue-property plots [i](#)

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

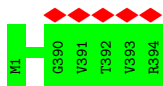
- Molecule 1: Actin-related protein 3

Chain A:  99%



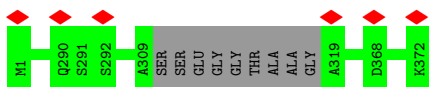
- Molecule 2: Actin-related protein 2

Chain B:  100%



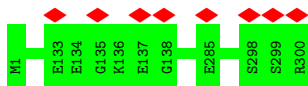
- Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:  98%



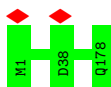
- Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:  100%



- Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:  100%



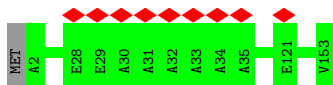
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:  99%



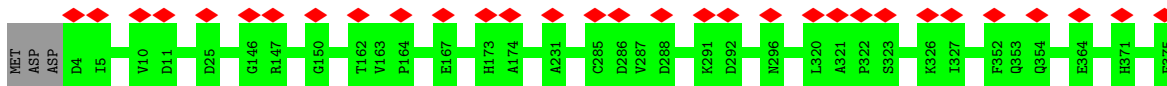
- Molecule 7: Actin-related protein 2/3 complex subunit 5-like protein

Chain G:  99%



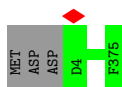
- Molecule 8: Actin, cytoplasmic 1

Chain H:  99%



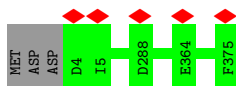
- Molecule 8: Actin, cytoplasmic 1

Chain J:  99%



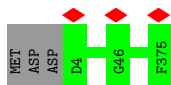
- Molecule 8: Actin, cytoplasmic 1

Chain K:  99%



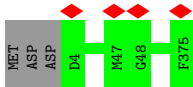
- Molecule 8: Actin, cytoplasmic 1

Chain N:  99%



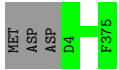
- Molecule 8: Actin, cytoplasmic 1

Chain O:  99%



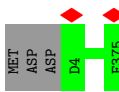
- Molecule 8: Actin, cytoplasmic 1

Chain P: 99%



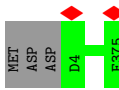
- Molecule 8: Actin, cytoplasmic 1

Chain Q: 99%



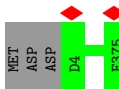
- Molecule 8: Actin, cytoplasmic 1

Chain R: 99%



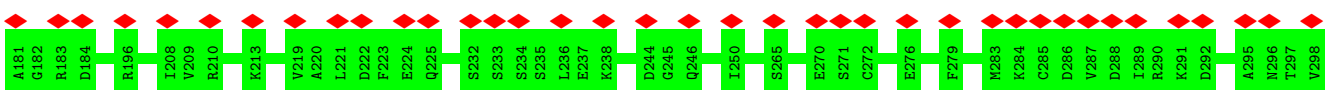
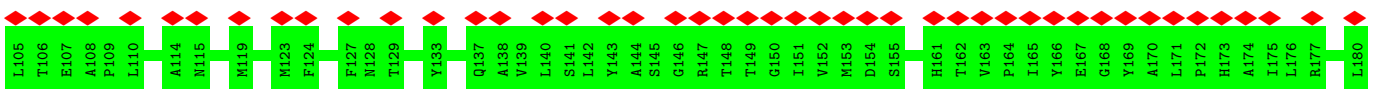
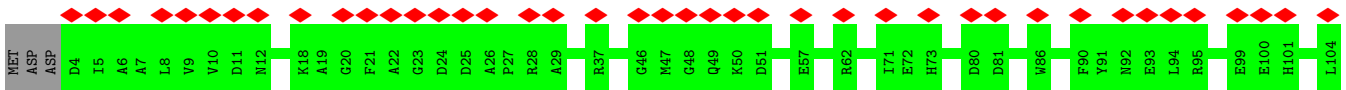
- Molecule 8: Actin, cytoplasmic 1

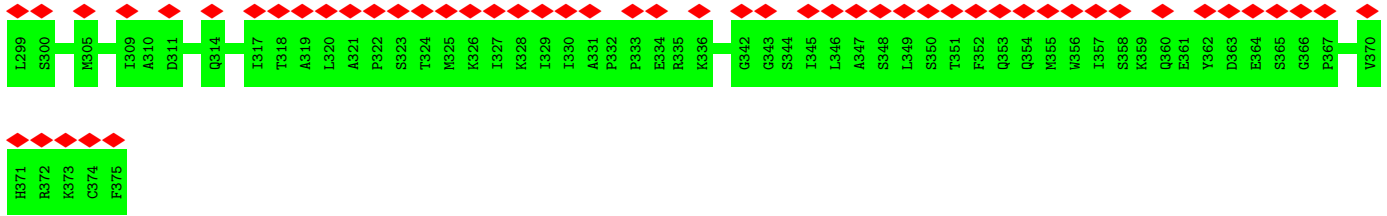
Chain S: 99%



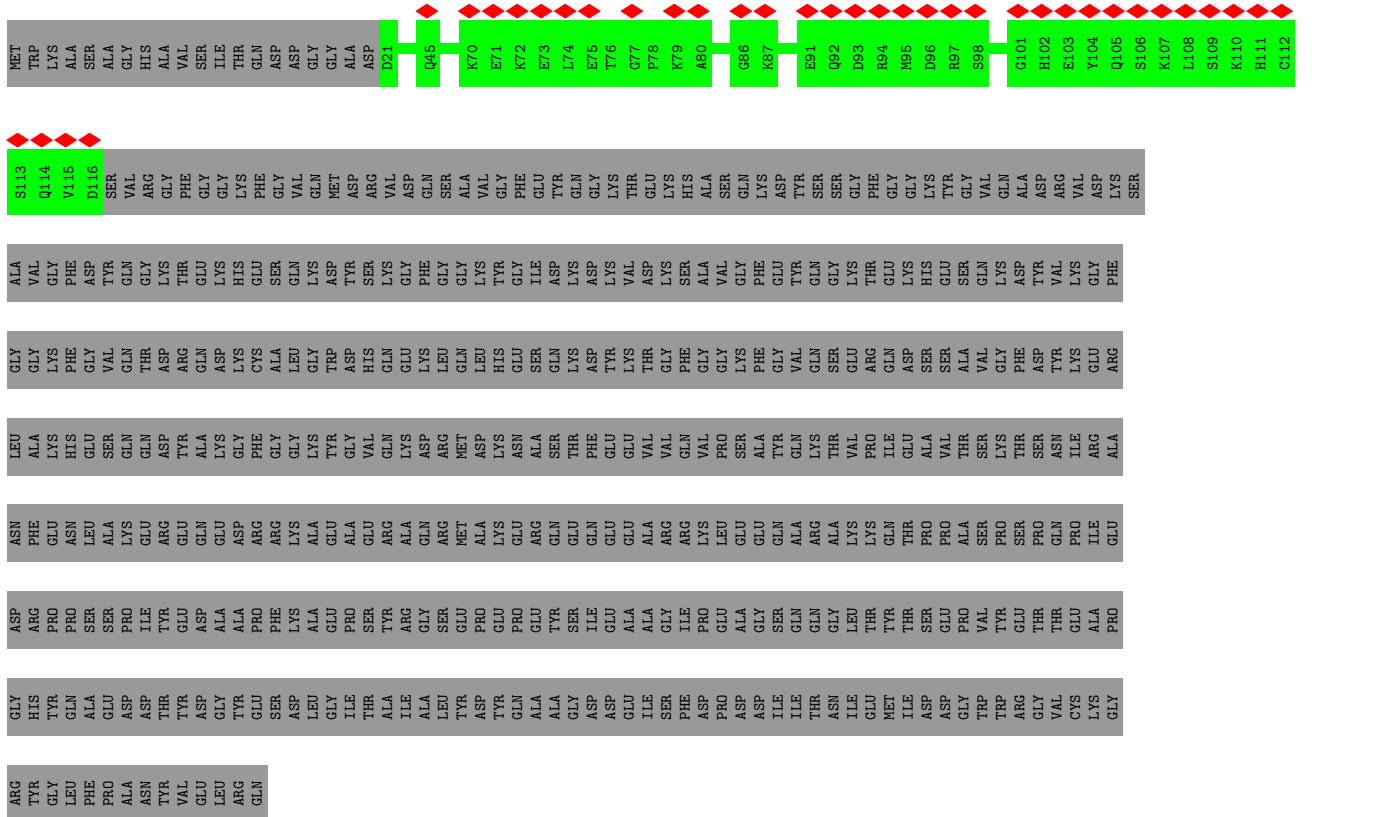
- Molecule 8: Actin, cytoplasmic 1

Chain W: 47% 99%

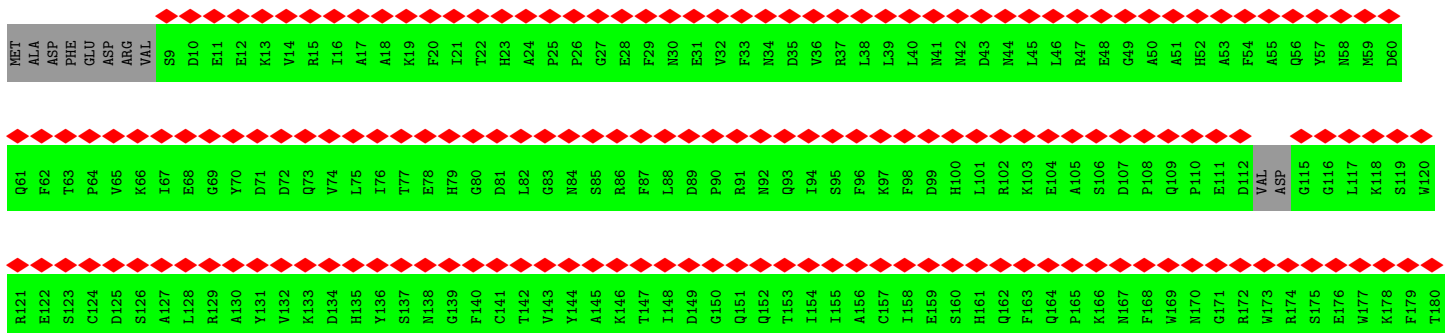


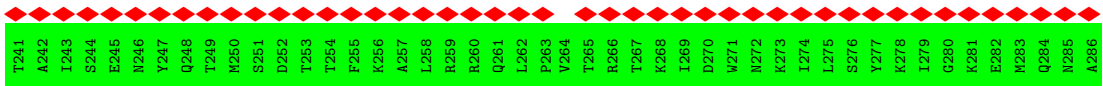
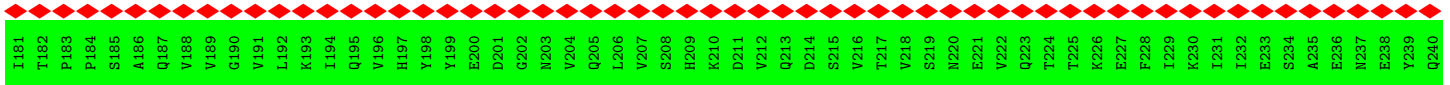


- Molecule 9: Src substrate cortactin

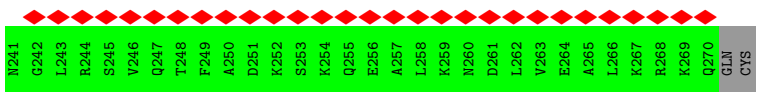
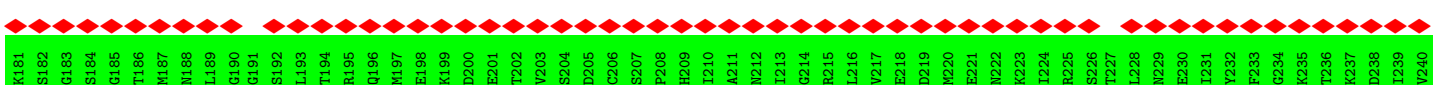
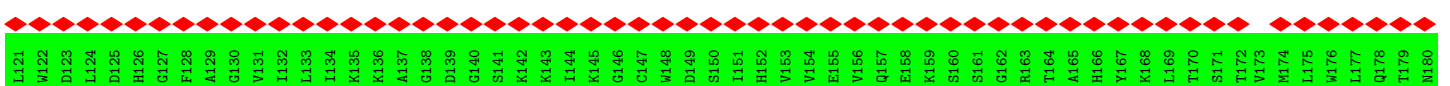
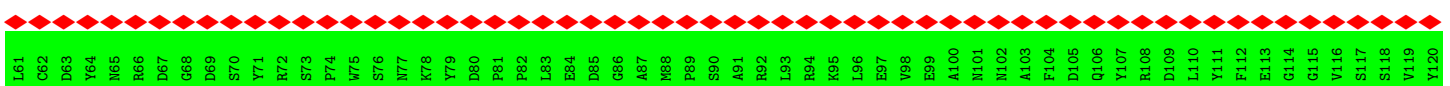
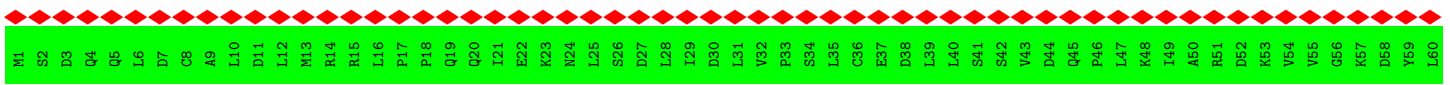


- Molecule 10: F-actin-capping protein subunit alpha-1





• Molecule 11: Isoform 2 of F-actin-capping protein subunit beta



• Molecule 12: Phalloidin



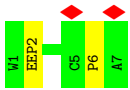
• Molecule 12: Phalloidin



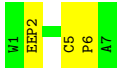
• Molecule 12: Phalloidin



● Molecule 12: Phalloidin



● Molecule 12: Phalloidin



● Molecule 12: Phalloidin



● Molecule 12: Phalloidin



● Molecule 12: Phalloidin



● Molecule 12: Phalloidin



● Molecule 12: Phalloidin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CryoSPARC Patch CTF	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.751	Depositor
Minimum map value	-0.283	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	469.48, 469.48, 469.48	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, DTH, HYP, MG, EEP

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	0.32	0/3393	0.45	0/4602
2	B	0.30	0/3210	0.46	0/4336
3	C	0.28	0/2886	0.46	0/3910
4	D	0.31	0/2470	0.44	0/3329
5	E	0.28	0/1479	0.41	0/1994
6	F	0.29	0/1393	0.44	0/1868
7	G	0.27	0/1194	0.41	0/1610
8	H	0.31	0/2946	0.46	0/3992
8	J	0.31	0/2964	0.45	0/4013
8	K	0.30	0/2961	0.43	0/4010
8	N	0.28	0/2964	0.43	0/4013
8	O	0.29	0/2964	0.43	0/4013
8	P	0.30	0/2964	0.43	0/4013
8	Q	0.30	0/2964	0.44	0/4013
8	R	0.29	0/2961	0.43	0/4009
8	S	0.27	0/2964	0.41	0/4013
8	W	0.35	0/2949	0.46	0/3996
9	I	0.44	0/794	0.57	0/1065
10	U	0.59	0/2269	0.81	0/3074
11	V	0.36	0/2152	0.56	0/2902
12	a	1.03	0/28	1.43	0/33
12	b	1.04	0/28	1.39	0/33
12	c	1.04	0/28	1.39	0/33
12	d	1.05	0/28	1.30	0/33
12	h	1.03	0/28	1.41	0/33
12	i	1.02	0/28	1.40	0/33
12	j	1.04	0/28	1.39	0/33
12	k	1.03	0/28	1.42	0/33
12	l	1.03	0/28	1.45	0/33
12	m	1.05	0/28	1.41	0/33
All	All	0.33	0/51121	0.48	0/69105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/418 (99%)	395 (96%)	17 (4%)	0	100	100
2	B	392/394 (100%)	378 (96%)	14 (4%)	0	100	100
3	C	359/372 (96%)	339 (94%)	20 (6%)	0	100	100
4	D	298/300 (99%)	289 (97%)	9 (3%)	0	100	100
5	E	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
6	F	165/168 (98%)	159 (96%)	6 (4%)	0	100	100
7	G	150/153 (98%)	145 (97%)	5 (3%)	0	100	100
8	H	370/375 (99%)	360 (97%)	10 (3%)	0	100	100
8	J	370/375 (99%)	361 (98%)	9 (2%)	0	100	100
8	K	370/375 (99%)	362 (98%)	8 (2%)	0	100	100
8	N	370/375 (99%)	364 (98%)	6 (2%)	0	100	100
8	O	370/375 (99%)	360 (97%)	10 (3%)	0	100	100
8	P	370/375 (99%)	364 (98%)	6 (2%)	0	100	100
8	Q	370/375 (99%)	363 (98%)	7 (2%)	0	100	100
8	R	370/375 (99%)	364 (98%)	6 (2%)	0	100	100
8	S	370/375 (99%)	360 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	W	370/375 (99%)	364 (98%)	6 (2%)	0	100	100
9	I	94/546 (17%)	89 (95%)	5 (5%)	0	100	100
10	U	272/286 (95%)	262 (96%)	10 (4%)	0	100	100
11	V	268/272 (98%)	260 (97%)	8 (3%)	0	100	100
12	a	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	b	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	c	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	d	2/7 (29%)	1 (50%)	1 (50%)	0	100	100
12	h	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	i	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	j	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	k	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	l	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
12	m	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	6306/6907 (91%)	6121 (97%)	176 (3%)	9 (0%)	54	81

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	a	5	CYS
12	b	5	CYS
12	c	5	CYS
12	h	5	CYS
12	i	5	CYS

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	360/363 (99%)	360 (100%)	0	100	100
2	B	345/345 (100%)	345 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	305/311 (98%)	305 (100%)	0	100	100
4	D	264/264 (100%)	264 (100%)	0	100	100
5	E	159/159 (100%)	159 (100%)	0	100	100
6	F	154/155 (99%)	154 (100%)	0	100	100
7	G	125/127 (98%)	125 (100%)	0	100	100
8	H	312/318 (98%)	312 (100%)	0	100	100
8	J	315/318 (99%)	315 (100%)	0	100	100
8	K	314/318 (99%)	314 (100%)	0	100	100
8	N	315/318 (99%)	315 (100%)	0	100	100
8	O	315/318 (99%)	315 (100%)	0	100	100
8	P	315/318 (99%)	315 (100%)	0	100	100
8	Q	315/318 (99%)	315 (100%)	0	100	100
8	R	314/318 (99%)	314 (100%)	0	100	100
8	S	315/318 (99%)	315 (100%)	0	100	100
8	W	312/318 (98%)	312 (100%)	0	100	100
9	I	84/448 (19%)	84 (100%)	0	100	100
10	U	242/255 (95%)	242 (100%)	0	100	100
11	V	237/241 (98%)	237 (100%)	0	100	100
12	a	2/2 (100%)	2 (100%)	0	100	100
12	b	2/2 (100%)	2 (100%)	0	100	100
12	c	2/2 (100%)	2 (100%)	0	100	100
12	d	2/2 (100%)	2 (100%)	0	100	100
12	h	2/2 (100%)	2 (100%)	0	100	100
12	i	2/2 (100%)	2 (100%)	0	100	100
12	j	2/2 (100%)	2 (100%)	0	100	100
12	k	2/2 (100%)	2 (100%)	0	100	100
12	l	2/2 (100%)	2 (100%)	0	100	100
12	m	2/2 (100%)	2 (100%)	0	100	100
All	All	5437/5868 (93%)	5437 (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 7 such

sidechains are listed below:

Mol	Chain	Res	Type
10	U	167	ASN
11	V	270	GLN
8	W	280	ASN
8	W	12	ASN
8	O	12	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](#)

30 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	HYP	h	6	12	6,8,9	0.49	0	5,10,12	1.29	1 (20%)
12	EEP	d	2	12	8,9,10	1.40	2 (25%)	5,12,14	0.98	0
12	HYP	a	6	12	6,8,9	0.51	0	5,10,12	1.26	1 (20%)
12	HYP	i	6	12	6,8,9	0.55	0	5,10,12	1.21	1 (20%)
12	HYP	d	6	12	6,8,9	0.48	0	5,10,12	1.27	1 (20%)
12	EEP	h	2	12	8,9,10	1.43	2 (25%)	5,12,14	1.01	0
12	HYP	b	6	12	6,8,9	0.51	0	5,10,12	1.24	1 (20%)
12	EEP	a	2	12	8,9,10	1.41	2 (25%)	5,12,14	1.01	0
12	HYP	m	6	12	6,8,9	0.54	0	5,10,12	1.29	1 (20%)
12	EEP	i	2	12	8,9,10	1.41	2 (25%)	5,12,14	1.06	0
12	HYP	k	6	12	6,8,9	0.58	0	5,10,12	1.24	1 (20%)
12	EEP	j	2	12	8,9,10	1.40	2 (25%)	5,12,14	1.00	0
12	EEP	c	2	12	8,9,10	1.36	2 (25%)	5,12,14	1.01	0
12	EEP	b	2	12	8,9,10	1.39	2 (25%)	5,12,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	EEP	l	2	12	8,9,10	1.39	2 (25%)	5,12,14	1.03	0
12	HYP	j	6	12	6,8,9	0.49	0	5,10,12	1.21	1 (20%)
12	EEP	m	2	12	8,9,10	1.39	2 (25%)	5,12,14	1.03	0
12	HYP	c	6	12	6,8,9	0.53	0	5,10,12	1.24	1 (20%)
12	EEP	k	2	12	8,9,10	1.43	2 (25%)	5,12,14	1.01	0
12	HYP	l	6	12	6,8,9	0.52	0	5,10,12	1.23	1 (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
12	HYP	h	6	12	-	0/0/11/13	0/1/1/1
12	EEP	d	2	12	-	3/9/10/12	-
12	HYP	a	6	12	-	0/0/11/13	0/1/1/1
12	HYP	i	6	12	-	0/0/11/13	0/1/1/1
12	HYP	d	6	12	-	0/0/11/13	0/1/1/1
12	EEP	h	2	12	-	3/9/10/12	-
12	HYP	b	6	12	-	0/0/11/13	0/1/1/1
12	EEP	a	2	12	-	3/9/10/12	-
12	HYP	m	6	12	-	0/0/11/13	0/1/1/1
12	EEP	i	2	12	-	3/9/10/12	-
12	HYP	k	6	12	-	0/0/11/13	0/1/1/1
12	EEP	j	2	12	-	3/9/10/12	-
12	EEP	c	2	12	-	3/9/10/12	-
12	EEP	b	2	12	-	3/9/10/12	-
12	EEP	l	2	12	-	3/9/10/12	-
12	HYP	j	6	12	-	0/0/11/13	0/1/1/1
12	EEP	m	2	12	-	3/9/10/12	-
12	HYP	c	6	12	-	0/0/11/13	0/1/1/1
12	EEP	k	2	12	-	3/9/10/12	-
12	HYP	l	6	12	-	0/0/11/13	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	i	2	EEP	CB-CA	-2.97	1.50	1.54
12	j	2	EEP	CB-CA	-2.86	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	d	2	EEP	CB-CA	-2.84	1.50	1.54
12	c	2	EEP	CB-CA	-2.83	1.50	1.54
12	k	2	EEP	CB-CA	-2.82	1.50	1.54

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	d	6	HYP	O-C-CA	-2.35	118.62	124.78
12	m	6	HYP	O-C-CA	-2.31	118.72	124.78
12	h	6	HYP	O-C-CA	-2.28	118.81	124.78
12	k	6	HYP	O-C-CA	-2.28	118.81	124.78
12	a	6	HYP	O-C-CA	-2.27	118.82	124.78

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	a	2	EEP	O2-CD1-CG-CB
12	a	2	EEP	O2-CD1-CG-O1
12	a	2	EEP	O2-CD1-CG-CD2
12	b	2	EEP	O2-CD1-CG-CB
12	b	2	EEP	O2-CD1-CG-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	ADP	N	401	14	24,29,29	0.92	1 (4%)	29,45,45	1.34	3 (10%)
13	ADP	H	401	14	24,29,29	0.98	1 (4%)	29,45,45	1.46	4 (13%)
13	ADP	B	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.40	4 (13%)
13	ADP	P	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
13	ADP	K	401	14	24,29,29	0.95	1 (4%)	29,45,45	1.52	3 (10%)
13	ADP	S	402	14	24,29,29	1.16	2 (8%)	29,45,45	1.63	7 (24%)
13	ADP	W	401	-	24,29,29	1.00	1 (4%)	29,45,45	1.40	4 (13%)
13	ADP	A	501	14	24,29,29	0.95	1 (4%)	29,45,45	1.40	3 (10%)
13	ADP	O	401	14	24,29,29	0.93	1 (4%)	29,45,45	1.35	3 (10%)
13	ADP	J	401	14	24,29,29	0.94	1 (4%)	29,45,45	1.49	4 (13%)
13	ADP	Q	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.52	4 (13%)
13	ADP	R	401	-	24,29,29	0.91	1 (4%)	29,45,45	1.36	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	N	401	14	-	5/12/32/32	0/3/3/3
13	ADP	H	401	14	-	5/12/32/32	0/3/3/3
13	ADP	B	501	-	-	3/12/32/32	0/3/3/3
13	ADP	P	401	-	-	2/12/32/32	0/3/3/3
13	ADP	K	401	14	-	2/12/32/32	0/3/3/3
13	ADP	S	402	14	-	0/12/32/32	0/3/3/3
13	ADP	W	401	-	-	2/12/32/32	0/3/3/3
13	ADP	A	501	14	-	1/12/32/32	0/3/3/3
13	ADP	O	401	14	-	6/12/32/32	0/3/3/3
13	ADP	J	401	14	-	3/12/32/32	0/3/3/3
13	ADP	Q	401	-	-	4/12/32/32	0/3/3/3
13	ADP	R	401	-	-	6/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	401	ADP	C5-C4	2.35	1.47	1.40
13	Q	401	ADP	C5-C4	2.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	401	ADP	C5-C4	2.31	1.47	1.40
13	S	402	ADP	PB-O3B	-2.29	1.46	1.54
13	J	401	ADP	C5-C4	2.29	1.47	1.40

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	402	ADP	C4-C5-N7	4.79	114.39	109.40
13	K	401	ADP	PA-O3A-PB	-4.53	117.28	132.83
13	P	401	ADP	PA-O3A-PB	-4.52	117.32	132.83
13	Q	401	ADP	PA-O3A-PB	-4.12	118.70	132.83
13	A	501	ADP	PA-O3A-PB	-4.05	118.94	132.83

There are no chirality outliers.

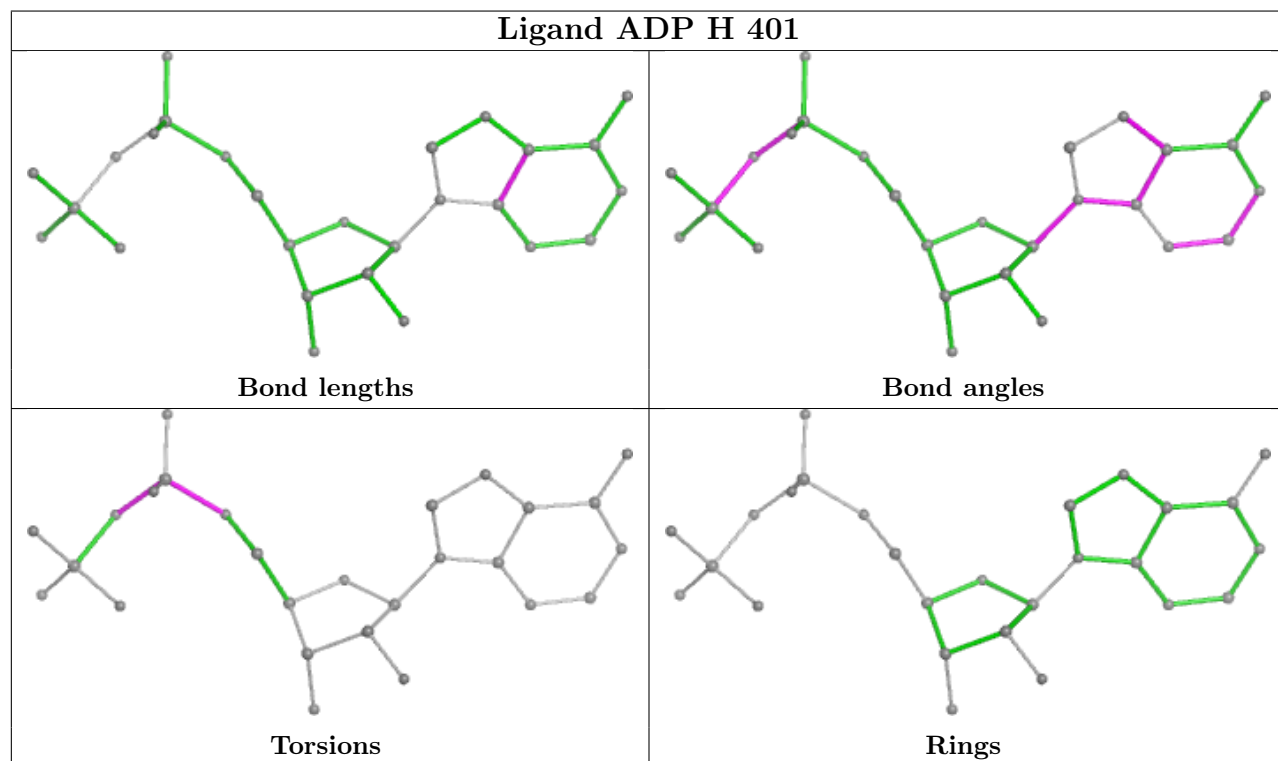
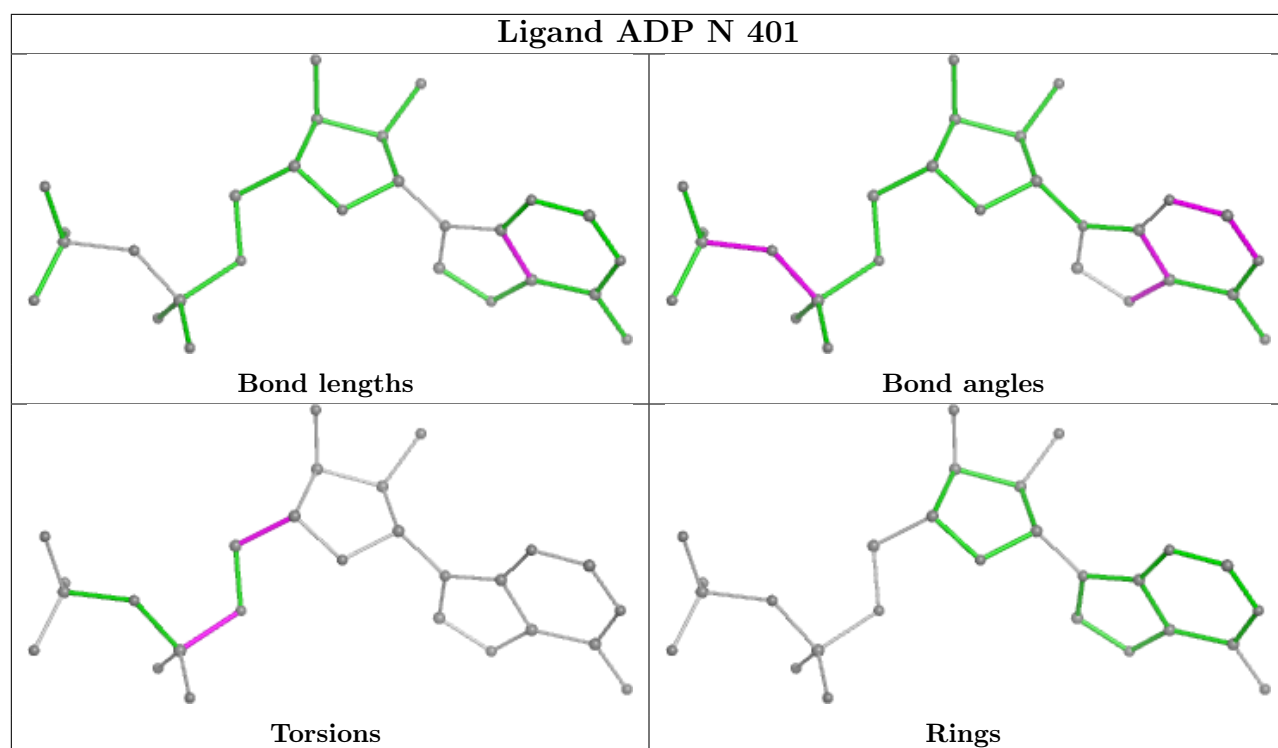
5 of 39 torsion outliers are listed below:

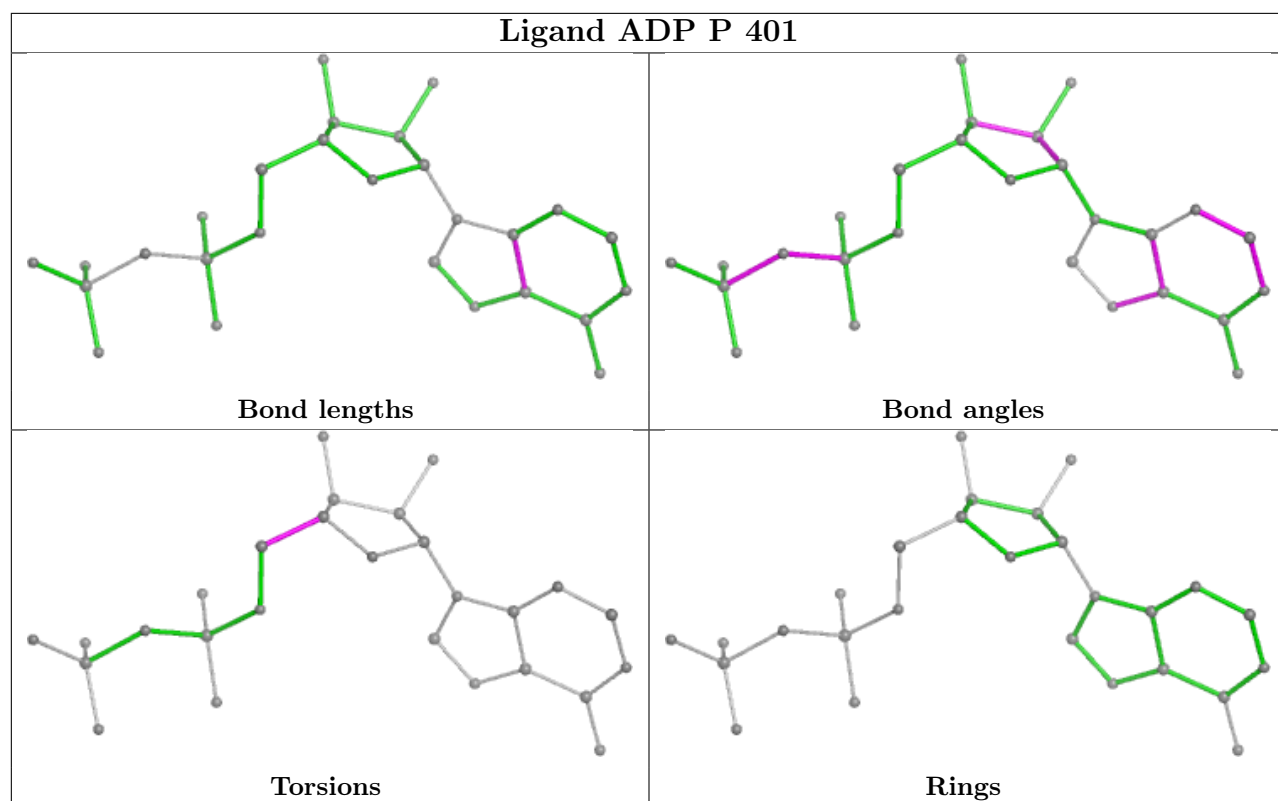
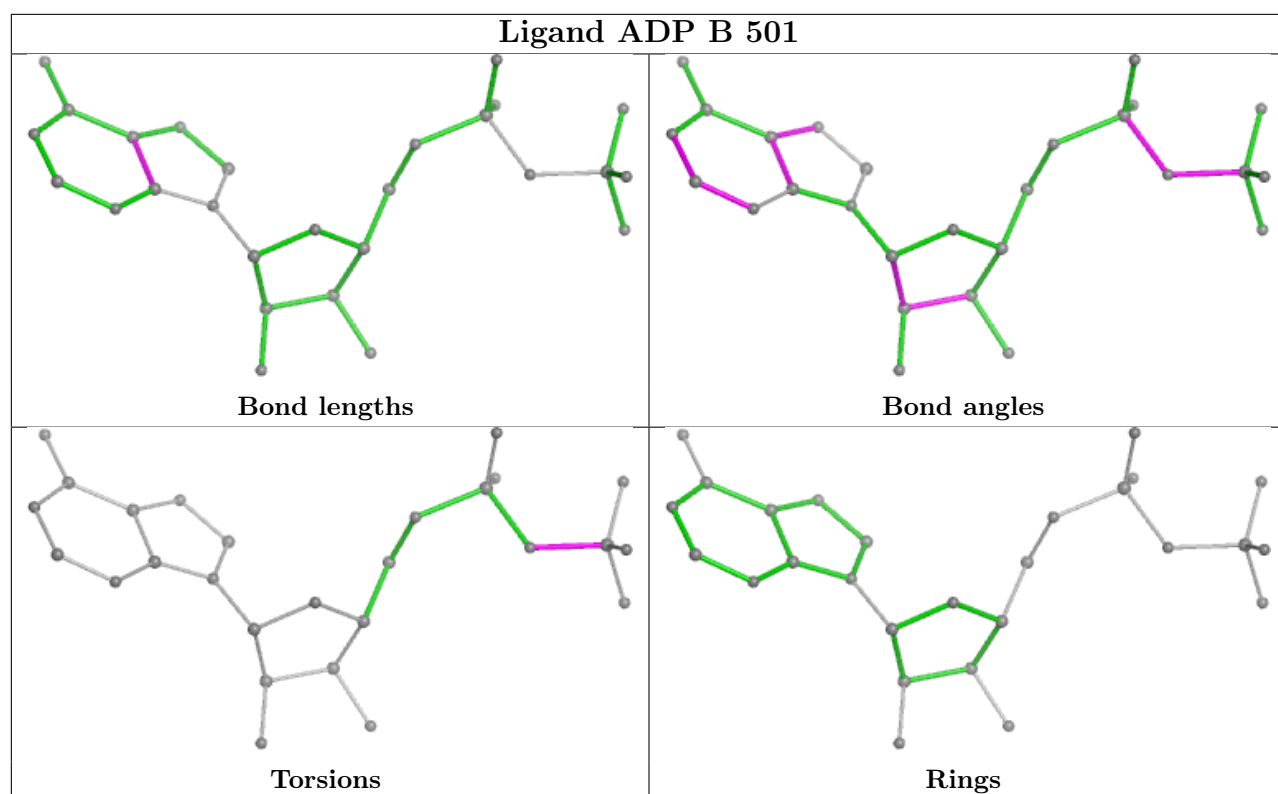
Mol	Chain	Res	Type	Atoms
13	B	501	ADP	PA-O3A-PB-O2B
13	H	401	ADP	C5'-O5'-PA-O1A
13	H	401	ADP	C5'-O5'-PA-O2A
13	J	401	ADP	C5'-O5'-PA-O2A
13	K	401	ADP	O4'-C4'-C5'-O5'

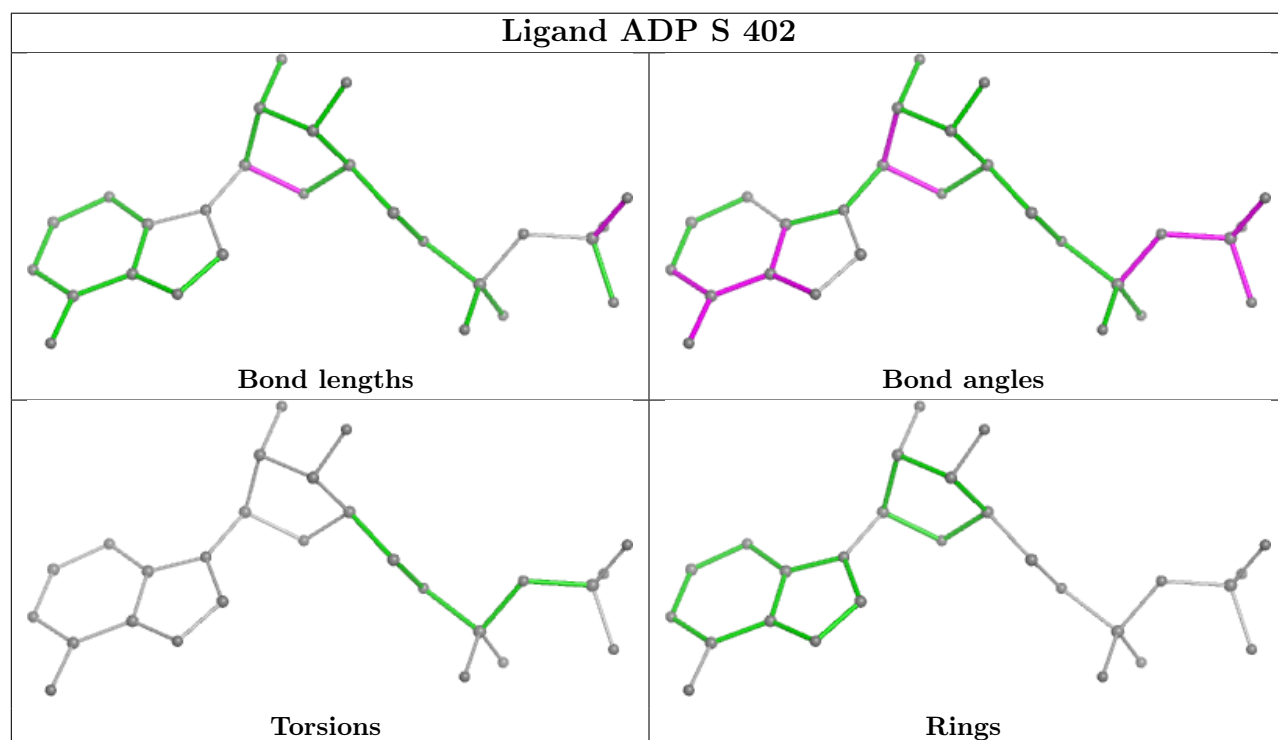
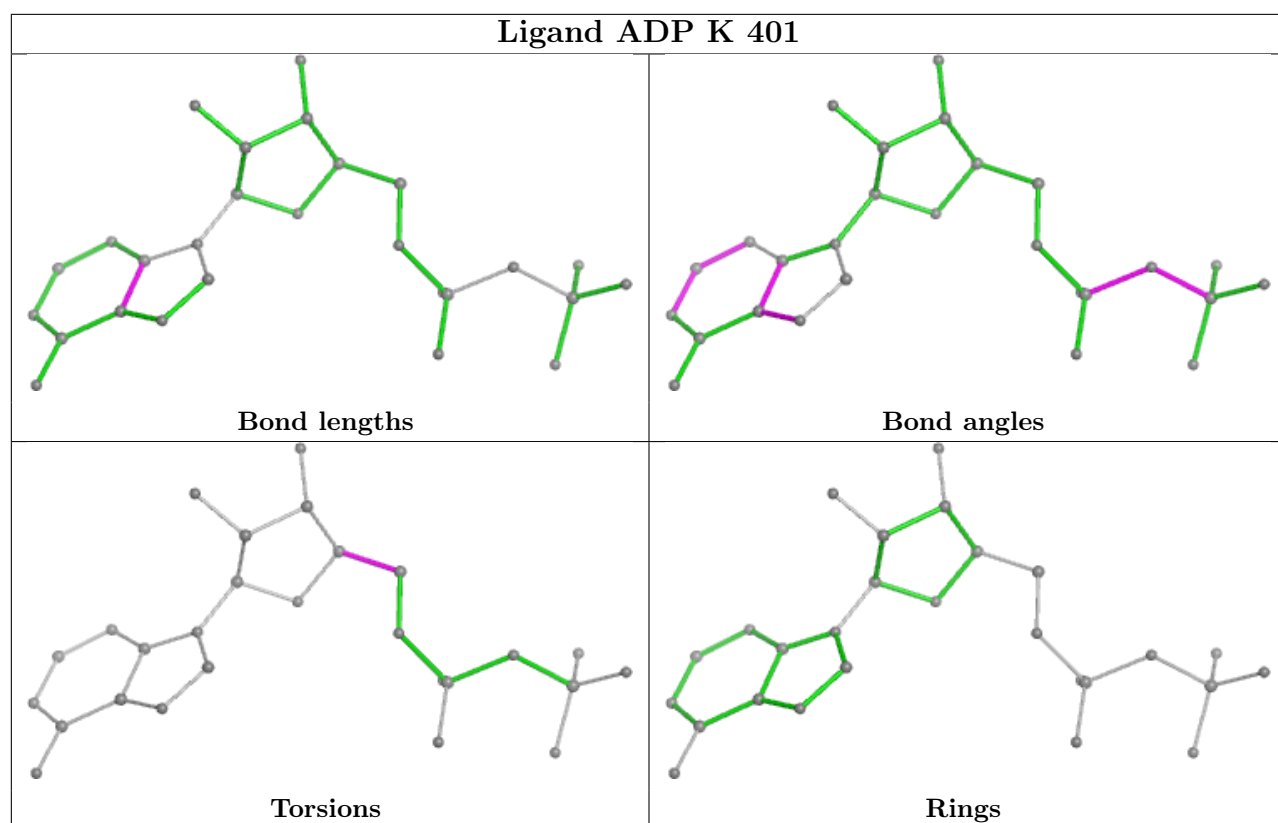
There are no ring outliers.

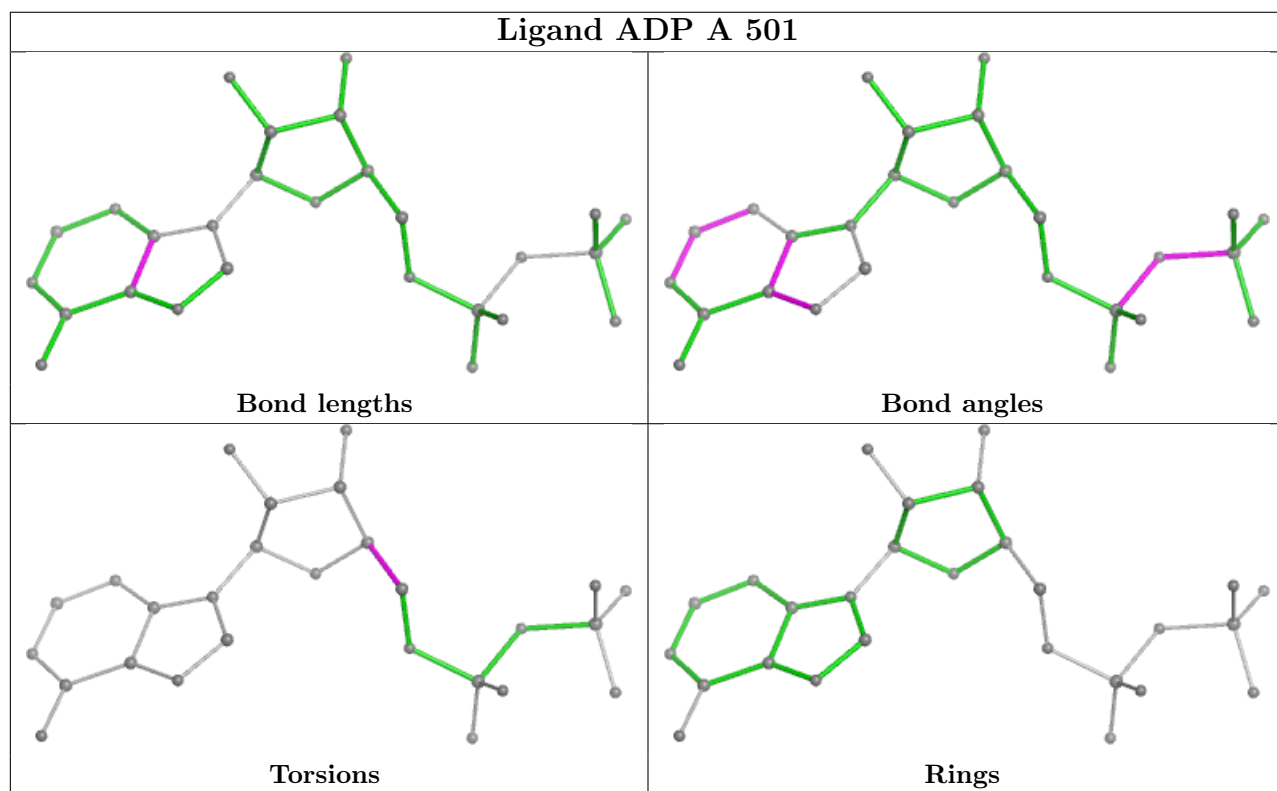
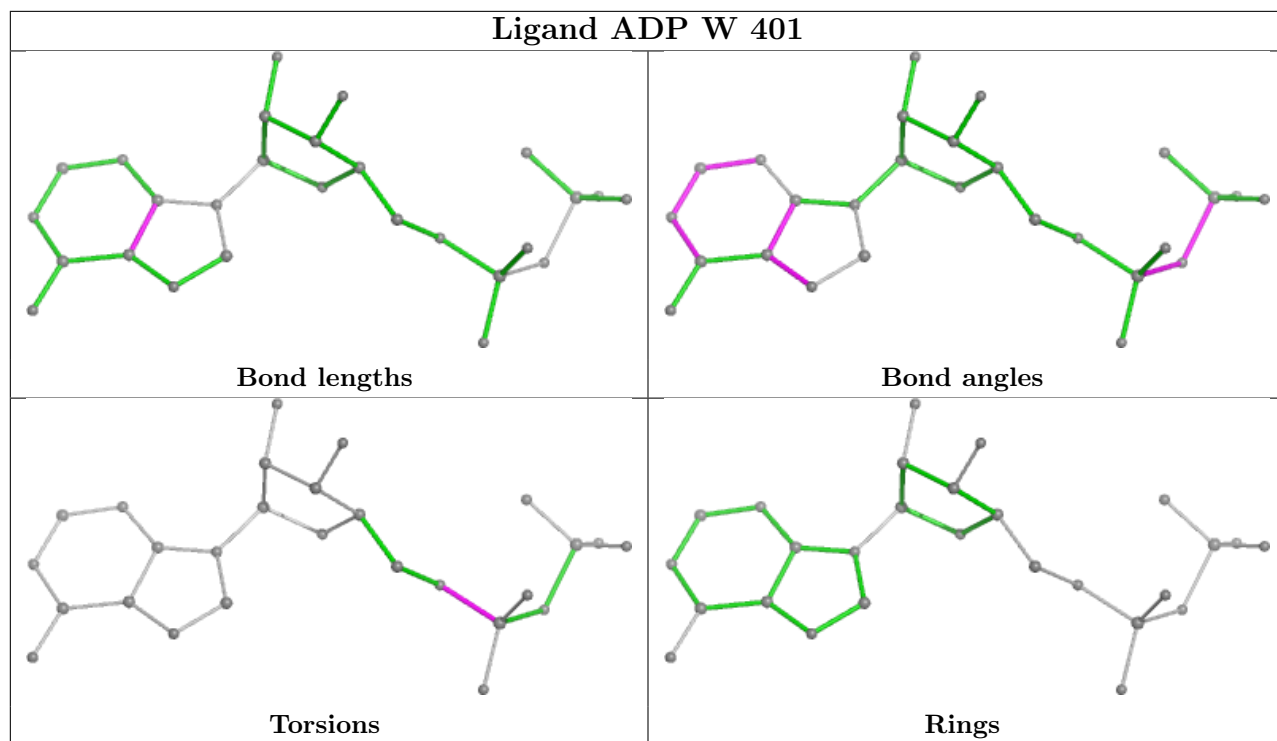
No monomer is involved in short contacts.

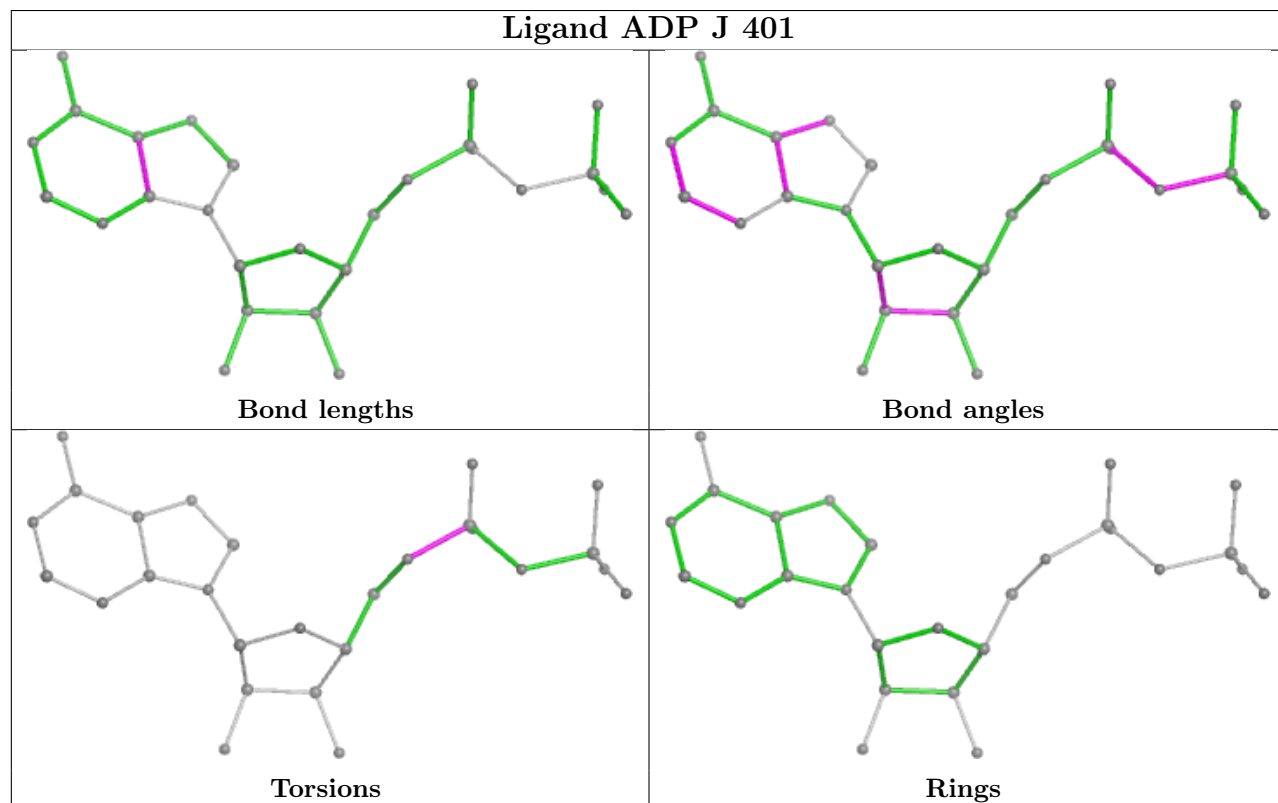
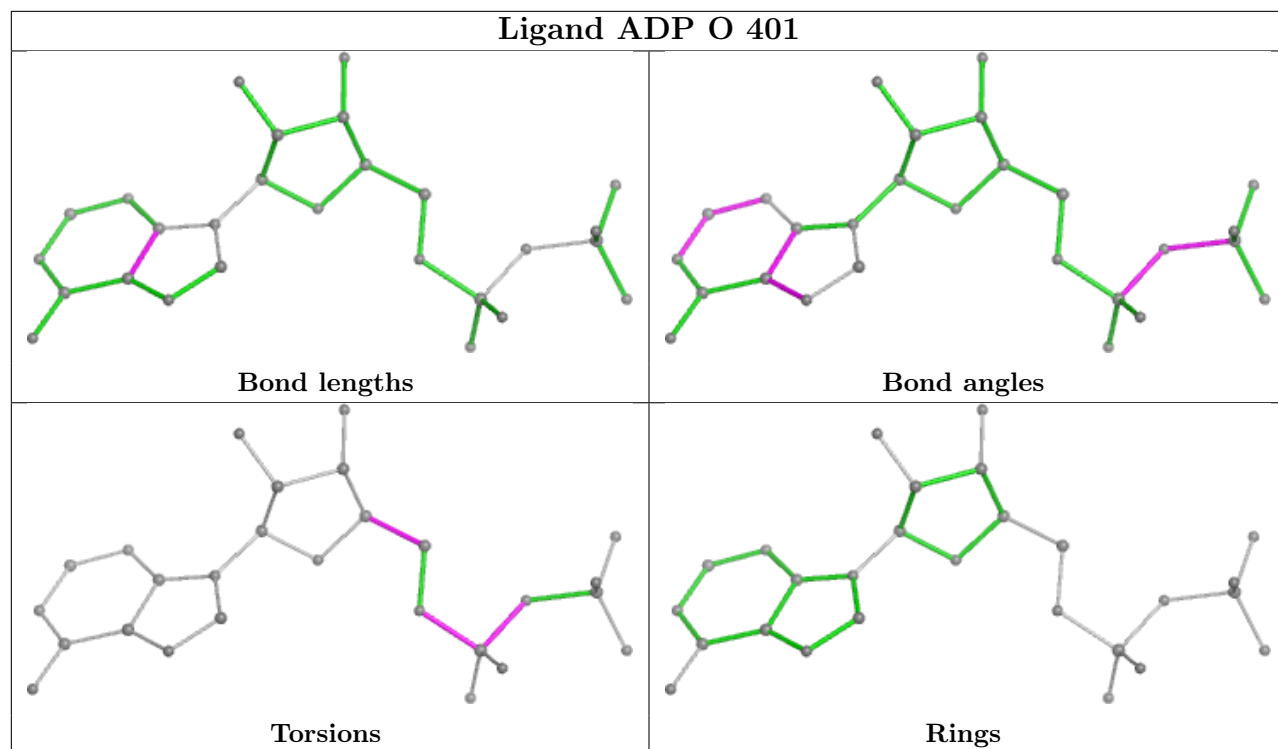
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

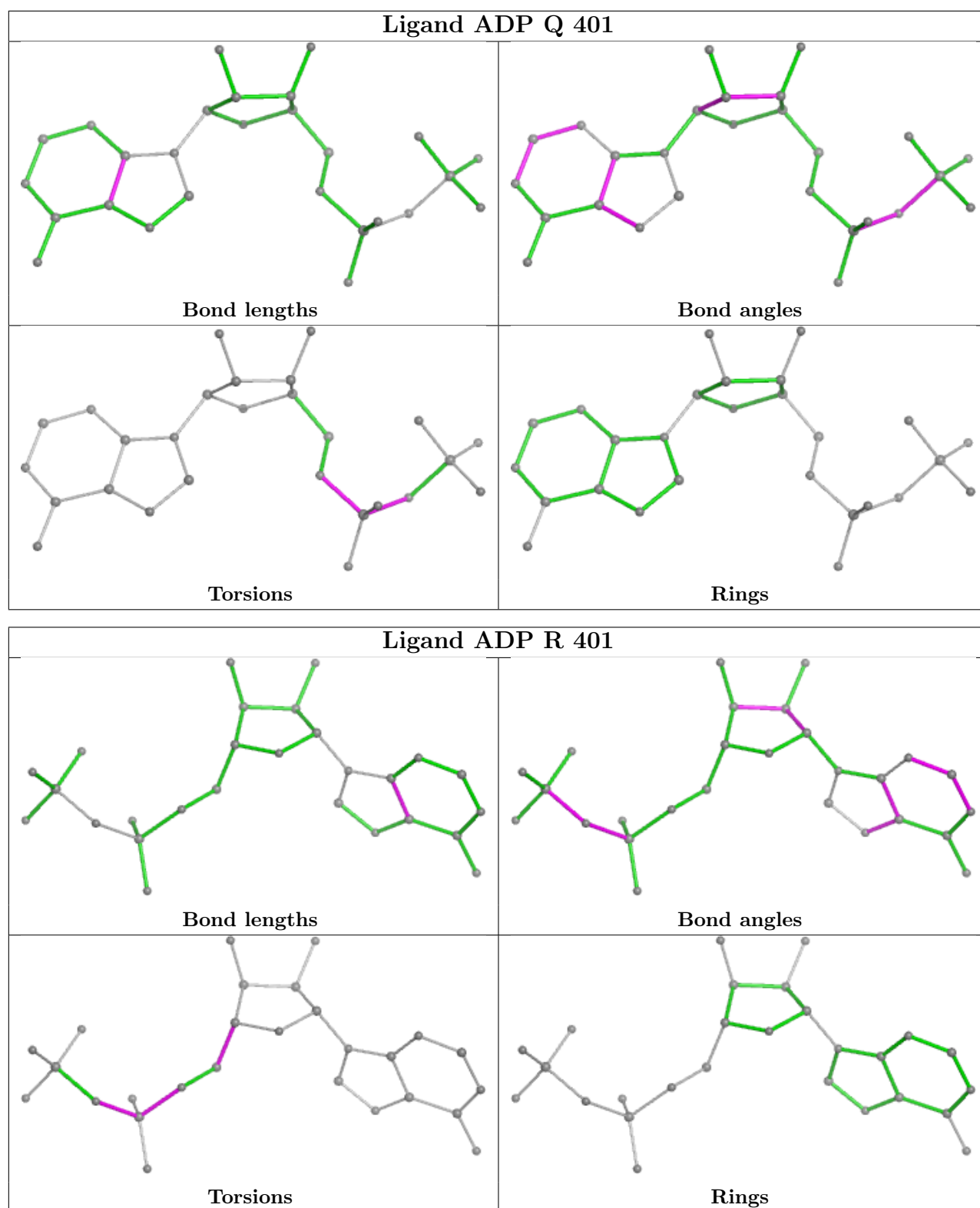












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

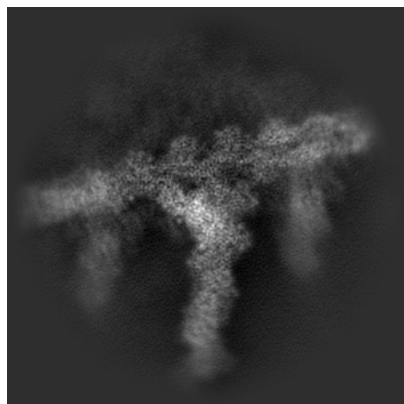
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17558. These allow visual inspection of the internal detail of the map and identification of artifacts.

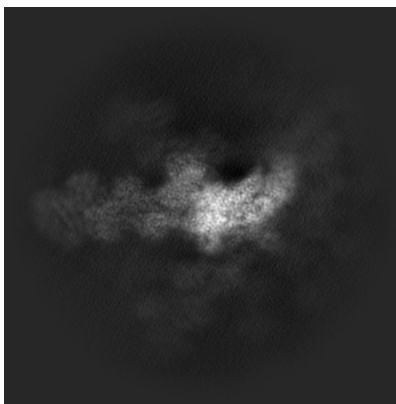
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

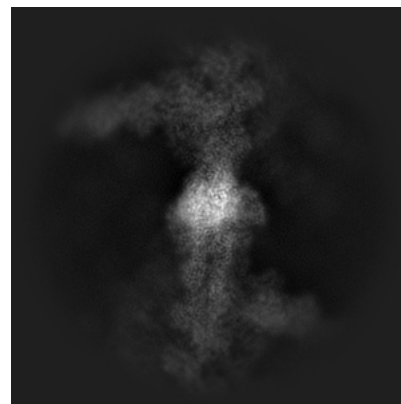
6.1.1 Primary map



X

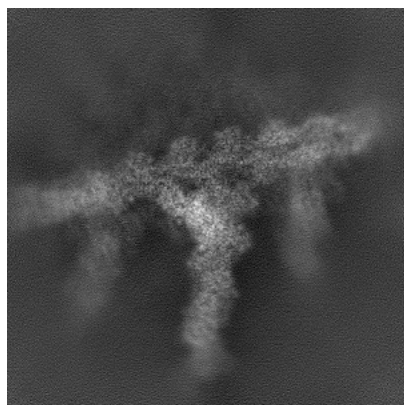


Y

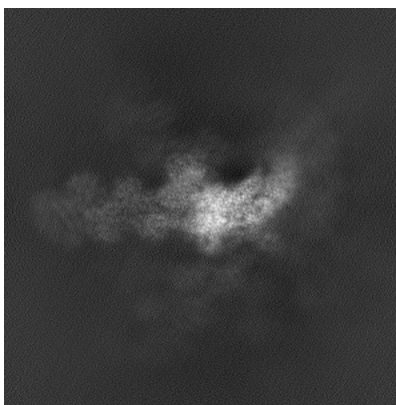


Z

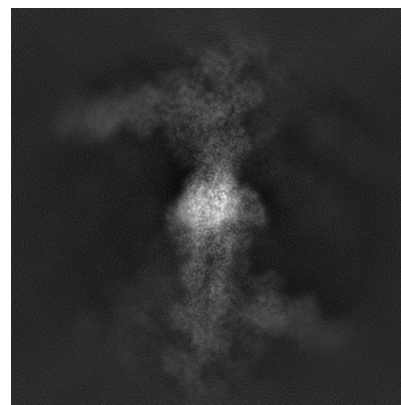
6.1.2 Raw map



X



Y

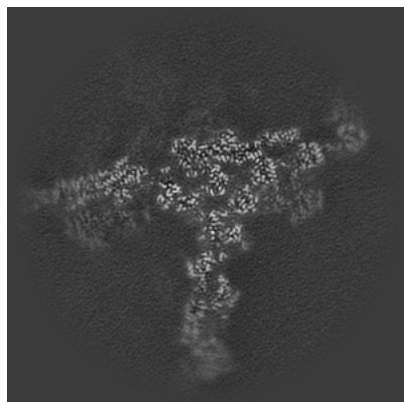


Z

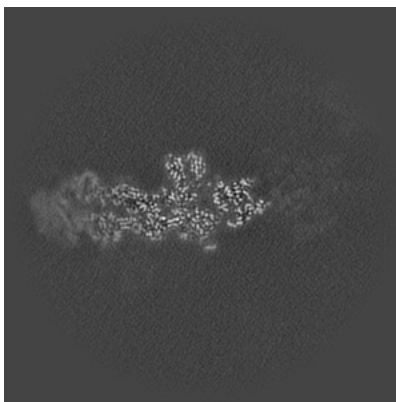
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

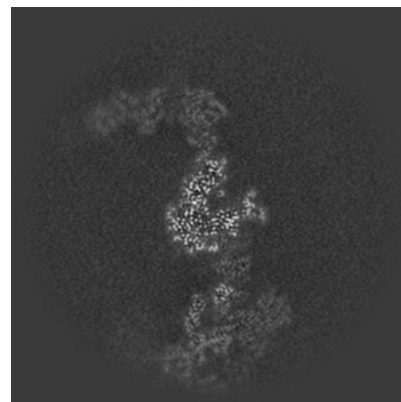
6.2.1 Primary map



X Index: 220

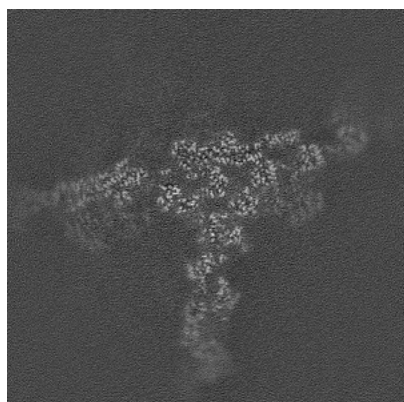


Y Index: 220

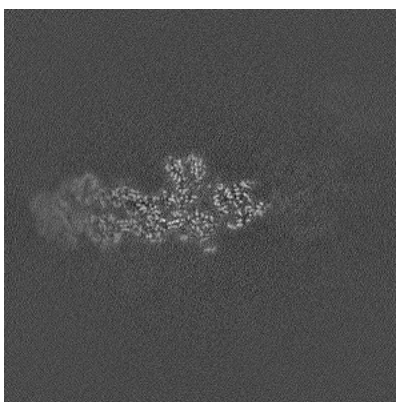


Z Index: 220

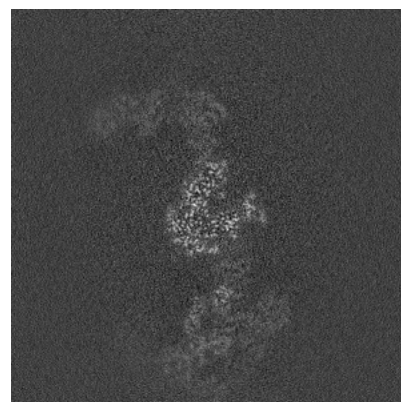
6.2.2 Raw map



X Index: 220



Y Index: 220

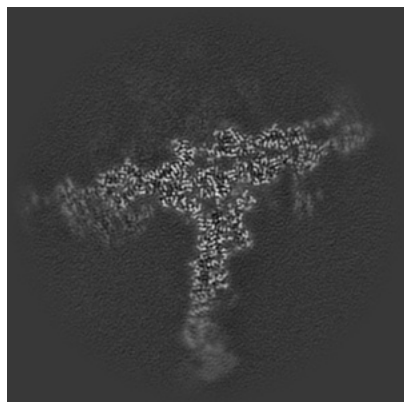


Z Index: 220

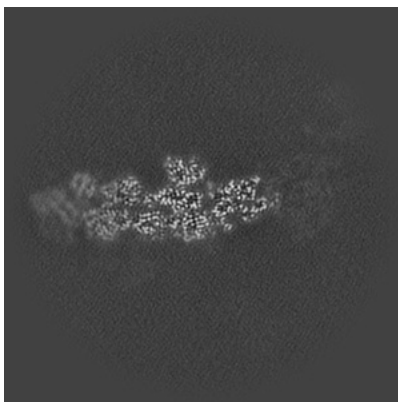
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

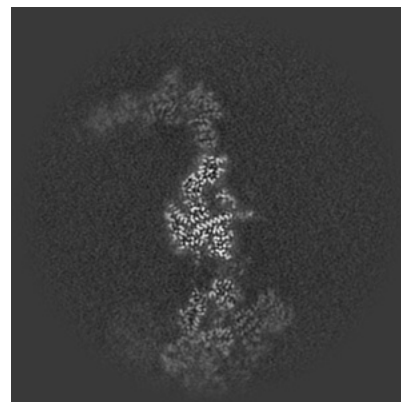
6.3.1 Primary map



X Index: 227



Y Index: 227

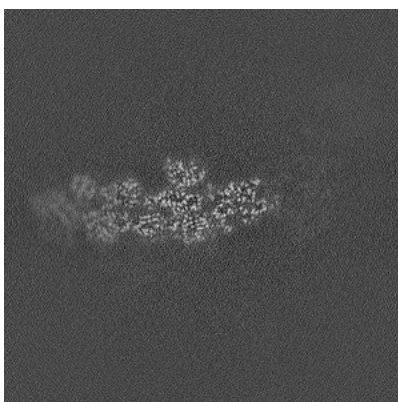


Z Index: 226

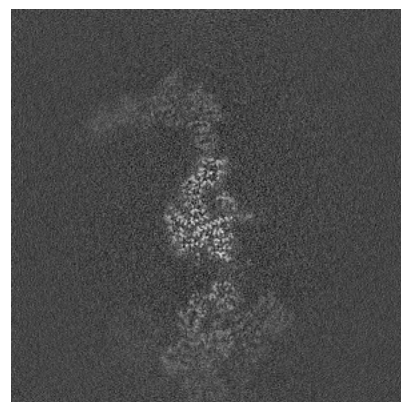
6.3.2 Raw map



X Index: 227



Y Index: 227

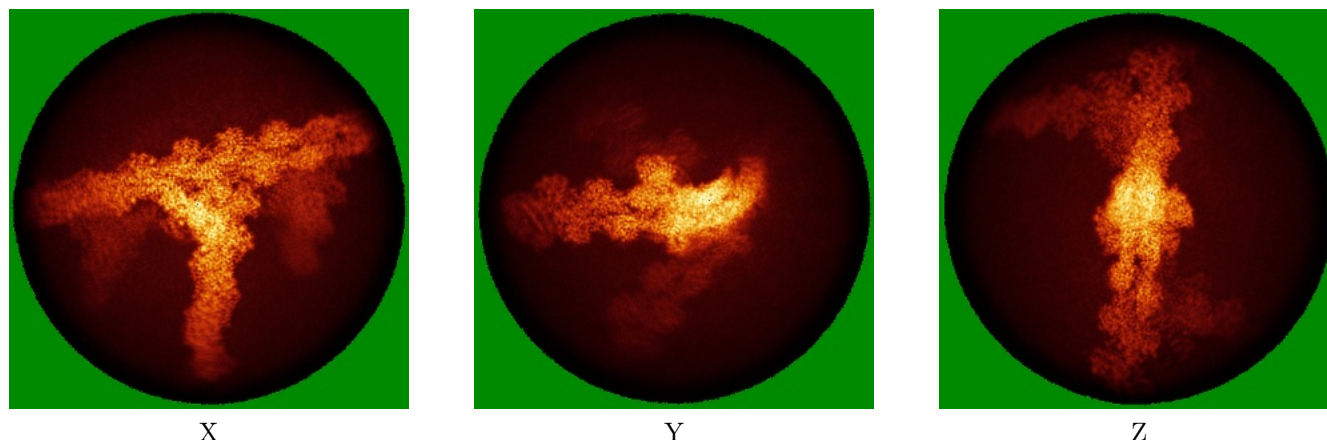


Z Index: 226

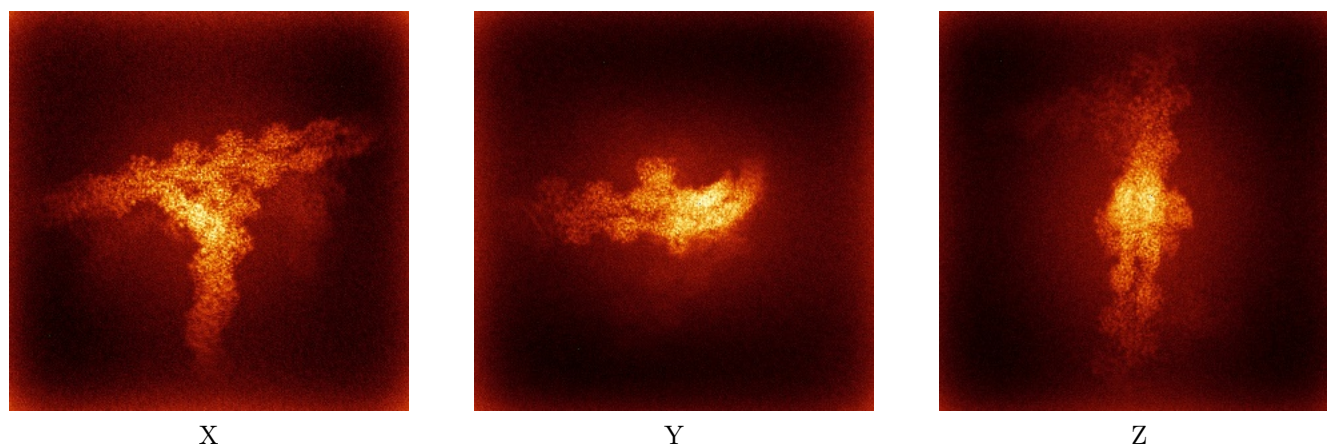
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



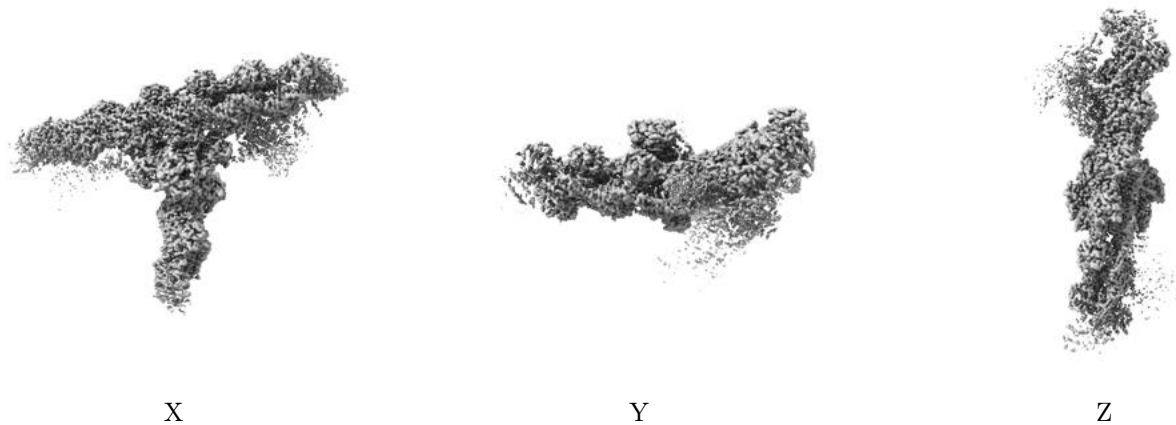
6.4.2 Raw map



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](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

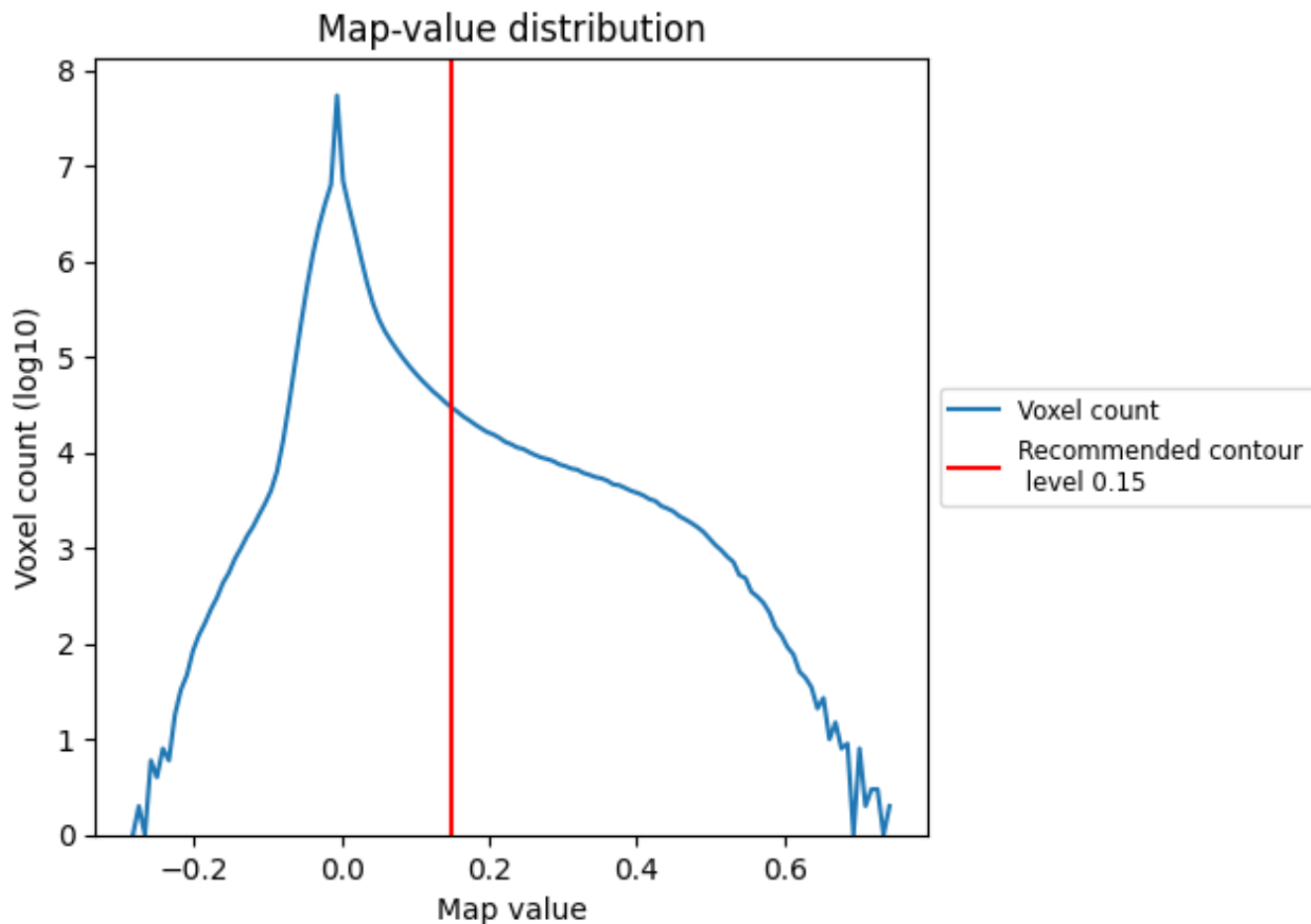
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

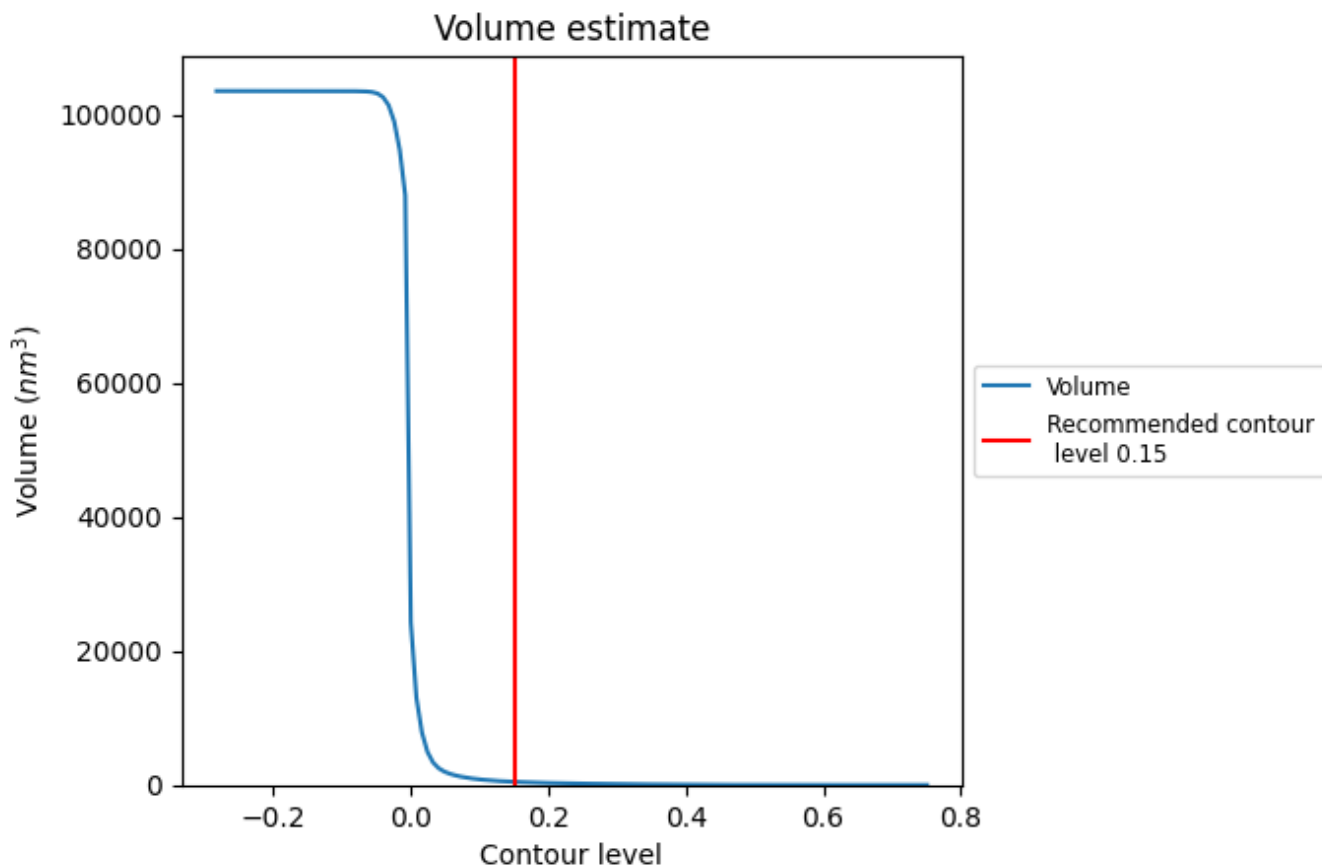
This section contains the results of statistical analysis of the map.

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.

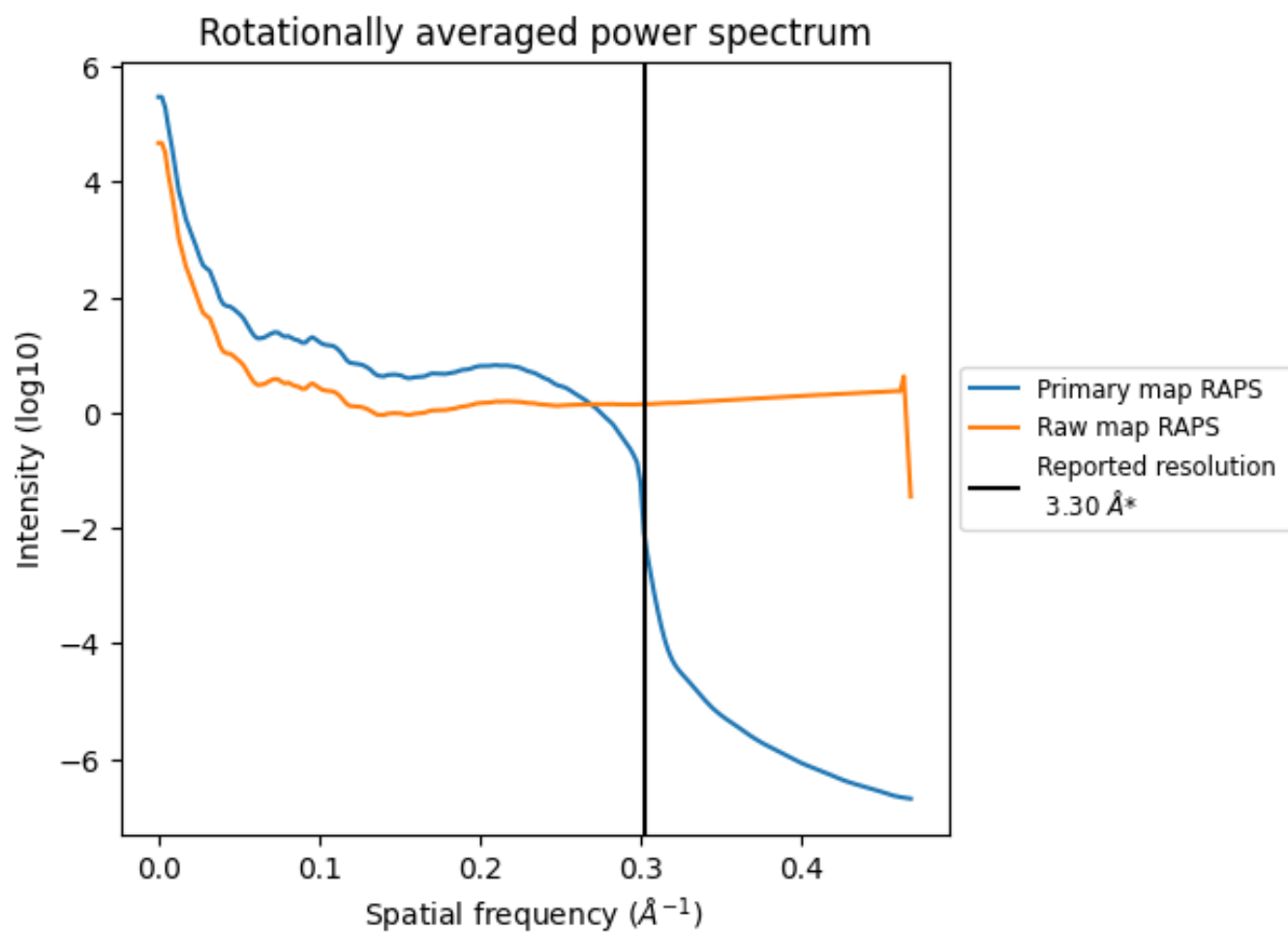
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 468 nm^3 ; this corresponds to an approximate mass of 423 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

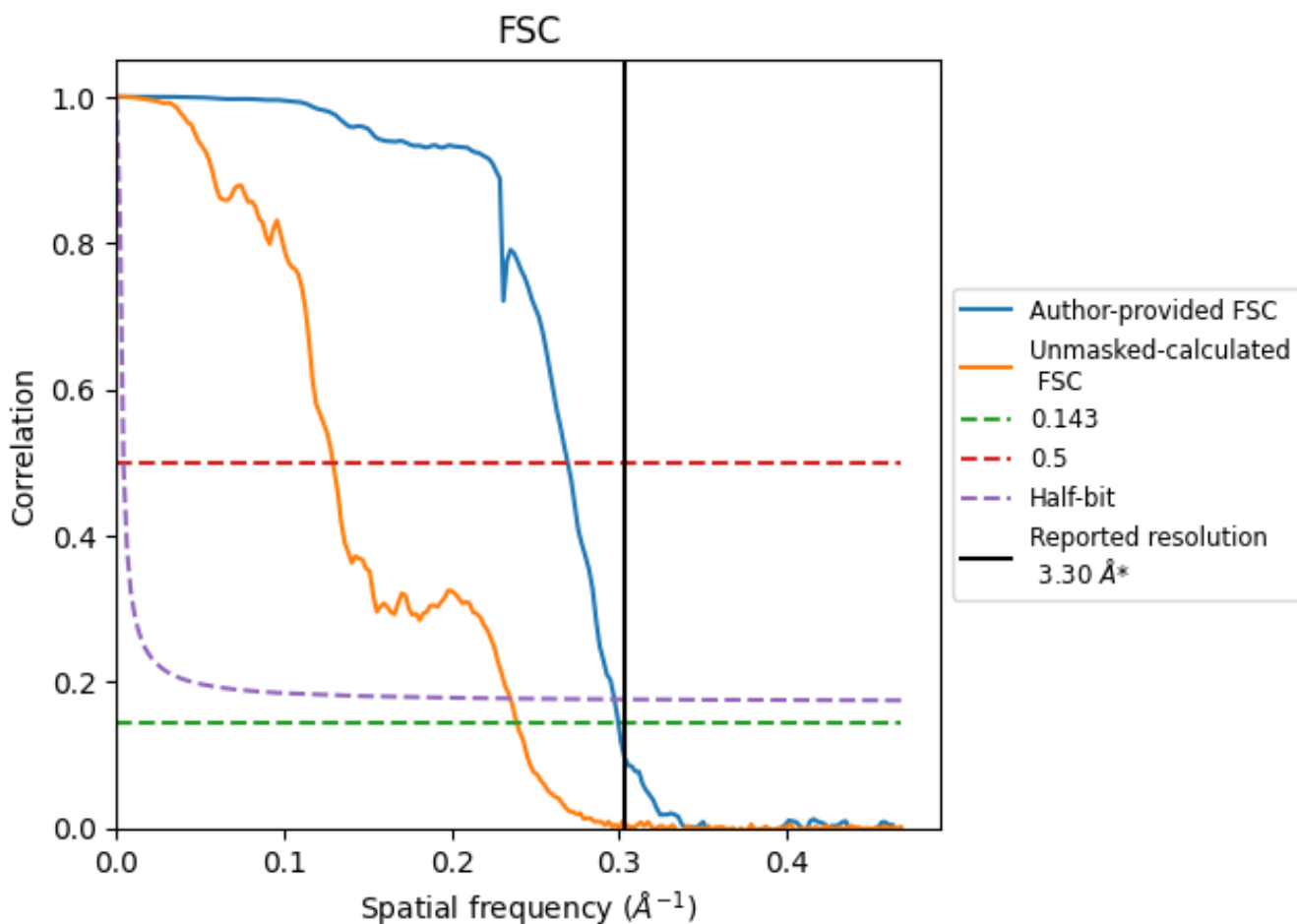


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates

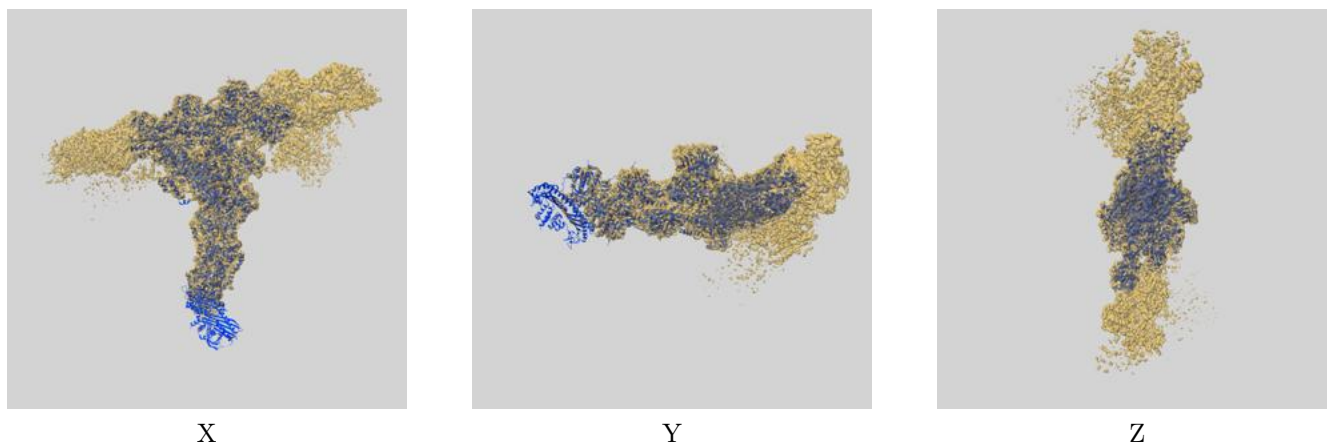
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.71	3.36
Unmasked-calculated*	4.18	7.73	4.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

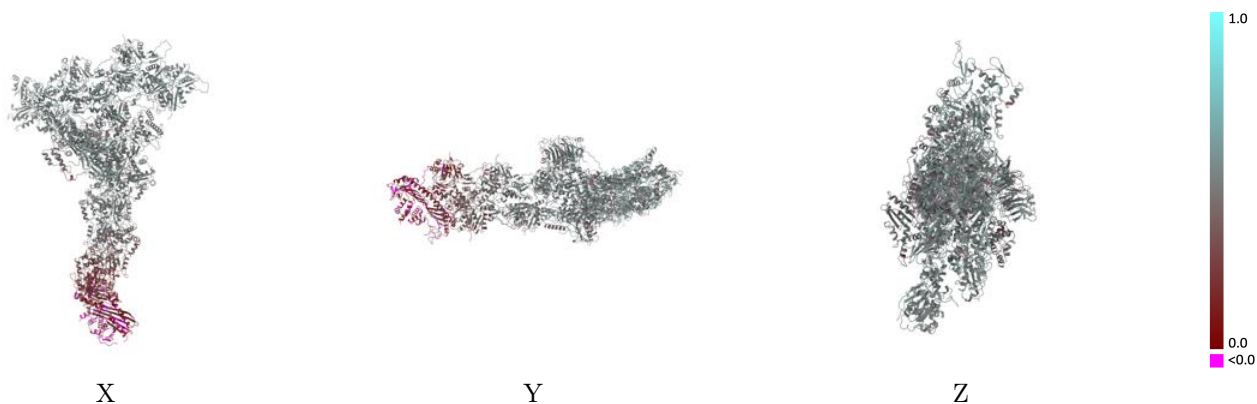
This section contains information regarding the fit between EMDB map EMD-17558 and PDB model 8P94. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



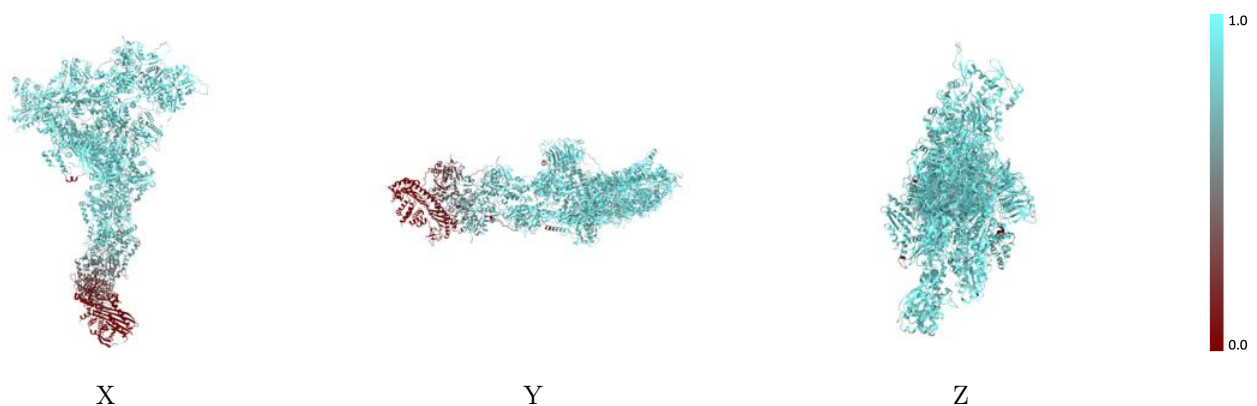
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



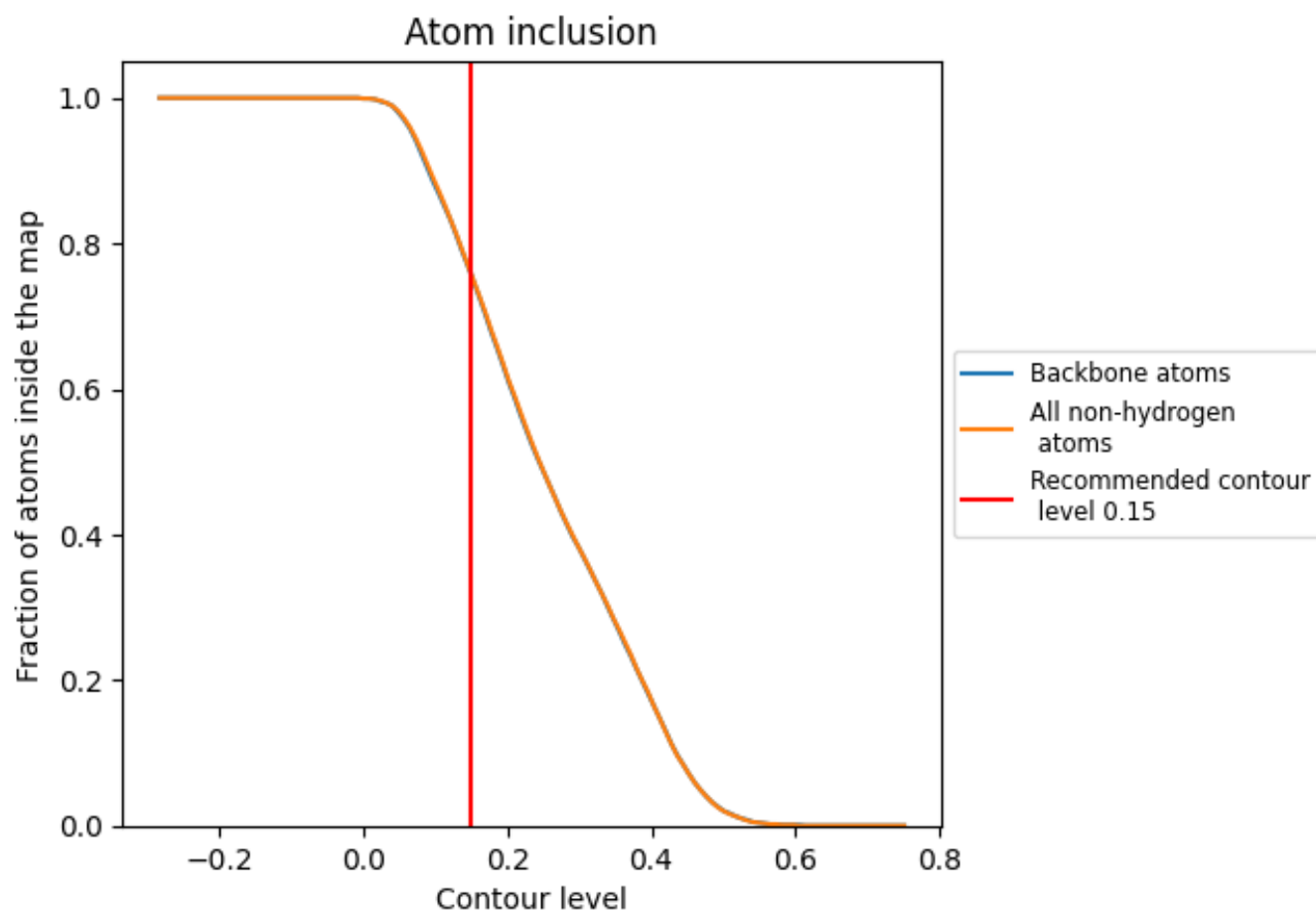
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.4520
A	 0.9240	 0.5150
B	 0.8890	 0.5050
C	 0.8950	 0.5000
D	 0.8670	 0.4850
E	 0.8770	 0.4910
F	 0.9140	 0.5170
G	 0.7900	 0.4570
H	 0.6860	 0.3920
I	 0.4990	 0.4160
J	 0.8810	 0.4970
K	 0.8290	 0.4730
N	 0.8660	 0.5160
O	 0.8590	 0.5170
P	 0.9090	 0.5270
Q	 0.8830	 0.5160
R	 0.9070	 0.5270
S	 0.8710	 0.5140
U	 0.0250	 0.1100
V	 0.0340	 0.1360
W	 0.4070	 0.2710
a	 0.8700	 0.4320
b	 0.9440	 0.5210
c	 0.9070	 0.5020
d	 0.6300	 0.3600
h	 0.9070	 0.5310
i	 0.9260	 0.5320
j	 0.9440	 0.5160
k	 0.9440	 0.5140
l	 0.8890	 0.5370
m	 0.8520	 0.5070

