wwPDB EM Validation Summary Report (i)

Apr 29, 2024 – 11:26 am BST

PDB ID	:	5AFU
EMDB ID	:	EMD-2860
Title	:	Cryo-EM structure of dynein tail-dynactin-BICD2N complex
Authors	:	Urnavicius, L.; Zhang, K.; Diamant, A.G.; Motz, C.; Schlager, M.A.; Yu, M.; Patel, N.A.; Robinson, C.V.; Carter, A.P.
Deposited on	:	2015-01-26
Resolution	:	8.20 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 (i) 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 (i)) were used in the production of this report:

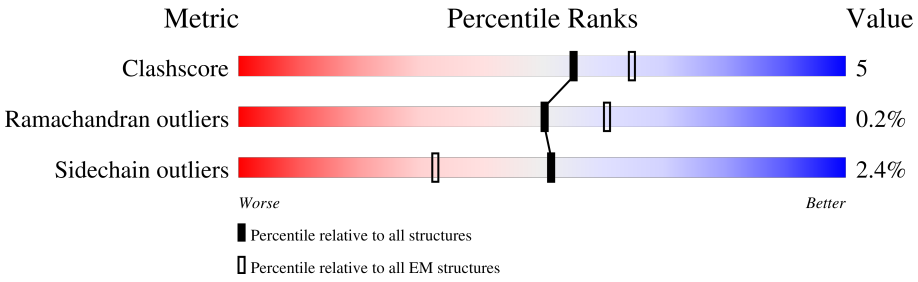
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.20 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)
Clashscore	158937	4297
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 <=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	1	361	8% 79% 21%
2	2	359	11% 80% 20%
3	3	350	11% 96%
3	4	350	11% 96%
4	5	275	17% 81% 19%
4	6	275	17% 80% 20%
5	A	370	96%
5	B	370	99%

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Mol	Chain	Length	Quality of chain
5	C	370	96%
5	D	370	97%
5	E	370	98%
5	F	370	98%
5	G	370	95% 5%
5	I	370	97%
6	H	370	99%
7	J	379	94%
8	K	275	78% 21%
9	L	270	82% 17%
10	M	587	99%
11	N	616	98%
12	O	65	91% 9%
12	P	65	5% 86% 14%
13	Q	87	80% 100%
13	R	87	100%
14	U	168	8% 96%
15	V	165	97%
16	Y	243	99%
17	Z	52	6% 98%
18	a	48	85% 12%
19	b	71	83% 17%
20	c	31	6% 94% 6%
21	d	20	15% 90% 5% 5%
22	z	53	23% 100%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 55952 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 DYNEIN TAIL.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	361	Total	C	N	O	0	0
			1810	1088	361	361		

- Molecule 2 is a protein called DYNEIN TAIL.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	359	Total	C	N	O	0	0
			1800	1082	359	359		

- Molecule 3 is a protein called DYNEIN TAIL.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	350	Total	C	N	O	0	0
			1723	1023	350	350		
3	4	350	Total	C	N	O	0	0
			1723	1023	350	350		

- Molecule 4 is a protein called DYNEIN TAIL.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	275	Total	C	N	O	0	0
			1375	825	275	275		
4	6	275	Total	C	N	O	0	0
			1375	825	275	275		

- Molecule 5 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
5	B	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
5	D	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
5	E	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
5	F	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
5	G	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
5	I	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		

- Molecule 6 is a protein called ACTIN, CYTOPLASMIC 1.

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

- Molecule 7 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	369	Total	C	N	O	S	0	0
			2879	1857	486	520	16		

- Molecule 8 is a protein called CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	275	Total	C	N	O	S	0	0
			2242	1415	393	429	5		

- Molecule 9 is a protein called F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	270	Total	C	N	O	S	0	0
			2137	1333	373	420	11		

- Molecule 10 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	587	Total 2935	C 1761	N 587	O 587	0	0

- Molecule 11 is a protein called DYNACTIN 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	N	616	Total 3080	C 1848	N 616	O 616	0	0

- Molecule 12 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	65	Total 323	C 193	N 65	O 65	0	0
12	P	65	Total 323	C 193	N 65	O 65	0	0

- Molecule 13 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Q	87	Total 435	C 261	N 87	O 87	0	0
13	R	87	Total 435	C 261	N 87	O 87	0	0

- Molecule 14 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	168	Total 826	C 490	N 168	O 168	0	0

- Molecule 15 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	165	Total 812	C 482	N 165	O 165	0	0

- Molecule 16 is a protein called F-ACTIN-CAPPING PROTEIN SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	243	Total 1215	C 729	N 243	O 243	0	0

- Molecule 17 is a protein called F-ACTIN-CAPPING PROTEIN SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Z	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 18 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	48	Total	C	N	O	S	0	0
			341	216	58	66	1		

- Molecule 19 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	71	Total	C	N	O	S	0	0
			517	324	93	99	1		

- Molecule 20 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	31	Total	C	N	O	S	0	0
			179	112	34	32	1		

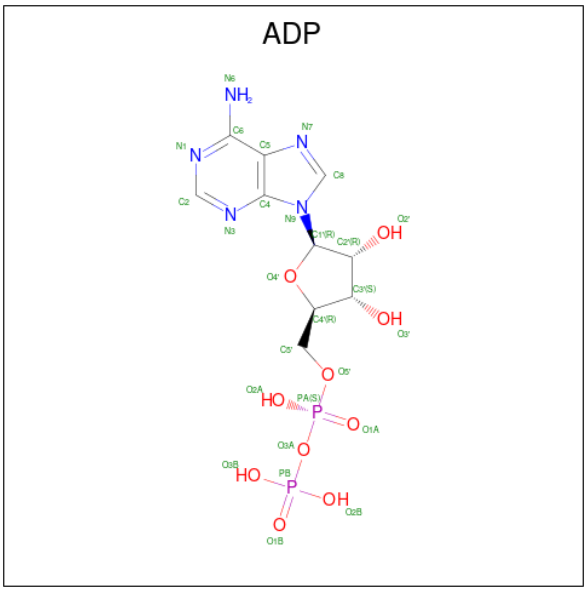
- Molecule 21 is a protein called DYNACTIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	20	Total	C	N	O	S	0	0
			127	80	23	23	1		

- Molecule 22 is a protein called F-ACTIN-CAPPING PROTEIN SUBUNIT BETA.

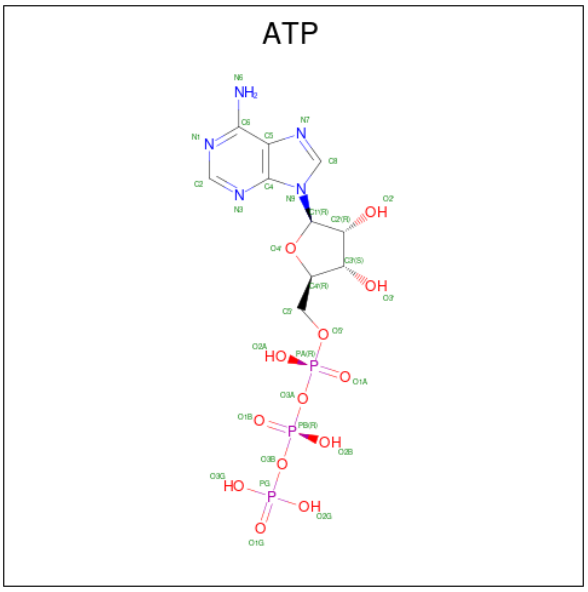
Mol	Chain	Residues	Atoms				AltConf	Trace
22	z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 24 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



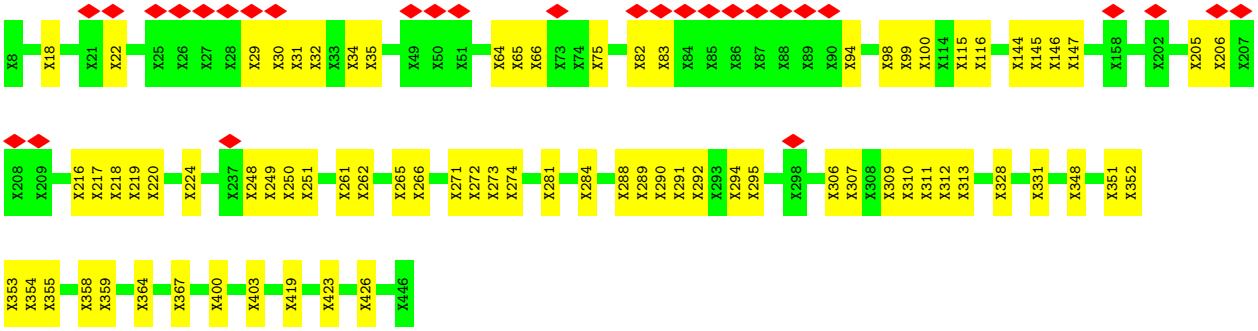
Mol	Chain	Residues	Atoms					AltConf
24	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

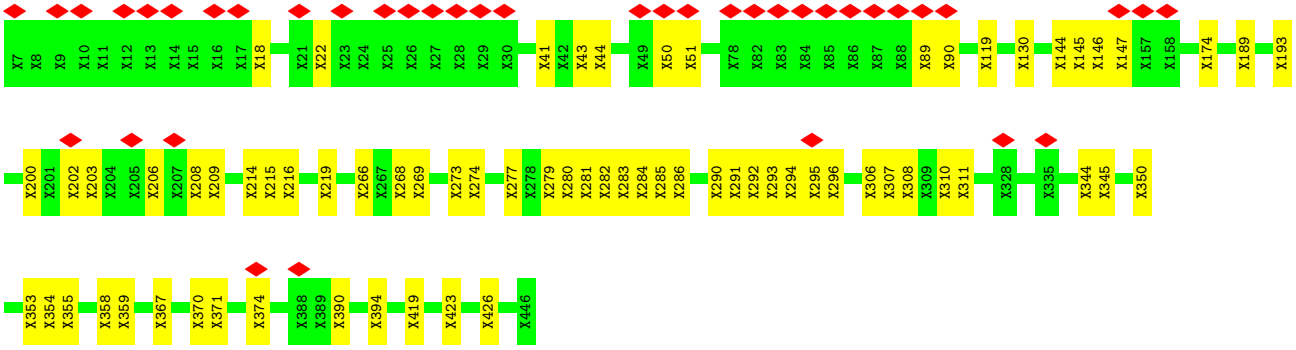
• Molecule 1: DYNEIN TAIL

Chain 1:



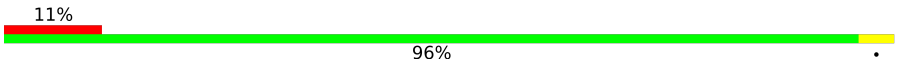
• Molecule 2: DYNEIN TAIL

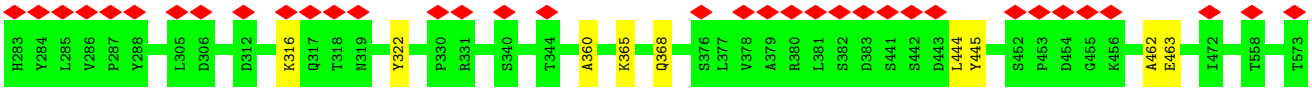
Chain 2:

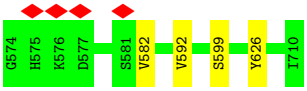


• Molecule 3: DYNEIN TAIL

Chain 3:

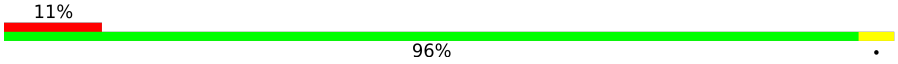


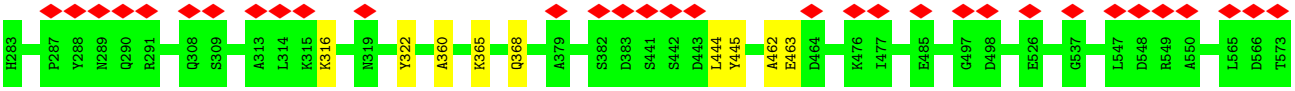


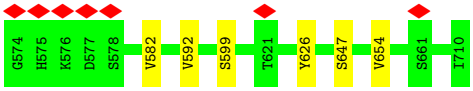


• Molecule 3: DYNEIN TAIL

Chain 4:

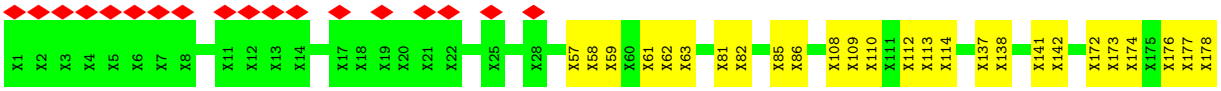


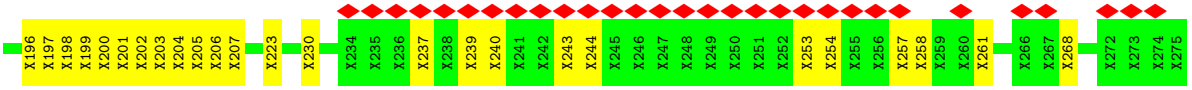




• Molecule 4: DYNEIN TAIL

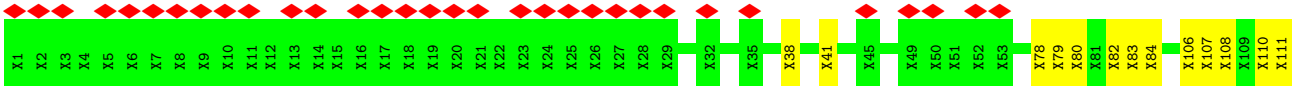
Chain 5:

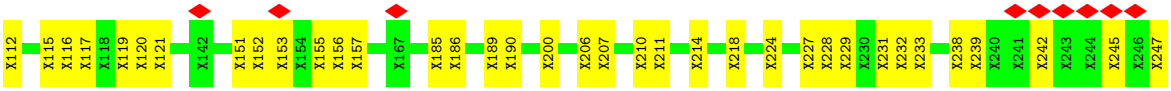


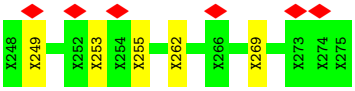


• Molecule 4: DYNEIN TAIL

Chain 6:

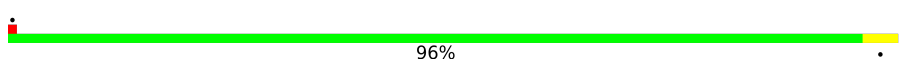


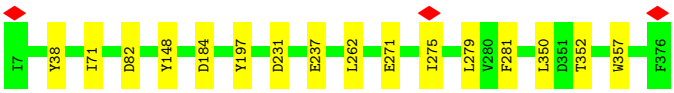




• Molecule 5: DYNACTIN

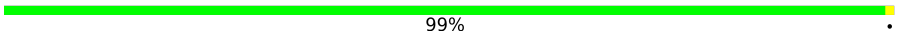
Chain A:





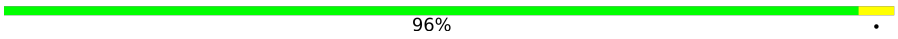
• Molecule 5: DYNACTIN

Chain B:



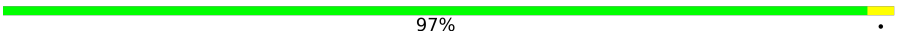
• Molecule 5: DYNACTIN

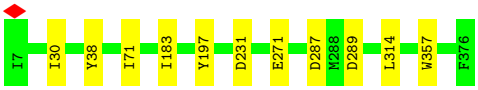
Chain C:



• Molecule 5: DYNACTIN

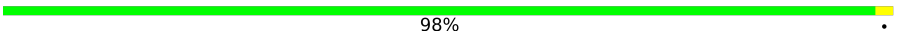
Chain D:





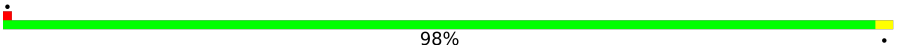
• Molecule 5: DYNACTIN

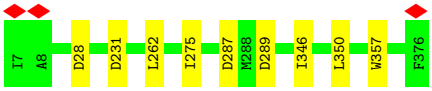
Chain E:



• Molecule 5: DYNACTIN

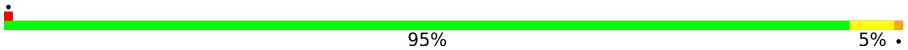
Chain F:

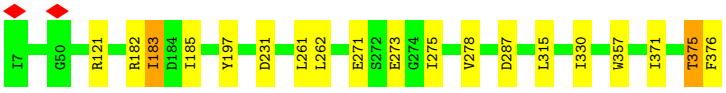




• Molecule 5: DYNACTIN

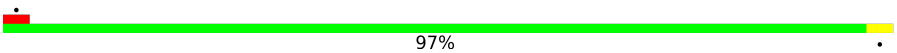
Chain G:

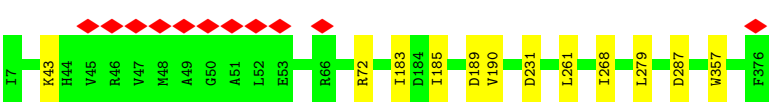




• Molecule 5: DYNACTIN

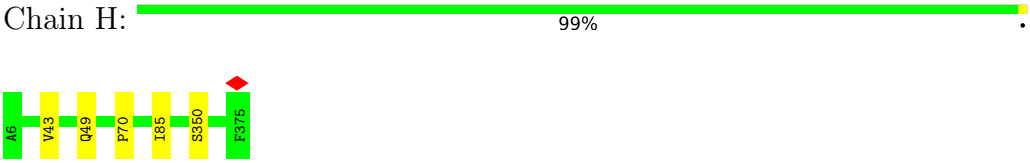
Chain I:





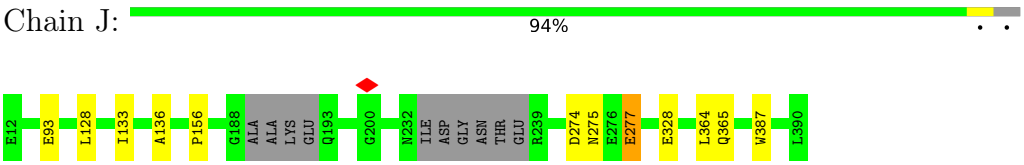
• Molecule 6: ACTIN, CYTOPLASMIC 1

Chain H:



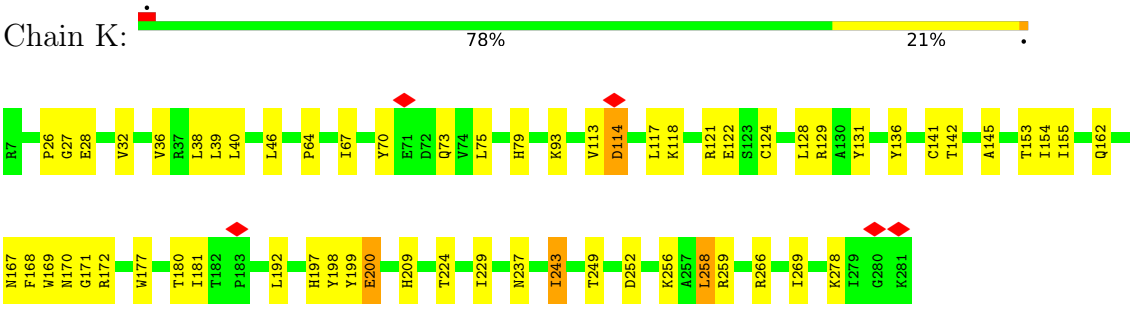
• Molecule 7: DYNACTIN

Chain J:



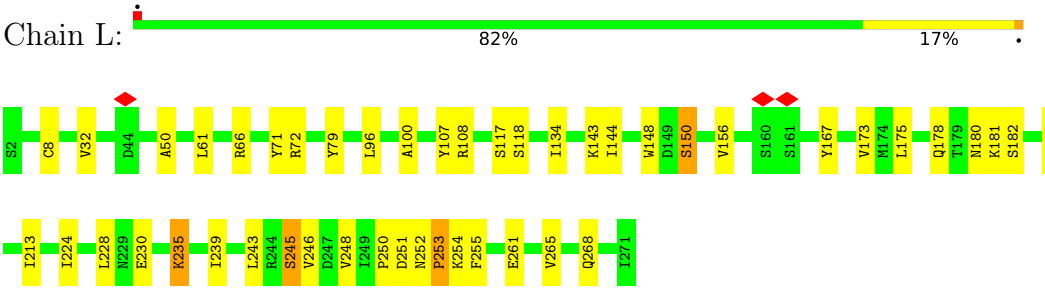
• Molecule 8: CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1

Chain K:



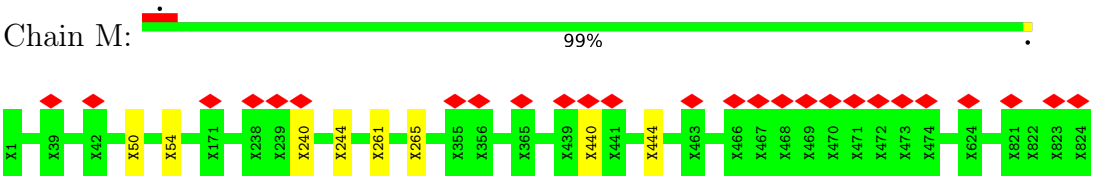
• Molecule 9: F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II

Chain L:



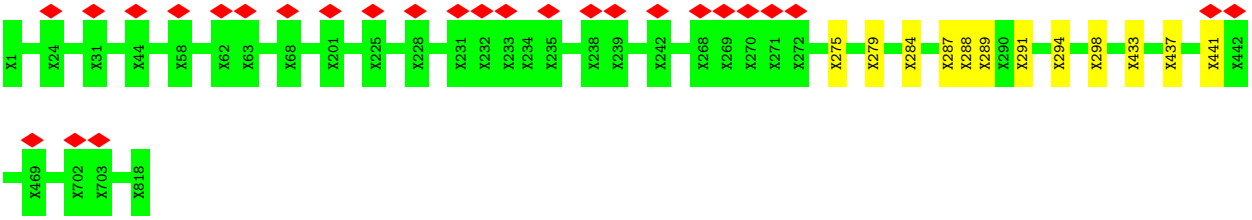
• Molecule 10: DYNACTIN

Chain M:



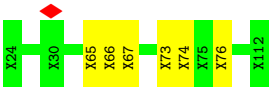
• Molecule 11: DYNACTIN 6

Chain N:



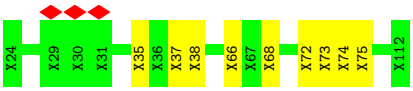
• Molecule 12: DYNACTIN

Chain O:



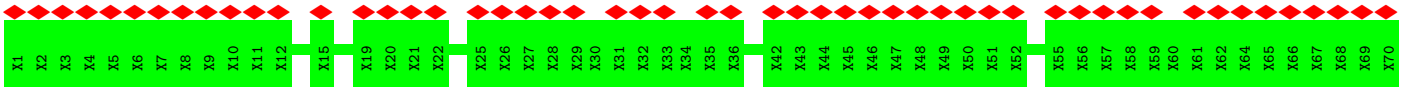
• Molecule 12: DYNACTIN

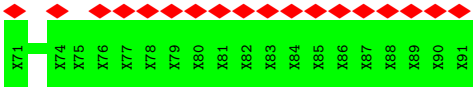
Chain P:



• Molecule 13: DYNACTIN

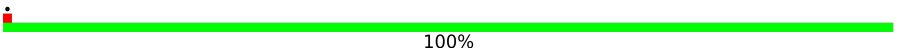
Chain Q:

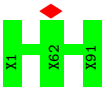




• Molecule 13: DYNACTIN

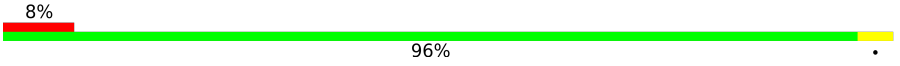
Chain R:

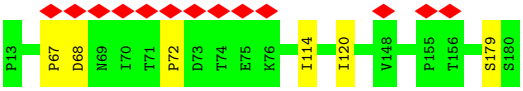




• Molecule 14: DYNACTIN

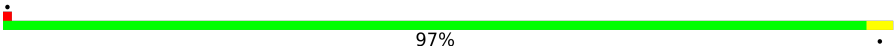
Chain U:

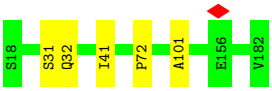




• Molecule 15: DYNACTIN

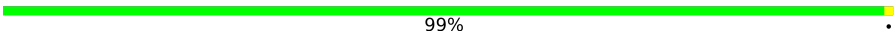
Chain V:

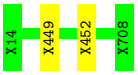




• Molecule 16: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA

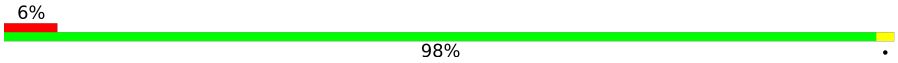
Chain Y:

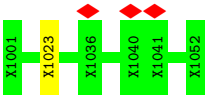




• Molecule 17: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA

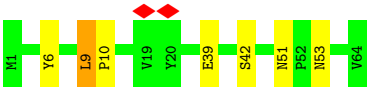
Chain Z:





• Molecule 18: DYNACTIN

Chain a:

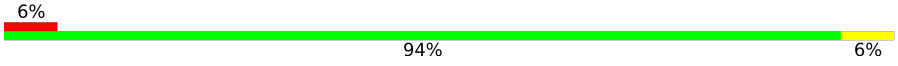


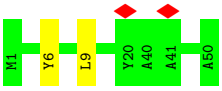
• Molecule 19: DYNACTIN

Chain b:

• Molecule 20: DYNACTIN

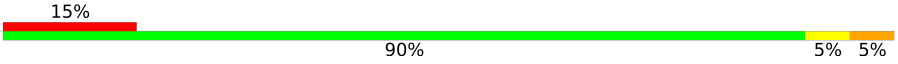
Chain c:

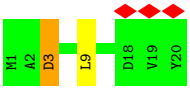




• Molecule 21: DYNACTIN

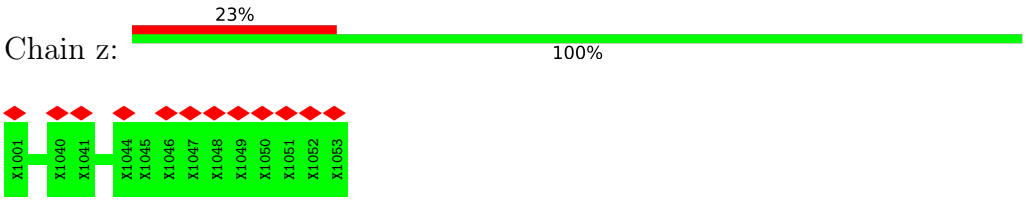
Chain d:





• Molecule 22: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85744	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	82353	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	578.88, 578.88, 578.88	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
3	3	0.39	0/1719	0.78	0/2384
3	4	0.39	0/1719	0.78	0/2384
5	A	0.37	0/3026	0.51	0/4086
5	B	0.37	0/3026	0.51	0/4086
5	C	0.37	0/3026	0.52	0/4086
5	D	0.37	0/3026	0.52	0/4086
5	E	0.37	0/3026	0.53	0/4086
5	F	0.37	0/3026	0.51	0/4086
5	G	0.37	0/3026	0.52	0/4086
5	I	0.37	0/3026	0.52	0/4086
6	H	0.37	0/2948	0.51	0/3991
7	J	0.37	0/2939	0.53	0/3987
8	K	0.39	0/2294	0.63	1/3106 (0.0%)
9	L	0.37	0/2173	0.60	1/2935 (0.0%)
14	U	0.28	0/825	0.51	0/1145
15	V	0.30	0/811	0.48	0/1126
18	a	0.52	1/347 (0.3%)	0.67	1/473 (0.2%)
19	b	0.43	0/524	0.72	0/705
20	c	0.40	0/181	0.65	0/249
21	d	0.46	0/130	0.73	0/179
All	All	0.37	1/40818 (0.0%)	0.56	3/55352 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	10	PRO	N-CD	5.05	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	253	PRO	CA-N-CD	-8.89	99.05	111.50
18	a	9	LEU	C-N-CD	5.78	140.54	128.40
8	K	114	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	375	THR	Peptide

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	1	1810	0	419	100	0
2	2	1800	0	417	78	0
3	3	1723	0	759	10	0
3	4	1723	0	759	12	0
4	5	1375	0	277	53	0
4	6	1375	0	277	52	0
5	A	2957	0	2952	9	0
5	B	2957	0	2952	2	0
5	C	2957	0	2952	2	0
5	D	2957	0	2952	1	0
5	E	2957	0	2952	1	0
5	F	2957	0	2952	19	0
5	G	2957	0	2952	15	0
5	I	2957	0	2952	5	0
6	H	2885	0	2856	3	0
7	J	2879	0	2970	7	0
8	K	2242	0	2169	69	0
9	L	2137	0	2122	74	0
10	M	2935	0	599	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	N	3080	0	633	7	0
12	O	323	0	76	3	0
12	P	323	0	76	10	0
13	Q	435	0	93	0	0
13	R	435	0	93	0	0
14	U	826	0	369	3	0
15	V	812	0	344	6	0
16	Y	1215	0	286	2	0
17	Z	260	0	57	1	0
18	a	341	0	310	0	0
19	b	517	0	489	0	0
20	c	179	0	155	0	0
21	d	127	0	103	0	0
22	z	265	0	57	0	0
23	A	27	0	12	0	0
23	B	27	0	12	0	0
23	C	27	0	12	0	0
23	D	27	0	12	0	0
23	E	27	0	12	0	0
23	F	27	0	12	0	0
23	G	27	0	12	0	0
23	I	27	0	12	0	0
23	J	27	0	12	0	0
24	H	31	0	12	0	0
All	All	55952	0	40501	480	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 5.

The worst 5 of 480 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)
2:2:355:UNK:CB	2:2:419:UNK:CB	1.80	1.52
4:5:268:UNK:CB	4:6:269:UNK:CB	1.95	1.44
4:6:253:UNK:CB	15:V:32:GLN:N	1.86	1.38
2:2:214:UNK:O	2:2:216:UNK:CA	1.71	1.38
1:1:31:UNK:CB	1:1:34:UNK:CB	2.01	1.38

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	342/350 (98%)	334 (98%)	8 (2%)	0	100	100
3	4	342/350 (98%)	334 (98%)	8 (2%)	0	100	100
5	A	368/370 (100%)	350 (95%)	18 (5%)	0	100	100
5	B	368/370 (100%)	348 (95%)	20 (5%)	0	100	100
5	C	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
5	D	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
5	E	368/370 (100%)	346 (94%)	22 (6%)	0	100	100
5	F	368/370 (100%)	341 (93%)	27 (7%)	0	100	100
5	G	368/370 (100%)	344 (94%)	24 (6%)	0	100	100
5	I	368/370 (100%)	346 (94%)	22 (6%)	0	100	100
6	H	368/370 (100%)	350 (95%)	18 (5%)	0	100	100
7	J	363/379 (96%)	331 (91%)	31 (8%)	1 (0%)	41	77
8	K	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
9	L	268/270 (99%)	257 (96%)	11 (4%)	0	100	100
14	U	166/168 (99%)	146 (88%)	15 (9%)	5 (3%)	4	28
15	V	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	25	66
18	a	44/48 (92%)	40 (91%)	3 (7%)	1 (2%)	6	34
19	b	65/71 (92%)	56 (86%)	8 (12%)	1 (2%)	10	46
20	c	27/31 (87%)	24 (89%)	2 (7%)	1 (4%)	3	24
21	d	18/20 (90%)	15 (83%)	1 (6%)	2 (11%)	0	7
All	All	5383/5457 (99%)	5060 (94%)	311 (6%)	12 (0%)	50	81

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	U	67	PRO

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Mol	Chain	Res	Type
14	U	72	PRO
18	a	9	LEU
19	b	9	LEU
20	c	9	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
5	A	318/318 (100%)	312 (98%)	6 (2%)	57 75
5	B	318/318 (100%)	314 (99%)	4 (1%)	69 81
5	C	318/318 (100%)	309 (97%)	9 (3%)	43 65
5	D	318/318 (100%)	309 (97%)	9 (3%)	43 65
5	E	318/318 (100%)	310 (98%)	8 (2%)	47 68
5	F	318/318 (100%)	313 (98%)	5 (2%)	62 79
5	G	318/318 (100%)	311 (98%)	7 (2%)	52 71
5	I	318/318 (100%)	312 (98%)	6 (2%)	57 75
6	H	313/313 (100%)	312 (100%)	1 (0%)	92 95
7	J	322/331 (97%)	318 (99%)	4 (1%)	71 83
8	K	245/245 (100%)	239 (98%)	6 (2%)	49 69
9	L	242/242 (100%)	236 (98%)	6 (2%)	47 68
18	a	31/41 (76%)	26 (84%)	5 (16%)	2 13
19	b	49/60 (82%)	38 (78%)	11 (22%)	1 5
20	c	7/16 (44%)	6 (86%)	1 (14%)	3 16
21	d	8/16 (50%)	7 (88%)	1 (12%)	4 19
All	All	3761/3808 (99%)	3672 (98%)	89 (2%)	51 69

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	J	277	GLU

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Mol	Chain	Res	Type
18	a	6	TYR
8	K	73	GLN
9	L	118	SER
18	a	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
8	K	79	HIS
8	K	84	ASN
19	b	51	ASN
9	L	209	HIS
18	a	51	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands 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	$\#\|Z\|>2$
23	ADP	A	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.45	4 (13%)
23	ADP	F	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.44	4 (13%)
23	ADP	B	800	-	24,29,29	1.05	2 (8%)	29,45,45	1.41	4 (13%)
23	ADP	E	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.44	4 (13%)
23	ADP	I	800	-	24,29,29	1.05	2 (8%)	29,45,45	1.47	4 (13%)
23	ADP	D	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.42	4 (13%)
24	ATP	H	401	-	26,33,33	1.02	2 (7%)	31,52,52	1.50	5 (16%)
23	ADP	G	800	-	24,29,29	1.05	2 (8%)	29,45,45	1.40	4 (13%)
23	ADP	J	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.48	5 (17%)
23	ADP	C	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.44	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
23	ADP	A	800	-	-	2/12/32/32	0/3/3/3
23	ADP	F	800	-	-	0/12/32/32	0/3/3/3
23	ADP	B	800	-	-	4/12/32/32	0/3/3/3
23	ADP	E	800	-	-	3/12/32/32	0/3/3/3
23	ADP	I	800	-	-	0/12/32/32	0/3/3/3
23	ADP	D	800	-	-	4/12/32/32	0/3/3/3
24	ATP	H	401	-	-	4/18/38/38	0/3/3/3
23	ADP	G	800	-	-	3/12/32/32	0/3/3/3
23	ADP	J	800	-	-	4/12/32/32	0/3/3/3
23	ADP	C	800	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	800	ADP	C5-C4	2.70	1.48	1.40
23	B	800	ADP	C5-C4	2.69	1.48	1.40
24	H	401	ATP	C5-C4	2.68	1.48	1.40
23	D	800	ADP	C5-C4	2.68	1.48	1.40
23	I	800	ADP	C5-C4	2.68	1.48	1.40

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	800	ADP	N3-C2-N1	-3.78	122.77	128.68
23	D	800	ADP	N3-C2-N1	-3.71	122.89	128.68
23	A	800	ADP	N3-C2-N1	-3.70	122.89	128.68
23	B	800	ADP	N3-C2-N1	-3.70	122.90	128.68
23	F	800	ADP	N3-C2-N1	-3.69	122.91	128.68

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

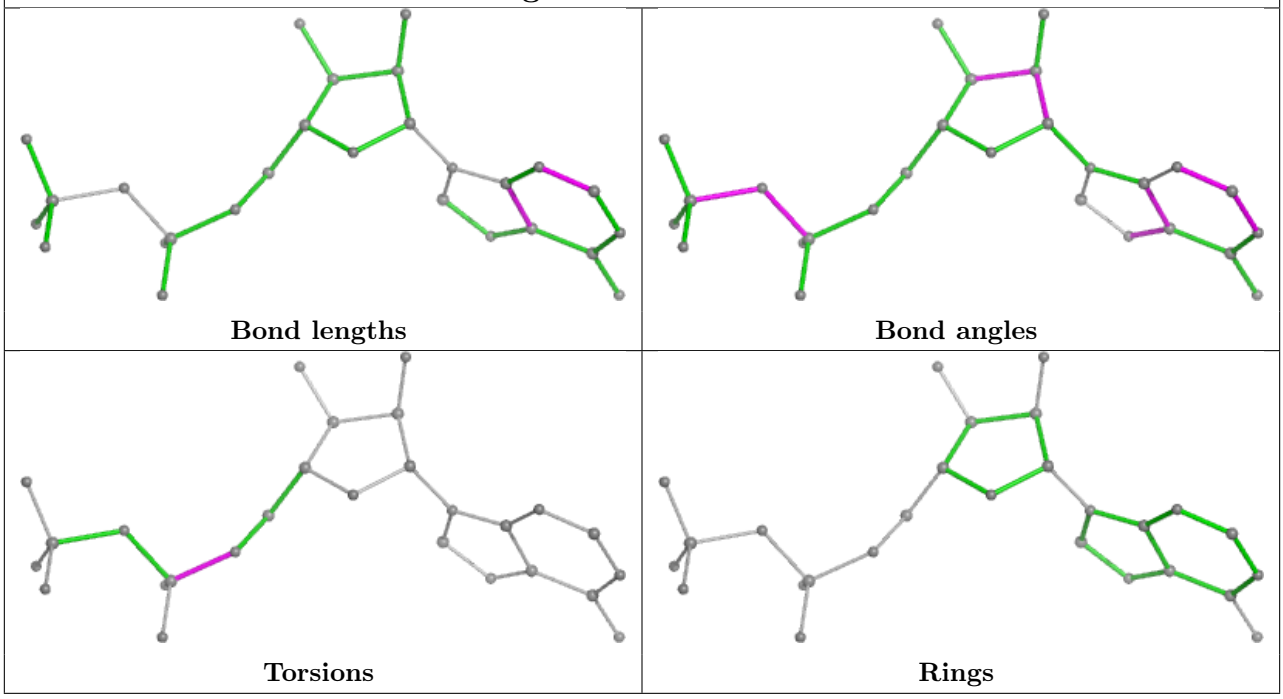
Mol	Chain	Res	Type	Atoms
23	B	800	ADP	C5'-O5'-PA-O3A
23	D	800	ADP	C5'-O5'-PA-O1A
23	D	800	ADP	C5'-O5'-PA-O2A
23	E	800	ADP	C5'-O5'-PA-O2A
23	J	800	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

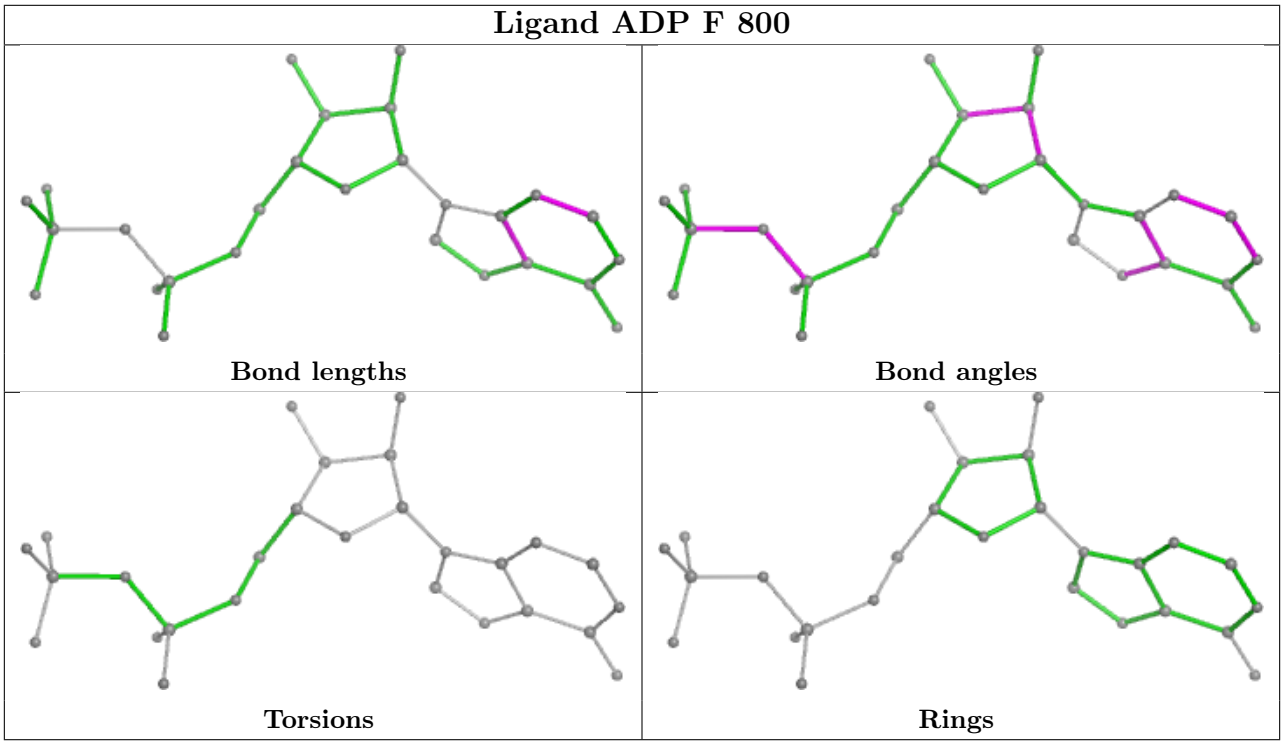
No monomer is involved in short contacts.

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 then 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.

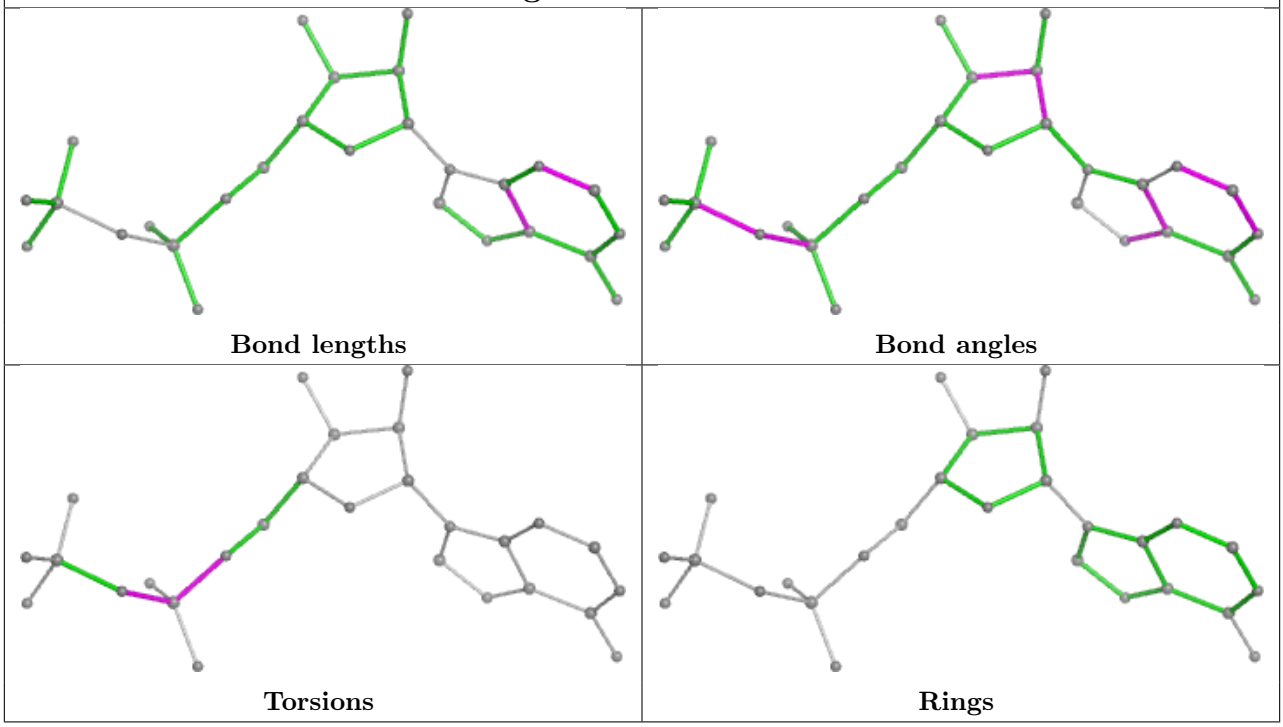
Ligand ADP A 800



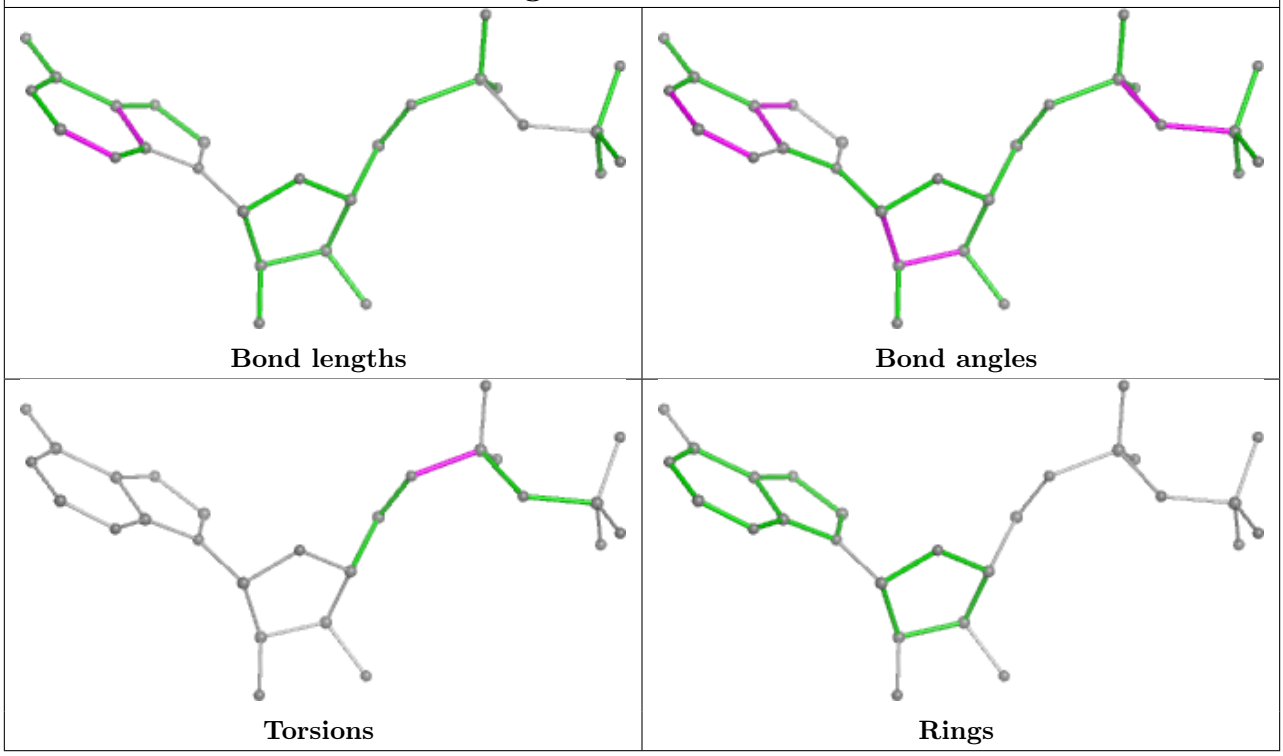
Ligand ADP F 800



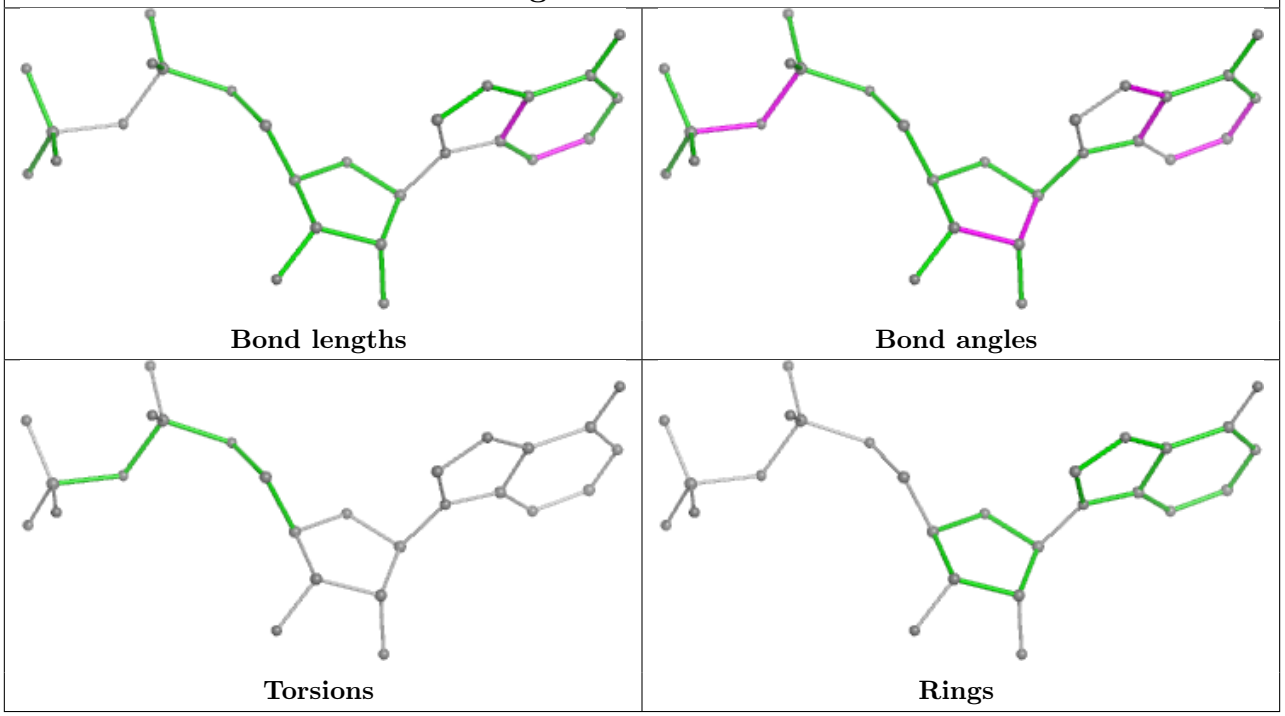
Ligand ADP B 800



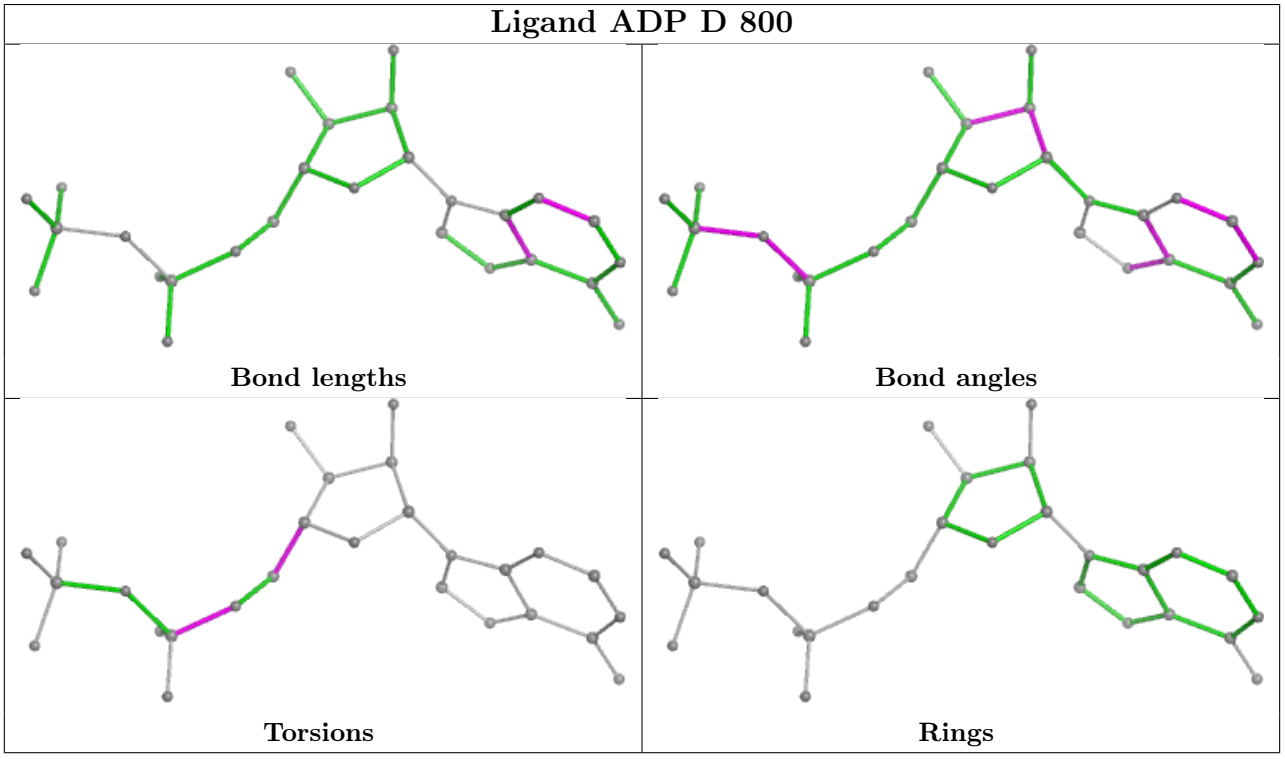
Ligand ADP E 800



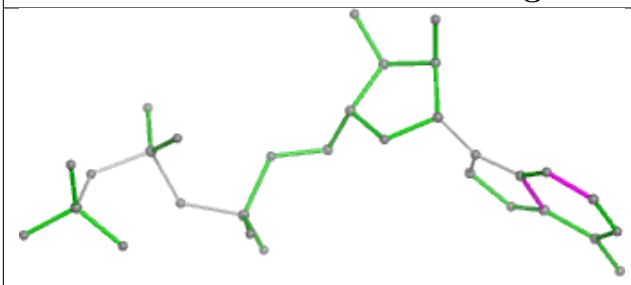
Ligand ADP I 800



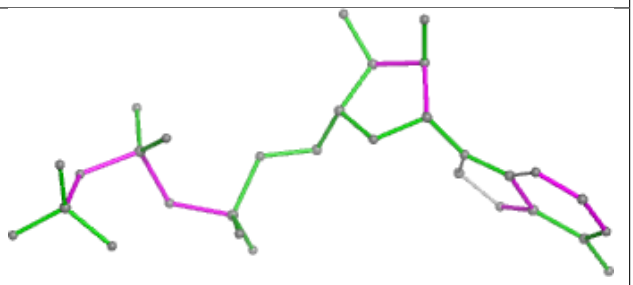
Ligand ADP D 800



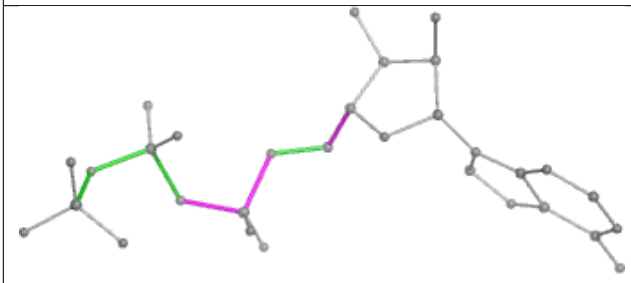
Ligand ATP H 401



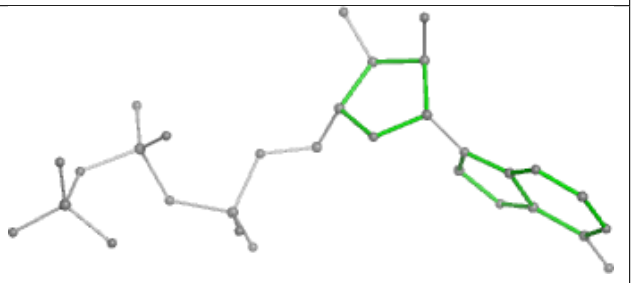
Bond lengths



Bond angles

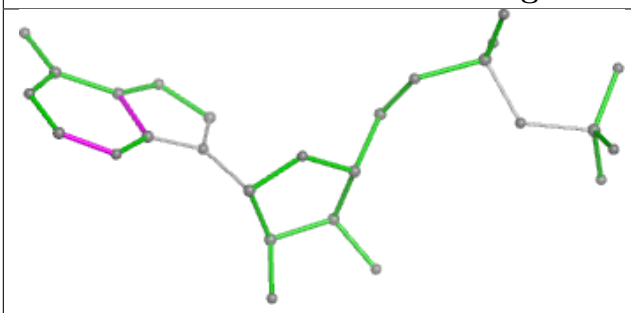


Torsions

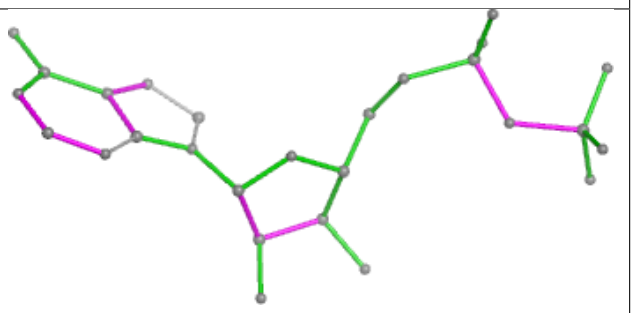


Rings

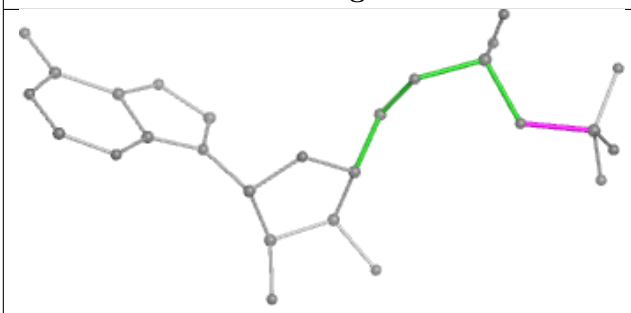
Ligand ADP G 800



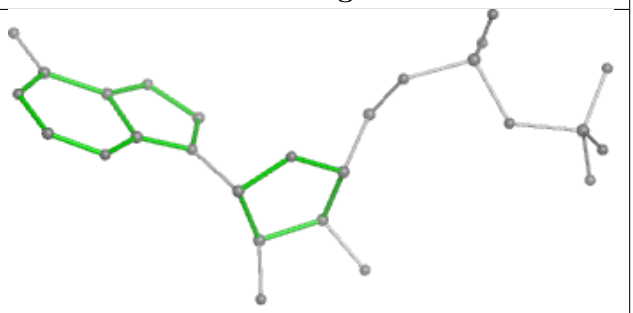
Bond lengths



Bond angles

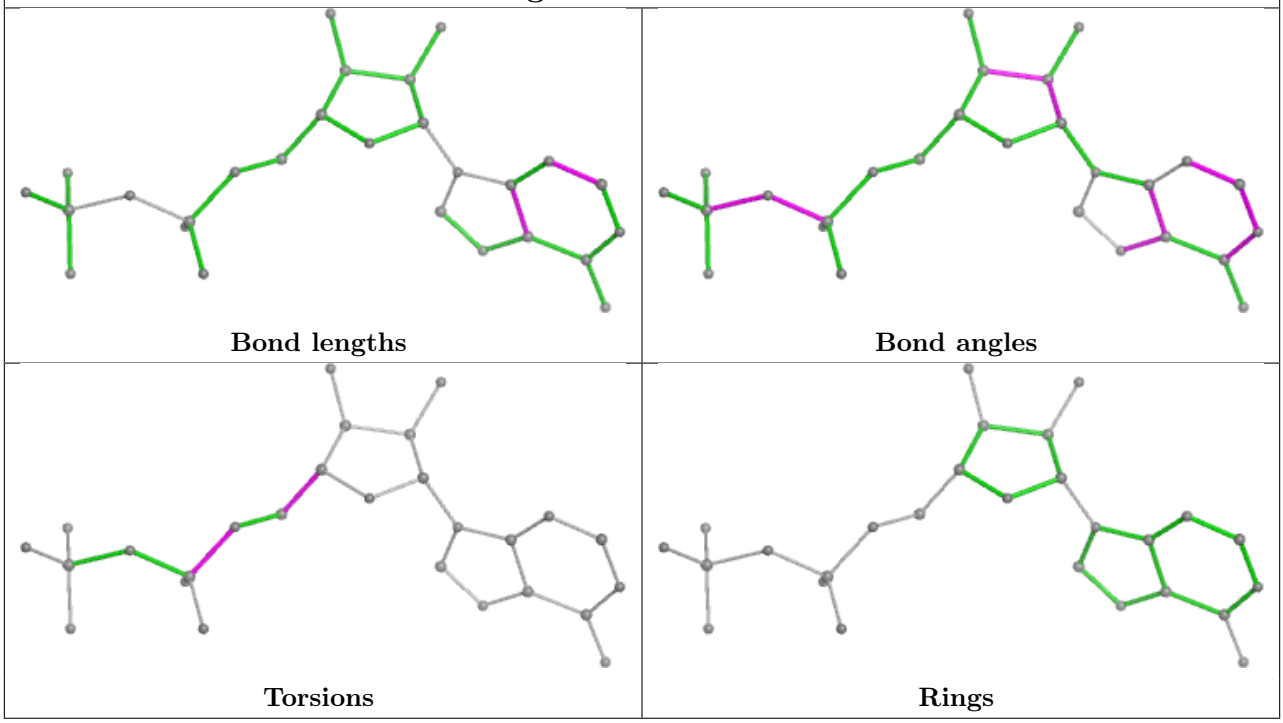


Torsions

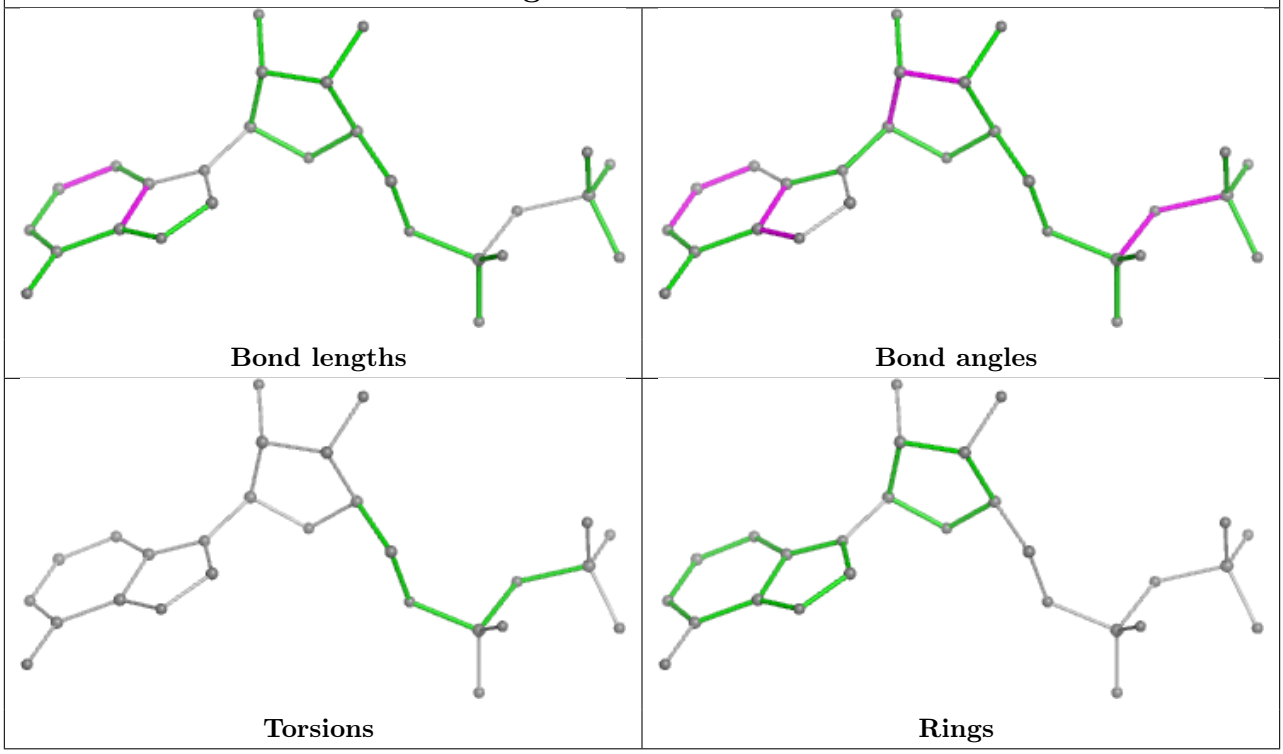


Rings

Ligand ADP J 800



Ligand ADP C 800



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	14
16	Y	12
2	2	12
11	N	5
10	M	5
12	O	3
12	P	3
3	3	3
3	4	3
13	Q	2
13	R	2
19	b	2
20	c	1
18	a	1

The worst 5 of 68 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	367:UNK	C	401:UNK	N	98.24
1	N	171:UNK	C	201:UNK	N	96.90
1	M	171:UNK	C	201:UNK	N	95.47
1	M	367:UNK	C	401:UNK	N	81.15
1	M	625:UNK	C	701:UNK	N	68.30

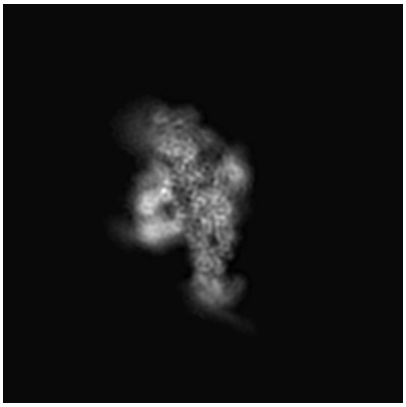
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2860. These allow visual inspection of the internal detail of the map and identification of artifacts.

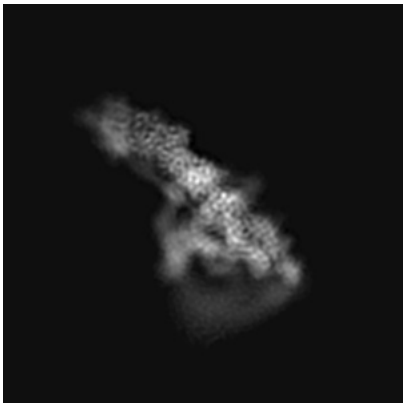
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

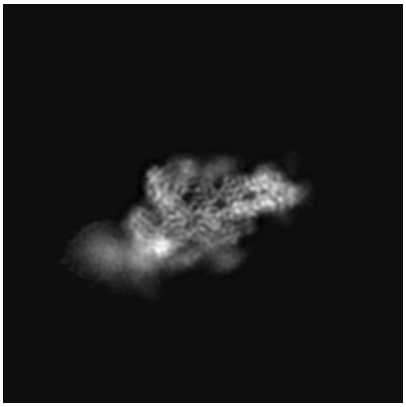
6.1.1 Primary map



X



Y

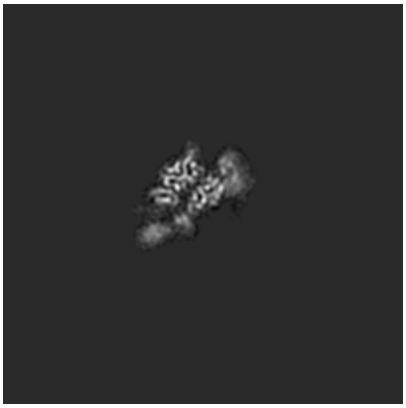


Z

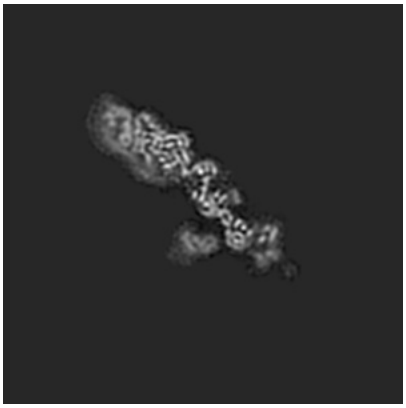
The images above show the map projected in three orthogonal directions.

6.2 Central slices

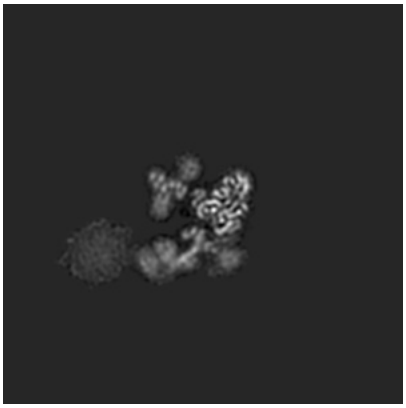
6.2.1 Primary map



X Index: 216



Y Index: 216

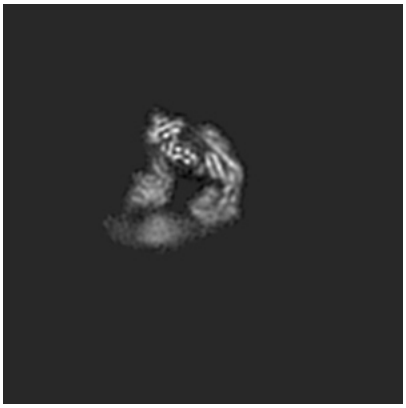


Z Index: 216

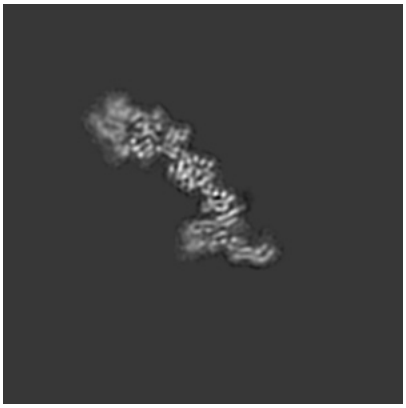
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

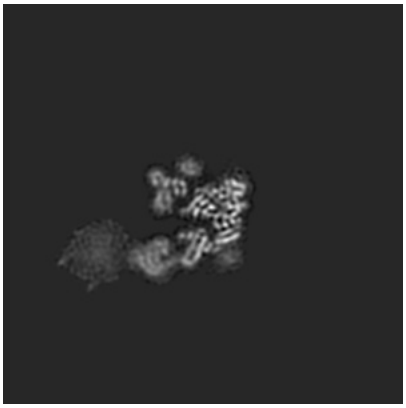
6.3.1 Primary map



X Index: 166



Y Index: 230

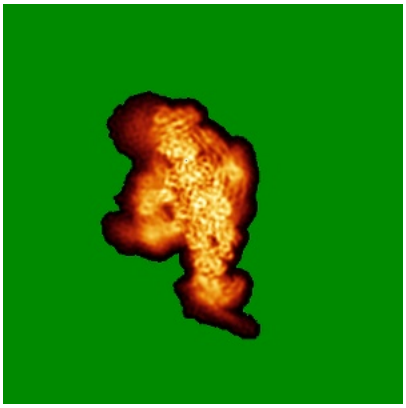


Z Index: 221

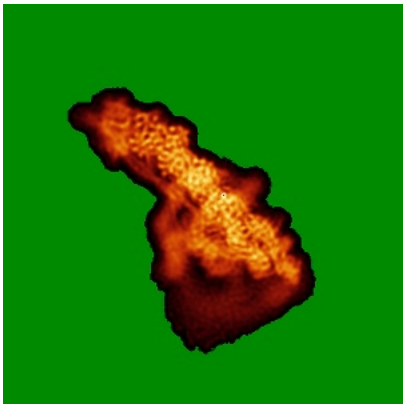
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

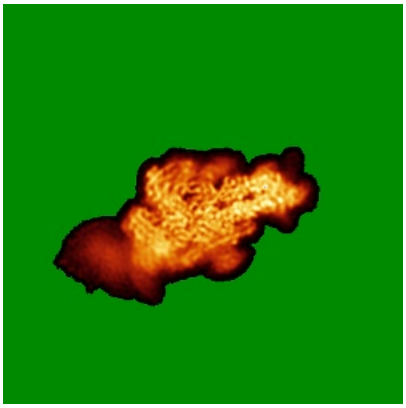
6.4.1 Primary map



X



Y

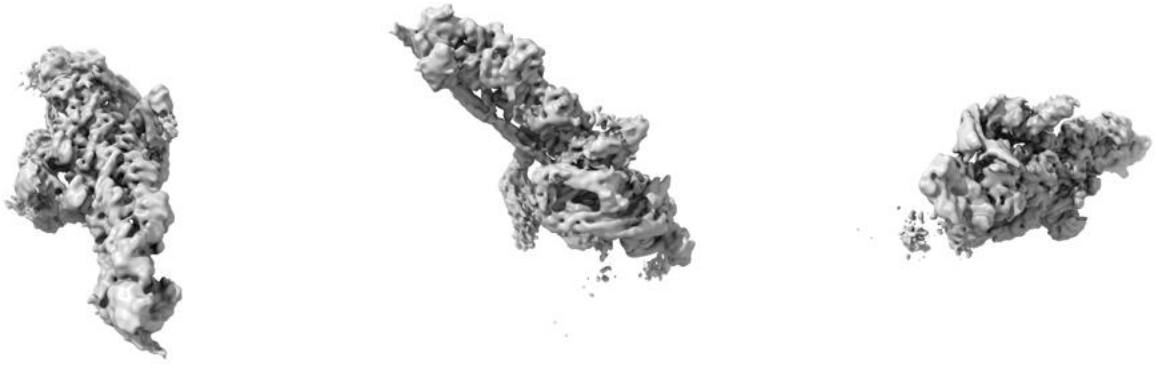


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

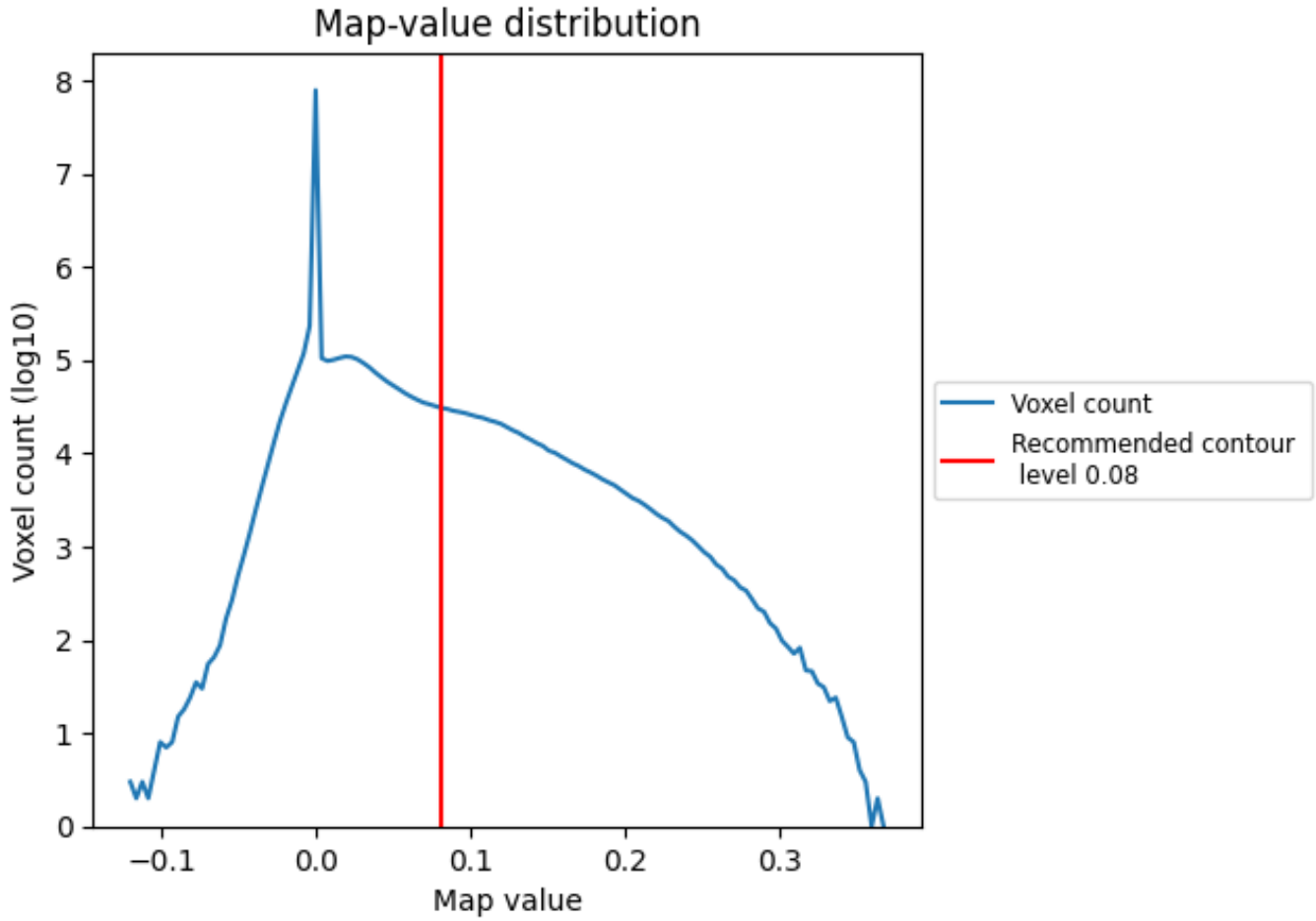
6.6 Mask visualisation (i)

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

7 Map analysis

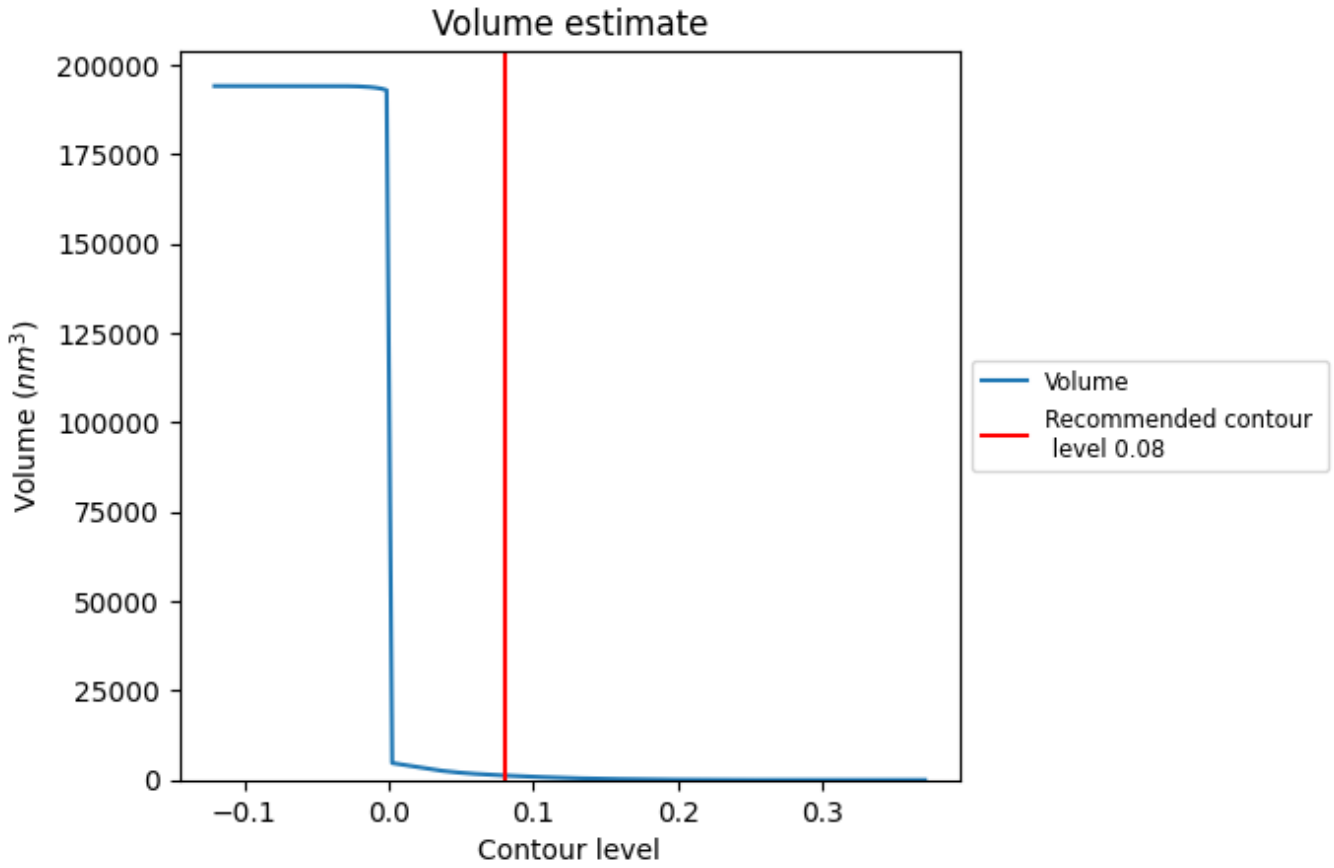
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

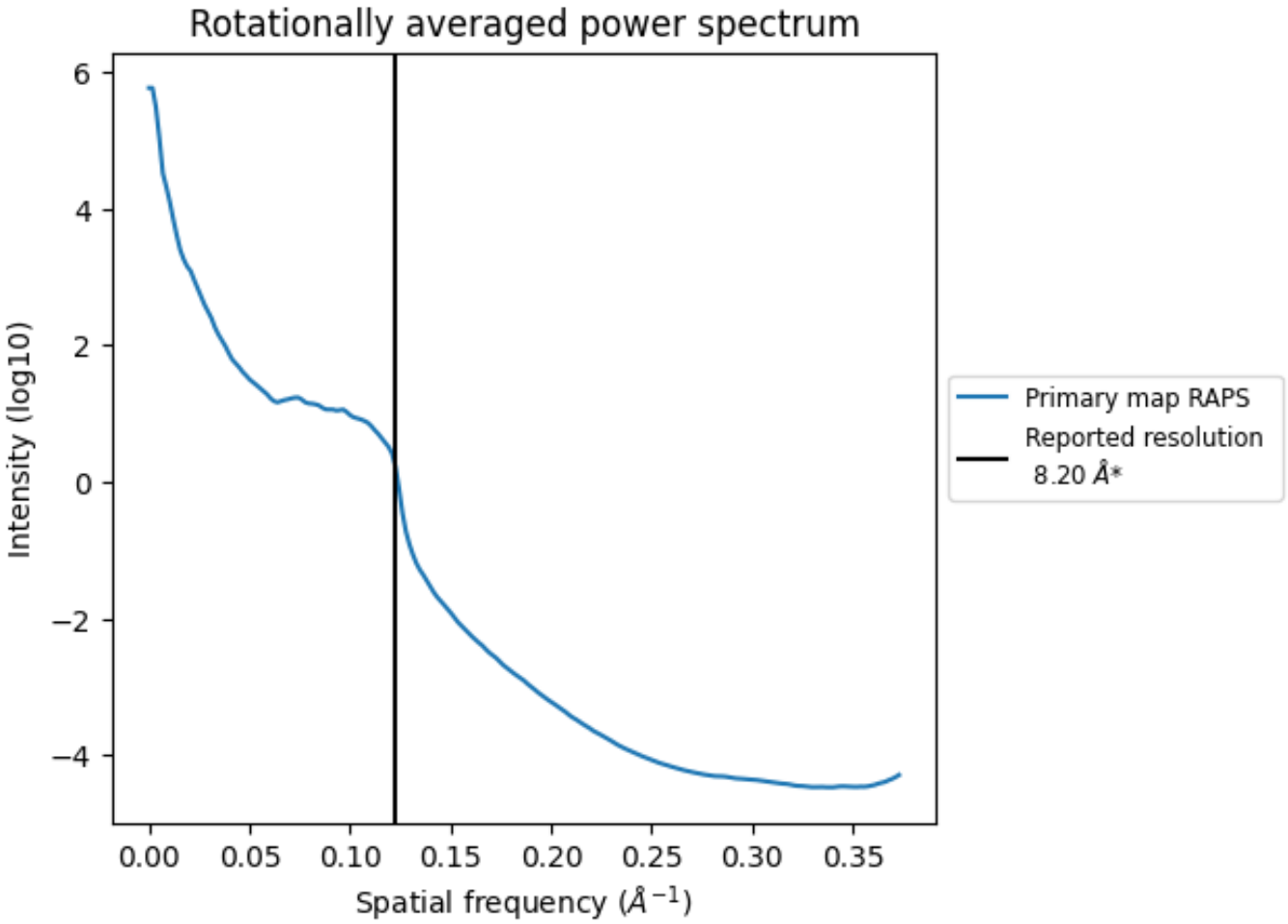
7.2 Volume estimate (i)



The volume at the recommended contour level is 1254 nm^3; this corresponds to an approximate mass of 1133 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 0.122 Å^{-1}

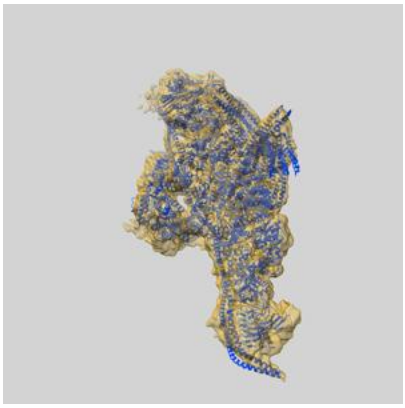
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

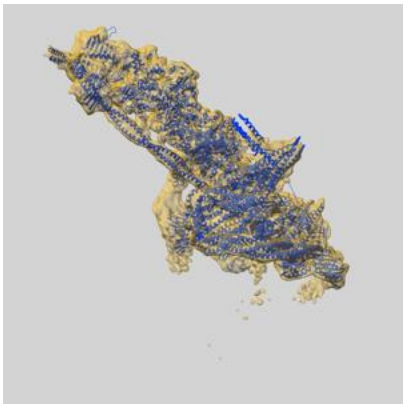
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2860 and PDB model 5AFU. Per-residue inclusion information can be found in section 3 on page 10.

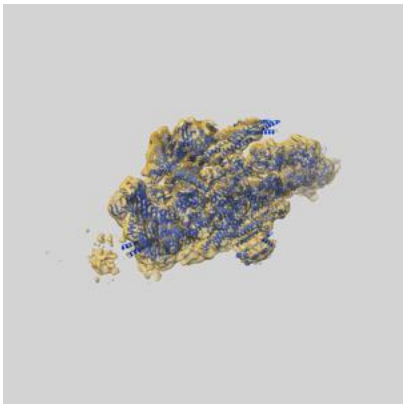
9.1 Map-model overlay



X



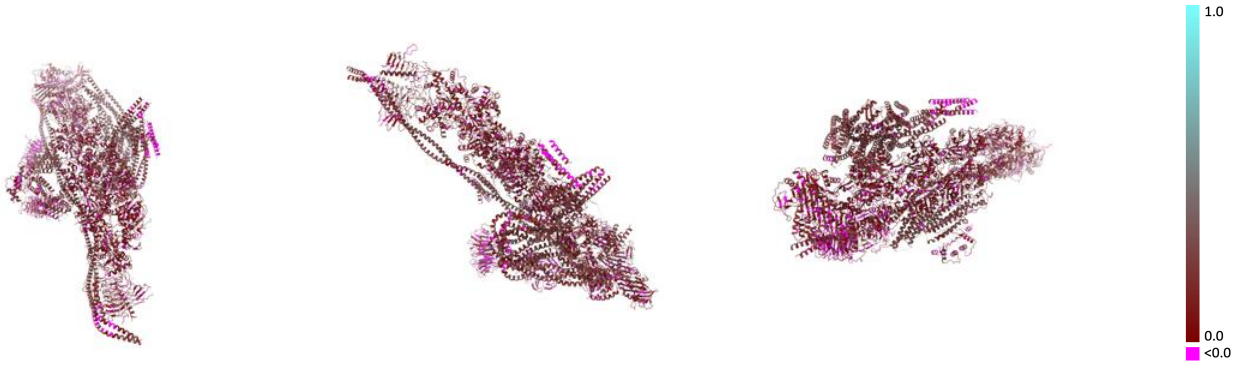
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

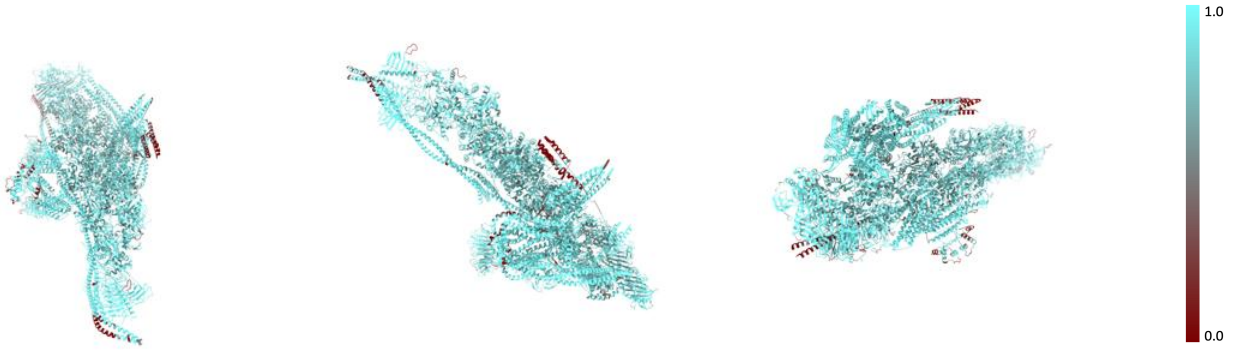
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

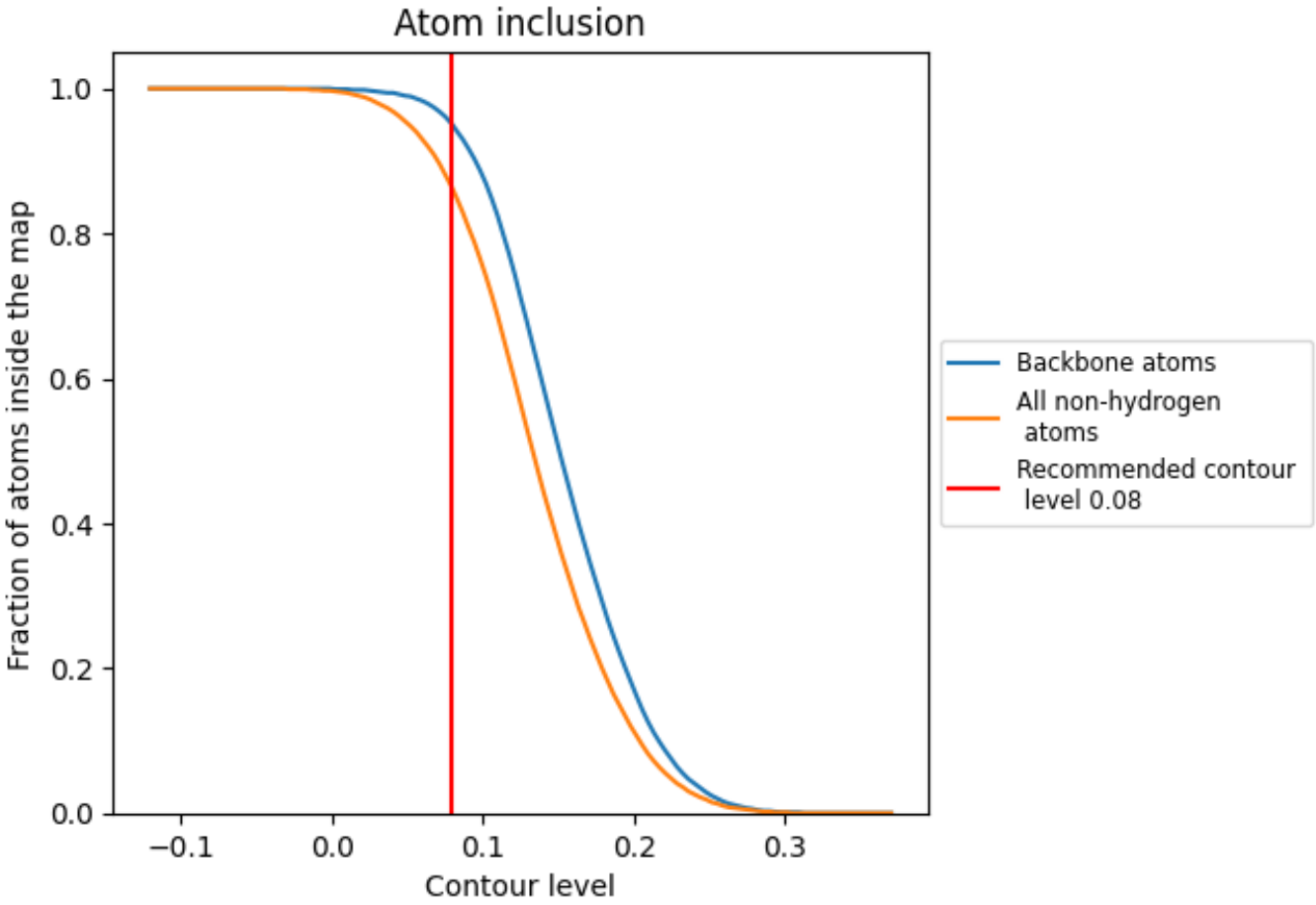
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 86% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.1480
1	0.9110	0.2280
2	0.8820	0.1940
3	0.8720	0.0470
4	0.8940	0.0530
5	0.8190	0.2310
6	0.8120	0.2120
A	0.8360	0.1200
B	0.8350	0.1290
C	0.8020	0.1270
D	0.8160	0.1270
E	0.8050	0.1290
F	0.8180	0.1250
G	0.8380	0.1260
H	0.8630	0.1330
I	0.8470	0.1220
J	0.8740	0.1370
K	0.9080	0.1300
L	0.8570	0.1240
M	0.9510	0.2100
N	0.9470	0.2140
O	0.9570	0.2000
P	0.9440	0.2100
Q	0.2090	0.0340
R	0.9840	0.2500
U	0.9140	0.1570
V	0.9910	0.1810
Y	0.9960	0.2110
Z	0.9230	0.1950
a	0.8460	0.2140
b	0.8790	0.1660
c	0.8980	0.1950
d	0.8390	0.1940
z	0.8000	0.1630