



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:19 pm GMT

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 : 3.50 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

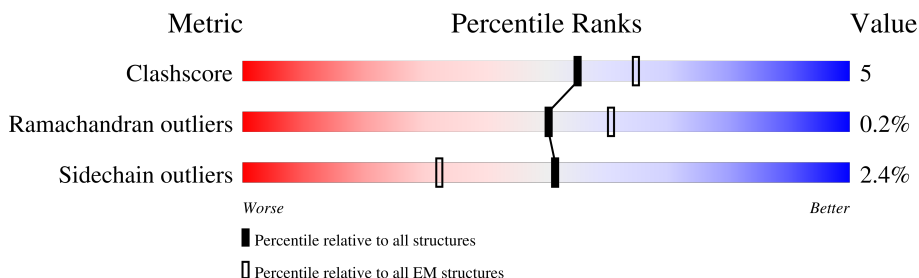
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



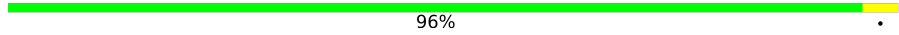
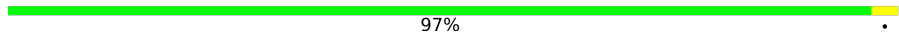
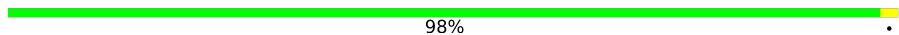
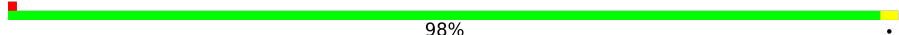
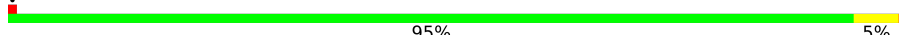
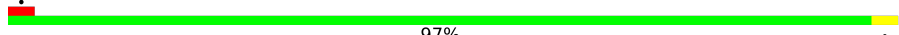
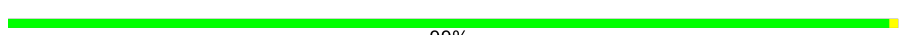




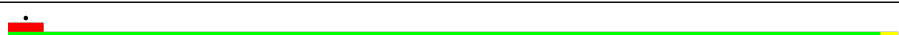

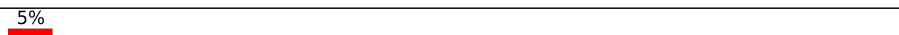

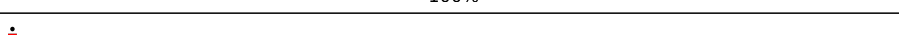
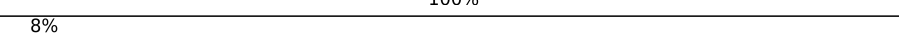
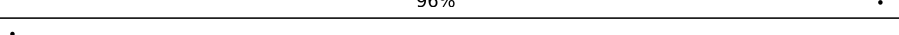
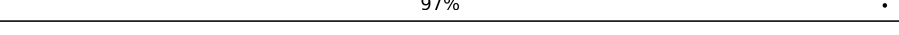
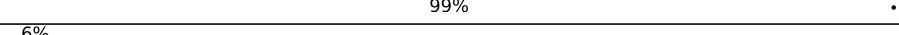
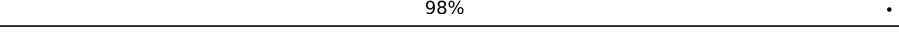


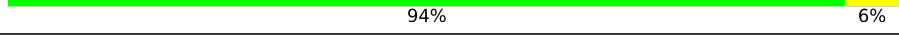

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	1	361	
2	2	359	
3	3	350	
3	4	350	
4	5	275	
4	6	275	
5	A	370	
5	B	370	

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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	 86% 14% 5%
13	Q	87	 100%
13	R	87	 100%
14	U	168	 96% 8%
15	V	165	 97%
16	Y	243	 99%
17	Z	52	 98% 6%
18	a	48	 85% 12%
19	b	71	 83% 17%
20	c	31	 94% 6% 6%
21	d	20	 90% 5% 5%
22	z	53	 100% 23%

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
			Total	C	N	O		
1	1	361	1810	1088	361	361	0	0

- Molecule 2 is a protein called DYNEIN TAIL.

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

- Molecule 3 is a protein called DYNEIN TAIL.

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

- Molecule 4 is a protein called DYNEIN TAIL.

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

- Molecule 5 is a protein called DYNACTIN.

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

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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 DYNAMACTIN.

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 DYNAMACTIN.

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

- Molecule 11 is a protein called DYNAMACTIN 6.

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

- Molecule 12 is a protein called DYNAMACTIN.

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

- Molecule 13 is a protein called DYNAMACTIN.

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

- Molecule 14 is a protein called DYNAMACTIN.

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

- Molecule 15 is a protein called DYNAMACTIN.

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

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

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

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

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

- Molecule 18 is a protein called DYNAMACTIN.

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

- Molecule 19 is a protein called DYNAMACTIN.

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

- Molecule 20 is a protein called DYNAMACTIN.

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

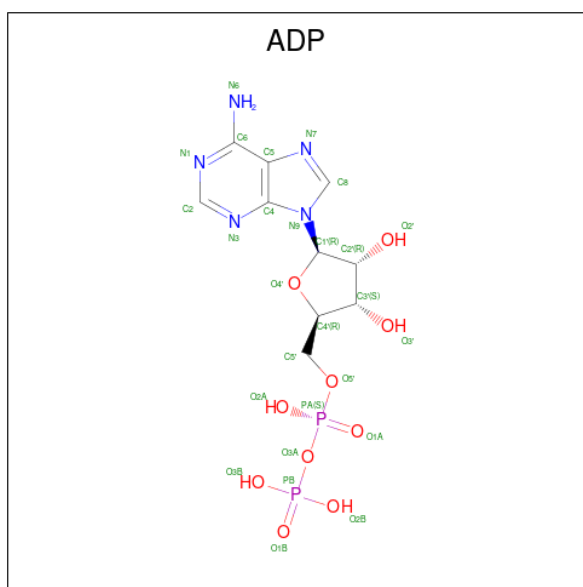
- Molecule 21 is a protein called DYNAMACTIN.

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

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

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

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



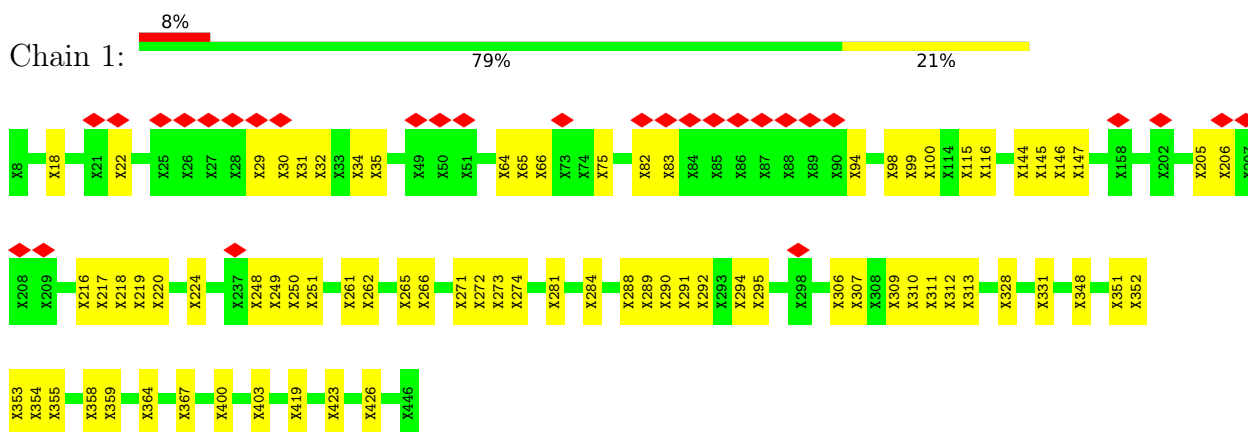
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	A	1	Total 27	C 10	N 5	O 10	P 2	0
23	B	1	Total 27	C 10	N 5	O 10	P 2	0
23	C	1	Total 27	C 10	N 5	O 10	P 2	0
23	D	1	Total 27	C 10	N 5	O 10	P 2	0
23	E	1	Total 27	C 10	N 5	O 10	P 2	0
23	F	1	Total 27	C 10	N 5	O 10	P 2	0
23	G	1	Total 27	C 10	N 5	O 10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

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

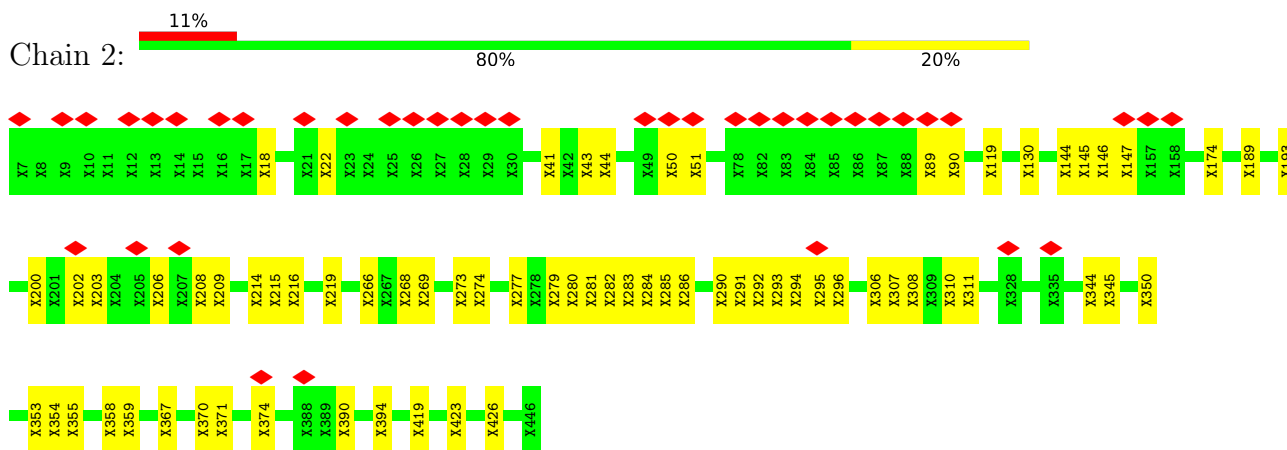
3 Residue-property plots [i](#)

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.

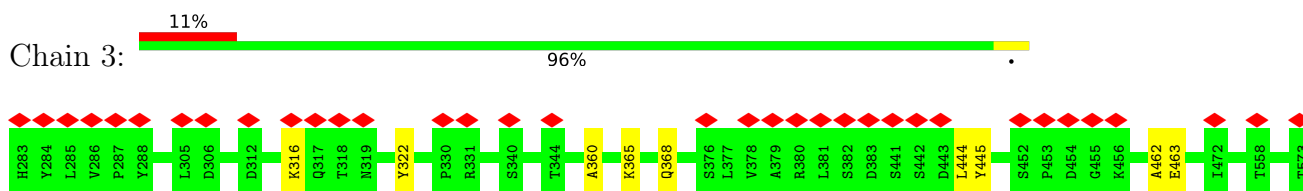
- Molecule 1: DYNEIN TAIL

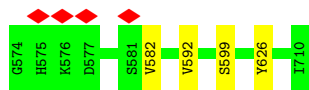


- Molecule 2: DYNEIN TAIL

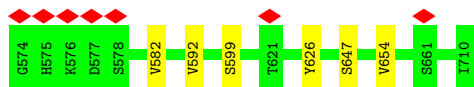
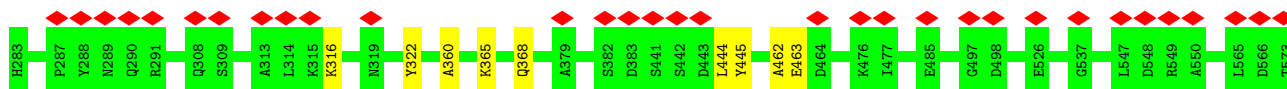


- Molecule 3: DYNEIN TAIL

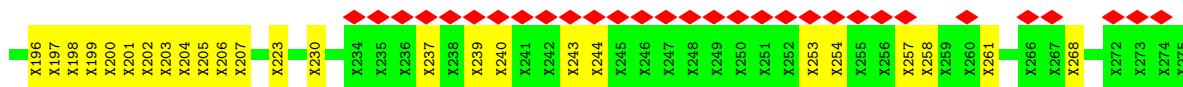
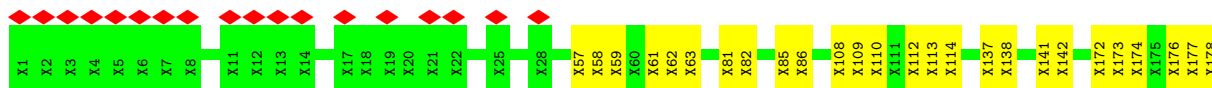
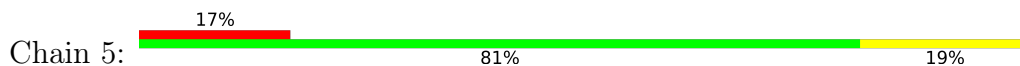




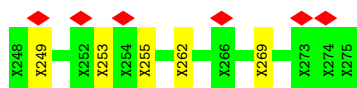
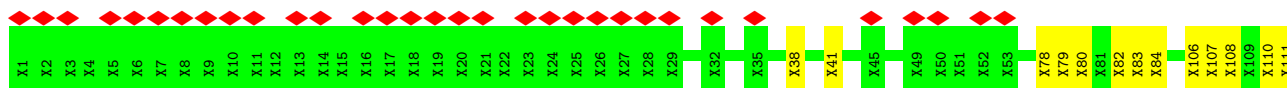
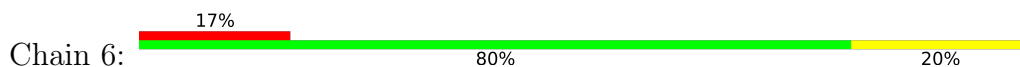
• Molecule 3: DYNEIN TAIL



• Molecule 4: DYNEIN TAIL



• Molecule 4: DYNEIN TAIL



• Molecule 5: DYNACTIN



• Molecule 5: DYNACTIN

Chain B:  99%



• Molecule 5: DYNAMICTIN

Chain C:  96%



• Molecule 5: DYNAMICTIN

Chain D:  97%



• Molecule 5: DYNAMICTIN

Chain E:  98%



• Molecule 5: DYNAMICTIN

Chain F:  98%



• Molecule 5: DYNAMICTIN

Chain G:  95% 5%



• Molecule 5: DYNAMICTIN

Chain I:  97%



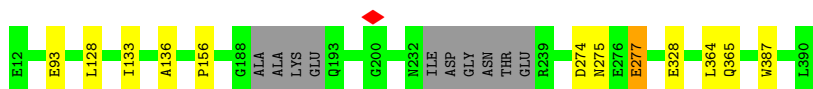
- Molecule 6: ACTIN, CYTOPLASMIC 1

Chain H:  99%




- Molecule 7: DYNAMICTIN

Chain J:  94%




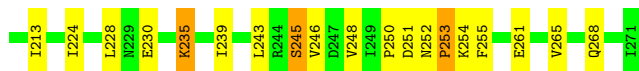
- Molecule 8: CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1

Chain K:  78%



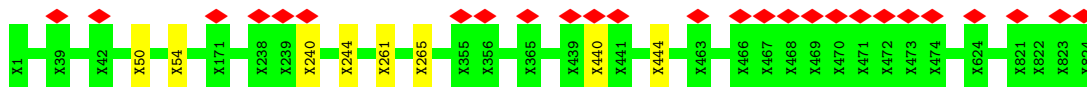
- Molecule 9: F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II

Chain L:  82%



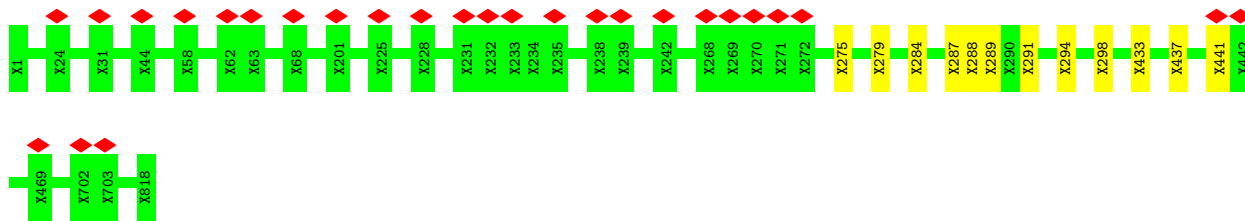
- Molecule 10: DYNAMICTIN

Chain M:  99%

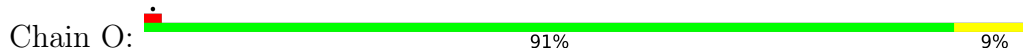


- Molecule 11: DYNAMICTIN 6

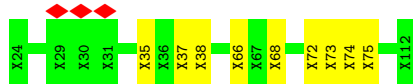
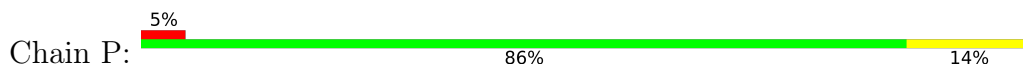
Chain N:  98%



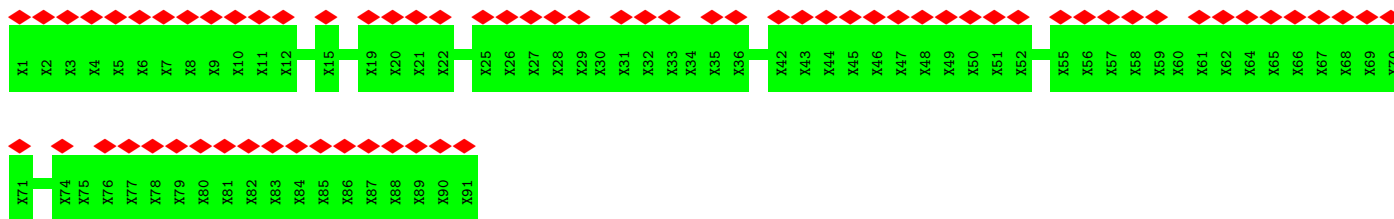
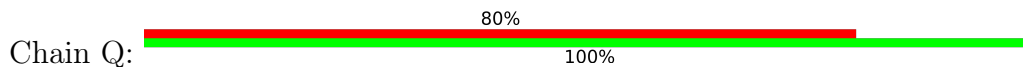
• Molecule 12: DYNACTIN



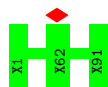
• Molecule 12: DYNACTIN



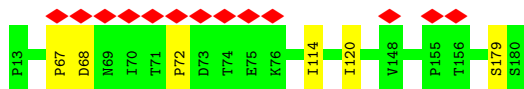
• Molecule 13: DYNACTIN



• Molecule 13: DYNACTIN



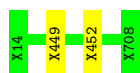
• Molecule 14: DYNACTIN



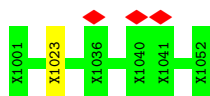
• Molecule 15: DYNACTIN



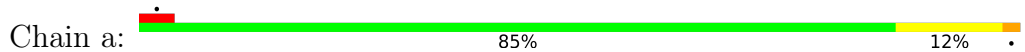
- Molecule 16: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA



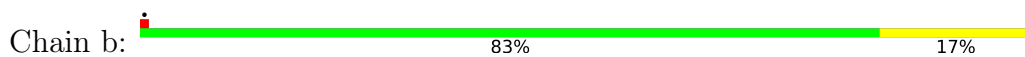
- Molecule 17: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA



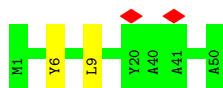
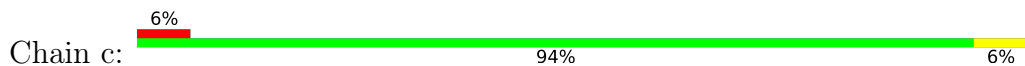
- Molecule 18: DYNACTIN



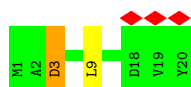
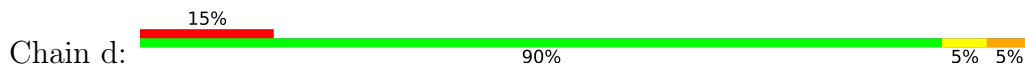
- Molecule 19: DYNACTIN



- Molecule 20: DYNACTIN

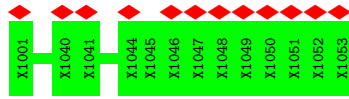


- Molecule 21: DYNACTIN



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

Chain z:  23%
100%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	578.88, 578.88, 578.88	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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.

All (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
1:1:355:UNK:CB	1:1:419:UNK:CB	2.03	1.36
9:L:251:ASP:CG	9:L:255:PHE:HE2	1.36	1.28
1:1:281:UNK:O	1:1:284:UNK:CB	1.83	1.27
1:1:31:UNK:O	1:1:34:UNK:N	1.67	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:UNK:O	2:2:22:UNK:CB	1.82	1.26
4:5:137:UNK:O	4:5:141:UNK:N	1.68	1.25
2:2:281:UNK:C	2:2:286:UNK:CB	2.14	1.25
4:6:238:UNK:O	4:6:242:UNK:N	1.70	1.24
2:2:281:UNK:O	2:2:286:UNK:CB	1.84	1.23
2:2:18:UNK:O	2:2:22:UNK:N	1.74	1.21
9:L:251:ASP:O	9:L:255:PHE:CD2	1.94	1.20
5:G:183:ILE:HD11	5:G:278:VAL:CG2	1.72	1.19
2:2:214:UNK:C	2:2:216:UNK:HA	1.71	1.18
9:L:253:PRO:HD2	9:L:254:LYS:H	1.08	1.17
2:2:370:UNK:O	2:2:374:UNK:N	1.77	1.17
1:1:359:UNK:CB	1:1:423:UNK:HA	1.75	1.16
1:1:271:UNK:O	1:1:274:UNK:N	1.79	1.14
1:1:281:UNK:O	1:1:284:UNK:CA	1.97	1.13
2:2:215:UNK:CB	2:2:219:UNK:CB	2.25	1.13
8:K:162:GLN:HG3	9:L:243:LEU:CD2	1.77	1.13
1:1:311:UNK:C	1:1:312:UNK:O	1.97	1.13
5:G:183:ILE:HD11	5:G:278:VAL:HG21	1.26	1.13
1:1:248:UNK:O	1:1:251:UNK:N	1.84	1.11
1:1:292:UNK:CB	5:F:350:LEU:HD23	1.80	1.10
9:L:245:SER:CB	9:L:248:VAL:HG23	1.82	1.10
2:2:306:UNK:O	2:2:310:UNK:N	1.86	1.09
1:1:311:UNK:C	1:1:312:UNK:C	2.30	1.09
8:K:93:LYS:HE3	8:K:122:GLU:OE2	1.51	1.08
9:L:245:SER:HB2	9:L:248:VAL:HG23	1.31	1.07
12:P:66:UNK:CB	12:P:74:UNK:O	2.03	1.07
9:L:245:SER:OG	9:L:248:VAL:CG2	2.02	1.07
9:L:251:ASP:CG	9:L:255:PHE:CE2	2.28	1.05
4:5:138:UNK:O	4:5:142:UNK:N	1.90	1.05
1:1:292:UNK:N	5:F:350:LEU:CD2	2.20	1.05
9:L:250:PRO:O	9:L:253:PRO:CD	2.05	1.04
8:K:162:GLN:HG3	9:L:243:LEU:HD21	1.37	1.03
2:2:215:UNK:CB	2:2:219:UNK:N	2.22	1.02
4:6:117:UNK:O	4:6:121:UNK:N	1.92	1.02
12:P:38:UNK:N	12:P:73:UNK:O	1.93	1.01
1:1:292:UNK:CA	5:F:350:LEU:CD2	2.37	1.01
2:2:274:UNK:CB	2:2:277:UNK:CB	2.38	1.01
2:2:307:UNK:O	2:2:311:UNK:N	1.93	1.00
1:1:281:UNK:O	1:1:284:UNK:N	1.94	1.00
1:1:312:UNK:C	1:1:313:UNK:N	2.25	1.00
4:5:82:UNK:O	4:5:86:UNK:N	1.95	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:292:UNK:N	5:F:350:LEU:HD21	1.77	0.99
4:5:109:UNK:O	4:5:113:UNK:N	1.94	0.99
4:6:253:UNK:CB	15:V:32:GLN:CA	2.40	0.98
1:1:292:UNK:CA	5:F:350:LEU:HD23	1.93	0.98
1:1:291:UNK:C	5:F:350:LEU:HD21	1.93	0.98
1:1:291:UNK:CB	5:F:350:LEU:HD11	1.94	0.97
4:6:253:UNK:CB	15:V:32:GLN:H	1.71	0.97
9:L:245:SER:OG	9:L:248:VAL:HG21	1.62	0.97
2:2:18:UNK:O	2:2:22:UNK:CA	2.12	0.97
1:1:291:UNK:CB	5:F:350:LEU:HD21	1.96	0.96
8:K:168:PHE:O	8:K:199:TYR:CD1	2.19	0.96
2:2:292:UNK:O	2:2:296:UNK:N	1.99	0.95
5:G:185:ILE:HD11	5:G:261:LEU:HG	1.45	0.95
9:L:251:ASP:OD1	9:L:255:PHE:HE2	1.48	0.95
4:5:174:UNK:O	4:5:178:UNK:N	1.98	0.95
5:G:183:ILE:CD1	5:G:278:VAL:HG21	1.95	0.95
9:L:251:ASP:OD1	9:L:255:PHE:CE2	2.19	0.94
4:5:240:UNK:O	4:5:244:UNK:N	2.01	0.94
8:K:93:LYS:NZ	8:K:122:GLU:OE1	2.01	0.93
1:1:216:UNK:O	1:1:219:UNK:N	2.00	0.93
2:2:214:UNK:O	2:2:216:UNK:HA	0.75	0.93
4:6:151:UNK:O	4:6:155:UNK:N	2.02	0.92
9:L:251:ASP:O	9:L:255:PHE:HD2	1.39	0.92
2:2:359:UNK:O	2:2:426:UNK:CB	2.18	0.91
4:5:110:UNK:O	4:5:114:UNK:N	2.03	0.91
8:K:93:LYS:CE	8:K:122:GLU:OE2	2.19	0.91
9:L:253:PRO:HD2	9:L:254:LYS:N	1.86	0.91
1:1:31:UNK:O	1:1:34:UNK:CA	2.19	0.90
4:5:174:UNK:O	4:5:178:UNK:CB	2.20	0.90
8:K:162:GLN:CG	9:L:243:LEU:HD21	2.03	0.89
2:2:215:UNK:CB	2:2:216:UNK:C	2.51	0.89
9:L:250:PRO:O	9:L:253:PRO:CG	2.19	0.89
1:1:271:UNK:O	1:1:274:UNK:CA	2.20	0.89
4:5:230:UNK:CB	4:6:231:UNK:CB	2.51	0.88
3:4:365:LYS:HA	3:4:444:LEU:CB	2.03	0.88
4:5:109:UNK:O	4:5:113:UNK:CB	2.20	0.88
2:2:390:UNK:O	2:2:394:UNK:HG2	1.74	0.88
2:2:144:UNK:O	2:2:145:UNK:C	2.21	0.88
8:K:162:GLN:CG	9:L:243:LEU:CD2	2.52	0.88
2:2:144:UNK:O	2:2:146:UNK:N	2.06	0.88
3:3:445:TYR:CB	3:3:463:GLU:CB	2.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:365:LYS:HA	3:3:444:LEU:CB	2.03	0.87
4:5:202:UNK:O	4:5:206:UNK:N	2.07	0.87
3:4:445:TYR:CB	3:4:463:GLU:CB	2.52	0.87
4:6:38:UNK:O	5:A:237:GLU:OE2	1.92	0.87
2:2:215:UNK:CB	2:2:216:UNK:O	2.23	0.86
9:L:251:ASP:CB	9:L:255:PHE:HE2	1.88	0.86
4:5:201:UNK:O	4:5:205:UNK:N	2.09	0.85
4:6:247:UNK:CB	14:U:179:SER:CB	2.54	0.85
4:5:199:UNK:O	4:5:203:UNK:N	2.10	0.84
1:1:289:UNK:CB	5:F:346:ILE:HG21	2.06	0.84
2:2:18:UNK:C	2:2:22:UNK:CB	2.55	0.84
12:P:38:UNK:O	12:P:73:UNK:N	2.11	0.84
1:1:281:UNK:C	1:1:284:UNK:CB	2.55	0.83
8:K:93:LYS:NZ	8:K:122:GLU:CD	2.32	0.83
3:3:445:TYR:O	3:3:462:ALA:HB1	1.79	0.83
9:L:251:ASP:CB	9:L:255:PHE:CE2	2.61	0.83
3:4:445:TYR:O	3:4:462:ALA:HB1	1.79	0.82
8:K:162:GLN:HG3	9:L:243:LEU:HD23	1.61	0.82
1:1:31:UNK:O	1:1:34:UNK:CB	2.28	0.82
9:L:252:ASN:N	9:L:253:PRO:HD3	1.95	0.82
9:L:253:PRO:CD	9:L:254:LYS:H	1.91	0.81
4:5:223:UNK:CB	4:6:224:UNK:CB	2.58	0.81
1:1:291:UNK:C	5:F:350:LEU:CD2	2.58	0.81
2:2:291:UNK:O	2:2:294:UNK:N	2.14	0.81
4:6:239:UNK:HA	4:6:242:UNK:CB	2.10	0.81
4:6:41:UNK:CB	5:A:237:GLU:OE1	2.29	0.81
5:G:185:ILE:HD11	5:G:261:LEU:CG	2.09	0.81
1:1:262:UNK:O	1:1:266:UNK:N	2.14	0.81
1:1:351:UNK:O	1:1:352:UNK:C	2.27	0.80
9:L:250:PRO:O	9:L:253:PRO:HG2	1.80	0.80
4:6:247:UNK:CB	14:U:179:SER:HA	2.12	0.80
4:6:228:UNK:O	4:6:232:UNK:N	2.15	0.80
4:6:253:UNK:CB	15:V:32:GLN:CB	2.60	0.80
5:G:183:ILE:HD11	5:G:278:VAL:HG23	1.61	0.80
8:K:168:PHE:O	8:K:199:TYR:CE1	2.34	0.80
1:1:115:UNK:CB	2:2:119:UNK:CB	2.61	0.79
2:2:50:UNK:O	2:2:51:UNK:O	2.01	0.79
1:1:291:UNK:O	1:1:295:UNK:N	2.15	0.79
9:L:251:ASP:C	9:L:255:PHE:CD2	2.56	0.78
1:1:351:UNK:O	1:1:353:UNK:N	2.16	0.78
4:5:81:UNK:O	4:5:85:UNK:N	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:350:UNK:CB	2:2:353:UNK:CB	2.62	0.78
2:2:268:UNK:O	2:2:273:UNK:CB	2.32	0.77
3:3:365:LYS:CA	3:3:444:LEU:CB	2.63	0.77
1:1:281:UNK:HA	1:1:284:UNK:CB	2.15	0.77
4:5:58:UNK:O	4:5:62:UNK:N	2.18	0.77
1:1:289:UNK:CB	5:F:346:ILE:CG2	2.63	0.77
3:4:365:LYS:CA	3:4:444:LEU:CB	2.63	0.76
8:K:168:PHE:CD2	8:K:200:GLU:HG3	2.20	0.76
2:2:359:UNK:CB	2:2:423:UNK:HA	2.16	0.76
1:1:292:UNK:HA	5:F:350:LEU:CD2	2.14	0.75
1:1:351:UNK:C	1:1:353:UNK:N	2.44	0.75
4:5:201:UNK:O	4:5:205:UNK:CB	2.34	0.75
4:6:106:UNK:O	4:6:110:UNK:N	2.19	0.75
9:L:251:ASP:C	9:L:255:PHE:HD2	1.89	0.75
1:1:65:UNK:CB	1:1:75:UNK:CB	2.64	0.74
1:1:281:UNK:O	1:1:284:UNK:C	2.34	0.74
4:6:247:UNK:CB	14:U:179:SER:CA	2.66	0.74
1:1:271:UNK:O	1:1:274:UNK:HA	1.87	0.74
4:5:244:UNK:CB	4:6:245:UNK:CB	2.65	0.74
4:5:138:UNK:O	4:5:142:UNK:CB	2.35	0.74
4:6:116:UNK:O	4:6:120:UNK:N	2.20	0.74
12:P:37:UNK:HA	12:P:73:UNK:O	1.88	0.74
4:5:173:UNK:O	4:5:177:UNK:N	2.20	0.73
4:6:238:UNK:O	4:6:242:UNK:CB	2.35	0.73
12:O:67:UNK:O	12:O:73:UNK:HA	1.89	0.73
4:5:203:UNK:O	4:5:207:UNK:N	2.21	0.73
9:L:251:ASP:HB2	9:L:255:PHE:CE2	2.24	0.73
1:1:292:UNK:HA	5:F:350:LEU:HD22	1.71	0.73
1:1:311:UNK:CB	1:1:312:UNK:H	2.01	0.73
1:1:311:UNK:CA	1:1:312:UNK:O	2.37	0.72
9:L:250:PRO:C	9:L:253:PRO:HD3	2.09	0.72
1:1:312:UNK:C	1:1:313:UNK:CA	2.68	0.72
9:L:245:SER:OG	9:L:248:VAL:HG23	1.80	0.71
4:5:108:UNK:O	4:5:112:UNK:N	2.23	0.71
1:1:359:UNK:CB	1:1:423:UNK:CA	2.63	0.71
1:1:144:UNK:O	1:1:145:UNK:C	2.34	0.71
8:K:168:PHE:HA	8:K:199:TYR:CE1	2.26	0.71
4:5:237:UNK:CB	4:6:238:UNK:CB	2.69	0.71
1:1:281:UNK:C	1:1:284:UNK:N	2.53	0.71
4:6:107:UNK:O	4:6:111:UNK:N	2.24	0.71
4:5:57:UNK:O	4:5:61:UNK:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:124:CYS:SG	8:K:224:THR:HG23	2.31	0.70
2:2:291:UNK:O	2:2:295:UNK:N	2.25	0.70
2:2:281:UNK:O	2:2:284:UNK:O	2.09	0.70
4:6:186:UNK:O	4:6:190:UNK:N	2.25	0.70
9:L:245:SER:CB	9:L:248:VAL:CG2	2.59	0.69
1:1:354:UNK:O	1:1:358:UNK:HG2	1.91	0.69
2:2:359:UNK:CA	2:2:423:UNK:HA	2.21	0.69
8:K:168:PHE:CA	8:K:199:TYR:CE1	2.74	0.69
4:6:116:UNK:O	4:6:120:UNK:CB	2.40	0.69
2:2:144:UNK:C	2:2:146:UNK:N	2.52	0.69
4:5:202:UNK:O	4:5:206:UNK:CB	2.41	0.69
1:1:248:UNK:O	1:1:249:UNK:C	2.40	0.69
4:6:79:UNK:O	4:6:83:UNK:N	2.25	0.69
8:K:118:LYS:O	8:K:122:GLU:HG3	1.94	0.68
2:2:215:UNK:CB	2:2:219:UNK:CA	2.71	0.68
8:K:93:LYS:HZ1	8:K:122:GLU:CD	1.91	0.68
9:L:252:ASN:N	9:L:253:PRO:CD	2.56	0.68
9:L:250:PRO:O	9:L:253:PRO:HD2	1.91	0.67
3:4:445:TYR:O	3:4:462:ALA:CB	2.43	0.67
4:6:227:UNK:O	4:6:231:UNK:N	2.27	0.67
2:2:203:UNK:O	2:2:206:UNK:N	2.28	0.67
4:6:238:UNK:O	4:6:242:UNK:CA	2.43	0.67
3:3:445:TYR:O	3:3:462:ALA:CB	2.43	0.67
1:1:291:UNK:CA	5:F:350:LEU:HD21	2.25	0.66
1:1:309:UNK:HA	1:1:348:UNK:CB	2.26	0.66
2:2:290:UNK:O	2:2:293:UNK:N	2.27	0.66
2:2:282:UNK:N	2:2:286:UNK:CB	2.58	0.66
1:1:281:UNK:CA	1:1:284:UNK:CB	2.73	0.66
4:6:207:UNK:O	4:6:211:UNK:N	2.29	0.66
5:G:375:THR:HG23	5:G:376:PHE:H	1.62	0.65
4:6:249:UNK:O	4:6:253:UNK:N	2.29	0.65
1:1:312:UNK:C	1:1:313:UNK:H2	2.06	0.65
1:1:288:UNK:O	1:1:289:UNK:C	2.40	0.65
5:G:121:ARG:HE	5:G:375:THR:HG21	1.61	0.65
4:6:253:UNK:CB	15:V:31:SER:C	2.64	0.64
8:K:168:PHE:C	8:K:199:TYR:CE1	2.71	0.64
12:O:66:UNK:HA	12:O:74:UNK:O	1.96	0.64
2:2:279:UNK:O	2:2:283:UNK:N	2.31	0.63
1:1:216:UNK:O	1:1:217:UNK:C	2.47	0.63
2:2:215:UNK:CB	2:2:216:UNK:CA	2.76	0.63
8:K:93:LYS:CE	8:K:122:GLU:CD	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:306:UNK:O	1:1:310:UNK:N	2.32	0.63
2:2:354:UNK:O	2:2:358:UNK:HG2	1.98	0.63
1:1:262:UNK:HA	1:1:265:UNK:CB	2.28	0.63
5:A:350:LEU:HD13	9:L:265:VAL:HG22	1.80	0.62
8:K:198:TYR:HB2	9:L:235:LYS:HG2	1.81	0.62
4:5:59:UNK:O	4:5:63:UNK:N	2.32	0.62
4:5:172:UNK:O	4:5:176:UNK:N	2.33	0.62
2:2:291:UNK:O	2:2:292:UNK:C	2.47	0.62
2:2:307:UNK:O	2:2:311:UNK:CB	2.47	0.62
8:K:153:THR:HG22	8:K:180:THR:HG22	1.81	0.61
9:L:250:PRO:C	9:L:253:PRO:CD	2.66	0.61
1:1:291:UNK:CB	5:F:350:LEU:CD1	2.77	0.61
2:2:355:UNK:CB	2:2:419:UNK:CA	2.74	0.61
4:5:198:UNK:O	4:5:202:UNK:N	2.33	0.61
4:6:80:UNK:O	4:6:84:UNK:CB	2.49	0.61
4:6:214:UNK:O	4:6:218:UNK:N	2.34	0.60
1:1:262:UNK:O	1:1:265:UNK:CB	2.50	0.60
1:1:359:UNK:CA	1:1:423:UNK:HA	2.32	0.60
4:5:137:UNK:O	4:5:141:UNK:CB	2.50	0.60
1:1:352:UNK:O	1:1:355:UNK:N	2.34	0.60
8:K:168:PHE:O	8:K:199:TYR:HD1	1.82	0.60
1:1:364:UNK:O	1:1:367:UNK:CB	2.50	0.60
4:6:152:UNK:O	4:6:156:UNK:N	2.34	0.60
1:1:281:UNK:O	1:1:284:UNK:O	2.20	0.60
3:3:599:SER:HA	3:3:626:TYR:O	2.03	0.59
5:G:185:ILE:HG23	5:G:185:ILE:O	2.02	0.59
12:P:35:UNK:HA	12:P:75:UNK:O	2.02	0.59
9:L:143:LYS:HB3	9:L:180:ASN:HB2	1.85	0.59
2:2:144:UNK:O	2:2:147:UNK:N	2.35	0.59
2:2:203:UNK:O	2:2:206:UNK:CA	2.51	0.59
2:2:359:UNK:HA	2:2:423:UNK:HA	1.85	0.59
3:4:599:SER:HA	3:4:626:TYR:O	2.02	0.59
5:A:271:GLU:OE2	8:K:266:ARG:NH1	2.36	0.59
1:1:248:UNK:C	1:1:250:UNK:N	2.62	0.59
2:2:130:UNK:CB	2:2:174:UNK:CB	2.81	0.58
4:5:110:UNK:O	4:5:114:UNK:CB	2.52	0.58
8:K:26:PRO:HB2	8:K:172:ARG:HD3	1.85	0.58
4:5:109:UNK:O	4:5:113:UNK:CA	2.51	0.58
2:2:290:UNK:C	2:2:292:UNK:N	2.63	0.58
8:K:168:PHE:HD2	8:K:200:GLU:HG3	1.65	0.58
4:6:78:UNK:O	4:6:82:UNK:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:27:GLY:HA3	8:K:170:ASN:ND2	2.19	0.58
1:1:272:UNK:C	1:1:274:UNK:N	2.60	0.57
4:5:240:UNK:HA	4:5:243:UNK:CB	2.34	0.57
8:K:167:ASN:HB3	8:K:169:TRP:CD1	2.40	0.57
2:2:41:UNK:O	2:2:44:UNK:CB	2.53	0.57
8:K:40:LEU:HB3	8:K:46:LEU:HD11	1.86	0.57
1:1:144:UNK:O	1:1:146:UNK:N	2.38	0.57
9:L:239:ILE:O	9:L:243:LEU:HG	2.04	0.57
9:L:251:ASP:C	9:L:253:PRO:CD	2.73	0.56
4:5:137:UNK:O	4:5:141:UNK:CA	2.53	0.56
8:K:79:HIS:CD2	8:K:155:ILE:HG21	2.40	0.56
4:5:174:UNK:O	4:5:178:UNK:CA	2.53	0.56
1:1:261:UNK:O	1:1:265:UNK:N	2.39	0.56
5:G:121:ARG:NE	5:G:375:THR:HG21	2.21	0.56
4:5:254:UNK:HA	4:5:257:UNK:CB	2.36	0.55
8:K:93:LYS:CE	8:K:122:GLU:OE1	2.54	0.55
8:K:121:ARG:NE	8:K:154:ILE:HG12	2.20	0.55
4:5:58:UNK:O	4:5:62:UNK:CB	2.54	0.55
11:N:437:UNK:O	11:N:441:UNK:N	2.40	0.55
8:K:168:PHE:HA	8:K:199:TYR:CZ	2.42	0.55
8:K:198:TYR:CZ	8:K:200:GLU:HB2	2.42	0.55
1:1:18:UNK:O	1:1:22:UNK:N	2.41	0.54
1:1:292:UNK:N	5:F:350:LEU:HD23	2.09	0.54
4:6:108:UNK:O	4:6:112:UNK:N	2.39	0.54
1:1:29:UNK:O	1:1:30:UNK:C	2.53	0.54
1:1:291:UNK:O	1:1:295:UNK:CB	2.55	0.54
2:2:214:UNK:C	2:2:216:UNK:CA	2.57	0.54
5:B:352:THR:HG21	8:K:278:LYS:CB	2.37	0.54
5:G:182:ARG:C	5:G:183:ILE:HG13	2.28	0.54
7:J:128:LEU:HD13	7:J:136:ALA:HB3	1.90	0.54
9:L:108:ARG:HD3	9:L:117:SER:HB3	1.89	0.54
9:L:253:PRO:CD	9:L:254:LYS:N	2.55	0.54
11:N:433:UNK:O	11:N:437:UNK:N	2.41	0.54
2:2:214:UNK:O	2:2:216:UNK:CB	2.51	0.53
1:1:291:UNK:CB	5:F:350:LEU:CD2	2.78	0.53
1:1:328:UNK:CB	1:1:331:UNK:CB	2.87	0.53
9:L:61:LEU:HD22	9:L:71:TYR:CD2	2.44	0.53
9:L:66:ARG:HD3	9:L:71:TYR:CE2	2.44	0.53
2:2:284:UNK:O	2:2:285:UNK:C	2.54	0.53
1:1:216:UNK:C	1:1:218:UNK:N	2.67	0.53
3:4:365:LYS:CB	3:4:444:LEU:CB	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:190:VAL:HG22	5:I:261:LEU:HD23	1.90	0.53
2:2:292:UNK:O	2:2:296:UNK:CB	2.56	0.53
9:L:50:ALA:HB2	9:L:61:LEU:HD21	1.91	0.53
3:3:365:LYS:CB	3:3:444:LEU:CB	2.87	0.53
9:L:100:ALA:HB2	9:L:210:ILE:HD13	1.91	0.53
4:5:81:UNK:O	4:5:85:UNK:CB	2.57	0.52
4:5:138:UNK:O	4:5:142:UNK:CA	2.57	0.52
4:6:80:UNK:O	4:6:84:UNK:N	2.42	0.52
4:5:239:UNK:O	4:5:243:UNK:N	2.42	0.52
1:1:262:UNK:O	1:1:265:UNK:CA	2.57	0.52
2:2:214:UNK:CB	2:2:216:UNK:HG2	2.39	0.52
9:L:96:LEU:HG	9:L:210:ILE:HD11	1.90	0.52
11:N:284:UNK:O	11:N:288:UNK:N	2.43	0.52
1:1:262:UNK:O	1:1:265:UNK:N	2.42	0.52
8:K:237:ASN:OD1	9:L:246:VAL:HG21	2.09	0.52
1:1:312:UNK:CA	1:1:313:UNK:N	2.73	0.52
8:K:118:LYS:HG2	8:K:145:ALA:HB1	1.90	0.52
4:6:229:UNK:O	4:6:233:UNK:N	2.43	0.52
2:2:291:UNK:C	2:2:293:UNK:N	2.64	0.51
2:2:308:UNK:O	2:2:311:UNK:O	2.28	0.51
2:2:344:UNK:O	2:2:345:UNK:C	2.55	0.51
11:N:287:UNK:O	11:N:291:UNK:N	2.43	0.51
5:I:185:ILE:HD11	5:I:261:LEU:HD21	1.92	0.51
12:P:37:UNK:CA	12:P:73:UNK:O	2.57	0.51
1:1:359:UNK:O	1:1:426:UNK:CB	2.58	0.51
2:2:214:UNK:O	2:2:216:UNK:CG	2.58	0.51
2:2:291:UNK:CB	6:H:350:SER:H	2.24	0.51
8:K:237:ASN:OD1	9:L:246:VAL:CG2	2.58	0.51
9:L:144:ILE:HG23	9:L:178:GLN:O	2.11	0.51
1:1:64:UNK:HA	1:1:75:UNK:O	2.11	0.51
12:P:38:UNK:O	12:P:73:UNK:CB	2.58	0.51
1:1:98:UNK:O	1:1:116:UNK:CB	2.58	0.50
8:K:67:ILE:HB	8:K:70:TYR:CD1	2.46	0.50
1:1:31:UNK:O	1:1:35:UNK:N	2.45	0.50
12:O:65:UNK:O	12:O:76:UNK:N	2.44	0.50
12:P:37:UNK:C	12:P:73:UNK:O	2.59	0.50
5:I:72:ARG:NH2	7:J:277:GLU:OE2	2.45	0.50
4:6:79:UNK:O	4:6:83:UNK:CB	2.60	0.49
4:6:206:UNK:O	4:6:210:UNK:N	2.45	0.49
8:K:39:LEU:HD21	9:L:32:VAL:CG2	2.42	0.49
8:K:64:PRO:HB3	8:K:75:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:131:TYR:CG	8:K:229:ILE:HG21	2.47	0.49
2:2:266:UNK:O	2:2:269:UNK:CB	2.60	0.49
4:6:107:UNK:O	4:6:111:UNK:CB	2.60	0.49
6:H:43:VAL:HG21	7:J:156:PRO:HG2	1.94	0.49
8:K:258:LEU:HD12	9:L:148:TRP:HB2	1.93	0.49
1:1:273:UNK:O	1:1:274:UNK:CB	2.60	0.49
4:5:59:UNK:O	4:5:63:UNK:CB	2.60	0.49
4:5:254:UNK:O	4:5:258:UNK:N	2.46	0.49
4:5:261:UNK:CB	4:6:262:UNK:CB	2.91	0.49
1:1:99:UNK:O	1:1:100:UNK:CB	2.60	0.49
10:M:240:UNK:O	10:M:244:UNK:N	2.45	0.49
4:5:199:UNK:CB	4:6:200:UNK:CB	2.91	0.49
8:K:192:LEU:O	8:K:209:HIS:HA	2.12	0.49
1:1:306:UNK:O	1:1:309:UNK:N	2.46	0.48
8:K:75:LEU:N	8:K:142:THR:OG1	2.46	0.48
1:1:307:UNK:O	1:1:311:UNK:N	2.45	0.48
1:1:289:UNK:CB	5:F:346:ILE:HG23	2.41	0.48
4:6:117:UNK:O	4:6:121:UNK:CB	2.61	0.48
5:A:281:PHE:CD2	9:L:230:GLU:OE2	2.67	0.48
9:L:251:ASP:C	9:L:253:PRO:HD3	2.32	0.48
1:1:352:UNK:O	1:1:353:UNK:C	2.62	0.48
4:5:253:UNK:O	4:5:257:UNK:N	2.47	0.48
11:N:294:UNK:O	11:N:298:UNK:N	2.46	0.48
1:1:205:UNK:O	1:1:206:UNK:CB	2.60	0.47
2:2:282:UNK:HA	2:2:286:UNK:CB	2.44	0.47
5:G:185:ILE:HD11	5:G:261:LEU:CD1	2.43	0.47
4:5:173:UNK:O	4:5:177:UNK:CB	2.63	0.47
9:L:134:ILE:HB	9:L:150:SER:HB2	1.97	0.47
3:4:360:ALA:HA	3:4:368:GLN:O	2.15	0.47
4:6:185:UNK:O	4:6:189:UNK:N	2.48	0.47
8:K:259:ARG:NH2	9:L:148:TRP:CH2	2.82	0.47
3:3:360:ALA:HA	3:3:368:GLN:O	2.15	0.47
4:5:254:UNK:CB	4:6:255:UNK:CB	2.92	0.47
5:A:148:TYR:CE1	9:L:265:VAL:HG11	2.50	0.47
6:H:70:PRO:HG3	6:H:85:ILE:HD12	1.97	0.47
8:K:197:HIS:CE1	8:K:199:TYR:HB3	2.50	0.47
8:K:198:TYR:OH	8:K:200:GLU:HB3	2.14	0.47
8:K:171:GLY:HA3	9:L:239:ILE:CG2	2.44	0.47
8:K:243:ILE:HG23	9:L:187:MET:HE1	1.96	0.47
1:1:31:UNK:O	1:1:32:UNK:C	2.63	0.46
2:2:189:UNK:O	2:2:193:UNK:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:82:UNK:O	1:1:83:UNK:CB	2.62	0.46
1:1:220:UNK:O	1:1:224:UNK:N	2.48	0.46
5:C:11:PRO:HG2	5:C:348:ALA:HB1	1.98	0.46
12:P:37:UNK:HA	12:P:74:UNK:HA	1.98	0.46
8:K:121:ARG:HB3	8:K:154:ILE:HG12	1.98	0.46
8:K:117:LEU:HG	8:K:121:ARG:CZ	2.46	0.46
1:1:272:UNK:O	1:1:273:UNK:C	2.63	0.46
2:2:290:UNK:O	2:2:293:UNK:CB	2.64	0.46
5:B:352:THR:HG21	8:K:278:LYS:HB3	1.97	0.46
8:K:131:TYR:CD2	8:K:229:ILE:HG21	2.51	0.46
12:P:68:UNK:CB	12:P:72:UNK:O	2.64	0.46
1:1:248:UNK:O	1:1:250:UNK:N	2.49	0.46
4:6:106:UNK:O	4:6:110:UNK:CB	2.64	0.46
9:L:148:TRP:CZ2	9:L:173:VAL:HG13	2.51	0.46
9:L:261:GLU:O	9:L:265:VAL:HG23	2.16	0.46
2:2:200:UNK:O	2:2:202:UNK:N	2.48	0.46
4:6:115:UNK:O	4:6:119:UNK:N	2.49	0.46
2:2:282:UNK:CA	2:2:286:UNK:CB	2.94	0.45
9:L:72:ARG:HB2	9:L:79:TYR:CE2	2.51	0.45
7:J:128:LEU:HD11	7:J:133:ILE:HG13	1.98	0.45
1:1:146:UNK:HA	1:1:147:UNK:HA	1.79	0.45
8:K:28:GLU:O	8:K:32:VAL:N	2.47	0.45
9:L:173:VAL:HG21	9:L:224:ILE:HG21	1.98	0.45
8:K:252:ASP:O	8:K:256:LYS:HB2	2.17	0.45
8:K:269:ILE:HD11	9:L:107:TYR:HD1	1.81	0.45
4:6:152:UNK:O	4:6:156:UNK:CB	2.64	0.45
15:V:72:PRO:CB	15:V:101:ALA:HB2	2.46	0.45
5:I:185:ILE:HD13	5:I:268:ILE:HD11	1.99	0.44
5:G:371:ILE:O	5:G:375:THR:HG22	2.16	0.44
8:K:121:ARG:HE	8:K:154:ILE:HG12	1.82	0.44
9:L:108:ARG:NH1	9:L:117:SER:OG	2.50	0.44
1:1:248:UNK:O	1:1:251:UNK:CA	2.63	0.44
2:2:307:UNK:O	2:2:311:UNK:CA	2.63	0.44
8:K:129:ARG:HG2	8:K:141:CYS:SG	2.57	0.44
1:1:400:UNK:O	1:1:403:UNK:CB	2.66	0.44
8:K:181:ILE:HD12	8:K:181:ILE:N	2.33	0.44
4:6:153:UNK:O	4:6:157:UNK:CB	2.66	0.43
4:5:197:UNK:O	4:5:201:UNK:N	2.51	0.43
5:D:38:TYR:CD1	5:D:71:ILE:HG23	2.53	0.43
11:N:275:UNK:O	11:N:279:UNK:N	2.50	0.43
8:K:177:TRP:CZ2	8:K:192:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:290:UNK:O	1:1:294:UNK:N	2.51	0.43
8:K:32:VAL:O	8:K:36:VAL:HG23	2.19	0.43
9:L:156:VAL:HG21	9:L:213:ILE:HD11	1.99	0.43
10:M:50:UNK:O	10:M:54:UNK:N	2.52	0.43
7:J:365:GLN:HE22	16:Y:452:UNK:C	2.32	0.43
8:K:198:TYR:CB	9:L:235:LYS:HG2	2.48	0.43
2:2:281:UNK:O	2:2:286:UNK:CA	2.60	0.43
8:K:38:LEU:HD23	9:L:8:CYS:SG	2.59	0.43
8:K:198:TYR:CZ	8:K:200:GLU:CB	3.02	0.43
10:M:440:UNK:O	10:M:444:UNK:N	2.52	0.43
2:2:206:UNK:O	2:2:208:UNK:N	2.52	0.42
7:J:364:LEU:HD11	16:Y:449:UNK:HA	2.01	0.42
8:K:168:PHE:HB3	8:K:199:TYR:CE1	2.53	0.42
2:2:367:UNK:O	2:2:371:UNK:N	2.53	0.42
5:C:315:LEU:HG	5:C:330:ILE:HD12	2.01	0.42
4:5:200:UNK:O	4:5:204:UNK:N	2.53	0.42
4:5:196:UNK:O	4:5:200:UNK:N	2.53	0.42
10:M:261:UNK:O	10:M:265:UNK:N	2.52	0.42
2:2:203:UNK:O	2:2:206:UNK:CB	2.67	0.42
4:5:200:UNK:O	4:5:204:UNK:CB	2.68	0.42
2:2:89:UNK:O	2:2:90:UNK:O	2.38	0.42
5:I:43:LYS:HA	7:J:275:ASN:HB3	2.01	0.42
8:K:237:ASN:ND2	9:L:246:VAL:HG21	2.35	0.42
9:L:61:LEU:HD22	9:L:71:TYR:CG	2.54	0.42
4:6:228:UNK:O	4:6:232:UNK:CB	2.68	0.42
9:L:156:VAL:HG22	9:L:167:TYR:CD1	2.55	0.42
2:2:43:UNK:O	2:2:44:UNK:C	2.69	0.41
5:A:352:THR:HG21	9:L:261:GLU:HA	2.03	0.41
5:F:262:LEU:HB3	5:F:275:ILE:HD12	2.00	0.41
5:A:38:TYR:CD1	5:A:71:ILE:HG23	2.56	0.41
9:L:181:LYS:O	9:L:182:SER:OG	2.33	0.41
9:L:148:TRP:CD1	9:L:175:LEU:CD2	3.04	0.41
1:1:289:UNK:C	1:1:291:UNK:N	2.80	0.41
2:2:89:UNK:C	2:2:90:UNK:O	2.67	0.41
2:2:370:UNK:O	2:2:374:UNK:CA	2.63	0.41
5:G:262:LEU:HB3	5:G:275:ILE:HD12	2.02	0.41
5:G:315:LEU:HG	5:G:330:ILE:HD12	2.03	0.41
2:2:50:UNK:O	2:2:51:UNK:C	2.67	0.41
5:A:262:LEU:HB3	5:A:275:ILE:HD12	2.03	0.41
9:L:173:VAL:HG11	9:L:228:LEU:HD11	2.03	0.41
5:E:185:ILE:HG23	5:E:185:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:93:LYS:NZ	8:K:122:GLU:OE2	2.43	0.40
2:2:208:UNK:O	2:2:209:UNK:C	2.69	0.40
4:5:108:UNK:O	4:5:112:UNK:CB	2.69	0.40
1:1:66:UNK:O	1:1:94:UNK:HA	2.21	0.40
1:1:312:UNK:CA	1:1:313:UNK:H2	2.34	0.40
2:2:280:UNK:HA	2:2:283:UNK:CB	2.52	0.40
3:3:316:LYS:O	3:3:322:TYR:HA	2.21	0.40
3:4:316:LYS:O	3:4:322:TYR:HA	2.21	0.40
3:4:599:SER:CA	3:4:626:TYR:O	2.70	0.40
9:L:251:ASP:C	9:L:255:PHE:CE2	2.94	0.40
1:1:311:UNK:CB	1:1:312:UNK:O	2.69	0.40
3:3:582:VAL:HA	3:3:592:VAL:O	2.22	0.40
4:5:201:UNK:O	4:5:205:UNK:CA	2.69	0.40
4:6:239:UNK:CA	4:6:242:UNK:CB	2.93	0.40
11:N:289:UNK:HA	17:Z:1023:UNK:HA	2.03	0.40
2:2:146:UNK:O	2:2:147:UNK:CB	2.69	0.40
3:4:582:VAL:HA	3:4:592:VAL:O	2.22	0.40
3:4:647:SER:O	3:4:654:VAL:HA	2.22	0.40
8:K:113:VAL:HG12	8:K:114:ASP:N	2.36	0.40
8:K:128:LEU:HB2	8:K:229:ILE:HD11	2.02	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	75
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	30
15	V	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	25	64
18	a	44/48 (92%)	40 (91%)	3 (7%)	1 (2%)	6	36
19	b	65/71 (92%)	56 (86%)	8 (12%)	1 (2%)	10	45
20	c	27/31 (87%)	24 (89%)	2 (7%)	1 (4%)	3	26
21	d	18/20 (90%)	15 (83%)	1 (6%)	2 (11%)	0	6
All	All	5383/5457 (99%)	5060 (94%)	311 (6%)	12 (0%)	50	81

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	U	67	PRO
14	U	72	PRO
18	a	9	LEU
19	b	9	LEU
20	c	9	LEU
21	d	3	ASP
21	d	9	LEU
14	U	68	ASP
14	U	120	ILE
7	J	387	TRP
14	U	114	ILE
15	V	41	ILE

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	80
5	B	318/318 (100%)	314 (99%)	4 (1%)	69	86
5	C	318/318 (100%)	309 (97%)	9 (3%)	43	72
5	D	318/318 (100%)	309 (97%)	9 (3%)	43	72
5	E	318/318 (100%)	310 (98%)	8 (2%)	47	75
5	F	318/318 (100%)	313 (98%)	5 (2%)	62	83
5	G	318/318 (100%)	311 (98%)	7 (2%)	52	78
5	I	318/318 (100%)	312 (98%)	6 (2%)	57	80
6	H	313/313 (100%)	312 (100%)	1 (0%)	92	97
7	J	322/331 (97%)	318 (99%)	4 (1%)	71	87
8	K	245/245 (100%)	239 (98%)	6 (2%)	49	76
9	L	242/242 (100%)	236 (98%)	6 (2%)	47	75
18	a	31/41 (76%)	26 (84%)	5 (16%)	2	14
19	b	49/60 (82%)	38 (78%)	11 (22%)	1	4
20	c	7/16 (44%)	6 (86%)	1 (14%)	3	19
21	d	8/16 (50%)	7 (88%)	1 (12%)	4	23
All	All	3761/3808 (99%)	3672 (98%)	89 (2%)	51	76

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	82	ASP
5	A	184	ASP
5	A	197	TYR
5	A	231	ASP
5	A	279	LEU
5	A	357	TRP
5	B	197	TYR
5	B	231	ASP

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Mol	Chain	Res	Type
5	B	279	LEU
5	B	357	TRP
5	C	16	ASN
5	C	82	ASP
5	C	197	TYR
5	C	231	ASP
5	C	271	GLU
5	C	279	LEU
5	C	287	ASP
5	C	304	SER
5	C	357	TRP
5	D	30	ILE
5	D	183	ILE
5	D	197	TYR
5	D	231	ASP
5	D	271	GLU
5	D	287	ASP
5	D	289	ASP
5	D	314	LEU
5	D	357	TRP
5	E	183	ILE
5	E	197	TYR
5	E	231	ASP
5	E	279	LEU
5	E	287	ASP
5	E	289	ASP
5	E	314	LEU
5	E	357	TRP
5	F	28	ASP
5	F	231	ASP
5	F	287	ASP
5	F	289	ASP
5	F	357	TRP
5	G	183	ILE
5	G	197	TYR
5	G	231	ASP
5	G	271	GLU
5	G	273	GLU
5	G	287	ASP
5	G	357	TRP
6	H	49	GLN
5	I	183	ILE

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Mol	Chain	Res	Type
5	I	189	ASP
5	I	231	ASP
5	I	279	LEU
5	I	287	ASP
5	I	357	TRP
7	J	93	GLU
7	J	274	ASP
7	J	277	GLU
7	J	328	GLU
8	K	73	GLN
8	K	136	TYR
8	K	200	GLU
8	K	243	ILE
8	K	249	THR
8	K	258	LEU
9	L	118	SER
9	L	150	SER
9	L	200	ASP
9	L	235	LYS
9	L	245	SER
9	L	268	GLN
18	a	6	TYR
18	a	39	GLU
18	a	42	SER
18	a	51	ASN
18	a	53	ASN
19	b	6	TYR
19	b	14	ARG
19	b	37	LEU
19	b	39	GLU
19	b	42	SER
19	b	51	ASN
19	b	53	ASN
19	b	67	LYS
19	b	69	LEU
19	b	70	ASP
19	b	78	THR
20	c	6	TYR
21	d	3	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	37	ASN
5	F	98	GLN
5	G	98	GLN
6	H	246	GLN
8	K	41	ASN
8	K	61	GLN
8	K	73	GLN
8	K	79	HIS
8	K	84	ASN
8	K	197	HIS
9	L	209	HIS
18	a	51	ASN
19	b	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	D	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.42	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	ADP	E	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.44	4 (13%)
24	ATP	H	401	-	26,33,33	1.02	2 (7%)	31,52,52	1.50	5 (16%)
23	ADP	B	800	-	24,29,29	1.05	2 (8%)	29,45,45	1.41	4 (13%)
23	ADP	A	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.45	4 (13%)
23	ADP	J	800	-	24,29,29	1.04	2 (8%)	29,45,45	1.48	5 (17%)
23	ADP	G	800	-	24,29,29	1.05	2 (8%)	29,45,45	1.40	4 (13%)
23	ADP	F	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	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	D	800	-	-	4/12/32/32	0/3/3/3
23	ADP	E	800	-	-	3/12/32/32	0/3/3/3
24	ATP	H	401	-	-	4/18/38/38	0/3/3/3
23	ADP	B	800	-	-	4/12/32/32	0/3/3/3
23	ADP	A	800	-	-	2/12/32/32	0/3/3/3
23	ADP	J	800	-	-	4/12/32/32	0/3/3/3
23	ADP	G	800	-	-	3/12/32/32	0/3/3/3
23	ADP	F	800	-	-	0/12/32/32	0/3/3/3
23	ADP	I	800	-	-	0/12/32/32	0/3/3/3
23	ADP	C	800	-	-	0/12/32/32	0/3/3/3

All (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
23	E	800	ADP	C5-C4	2.68	1.48	1.40
23	C	800	ADP	C5-C4	2.66	1.48	1.40
23	F	800	ADP	C5-C4	2.66	1.48	1.40
23	A	800	ADP	C5-C4	2.66	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	800	ADP	C5-C4	2.63	1.47	1.40
23	E	800	ADP	C2-N3	2.32	1.35	1.32
23	C	800	ADP	C2-N3	2.29	1.35	1.32
23	F	800	ADP	C2-N3	2.28	1.35	1.32
23	B	800	ADP	C2-N3	2.27	1.35	1.32
24	H	401	ATP	C2-N3	2.25	1.35	1.32
23	D	800	ADP	C2-N3	2.24	1.35	1.32
23	I	800	ADP	C2-N3	2.24	1.35	1.32
23	G	800	ADP	C2-N3	2.24	1.35	1.32
23	J	800	ADP	C2-N3	2.23	1.35	1.32
23	A	800	ADP	C2-N3	2.21	1.35	1.32

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
23	I	800	ADP	N3-C2-N1	-3.66	122.95	128.68
23	C	800	ADP	N3-C2-N1	-3.66	122.95	128.68
23	E	800	ADP	N3-C2-N1	-3.64	122.99	128.68
24	H	401	ATP	N3-C2-N1	-3.63	123.00	128.68
23	G	800	ADP	N3-C2-N1	-3.63	123.01	128.68
23	I	800	ADP	PA-O3A-PB	-3.35	121.33	132.83
23	J	800	ADP	C3'-C2'-C1'	3.28	105.92	100.98
23	E	800	ADP	PA-O3A-PB	-3.22	121.77	132.83
24	H	401	ATP	PA-O3A-PB	-3.19	121.87	132.83
23	A	800	ADP	PA-O3A-PB	-3.17	121.95	132.83
23	F	800	ADP	C3'-C2'-C1'	3.16	105.73	100.98
23	C	800	ADP	C3'-C2'-C1'	3.14	105.70	100.98
23	D	800	ADP	PA-O3A-PB	-3.11	122.14	132.83
23	C	800	ADP	PA-O3A-PB	-3.11	122.16	132.83
23	I	800	ADP	C3'-C2'-C1'	3.08	105.61	100.98
23	F	800	ADP	PA-O3A-PB	-3.05	122.37	132.83
23	E	800	ADP	C3'-C2'-C1'	3.04	105.56	100.98
23	B	800	ADP	C3'-C2'-C1'	3.03	105.54	100.98
24	H	401	ATP	PB-O3B-PG	-3.03	122.44	132.83
23	A	800	ADP	C3'-C2'-C1'	3.02	105.53	100.98
23	J	800	ADP	PA-O3A-PB	-3.01	122.51	132.83
23	G	800	ADP	C3'-C2'-C1'	2.91	105.35	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	800	ADP	C4-C5-N7	-2.81	106.47	109.40
23	G	800	ADP	PA-O3A-PB	-2.80	123.20	132.83
23	D	800	ADP	C3'-C2'-C1'	2.80	105.20	100.98
23	B	800	ADP	PA-O3A-PB	-2.80	123.22	132.83
23	J	800	ADP	C4-C5-N7	-2.79	106.49	109.40
23	B	800	ADP	C4-C5-N7	-2.78	106.50	109.40
23	I	800	ADP	C4-C5-N7	-2.77	106.52	109.40
23	A	800	ADP	C4-C5-N7	-2.76	106.53	109.40
24	H	401	ATP	C4-C5-N7	-2.75	106.53	109.40
23	C	800	ADP	C4-C5-N7	-2.74	106.55	109.40
23	F	800	ADP	C4-C5-N7	-2.74	106.55	109.40
24	H	401	ATP	C3'-C2'-C1'	2.73	105.08	100.98
23	D	800	ADP	C4-C5-N7	-2.72	106.57	109.40
23	E	800	ADP	C4-C5-N7	-2.69	106.59	109.40
23	J	800	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (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
23	J	800	ADP	C3'-C4'-C5'-O5'
24	H	401	ATP	C3'-C4'-C5'-O5'
24	H	401	ATP	O4'-C4'-C5'-O5'
23	J	800	ADP	O4'-C4'-C5'-O5'
24	H	401	ATP	PB-O3A-PA-O5'
23	G	800	ADP	PA-O3A-PB-O1B
23	D	800	ADP	C5'-O5'-PA-O3A
23	E	800	ADP	C5'-O5'-PA-O3A
23	B	800	ADP	PB-O3A-PA-O2A
23	B	800	ADP	C5'-O5'-PA-O1A
23	J	800	ADP	C5'-O5'-PA-O1A
23	B	800	ADP	PB-O3A-PA-O1A
23	D	800	ADP	C3'-C4'-C5'-O5'
23	G	800	ADP	PA-O3A-PB-O2B
23	G	800	ADP	PA-O3A-PB-O3B
23	A	800	ADP	C5'-O5'-PA-O3A
24	H	401	ATP	C5'-O5'-PA-O3A

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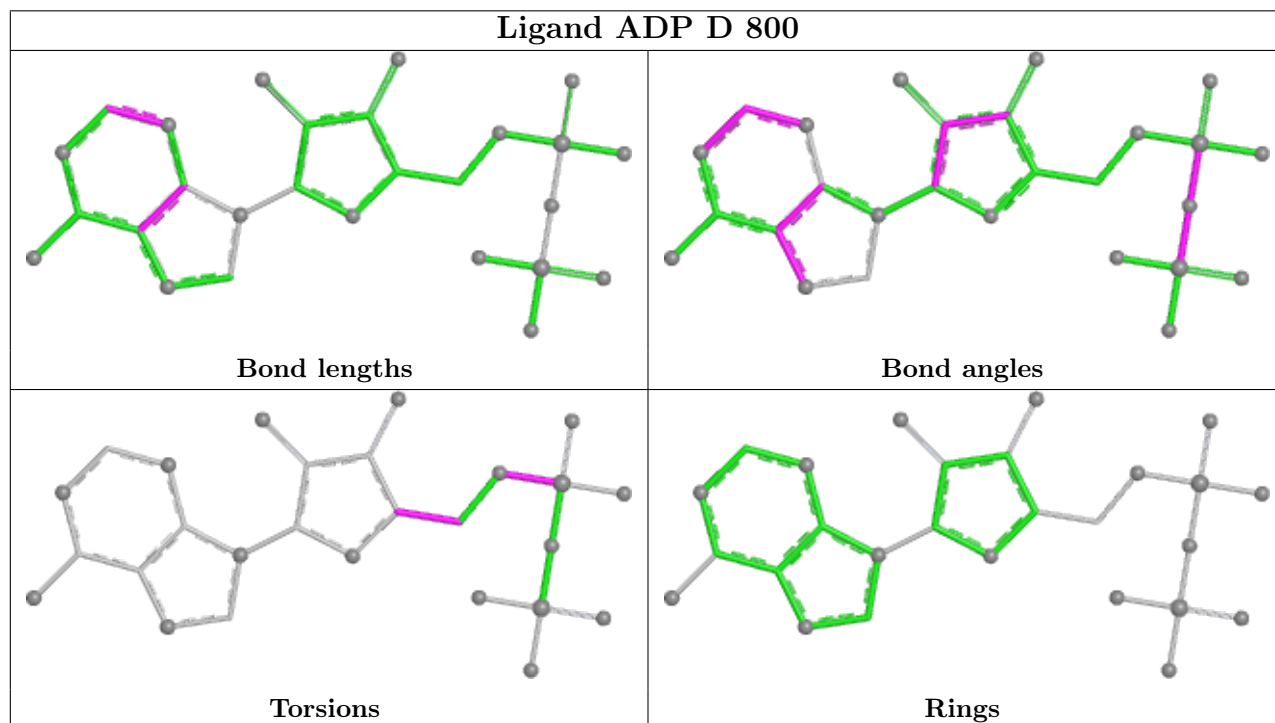
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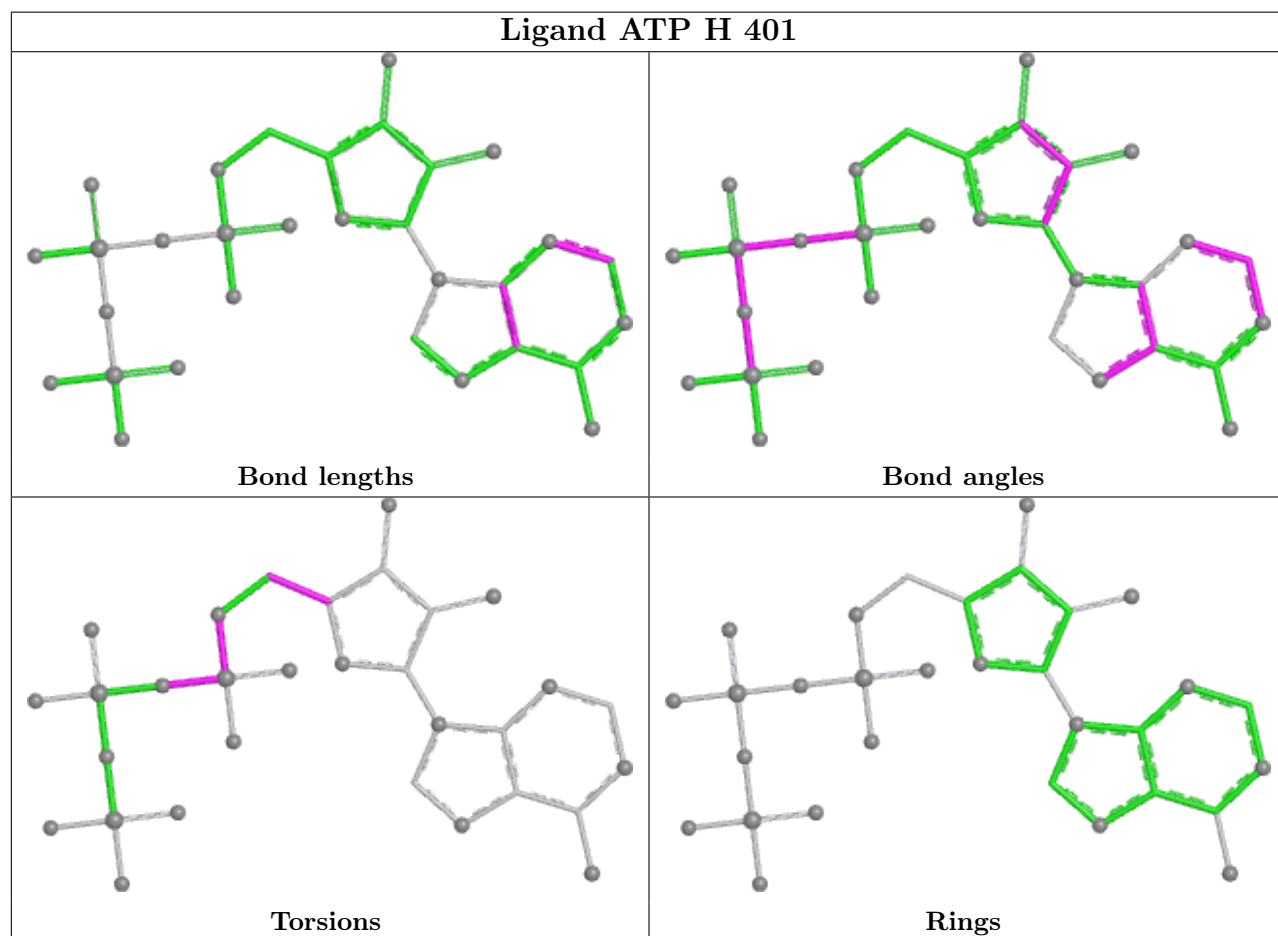
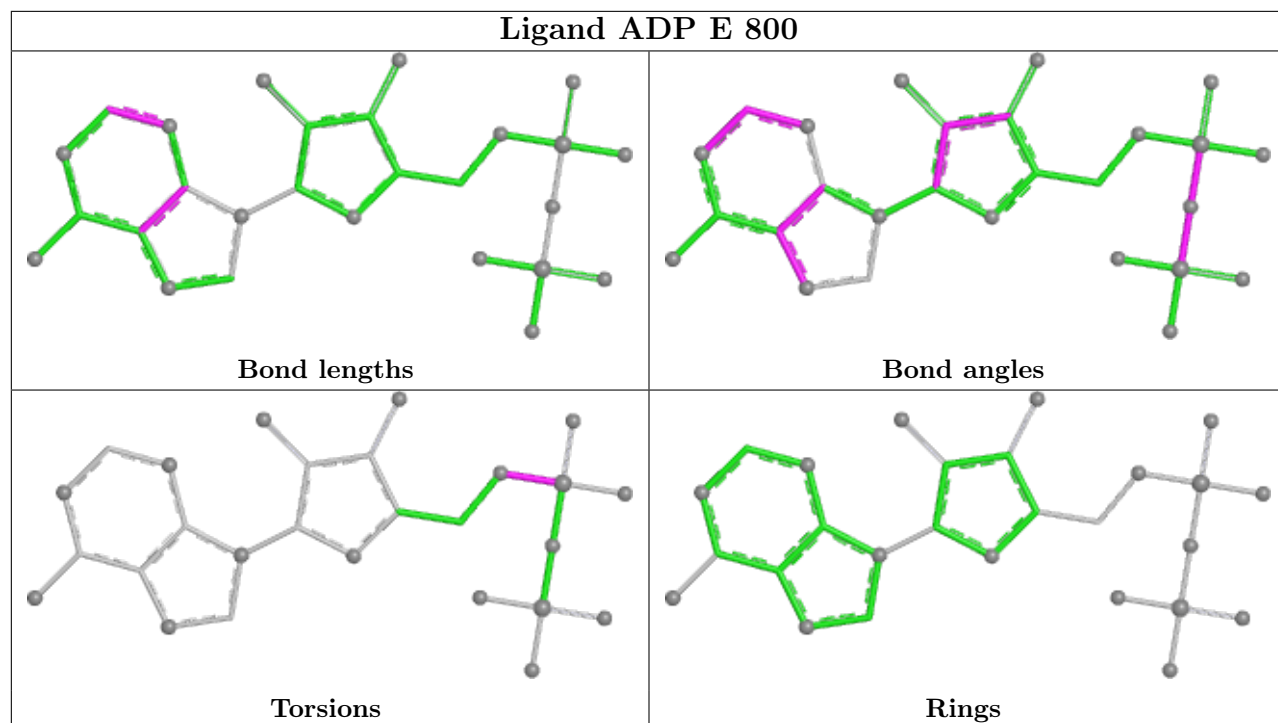
Mol	Chain	Res	Type	Atoms
23	A	800	ADP	C5'-O5'-PA-O1A
23	E	800	ADP	C5'-O5'-PA-O1A

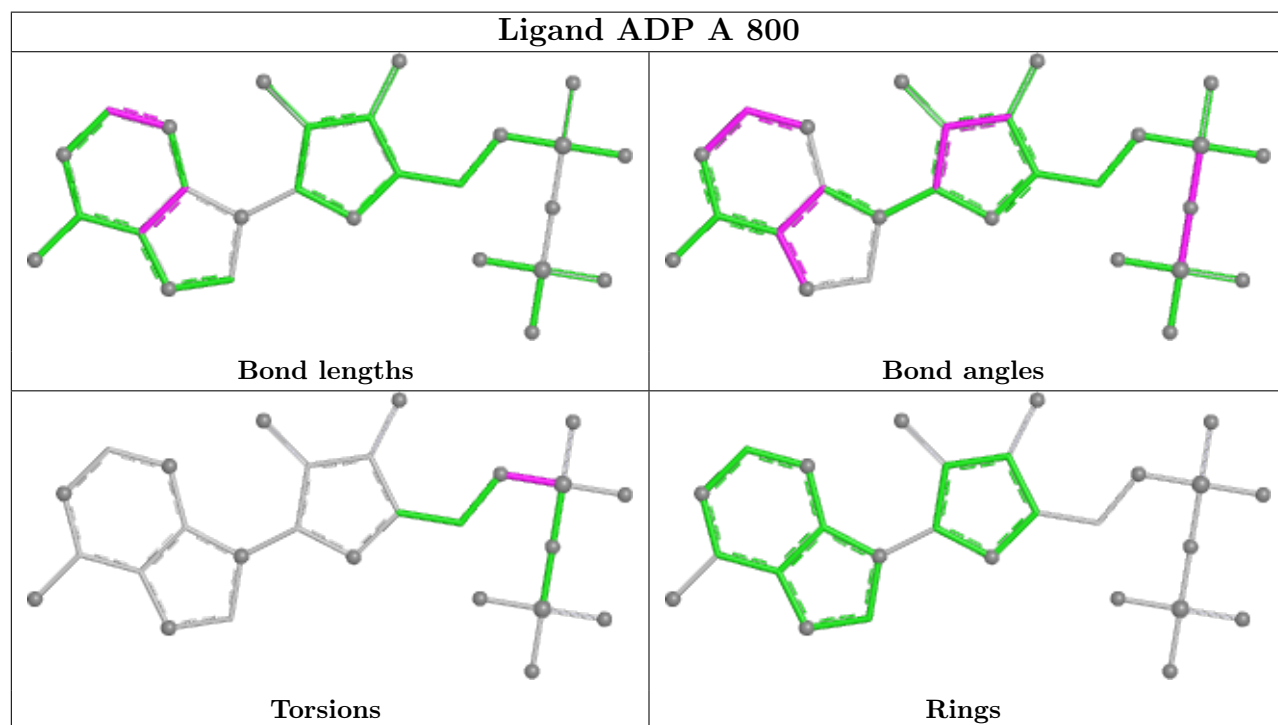
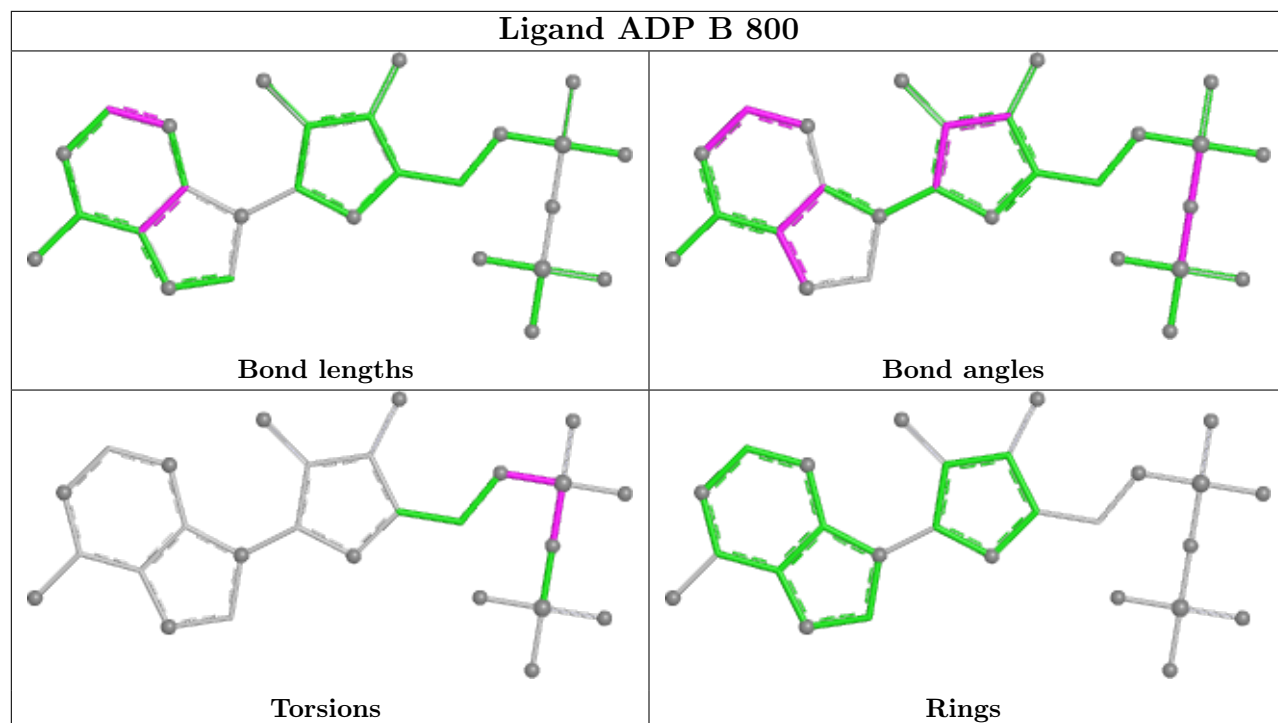
There are no ring outliers.

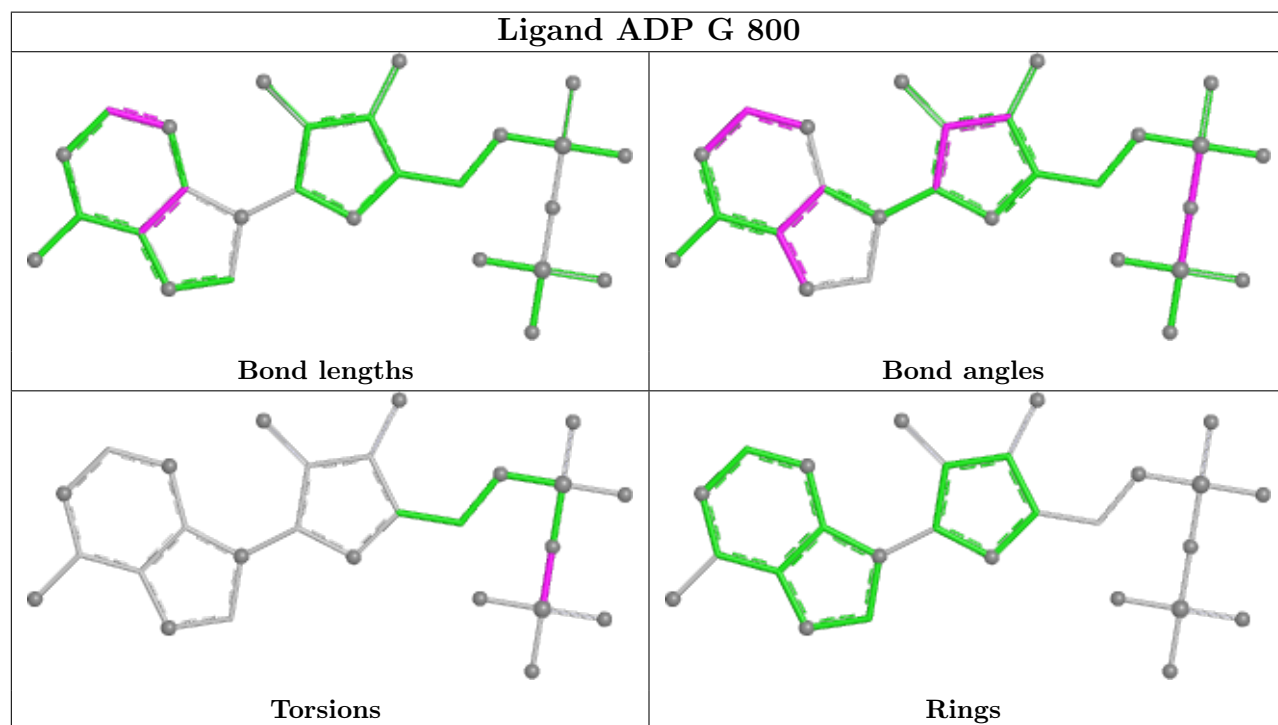
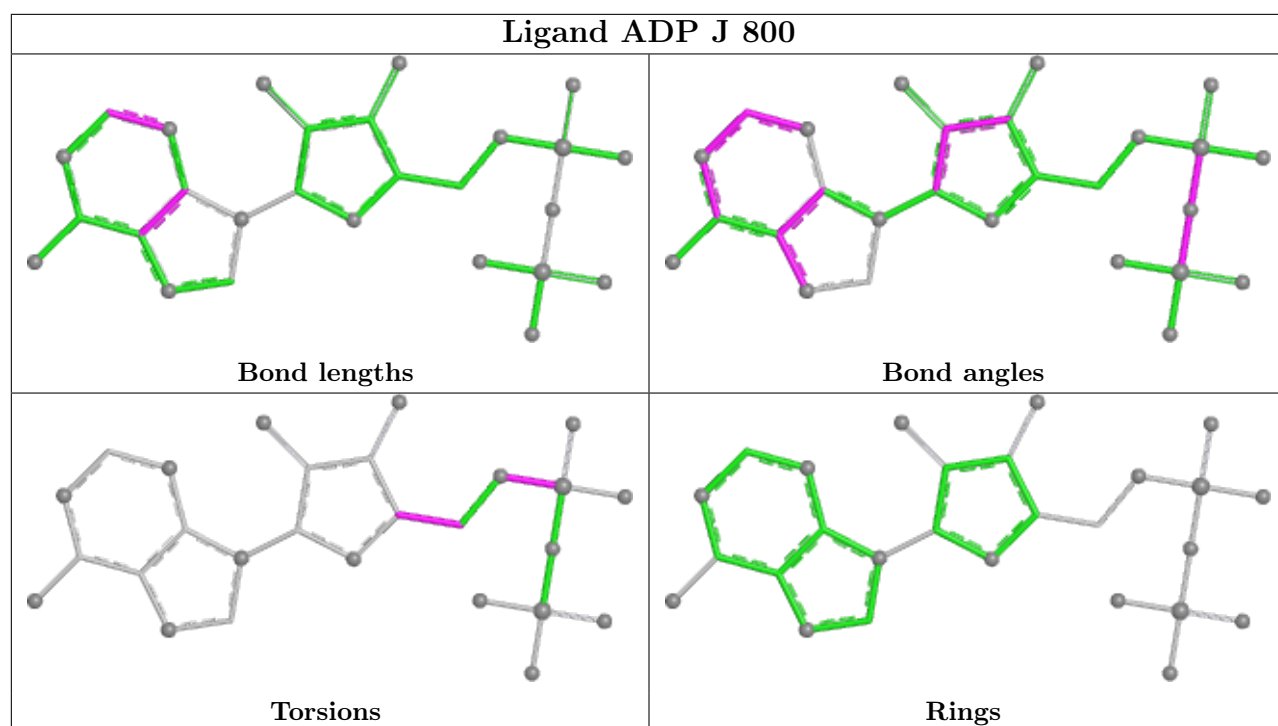
No monomer is involved in short contacts.

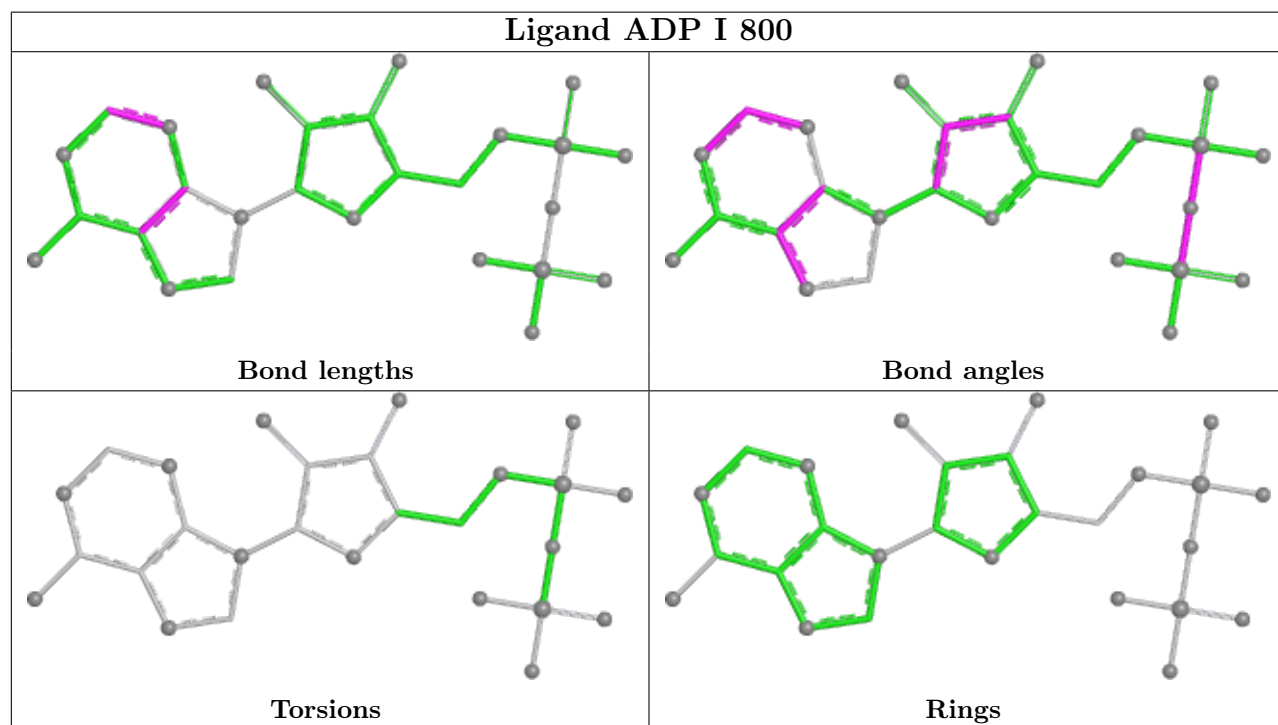
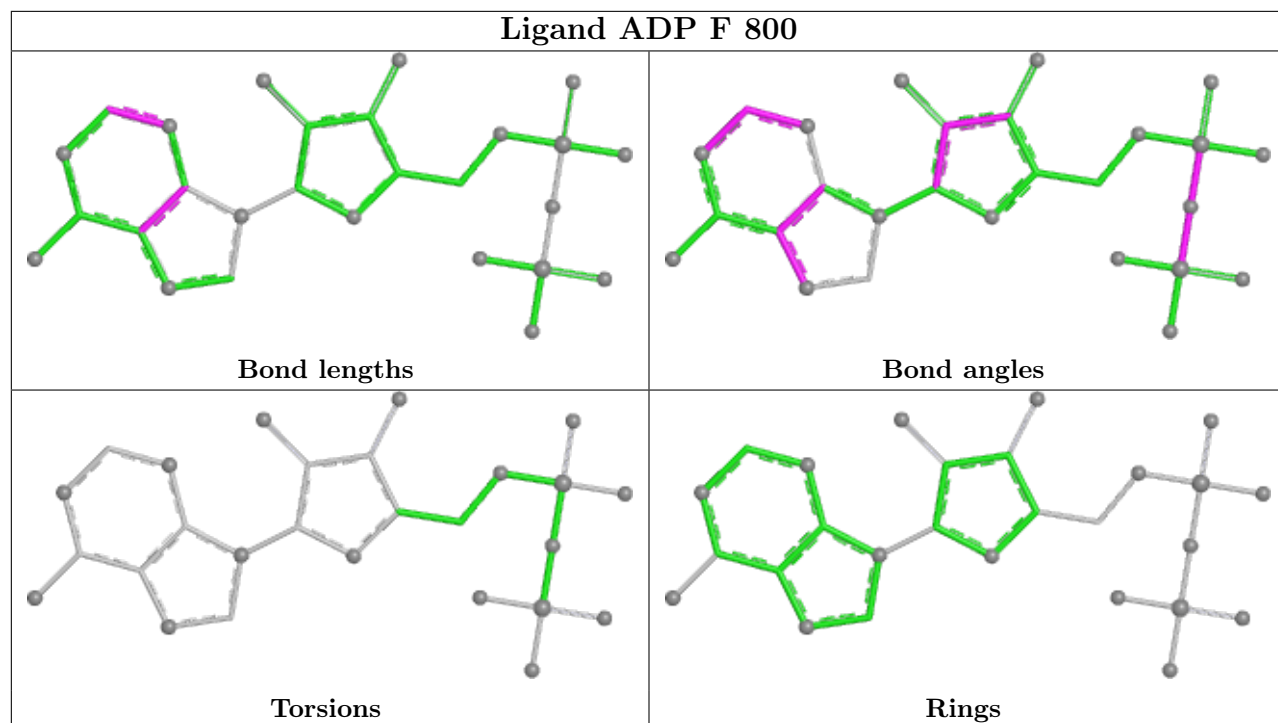
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

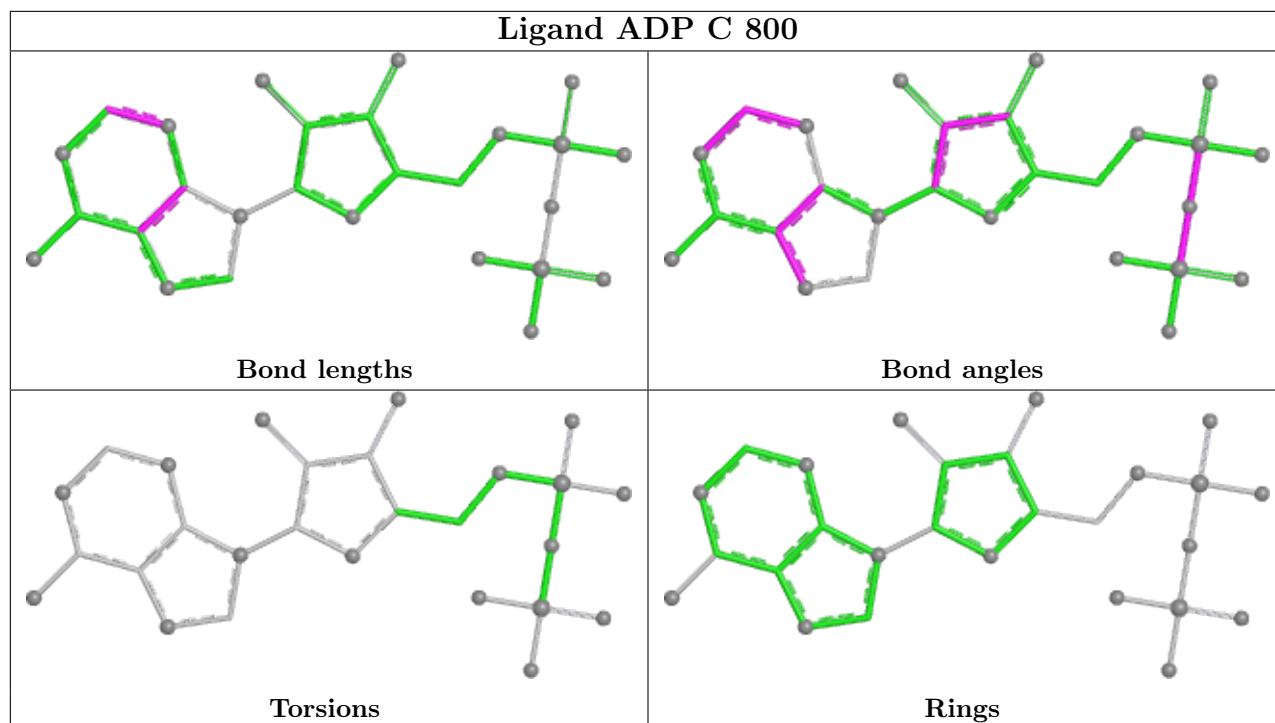












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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

All 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
1	N	634:UNK	C	701:UNK	N	67.12
1	Y	467:UNK	C	508:UNK	N	67.04
1	Y	40:UNK	C	155:UNK	N	62.15
1	Q	38:UNK	C	42:UNK	N	56.21
1	R	38:UNK	C	42:UNK	N	55.17
1	Y	359:UNK	C	415:UNK	N	40.33
1	M	741:UNK	C	801:UNK	N	35.77
1	N	768:UNK	C	801:UNK	N	29.90
1	Y	193:UNK	C	282:UNK	N	28.74
1	c	20:TYR	C	40:ALA	N	26.28
1	M	559:UNK	C	601:UNK	N	26.08
1	N	559:UNK	C	602:UNK	N	25.47
1	Y	160:UNK	C	181:UNK	N	25.09
1	Y	620:UNK	C	703:UNK	N	23.12
1	a	20:TYR	C	37:LEU	N	22.89
1	b	20:TYR	C	37:LEU	N	22.79
1	O	41:UNK	C	64:UNK	N	22.15
1	P	41:UNK	C	64:UNK	N	22.14
1	1	51:UNK	C	61:UNK	N	19.81
1	2	78:UNK	C	82:UNK	N	19.13
1	2	51:UNK	C	61:UNK	N	18.63
1	P	94:UNK	C	96:UNK	N	17.25
1	O	94:UNK	C	96:UNK	N	17.13
1	Q	62:UNK	C	64:UNK	N	16.54
1	R	62:UNK	C	64:UNK	N	16.50
1	P	78:UNK	C	80:UNK	N	15.76
1	O	78:UNK	C	80:UNK	N	15.75
1	2	374:UNK	C	381:UNK	N	15.54
1	2	236:UNK	C	248:UNK	N	15.23
1	3	383:ASP	C	441:SER	N	14.69
1	4	383:ASP	C	441:SER	N	14.69
1	1	374:UNK	C	381:UNK	N	14.50
1	1	237:UNK	C	248:UNK	N	14.47
1	Y	535:UNK	C	580:UNK	N	14.47
1	1	119:UNK	C	125:UNK	N	13.52
1	Y	611:UNK	C	615:UNK	N	13.18
1	2	90:UNK	C	94:UNK	N	12.85
1	1	179:UNK	C	180:UNK	N	12.49

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	410:UNK	C	418:UNK	N	12.43
1	2	410:UNK	C	418:UNK	N	12.28
1	2	119:UNK	C	125:UNK	N	11.74
1	1	78:UNK	C	82:UNK	N	11.27
1	2	319:UNK	C	328:UNK	N	9.52
1	2	147:UNK	C	157:UNK	N	8.69
1	1	90:UNK	C	94:UNK	N	8.37
1	Y	421:UNK	C	423:UNK	N	8.18
1	Y	597:UNK	C	601:UNK	N	7.90
1	1	319:UNK	C	328:UNK	N	7.73
1	1	148:UNK	C	157:UNK	N	7.15
1	1	66:UNK	C	73:UNK	N	7.13
1	Y	586:UNK	C	588:UNK	N	7.02
1	2	179:UNK	C	180:UNK	N	6.93
1	3	566:ASP	C	573:THR	N	6.80
1	4	566:ASP	C	573:THR	N	6.80
1	3	605:LEU	C	621:THR	N	6.16
1	4	605:LEU	C	621:THR	N	6.16
1	2	66:UNK	C	73:UNK	N	6.08
1	2	99:UNK	C	114:UNK	N	5.30
1	1	100:UNK	C	114:UNK	N	5.09
1	Y	298:UNK	C	300:UNK	N	4.19
1	1	311:UNK	C	312:UNK	N	3.91
1	b	64:VAL	C	65:GLY	N	3.04
1	1	312:UNK	C	313:UNK	N	2.25

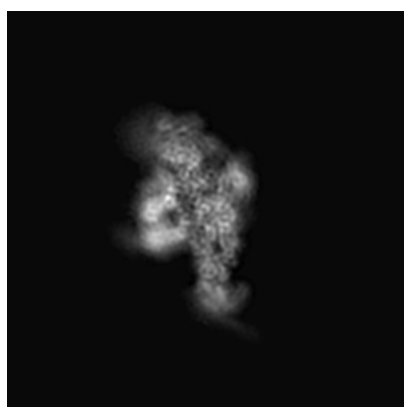
6 Map visualisation [i](#)

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.

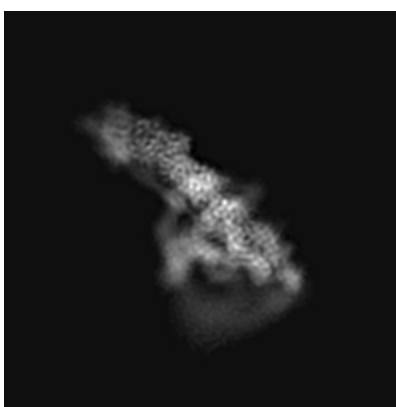
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

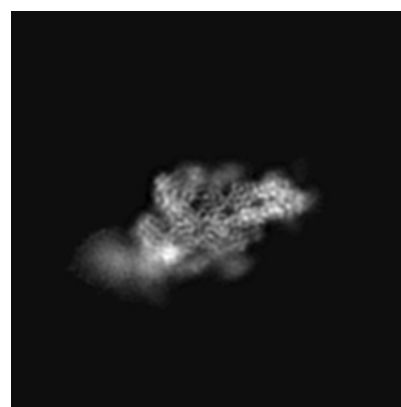
6.1.1 Primary map



X



Y

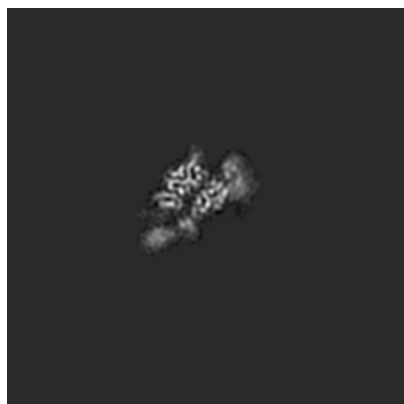


Z

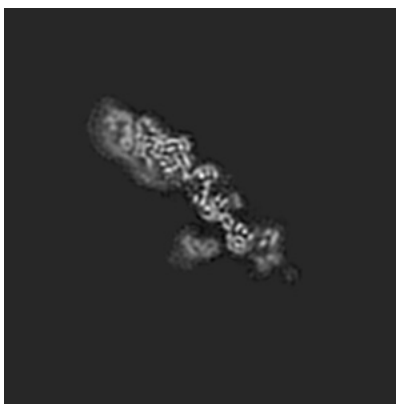
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

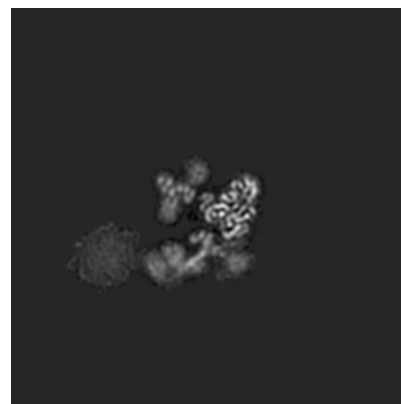
6.2.1 Primary map



X Index: 216



Y Index: 216

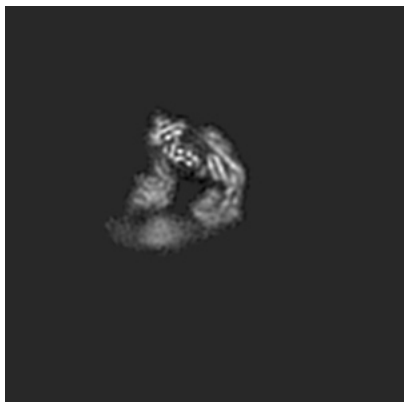


Z Index: 216

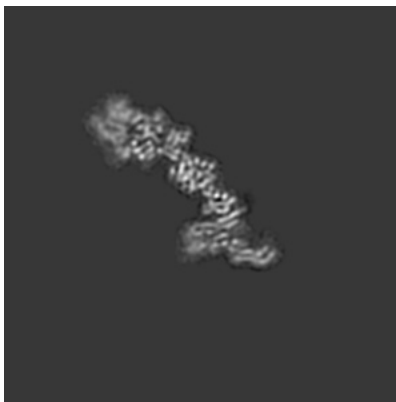
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

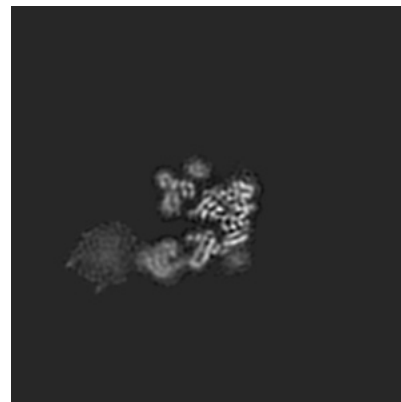
6.3.1 Primary map



X Index: 166



Y Index: 230



Z Index: 221

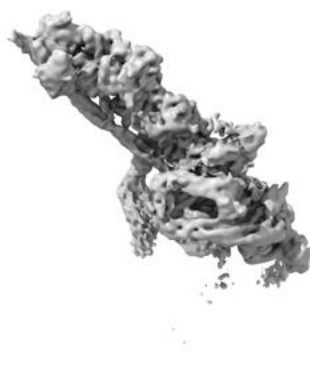
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 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.

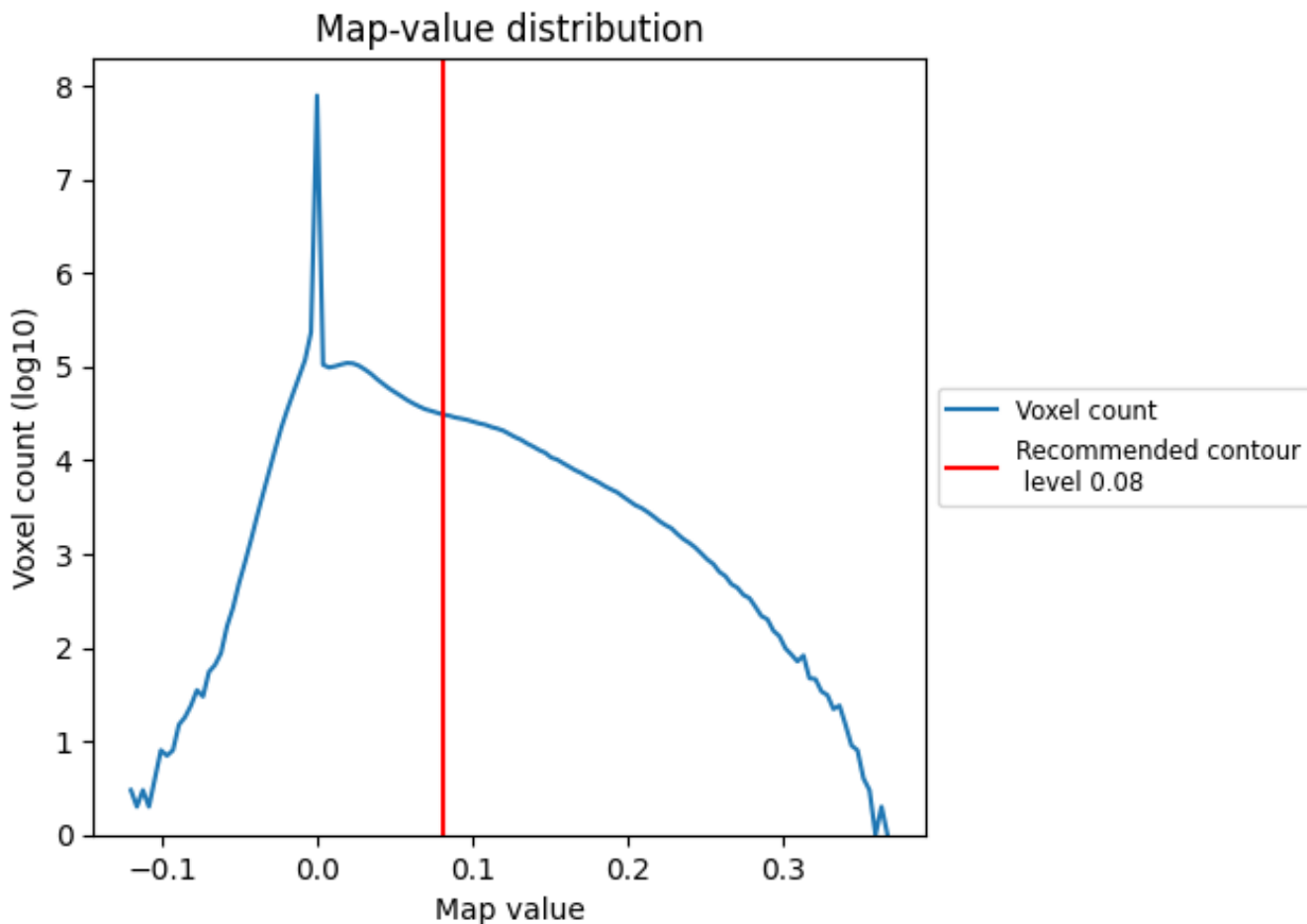
6.5 Mask visualisation

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

7 Map analysis [i](#)

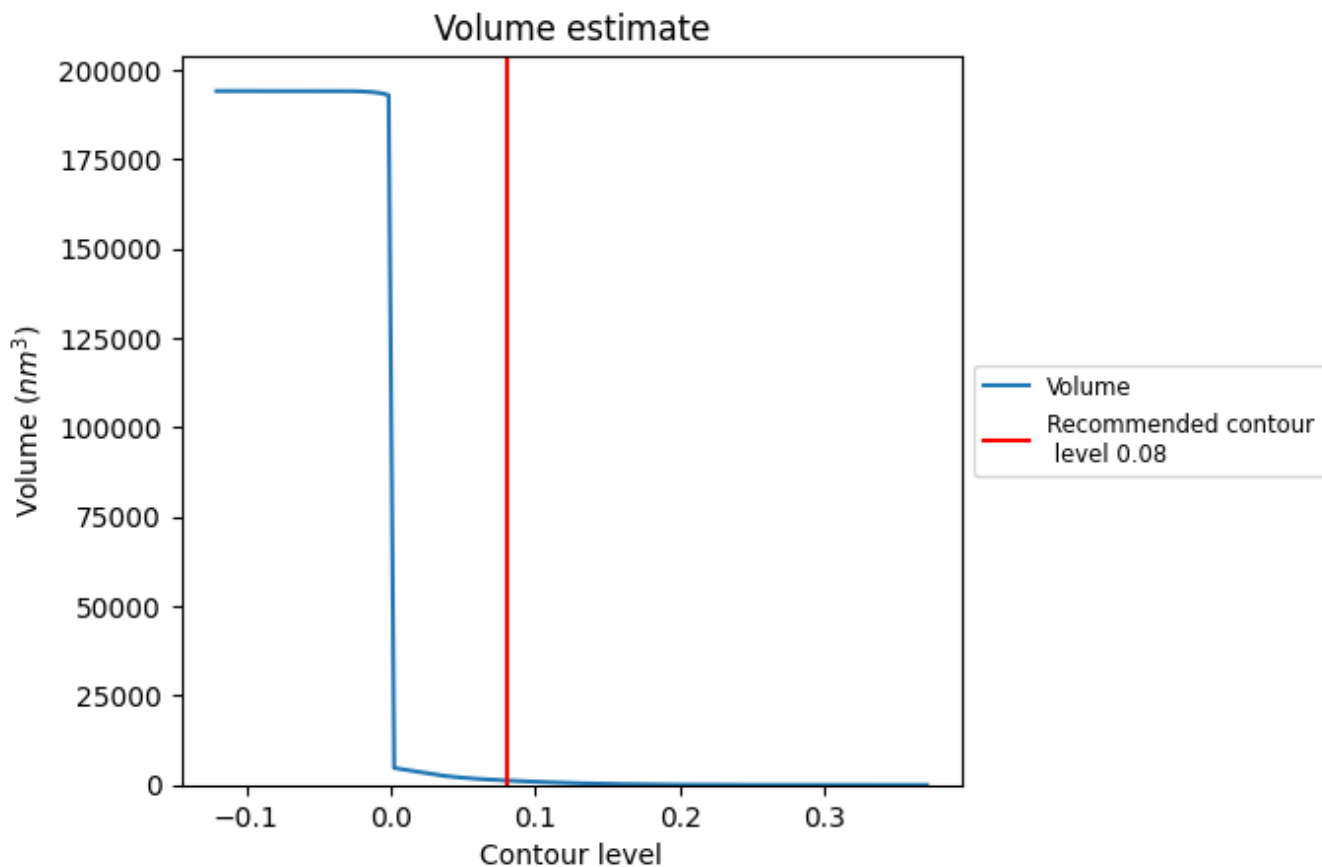
This section contains the results of statistical analysis of the map.

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.

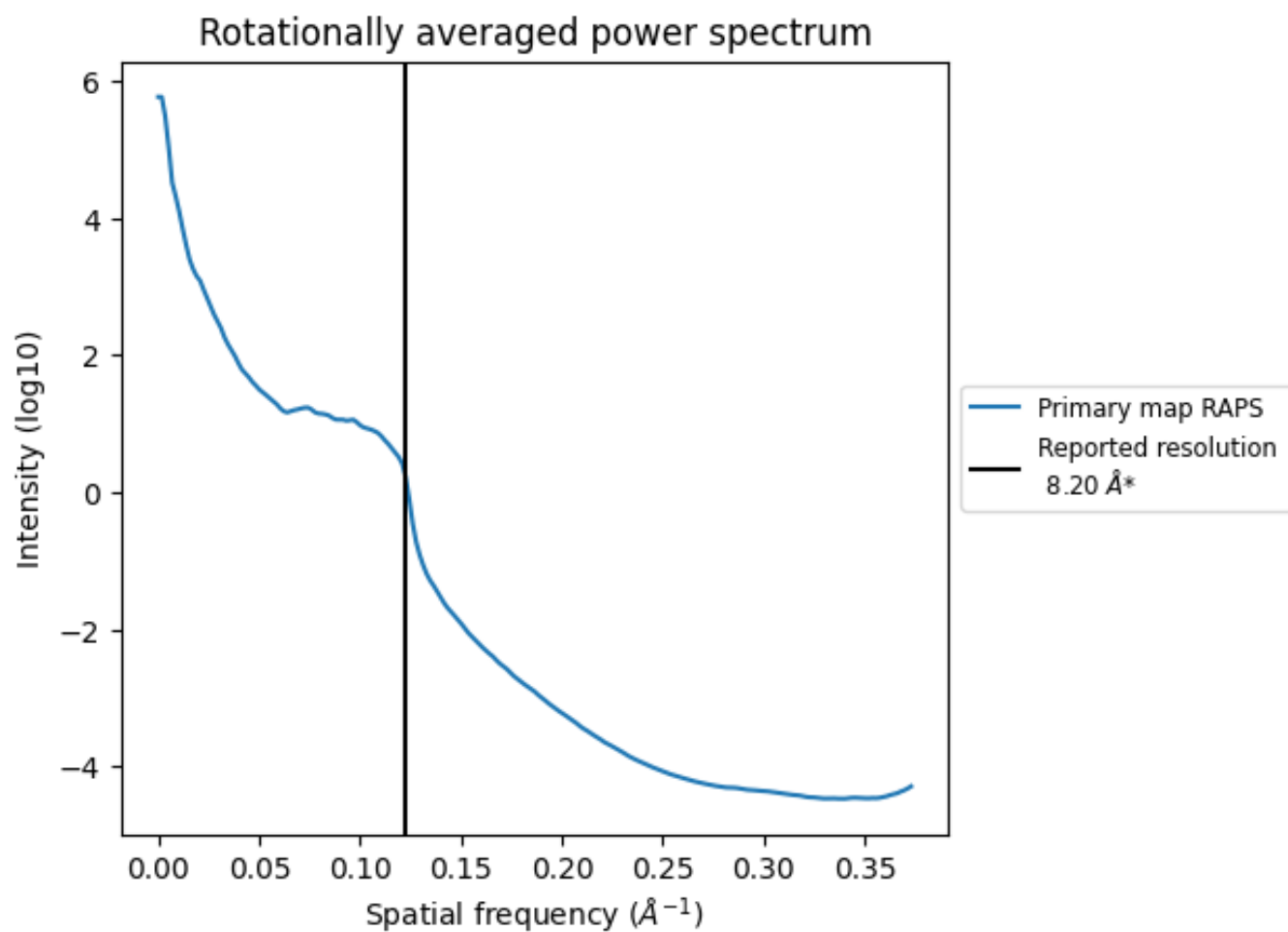
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1254 nm³; 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\AA^{-1}

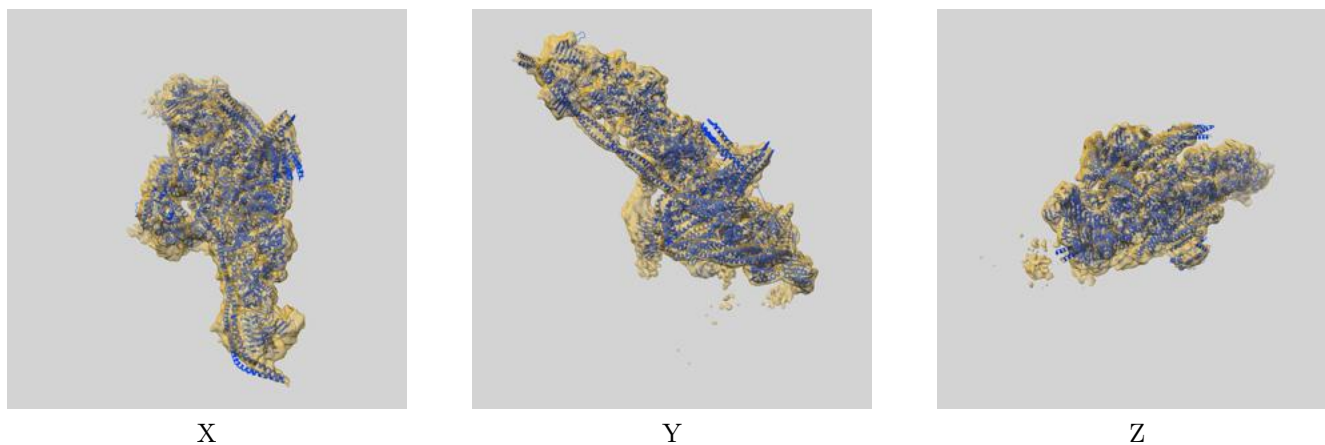
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

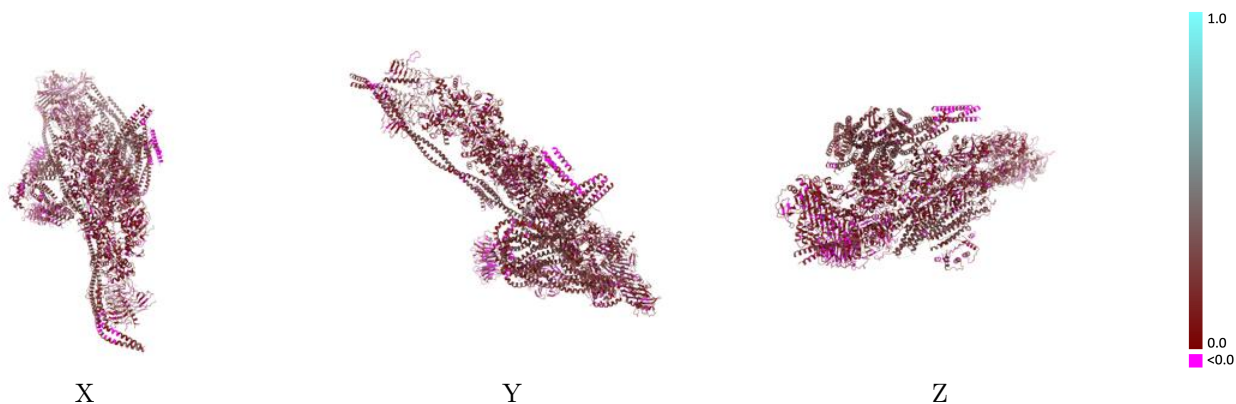
This section contains information regarding the fit between EMDB map EMD-2860 and PDB model 5AFU. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



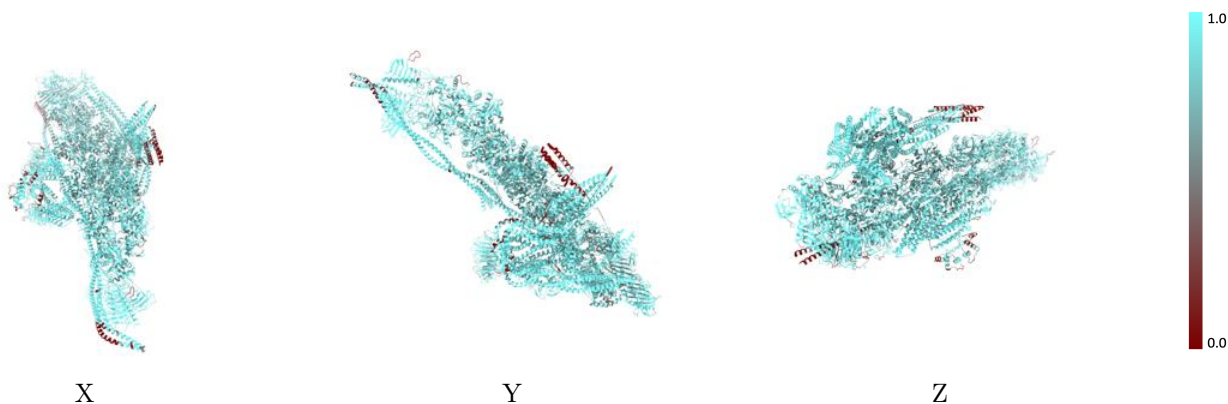
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



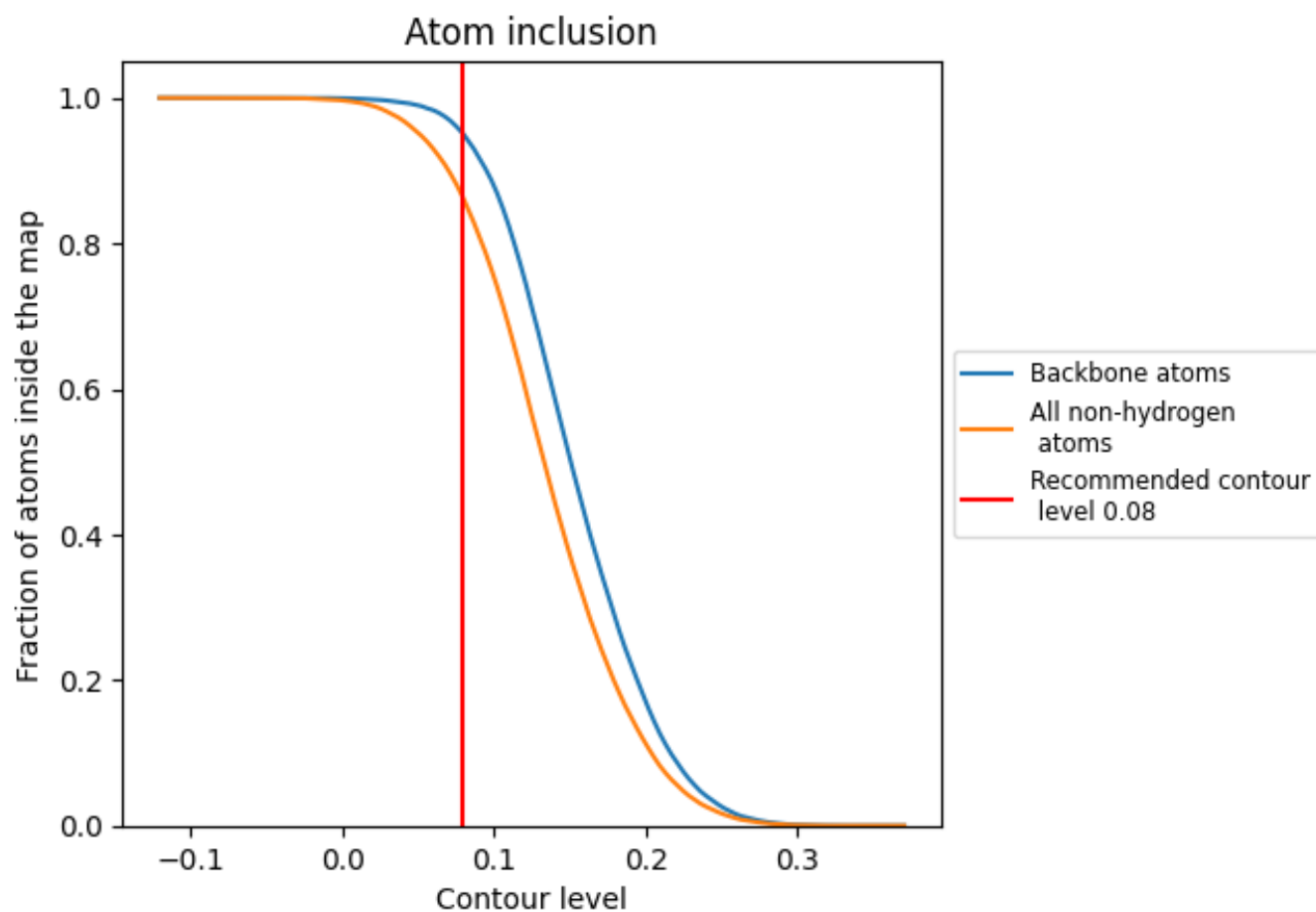
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).





































































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	 0.8617	 0.1480
1	 0.9110	 0.2280
2	 0.8817	 0.1940
3	 0.8723	 0.0470
4	 0.8938	 0.0530
5	 0.8189	 0.2310
6	 0.8116	 0.2120
A	 0.8361	 0.1200
B	 0.8347	 0.1290
C	 0.8025	 0.1270
D	 0.8155	 0.1270
E	 0.8052	 0.1290
F	 0.8176	 0.1250
G	 0.8378	 0.1260
H	 0.8626	 0.1330
I	 0.8474	 0.1220
J	 0.8736	 0.1370
K	 0.9081	 0.1300
L	 0.8567	 0.1240
M	 0.9506	 0.2100
N	 0.9471	 0.2140
O	 0.9567	 0.2000
P	 0.9443	 0.2100
Q	 0.2092	 0.0340
R	 0.9839	 0.2500
U	 0.9140	 0.1570
V	 0.9914	 0.1810
Y	 0.9959	 0.2110
Z	 0.9231	 0.1950
a	 0.8457	 0.2140
b	 0.8794	 0.1660
c	 0.8977	 0.1950
d	 0.8387	 0.1940
z	 0.8000	 0.1630

