wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:24 PM 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	:	3.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

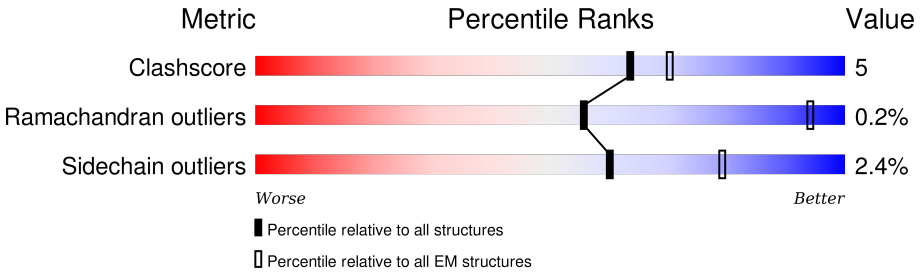
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	1	361	79% 21%
2	2	359	80% 20%
3	3	350	96% .
3	4	350	96% .
4	5	275	81% 19%
4	6	275	80% 20%
5	A	370	96% .
5	B	370	99% .
5	C	370	96% .

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	C	N	O	0	0
			2935	1761	587	587		

- Molecule 11 is a protein called DYNACTIN 6.

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

- Molecule 12 is a protein called DYNACTIN.

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

- Molecule 13 is a protein called DYNACTIN.

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

- Molecule 14 is a protein called DYNACTIN.

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

- Molecule 15 is a protein called DYNACTIN.

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

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

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

- 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		

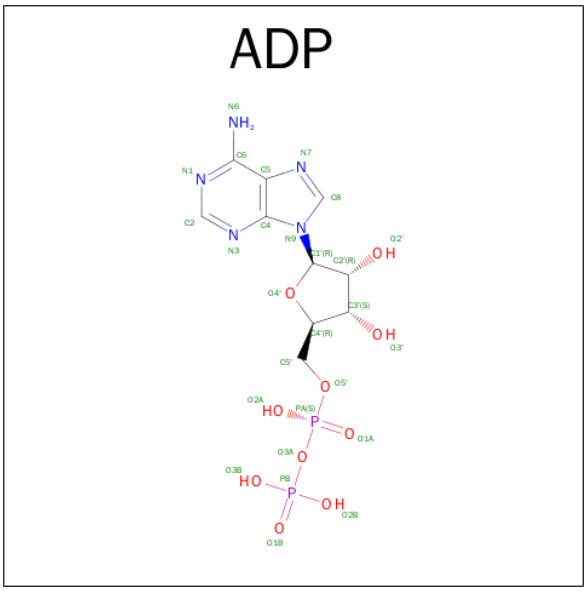
- Molecule 21 is a protein called DYNACTIN.

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.

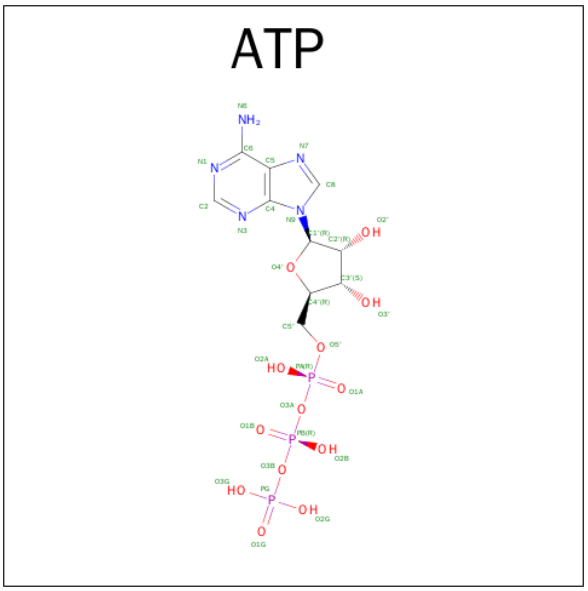
Mol	Chain	Residues	Atoms				AltConf	Trace
22	z	53	Total	C	N	O	0	0
			265	159	53	53		

- 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: $C_{10}H_{16}N_5O_{13}P_3$).



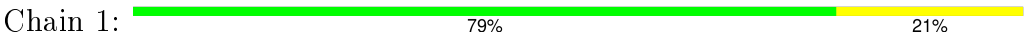
Mol	Chain	Residues	Atoms					AltConf
24	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

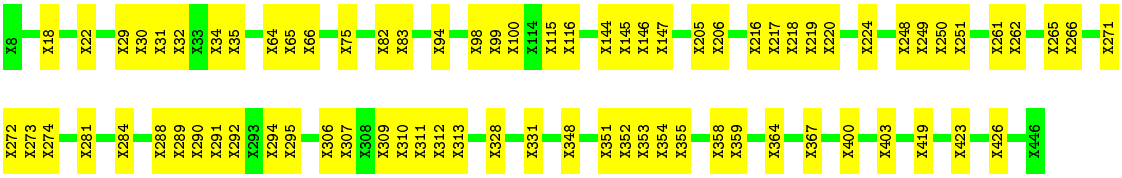
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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

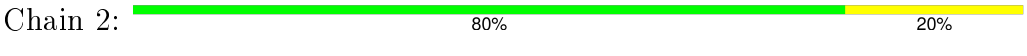
Chain 1:

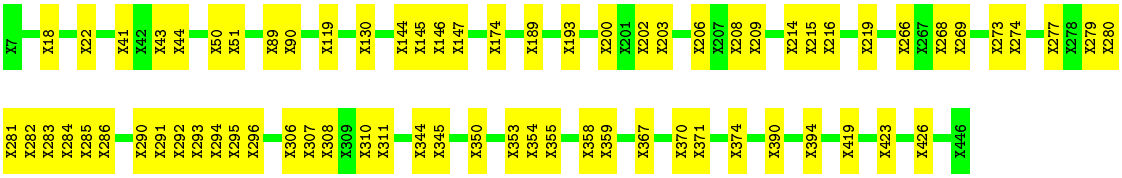




- Molecule 2: DYNEIN TAIL

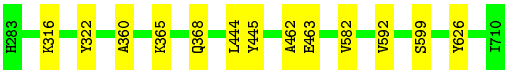
Chain 2:





- Molecule 3: DYNEIN TAIL

Chain 3:

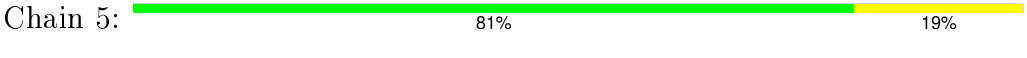


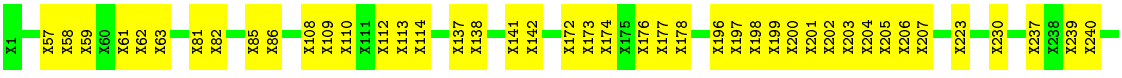
- Molecule 3: DYNEIN TAIL

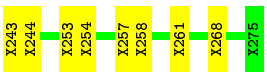
Chain 4:

- Molecule 4: DYNEIN TAIL

Chain 5:

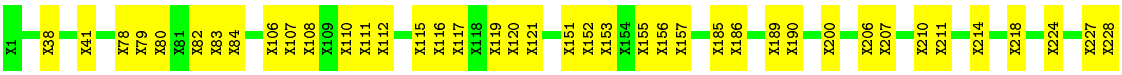






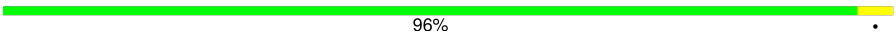
• Molecule 4: DYNEIN TAIL

Chain 6:



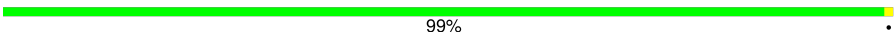
• Molecule 5: DYNACTIN

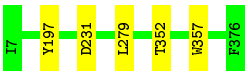
Chain A:



• Molecule 5: DYNACTIN

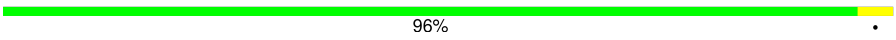
Chain B:

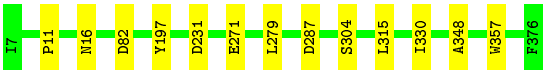




• Molecule 5: DYNACTIN

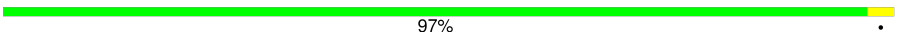
Chain C:





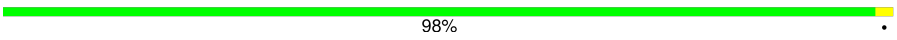
• Molecule 5: DYNACTIN

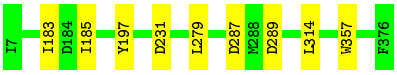
Chain D:



• Molecule 5: DYNACTIN

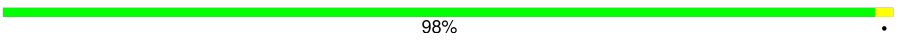
Chain E:





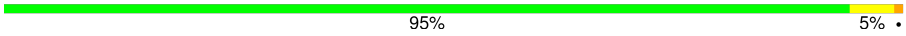
• Molecule 5: DYNACTIN

Chain F:



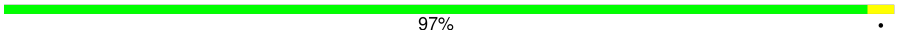
• Molecule 5: DYNACTIN

Chain G:



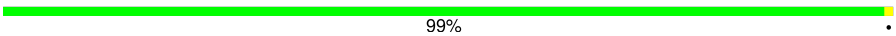
• Molecule 5: DYNACTIN

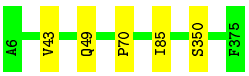
Chain I:



• Molecule 6: ACTIN, CYTOPLASMIC 1

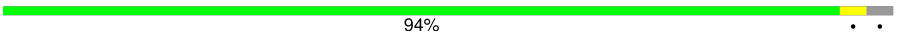
Chain H:

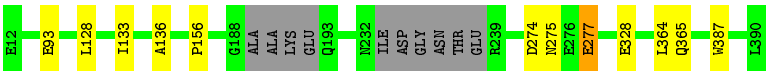




• Molecule 7: DYNACTIN

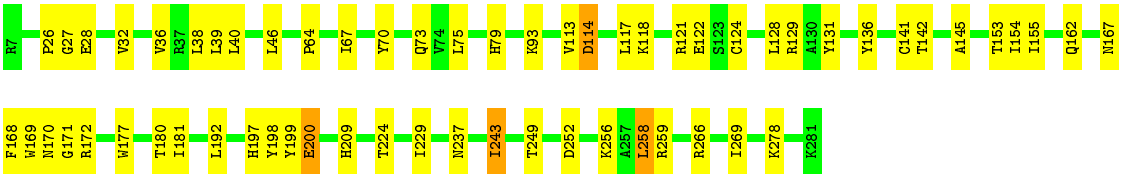
Chain J:





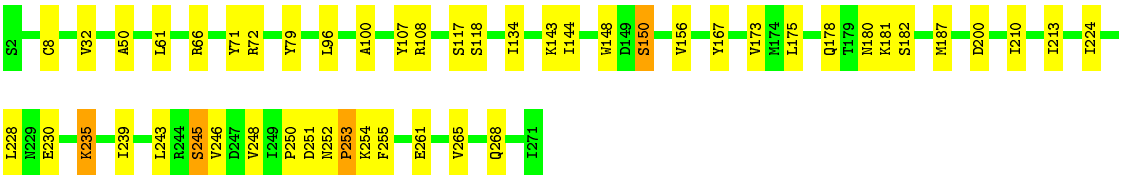
• Molecule 8: CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1

Chain K:



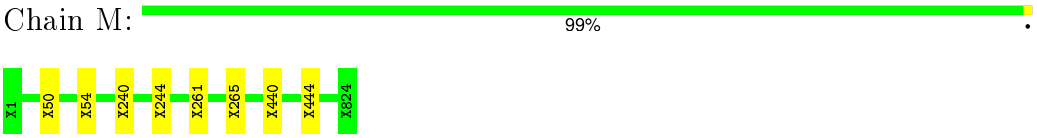
• Molecule 9: F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II

Chain L:



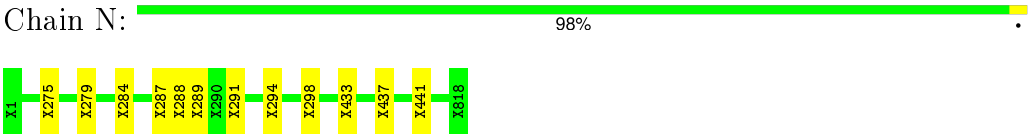
• Molecule 10: DYNACTIN

Chain M:



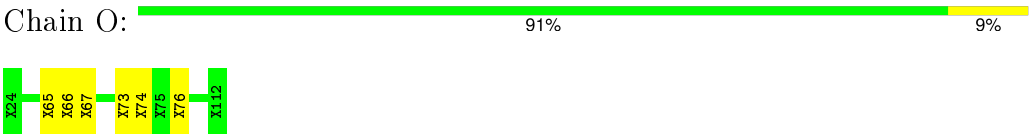
• Molecule 11: DYNACTIN 6

Chain N:



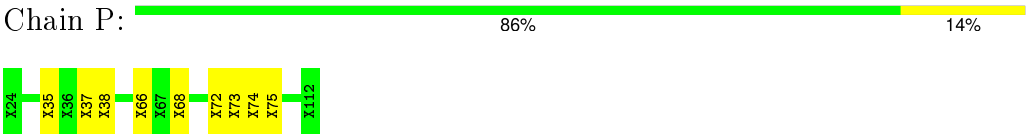
• Molecule 12: DYNACTIN

Chain O:



• Molecule 12: DYNACTIN

Chain P:



• Molecule 13: DYNACTIN

Chain Q:

There are no outlier residues recorded for this chain.

• Molecule 13: DYNACTIN

Chain R:

There are no outlier residues recorded for this chain.

• Molecule 14: DYNACTIN

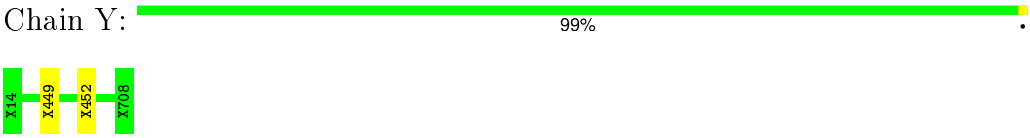
Chain U:

• Molecule 15: DYNACTIN

Chain V:

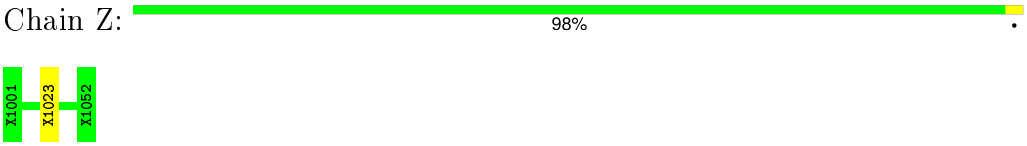
• Molecule 16: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA

Chain Y:



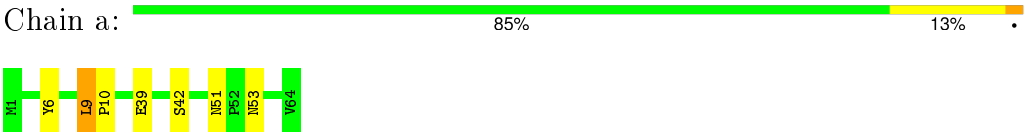
• Molecule 17: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA

Chain Z:



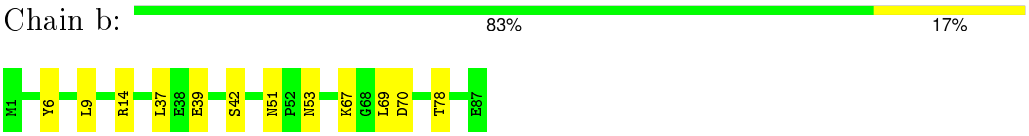
• Molecule 18: DYNACTIN

Chain a:



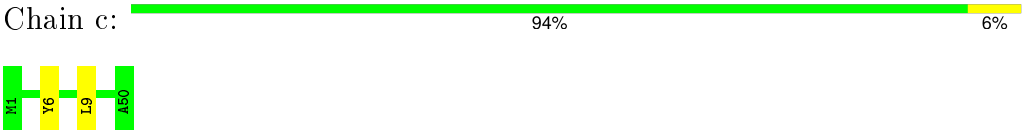
• Molecule 19: DYNACTIN

Chain b:



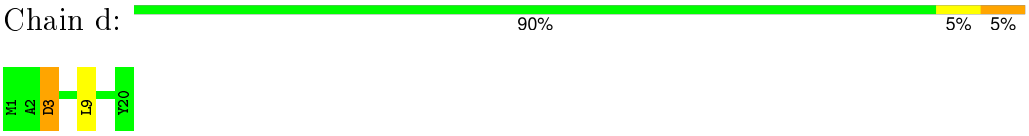
• Molecule 20: DYNACTIN

Chain c:



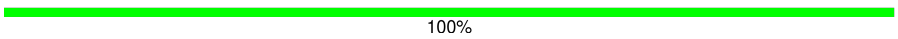
• Molecule 21: DYNACTIN

Chain d:



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

Chain z:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
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	47000	Depositor
Image detector	FEI FALCON II	Depositor

5 Model quality

5.1 Standard geometry

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

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
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
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%)
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
2:2:215:UNK:CB	2:2:219:UNK:CB	2.25	1.13
1:1:281:UNK:O	1:1:284:UNK:CA	1.97	1.13
8:K:162:GLN:HG3	9:L:243:LEU:CD2	1.77	1.13
5:G:183:ILE:HD11	5:G:278:VAL:HG21	1.26	1.13
1:1:311:UNK:C	1:1:312:UNK:O	1.97	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

Continued on next page...

Continued from previous page...

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
9:L:251:ASP:O	9:L:255:PHE:HD2	1.39	0.92
4:6:151:UNK:O	4:6:155:UNK:N	2.02	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
9:L:253:PRO:HD2	9:L:254:LYS:N	1.86	0.91
8:K:93:LYS:CE	8:K:122:GLU:OE2	2.19	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
8:K:162:GLN:CG	9:L:243:LEU:CD2	2.52	0.88
2:2:144:UNK:O	2:2:145:UNK:C	2.21	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

Continued on next page...

Continued from previous page...

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
2:2:18:UNK:C	2:2:22:UNK:CB	2.55	0.84
1:1:289:UNK:CB	5:F:346:ILE:HG21	2.06	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
8:K:162:GLN:HG3	9:L:243:LEU:HD23	1.61	0.82
3:4:445:TYR:O	3:4:462:ALA:HB1	1.79	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

Continued on next page...

Continued from previous page...

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
8:K:168:PHE:CD2	8:K:200:GLU:HG3	2.20	0.76
3:4:365:LYS:CA	3:4:444:LEU:CB	2.63	0.76
2:2:359:UNK:CB	2:2:423:UNK:HA	2.16	0.76
1:1:351:UNK:C	1:1:353:UNK:N	2.44	0.75
1:1:292:UNK:HA	5:F:350:LEU:CD2	2.14	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
12:P:37:UNK:HA	12:P:73:UNK:O	1.88	0.74
4:6:116:UNK:O	4:6:120:UNK:N	2.20	0.74
4:6:238:UNK:O	4:6:242:UNK:CB	2.35	0.73
4:5:173:UNK:O	4:5:177:UNK:N	2.20	0.73
12:O:67:UNK:O	12:O:73:UNK:HA	1.89	0.73
9:L:251:ASP:HB2	9:L:255:PHE:CE2	2.24	0.73
4:5:203:UNK:O	4:5:207:UNK:N	2.21	0.73
1:1:311:UNK:CB	1:1:312:UNK:H	2.01	0.73
1:1:292:UNK:HA	5:F:350:LEU:HD22	1.71	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

Continued on next page...

Continued from previous page...

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
8:K:168:PHE:CA	8:K:199:TYR:CE1	2.74	0.69
2:2:359:UNK:CA	2:2:423:UNK:HA	2.21	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
4:6:238:UNK:O	4:6:242:UNK:CA	2.43	0.67
2:2:203:UNK:O	2:2:206:UNK:N	2.28	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

Continued on next page...

Continued from previous page...

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
8:K:198:TYR:HB2	9:L:235:LYS:HG2	1.81	0.62
5:A:350:LEU:HD13	9:L:265:VAL:HG22	1.80	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
9:L:250:PRO:C	9:L:253:PRO:CD	2.66	0.61
8:K:153:THR:HG22	8:K:180:THR:HG22	1.81	0.61
2:2:355:UNK:CB	2:2:419:UNK:CA	2.74	0.61
1:1:291:UNK:CB	5:F:350:LEU:CD1	2.77	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
4:5:137:UNK:O	4:5:141:UNK:CB	2.50	0.60
1:1:359:UNK:CA	1:1:423:UNK:HA	2.32	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
4:6:152:UNK:O	4:6:156:UNK:N	2.34	0.60
1:1:364:UNK:O	1:1:367:UNK:CB	2.50	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:O	5:G:185:ILE:HG23	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
5:A:271:GLU:OE2	8:K:266:ARG:NH1	2.36	0.59
3:4:599:SER:HA	3:4:626:TYR:O	2.02	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
8:K:27:GLY:HA3	8:K:170:ASN:ND2	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:78:UNK:O	4:6:82:UNK:N	2.37	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
9:L:239:ILE:O	9:L:243:LEU:HG	2.04	0.57
1:1:144:UNK:O	1:1:146:UNK:N	2.38	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
8:K:93:LYS:CE	8:K:122:GLU:OE1	2.54	0.55
4:5:254:UNK:HA	4:5:257:UNK:CB	2.36	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
1:1:292:UNK:N	5:F:350:LEU:HD23	2.09	0.54
1:1:18:UNK:O	1:1:22:UNK:N	2.41	0.54
4:6:108:UNK:O	4:6:112:UNK:N	2.39	0.54
1:1:291:UNK:O	1:1:295:UNK:CB	2.55	0.54
1:1:29:UNK:O	1:1:30:UNK:C	2.53	0.54
2:2:214:UNK:C	2:2:216:UNK:CA	2.57	0.54
5:G:182:ARG:C	5:G:183:ILE:HG13	2.28	0.54
5:B:352:THR:HG21	8:K:278:LYS:CB	2.37	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

Continued on next page...

Continued from previous page...

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
4:5:138:UNK:O	4:5:142:UNK:CA	2.57	0.52
4:5:81:UNK:O	4:5:85:UNK:CB	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
2:2:214:UNK:CB	2:2:216:UNK:HG2	2.39	0.52
1:1:262:UNK:O	1:1:265:UNK:CA	2.57	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
2:2:308:UNK:O	2:2:311:UNK:O	2.28	0.51
2:2:291:UNK:C	2:2:293:UNK:N	2.64	0.51
11:N:287:UNK:O	11:N:291:UNK:N	2.43	0.51
2:2:344:UNK:O	2:2:345:UNK:C	2.55	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
2:2:214:UNK:O	2:2:216:UNK:CG	2.58	0.51
1:1:359:UNK:O	1:1:426:UNK:CB	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
12:P:38:UNK:O	12:P:73:UNK:CB	2.58	0.51
1:1:64:UNK:HA	1:1:75:UNK:O	2.11	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:P:37:UNK:C	12:P:73:UNK:O	2.59	0.50
12:O:65:UNK:O	12:O:76:UNK:N	2.44	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
8:K:64:PRO:HB3	8:K:75:LEU:HD23	1.93	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

Continued on next page...

Continued from previous page...

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
8:K:258:LEU:HD12	9:L:148:TRP:HB2	1.93	0.49
6:H:43:VAL:HG21	7:J:156:PRO:HG2	1.94	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
2:2:282:UNK:HA	2:2:286:UNK:CB	2.44	0.47
1:1:205:UNK:O	1:1:206:UNK:CB	2.60	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
8:K:259:ARG:NH2	9:L:148:TRP:CH2	2.82	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: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
5:A:148:TYR:CE1	9:L:265:VAL:HG11	2.50	0.47
4:5:254:UNK:CB	4:6:255:UNK:CB	2.92	0.47
6:H:70:PRO:HG3	6:H:85:ILE:HD12	1.97	0.47
3:3:360:ALA:HA	3:3:368:GLN:O	2.15	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

Continued on next page...

Continued from previous page...

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
9:L:173:VAL:HG21	9:L:224:ILE:HG21	1.98	0.45
8:K:28:GLU:O	8:K:32:VAL:N	2.47	0.45
8:K:269:ILE:HD11	9:L:107:TYR:HD1	1.81	0.45
8:K:252:ASP:O	8:K:256:LYS:HB2	2.17	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:N	8:K:181:ILE:HD12	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
11:N:275:UNK:O	11:N:279:UNK:N	2.50	0.43
5:D:38:TYR:CD1	5:D:71:ILE:HG23	2.53	0.43
8:K:177:TRP:CZ2	8:K:192:LEU:HD11	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:32:VAL:O	8:K:36:VAL:HG23	2.19	0.43
1:1:290:UNK:O	1:1:294:UNK:N	2.51	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
8:K:198:TYR:CB	9:L:235:LYS:HG2	2.48	0.43
7:J:365:GLN:HE22	16:Y:452:UNK:C	2.32	0.43
2:2:281:UNK:O	2:2:286:UNK:CA	2.60	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
8:K:38:LEU:HD23	9:L:8:CYS:SG	2.59	0.43
8:K:168:PHE:HB3	8:K:199:TYR:CE1	2.53	0.42
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
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
8:K:237:ASN:ND2	9:L:246:VAL:HG21	2.35	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
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:315:LEU:HG	5:G:330:ILE:HD12	2.03	0.41
5:G:262:LEU:HB3	5:G:275:ILE:HD12	2.02	0.41
2:2:50:UNK:O	2:2:51:UNK:C	2.67	0.41
9:L:173:VAL:HG11	9:L:228:LEU:HD11	2.03	0.41
5:A:262:LEU:HB3	5:A:275:ILE:HD12	2.03	0.41
8:K:93:LYS:NZ	8:K:122:GLU:OE2	2.43	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:ILE:O	5:E:185:ILE:HG23	2.21	0.40
4:5:108:UNK:O	4:5:112:UNK:CB	2.69	0.40
2:2:208:UNK:O	2:2:209:UNK:C	2.69	0.40
9:L:251:ASP:C	9:L:255:PHE:CE2	2.94	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
3:4:599:SER:CA	3:4:626:TYR:O	2.70	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
1:1:66:UNK:O	1:1:94:UNK:HA	2.21	0.40
4:6:239:UNK:CA	4:6:242:UNK:CB	2.93	0.40
1:1:311:UNK:CB	1:1:312:UNK:O	2.69	0.40
4:5:201:UNK:O	4:5:205:UNK:CA	2.69	0.40
11:N:289:UNK:HA	17:Z:1023:UNK:HA	2.03	0.40
3:3:582:VAL:HA	3:3:592:VAL:O	2.22	0.40
2:2:146:UNK:O	2:2:147:UNK:CB	2.69	0.40
8:K:128:LEU:HB2	8:K:229:ILE:HD11	2.02	0.40
8:K:113:VAL:HG12	8:K:114:ASP:N	2.36	0.40
3:4:647:SER:O	3:4:654:VAL:HA	2.22	0.40
3:4:582:VAL:HA	3:4:592:VAL:O	2.22	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

Continued on next page...

Continued from previous page...

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%)	46 84
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%)	5 42
15	V	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	30 75
18	a	44/48 (92%)	40 (91%)	3 (7%)	1 (2%)	8 48
19	b	65/71 (92%)	56 (86%)	8 (12%)	1 (2%)	13 56
20	c	27/31 (87%)	24 (89%)	2 (7%)	1 (4%)	4 36
21	d	18/20 (90%)	15 (83%)	1 (6%)	2 (11%)	0 7
All	All	5383/5457 (99%)	5060 (94%)	311 (6%)	12 (0%)	56 88

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%)	65 87
5	B	318/318 (100%)	314 (99%)	4 (1%)	76 91
5	C	318/318 (100%)	309 (97%)	9 (3%)	51 82
5	D	318/318 (100%)	309 (97%)	9 (3%)	51 82
5	E	318/318 (100%)	310 (98%)	8 (2%)	55 84
5	F	318/318 (100%)	313 (98%)	5 (2%)	70 89
5	G	318/318 (100%)	311 (98%)	7 (2%)	60 85
5	I	318/318 (100%)	312 (98%)	6 (2%)	65 87
6	H	313/313 (100%)	312 (100%)	1 (0%)	94 99
7	J	322/331 (97%)	318 (99%)	4 (1%)	78 92
8	K	245/245 (100%)	239 (98%)	6 (2%)	57 85
9	L	242/242 (100%)	236 (98%)	6 (2%)	55 84
18	a	31/41 (76%)	26 (84%)	5 (16%)	3 18
19	b	49/60 (82%)	38 (78%)	11 (22%)	1 6
20	c	7/16 (44%)	6 (86%)	1 (14%)	4 24
21	d	8/16 (50%)	7 (88%)	1 (12%)	6 29
All	All	3761/3808 (99%)	3672 (98%)	89 (2%)	60 85

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Some 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	1.06	1 (4%)	23,45,45	1.90	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	ADP	B	800	-	24,29,29	1.07	2 (8%)	23,45,45	1.90	1 (4%)
23	ADP	C	800	-	24,29,29	1.06	2 (8%)	23,45,45	1.89	2 (8%)
23	ADP	D	800	-	24,29,29	1.07	2 (8%)	23,45,45	1.89	1 (4%)
23	ADP	E	800	-	24,29,29	1.07	2 (8%)	23,45,45	1.88	2 (8%)
23	ADP	F	800	-	24,29,29	1.07	2 (8%)	23,45,45	1.90	2 (8%)
23	ADP	G	800	-	24,29,29	1.07	2 (8%)	23,45,45	1.88	2 (8%)
24	ATP	H	401	-	26,33,33	1.04	2 (7%)	26,52,52	1.79	2 (7%)
23	ADP	I	800	-	24,29,29	1.07	2 (8%)	23,45,45	1.90	2 (8%)
23	ADP	J	800	-	24,29,29	1.06	2 (8%)	23,45,45	1.98	2 (8%)

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	-	-	0/12/32/32	0/3/3/3
23	ADP	B	800	-	-	0/12/32/32	0/3/3/3
23	ADP	C	800	-	-	0/12/32/32	0/3/3/3
23	ADP	D	800	-	-	0/12/32/32	0/3/3/3
23	ADP	E	800	-	-	0/12/32/32	0/3/3/3
23	ADP	F	800	-	-	0/12/32/32	0/3/3/3
23	ADP	G	800	-	-	0/12/32/32	0/3/3/3
24	ATP	H	401	-	-	0/18/38/38	0/3/3/3
23	ADP	I	800	-	-	0/12/32/32	0/3/3/3
23	ADP	J	800	-	-	0/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	800	ADP	C2-N3	2.00	1.35	1.32
23	G	800	ADP	C2-N3	2.00	1.35	1.32
23	I	800	ADP	C2-N3	2.01	1.35	1.32
23	D	800	ADP	C2-N3	2.01	1.35	1.32
24	H	401	ATP	C2-N3	2.02	1.35	1.32
23	B	800	ADP	C2-N3	2.03	1.35	1.32
23	F	800	ADP	C2-N3	2.04	1.35	1.32
23	C	800	ADP	C2-N3	2.05	1.35	1.32
23	E	800	ADP	C2-N3	2.08	1.35	1.32
23	J	800	ADP	C5-C4	3.28	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	800	ADP	C5-C4	3.31	1.48	1.40
23	F	800	ADP	C5-C4	3.31	1.48	1.40
23	C	800	ADP	C5-C4	3.32	1.48	1.40
23	E	800	ADP	C5-C4	3.33	1.48	1.40
23	I	800	ADP	C5-C4	3.33	1.48	1.40
23	D	800	ADP	C5-C4	3.33	1.48	1.40
24	H	401	ATP	C5-C4	3.34	1.48	1.40
23	B	800	ADP	C5-C4	3.35	1.48	1.40
23	G	800	ADP	C5-C4	3.36	1.48	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	800	ADP	N3-C2-N1	-7.77	122.77	128.87
23	D	800	ADP	N3-C2-N1	-7.62	122.89	128.87
23	A	800	ADP	N3-C2-N1	-7.61	122.89	128.87
23	B	800	ADP	N3-C2-N1	-7.60	122.90	128.87
23	F	800	ADP	N3-C2-N1	-7.59	122.91	128.87
23	I	800	ADP	N3-C2-N1	-7.54	122.95	128.87
23	C	800	ADP	N3-C2-N1	-7.53	122.95	128.87
23	E	800	ADP	N3-C2-N1	-7.49	122.99	128.87
24	H	401	ATP	N3-C2-N1	-7.48	123.00	128.87
23	G	800	ADP	N3-C2-N1	-7.46	123.01	128.87
24	H	401	ATP	C4'-O4'-C1'	2.01	111.77	109.64
23	E	800	ADP	C4'-O4'-C1'	2.02	111.78	109.64
23	F	800	ADP	C4'-O4'-C1'	2.08	111.85	109.64
23	G	800	ADP	C4'-O4'-C1'	2.12	111.89	109.64
23	I	800	ADP	C4'-O4'-C1'	2.13	111.90	109.64
23	C	800	ADP	C4'-O4'-C1'	2.17	111.94	109.64
23	J	800	ADP	C4'-O4'-C1'	2.82	112.63	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.