



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:22 PM BST

PDB ID : 5ADX
EMDB ID: : EMD-2856
Title : CryoEM structure of dynactin complex at 4.0 angstrom resolution
Authors : Zhang, K.; Urnavicius, L.; Diamant, A.G.; Motz, C.; Schlage, M.A.; Yu, M.;
Patel, N.A.; Robinson, C.V.; Carter, A.P.
Deposited on : 2015-08-24
Resolution : 4.00 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 : unknown
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

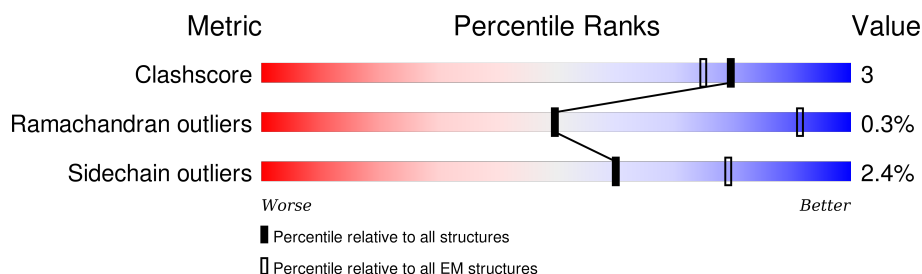
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.










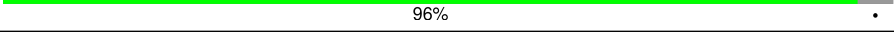
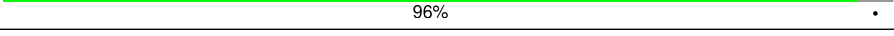
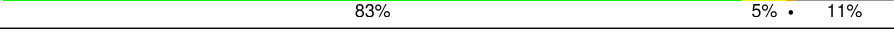
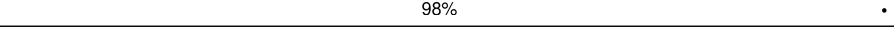
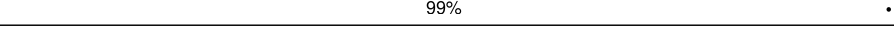
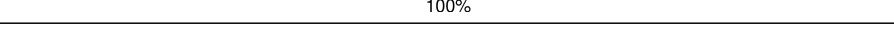
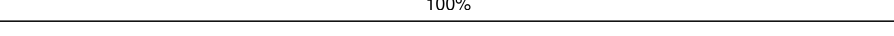


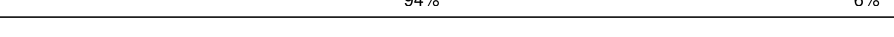

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	370	96% .
1	B	370	98% .
1	C	370	96% .
1	D	370	97% .
1	E	370	98% .
1	F	370	98% .
1	G	370	95% 5% .
1	I	370	94% 6% .
2	H	370	99% .

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Mol	Chain	Length	Quality of chain
3	J	417	 85% 12%
4	K	275	 78% 21%
5	L	270	 82% 17%
6	M	824	 67% 31%
7	N	818	 71% 26%
8	O	88	 67% 7% 26%
8	P	88	 64% 10% 26%
9	Q	91	 96%
9	R	91	 96%
10	U	190	 83% 5% 11%
11	V	165	 98%
12	Y	243	 99%
13	Z	419	 100%
13	z	419	 100%
14	a	48	 85% 13%
15	b	71	 83% 17%
16	c	31	 94% 6%
17	d	20	 90% 5% 5%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49392 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 ACTIN RELATED PROTEIN 1.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	GLU	ASP	CONFLICT	UNP F2Z5G5
B	97	GLU	ASP	CONFLICT	UNP F2Z5G5
C	97	GLU	ASP	CONFLICT	UNP F2Z5G5
D	97	GLU	ASP	CONFLICT	UNP F2Z5G5
E	97	GLU	ASP	CONFLICT	UNP F2Z5G5
F	97	GLU	ASP	CONFLICT	UNP F2Z5G5
G	97	GLU	ASP	CONFLICT	UNP F2Z5G5
I	97	GLU	ASP	CONFLICT	UNP F2Z5G5

- Molecule 2 is a protein called ACTIN, CYTOPLASMIC 1.

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

- Molecule 3 is a protein called ACTIN RELATED PROTEIN 11.

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

- Molecule 4 is a protein called CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1.

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

- Molecule 5 is a protein called F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II.

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

- Molecule 6 is a protein called DYNAMACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	571	Total	C	N	O	0	0
			2855	1713	571	571		

- Molecule 7 is a protein called DYNAMACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	602	Total	C	N	O	0	0
			3010	1806	602	602		

- Molecule 8 is a protein called DYNAMACTIN SUBUNIT 3.

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

- Molecule 9 is a protein called DYNAMACTIN SUBUNIT 2.

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

- Molecule 10 is a protein called DYNAMACTIN 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	169	Total	C	N	O	0	0
			831	493	169	169		

- Molecule 11 is a protein called DYNAMACTIN SUBUNIT 6.

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

- Molecule 12 is a protein called DYNAMACTIN SUBUNIT 2.

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

- Molecule 13 is a protein called DYNAMACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Z	419	Total	C	N	O	0	0
			2095	1257	419	419		
13	z	419	Total	C	N	O	0	0
			2095	1257	419	419		

- Molecule 14 is a protein called DYNAMACTIN SUBUNIT 2.

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

- Molecule 15 is a protein called DYNAMACTIN SUBUNIT 2.

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

- Molecule 16 is a protein called DYNAMACTIN SUBUNIT 2.

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

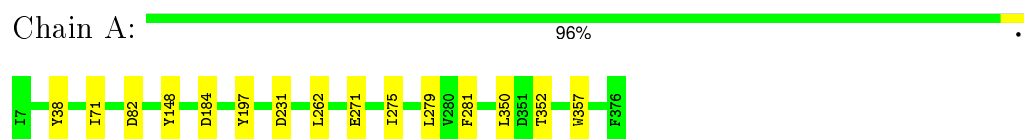
- Molecule 17 is a protein called DYNAMACTIN SUBUNIT 2.

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

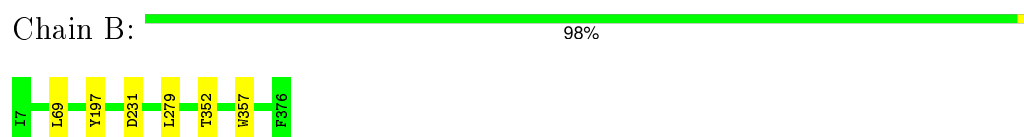
3 Residue-property plots [i](#)

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.

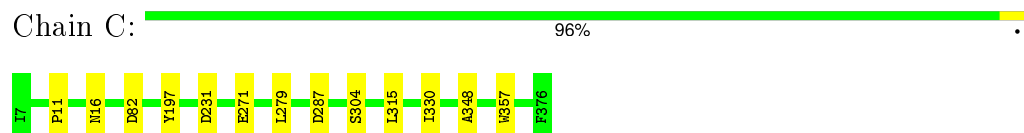
- Molecule 1: ACTIN RELATED PROTEIN 1



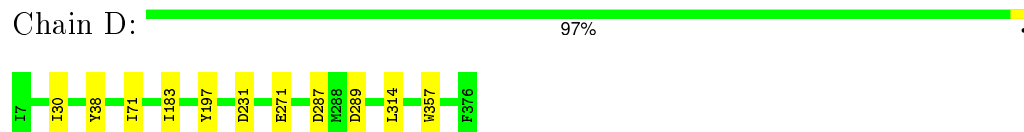
- Molecule 1: ACTIN RELATED PROTEIN 1



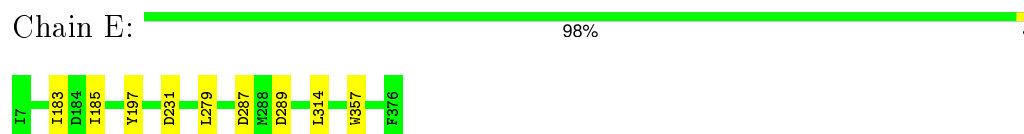
- Molecule 1: ACTIN RELATED PROTEIN 1



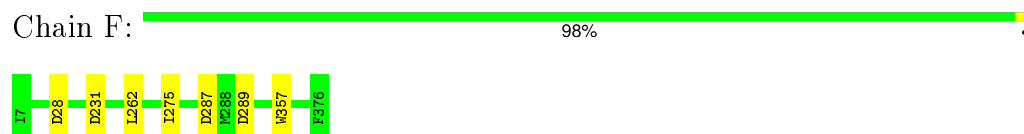
- Molecule 1: ACTIN RELATED PROTEIN 1



- Molecule 1: ACTIN RELATED PROTEIN 1



- Molecule 1: ACTIN RELATED PROTEIN 1



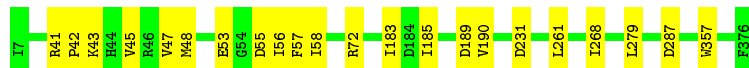
- Molecule 1: ACTIN RELATED PROTEIN 1

Chain G:  95% 5% •



- Molecule 1: ACTIN RELATED PROTEIN 1

Chain I:  94% 6% •




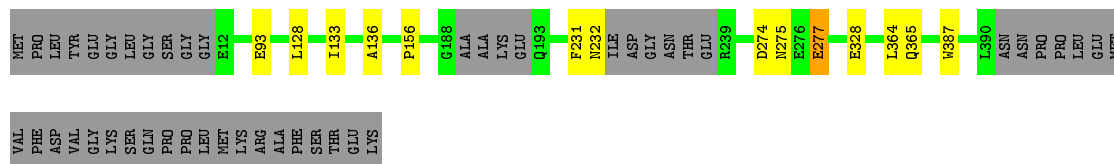
- Molecule 2: ACTIN, CYTOPLASMIC 1

Chain H:  99% •




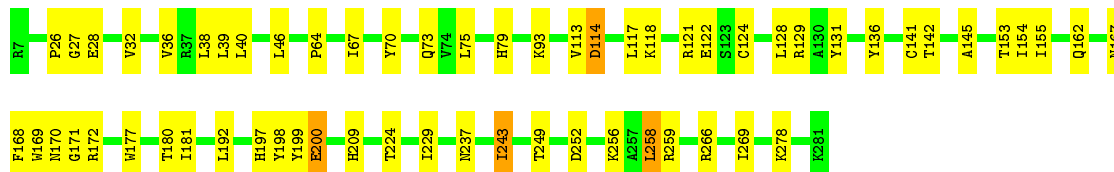
- Molecule 3: ACTIN RELATED PROTEIN 11

Chain J:  85% 12% •




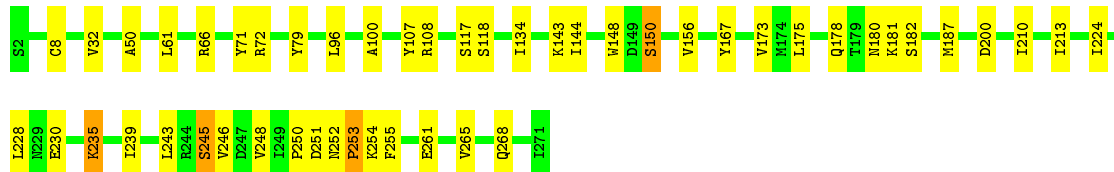
- Molecule 4: CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1

Chain K:  78% 21% •

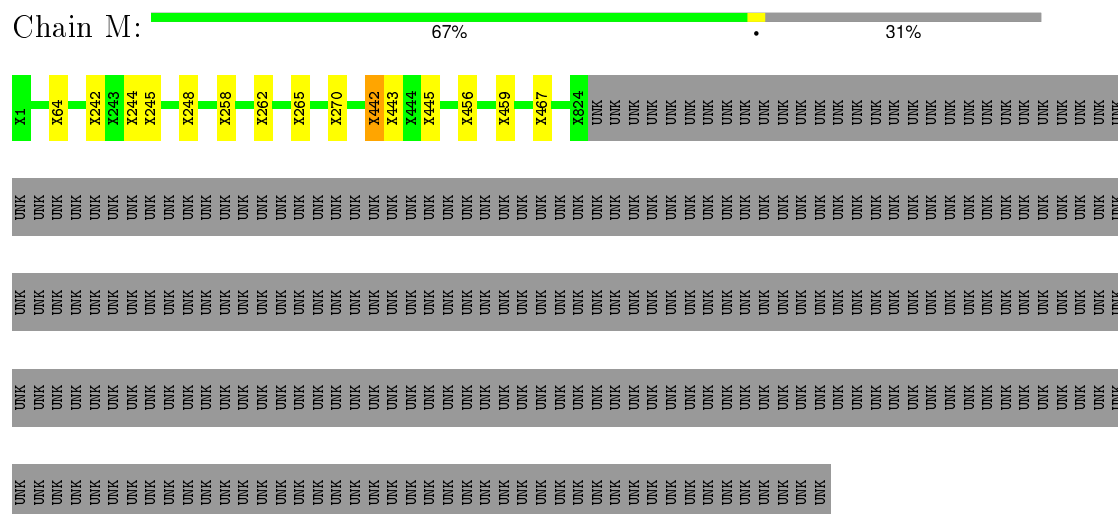


- Molecule 5: F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II

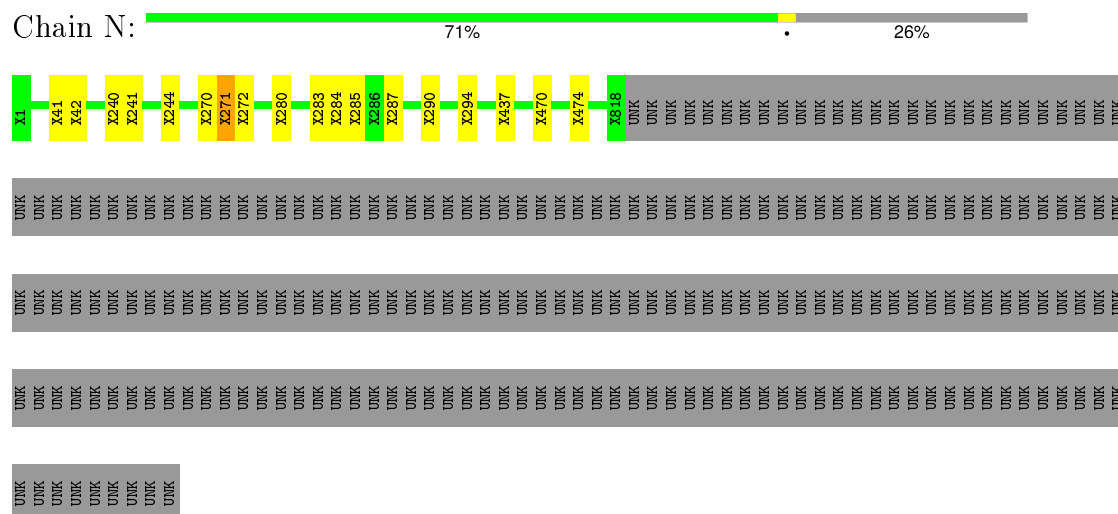
Chain L:  82% 17% •



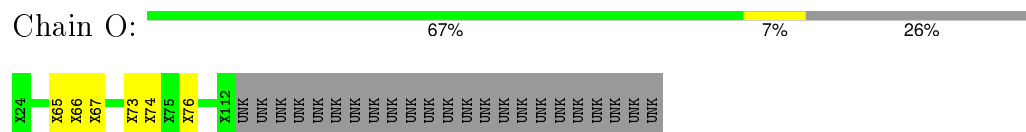
- Molecule 6: DYNAMACTIN SUBUNIT 2



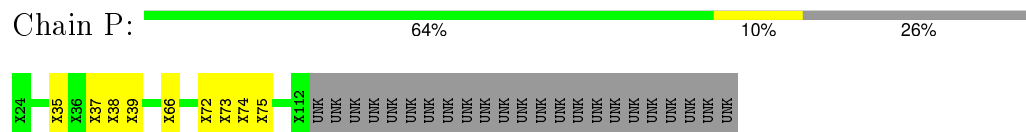
- Molecule 7: DYNAMICTIN SUBUNIT 2



- Molecule 8: DYNAMICTIN SUBUNIT 3

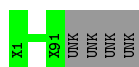


- Molecule 8: DYNAMICTIN SUBUNIT 3



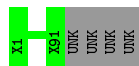
- Molecule 9: DYNAMICTIN SUBUNIT 2





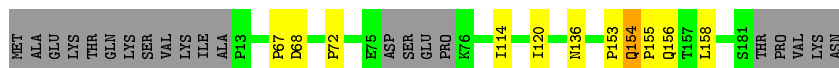
- Molecule 9: DYNAMICTIN SUBUNIT 2

Chain R: 96%



- Molecule 10: DYNAMICTIN 5

Chain U: 83% 5% 11%



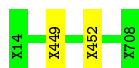
- Molecule 11: DYNAMICTIN SUBUNIT 6

Chain V: 98%



- Molecule 12: DYNAMICTIN SUBUNIT 2

Chain Y: 99%



- Molecule 13: DYNAMICTIN SUBUNIT 2

Chain Z: 100%



- Molecule 13: DYNAMICTIN SUBUNIT 2

Chain z: 100%

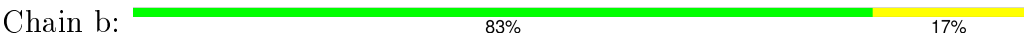
There are no outlier residues recorded for this chain.

- Molecule 14: DYNAMICTIN SUBUNIT 2

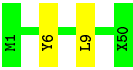
Chain a: 85% 13%



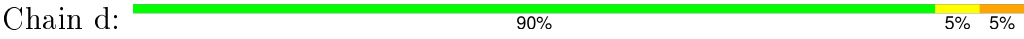
- Molecule 15: DYNAMICTIN SUBUNIT 2



• Molecule 16: DYNAMACTIN SUBUNIT 2



• Molecule 17: DYNAMACTIN SUBUNIT 2



4 Experimental information

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	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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
1	A	0.37	0/3026	0.51	0/4086
1	B	0.37	0/3026	0.51	0/4086
1	C	0.37	0/3026	0.52	0/4086
1	D	0.37	0/3026	0.52	0/4086
1	E	0.37	0/3026	0.53	0/4086
1	F	0.37	0/3026	0.51	0/4086
1	G	0.37	0/3026	0.52	0/4086
1	I	0.38	0/3026	0.52	0/4086
10	U	0.28	0/830	0.50	0/1152
11	V	0.30	0/811	0.48	0/1126
14	a	0.52	1/347 (0.3%)	0.67	1/473 (0.2%)
15	b	0.41	0/525	0.66	0/708
16	c	0.45	0/127	0.71	0/175
17	d	0.46	0/130	0.73	0/179
2	H	0.37	0/2948	0.51	0/3991
3	J	0.37	0/2939	0.53	0/3987
4	K	0.39	0/2294	0.63	1/3106 (0.0%)
5	L	0.37	0/2173	0.60	1/2935 (0.0%)
All	All	0.37	1/37332 (0.0%)	0.53	3/50520 (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
1	G	0	1
6	M	0	1
7	N	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	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(°)
5	L	253	PRO	CA-N-CD	-8.89	99.05	111.50
14	a	9	LEU	C-N-CD	5.78	140.54	128.40
4	K	114	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	375	THR	Peptide
6	M	442	UNK	Peptide
7	N	270	UNK	Peptide
7	N	271	UNK	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2957	0	2952	7	0
1	B	2957	0	2952	7	0
1	C	2957	0	2952	2	0
1	D	2957	0	2952	1	0
1	E	2957	0	2952	1	0
1	F	2957	0	2952	1	0
1	G	2957	0	2952	15	0
1	I	2957	0	2952	25	0
2	H	2885	0	2856	2	0
3	J	2879	0	2969	18	0
4	K	2242	0	2169	69	0
5	L	2137	0	2122	74	0
6	M	2855	0	585	12	0
7	N	3010	0	619	13	0
8	O	323	0	76	3	0
8	P	323	0	77	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Q	435	0	93	0	0
9	R	435	0	93	0	0
10	U	831	0	374	6	0
11	V	812	0	344	1	0
12	Y	1215	0	286	2	0
13	Z	2095	0	429	1	0
13	z	2095	0	427	0	0
14	a	341	0	310	0	0
15	b	517	0	490	0	0
16	c	179	0	116	0	0
17	d	127	0	103	0	0
All	All	49392	0	38154	229	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 3.

All (229) 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)
5:L:251:ASP:CG	5:L:255:PHE:HE2	1.36	1.28
5:L:251:ASP:O	5:L:255:PHE:CD2	1.94	1.20
1:G:183:ILE:HD11	1:G:278:VAL:CG2	1.72	1.19
5:L:253:PRO:HD2	5:L:254:LYS:H	1.08	1.17
4:K:162:GLN:HG3	5:L:243:LEU:CD2	1.77	1.13
1:G:183:ILE:HD11	1:G:278:VAL:HG21	1.26	1.13
5:L:245:SER:CB	5:L:248:VAL:HG23	1.82	1.10
4:K:93:LYS:HE3	4:K:122:GLU:OE2	1.51	1.08
5:L:245:SER:HB2	5:L:248:VAL:HG23	1.31	1.07
8:P:66:UNK:CB	8:P:74:UNK:O	2.03	1.07
5:L:245:SER:OG	5:L:248:VAL:CG2	2.02	1.07
5:L:251:ASP:CG	5:L:255:PHE:CE2	2.28	1.05
5:L:250:PRO:O	5:L:253:PRO:CD	2.05	1.04
4:K:162:GLN:HG3	5:L:243:LEU:HD21	1.37	1.03
1:I:43:LYS:HA	3:J:275:ASN:HB3	1.39	1.02
1:I:41:ARG:NH1	1:I:72:ARG:HD2	1.75	1.02
8:P:38:UNK:N	8:P:73:UNK:O	1.93	1.01
1:I:41:ARG:HH12	1:I:72:ARG:HD2	1.22	1.01
1:I:45:VAL:H	3:J:275:ASN:HD21	1.12	0.97
5:L:245:SER:OG	5:L:248:VAL:HG21	1.62	0.97
4:K:168:PHE:O	4:K:199:TYR:CD1	2.19	0.96
1:G:185:ILE:HD11	1:G:261:LEU:HG	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:251:ASP:OD1	5:L:255:PHE:HE2	1.48	0.95
1:G:183:ILE:CD1	1:G:278:VAL:HG21	1.95	0.95
1:I:45:VAL:N	3:J:275:ASN:HD21	1.65	0.94
5:L:251:ASP:OD1	5:L:255:PHE:CE2	2.19	0.94
4:K:93:LYS:NZ	4:K:122:GLU:OE1	2.01	0.93
5:L:251:ASP:O	5:L:255:PHE:HD2	1.39	0.92
6:M:442:UNK:HA	6:M:443:UNK:CB	1.98	0.91
5:L:253:PRO:HD2	5:L:254:LYS:N	1.86	0.91
4:K:93:LYS:CE	4:K:122:GLU:OE2	2.19	0.91
1:I:47:VAL:HG21	3:J:232:ASN:HB2	1.53	0.90
1:I:45:VAL:H	3:J:275:ASN:ND2	1.68	0.90
4:K:162:GLN:CG	5:L:243:LEU:HD21	2.03	0.89
5:L:250:PRO:O	5:L:253:PRO:CG	2.19	0.89
4:K:162:GLN:CG	5:L:243:LEU:CD2	2.52	0.88
1:I:57:PHE:C	1:I:58:ILE:HD12	1.95	0.86
5:L:251:ASP:CB	5:L:255:PHE:HE2	1.88	0.86
10:U:153:PRO:O	10:U:154:GLN:O	1.94	0.85
8:P:38:UNK:O	8:P:73:UNK:N	2.11	0.84
1:I:43:LYS:CA	3:J:275:ASN:HB3	2.06	0.84
4:K:93:LYS:NZ	4:K:122:GLU:CD	2.32	0.83
5:L:251:ASP:CB	5:L:255:PHE:CE2	2.61	0.83
4:K:162:GLN:HG3	5:L:243:LEU:HD23	1.61	0.82
5:L:252:ASN:N	5:L:253:PRO:HD3	1.95	0.82
5:L:253:PRO:CD	5:L:254:LYS:H	1.91	0.81
1:I:56:ILE:HG22	1:I:58:ILE:CD1	2.10	0.81
1:I:45:VAL:N	3:J:275:ASN:ND2	2.28	0.81
1:G:185:ILE:HD11	1:G:261:LEU:CG	2.09	0.81
7:N:240:UNK:HA	7:N:241:UNK:CB	2.10	0.80
5:L:250:PRO:O	5:L:253:PRO:HG2	1.80	0.80
1:G:183:ILE:HD11	1:G:278:VAL:HG23	1.61	0.80
4:K:168:PHE:O	4:K:199:TYR:CE1	2.34	0.80
5:L:251:ASP:C	5:L:255:PHE:CD2	2.56	0.78
4:K:168:PHE:CD2	4:K:200:GLU:HG3	2.20	0.76
1:I:56:ILE:HG22	1:I:58:ILE:HD11	1.68	0.75
5:L:251:ASP:C	5:L:255:PHE:HD2	1.89	0.75
1:I:56:ILE:CG2	1:I:58:ILE:HD11	2.16	0.74
8:P:37:UNK:HA	8:P:73:UNK:O	1.88	0.74
8:O:67:UNK:O	8:O:73:UNK:HA	1.89	0.73
5:L:251:ASP:HB2	5:L:255:PHE:CE2	2.24	0.73
5:L:250:PRO:C	5:L:253:PRO:HD3	2.09	0.72
5:L:245:SER:OG	5:L:248:VAL:HG23	1.80	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:168:PHE:HA	4:K:199:TYR:CE1	2.26	0.71
1:I:58:ILE:N	1:I:58:ILE:HD12	2.06	0.71
6:M:244:UNK:O	6:M:248:UNK:N	2.24	0.71
6:M:265:UNK:CB	6:M:467:UNK:CB	2.69	0.71
4:K:124:CYS:SG	4:K:224:THR:HG23	2.31	0.70
5:L:245:SER:CB	5:L:248:VAL:CG2	2.59	0.69
4:K:168:PHE:CA	4:K:199:TYR:CE1	2.74	0.69
1:B:69:LEU:O	1:B:69:LEU:HD22	5.51	0.69
1:B:69:LEU:HD13	1:B:69:LEU:O	5.43	0.69
4:K:118:LYS:O	4:K:122:GLU:HG3	1.94	0.68
4:K:93:LYS:HZ1	4:K:122:GLU:CD	1.91	0.68
5:L:252:ASN:N	5:L:253:PRO:CD	2.56	0.68
5:L:250:PRO:O	5:L:253:PRO:HD2	1.91	0.67
1:I:47:VAL:HG23	3:J:231:PHE:O	1.94	0.66
1:G:375:THR:HG23	1:G:376:PHE:H	1.62	0.65
1:G:121:ARG:HE	1:G:375:THR:HG21	1.61	0.65
4:K:168:PHE:C	4:K:199:TYR:CE1	2.71	0.64
8:O:66:UNK:HA	8:O:74:UNK:O	1.96	0.64
4:K:93:LYS:CE	4:K:122:GLU:CD	2.66	0.63
10:U:156:GLN:O	10:U:158:LEU:N	2.26	0.63
4:K:198:TYR:HB2	5:L:235:LYS:HG2	1.81	0.62
1:A:350:LEU:HD13	5:L:265:VAL:HG22	1.80	0.62
5:L:250:PRO:C	5:L:253:PRO:CD	2.66	0.61
4:K:153:THR:HG22	4:K:180:THR:HG22	1.81	0.61
4:K:168:PHE:O	4:K:199:TYR:HD1	1.82	0.60
1:G:185:ILE:O	1:G:185:ILE:HG23	2.02	0.59
8:P:35:UNK:HA	8:P:75:UNK:O	2.02	0.59
5:L:143:LYS:HB3	5:L:180:ASN:HB2	1.85	0.59
1:A:271:GLU:OE2	4:K:266:ARG:NH1	2.36	0.59
4:K:26:PRO:HB2	4:K:172:ARG:HD3	1.85	0.58
4:K:168:PHE:HD2	4:K:200:GLU:HG3	1.65	0.58
4:K:27:GLY:HA3	4:K:170:ASN:ND2	2.19	0.58
4:K:167:ASN:HB3	4:K:169:TRP:CD1	2.40	0.57
4:K:40:LEU:HB3	4:K:46:LEU:HD11	1.86	0.57
5:L:239:ILE:O	5:L:243:LEU:HG	2.04	0.57
6:M:64:UNK:O	6:M:270:UNK:CB	2.53	0.56
5:L:251:ASP:C	5:L:253:PRO:CD	2.73	0.56
4:K:79:HIS:CD2	4:K:155:ILE:HG21	2.40	0.56
6:M:265:UNK:CB	6:M:467:UNK:HA	2.36	0.56
1:G:121:ARG:NE	1:G:375:THR:HG21	2.21	0.56
4:K:93:LYS:CE	4:K:122:GLU:OE1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:271:UNK:CB	7:N:272:UNK:HA	2.35	0.55
4:K:121:ARG:NE	4:K:154:ILE:HG12	2.20	0.55
7:N:240:UNK:CA	7:N:241:UNK:CB	2.84	0.55
4:K:168:PHE:HA	4:K:199:TYR:CZ	2.42	0.55
7:N:41:UNK:CA	7:N:42:UNK:CB	2.85	0.55
4:K:198:TYR:CZ	4:K:200:GLU:HB2	2.42	0.55
6:M:442:UNK:CB	6:M:445:UNK:CB	2.85	0.54
1:G:182:ARG:C	1:G:183:ILE:HG13	2.28	0.54
1:B:352:THR:HG21	4:K:278:LYS:CB	2.37	0.54
3:J:128:LEU:HD13	3:J:136:ALA:HB3	1.90	0.54
5:L:108:ARG:HD3	5:L:117:SER:HB3	1.89	0.54
1:B:69:LEU:HD22	1:B:69:LEU:C	4.64	0.54
5:L:253:PRO:CD	5:L:254:LYS:N	2.55	0.54
5:L:61:LEU:HD22	5:L:71:TYR:CD2	2.44	0.53
7:N:41:UNK:N	7:N:42:UNK:CB	2.72	0.53
5:L:66:ARG:HD3	5:L:71:TYR:CE2	2.44	0.53
1:I:190:VAL:HG22	1:I:261:LEU:HD23	1.90	0.53
5:L:50:ALA:HB2	5:L:61:LEU:HD21	1.91	0.53
5:L:100:ALA:HB2	5:L:210:ILE:HD13	1.91	0.53
5:L:96:LEU:HG	5:L:210:ILE:HD11	1.90	0.52
7:N:280:UNK:O	7:N:284:UNK:N	2.43	0.52
4:K:237:ASN:OD1	5:L:246:VAL:HG21	2.09	0.52
4:K:118:LYS:HG2	4:K:145:ALA:HB1	1.90	0.52
7:N:283:UNK:O	7:N:287:UNK:N	2.43	0.51
1:I:185:ILE:HD11	1:I:261:LEU:HD21	1.92	0.51
8:P:37:UNK:CA	8:P:73:UNK:O	2.57	0.51
4:K:237:ASN:OD1	5:L:246:VAL:CG2	2.58	0.51
5:L:144:ILE:HG23	5:L:178:GLN:O	2.11	0.51
8:P:38:UNK:O	8:P:73:UNK:CB	2.58	0.51
4:K:67:ILE:HB	4:K:70:TYR:CD1	2.46	0.50
6:M:265:UNK:CB	6:M:467:UNK:CA	2.90	0.50
1:B:69:LEU:H	1:B:69:LEU:CD1	4.03	0.50
8:P:37:UNK:C	8:P:73:UNK:O	2.59	0.50
1:I:45:VAL:HB	3:J:275:ASN:HD21	1.75	0.50
8:O:65:UNK:O	8:O:76:UNK:N	2.44	0.50
1:I:72:ARG:NH2	3:J:277:GLU:OE2	2.45	0.50
4:K:39:LEU:HD21	5:L:32:VAL:CG2	2.42	0.49
4:K:64:PRO:HB3	4:K:75:LEU:HD23	1.93	0.49
10:U:153:PRO:O	10:U:154:GLN:C	2.48	0.49
4:K:131:TYR:CG	4:K:229:ILE:HG21	2.47	0.49
1:I:58:ILE:N	1:I:58:ILE:CD1	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:258:LEU:HD12	5:L:148:TRP:HB2	1.93	0.49
2:H:43:VAL:HG21	3:J:156:PRO:HG2	1.94	0.49
7:N:470:UNK:O	7:N:474:UNK:N	2.46	0.49
4:K:192:LEU:O	4:K:209:HIS:HA	2.12	0.49
4:K:75:LEU:N	4:K:142:THR:OG1	2.46	0.48
1:A:281:PHE:CD2	5:L:230:GLU:OE2	2.67	0.48
5:L:251:ASP:C	5:L:253:PRO:HD3	2.32	0.48
7:N:290:UNK:O	7:N:294:UNK:N	2.46	0.48
6:M:456:UNK:HA	6:M:459:UNK:CB	2.44	0.47
1:I:43:LYS:C	3:J:275:ASN:HB3	2.24	0.47
1:G:185:ILE:HD11	1:G:261:LEU:CD1	2.43	0.47
10:U:153:PRO:C	10:U:154:GLN:O	2.51	0.47
1:I:47:VAL:CG2	3:J:232:ASN:HB2	2.33	0.47
5:L:134:ILE:HB	5:L:150:SER:HB2	1.97	0.47
4:K:259:ARG:NH2	5:L:148:TRP:CH2	2.82	0.47
4:K:197:HIS:CE1	4:K:199:TYR:HB3	2.50	0.47
4:K:198:TYR:OH	4:K:200:GLU:HB3	2.14	0.47
1:A:148:TYR:CE1	5:L:265:VAL:HG11	2.50	0.47
2:H:70:PRO:HG3	2:H:85:ILE:HD12	1.97	0.47
4:K:171:GLY:HA3	5:L:239:ILE:CG2	2.44	0.47
4:K:243:ILE:HG23	5:L:187:MET:HE1	1.96	0.47
1:C:11:PRO:HG2	1:C:348:ALA:HB1	1.98	0.46
8:P:37:UNK:HA	8:P:74:UNK:HA	1.98	0.46
4:K:121:ARG:HB3	4:K:154:ILE:HG12	1.98	0.46
4:K:117:LEU:HG	4:K:121:ARG:CZ	2.46	0.46
1:B:352:THR:HG21	4:K:278:LYS:HB3	1.97	0.46
4:K:131:TYR:CD2	4:K:229:ILE:HG21	2.51	0.46
6:M:242:UNK:O	6:M:245:UNK:N	2.49	0.46
7:N:41:UNK:HA	7:N:42:UNK:CB	2.46	0.46
5:L:148:TRP:CZ2	5:L:173:VAL:HG13	2.51	0.46
5:L:261:GLU:O	5:L:265:VAL:HG23	2.16	0.46
6:M:242:UNK:C	6:M:244:UNK:N	2.76	0.45
5:L:72:ARG:HB2	5:L:79:TYR:CE2	2.51	0.45
3:J:128:LEU:HD11	3:J:133:ILE:HG13	1.98	0.45
5:L:173:VAL:HG21	5:L:224:ILE:HG21	1.98	0.45
4:K:28:GLU:O	4:K:32:VAL:N	2.47	0.45
10:U:136:ASN:CB	10:U:155:PRO:N	2.80	0.45
4:K:269:ILE:HD11	5:L:107:TYR:HD1	1.81	0.45
4:K:252:ASP:O	4:K:256:LYS:HB2	2.17	0.45
11:V:72:PRO:CB	11:V:101:ALA:HB2	2.46	0.45
8:P:39:UNK:HA	8:P:72:UNK:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:ILE:HD13	1:I:268:ILE:HD11	1.99	0.44
1:I:45:VAL:CB	3:J:275:ASN:HD21	2.29	0.44
1:G:371:ILE:O	1:G:375:THR:HG22	2.16	0.44
4:K:121:ARG:HE	4:K:154:ILE:HG12	1.82	0.44
5:L:108:ARG:NH1	5:L:117:SER:OG	2.50	0.44
4:K:129:ARG:HG2	4:K:141:CYS:SG	2.57	0.44
4:K:181:ILE:N	4:K:181:ILE:HD12	2.33	0.44
7:N:271:UNK:CB	7:N:272:UNK:CA	2.96	0.43
1:D:38:TYR:CD1	1:D:71:ILE:HG23	2.53	0.43
4:K:177:TRP:CZ2	4:K:192:LEU:HD11	2.54	0.43
4:K:32:VAL:O	4:K:36:VAL:HG23	2.19	0.43
5:L:156:VAL:HG21	5:L:213:ILE:HD11	1.99	0.43
4:K:198:TYR:CB	5:L:235:LYS:HG2	2.48	0.43
3:J:365:GLN:HE22	12:Y:452:UNK:C	2.32	0.43
4:K:198:TYR:CZ	4:K:200:GLU:CB	3.02	0.43
4:K:38:LEU:HD23	5:L:8:CYS:SG	2.59	0.43
4:K:168:PHE:HB3	4:K:199:TYR:CE1	2.53	0.42
3:J:364:LEU:HD11	12:Y:449:UNK:HA	2.01	0.42
6:M:442:UNK:CB	6:M:445:UNK:N	2.82	0.42
1:C:315:LEU:HG	1:C:330:ILE:HD12	2.01	0.42
6:M:258:UNK:O	6:M:262:UNK:N	2.52	0.42
10:U:156:GLN:C	10:U:158:LEU:H	2.17	0.42
4:K:237:ASN:ND2	5:L:246:VAL:HG21	2.35	0.42
5:L:61:LEU:HD22	5:L:71:TYR:CG	2.54	0.42
5:L:156:VAL:HG22	5:L:167:TYR:CD1	2.55	0.42
1:A:352:THR:HG21	5:L:261:GLU:HA	2.03	0.41
1:F:262:LEU:HB3	1:F:275:ILE:HD12	2.00	0.41
5:L:181:LYS:O	5:L:182:SER:OG	2.33	0.41
1:A:38:TYR:CD1	1:A:71:ILE:HG23	2.56	0.41
1:B:69:LEU:HD13	1:B:69:LEU:H	4.67	0.41
5:L:148:TRP:CD1	5:L:175:LEU:CD2	3.04	0.41
1:G:315:LEU:HG	1:G:330:ILE:HD12	2.03	0.41
1:G:262:LEU:HB3	1:G:275:ILE:HD12	2.02	0.41
5:L:173:VAL:HG11	5:L:228:LEU:HD11	2.03	0.41
1:A:262:LEU:HB3	1:A:275:ILE:HD12	2.03	0.41
1:I:42:PRO:HD3	1:I:55:ASP:HB3	2.02	0.41
4:K:93:LYS:NZ	4:K:122:GLU:OE2	2.43	0.40
1:E:185:ILE:HG23	1:E:185:ILE:O	2.21	0.40
5:L:251:ASP:C	5:L:255:PHE:CE2	2.94	0.40
7:N:285:UNK:HA	13:Z:1023:UNK:HA	2.03	0.40
4:K:128:LEU:HB2	4:K:229:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:244:UNK:CB	7:N:437:UNK:CB	3.00	0.40
4:K:113:VAL:HG12	4:K:114:ASP:N	2.36	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	
1	A	368/370 (100%)	350 (95%)	18 (5%)	0	100	100
1	B	368/370 (100%)	348 (95%)	20 (5%)	0	100	100
1	C	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
1	D	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
1	E	368/370 (100%)	346 (94%)	22 (6%)	0	100	100
1	F	368/370 (100%)	341 (93%)	27 (7%)	0	100	100
1	G	368/370 (100%)	344 (94%)	24 (6%)	0	100	100
1	I	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
2	H	368/370 (100%)	350 (95%)	18 (5%)	0	100	100
3	J	363/417 (87%)	331 (91%)	31 (8%)	1 (0%)	46	82
4	K	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
5	L	268/270 (99%)	257 (96%)	11 (4%)	0	100	100
10	U	167/190 (88%)	145 (87%)	16 (10%)	6 (4%)	4	41
11	V	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	30	73
14	a	44/48 (92%)	40 (91%)	3 (7%)	1 (2%)	8	51
15	b	67/71 (94%)	58 (87%)	8 (12%)	1 (2%)	13	58
16	c	18/31 (58%)	16 (89%)	1 (6%)	1 (6%)	2	29
17	d	18/20 (90%)	15 (83%)	1 (6%)	2 (11%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4693/4817 (97%)	4386 (94%)	294 (6%)	13 (0%)	50 82

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	U	67	PRO
10	U	72	PRO
10	U	154	GLN
14	a	9	LEU
15	b	9	LEU
16	c	9	LEU
17	d	3	ASP
17	d	9	LEU
10	U	68	ASP
10	U	120	ILE
3	J	387	TRP
10	U	114	ILE
11	V	41	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	318/318 (100%)	312 (98%)	6 (2%)	65 86
1	B	318/318 (100%)	314 (99%)	4 (1%)	76 90
1	C	318/318 (100%)	309 (97%)	9 (3%)	51 79
1	D	318/318 (100%)	309 (97%)	9 (3%)	51 79
1	E	318/318 (100%)	310 (98%)	8 (2%)	55 82
1	F	318/318 (100%)	313 (98%)	5 (2%)	70 88
1	G	318/318 (100%)	311 (98%)	7 (2%)	60 84
1	I	318/318 (100%)	310 (98%)	8 (2%)	55 82
2	H	313/313 (100%)	312 (100%)	1 (0%)	94 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	322/363 (89%)	318 (99%)	4 (1%)	78	90
4	K	245/245 (100%)	239 (98%)	6 (2%)	57	82
5	L	242/242 (100%)	236 (98%)	6 (2%)	55	82
14	a	31/41 (76%)	26 (84%)	5 (16%)	3	22
15	b	49/60 (82%)	38 (78%)	11 (22%)	1	10
16	c	7/16 (44%)	6 (86%)	1 (14%)	4	28
17	d	8/16 (50%)	7 (88%)	1 (12%)	6	32
All	All	3761/3840 (98%)	3670 (98%)	91 (2%)	60	82

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	184	ASP
1	A	197	TYR
1	A	231	ASP
1	A	279	LEU
1	A	357	TRP
1	B	197	TYR
1	B	231	ASP
1	B	279	LEU
1	B	357	TRP
1	C	16	ASN
1	C	82	ASP
1	C	197	TYR
1	C	231	ASP
1	C	271	GLU
1	C	279	LEU
1	C	287	ASP
1	C	304	SER
1	C	357	TRP
1	D	30	ILE
1	D	183	ILE
1	D	197	TYR
1	D	231	ASP
1	D	271	GLU
1	D	287	ASP
1	D	289	ASP
1	D	314	LEU
1	D	357	TRP

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Mol	Chain	Res	Type
1	E	183	ILE
1	E	197	TYR
1	E	231	ASP
1	E	279	LEU
1	E	287	ASP
1	E	289	ASP
1	E	314	LEU
1	E	357	TRP
1	F	28	ASP
1	F	231	ASP
1	F	287	ASP
1	F	289	ASP
1	F	357	TRP
1	G	183	ILE
1	G	197	TYR
1	G	231	ASP
1	G	271	GLU
1	G	273	GLU
1	G	287	ASP
1	G	357	TRP
2	H	49	GLN
1	I	48	MET
1	I	53	GLU
1	I	183	ILE
1	I	189	ASP
1	I	231	ASP
1	I	279	LEU
1	I	287	ASP
1	I	357	TRP
3	J	93	GLU
3	J	274	ASP
3	J	277	GLU
3	J	328	GLU
4	K	73	GLN
4	K	136	TYR
4	K	200	GLU
4	K	243	ILE
4	K	249	THR
4	K	258	LEU
5	L	118	SER
5	L	150	SER
5	L	200	ASP

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Mol	Chain	Res	Type
5	L	235	LYS
5	L	245	SER
5	L	268	GLN
14	a	6	TYR
14	a	39	GLU
14	a	42	SER
14	a	51	ASN
14	a	53	ASN
15	b	6	TYR
15	b	14	ARG
15	b	37	LEU
15	b	39	GLU
15	b	42	SER
15	b	51	ASN
15	b	53	ASN
15	b	61	ASP
15	b	67	LYS
15	b	69	LEU
15	b	78	THR
16	c	6	TYR
17	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
1	D	37	ASN
1	F	98	GLN
1	G	98	GLN
2	H	246	GLN
4	K	41	ASN
4	K	61	GLN
4	K	73	GLN
4	K	79	HIS
4	K	84	ASN
4	K	197	HIS
5	L	209	HIS
14	a	51	ASN
15	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.