Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 7, 2019 – 10:37 AM EST

PDB ID	:	5H3D
EMDB ID:	:	EMD-2546
Title	:	Helical structure of membrane tubules decorated by ACAP1 (BARPH doamin) protein by cryo-electron microscopy and MD simulation
Authors	:	Chan, C.; Pang, X.Y.; Zhang, Y.; Sun, F.; Fan, J.
Deposited on	:	2016-10-22
Resolution	:	14.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

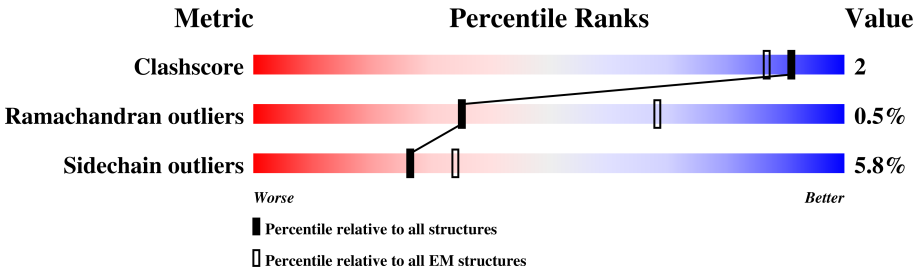
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 14.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	A	382	66% 24% • • 5%
1	B	382	70% 19% • 5%
1	C	382	70% 20% 6% 5%
1	D	382	67% 23% • • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23314 atoms, of which 11698 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 Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	364	Total	C	H	N	O	S	0	0
			5849	1825	2934	534	543	13		
1	B	361	Total	C	H	N	O	S	0	0
			5808	1810	2915	531	539	13		
1	C	364	Total	C	H	N	O	S	0	0
			5849	1825	2934	534	543	13		
1	D	361	Total	C	H	N	O	S	0	0
			5808	1810	2915	531	539	13		

There are 20 discrepancies between the modelled and reference sequences:

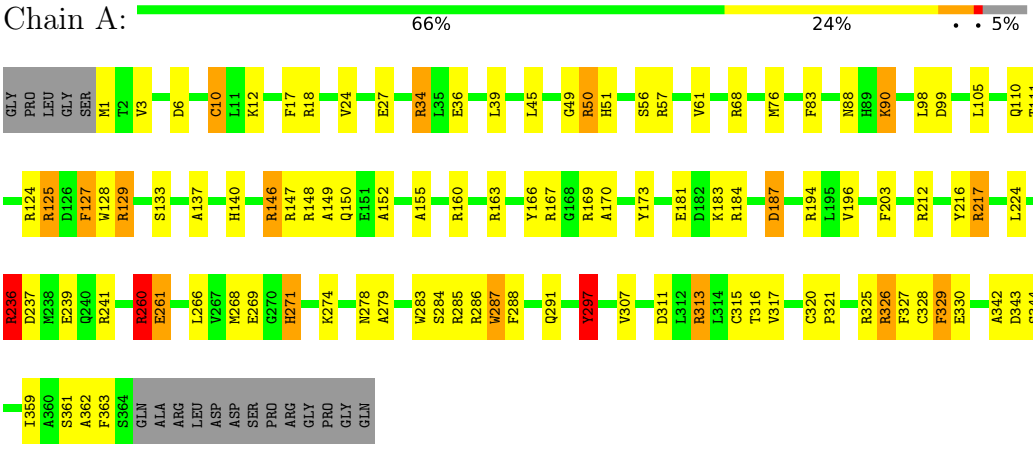
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q15027
A	-3	PRO	-	expression tag	UNP Q15027
A	-2	LEU	-	expression tag	UNP Q15027
A	-1	GLY	-	expression tag	UNP Q15027
A	0	SER	-	expression tag	UNP Q15027
B	-4	GLY	-	expression tag	UNP Q15027
B	-3	PRO	-	expression tag	UNP Q15027
B	-2	LEU	-	expression tag	UNP Q15027
B	-1	GLY	-	expression tag	UNP Q15027
B	0	SER	-	expression tag	UNP Q15027
C	-4	GLY	-	expression tag	UNP Q15027
C	-3	PRO	-	expression tag	UNP Q15027
C	-2	LEU	-	expression tag	UNP Q15027
C	-1	GLY	-	expression tag	UNP Q15027
C	0	SER	-	expression tag	UNP Q15027
D	-4	GLY	-	expression tag	UNP Q15027
D	-3	PRO	-	expression tag	UNP Q15027
D	-2	LEU	-	expression tag	UNP Q15027
D	-1	GLY	-	expression tag	UNP Q15027
D	0	SER	-	expression tag	UNP Q15027

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 the various outlier classes 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.

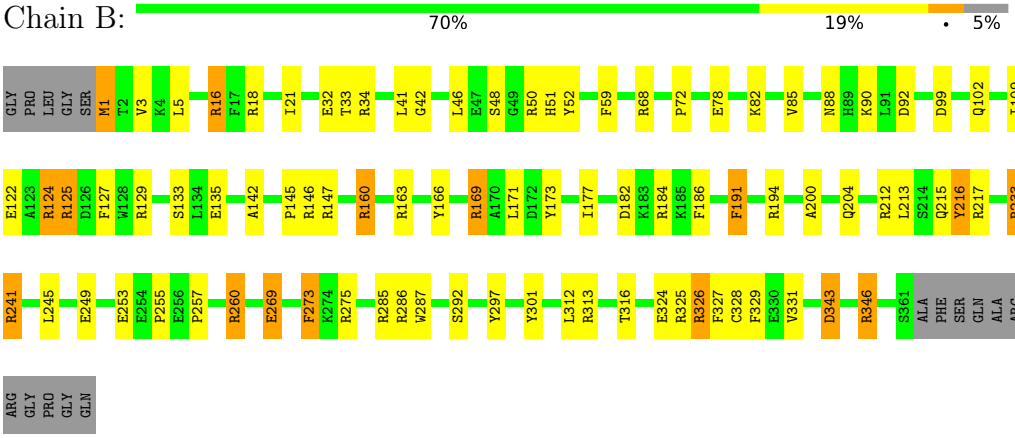
• Molecule 1: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1

Chain A:



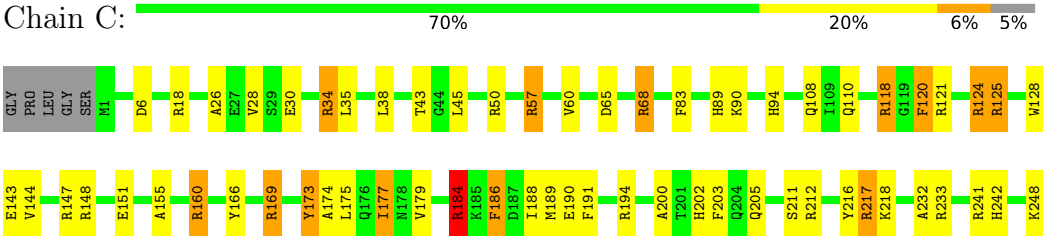
• Molecule 1: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1

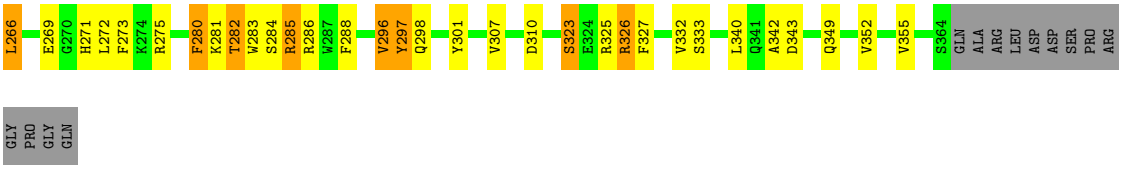
Chain B:



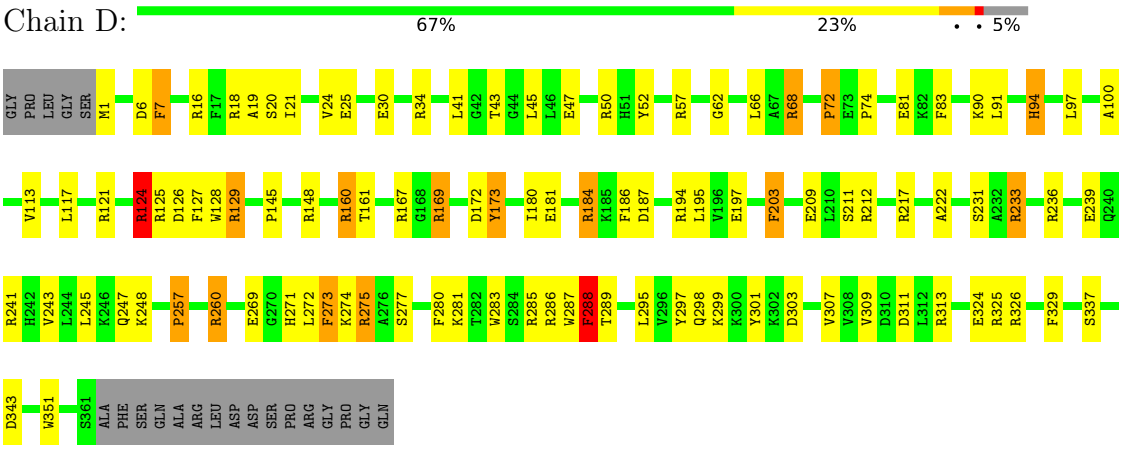
• Molecule 1: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1

Chain C:





• Molecule 1: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=42.72°, rise=23.20 Å, axial sym=C3	Depositor
Number of segments used	304	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	1.62	16/2963 (0.5%)	2.28	114/3987 (2.9%)
1	B	1.64	18/2940 (0.6%)	2.18	92/3956 (2.3%)
1	C	1.60	15/2963 (0.5%)	2.21	94/3987 (2.4%)
1	D	1.61	16/2940 (0.5%)	2.16	92/3956 (2.3%)
All	All	1.62	65/11806 (0.6%)	2.21	392/15886 (2.5%)

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	A	0	12
1	B	0	10
1	C	0	12
1	D	0	15
All	All	0	49

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	TRP	CD2-CE2	8.13	1.51	1.41
1	B	78	GLU	CB-CG	7.08	1.65	1.52
1	A	239	GLU	CD-OE1	6.70	1.33	1.25
1	C	151	GLU	CB-CG	6.64	1.64	1.52
1	B	48	SER	CA-CB	6.54	1.62	1.52
1	A	166	TYR	CG-CD1	6.35	1.47	1.39
1	B	122	GLU	CB-CG	6.30	1.64	1.52
1	A	361	SER	CA-CB	6.18	1.62	1.52
1	C	191	PHE	CB-CG	-6.17	1.40	1.51
1	B	326	ARG	CZ-NH1	-6.06	1.25	1.33
1	C	169	ARG	N-CA	-6.01	1.34	1.46
1	A	297	TYR	CG-CD2	5.95	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	ARG	CZ-NH1	-5.93	1.25	1.33
1	A	288	PHE	CG-CD2	5.90	1.47	1.38
1	C	148	ARG	CZ-NH1	-5.90	1.25	1.33
1	B	133	SER	CA-CB	-5.88	1.44	1.52
1	B	52	TYR	CB-CG	-5.86	1.42	1.51
1	C	326	ARG	CD-NE	5.82	1.56	1.46
1	D	52	TYR	CZ-OH	5.78	1.47	1.37
1	D	297	TYR	CB-CG	-5.74	1.43	1.51
1	A	216	TYR	CB-CG	-5.70	1.43	1.51
1	D	301	TYR	CZ-OH	5.70	1.47	1.37
1	C	355	VAL	CA-CB	-5.69	1.42	1.54
1	D	145	PRO	N-CD	-5.67	1.40	1.47
1	A	330	GLU	CB-CG	5.65	1.62	1.52
1	C	190	GLU	CD-OE1	5.65	1.31	1.25
1	A	128	TRP	CD2-CE2	-5.64	1.34	1.41
1	B	41	LEU	C-N	5.62	1.43	1.33
1	C	285	ARG	CZ-NH2	-5.60	1.25	1.33
1	C	143	GLU	CA-CB	5.59	1.66	1.53
1	C	155	ALA	CA-CB	5.59	1.64	1.52
1	D	239	GLU	CG-CD	-5.57	1.43	1.51
1	D	203	PHE	CG-CD2	5.51	1.47	1.38
1	A	36	GLU	CG-CD	-5.51	1.43	1.51
1	A	345	GLU	CD-OE1	-5.49	1.19	1.25
1	D	81	GLU	CB-CG	5.46	1.62	1.52
1	B	324	GLU	CG-CD	5.45	1.60	1.51
1	D	211	SER	CA-CB	5.43	1.61	1.52
1	A	163	ARG	CZ-NH2	-5.40	1.26	1.33
1	B	327	PHE	CE2-CZ	5.38	1.47	1.37
1	B	236	ARG	CD-NE	5.25	1.55	1.46
1	B	313	ARG	CD-NE	5.24	1.55	1.46
1	D	47	GLU	CD-OE1	-5.24	1.19	1.25
1	B	127	PHE	CB-CG	5.24	1.60	1.51
1	B	169	ARG	CD-NE	5.22	1.55	1.46
1	D	288	PHE	CG-CD1	5.20	1.46	1.38
1	B	173	TYR	CB-CG	5.20	1.59	1.51
1	D	287	TRP	CE2-CZ2	-5.19	1.30	1.39
1	D	324	GLU	CG-CD	-5.17	1.44	1.51
1	A	49	GLY	CA-C	-5.17	1.43	1.51
1	C	57	ARG	CZ-NH1	-5.16	1.26	1.33
1	C	169	ARG	CG-CD	5.14	1.64	1.51
1	C	128	TRP	NE1-CE2	-5.13	1.30	1.37
1	B	18	ARG	NE-CZ	5.13	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	277	SER	CA-CB	5.11	1.60	1.52
1	B	16	ARG	CZ-NH1	-5.09	1.26	1.33
1	C	173	TYR	CG-CD1	5.08	1.45	1.39
1	A	166	TYR	CA-CB	5.06	1.65	1.53
1	C	166	TYR	CA-CB	5.06	1.65	1.53
1	A	283	TRP	CG-CD1	5.06	1.43	1.36
1	D	128	TRP	CD2-CE2	5.05	1.47	1.41
1	D	181	GLU	CD-OE2	-5.05	1.20	1.25
1	A	321	PRO	N-CD	-5.04	1.40	1.47
1	A	27	GLU	CD-OE2	5.04	1.31	1.25
1	B	297	TYR	CD2-CE2	5.03	1.46	1.39

All (392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	ARG	NE-CZ-NH1	24.61	132.60	120.30
1	A	148	ARG	NE-CZ-NH2	21.06	130.83	120.30
1	D	124	ARG	NE-CZ-NH1	20.73	130.66	120.30
1	D	16	ARG	NE-CZ-NH2	20.09	130.34	120.30
1	C	325	ARG	NE-CZ-NH1	19.80	130.20	120.30
1	B	275	ARG	NE-CZ-NH1	19.33	129.97	120.30
1	A	163	ARG	NE-CZ-NH2	18.02	129.31	120.30
1	D	124	ARG	NE-CZ-NH2	-17.40	111.60	120.30
1	A	121	ARG	NE-CZ-NH1	17.18	128.89	120.30
1	D	169	ARG	NE-CZ-NH1	17.17	128.88	120.30
1	C	124	ARG	NE-CZ-NH1	16.76	128.68	120.30
1	D	50	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	C	212	ARG	NE-CZ-NH1	16.57	128.58	120.30
1	A	285	ARG	NE-CZ-NH2	-16.55	112.02	120.30
1	D	18	ARG	NE-CZ-NH1	16.37	128.48	120.30
1	D	194	ARG	NE-CZ-NH1	16.26	128.43	120.30
1	C	50	ARG	NE-CZ-NH2	16.18	128.39	120.30
1	B	125	ARG	NE-CZ-NH2	-16.09	112.25	120.30
1	B	118	ARG	NE-CZ-NH1	15.51	128.05	120.30
1	A	260	ARG	NE-CZ-NH1	15.47	128.04	120.30
1	D	68	ARG	NE-CZ-NH1	15.34	127.97	120.30
1	C	57	ARG	NE-CZ-NH1	15.31	127.96	120.30
1	A	166	TYR	CB-CG-CD2	-15.28	111.83	121.00
1	C	260	ARG	NE-CZ-NH1	15.17	127.89	120.30
1	A	167	ARG	NE-CZ-NH2	15.12	127.86	120.30
1	C	147	ARG	NE-CZ-NH2	14.87	127.74	120.30
1	B	233	ARG	NE-CZ-NH2	14.82	127.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ARG	NE-CZ-NH2	-14.69	112.95	120.30
1	C	241	ARG	NE-CZ-NH1	14.65	127.63	120.30
1	B	260	ARG	NE-CZ-NH1	14.47	127.53	120.30
1	D	236	ARG	NE-CZ-NH1	14.36	127.48	120.30
1	A	184	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	D	236	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	B	326	ARG	NE-CZ-NH2	14.09	127.35	120.30
1	B	184	ARG	NE-CZ-NH2	14.09	127.34	120.30
1	C	160	ARG	NE-CZ-NH2	13.83	127.22	120.30
1	A	241	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	C	121	ARG	NE-CZ-NH2	-13.78	113.41	120.30
1	A	147	ARG	NE-CZ-NH1	-13.74	113.43	120.30
1	C	57	ARG	NE-CZ-NH2	-13.71	113.44	120.30
1	B	68	ARG	NE-CZ-NH1	13.65	127.13	120.30
1	C	18	ARG	NE-CZ-NH2	-13.65	113.48	120.30
1	A	146	ARG	NE-CZ-NH1	13.62	127.11	120.30
1	D	169	ARG	NE-CZ-NH2	-13.61	113.50	120.30
1	C	184	ARG	NE-CZ-NH1	13.41	127.01	120.30
1	A	194	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	A	18	ARG	NE-CZ-NH2	-13.11	113.74	120.30
1	A	236	ARG	NE-CZ-NH1	13.06	126.83	120.30
1	B	346	ARG	NE-CZ-NH1	12.97	126.79	120.30
1	B	285	ARG	NE-CZ-NH1	12.97	126.78	120.30
1	B	68	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	B	191	PHE	CB-CG-CD2	-12.73	111.89	120.80
1	B	160	ARG	NE-CZ-NH2	12.70	126.65	120.30
1	C	68	ARG	NE-CZ-NH2	12.68	126.64	120.30
1	B	166	TYR	CB-CG-CD1	-12.51	113.50	121.00
1	C	121	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	B	194	ARG	NE-CZ-NH2	-12.41	114.10	120.30
1	A	326	ARG	NE-CZ-NH2	-12.39	114.11	120.30
1	B	346	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	C	217	ARG	NE-CZ-NH1	-12.13	114.24	120.30
1	C	327	PHE	CB-CG-CD2	12.04	129.23	120.80
1	A	233	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	A	148	ARG	NE-CZ-NH1	-11.81	114.40	120.30
1	A	18	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	D	50	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	B	326	ARG	NH1-CZ-NH2	-11.33	106.94	119.40
1	C	297	TYR	CB-CG-CD2	-11.32	114.21	121.00
1	A	160	ARG	NE-CZ-NH2	11.27	125.94	120.30
1	B	194	ARG	NE-CZ-NH1	11.26	125.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	C	147	ARG	NE-CZ-NH1	-10.93	114.84	120.30
1	A	216	TYR	CB-CG-CD1	-10.87	114.48	121.00
1	B	325	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	D	187	ASP	CB-CG-OD1	10.84	128.05	118.30
1	B	326	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	A	363	PHE	CB-CG-CD1	10.80	128.36	120.80
1	A	325	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	C	194	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	A	212	ARG	NE-CZ-NH2	10.73	125.67	120.30
1	C	327	PHE	CB-CG-CD1	-10.69	113.32	120.80
1	B	166	TYR	CB-CG-CD2	10.54	127.33	121.00
1	B	18	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	C	203	PHE	CB-CG-CD1	10.42	128.10	120.80
1	A	326	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	C	275	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	A	34	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	A	147	ARG	NE-CZ-NH2	10.30	125.45	120.30
1	A	237	ASP	CB-CG-OD1	10.27	127.54	118.30
1	C	326	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	D	173	TYR	CB-CG-CD2	-10.23	114.86	121.00
1	B	125	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	D	217	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	C	160	ARG	NE-CZ-NH1	-10.08	115.26	120.30
1	A	216	TYR	CB-CG-CD2	10.07	127.04	121.00
1	B	163	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	D	260	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	D	233	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	D	313	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	166	TYR	CB-CG-CD1	9.79	126.88	121.00
1	B	129	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	D	212	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	C	326	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	241	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	A	237	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	D	121	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	C	184	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	163	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	C	217	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	C	186	PHE	CB-CG-CD2	-9.20	114.36	120.80
1	A	127	PHE	CB-CG-CD1	-9.12	114.42	120.80
1	B	343	ASP	CB-CG-OD1	9.09	126.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	B	169	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	D	125	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	D	286	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	311	ASP	CB-CG-OD2	8.81	126.23	118.30
1	A	363	PHE	CB-CG-CD2	-8.80	114.64	120.80
1	A	68	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	B	325	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	285	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	D	187	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	A	76	MET	CG-SD-CE	-8.60	86.44	100.20
1	B	313	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	D	129	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	233	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	D	325	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	C	301	TYR	CB-CG-CD2	8.48	126.09	121.00
1	D	343	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	D	34	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	B	216	TYR	CG-CD1-CE1	-8.38	114.60	121.30
1	D	233	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	B	118	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	241	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	B	34	ARG	NE-CZ-NH2	8.19	124.39	120.30
1	D	273	PHE	CB-CG-CD2	8.14	126.50	120.80
1	B	146	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	297	TYR	CB-CG-CD2	-8.11	116.14	121.00
1	B	275	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C	124	ARG	NH1-CZ-NH2	-8.09	110.50	119.40
1	A	286	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	C	285	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	B	52	TYR	CG-CD2-CE2	-7.95	114.94	121.30
1	D	18	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	C	301	TYR	CB-CG-CD1	-7.85	116.29	121.00
1	B	121	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	D	309	VAL	CA-CB-CG2	7.84	122.66	110.90
1	C	125	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	C	323	SER	N-CA-CB	7.78	122.18	110.50
1	B	124	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	6	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	D	313	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	C	297	TYR	CB-CG-CD1	7.69	125.61	121.00
1	B	301	TYR	CD1-CE1-CZ	7.69	126.72	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	160	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	216	TYR	CZ-CE2-CD2	-7.65	112.91	119.80
1	B	233	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	184	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	50	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	C	285	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	A	343	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	18	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	C	194	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	217	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	C	285	ARG	NH1-CZ-NH2	-7.46	111.19	119.40
1	A	125	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	D	241	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	160	ARG	NH1-CZ-NH2	-7.41	111.25	119.40
1	B	142	ALA	CB-CA-C	7.41	121.21	110.10
1	C	232	ALA	N-CA-CB	-7.40	99.75	110.10
1	B	241	ARG	NH1-CZ-NH2	-7.39	111.28	119.40
1	D	194	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	C	129	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	191	PHE	CB-CG-CD1	7.35	125.94	120.80
1	B	99	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	A	27	GLU	OE1-CD-OE2	-7.32	114.51	123.30
1	A	329	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	B	142	ALA	N-CA-CB	-7.30	99.88	110.10
1	B	313	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	313	ARG	CD-NE-CZ	-7.26	113.44	123.60
1	A	343	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	83	PHE	CB-CG-CD1	-7.24	115.73	120.80
1	C	120	PHE	CB-CG-CD2	-7.19	115.77	120.80
1	D	343	ASP	CB-CG-OD1	7.18	124.76	118.30
1	D	329	PHE	CB-CG-CD2	7.16	125.81	120.80
1	A	68	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	B	163	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	194	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	236	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	125	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	269	GLU	N-CA-CB	7.07	123.32	110.60
1	B	241	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	16	ARG	NH1-CZ-NH2	-7.00	111.70	119.40
1	A	328	CYS	O-C-N	-6.93	111.61	122.70
1	D	83	PHE	CB-CG-CD2	6.93	125.65	120.80
1	C	118	ARG	NE-CZ-NH2	6.91	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	343	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	B	186	PHE	CB-CG-CD1	-6.85	116.01	120.80
1	A	329	PHE	CB-CG-CD2	6.84	125.59	120.80
1	B	32	GLU	N-CA-CB	-6.84	98.29	110.60
1	C	68	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	C	189	MET	CG-SD-CE	-6.81	89.31	100.20
1	C	34	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	313	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	83	PHE	CB-CG-CD2	6.74	125.52	120.80
1	A	346	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	83	PHE	CB-CG-CD2	6.74	125.52	120.80
1	D	160	ARG	NH1-CZ-NH2	-6.72	112.01	119.40
1	A	260	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
1	B	88	ASN	CB-CA-C	6.69	123.77	110.40
1	D	329	PHE	CB-CG-CD1	-6.68	116.12	120.80
1	D	126	ASP	CB-CG-OD2	6.67	124.31	118.30
1	B	217	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	146	ARG	NH1-CZ-NH2	-6.63	112.11	119.40
1	D	184	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	284	SER	N-CA-CB	6.62	120.43	110.50
1	B	212	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	287	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	167	ARG	NH1-CZ-NH2	-6.59	112.15	119.40
1	A	51	HIS	CA-CB-CG	6.58	124.79	113.60
1	B	312	LEU	O-C-N	-6.55	112.23	122.70
1	B	286	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	C	203	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	D	222	ALA	O-C-N	-6.50	112.30	122.70
1	A	160	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
1	D	260	ARG	NH1-CZ-NH2	-6.47	112.29	119.40
1	C	325	ARG	NH1-CZ-NH2	-6.46	112.30	119.40
1	D	337	SER	N-CA-CB	6.46	120.19	110.50
1	C	50	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	C	174	ALA	N-CA-CB	-6.44	101.08	110.10
1	D	121	ARG	CG-CD-NE	-6.44	98.28	111.80
1	C	241	ARG	CD-NE-CZ	6.43	132.60	123.60
1	B	1	MET	CG-SD-CE	-6.42	89.93	100.20
1	C	343	ASP	CB-CG-OD1	6.41	124.07	118.30
1	D	325	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	28	VAL	CG1-CB-CG2	-6.38	100.69	110.90
1	A	327	PHE	CB-CG-CD1	-6.37	116.34	120.80
1	D	127	PHE	CB-CG-CD2	-6.30	116.39	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	233	ARG	CD-NE-CZ	6.29	132.41	123.60
1	D	160	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	C	271	HIS	CA-CB-CG	6.29	124.29	113.60
1	C	65	ASP	CB-CG-OD1	6.28	123.96	118.30
1	D	326	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	173	TYR	CB-CG-CD1	6.26	124.75	121.00
1	D	161	THR	CA-CB-CG2	-6.25	103.66	112.40
1	C	325	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	83	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	A	187	ASP	CB-CG-OD2	6.23	123.91	118.30
1	C	273	PHE	CB-CG-CD1	-6.19	116.47	120.80
1	D	217	ARG	CD-NE-CZ	-6.19	114.94	123.60
1	C	280	PHE	CB-CG-CD1	-6.18	116.47	120.80
1	B	260	ARG	NH1-CZ-NH2	-6.17	112.61	119.40
1	D	19	ALA	N-CA-CB	-6.17	101.46	110.10
1	C	349	GLN	CG-CD-OE1	-6.14	109.32	121.60
1	B	182	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	187	ASP	N-CA-CB	6.10	121.59	110.60
1	D	186	PHE	CB-CG-CD2	6.09	125.06	120.80
1	D	184	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	57	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	A	278	ASN	O-C-N	-6.03	113.05	122.70
1	D	212	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	26	ALA	N-CA-CB	-6.01	101.68	110.10
1	A	344	SER	N-CA-CB	-6.00	101.50	110.50
1	A	99	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	C	43	THR	CA-CB-CG2	-5.99	104.02	112.40
1	A	320	CYS	O-C-N	-5.94	109.81	121.10
1	D	273	PHE	CB-CG-CD1	-5.94	116.64	120.80
1	D	326	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	B	285	ARG	CD-NE-CZ	-5.91	115.32	123.60
1	A	342	ALA	CB-CA-C	-5.91	101.24	110.10
1	D	172	ASP	O-C-N	-5.90	113.26	122.70
1	A	268	MET	CG-SD-CE	-5.89	90.77	100.20
1	A	194	ARG	CB-CA-C	-5.89	98.62	110.40
1	D	100	ALA	CB-CA-C	-5.88	101.28	110.10
1	D	125	ARG	NH1-CZ-NH2	-5.87	112.95	119.40
1	D	311	ASP	CB-CG-OD1	-5.86	113.02	118.30
1	B	50	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	307	VAL	CG1-CB-CG2	-5.86	101.53	110.90
1	B	273	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	B	3	VAL	CG1-CB-CG2	-5.81	101.60	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	173	TYR	CB-CG-CD1	5.80	124.48	121.00
1	C	212	ARG	NH1-CZ-NH2	-5.80	113.03	119.40
1	D	209	GLU	CB-CA-C	5.76	121.93	110.40
1	A	194	ARG	CD-NE-CZ	5.76	131.66	123.60
1	C	212	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	238	MET	CG-SD-CE	-5.74	91.01	100.20
1	D	241	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	B	217	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	A	124	ARG	CG-CD-NE	-5.70	99.84	111.80
1	A	173	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	C	18	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	326	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
1	B	147	ARG	O-C-N	-5.66	113.65	122.70
1	D	184	ARG	CA-CB-CG	5.65	125.84	113.40
1	B	327	PHE	CG-CD1-CE1	5.65	127.01	120.80
1	C	332	VAL	CG1-CB-CG2	-5.64	101.87	110.90
1	D	280	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	D	7	PHE	CG-CD2-CE2	5.62	126.98	120.80
1	B	59	PHE	CB-CG-CD2	-5.61	116.87	120.80
1	C	200	ALA	N-CA-CB	-5.61	102.25	110.10
1	A	34	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	3	VAL	CA-CB-CG1	5.60	119.31	110.90
1	A	216	TYR	CA-CB-CG	-5.60	102.75	113.40
1	B	135	GLU	O-C-N	-5.60	113.74	122.70
1	A	137	ALA	N-CA-CB	5.60	117.94	110.10
1	A	181	GLU	O-C-N	5.57	131.62	122.70
1	D	20	SER	N-CA-CB	5.57	118.86	110.50
1	D	125	ARG	CD-NE-CZ	-5.56	115.82	123.60
1	A	315	CYS	O-C-N	-5.55	113.82	122.70
1	A	327	PHE	CB-CG-CD2	5.55	124.68	120.80
1	C	286	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	1	MET	CA-CB-CG	5.55	122.73	113.30
1	D	243	VAL	CA-CB-CG1	-5.54	102.59	110.90
1	D	72	PRO	N-CA-CB	-5.54	96.50	102.60
1	D	231	SER	O-C-N	-5.53	113.85	122.70
1	A	173	TYR	CD1-CE1-CZ	-5.52	114.83	119.80
1	B	135	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	A	148	ARG	CD-NE-CZ	5.50	131.31	123.60
1	B	3	VAL	CA-CB-CG1	5.48	119.12	110.90
1	C	352	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	D	301	TYR	CG-CD1-CE1	-5.48	116.92	121.30
1	D	41	LEU	CB-CG-CD2	5.47	120.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	52	TYR	CZ-CE2-CD2	5.47	124.72	119.80
1	B	124	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
1	B	301	TYR	CG-CD1-CE1	-5.45	116.94	121.30
1	B	120	PHE	CB-CA-C	5.45	121.30	110.40
1	A	133	SER	N-CA-CB	5.44	118.66	110.50
1	C	283	TRP	CE3-CZ3-CH2	-5.43	115.23	121.20
1	D	43	THR	CA-CB-OG1	5.42	120.38	109.00
1	A	149	ALA	N-CA-CB	-5.41	102.53	110.10
1	C	259	LEU	CA-CB-CG	5.38	127.68	115.30
1	C	173	TYR	CG-CD1-CE1	-5.38	117.00	121.30
1	D	30	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	A	297	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	B	92	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	56	SER	N-CA-CB	5.36	118.54	110.50
1	A	228	VAL	CA-CB-CG2	-5.34	102.88	110.90
1	A	224	LEU	CB-CG-CD1	5.34	120.08	111.00
1	A	311	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	292	SER	N-CA-CB	5.34	118.51	110.50
1	C	177	ILE	O-C-N	-5.33	114.16	122.70
1	B	328	CYS	CA-CB-SG	5.33	123.60	114.00
1	C	108	GLN	O-C-N	-5.33	114.17	122.70
1	C	6	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	30	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	D	91	LEU	C-N-CA	5.32	135.00	121.70
1	A	325	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	126	ASP	CB-CG-OD1	-5.29	113.53	118.30
1	B	169	ARG	O-C-N	-5.29	114.24	122.70
1	D	128	TRP	CB-CA-C	5.29	120.97	110.40
1	A	313	ARG	NH1-CZ-NH2	-5.28	113.60	119.40
1	A	88	ASN	N-CA-CB	-5.26	101.12	110.60
1	A	152	ALA	O-C-N	-5.25	114.30	122.70
1	A	212	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	B	52	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	34	ARG	CG-CD-NE	-5.24	100.81	111.80
1	B	171	LEU	O-C-N	-5.22	114.34	122.70
1	D	45	LEU	N-CA-CB	-5.22	99.96	110.40
1	D	43	THR	N-CA-CB	5.22	120.22	110.30
1	A	241	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	C	211	SER	O-C-N	-5.20	114.38	122.70
1	C	173	TYR	CD1-CE1-CZ	5.20	124.48	119.80
1	C	286	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	355	VAL	CG1-CB-CG2	-5.19	102.59	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	ALA	CB-CA-C	-5.18	102.33	110.10
1	C	296	VAL	O-C-N	-5.16	114.44	122.70
1	D	62	GLY	O-C-N	-5.15	114.46	122.70
1	D	298	GLN	CB-CA-C	-5.14	100.12	110.40
1	A	297	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	B	275	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	D	68	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	24	VAL	O-C-N	-5.13	114.49	122.70
1	D	326	ARG	O-C-N	5.13	130.90	122.70
1	D	307	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	B	5	LEU	O-C-N	-5.11	114.52	122.70
1	A	203	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	317	VAL	CG1-CB-CG2	-5.11	102.73	110.90
1	C	342	ALA	CB-CA-C	-5.09	102.47	110.10
1	C	282	THR	N-CA-C	5.09	124.73	111.00
1	A	111	THR	CA-CB-CG2	5.08	119.52	112.40
1	A	196	VAL	CA-CB-CG2	5.08	118.52	110.90
1	C	233	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	A	347	LEU	CB-CG-CD1	5.07	119.62	111.00
1	B	297	TYR	CD1-CE1-CZ	5.07	124.36	119.80
1	B	217	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	362	ALA	O-C-N	-5.05	114.62	122.70
1	B	34	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	C	110	GLN	CB-CA-C	-5.05	100.30	110.40
1	D	297	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
1	C	144	VAL	CA-CB-CG2	-5.03	103.36	110.90
1	C	35	LEU	CB-CG-CD2	5.03	119.55	111.00
1	C	333	SER	CA-C-O	5.02	130.64	120.10
1	C	284	SER	N-CA-CB	5.01	118.02	110.50

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLU	Peptide
1	A	125	ARG	Sidechain
1	A	127	PHE	Sidechain
1	A	129	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	17	PHE	Sidechain
1	A	236	ARG	Sidechain
1	A	260	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	271	HIS	Sidechain
1	A	297	TYR	Sidechain
1	A	313	ARG	Sidechain
1	A	34	ARG	Sidechain
1	B	120	PHE	Sidechain
1	B	121	ARG	Sidechain
1	B	124	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	169	ARG	Sidechain
1	B	216	TYR	Sidechain
1	B	241	ARG	Sidechain
1	B	273	PHE	Sidechain
1	B	346	ARG	Sidechain
1	B	51	HIS	Sidechain
1	C	118	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	160	ARG	Sidechain
1	C	169	ARG	Sidechain
1	C	184	ARG	Sidechain
1	C	186	PHE	Sidechain
1	C	216	TYR	Sidechain
1	C	280	PHE	Peptide
1	C	285	ARG	Sidechain
1	C	34	ARG	Sidechain
1	C	57	ARG	Sidechain
1	C	68	ARG	Sidechain
1	D	129	ARG	Sidechain
1	D	148	ARG	Sidechain
1	D	167	ARG	Sidechain
1	D	173	TYR	Sidechain
1	D	184	ARG	Sidechain
1	D	233	ARG	Sidechain
1	D	271	HIS	Sidechain
1	D	273	PHE	Sidechain
1	D	275	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	288	PHE	Sidechain
1	D	57	ARG	Sidechain
1	D	6	ASP	Peptide
1	D	68	ARG	Sidechain
1	D	7	PHE	Sidechain

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	A	2915	2934	2936	10	0
1	B	2893	2915	2917	8	0
1	C	2915	2934	2936	13	0
1	D	2893	2915	2917	14	0
All	All	11616	11698	11706	39	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 2.

All (39) 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)
1:D:94:HIS:CD2	1:D:97:LEU:HD23	2.31	0.65
1:C:202:HIS:CE1	1:D:203:PHE:CE2	2.91	0.57
1:C:202:HIS:CE1	1:D:203:PHE:CZ	2.97	0.52
1:A:271:HIS:CE1	1:A:287:TRP:CE3	3.00	0.49
1:C:296:VAL:HG12	1:C:307:VAL:HA	1.95	0.49
1:C:217:ARG:HH11	1:D:197:GLU:CD	2.17	0.49
1:C:38:LEU:CD2	1:D:66:LEU:HD11	2.43	0.48
1:B:109:ILE:HD11	1:B:191:PHE:CD2	2.48	0.48
1:C:120:PHE:CE2	1:C:177:ILE:HD11	2.48	0.47
1:D:288:PHE:HB3	1:D:295:LEU:HD11	1.97	0.47
1:D:272:LEU:HD21	1:D:351:TRP:CD1	2.49	0.47
1:A:140:HIS:CD2	1:A:155:ALA:HB2	2.50	0.47
1:C:307:VAL:HG11	1:C:310:ASP:HB3	1.97	0.47
1:A:39:LEU:HA	1:A:105:LEU:HD11	1.99	0.45
1:C:272:LEU:HB2	1:C:288:PHE:CE1	2.52	0.45
1:B:253:GLU:H	1:B:253:GLU:CD	2.21	0.44
1:D:289:THR:O	1:D:295:LEU:HD12	2.18	0.44
1:C:89:HIS:HE1	1:C:205:GLN:O	2.00	0.44
1:B:245:LEU:HA	1:B:249:GLU:HG2	2.00	0.43
1:D:169:ARG:HA	1:D:169:ARG:CZ	2.48	0.43
1:C:175:LEU:O	1:C:179:VAL:HG23	2.19	0.43
1:C:45:LEU:HD23	1:C:45:LEU:C	2.39	0.43
1:C:94:HIS:HD1	1:C:202:HIS:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HG3	1:A:98:LEU:HD13	2.00	0.42
1:A:90:LYS:HE2	1:B:200:ALA:HA	2.00	0.42
1:C:340:LEU:HA	1:C:340:LEU:HD23	1.90	0.42
1:D:25:GLU:CD	1:D:124:ARG:HE	2.23	0.42
1:D:247:GLN:HG3	1:D:248:LYS:HG2	2.02	0.42
1:D:21:ILE:HA	1:D:24:VAL:HG12	2.02	0.42
1:A:183:LYS:HE3	1:A:187:ASP:OD1	2.20	0.41
1:B:42:GLY:O	1:B:46:LEU:HG	2.20	0.41
1:A:316:THR:HA	1:A:359:ILE:HD13	2.02	0.41
1:A:10:CYS:HB2	1:A:170:ALA:HB1	2.01	0.41
1:A:146:ARG:HG3	1:B:326:ARG:HA	2.02	0.41
1:D:274:LYS:O	1:D:283:TRP:HA	2.21	0.41
1:B:21:ILE:HG22	1:B:177:ILE:CD1	2.50	0.40
1:B:82:LYS:HA	1:B:85:VAL:HG12	2.03	0.40
1:D:117:LEU:HA	1:D:180:ILE:HD12	2.02	0.40
1:A:260:ARG:O	1:A:261:GLU:HB2	2.21	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	362/382 (95%)	352 (97%)	8 (2%)	2 (1%)	27	70
1	B	359/382 (94%)	348 (97%)	9 (2%)	2 (1%)	27	70
1	C	362/382 (95%)	345 (95%)	15 (4%)	2 (1%)	27	70
1	D	359/382 (94%)	340 (95%)	18 (5%)	1 (0%)	43	81
All	All	1442/1528 (94%)	1385 (96%)	50 (4%)	7 (0%)	35	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LEU
1	C	323	SER
1	B	257	PRO
1	C	266	LEU
1	D	257	PRO
1	A	261	GLU
1	B	255	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/325 (96%)	293 (94%)	19 (6%)	20	52
1	B	310/325 (95%)	291 (94%)	19 (6%)	20	52
1	C	312/325 (96%)	294 (94%)	18 (6%)	22	52
1	D	310/325 (95%)	294 (95%)	16 (5%)	25	56
All	All	1244/1300 (96%)	1172 (94%)	72 (6%)	26	52

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	CYS
1	A	12	LYS
1	A	45	LEU
1	A	61	VAL
1	A	90	LYS
1	A	110	GLN
1	A	150	GLN
1	A	217	ARG
1	A	236	ARG
1	A	260	ARG
1	A	269	GLU
1	A	274	LYS
1	A	287	TRP
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	297	TYR
1	A	326	ARG
1	A	329	PHE
1	A	348	LEU
1	B	1	MET
1	B	16	ARG
1	B	33	THR
1	B	72	PRO
1	B	90	LYS
1	B	102	GLN
1	B	120	PHE
1	B	125	ARG
1	B	145	PRO
1	B	204	GLN
1	B	213	LEU
1	B	215	GLN
1	B	233	ARG
1	B	260	ARG
1	B	269	GLU
1	B	316	THR
1	B	329	PHE
1	B	331	VAL
1	B	343	ASP
1	C	60	VAL
1	C	90	LYS
1	C	124	ARG
1	C	134	LEU
1	C	173	TYR
1	C	184	ARG
1	C	188	ILE
1	C	218	LYS
1	C	242	HIS
1	C	248	LYS
1	C	260	ARG
1	C	266	LEU
1	C	269	GLU
1	C	281	LYS
1	C	282	THR
1	C	297	TYR
1	C	298	GLN
1	C	326	ARG
1	D	72	PRO

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Mol	Chain	Res	Type
1	D	74	PRO
1	D	90	LYS
1	D	94	HIS
1	D	113	VAL
1	D	124	ARG
1	D	160	ARG
1	D	195	LEU
1	D	245	LEU
1	D	257	PRO
1	D	260	ARG
1	D	269	GLU
1	D	275	ARG
1	D	281	LYS
1	D	299	LYS
1	D	303	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	B	51	HIS
1	B	89	HIS
1	B	207	HIS
1	C	225	HIS
1	D	51	HIS
1	D	207	HIS

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 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.