Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 12:12 pm GMT

PDB ID	:	9HVM
EMDB ID	:	EMD-52438
Title	:	In-cell Structure of Pyrenoid Rubisco
Authors	:	Nadav, E.; Zhen, H.; Maud, D.; Alireza, R.; Juan R, P.; Peijun, P.
Deposited on	:	2024-12-30
Resolution	:	8.10 Å(reported)
Based on initial models	:	1GK8, 1EJ7

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

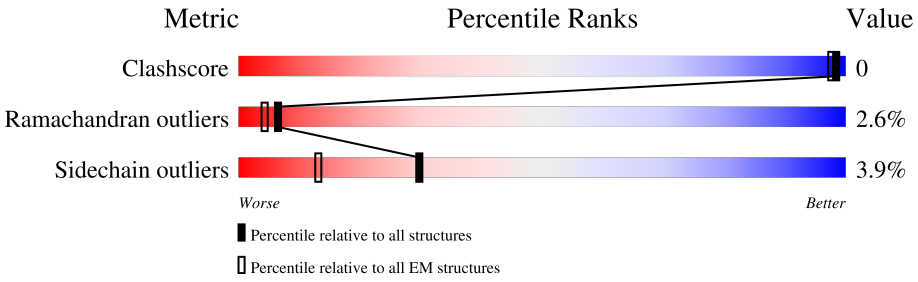
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 8.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	469	85% 12% •
1	C	469	84% 13% •
1	E	469	85% 13% •
1	G	469	84% 14% •
1	I	469	84% 14% •
1	K	469	85% 13% •
1	M	469	85% 12% •
1	O	469	85% 13% •
2	B	132	92% 6% •

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Mol	Chain	Length	Quality of chain
2	D	132	93% 6%
2	F	132	93% 6%
2	H	132	92% 7%
2	J	132	92% 8%
2	L	132	93% 6%
2	N	132	93% 6%
2	P	132	92% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 37816 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 Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	C	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	E	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	G	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	I	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	K	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	M	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		
1	O	469	Total	C	N	O	S	0	0
			3647	2308	642	673	24		

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase small subunit, chloroplastic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	D	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	F	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	H	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	J	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	L	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		

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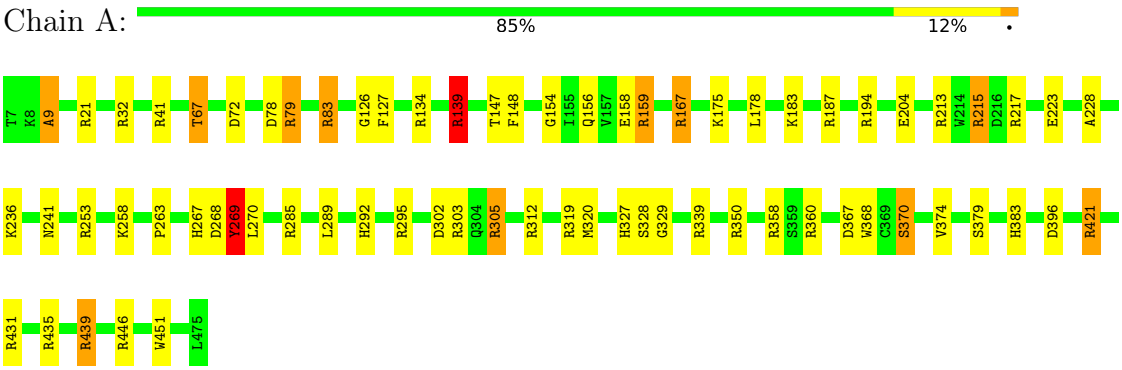
Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		
2	P	132	Total	C	N	O	S	0	0
			1080	701	176	192	11		

3 Residue-property plots (i)

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

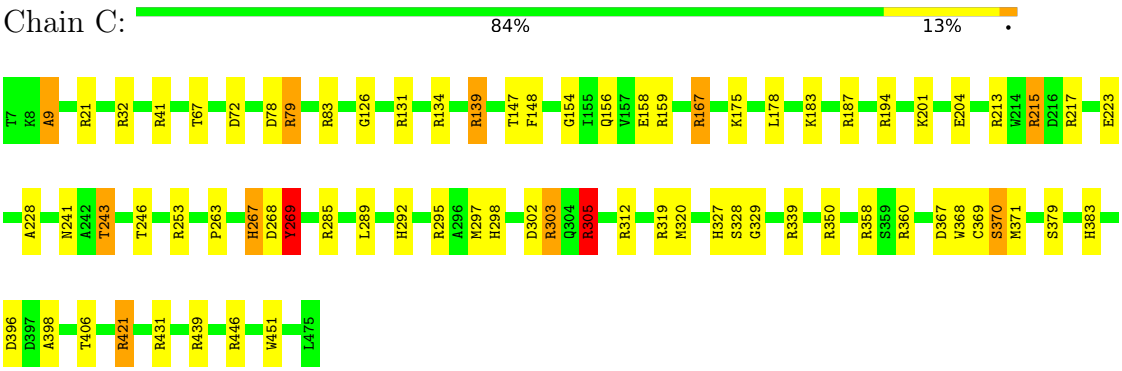
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A:



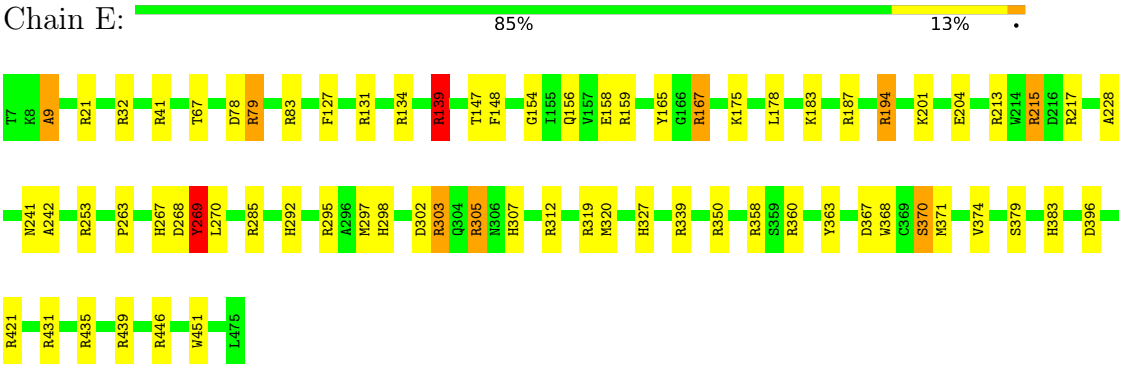
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain C:



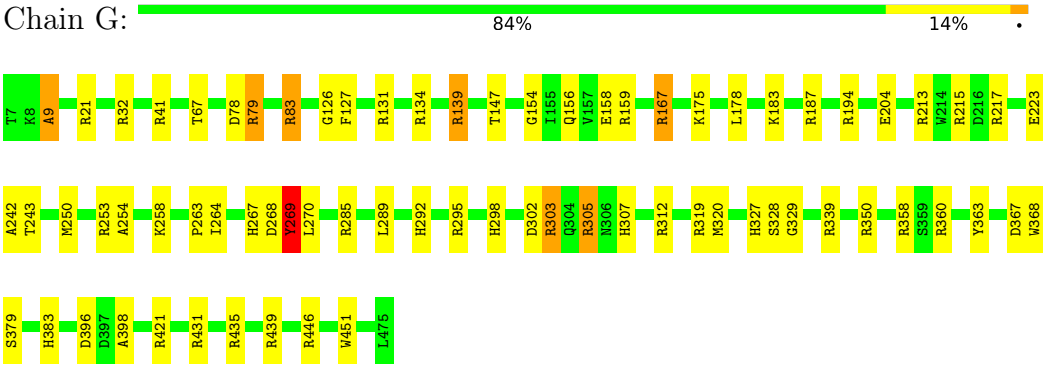
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E:



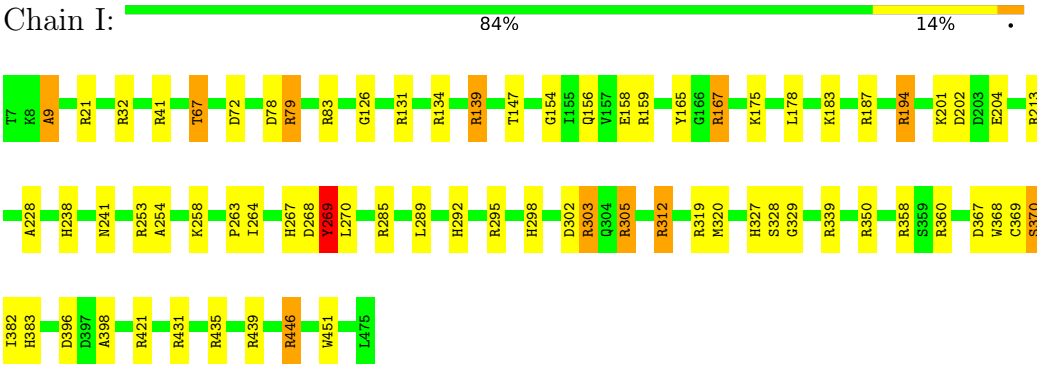
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G:



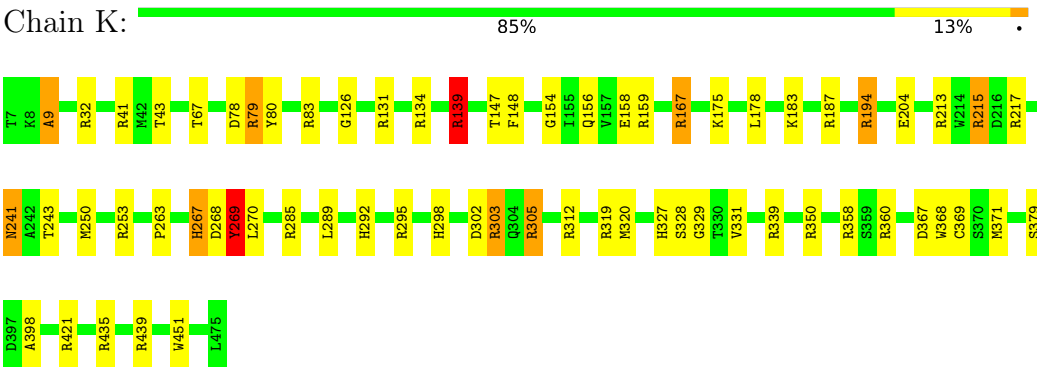
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain I:



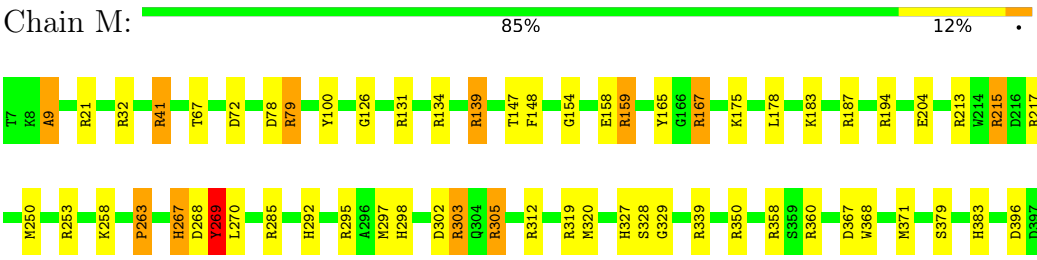
• Molecule 1: Ribulose bisphosphate carboxylase large chain

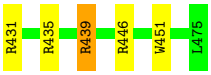
Chain K:



• Molecule 1: Ribulose bisphosphate carboxylase large chain

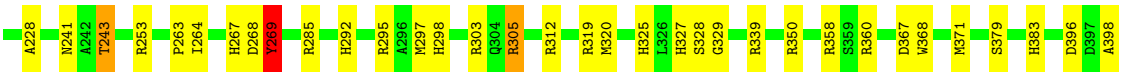
Chain M:





• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain O:

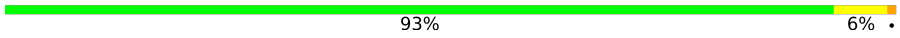


• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

Chain B:

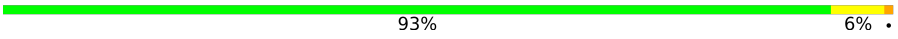
• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

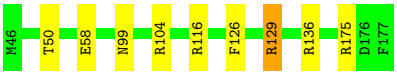
Chain D:



• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

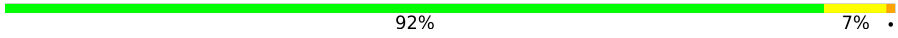
Chain F:





• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

Chain H:

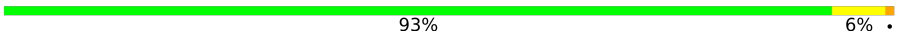


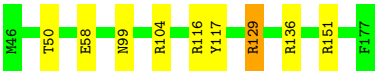
• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

Chain J:

• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

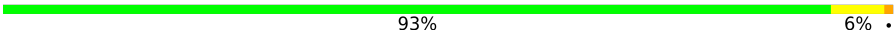
Chain L:





• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

Chain N:



• Molecule 2: Ribulose bisphosphate carboxylase small subunit, chloroplastic 1

Chain P:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of subtomograms used	17713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	120	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.72	0/3733	1.27	46/5054 (0.9%)
1	C	0.72	0/3733	1.28	46/5054 (0.9%)
1	E	0.72	0/3733	1.29	46/5054 (0.9%)
1	G	0.72	0/3733	1.28	51/5054 (1.0%)
1	I	0.72	0/3733	1.25	43/5054 (0.9%)
1	K	0.72	0/3733	1.22	37/5054 (0.7%)
1	M	0.72	0/3733	1.24	45/5054 (0.9%)
1	O	0.72	0/3733	1.27	44/5054 (0.9%)
2	B	0.73	0/1111	1.14	10/1509 (0.7%)
2	D	0.74	0/1111	1.10	7/1509 (0.5%)
2	F	0.74	0/1111	1.10	7/1509 (0.5%)
2	H	0.74	0/1111	1.09	7/1509 (0.5%)
2	J	0.74	0/1111	1.10	6/1509 (0.4%)
2	L	0.74	0/1111	1.09	7/1509 (0.5%)
2	N	0.74	0/1111	1.11	7/1509 (0.5%)
2	P	0.74	0/1111	1.08	4/1509 (0.3%)
All	All	0.72	0/38752	1.23	413/52504 (0.8%)

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	19
1	C	0	16
1	E	0	20
1	G	0	18
1	I	0	20
1	K	0	19
1	M	0	18
1	O	0	19
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	F	0	1
2	H	0	2
2	J	0	1
2	L	0	2
2	N	0	2
2	P	0	2
All	All	0	161

There are no bond length outliers.

All (413) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	253	ARG	NE-CZ-NH1	13.27	126.93	120.30
1	M	253	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	A	253	ARG	NE-CZ-NH1	12.51	126.56	120.30
1	C	446	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	C	421	ARG	NE-CZ-NH1	11.99	126.30	120.30
1	A	421	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	I	350	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	I	253	ARG	NE-CZ-NH1	11.71	126.15	120.30
1	G	253	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	E	421	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	G	421	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	O	253	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	K	253	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	C	350	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	C	253	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	K	421	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	M	421	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	O	350	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	O	350	ARG	NE-CZ-NH1	11.05	125.82	120.30
1	I	421	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	E	79	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	O	131	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	G	139	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	A	295	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	K	285	ARG	NE-CZ-NH1	10.52	125.56	120.30
2	B	136	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	E	446	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	194	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	350	ARG	NE-CZ-NH1	10.21	125.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	431	ARG	NE-CZ-NH1	10.13	125.37	120.30
1	O	421	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	G	79	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	E	194	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	E	295	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	A	339	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	C	79	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	M	215	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	K	358	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	O	295	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	305	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	O	305	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	O	215	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	C	215	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	O	431	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	I	350	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	I	285	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	G	215	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	M	446	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	E	446	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	215	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	O	285	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	G	269	TYR	CB-CG-CD2	9.51	126.71	121.00
2	J	136	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	E	41	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	E	134	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	E	305	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	G	134	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	G	194	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	K	295	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	K	350	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	O	358	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	G	312	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	I	131	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	I	358	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	M	339	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	G	285	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	K	312	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	C	285	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	M	305	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	E	439	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	A	358	ARG	NE-CZ-NH1	8.87	124.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	41	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	A	187	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	K	305	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	G	446	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	C	131	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	C	358	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	M	32	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	C	339	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	E	139	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	I	435	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	G	285	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	350	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	339	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	I	435	ARG	NE-CZ-NH1	8.51	124.55	120.30
2	D	136	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	E	350	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	J	170	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	E	139	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	E	215	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	G	131	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	G	139	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	I	269	TYR	CB-CG-CD2	8.39	126.04	121.00
1	E	285	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	G	358	ARG	NE-CZ-NH1	8.37	124.49	120.30
2	F	136	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	O	446	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	G	269	TYR	CB-CG-CD1	-8.31	116.01	121.00
1	I	187	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	C	312	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	K	285	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	O	269	TYR	CB-CG-CD2	8.29	125.97	121.00
2	P	136	ARG	NE-CZ-NH1	8.29	124.44	120.30
2	N	136	ARG	NE-CZ-NH2	-8.27	116.16	120.30
2	N	136	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	435	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	295	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	I	339	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	M	269	TYR	CB-CG-CD2	8.21	125.93	121.00
1	C	139	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	E	358	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	269	TYR	CB-CG-CD2	8.12	125.87	121.00
1	E	269	TYR	CB-CG-CD2	8.11	125.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	312	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	O	446	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	I	21	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	213	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	N	116	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	K	41	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	E	350	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	M	358	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	G	303	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	C	83	ARG	NE-CZ-NH1	7.99	124.30	120.30
2	L	136	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	C	194	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	G	350	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	I	32	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	C	305	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	C	32	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	K	187	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	G	360	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	M	131	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	G	213	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	C	187	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	G	215	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	I	215	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	I	360	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	269	TYR	CB-CG-CD2	7.80	125.68	121.00
1	A	167	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	M	350	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	O	187	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	I	213	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	O	79	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	G	21	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	K	32	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	K	269	TYR	CB-CG-CD2	7.74	125.65	121.00
2	B	175	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	E	339	ARG	NE-CZ-NH1	7.71	124.15	120.30
2	B	104	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	H	136	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	K	131	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	C	319	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	F	116	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	431	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	167	ARG	NE-CZ-NH1	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	269	TYR	CB-CG-CD1	-7.66	116.41	121.00
1	K	350	ARG	NE-CZ-NH2	-7.63	116.48	120.30
2	L	116	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	439	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	K	303	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	M	303	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	I	446	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	446	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	K	79	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	360	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	I	305	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	O	167	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	O	269	TYR	CB-CG-CD1	-7.54	116.48	121.00
2	P	116	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	G	295	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	E	131	ARG	NE-CZ-NH1	7.49	124.05	120.30
2	N	104	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	21	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	M	285	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	A	134	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	I	446	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	M	360	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	G	187	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	M	41	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	I	319	ARG	NE-CZ-NH1	7.43	124.02	120.30
2	L	104	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	21	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	B	175	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	I	269	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	E	187	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	F	129	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	134	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	E	215	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	285	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	G	360	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	C	269	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	C	360	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	K	213	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	N	129	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	E	167	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	M	79	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	O	319	ARG	NE-CZ-NH1	7.26	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	435	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	303	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	312	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	C	139	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	G	83	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	I	79	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	G	350	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	E	21	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	D	175	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	M	167	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	I	303	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	C	215	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	D	104	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	I	217	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	G	134	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	O	41	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	E	32	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	I	134	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	G	167	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	K	159	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	M	295	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	M	350	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	E	21	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	E	213	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	K	194	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	I	167	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	C	439	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	G	305	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	L	151	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	C	217	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	K	269	TYR	CB-CG-CD1	-6.96	116.82	121.00
1	M	435	ARG	NE-CZ-NH2	-6.95	116.82	120.30
2	B	116	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	O	213	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	M	187	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	E	134	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	J	116	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	360	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	G	431	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	E	269	TYR	CB-CG-CD1	-6.91	116.86	121.00
1	G	312	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	C	159	ARG	NE-CZ-NH1	6.89	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	319	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	O	439	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	269	TYR	CB-CG-CD1	-6.88	116.87	121.00
1	I	134	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	K	339	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	159	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	L	151	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	32	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	370	SER	N-CA-CB	6.82	120.73	110.50
1	A	79	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	E	360	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	G	305	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	G	217	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	I	295	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	E	435	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	K	312	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	312	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	21	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	O	83	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	G	21	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	O	41	ARG	NE-CZ-NH2	-6.75	116.93	120.30
2	H	151	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	O	194	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	I	285	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	M	435	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	M	312	ARG	NE-CZ-NH2	-6.71	116.95	120.30
2	D	175	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	213	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	G	319	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	I	139	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	M	194	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	159	ARG	NE-CZ-NH2	-6.63	116.98	120.30
2	H	116	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	41	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	B	129	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	E	303	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	M	339	ARG	NE-CZ-NH2	-6.60	117.00	120.30
2	B	129	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	O	312	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	E	41	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	E	319	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	E	312	ARG	NE-CZ-NH1	6.58	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	134	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	G	370	SER	N-CA-CB	6.56	120.33	110.50
1	C	285	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	295	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	421	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	41	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	K	435	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	H	104	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	319	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	O	21	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	E	83	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	O	339	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	134	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	M	439	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	E	370	SER	N-CA-CB	6.40	120.10	110.50
1	E	217	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	K	215	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	O	32	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	O	139	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	M	21	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	I	439	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	L	129	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	M	159	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	G	435	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	G	339	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	213	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	P	104	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	41	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	O	217	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	I	370	SER	N-CA-CB	6.26	119.90	110.50
1	A	217	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	350	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	41	ARG	NE-CZ-NH2	-6.25	117.17	120.30
2	F	104	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	G	217	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	K	319	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	M	360	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	O	295	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	J	104	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	I	194	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	79	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	D	116	ARG	NE-CZ-NH1	6.19	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	9	ALA	N-CA-CB	6.19	118.76	110.10
2	N	129	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	I	312	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	G	435	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	P	151	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	K	167	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	M	79	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	312	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	G	421	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	O	9	ALA	N-CA-CB	6.07	118.60	110.10
1	O	213	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	E	421	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	E	9	ALA	N-CA-CB	6.04	118.56	110.10
1	M	21	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	194	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	421	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	I	9	ALA	N-CA-CB	5.98	118.47	110.10
1	A	139	ARG	NE-CZ-NH1	5.97	123.28	120.30
2	B	151	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	83	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	9	ALA	N-CA-CB	5.93	118.41	110.10
1	C	134	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	M	421	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	J	170	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	K	159	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	O	360	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	I	213	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	G	194	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	G	83	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	O	421	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	C	9	ALA	N-CA-CB	5.83	118.26	110.10
1	C	446	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	O	435	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	M	9	ALA	N-CA-CB	5.79	118.20	110.10
1	O	360	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	K	217	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	B	104	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	E	213	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	G	32	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	H	170	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	M	303	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	M	217	ARG	NE-CZ-NH1	5.67	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	303	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	M	213	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	K	360	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	G	303	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	C	431	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	K	421	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	B	170	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	D	129	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	F	129	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	K	79	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	M	139	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	N	151	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	F	175	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	L	104	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	I	319	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	K	9	ALA	N-CA-CB	5.46	117.75	110.10
2	H	129	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	435	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	194	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	O	312	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	M	215	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	I	421	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	I	431	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	M	431	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	370	SER	N-CA-CB	5.31	118.46	110.50
1	O	319	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	D	151	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	H	126	PHE	CB-CG-CD1	5.24	124.47	120.80
1	E	431	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	398	ALA	C-N-CA	5.22	134.76	121.70
1	G	439	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	K	398	ALA	C-N-CA	5.14	134.54	121.70
1	M	134	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	F	126	PHE	CB-CG-CD1	5.13	124.39	120.80
1	I	398	ALA	C-N-CA	5.11	134.48	121.70
1	M	250	MET	CG-SD-CE	-5.08	92.06	100.20
1	M	398	ALA	C-N-CA	5.08	134.40	121.70
1	K	139	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	398	ALA	C-N-CA	5.07	134.38	121.70
1	E	253	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	I	67	THR	N-CA-CB	5.04	119.89	110.30
1	O	398	ALA	C-N-CA	5.04	134.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	79	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	O	134	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	G	250	MET	CG-SD-CE	-5.02	92.17	100.20
1	A	67	THR	N-CA-CB	5.01	119.82	110.30
1	K	250	MET	CG-SD-CE	-5.01	92.19	100.20
2	J	151	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (161) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	147	THR	Peptide
1	A	178	LEU	Peptide
1	A	215	ARG	Sidechain
1	A	228	ALA	Peptide
1	A	236	LYS	Peptide
1	A	263	PRO	Peptide
1	A	268	ASP	Peptide
1	A	269	TYR	Sidechain
1	A	320	MET	Peptide
1	A	327	HIS	Peptide
1	A	367	ASP	Peptide
1	A	374	VAL	Peptide
1	A	379	SER	Peptide
1	A	383	HIS	Peptide
1	A	396	ASP	Peptide
1	A	421	ARG	Sidechain
1	A	451	TRP	Peptide
1	A	83	ARG	Sidechain
2	B	129	ARG	Sidechain
1	C	147	THR	Peptide
1	C	178	LEU	Peptide
1	C	215	ARG	Sidechain
1	C	228	ALA	Peptide
1	C	241	ASN	Peptide
1	C	263	PRO	Peptide
1	C	268	ASP	Peptide
1	C	305	ARG	Sidechain
1	C	320	MET	Peptide
1	C	327	HIS	Peptide
1	C	367	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	C	379	SER	Peptide
1	C	383	HIS	Peptide
1	C	396	ASP	Peptide
1	C	421	ARG	Sidechain
1	C	451	TRP	Peptide
2	D	129	ARG	Sidechain
1	E	139	ARG	Sidechain
1	E	147	THR	Peptide
1	E	178	LEU	Peptide
1	E	194	ARG	Sidechain
1	E	215	ARG	Sidechain
1	E	228	ALA	Peptide
1	E	241	ASN	Peptide
1	E	263	PRO	Peptide
1	E	268	ASP	Peptide
1	E	269	TYR	Sidechain
1	E	320	MET	Peptide
1	E	327	HIS	Peptide,Sidechain
1	E	363	TYR	Sidechain
1	E	367	ASP	Peptide
1	E	374	VAL	Peptide
1	E	379	SER	Peptide
1	E	383	HIS	Peptide
1	E	396	ASP	Peptide
1	E	451	TRP	Peptide
2	F	129	ARG	Sidechain
1	G	139	ARG	Sidechain
1	G	147	THR	Peptide
1	G	178	LEU	Peptide
1	G	228	ALA	Peptide
1	G	241	ASN	Peptide
1	G	254	ALA	Mainchain
1	G	263	PRO	Peptide
1	G	268	ASP	Peptide
1	G	269	TYR	Sidechain
1	G	320	MET	Peptide
1	G	327	HIS	Peptide
1	G	363	TYR	Sidechain
1	G	367	ASP	Peptide
1	G	379	SER	Peptide
1	G	383	HIS	Peptide
1	G	396	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	G	451	TRP	Peptide
1	G	83	ARG	Sidechain
2	H	117	TYR	Sidechain
2	H	129	ARG	Sidechain
1	I	147	THR	Peptide
1	I	178	LEU	Peptide
1	I	194	ARG	Sidechain
1	I	215	ARG	Sidechain
1	I	228	ALA	Peptide
1	I	241	ASN	Peptide
1	I	254	ALA	Mainchain
1	I	263	PRO	Peptide
1	I	268	ASP	Peptide
1	I	269	TYR	Sidechain
1	I	312	ARG	Sidechain
1	I	320	MET	Peptide
1	I	327	HIS	Peptide
1	I	367	ASP	Peptide
1	I	379	SER	Peptide
1	I	383	HIS	Peptide
1	I	396	ASP	Peptide
1	I	446	ARG	Sidechain
1	I	451	TRP	Peptide
1	I	83	ARG	Sidechain
2	J	129	ARG	Sidechain
1	K	139	ARG	Sidechain
1	K	147	THR	Peptide
1	K	178	LEU	Peptide
1	K	194	ARG	Sidechain
1	K	215	ARG	Sidechain
1	K	228	ALA	Peptide
1	K	241	ASN	Peptide
1	K	263	PRO	Peptide
1	K	268	ASP	Peptide
1	K	269	TYR	Sidechain
1	K	320	MET	Peptide
1	K	327	HIS	Peptide
1	K	367	ASP	Peptide
1	K	379	SER	Peptide
1	K	383	HIS	Peptide
1	K	396	ASP	Peptide
1	K	451	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	K	80	TYR	Sidechain
1	K	83	ARG	Sidechain
2	L	117	TYR	Sidechain
2	L	129	ARG	Sidechain
1	M	100	TYR	Sidechain
1	M	147	THR	Peptide
1	M	159	ARG	Sidechain
1	M	178	LEU	Peptide
1	M	215	ARG	Sidechain
1	M	228	ALA	Peptide
1	M	241	ASN	Peptide
1	M	263	PRO	Peptide
1	M	268	ASP	Peptide
1	M	269	TYR	Sidechain
1	M	320	MET	Peptide
1	M	327	HIS	Peptide
1	M	367	ASP	Peptide
1	M	379	SER	Peptide
1	M	383	HIS	Peptide
1	M	396	ASP	Peptide
1	M	41	ARG	Sidechain
1	M	451	TRP	Peptide
2	N	129	ARG	Sidechain
2	N	170	ARG	Sidechain
1	O	139	ARG	Sidechain
1	O	147	THR	Peptide
1	O	178	LEU	Peptide
1	O	194	ARG	Sidechain
1	O	215	ARG	Sidechain
1	O	228	ALA	Peptide
1	O	241	ASN	Peptide
1	O	263	PRO	Peptide
1	O	268	ASP	Peptide
1	O	269	TYR	Sidechain
1	O	320	MET	Peptide
1	O	327	HIS	Peptide
1	O	367	ASP	Peptide
1	O	379	SER	Peptide
1	O	383	HIS	Peptide
1	O	396	ASP	Peptide
1	O	421	ARG	Sidechain
1	O	451	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	O	83	ARG	Sidechain
2	P	129	ARG	Sidechain
2	P	170	ARG	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	3647	0	3570	0	0
1	C	3647	0	3570	2	0
1	E	3647	0	3570	2	0
1	G	3647	0	3570	2	0
1	I	3647	0	3570	3	0
1	K	3647	0	3570	2	0
1	M	3647	0	3570	2	0
1	O	3647	0	3570	1	0
2	B	1080	0	1052	0	0
2	D	1080	0	1052	0	0
2	F	1080	0	1052	0	0
2	H	1080	0	1052	0	0
2	J	1080	0	1052	1	0
2	L	1080	0	1052	0	0
2	N	1080	0	1052	0	0
2	P	1080	0	1052	0	0
All	All	37816	0	36976	14	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 0.

All (14) 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:E:307:HIS:CE1	1:G:307:HIS:CE1	2.99	0.51
1:I:202:ASP:OD2	1:I:238:HIS:HE1	1.97	0.48
1:M:298:HIS:CE1	1:M:303:ARG:HD2	2.50	0.47
1:G:298:HIS:CE1	1:G:303:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:298:HIS:CE1	1:I:303:ARG:HD2	2.51	0.46
1:M:267:HIS:CD2	1:M:269:TYR:CD1	3.03	0.46
1:K:267:HIS:CD2	1:K:269:TYR:CD1	3.04	0.46
1:O:298:HIS:CE1	1:O:303:ARG:HD2	2.53	0.44
1:C:298:HIS:CE1	1:C:303:ARG:HD2	2.52	0.44
1:C:267:HIS:CD2	1:C:269:TYR:CD1	3.07	0.43
1:K:298:HIS:CE1	1:K:303:ARG:HD2	2.54	0.43
2:J:83:TRP:CZ3	2:J:156:ASP:HB2	2.55	0.42
1:I:202:ASP:OD2	1:I:238:HIS:CE1	2.73	0.41
1:E:298:HIS:CE1	1:E:303:ARG:HD2	2.56	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	467/469 (100%)	420 (90%)	33 (7%)	14 (3%)	3 23
1	C	467/469 (100%)	420 (90%)	30 (6%)	17 (4%)	3 20
1	E	467/469 (100%)	418 (90%)	36 (8%)	13 (3%)	4 24
1	G	467/469 (100%)	419 (90%)	33 (7%)	15 (3%)	3 21
1	I	467/469 (100%)	416 (89%)	36 (8%)	15 (3%)	3 21
1	K	467/469 (100%)	425 (91%)	28 (6%)	14 (3%)	3 23
1	M	467/469 (100%)	420 (90%)	33 (7%)	14 (3%)	3 23
1	O	467/469 (100%)	418 (90%)	34 (7%)	15 (3%)	3 21
2	B	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	8 40
2	D	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16 55
2	F	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16 55
2	H	130/132 (98%)	121 (93%)	9 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	J	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16 55
2	L	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	16 55
2	N	130/132 (98%)	121 (93%)	9 (7%)	0	100 100
2	P	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8 40
All	All	4776/4808 (99%)	4314 (90%)	337 (7%)	125 (3%)	6 26

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ALA
1	A	67	THR
1	A	78	ASP
1	A	269	TYR
1	A	305	ARG
1	A	368	TRP
1	A	370	SER
1	C	9	ALA
1	C	67	THR
1	C	78	ASP
1	C	269	TYR
1	C	305	ARG
1	C	368	TRP
1	E	9	ALA
1	E	67	THR
1	E	78	ASP
1	E	242	ALA
1	E	269	TYR
1	E	305	ARG
1	E	368	TRP
1	E	370	SER
1	G	9	ALA
1	G	67	THR
1	G	269	TYR
1	G	305	ARG
1	G	368	TRP
1	G	370	SER
1	I	9	ALA
1	I	67	THR
1	I	78	ASP
1	I	269	TYR
1	I	305	ARG

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Mol	Chain	Res	Type
1	I	368	TRP
1	I	370	SER
1	K	9	ALA
1	K	78	ASP
1	K	269	TYR
1	K	305	ARG
1	K	368	TRP
1	M	9	ALA
1	M	67	THR
1	M	78	ASP
1	M	269	TYR
1	M	305	ARG
1	M	368	TRP
1	O	9	ALA
1	O	67	THR
1	O	78	ASP
1	O	269	TYR
1	O	305	ARG
1	O	368	TRP
1	A	154	GLY
1	A	328	SER
1	A	329	GLY
1	C	243	THR
1	C	328	SER
1	C	329	GLY
1	E	154	GLY
1	G	78	ASP
1	G	154	GLY
1	G	328	SER
1	G	329	GLY
1	I	165	TYR
1	I	329	GLY
1	K	328	SER
1	K	329	GLY
1	K	369	CYS
1	M	328	SER
1	M	329	GLY
1	O	154	GLY
1	O	328	SER
1	O	329	GLY
1	C	370	SER
2	D	50	THR

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Mol	Chain	Res	Type
1	E	127	PHE
1	E	148	PHE
1	E	165	TYR
1	G	127	PHE
1	I	154	GLY
1	I	369	CYS
1	K	67	THR
1	K	148	PHE
1	K	154	GLY
1	K	289	LEU
1	M	154	GLY
1	M	165	TYR
1	M	297	MET
1	O	165	TYR
1	O	243	THR
1	O	297	MET
1	A	148	PHE
1	C	154	GLY
1	C	289	LEU
1	C	297	MET
1	C	406	THR
1	E	297	MET
1	G	242	ALA
1	I	264	ILE
1	I	289	LEU
1	I	328	SER
1	M	148	PHE
1	O	148	PHE
2	P	175	ARG
1	A	126	GLY
1	A	127	PHE
2	B	175	ARG
1	C	148	PHE
1	G	126	GLY
1	G	289	LEU
2	L	50	THR
2	P	50	THR
1	A	289	LEU
1	C	126	GLY
1	C	369	CYS
2	F	50	THR
1	G	264	ILE

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Mol	Chain	Res	Type
1	I	126	GLY
1	K	126	GLY
1	O	126	GLY
1	O	264	ILE
2	B	50	THR
2	J	50	THR
1	M	126	GLY
1	K	331	VAL
1	M	263	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	375/375 (100%)	357 (95%)	18 (5%)	21	43
1	C	375/375 (100%)	358 (96%)	17 (4%)	23	45
1	E	375/375 (100%)	360 (96%)	15 (4%)	27	47
1	G	375/375 (100%)	359 (96%)	16 (4%)	25	46
1	I	375/375 (100%)	357 (95%)	18 (5%)	21	43
1	K	375/375 (100%)	357 (95%)	18 (5%)	21	43
1	M	375/375 (100%)	359 (96%)	16 (4%)	25	46
1	O	375/375 (100%)	358 (96%)	17 (4%)	23	45
2	B	116/116 (100%)	114 (98%)	2 (2%)	56	72
2	D	116/116 (100%)	114 (98%)	2 (2%)	56	72
2	F	116/116 (100%)	114 (98%)	2 (2%)	56	72
2	H	116/116 (100%)	114 (98%)	2 (2%)	56	72
2	J	116/116 (100%)	114 (98%)	2 (2%)	56	72
2	L	116/116 (100%)	114 (98%)	2 (2%)	56	72
2	N	116/116 (100%)	113 (97%)	3 (3%)	41	59
2	P	116/116 (100%)	113 (97%)	3 (3%)	41	59
All	All	3928/3928 (100%)	3775 (96%)	153 (4%)	30	48

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	79	ARG
1	A	139	ARG
1	A	156	GLN
1	A	158	GLU
1	A	159	ARG
1	A	167	ARG
1	A	175	LYS
1	A	183	LYS
1	A	204	GLU
1	A	223	GLU
1	A	241	ASN
1	A	258	LYS
1	A	267	HIS
1	A	270	LEU
1	A	292	HIS
1	A	302	ASP
1	A	439	ARG
2	B	58	GLU
2	B	99	ASN
1	C	72	ASP
1	C	79	ARG
1	C	139	ARG
1	C	156	GLN
1	C	158	GLU
1	C	167	ARG
1	C	175	LYS
1	C	183	LYS
1	C	201	LYS
1	C	204	GLU
1	C	223	GLU
1	C	243	THR
1	C	246	THR
1	C	267	HIS
1	C	292	HIS
1	C	302	ASP
1	C	371	MET
2	D	58	GLU
2	D	99	ASN
1	E	79	ARG
1	E	139	ARG
1	E	156	GLN

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Mol	Chain	Res	Type
1	E	158	GLU
1	E	159	ARG
1	E	167	ARG
1	E	175	LYS
1	E	183	LYS
1	E	201	LYS
1	E	204	GLU
1	E	267	HIS
1	E	270	LEU
1	E	292	HIS
1	E	302	ASP
1	E	371	MET
2	F	58	GLU
2	F	99	ASN
1	G	79	ARG
1	G	156	GLN
1	G	158	GLU
1	G	159	ARG
1	G	167	ARG
1	G	175	LYS
1	G	183	LYS
1	G	204	GLU
1	G	223	GLU
1	G	243	THR
1	G	258	LYS
1	G	267	HIS
1	G	270	LEU
1	G	292	HIS
1	G	302	ASP
1	G	371	MET
2	H	58	GLU
2	H	99	ASN
1	I	72	ASP
1	I	79	ARG
1	I	139	ARG
1	I	156	GLN
1	I	158	GLU
1	I	159	ARG
1	I	167	ARG
1	I	175	LYS
1	I	183	LYS
1	I	201	LYS

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Mol	Chain	Res	Type
1	I	204	GLU
1	I	258	LYS
1	I	267	HIS
1	I	270	LEU
1	I	292	HIS
1	I	302	ASP
1	I	371	MET
1	I	382	ILE
2	J	58	GLU
2	J	99	ASN
1	K	43	THR
1	K	79	ARG
1	K	139	ARG
1	K	156	GLN
1	K	158	GLU
1	K	167	ARG
1	K	175	LYS
1	K	183	LYS
1	K	204	GLU
1	K	223	GLU
1	K	241	ASN
1	K	243	THR
1	K	267	HIS
1	K	270	LEU
1	K	292	HIS
1	K	302	ASP
1	K	371	MET
1	K	439	ARG
2	L	58	GLU
2	L	99	ASN
1	M	72	ASP
1	M	79	ARG
1	M	139	ARG
1	M	158	GLU
1	M	167	ARG
1	M	175	LYS
1	M	183	LYS
1	M	204	GLU
1	M	241	ASN
1	M	258	LYS
1	M	267	HIS
1	M	270	LEU

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Mol	Chain	Res	Type
1	M	292	HIS
1	M	302	ASP
1	M	371	MET
1	M	439	ARG
2	N	58	GLU
2	N	99	ASN
2	N	173	THR
1	O	72	ASP
1	O	79	ARG
1	O	139	ARG
1	O	156	GLN
1	O	158	GLU
1	O	159	ARG
1	O	167	ARG
1	O	175	LYS
1	O	183	LYS
1	O	204	GLU
1	O	223	GLU
1	O	243	THR
1	O	267	HIS
1	O	292	HIS
1	O	325	HIS
1	O	371	MET
1	O	439	ARG
2	P	49	TRP
2	P	58	GLU
2	P	99	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	327	HIS
1	C	267	HIS
2	H	99	ASN
1	K	241	ASN
1	K	267	HIS
1	K	386	HIS
2	L	99	ASN
2	P	99	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 oligosaccharides 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.