

wwPDB EM Map/Model Validation Report ⓘ

Jul 7, 2016 – 05:36 PM EDT

PDB ID : 5G06
EMDB ID: : 3366
Title : Cryo-EM structure of yeast cytoplasmic exosome
Authors : Liu, J.J.; Niu, C.Y.; Wu, Y.; Tan, D.; Wang, Y.; Ye, M.D.; Liu, Y.; Zhao, W.W.; Zhou, K.; Liu, Q.S.; Dai, J.B.; Yang, X.R.; Dong, M.Q.; Huang, N.; Wang, H.W.
Deposited on : 2016-03-17
Resolution : 4.20 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) : rb-20027790

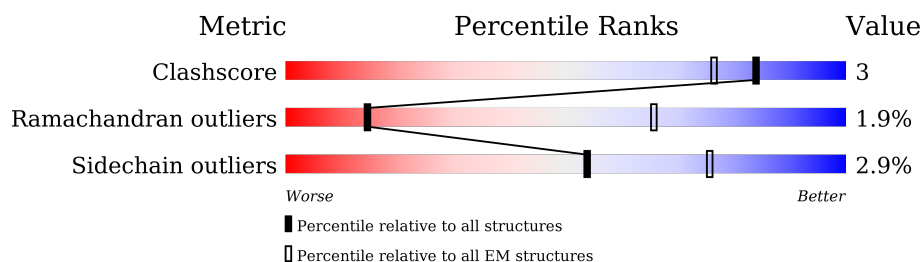
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	305	79% 19% ..
2	B	246	73% 21% . .
3	C	394	64% 17% . . 15%
4	D	223	81% 18% .
5	E	265	79% 19% .
6	F	250	61% 20% . . 16%
7	G	240	75% 20% . .
8	H	359	58% 21% . 18%
9	I	292	57% 18% . . 22%

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Mol	Chain	Length	Quality of chain
10	J	1001	<div><div></div><div>74%</div><div>22%</div><div>• •</div></div>
11	P	747	<div><div>8%</div><div>• •</div><div>87%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26794 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 EXOSOME COMPLEX COMPONENT RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	302	Total	C	N	O	S	0	0
			2350	1474	402	457	17		

- Molecule 2 is a protein called EXOSOME COMPLEX COMPONENT SKI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	240	Total	C	N	O	S	0	0
			1890	1182	338	362	8		

- Molecule 3 is a protein called EXOSOME COMPLEX COMPONENT RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2622	1653	455	503	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	363	MET	VAL	CONFLICT	UNP P25359

- Molecule 4 is a protein called EXOSOME COMPLEX COMPONENT RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	223	Total	C	N	O	S	0	0
			1707	1073	289	335	10		

- Molecule 5 is a protein called EXOSOME COMPLEX COMPONENT RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	265	Total	C	N	O	S	0	0
			2048	1307	336	400	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	138	ILE	VAL	CONFLICT	UNP Q12277

- Molecule 6 is a protein called EXOSOME COMPLEX COMPONENT MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	211	Total	C	N	O	S	0	0
			1627	1018	276	323	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	75	SER	THR	CONFLICT	UNP P48240

- Molecule 7 is a protein called EXOSOME COMPLEX COMPONENT RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	236	Total	C	N	O	S	0	0
			1831	1169	301	350	11		

- Molecule 8 is a protein called EXOSOME COMPLEX COMPONENT RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	293	Total	C	N	O	S	0	0
			2277	1419	411	435	12		

- Molecule 9 is a protein called EXOSOME COMPLEX COMPONENT CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	227	Total	C	N	O	S	0	0
			1750	1093	310	338	9		

- Molecule 10 is a protein called EXOSOME COMPLEX EXONUCLEASE DIS3.

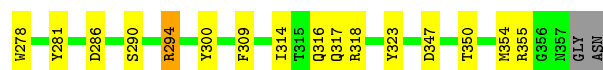
Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	993	Total	C	N	O	S	0	0
			7942	5002	1395	1509	36		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	171	ASN	ASP	CONFLICT	UNP Q08162
J	551	ASN	ASP	CONFLICT	UNP Q08162

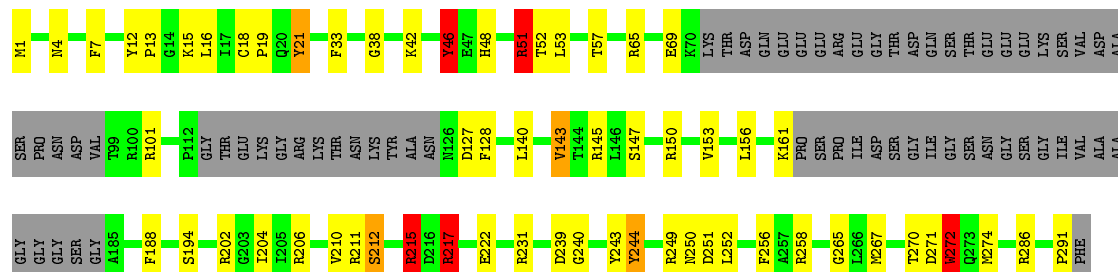
- Molecule 11 is a protein called SUPERKILLER PROTEIN 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	95	750	475	128	146	1	0	0



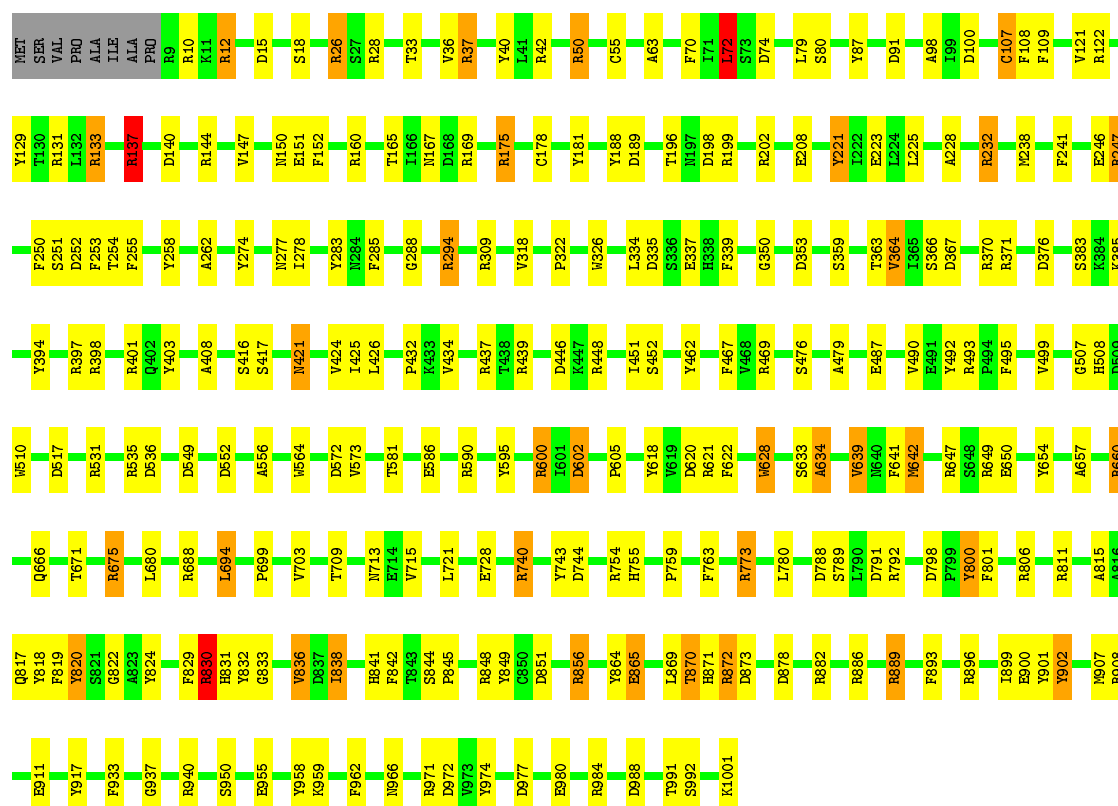
• Molecule 9: EXOSOME COMPLEX COMPONENT CSL4

Chain I: 57% 18% 22%



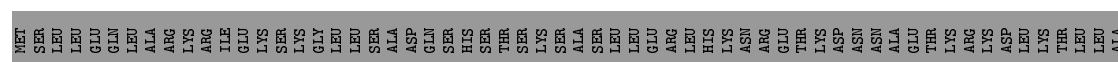
• Molecule 10: EXOSOME COMPLEX EXONUCLEASE DIS3

Chain J: 74% 22%



• Molecule 11: SUPERKILLER PROTEIN 7

Chain P: 8% 87%



[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPHS	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (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	1.70	14/2386 (0.6%)	1.91	46/3218 (1.4%)
10	J	1.75	90/8097 (1.1%)	1.98	214/10972 (2.0%)
11	P	1.69	6/763 (0.8%)	1.87	15/1031 (1.5%)
2	B	1.75	25/1914 (1.3%)	1.91	33/2577 (1.3%)
3	C	1.69	23/2659 (0.9%)	2.01	69/3596 (1.9%)
4	D	1.67	9/1725 (0.5%)	1.86	27/2339 (1.2%)
5	E	1.68	11/2087 (0.5%)	1.90	42/2836 (1.5%)
6	F	1.79	16/1649 (1.0%)	2.04	48/2222 (2.2%)
7	G	1.76	17/1868 (0.9%)	1.99	53/2531 (2.1%)
8	H	1.80	30/2311 (1.3%)	2.02	61/3118 (2.0%)
9	I	1.78	26/1774 (1.5%)	1.98	42/2398 (1.8%)
All	All	1.74	267/27233 (1.0%)	1.96	650/36838 (1.8%)

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	3
10	J	0	26
11	P	0	1
2	B	0	7
3	C	0	10
4	D	0	2
5	E	0	4
6	F	0	5
7	G	0	7
8	H	0	5
9	I	0	6
All	All	0	76

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	110	ARG	CZ-NH2	9.83	1.45	1.33
10	J	886	ARG	CZ-NH2	9.40	1.45	1.33
8	H	74	TYR	CZ-OH	8.53	1.52	1.37
10	J	590	ARG	NE-CZ	8.02	1.43	1.33
1	A	34	ARG	CZ-NH2	7.95	1.43	1.33
5	E	143	PHE	CB-CG	7.94	1.64	1.51
8	H	96	SER	CA-CB	7.86	1.64	1.52
10	J	740	ARG	CZ-NH2	7.79	1.43	1.33
8	H	281	TYR	CG-CD2	7.72	1.49	1.39
7	G	99	TYR	CG-CD1	7.67	1.49	1.39
5	E	120	TYR	CD1-CE1	7.59	1.50	1.39
10	J	188	TYR	CG-CD1	7.51	1.49	1.39
3	C	298	GLY	CA-C	-7.50	1.39	1.51
9	I	249	ARG	NE-CZ	7.44	1.42	1.33
7	G	195	TRP	CB-CG	7.40	1.63	1.50
3	C	50	ARG	NE-CZ	7.28	1.42	1.33
1	A	24	ARG	CD-NE	7.26	1.58	1.46
10	J	469	ARG	NE-CZ	7.26	1.42	1.33
2	B	21	GLU	CD-OE2	7.15	1.33	1.25
10	J	288	GLY	CA-C	7.11	1.63	1.51
10	J	660	ARG	CZ-NH1	7.11	1.42	1.33
10	J	401	ARG	CZ-NH2	7.09	1.42	1.33
10	J	122	ARG	CZ-NH2	7.08	1.42	1.33
10	J	37	ARG	CZ-NH1	7.08	1.42	1.33
8	H	10	ARG	CZ-NH1	7.02	1.42	1.33
10	J	417	SER	CA-CB	6.95	1.63	1.52
10	J	87	TYR	CE2-CZ	6.93	1.47	1.38
9	I	212	SER	CA-CB	6.89	1.63	1.52
3	C	222	ARG	CZ-NH1	6.87	1.42	1.33
2	B	188	GLY	CA-C	-6.86	1.40	1.51
6	F	129	ARG	CD-NE	6.84	1.58	1.46
10	J	42	ARG	NE-CZ	6.83	1.42	1.33
2	B	3	ARG	CD-NE	6.76	1.57	1.46
3	C	384	ARG	NE-CZ	6.75	1.41	1.33
10	J	309	ARG	NE-CZ	6.75	1.41	1.33
10	J	28	ARG	NE-CZ	6.73	1.41	1.33
3	C	381	SER	CA-CB	6.72	1.63	1.52
10	J	80	SER	CA-CB	6.71	1.63	1.52
9	I	258	ARG	CD-NE	6.67	1.57	1.46
1	A	114	ARG	CD-NE	6.62	1.57	1.46
10	J	232	ARG	CZ-NH1	6.61	1.41	1.33
9	I	18	CYS	CA-CB	6.59	1.68	1.53
8	H	150	ARG	CZ-NH1	6.54	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	917	TYR	CB-CG	6.54	1.61	1.51
1	A	135	ARG	NE-CZ	6.54	1.41	1.33
9	I	202	ARG	NE-CZ	6.51	1.41	1.33
3	C	301	GLU	CD-OE2	6.50	1.32	1.25
8	H	195	ARG	CD-NE	6.47	1.57	1.46
10	J	394	TYR	CZ-OH	6.46	1.48	1.37
10	J	743	TYR	CE2-CZ	6.45	1.47	1.38
7	G	143	ARG	CD-NE	6.41	1.57	1.46
5	E	175	TYR	CB-CG	-6.41	1.42	1.51
10	J	137	ARG	CD-NE	6.41	1.57	1.46
7	G	122	ARG	CZ-NH2	6.39	1.41	1.33
1	A	267	GLU	CD-OE1	6.39	1.32	1.25
10	J	144	ARG	CD-NE	6.36	1.57	1.46
10	J	199	ARG	CZ-NH2	6.35	1.41	1.33
10	J	811	ARG	CZ-NH1	6.35	1.41	1.33
7	G	231	PHE	CG-CD1	6.34	1.48	1.38
10	J	108	PHE	CE1-CZ	6.34	1.49	1.37
6	F	109	GLU	CD-OE1	6.33	1.32	1.25
8	H	323	TYR	CZ-OH	6.32	1.48	1.37
6	F	234	TYR	CG-CD2	6.31	1.47	1.39
10	J	535	ARG	NE-CZ	6.29	1.41	1.33
10	J	350	GLY	N-CA	-6.29	1.36	1.46
8	H	58	GLY	CA-C	-6.29	1.41	1.51
10	J	448	ARG	CZ-NH1	6.27	1.41	1.33
10	J	958	TYR	CE2-CZ	6.27	1.46	1.38
10	J	896	ARG	CZ-NH1	6.24	1.41	1.33
8	H	318	ARG	NE-CZ	6.21	1.41	1.33
9	I	222	GLU	CD-OE1	6.18	1.32	1.25
2	B	13	ARG	CZ-NH2	6.18	1.41	1.33
10	J	622	PHE	CG-CD2	6.17	1.48	1.38
2	B	223	ARG	CZ-NH2	6.14	1.41	1.33
5	E	227	ARG	NE-CZ	6.10	1.41	1.33
2	B	108	PHE	CG-CD1	6.09	1.47	1.38
9	I	69	GLU	CG-CD	6.06	1.61	1.51
9	I	69	GLU	CD-OE2	6.05	1.32	1.25
10	J	618	TYR	CE2-CZ	6.05	1.46	1.38
6	F	238	ARG	CZ-NH2	6.03	1.40	1.33
6	F	229	ARG	CZ-NH2	6.03	1.40	1.33
10	J	980	GLU	CD-OE1	6.03	1.32	1.25
9	I	265	GLY	CA-C	-6.02	1.42	1.51
2	B	157	TYR	CG-CD1	5.99	1.47	1.39
3	C	382	ARG	CZ-NH1	5.98	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	147	SER	CA-CB	5.95	1.61	1.52
8	H	162	PHE	CG-CD1	5.92	1.47	1.38
10	J	864	TYR	CE1-CZ	5.92	1.46	1.38
5	E	251	VAL	CA-C	-5.90	1.37	1.52
5	E	216	SER	CA-CB	5.89	1.61	1.52
3	C	269	ARG	CZ-NH2	5.89	1.40	1.33
8	H	300	TYR	CD1-CE1	5.89	1.48	1.39
6	F	238	ARG	CD-NE	5.89	1.56	1.46
8	H	350	THR	N-CA	-5.89	1.34	1.46
1	A	243	ARG	NE-CZ	5.88	1.40	1.33
2	B	86	ARG	CZ-NH1	5.88	1.40	1.33
7	G	26	TYR	CG-CD1	5.87	1.46	1.39
7	G	229	ARG	CZ-NH1	5.87	1.40	1.33
8	H	281	TYR	CE1-CZ	5.87	1.46	1.38
10	J	398	ARG	NE-CZ	5.86	1.40	1.33
2	B	26	GLU	CD-OE2	5.86	1.32	1.25
8	H	81	TYR	CG-CD1	5.85	1.46	1.39
10	J	740	ARG	CZ-NH1	5.85	1.40	1.33
10	J	754	ARG	NE-CZ	5.84	1.40	1.33
9	I	145	ARG	NE-CZ	5.82	1.40	1.33
10	J	12	ARG	NE-CZ	5.82	1.40	1.33
10	J	492	TYR	CE2-CZ	5.80	1.46	1.38
6	F	213	PHE	CB-CG	-5.80	1.41	1.51
10	J	822	GLY	CA-C	-5.80	1.42	1.51
8	H	195	ARG	CZ-NH2	5.78	1.40	1.33
10	J	940	ARG	CZ-NH2	5.76	1.40	1.33
8	H	290	SER	CA-CB	5.75	1.61	1.52
6	F	6	ARG	NE-CZ	5.75	1.40	1.33
8	H	199	PHE	CG-CD2	5.74	1.47	1.38
10	J	800	TYR	CZ-OH	5.73	1.47	1.37
10	J	830	ARG	CD-NE	5.72	1.56	1.46
10	J	221	TYR	CE1-CZ	5.71	1.46	1.38
10	J	476	SER	CA-CB	5.71	1.61	1.52
10	J	950	SER	CA-CB	5.70	1.61	1.52
4	D	39	ARG	NE-CZ	5.70	1.40	1.33
9	I	51	ARG	NE-CZ	5.70	1.40	1.33
10	J	974	TYR	CG-CD1	5.70	1.46	1.39
8	H	294	ARG	CD-NE	5.69	1.56	1.46
8	H	209	ARG	CD-NE	5.68	1.56	1.46
10	J	649	ARG	CD-NE	5.67	1.56	1.46
3	C	245	ARG	CZ-NH2	5.66	1.40	1.33
5	E	32	ARG	CD-NE	5.66	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	286	ARG	CZ-NH2	5.66	1.40	1.33
9	I	252	LEU	C-N	5.66	1.43	1.33
6	F	237	TYR	CE1-CZ	5.65	1.45	1.38
10	J	792	ARG	CZ-NH1	5.65	1.40	1.33
10	J	255	PHE	CE2-CZ	5.65	1.48	1.37
2	B	33	PRO	N-CD	-5.63	1.40	1.47
10	J	283	TYR	CD2-CE2	5.63	1.47	1.39
3	C	391	ARG	CZ-NH1	5.63	1.40	1.33
9	I	211	ARG	CZ-NH1	5.63	1.40	1.33
9	I	101	ARG	NE-CZ	5.62	1.40	1.33
10	J	202	ARG	NE-CZ	5.62	1.40	1.33
1	A	207	GLU	CG-CD	-5.62	1.43	1.51
9	I	206	ARG	CZ-NH1	5.62	1.40	1.33
10	J	600	ARG	CD-NE	5.62	1.55	1.46
4	D	6	GLU	CD-OE2	5.61	1.31	1.25
5	E	25	GLY	N-CA	-5.60	1.37	1.46
5	E	234	SER	CA-CB	5.60	1.61	1.52
8	H	323	TYR	CB-CG	-5.60	1.43	1.51
6	F	225	GLU	CD-OE1	5.59	1.31	1.25
10	J	908	ARG	CZ-NH2	5.59	1.40	1.33
11	P	73	SER	CB-OG	-5.58	1.34	1.42
10	J	50	ARG	CZ-NH1	5.57	1.40	1.33
2	B	45	GLY	N-CA	-5.56	1.37	1.46
9	I	194	SER	CA-CB	5.56	1.61	1.52
10	J	721	LEU	N-CA	-5.56	1.35	1.46
3	C	207	ARG	NE-CZ	5.56	1.40	1.33
9	I	215	ARG	CD-NE	5.55	1.55	1.46
8	H	278	TRP	CE3-CZ3	5.55	1.47	1.38
3	C	357	TYR	CE2-CZ	5.54	1.45	1.38
8	H	82	SER	CA-CB	5.53	1.61	1.52
8	H	103	ARG	CD-NE	5.52	1.55	1.46
1	A	28	ARG	NE-CZ	5.51	1.40	1.33
3	C	132	PRO	N-CD	-5.51	1.40	1.47
9	I	256	PHE	CG-CD2	5.50	1.47	1.38
7	G	229	ARG	NE-CZ	5.50	1.40	1.33
2	B	225	ARG	NE-CZ	5.50	1.40	1.33
10	J	848	ARG	CZ-NH2	5.50	1.40	1.33
10	J	467	PHE	CE2-CZ	5.47	1.47	1.37
2	B	99	GLU	CD-OE1	5.46	1.31	1.25
4	D	85	ARG	CZ-NH1	5.45	1.40	1.33
3	C	46	TYR	CZ-OH	5.44	1.47	1.37
10	J	531	ARG	CZ-NH1	5.44	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	85	GLU	CB-CG	5.43	1.62	1.52
7	G	208	TYR	CG-CD2	5.43	1.46	1.39
10	J	283	TYR	CD1-CE1	5.43	1.47	1.39
11	P	64	ARG	NE-CZ	5.43	1.40	1.33
7	G	114	GLN	CG-CD	5.41	1.63	1.51
10	J	337	GLU	CB-CG	5.41	1.62	1.52
7	G	80	PHE	CG-CD2	5.41	1.46	1.38
9	I	217	ARG	CZ-NH2	5.41	1.40	1.33
1	A	171	GLY	CA-C	-5.40	1.43	1.51
3	C	207	ARG	CZ-NH2	5.39	1.40	1.33
9	I	12	TYR	CE2-CZ	5.39	1.45	1.38
3	C	337	GLU	CB-CG	5.38	1.62	1.52
8	H	243	ARG	CZ-NH1	5.37	1.40	1.33
2	B	95	ARG	CD-NE	5.37	1.55	1.46
11	P	48	CYS	CB-SG	-5.37	1.73	1.81
4	D	39	ARG	CD-NE	5.37	1.55	1.46
6	F	238	ARG	NE-CZ	5.37	1.40	1.33
3	C	264	ARG	CZ-NH1	5.33	1.40	1.33
10	J	36	VAL	CB-CG1	5.33	1.64	1.52
1	A	162	PHE	CG-CD2	5.32	1.46	1.38
10	J	882	ARG	CZ-NH2	5.32	1.40	1.33
7	G	122	ARG	NE-CZ	5.32	1.40	1.33
2	B	85	GLU	CD-OE2	-5.31	1.19	1.25
6	F	165	ILE	N-CA	-5.30	1.35	1.46
9	I	150	ARG	CZ-NH1	5.29	1.40	1.33
3	C	163	ARG	CD-NE	5.29	1.55	1.46
10	J	437	ARG	CZ-NH2	5.29	1.40	1.33
3	C	262	ARG	CD-NE	5.28	1.55	1.46
4	D	45	GLN	N-CA	-5.28	1.35	1.46
10	J	675	ARG	CZ-NH1	5.28	1.40	1.33
3	C	24	ARG	CZ-NH2	5.28	1.40	1.33
10	J	160	ARG	CZ-NH1	5.28	1.40	1.33
10	J	819	PHE	CG-CD1	5.27	1.46	1.38
1	A	213	GLU	CD-OE2	5.26	1.31	1.25
1	A	267	GLU	CB-CG	5.26	1.62	1.52
10	J	590	ARG	CD-NE	5.25	1.55	1.46
6	F	12	PRO	N-CD	-5.25	1.40	1.47
7	G	168	PHE	CG-CD1	5.25	1.46	1.38
8	H	205	SER	CA-CB	5.25	1.60	1.52
10	J	137	ARG	NE-CZ	5.23	1.39	1.33
4	D	62	ARG	NE-CZ	5.22	1.39	1.33
10	J	660	ARG	NE-CZ	5.22	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	937	GLY	CA-C	-5.22	1.43	1.51
7	G	143	ARG	NE-CZ	5.21	1.39	1.33
10	J	849	TYR	CG-CD2	5.21	1.46	1.39
2	B	95	ARG	NE-CZ	5.20	1.39	1.33
11	P	81	GLU	CG-CD	5.18	1.59	1.51
2	B	223	ARG	NE-CZ	5.18	1.39	1.33
10	J	383	SER	CA-CB	5.17	1.60	1.52
10	J	984	ARG	CZ-NH1	5.17	1.39	1.33
7	G	59	TYR	CE2-CZ	5.16	1.45	1.38
10	J	15	ASP	CA-CB	5.15	1.65	1.53
10	J	403	TYR	CD1-CE1	5.15	1.47	1.39
10	J	759	PRO	N-CA	-5.15	1.38	1.47
1	A	130	LYS	CA-C	-5.14	1.39	1.52
8	H	67	TRP	CB-CG	5.14	1.59	1.50
7	G	22	GLY	CA-C	-5.14	1.43	1.51
3	C	177	ARG	NE-CZ	5.12	1.39	1.33
8	H	10	ARG	CA-CB	5.11	1.65	1.53
10	J	900	GLU	CG-CD	5.11	1.59	1.51
6	F	43	GLU	CG-CD	5.11	1.59	1.51
8	H	101	LYS	N-CA	-5.10	1.36	1.46
2	B	197	SER	CA-CB	5.10	1.60	1.52
2	B	44	GLN	C-N	5.09	1.42	1.33
4	D	19	PHE	CE2-CZ	5.09	1.47	1.37
8	H	75	PHE	CG-CD1	5.09	1.46	1.38
6	F	8	ARG	CZ-NH1	5.08	1.39	1.33
3	C	297	TYR	CG-CD1	5.08	1.45	1.39
2	B	119	ARG	CZ-NH1	5.08	1.39	1.33
4	D	107	ARG	CZ-NH1	5.08	1.39	1.33
5	E	21	ILE	N-CA	-5.08	1.36	1.46
6	F	54	GLU	CD-OE2	5.07	1.31	1.25
2	B	60	ARG	CZ-NH1	5.07	1.39	1.33
1	A	44	PHE	CG-CD2	5.07	1.46	1.38
8	H	281	TYR	CZ-OH	5.07	1.46	1.37
10	J	397	ARG	CZ-NH1	5.07	1.39	1.33
3	C	150	THR	CA-CB	-5.07	1.40	1.53
10	J	801	PHE	CG-CD2	5.07	1.46	1.38
9	I	38	GLY	N-CA	-5.07	1.38	1.46
9	I	65	ARG	NE-CZ	5.07	1.39	1.33
10	J	247	ARG	NE-CZ	5.06	1.39	1.33
11	P	46	VAL	CB-CG2	5.06	1.63	1.52
10	J	763	PHE	CB-CG	5.06	1.59	1.51
9	I	231	ARG	NE-CZ	5.05	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GLU	CG-CD	5.05	1.59	1.51
4	D	83	TYR	CD1-CE1	5.04	1.47	1.39
10	J	151	GLU	CG-CD	5.04	1.59	1.51
5	E	153	TYR	CG-CD2	5.03	1.45	1.39
10	J	274	TYR	CE2-CZ	5.03	1.45	1.38
10	J	728	GLU	CD-OE2	5.03	1.31	1.25
10	J	223	GLU	CB-CG	5.02	1.61	1.52
2	B	239	ARG	NE-CZ	5.02	1.39	1.33
10	J	232	ARG	NE-CZ	5.02	1.39	1.33
10	J	649	ARG	NE-CZ	5.02	1.39	1.33
11	P	81	GLU	CD-OE2	-5.02	1.20	1.25
2	B	175	ASN	C-N	5.01	1.45	1.34
10	J	294	ARG	CZ-NH2	5.00	1.39	1.33
10	J	586	GLU	CD-OE1	-5.00	1.20	1.25

All (650) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	TYR	CB-CG-CD2	20.64	133.39	121.00
8	H	281	TYR	CB-CG-CD2	-16.23	111.26	121.00
3	C	44	ARG	NE-CZ-NH2	-15.84	112.38	120.30
7	G	110	ARG	NE-CZ-NH1	15.73	128.16	120.30
3	C	262	ARG	NE-CZ-NH1	15.64	128.12	120.30
10	J	169	ARG	NE-CZ-NH2	-15.37	112.61	120.30
9	I	150	ARG	NE-CZ-NH2	14.88	127.74	120.30
6	F	229	ARG	NE-CZ-NH1	14.84	127.72	120.30
2	B	7	TYR	CB-CG-CD1	-14.58	112.25	121.00
7	G	64	TYR	CB-CG-CD2	13.76	129.25	121.00
10	J	848	ARG	NE-CZ-NH1	13.71	127.16	120.30
7	G	143	ARG	NE-CZ-NH2	-12.62	113.99	120.30
5	E	49	ARG	NE-CZ-NH2	-12.59	114.01	120.30
6	F	238	ARG	NE-CZ-NH2	-12.48	114.06	120.30
8	H	103	ARG	NE-CZ-NH2	-12.46	114.07	120.30
10	J	754	ARG	NE-CZ-NH1	-12.34	114.13	120.30
10	J	773	ARG	NE-CZ-NH1	-12.32	114.14	120.30
10	J	743	TYR	CB-CG-CD1	12.18	128.31	121.00
3	C	163	ARG	NE-CZ-NH1	11.98	126.29	120.30
10	J	872	ARG	NE-CZ-NH2	-11.94	114.33	120.30
10	J	401	ARG	NE-CZ-NH1	11.88	126.24	120.30
3	C	33	ARG	NE-CZ-NH2	11.86	126.23	120.30
6	F	238	ARG	NE-CZ-NH1	11.83	126.22	120.30
8	H	234	ARG	NE-CZ-NH1	11.74	126.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	819	PHE	CB-CG-CD1	-11.64	112.65	120.80
3	C	260	ARG	NE-CZ-NH2	-11.58	114.51	120.30
10	J	940	ARG	NE-CZ-NH1	11.54	126.07	120.30
6	F	116	PHE	CB-CG-CD2	-11.44	112.80	120.80
8	H	150	ARG	NE-CZ-NH1	-11.42	114.59	120.30
5	E	26	ARG	NE-CZ-NH1	11.35	125.98	120.30
5	E	122	PHE	CB-CG-CD1	-11.18	112.97	120.80
8	H	318	ARG	NE-CZ-NH2	-11.15	114.72	120.30
10	J	654	TYR	CB-CG-CD2	-11.06	114.36	121.00
10	J	181	TYR	CB-CG-CD2	-10.95	114.43	121.00
1	A	20	ARG	NE-CZ-NH1	10.93	125.77	120.30
10	J	829	PHE	CB-CG-CD1	10.81	128.37	120.80
10	J	896	ARG	NE-CZ-NH1	10.78	125.69	120.30
6	F	7	ARG	NE-CZ-NH2	-10.77	114.91	120.30
3	C	24	ARG	NE-CZ-NH2	-10.77	114.92	120.30
5	E	260	ARG	NE-CZ-NH2	-10.73	114.93	120.30
8	H	230	TYR	CB-CG-CD1	10.73	127.44	121.00
1	A	277	ASP	CB-CG-OD2	-10.71	108.66	118.30
1	A	71	ARG	NE-CZ-NH1	10.69	125.65	120.30
8	H	281	TYR	CB-CG-CD1	10.69	127.41	121.00
2	B	81	PHE	CB-CG-CD2	-10.66	113.34	120.80
10	J	12	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	A	303	ARG	NE-CZ-NH1	-10.46	115.07	120.30
3	C	189	TYR	CB-CG-CD1	-10.46	114.73	121.00
7	G	122	ARG	NE-CZ-NH2	-10.45	115.08	120.30
6	F	190	MET	CG-SD-CE	-10.45	83.49	100.20
6	F	129	ARG	NE-CZ-NH2	10.41	125.50	120.30
10	J	917	TYR	CB-CG-CD1	-10.34	114.80	121.00
10	J	820	TYR	CB-CG-CD1	10.30	127.18	121.00
3	C	177	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	A	24	ARG	NE-CZ-NH2	10.29	125.44	120.30
10	J	232	ARG	NE-CZ-NH2	-10.23	115.19	120.30
10	J	10	ARG	NE-CZ-NH2	-10.22	115.19	120.30
3	C	251	ARG	NE-CZ-NH1	10.19	125.39	120.30
5	E	81	ASP	CB-CG-OD2	-10.07	109.23	118.30
3	C	260	ARG	NE-CZ-NH1	10.06	125.33	120.30
8	H	243	ARG	NE-CZ-NH1	10.06	125.33	120.30
8	H	149	ARG	NE-CZ-NH1	10.05	125.33	120.30
8	H	230	TYR	CB-CG-CD2	-10.03	114.98	121.00
10	J	743	TYR	CB-CG-CD2	-10.00	115.00	121.00
9	I	206	ARG	NE-CZ-NH1	9.98	125.29	120.30
8	H	191	TYR	CB-CG-CD1	9.95	126.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	20	ARG	NE-CZ-NH2	-9.90	115.35	120.30
9	I	256	PHE	CB-CG-CD1	9.89	127.72	120.80
8	H	149	ARG	NE-CZ-NH2	-9.79	115.40	120.30
10	J	549	ASP	CB-CG-OD1	-9.61	109.65	118.30
3	C	140	ARG	NE-CZ-NH1	9.54	125.07	120.30
10	J	811	ARG	NE-CZ-NH1	9.54	125.07	120.30
10	J	974	TYR	CB-CG-CD2	-9.50	115.30	121.00
7	G	229	ARG	NE-CZ-NH1	-9.49	115.56	120.30
10	J	621	ARG	NE-CZ-NH2	-9.47	115.56	120.30
8	H	90	ARG	NE-CZ-NH2	-9.47	115.56	120.30
8	H	51	ASP	CB-CG-OD1	9.45	126.81	118.30
10	J	882	ARG	NE-CZ-NH2	9.33	124.97	120.30
10	J	933	PHE	CB-CG-CD2	-9.27	114.31	120.80
5	E	260	ARG	NE-CZ-NH1	9.16	124.88	120.30
7	G	6	PHE	CB-CG-CD2	-9.12	114.42	120.80
9	I	256	PHE	CB-CG-CD2	-9.11	114.42	120.80
3	C	215	ALA	N-CA-CB	9.06	122.79	110.10
8	H	103	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	23	TYR	CB-CG-CD2	-9.01	115.59	121.00
5	E	122	PHE	CB-CG-CD2	9.01	127.10	120.80
10	J	977	ASP	CB-CG-OD2	-8.99	110.21	118.30
3	C	297	TYR	CB-CG-CD1	-8.90	115.66	121.00
4	D	62	ARG	NE-CZ-NH2	-8.90	115.85	120.30
10	J	70	PHE	CB-CG-CD2	-8.90	114.57	120.80
7	G	6	PHE	CB-CG-CD1	8.88	127.02	120.80
8	H	110	ASP	CB-CG-OD1	8.82	126.24	118.30
10	J	144	ARG	NE-CZ-NH2	-8.79	115.91	120.30
7	G	64	TYR	CB-CG-CD1	-8.71	115.77	121.00
9	I	145	ARG	NE-CZ-NH1	-8.67	115.96	120.30
10	J	870	THR	CA-CB-CG2	-8.66	100.27	112.40
5	E	49	ARG	NE-CZ-NH1	8.62	124.61	120.30
8	H	234	ARG	NE-CZ-NH2	-8.62	115.99	120.30
10	J	144	ARG	NE-CZ-NH1	8.62	124.61	120.30
9	I	217	ARG	NE-CZ-NH2	-8.59	116.00	120.30
10	J	971	ARG	NE-CZ-NH1	8.53	124.56	120.30
10	J	908	ARG	NE-CZ-NH1	8.51	124.56	120.30
7	G	35	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	277	ASP	CB-CG-OD1	8.47	125.92	118.30
2	B	81	PHE	CB-CG-CD1	8.40	126.68	120.80
10	J	189	ASP	CB-CG-OD2	-8.37	110.77	118.30
10	J	660	ARG	NE-CZ-NH1	-8.35	116.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PHE	CB-CG-CD2	-8.34	114.96	120.80
9	I	202	ARG	NE-CZ-NH2	-8.33	116.13	120.30
10	J	283	TYR	CB-CG-CD1	-8.31	116.01	121.00
7	G	168	PHE	CB-CG-CD2	-8.31	114.98	120.80
6	F	121	PHE	CB-CG-CD2	-8.28	115.01	120.80
5	E	13	ASP	CB-CG-OD2	-8.26	110.87	118.30
10	J	974	TYR	CB-CG-CD1	8.26	125.95	121.00
10	J	70	PHE	CB-CG-CD1	8.25	126.58	120.80
11	P	55	ARG	NE-CZ-NH2	-8.23	116.19	120.30
10	J	87	TYR	CB-CG-CD2	-8.20	116.08	121.00
10	J	886	ARG	NE-CZ-NH1	8.21	124.40	120.30
7	G	209	ARG	NE-CZ-NH2	-8.18	116.21	120.30
6	F	52	PHE	CB-CG-CD1	8.18	126.52	120.80
9	I	202	ARG	NE-CZ-NH1	8.09	124.34	120.30
10	J	448	ARG	NE-CZ-NH2	-8.07	116.27	120.30
10	J	622	PHE	CB-CG-CD1	8.07	126.45	120.80
2	B	3	ARG	NE-CZ-NH2	-8.04	116.28	120.30
10	J	437	ARG	NE-CZ-NH1	8.02	124.31	120.30
9	I	286	ARG	NE-CZ-NH2	7.96	124.28	120.30
10	J	397	ARG	NE-CZ-NH2	7.95	124.28	120.30
6	F	52	PHE	CB-CG-CD2	-7.93	115.25	120.80
10	J	371	ARG	NE-CZ-NH2	-7.92	116.34	120.30
3	C	44	ARG	NE-CZ-NH1	7.91	124.25	120.30
7	G	26	TYR	CB-CG-CD1	7.87	125.72	121.00
10	J	549	ASP	CB-CG-OD2	7.86	125.37	118.30
1	A	198	PHE	CB-CG-CD2	7.85	126.30	120.80
11	P	64	ARG	NE-CZ-NH1	-7.85	116.38	120.30
9	I	188	PHE	CB-CG-CD1	-7.83	115.31	120.80
10	J	917	TYR	CG-CD2-CE2	-7.83	115.03	121.30
10	J	634	ALA	N-CA-CB	7.75	120.96	110.10
7	G	84	TYR	CB-CG-CD2	-7.74	116.36	121.00
8	H	110	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	A	162	PHE	CB-CG-CD1	7.65	126.15	120.80
8	H	10	ARG	NE-CZ-NH1	7.63	124.11	120.30
10	J	740	ARG	NE-CZ-NH1	7.62	124.11	120.30
10	J	131	ARG	NE-CZ-NH1	7.60	124.10	120.30
8	H	10	ARG	NE-CZ-NH2	-7.59	116.50	120.30
6	F	78	TYR	CB-CG-CD2	7.59	125.55	121.00
6	F	229	ARG	NE-CZ-NH2	-7.56	116.52	120.30
7	G	147	PHE	CB-CG-CD1	7.56	126.09	120.80
7	G	117	ASP	CB-CG-OD2	-7.56	111.50	118.30
3	C	370	THR	CA-CB-CG2	-7.52	101.88	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	PHE	CB-CG-CD2	7.51	126.06	120.80
10	J	467	PHE	CB-CG-CD1	7.51	126.06	120.80
7	G	58	ASP	CB-CG-OD1	-7.50	111.55	118.30
10	J	26	ARG	NE-CZ-NH2	-7.48	116.56	120.30
6	F	84	ARG	NE-CZ-NH2	-7.46	116.57	120.30
3	C	138	ARG	NE-CZ-NH2	7.45	124.03	120.30
2	B	17	ARG	NE-CZ-NH2	7.45	124.02	120.30
10	J	754	ARG	NE-CZ-NH2	7.43	124.02	120.30
8	H	67	TRP	CB-CG-CD2	-7.43	116.94	126.60
10	J	819	PHE	CB-CG-CD2	7.41	125.99	120.80
8	H	203	PRO	N-CA-CB	7.40	112.18	103.30
8	H	191	TYR	CB-CG-CD2	-7.40	116.56	121.00
4	D	144	ASP	CB-CG-OD1	-7.39	111.65	118.30
9	I	145	ARG	NE-CZ-NH2	-7.39	116.61	120.30
3	C	131	TYR	CB-CG-CD2	-7.37	116.58	121.00
6	F	78	TYR	CB-CG-CD1	-7.34	116.59	121.00
10	J	152	PHE	CB-CG-CD2	-7.32	115.67	120.80
6	F	203	PHE	CB-CG-CD2	-7.31	115.68	120.80
11	P	64	ARG	NE-CZ-NH2	7.29	123.95	120.30
9	I	145	ARG	NH1-CZ-NH2	7.29	127.42	119.40
1	A	23	TYR	CG-CD1-CE1	-7.27	115.48	121.30
7	G	91	PHE	CB-CG-CD2	7.26	125.88	120.80
2	B	41	TYR	CB-CG-CD2	-7.25	116.65	121.00
7	G	64	TYR	CG-CD2-CE2	7.25	127.10	121.30
10	J	510	TRP	CB-CG-CD1	7.23	136.40	127.00
2	B	95	ARG	NE-CZ-NH1	7.23	123.91	120.30
3	C	207	ARG	NE-CZ-NH2	-7.22	116.69	120.30
10	J	618	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	91	PHE	CB-CG-CD1	-7.19	115.77	120.80
10	J	255	PHE	CB-CG-CD1	7.17	125.82	120.80
10	J	893	PHE	CB-CG-CD1	7.17	125.82	120.80
5	E	126	VAL	CA-CB-CG2	-7.12	100.22	110.90
10	J	971	ARG	NE-CZ-NH2	-7.10	116.75	120.30
6	F	222	ASP	CB-CG-OD1	7.10	124.69	118.30
10	J	147	VAL	CG1-CB-CG2	7.08	122.24	110.90
5	E	144	ALA	CB-CA-C	-7.06	99.51	110.10
10	J	437	ARG	NE-CZ-NH2	-7.05	116.77	120.30
3	C	187	VAL	N-CA-C	-7.05	91.97	111.00
8	H	355	ARG	NE-CZ-NH1	7.05	123.82	120.30
9	I	13	PRO	N-CA-CB	7.03	111.74	103.30
5	E	181	ASP	CB-CG-OD2	-7.03	111.97	118.30
7	G	71	PHE	CB-CG-CD2	-7.03	115.88	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	680	LEU	CB-CG-CD2	7.03	122.94	111.00
3	C	140	ARG	NE-CZ-NH2	-7.02	116.79	120.30
10	J	602	ASP	CB-CG-OD2	-7.02	111.98	118.30
5	E	110	ASP	CB-CG-OD1	-7.00	112.00	118.30
6	F	193	ALA	N-CA-CB	7.00	119.89	110.10
10	J	452	SER	N-CA-CB	6.99	120.99	110.50
10	J	160	ARG	NE-CZ-NH1	6.99	123.80	120.30
3	C	376	ARG	NE-CZ-NH2	-6.94	116.83	120.30
10	J	535	ARG	NE-CZ-NH1	6.93	123.77	120.30
3	C	62	TYR	CB-CG-CD1	-6.93	116.84	121.00
10	J	572	ASP	CB-CG-OD2	6.93	124.54	118.30
10	J	572	ASP	CB-CG-OD1	-6.92	112.07	118.30
3	C	49	PHE	CB-CG-CD1	-6.90	115.97	120.80
3	C	297	TYR	CG-CD2-CE2	-6.87	115.80	121.30
1	A	46	ASP	CB-CG-OD2	-6.85	112.13	118.30
4	D	62	ARG	NE-CZ-NH1	6.83	123.72	120.30
7	G	168	PHE	CB-CG-CD1	6.82	125.58	120.80
1	A	119	ASP	CB-CG-OD1	6.82	124.44	118.30
2	B	139	LEU	CB-CA-C	-6.81	97.26	110.20
8	H	347	ASP	CB-CG-OD2	-6.81	112.17	118.30
10	J	622	PHE	CB-CA-C	-6.81	96.78	110.40
3	C	262	ARG	C-N-CA	6.80	136.58	122.30
7	G	208	TYR	CG-CD2-CE2	-6.80	115.86	121.30
9	I	65	ARG	NE-CZ-NH1	6.78	123.69	120.30
3	C	228	ASP	CB-CG-OD2	-6.77	112.21	118.30
10	J	856	ARG	NE-CZ-NH2	6.76	123.68	120.30
10	J	977	ASP	CB-CG-OD1	6.76	124.38	118.30
10	J	247	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	243	ARG	NE-CZ-NH1	6.74	123.67	120.30
9	I	7	PHE	CB-CG-CD2	-6.74	116.08	120.80
9	I	101	ARG	NE-CZ-NH1	6.72	123.66	120.30
7	G	143	ARG	NE-CZ-NH1	6.72	123.66	120.30
7	G	102	PHE	CB-CG-CD1	-6.71	116.10	120.80
3	C	63	ALA	N-CA-CB	6.71	119.49	110.10
10	J	688	ARG	NE-CZ-NH1	6.70	123.65	120.30
8	H	87	THR	CA-CB-CG2	-6.69	103.03	112.40
8	H	53	GLN	O-C-N	6.69	133.40	122.70
6	F	98	LYS	O-C-N	6.68	133.39	122.70
10	J	600	ARG	NE-CZ-NH1	6.67	123.63	120.30
3	C	33	ARG	NE-CZ-NH1	-6.62	116.99	120.30
6	F	146	ASP	CB-CG-OD1	-6.62	112.34	118.30
11	P	31	PHE	CB-CG-CD1	-6.58	116.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	81	TYR	CB-CG-CD2	6.57	124.94	121.00
2	B	209	ARG	NE-CZ-NH1	6.56	123.58	120.30
8	H	309	PHE	CB-CG-CD1	6.55	125.39	120.80
3	C	297	TYR	CG-CD1-CE1	-6.55	116.06	121.30
10	J	188	TYR	CG-CD2-CE2	6.55	126.54	121.30
6	F	75	SER	N-CA-CB	6.54	120.31	110.50
8	H	51	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	A	140	PHE	CB-CG-CD1	-6.53	116.23	120.80
10	J	666	GLN	N-CA-C	-6.53	93.37	111.00
11	P	55	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	262	MET	CG-SD-CE	6.52	110.63	100.20
10	J	371	ARG	NE-CZ-NH1	6.51	123.56	120.30
11	P	62	PHE	CB-CG-CD1	6.51	125.35	120.80
3	C	50	ARG	NE-CZ-NH2	-6.50	117.05	120.30
6	F	65	ARG	NE-CZ-NH1	6.48	123.54	120.30
5	E	181	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	147	PHE	CB-CG-CD2	6.47	125.33	120.80
10	J	842	PHE	CB-CG-CD1	-6.46	116.28	120.80
10	J	490	VAL	CA-CB-CG2	-6.45	101.23	110.90
1	A	86	MET	CG-SD-CE	-6.44	89.89	100.20
11	P	74	ALA	N-CA-CB	6.44	119.12	110.10
3	C	11	GLU	C-N-CA	6.44	137.79	121.70
2	B	226	ASP	CB-CG-OD2	-6.43	112.51	118.30
10	J	556	ALA	N-CA-CB	6.43	119.10	110.10
9	I	7	PHE	CB-CG-CD1	6.42	125.29	120.80
8	H	100	LEU	CB-CG-CD1	6.40	121.89	111.00
7	G	196	VAL	CA-CB-CG1	6.40	120.50	110.90
10	J	647	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	232	ASP	CB-CG-OD1	-6.37	112.56	118.30
10	J	564	TRP	CB-CG-CD1	6.37	135.28	127.00
7	G	147	PHE	CB-CG-CD2	-6.37	116.34	120.80
4	D	100	ASP	CB-CG-OD1	-6.35	112.58	118.30
5	E	12	TYR	CB-CG-CD1	-6.35	117.19	121.00
10	J	958	TYR	CB-CG-CD2	-6.34	117.19	121.00
10	J	188	TYR	CZ-CE2-CD2	-6.34	114.09	119.80
10	J	798	ASP	CB-CA-C	-6.34	97.73	110.40
6	F	178	LEU	CB-CG-CD1	6.33	121.77	111.00
6	F	203	PHE	CD1-CE1-CZ	-6.33	112.50	120.10
7	G	231	PHE	CB-CG-CD1	6.32	125.22	120.80
6	F	53	ILE	O-C-N	-6.31	112.61	122.70
10	J	820	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	A	136	ALA	N-CA-CB	6.30	118.92	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	ARG	NE-CZ-NH2	-6.30	117.15	120.30
10	J	878	ASP	CB-CG-OD1	6.29	123.97	118.30
7	G	11	PHE	CB-CG-CD2	-6.28	116.40	120.80
5	E	228	SER	N-CA-CB	6.27	119.90	110.50
10	J	421	ASN	CB-CG-OD1	-6.27	109.06	121.60
10	J	189	ASP	CB-CG-OD1	6.24	123.92	118.30
4	D	114	ASN	CB-CA-C	-6.24	97.92	110.40
9	I	272	TRP	CB-CG-CD1	6.24	135.11	127.00
10	J	886	ARG	NE-CZ-NH2	-6.24	117.18	120.30
3	C	42	CYS	C-N-CA	6.24	137.29	121.70
6	F	145	LYS	N-CA-CB	6.23	121.81	110.60
5	E	143	PHE	CB-CG-CD2	-6.23	116.44	120.80
10	J	842	PHE	CB-CG-CD2	6.23	125.16	120.80
4	D	85	ARG	NE-CZ-NH1	6.22	123.41	120.30
10	J	262	ALA	N-CA-CB	6.22	118.81	110.10
7	G	122	ARG	NE-CZ-NH1	6.22	123.41	120.30
10	J	370	ARG	NE-CZ-NH2	6.22	123.41	120.30
3	C	262	ARG	NE-CZ-NH2	-6.22	117.19	120.30
10	J	654	TYR	CB-CG-CD1	6.22	124.73	121.00
3	C	127	TYR	CB-CG-CD1	-6.21	117.27	121.00
8	H	314	ILE	CA-CB-CG1	-6.21	99.21	111.00
10	J	836	VAL	CA-CB-CG1	-6.20	101.60	110.90
9	I	231	ARG	O-C-N	-6.18	112.80	122.70
10	J	37	ARG	NE-CZ-NH2	6.18	123.39	120.30
10	J	79	LEU	N-CA-CB	6.18	122.75	110.40
1	A	68	TYR	CB-CG-CD2	-6.17	117.30	121.00
11	P	4	PHE	CG-CD2-CE2	-6.17	114.01	120.80
2	B	18	ARG	NE-CZ-NH2	-6.17	117.22	120.30
6	F	8	ARG	NE-CZ-NH1	6.17	123.38	120.30
10	J	889	ARG	NE-CZ-NH1	-6.17	117.22	120.30
10	J	241	PHE	CB-CG-CD1	-6.16	116.49	120.80
6	F	203	PHE	CB-CG-CD1	6.16	125.11	120.80
10	J	258	TYR	CB-CG-CD1	6.16	124.70	121.00
10	J	780	LEU	CB-CG-CD1	6.15	121.45	111.00
9	I	271	ASP	N-CA-C	-6.14	94.42	111.00
10	J	836	VAL	CA-CB-CG2	6.14	120.11	110.90
10	J	564	TRP	CB-CG-CD2	-6.14	118.62	126.60
10	J	175	ARG	NE-CZ-NH1	-6.13	117.23	120.30
7	G	208	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	A	243	ARG	N-CA-CB	6.12	121.61	110.60
7	G	184	PHE	CB-CG-CD2	-6.11	116.52	120.80
10	J	178	CYS	CA-CB-SG	-6.11	103.00	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	824	TYR	CB-CG-CD2	6.11	124.67	121.00
6	F	115	SER	N-CA-CB	6.11	119.66	110.50
8	H	152	SER	CB-CA-C	-6.10	98.51	110.10
5	E	233	ASP	CB-CG-OD2	-6.10	112.81	118.30
3	C	163	ARG	NE-CZ-NH2	-6.09	117.25	120.30
5	E	39	ASP	CB-CG-OD2	6.08	123.78	118.30
9	I	38	GLY	N-CA-C	-6.07	97.92	113.10
5	E	153	TYR	N-CA-C	-6.07	94.62	111.00
7	G	19	VAL	CA-CB-CG1	-6.07	101.80	110.90
8	H	209	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	116	GLY	N-CA-C	-6.06	97.95	113.10
10	J	657	ALA	CB-CA-C	-6.06	101.01	110.10
9	I	286	ARG	NH1-CZ-NH2	-6.04	112.75	119.40
10	J	398	ARG	NE-CZ-NH1	6.03	123.31	120.30
10	J	581	THR	CA-CB-CG2	-6.03	103.96	112.40
10	J	100	ASP	CB-CG-OD1	-6.02	112.88	118.30
10	J	462	TYR	CB-CG-CD1	-6.02	117.39	121.00
10	J	285	PHE	CG-CD1-CE1	6.01	127.42	120.80
10	J	367	ASP	CB-CG-OD2	6.01	123.71	118.30
9	I	21	TYR	CZ-CE2-CD2	-6.01	114.39	119.80
7	G	163	ALA	CB-CA-C	-6.00	101.09	110.10
9	I	128	PHE	CG-CD2-CE2	-6.00	114.20	120.80
9	I	46	TYR	CZ-CE2-CD2	-6.00	114.40	119.80
10	J	493	ARG	NE-CZ-NH2	-5.99	117.31	120.30
7	G	152	ASP	CB-CG-OD1	-5.98	112.91	118.30
10	J	641	PHE	CA-CB-CG	-5.98	99.54	113.90
5	E	13	ASP	CB-CG-OD1	5.98	123.68	118.30
3	C	207	ARG	CG-CD-NE	-5.97	99.27	111.80
5	E	218	SER	N-CA-CB	5.96	119.44	110.50
2	B	208	ASP	CB-CA-C	-5.95	98.50	110.40
5	E	188	PHE	CB-CG-CD2	5.95	124.96	120.80
10	J	446	ASP	CB-CG-OD1	5.95	123.65	118.30
10	J	376	ASP	CB-CG-OD1	-5.93	112.96	118.30
10	J	50	ARG	CD-NE-CZ	-5.93	115.29	123.60
3	C	334	LEU	CB-CG-CD2	5.93	121.08	111.00
6	F	54	GLU	C-N-CA	5.93	136.52	121.70
2	B	60	ARG	NE-CZ-NH1	-5.92	117.34	120.30
10	J	641	PHE	CB-CG-CD1	-5.91	116.66	120.80
6	F	6	ARG	NE-CZ-NH1	5.91	123.25	120.30
9	I	267	MET	CG-SD-CE	-5.91	90.75	100.20
1	A	61	SER	N-CA-CB	5.90	119.35	110.50
8	H	209	ARG	NE-CZ-NH1	5.90	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	237	TYR	CB-CG-CD2	-5.88	117.47	121.00
3	C	125	ALA	CB-CA-C	-5.87	101.29	110.10
10	J	376	ASP	CB-CG-OD2	5.86	123.57	118.30
2	B	65	MET	CG-SD-CE	-5.86	90.83	100.20
6	F	200	VAL	CA-CB-CG2	-5.85	102.12	110.90
5	E	146	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	A	62	CYS	N-CA-CB	5.83	121.10	110.60
7	G	110	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
6	F	222	ASP	CB-CG-OD2	-5.83	113.06	118.30
10	J	510	TRP	CB-CG-CD2	-5.82	119.03	126.60
10	J	829	PHE	CG-CD1-CE1	5.82	127.20	120.80
5	E	172	PHE	CB-CG-CD1	-5.80	116.74	120.80
5	E	7	GLU	N-CA-CB	5.80	121.05	110.60
2	B	23	ARG	NE-CZ-NH1	5.80	123.20	120.30
3	C	51	ASP	CB-CG-OD1	-5.78	113.10	118.30
10	J	232	ARG	N-CA-CB	5.78	121.00	110.60
3	C	273	GLU	N-CA-C	-5.77	95.42	111.00
10	J	40	TYR	CZ-CE2-CD2	5.77	124.99	119.80
10	J	401	ARG	NE-CZ-NH2	-5.77	117.42	120.30
5	E	22	ARG	NE-CZ-NH1	-5.76	117.42	120.30
3	C	235	MET	CB-CA-C	-5.76	98.89	110.40
5	E	86	ARG	NE-CZ-NH1	5.75	123.18	120.30
3	C	251	ARG	NE-CZ-NH2	-5.74	117.43	120.30
7	G	68	VAL	CA-CB-CG1	-5.74	102.29	110.90
10	J	788	ASP	CB-CA-C	-5.74	98.92	110.40
10	J	334	LEU	CB-CG-CD2	5.74	120.75	111.00
3	C	70	THR	O-C-N	5.73	131.87	122.70
2	B	226	ASP	CB-CG-OD1	5.73	123.46	118.30
10	J	675	ARG	NE-CZ-NH1	-5.73	117.44	120.30
6	F	215	LYS	N-CA-CB	5.73	120.91	110.60
3	C	123	ILE	N-CA-C	-5.72	95.56	111.00
5	E	125	PHE	CG-CD1-CE1	-5.72	114.51	120.80
10	J	12	ARG	NE-CZ-NH1	5.72	123.16	120.30
7	G	117	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	179	VAL	CG1-CB-CG2	-5.71	101.77	110.90
10	J	87	TYR	CD1-CE1-CZ	5.70	124.93	119.80
2	B	3	ARG	NE-CZ-NH1	5.70	123.15	120.30
4	D	75	THR	CA-C-N	5.70	133.06	117.10
8	H	76	LEU	N-CA-C	-5.70	95.60	111.00
1	A	21	GLN	CB-CA-C	-5.69	99.02	110.40
10	J	901	TYR	CB-CG-CD2	5.69	124.41	121.00
8	H	93	ARG	NE-CZ-NH2	5.68	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	VAL	CG1-CB-CG2	5.68	119.99	110.90
10	J	896	ARG	NE-CZ-NH2	-5.68	117.46	120.30
7	G	35	ARG	NE-CZ-NH2	-5.67	117.46	120.30
10	J	984	ARG	NE-CZ-NH2	5.67	123.14	120.30
4	D	100	ASP	CB-CG-OD2	5.66	123.39	118.30
6	F	81	ARG	CD-NE-CZ	5.65	131.51	123.60
9	I	127	ASP	N-CA-CB	5.65	120.77	110.60
3	C	68	ILE	N-CA-C	-5.64	95.77	111.00
3	C	382	ARG	NE-CZ-NH2	5.64	123.12	120.30
7	G	42	LEU	CB-CG-CD2	5.64	120.59	111.00
7	G	1	MET	CG-SD-CE	-5.64	91.18	100.20
3	C	272	TYR	CB-CG-CD2	-5.63	117.62	121.00
6	F	189	ASP	N-CA-C	-5.63	95.80	111.00
10	J	165	THR	CA-CB-CG2	-5.63	104.52	112.40
8	H	79	MET	CG-SD-CE	-5.63	91.19	100.20
10	J	851	ASP	CB-CG-OD2	-5.62	113.24	118.30
10	J	258	TYR	CB-CG-CD2	-5.62	117.63	121.00
10	J	394	TYR	CB-CG-CD1	5.62	124.37	121.00
3	C	254	ASP	N-CA-CB	5.62	120.71	110.60
3	C	269	ARG	NE-CZ-NH1	5.62	123.11	120.30
10	J	225	LEU	CA-C-O	-5.61	108.32	120.10
10	J	359	SER	N-CA-CB	5.61	118.92	110.50
3	C	127	TYR	CB-CG-CD2	5.61	124.36	121.00
4	D	127	LEU	CA-CB-CG	-5.61	102.40	115.30
1	A	30	PHE	CB-CG-CD1	5.61	124.73	120.80
3	C	391	ARG	NE-CZ-NH1	5.60	123.10	120.30
8	H	115	ARG	NE-CZ-NH2	-5.60	117.50	120.30
8	H	124	TRP	CE3-CZ3-CH2	5.59	127.35	121.20
10	J	181	TYR	CZ-CE2-CD2	5.59	124.83	119.80
4	D	9	ILE	CA-CB-CG1	5.58	121.60	111.00
9	I	33	PHE	CB-CG-CD2	-5.58	116.89	120.80
6	F	234	TYR	CA-CB-CG	5.57	123.98	113.40
8	H	104	TYR	CB-CG-CD1	5.57	124.34	121.00
10	J	848	ARG	NE-CZ-NH2	-5.56	117.52	120.30
10	J	901	TYR	CD1-CE1-CZ	-5.56	114.79	119.80
1	A	246	VAL	CA-CB-CG2	-5.56	102.56	110.90
4	D	189	ASP	CB-CA-C	-5.55	99.30	110.40
11	P	50	LEU	CB-CG-CD2	5.55	120.44	111.00
9	I	140	LEU	N-CA-CB	5.55	121.50	110.40
10	J	434	VAL	CB-CA-C	-5.55	100.86	111.40
3	C	189	TYR	CB-CG-CD2	5.54	124.33	121.00
10	J	639	VAL	CA-CB-CG1	5.54	119.21	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	193	VAL	N-CA-C	-5.53	96.06	111.00
10	J	285	PHE	CB-CA-C	-5.53	99.34	110.40
10	J	169	ARG	NE-CZ-NH1	5.53	123.06	120.30
8	H	223	VAL	CG1-CB-CG2	-5.52	102.06	110.90
10	J	55	CYS	CA-CB-SG	-5.52	104.06	114.00
7	G	99	TYR	CB-CG-CD2	-5.52	117.69	121.00
8	H	286	ASP	N-CA-CB	5.52	120.53	110.60
9	I	1	MET	CG-SD-CE	-5.51	91.38	100.20
11	P	91	VAL	CA-CB-CG1	5.50	119.15	110.90
10	J	620	ASP	CB-CG-OD1	5.50	123.25	118.30
9	I	57	THR	CA-CB-CG2	-5.50	104.70	112.40
2	B	31	THR	CA-CB-CG2	-5.49	104.71	112.40
4	D	81	HIS	CA-CB-CG	-5.49	104.27	113.60
7	G	187	ALA	N-CA-CB	5.49	117.79	110.10
10	J	838	ILE	CA-CB-CG1	5.49	121.43	111.00
10	J	98	ALA	N-CA-CB	5.49	117.78	110.10
2	B	19	TRP	CB-CA-C	-5.48	99.44	110.40
3	C	382	ARG	N-CA-CB	-5.48	100.74	110.60
4	D	121	VAL	CG1-CB-CG2	-5.47	102.14	110.90
7	G	84	TYR	N-CA-C	-5.47	96.23	111.00
10	J	517	ASP	CB-CG-OD2	-5.47	113.38	118.30
10	J	829	PHE	CB-CG-CD2	-5.47	116.97	120.80
2	B	47	ASN	N-CA-CB	5.46	120.44	110.60
2	B	157	TYR	CB-CG-CD1	-5.46	117.72	121.00
11	P	4	PHE	CB-CA-C	-5.46	99.47	110.40
10	J	642	MET	CA-CB-CG	5.46	122.58	113.30
8	H	183	SER	N-CA-CB	5.46	118.69	110.50
8	H	243	ARG	NE-CZ-NH2	-5.45	117.57	120.30
3	C	209	TRP	CG-CD2-CE3	-5.44	129.00	133.90
8	H	127	ASP	N-CA-CB	5.44	120.39	110.60
10	J	167	ASN	CB-CA-C	-5.44	99.52	110.40
5	E	188	PHE	CB-CG-CD1	-5.44	116.99	120.80
8	H	74	TYR	CG-CD2-CE2	-5.43	116.95	121.30
2	B	184	THR	CA-CB-CG2	-5.43	104.79	112.40
9	I	270	THR	CA-CB-CG2	-5.43	104.80	112.40
1	A	200	PHE	CB-CA-C	-5.43	99.54	110.40
10	J	318	VAL	CA-CB-CG2	5.42	119.03	110.90
2	B	155	PHE	CB-CG-CD2	5.42	124.59	120.80
10	J	487	GLU	O-C-N	-5.41	114.05	122.70
5	E	200	ASP	CA-CB-CG	-5.40	101.51	113.40
10	J	33	THR	N-CA-CB	5.40	120.56	110.30
10	J	72	LEU	N-CA-CB	5.40	121.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	439	ARG	NE-CZ-NH1	-5.40	117.60	120.30
6	F	168	LEU	CB-CG-CD2	5.40	120.17	111.00
5	E	153	TYR	N-CA-CB	5.40	120.31	110.60
9	I	128	PHE	CZ-CE2-CD2	5.39	126.57	120.10
10	J	495	PHE	CB-CG-CD1	5.39	124.58	120.80
1	A	77	PHE	CB-CG-CD2	-5.39	117.03	120.80
2	B	36	ALA	N-CA-CB	5.39	117.65	110.10
5	E	125	PHE	CB-CG-CD2	-5.38	117.03	120.80
9	I	274	MET	CG-SD-CE	-5.38	91.59	100.20
10	J	479	ALA	N-CA-CB	5.38	117.63	110.10
3	C	394	ILE	CA-CB-CG1	-5.37	100.79	111.00
10	J	650	GLU	OE1-CD-OE2	5.37	129.75	123.30
10	J	536	ASP	CB-CG-OD1	-5.37	113.47	118.30
10	J	499	VAL	CA-CB-CG2	-5.37	102.85	110.90
2	B	132	ASP	N-CA-C	-5.36	96.52	111.00
6	F	76	ALA	N-CA-CB	5.36	117.61	110.10
1	A	205	ASP	CA-CB-CG	-5.36	101.61	113.40
10	J	789	SER	N-CA-CB	5.36	118.54	110.50
7	G	38	ASN	CA-CB-CG	-5.35	101.62	113.40
3	C	189	TYR	CG-CD2-CE2	-5.35	117.02	121.30
10	J	277	ASN	O-C-N	5.35	131.26	122.70
6	F	191	ALA	N-CA-CB	5.35	117.59	110.10
6	F	129	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
10	J	152	PHE	CB-CG-CD1	5.34	124.54	120.80
7	G	56	TYR	CG-CD2-CE2	-5.34	117.03	121.30
9	I	244	TYR	CB-CG-CD1	5.34	124.21	121.00
8	H	147	ILE	N-CA-CB	5.34	123.08	110.80
5	E	30	GLN	N-CA-CB	5.34	120.21	110.60
10	J	1001	LYS	CA-CB-CG	5.34	125.14	113.40
3	C	12	ILE	CB-CA-C	5.33	122.27	111.60
1	A	231	ARG	NE-CZ-NH2	-5.33	117.63	120.30
5	E	39	ASP	CB-CG-OD1	-5.33	113.50	118.30
5	E	102	VAL	CA-CB-CG2	-5.33	102.90	110.90
4	D	18	GLU	N-CA-C	-5.33	96.62	111.00
10	J	641	PHE	CB-CA-C	-5.33	99.75	110.40
10	J	133	ARG	NE-CZ-NH2	5.32	122.96	120.30
11	P	4	PHE	CB-CG-CD2	-5.32	117.07	120.80
4	D	203	GLN	CB-CA-C	-5.32	99.76	110.40
2	B	141	ASN	N-CA-CB	5.32	120.17	110.60
10	J	873	ASP	CB-CG-OD2	-5.32	113.52	118.30
2	B	166	TYR	CB-CG-CD2	-5.31	117.81	121.00
4	D	195	LEU	CB-CA-C	-5.31	100.11	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	214	TRP	CA-CB-CG	5.31	123.78	113.70
6	F	174	THR	CA-CB-CG2	-5.30	104.98	112.40
2	B	4	LEU	N-CA-CB	5.30	121.00	110.40
4	D	105	SER	N-CA-CB	5.30	118.45	110.50
8	H	67	TRP	CE2-CD2-CG	-5.29	103.07	107.30
10	J	129	TYR	CB-CG-CD2	-5.29	117.83	121.00
10	J	253	PHE	CB-CG-CD2	5.29	124.50	120.80
1	A	53	ASN	CB-CA-C	-5.29	99.83	110.40
10	J	896	ARG	N-CA-CB	5.29	120.11	110.60
10	J	773	ARG	NE-CZ-NH2	5.28	122.94	120.30
10	J	383	SER	N-CA-CB	5.28	118.42	110.50
11	P	74	ALA	CB-CA-C	-5.28	102.19	110.10
2	B	157	TYR	N-CA-CB	5.27	120.09	110.60
10	J	446	ASP	CB-CG-OD2	-5.27	113.56	118.30
4	D	23	ASP	N-CA-CB	5.27	120.08	110.60
10	J	416	SER	N-CA-CB	5.27	118.40	110.50
1	A	179	VAL	CA-CB-CG2	5.26	118.80	110.90
10	J	917	TYR	CD1-CG-CD2	5.26	123.68	117.90
6	F	143	TYR	CA-CB-CG	5.26	123.39	113.40
7	G	144	ASP	CB-CG-OD1	-5.26	113.57	118.30
10	J	198	ASP	N-CA-C	-5.26	96.81	111.00
10	J	18	SER	N-CA-CB	5.25	118.38	110.50
3	C	212	VAL	CG1-CB-CG2	5.25	119.30	110.90
7	G	123	VAL	N-CA-C	-5.25	96.84	111.00
10	J	278	ILE	CA-C-O	5.24	131.10	120.10
10	J	122	ARG	NE-CZ-NH2	5.24	122.92	120.30
7	G	131	GLU	CB-CA-C	-5.23	99.93	110.40
9	I	243	TYR	CB-CG-CD1	5.23	124.14	121.00
10	J	893	PHE	CD1-CE1-CZ	-5.23	113.83	120.10
1	A	40	PHE	CB-CG-CD1	5.23	124.46	120.80
10	J	907	MET	N-CA-CB	5.23	120.01	110.60
7	G	149	ILE	N-CA-C	-5.23	96.89	111.00
1	A	59	ARG	NE-CZ-NH2	5.22	122.91	120.30
8	H	318	ARG	CG-CD-NE	-5.22	100.84	111.80
10	J	467	PHE	CB-CG-CD2	-5.22	117.15	120.80
8	H	196	ASN	O-C-N	-5.22	114.33	123.20
8	H	63	ASP	CB-CG-OD2	-5.21	113.61	118.30
4	D	110	SER	N-CA-CB	5.21	118.31	110.50
9	I	150	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
10	J	367	ASP	CB-CG-OD1	-5.21	113.61	118.30
10	J	899	ILE	CB-CA-C	-5.21	101.19	111.60
5	E	175	TYR	CB-CG-CD1	5.21	124.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	27	PRO	N-CA-CB	5.20	109.54	103.30
3	C	376	ARG	NE-CZ-NH1	5.20	122.90	120.30
7	G	99	TYR	CB-CG-CD1	5.19	124.12	121.00
1	A	39	THR	N-CA-CB	5.19	120.16	110.30
4	D	61	THR	OG1-CB-CG2	-5.19	98.06	110.00
10	J	911	GLU	OE1-CD-OE2	5.19	129.53	123.30
8	H	90	ARG	NE-CZ-NH1	5.18	122.89	120.30
10	J	791	ASP	N-CA-CB	5.18	119.92	110.60
9	I	143	VAL	CA-CB-CG2	5.18	118.67	110.90
10	J	699	PRO	O-C-N	5.18	130.98	122.70
2	B	58	GLU	CB-CA-C	5.17	120.75	110.40
9	I	239	ASP	O-C-N	-5.17	114.41	123.20
6	F	47	SER	N-CA-C	-5.16	97.06	111.00
6	F	197	ASN	O-C-N	-5.16	114.42	123.20
8	H	347	ASP	CB-CG-OD1	5.16	122.95	118.30
10	J	339	PHE	CB-CG-CD1	5.16	124.41	120.80
8	H	150	ARG	NH1-CZ-NH2	5.16	125.07	119.40
10	J	917	TYR	CZ-CE2-CD2	5.16	124.44	119.80
5	E	181	ASP	N-CA-CB	5.16	119.88	110.60
9	I	204	ILE	N-CA-CB	5.15	122.64	110.80
10	J	865	GLU	N-CA-C	-5.14	97.11	111.00
6	F	214	TRP	CB-CG-CD2	-5.14	119.91	126.60
4	D	160	VAL	CG1-CB-CG2	-5.14	102.68	110.90
8	H	81	TYR	CB-CG-CD1	-5.14	117.92	121.00
3	C	263	GLY	C-N-CA	5.13	134.53	121.70
10	J	639	VAL	CA-CB-CG2	-5.13	103.20	110.90
3	C	335	ASP	CB-CG-OD1	5.13	122.92	118.30
5	E	26	ARG	NE-CZ-NH2	-5.12	117.74	120.30
11	P	49	ASN	CB-CA-C	-5.12	100.17	110.40
10	J	252	ASP	CB-CA-C	-5.12	100.17	110.40
1	A	191	HIS	N-CA-CB	5.11	119.81	110.60
10	J	335	ASP	CB-CG-OD1	5.11	122.90	118.30
8	H	317	GLN	N-CA-CB	5.11	119.80	110.60
5	E	197	MET	CG-SD-CE	-5.11	92.02	100.20
8	H	186	THR	N-CA-CB	5.11	120.01	110.30
10	J	703	VAL	CA-CB-CG2	5.11	118.57	110.90
7	G	155	ILE	CG1-CB-CG2	5.11	122.63	111.40
10	J	188	TYR	CB-CG-CD1	5.11	124.06	121.00
5	E	209	ALA	CB-CA-C	5.10	117.76	110.10
3	C	131	TYR	CG-CD2-CE2	-5.10	117.22	121.30
10	J	744	ASP	CB-CG-OD2	5.09	122.89	118.30
11	P	80	ASN	CB-CA-C	-5.09	100.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	121	VAL	CA-CB-CG1	-5.09	103.27	110.90
10	J	426	LEU	CB-CG-CD2	5.08	119.64	111.00
3	C	297	TYR	CD1-CG-CD2	5.08	123.49	117.90
1	A	290	ARG	N-CA-CB	5.08	119.74	110.60
3	C	134	VAL	N-CA-C	-5.08	97.29	111.00
3	C	393	ASN	CA-CB-CG	-5.08	102.23	113.40
4	D	167	PHE	CB-CG-CD1	-5.08	117.25	120.80
10	J	353	ASP	CB-CG-OD2	5.07	122.87	118.30
10	J	958	TYR	N-CA-CB	5.07	119.72	110.60
4	D	120	LEU	CB-CA-C	-5.06	100.58	110.20
7	G	139	SER	CB-CA-C	-5.06	100.49	110.10
1	A	252	GLY	N-CA-C	-5.06	100.45	113.10
4	D	109	LEU	N-CA-CB	5.06	120.51	110.40
6	F	214	TRP	CB-CG-CD1	5.06	133.57	127.00
1	A	37	GLU	OE1-CD-OE2	-5.05	117.23	123.30
7	G	76	ILE	CA-CB-CG1	-5.05	101.40	111.00
10	J	882	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
10	J	800	TYR	CB-CG-CD1	-5.05	117.97	121.00
10	J	851	ASP	CB-CG-OD1	5.05	122.84	118.30
10	J	972	ASP	CB-CA-C	-5.05	100.30	110.40
4	D	182	SER	N-CA-C	-5.05	97.38	111.00
8	H	152	SER	N-CA-CB	5.04	118.06	110.50
3	C	70	THR	CA-CB-CG2	-5.04	105.34	112.40
9	I	272	TRP	CE3-CZ3-CH2	-5.04	115.66	121.20
10	J	326	TRP	CB-CG-CD2	-5.04	120.05	126.60
10	J	962	PHE	CB-CG-CD1	-5.03	117.28	120.80
3	C	263	GLY	N-CA-C	-5.03	100.52	113.10
10	J	728	GLU	OE1-CD-OE2	5.03	129.34	123.30
10	J	988	ASP	CB-CG-OD1	5.03	122.83	118.30
4	D	67	GLU	CA-CB-CG	5.03	124.46	113.40
8	H	7	ILE	N-CA-C	-5.03	97.42	111.00
9	I	210	VAL	CA-CB-CG1	5.03	118.44	110.90
10	J	902	TYR	CZ-CE2-CD2	5.02	124.32	119.80
7	G	92	SER	C-N-CA	5.02	134.25	121.70
4	D	167	PHE	CB-CG-CD2	5.01	124.31	120.80
8	H	135	VAL	CA-CB-CG2	5.01	118.42	110.90
10	J	815	ALA	O-C-N	-5.01	114.68	122.70
3	C	127	TYR	CA-CB-CG	-5.00	103.90	113.40

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Sidechain
1	A	303	ARG	Sidechain
1	A	44	PHE	Sidechain
2	B	106	ARG	Sidechain
2	B	155	PHE	Sidechain
2	B	225	ARG	Sidechain
2	B	23	ARG	Sidechain
2	B	3	ARG	Sidechain
2	B	41	TYR	Sidechain
2	B	96	ARG	Sidechain
3	C	127	TYR	Sidechain
3	C	131	TYR	Sidechain
3	C	222	ARG	Sidechain
3	C	236	TYR	Sidechain
3	C	256	ARG	Sidechain
3	C	269	ARG	Sidechain
3	C	382	ARG	Sidechain
3	C	40	ARG	Sidechain
3	C	44	ARG	Sidechain
3	C	46	TYR	Sidechain
4	D	36	PRO	Peptide
4	D	71	ARG	Sidechain
5	E	12	TYR	Sidechain
5	E	175	TYR	Sidechain
5	E	22	ARG	Sidechain
5	E	40	PHE	Sidechain
6	F	138	PHE	Sidechain
6	F	140	TYR	Sidechain
6	F	20	PHE	Sidechain
6	F	222	ASP	Peptide
6	F	84	ARG	Sidechain
7	G	120	TYR	Sidechain
7	G	143	ARG	Sidechain
7	G	147	PHE	Sidechain
7	G	231	PHE	Sidechain
7	G	26	TYR	Sidechain
7	G	35	ARG	Sidechain
7	G	59	TYR	Sidechain
8	H	10	ARG	Sidechain
8	H	104	TYR	Sidechain
8	H	209	ARG	Sidechain
8	H	294	ARG	Sidechain
8	H	71	HIS	Sidechain

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Mol	Chain	Res	Type	Group
9	I	21	TYR	Sidechain
9	I	215	ARG	Sidechain
9	I	217	ARG	Sidechain
9	I	244	TYR	Sidechain
9	I	46	TYR	Sidechain
9	I	51	ARG	Sidechain
10	J	109	PHE	Sidechain
10	J	12	ARG	Sidechain
10	J	133	ARG	Sidechain
10	J	137	ARG	Sidechain
10	J	175	ARG	Sidechain
10	J	221	TYR	Sidechain
10	J	247	ARG	Sidechain
10	J	250	PHE	Sidechain
10	J	26	ARG	Sidechain
10	J	37	ARG	Sidechain
10	J	50	ARG	Sidechain
10	J	595	TYR	Sidechain
10	J	600	ARG	Sidechain
10	J	633	SER	Peptide
10	J	660	ARG	Sidechain
10	J	675	ARG	Sidechain
10	J	72	LEU	Peptide
10	J	740	ARG	Sidechain
10	J	773	ARG	Sidechain
10	J	800	TYR	Sidechain
10	J	806	ARG	Sidechain
10	J	818	TYR	Sidechain
10	J	830	ARG	Sidechain
10	J	832	TYR	Sidechain
10	J	865	GLU	Peptide
10	J	889	ARG	Sidechain
11	P	4	PHE	Sidechain

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	2350	0	2345	4	0
2	B	1890	0	1943	5	0
3	C	2622	0	2688	25	0
4	D	1707	0	1766	4	0
5	E	2048	0	2079	4	0
6	F	1627	0	1607	50	0
7	G	1831	0	1829	2	0
8	H	2277	0	2283	9	0
9	I	1750	0	1755	45	0
10	J	7942	0	7947	12	0
11	P	750	0	759	112	0
All	All	26794	0	27001	157	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 (157) 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)
6:F:49:HIS:NE2	11:P:36:LYS:HD2	1.28	1.43
3:C:51:ASP:CB	11:P:47:PRO:HD3	1.49	1.41
9:I:250:ASN:OD1	11:P:86:LEU:CD1	1.71	1.38
3:C:81:LYS:HE2	11:P:35:LYS:CB	1.45	1.38
6:F:52:PHE:CD2	11:P:32:LEU:HD22	1.61	1.34
3:C:51:ASP:HB2	11:P:47:PRO:CD	1.56	1.33
3:C:81:LYS:CE	11:P:35:LYS:HB3	1.65	1.27
9:I:272:TRP:CZ3	11:P:86:LEU:HD21	1.72	1.24
6:F:52:PHE:CE2	11:P:32:LEU:HD22	1.76	1.21
6:F:61:LEU:HD22	11:P:32:LEU:HD13	1.23	1.15
9:I:250:ASN:ND2	11:P:86:LEU:HD13	1.63	1.14
9:I:272:TRP:CD1	11:P:82:LYS:HE2	1.80	1.13
9:I:250:ASN:CG	11:P:86:LEU:CD1	2.17	1.13
6:F:49:HIS:NE2	11:P:36:LYS:CD	2.12	1.12
9:I:272:TRP:HZ3	11:P:86:LEU:HD21	0.96	1.10
9:I:250:ASN:OD1	11:P:86:LEU:HD11	0.92	1.10
6:F:52:PHE:CE2	11:P:32:LEU:CD2	2.38	1.06
9:I:272:TRP:CD1	11:P:82:LYS:CE	2.27	1.02
9:I:272:TRP:CZ3	11:P:86:LEU:CD2	2.42	1.02
6:F:238:ARG:HD3	11:P:18:LEU:CD2	1.89	1.01
9:I:250:ASN:CG	11:P:86:LEU:HD13	1.82	0.99
6:F:206:ASN:OD1	11:P:18:LEU:HD22	1.62	0.99
6:F:239:ASP:CG	11:P:19:SER:HA	1.82	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:LEU:HD13	11:P:61:ASN:HD22	1.26	0.98
9:I:291:PRO:HD2	11:P:79:PHE:HE2	1.30	0.96
6:F:239:ASP:HB3	11:P:19:SER:O	1.65	0.95
6:F:61:LEU:HD22	11:P:32:LEU:CD1	1.95	0.95
6:F:239:ASP:CB	11:P:19:SER:HA	1.96	0.95
6:F:52:PHE:CD2	11:P:32:LEU:CD2	2.49	0.95
6:F:239:ASP:OD1	11:P:19:SER:HA	1.67	0.94
9:I:250:ASN:CG	11:P:86:LEU:HD11	1.84	0.94
9:I:48:HIS:CD2	11:P:11:ILE:HD11	2.03	0.93
9:I:19:PRO:HB3	11:P:8:ASN:HD21	1.35	0.91
9:I:272:TRP:HZ3	11:P:86:LEU:CD2	1.78	0.90
3:C:48:GLU:HB3	11:P:49:ASN:ND2	1.86	0.90
6:F:52:PHE:HE2	11:P:32:LEU:CD2	1.84	0.90
6:F:239:ASP:OD2	11:P:18:LEU:O	1.94	0.85
9:I:291:PRO:HB2	11:P:73:SER:HB2	1.59	0.84
6:F:52:PHE:HE2	11:P:32:LEU:HD21	1.43	0.84
6:F:52:PHE:HD2	11:P:32:LEU:HD22	1.39	0.83
6:F:238:ARG:HD3	11:P:18:LEU:HD21	1.60	0.83
6:F:238:ARG:HD3	11:P:18:LEU:HD23	1.61	0.82
6:F:238:ARG:NH1	11:P:18:LEU:HD23	1.94	0.82
3:C:37:LEU:HD13	11:P:61:ASN:ND2	1.94	0.81
6:F:206:ASN:OD1	11:P:18:LEU:CD2	2.27	0.81
6:F:239:ASP:CG	11:P:18:LEU:O	2.20	0.80
9:I:250:ASN:HD21	11:P:86:LEU:HD13	1.43	0.80
9:I:19:PRO:HB3	11:P:8:ASN:ND2	1.97	0.78
6:F:238:ARG:CD	11:P:18:LEU:HD21	2.14	0.77
6:F:61:LEU:CD2	11:P:32:LEU:CD1	2.62	0.77
6:F:239:ASP:CG	11:P:19:SER:CA	2.53	0.77
6:F:239:ASP:OD1	11:P:18:LEU:C	2.24	0.76
6:F:239:ASP:HB3	11:P:19:SER:CA	2.16	0.76
6:F:239:ASP:OD1	11:P:19:SER:N	2.20	0.75
3:C:81:LYS:HE2	11:P:35:LYS:HB3	0.78	0.75
6:F:61:LEU:CD2	11:P:32:LEU:HD13	2.10	0.75
3:C:81:LYS:HB3	11:P:35:LYS:NZ	2.02	0.75
9:I:291:PRO:HD2	11:P:79:PHE:CE2	2.20	0.74
9:I:272:TRP:HB3	11:P:82:LYS:HE3	1.66	0.74
6:F:239:ASP:HB3	11:P:19:SER:HA	1.69	0.74
3:C:51:ASP:OD2	11:P:47:PRO:HB3	1.87	0.74
6:F:239:ASP:OD1	11:P:19:SER:CA	2.34	0.73
6:F:238:ARG:CD	11:P:18:LEU:CD2	2.65	0.73
6:F:239:ASP:HB3	11:P:19:SER:C	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:16:LEU:HG	11:P:15:LYS:NZ	2.06	0.71
6:F:238:ARG:HH11	11:P:18:LEU:HD23	1.56	0.71
9:I:291:PRO:HG2	11:P:73:SER:O	1.90	0.70
10:J:831:HIS:CD2	10:J:836:VAL:HG23	2.26	0.70
6:F:239:ASP:CB	11:P:19:SER:CA	2.70	0.69
3:C:37:LEU:CD1	11:P:61:ASN:HD22	2.03	0.68
10:J:991:THR:HG22	10:J:992:SER:H	1.59	0.67
3:C:51:ASP:CG	11:P:47:PRO:HD3	2.15	0.67
6:F:239:ASP:CB	11:P:19:SER:O	2.42	0.65
9:I:15:LYS:NZ	11:P:16:ASN:HD21	1.97	0.63
10:J:628:TRP:HB3	10:J:639:VAL:HG23	1.80	0.63
10:J:694:LEU:H	10:J:694:LEU:HD23	1.66	0.61
9:I:272:TRP:CH2	11:P:86:LEU:HD23	2.36	0.60
6:F:49:HIS:CD2	11:P:36:LYS:HD2	2.28	0.60
6:F:61:LEU:CD2	11:P:32:LEU:HD12	2.32	0.60
3:C:81:LYS:HB3	11:P:35:LYS:HZ1	1.65	0.59
6:F:49:HIS:CE1	11:P:36:LYS:HB2	2.39	0.58
9:I:272:TRP:CB	11:P:82:LYS:HE3	2.06	0.58
8:H:67:TRP:CD2	8:H:95:LEU:HD12	2.38	0.57
3:C:11:GLU:HG2	11:P:79:PHE:HD2	1.69	0.56
9:I:15:LYS:CE	11:P:16:ASN:ND2	2.68	0.56
6:F:238:ARG:CZ	11:P:18:LEU:HD23	2.35	0.56
9:I:272:TRP:CH2	11:P:86:LEU:CD2	2.88	0.56
3:C:81:LYS:CE	11:P:35:LYS:CB	2.39	0.56
9:I:19:PRO:CB	11:P:8:ASN:HD21	2.12	0.56
3:C:51:ASP:HB2	11:P:47:PRO:HD3	0.67	0.56
6:F:61:LEU:HD21	11:P:32:LEU:HD12	1.88	0.55
8:H:128:ILE:HD13	8:H:128:ILE:H	1.70	0.55
5:E:21:ILE:HD13	5:E:21:ILE:H	1.72	0.54
2:B:79:THR:HG21	5:E:129:LEU:HD22	1.91	0.53
9:I:19:PRO:CB	11:P:8:ASN:ND2	2.71	0.53
3:C:81:LYS:HB3	11:P:35:LYS:HZ2	1.74	0.53
9:I:16:LEU:HD12	11:P:11:ILE:CG2	2.39	0.53
9:I:16:LEU:CD1	11:P:11:ILE:HG21	2.39	0.52
6:F:242:ILE:HD13	11:P:19:SER:OG	2.08	0.52
6:F:239:ASP:CG	11:P:18:LEU:C	2.68	0.52
6:F:49:HIS:HE1	11:P:36:LYS:HB2	1.75	0.51
10:J:573:VAL:HG21	10:J:845:PRO:HB2	1.93	0.51
10:J:869:LEU:HA	10:J:872:ARG:HE	1.76	0.50
9:I:15:LYS:HD2	11:P:15:LYS:HE3	1.93	0.50
6:F:236:ARG:HH12	11:P:22:ILE:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:238:ARG:CD	11:P:18:LEU:HD23	2.35	0.49
9:I:272:TRP:NE1	11:P:82:LYS:CE	2.70	0.49
9:I:15:LYS:NZ	11:P:16:ASN:ND2	2.61	0.48
8:H:145:GLY:HA3	8:H:150:ARG:HG2	1.95	0.48
5:E:154:LEU:HD11	5:E:180:LEU:HD13	1.94	0.48
10:J:856:ARG:HB2	10:J:871:HIS:CE1	2.48	0.47
3:C:263:GLY:HA2	3:C:264:ARG:HB2	1.96	0.47
7:G:99:TYR:CD2	7:G:111:PRO:HD2	2.50	0.47
9:I:16:LEU:HD12	11:P:11:ILE:HG22	1.97	0.47
2:B:108:PHE:CE1	2:B:158:ILE:HD12	2.50	0.47
1:A:12:SER:HA	1:A:230:LEU:HD21	1.97	0.47
9:I:16:LEU:HG	11:P:15:LYS:CE	2.44	0.46
8:H:107:GLU:HA	8:H:176:LEU:HD22	1.98	0.46
9:I:16:LEU:HD11	11:P:11:ILE:HG21	1.98	0.46
7:G:224:LYS:HD2	7:G:224:LYS:H	1.81	0.46
9:I:272:TRP:CZ3	11:P:86:LEU:HD23	2.39	0.46
10:J:424:VAL:HG21	10:J:451:ILE:HG21	1.97	0.45
8:H:106:PRO:HB2	8:H:176:LEU:HD13	1.98	0.45
4:D:50:ILE:HB	4:D:67:GLU:HG3	1.98	0.45
11:P:59:ILE:HA	11:P:62:PHE:CD2	2.51	0.45
3:C:48:GLU:CB	11:P:49:ASN:ND2	2.66	0.45
3:C:39:ILE:HD12	3:C:43:LEU:HA	1.99	0.45
6:F:102:LEU:O	6:F:102:LEU:HG	2.17	0.45
9:I:272:TRP:NE1	11:P:82:LYS:HE2	2.26	0.45
6:F:52:PHE:CE2	11:P:32:LEU:HD21	2.24	0.44
11:P:20:THR:HG22	11:P:21:SER:H	1.82	0.44
8:H:160:ARG:HH12	9:I:240:GLY:H	1.63	0.44
3:C:81:LYS:CB	11:P:35:LYS:NZ	2.75	0.44
3:C:87:VAL:HG22	3:C:219:VAL:HG22	2.00	0.44
1:A:303:ARG:HH22	10:J:715:VAL:HG13	1.83	0.43
8:H:62:THR:HG21	8:H:68:MET:SD	2.58	0.43
9:I:16:LEU:HG	11:P:15:LYS:HE2	2.00	0.43
4:D:46:LEU:HD23	4:D:78:ILE:HG21	2.00	0.43
9:I:46:TYR:HB2	9:I:53:LEU:HB3	2.00	0.43
3:C:51:ASP:OD2	11:P:47:PRO:CB	2.62	0.42
9:I:143:VAL:HG22	9:I:153:VAL:HG12	2.00	0.42
10:J:408:ALA:HA	10:J:425:ILE:HD11	2.00	0.42
1:A:120:VAL:HA	1:A:123:LEU:HG	2.02	0.42
1:A:179:VAL:HG12	1:A:184:PRO:HB3	2.01	0.42
3:C:269:ARG:HG2	3:C:270:GLU:H	1.85	0.42
5:E:255:ALA:HB3	5:E:256:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:213:HIS:CE1	8:H:316:GLN:HE21	2.38	0.41
2:B:169:THR:HG23	10:J:63:ALA:CB	2.50	0.41
2:B:20:ASN:HD22	2:B:20:ASN:H	1.68	0.41
4:D:202:CYS:O	4:D:206:VAL:HG23	2.20	0.41
8:H:214:THR:HG23	8:H:224:VAL:HA	2.02	0.41
10:J:91:ASP:HB2	10:J:196:THR:HA	2.03	0.41
3:C:24:ARG:HG3	9:I:156:LEU:HB3	2.03	0.41
6:F:52:PHE:HD2	11:P:32:LEU:CD2	2.12	0.40
2:B:156:ASP:HB2	2:B:190:VAL:HG22	2.03	0.40
9:I:15:LYS:HE2	11:P:16:ASN:ND2	2.37	0.40
4:D:28:CYS:HB2	4:D:115:ALA:HB1	2.03	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	300/305 (98%)	278 (93%)	18 (6%)	4 (1%)	15 60
2	B	238/246 (97%)	223 (94%)	11 (5%)	4 (2%)	11 56
3	C	327/394 (83%)	294 (90%)	22 (7%)	11 (3%)	5 42
4	D	221/223 (99%)	211 (96%)	9 (4%)	1 (0%)	34 77
5	E	263/265 (99%)	248 (94%)	10 (4%)	5 (2%)	10 54
6	F	205/250 (82%)	194 (95%)	8 (4%)	3 (2%)	13 58
7	G	234/240 (98%)	219 (94%)	14 (6%)	1 (0%)	39 80
8	H	287/359 (80%)	263 (92%)	15 (5%)	9 (3%)	5 44
9	I	219/292 (75%)	200 (91%)	14 (6%)	5 (2%)	8 50
10	J	991/1001 (99%)	905 (91%)	68 (7%)	18 (2%)	11 55
11	P	93/747 (12%)	82 (88%)	9 (10%)	2 (2%)	8 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3378/4322 (78%)	3117 (92%)	198 (6%)	63 (2%)	14	54

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ALA
3	C	10	ILE
3	C	11	GLU
3	C	12	ILE
3	C	143	ALA
3	C	191	ASP
5	E	182	ILE
6	F	55	ASN
6	F	80	PRO
8	H	54	ILE
8	H	148	LEU
10	J	238	MET
10	J	838	ILE
10	J	966	ASN
3	C	73	ASN
3	C	353	PRO
5	E	29	HIS
5	E	166	VAL
6	F	84	ARG
8	H	92	ASN
8	H	147	ILE
9	I	4	ASN
10	J	385	LYS
10	J	508	HIS
10	J	634	ALA
1	A	117	ALA
2	B	35	ALA
2	B	167	ASP
5	E	112	SER
5	E	134	HIS
8	H	77	ASP
9	I	217	ARG
9	I	251	ASP
10	J	150	ASN
10	J	833	GLY
11	P	53	THR
1	A	242	ASN

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Mol	Chain	Res	Type
3	C	190	PRO
3	C	359	GLN
7	G	145	ALA
8	H	122	LYS
8	H	151	LYS
8	H	187	ARG
8	H	277	SER
9	I	215	ARG
10	J	107	CYS
10	J	246	GLU
10	J	363	THR
10	J	507	GLY
10	J	605	PRO
11	P	20	THR
3	C	8	GLU
3	C	366	GLY
9	I	212	SER
10	J	228	ALA
10	J	364	VAL
10	J	844	SER
1	A	96	ILE
2	B	93	ASN
2	B	33	PRO
10	J	322	PRO
4	D	135	PRO
10	J	432	PRO

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	263/266 (99%)	259 (98%)	4 (2%)	72	89
2	B	214/218 (98%)	207 (97%)	7 (3%)	45	78
3	C	294/349 (84%)	286 (97%)	8 (3%)	52	80
4	D	197/197 (100%)	193 (98%)	4 (2%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	240/240 (100%)	233 (97%)	7 (3%)	50	79
6	F	181/219 (83%)	174 (96%)	7 (4%)	39	74
7	G	205/209 (98%)	197 (96%)	8 (4%)	39	74
8	H	252/311 (81%)	245 (97%)	7 (3%)	51	80
9	I	190/240 (79%)	184 (97%)	6 (3%)	46	78
10	J	895/901 (99%)	865 (97%)	30 (3%)	44	77
11	P	89/702 (13%)	88 (99%)	1 (1%)	80	91
All	All	3020/3852 (78%)	2931 (97%)	89 (3%)	54	79

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

Mol	Chain	Res	Type
1	A	73	PHE
1	A	96	ILE
1	A	142	ASP
1	A	167	ILE
2	B	20	ASN
2	B	34	HIS
2	B	173	ASP
2	B	180	ASN
2	B	187	LEU
2	B	196	LEU
2	B	225	ARG
3	C	10	ILE
3	C	24	ARG
3	C	58	THR
3	C	80	LEU
3	C	159	ILE
3	C	191	ASP
3	C	212	VAL
3	C	289	LYS
4	D	9	ILE
4	D	136	ILE
4	D	148	ASP
4	D	193	SER
5	E	21	ILE
5	E	54	ASP
5	E	76	LEU
5	E	86	ARG
5	E	90	LEU

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Mol	Chain	Res	Type
5	E	116	LEU
5	E	232	ASN
6	F	7	ARG
6	F	52	PHE
6	F	80	PRO
6	F	84	ARG
6	F	175	SER
6	F	189	ASP
6	F	195	GLU
7	G	29	PRO
7	G	68	VAL
7	G	70	ASP
7	G	96	SER
7	G	99	TYR
7	G	119	VAL
7	G	218	ASN
7	G	234	ILE
8	H	68	MET
8	H	80	THR
8	H	128	ILE
8	H	169	LEU
8	H	195	ARG
8	H	225	LEU
8	H	354	MET
9	I	42	LYS
9	I	51	ARG
9	I	52	THR
9	I	161	LYS
9	I	215	ARG
9	I	272	TRP
10	J	72	LEU
10	J	74	ASP
10	J	107	CYS
10	J	137	ARG
10	J	140	ASP
10	J	208	GLU
10	J	232	ARG
10	J	251	SER
10	J	254	THR
10	J	294	ARG
10	J	364	VAL
10	J	366	SER

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Mol	Chain	Res	Type
10	J	421	ASN
10	J	552	ASP
10	J	602	ASP
10	J	628	TRP
10	J	642	MET
10	J	671	THR
10	J	694	LEU
10	J	709	THR
10	J	713	ASN
10	J	755	HIS
10	J	817	GLN
10	J	820	TYR
10	J	830	ARG
10	J	841	HIS
10	J	870	THR
10	J	902	TYR
10	J	955	GLU
10	J	959	LYS
11	P	46	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	247	GLN
1	A	291	ASN
2	B	20	ASN
2	B	32	HIS
2	B	111	ASN
2	B	131	GLN
3	C	78	ASN
4	D	81	HIS
5	E	232	ASN
6	F	44	GLN
6	F	99	ASN
6	F	171	HIS
6	F	235	ASN
7	G	43	HIS
8	H	185	HIS
8	H	196	ASN
8	H	302	ASN
8	H	316	GLN

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Mol	Chain	Res	Type
9	I	126	ASN
9	I	192	GLN
10	J	155	HIS
10	J	275	GLN
10	J	421	ASN
10	J	555	HIS
10	J	667	ASN
10	J	713	ASN
10	J	841	HIS
10	J	871	HIS
10	J	888	HIS
10	J	890	ASN
11	P	8	ASN
11	P	16	ASN
11	P	61	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.