Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 09:18 PM BST

PDB ID	:	2JOJ
Title	:	NMR solution structure of N-terminal domain of Euplotes octocarinatus centrin
Authors	:	Hong, J.; Guo, C.; Lin, D.
Deposited on	:	2007-03-14

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

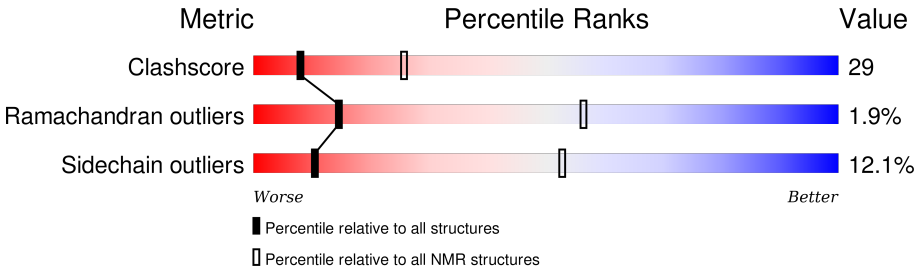
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	77	43% 44% . 9%

2 Ensemble composition and analysis (i)

This entry contains 16 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:27-A:77, A:82-A:100 (70)	0.44	16

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1253 atoms, of which 617 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Centrin protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	77	1253	401	617	102	130	3	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Centrin protein

Chain A:

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Centrin protein

Chain A:

4.2.2 Score per residue for model 2

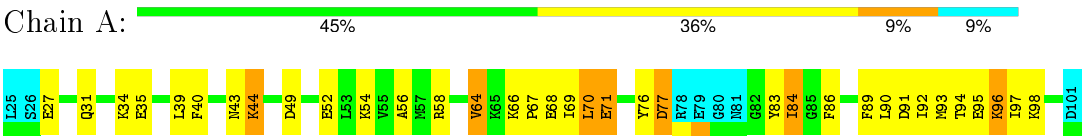
- Molecule 1: Centrin protein

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Centrin protein

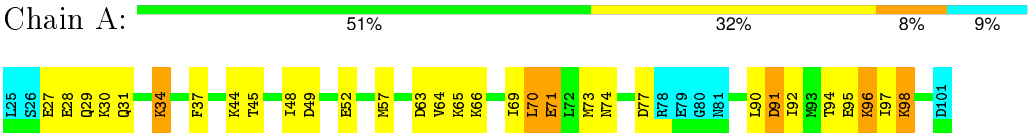
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Centrin protein

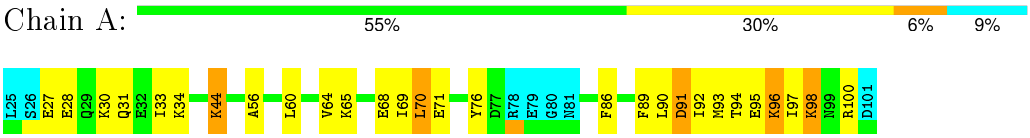
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Centrin protein

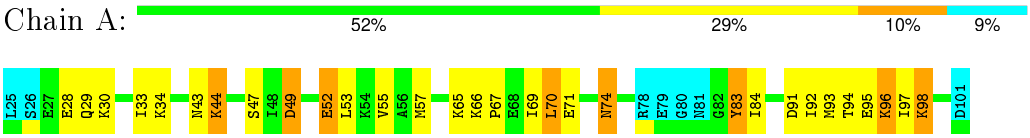
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Centrin protein

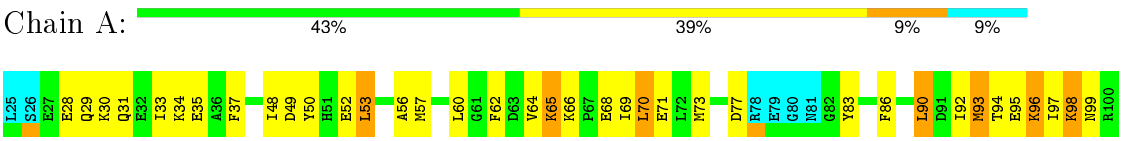
Chain A:



4.2.7 Score per residue for model 7

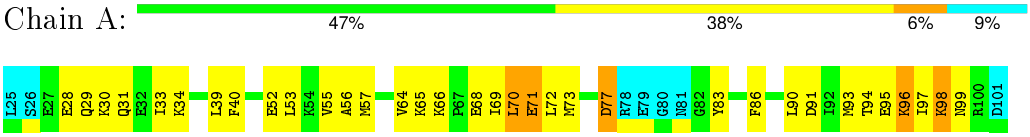
• Molecule 1: Centrin protein

Chain A:



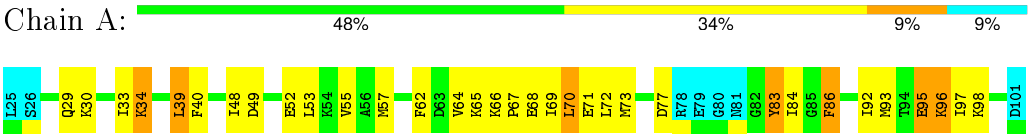
4.2.8 Score per residue for model 8

• Molecule 1: Centrin protein



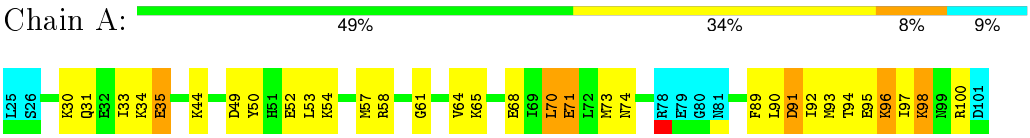
4.2.9 Score per residue for model 9

• Molecule 1: Centrin protein



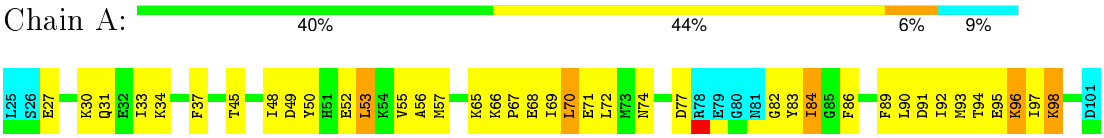
4.2.10 Score per residue for model 10

• Molecule 1: Centrin protein



4.2.11 Score per residue for model 11

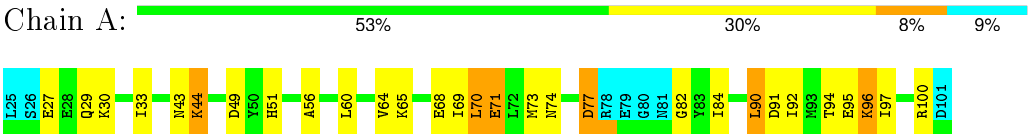
• Molecule 1: Centrin protein



4.2.12 Score per residue for model 12

• Molecule 1: Centrin protein

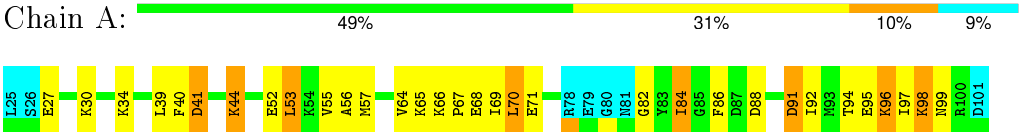
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Centrin protein

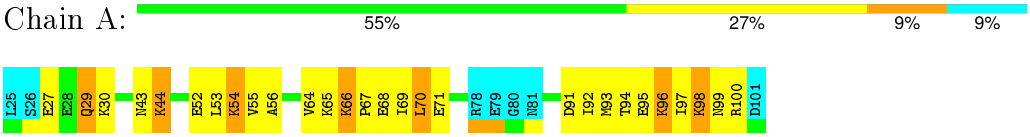
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Centrin protein

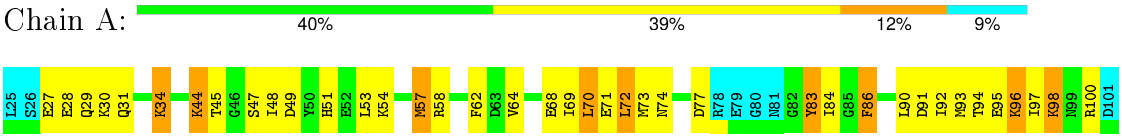
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Centrin protein

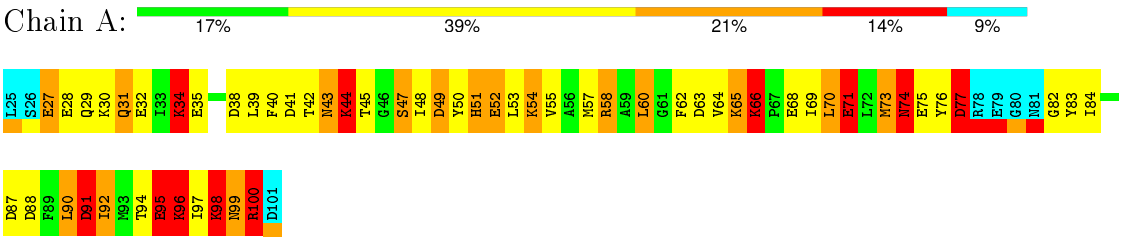
Chain A:



4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Centrin protein

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 16 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 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 (average) 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	1.22±3.06	12±46/591 (2.1±7.7%)	0.89±1.50	9±35/791 (1.2±4.5%)
All	All	3.30	196/9456 (2.1%)	1.74	146/12656 (1.2%)

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	Planarity
1	A	0.0±0.0	0.2±0.4
All	All	0	3

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	32	GLU	CD-OE2	-65.68	0.53	1.25	16	1
1	A	95	GLU	CD-OE2	-61.98	0.57	1.25	16	1
1	A	75	GLU	CD-OE2	-59.84	0.59	1.25	16	1
1	A	68	GLU	CD-OE2	-56.25	0.63	1.25	16	1
1	A	58	ARG	CZ-NH2	-51.64	0.66	1.33	16	1
1	A	100	ARG	CZ-NH2	-48.83	0.69	1.33	16	1
1	A	27	GLU	CD-OE1	-48.61	0.72	1.25	16	1
1	A	58	ARG	CZ-NH1	-48.31	0.70	1.33	16	1
1	A	27	GLU	CG-CD	-47.76	0.80	1.51	16	1
1	A	27	GLU	CD-OE2	-46.01	0.75	1.25	16	1
1	A	71	GLU	CD-OE2	-41.40	0.80	1.25	16	1
1	A	35	GLU	CD-OE2	-41.18	0.80	1.25	16	1
1	A	100	ARG	CZ-NH1	-41.15	0.79	1.33	16	1
1	A	58	ARG	CD-NE	-40.91	0.77	1.46	16	1
1	A	100	ARG	CD-NE	-39.71	0.79	1.46	16	1
1	A	95	GLU	CG-CD	-38.95	0.93	1.51	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	51	HIS	CG-ND1	-38.58	0.53	1.38	16	1
1	A	29	GLN	CD-OE1	-38.03	0.40	1.24	16	1
1	A	75	GLU	CD-OE1	-37.27	0.84	1.25	16	1
1	A	74	ASN	CG-ND2	-36.79	0.40	1.32	16	1
1	A	51	HIS	CE1-NE2	-36.68	0.48	1.32	16	1
1	A	32	GLU	CG-CD	-35.79	0.98	1.51	16	1
1	A	66	LYS	CE-NZ	-35.39	0.60	1.49	16	1
1	A	87	ASP	CB-CG	-35.36	0.77	1.51	16	1
1	A	47	SER	CB-OG	-34.17	0.97	1.42	16	1
1	A	31	GLN	CD-OE1	-32.96	0.51	1.24	16	1
1	A	29	GLN	CD-NE2	-32.41	0.51	1.32	16	1
1	A	77	ASP	C-O	-31.89	0.62	1.23	16	1
1	A	68	GLU	CG-CD	-31.78	1.04	1.51	16	1
1	A	35	GLU	CG-CD	-31.64	1.04	1.51	16	1
1	A	54	LYS	CE-NZ	-31.34	0.70	1.49	16	1
1	A	51	HIS	CG-CD2	-30.50	0.83	1.35	16	1
1	A	54	LYS	CD-CE	-30.00	0.76	1.51	16	1
1	A	95	GLU	CD-OE1	-29.30	0.93	1.25	16	1
1	A	76	TYR	CE1-CZ	-28.39	1.01	1.38	16	2
1	A	75	GLU	CG-CD	-27.95	1.10	1.51	16	1
1	A	76	TYR	CG-CD2	-27.93	1.02	1.39	16	1
1	A	91	ASP	CB-CG	-27.14	0.94	1.51	16	1
1	A	29	GLN	CG-CD	-26.88	0.89	1.51	16	1
1	A	77	ASP	C-N	-26.46	0.73	1.34	16	1
1	A	43	ASN	CB-CG	-26.27	0.90	1.51	16	1
1	A	100	ARG	NE-CZ	-26.26	0.98	1.33	16	1
1	A	66	LYS	CD-CE	-26.06	0.86	1.51	16	1
1	A	35	GLU	CD-OE1	-25.86	0.97	1.25	16	1
1	A	57	MET	CG-SD	-25.36	1.15	1.81	16	1
1	A	31	GLN	CG-CD	-25.00	0.93	1.51	16	1
1	A	45	THR	C-O	-24.74	0.76	1.23	16	1
1	A	43	ASN	CG-ND2	-24.58	0.71	1.32	16	1
1	A	34	LYS	CB-CG	-24.51	0.86	1.52	16	1
1	A	44	LYS	CE-NZ	-24.48	0.87	1.49	16	1
1	A	58	ARG	CB-CG	-24.08	0.87	1.52	16	1
1	A	65	LYS	CE-NZ	-23.92	0.89	1.49	16	1
1	A	51	HIS	CB-CG	-23.67	1.07	1.50	16	1
1	A	31	GLN	CD-NE2	-23.67	0.73	1.32	16	1
1	A	51	HIS	CD2-NE2	-23.67	0.85	1.38	16	1
1	A	88	ASP	CG-OD2	-23.62	0.71	1.25	16	1
1	A	44	LYS	CB-CG	-23.56	0.89	1.52	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	88	ASP	CB-CG	-22.23	1.05	1.51	16	1
1	A	91	ASP	CG-OD2	-22.21	0.74	1.25	16	1
1	A	52	GLU	CB-CG	-22.19	1.09	1.52	16	1
1	A	63	ASP	CB-CG	-22.19	1.05	1.51	16	1
1	A	54	LYS	CB-CG	-22.16	0.92	1.52	16	1
1	A	43	ASN	CG-OD1	-22.09	0.75	1.24	16	1
1	A	55	VAL	CB-CG1	-22.02	1.06	1.52	16	1
1	A	38	ASP	CB-CG	-21.90	1.05	1.51	16	1
1	A	75	GLU	CB-CG	-21.54	1.11	1.52	16	1
1	A	55	VAL	CB-CG2	-20.92	1.08	1.52	16	1
1	A	60	LEU	CG-CD1	-20.80	0.74	1.51	16	1
1	A	91	ASP	CG-OD1	-20.66	0.77	1.25	16	1
1	A	68	GLU	CB-CG	-20.41	1.13	1.52	16	1
1	A	38	ASP	CG-OD2	-19.90	0.79	1.25	16	1
1	A	99	ASN	CG-OD1	-19.90	0.80	1.24	16	1
1	A	100	ARG	CB-CG	-19.64	0.99	1.52	16	1
1	A	71	GLU	CD-OE1	-19.58	1.04	1.25	16	1
1	A	45	THR	C-N	-19.49	0.97	1.33	16	1
1	A	43	ASN	C-O	-19.48	0.86	1.23	16	1
1	A	87	ASP	CG-OD2	-19.38	0.80	1.25	16	1
1	A	66	LYS	CG-CD	-18.85	0.88	1.52	16	1
1	A	44	LYS	CD-CE	-18.59	1.04	1.51	16	1
1	A	76	TYR	CE2-CZ	-18.55	1.14	1.38	16	2
1	A	52	GLU	CG-CD	-18.51	1.24	1.51	16	1
1	A	74	ASN	CG-OD1	-18.44	0.83	1.24	16	1
1	A	73	MET	CG-SD	-18.39	1.33	1.81	16	1
1	A	76	TYR	CG-CD1	-18.22	1.15	1.39	16	1
1	A	65	LYS	CG-CD	-18.12	0.90	1.52	16	1
1	A	73	MET	CB-CG	-18.10	0.93	1.51	16	1
1	A	99	ASN	CG-ND2	-17.91	0.88	1.32	16	1
1	A	44	LYS	CA-CB	-17.62	1.15	1.53	16	1
1	A	44	LYS	C-O	-17.62	0.89	1.23	16	1
1	A	83	TYR	CG-CD2	-17.58	1.16	1.39	16	1
1	A	58	ARG	NE-CZ	-17.23	1.10	1.33	16	1
1	A	32	GLU	CD-OE1	-17.03	1.06	1.25	16	1
1	A	28	GLU	CD-OE2	-16.61	1.07	1.25	16	1
1	A	82	GLY	N-CA	-16.61	1.21	1.46	16	1
1	A	44	LYS	CG-CD	-16.57	0.96	1.52	16	1
1	A	29	GLN	CB-CG	-16.55	1.07	1.52	16	1
1	A	60	LEU	CG-CD2	-16.02	0.92	1.51	16	1
1	A	77	ASP	CG-OD2	-15.94	0.88	1.25	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	83	TYR	CE1-CZ	-15.66	1.18	1.38	16	2
1	A	71	GLU	CG-CD	-15.64	1.28	1.51	16	1
1	A	87	ASP	CG-OD1	-15.42	0.89	1.25	16	1
1	A	100	ARG	C-N	-15.12	0.99	1.34	16	1
1	A	66	LYS	CB-CG	-15.00	1.12	1.52	16	1
1	A	51	HIS	ND1-CE1	-14.92	0.97	1.34	16	1
1	A	49	ASP	CG-OD2	-14.76	0.91	1.25	16	1
1	A	90	LEU	CG-CD1	-14.75	0.97	1.51	16	1
1	A	28	GLU	CD-OE1	-14.75	1.09	1.25	16	1
1	A	83	TYR	CB-CG	-14.62	1.29	1.51	16	1
1	A	53	LEU	CG-CD2	-14.60	0.97	1.51	16	1
1	A	43	ASN	C-N	-14.52	1.00	1.34	16	1
1	A	65	LYS	CD-CE	-14.47	1.15	1.51	16	1
1	A	63	ASP	CG-OD1	-14.18	0.92	1.25	16	1
1	A	35	GLU	CB-CG	-14.16	1.25	1.52	16	1
1	A	50	TYR	CB-CG	-13.96	1.30	1.51	16	1
1	A	83	TYR	CD2-CE2	-13.91	1.18	1.39	16	1
1	A	41	ASP	CG-OD1	-13.89	0.93	1.25	16	1
1	A	30	LYS	CB-CG	-13.75	1.15	1.52	16	1
1	A	83	TYR	CD1-CE1	-13.74	1.18	1.39	16	1
1	A	44	LYS	C-N	-13.72	1.02	1.34	16	1
1	A	50	TYR	CD2-CE2	-13.50	1.19	1.39	16	1
1	A	50	TYR	CD1-CE1	-13.46	1.19	1.39	16	1
1	A	41	ASP	C-O	-13.41	0.97	1.23	16	1
1	A	41	ASP	CG-OD2	-13.29	0.94	1.25	16	1
1	A	63	ASP	C-O	-13.09	0.98	1.23	16	1
1	A	98	LYS	CB-CG	-13.07	1.17	1.52	16	1
1	A	90	LEU	CG-CD2	-13.04	1.03	1.51	16	1
1	A	52	GLU	CD-OE1	-12.63	1.11	1.25	16	1
1	A	77	ASP	CG-OD1	-12.54	0.96	1.25	16	1
1	A	52	GLU	CD-OE2	-12.34	1.12	1.25	16	1
1	A	32	GLU	CB-CG	-12.25	1.28	1.52	16	1
1	A	28	GLU	CG-CD	-11.50	1.34	1.51	16	1
1	A	40	PHE	CG-CD1	-11.48	1.21	1.38	16	1
1	A	53	LEU	CG-CD1	-11.39	1.09	1.51	16	1
1	A	50	TYR	CZ-OH	-11.18	1.18	1.37	16	1
1	A	83	TYR	CZ-OH	-11.04	1.19	1.37	16	1
1	A	41	ASP	C-N	-10.87	1.09	1.34	16	1
1	A	39	LEU	CG-CD2	-10.70	1.12	1.51	16	1
1	A	39	LEU	CG-CD1	-10.54	1.12	1.51	16	1
1	A	77	ASP	CB-CG	-10.24	1.30	1.51	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	50	TYR	CE1-CZ	-10.11	1.25	1.38	16	1
1	A	50	TYR	CG-CD2	-9.93	1.26	1.39	16	1
1	A	30	LYS	CG-CD	-9.89	1.18	1.52	16	1
1	A	64	VAL	CB-CG2	-9.71	1.32	1.52	16	1
1	A	63	ASP	C-N	-9.54	1.12	1.34	16	1
1	A	49	ASP	CB-CG	-9.41	1.31	1.51	16	1
1	A	34	LYS	CE-NZ	-9.27	1.25	1.49	16	1
1	A	76	TYR	CB-CG	-9.20	1.37	1.51	16	1
1	A	76	TYR	CD2-CE2	-9.03	1.25	1.39	16	1
1	A	76	TYR	CD1-CE1	-8.98	1.25	1.39	16	1
1	A	68	GLU	CD-OE1	-8.94	1.15	1.25	16	1
1	A	98	LYS	CG-CD	-8.69	1.23	1.52	16	1
1	A	99	ASN	C-O	-8.69	1.06	1.23	16	1
1	A	27	GLU	CB-CG	-8.67	1.35	1.52	16	1
1	A	62	PHE	C-N	-8.59	1.14	1.34	16	1
1	A	83	TYR	CE2-CZ	-8.41	1.27	1.38	16	4
1	A	100	ARG	C-O	-8.34	1.07	1.23	16	1
1	A	40	PHE	CE2-CZ	-8.10	1.22	1.37	16	1
1	A	57	MET	CB-CG	-8.08	1.25	1.51	16	1
1	A	48	ILE	CB-CG1	-7.80	1.32	1.54	16	1
1	A	71	GLU	CB-CG	-7.66	1.37	1.52	16	1
1	A	45	THR	N-CA	-7.43	1.31	1.46	16	1
1	A	92	ILE	CG1-CD1	-7.42	0.99	1.50	16	1
1	A	63	ASP	CG-OD2	-7.34	1.08	1.25	16	1
1	A	76	TYR	CZ-OH	-7.29	1.25	1.37	16	1
1	A	58	ARG	CG-CD	-7.17	1.34	1.51	16	1
1	A	30	LYS	CE-NZ	-7.10	1.31	1.49	16	1
1	A	40	PHE	CB-CG	-6.87	1.39	1.51	16	1
1	A	64	VAL	CB-CG1	-6.85	1.38	1.52	16	1
1	A	98	LYS	CE-NZ	-6.70	1.32	1.49	16	1
1	A	31	GLN	CB-CG	-6.59	1.34	1.52	16	1
1	A	48	ILE	CB-CG2	-6.53	1.32	1.52	16	1
1	A	96	LYS	CD-CE	-6.46	1.35	1.51	16	1
1	A	44	LYS	CA-C	-6.44	1.36	1.52	16	1
1	A	30	LYS	CD-CE	-6.22	1.35	1.51	16	1
1	A	62	PHE	C-O	-6.17	1.11	1.23	16	1
1	A	99	ASN	C-N	-6.09	1.20	1.34	16	1
1	A	83	TYR	CG-CD1	-5.89	1.31	1.39	16	1
1	A	34	LYS	CG-CD	-5.71	1.33	1.52	16	1
1	A	50	TYR	CE2-CZ	-5.65	1.31	1.38	16	1
1	A	100	ARG	CG-CD	-5.62	1.37	1.51	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	45	THR	CA-CB	-5.58	1.38	1.53	16	1
1	A	63	ASP	CA-CB	-5.53	1.41	1.53	16	1
1	A	42	THR	C-N	-5.48	1.21	1.34	16	1
1	A	62	PHE	CE1-CZ	5.44	1.47	1.37	15	1
1	A	40	PHE	CD1-CE1	-5.39	1.28	1.39	16	1
1	A	40	PHE	CD2-CE2	-5.33	1.28	1.39	16	1
1	A	96	LYS	CE-NZ	-5.27	1.35	1.49	16	1
1	A	50	TYR	CG-CD1	-5.19	1.32	1.39	16	1
1	A	64	VAL	CA-CB	-5.17	1.43	1.54	16	1
1	A	41	ASP	CB-CG	-5.15	1.41	1.51	16	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	58	ARG	NE-CZ-NH1	51.27	145.94	120.30	16	1
1	A	88	ASP	CB-CG-OD2	-47.97	75.12	118.30	16	1
1	A	58	ARG	NE-CZ-NH2	44.88	142.74	120.30	16	1
1	A	58	ARG	NH1-CZ-NH2	-43.71	71.32	119.40	16	1
1	A	38	ASP	CB-CG-OD2	-39.96	82.33	118.30	16	1
1	A	77	ASP	O-C-N	-33.61	68.92	122.70	16	1
1	A	74	ASN	OD1-CG-ND2	-31.26	50.00	121.90	16	1
1	A	100	ARG	NE-CZ-NH1	31.18	135.89	120.30	16	1
1	A	88	ASP	CB-CG-OD1	30.86	146.08	118.30	16	1
1	A	51	HIS	ND1-CG-CD2	-29.57	64.60	106.00	16	1
1	A	38	ASP	CB-CG-OD1	24.03	139.93	118.30	16	1
1	A	32	GLU	CG-CD-OE2	-23.03	72.25	118.30	16	1
1	A	34	LYS	CA-CB-CG	21.57	160.87	113.40	16	1
1	A	74	ASN	CB-CG-OD1	21.33	164.27	121.60	16	1
1	A	68	GLU	CG-CD-OE2	-21.29	75.72	118.30	16	1
1	A	57	MET	CG-SD-CE	20.78	133.45	100.20	16	1
1	A	98	LYS	CB-CG-CD	20.51	164.92	111.60	16	1
1	A	29	GLN	OE1-CD-NE2	-19.99	75.93	121.90	16	1
1	A	100	ARG	NH1-CZ-NH2	-19.78	97.65	119.40	16	1
1	A	73	MET	CG-SD-CE	19.67	131.67	100.20	16	1
1	A	51	HIS	CG-CD2-NE2	19.41	146.08	109.20	16	1
1	A	60	LEU	CB-CG-CD2	18.44	142.34	111.00	16	1
1	A	66	LYS	CG-CD-CE	18.21	166.53	111.90	16	1
1	A	65	LYS	CB-CG-CD	17.23	156.39	111.60	16	1
1	A	51	HIS	CG-ND1-CE1	17.03	132.04	108.20	16	1
1	A	73	MET	CA-CB-CG	16.98	142.17	113.30	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	58	ARG	CD-NE-CZ	16.88	147.24	123.60	16	1
1	A	87	ASP	CB-CG-OD2	-16.86	103.12	118.30	16	1
1	A	54	LYS	CD-CE-NZ	16.81	150.37	111.70	16	1
1	A	76	TYR	CB-CG-CD1	16.74	131.05	121.00	16	1
1	A	32	GLU	CG-CD-OE1	16.57	151.44	118.30	16	1
1	A	54	LYS	CG-CD-CE	16.50	161.41	111.90	16	1
1	A	45	THR	O-C-N	-16.40	95.31	123.20	16	1
1	A	49	ASP	CB-CG-OD1	16.24	132.92	118.30	16	1
1	A	66	LYS	CD-CE-NZ	16.15	148.85	111.70	16	1
1	A	63	ASP	CB-CG-OD1	-15.88	104.00	118.30	16	1
1	A	58	ARG	CG-CD-NE	15.11	143.53	111.80	16	1
1	A	68	GLU	CG-CD-OE1	14.85	148.01	118.30	16	1
1	A	99	ASN	OD1-CG-ND2	-14.66	88.19	121.90	16	1
1	A	27	GLU	CB-CG-CD	14.55	153.48	114.20	16	1
1	A	49	ASP	CB-CG-OD2	-14.54	105.21	118.30	16	1
1	A	51	HIS	CE1-NE2-CD2	-14.51	70.33	106.60	16	1
1	A	44	LYS	CB-CG-CD	14.12	148.31	111.60	16	1
1	A	95	GLU	CG-CD-OE2	-14.03	90.24	118.30	16	1
1	A	43	ASN	CA-CB-CG	13.81	143.79	113.40	16	1
1	A	58	ARG	CA-CB-CG	13.48	143.06	113.40	16	1
1	A	87	ASP	CA-CB-CG	13.46	143.00	113.40	16	1
1	A	52	GLU	CA-CB-CG	13.25	142.55	113.40	16	1
1	A	77	ASP	CA-C-N	13.18	146.20	117.20	16	1
1	A	58	ARG	CB-CG-CD	13.01	145.42	111.60	16	1
1	A	75	GLU	OE1-CD-OE2	-12.99	107.71	123.30	16	1
1	A	90	LEU	CB-CG-CD2	12.84	132.82	111.00	16	1
1	A	83	TYR	CB-CG-CD2	-12.79	113.33	121.00	16	1
1	A	68	GLU	CB-CG-CD	12.34	147.53	114.20	16	1
1	A	100	ARG	NE-CZ-NH2	12.33	126.46	120.30	16	1
1	A	76	TYR	CG-CD1-CE1	12.31	131.15	121.30	16	1
1	A	74	ASN	CB-CG-ND2	12.10	145.74	116.70	16	1
1	A	95	GLU	CG-CD-OE1	12.04	142.38	118.30	16	1
1	A	29	GLN	CG-CD-NE2	11.81	145.04	116.70	16	1
1	A	77	ASP	CA-C-O	11.79	144.85	120.10	16	1
1	A	30	LYS	CB-CG-CD	11.74	142.14	111.60	16	1
1	A	100	ARG	CA-CB-CG	11.63	138.99	113.40	16	1
1	A	60	LEU	CD1-CG-CD2	-11.54	75.86	110.50	16	1
1	A	43	ASN	O-C-N	-11.15	104.86	122.70	16	1
1	A	51	HIS	CA-CB-CG	11.14	132.53	113.60	16	1
1	A	76	TYR	CZ-CE2-CD2	11.07	129.76	119.80	16	1
1	A	77	ASP	C-N-CA	10.96	149.10	121.70	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	32	GLU	OE1-CD-OE2	10.84	136.31	123.30	16	1
1	A	68	GLU	OE1-CD-OE2	10.81	136.27	123.30	16	1
1	A	35	GLU	CB-CG-CD	10.73	143.16	114.20	16	1
1	A	60	LEU	CB-CG-CD1	10.62	129.05	111.00	16	1
1	A	75	GLU	CG-CD-OE1	10.59	139.48	118.30	16	1
1	A	53	LEU	CB-CG-CD1	10.57	128.96	111.00	16	1
1	A	90	LEU	CB-CG-CD1	10.30	128.51	111.00	16	1
1	A	45	THR	CA-C-N	10.29	136.78	116.20	16	1
1	A	77	ASP	CB-CG-OD1	10.03	127.33	118.30	16	1
1	A	76	TYR	CD1-CG-CD2	-9.87	107.04	117.90	16	1
1	A	66	LYS	CB-CG-CD	9.85	137.21	111.60	16	1
1	A	83	TYR	CD1-CE1-CZ	-9.84	110.94	119.80	16	1
1	A	55	VAL	CG1-CB-CG2	-9.79	95.24	110.90	16	1
1	A	83	TYR	CG-CD2-CE2	-9.76	113.50	121.30	16	1
1	A	34	LYS	CB-CG-CD	9.66	136.71	111.60	16	1
1	A	90	LEU	CD1-CG-CD2	-9.37	82.40	110.50	16	1
1	A	41	ASP	CB-CG-OD2	9.29	126.66	118.30	16	1
1	A	40	PHE	CB-CG-CD1	-9.01	114.50	120.80	16	1
1	A	51	HIS	CB-CG-CD2	8.95	158.53	130.80	16	1
1	A	41	ASP	CB-CG-OD1	8.77	126.19	118.30	16	1
1	A	55	VAL	CA-CB-CG2	8.73	124.00	110.90	16	1
1	A	29	GLN	CG-CD-OE1	8.71	139.03	121.60	16	1
1	A	41	ASP	O-C-N	-8.56	109.00	122.70	16	1
1	A	91	ASP	CA-CB-CG	8.53	132.16	113.40	16	1
1	A	41	ASP	OD1-CG-OD2	-8.50	107.14	123.30	16	1
1	A	50	TYR	CB-CG-CD2	-8.41	115.95	121.00	16	1
1	A	65	LYS	CD-CE-NZ	-8.36	92.47	111.70	16	1
1	A	31	GLN	CG-CD-NE2	8.31	136.65	116.70	16	1
1	A	71	GLU	CG-CD-OE1	8.21	134.72	118.30	16	1
1	A	88	ASP	OD1-CG-OD2	8.16	138.80	123.30	16	1
1	A	99	ASN	CB-CG-ND2	7.93	135.73	116.70	16	1
1	A	87	ASP	OD1-CG-OD2	7.85	138.22	123.30	16	1
1	A	98	LYS	CA-CB-CG	7.81	130.59	113.40	16	1
1	A	40	PHE	CB-CG-CD2	7.77	126.24	120.80	16	1
1	A	51	HIS	ND1-CE1-NE2	7.75	126.94	109.90	16	1
1	A	83	TYR	CB-CG-CD1	7.73	125.64	121.00	16	1
1	A	71	GLU	CB-CG-CD	7.70	134.98	114.20	16	1
1	A	45	THR	C-N-CA	7.67	138.41	122.30	16	1
1	A	95	GLU	CB-CG-CD	7.67	134.90	114.20	16	1
1	A	38	ASP	OD1-CG-OD2	7.60	137.74	123.30	16	1
1	A	44	LYS	CD-CE-NZ	7.46	128.85	111.70	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	71	GLU	OE1-CD-OE2	-7.46	114.35	123.30	16	1
1	A	31	GLN	OE1-CD-NE2	-7.34	105.02	121.90	16	1
1	A	44	LYS	O-C-N	-7.31	111.01	122.70	16	1
1	A	99	ASN	CB-CG-OD1	7.24	136.08	121.60	16	1
1	A	57	MET	CB-CG-SD	-7.14	90.98	112.40	16	1
1	A	54	LYS	CA-CB-CG	7.03	128.86	113.40	16	1
1	A	55	VAL	CA-CB-CG1	7.02	121.43	110.90	16	1
1	A	100	ARG	CB-CG-CD	6.88	129.50	111.60	16	1
1	A	50	TYR	CG-CD2-CE2	-6.60	116.02	121.30	16	1
1	A	76	TYR	CE1-CZ-CE2	-6.58	109.27	119.80	16	1
1	A	63	ASP	CB-CG-OD2	6.55	124.19	118.30	16	1
1	A	57	MET	CA-CB-CG	6.46	124.28	113.30	16	1
1	A	63	ASP	O-C-N	-6.44	112.39	122.70	16	1
1	A	83	TYR	CA-CB-CG	6.39	125.55	113.40	16	1
1	A	29	GLN	CB-CG-CD	-6.36	95.08	111.60	16	1
1	A	50	TYR	CD1-CE1-CZ	-5.96	114.44	119.80	16	1
1	A	100	ARG	CA-C-O	5.91	132.51	120.10	16	1
1	A	44	LYS	CG-CD-CE	5.88	129.55	111.90	16	1
1	A	35	GLU	CG-CD-OE2	-5.78	106.73	118.30	16	1
1	A	83	TYR	CZ-CE2-CD2	5.77	124.99	119.80	16	1
1	A	100	ARG	O-C-N	-5.75	113.50	122.70	16	1
1	A	83	TYR	CG-CD1-CE1	5.70	125.86	121.30	16	1
1	A	40	PHE	CG-CD1-CE1	-5.63	114.61	120.80	16	1
1	A	77	ASP	OD1-CG-OD2	-5.60	112.67	123.30	16	1
1	A	39	LEU	CB-CG-CD1	5.53	120.39	111.00	16	1
1	A	40	PHE	CZ-CE2-CD2	-5.50	113.49	120.10	16	1
1	A	66	LYS	CA-CB-CG	5.48	125.46	113.40	16	1
1	A	51	HIS	CB-CG-ND1	5.46	136.85	123.20	16	1
1	A	53	LEU	CD1-CG-CD2	-5.46	94.13	110.50	16	1
1	A	31	GLN	CB-CG-CD	5.27	125.30	111.60	16	1
1	A	29	GLN	CA-CB-CG	5.19	124.81	113.40	16	1
1	A	54	LYS	CB-CG-CD	5.15	125.00	111.60	16	1
1	A	92	ILE	CB-CG1-CD1	5.14	128.28	113.90	16	1
1	A	40	PHE	CG-CD2-CE2	5.13	126.45	120.80	16	1
1	A	38	ASP	CA-CB-CG	5.09	124.61	113.40	16	1
1	A	65	LYS	CG-CD-CE	-5.05	96.74	111.90	16	1
1	A	48	ILE	CB-CG1-CD1	5.04	128.00	113.90	16	1
1	A	43	ASN	CA-C-N	5.03	128.26	117.20	16	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	86	PHE	Sidechain	2
1	A	83	TYR	Sidechain	1

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	581	567	558	33±33
All	All	9296	9072	9048	528

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 29.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:CA	1:A:44:LYS:CG	1.60	1.80	16	1
1:A:66:LYS:CD	1:A:66:LYS:CB	1.52	1.86	16	1
1:A:44:LYS:CB	1:A:44:LYS:CD	1.52	1.77	16	1
1:A:58:ARG:CZ	1:A:58:ARG:CD	1.51	1.79	16	1
1:A:51:HIS:CB	1:A:51:HIS:CD2	1.49	1.87	16	1
1:A:74:ASN:CB	1:A:74:ASN:ND2	1.43	1.79	16	1
1:A:58:ARG:NE	1:A:58:ARG:NH2	1.41	1.67	16	1
1:A:71:GLU:OE2	1:A:71:GLU:CG	1.35	1.73	16	1
1:A:34:LYS:CD	1:A:34:LYS:CB	1.33	2.04	16	1
1:A:58:ARG:NE	1:A:58:ARG:NH1	1.33	1.73	16	1
1:A:60:LEU:CD1	1:A:60:LEU:CB	1.33	2.03	16	1
1:A:44:LYS:O	1:A:44:LYS:HG2	1.30	1.11	16	1
1:A:54:LYS:CB	1:A:54:LYS:CD	1.30	2.07	16	1
1:A:31:GLN:CD	1:A:31:GLN:CB	1.27	2.03	16	1
1:A:58:ARG:CD	1:A:58:ARG:CB	1.26	2.11	16	1
1:A:54:LYS:CG	1:A:54:LYS:CE	1.25	2.13	16	1
1:A:58:ARG:NE	1:A:58:ARG:CG	1.24	2.00	16	1
1:A:71:GLU:OE1	1:A:71:GLU:OE2	1.22	1.55	16	1
1:A:44:LYS:C	1:A:44:LYS:HG2	1.21	1.52	16	1
1:A:27:GLU:CD	1:A:27:GLU:CB	1.20	2.10	16	1
1:A:54:LYS:CG	1:A:54:LYS:CA	1.18	2.21	16	1
1:A:77:ASP:CA	1:A:77:ASP:O	1.13	1.94	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ARG:CG	1:A:58:ARG:CA	1.11	2.27	16	1
1:A:44:LYS:C	1:A:44:LYS:CG	1.10	2.17	16	1
1:A:34:LYS:CG	1:A:34:LYS:CA	1.09	2.31	16	1
1:A:31:GLN:CD	1:A:31:GLN:HG2	1.08	1.52	16	1
1:A:43:ASN:CG	1:A:43:ASN:CA	1.06	2.22	16	1
1:A:31:GLN:CD	1:A:31:GLN:HG3	1.03	1.52	16	1
1:A:74:ASN:OD1	1:A:74:ASN:CG	1.03	0.83	16	1
1:A:31:GLN:CD	1:A:31:GLN:CG	1.03	0.93	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD23	1.01	1.54	16	1
1:A:43:ASN:CG	1:A:43:ASN:HB3	1.01	1.44	16	1
1:A:60:LEU:CD2	1:A:60:LEU:CB	1.00	2.28	16	1
1:A:60:LEU:HD22	1:A:60:LEU:CG	1.00	1.55	16	1
1:A:60:LEU:CD1	1:A:60:LEU:HG	0.99	1.61	16	1
1:A:71:GLU:CD	1:A:71:GLU:OE2	0.99	0.80	16	1
1:A:43:ASN:CG	1:A:43:ASN:CB	0.99	0.90	16	1
1:A:43:ASN:CG	1:A:43:ASN:HB2	0.97	1.44	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD21	0.96	1.54	16	1
1:A:54:LYS:HB2	1:A:54:LYS:CG	0.96	1.50	16	1
1:A:54:LYS:HB3	1:A:54:LYS:CG	0.96	1.50	16	1
1:A:54:LYS:CB	1:A:54:LYS:HG2	0.96	1.51	16	1
1:A:58:ARG:NE	1:A:58:ARG:HD3	0.96	1.34	16	1
1:A:54:LYS:CB	1:A:54:LYS:HG3	0.95	1.51	16	1
1:A:60:LEU:CD2	1:A:60:LEU:HG	0.95	1.67	16	1
1:A:44:LYS:HB2	1:A:44:LYS:CG	0.94	1.48	16	1
1:A:44:LYS:HB3	1:A:44:LYS:CG	0.94	1.48	16	1
1:A:58:ARG:NE	1:A:58:ARG:HD2	0.93	1.34	16	1
1:A:60:LEU:CG	1:A:60:LEU:CD2	0.92	0.92	16	1
1:A:54:LYS:CB	1:A:54:LYS:CG	0.92	0.92	16	1
1:A:58:ARG:NE	1:A:58:ARG:CD	0.91	0.76	16	1
1:A:66:LYS:CD	1:A:66:LYS:HG2	0.91	1.44	16	1
1:A:66:LYS:HG3	1:A:66:LYS:CD	0.89	1.44	16	1
1:A:34:LYS:HG2	1:A:34:LYS:CB	0.89	1.43	16	1
1:A:50:TYR:HA	1:A:53:LEU:HB2	0.89	1.43	11	2
1:A:27:GLU:CD	1:A:27:GLU:CG	0.88	0.80	16	1
1:A:34:LYS:HG3	1:A:34:LYS:CB	0.88	1.43	16	1
1:A:27:GLU:CD	1:A:27:GLU:HG2	0.88	1.34	16	1
1:A:44:LYS:CB	1:A:44:LYS:CG	0.88	0.88	16	1
1:A:58:ARG:CG	1:A:58:ARG:HB2	0.88	1.42	16	1
1:A:58:ARG:NH1	1:A:58:ARG:HH21	0.88	1.65	16	1
1:A:27:GLU:CD	1:A:27:GLU:HG3	0.88	1.34	16	1
1:A:66:LYS:CD	1:A:66:LYS:CG	0.87	0.88	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:CG	1:A:60:LEU:HD11	0.87	1.41	16	1
1:A:60:LEU:HD12	1:A:60:LEU:CG	0.87	1.41	16	1
1:A:58:ARG:CG	1:A:58:ARG:CB	0.87	0.87	16	1
1:A:44:LYS:CB	1:A:44:LYS:HG3	0.87	1.42	16	1
1:A:58:ARG:HG3	1:A:58:ARG:CB	0.86	1.41	16	1
1:A:64:VAL:HB	1:A:68:GLU:HB2	0.86	1.47	15	6
1:A:58:ARG:CG	1:A:58:ARG:HB3	0.86	1.42	16	1
1:A:51:HIS:HE2	1:A:51:HIS:CD2	0.86	1.63	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD13	0.86	1.41	16	1
1:A:58:ARG:NH2	1:A:58:ARG:HH11	0.85	1.65	16	1
1:A:34:LYS:CG	1:A:34:LYS:CB	0.85	0.86	16	1
1:A:58:ARG:CB	1:A:58:ARG:HG2	0.85	1.41	16	1
1:A:51:HIS:HE1	1:A:51:HIS:CD2	0.83	1.74	16	1
1:A:58:ARG:CZ	1:A:58:ARG:NH1	0.83	0.70	16	1
1:A:34:LYS:HB2	1:A:34:LYS:CG	0.83	1.36	16	1
1:A:51:HIS:CD2	1:A:51:HIS:CE1	0.82	0.83	16	1
1:A:34:LYS:CG	1:A:34:LYS:HB3	0.82	1.36	16	1
1:A:96:LYS:HE2	1:A:97:ILE:HG23	0.81	1.51	15	1
1:A:48:ILE:HG22	1:A:84:ILE:HG12	0.81	1.51	11	1
1:A:58:ARG:CD	1:A:58:ARG:NH1	0.80	2.32	16	1
1:A:58:ARG:NH2	1:A:58:ARG:CZ	0.79	0.65	16	1
1:A:58:ARG:NH2	1:A:58:ARG:NH1	0.79	0.79	16	1
1:A:31:GLN:CD	1:A:31:GLN:HE22	0.78	1.38	16	1
1:A:74:ASN:OD1	1:A:74:ASN:ND2	0.77	0.65	16	1
1:A:54:LYS:HE2	1:A:54:LYS:CD	0.77	1.32	16	1
1:A:54:LYS:HE3	1:A:54:LYS:CD	0.76	1.32	16	1
1:A:44:LYS:CB	1:A:44:LYS:HD3	0.76	2.05	16	1
1:A:43:ASN:CG	1:A:43:ASN:HD22	0.76	1.36	16	1
1:A:54:LYS:HE2	1:A:54:LYS:NZ	0.76	1.28	16	1
1:A:31:GLN:CD	1:A:31:GLN:HE21	0.76	1.38	16	1
1:A:66:LYS:HE2	1:A:66:LYS:NZ	0.75	1.22	16	1
1:A:54:LYS:CE	1:A:54:LYS:HD2	0.75	1.29	16	1
1:A:54:LYS:HD3	1:A:54:LYS:CE	0.75	1.29	16	1
1:A:60:LEU:CG	1:A:60:LEU:CD1	0.74	0.74	16	1
1:A:54:LYS:CB	1:A:54:LYS:HD3	0.73	2.12	16	1
1:A:96:LYS:O	1:A:100:ARG:HA	0.73	1.83	12	5
1:A:77:ASP:HA	1:A:84:ILE:HG22	0.73	1.59	3	1
1:A:43:ASN:CG	1:A:43:ASN:HD21	0.73	1.36	16	1
1:A:66:LYS:CD	1:A:66:LYS:HE3	0.72	1.39	16	1
1:A:51:HIS:CG	1:A:51:HIS:CD2	0.72	0.83	16	1
1:A:91:ASP:HA	1:A:94:THR:OG1	0.72	1.85	13	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LYS:HG2	1:A:69:ILE:HD13	0.71	1.60	3	2
1:A:71:GLU:OE2	1:A:71:GLU:HG2	0.71	1.80	16	1
1:A:66:LYS:HD2	1:A:66:LYS:CE	0.71	1.34	16	1
1:A:54:LYS:HE3	1:A:54:LYS:NZ	0.71	1.28	16	1
1:A:66:LYS:HE2	1:A:66:LYS:CD	0.70	1.39	16	1
1:A:54:LYS:CE	1:A:54:LYS:CD	0.70	0.76	16	1
1:A:66:LYS:CD	1:A:66:LYS:HB3	0.69	2.11	16	1
1:A:66:LYS:NZ	1:A:66:LYS:HE3	0.69	1.22	16	1
1:A:64:VAL:O	1:A:68:GLU:HB3	0.69	1.88	5	2
1:A:66:LYS:HD3	1:A:66:LYS:CE	0.69	1.34	16	1
1:A:57:MET:HE3	1:A:64:VAL:HG21	0.68	1.66	13	1
1:A:31:GLN:CD	1:A:31:GLN:NE2	0.67	0.73	16	1
1:A:27:GLU:HA	1:A:30:LYS:HG3	0.66	1.68	11	2
1:A:51:HIS:HD2	1:A:51:HIS:CG	0.66	1.42	16	1
1:A:43:ASN:CG	1:A:43:ASN:ND2	0.65	0.71	16	1
1:A:51:HIS:CD2	1:A:51:HIS:NE2	0.65	0.85	16	1
1:A:92:ILE:HA	1:A:95:GLU:HB2	0.65	1.68	10	15
1:A:97:ILE:HD12	1:A:98:LYS:N	0.65	2.06	8	15
1:A:58:ARG:CZ	1:A:58:ARG:HH12	0.65	1.35	16	1
1:A:96:LYS:HE3	1:A:97:ILE:HG23	0.65	1.67	16	7
1:A:44:LYS:O	1:A:44:LYS:CG	0.64	2.03	16	1
1:A:58:ARG:CZ	1:A:58:ARG:HH11	0.63	1.35	16	1
1:A:54:LYS:HE2	1:A:54:LYS:HD3	0.63	1.10	16	1
1:A:66:LYS:CG	1:A:66:LYS:HD2	0.62	1.35	16	1
1:A:34:LYS:HB2	1:A:34:LYS:HG2	0.62	1.18	16	1
1:A:27:GLU:HA	1:A:30:LYS:CG	0.61	2.25	5	2
1:A:64:VAL:C	1:A:65:LYS:HE3	0.61	2.15	5	2
1:A:65:LYS:O	1:A:69:ILE:HB	0.60	1.96	11	10
1:A:73:MET:HA	1:A:76:TYR:CE2	0.60	2.31	1	1
1:A:27:GLU:HA	1:A:30:LYS:CD	0.60	2.26	12	1
1:A:58:ARG:CZ	1:A:58:ARG:HH21	0.60	1.32	16	1
1:A:34:LYS:HD3	1:A:86:PHE:CZ	0.60	2.31	15	4
1:A:66:LYS:HG2	1:A:66:LYS:HD2	0.60	1.25	16	1
1:A:66:LYS:HD3	1:A:66:LYS:CG	0.60	1.35	16	1
1:A:34:LYS:HG3	1:A:34:LYS:HB3	0.59	1.17	16	1
1:A:58:ARG:CZ	1:A:58:ARG:HH22	0.59	1.32	16	1
1:A:54:LYS:HZ2	1:A:54:LYS:CE	0.59	1.31	16	1
1:A:54:LYS:HZ3	1:A:54:LYS:CE	0.59	1.30	16	1
1:A:54:LYS:HZ1	1:A:54:LYS:CE	0.59	1.30	16	1
1:A:49:ASP:HB2	1:A:83:TYR:CE2	0.59	2.33	3	4
1:A:56:ALA:O	1:A:60:LEU:HG	0.58	1.98	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:C	1:A:70:LEU:HD22	0.58	2.19	15	11
1:A:58:ARG:CD	1:A:58:ARG:HE	0.58	1.30	16	1
1:A:27:GLU:HA	1:A:30:LYS:HD2	0.58	1.76	1	1
1:A:49:ASP:OD2	1:A:51:HIS:HB3	0.58	1.98	15	1
1:A:53:LEU:HD22	1:A:73:MET:HG2	0.58	1.75	9	1
1:A:44:LYS:CE	1:A:44:LYS:CB	0.57	2.54	16	1
1:A:51:HIS:HD2	1:A:51:HIS:NE2	0.57	1.43	16	1
1:A:51:HIS:ND1	1:A:51:HIS:CD2	0.57	0.77	16	1
1:A:74:ASN:CA	1:A:74:ASN:ND2	0.57	2.65	16	1
1:A:30:LYS:HE3	1:A:86:PHE:HE2	0.57	1.59	5	1
1:A:66:LYS:O	1:A:70:LEU:HD12	0.57	1.99	4	3
1:A:96:LYS:C	1:A:96:LYS:HD2	0.57	2.19	12	6
1:A:70:LEU:HD13	1:A:71:GLU:N	0.57	2.14	15	11
1:A:96:LYS:HD2	1:A:96:LYS:C	0.57	2.20	14	5
1:A:65:LYS:HE2	1:A:65:LYS:N	0.56	2.15	7	1
1:A:58:ARG:NH1	1:A:58:ARG:HH22	0.56	0.87	16	1
1:A:71:GLU:HA	1:A:74:ASN:HB3	0.56	1.77	4	2
1:A:30:LYS:HB3	1:A:34:LYS:HE2	0.56	1.75	5	2
1:A:77:ASP:O	1:A:77:ASP:C	0.56	0.62	16	1
1:A:44:LYS:HE3	1:A:44:LYS:HA	0.56	1.78	13	1
1:A:73:MET:O	1:A:77:ASP:HB3	0.56	2.01	16	5
1:A:64:VAL:O	1:A:68:GLU:HB2	0.55	2.00	14	3
1:A:70:LEU:HD22	1:A:70:LEU:C	0.55	2.22	9	5
1:A:33:ILE:HA	1:A:93:MET:SD	0.55	2.41	6	4
1:A:54:LYS:CE	1:A:54:LYS:NZ	0.55	0.70	16	1
1:A:33:ILE:HG21	1:A:90:LEU:HD22	0.55	1.78	12	1
1:A:97:ILE:HA	1:A:100:ARG:HB2	0.55	1.78	2	1
1:A:65:LYS:O	1:A:69:ILE:HG22	0.55	2.02	4	1
1:A:91:ASP:O	1:A:95:GLU:HB2	0.54	2.02	15	11
1:A:27:GLU:CD	1:A:27:GLU:OE2	0.54	0.75	16	1
1:A:43:ASN:CG	1:A:43:ASN:OD1	0.54	0.75	16	1
1:A:63:ASP:O	1:A:65:LYS:HG2	0.53	2.02	4	1
1:A:30:LYS:O	1:A:34:LYS:HG2	0.53	2.03	11	2
1:A:96:LYS:CE	1:A:97:ILE:HG23	0.53	2.30	15	2
1:A:66:LYS:N	1:A:67:PRO:HD2	0.53	2.18	11	5
1:A:66:LYS:HZ1	1:A:66:LYS:CE	0.53	1.23	16	1
1:A:52:GLU:O	1:A:55:VAL:HG22	0.53	2.04	11	6
1:A:48:ILE:HG22	1:A:84:ILE:CG1	0.53	2.32	11	1
1:A:66:LYS:O	1:A:69:ILE:HG22	0.52	2.04	7	4
1:A:53:LEU:O	1:A:57:MET:HG3	0.52	2.05	7	3
1:A:66:LYS:HZ3	1:A:66:LYS:CE	0.52	1.23	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLU:O	1:A:39:LEU:HB2	0.52	2.05	3	1
1:A:48:ILE:O	1:A:83:TYR:HB2	0.52	2.04	11	2
1:A:39:LEU:HD13	1:A:40:PHE:N	0.52	2.19	9	1
1:A:49:ASP:HB3	1:A:52:GLU:OE2	0.52	2.03	11	2
1:A:29:GLN:O	1:A:33:ILE:HG13	0.52	2.05	9	4
1:A:53:LEU:HD22	1:A:73:MET:HB3	0.52	1.81	1	1
1:A:48:ILE:CG2	1:A:84:ILE:HG13	0.52	2.35	1	1
1:A:31:GLN:O	1:A:35:GLU:HB2	0.52	2.05	7	2
1:A:27:GLU:O	1:A:31:GLN:HG2	0.52	2.05	1	4
1:A:70:LEU:HD13	1:A:71:GLU:H	0.52	1.65	2	12
1:A:66:LYS:HZ2	1:A:66:LYS:CE	0.52	1.23	16	1
1:A:30:LYS:O	1:A:34:LYS:HB3	0.52	2.05	5	2
1:A:54:LYS:O	1:A:58:ARG:HG3	0.51	2.05	3	1
1:A:57:MET:SD	1:A:69:ILE:HG13	0.51	2.45	4	1
1:A:44:LYS:O	1:A:44:LYS:HD3	0.51	2.06	4	1
1:A:66:LYS:HD3	1:A:66:LYS:HG3	0.51	1.23	16	1
1:A:27:GLU:CD	1:A:27:GLU:OE1	0.51	0.72	16	1
1:A:58:ARG:NH2	1:A:58:ARG:HH12	0.51	0.93	16	1
1:A:40:PHE:HB2	1:A:55:VAL:CG2	0.51	2.36	9	1
1:A:95:GLU:HA	1:A:98:LYS:CE	0.51	2.36	2	6
1:A:48:ILE:HG23	1:A:52:GLU:HB2	0.51	1.82	7	2
1:A:33:ILE:HG23	1:A:93:MET:SD	0.51	2.45	11	2
1:A:74:ASN:HD22	1:A:74:ASN:CG	0.51	1.12	16	1
1:A:98:LYS:HD2	1:A:99:ASN:N	0.51	2.21	14	3
1:A:53:LEU:O	1:A:57:MET:HG2	0.50	2.05	9	4
1:A:53:LEU:HD13	1:A:56:ALA:HB3	0.50	1.82	11	1
1:A:65:LYS:HA	1:A:65:LYS:HE2	0.50	1.81	10	1
1:A:68:GLU:O	1:A:72:LEU:HB2	0.50	2.06	1	3
1:A:96:LYS:HD2	1:A:97:ILE:N	0.50	2.22	2	5
1:A:30:LYS:O	1:A:34:LYS:HE3	0.50	2.06	10	4
1:A:34:LYS:HA	1:A:37:PHE:CB	0.50	2.36	11	2
1:A:94:THR:O	1:A:98:LYS:HE2	0.50	2.07	14	4
1:A:41:ASP:OD2	1:A:44:LYS:HA	0.49	2.07	13	1
1:A:50:TYR:HB3	1:A:73:MET:SD	0.49	2.46	10	1
1:A:50:TYR:HD2	1:A:69:ILE:HG13	0.49	1.66	11	1
1:A:95:GLU:O	1:A:98:LYS:HE2	0.49	2.07	15	1
1:A:27:GLU:O	1:A:31:GLN:HG3	0.49	2.08	5	3
1:A:95:GLU:HA	1:A:98:LYS:HE2	0.49	1.83	7	2
1:A:70:LEU:HD22	1:A:71:GLU:N	0.49	2.23	7	7
1:A:48:ILE:HG23	1:A:52:GLU:HG3	0.49	1.83	4	1
1:A:54:LYS:HA	1:A:57:MET:SD	0.49	2.48	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PHE:HE1	1:A:96:LYS:HB3	0.48	1.68	7	1
1:A:71:GLU:OE1	1:A:74:ASN:HB3	0.48	2.08	6	1
1:A:40:PHE:CE2	1:A:56:ALA:HA	0.48	2.43	3	1
1:A:97:ILE:HD12	1:A:98:LYS:H	0.48	1.68	14	2
1:A:96:LYS:O	1:A:100:ARG:HB3	0.48	2.09	14	1
1:A:93:MET:O	1:A:96:LYS:HE2	0.48	2.09	14	5
1:A:62:PHE:HZ	1:A:96:LYS:HG2	0.48	1.68	9	1
1:A:53:LEU:HD21	1:A:72:LEU:HD22	0.47	1.84	9	1
1:A:50:TYR:HE2	1:A:72:LEU:HD22	0.47	1.69	11	1
1:A:66:LYS:HD2	1:A:66:LYS:HE3	0.47	1.24	16	1
1:A:40:PHE:CE1	1:A:56:ALA:HA	0.47	2.44	8	2
1:A:73:MET:HE2	1:A:77:ASP:HB3	0.47	1.86	4	1
1:A:54:LYS:HA	1:A:69:ILE:HD11	0.47	1.85	1	1
1:A:43:ASN:O	1:A:44:LYS:HB2	0.47	2.10	14	3
1:A:39:LEU:HD13	1:A:39:LEU:C	0.47	2.29	13	2
1:A:27:GLU:HA	1:A:30:LYS:HD3	0.47	1.85	12	2
1:A:34:LYS:HD3	1:A:86:PHE:CE1	0.47	2.45	15	4
1:A:84:ILE:HB	1:A:88:ASP:HB2	0.47	1.85	13	1
1:A:54:LYS:O	1:A:58:ARG:HB2	0.47	2.10	15	1
1:A:28:GLU:HG3	1:A:29:GLN:N	0.46	2.24	6	3
1:A:49:ASP:HB3	1:A:83:TYR:CD2	0.46	2.45	6	1
1:A:57:MET:HG3	1:A:69:ILE:HD11	0.46	1.88	11	1
1:A:89:PHE:O	1:A:92:ILE:HB	0.46	2.11	11	3
1:A:94:THR:O	1:A:98:LYS:HB3	0.45	2.11	4	3
1:A:34:LYS:HA	1:A:37:PHE:HB3	0.45	1.89	4	1
1:A:50:TYR:HD2	1:A:82:GLY:HA2	0.45	1.71	1	1
1:A:94:THR:O	1:A:98:LYS:HG3	0.45	2.11	7	2
1:A:66:LYS:NZ	1:A:66:LYS:CE	0.45	0.60	16	1
1:A:34:LYS:HA	1:A:86:PHE:CE1	0.45	2.47	13	1
1:A:64:VAL:HB	1:A:68:GLU:HB3	0.45	1.87	2	1
1:A:44:LYS:CB	1:A:44:LYS:HG2	0.45	1.42	16	1
1:A:44:LYS:HE2	1:A:44:LYS:O	0.44	2.12	15	1
1:A:54:LYS:CG	1:A:69:ILE:HD13	0.44	2.37	3	1
1:A:89:PHE:HA	1:A:92:ILE:HD12	0.44	1.90	5	2
1:A:88:ASP:O	1:A:92:ILE:HG13	0.44	2.13	2	1
1:A:96:LYS:HE3	1:A:96:LYS:C	0.43	2.33	15	1
1:A:66:LYS:HB2	1:A:67:PRO:HD3	0.43	1.89	2	1
1:A:33:ILE:HG21	1:A:90:LEU:HG	0.43	1.89	7	1
1:A:30:LYS:O	1:A:34:LYS:N	0.43	2.50	5	1
1:A:53:LEU:HD12	1:A:69:ILE:HG12	0.43	1.89	14	1
1:A:53:LEU:HG	1:A:73:MET:HB3	0.43	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLU:O	1:A:31:GLN:HG2	0.43	2.14	8	1
1:A:44:LYS:HD3	1:A:47:SER:HB2	0.43	1.90	15	1
1:A:29:GLN:HE21	1:A:30:LYS:HG3	0.43	1.74	2	1
1:A:43:ASN:O	1:A:44:LYS:HB3	0.43	2.14	6	1
1:A:30:LYS:HE3	1:A:86:PHE:CE2	0.42	2.46	5	1
1:A:97:ILE:HA	1:A:100:ARG:HB3	0.42	1.90	5	1
1:A:66:LYS:CD	1:A:66:LYS:CE	0.42	0.86	16	1
1:A:44:LYS:HB3	1:A:47:SER:O	0.42	2.14	15	1
1:A:74:ASN:ND2	1:A:74:ASN:CG	0.42	0.40	16	1
1:A:37:PHE:CZ	1:A:86:PHE:HB2	0.42	2.50	7	1
1:A:97:ILE:HD12	1:A:98:LYS:HG3	0.42	1.90	14	1
1:A:53:LEU:HD22	1:A:56:ALA:HB3	0.42	1.91	14	1
1:A:62:PHE:CZ	1:A:96:LYS:HG2	0.42	2.48	9	1
1:A:64:VAL:HG23	1:A:69:ILE:HB	0.42	1.90	5	1
1:A:98:LYS:C	1:A:98:LYS:HD2	0.42	2.35	15	1
1:A:92:ILE:HA	1:A:95:GLU:CB	0.42	2.45	2	3
1:A:30:LYS:HB3	1:A:34:LYS:CE	0.41	2.45	7	1
1:A:53:LEU:HD22	1:A:57:MET:HG2	0.41	1.90	13	1
1:A:76:TYR:N	1:A:76:TYR:CD1	0.41	2.89	5	1
1:A:50:TYR:HE1	1:A:84:ILE:HD13	0.41	1.75	11	1
1:A:34:LYS:HG2	1:A:86:PHE:CE1	0.41	2.50	3	1
1:A:71:GLU:HA	1:A:74:ASN:HB2	0.41	1.90	15	1
1:A:98:LYS:HE2	1:A:98:LYS:HB3	0.41	1.80	2	1
1:A:73:MET:HE3	1:A:77:ASP:HB2	0.41	1.92	9	1
1:A:30:LYS:O	1:A:34:LYS:HB2	0.41	2.16	15	1
1:A:54:LYS:HZ1	1:A:54:LYS:HE2	0.41	1.20	16	1
1:A:34:LYS:HB3	1:A:86:PHE:CZ	0.41	2.51	11	1
1:A:54:LYS:O	1:A:58:ARG:HG2	0.41	2.15	10	1
1:A:96:LYS:HE3	1:A:97:ILE:N	0.41	2.30	9	1
1:A:66:LYS:HB3	1:A:67:PRO:HD3	0.41	1.93	3	1
1:A:27:GLU:HA	1:A:30:LYS:HB2	0.40	1.94	14	1
1:A:69:ILE:O	1:A:72:LEU:HB3	0.40	2.16	15	1
1:A:48:ILE:HG23	1:A:52:GLU:CB	0.40	2.47	9	1

6.3 Torsion angles

6.3.1 Protein backbone

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 NMR 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	70/77 (91%)	63±2 (89±3%)	6±2 (9±3%)	1±1 (2±1%)	14 56
All	All	1120/1232 (91%)	1001 (89%)	98 (9%)	21 (2%)	14 56

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	44	LYS	7
1	A	45	THR	4
1	A	82	GLY	3
1	A	64	VAL	2
1	A	77	ASP	2
1	A	41	ASP	1
1	A	61	GLY	1
1	A	100	ARG	1

6.3.2 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 NMR 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	63/69 (91%)	55±2 (88±4%)	8±2 (12±4%)	10 53
All	All	1008/1104 (91%)	886 (88%)	122 (12%)	10 53

All 27 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	70	LEU	16
1	A	96	LYS	16
1	A	98	LYS	13
1	A	90	LEU	12
1	A	84	ILE	9
1	A	71	GLU	6
1	A	91	ASP	5
1	A	77	ASP	4
1	A	34	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	49	ASP	4
1	A	65	LYS	3
1	A	44	LYS	3
1	A	52	GLU	3
1	A	53	LEU	3
1	A	29	GLN	2
1	A	47	SER	2
1	A	66	LYS	2
1	A	35	GLU	2
1	A	93	MET	2
1	A	99	ASN	2
1	A	95	GLU	2
1	A	74	ASN	2
1	A	51	HIS	1
1	A	57	MET	1
1	A	54	LYS	1
1	A	39	LEU	1
1	A	72	LEU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided