



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:01 AM UTC

PDB ID : 2JOJ / pdb_00002joj
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

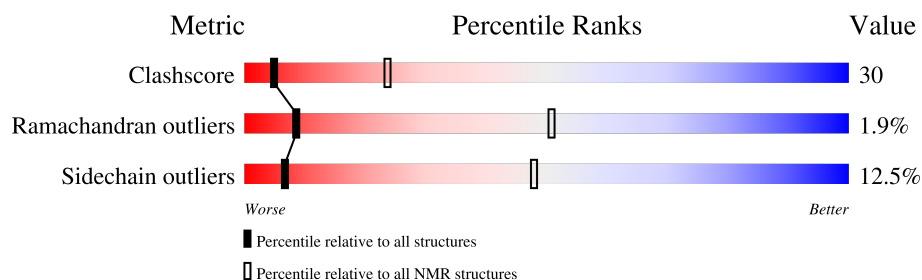
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	77	45% 40% 5% 9%

2 Ensemble composition and analysis

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)	0.76	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.

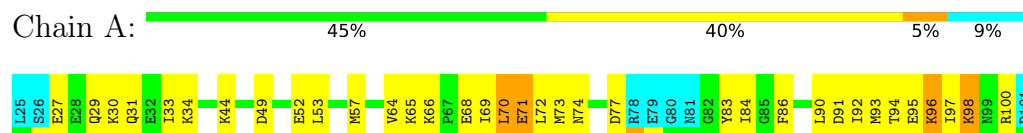
Mol	Chain	Residues	Atoms						Trace
1	A	77	Total	C	H	N	O	S	0
			1253	401	617	102	130	3	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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

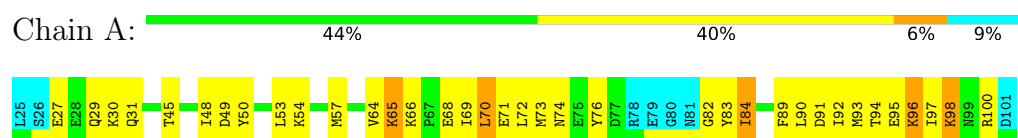


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

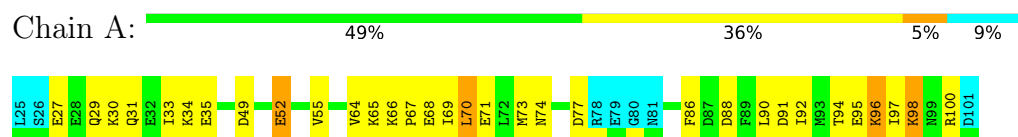
4.2.1 Score per residue for model 1

- Molecule 1: Centrin protein



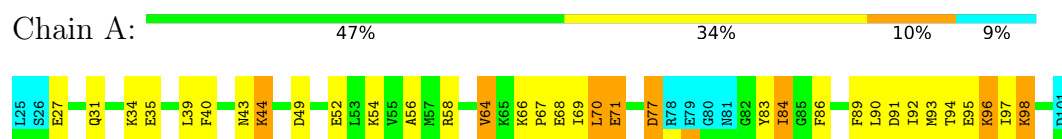
4.2.2 Score per residue for model 2

- Molecule 1: Centrin protein



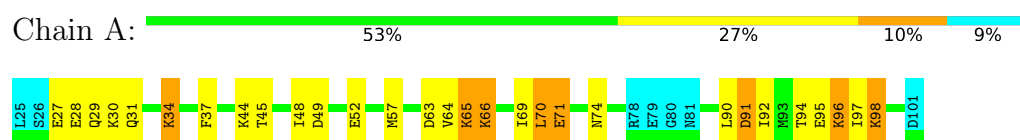
4.2.3 Score per residue for model 3

- Molecule 1: Centrin protein



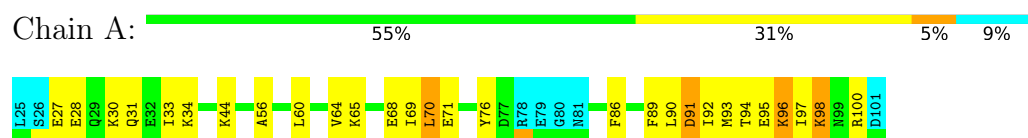
4.2.4 Score per residue for model 4

- Molecule 1: Centrin protein



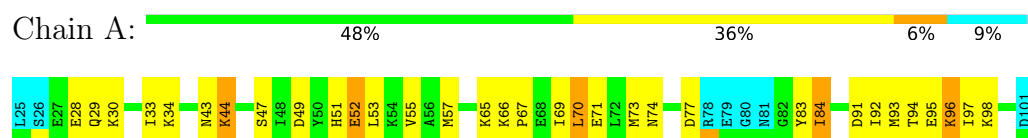
4.2.5 Score per residue for model 5

- Molecule 1: Centrin protein



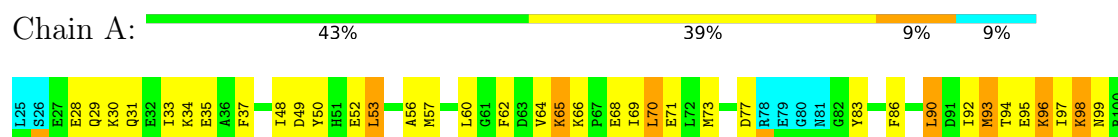
4.2.6 Score per residue for model 6

- Molecule 1: Centrin protein



4.2.7 Score per residue for model 7

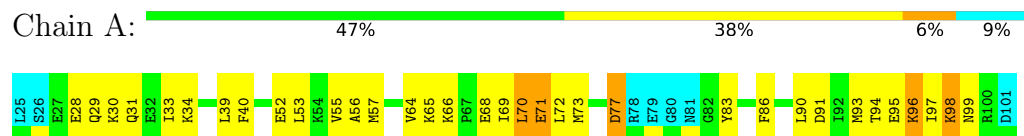
- Molecule 1: Centrin protein



D101

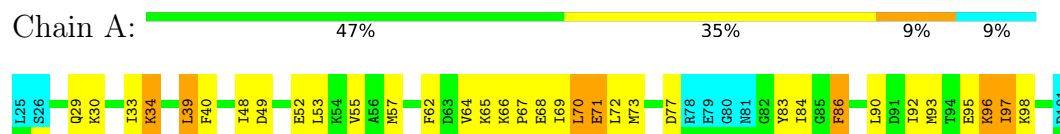
4.2.8 Score per residue for model 8

- Molecule 1: Centrin protein



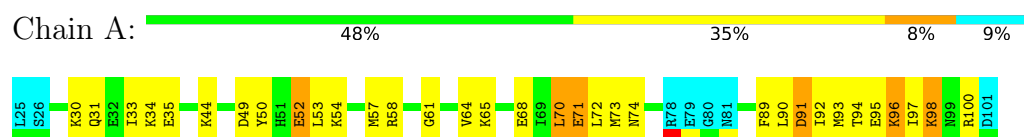
4.2.9 Score per residue for model 9

- Molecule 1: Centrin protein



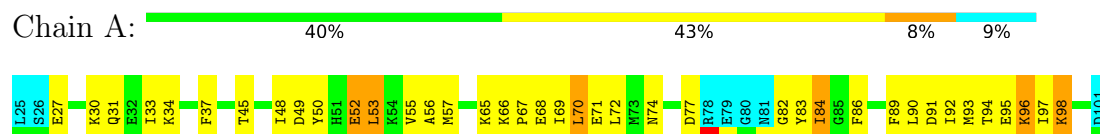
4.2.10 Score per residue for model 10

- Molecule 1: Centrin protein



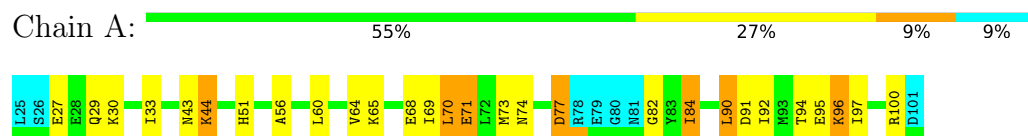
4.2.11 Score per residue for model 11

- Molecule 1: Centrin protein



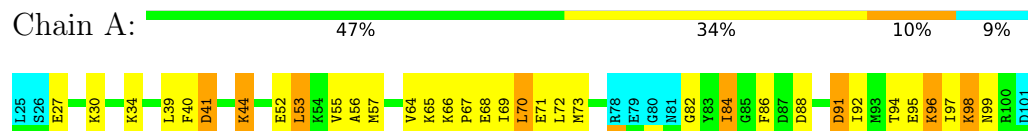
4.2.12 Score per residue for model 12

- Molecule 1: Centrin protein



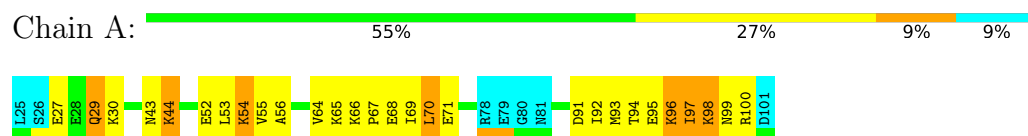
4.2.13 Score per residue for model 13

- Molecule 1: Centrin protein



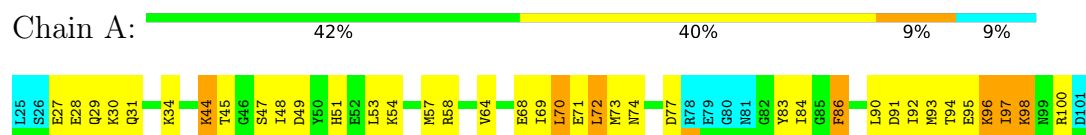
4.2.14 Score per residue for model 14

- Molecule 1: Centrin protein



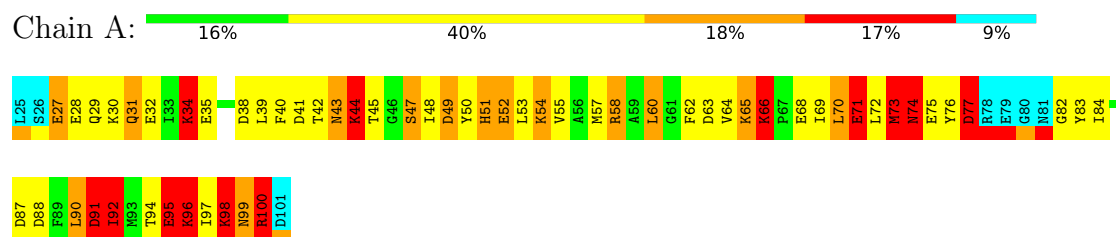
4.2.15 Score per residue for model 15

- Molecule 1: Centrin protein



4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Centrin protein



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.

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	1.26±3.01	12±46/591 (2.0± 7.7%)	1.19±1.55	9±34/791 (1.1± 4.3%)
All	All	3.26	188/9456 (2.0%)	1.95	139/12656 (1.1%)

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	51	HIS	CE1-NE2	-84.27	0.48	1.32	16	1
1	A	51	HIS	CG-ND1	-76.70	0.53	1.38	16	1
1	A	58	ARG	CZ-NH2	-51.95	0.66	1.33	16	1
1	A	58	ARG	CD-NE	-49.53	0.77	1.46	16	1
1	A	100	ARG	CZ-NH2	-49.14	0.69	1.33	16	1
1	A	77	ASP	C-N	-48.87	0.73	1.33	16	1
1	A	77	ASP	C-O	-48.10	0.62	1.23	16	1
1	A	100	ARG	CD-NE	-48.08	0.79	1.46	16	1
1	A	51	HIS	CD2-NE2	-47.25	0.85	1.37	16	1
1	A	51	HIS	CG-CD2	-47.22	0.83	1.35	16	1
1	A	58	ARG	CZ-NH1	-44.65	0.70	1.32	16	1
1	A	74	ASN	CG-ND2	-43.99	0.40	1.33	16	1
1	A	29	GLN	CD-OE1	-43.83	0.40	1.23	16	1
1	A	29	GLN	CD-NE2	-38.78	0.51	1.33	16	1
1	A	100	ARG	CZ-NH1	-37.99	0.79	1.32	16	1
1	A	31	GLN	CD-OE1	-37.96	0.51	1.23	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	32	GLU	CD-OE2	-37.87	0.53	1.25	16	1
1	A	45	THR	C-O	-36.97	0.76	1.24	16	1
1	A	95	GLU	CD-OE2	-35.73	0.57	1.25	16	1
1	A	51	HIS	ND1-CE1	-35.09	0.97	1.32	16	1
1	A	75	GLU	CD-OE2	-34.48	0.59	1.25	16	1
1	A	45	THR	C-N	-32.43	0.97	1.33	16	1
1	A	68	GLU	CD-OE2	-32.41	0.63	1.25	16	1
1	A	100	ARG	NE-CZ	-31.03	0.98	1.33	16	1
1	A	51	HIS	CB-CG	-30.51	1.07	1.50	16	1
1	A	87	ASP	CB-CG	-29.82	0.77	1.52	16	1
1	A	66	LYS	CE-NZ	-29.59	0.60	1.49	16	1
1	A	43	ASN	CG-ND2	-29.45	0.71	1.33	16	1
1	A	27	GLU	CG-CD	-28.70	0.80	1.52	16	1
1	A	88	ASP	CG-OD2	-28.59	0.71	1.25	16	1
1	A	31	GLN	CD-NE2	-28.37	0.73	1.33	16	1
1	A	27	GLU	CD-OE1	-27.99	0.72	1.25	16	1
1	A	43	ASN	C-O	-27.81	0.86	1.23	16	1
1	A	44	LYS	C-O	-27.07	0.89	1.24	16	1
1	A	91	ASP	CG-OD2	-26.89	0.74	1.25	16	1
1	A	27	GLU	CD-OE2	-26.48	0.75	1.25	16	1
1	A	54	LYS	CE-NZ	-26.22	0.70	1.49	16	1
1	A	57	MET	CG-SD	-26.22	1.15	1.80	16	1
1	A	54	LYS	CD-CE	-25.40	0.76	1.52	16	1
1	A	43	ASN	CG-OD1	-25.37	0.75	1.23	16	1
1	A	29	GLN	CG-CD	-25.12	0.89	1.52	16	1
1	A	91	ASP	CG-OD1	-25.01	0.77	1.25	16	1
1	A	43	ASN	CB-CG	-24.57	0.90	1.52	16	1
1	A	41	ASP	C-O	-24.45	0.97	1.23	16	1
1	A	100	ARG	C-N	-24.34	0.99	1.33	16	1
1	A	38	ASP	CG-OD2	-24.09	0.79	1.25	16	1
1	A	71	GLU	CD-OE2	-23.81	0.80	1.25	16	1
1	A	35	GLU	CD-OE2	-23.69	0.80	1.25	16	1
1	A	43	ASN	C-N	-23.60	1.00	1.33	16	1
1	A	60	LEU	CG-CD1	-23.53	0.74	1.52	16	1
1	A	87	ASP	CG-OD2	-23.46	0.80	1.25	16	1
1	A	95	GLU	CG-CD	-23.41	0.93	1.52	16	1
1	A	31	GLN	CG-CD	-23.40	0.93	1.52	16	1
1	A	91	ASP	CB-CG	-22.92	0.94	1.52	16	1
1	A	99	ASN	CG-OD1	-22.83	0.80	1.23	16	1
1	A	44	LYS	CA-CB	-22.65	1.15	1.53	16	1
1	A	47	SER	CB-OG	-22.16	0.97	1.42	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	66	LYS	CD-CE	-22.12	0.86	1.52	16	1
1	A	34	LYS	CB-CG	-22.03	0.86	1.52	16	1
1	A	58	ARG	CB-CG	-21.64	0.87	1.52	16	1
1	A	32	GLU	CG-CD	-21.52	0.98	1.52	16	1
1	A	99	ASN	CG-ND2	-21.52	0.88	1.33	16	1
1	A	75	GLU	CD-OE1	-21.42	0.84	1.25	16	1
1	A	66	LYS	CG-CD	-21.36	0.88	1.52	16	1
1	A	44	LYS	CB-CG	-21.17	0.89	1.52	16	1
1	A	74	ASN	CG-OD1	-21.14	0.83	1.23	16	1
1	A	65	LYS	CG-CD	-20.54	0.90	1.52	16	1
1	A	44	LYS	CE-NZ	-20.50	0.87	1.49	16	1
1	A	58	ARG	NE-CZ	-20.36	1.10	1.33	16	1
1	A	65	LYS	CE-NZ	-20.03	0.89	1.49	16	1
1	A	54	LYS	CB-CG	-19.91	0.92	1.52	16	1
1	A	73	MET	CB-CG	-19.68	0.93	1.52	16	1
1	A	77	ASP	CG-OD2	-19.29	0.88	1.25	16	1
1	A	44	LYS	C-N	-19.24	1.02	1.33	16	1
1	A	68	GLU	CG-CD	-19.11	1.04	1.52	16	1
1	A	35	GLU	CG-CD	-19.02	1.04	1.52	16	1
1	A	73	MET	CG-SD	-18.97	1.33	1.80	16	1
1	A	88	ASP	CB-CG	-18.80	1.05	1.52	16	1
1	A	44	LYS	CG-CD	-18.77	0.96	1.52	16	1
1	A	63	ASP	CB-CG	-18.76	1.05	1.52	16	1
1	A	87	ASP	CG-OD1	-18.67	0.89	1.25	16	1
1	A	63	ASP	C-N	-18.60	1.12	1.33	16	1
1	A	63	ASP	C-O	-18.58	0.98	1.23	16	1
1	A	38	ASP	CB-CG	-18.52	1.05	1.52	16	1
1	A	60	LEU	CG-CD2	-18.17	0.92	1.52	16	1
1	A	49	ASP	CG-OD2	-17.86	0.91	1.25	16	1
1	A	100	ARG	CB-CG	-17.64	0.99	1.52	16	1
1	A	76	TYR	CG-CD2	-17.38	1.02	1.39	16	1
1	A	63	ASP	CG-OD1	-17.17	0.92	1.25	16	1
1	A	41	ASP	CG-OD1	-16.81	0.93	1.25	16	1
1	A	75	GLU	CG-CD	-16.81	1.10	1.52	16	1
1	A	95	GLU	CD-OE1	-16.80	0.93	1.25	16	1
1	A	90	LEU	CG-CD1	-16.75	0.97	1.52	16	1
1	A	82	GLY	N-CA	-16.71	1.21	1.45	16	1
1	A	53	LEU	CG-CD2	-16.58	0.97	1.52	16	1
1	A	41	ASP	C-N	-16.53	1.09	1.33	16	1
1	A	41	ASP	CG-OD2	-16.09	0.94	1.25	16	1
1	A	44	LYS	CD-CE	-15.89	1.04	1.52	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	76	TYR	CE1-CZ	-15.25	1.01	1.38	16	1
1	A	77	ASP	CG-OD1	-15.18	0.96	1.25	16	1
1	A	29	GLN	CB-CG	-14.86	1.07	1.52	16	1
1	A	90	LEU	CG-CD2	-14.83	1.03	1.52	16	1
1	A	35	GLU	CD-OE1	-14.82	0.97	1.25	16	1
1	A	52	GLU	CB-CG	-14.15	1.09	1.52	16	1
1	A	55	VAL	CB-CG1	-13.93	1.06	1.52	16	1
1	A	75	GLU	CB-CG	-13.74	1.11	1.52	16	1
1	A	92	ILE	CG1-CD1	-13.47	0.99	1.51	16	1
1	A	66	LYS	CB-CG	-13.47	1.12	1.52	16	1
1	A	55	VAL	CB-CG2	-13.22	1.08	1.52	16	1
1	A	100	ARG	C-O	-13.07	1.07	1.24	16	1
1	A	99	ASN	C-O	-13.03	1.06	1.23	16	1
1	A	68	GLU	CB-CG	-13.03	1.13	1.52	16	1
1	A	53	LEU	CG-CD1	-12.98	1.09	1.52	16	1
1	A	65	LYS	CD-CE	-12.46	1.15	1.52	16	1
1	A	44	LYS	CA-C	-12.36	1.36	1.52	16	1
1	A	30	LYS	CB-CG	-12.34	1.15	1.52	16	1
1	A	39	LEU	CG-CD2	-12.21	1.12	1.52	16	1
1	A	39	LEU	CG-CD1	-12.04	1.12	1.52	16	1
1	A	98	LYS	CB-CG	-11.73	1.17	1.52	16	1
1	A	76	TYR	CG-CD1	-11.38	1.15	1.39	16	1
1	A	30	LYS	CG-CD	-11.21	1.18	1.52	16	1
1	A	71	GLU	CD-OE1	-11.18	1.04	1.25	16	1
1	A	52	GLU	CG-CD	-11.14	1.24	1.52	16	1
1	A	83	TYR	CG-CD2	-10.98	1.16	1.39	16	1
1	A	48	ILE	CB-CG1	-10.62	1.32	1.53	16	1
1	A	62	PHE	C-N	-10.57	1.14	1.34	16	1
1	A	45	THR	N-CA	-10.26	1.31	1.45	16	1
1	A	73	MET	SD-CE	-10.10	1.54	1.79	16	1
1	A	83	TYR	CB-CG	-9.97	1.29	1.51	16	1
1	A	76	TYR	CE2-CZ	-9.92	1.14	1.38	16	1
1	A	98	LYS	CG-CD	-9.85	1.23	1.52	16	1
1	A	99	ASN	C-N	-9.75	1.20	1.33	16	1
1	A	32	GLU	CD-OE1	-9.70	1.06	1.25	16	1
1	A	77	ASP	CA-C	-9.69	1.40	1.52	16	1
1	A	45	THR	CA-CB	-9.64	1.38	1.54	16	1
1	A	62	PHE	C-O	-9.56	1.11	1.23	16	1
1	A	50	TYR	CB-CG	-9.52	1.30	1.51	16	1
1	A	42	THR	C-N	-9.50	1.21	1.33	16	1
1	A	28	GLU	CD-OE2	-9.46	1.07	1.25	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	71	GLU	CG-CD	-9.42	1.28	1.52	16	1
1	A	50	TYR	CZ-OH	-9.15	1.18	1.38	16	1
1	A	57	MET	SD-CE	-9.07	1.56	1.79	16	1
1	A	35	GLU	CB-CG	-9.07	1.25	1.52	16	1
1	A	83	TYR	CZ-OH	-9.03	1.19	1.38	16	1
1	A	57	MET	CB-CG	-8.98	1.25	1.52	16	1
1	A	63	ASP	CG-OD2	-8.88	1.08	1.25	16	1
1	A	43	ASN	CA-C	-8.72	1.42	1.52	16	1
1	A	77	ASP	CB-CG	-8.72	1.30	1.52	16	1
1	A	64	VAL	CA-CB	-8.54	1.43	1.54	16	1
1	A	28	GLU	CD-OE1	-8.38	1.09	1.25	16	1
1	A	83	TYR	CE1-CZ	-8.36	1.18	1.38	16	1
1	A	40	PHE	CG-CD1	-8.25	1.21	1.38	16	1
1	A	49	ASP	CB-CG	-8.02	1.31	1.52	16	1
1	A	32	GLU	CB-CG	-7.86	1.28	1.52	16	1
1	A	34	LYS	CE-NZ	-7.82	1.25	1.49	16	1
1	A	44	LYS	N-CA	-7.56	1.36	1.46	16	1
1	A	52	GLU	CD-OE1	-7.15	1.11	1.25	16	1
1	A	52	GLU	CD-OE2	-6.99	1.12	1.25	16	1
1	A	28	GLU	CG-CD	-6.94	1.34	1.52	16	1
1	A	43	ASN	CA-CB	-6.78	1.43	1.53	16	1
1	A	83	TYR	CD2-CE2	-6.72	1.18	1.38	16	1
1	A	83	TYR	CD1-CE1	-6.64	1.18	1.38	16	1
1	A	50	TYR	CD2-CE2	-6.52	1.19	1.38	16	1
1	A	50	TYR	CD1-CE1	-6.50	1.19	1.38	16	1
1	A	34	LYS	CG-CD	-6.47	1.33	1.52	16	1
1	A	45	THR	CB-OG1	-6.44	1.33	1.43	16	1
1	A	76	TYR	CB-CG	-6.28	1.37	1.51	16	1
1	A	50	TYR	CG-CD2	-6.24	1.26	1.39	16	1
1	A	100	ARG	CA-C	-6.17	1.44	1.52	16	1
1	A	58	ARG	CG-CD	-6.14	1.34	1.52	16	1
1	A	64	VAL	CB-CG2	-6.09	1.32	1.52	16	1
1	A	48	ILE	CB-CG2	-6.04	1.32	1.52	16	1
1	A	30	LYS	CE-NZ	-6.02	1.31	1.49	16	1
1	A	76	TYR	CZ-OH	-6.00	1.25	1.38	16	1
1	A	31	GLN	CB-CG	-5.90	1.34	1.52	16	1
1	A	45	THR	CA-C	-5.85	1.45	1.52	16	1
1	A	96	LYS	CD-CE	-5.79	1.35	1.52	16	1
1	A	98	LYS	CE-NZ	-5.68	1.32	1.49	16	1
1	A	48	ILE	CG1-CD1	-5.65	1.29	1.51	16	1
1	A	27	GLU	CB-CG	-5.59	1.35	1.52	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	30	LYS	CD-CE	-5.59	1.35	1.52	16	1
1	A	40	PHE	CE2-CZ	-5.56	1.22	1.38	16	1
1	A	72	LEU	CG-CD2	-5.48	1.34	1.52	16	1
1	A	50	TYR	CE1-CZ	-5.35	1.25	1.38	16	1
1	A	72	LEU	CG-CD1	-5.32	1.35	1.52	16	1
1	A	42	THR	C-O	-5.17	1.17	1.24	16	1
1	A	64	VAL	C-O	-5.02	1.19	1.24	16	1
1	A	68	GLU	CD-OE1	-5.01	1.15	1.25	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(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	ASN	OD1-CG-ND2	-72.60	50.00	122.60	16	1
1	A	29	GLN	OE1-CD-NE2	-46.67	75.93	122.60	16	1
1	A	77	ASP	O-C-N	-45.71	68.92	122.86	16	1
1	A	51	HIS	ND1-CG-CD2	-41.50	64.60	106.10	16	1
1	A	51	HIS	CG-CD2-NE2	38.88	146.08	107.20	16	1
1	A	51	HIS	CE1-NE2-CD2	-38.67	70.33	109.00	16	1
1	A	58	ARG	NH1-CZ-NH2	-36.91	71.32	119.30	16	1
1	A	99	ASN	OD1-CG-ND2	-34.41	88.19	122.60	16	1
1	A	43	ASN	CA-CB-CG	31.19	143.79	112.60	16	1
1	A	87	ASP	CA-CB-CG	30.40	143.00	112.60	16	1
1	A	58	ARG	NE-CZ-NH2	26.16	142.74	119.20	16	1
1	A	45	THR	O-C-N	-24.69	95.31	122.23	16	1
1	A	58	ARG	NE-CZ-NH1	24.44	145.94	121.50	16	1
1	A	27	GLU	CB-CG-CD	24.05	153.48	112.60	16	1
1	A	66	LYS	CG-CD-CE	24.01	166.53	111.30	16	1
1	A	34	LYS	CA-CB-CG	23.38	160.87	114.10	16	1
1	A	98	LYS	CB-CG-CD	23.31	164.92	111.30	16	1
1	A	54	LYS	CG-CD-CE	21.79	161.41	111.30	16	1
1	A	74	ASN	CB-CG-OD1	21.73	164.27	120.80	16	1
1	A	77	ASP	CA-C-O	21.37	144.85	121.56	16	1
1	A	51	HIS	CB-CG-CD2	21.02	158.53	131.20	16	1
1	A	68	GLU	CB-CG-CD	20.55	147.53	112.60	16	1
1	A	32	GLU	CG-CD-OE2	-20.07	72.25	118.40	16	1
1	A	65	LYS	CB-CG-CD	19.61	156.39	111.30	16	1
1	A	91	ASP	CA-CB-CG	19.56	132.16	112.60	16	1
1	A	74	ASN	CB-CG-ND2	19.56	145.74	116.40	16	1
1	A	29	GLN	CG-CD-NE2	19.10	145.04	116.40	16	1
1	A	88	ASP	CB-CG-OD2	-18.82	75.12	118.40	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	77	ASP	CA-C-N	18.81	149.10	120.89	16	1
1	A	77	ASP	C-N-CA	18.81	149.10	120.89	16	1
1	A	51	HIS	CA-CB-CG	18.73	132.53	113.80	16	1
1	A	68	GLU	CG-CD-OE2	-18.55	75.72	118.40	16	1
1	A	51	HIS	ND1-CE1-NE2	18.55	126.94	108.40	16	1
1	A	35	GLU	CB-CG-CD	17.98	143.16	112.60	16	1
1	A	31	GLN	OE1-CD-NE2	-17.58	105.02	122.60	16	1
1	A	100	ARG	NH1-CZ-NH2	-16.66	97.65	119.30	16	1
1	A	58	ARG	CD-NE-CZ	16.31	147.24	124.40	16	1
1	A	44	LYS	CB-CG-CD	16.09	148.31	111.30	16	1
1	A	60	LEU	CD1-CG-CD2	-15.88	75.86	110.80	16	1
1	A	38	ASP	CB-CG-OD2	-15.68	82.33	118.40	16	1
1	A	58	ARG	CB-CG-CD	14.84	145.42	111.30	16	1
1	A	57	MET	CG-SD-CE	14.80	133.45	100.90	16	1
1	A	58	ARG	CA-CB-CG	14.48	143.06	114.10	16	1
1	A	100	ARG	NE-CZ-NH1	14.39	135.89	121.50	16	1
1	A	32	GLU	CG-CD-OE1	14.37	151.44	118.40	16	1
1	A	58	ARG	CG-CD-NE	14.33	143.53	112.00	16	1
1	A	52	GLU	CA-CB-CG	14.23	142.55	114.10	16	1
1	A	73	MET	CA-CB-CG	14.03	142.17	114.10	16	1
1	A	73	MET	CG-SD-CE	13.99	131.67	100.90	16	1
1	A	31	GLN	CG-CD-NE2	13.50	136.65	116.40	16	1
1	A	30	LYS	CB-CG-CD	13.41	142.14	111.30	16	1
1	A	51	HIS	CG-ND1-CE1	13.38	132.04	109.30	16	1
1	A	43	ASN	O-C-N	-13.23	104.86	122.19	16	1
1	A	71	GLU	CB-CG-CD	13.16	134.98	112.60	16	1
1	A	95	GLU	CB-CG-CD	13.12	134.90	112.60	16	1
1	A	90	LEU	CD1-CG-CD2	-12.91	82.40	110.80	16	1
1	A	99	ASN	CB-CG-ND2	12.89	135.73	116.40	16	1
1	A	68	GLU	CG-CD-OE1	12.87	148.01	118.40	16	1
1	A	100	ARG	CA-CB-CG	12.45	138.99	114.10	16	1
1	A	95	GLU	CG-CD-OE2	-12.24	90.24	118.40	16	1
1	A	88	ASP	CB-CG-OD1	12.03	146.08	118.40	16	1
1	A	54	LYS	CD-CE-NZ	12.02	150.37	111.90	16	1
1	A	38	ASP	CA-CB-CG	12.01	124.61	112.60	16	1
1	A	66	LYS	CD-CE-NZ	11.55	148.85	111.90	16	1
1	A	66	LYS	CB-CG-CD	11.26	137.21	111.30	16	1
1	A	34	LYS	CB-CG-CD	11.05	136.71	111.30	16	1
1	A	60	LEU	CB-CG-CD2	10.55	142.34	110.70	16	1
1	A	95	GLU	CG-CD-OE1	10.43	142.38	118.40	16	1
1	A	29	GLN	CB-CG-CD	-10.31	95.08	112.60	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	49	ASP	CA-CB-CG	10.11	122.71	112.60	16	1
1	A	41	ASP	O-C-N	-9.49	109.00	122.29	16	1
1	A	51	HIS	CB-CG-ND1	9.44	136.85	122.70	16	1
1	A	38	ASP	CB-CG-OD1	9.36	139.93	118.40	16	1
1	A	75	GLU	CG-CD-OE1	9.16	139.48	118.40	16	1
1	A	29	GLN	CG-CD-OE1	9.11	139.03	120.80	16	1
1	A	44	LYS	O-C-N	-8.71	111.01	122.59	16	1
1	A	52	GLU	CB-CG-CD	8.66	127.32	112.60	16	1
1	A	45	THR	CA-C-N	8.50	138.41	121.06	16	1
1	A	45	THR	C-N-CA	8.50	138.41	121.06	16	1
1	A	100	ARG	CA-C-O	8.39	132.51	120.51	16	1
1	A	98	LYS	CA-CB-CG	8.24	130.59	114.10	16	1
1	A	100	ARG	NE-CZ-NH2	8.07	126.46	119.20	16	1
1	A	55	VAL	CA-CB-CG2	8.00	124.00	110.40	16	1
1	A	44	LYS	CG-CD-CE	7.93	129.55	111.30	16	1
1	A	63	ASP	CA-CB-CG	7.92	120.52	112.60	16	1
1	A	100	ARG	CB-CG-CD	7.91	129.50	111.30	16	1
1	A	45	THR	CA-C-O	7.86	127.91	119.03	16	1
1	A	99	ASN	CB-CG-OD1	7.64	136.08	120.80	16	1
1	A	53	LEU	CD1-CG-CD2	-7.58	94.13	110.80	16	1
1	A	31	GLN	CB-CG-CD	7.47	125.30	112.60	16	1
1	A	54	LYS	CA-CB-CG	7.38	128.86	114.10	16	1
1	A	76	TYR	CD1-CG-CD2	-7.38	107.04	118.10	16	1
1	A	90	LEU	CB-CG-CD2	7.37	132.82	110.70	16	1
1	A	88	ASP	CA-CB-CG	7.29	119.89	112.60	16	1
1	A	57	MET	CB-CG-SD	-7.24	90.98	112.70	16	1
1	A	71	GLU	CG-CD-OE1	7.09	134.72	118.40	16	1
1	A	55	VAL	CG1-CB-CG2	-7.07	95.24	110.80	16	1
1	A	92	ILE	CB-CG1-CD1	6.89	128.28	113.80	16	1
1	A	100	ARG	O-C-N	-6.83	113.50	122.59	16	1
1	A	76	TYR	CB-CG-CD1	6.83	131.05	120.80	16	1
1	A	63	ASP	O-C-N	-6.81	112.39	122.81	16	1
1	A	48	ILE	CB-CG1-CD1	6.76	128.00	113.80	16	1
1	A	47	SER	CA-CB-OG	6.71	124.53	111.10	16	1
1	A	87	ASP	CB-CG-OD2	-6.64	103.12	118.40	16	1
1	A	76	TYR	CG-CD1-CE1	6.63	131.15	121.20	16	1
1	A	88	ASP	OD1-CG-OD2	6.62	138.80	122.90	16	1
1	A	41	ASP	OD1-CG-OD2	-6.57	107.14	122.90	16	1
1	A	63	ASP	CA-C-N	6.55	129.24	121.84	16	1
1	A	63	ASP	C-N-CA	6.55	129.24	121.84	16	1
1	A	55	VAL	CA-CB-CG1	6.49	121.43	110.40	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	83	TYR	CA-CB-CG	6.47	125.55	113.90	16	1
1	A	87	ASP	OD1-CG-OD2	6.38	138.22	122.90	16	1
1	A	65	LYS	CG-CD-CE	-6.33	96.74	111.30	16	1
1	A	75	GLU	OE1-CD-OE2	-6.33	107.71	122.90	16	1
1	A	49	ASP	CB-CG-OD1	6.31	132.92	118.40	16	1
1	A	63	ASP	CB-CG-OD1	-6.26	104.00	118.40	16	1
1	A	38	ASP	OD1-CG-OD2	6.18	137.74	122.90	16	1
1	A	60	LEU	CB-CG-CD1	6.12	129.05	110.70	16	1
1	A	44	LYS	N-CA-C	6.10	123.80	110.80	16	1
1	A	53	LEU	CB-CG-CD1	6.09	128.96	110.70	16	1
1	A	65	LYS	CD-CE-NZ	-6.07	92.47	111.90	16	1
1	A	54	LYS	CB-CG-CD	5.96	125.00	111.30	16	1
1	A	43	ASN	CA-C-N	5.94	132.89	121.54	16	1
1	A	43	ASN	C-N-CA	5.94	132.89	121.54	16	1
1	A	90	LEU	CB-CG-CD1	5.94	128.51	110.70	16	1
1	A	49	ASP	CB-CG-OD2	-5.73	105.21	118.40	16	1
1	A	66	LYS	CA-CB-CG	5.68	125.46	114.10	16	1
1	A	76	TYR	CZ-CE2-CD2	5.65	129.76	119.60	16	1
1	A	32	GLU	OE1-CD-OE2	5.59	136.31	122.90	16	1
1	A	68	GLU	OE1-CD-OE2	5.57	136.27	122.90	16	1
1	A	76	TYR	CE1-CZ-CE2	-5.52	109.27	120.30	16	1
1	A	29	GLN	CA-CB-CG	5.35	124.81	114.10	16	1
1	A	44	LYS	CD-CE-NZ	5.30	128.85	111.90	16	1
1	A	62	PHE	O-C-N	-5.20	116.39	123.10	16	1
1	A	83	TYR	CG-CD2-CE2	-5.14	113.50	121.20	16	1
1	A	39	LEU	CD1-CG-CD2	-5.13	99.51	110.80	16	1
1	A	57	MET	CA-CB-CG	5.09	124.28	114.10	16	1
1	A	35	GLU	CG-CD-OE2	-5.07	106.73	118.40	16	1
1	A	44	LYS	CA-CB-CG	5.01	124.13	114.10	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 ⓘ

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	559	34±33
All	All	9296	9072	9049	545

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 30.

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:CG	1:A:44:LYS:CA	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:CD	1:A:58:ARG:CZ	1.51	1.79	16	1
1:A:51:HIS:CD2	1:A:51:HIS:CB	1.49	1.87	16	1
1:A:74:ASN:ND2	1:A:74:ASN:CB	1.43	1.79	16	1
1:A:58:ARG:NH2	1:A:58:ARG:NE	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:CB	1:A:34:LYS:CD	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:31:GLN:CD	1:A:31:GLN:CB	1.31	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:44:LYS:HG2	1:A:44:LYS:C	1.26	1.52	16	1
1:A:58:ARG:CD	1:A:58:ARG:CB	1.26	2.11	16	1
1:A:27:GLU:CD	1:A:27:GLU:CB	1.25	2.10	16	1
1:A:54:LYS:CE	1:A:54:LYS:CG	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:OE2	1:A:71:GLU:OE1	1.22	1.55	16	1
1:A:54:LYS:CG	1:A:54:LYS:CA	1.18	2.21	16	1
1:A:44:LYS:CG	1:A:44:LYS:C	1.15	2.17	16	1
1:A:77:ASP:CA	1:A:77:ASP:O	1.13	1.94	16	1
1:A:43:ASN:CG	1:A:43:ASN:CA	1.11	2.22	16	1
1:A:58:ARG:CG	1:A:58:ARG:CA	1.11	2.27	16	1
1:A:34:LYS:CG	1:A:34:LYS:CA	1.09	2.31	16	1
1:A:74:ASN:CG	1:A:74:ASN:OD1	1.07	0.83	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLU:OE2	1:A:71:GLU:CD	1.04	0.80	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD23	1.01	1.54	16	1
1:A:31:GLN:CD	1:A:31:GLN:HG2	1.01	1.52	16	1
1:A:60:LEU:CB	1:A:60:LEU:CD2	1.00	2.28	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD22	1.00	1.55	16	1
1:A:60:LEU:CD1	1:A:60:LEU:HG	0.99	1.61	16	1
1:A:31:GLN:CD	1:A:31:GLN:HG3	0.99	1.52	16	1
1:A:31:GLN:CD	1:A:31:GLN:CG	0.98	0.93	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD21	0.96	1.54	16	1
1:A:54:LYS:CG	1:A:54:LYS:HB2	0.96	1.50	16	1
1:A:54:LYS:CG	1:A:54:LYS:HB3	0.96	1.50	16	1
1:A:54:LYS:CB	1:A:54:LYS:HG2	0.96	1.51	16	1
1:A:43:ASN:CG	1:A:43:ASN:HB3	0.96	1.44	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:43:ASN:CG	1:A:43:ASN:CB	0.94	0.90	16	1
1:A:44:LYS:CG	1:A:44:LYS:HB2	0.94	1.48	16	1
1:A:44:LYS:CG	1:A:44:LYS:HB3	0.94	1.48	16	1
1:A:43:ASN:CG	1:A:43:ASN:HB2	0.93	1.44	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:CD	1:A:58:ARG:NE	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:CD	1:A:66:LYS:HG3	0.89	1.44	16	1
1:A:34:LYS:CB	1:A:34:LYS:HG2	0.89	1.43	16	1
1:A:50:TYR:HA	1:A:53:LEU:HB2	0.89	1.43	11	2
1:A:34:LYS:CB	1:A:34:LYS:HG3	0.88	1.43	16	1
1:A:44:LYS:CG	1:A:44:LYS:CB	0.88	0.88	16	1
1:A:58:ARG:NH1	1:A:58:ARG:HH21	0.88	1.65	16	1
1:A:58:ARG:CG	1:A:58:ARG:HB2	0.88	1.42	16	1
1:A:66:LYS:CD	1:A:66:LYS:CG	0.87	0.88	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD11	0.87	1.41	16	1
1:A:60:LEU:CG	1:A:60:LEU:HD12	0.87	1.41	16	1
1:A:58:ARG:CB	1:A:58:ARG:CG	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:CB	1:A:58:ARG:HG3	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:CD2	1:A:51:HIS:HE2	0.86	1.63	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:HD13	0.86	1.41	16	1
1:A:34:LYS:CB	1:A:34:LYS:CG	0.85	0.86	16	1
1:A:58:ARG:NH2	1:A:58:ARG:HH11	0.85	1.65	16	1
1:A:58:ARG:CB	1:A:58:ARG:HG2	0.85	1.41	16	1
1:A:27:GLU:CD	1:A:27:GLU:HG2	0.85	1.34	16	1
1:A:51:HIS:CD2	1:A:51:HIS:HE1	0.83	1.74	16	1
1:A:27:GLU:CD	1:A:27:GLU:HG3	0.83	1.34	16	1
1:A:58:ARG:CZ	1:A:58:ARG:NH1	0.83	0.70	16	1
1:A:27:GLU:CD	1:A:27:GLU:CG	0.83	0.80	16	1
1:A:34:LYS:CG	1:A:34:LYS:HB2	0.83	1.36	16	1
1:A:34:LYS:CG	1:A:34:LYS:HB3	0.82	1.36	16	1
1:A:51:HIS:CD2	1:A:51:HIS:CE1	0.82	0.83	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:CZ	1:A:58:ARG:NH2	0.79	0.65	16	1
1:A:58:ARG:NH2	1:A:58:ARG:NH1	0.79	0.79	16	1
1:A:74:ASN:ND2	1:A:74:ASN:OD1	0.77	0.65	16	1
1:A:54:LYS:CD	1:A:54:LYS:HE2	0.77	1.32	16	1
1:A:54:LYS:CD	1:A:54:LYS:HE3	0.76	1.32	16	1
1:A:44:LYS:CB	1:A:44:LYS:HD3	0.76	2.05	16	1
1:A:54:LYS:HE2	1:A:54:LYS:NZ	0.76	1.28	16	1
1:A:66:LYS:NZ	1:A:66:LYS:HE2	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:CE	1:A:54:LYS:HD3	0.75	1.29	16	1
1:A:60:LEU:CD1	1:A:60:LEU:CG	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:31:GLN:CD	1:A:31:GLN:HE22	0.73	1.38	16	1
1:A:66:LYS:CD	1:A:66:LYS:HE3	0.72	1.39	16	1
1:A:91:ASP:HA	1:A:94:THR:OG1	0.72	1.85	13	12
1:A:51:HIS:CD2	1:A:51:HIS:CG	0.72	0.83	16	1
1:A:54:LYS:HG2	1:A:69:ILE:HD13	0.71	1.60	3	2
1:A:31:GLN:CD	1:A:31:GLN:HE21	0.71	1.38	16	1
1:A:43:ASN:CG	1:A:43:ASN:HD22	0.71	1.36	16	1
1:A:71:GLU:OE2	1:A:71:GLU:HG2	0.71	1.80	16	1
1:A:54:LYS:HE3	1:A:54:LYS:NZ	0.71	1.28	16	1
1:A:66:LYS:CE	1:A:66:LYS:HD2	0.71	1.34	16	1
1:A:43:ASN:CG	1:A:43:ASN:HD21	0.71	1.36	16	1
1:A:54:LYS:CD	1:A:54:LYS:CE	0.70	0.76	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LYS:CD	1:A:66:LYS:HE2	0.70	1.39	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:CE	1:A:66:LYS:HD3	0.69	1.34	16	1
1:A:27:GLU:HA	1:A:30:LYS:HG3	0.66	1.68	11	2
1:A:51:HIS:CG	1:A:51:HIS:HD2	0.66	1.42	16	1
1:A:64:VAL:C	1:A:65:LYS:HE3	0.65	2.15	5	2
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:73:MET:HE3	1:A:84:ILE:HG23	0.65	1.69	12	3
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:CG	1:A:44:LYS:O	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:31:GLN:CD	1:A:31:GLN:NE2	0.63	0.73	16	1
1:A:70:LEU:C	1:A:70:LEU:HD22	0.63	2.19	15	16
1:A:66:LYS:CG	1:A:66:LYS:HD2	0.62	1.35	16	1
1:A:96:LYS:HD2	1:A:96:LYS:C	0.62	2.20	14	12
1:A:34:LYS:HG2	1:A:34:LYS:HB2	0.62	1.18	16	1
1:A:49:ASP:HA	1:A:73:MET:HE1	0.61	1.72	2	2
1:A:27:GLU:HA	1:A:30:LYS:CG	0.61	2.25	5	2
1:A:77:ASP:C	1:A:77:ASP:O	0.61	0.62	16	1
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:43:ASN:CG	1:A:43:ASN:ND2	0.60	0.71	16	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:CG	1:A:66:LYS:HD3	0.60	1.35	16	1
1:A:34:LYS:HG3	1:A:34:LYS:HB3	0.59	1.17	16	1
1:A:54:LYS:CE	1:A:54:LYS:HZ2	0.59	1.31	16	1
1:A:54:LYS:CE	1:A:54:LYS:HZ3	0.59	1.30	16	1
1:A:58:ARG:CZ	1:A:58:ARG:HH22	0.59	1.32	16	1
1:A:54:LYS:CE	1:A:54:LYS:HZ1	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
1:A:58:ARG:CD	1:A:58:ARG:HE	0.58	1.30	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:CB	1:A:44:LYS:CE	0.57	2.54	16	1
1:A:51:HIS:HD2	1:A:51:HIS:NE2	0.57	1.43	16	1
1:A:30:LYS:HE3	1:A:86:PHE:HE2	0.57	1.59	5	1
1:A:51:HIS:CD2	1:A:51:HIS:ND1	0.57	0.77	16	1
1:A:74:ASN:ND2	1:A:74:ASN:CA	0.57	2.65	16	1
1:A:66:LYS:O	1:A:70:LEU:HD12	0.57	1.99	4	3
1:A:57:MET:HE3	1:A:64:VAL:HG21	0.57	1.75	13	1
1:A:70:LEU:HD13	1:A:71:GLU:N	0.57	2.14	15	11
1:A:65:LYS:HE2	1:A:65:LYS:N	0.56	2.15	7	1
1:A:71:GLU:HA	1:A:74:ASN:HB3	0.56	1.77	4	2
1:A:58:ARG:NH1	1:A:58:ARG:HH22	0.56	0.87	16	1
1:A:30:LYS:HB3	1:A:34:LYS:HE2	0.56	1.75	5	2
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: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: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:66:LYS:N	1:A:67:PRO:HD2	0.53	2.18	11	5
1:A:96:LYS:CE	1:A:97:ILE:HG23	0.53	2.30	15	2
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:CE	1:A:66:LYS:HZ1	0.53	1.23	16	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:CE	1:A:66:LYS:HZ3	0.52	1.23	16	1
1:A:35:GLU:O	1:A:39:LEU:HB2	0.52	2.05	3	1
1:A:39:LEU:C	1:A:39:LEU:HD13	0.52	2.29	13	2
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:48:ILE:CG2	1:A:84:ILE:HG13	0.52	2.35	1	1
1:A:53:LEU:HD22	1:A:73:MET:HB3	0.52	1.81	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:GLN:O	1:A:33:ILE:HG13	0.52	2.05	9	4
1:A:27:GLU:O	1:A:31:GLN:HG2	0.52	2.05	1	4
1:A:31:GLN:O	1:A:35:GLU:HB2	0.52	2.05	7	2
1:A:70:LEU:HD13	1:A:71:GLU:H	0.52	1.65	2	12
1:A:30:LYS:O	1:A:34:LYS:HB3	0.52	2.05	5	2
1:A:66:LYS:CE	1:A:66:LYS:HZ2	0.52	1.23	16	1
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:HG3	1:A:66:LYS:HD3	0.51	1.23	16	1
1:A:40:PHE:HB2	1:A:55:VAL:CG2	0.51	2.36	9	1
1:A:58:ARG:NH2	1:A:58:ARG:HH12	0.51	0.93	16	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: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:HE2	1:A:65:LYS:HA	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:43:ASN:CG	1:A:43:ASN:OD1	0.50	0.75	16	1
1:A:50:TYR:HB3	1:A:73:MET:SD	0.49	2.46	10	1
1:A:41:ASP:OD2	1:A:44:LYS:HA	0.49	2.07	13	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:CD	1:A:27:GLU:OE2	0.49	0.75	16	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
1:A:71:GLU:OE1	1:A:74:ASN:HB3	0.48	2.08	6	1
1:A:62:PHE:HE1	1:A:96:LYS:HB3	0.48	1.68	7	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:HE3	1:A:96:LYS:C	0.48	2.33	15	1
1:A:74:ASN:ND2	1:A:74:ASN:CG	0.48	0.40	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:31:GLN:CD	1:A:31:GLN:HB3	0.48	2.19	16	1
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:40:PHE:CE1	1:A:56:ALA:HA	0.47	2.44	8	2
1:A:66:LYS:HE3	1:A:66:LYS:HD2	0.47	1.24	16	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: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:27:GLU:CD	1:A:27:GLU:OE1	0.47	0.72	16	1
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	2.25	4	3
1:A:98:LYS:HD2	1:A:98:LYS:C	0.46	2.35	15	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:74:ASN:CG	1:A:74:ASN:HD22	0.46	1.12	16	1
1:A:89:PHE:O	1:A:92:ILE:HB	0.46	2.11	11	3
1:A:73:MET:HE3	1:A:77:ASP:HB2	0.46	1.87	9	2
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: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: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:39:LEU:HD22	1:A:39:LEU:C	0.44	2.38	9	1
1:A:44:LYS:O	1:A:44:LYS:HE2	0.44	2.12	15	1
1:A:54:LYS:CG	1:A:69:ILE:HD13	0.44	2.37	3	1
1:A:49:ASP:CG	1:A:51:HIS:HD1	0.44	2.21	6	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:66:LYS:HB2	1:A:67:PRO:HD3	0.43	1.89	2	1
1:A:30:LYS:O	1:A:34:LYS:N	0.43	2.50	5	1
1:A:33:ILE:HG21	1:A:90:LEU:HG	0.43	1.89	7	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:70:LEU:C	1:A:70:LEU:CD2	0.42	2.92	15	1
1:A:97:ILE:HA	1:A:100:ARG:HB3	0.42	1.90	5	1
1:A:52:GLU:H	1:A:52:GLU:CD	0.42	2.22	10	1
1:A:44:LYS:HB3	1:A:47:SER:O	0.42	2.14	15	1
1:A:66:LYS:CD	1:A:66:LYS:CE	0.42	0.86	16	1
1:A:57:MET:HE1	1:A:72:LEU:HD13	0.42	1.92	13	1
1:A:37:PHE:CZ	1:A:86:PHE:HB2	0.42	2.50	7	1
1:A:53:LEU:HD22	1:A:56:ALA:HB3	0.42	1.91	14	1
1:A:97:ILE:HD12	1:A:98:LYS:HG3	0.42	1.90	14	1
1:A:57:MET:HE3	1:A:64:VAL:HG22	0.42	1.91	15	1
1:A:64:VAL:HG23	1:A:69:ILE:HB	0.42	1.90	5	1
1:A:62:PHE:CZ	1:A:96:LYS:HG2	0.42	2.48	9	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:73:MET:HE3	1:A:77:ASP:CB	0.41	2.45	15	1
1:A:76:TYR:N	1:A:76:TYR:CD1	0.41	2.89	5	1
1:A:34:LYS:HG2	1:A:86:PHE:CE1	0.41	2.50	3	1
1:A:50:TYR:HE1	1:A:84:ILE:HD13	0.41	1.75	11	1
1:A:71:GLU:HA	1:A:74:ASN:HB2	0.41	1.90	15	1
1:A:98:LYS:HB3	1:A:98:LYS:HE2	0.41	1.80	2	1
1:A:30:LYS:O	1:A:34:LYS:HB2	0.41	2.16	15	1
1:A:54:LYS:O	1:A:58:ARG:HG2	0.41	2.15	10	1
1:A:72:LEU:C	1:A:72:LEU:HD23	0.41	2.41	10	1
1:A:34:LYS:HB3	1:A:86:PHE:CZ	0.41	2.51	11	1
1:A:54:LYS:HE2	1:A:54:LYS:HZ1	0.41	1.20	16	1
1:A:66:LYS:HB3	1:A:67:PRO:HD3	0.41	1.93	3	1
1:A:96:LYS:HE3	1:A:97:ILE:N	0.41	2.30	9	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 [i](#)

6.3.1 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 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%)	8	51
All	All	1120/1232 (91%)	1001 (89%)	98 (9%)	21 (2%)	8	51

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	61	GLY	1
1	A	41	ASP	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±3 (88±4%)	8±3 (12±4%)	7	48
All	All	1008/1104 (91%)	882 (88%)	126 (12%)	7	48

All 29 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

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Mol	Chain	Res	Type	Models (Total)
1	A	90	LEU	13
1	A	98	LYS	13
1	A	84	ILE	9
1	A	71	GLU	7
1	A	52	GLU	6
1	A	91	ASP	5
1	A	65	LYS	4
1	A	77	ASP	4
1	A	74	ASN	3
1	A	34	LYS	3
1	A	53	LEU	3
1	A	97	ILE	3
1	A	49	ASP	2
1	A	66	LYS	2
1	A	47	SER	2
1	A	93	MET	2
1	A	29	GLN	2
1	A	44	LYS	2
1	A	35	GLU	1
1	A	99	ASN	1
1	A	39	LEU	1
1	A	51	HIS	1
1	A	54	LYS	1
1	A	72	LEU	1
1	A	73	MET	1
1	A	92	ILE	1
1	A	95	GLU	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	16-A	13

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
16	A	99:ASN	C	100:ARG	N	1.20
16	A	62:PHE	C	63:ASP	N	1.14
16	A	63:ASP	C	64:VAL	N	1.12
16	A	41:ASP	C	42:THR	N	1.09
16	A	44:LYS	C	45:THR	N	1.02
16	A	79:GLU	C	80:GLY	N	1.01
16	A	43:ASN	C	44:LYS	N	1.00
16	A	100:ARG	C	101:ASP	N	0.99
16	A	45:THR	C	46:GLY	N	0.98
16	A	80:GLY	C	81:ASN	N	0.79
16	A	81:ASN	C	82:GLY	N	0.79
16	A	77:ASP	C	78:ARG	N	0.73
16	A	78:ARG	C	79:GLU	N	0.36

7 Chemical shift validation

No chemical shift data were provided