



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:04 AM UTC

PDB ID : 1COD / pdb_00001cod
Title : SOLUTION CONFORMATION OF COBROTOXIN: A NUCLEAR
MAGNETIC RESONANCE AND HYBRID DISTANCE GEOMETRY-
DYNAMICAL SIMULATED ANNEALING STUDY
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Deposited on : 1994-05-11

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

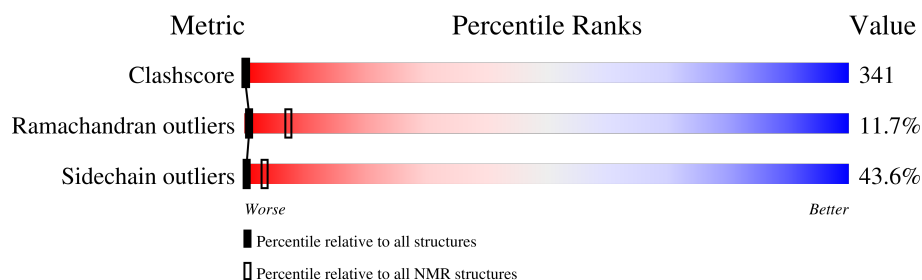
1 Overall quality at a glance

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	62	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

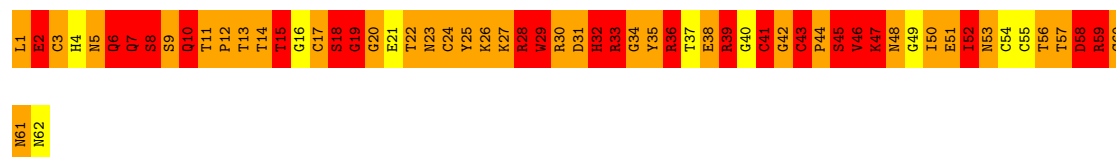
3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 918 atoms, of which 438 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COBROTOXIN.

Mol	Chain	Residues	Atoms						Trace
1	A	62	Total	C	H	N	O	S	0
			918	277	438	97	98	8	

- Molecule 1: COBROTOXIN



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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	26.00	322/487 (66.1%)	15.83	267/653 (40.9%)
All	All	26.00	322/487 (66.1%)	15.83	267/653 (40.9%)

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	6	2
All	All	6	2

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	HIS	CE1-NE2	-119.56	0.12	1.32
1	A	33	ARG	CZ-NH2	-73.09	0.38	1.33
1	A	32	HIS	CG-ND1	-73.09	0.57	1.38
1	A	32	HIS	CG-CD2	-71.55	0.57	1.35
1	A	45	SER	CA-CB	-68.54	0.38	1.53
1	A	45	SER	C-O	-68.25	0.43	1.23
1	A	39	ARG	NE-CZ	-66.97	0.59	1.33
1	A	4	HIS	CG-CD2	-65.53	0.63	1.35
1	A	59	ARG	CZ-NH2	-65.28	0.48	1.33
1	A	59	ARG	CZ-NH1	-63.75	0.43	1.32
1	A	30	ARG	CZ-NH2	-63.46	0.51	1.33
1	A	33	ARG	CD-NE	-62.58	0.58	1.46
1	A	36	ARG	CZ-NH1	-62.48	0.45	1.32
1	A	9	SER	C-O	-61.39	0.46	1.24
1	A	22	THR	CB-OG1	-61.30	0.45	1.43
1	A	4	HIS	CE1-NE2	-61.02	0.71	1.32
1	A	18	SER	C-O	-60.60	0.47	1.24
1	A	51	GLU	CD-OE2	-60.46	0.10	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ARG	CZ-NH2	-60.34	0.55	1.33
1	A	39	ARG	CD-NE	-58.63	0.64	1.46
1	A	28	ARG	CZ-NH1	-58.59	0.50	1.32
1	A	15	THR	CB-OG1	-58.19	0.50	1.43
1	A	61	ASN	CG-OD1	-57.75	0.13	1.23
1	A	8	SER	C-O	-57.66	0.51	1.24
1	A	45	SER	C-N	-57.45	0.55	1.33
1	A	9	SER	CB-OG	-55.25	0.31	1.42
1	A	33	ARG	CZ-NH1	-55.12	0.55	1.32
1	A	4	HIS	ND1-CE1	-54.73	0.77	1.32
1	A	30	ARG	CD-NE	-54.36	0.70	1.46
1	A	10	GLN	CD-OE1	-52.45	0.23	1.23
1	A	33	ARG	NE-CZ	-52.05	0.75	1.33
1	A	23	ASN	CG-OD1	-52.02	0.24	1.23
1	A	30	ARG	NE-CZ	-51.28	0.76	1.33
1	A	62	ASN	C-OXT	-50.44	0.22	1.23
1	A	46	VAL	C-O	-50.29	0.64	1.24
1	A	28	ARG	CD-NE	-49.72	0.76	1.46
1	A	34	GLY	C-O	-49.26	0.57	1.23
1	A	25	TYR	CG-CD2	-49.04	0.36	1.39
1	A	44	PRO	C-O	-48.83	0.47	1.23
1	A	5	ASN	CG-OD1	-48.72	0.30	1.23
1	A	21	GLU	CD-OE2	-48.28	0.33	1.25
1	A	46	VAL	CA-CB	-48.16	0.89	1.54
1	A	30	ARG	CZ-NH1	-48.11	0.65	1.32
1	A	62	ASN	CA-C	-47.01	0.54	1.52
1	A	28	ARG	CZ-NH2	-46.87	0.72	1.33
1	A	45	SER	CB-OG	-46.74	0.48	1.42
1	A	61	ASN	CB-CG	-46.66	0.35	1.52
1	A	61	ASN	CG-ND2	-46.63	0.35	1.33
1	A	18	SER	C-N	-46.60	0.65	1.33
1	A	32	HIS	ND1-CE1	-46.38	0.86	1.32
1	A	7	GLN	CD-OE1	-46.17	0.35	1.23
1	A	8	SER	C-N	-45.89	0.69	1.33
1	A	36	ARG	CD-NE	-45.85	0.82	1.46
1	A	2	GLU	CD-OE1	-45.37	0.39	1.25
1	A	32	HIS	CA-CB	-45.00	0.77	1.53
1	A	31	ASP	CG-OD1	-44.31	0.41	1.25
1	A	36	ARG	CZ-NH2	-43.99	0.76	1.33
1	A	59	ARG	NE-CZ	-43.90	0.84	1.33
1	A	44	PRO	CA-C	-43.90	1.03	1.53
1	A	8	SER	CB-OG	-43.31	0.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	HIS	CD2-NE2	-43.26	0.90	1.37
1	A	9	SER	C-N	-43.22	0.73	1.33
1	A	7	GLN	CD-NE2	-42.92	0.43	1.33
1	A	62	ASN	CG-OD1	-42.84	0.42	1.23
1	A	25	TYR	CE1-CZ	-42.48	0.36	1.38
1	A	36	ARG	NE-CZ	-41.97	0.86	1.33
1	A	39	ARG	CZ-NH1	-40.34	0.76	1.32
1	A	35	TYR	CG-CD1	-40.34	0.54	1.39
1	A	33	ARG	C-O	-39.97	0.73	1.24
1	A	21	GLU	CG-CD	-39.22	0.54	1.52
1	A	62	ASN	CA-CB	-39.18	0.75	1.53
1	A	38	GLU	CD-OE1	-38.78	0.51	1.25
1	A	4	HIS	CG-ND1	-38.44	0.95	1.38
1	A	48	ASN	CG-ND2	-38.42	0.52	1.33
1	A	4	HIS	CB-CG	-38.37	0.96	1.50
1	A	48	ASN	CG-OD1	-38.08	0.51	1.23
1	A	44	PRO	CA-CB	-37.45	0.91	1.53
1	A	18	SER	CB-OG	-37.43	0.67	1.42
1	A	2	GLU	CD-OE2	-37.31	0.54	1.25
1	A	31	ASP	CG-OD2	-37.28	0.54	1.25
1	A	1	LEU	CB-CG	-36.95	0.79	1.53
1	A	53	ASN	CG-OD1	-36.86	0.53	1.23
1	A	21	GLU	CD-OE1	-36.29	0.56	1.25
1	A	32	HIS	C-N	-35.95	0.83	1.33
1	A	59	ARG	CD-NE	-35.86	0.96	1.46
1	A	4	HIS	CD2-NE2	-35.61	0.98	1.37
1	A	45	SER	N-CA	-35.40	1.05	1.46
1	A	25	TYR	CG-CD1	-35.26	0.65	1.39
1	A	34	GLY	C-N	-34.95	0.88	1.33
1	A	17	CYS	C-O	-34.84	0.81	1.24
1	A	35	TYR	CE2-CZ	-34.80	0.54	1.38
1	A	13	THR	CB-OG1	-34.63	0.88	1.43
1	A	32	HIS	CB-CG	-34.54	1.01	1.50
1	A	62	ASN	C-O	-34.29	0.55	1.23
1	A	44	PRO	N-CD	-33.53	1.00	1.47
1	A	47	LYS	CD-CE	-33.27	0.52	1.52
1	A	57	THR	C-O	-33.27	0.77	1.23
1	A	51	GLU	CD-OE1	-33.24	0.62	1.25
1	A	40	GLY	C-O	-33.21	0.79	1.23
1	A	6	GLN	CD-NE2	-32.91	0.64	1.33
1	A	6	GLN	CD-OE1	-32.78	0.61	1.23
1	A	43	CYS	C-O	-32.54	0.82	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	GLN	CG-CD	-32.44	0.70	1.52
1	A	47	LYS	CG-CD	-32.33	0.55	1.52
1	A	1	LEU	CG-CD1	-32.26	0.46	1.52
1	A	35	TYR	CB-CG	-32.18	0.80	1.51
1	A	32	HIS	C-O	-32.05	0.83	1.24
1	A	5	ASN	CG-ND2	-31.94	0.66	1.33
1	A	10	GLN	C-O	-31.86	0.83	1.24
1	A	38	GLU	CD-OE2	-31.75	0.65	1.25
1	A	58	ASP	CG-OD1	-31.55	0.65	1.25
1	A	6	GLN	CB-CG	-31.53	0.57	1.52
1	A	33	ARG	CB-CG	-31.15	0.59	1.52
1	A	33	ARG	CA-C	-31.13	1.11	1.52
1	A	6	GLN	C-O	-31.05	0.87	1.23
1	A	47	LYS	CE-NZ	-30.98	0.56	1.49
1	A	53	ASN	CG-ND2	-30.85	0.68	1.33
1	A	35	TYR	CZ-OH	-30.52	0.73	1.38
1	A	31	ASP	C-O	-30.44	0.84	1.23
1	A	25	TYR	CE2-CZ	-30.39	0.65	1.38
1	A	33	ARG	CA-CB	-30.15	1.02	1.53
1	A	19	GLY	CA-C	-30.09	1.09	1.51
1	A	21	GLU	CA-CB	-30.03	1.05	1.53
1	A	32	HIS	CA-C	-30.00	1.12	1.52
1	A	41	CYS	CB-SG	-29.71	0.83	1.81
1	A	19	GLY	C-N	-29.64	0.90	1.33
1	A	47	LYS	CB-CG	-29.60	0.63	1.52
1	A	14	THR	CB-OG1	-29.10	0.97	1.43
1	A	33	ARG	N-CA	-28.72	1.09	1.46
1	A	20	GLY	C-O	-28.71	0.85	1.23
1	A	35	TYR	CG-CD2	-28.70	0.79	1.39
1	A	40	GLY	C-N	-28.45	0.94	1.33
1	A	43	CYS	C-N	-28.42	0.92	1.33
1	A	57	THR	C-N	-28.25	0.94	1.33
1	A	16	GLY	C-O	-28.18	0.85	1.23
1	A	15	THR	CB-CG2	-27.50	0.61	1.52
1	A	51	GLU	CG-CD	-27.35	0.83	1.52
1	A	20	GLY	N-CA	-27.30	1.05	1.45
1	A	6	GLN	C-N	-27.20	0.94	1.33
1	A	23	ASN	CG-ND2	-27.13	0.76	1.33
1	A	39	ARG	CG-CD	-26.78	0.72	1.52
1	A	59	ARG	CB-CG	-26.63	0.72	1.52
1	A	47	LYS	C-O	-26.62	0.90	1.24
1	A	17	CYS	C-N	-26.33	0.96	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	LYS	CD-CE	-26.14	0.74	1.52
1	A	28	ARG	NE-CZ	-26.00	1.04	1.33
1	A	17	CYS	CA-CB	-25.70	1.16	1.53
1	A	7	GLN	CG-CD	-25.64	0.88	1.52
1	A	18	SER	CA-CB	-25.63	1.10	1.53
1	A	1	LEU	CG-CD2	-25.35	0.68	1.52
1	A	7	GLN	C-O	-25.23	0.94	1.24
1	A	45	SER	CA-C	-25.21	1.22	1.52
1	A	27	LYS	CB-CG	-25.09	0.77	1.52
1	A	2	GLU	CB-CG	-25.04	0.77	1.52
1	A	30	ARG	CB-CG	-24.94	0.77	1.52
1	A	57	THR	CB-OG1	-24.68	1.04	1.43
1	A	35	TYR	CE1-CZ	-24.59	0.79	1.38
1	A	5	ASN	CB-CG	-24.57	0.90	1.52
1	A	16	GLY	C-N	-24.55	0.98	1.33
1	A	58	ASP	CG-OD2	-24.08	0.79	1.25
1	A	61	ASN	C-N	-24.01	0.99	1.33
1	A	5	ASN	C-N	-23.96	1.03	1.33
1	A	22	THR	CB-CG2	-23.84	0.73	1.52
1	A	34	GLY	N-CA	-23.70	1.10	1.45
1	A	46	VAL	N-CA	-23.52	1.17	1.46
1	A	15	THR	C-O	-23.34	0.97	1.23
1	A	11	THR	CB-OG1	-23.14	1.06	1.43
1	A	48	ASN	CB-CG	-23.06	0.94	1.52
1	A	10	GLN	CD-NE2	-22.98	0.85	1.33
1	A	47	LYS	CA-CB	-22.94	1.14	1.53
1	A	62	ASN	CG-ND2	-22.62	0.85	1.33
1	A	21	GLU	CB-CG	-22.35	0.85	1.52
1	A	36	ARG	CG-CD	-22.06	0.86	1.52
1	A	5	ASN	C-O	-22.05	0.95	1.23
1	A	10	GLN	C-N	-21.93	0.98	1.33
1	A	62	ASN	CB-CG	-21.84	0.97	1.52
1	A	61	ASN	C-O	-21.72	0.93	1.23
1	A	31	ASP	CB-CG	-21.64	0.97	1.52
1	A	38	GLU	CB-CG	-21.36	0.88	1.52
1	A	17	CYS	CA-C	-21.24	1.26	1.52
1	A	35	TYR	CD1-CE1	-21.24	0.74	1.38
1	A	35	TYR	CD2-CE2	-21.17	0.75	1.38
1	A	26	LYS	CE-NZ	-21.13	0.85	1.49
1	A	25	TYR	CB-CG	-20.89	1.05	1.51
1	A	31	ASP	C-N	-20.54	1.04	1.33
1	A	46	VAL	CB-CG2	-20.50	0.84	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ARG	CG-CD	-20.39	0.91	1.52
1	A	19	GLY	C-O	-19.86	0.97	1.23
1	A	39	ARG	CB-CG	-19.72	0.93	1.52
1	A	25	TYR	CZ-OH	-19.68	0.96	1.38
1	A	26	LYS	CB-CG	-19.45	0.94	1.52
1	A	7	GLN	CB-CG	-19.01	0.95	1.52
1	A	27	LYS	CD-CE	-18.98	0.95	1.52
1	A	23	ASN	CB-CG	-18.50	1.05	1.52
1	A	38	GLU	CG-CD	-17.91	1.07	1.52
1	A	3	CYS	CB-SG	-17.59	1.23	1.81
1	A	18	SER	N-CA	-17.47	1.23	1.46
1	A	46	VAL	C-N	-17.33	1.09	1.33
1	A	14	THR	CB-CG2	-17.16	0.95	1.52
1	A	47	LYS	C-N	-17.07	1.09	1.33
1	A	46	VAL	CA-C	-16.54	1.31	1.52
1	A	30	ARG	CG-CD	-16.50	1.02	1.52
1	A	52	ILE	CB-CG1	-16.45	1.20	1.53
1	A	20	GLY	C-N	-16.29	1.11	1.33
1	A	27	LYS	CE-NZ	-16.04	1.01	1.49
1	A	13	THR	CB-CG2	-15.59	1.01	1.52
1	A	2	GLU	CG-CD	-15.38	1.13	1.52
1	A	18	SER	CA-C	-14.80	1.32	1.52
1	A	20	GLY	CA-C	-14.79	1.31	1.51
1	A	55	CYS	CB-SG	-14.56	1.33	1.81
1	A	26	LYS	CG-CD	-14.25	1.09	1.52
1	A	21	GLU	C-O	-14.14	1.05	1.23
1	A	7	GLN	C-N	-14.12	1.14	1.33
1	A	22	THR	C-O	-13.93	1.06	1.24
1	A	30	ARG	C-O	-13.80	1.07	1.24
1	A	25	TYR	CD2-CE2	-13.48	0.98	1.38
1	A	25	TYR	CD1-CE1	-13.46	0.98	1.38
1	A	15	THR	CA-CB	-13.34	1.32	1.53
1	A	1	LEU	CA-CB	-13.00	1.27	1.53
1	A	15	THR	C-N	-12.86	1.14	1.33
1	A	21	GLU	N-CA	-12.86	1.29	1.45
1	A	59	ARG	CG-CD	-12.83	1.14	1.52
1	A	60	CYS	CB-SG	-12.61	1.39	1.81
1	A	42	GLY	C-O	-12.56	1.07	1.23
1	A	46	VAL	CB-CG1	-12.54	1.11	1.52
1	A	30	ARG	C-N	-12.46	1.17	1.33
1	A	47	LYS	N-CA	-12.29	1.30	1.46
1	A	57	THR	CB-CG2	-12.16	1.12	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	CYS	CB-SG	-12.13	1.41	1.81
1	A	11	THR	CB-CG2	-12.09	1.12	1.52
1	A	29	TRP	NE1-CE2	-12.07	1.24	1.37
1	A	50	ILE	CG1-CD1	-11.73	1.06	1.51
1	A	29	TRP	CD2-CE3	-11.65	1.21	1.40
1	A	29	TRP	C-O	-11.61	1.11	1.23
1	A	47	LYS	CA-C	-11.35	1.37	1.52
1	A	27	LYS	CG-CD	-11.28	1.18	1.52
1	A	48	ASN	CA-CB	-11.19	1.34	1.53
1	A	29	TRP	C-N	-11.18	1.18	1.33
1	A	58	ASP	CB-CG	-11.08	1.24	1.52
1	A	10	GLN	CB-CG	-10.94	1.19	1.52
1	A	14	THR	C-O	-10.74	1.10	1.23
1	A	30	ARG	CA-C	-10.67	1.40	1.52
1	A	31	ASP	CA-CB	-10.63	1.35	1.53
1	A	19	GLY	N-CA	-10.62	1.29	1.45
1	A	15	THR	CA-C	-10.61	1.40	1.52
1	A	21	GLU	CA-C	-10.51	1.39	1.52
1	A	31	ASP	CA-C	-10.29	1.39	1.52
1	A	44	PRO	C-N	-10.26	1.20	1.33
1	A	22	THR	CA-CB	-9.91	1.35	1.53
1	A	28	ARG	CG-CD	-9.82	1.23	1.52
1	A	10	GLN	CA-CB	-9.81	1.36	1.53
1	A	36	ARG	CB-CG	-9.76	1.23	1.52
1	A	28	ARG	CB-CG	-9.75	1.23	1.52
1	A	29	TRP	CG-CD1	-9.43	1.13	1.36
1	A	52	ILE	CB-CG2	-9.31	1.21	1.52
1	A	9	SER	CA-CB	-9.15	1.38	1.53
1	A	53	ASN	CB-CG	-9.06	1.29	1.52
1	A	30	ARG	CA-CB	-9.01	1.39	1.53
1	A	21	GLU	C-N	-8.99	1.18	1.34
1	A	11	THR	C-N	-8.96	1.23	1.33
1	A	1	LEU	N-CA	-8.92	1.29	1.46
1	A	48	ASN	N-CA	-8.89	1.34	1.46
1	A	23	ASN	CA-CB	-8.75	1.38	1.53
1	A	29	TRP	CD2-CE2	-8.65	1.26	1.41
1	A	11	THR	CA-CB	-8.62	1.39	1.52
1	A	29	TRP	CZ2-CH2	-8.59	1.21	1.37
1	A	4	HIS	C-O	-8.51	1.13	1.23
1	A	22	THR	N-CA	-8.33	1.35	1.46
1	A	55	CYS	C-O	-8.26	1.13	1.23
1	A	12	PRO	CA-CB	-8.08	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	CYS	CB-SG	-7.87	1.55	1.81
1	A	35	TYR	CA-CB	-7.81	1.39	1.53
1	A	34	GLY	CA-C	-7.46	1.41	1.51
1	A	61	ASN	CA-C	-7.37	1.42	1.52
1	A	11	THR	C-O	-7.33	1.15	1.24
1	A	25	TYR	C-O	-7.29	1.14	1.23
1	A	43	CYS	CB-SG	-7.22	1.57	1.81
1	A	32	HIS	N-CA	-7.21	1.36	1.46
1	A	33	ARG	C-N	-7.13	1.23	1.33
1	A	7	GLN	CA-CB	-7.03	1.43	1.53
1	A	60	CYS	C-O	-7.00	1.14	1.23
1	A	14	THR	C-N	-6.89	1.25	1.33
1	A	31	ASP	N-CA	-6.80	1.36	1.45
1	A	22	THR	CA-C	-6.75	1.43	1.52
1	A	24	CYS	CB-SG	-6.69	1.59	1.81
1	A	48	ASN	C-O	-6.68	1.15	1.24
1	A	9	SER	CA-C	-6.64	1.43	1.52
1	A	44	PRO	CG-CD	-6.64	1.28	1.50
1	A	56	THR	C-N	-6.54	1.25	1.33
1	A	8	SER	CA-CB	-6.49	1.42	1.53
1	A	52	ILE	CG1-CD1	-6.49	1.26	1.51
1	A	39	ARG	C-O	-6.44	1.16	1.23
1	A	35	TYR	N-CA	-6.39	1.38	1.46
1	A	22	THR	C-N	-6.33	1.25	1.33
1	A	51	GLU	CB-CG	-6.26	1.33	1.52
1	A	6	GLN	CG-CD	-6.18	1.36	1.52
1	A	10	GLN	CA-C	-6.17	1.44	1.52
1	A	29	TRP	CZ3-CH2	-6.14	1.25	1.40
1	A	12	PRO	C-O	-6.11	1.17	1.23
1	A	8	SER	CA-C	-6.06	1.44	1.52
1	A	48	ASN	C-N	-6.04	1.24	1.33
1	A	25	TYR	C-N	-5.92	1.26	1.33
1	A	7	GLN	CA-C	-5.88	1.45	1.52
1	A	61	ASN	CA-CB	-5.86	1.44	1.52
1	A	36	ARG	C-O	-5.81	1.17	1.23
1	A	1	LEU	C-N	-5.75	1.26	1.33
1	A	60	CYS	C-N	-5.74	1.25	1.33
1	A	49	GLY	C-O	-5.70	1.16	1.23
1	A	42	GLY	C-N	-5.67	1.21	1.33
1	A	16	GLY	N-CA	-5.62	1.37	1.45
1	A	4	HIS	C-N	-5.61	1.25	1.33
1	A	35	TYR	C-N	-5.58	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	PRO	N-CD	-5.56	1.40	1.47
1	A	41	CYS	C-O	-5.53	1.17	1.23
1	A	55	CYS	C-N	-5.49	1.22	1.34
1	A	49	GLY	C-N	-5.42	1.26	1.33
1	A	2	GLU	CA-CB	-5.34	1.44	1.53
1	A	56	THR	C-O	-5.23	1.16	1.23
1	A	12	PRO	C-N	-5.18	1.25	1.33
1	A	1	LEU	C-O	-5.12	1.13	1.23
1	A	58	ASP	C-O	-5.08	1.17	1.24
1	A	39	ARG	C-N	-5.04	1.26	1.33

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	SER	O-C-N	-102.65	15.48	123.26
1	A	32	HIS	ND1-CG-CD2	-85.97	20.13	106.10
1	A	7	GLN	OE1-CD-NE2	-77.53	45.07	122.60
1	A	9	SER	O-C-N	-76.94	20.26	122.59
1	A	8	SER	O-C-N	-72.99	25.51	122.59
1	A	6	GLN	OE1-CD-NE2	-70.72	51.88	122.60
1	A	18	SER	O-C-N	-67.90	32.29	122.59
1	A	53	ASN	OD1-CG-ND2	-66.41	56.19	122.60
1	A	32	HIS	CG-CD2-NE2	60.26	167.46	107.20
1	A	25	TYR	CD1-CG-CD2	-59.21	29.29	118.10
1	A	23	ASN	OD1-CG-ND2	-58.77	63.83	122.60
1	A	59	ARG	NH1-CZ-NH2	-57.17	44.98	119.30
1	A	45	SER	N-CA-CB	-53.05	29.77	111.46
1	A	10	GLN	CG-CD-OE1	-48.89	23.01	120.80
1	A	45	SER	CA-C-O	47.16	171.37	121.38
1	A	25	TYR	CE1-CZ-CE2	-45.57	29.16	120.30
1	A	59	ARG	NE-CZ-NH2	44.06	158.86	119.20
1	A	28	ARG	NH1-CZ-NH2	-41.93	64.79	119.30
1	A	10	GLN	OE1-CD-NE2	41.22	163.82	122.60
1	A	45	SER	N-CA-C	41.08	168.57	108.60
1	A	5	ASN	OD1-CG-ND2	-40.30	82.30	122.60
1	A	48	ASN	OD1-CG-ND2	-39.56	83.04	122.60
1	A	1	LEU	CD1-CG-CD2	-39.37	24.19	110.80
1	A	44	PRO	CA-C-O	-39.28	64.15	121.90
1	A	28	ARG	NE-CZ-NH2	38.65	153.99	119.20
1	A	2	GLU	CB-CG-CD	37.90	177.03	112.60
1	A	10	GLN	CG-CD-NE2	37.84	173.17	116.40
1	A	61	ASN	CA-CB-CG	37.44	150.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	GLY	O-C-N	-35.68	76.31	122.70
1	A	33	ARG	NH1-CZ-NH2	-35.12	73.64	119.30
1	A	59	ARG	NE-CZ-NH1	34.66	156.16	121.50
1	A	32	HIS	CG-ND1-CE1	34.09	167.26	109.30
1	A	45	SER	CA-CB-OG	-34.00	43.10	111.10
1	A	9	SER	CA-C-O	33.32	168.15	120.51
1	A	36	ARG	NE-CZ-NH2	32.89	148.80	119.20
1	A	28	ARG	CD-NE-CZ	32.65	170.11	124.40
1	A	25	TYR	CB-CG-CD1	32.60	169.70	120.80
1	A	25	TYR	CG-CD1-CE1	32.36	169.75	121.20
1	A	32	HIS	CE1-NE2-CD2	-32.28	76.72	109.00
1	A	23	ASN	CB-CG-ND2	32.27	164.81	116.40
1	A	5	ASN	CA-CB-CG	32.26	144.86	112.60
1	A	8	SER	CA-C-O	31.84	166.04	120.51
1	A	32	HIS	CB-CG-ND1	31.12	169.37	122.70
1	A	2	GLU	OE1-CD-OE2	-30.88	48.79	122.90
1	A	32	HIS	CB-CG-CD2	30.22	170.49	131.20
1	A	2	GLU	CA-CB-CG	30.08	174.25	114.10
1	A	33	ARG	NE-CZ-NH1	29.38	150.88	121.50
1	A	18	SER	CA-C-O	29.11	162.14	120.51
1	A	45	SER	CA-C-N	28.59	173.43	121.97
1	A	45	SER	C-N-CA	28.59	173.43	121.97
1	A	8	SER	CA-CB-OG	28.41	167.91	111.10
1	A	6	GLN	CB-CG-CD	28.13	160.42	112.60
1	A	7	GLN	CG-CD-NE2	28.13	158.59	116.40
1	A	25	TYR	CZ-CE2-CD2	27.87	169.76	119.60
1	A	27	LYS	CG-CD-CE	27.48	174.50	111.30
1	A	10	GLN	CB-CG-CD	27.23	158.90	112.60
1	A	25	TYR	CB-CG-CD2	26.79	160.99	120.80
1	A	25	TYR	CG-CD2-CE2	26.48	160.91	121.20
1	A	9	SER	CA-C-N	26.34	171.85	121.54
1	A	9	SER	C-N-CA	26.34	171.85	121.54
1	A	61	ASN	CB-CG-ND2	26.17	155.65	116.40
1	A	5	ASN	CB-CG-ND2	25.65	154.87	116.40
1	A	40	GLY	O-C-N	-25.49	89.57	122.70
1	A	53	ASN	CB-CG-ND2	25.31	154.37	116.40
1	A	39	ARG	NE-CZ-NH2	-25.01	96.69	119.20
1	A	8	SER	CA-C-N	24.83	168.97	121.54
1	A	8	SER	C-N-CA	24.83	168.97	121.54
1	A	6	GLN	CG-CD-NE2	24.77	153.55	116.40
1	A	26	LYS	CG-CD-CE	24.41	167.45	111.30
1	A	47	LYS	CA-CB-CG	-24.09	65.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	GLN	CA-CB-CG	23.87	161.85	114.10
1	A	45	SER	CB-CA-C	23.32	156.87	111.17
1	A	59	ARG	CG-CD-NE	23.13	162.89	112.00
1	A	25	TYR	CD1-CE1-CZ	23.07	161.13	119.60
1	A	43	CYS	O-C-N	-22.95	94.93	121.32
1	A	51	GLU	CG-CD-OE1	22.80	170.83	118.40
1	A	18	SER	CA-C-N	22.75	165.99	121.41
1	A	18	SER	C-N-CA	22.75	165.99	121.41
1	A	62	ASN	CA-CB-CG	22.41	135.01	112.60
1	A	32	HIS	CA-CB-CG	22.34	136.14	113.80
1	A	41	CYS	CA-CB-SG	21.81	164.56	114.40
1	A	62	ASN	CB-CG-ND2	21.53	148.69	116.40
1	A	44	PRO	CA-C-N	21.46	158.50	121.80
1	A	44	PRO	C-N-CA	21.46	158.50	121.80
1	A	28	ARG	CG-CD-NE	21.35	158.98	112.00
1	A	4	HIS	ND1-CE1-NE2	-21.28	87.12	108.40
1	A	6	GLN	O-C-N	-21.22	97.90	123.36
1	A	59	ARG	CB-CG-CD	21.14	159.93	111.30
1	A	36	ARG	NH1-CZ-NH2	-20.73	92.35	119.30
1	A	35	TYR	CA-CB-CG	20.30	150.45	113.90
1	A	33	ARG	CA-C-O	-19.96	91.96	120.51
1	A	28	ARG	NE-CZ-NH1	19.73	141.23	121.50
1	A	59	ARG	CA-CB-CG	19.57	153.24	114.10
1	A	1	LEU	CB-CG-CD2	19.54	169.31	110.70
1	A	59	ARG	CD-NE-CZ	19.42	151.59	124.40
1	A	61	ASN	CB-CG-OD1	-19.04	82.72	120.80
1	A	46	VAL	N-CA-CB	-18.93	80.00	111.23
1	A	33	ARG	CG-CD-NE	18.92	153.62	112.00
1	A	62	ASN	N-CA-CB	18.52	141.99	110.50
1	A	26	LYS	CB-CG-CD	18.19	153.15	111.30
1	A	33	ARG	NE-CZ-NH2	18.08	135.47	119.20
1	A	57	THR	O-C-N	-18.06	88.40	121.63
1	A	62	ASN	CB-CA-C	-18.00	75.91	110.10
1	A	2	GLU	CG-CD-OE2	17.97	159.74	118.40
1	A	44	PRO	N-CD-CG	-17.96	76.26	103.20
1	A	34	GLY	CA-C-N	17.95	150.22	121.86
1	A	34	GLY	C-N-CA	17.95	150.22	121.86
1	A	31	ASP	OD1-CG-OD2	-17.86	80.04	122.90
1	A	7	GLN	CG-CD-OE1	17.77	156.34	120.80
1	A	51	GLU	CB-CG-CD	17.77	142.81	112.60
1	A	30	ARG	NE-CZ-NH1	17.61	139.11	121.50
1	A	22	THR	CA-CB-CG2	17.48	140.21	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ILE	CB-CG1-CD1	17.47	150.48	113.80
1	A	15	THR	OG1-CB-CG2	-17.43	74.44	109.30
1	A	16	GLY	O-C-N	-17.31	100.20	122.70
1	A	21	GLU	CA-CB-CG	-17.15	79.80	114.10
1	A	10	GLN	O-C-N	-17.03	99.95	122.59
1	A	6	GLN	CG-CD-OE1	16.88	154.57	120.80
1	A	27	LYS	CA-CB-CG	16.72	147.55	114.10
1	A	25	TYR	OH-CZ-CE2	16.62	169.77	119.90
1	A	4	HIS	CA-CB-CG	16.53	130.33	113.80
1	A	15	THR	CA-CB-CG2	16.30	138.21	110.50
1	A	47	LYS	CG-CD-CE	-16.26	73.90	111.30
1	A	21	GLU	CB-CG-CD	16.23	140.19	112.60
1	A	21	GLU	CG-CD-OE2	-16.20	81.15	118.40
1	A	30	ARG	NH1-CZ-NH2	-15.87	98.66	119.30
1	A	36	ARG	CG-CD-NE	15.18	145.40	112.00
1	A	15	THR	CA-CB-OG1	15.15	132.33	109.60
1	A	5	ASN	O-C-N	-14.89	103.83	123.19
1	A	47	LYS	CB-CG-CD	-14.73	77.42	111.30
1	A	38	GLU	CB-CG-CD	14.72	137.63	112.60
1	A	62	ASN	OD1-CG-ND2	-14.46	108.14	122.60
1	A	2	GLU	CG-CD-OE1	14.38	151.48	118.40
1	A	53	ASN	CB-CG-OD1	14.32	149.44	120.80
1	A	43	CYS	CA-C-N	14.24	136.22	120.98
1	A	43	CYS	C-N-CA	14.24	136.22	120.98
1	A	7	GLN	CB-CG-CD	14.01	136.41	112.60
1	A	51	GLU	OE1-CD-OE2	-13.97	89.38	122.90
1	A	25	TYR	CE1-CZ-OH	13.72	161.06	119.90
1	A	48	ASN	CB-CG-ND2	13.70	136.95	116.40
1	A	36	ARG	CB-CG-CD	13.34	141.98	111.30
1	A	25	TYR	CA-CB-CG	13.26	137.76	113.90
1	A	26	LYS	CD-CE-NZ	13.18	154.07	111.90
1	A	4	HIS	CE1-NE2-CD2	13.11	122.11	109.00
1	A	31	ASP	CA-CB-CG	12.96	125.56	112.60
1	A	46	VAL	N-CA-C	12.78	135.92	109.34
1	A	39	ARG	NE-CZ-NH1	12.76	134.26	121.50
1	A	33	ARG	CD-NE-CZ	12.65	142.11	124.40
1	A	62	ASN	CA-C-O	12.64	158.92	121.00
1	A	22	THR	OG1-CB-CG2	-12.60	84.11	109.30
1	A	44	PRO	O-C-N	12.56	138.59	122.89
1	A	31	ASP	O-C-N	-12.52	107.18	122.96
1	A	46	VAL	O-C-N	-12.51	106.94	122.57
1	A	31	ASP	CB-CG-OD2	12.34	146.79	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	LEU	CB-CG-CD1	12.31	147.63	110.70
1	A	38	GLU	OE1-CD-OE2	-12.27	93.44	122.90
1	A	44	PRO	CA-N-CD	12.22	129.10	112.00
1	A	39	ARG	CG-CD-NE	12.15	138.74	112.00
1	A	4	HIS	CB-CG-ND1	12.00	140.69	122.70
1	A	35	TYR	CB-CG-CD2	11.87	138.60	120.80
1	A	17	CYS	O-C-N	-11.82	109.74	123.22
1	A	46	VAL	CA-C-N	11.82	144.12	121.54
1	A	46	VAL	C-N-CA	11.82	144.12	121.54
1	A	32	HIS	N-CA-C	11.75	135.83	110.80
1	A	33	ARG	N-CA-C	-11.63	86.03	110.80
1	A	35	TYR	CG-CD2-CE2	11.63	138.64	121.20
1	A	27	LYS	CB-CG-CD	11.35	137.40	111.30
1	A	61	ASN	O-C-N	-11.26	106.87	122.41
1	A	21	GLU	CG-CD-OE1	11.22	144.21	118.40
1	A	18	SER	N-CA-CB	-10.88	92.11	110.49
1	A	4	HIS	CG-ND1-CE1	10.73	127.54	109.30
1	A	35	TYR	CD1-CE1-CZ	10.63	138.74	119.60
1	A	4	HIS	ND1-CG-CD2	-10.59	95.51	106.10
1	A	6	GLN	CA-C-O	10.32	132.05	119.98
1	A	36	ARG	CD-NE-CZ	10.13	138.58	124.40
1	A	21	GLU	N-CA-C	10.12	125.46	110.48
1	A	33	ARG	CA-C-N	9.92	140.86	121.41
1	A	33	ARG	C-N-CA	9.92	140.86	121.41
1	A	27	LYS	CD-CE-NZ	9.89	143.56	111.90
1	A	13	THR	CA-CB-CG2	9.88	127.30	110.50
1	A	44	PRO	N-CA-C	9.87	126.29	110.40
1	A	28	ARG	CB-CG-CD	9.68	133.57	111.30
1	A	38	GLU	CA-CB-CG	9.67	133.44	114.10
1	A	57	THR	CA-C-N	9.61	139.89	121.54
1	A	57	THR	C-N-CA	9.61	139.89	121.54
1	A	48	ASN	CB-CG-OD1	9.61	140.01	120.80
1	A	35	TYR	CG-CD1-CE1	-9.59	106.82	121.20
1	A	40	GLY	CA-C-N	9.58	138.30	122.87
1	A	40	GLY	C-N-CA	9.58	138.30	122.87
1	A	38	GLU	CG-CD-OE2	9.45	140.14	118.40
1	A	29	TRP	NE1-CE2-CD2	-9.44	95.13	107.40
1	A	58	ASP	OD1-CG-OD2	-9.36	100.43	122.90
1	A	35	TYR	CB-CG-CD1	-9.32	106.82	120.80
1	A	26	LYS	CA-CB-CG	9.31	132.72	114.10
1	A	43	CYS	CA-C-O	9.20	132.77	120.16
1	A	7	GLN	O-C-N	-9.10	111.49	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	TRP	CE2-CD2-CE3	-9.05	109.75	118.80
1	A	13	THR	OG1-CB-CG2	-8.88	91.53	109.30
1	A	30	ARG	CA-CB-CG	8.82	131.74	114.10
1	A	62	ASN	CB-CG-OD1	-8.82	103.16	120.80
1	A	46	VAL	CB-CA-C	8.67	125.52	111.29
1	A	9	SER	CA-CB-OG	8.33	127.75	111.10
1	A	44	PRO	CB-CG-CD	8.16	132.20	106.10
1	A	51	GLU	CG-CD-OE2	-8.09	99.79	118.40
1	A	34	GLY	CA-C-O	7.98	134.46	120.57
1	A	46	VAL	CA-C-O	-7.90	110.91	120.78
1	A	58	ASP	CB-CG-OD2	7.88	136.53	118.40
1	A	14	THR	CA-CB-OG1	7.72	121.18	109.60
1	A	47	LYS	O-C-N	-7.72	112.33	122.59
1	A	29	TRP	CZ3-CH2-CZ2	-7.66	111.54	121.50
1	A	13	THR	CA-CB-OG1	7.64	121.06	109.60
1	A	10	GLN	CA-C-N	7.54	133.59	121.83
1	A	10	GLN	C-N-CA	7.54	133.59	121.83
1	A	39	ARG	NH1-CZ-NH2	7.50	129.04	119.30
1	A	43	CYS	C-N-CD	-7.39	94.68	125.00
1	A	40	GLY	CA-C-O	7.33	133.32	120.57
1	A	6	GLN	CA-C-N	7.29	131.74	121.24
1	A	6	GLN	C-N-CA	7.29	131.74	121.24
1	A	44	PRO	CA-CB-CG	-7.28	90.66	104.50
1	A	29	TRP	O-C-N	-7.28	115.20	122.99
1	A	16	GLY	CA-C-N	7.28	132.45	122.19
1	A	16	GLY	C-N-CA	7.28	132.45	122.19
1	A	29	TRP	CE2-CD2-CG	7.27	115.92	107.20
1	A	57	THR	CA-C-O	7.26	133.28	122.32
1	A	35	TYR	CZ-CE2-CD2	-7.12	106.79	119.60
1	A	5	ASN	CA-C-O	7.03	129.05	121.11
1	A	39	ARG	CA-CB-CG	6.93	127.97	114.10
1	A	18	SER	N-CA-C	6.85	125.39	110.80
1	A	33	ARG	CB-CG-CD	6.79	126.93	111.30
1	A	34	GLY	N-CA-C	6.54	128.69	113.18
1	A	62	ASN	N-CA-C	6.50	129.21	111.00
1	A	31	ASP	CB-CG-OD1	6.42	133.18	118.40
1	A	30	ARG	CB-CG-CD	6.42	126.06	111.30
1	A	29	TRP	CB-CG-CD2	6.40	135.77	126.80
1	A	20	GLY	CA-C-N	6.39	132.00	121.39
1	A	20	GLY	C-N-CA	6.39	132.00	121.39
1	A	35	TYR	CE1-CZ-OH	6.33	138.90	119.90
1	A	32	HIS	O-C-N	-6.26	114.27	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ARG	CG-CD-NE	6.24	125.74	112.00
1	A	15	THR	O-C-N	-6.24	115.30	123.28
1	A	33	ARG	N-CA-CB	6.17	120.92	110.49
1	A	44	PRO	CB-CA-C	-6.17	100.72	110.96
1	A	3	CYS	CA-CB-SG	6.15	128.55	114.40
1	A	20	GLY	O-C-N	-6.05	114.84	122.70
1	A	31	ASP	CA-C-N	5.86	132.74	121.54
1	A	31	ASP	C-N-CA	5.86	132.74	121.54
1	A	46	VAL	CG1-CB-CG2	-5.85	97.94	110.80
1	A	39	ARG	CB-CG-CD	5.84	124.74	111.30
1	A	55	CYS	O-C-N	-5.79	116.88	123.48
1	A	61	ASN	CA-C-O	5.70	128.33	121.66
1	A	4	HIS	CB-CG-CD2	-5.70	123.80	131.20
1	A	11	THR	CA-CB-CG2	5.64	120.09	110.50
1	A	19	GLY	CA-C-N	-5.63	110.37	121.41
1	A	19	GLY	C-N-CA	-5.63	110.37	121.41
1	A	29	TRP	CD1-NE1-CE2	5.57	118.92	108.90
1	A	10	GLN	CA-C-O	5.39	128.21	120.51
1	A	48	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	32	HIS	CB-CA-C	-5.32	99.84	110.42
1	A	33	ARG	O-C-N	5.31	129.65	122.59
1	A	30	ARG	CD-NE-CZ	-5.30	116.99	124.40
1	A	23	ASN	CB-CG-OD1	5.28	131.37	120.80
1	A	29	TRP	NE1-CE2-CZ2	5.16	137.85	130.10
1	A	46	VAL	CA-CB-CG1	-5.16	101.62	110.40
1	A	5	ASN	CA-C-N	5.12	129.18	121.40
1	A	5	ASN	C-N-CA	5.12	129.18	121.40
1	A	32	HIS	CA-C-O	5.05	127.73	120.51
1	A	14	THR	OG1-CB-CG2	-5.04	99.21	109.30

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	15	THR	CB
1	A	22	THR	CB
1	A	32	HIS	CA
1	A	45	SER	CA
1	A	46	VAL	CA
1	A	62	ASN	CA

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	33	ARG	Sidechain
1	A	39	ARG	Sidechain

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	480	438	414	305
All	All	480	438	414	305

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 341.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:59:ARG:CZ	1:A:59:ARG:CD	1.65	1.74
1:A:27:LYS:CB	1:A:27:LYS:CD	1.57	1.82
1:A:59:ARG:CD	1:A:59:ARG:CB	1.57	1.83
1:A:15:THR:CG2	1:A:15:THR:CA	1.55	1.82
1:A:61:ASN:CG	1:A:61:ASN:CA	1.55	1.76
1:A:26:LYS:CE	1:A:26:LYS:CG	1.54	1.82
1:A:28:ARG:CD	1:A:28:ARG:CZ	1.53	1.80
1:A:38:GLU:CB	1:A:38:GLU:CD	1.48	1.82
1:A:1:LEU:HG	1:A:1:LEU:CA	1.45	0.97
1:A:2:GLU:CB	1:A:2:GLU:CD	1.45	1.90
1:A:2:GLU:OE2	1:A:2:GLU:CG	1.45	1.65
1:A:10:GLN:CD	1:A:10:GLN:CB	1.44	1.87
1:A:23:ASN:ND2	1:A:23:ASN:CB	1.44	1.80
1:A:22:THR:CG2	1:A:22:THR:CA	1.43	1.97
1:A:6:GLN:CB	1:A:6:GLN:CD	1.42	1.91
1:A:18:SER:C	1:A:19:GLY:CA	1.41	1.93
1:A:26:LYS:CB	1:A:26:LYS:CD	1.41	1.97
1:A:15:THR:CA	1:A:15:THR:OG1	1.40	1.70
1:A:36:ARG:CD	1:A:36:ARG:CB	1.39	1.98
1:A:58:ASP:OD1	1:A:58:ASP:CB	1.39	1.68
1:A:9:SER:O	1:A:10:GLN:CA	1.38	1.68
1:A:6:GLN:CG	1:A:6:GLN:CA	1.36	2.00
1:A:48:ASN:CG	1:A:48:ASN:CA	1.35	1.97

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:28:ARG:NH2	1:A:28:ARG:NE	1.34	1.72
1:A:61:ASN:CA	1:A:61:ASN:OD1	1.34	1.74
1:A:53:ASN:ND2	1:A:53:ASN:CB	1.32	1.93
1:A:53:ASN:CB	1:A:53:ASN:OD1	1.31	1.77
1:A:18:SER:O	1:A:18:SER:CA	1.31	1.78
1:A:6:GLN:CG	1:A:6:GLN:NE2	1.30	1.95
1:A:51:GLU:CD	1:A:51:GLU:CB	1.29	2.06
1:A:28:ARG:NE	1:A:28:ARG:CG	1.28	1.96
1:A:17:CYS:SG	1:A:41:CYS:CB	1.28	2.22
1:A:8:SER:C	1:A:9:SER:CA	1.25	2.09
1:A:59:ARG:CG	1:A:59:ARG:CA	1.23	2.15
1:A:9:SER:C	1:A:10:GLN:CA	1.22	2.13
1:A:27:LYS:CG	1:A:27:LYS:CA	1.21	2.18
1:A:18:SER:CA	1:A:19:GLY:N	1.21	1.96
1:A:9:SER:O	1:A:9:SER:CA	1.20	1.89
1:A:38:GLU:CG	1:A:38:GLU:CA	1.20	2.19
1:A:39:ARG:CG	1:A:39:ARG:CA	1.20	2.19
1:A:58:ASP:CB	1:A:58:ASP:OD2	1.19	1.89
1:A:61:ASN:CA	1:A:61:ASN:ND2	1.18	2.06
1:A:2:GLU:CG	1:A:2:GLU:CA	1.17	2.21
1:A:41:CYS:SG	1:A:41:CYS:CA	1.15	2.32
1:A:8:SER:O	1:A:8:SER:CA	1.15	1.94
1:A:6:GLN:CG	1:A:6:GLN:OE1	1.14	1.93
1:A:26:LYS:CG	1:A:26:LYS:CA	1.14	2.23
1:A:8:SER:CA	1:A:8:SER:OG	1.12	1.96
1:A:5:ASN:CG	1:A:5:ASN:CA	1.07	2.27
1:A:8:SER:CA	1:A:9:SER:N	1.07	2.12
1:A:9:SER:CA	1:A:10:GLN:N	1.07	2.16
1:A:48:ASN:CG	1:A:48:ASN:HB3	1.06	1.54
1:A:48:ASN:CG	1:A:48:ASN:HB2	1.06	1.54
1:A:15:THR:OG1	1:A:15:THR:HB	1.05	1.37
1:A:59:ARG:CZ	1:A:59:ARG:HD3	0.99	1.87
1:A:15:THR:OG1	1:A:15:THR:HG23	0.98	1.23
1:A:48:ASN:CG	1:A:48:ASN:CB	0.98	0.94
1:A:46:VAL:O	1:A:46:VAL:HG12	0.98	1.46
1:A:15:THR:CG2	1:A:15:THR:OG1	0.98	0.68
1:A:27:LYS:CB	1:A:27:LYS:HD3	0.96	1.89
1:A:61:ASN:ND2	1:A:61:ASN:HB2	0.96	1.35
1:A:39:ARG:CG	1:A:39:ARG:HB3	0.95	1.51
1:A:61:ASN:OD1	1:A:61:ASN:HB3	0.95	1.18
1:A:5:ASN:CG	1:A:5:ASN:HB3	0.94	1.44
1:A:5:ASN:CG	1:A:5:ASN:CB	0.94	0.90

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:26:LYS:CG	1:A:26:LYS:HB3	0.94	1.50
1:A:26:LYS:CG	1:A:26:LYS:HB2	0.94	1.50
1:A:39:ARG:CG	1:A:39:ARG:HB2	0.94	1.51
1:A:1:LEU:HG	1:A:1:LEU:HA	0.93	1.37
1:A:26:LYS:CG	1:A:26:LYS:CB	0.93	0.94
1:A:39:ARG:CG	1:A:39:ARG:CB	0.93	0.93
1:A:5:ASN:CG	1:A:5:ASN:HB2	0.93	1.44
1:A:38:GLU:CG	1:A:38:GLU:HB2	0.92	1.45
1:A:17:CYS:HG	1:A:41:CYS:CB	0.92	1.67
1:A:15:THR:OG1	1:A:15:THR:HG22	0.92	1.60
1:A:28:ARG:NH2	1:A:28:ARG:HH11	0.91	1.53
1:A:38:GLU:CG	1:A:38:GLU:HB3	0.91	1.45
1:A:38:GLU:CB	1:A:38:GLU:HG2	0.91	1.44
1:A:28:ARG:NE	1:A:28:ARG:HD3	0.90	1.30
1:A:41:CYS:CB	1:A:41:CYS:SG	0.90	0.83
1:A:51:GLU:CD	1:A:51:GLU:HG3	0.90	1.39
1:A:38:GLU:CB	1:A:38:GLU:HG3	0.90	1.44
1:A:51:GLU:CD	1:A:51:GLU:HG2	0.90	1.39
1:A:28:ARG:NE	1:A:28:ARG:HD2	0.89	1.30
1:A:8:SER:OG	1:A:8:SER:HB2	0.89	1.15
1:A:26:LYS:CB	1:A:26:LYS:HG2	0.89	1.44
1:A:36:ARG:CD	1:A:36:ARG:HG2	0.88	1.41
1:A:8:SER:OG	1:A:8:SER:HB3	0.88	1.15
1:A:51:GLU:CD	1:A:51:GLU:CG	0.88	0.83
1:A:38:GLU:CB	1:A:38:GLU:CG	0.88	0.88
1:A:15:THR:CG2	1:A:15:THR:HB	0.87	1.44
1:A:26:LYS:CB	1:A:26:LYS:HG3	0.87	1.44
1:A:36:ARG:CD	1:A:36:ARG:HG3	0.87	1.41
1:A:22:THR:CB	1:A:22:THR:HG22	0.86	1.40
1:A:22:THR:CG2	1:A:22:THR:HB	0.86	1.41
1:A:41:CYS:CB	1:A:41:CYS:HG	0.86	1.67
1:A:47:LYS:CD	1:A:50:ILE:HD11	0.86	2.01
1:A:36:ARG:CG	1:A:36:ARG:HD3	0.86	1.40
1:A:22:THR:CB	1:A:22:THR:HG21	0.85	1.40
1:A:22:THR:CB	1:A:22:THR:HG23	0.85	1.40
1:A:1:LEU:CG	1:A:1:LEU:HB3	0.85	1.39
1:A:6:GLN:CD	1:A:6:GLN:OE1	0.85	0.61
1:A:28:ARG:CD	1:A:28:ARG:NE	0.85	0.76
1:A:36:ARG:CG	1:A:36:ARG:HD2	0.85	1.40
1:A:1:LEU:CG	1:A:1:LEU:HB2	0.85	1.39
1:A:28:ARG:CZ	1:A:28:ARG:NH2	0.85	0.72
1:A:27:LYS:HD3	1:A:27:LYS:HB2	0.84	1.42

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:36:ARG:CD	1:A:36:ARG:CG	0.84	0.86
1:A:1:LEU:CG	1:A:1:LEU:HD21	0.83	1.36
1:A:22:THR:HG23	1:A:22:THR:HG1	0.83	0.86
1:A:61:ASN:ND2	1:A:61:ASN:CB	0.83	0.68
1:A:10:GLN:CD	1:A:10:GLN:HE22	0.82	1.48
1:A:1:LEU:CG	1:A:1:LEU:HD23	0.82	1.36
1:A:27:LYS:CB	1:A:27:LYS:HG3	0.82	1.36
1:A:1:LEU:HG	1:A:1:LEU:C	0.82	1.95
1:A:10:GLN:CD	1:A:10:GLN:HE21	0.81	1.48
1:A:8:SER:OG	1:A:8:SER:CB	0.81	0.55
1:A:47:LYS:HB3	1:A:50:ILE:HD11	0.81	1.53
1:A:59:ARG:CB	1:A:59:ARG:HD3	0.81	2.03
1:A:1:LEU:CG	1:A:1:LEU:HD22	0.81	1.36
1:A:27:LYS:CB	1:A:27:LYS:HG2	0.81	1.36
1:A:15:THR:OG1	1:A:15:THR:CB	0.80	0.50
1:A:27:LYS:CG	1:A:27:LYS:HB3	0.79	1.33
1:A:36:ARG:HD2	1:A:36:ARG:NE	0.79	1.37
1:A:1:LEU:CG	1:A:1:LEU:CB	0.79	0.79
1:A:15:THR:OG1	1:A:15:THR:HG21	0.79	1.03
1:A:36:ARG:HD3	1:A:36:ARG:NE	0.79	1.37
1:A:27:LYS:CG	1:A:27:LYS:HB2	0.79	1.33
1:A:61:ASN:CG	1:A:61:ASN:C	0.78	2.50
1:A:39:ARG:CB	1:A:39:ARG:HG2	0.78	1.52
1:A:61:ASN:ND2	1:A:61:ASN:HB3	0.78	1.17
1:A:10:GLN:CD	1:A:10:GLN:HG3	0.78	1.26
1:A:15:THR:HG23	1:A:15:THR:CB	0.77	1.31
1:A:10:GLN:CD	1:A:10:GLN:HG2	0.77	1.26
1:A:15:THR:HG22	1:A:15:THR:CB	0.76	1.31
1:A:9:SER:C	1:A:10:GLN:N	0.76	0.73
1:A:44:PRO:O	1:A:45:SER:HB3	0.76	1.55
1:A:53:ASN:OD1	1:A:53:ASN:CG	0.76	0.53
1:A:15:THR:CB	1:A:15:THR:HG21	0.76	1.31
1:A:27:LYS:CB	1:A:27:LYS:CG	0.76	0.77
1:A:59:ARG:CG	1:A:59:ARG:HB2	0.75	1.29
1:A:38:GLU:CB	1:A:38:GLU:OE1	0.75	2.07
1:A:58:ASP:OD1	1:A:58:ASP:CA	0.75	2.34
1:A:26:LYS:CD	1:A:26:LYS:HE2	0.75	1.29
1:A:59:ARG:CG	1:A:59:ARG:HB3	0.74	1.29
1:A:61:ASN:OD1	1:A:61:ASN:HB2	0.74	0.98
1:A:10:GLN:CD	1:A:10:GLN:NE2	0.74	0.85
1:A:15:THR:CG2	1:A:15:THR:HG1	0.74	1.45
1:A:39:ARG:CB	1:A:39:ARG:HG3	0.74	1.52

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:47:LYS:HD2	1:A:50:ILE:HD11	0.74	1.59
1:A:53:ASN:ND2	1:A:53:ASN:CG	0.74	0.68
1:A:22:THR:HG21	1:A:22:THR:HG1	0.74	0.82
1:A:23:ASN:CG	1:A:23:ASN:HD22	0.74	1.40
1:A:59:ARG:CB	1:A:59:ARG:HG2	0.73	1.27
1:A:59:ARG:CB	1:A:59:ARG:HG3	0.73	1.27
1:A:22:THR:CG2	1:A:22:THR:CB	0.73	0.73
1:A:23:ASN:CG	1:A:23:ASN:HD21	0.73	1.40
1:A:47:LYS:CB	1:A:50:ILE:HD11	0.73	2.12
1:A:26:LYS:CE	1:A:26:LYS:HZ1	0.72	1.43
1:A:2:GLU:CG	1:A:2:GLU:HB2	0.72	1.26
1:A:26:LYS:CD	1:A:26:LYS:HE3	0.72	1.29
1:A:2:GLU:CG	1:A:2:GLU:HB3	0.72	1.26
1:A:23:ASN:ND2	1:A:23:ASN:CG	0.72	0.76
1:A:26:LYS:CB	1:A:26:LYS:HD3	0.72	2.11
1:A:53:ASN:ND2	1:A:53:ASN:OD1	0.72	0.59
1:A:26:LYS:HE2	1:A:26:LYS:NZ	0.72	1.38
1:A:26:LYS:CE	1:A:26:LYS:HD3	0.71	1.25
1:A:2:GLU:CB	1:A:2:GLU:HG3	0.71	1.25
1:A:2:GLU:CB	1:A:2:GLU:HG2	0.71	1.25
1:A:26:LYS:CE	1:A:26:LYS:HD2	0.71	1.25
1:A:26:LYS:CE	1:A:26:LYS:HZ3	0.71	1.43
1:A:31:ASP:O	1:A:34:GLY:N	0.70	2.24
1:A:26:LYS:CE	1:A:26:LYS:HZ2	0.70	1.43
1:A:36:ARG:CZ	1:A:36:ARG:HH21	0.70	1.40
1:A:26:LYS:CE	1:A:26:LYS:NZ	0.70	0.86
1:A:2:GLU:CD	1:A:2:GLU:OE2	0.70	0.54
1:A:59:ARG:CB	1:A:59:ARG:CG	0.70	0.72
1:A:6:GLN:CD	1:A:6:GLN:NE2	0.70	0.64
1:A:41:CYS:SG	1:A:41:CYS:HB2	0.69	1.32
1:A:58:ASP:OD1	1:A:58:ASP:CG	0.69	0.65
1:A:22:THR:CG2	1:A:22:THR:HG1	0.69	0.66
1:A:59:ARG:HB3	1:A:59:ARG:HG2	0.69	0.96
1:A:1:LEU:HG	1:A:1:LEU:CB	0.69	0.63
1:A:36:ARG:HD3	1:A:36:ARG:NH1	0.69	1.68
1:A:61:ASN:CB	1:A:61:ASN:HD21	0.69	1.41
1:A:36:ARG:CZ	1:A:36:ARG:HH22	0.69	1.40
1:A:26:LYS:HE3	1:A:26:LYS:NZ	0.69	1.38
1:A:1:LEU:CG	1:A:1:LEU:CD2	0.68	0.68
1:A:41:CYS:SG	1:A:41:CYS:HB3	0.68	1.32
1:A:6:GLN:NE2	1:A:6:GLN:OE1	0.67	0.55
1:A:53:ASN:CG	1:A:53:ASN:HD21	0.67	1.34

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:10:GLN:CD	1:A:10:GLN:CG	0.67	0.71
1:A:1:LEU:CG	1:A:1:LEU:HD11	0.67	1.20
1:A:1:LEU:CG	1:A:1:LEU:HD13	0.67	1.20
1:A:1:LEU:CG	1:A:1:LEU:HD12	0.67	1.20
1:A:28:ARG:CZ	1:A:28:ARG:HH21	0.67	1.37
1:A:5:ASN:CG	1:A:5:ASN:HD21	0.67	1.32
1:A:26:LYS:CE	1:A:26:LYS:HG2	0.66	2.12
1:A:28:ARG:NH2	1:A:28:ARG:NH1	0.66	0.68
1:A:5:ASN:CG	1:A:5:ASN:HD22	0.66	1.32
1:A:47:LYS:HD3	1:A:50:ILE:HD11	0.66	1.67
1:A:3:CYS:SG	1:A:24:CYS:CB	0.66	2.70
1:A:53:ASN:CG	1:A:53:ASN:HD22	0.65	1.34
1:A:58:ASP:OD2	1:A:58:ASP:CG	0.65	0.79
1:A:61:ASN:OD1	1:A:61:ASN:CB	0.65	0.36
1:A:6:GLN:CD	1:A:6:GLN:HE21	0.65	1.30
1:A:9:SER:O	1:A:9:SER:C	0.65	0.46
1:A:23:ASN:HA	1:A:56:THR:HG22	0.65	1.68
1:A:6:GLN:CB	1:A:6:GLN:HG3	0.65	1.18
1:A:28:ARG:HD2	1:A:28:ARG:HE	0.65	0.95
1:A:2:GLU:CB	1:A:2:GLU:CG	0.64	0.77
1:A:6:GLN:CD	1:A:6:GLN:HE22	0.64	1.30
1:A:1:LEU:CA	1:A:1:LEU:CG	0.64	1.90
1:A:59:ARG:CZ	1:A:59:ARG:HE	0.64	1.34
1:A:6:GLN:CG	1:A:6:GLN:HB3	0.64	1.17
1:A:6:GLN:CB	1:A:6:GLN:HG2	0.64	1.18
1:A:6:GLN:CG	1:A:6:GLN:HB2	0.63	1.17
1:A:28:ARG:NH2	1:A:28:ARG:HE	0.63	1.88
1:A:29:TRP:CD1	1:A:29:TRP:N	0.62	2.61
1:A:36:ARG:CD	1:A:36:ARG:HE	0.62	1.38
1:A:8:SER:C	1:A:9:SER:N	0.62	0.69
1:A:59:ARG:CZ	1:A:59:ARG:HD2	0.62	2.12
1:A:36:ARG:CZ	1:A:36:ARG:HE	0.62	1.42
1:A:8:SER:C	1:A:8:SER:O	0.62	0.51
1:A:18:SER:C	1:A:20:GLY:N	0.61	2.57
1:A:2:GLU:HB2	1:A:2:GLU:HG2	0.61	0.99
1:A:15:THR:CG2	1:A:15:THR:CB	0.61	0.61
1:A:8:SER:HA	1:A:37:THR:OG1	0.61	1.96
1:A:36:ARG:CZ	1:A:36:ARG:NH2	0.60	0.76
1:A:2:GLU:OE2	1:A:2:GLU:HG2	0.60	1.88
1:A:61:ASN:CG	1:A:61:ASN:HB2	0.59	1.08
1:A:61:ASN:CG	1:A:61:ASN:HB3	0.59	1.08
1:A:18:SER:HA	1:A:19:GLY:N	0.59	2.08

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:61:ASN:OD1	1:A:61:ASN:ND2	0.58	0.43
1:A:2:GLU:HB3	1:A:2:GLU:HG3	0.58	0.99
1:A:52:ILE:HD13	1:A:52:ILE:N	0.58	2.13
1:A:6:GLN:HB3	1:A:6:GLN:HG2	0.58	0.86
1:A:61:ASN:OD1	1:A:61:ASN:C	0.58	2.45
1:A:23:ASN:HA	1:A:56:THR:CG2	0.57	2.29
1:A:26:LYS:CE	1:A:26:LYS:CD	0.56	0.74
1:A:31:ASP:O	1:A:33:ARG:N	0.56	2.35
1:A:42:GLY:O	1:A:43:CYS:HB2	0.56	2.00
1:A:52:ILE:N	1:A:52:ILE:CD1	0.56	2.69
1:A:22:THR:CG2	1:A:22:THR:N	0.56	2.65
1:A:5:ASN:CG	1:A:5:ASN:ND2	0.56	0.66
1:A:2:GLU:OE2	1:A:2:GLU:HG3	0.56	1.86
1:A:48:ASN:CG	1:A:48:ASN:HD21	0.56	1.21
1:A:1:LEU:CG	1:A:1:LEU:C	0.55	2.67
1:A:61:ASN:CB	1:A:61:ASN:HD22	0.55	1.25
1:A:48:ASN:CG	1:A:48:ASN:HD22	0.54	1.21
1:A:18:SER:C	1:A:19:GLY:N	0.54	0.65
1:A:44:PRO:C	1:A:45:SER:HB3	0.53	1.42
1:A:47:LYS:O	1:A:48:ASN:HB2	0.53	2.03
1:A:28:ARG:NH2	1:A:28:ARG:HH12	0.53	0.63
1:A:15:THR:CG2	1:A:15:THR:N	0.53	2.65
1:A:33:ARG:CZ	1:A:33:ARG:HH11	0.53	1.23
1:A:26:LYS:CG	1:A:26:LYS:C	0.52	2.81
1:A:6:GLN:CG	1:A:6:GLN:C	0.52	2.78
1:A:22:THR:CG2	1:A:22:THR:OG1	0.52	0.82
1:A:36:ARG:HD3	1:A:36:ARG:HH11	0.52	1.25
1:A:7:GLN:O	1:A:8:SER:C	0.52	2.40
1:A:8:SER:C	1:A:9:SER:CB	0.51	2.78
1:A:59:ARG:CZ	1:A:59:ARG:NE	0.51	0.84
1:A:36:ARG:HD2	1:A:36:ARG:HH11	0.50	1.40
1:A:18:SER:C	1:A:18:SER:O	0.50	0.47
1:A:6:GLN:CB	1:A:6:GLN:CG	0.50	0.57
1:A:28:ARG:CD	1:A:28:ARG:HE	0.49	1.20
1:A:47:LYS:CD	1:A:50:ILE:CD1	0.49	2.83
1:A:59:ARG:CB	1:A:59:ARG:HD2	0.49	2.18
1:A:26:LYS:HG2	1:A:26:LYS:C	0.48	2.31
1:A:47:LYS:HD3	1:A:50:ILE:CD1	0.48	2.36
1:A:9:SER:O	1:A:10:GLN:CB	0.48	2.47
1:A:36:ARG:CD	1:A:36:ARG:HH11	0.48	1.42
1:A:51:GLU:C	1:A:52:ILE:HD13	0.48	2.34
1:A:9:SER:C	1:A:10:GLN:CB	0.48	2.83

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:26:LYS:HE2	1:A:26:LYS:HD3	0.47	1.14
1:A:48:ASN:CG	1:A:48:ASN:C	0.47	2.77
1:A:59:ARG:CZ	1:A:59:ARG:HH21	0.47	1.18
1:A:15:THR:OG1	1:A:15:THR:C	0.47	2.48
1:A:59:ARG:CZ	1:A:59:ARG:HH22	0.47	1.18
1:A:18:SER:O	1:A:18:SER:CB	0.46	2.44
1:A:50:ILE:HG13	1:A:52:ILE:CD1	0.46	2.40
1:A:59:ARG:HD3	1:A:59:ARG:HB2	0.46	1.73
1:A:15:THR:OG1	1:A:15:THR:N	0.45	2.40
1:A:48:ASN:CG	1:A:48:ASN:HA	0.45	2.19
1:A:9:SER:O	1:A:10:GLN:N	0.45	0.33
1:A:60:CYS:O	1:A:60:CYS:SG	0.45	2.75
1:A:42:GLY:O	1:A:43:CYS:CB	0.44	2.59
1:A:36:ARG:CZ	1:A:36:ARG:HH12	0.44	1.15
1:A:59:ARG:CZ	1:A:59:ARG:HH11	0.44	1.14
1:A:8:SER:CB	1:A:8:SER:HG	0.44	1.15
1:A:31:ASP:O	1:A:34:GLY:CA	0.43	2.65
1:A:59:ARG:CZ	1:A:59:ARG:HH12	0.43	1.14
1:A:22:THR:C	1:A:23:ASN:CG	0.43	2.80
1:A:36:ARG:CZ	1:A:36:ARG:HH11	0.43	1.15
1:A:50:ILE:HG13	1:A:52:ILE:HD12	0.42	1.90
1:A:48:ASN:CG	1:A:48:ASN:ND2	0.42	0.52
1:A:61:ASN:CG	1:A:61:ASN:HD21	0.42	1.08
1:A:61:ASN:CG	1:A:61:ASN:HD22	0.42	1.08
1:A:58:ASP:O	1:A:59:ARG:C	0.42	2.60
1:A:61:ASN:CG	1:A:61:ASN:N	0.41	2.67
1:A:6:GLN:HB3	1:A:12:PRO:HA	0.40	1.93
1:A:15:THR:CB	1:A:15:THR:HG1	0.40	1.11
1:A:39:ARG:CA	1:A:39:ARG:HG3	0.40	2.16
1:A:53:ASN:OD1	1:A:53:ASN:CA	0.40	2.60

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	60/62 (97%)	42 (70%)	11 (18%)	7 (12%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	60/62 (97%)	42 (70%)	11 (18%)	7 (12%)	1 7

All 7 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	8	SER
1	A	19	GLY
1	A	32	HIS
1	A	43	CYS
1	A	46	VAL
1	A	47	LYS
1	A	58	ASP

6.3.2 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 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	55/55 (100%)	31 (56%)	24 (44%)	0 3
All	All	55/55 (100%)	31 (56%)	24 (44%)	0 3

All 24 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	2	GLU
1	A	6	GLN
1	A	7	GLN
1	A	8	SER
1	A	10	GLN
1	A	11	THR
1	A	13	THR
1	A	14	THR
1	A	15	THR
1	A	18	SER
1	A	25	TYR
1	A	28	ARG

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Mol	Chain	Res	Type
1	A	29	TRP
1	A	30	ARG
1	A	32	HIS
1	A	35	TYR
1	A	36	ARG
1	A	41	CYS
1	A	43	CYS
1	A	45	SER
1	A	46	VAL
1	A	52	ILE
1	A	57	THR
1	A	59	ARG

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

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	A	25

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	21:GLU	C	22:THR	N	1.18
1	A	29:TRP	C	30:ARG	N	1.18
1	A	30:ARG	C	31:ASP	N	1.17
1	A	15:THR	C	16:GLY	N	1.14
1	A	7:GLN	C	8:SER	N	1.13
1	A	20:GLY	C	21:GLU	N	1.11
1	A	46:VAL	C	47:LYS	N	1.09
1	A	47:LYS	C	48:ASN	N	1.09
1	A	31:ASP	C	32:HIS	N	1.04
1	A	5:ASN	C	6:GLN	N	1.03
1	A	61:ASN	C	62:ASN	N	0.99
1	A	10:GLN	C	11:THR	N	0.98
1	A	16:GLY	C	17:CYS	N	0.98
1	A	17:CYS	C	18:SER	N	0.96
1	A	6:GLN	C	7:GLN	N	0.94
1	A	40:GLY	C	41:CYS	N	0.94
1	A	57:THR	C	58:ASP	N	0.94
1	A	43:CYS	C	44:PRO	N	0.92
1	A	19:GLY	C	20:GLY	N	0.90
1	A	34:GLY	C	35:TYR	N	0.88
1	A	32:HIS	C	33:ARG	N	0.83
1	A	9:SER	C	10:GLN	N	0.73
1	A	8:SER	C	9:SER	N	0.69
1	A	18:SER	C	19:GLY	N	0.65
1	A	45:SER	C	46:VAL	N	0.55

7 Chemical shift validation

No chemical shift data were provided