



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 01:52 PM BST

PDB ID : 1COD
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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

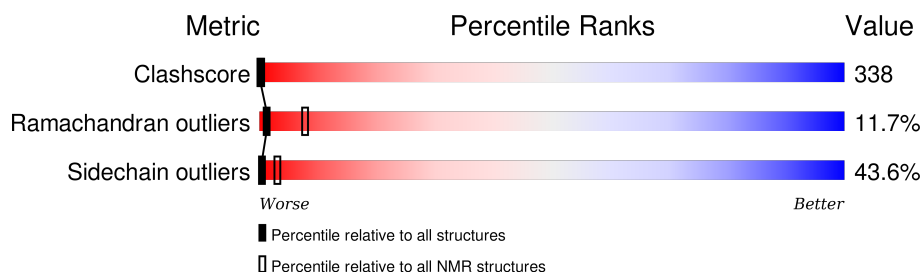
1 Overall quality at a glance

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 $\leq 5\%$

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.

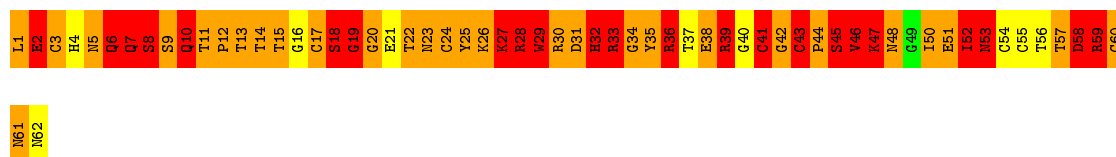
Mol	Chain	Residues	Atoms						Trace
1	A	62	Total	C	H	N	O	S	0
			918	277	438	97	98	8	

4 Residue-property plots

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: COBROTOXIN

Chain A:  15% 47% 37%



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. 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	25.51	282/487 (57.9%)	15.52	245/653 (37.5%)
All	All	25.51	282/487 (57.9%)	15.52	245/653 (37.5%)

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	51	GLU	CD-OE2	-104.71	0.10	1.25
1	A	9	SER	CB-OG	-85.08	0.31	1.42
1	A	21	GLU	CD-OE2	-83.67	0.33	1.25
1	A	25	TYR	CG-CD2	-79.06	0.36	1.39
1	A	25	TYR	CE1-CZ	-78.66	0.36	1.38
1	A	2	GLU	CD-OE1	-78.63	0.39	1.25
1	A	45	SER	CA-CB	-76.28	0.38	1.52
1	A	33	ARG	CZ-NH2	-72.79	0.38	1.33
1	A	45	SER	CB-OG	-71.99	0.48	1.42
1	A	59	ARG	CZ-NH1	-68.88	0.43	1.33
1	A	36	ARG	CZ-NH1	-67.52	0.45	1.33
1	A	38	GLU	CD-OE1	-67.26	0.51	1.25
1	A	8	SER	CB-OG	-66.70	0.55	1.42
1	A	21	GLU	CG-CD	-65.29	0.54	1.51
1	A	35	TYR	CG-CD1	-65.00	0.54	1.39
1	A	59	ARG	CZ-NH2	-64.97	0.48	1.33
1	A	2	GLU	CD-OE2	-64.72	0.54	1.25
1	A	35	TYR	CE2-CZ	-64.47	0.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ARG	CZ-NH1	-63.32	0.50	1.33
1	A	30	ARG	CZ-NH2	-63.15	0.51	1.33
1	A	21	GLU	CD-OE1	-62.96	0.56	1.25
1	A	39	ARG	CZ-NH2	-60.03	0.55	1.33
1	A	33	ARG	CZ-NH1	-59.59	0.55	1.33
1	A	41	CYS	CB-SG	-58.25	0.83	1.82
1	A	51	GLU	CD-OE1	-57.69	0.62	1.25
1	A	18	SER	CB-OG	-57.66	0.67	1.42
1	A	25	TYR	CG-CD1	-56.80	0.65	1.39
1	A	39	ARG	NE-CZ	-56.67	0.59	1.33
1	A	25	TYR	CE2-CZ	-56.33	0.65	1.38
1	A	38	GLU	CD-OE2	-55.12	0.65	1.25
1	A	62	ASN	C-OXT	-52.98	0.22	1.23
1	A	30	ARG	CZ-NH1	-52.05	0.65	1.33
1	A	32	HIS	CE1-NE2	-52.02	0.12	1.32
1	A	33	ARG	CD-NE	-51.65	0.58	1.46
1	A	61	ASN	CB-CG	-50.28	0.35	1.51
1	A	61	ASN	CG-OD1	-50.05	0.13	1.24
1	A	22	THR	CB-OG1	-48.79	0.45	1.43
1	A	39	ARG	CD-NE	-48.41	0.64	1.46
1	A	35	TYR	CB-CG	-47.20	0.80	1.51
1	A	28	ARG	CZ-NH2	-46.56	0.72	1.33
1	A	15	THR	CB-OG1	-46.30	0.50	1.43
1	A	32	HIS	CG-CD2	-46.24	0.57	1.35
1	A	35	TYR	CG-CD2	-46.21	0.79	1.39
1	A	35	TYR	CE1-CZ	-45.62	0.79	1.38
1	A	51	GLU	CG-CD	-45.52	0.83	1.51
1	A	10	GLN	CD-OE1	-45.48	0.23	1.24
1	A	23	ASN	CG-OD1	-45.11	0.24	1.24
1	A	30	ARG	CD-NE	-44.89	0.70	1.46
1	A	33	ARG	NE-CZ	-44.04	0.75	1.33
1	A	36	ARG	CZ-NH2	-43.68	0.76	1.33
1	A	39	ARG	CZ-NH1	-43.68	0.76	1.33
1	A	30	ARG	NE-CZ	-43.39	0.76	1.33
1	A	35	TYR	CD1-CE1	-42.95	0.74	1.39
1	A	35	TYR	CD2-CE2	-42.82	0.75	1.39
1	A	4	HIS	CG-CD2	-42.34	0.63	1.35
1	A	5	ASN	CG-OD1	-42.26	0.30	1.24
1	A	45	SER	C-O	-41.80	0.43	1.23
1	A	34	GLY	C-O	-41.40	0.57	1.23
1	A	28	ARG	CD-NE	-41.06	0.76	1.46
1	A	9	SER	C-O	-40.38	0.46	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	GLN	CD-OE1	-40.06	0.35	1.24
1	A	18	SER	C-O	-39.86	0.47	1.23
1	A	47	LYS	CD-CE	-39.45	0.52	1.51
1	A	2	GLU	CB-CG	-39.38	0.77	1.52
1	A	61	ASN	CG-ND2	-39.01	0.35	1.32
1	A	44	PRO	C-O	-38.01	0.47	1.23
1	A	62	ASN	CA-C	-37.97	0.54	1.52
1	A	8	SER	C-O	-37.90	0.51	1.23
1	A	36	ARG	CD-NE	-37.87	0.82	1.46
1	A	35	TYR	CZ-OH	-37.59	0.73	1.37
1	A	18	SER	C-N	-37.55	0.65	1.33
1	A	62	ASN	CG-OD1	-37.18	0.42	1.24
1	A	59	ARG	NE-CZ	-37.15	0.84	1.33
1	A	47	LYS	CE-NZ	-37.06	0.56	1.49
1	A	32	HIS	CG-ND1	-36.77	0.57	1.38
1	A	31	ASP	CG-OD1	-36.60	0.41	1.25
1	A	62	ASN	C-O	-35.99	0.55	1.23
1	A	7	GLN	CD-NE2	-35.89	0.43	1.32
1	A	36	ARG	NE-CZ	-35.51	0.86	1.33
1	A	21	GLU	CB-CG	-35.13	0.85	1.52
1	A	6	GLN	CB-CG	-35.07	0.57	1.52
1	A	10	GLN	CG-CD	-34.83	0.70	1.51
1	A	32	HIS	CA-CB	-34.78	0.77	1.53
1	A	3	CYS	CB-SG	-34.74	1.23	1.82
1	A	33	ARG	CB-CG	-34.64	0.59	1.52
1	A	45	SER	C-N	-34.15	0.55	1.34
1	A	44	PRO	N-CD	-33.60	1.00	1.47
1	A	38	GLU	CB-CG	-33.57	0.88	1.52
1	A	48	ASN	CG-OD1	-33.07	0.51	1.24
1	A	47	LYS	CB-CG	-32.93	0.63	1.52
1	A	46	VAL	CB-CG2	-32.35	0.84	1.52
1	A	48	ASN	CG-ND2	-32.11	0.52	1.32
1	A	53	ASN	CG-OD1	-32.02	0.53	1.24
1	A	39	ARG	CG-CD	-31.93	0.72	1.51
1	A	46	VAL	CA-CB	-31.33	0.89	1.54
1	A	44	PRO	CA-CB	-31.29	0.91	1.53
1	A	46	VAL	C-O	-31.12	0.64	1.23
1	A	26	LYS	CD-CE	-30.89	0.74	1.51
1	A	31	ASP	CG-OD2	-30.80	0.54	1.25
1	A	25	TYR	CB-CG	-30.63	1.05	1.51
1	A	62	ASN	CA-CB	-30.02	0.75	1.53
1	A	4	HIS	CB-CG	-29.79	0.96	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLU	CG-CD	-29.79	1.07	1.51
1	A	59	ARG	CD-NE	-29.65	0.96	1.46
1	A	59	ARG	CB-CG	-29.62	0.72	1.52
1	A	55	CYS	CB-SG	-28.85	1.33	1.82
1	A	1	LEU	CG-CD1	-28.59	0.46	1.51
1	A	47	LYS	CG-CD	-28.53	0.55	1.52
1	A	18	SER	CA-CB	-28.52	1.10	1.52
1	A	6	GLN	CD-OE1	-28.49	0.61	1.24
1	A	8	SER	C-N	-28.09	0.69	1.34
1	A	27	LYS	CB-CG	-27.91	0.77	1.52
1	A	40	GLY	C-O	-27.85	0.79	1.23
1	A	30	ARG	CB-CG	-27.75	0.77	1.52
1	A	6	GLN	CD-NE2	-27.48	0.64	1.32
1	A	13	THR	CB-OG1	-27.45	0.88	1.43
1	A	15	THR	CB-CG2	-27.44	0.61	1.52
1	A	7	GLN	CG-CD	-27.43	0.88	1.51
1	A	25	TYR	CD2-CE2	-27.43	0.98	1.39
1	A	25	TYR	CD1-CE1	-27.39	0.98	1.39
1	A	20	GLY	N-CA	-26.84	1.05	1.46
1	A	32	HIS	CB-CG	-26.81	1.01	1.50
1	A	5	ASN	CG-ND2	-26.67	0.66	1.32
1	A	4	HIS	CE1-NE2	-26.57	0.71	1.32
1	A	19	GLY	CA-C	-26.50	1.09	1.51
1	A	9	SER	C-N	-26.46	0.73	1.34
1	A	5	ASN	CB-CG	-26.28	0.90	1.51
1	A	36	ARG	CG-CD	-26.27	0.86	1.51
1	A	33	ARG	C-O	-26.18	0.73	1.23
1	A	58	ASP	CG-OD1	-26.07	0.65	1.25
1	A	53	ASN	CG-ND2	-25.75	0.68	1.32
1	A	31	ASP	CB-CG	-25.62	0.97	1.51
1	A	2	GLU	CG-CD	-25.57	1.13	1.51
1	A	26	LYS	CE-NZ	-25.24	0.85	1.49
1	A	1	LEU	CB-CG	-25.17	0.79	1.52
1	A	60	CYS	CB-SG	-25.06	1.39	1.82
1	A	44	PRO	CA-C	-24.72	1.03	1.52
1	A	48	ASN	CB-CG	-24.63	0.94	1.51
1	A	57	THR	C-O	-24.41	0.77	1.23
1	A	33	ARG	CG-CD	-24.27	0.91	1.51
1	A	25	TYR	CZ-OH	-24.19	0.96	1.37
1	A	17	CYS	CB-SG	-24.14	1.41	1.82
1	A	20	GLY	C-O	-24.06	0.85	1.23
1	A	19	GLY	C-N	-23.79	0.90	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	THR	CB-CG2	-23.78	0.73	1.52
1	A	16	GLY	C-O	-23.61	0.85	1.23
1	A	33	ARG	CA-CB	-23.38	1.02	1.53
1	A	34	GLY	N-CA	-23.37	1.10	1.46
1	A	62	ASN	CB-CG	-23.30	0.97	1.51
1	A	14	THR	CB-OG1	-23.03	0.97	1.43
1	A	4	HIS	ND1-CE1	-22.77	0.77	1.34
1	A	23	ASN	CG-ND2	-22.63	0.76	1.32
1	A	1	LEU	CG-CD2	-22.42	0.68	1.51
1	A	27	LYS	CD-CE	-22.30	0.95	1.51
1	A	43	CYS	C-N	-22.16	0.92	1.34
1	A	32	HIS	C-N	-22.04	0.83	1.34
1	A	17	CYS	C-O	-22.04	0.81	1.23
1	A	28	ARG	NE-CZ	-22.00	1.04	1.33
1	A	39	ARG	CB-CG	-21.95	0.93	1.52
1	A	21	GLU	CA-CB	-21.84	1.05	1.53
1	A	32	HIS	CD2-NE2	-21.68	0.90	1.38
1	A	26	LYS	CB-CG	-21.64	0.94	1.52
1	A	43	CYS	C-O	-21.46	0.82	1.23
1	A	7	GLN	CB-CG	-21.16	0.95	1.52
1	A	32	HIS	C-O	-20.92	0.83	1.23
1	A	10	GLN	C-O	-20.80	0.83	1.23
1	A	45	SER	N-CA	-20.66	1.05	1.46
1	A	31	ASP	C-O	-20.40	0.84	1.23
1	A	58	ASP	CG-OD2	-19.89	0.79	1.25
1	A	46	VAL	CB-CG1	-19.86	1.11	1.52
1	A	23	ASN	CB-CG	-19.67	1.05	1.51
1	A	34	GLY	C-N	-19.66	0.88	1.34
1	A	30	ARG	CG-CD	-19.60	1.02	1.51
1	A	57	THR	CB-OG1	-19.50	1.04	1.43
1	A	4	HIS	CG-ND1	-19.45	0.95	1.38
1	A	32	HIS	ND1-CE1	-19.43	0.86	1.34
1	A	10	GLN	CD-NE2	-19.14	0.85	1.32
1	A	27	LYS	CE-NZ	-19.13	1.01	1.49
1	A	6	GLN	C-O	-18.97	0.87	1.23
1	A	62	ASN	CG-ND2	-18.84	0.85	1.32
1	A	33	ARG	N-CA	-18.60	1.09	1.46
1	A	11	THR	CB-OG1	-18.26	1.06	1.43
1	A	4	HIS	CD2-NE2	-17.85	0.98	1.38
1	A	47	LYS	CA-CB	-17.84	1.14	1.53
1	A	40	GLY	C-N	-17.36	0.94	1.34
1	A	57	THR	C-N	-17.35	0.94	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	LYS	C-O	-17.32	0.90	1.23
1	A	6	GLN	C-N	-17.27	0.94	1.34
1	A	14	THR	CB-CG2	-17.09	0.95	1.52
1	A	17	CYS	CA-CB	-16.96	1.16	1.53
1	A	29	TRP	CG-CD1	-16.69	1.13	1.36
1	A	19	GLY	C-O	-16.59	0.97	1.23
1	A	17	CYS	C-N	-16.18	0.96	1.34
1	A	33	ARG	CA-C	-16.11	1.11	1.52
1	A	54	CYS	CB-SG	-15.86	1.55	1.82
1	A	32	HIS	CA-C	-15.53	1.12	1.52
1	A	13	THR	CB-CG2	-15.52	1.01	1.52
1	A	61	ASN	C-O	-15.51	0.93	1.23
1	A	10	GLN	C-N	-15.47	0.98	1.34
1	A	16	GLY	C-N	-15.40	0.98	1.34
1	A	59	ARG	CG-CD	-15.19	1.14	1.51
1	A	7	GLN	C-O	-15.19	0.94	1.23
1	A	61	ASN	C-N	-14.92	0.99	1.34
1	A	5	ASN	C-O	-14.78	0.95	1.23
1	A	46	VAL	N-CA	-14.70	1.17	1.46
1	A	43	CYS	CB-SG	-14.60	1.57	1.82
1	A	15	THR	C-O	-13.58	0.97	1.23
1	A	24	CYS	CB-SG	-13.57	1.59	1.82
1	A	5	ASN	C-N	-13.30	1.03	1.34
1	A	58	ASP	CB-CG	-13.04	1.24	1.51
1	A	20	GLY	CA-C	-13.01	1.31	1.51
1	A	31	ASP	C-N	-12.66	1.04	1.34
1	A	26	LYS	CG-CD	-12.57	1.09	1.52
1	A	29	TRP	CD2-CE3	-12.50	1.21	1.40
1	A	29	TRP	CD2-CE2	-12.26	1.26	1.41
1	A	10	GLN	CB-CG	-12.19	1.19	1.52
1	A	57	THR	CB-CG2	-12.10	1.12	1.52
1	A	11	THR	CB-CG2	-12.02	1.12	1.52
1	A	52	ILE	CB-CG1	-11.97	1.20	1.54
1	A	45	SER	CA-C	-11.76	1.22	1.52
1	A	28	ARG	CG-CD	-11.59	1.23	1.51
1	A	1	LEU	CA-CB	-11.44	1.27	1.53
1	A	18	SER	N-CA	-11.35	1.23	1.46
1	A	36	ARG	CB-CG	-10.88	1.23	1.52
1	A	28	ARG	CB-CG	-10.87	1.23	1.52
1	A	19	GLY	N-CA	-10.72	1.29	1.46
1	A	46	VAL	C-N	-10.71	1.09	1.34
1	A	47	LYS	C-N	-10.55	1.09	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	TRP	NE1-CE2	-10.29	1.24	1.37
1	A	17	CYS	CA-C	-10.20	1.26	1.52
1	A	42	GLY	C-O	-10.19	1.07	1.23
1	A	15	THR	C-N	-10.18	1.14	1.33
1	A	52	ILE	CB-CG2	-10.01	1.21	1.52
1	A	9	SER	CA-CB	-9.96	1.38	1.52
1	A	27	LYS	CG-CD	-9.95	1.18	1.52
1	A	20	GLY	C-N	-9.91	1.11	1.34
1	A	51	GLU	CB-CG	-9.72	1.33	1.52
1	A	53	ASN	CB-CG	-9.41	1.29	1.51
1	A	29	TRP	CZ3-CH2	-9.34	1.25	1.40
1	A	21	GLU	C-O	-9.17	1.05	1.23
1	A	22	THR	C-O	-8.87	1.06	1.23
1	A	7	GLN	C-N	-8.75	1.14	1.34
1	A	21	GLU	N-CA	-8.66	1.29	1.46
1	A	29	TRP	CZ2-CH2	-8.64	1.21	1.37
1	A	31	ASP	CA-CB	-8.58	1.35	1.53
1	A	1	LEU	N-CA	-8.52	1.29	1.46
1	A	30	ARG	C-O	-8.33	1.07	1.23
1	A	15	THR	CA-CB	-8.18	1.32	1.53
1	A	46	VAL	CA-C	-8.16	1.31	1.52
1	A	47	LYS	N-CA	-8.01	1.30	1.46
1	A	10	GLN	CA-CB	-7.75	1.36	1.53
1	A	18	SER	CA-C	-7.70	1.32	1.52
1	A	30	ARG	C-N	-7.41	1.17	1.34
1	A	48	ASN	CA-CB	-7.15	1.34	1.53
1	A	22	THR	CA-CB	-6.97	1.35	1.53
1	A	8	SER	CA-CB	-6.97	1.42	1.52
1	A	44	PRO	CG-CD	-6.81	1.28	1.50
1	A	35	TYR	CA-CB	-6.69	1.39	1.53
1	A	29	TRP	C-N	-6.65	1.18	1.34
1	A	14	THR	C-O	-6.59	1.10	1.23
1	A	21	GLU	C-N	-6.59	1.18	1.34
1	A	30	ARG	CA-CB	-6.56	1.39	1.53
1	A	34	GLY	CA-C	-6.55	1.41	1.51
1	A	29	TRP	C-O	-6.45	1.11	1.23
1	A	50	ILE	CG1-CD1	-6.44	1.06	1.50
1	A	6	GLN	CG-CD	-6.28	1.36	1.51
1	A	47	LYS	CA-C	-5.92	1.37	1.52
1	A	16	GLY	N-CA	-5.88	1.37	1.46
1	A	44	PRO	C-N	-5.88	1.20	1.34
1	A	48	ASN	N-CA	-5.81	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ASN	CA-CB	-5.66	1.38	1.53
1	A	12	PRO	N-CD	-5.63	1.40	1.47
1	A	33	ARG	C-N	-5.53	1.23	1.33
1	A	11	THR	C-N	-5.45	1.23	1.34
1	A	55	CYS	C-O	-5.41	1.13	1.23
1	A	21	GLU	CA-C	-5.33	1.39	1.52
1	A	42	GLY	C-N	-5.33	1.21	1.34
1	A	11	THR	CA-CB	-5.32	1.39	1.53
1	A	1	LEU	C-O	-5.29	1.13	1.23
1	A	22	THR	N-CA	-5.28	1.35	1.46
1	A	55	CYS	C-N	-5.17	1.22	1.34
1	A	31	ASP	CA-C	-5.14	1.39	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	TYR	CB-CG-CD1	81.17	169.70	121.00
1	A	25	TYR	CD1-CG-CD2	-80.55	29.29	117.90
1	A	59	ARG	NE-CZ-NH2	77.11	158.86	120.30
1	A	59	ARG	NE-CZ-NH1	71.72	156.16	120.30
1	A	59	ARG	NH1-CZ-NH2	-67.65	44.98	119.40
1	A	28	ARG	NE-CZ-NH2	67.37	153.99	120.30
1	A	45	SER	O-C-N	-67.01	15.48	122.70
1	A	25	TYR	CB-CG-CD2	66.65	160.99	121.00
1	A	9	SER	O-C-N	-64.03	20.26	122.70
1	A	2	GLU	OE1-CD-OE2	-62.09	48.79	123.30
1	A	32	HIS	ND1-CG-CD2	-61.33	20.13	106.00
1	A	33	ARG	NE-CZ-NH1	61.17	150.88	120.30
1	A	8	SER	O-C-N	-60.74	25.51	122.70
1	A	25	TYR	CG-CD1-CE1	60.56	169.75	121.30
1	A	36	ARG	NE-CZ-NH2	57.00	148.80	120.30
1	A	25	TYR	CE1-CZ-CE2	-56.65	29.16	119.80
1	A	25	TYR	CZ-CE2-CD2	55.51	169.76	119.80
1	A	45	SER	N-CA-CB	-53.82	29.77	110.50
1	A	18	SER	O-C-N	-53.48	32.29	123.20
1	A	28	ARG	NH1-CZ-NH2	-49.65	64.79	119.40
1	A	25	TYR	CG-CD2-CE2	49.52	160.91	121.30
1	A	10	GLN	CG-CD-OE1	-49.29	23.01	121.60
1	A	39	ARG	NE-CZ-NH2	-47.21	96.69	120.30
1	A	25	TYR	CD1-CE1-CZ	45.92	161.13	119.80
1	A	32	HIS	CG-ND1-CE1	42.19	167.26	108.20
1	A	28	ARG	NE-CZ-NH1	41.86	141.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ARG	NH1-CZ-NH2	-41.60	73.64	119.40
1	A	30	ARG	NE-CZ-NH1	37.62	139.11	120.30
1	A	1	LEU	CB-CG-CD2	34.30	169.31	111.00
1	A	7	GLN	OE1-CD-NE2	-33.40	45.07	121.90
1	A	28	ARG	CD-NE-CZ	33.22	170.11	123.60
1	A	31	ASP	CB-CG-OD2	31.65	146.79	118.30
1	A	32	HIS	CG-CD2-NE2	30.66	167.46	109.20
1	A	6	GLN	OE1-CD-NE2	-30.44	51.88	121.90
1	A	33	ARG	NE-CZ-NH2	30.35	135.47	120.30
1	A	35	TYR	CB-CG-CD2	29.34	138.60	121.00
1	A	34	GLY	O-C-N	-28.99	76.31	122.70
1	A	1	LEU	CD1-CG-CD2	-28.77	24.19	110.50
1	A	53	ASN	OD1-CG-ND2	-28.57	56.19	121.90
1	A	51	GLU	OE1-CD-OE2	-28.27	89.38	123.30
1	A	41	CYS	CA-CB-SG	28.09	164.56	114.00
1	A	39	ARG	NE-CZ-NH1	27.92	134.26	120.30
1	A	2	GLU	CA-CB-CG	27.66	174.25	113.40
1	A	51	GLU	CG-CD-OE1	26.26	170.83	118.30
1	A	45	SER	CA-C-N	25.43	173.15	117.20
1	A	23	ASN	OD1-CG-ND2	-25.25	63.83	121.90
1	A	45	SER	CA-CB-OG	-25.22	43.10	111.20
1	A	38	GLU	OE1-CD-OE2	-24.88	93.44	123.30
1	A	9	SER	CA-C-N	24.72	171.59	117.20
1	A	18	SER	CA-C-N	24.69	165.57	116.20
1	A	45	SER	CB-CA-C	24.62	156.87	110.10
1	A	36	ARG	NH1-CZ-NH2	-24.59	92.35	119.40
1	A	45	SER	CA-C-O	24.41	171.37	120.10
1	A	59	ARG	CG-CD-NE	24.33	162.89	111.80
1	A	35	TYR	CB-CG-CD1	-23.63	106.82	121.00
1	A	10	GLN	CG-CD-NE2	23.53	173.17	116.70
1	A	44	PRO	CA-C-O	-23.35	64.15	120.20
1	A	8	SER	CA-C-N	23.30	168.45	117.20
1	A	2	GLU	CB-CG-CD	23.27	177.03	114.20
1	A	9	SER	CA-C-O	22.88	168.15	120.10
1	A	31	ASP	OD1-CG-OD2	-22.77	80.04	123.30
1	A	28	ARG	CG-CD-NE	22.47	158.98	111.80
1	A	6	GLN	CA-CB-CG	22.02	161.85	113.40
1	A	8	SER	CA-C-O	21.88	166.04	120.10
1	A	35	TYR	CG-CD2-CE2	21.68	138.64	121.30
1	A	47	LYS	CA-CB-CG	-21.58	65.93	113.40
1	A	1	LEU	CB-CG-CD1	21.55	147.63	111.00
1	A	57	THR	O-C-N	-21.44	88.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	SER	N-CA-C	21.32	168.57	111.00
1	A	35	TYR	CD1-CE1-CZ	21.04	138.74	119.80
1	A	8	SER	CA-CB-OG	21.00	167.91	111.20
1	A	27	LYS	CG-CD-CE	20.87	174.50	111.90
1	A	18	SER	C-N-CA	20.80	165.99	122.30
1	A	2	GLU	CG-CD-OE2	20.72	159.74	118.30
1	A	40	GLY	O-C-N	-20.71	89.57	122.70
1	A	45	SER	C-N-CA	20.69	173.43	121.70
1	A	58	ASP	CB-CG-OD2	20.26	136.53	118.30
1	A	9	SER	C-N-CA	20.06	171.85	121.70
1	A	23	ASN	CB-CG-ND2	20.04	164.81	116.70
1	A	18	SER	CA-C-O	20.02	162.14	120.10
1	A	59	ARG	CD-NE-CZ	20.00	151.59	123.60
1	A	33	ARG	CG-CD-NE	19.91	153.62	111.80
1	A	22	THR	CA-CB-CG2	19.86	140.21	112.40
1	A	35	TYR	CA-CB-CG	19.50	150.45	113.40
1	A	61	ASN	CB-CG-OD1	-19.44	82.72	121.60
1	A	8	SER	C-N-CA	18.91	168.97	121.70
1	A	30	ARG	NH1-CZ-NH2	-18.85	98.66	119.40
1	A	6	GLN	CB-CG-CD	18.77	160.42	111.60
1	A	59	ARG	CB-CG-CD	18.59	159.93	111.60
1	A	21	GLU	CG-CD-OE2	-18.57	81.15	118.30
1	A	26	LYS	CG-CD-CE	18.52	167.45	111.90
1	A	62	ASN	CA-C-O	18.49	158.92	120.10
1	A	32	HIS	CB-CG-ND1	18.47	169.37	123.20
1	A	15	THR	CA-CB-CG2	18.43	138.21	112.40
1	A	26	LYS	CD-CE-NZ	18.42	154.07	111.70
1	A	25	TYR	OH-CZ-CE2	18.40	169.77	120.10
1	A	10	GLN	OE1-CD-NE2	18.23	163.82	121.90
1	A	44	PRO	CA-C-N	18.21	157.25	117.20
1	A	10	GLN	CB-CG-CD	18.19	158.90	111.60
1	A	59	ARG	CA-CB-CG	18.11	153.24	113.40
1	A	35	TYR	CG-CD1-CE1	-18.10	106.82	121.30
1	A	44	PRO	N-CD-CG	-17.96	76.26	103.20
1	A	7	GLN	CG-CD-NE2	17.45	158.59	116.70
1	A	62	ASN	N-CA-CB	17.44	141.99	110.60
1	A	7	GLN	CG-CD-OE1	17.37	156.34	121.60
1	A	62	ASN	CB-CA-C	-17.25	75.91	110.40
1	A	5	ASN	OD1-CG-ND2	-17.22	82.30	121.90
1	A	48	ASN	OD1-CG-ND2	-16.89	83.04	121.90
1	A	61	ASN	CA-CB-CG	16.66	150.04	113.40
1	A	2	GLU	CG-CD-OE1	16.59	151.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASP	CB-CG-OD1	16.53	133.18	118.30
1	A	6	GLN	CG-CD-OE1	16.48	154.57	121.60
1	A	61	ASN	CB-CG-ND2	16.23	155.65	116.70
1	A	36	ARG	CG-CD-NE	16.00	145.40	111.80
1	A	26	LYS	CB-CG-CD	15.98	153.15	111.60
1	A	5	ASN	CB-CG-ND2	15.90	154.87	116.70
1	A	53	ASN	CB-CG-ND2	15.70	154.37	116.70
1	A	27	LYS	CA-CB-CG	15.52	147.55	113.40
1	A	6	GLN	O-C-N	-15.50	97.90	122.70
1	A	15	THR	OG1-CB-CG2	-15.46	74.44	110.00
1	A	6	GLN	CG-CD-NE2	15.36	153.55	116.70
1	A	21	GLU	CA-CB-CG	-15.27	79.80	113.40
1	A	25	TYR	CE1-CZ-OH	15.17	161.06	120.10
1	A	44	PRO	C-N-CA	14.72	158.50	121.70
1	A	34	GLY	CA-C-N	14.56	149.23	117.20
1	A	35	TYR	CZ-CE2-CD2	-14.46	106.79	119.80
1	A	46	VAL	N-CA-CB	-14.32	80.00	111.50
1	A	5	ASN	CA-CB-CG	14.30	144.86	113.40
1	A	10	GLN	O-C-N	-14.22	99.95	122.70
1	A	16	GLY	O-C-N	-14.06	100.20	122.70
1	A	53	ASN	CB-CG-OD1	13.92	149.44	121.60
1	A	27	LYS	CD-CE-NZ	13.85	143.56	111.70
1	A	4	HIS	CG-ND1-CE1	13.81	127.54	108.20
1	A	43	CYS	O-C-N	-13.77	94.93	121.10
1	A	33	ARG	CA-C-O	-13.40	91.96	120.10
1	A	62	ASN	CB-CG-ND2	13.33	148.69	116.70
1	A	32	HIS	CA-CB-CG	13.26	136.14	113.60
1	A	33	ARG	CD-NE-CZ	13.22	142.11	123.60
1	A	47	LYS	CB-CG-CD	-13.15	77.42	111.60
1	A	52	ILE	CB-CG1-CD1	13.06	150.48	113.90
1	A	21	GLU	CG-CD-OE1	12.96	144.21	118.30
1	A	39	ARG	CG-CD-NE	12.83	138.74	111.80
1	A	25	TYR	CA-CB-CG	12.82	137.76	113.40
1	A	32	HIS	CB-CG-CD2	12.80	170.49	130.80
1	A	47	LYS	CG-CD-CE	-12.67	73.90	111.90
1	A	44	PRO	CA-N-CD	12.43	129.10	111.70
1	A	18	SER	N-CA-CB	-12.26	92.11	110.50
1	A	29	TRP	NE1-CE2-CD2	-12.17	95.13	107.30
1	A	58	ASP	OD1-CG-OD2	-12.04	100.43	123.30
1	A	32	HIS	CE1-NE2-CD2	-11.95	76.72	106.60
1	A	5	ASN	O-C-N	-11.80	103.83	122.70
1	A	43	CYS	C-N-CD	-11.78	94.68	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	CB-CG-CD	11.68	141.98	111.60
1	A	34	GLY	C-N-CA	11.41	150.22	121.70
1	A	46	VAL	CA-C-N	11.34	142.15	117.20
1	A	22	THR	OG1-CB-CG2	-11.26	84.11	110.00
1	A	15	THR	CA-CB-OG1	11.11	132.33	109.00
1	A	33	ARG	CA-C-N	11.09	138.38	116.20
1	A	29	TRP	CD1-NE1-CE2	11.02	118.92	109.00
1	A	38	GLU	CG-CD-OE2	10.92	140.14	118.30
1	A	29	TRP	CE2-CD2-CG	10.78	115.92	107.30
1	A	36	ARG	CD-NE-CZ	10.70	138.58	123.60
1	A	13	THR	CA-CB-CG2	10.64	127.30	112.40
1	A	51	GLU	CB-CG-CD	10.60	142.81	114.20
1	A	4	HIS	ND1-CE1-NE2	-10.36	87.12	109.90
1	A	44	PRO	O-C-N	9.93	138.59	122.70
1	A	27	LYS	CB-CG-CD	9.92	137.40	111.60
1	A	61	ASN	O-C-N	-9.89	106.87	122.70
1	A	46	VAL	O-C-N	-9.85	106.94	122.70
1	A	4	HIS	CA-CB-CG	9.84	130.33	113.60
1	A	62	ASN	CA-CB-CG	9.82	135.01	113.40
1	A	31	ASP	O-C-N	-9.70	107.18	122.70
1	A	21	GLU	CB-CG-CD	9.63	140.19	114.20
1	A	57	THR	CA-C-N	9.60	138.31	117.20
1	A	7	GLN	CB-CG-CD	9.54	136.41	111.60
1	A	21	GLU	OE1-CD-OE2	9.45	134.64	123.30
1	A	51	GLU	CG-CD-OE2	-9.25	99.79	118.30
1	A	33	ARG	N-CA-C	-9.25	86.03	111.00
1	A	46	VAL	N-CA-C	9.23	135.92	111.00
1	A	62	ASN	CB-CG-OD1	-9.22	103.16	121.60
1	A	48	ASN	CB-CG-OD1	9.21	140.01	121.60
1	A	32	HIS	N-CA-C	9.20	135.83	111.00
1	A	38	GLU	CA-CB-CG	9.11	133.44	113.40
1	A	40	GLY	CA-C-N	9.05	137.11	117.20
1	A	46	VAL	C-N-CA	8.97	144.12	121.70
1	A	33	ARG	C-N-CA	8.84	140.86	122.30
1	A	26	LYS	CA-CB-CG	8.78	132.72	113.40
1	A	39	ARG	NH1-CZ-NH2	8.77	129.04	119.40
1	A	38	GLU	CB-CG-CD	8.68	137.63	114.20
1	A	28	ARG	CB-CG-CD	8.45	133.57	111.60
1	A	48	ASN	CB-CG-ND2	8.44	136.95	116.70
1	A	29	TRP	CZ3-CH2-CZ2	-8.39	111.54	121.60
1	A	30	ARG	CA-CB-CG	8.34	131.74	113.40
1	A	46	VAL	CG1-CB-CG2	-8.10	97.94	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	CYS	O-C-N	-8.10	109.74	122.70
1	A	3	CYS	CA-CB-SG	8.09	128.55	114.00
1	A	13	THR	OG1-CB-CG2	-8.03	91.53	110.00
1	A	34	GLY	CA-C-O	7.70	134.46	120.60
1	A	1	LEU	CA-CB-CG	7.56	132.68	115.30
1	A	4	HIS	ND1-CG-CD2	-7.49	95.51	106.00
1	A	29	TRP	CE2-CD2-CE3	-7.46	109.75	118.70
1	A	46	VAL	CB-CA-C	7.43	125.52	111.40
1	A	57	THR	C-N-CA	7.28	139.89	121.70
1	A	40	GLY	CA-C-O	7.07	133.32	120.60
1	A	29	TRP	CB-CG-CD2	7.05	135.77	126.60
1	A	44	PRO	CA-CB-CG	-7.02	90.66	104.00
1	A	7	GLN	O-C-N	-7.00	111.49	122.70
1	A	4	HIS	CB-CG-ND1	7.00	140.69	123.20
1	A	35	TYR	CE1-CZ-OH	6.96	138.90	120.10
1	A	29	TRP	NE1-CE2-CZ2	6.77	137.85	130.40
1	A	62	ASN	N-CA-C	6.74	129.21	111.00
1	A	10	GLN	CA-C-N	6.65	131.84	117.20
1	A	40	GLY	C-N-CA	6.64	138.30	121.70
1	A	30	ARG	CG-CD-NE	6.64	125.74	111.80
1	A	39	ARG	CA-CB-CG	6.62	127.97	113.40
1	A	44	PRO	CB-CG-CD	6.59	132.20	106.50
1	A	47	LYS	O-C-N	-6.48	112.33	122.70
1	A	57	THR	CA-C-O	6.28	133.28	120.10
1	A	34	GLY	N-CA-C	6.24	128.69	113.10
1	A	16	GLY	CA-C-N	6.21	130.86	117.20
1	A	4	HIS	CE1-NE2-CD2	6.20	122.11	106.60
1	A	46	VAL	CA-CB-CG1	-6.18	101.62	110.90
1	A	9	SER	CA-CB-OG	6.13	127.75	111.20
1	A	31	ASP	CA-C-N	6.04	130.48	117.20
1	A	43	CYS	CA-C-O	6.03	132.77	120.10
1	A	62	ASN	OD1-CG-ND2	-5.98	108.14	121.90
1	A	33	ARG	CB-CG-CD	5.89	126.93	111.60
1	A	6	GLN	CA-C-N	5.84	130.05	117.20
1	A	14	THR	CA-CB-OG1	5.80	121.18	109.00
1	A	13	THR	CA-CB-OG1	5.74	121.06	109.00
1	A	33	ARG	N-CA-CB	5.73	120.92	110.60
1	A	6	GLN	CA-C-O	5.69	132.05	120.10
1	A	19	GLY	C-N-CA	-5.68	110.37	122.30
1	A	20	GLY	CA-C-N	5.63	129.58	117.20
1	A	30	ARG	CB-CG-CD	5.56	126.06	111.60
1	A	31	ASP	CA-CB-CG	5.53	125.56	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	THR	CA-CB-CG2	5.49	120.09	112.40
1	A	44	PRO	N-CA-C	5.46	126.29	112.10
1	A	43	CYS	CA-C-N	5.43	132.30	117.10
1	A	21	GLU	N-CA-C	5.36	125.46	111.00
1	A	18	SER	N-CA-C	5.33	125.39	111.00
1	A	32	HIS	CB-CA-C	-5.28	99.84	110.40
1	A	32	HIS	O-C-N	-5.27	114.27	122.70
1	A	58	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	39	ARG	CB-CG-CD	5.05	124.74	111.60

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	39	ARG	Sidechain
1	A	33	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	410	301
All	All	480	438	410	301

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 338.

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:CD	1:A:27:LYS:CB	1.57	1.82
1:A:59:ARG:CB	1:A:59:ARG:CD	1.57	1.83
1:A:15:THR:CG2	1:A:15:THR:CA	1.55	1.82
1:A:26:LYS:CG	1:A:26:LYS:CE	1.54	1.82
1:A:28:ARG:CD	1:A:28:ARG:CZ	1.53	1.80
1:A:61:ASN:CA	1:A:61:ASN:CG	1.51	1.76
1:A:1:LEU:HG	1:A:1:LEU:CA	1.45	0.97
1:A:2:GLU:CG	1:A:2:GLU:OE2	1.45	1.65
1:A:23:ASN:CB	1:A:23:ASN:ND2	1.44	1.80
1:A:38:GLU:CB	1:A:38:GLU:CD	1.43	1.82
1:A:22:THR:CG2	1:A:22:THR:CA	1.43	1.97
1:A:10:GLN:CD	1:A:10:GLN:CB	1.42	1.87
1:A:26:LYS:CD	1:A:26:LYS:CB	1.41	1.97
1:A:2:GLU:CD	1:A:2:GLU:CB	1.40	1.90
1:A:15:THR:OG1	1:A:15:THR:CA	1.40	1.70
1:A:36:ARG:CB	1:A:36:ARG:CD	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:CD	1:A:6:GLN:CB	1.38	1.91
1:A:18:SER:C	1:A:19:GLY:CA	1.37	1.93
1:A:6:GLN:CA	1:A:6:GLN:CG	1.36	2.00
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:48:ASN:CG	1:A:48:ASN:CA	1.32	1.97
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:NE2	1:A:6:GLN:CG	1.30	1.95
1:A:28:ARG:CG	1:A:28:ARG:NE	1.28	1.96
1:A:17:CYS:SG	1:A:41:CYS:CB	1.28	2.22
1:A:59:ARG:CA	1:A:59:ARG:CG	1.23	2.15
1:A:51:GLU:CB	1:A:51:GLU:CD	1.23	2.06
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:38:GLU:CA	1:A:38:GLU:CG	1.20	2.19
1:A:9:SER:O	1:A:9:SER:CA	1.20	1.89
1:A:39:ARG:CG	1:A:39:ARG:CA	1.20	2.19
1:A:8:SER:C	1:A:9:SER:CA	1.20	2.09
1:A:58:ASP:OD2	1:A:58:ASP:CB	1.19	1.89
1:A:61:ASN:CA	1:A:61:ASN:ND2	1.18	2.06
1:A:9:SER:C	1:A:10:GLN:CA	1.17	2.13
1:A:2:GLU:CG	1:A:2:GLU:CA	1.17	2.21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:26:LYS:CG	1:A:26:LYS:CA	1.14	2.23
1:A:6:GLN:OE1	1:A:6:GLN:CG	1.14	1.93
1:A:8:SER:OG	1:A:8:SER:CA	1.12	1.96
1:A:48:ASN:CG	1:A:48:ASN:HB3	1.11	1.54
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:46:VAL:O	1:A:46:VAL:HG12	1.06	1.46
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:48:ASN:CG	1:A:48:ASN:CB	1.03	0.94
1:A:5:ASN:CA	1:A:5:ASN:CG	1.02	2.27
1:A:59:ARG:CZ	1:A:59:ARG:HD3	0.99	1.87
1:A:5:ASN:CB	1:A:5:ASN:CG	0.99	0.90
1:A:15:THR:HG23	1:A:15:THR:OG1	0.98	1.23
1:A:15:THR:CG2	1:A:15:THR:OG1	0.98	0.68
1:A:5:ASN:HB3	1:A:5:ASN:CG	0.97	1.44
1:A:5:ASN:HB2	1:A:5:ASN:CG	0.97	1.44
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: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:51:GLU:HG3	1:A:51:GLU:CD	0.94	1.39
1:A:1:LEU:HA	1:A:1:LEU:HG	0.93	1.37
1:A:26:LYS:CG	1:A:26:LYS:CB	0.93	0.94
1:A:51:GLU:CG	1:A:51:GLU:CD	0.93	0.83
1:A:39:ARG:CB	1:A:39:ARG:CG	0.93	0.93
1:A:38:GLU:HB2	1:A:38:GLU:CG	0.92	1.45
1:A:51:GLU:HG2	1:A:51:GLU:CD	0.92	1.39
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:HD3	1:A:28:ARG:NE	0.90	1.30
1:A:41:CYS:SG	1:A:41:CYS:CB	0.90	0.83
1:A:38:GLU:CB	1:A:38:GLU:HG3	0.90	1.44
1:A:28:ARG:NE	1:A:28:ARG:HD2	0.89	1.30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:8:SER:OG	1:A:8:SER:HB2	0.89	1.15
1:A:26:LYS:HG2	1:A:26:LYS:CB	0.89	1.44
1:A:36:ARG:HG2	1:A:36:ARG:CD	0.88	1.41
1:A:8:SER:HB3	1:A:8:SER:OG	0.88	1.15
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:HG3	1:A:36:ARG:CD	0.87	1.41
1:A:22:THR:HG22	1:A:22:THR:CB	0.86	1.40
1:A:22:THR:HB	1:A:22:THR:CG2	0.86	1.41
1:A:41:CYS:HG	1:A:41:CYS:CB	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:10:GLN:CD	1:A:10:GLN:HE22	0.86	1.48
1:A:22:THR:HG21	1:A:22:THR:CB	0.85	1.40
1:A:22:THR:HG23	1:A:22:THR:CB	0.85	1.40
1:A:1:LEU:CG	1:A:1:LEU:HB3	0.85	1.39
1:A:28:ARG:CD	1:A:28:ARG:NE	0.85	0.76
1:A:36:ARG:HD2	1:A:36:ARG:CG	0.85	1.40
1:A:28:ARG:NH2	1:A:28:ARG:CZ	0.85	0.72
1:A:1:LEU:HB2	1:A:1:LEU:CG	0.85	1.39
1:A:27:LYS:HB2	1:A:27:LYS:HD3	0.84	1.42
1:A:10:GLN:HE21	1:A:10:GLN:CD	0.84	1.48
1:A:36:ARG:CG	1:A:36:ARG:CD	0.84	0.86
1:A:1:LEU:CG	1:A:1:LEU:HD21	0.83	1.36
1:A:22:THR:HG1	1:A:22:THR:HG23	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:HG3	0.83	1.26
1:A:1:LEU:HD23	1:A:1:LEU:CG	0.82	1.36
1:A:27:LYS:HG3	1:A:27:LYS:CB	0.82	1.36
1:A:10:GLN:CD	1:A:10:GLN:HG2	0.81	1.26
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:38:GLU:CB	1:A:38:GLU:OE1	0.81	2.07
1:A:27:LYS:HG2	1:A:27:LYS:CB	0.81	1.36
1:A:1:LEU:HD22	1:A:1:LEU:CG	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:23:ASN:HD21	1:A:23:ASN:CG	0.79	1.40

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:15:THR:OG1	1:A:15:THR:HG21	0.79	1.03
1:A:36:ARG:NE	1:A:36:ARG:HD3	0.79	1.37
1:A:10:GLN:NE2	1:A:10:GLN:CD	0.79	0.85
1:A:27:LYS:HB2	1:A:27:LYS:CG	0.79	1.33
1:A:61:ASN:ND2	1:A:61:ASN:HB3	0.78	1.17
1:A:39:ARG:CB	1:A:39:ARG:HG2	0.78	1.52
1:A:6:GLN:OE1	1:A:6:GLN:CD	0.78	0.61
1:A:15:THR:HG23	1:A:15:THR:CB	0.77	1.31
1:A:1:LEU:C	1:A:1:LEU:HG	0.77	1.95
1:A:23:ASN:HD22	1:A:23:ASN:CG	0.77	1.40
1:A:15:THR:CB	1:A:15:THR:HG22	0.76	1.31
1:A:44:PRO:O	1:A:45:SER:HB3	0.76	1.55
1:A:15:THR:CB	1:A:15:THR:HG21	0.76	1.31
1:A:27:LYS:CG	1:A:27:LYS:CB	0.76	0.77
1:A:59:ARG:HB2	1:A:59:ARG:CG	0.75	1.29
1:A:58:ASP:CA	1:A:58:ASP:OD1	0.75	2.34
1:A:26:LYS:CD	1:A:26:LYS:HE2	0.75	1.29
1:A:59:ARG:HB3	1:A:59:ARG:CG	0.74	1.29
1:A:61:ASN:OD1	1:A:61:ASN:HB2	0.74	0.98
1:A:15:THR:HG1	1:A:15:THR:CG2	0.74	1.45
1:A:39:ARG:CB	1:A:39:ARG:HG3	0.74	1.52
1:A:47:LYS:HD2	1:A:50:ILE:HD11	0.74	1.59
1:A:22:THR:HG21	1:A:22:THR:HG1	0.74	0.82
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:47:LYS:CB	1:A:50:ILE:HD11	0.73	2.12
1:A:10:GLN:CG	1:A:10:GLN:CD	0.73	0.71
1:A:26:LYS:HZ1	1:A:26:LYS:CE	0.72	1.43
1:A:26:LYS:CD	1:A:26:LYS:HE3	0.72	1.29
1:A:2:GLU:HB2	1:A:2:GLU:CG	0.72	1.26
1:A:2:GLU:CG	1:A:2:GLU:HB3	0.72	1.26
1:A:26:LYS:HD3	1:A:26:LYS:CB	0.72	2.11
1:A:53:ASN:ND2	1:A:53:ASN:OD1	0.72	0.59
1:A:26:LYS:NZ	1:A:26:LYS:HE2	0.72	1.38
1:A:53:ASN:HD21	1:A:53:ASN:CG	0.71	1.34
1:A:5:ASN:HD21	1:A:5:ASN:CG	0.71	1.32
1:A:26:LYS:HD3	1:A:26:LYS:CE	0.71	1.25
1:A:2:GLU:HG3	1:A:2:GLU:CB	0.71	1.25
1:A:26:LYS:HD2	1:A:26:LYS:CE	0.71	1.25
1:A:2:GLU:CB	1:A:2:GLU:HG2	0.71	1.25
1:A:5:ASN:HD22	1:A:5:ASN:CG	0.71	1.32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:26:LYS:HZ3	1:A:26:LYS:CE	0.71	1.43
1:A:31:ASP:O	1:A:34:GLY:N	0.70	2.24
1:A:26:LYS:HZ2	1:A:26:LYS:CE	0.70	1.43
1:A:53:ASN:HD22	1:A:53:ASN:CG	0.70	1.34
1:A:9:SER:C	1:A:10:GLN:N	0.70	0.73
1:A:23:ASN:ND2	1:A:23:ASN:CG	0.70	0.76
1:A:36:ARG:HH21	1:A:36:ARG:CZ	0.70	1.40
1:A:26:LYS:NZ	1:A:26:LYS:CE	0.70	0.86
1:A:59:ARG:CB	1:A:59:ARG:CG	0.70	0.72
1:A:6:GLN:CD	1:A:6:GLN:HE21	0.69	1.30
1:A:41:CYS:HB2	1:A:41:CYS:SG	0.69	1.32
1:A:6:GLN:CD	1:A:6:GLN:HE22	0.69	1.30
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:61:ASN:HD21	1:A:61:ASN:CB	0.69	1.41
1:A:61:ASN:C	1:A:61:ASN:CG	0.69	2.50
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:36:ARG:HH22	1:A:36:ARG:CZ	0.69	1.40
1:A:26:LYS:NZ	1:A:26:LYS:HE3	0.69	1.38
1:A:53:ASN:OD1	1:A:53:ASN:CG	0.69	0.53
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:ND2	1:A:53:ASN:CG	0.67	0.68
1:A:1:LEU:CG	1:A:1:LEU:HD11	0.67	1.20
1:A:1:LEU:HD13	1:A:1:LEU:CG	0.67	1.20
1:A:28:ARG:HH21	1:A:28:ARG:CZ	0.67	1.37
1:A:1:LEU:HD12	1:A:1:LEU:CG	0.67	1.20
1:A:26:LYS:HG2	1:A:26:LYS:CE	0.66	2.12
1:A:28:ARG:NH2	1:A:28:ARG:NH1	0.66	0.68
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:61:ASN:OD1	1:A:61:ASN:CB	0.65	0.36
1:A:2:GLU:CD	1:A:2:GLU:OE2	0.65	0.54
1:A:6:GLN:NE2	1:A:6:GLN:CD	0.65	0.64
1:A:23:ASN:HA	1:A:56:THR:HG22	0.65	1.68
1:A:28:ARG:HE	1:A:28:ARG:HD2	0.65	0.95
1:A:6:GLN:HG3	1:A:6:GLN:CB	0.65	1.18
1:A:2:GLU:CG	1:A:2:GLU:CB	0.64	0.77
1:A:59:ARG:CZ	1:A:59:ARG:HE	0.64	1.34
1:A:1:LEU:CG	1:A:1:LEU:CA	0.64	1.90

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:61:ASN:CG	1:A:61:ASN:HB2	0.64	1.08
1:A:61:ASN:HB3	1:A:61:ASN:CG	0.64	1.08
1:A:6:GLN:HB3	1:A:6:GLN:CG	0.64	1.17
1:A:6:GLN:HG2	1:A:6:GLN:CB	0.64	1.18
1:A:28:ARG:HE	1:A:28:ARG:NH2	0.63	1.88
1:A:6:GLN:HB2	1:A:6:GLN:CG	0.63	1.17
1:A:29:TRP:CD1	1:A:29:TRP:N	0.62	2.61
1:A:36:ARG:HE	1:A:36:ARG:CD	0.62	1.38
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: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:58:ASP:CG	1:A:58:ASP:OD2	0.61	0.79
1:A:36:ARG:NH2	1:A:36:ARG:CZ	0.60	0.76
1:A:5:ASN:ND2	1:A:5:ASN:CG	0.60	0.66
1:A:2:GLU:HG2	1:A:2:GLU:OE2	0.60	1.88
1:A:48:ASN:CG	1:A:48:ASN:HD21	0.60	1.21
1:A:18:SER:HA	1:A:19:GLY:N	0.59	2.08
1:A:48:ASN:CG	1:A:48:ASN:HD22	0.58	1.21
1:A:61:ASN:OD1	1:A:61:ASN:ND2	0.58	0.43
1:A:2:GLU:HG3	1:A:2:GLU:HB3	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:23:ASN:HA	1:A:56:THR:CG2	0.57	2.29
1:A:9:SER:O	1:A:9:SER:C	0.57	0.46
1:A:18:SER:C	1:A:20:GLY:N	0.57	2.57
1:A:26:LYS:CD	1:A:26:LYS:CE	0.56	0.74
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:31:ASP:O	1:A:33:ARG:N	0.56	2.35
1:A:22:THR:CG2	1:A:22:THR:N	0.56	2.65
1:A:2:GLU:HG3	1:A:2:GLU:OE2	0.56	1.86
1:A:61:ASN:HD22	1:A:61:ASN:CB	0.55	1.25
1:A:47:LYS:O	1:A:48:ASN:HB2	0.53	2.03
1:A:28:ARG:HH12	1:A:28:ARG:NH2	0.53	0.63
1:A:8:SER:C	1:A:9:SER:N	0.53	0.69
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:8:SER:C	1:A:8:SER:O	0.53	0.51
1:A:58:ASP:CG	1:A:58:ASP:OD1	0.52	0.65
1:A:22:THR:CG2	1:A:22:THR:OG1	0.52	0.82

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:36:ARG:HD3	1:A:36:ARG:HH11	0.52	1.25
1:A:59:ARG:CZ	1:A:59:ARG:NE	0.51	0.84
1:A:1:LEU:C	1:A:1:LEU:CG	0.50	2.67
1:A:36:ARG:HD2	1:A:36:ARG:HH11	0.50	1.40
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:44:PRO:C	1:A:45:SER:HB3	0.49	1.42
1:A:47:LYS:HD3	1:A:50:ILE:CD1	0.48	2.36
1:A:8:SER:C	1:A:9:SER:CB	0.48	2.78
1:A:9:SER:O	1:A:10:GLN:CB	0.48	2.47
1:A:36:ARG:HH11	1:A:36:ARG:CD	0.48	1.42
1:A:26:LYS:CG	1:A:26:LYS:C	0.47	2.81
1:A:26:LYS:HD3	1:A:26:LYS:HE2	0.47	1.14
1:A:6:GLN:C	1:A:6:GLN:CG	0.47	2.78
1:A:59:ARG:CZ	1:A:59:ARG:HH21	0.47	1.18
1:A:7:GLN:O	1:A:8:SER:C	0.47	2.40
1:A:59:ARG:CZ	1:A:59:ARG:HH22	0.47	1.18
1:A:61:ASN:HD21	1:A:61:ASN:CG	0.47	1.08
1:A:48:ASN:CG	1:A:48:ASN:ND2	0.47	0.52
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:61:ASN:HD22	1:A:61:ASN:CG	0.46	1.08
1:A:61:ASN:OD1	1:A:61:ASN:C	0.46	2.45
1:A:15:THR:OG1	1:A:15:THR:N	0.45	2.40
1:A:18:SER:O	1:A:18:SER:C	0.45	0.47
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:HH12	1:A:36:ARG:CZ	0.44	1.15
1:A:59:ARG:CZ	1:A:59:ARG:HH11	0.44	1.14
1:A:26:LYS:C	1:A:26:LYS:HG2	0.44	2.31
1:A:8:SER:CB	1:A:8:SER:HG	0.44	1.15
1:A:51:GLU:C	1:A:52:ILE:HD13	0.43	2.34
1:A:59:ARG:CZ	1:A:59:ARG:HH12	0.43	1.14
1:A:31:ASP:O	1:A:34:GLY:CA	0.43	2.65
1:A:36:ARG:CZ	1:A:36:ARG:HH11	0.43	1.15
1:A:18:SER:C	1:A:19:GLY:N	0.43	0.65
1:A:50:ILE:HG13	1:A:52:ILE:HD12	0.42	1.90
1:A:51:GLU:OE1	1:A:51:GLU:CD	0.41	0.62

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:61:ASN:CG	1:A:61:ASN:CB	0.41	0.35
1:A:6:GLN:HB3	1:A:12:PRO:HA	0.40	1.93
1:A:15:THR:HG1	1:A:15:THR:CB	0.40	1.11
1:A:48:ASN:CG	1:A:48:ASN:HA	0.40	2.19
1:A:53:ASN:CA	1:A:53:ASN:OD1	0.40	2.60
1:A:39:ARG:HG3	1:A:39:ARG:CA	0.40	2.16

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	60/62 (97%)	42 (70%)	11 (18%)	7 (12%)	1	8
All	All	60/62 (97%)	42 (70%)	11 (18%)	7 (12%)	1	8

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

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

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	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	41	CYS
1	A	6	GLN
1	A	52	ILE
1	A	57	THR
1	A	27	LYS
1	A	11	THR
1	A	45	SER
1	A	18	SER
1	A	7	GLN
1	A	32	HIS
1	A	10	GLN
1	A	13	THR
1	A	14	THR
1	A	36	ARG
1	A	43	CYS
1	A	8	SER
1	A	53	ASN
1	A	25	TYR
1	A	35	TYR
1	A	29	TRP
1	A	2	GLU
1	A	28	ARG
1	A	30	ARG
1	A	59	ARG

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 [i](#)

There are no carbohydrates 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](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided