



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:42 AM UTC

PDB ID : 1HDP / pdb_00001hdp
Title : SOLUTION STRUCTURE OF A POU-SPECIFIC HOMEODOMAIN: 3D-NMR STUDIES OF HUMAN B-CELL TRANSCRIPTION FACTOR OCT-2
Authors : Sivaraja, M.; Botfield, M.C.; Mueller, M.; Jancso, A.; Weiss, M.A.
Deposited on : 1994-03-08

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

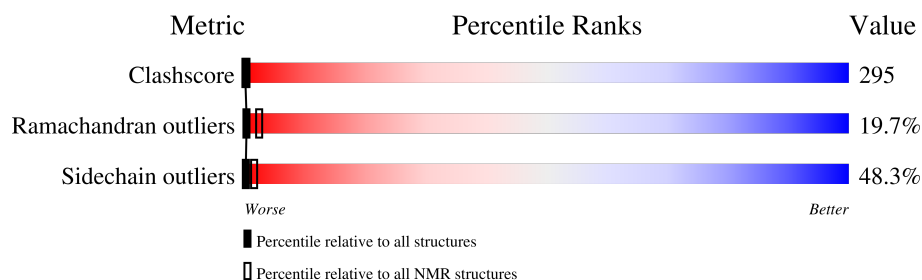
1 Overall quality at a glance

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	63	

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 1097 atoms, of which 563 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called OCT-2 POU HOMEODOMAIN.

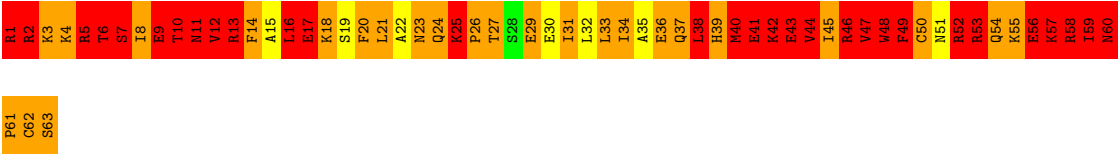
Mol	Chain	Residues	Atoms						Trace
1	A	63	Total	C	H	N	O	S	0
			1097	334	563	104	93	3	

4 Residue-property plots

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: OCT-2 POU HOMEODOMAIN

Chain A:  11% 40% 48%



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
DGII	refinement	

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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	32.51	378/541 (69.9%)	15.33	281/721 (39.0%)
All	All	32.51	378/541 (69.9%)	15.33	281/721 (39.0%)

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	18	4
All	All	18	4

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	62	CYS	N-CA	-99.28	0.18	1.46
1	A	2	ARG	NE-CZ	-98.96	0.24	1.33
1	A	61	PRO	N-CD	-97.99	0.10	1.47
1	A	61	PRO	CA-C	-95.57	0.16	1.52
1	A	39	HIS	CE1-NE2	-90.76	0.41	1.32
1	A	60	ASN	C-O	-89.56	0.09	1.24
1	A	2	ARG	CD-NE	-89.25	0.21	1.46
1	A	58	ARG	C-N	-85.41	0.34	1.33
1	A	61	PRO	C-O	-85.37	0.12	1.24
1	A	1	ARG	CD-NE	-84.02	0.28	1.46
1	A	62	CYS	C-N	-82.26	0.18	1.33
1	A	2	ARG	CZ-NH2	-81.46	0.27	1.33
1	A	39	HIS	CG-ND1	-80.49	0.49	1.38
1	A	62	CYS	CA-C	-79.04	0.46	1.52
1	A	8	ILE	C-O	-79.01	0.30	1.24
1	A	3	LYS	C-O	-78.99	0.15	1.23
1	A	3	LYS	CA-CB	-78.15	0.35	1.53
1	A	5	ARG	CZ-NH2	-76.99	0.33	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	PRO	C-N	-76.69	0.26	1.33
1	A	1	ARG	NE-CZ	-76.30	0.49	1.33
1	A	58	ARG	C-O	-75.90	0.28	1.24
1	A	2	ARG	CA-C	-75.84	0.51	1.52
1	A	59	ILE	CA-CB	-74.87	0.56	1.54
1	A	39	HIS	CG-CD2	-74.29	0.54	1.35
1	A	5	ARG	CA-CB	-73.28	0.61	1.53
1	A	3	LYS	CA-C	-71.90	0.62	1.53
1	A	7	SER	C-N	-70.82	0.37	1.33
1	A	39	HIS	CD2-NE2	-70.09	0.60	1.37
1	A	39	HIS	ND1-CE1	-69.46	0.63	1.32
1	A	61	PRO	CA-CB	-68.79	0.56	1.53
1	A	6	THR	C-O	-67.23	0.39	1.24
1	A	60	ASN	CA-CB	-67.03	0.47	1.53
1	A	13	ARG	CZ-NH2	-66.63	0.46	1.33
1	A	2	ARG	C-O	-64.99	0.42	1.24
1	A	2	ARG	N-CA	-64.72	0.62	1.46
1	A	10	THR	CA-CB	-64.17	0.45	1.53
1	A	10	THR	CB-OG1	-63.23	0.42	1.43
1	A	63	SER	CA-CB	-63.06	0.27	1.53
1	A	58	ARG	CD-NE	-63.01	0.58	1.46
1	A	58	ARG	CZ-NH1	-62.97	0.44	1.32
1	A	5	ARG	NE-CZ	-62.52	0.64	1.33
1	A	6	THR	C-N	-62.34	0.46	1.33
1	A	3	LYS	N-CA	-62.10	0.56	1.46
1	A	2	ARG	CZ-NH1	-62.08	0.45	1.32
1	A	6	THR	CA-C	-61.52	0.70	1.52
1	A	7	SER	N-CA	-61.18	0.67	1.46
1	A	58	ARG	CZ-NH2	-60.29	0.55	1.33
1	A	60	ASN	CG-ND2	-59.71	0.07	1.33
1	A	60	ASN	CA-C	-59.44	0.78	1.52
1	A	62	CYS	C-O	-59.06	0.49	1.24
1	A	1	ARG	CZ-NH1	-58.99	0.50	1.32
1	A	7	SER	CA-CB	-58.78	0.54	1.53
1	A	46	ARG	CZ-NH2	-58.69	0.57	1.33
1	A	37	GLN	CD-OE1	-58.41	0.12	1.23
1	A	9	GLU	C-O	-58.32	0.50	1.24
1	A	53	ARG	CD-NE	-58.04	0.65	1.46
1	A	4	LYS	CA-CB	-57.96	0.47	1.53
1	A	59	ILE	CB-CG1	-57.76	0.38	1.53
1	A	62	CYS	CA-CB	-57.53	0.56	1.53
1	A	3	LYS	C-N	-57.22	0.56	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	GLN	CD-OE1	-56.61	0.15	1.23
1	A	58	ARG	CA-C	-56.33	0.77	1.52
1	A	59	ILE	N-CA	-56.09	0.73	1.46
1	A	63	SER	N-CA	-55.91	0.40	1.46
1	A	1	ARG	CZ-NH2	-55.66	0.61	1.33
1	A	4	LYS	N-CA	-55.38	0.62	1.46
1	A	1	ARG	C-N	-55.17	0.56	1.33
1	A	63	SER	CA-C	-54.98	0.37	1.52
1	A	5	ARG	CD-NE	-54.38	0.70	1.46
1	A	61	PRO	N-CA	-54.08	0.78	1.47
1	A	1	ARG	N-CA	-53.90	0.43	1.46
1	A	53	ARG	NE-CZ	-53.79	0.73	1.33
1	A	39	HIS	CB-CG	-53.79	0.74	1.50
1	A	7	SER	CB-OG	-53.60	0.34	1.42
1	A	6	THR	CA-CB	-53.32	0.63	1.53
1	A	2	ARG	CA-CB	-53.02	0.63	1.53
1	A	58	ARG	CA-CB	-52.71	0.64	1.53
1	A	38	LEU	C-N	-52.65	0.73	1.33
1	A	59	ILE	CA-C	-52.61	0.83	1.52
1	A	58	ARG	NE-CZ	-52.56	0.75	1.33
1	A	6	THR	CB-OG1	-52.23	0.60	1.43
1	A	56	GLU	CD-OE2	-51.82	0.26	1.25
1	A	9	GLU	CD-OE1	-51.63	0.27	1.25
1	A	9	GLU	CA-CB	-51.21	0.67	1.53
1	A	4	LYS	C-O	-50.82	0.65	1.23
1	A	13	ARG	CZ-NH1	-50.27	0.62	1.32
1	A	60	ASN	N-CA	-50.27	0.75	1.46
1	A	60	ASN	CG-OD1	-50.02	0.28	1.23
1	A	7	SER	C-O	-49.92	0.61	1.24
1	A	5	ARG	N-CA	-49.42	0.83	1.46
1	A	30	GLU	CD-OE2	-48.62	0.33	1.25
1	A	36	GLU	CD-OE1	-48.38	0.33	1.25
1	A	1	ARG	CA-CB	-48.35	0.56	1.53
1	A	4	LYS	CA-C	-48.23	0.83	1.53
1	A	24	GLN	CD-NE2	-47.97	0.32	1.33
1	A	57	LYS	C-O	-47.62	0.67	1.23
1	A	38	LEU	CB-CG	-47.38	0.58	1.53
1	A	59	ILE	C-N	-46.60	0.37	1.33
1	A	60	ASN	CB-CG	-46.49	0.35	1.52
1	A	17	GLU	CD-OE2	-45.69	0.38	1.25
1	A	5	ARG	CA-C	-45.56	0.94	1.52
1	A	63	SER	CB-OG	-45.55	0.51	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	THR	N-CA	-45.41	0.87	1.46
1	A	36	GLU	CD-OE2	-45.20	0.39	1.25
1	A	52	ARG	CZ-NH2	-44.49	0.75	1.33
1	A	57	LYS	C-N	-44.48	0.71	1.33
1	A	56	GLU	CD-OE1	-44.37	0.41	1.25
1	A	8	ILE	C-N	-44.07	0.71	1.33
1	A	5	ARG	C-N	-44.00	0.72	1.33
1	A	63	SER	C-O	-43.88	0.35	1.23
1	A	30	GLU	CG-CD	-43.27	0.43	1.52
1	A	24	GLN	CD-OE1	-42.82	0.42	1.23
1	A	62	CYS	CB-SG	-42.66	0.40	1.81
1	A	11	ASN	CB-CG	-42.38	0.46	1.52
1	A	11	ASN	CG-OD1	-42.27	0.43	1.23
1	A	9	GLU	C-N	-42.08	0.74	1.33
1	A	1	ARG	CA-C	-41.90	0.65	1.52
1	A	11	ASN	CG-ND2	-41.20	0.46	1.33
1	A	30	GLU	CD-OE1	-40.74	0.47	1.25
1	A	3	LYS	CB-CG	-40.30	0.31	1.52
1	A	41	GLU	CD-OE2	-40.27	0.48	1.25
1	A	57	LYS	CD-CE	-39.92	0.32	1.52
1	A	1	ARG	C-O	-39.65	0.44	1.23
1	A	58	ARG	CB-CG	-39.65	0.33	1.52
1	A	23	ASN	C-O	-39.61	0.75	1.23
1	A	6	THR	CB-CG2	-39.21	0.23	1.52
1	A	18	LYS	CE-NZ	-38.91	0.32	1.49
1	A	38	LEU	CG-CD1	-38.78	0.24	1.52
1	A	57	LYS	CE-NZ	-38.65	0.33	1.49
1	A	43	GLU	CD-OE1	-38.38	0.52	1.25
1	A	38	LEU	C-O	-38.34	0.75	1.24
1	A	53	ARG	CZ-NH2	-38.34	0.83	1.33
1	A	5	ARG	C-O	-38.31	0.80	1.24
1	A	51	ASN	CG-OD1	-38.10	0.51	1.23
1	A	4	LYS	CG-CD	-37.80	0.39	1.52
1	A	3	LYS	CG-CD	-37.67	0.39	1.52
1	A	59	ILE	C-O	-37.57	0.68	1.24
1	A	3	LYS	CD-CE	-37.51	0.40	1.52
1	A	4	LYS	CE-NZ	-37.47	0.36	1.49
1	A	46	ARG	NE-CZ	-37.20	0.92	1.33
1	A	5	ARG	CZ-NH1	-36.90	0.81	1.32
1	A	14	PHE	CG-CD2	-36.35	0.62	1.38
1	A	2	ARG	C-N	-36.28	0.86	1.33
1	A	52	ARG	CZ-NH1	-36.15	0.82	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	ARG	CG-CD	-35.47	0.46	1.52
1	A	37	GLN	CD-NE2	-35.37	0.58	1.33
1	A	17	GLU	CD-OE1	-35.35	0.58	1.25
1	A	9	GLU	CD-OE2	-34.73	0.59	1.25
1	A	2	ARG	CG-CD	-34.10	0.50	1.52
1	A	40	MET	SD-CE	-33.93	0.94	1.79
1	A	58	ARG	CG-CD	-33.64	0.51	1.52
1	A	23	ASN	C-N	-33.59	0.87	1.33
1	A	43	GLU	CD-OE2	-33.49	0.61	1.25
1	A	9	GLU	CB-CG	-33.07	0.53	1.52
1	A	57	LYS	CB-CG	-32.96	0.53	1.52
1	A	13	ARG	NE-CZ	-32.68	0.97	1.33
1	A	57	LYS	CG-CD	-32.62	0.54	1.52
1	A	4	LYS	CB-CG	-32.53	0.54	1.52
1	A	40	MET	C-O	-32.05	0.87	1.23
1	A	5	ARG	CB-CG	-31.95	0.56	1.52
1	A	53	ARG	CZ-NH1	-31.33	0.88	1.32
1	A	18	LYS	CB-CG	-30.82	0.59	1.52
1	A	5	ARG	CG-CD	-30.57	0.60	1.52
1	A	60	ASN	C-N	-30.11	0.63	1.33
1	A	46	ARG	CZ-NH1	-29.90	0.90	1.32
1	A	29	GLU	CD-OE2	-29.76	0.68	1.25
1	A	37	GLN	CG-CD	-29.47	0.78	1.52
1	A	33	LEU	CB-CG	-28.99	0.95	1.53
1	A	54	GLN	CG-CD	-28.99	0.79	1.52
1	A	4	LYS	C-N	-28.76	0.92	1.33
1	A	46	ARG	CD-NE	-28.40	1.06	1.46
1	A	21	LEU	CB-CG	-28.04	0.97	1.53
1	A	23	ASN	CG-ND2	-28.02	0.74	1.33
1	A	41	GLU	CD-OE1	-27.84	0.72	1.25
1	A	33	LEU	CG-CD2	-27.80	0.60	1.52
1	A	19	SER	CB-OG	-27.77	0.86	1.42
1	A	25	LYS	CD-CE	-27.72	0.69	1.52
1	A	23	ASN	CG-OD1	-27.63	0.71	1.23
1	A	13	ARG	CD-NE	-27.46	1.07	1.46
1	A	59	ILE	CB-CG2	-27.41	0.62	1.52
1	A	9	GLU	CA-C	-26.93	1.16	1.52
1	A	12	VAL	CA-CB	-26.93	1.22	1.54
1	A	10	THR	N-CA	-26.77	1.11	1.46
1	A	38	LEU	CA-CB	-26.56	1.08	1.53
1	A	3	LYS	CE-NZ	-26.13	0.70	1.49
1	A	29	GLU	CD-OE1	-26.12	0.75	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	THR	CB-CG2	-25.87	0.67	1.52
1	A	59	ILE	CG1-CD1	-25.84	0.51	1.51
1	A	25	LYS	CB-CG	-25.84	0.74	1.52
1	A	56	GLU	CG-CD	-25.81	0.87	1.52
1	A	8	ILE	N-CA	-25.62	1.14	1.46
1	A	46	ARG	CB-CG	-25.62	0.75	1.52
1	A	2	ARG	CB-CG	-25.54	0.75	1.52
1	A	14	PHE	CE1-CZ	-25.34	0.62	1.38
1	A	24	GLN	CG-CD	-24.71	0.90	1.52
1	A	30	GLU	CB-CG	-24.65	0.78	1.52
1	A	18	LYS	CG-CD	-24.29	0.79	1.52
1	A	8	ILE	CB-CG1	-24.13	1.05	1.53
1	A	52	ARG	NE-CZ	-24.02	1.06	1.33
1	A	57	LYS	CA-C	-23.64	1.23	1.52
1	A	25	LYS	CE-NZ	-23.33	0.79	1.49
1	A	36	GLU	CG-CD	-23.31	0.93	1.52
1	A	36	GLU	CB-CG	-23.13	0.83	1.52
1	A	53	ARG	CB-CG	-23.12	0.83	1.52
1	A	4	LYS	CD-CE	-23.12	0.83	1.52
1	A	58	ARG	N-CA	-23.04	1.16	1.46
1	A	33	LEU	CG-CD1	-22.97	0.76	1.52
1	A	20	PHE	CG-CD2	-22.93	0.90	1.38
1	A	55	LYS	CE-NZ	-22.77	0.81	1.49
1	A	54	GLN	CD-NE2	-22.76	0.85	1.33
1	A	7	SER	CA-C	-22.63	1.22	1.52
1	A	29	GLU	CB-CG	-22.44	0.85	1.52
1	A	20	PHE	CG-CD1	-22.11	0.92	1.38
1	A	18	LYS	CD-CE	-22.09	0.86	1.52
1	A	42	LYS	CE-NZ	-21.97	0.83	1.49
1	A	55	LYS	CB-CG	-21.66	0.87	1.52
1	A	41	GLU	CB-CG	-21.65	0.87	1.52
1	A	51	ASN	CG-ND2	-21.61	0.87	1.33
1	A	1	ARG	CB-CG	-20.80	0.90	1.52
1	A	8	ILE	CA-C	-20.77	1.26	1.52
1	A	61	PRO	CB-CG	-20.74	0.46	1.49
1	A	40	MET	CB-CG	-20.52	0.90	1.52
1	A	11	ASN	C-N	-20.49	1.08	1.33
1	A	9	GLU	CG-CD	-20.12	1.01	1.52
1	A	40	MET	C-N	-20.11	1.05	1.33
1	A	38	LEU	CA-C	-19.97	1.26	1.52
1	A	11	ASN	N-CA	-19.63	1.21	1.46
1	A	21	LEU	CG-CD1	-19.34	0.88	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	LYS	CD-CE	-19.05	0.95	1.52
1	A	42	LYS	CD-CE	-18.98	0.95	1.52
1	A	21	LEU	CG-CD2	-18.93	0.90	1.52
1	A	27	THR	CB-OG1	-18.80	1.13	1.43
1	A	10	THR	CA-C	-18.77	1.27	1.52
1	A	9	GLU	N-CA	-18.37	1.22	1.46
1	A	42	LYS	CG-CD	-18.30	0.97	1.52
1	A	61	PRO	CG-CD	-18.27	0.88	1.50
1	A	38	LEU	CG-CD2	-18.15	0.92	1.52
1	A	24	GLN	CA-CB	-18.11	1.28	1.53
1	A	31	ILE	CG1-CD1	-17.45	0.83	1.51
1	A	39	HIS	N-CA	-17.25	1.18	1.46
1	A	57	LYS	CA-CB	-17.07	1.24	1.53
1	A	53	ARG	CG-CD	-16.92	1.01	1.52
1	A	23	ASN	CB-CG	-16.26	1.11	1.52
1	A	8	ILE	CA-CB	-16.19	1.32	1.54
1	A	40	MET	CG-SD	-16.18	1.40	1.80
1	A	14	PHE	CG-CD1	-16.13	1.04	1.38
1	A	20	PHE	CE1-CZ	-16.03	0.90	1.38
1	A	46	ARG	CG-CD	-15.99	1.04	1.52
1	A	42	LYS	CB-CG	-15.63	1.05	1.52
1	A	20	PHE	CE2-CZ	-15.45	0.92	1.38
1	A	8	ILE	CG1-CD1	-15.38	0.91	1.51
1	A	20	PHE	C-N	-15.33	1.13	1.34
1	A	24	GLN	C-O	-15.16	1.02	1.24
1	A	56	GLU	C-N	-15.15	1.13	1.33
1	A	24	GLN	N-CA	-14.69	1.29	1.46
1	A	55	LYS	CG-CD	-14.53	1.08	1.52
1	A	56	GLU	C-O	-14.45	1.06	1.24
1	A	17	GLU	CG-CD	-14.30	1.16	1.52
1	A	23	ASN	CA-CB	-14.27	1.29	1.53
1	A	23	ASN	N-CA	-14.03	1.28	1.46
1	A	14	PHE	CB-CG	-13.74	1.19	1.50
1	A	21	LEU	CA-CB	-13.65	1.30	1.53
1	A	39	HIS	CA-CB	-13.14	1.14	1.53
1	A	23	ASN	CA-C	-12.99	1.36	1.52
1	A	25	LYS	CA-CB	-12.92	1.38	1.53
1	A	22	ALA	CA-C	-12.82	1.36	1.52
1	A	22	ALA	C-N	-12.77	1.17	1.33
1	A	43	GLU	CG-CD	-12.64	1.20	1.52
1	A	8	ILE	CB-CG2	-12.53	1.11	1.52
1	A	52	ARG	CG-CD	-12.44	1.15	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	LEU	C-N	-12.39	1.17	1.33
1	A	22	ALA	CA-CB	-12.22	1.33	1.53
1	A	26	PRO	N-CA	-12.21	1.32	1.47
1	A	11	ASN	C-O	-11.38	1.09	1.24
1	A	20	PHE	C-O	-11.33	1.11	1.24
1	A	14	PHE	CE2-CZ	-11.25	1.04	1.38
1	A	16	LEU	C-N	-11.21	1.20	1.33
1	A	26	PRO	C-O	-11.11	1.11	1.23
1	A	25	LYS	CA-C	-10.85	1.39	1.52
1	A	25	LYS	N-CA	-10.38	1.35	1.46
1	A	24	GLN	C-N	-10.33	1.19	1.33
1	A	26	PRO	CA-CB	-9.86	1.40	1.53
1	A	37	GLN	C-O	-9.65	1.12	1.24
1	A	12	VAL	N-CA	-9.45	1.35	1.46
1	A	14	PHE	CD1-CE1	-9.38	1.10	1.38
1	A	24	GLN	CA-C	-9.38	1.40	1.52
1	A	14	PHE	CD2-CE2	-9.34	1.10	1.38
1	A	29	GLU	CG-CD	-9.29	1.28	1.52
1	A	39	HIS	CA-C	-9.09	1.44	1.53
1	A	21	LEU	N-CA	-8.85	1.35	1.46
1	A	26	PRO	N-CD	-8.71	1.35	1.47
1	A	57	LYS	N-CA	-8.71	1.35	1.46
1	A	11	ASN	CA-CB	-8.64	1.38	1.53
1	A	18	LYS	C-N	-8.51	1.21	1.33
1	A	51	ASN	CB-CG	-8.47	1.30	1.52
1	A	27	THR	CB-CG2	-8.42	1.24	1.52
1	A	36	GLU	C-N	-8.41	1.22	1.33
1	A	25	LYS	CG-CD	-8.41	1.27	1.52
1	A	25	LYS	C-O	-8.39	1.14	1.24
1	A	10	THR	C-N	-8.32	1.23	1.34
1	A	13	ARG	N-CA	-8.25	1.36	1.46
1	A	19	SER	CA-CB	-8.03	1.40	1.53
1	A	24	GLN	CB-CG	-8.03	1.28	1.52
1	A	37	GLN	N-CA	-7.93	1.36	1.46
1	A	14	PHE	N-CA	-7.91	1.36	1.46
1	A	22	ALA	N-CA	-7.77	1.36	1.46
1	A	56	GLU	CA-C	-7.71	1.43	1.52
1	A	25	LYS	C-N	-7.62	1.24	1.33
1	A	56	GLU	CB-CG	-7.58	1.29	1.52
1	A	20	PHE	CA-C	-7.53	1.43	1.52
1	A	19	SER	C-N	-7.49	1.24	1.33
1	A	34	ILE	CG1-CD1	-7.49	1.22	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	CYS	CB-SG	-7.43	1.56	1.81
1	A	40	MET	CA-CB	-7.38	1.41	1.53
1	A	22	ALA	C-O	-7.36	1.15	1.24
1	A	52	ARG	CD-NE	-7.30	1.36	1.46
1	A	13	ARG	CG-CD	-7.21	1.30	1.52
1	A	12	VAL	CA-C	-7.16	1.44	1.52
1	A	21	LEU	C-O	-7.05	1.15	1.24
1	A	37	GLN	CA-CB	-6.99	1.42	1.53
1	A	40	MET	CA-C	-6.96	1.44	1.52
1	A	38	LEU	N-CA	-6.87	1.37	1.46
1	A	37	GLN	CA-C	-6.79	1.44	1.52
1	A	41	GLU	CA-CB	-6.72	1.41	1.53
1	A	13	ARG	CA-C	-6.66	1.43	1.52
1	A	40	MET	N-CA	-6.63	1.38	1.46
1	A	11	ASN	CA-C	-6.53	1.43	1.52
1	A	20	PHE	N-CA	-6.50	1.38	1.46
1	A	42	LYS	C-O	-6.45	1.16	1.24
1	A	19	SER	N-CA	-6.44	1.37	1.46
1	A	17	GLU	C-N	-6.43	1.25	1.34
1	A	50	CYS	N-CA	-6.39	1.38	1.46
1	A	36	GLU	CA-C	-6.32	1.43	1.52
1	A	16	LEU	C-O	-6.21	1.16	1.24
1	A	36	GLU	C-O	-6.15	1.16	1.24
1	A	55	LYS	C-O	-6.15	1.16	1.24
1	A	52	ARG	C-O	-6.13	1.17	1.24
1	A	41	GLU	CG-CD	-6.13	1.36	1.52
1	A	41	GLU	N-CA	-6.12	1.38	1.45
1	A	26	PRO	C-N	-6.11	1.23	1.33
1	A	56	GLU	N-CA	-6.06	1.38	1.46
1	A	41	GLU	C-O	-6.05	1.16	1.23
1	A	55	LYS	N-CA	-6.02	1.38	1.46
1	A	17	GLU	N-CA	-5.97	1.39	1.46
1	A	12	VAL	C-N	-5.95	1.26	1.34
1	A	13	ARG	CB-CG	-5.88	1.34	1.52
1	A	21	LEU	CA-C	-5.81	1.44	1.52
1	A	26	PRO	CA-C	-5.74	1.46	1.52
1	A	31	ILE	CA-CB	-5.72	1.47	1.54
1	A	27	THR	N-CA	-5.71	1.39	1.45
1	A	14	PHE	C-N	-5.70	1.26	1.34
1	A	10	THR	C-O	-5.67	1.16	1.24
1	A	54	GLN	CA-C	-5.67	1.45	1.52
1	A	15	ALA	C-N	-5.65	1.26	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	ARG	N-CA	-5.63	1.39	1.46
1	A	54	GLN	C-O	-5.63	1.17	1.24
1	A	35	ALA	C-O	-5.59	1.17	1.24
1	A	49	PHE	C-N	-5.58	1.26	1.33
1	A	50	CYS	C-O	-5.52	1.17	1.24
1	A	37	GLN	C-N	-5.47	1.26	1.33
1	A	14	PHE	C-O	-5.44	1.17	1.24
1	A	13	ARG	C-N	-5.43	1.26	1.33
1	A	35	ALA	C-N	-5.42	1.26	1.33
1	A	27	THR	C-N	-5.40	1.26	1.33
1	A	44	VAL	N-CA	-5.39	1.39	1.46
1	A	18	LYS	CA-CB	-5.37	1.44	1.53
1	A	29	GLU	N-CA	-5.34	1.39	1.46
1	A	54	GLN	N-CA	-5.33	1.39	1.46
1	A	47	VAL	C-O	-5.33	1.17	1.24
1	A	53	ARG	CA-CB	-5.30	1.44	1.53
1	A	46	ARG	N-CA	-5.24	1.40	1.46
1	A	51	ASN	C-N	-5.24	1.26	1.33
1	A	33	LEU	C-N	-5.22	1.28	1.34
1	A	56	GLU	CA-CB	-5.21	1.45	1.53
1	A	47	VAL	CA-CB	-5.14	1.48	1.54
1	A	48	TRP	N-CA	-5.12	1.39	1.46
1	A	53	ARG	CA-C	-5.07	1.45	1.52
1	A	39	HIS	C-N	-5.06	1.27	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	8	ILE	O-C-N	-86.88	13.97	122.57
1	A	24	GLN	OE1-CD-NE2	-82.78	39.82	122.60
1	A	58	ARG	O-C-N	-73.98	24.19	122.59
1	A	2	ARG	NE-CZ-NH2	-73.56	53.00	119.20
1	A	7	SER	O-C-N	-67.32	33.05	122.59
1	A	2	ARG	CA-C-O	-62.66	30.91	120.51
1	A	37	GLN	OE1-CD-NE2	-60.41	62.19	122.60
1	A	63	SER	N-CA-CB	-58.45	11.14	110.50
1	A	61	PRO	N-CA-CB	58.21	164.37	103.25
1	A	62	CYS	CA-C-N	-56.20	20.54	121.70
1	A	62	CYS	C-N-CA	-56.20	20.54	121.70
1	A	5	ARG	NE-CZ-NH2	-54.96	69.74	119.20
1	A	54	GLN	CG-CD-OE1	-53.03	14.73	120.80
1	A	13	ARG	NH1-CZ-NH2	-46.92	58.30	119.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLN	OE1-CD-NE2	45.78	168.38	122.60
1	A	60	ASN	CA-CB-CG	-45.63	66.97	112.60
1	A	61	PRO	CA-CB-CG	-43.25	22.33	104.50
1	A	11	ASN	CA-CB-CG	42.95	155.55	112.60
1	A	10	THR	CA-CB-CG2	-42.43	38.37	110.50
1	A	61	PRO	CA-C-O	-42.02	44.12	120.60
1	A	60	ASN	CA-C-N	41.55	171.77	119.84
1	A	60	ASN	C-N-CA	41.55	171.77	119.84
1	A	54	GLN	CG-CD-NE2	40.32	176.88	116.40
1	A	3	LYS	CB-CA-C	-39.74	50.90	112.09
1	A	8	ILE	CA-C-O	39.71	170.41	120.78
1	A	3	LYS	N-CA-CB	39.17	173.54	111.65
1	A	51	ASN	OD1-CG-ND2	-38.80	83.80	122.60
1	A	33	LEU	CD1-CG-CD2	-38.46	26.19	110.80
1	A	60	ASN	O-C-N	-38.28	77.30	121.32
1	A	3	LYS	CA-CB-CG	-38.25	37.60	114.10
1	A	56	GLU	OE1-CD-OE2	-37.98	31.76	122.90
1	A	36	GLU	OE1-CD-OE2	-37.91	31.93	122.90
1	A	62	CYS	CA-C-O	37.41	174.00	120.51
1	A	5	ARG	NE-CZ-NH1	35.84	157.34	121.50
1	A	58	ARG	CB-CG-CD	-35.82	28.91	111.30
1	A	37	GLN	CG-CD-NE2	35.08	169.02	116.40
1	A	13	ARG	NE-CZ-NH1	34.07	155.57	121.50
1	A	7	SER	CA-C-O	33.74	168.76	120.51
1	A	30	GLU	CB-CG-CD	33.44	169.45	112.60
1	A	62	CYS	O-C-N	33.10	166.61	122.59
1	A	39	HIS	CA-CB-CG	33.00	146.80	113.80
1	A	58	ARG	CA-C-O	32.96	167.64	120.51
1	A	58	ARG	CD-NE-CZ	32.11	169.36	124.40
1	A	2	ARG	O-C-N	32.09	165.27	122.59
1	A	59	ILE	CA-C-O	32.06	151.65	119.91
1	A	6	THR	CA-CB-OG1	30.87	155.90	109.60
1	A	5	ARG	CB-CA-C	-30.84	63.79	110.67
1	A	2	ARG	CA-C-N	30.00	166.78	122.68
1	A	2	ARG	C-N-CA	30.00	166.78	122.68
1	A	13	ARG	NE-CZ-NH2	29.93	146.13	119.20
1	A	53	ARG	CG-CD-NE	29.85	177.68	112.00
1	A	2	ARG	NE-CZ-NH1	29.80	151.29	121.50
1	A	58	ARG	CA-C-N	29.51	169.10	122.76
1	A	58	ARG	C-N-CA	29.51	169.10	122.76
1	A	60	ASN	CB-CG-ND2	-29.39	72.31	116.40
1	A	3	LYS	CA-C-O	-28.99	86.19	122.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLU	OE1-CD-OE2	-28.78	53.82	122.90
1	A	38	LEU	CD1-CG-CD2	-28.75	47.54	110.80
1	A	3	LYS	CA-C-N	28.59	164.03	122.87
1	A	3	LYS	C-N-CA	28.59	164.03	122.87
1	A	8	ILE	CA-C-N	28.45	175.88	121.54
1	A	8	ILE	C-N-CA	28.45	175.88	121.54
1	A	37	GLN	CB-CG-CD	28.20	160.55	112.60
1	A	2	ARG	NH1-CZ-NH2	28.00	155.71	119.30
1	A	9	GLU	O-C-N	-27.25	86.35	122.59
1	A	58	ARG	NH1-CZ-NH2	-26.75	84.53	119.30
1	A	61	PRO	O-C-N	26.69	158.67	122.64
1	A	42	LYS	CG-CD-CE	26.55	172.38	111.30
1	A	58	ARG	NE-CZ-NH2	26.46	143.01	119.20
1	A	9	GLU	CB-CG-CD	26.32	157.34	112.60
1	A	24	GLN	CG-CD-NE2	26.29	155.83	116.40
1	A	18	LYS	CG-CD-CE	26.11	171.35	111.30
1	A	10	THR	CA-CB-OG1	-25.92	70.72	109.60
1	A	4	LYS	N-CA-C	25.68	144.72	109.54
1	A	9	GLU	OE1-CD-OE2	-25.36	62.04	122.90
1	A	62	CYS	N-CA-C	-25.27	56.98	110.80
1	A	39	HIS	ND1-CG-CD2	-25.23	80.87	106.10
1	A	57	LYS	O-C-N	-25.17	91.91	122.87
1	A	60	ASN	N-CA-CB	-25.15	65.61	110.37
1	A	13	ARG	CD-NE-CZ	24.55	158.78	124.40
1	A	7	SER	N-CA-CB	-24.32	69.38	110.49
1	A	3	LYS	CB-CG-CD	24.11	166.76	111.30
1	A	60	ASN	CB-CG-OD1	23.62	168.05	120.80
1	A	41	GLU	OE1-CD-OE2	-22.98	67.75	122.90
1	A	36	GLU	CB-CG-CD	22.93	151.59	112.60
1	A	39	HIS	CG-CD2-NE2	22.55	129.75	107.20
1	A	10	THR	N-CA-C	22.38	158.47	110.80
1	A	4	LYS	CB-CG-CD	-22.25	60.12	111.30
1	A	24	GLN	CG-CD-OE1	21.77	164.34	120.80
1	A	46	ARG	NE-CZ-NH1	21.64	143.14	121.50
1	A	31	ILE	CB-CG1-CD1	21.44	158.83	113.80
1	A	56	GLU	CG-CD-OE1	21.43	167.68	118.40
1	A	53	ARG	CD-NE-CZ	21.39	154.34	124.40
1	A	23	ASN	O-C-N	-21.31	98.48	123.41
1	A	59	ILE	CB-CA-C	21.25	138.84	111.85
1	A	60	ASN	N-CA-C	21.13	156.51	109.81
1	A	61	PRO	CA-C-N	21.11	161.86	121.54
1	A	61	PRO	C-N-CA	21.11	161.86	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ARG	CA-CB-CG	21.00	156.10	114.10
1	A	63	SER	CA-CB-OG	20.92	152.93	111.10
1	A	62	CYS	CB-CA-C	20.91	152.03	110.42
1	A	51	ASN	CB-CG-ND2	20.89	147.73	116.40
1	A	63	SER	CB-CA-C	-20.62	70.92	110.10
1	A	7	SER	CA-C-N	20.46	158.80	121.97
1	A	7	SER	C-N-CA	20.46	158.80	121.97
1	A	36	GLU	CG-CD-OE2	20.42	165.36	118.40
1	A	5	ARG	N-CA-C	20.24	138.30	109.15
1	A	33	LEU	CB-CG-CD1	19.92	170.45	110.70
1	A	46	ARG	CD-NE-CZ	19.91	152.28	124.40
1	A	56	GLU	CB-CG-CD	19.41	145.60	112.60
1	A	43	GLU	OE1-CD-OE2	-19.38	76.40	122.90
1	A	36	GLU	CG-CD-OE1	19.27	162.72	118.40
1	A	59	ILE	N-CA-C	19.14	130.35	112.17
1	A	59	ILE	N-CA-CB	-18.97	87.05	112.28
1	A	6	THR	OG1-CB-CG2	-18.85	71.60	109.30
1	A	9	GLU	CG-CD-OE2	18.74	161.50	118.40
1	A	20	PHE	CD1-CG-CD2	-18.70	90.55	118.60
1	A	61	PRO	CB-CG-CD	18.70	165.95	106.10
1	A	38	LEU	O-C-N	-18.65	97.78	122.59
1	A	55	LYS	CD-CE-NZ	18.50	171.12	111.90
1	A	5	ARG	N-CA-CB	18.33	139.66	109.60
1	A	56	GLU	CG-CD-OE2	18.33	160.56	118.40
1	A	1	ARG	NE-CZ-NH1	-18.04	103.46	121.50
1	A	17	GLU	CG-CD-OE1	17.69	159.09	118.40
1	A	2	ARG	N-CA-CB	17.48	140.02	110.49
1	A	1	ARG	CD-NE-CZ	17.47	148.85	124.40
1	A	21	LEU	CD1-CG-CD2	-17.44	72.44	110.80
1	A	38	LEU	CB-CG-CD2	17.37	162.82	110.70
1	A	52	ARG	NH1-CZ-NH2	-17.33	96.78	119.30
1	A	33	LEU	CB-CG-CD2	17.25	162.46	110.70
1	A	6	THR	O-C-N	-16.98	100.01	122.59
1	A	13	ARG	CG-CD-NE	16.87	149.12	112.00
1	A	55	LYS	CB-CG-CD	16.85	150.06	111.30
1	A	40	MET	CB-CG-SD	16.68	162.75	112.70
1	A	53	ARG	CB-CG-CD	16.50	149.26	111.30
1	A	1	ARG	CB-CG-CD	-16.47	73.42	111.30
1	A	25	LYS	CG-CD-CE	16.46	149.16	111.30
1	A	20	PHE	CE1-CZ-CE2	-16.27	90.72	120.00
1	A	23	ASN	OD1-CG-ND2	-16.25	106.35	122.60
1	A	46	ARG	CG-CD-NE	16.18	147.60	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	N-CA-C	15.80	144.46	110.80
1	A	9	GLU	N-CA-C	15.62	144.07	110.80
1	A	46	ARG	CB-CG-CD	15.54	147.03	111.30
1	A	25	LYS	CA-CB-CG	15.41	144.91	114.10
1	A	62	CYS	N-CA-CB	15.33	136.40	110.49
1	A	41	GLU	CG-CD-OE1	15.30	153.59	118.40
1	A	7	SER	N-CA-C	14.87	142.47	110.80
1	A	18	LYS	CA-CB-CG	14.71	143.53	114.10
1	A	14	PHE	CB-CG-CD1	14.66	145.62	120.70
1	A	14	PHE	CG-CD1-CE1	14.65	145.60	120.70
1	A	36	GLU	CA-CB-CG	14.52	143.15	114.10
1	A	7	SER	CB-CA-C	14.45	139.17	110.42
1	A	30	GLU	CG-CD-OE2	-14.25	85.63	118.40
1	A	57	LYS	CD-CE-NZ	-14.20	66.45	111.90
1	A	14	PHE	CZ-CE2-CD2	14.20	145.55	120.00
1	A	40	MET	CG-SD-CE	14.19	132.13	100.90
1	A	57	LYS	CA-C-O	13.69	136.25	121.19
1	A	4	LYS	CA-C-O	-13.55	99.17	121.94
1	A	61	PRO	N-CA-C	-13.55	84.56	112.47
1	A	29	GLU	CB-CG-CD	13.50	135.56	112.60
1	A	60	ASN	CB-CA-C	13.29	136.35	110.17
1	A	9	GLU	CA-C-N	13.27	146.89	121.54
1	A	9	GLU	C-N-CA	13.27	146.89	121.54
1	A	12	VAL	N-CA-C	12.80	122.70	110.42
1	A	4	LYS	CA-CB-CG	-12.75	88.60	114.10
1	A	52	ARG	NE-CZ-NH1	12.55	134.05	121.50
1	A	17	GLU	CG-CD-OE2	12.47	147.08	118.40
1	A	55	LYS	CA-CB-CG	12.34	138.79	114.10
1	A	40	MET	O-C-N	-12.21	108.42	123.44
1	A	46	ARG	NE-CZ-NH2	-12.20	108.22	119.20
1	A	59	ILE	CA-CB-CG2	12.05	130.98	110.50
1	A	39	HIS	CE1-NE2-CD2	-11.98	97.02	109.00
1	A	43	GLU	CG-CD-OE2	11.79	145.52	118.40
1	A	3	LYS	N-CA-C	11.65	127.32	111.24
1	A	10	THR	N-CA-CB	-11.49	91.08	110.49
1	A	42	LYS	CD-CE-NZ	11.47	148.61	111.90
1	A	9	GLU	CB-CA-C	-11.31	87.90	110.42
1	A	25	LYS	CB-CG-CD	11.31	137.32	111.30
1	A	57	LYS	CA-CB-CG	-11.16	91.78	114.10
1	A	59	ILE	CA-C-N	-11.10	94.72	121.80
1	A	59	ILE	C-N-CA	-11.10	94.72	121.80
1	A	52	ARG	NE-CZ-NH2	11.08	129.17	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	LEU	CA-C-O	11.00	136.25	120.51
1	A	58	ARG	NE-CZ-NH1	10.96	132.46	121.50
1	A	40	MET	CA-CB-CG	10.93	135.95	114.10
1	A	29	GLU	OE1-CD-OE2	-10.67	97.29	122.90
1	A	7	SER	CA-CB-OG	10.48	132.06	111.10
1	A	5	ARG	NH1-CZ-NH2	10.48	132.92	119.30
1	A	10	THR	OG1-CB-CG2	-10.47	88.35	109.30
1	A	18	LYS	CB-CG-CD	10.45	135.33	111.30
1	A	4	LYS	N-CA-CB	-10.43	86.59	111.74
1	A	63	SER	N-CA-C	-10.41	81.84	111.00
1	A	61	PRO	CA-N-CD	-10.24	97.67	112.00
1	A	11	ASN	OD1-CG-ND2	10.20	132.80	122.60
1	A	61	PRO	CB-CA-C	-10.17	94.77	111.56
1	A	39	HIS	N-CA-C	10.09	123.43	109.11
1	A	2	ARG	CB-CG-CD	10.06	134.43	111.30
1	A	8	ILE	CB-CG1-CD1	9.94	134.66	113.80
1	A	46	ARG	CA-CB-CG	9.77	133.63	114.10
1	A	61	PRO	N-CD-CG	-9.74	88.59	103.20
1	A	23	ASN	CA-CB-CG	9.60	122.20	112.60
1	A	39	HIS	CG-ND1-CE1	9.55	125.53	109.30
1	A	39	HIS	CB-CG-CD2	9.30	143.29	131.20
1	A	3	LYS	O-C-N	-8.93	111.87	122.86
1	A	41	GLU	CG-CD-OE2	8.81	138.66	118.40
1	A	39	HIS	CB-CG-ND1	8.73	135.80	122.70
1	A	38	LEU	CA-CB-CG	8.69	146.72	116.30
1	A	55	LYS	CG-CD-CE	8.67	131.25	111.30
1	A	2	ARG	CG-CD-NE	-8.62	93.04	112.00
1	A	53	ARG	NE-CZ-NH2	-8.60	111.46	119.20
1	A	20	PHE	CG-CD1-CE1	8.60	135.31	120.70
1	A	25	LYS	CD-CE-NZ	8.59	139.38	111.90
1	A	43	GLU	CG-CD-OE1	8.56	138.08	118.40
1	A	20	PHE	CB-CG-CD1	8.55	135.23	120.70
1	A	21	LEU	CB-CG-CD2	8.55	136.35	110.70
1	A	53	ARG	NH1-CZ-NH2	8.52	130.38	119.30
1	A	47	VAL	N-CA-CB	8.48	121.07	110.47
1	A	4	LYS	CA-C-N	8.47	134.88	121.66
1	A	4	LYS	C-N-CA	8.47	134.88	121.66
1	A	20	PHE	CZ-CE2-CD2	8.46	135.22	120.00
1	A	24	GLN	CB-CG-CD	-8.44	98.25	112.60
1	A	60	ASN	C-N-CD	-8.40	90.55	125.00
1	A	1	ARG	NE-CZ-NH2	8.37	126.73	119.20
1	A	5	ARG	CD-NE-CZ	8.34	136.07	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	LEU	CB-CG-CD1	8.31	135.65	110.70
1	A	17	GLU	CB-CG-CD	8.27	126.66	112.60
1	A	46	ARG	NH1-CZ-NH2	-8.20	108.64	119.30
1	A	14	PHE	CD1-CG-CD2	-8.14	106.38	118.60
1	A	14	PHE	CA-CB-CG	8.13	121.94	113.80
1	A	1	ARG	NH1-CZ-NH2	8.08	129.81	119.30
1	A	30	GLU	CG-CD-OE1	8.01	136.82	118.40
1	A	58	ARG	CB-CA-C	-7.99	94.52	110.42
1	A	23	ASN	CA-C-N	7.96	134.99	122.49
1	A	23	ASN	C-N-CA	7.96	134.99	122.49
1	A	20	PHE	CB-CG-CD2	7.95	134.22	120.70
1	A	20	PHE	CG-CD2-CE2	7.91	134.14	120.70
1	A	23	ASN	CA-C-O	7.86	130.21	120.54
1	A	9	GLU	CG-CD-OE1	7.85	136.45	118.40
1	A	20	PHE	CD1-CE1-CZ	7.81	134.05	120.00
1	A	5	ARG	CA-C-O	7.69	129.77	120.62
1	A	42	LYS	CA-CB-CG	7.67	129.45	114.10
1	A	38	LEU	CB-CG-CD1	7.64	133.63	110.70
1	A	4	LYS	O-C-N	7.62	132.18	122.28
1	A	14	PHE	CE1-CZ-CE2	-7.57	106.38	120.00
1	A	29	GLU	CA-CB-CG	7.49	129.07	114.10
1	A	14	PHE	CB-CG-CD2	-7.47	108.00	120.70
1	A	6	THR	CA-CB-CG2	-7.45	97.84	110.50
1	A	14	PHE	CG-CD2-CE2	-7.44	108.05	120.70
1	A	1	ARG	N-CA-C	-7.38	90.33	111.00
1	A	57	LYS	CA-C-N	7.33	135.55	121.54
1	A	57	LYS	C-N-CA	7.33	135.55	121.54
1	A	4	LYS	CB-CA-C	7.23	128.68	111.83
1	A	6	THR	CA-C-N	7.13	135.15	121.54
1	A	6	THR	C-N-CA	7.13	135.15	121.54
1	A	13	ARG	CB-CG-CD	7.03	127.46	111.30
1	A	29	GLU	CG-CD-OE1	7.01	134.51	118.40
1	A	58	ARG	CA-CB-CG	-6.72	100.66	114.10
1	A	14	PHE	CD1-CE1-CZ	-6.65	108.03	120.00
1	A	1	ARG	CG-CD-NE	-6.63	97.42	112.00
1	A	21	LEU	N-CA-C	6.56	119.25	111.71
1	A	11	ASN	CA-C-O	6.47	127.44	120.20
1	A	2	ARG	CA-CB-CG	6.46	127.02	114.10
1	A	8	ILE	CA-CB-CG2	6.40	121.38	110.50
1	A	60	ASN	CA-C-O	-6.39	111.41	120.16
1	A	10	THR	O-C-N	6.30	130.97	122.59
1	A	9	GLU	CA-C-O	6.21	129.39	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	CG-CD-NE	-6.18	98.40	112.00
1	A	38	LEU	N-CA-C	6.13	123.86	110.80
1	A	30	GLU	OE1-CD-OE2	6.10	137.54	122.90
1	A	40	MET	CA-C-N	6.02	132.93	122.81
1	A	40	MET	C-N-CA	6.02	132.93	122.81
1	A	33	LEU	CA-CB-CG	5.92	137.01	116.30
1	A	6	THR	CA-C-O	5.50	128.38	120.51
1	A	5	ARG	CB-CG-CD	-5.26	99.21	111.30
1	A	8	ILE	CB-CA-C	5.21	119.83	111.29
1	A	23	ASN	CB-CG-OD1	5.20	131.20	120.80
1	A	11	ASN	CB-CG-ND2	-5.18	108.63	116.40
1	A	1	ARG	CA-CB-CG	-5.16	103.78	114.10
1	A	1	ARG	CA-C-N	5.15	131.37	121.54
1	A	1	ARG	C-N-CA	5.15	131.37	121.54
1	A	1	ARG	CB-CA-C	-5.01	100.58	110.10

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	1	ARG	CA
1	A	2	ARG	CA
1	A	3	LYS	CA
1	A	4	LYS	CA
1	A	5	ARG	CA
1	A	6	THR	CB,CA
1	A	7	SER	CA
1	A	9	GLU	CA
1	A	10	THR	CB,CA
1	A	58	ARG	CA
1	A	59	ILE	CB,CA
1	A	60	ASN	CA
1	A	61	PRO	CA
1	A	62	CYS	CA
1	A	63	SER	CA

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	5	ARG	Sidechain
1	A	13	ARG	Sidechain
1	A	46	ARG	Sidechain
1	A	52	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	534	563	526	313
All	All	534	563	526	313

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 295.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:53:ARG:CB	1:A:53:ARG:CD	1.59	1.77
1:A:8:ILE:CD1	1:A:8:ILE:CB	1.57	1.81
1:A:38:LEU:CD1	1:A:38:LEU:CA	1.52	1.81
1:A:11:ASN:CG	1:A:11:ASN:CA	1.51	1.81
1:A:42:LYS:NZ	1:A:42:LYS:CD	1.50	1.71
1:A:55:LYS:NZ	1:A:55:LYS:CD	1.49	1.75
1:A:25:LYS:CB	1:A:25:LYS:CD	1.49	1.88
1:A:25:LYS:CE	1:A:25:LYS:CG	1.48	1.89
1:A:55:LYS:CD	1:A:55:LYS:CB	1.48	1.89
1:A:8:ILE:O	1:A:9:GLU:CA	1.45	1.65
1:A:18:LYS:CG	1:A:18:LYS:CA	1.42	1.95
1:A:20:PHE:CZ	1:A:20:PHE:CD1	1.42	2.07
1:A:20:PHE:CG	1:A:20:PHE:CE2	1.42	2.07
1:A:52:ARG:NH2	1:A:52:ARG:NE	1.41	1.64
1:A:54:GLN:CD	1:A:54:GLN:CB	1.39	1.95
1:A:20:PHE:CZ	1:A:20:PHE:CD2	1.38	2.09
1:A:20:PHE:CG	1:A:20:PHE:CE1	1.38	2.09
1:A:41:GLU:CG	1:A:41:GLU:CA	1.37	2.01
1:A:53:ARG:CG	1:A:53:ARG:CA	1.37	1.99
1:A:17:GLU:OE1	1:A:17:GLU:CG	1.37	1.71
1:A:43:GLU:OE2	1:A:43:GLU:CG	1.36	1.74
1:A:29:GLU:CB	1:A:29:GLU:CD	1.35	1.98
1:A:41:GLU:CB	1:A:41:GLU:CD	1.35	1.96
1:A:25:LYS:CG	1:A:25:LYS:CA	1.33	2.04
1:A:41:GLU:CG	1:A:41:GLU:OE2	1.33	1.76
1:A:23:ASN:C	1:A:24:GLN:CA	1.32	2.00
1:A:52:ARG:NE	1:A:52:ARG:NH1	1.31	1.73
1:A:29:GLU:OE2	1:A:29:GLU:CG	1.30	1.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:11:ASN:CA	1:A:11:ASN:ND2	1.28	1.97
1:A:8:ILE:CA	1:A:9:GLU:N	1.27	1.97
1:A:20:PHE:CD2	1:A:20:PHE:CB	1.27	2.17
1:A:29:GLU:CG	1:A:29:GLU:CA	1.26	2.13
1:A:56:GLU:CD	1:A:56:GLU:CB	1.26	2.07
1:A:40:MET:CE	1:A:40:MET:CG	1.24	2.15
1:A:20:PHE:CD1	1:A:20:PHE:CB	1.23	2.19
1:A:40:MET:CG	1:A:40:MET:CA	1.23	2.15
1:A:36:GLU:CG	1:A:36:GLU:CA	1.22	2.17
1:A:40:MET:CB	1:A:40:MET:SD	1.21	2.28
1:A:23:ASN:CA	1:A:24:GLN:N	1.19	2.04
1:A:55:LYS:CG	1:A:55:LYS:CA	1.18	2.21
1:A:37:GLN:CD	1:A:37:GLN:CB	1.18	2.16
1:A:23:ASN:CA	1:A:23:ASN:O	1.17	1.93
1:A:31:ILE:CD1	1:A:31:ILE:CB	1.15	2.23
1:A:29:GLU:CG	1:A:29:GLU:OE1	1.14	1.89
1:A:58:ARG:NH2	1:A:60:ASN:HB2	1.12	1.15
1:A:8:ILE:C	1:A:9:GLU:CA	1.06	1.93
1:A:41:GLU:CG	1:A:41:GLU:OE1	1.06	2.03
1:A:8:ILE:O	1:A:9:GLU:CB	1.04	2.01
1:A:40:MET:CE	1:A:40:MET:SD	1.04	0.94
1:A:12:VAL:HG23	1:A:16:LEU:HD22	1.02	1.23
1:A:5:ARG:CZ	1:A:7:SER:HB3	1.00	1.58
1:A:8:ILE:CG1	1:A:8:ILE:HD11	1.00	1.54
1:A:8:ILE:CG1	1:A:8:ILE:HD13	1.00	1.54
1:A:42:LYS:NZ	1:A:42:LYS:HE2	0.99	1.37
1:A:38:LEU:HD23	1:A:39:HIS:HD2	0.99	1.16
1:A:42:LYS:NZ	1:A:42:LYS:HE3	0.98	1.37
1:A:41:GLU:CD	1:A:41:GLU:OE1	0.97	0.72
1:A:38:LEU:HD23	1:A:39:HIS:CD2	0.96	1.95
1:A:53:ARG:CB	1:A:53:ARG:HD2	0.96	1.89
1:A:8:ILE:CG1	1:A:8:ILE:HD12	0.96	1.54
1:A:53:ARG:HG2	1:A:53:ARG:C	0.96	1.85
1:A:41:GLU:CB	1:A:41:GLU:HG3	0.95	1.48
1:A:42:LYS:NZ	1:A:42:LYS:CE	0.95	0.83
1:A:31:ILE:CG1	1:A:31:ILE:HD11	0.94	1.47
1:A:41:GLU:CG	1:A:41:GLU:HB3	0.94	1.48
1:A:54:GLN:CD	1:A:54:GLN:HG3	0.94	1.43
1:A:31:ILE:CG1	1:A:31:ILE:HD13	0.94	1.47
1:A:41:GLU:CG	1:A:41:GLU:HB2	0.94	1.48
1:A:41:GLU:CB	1:A:41:GLU:HG2	0.94	1.48
1:A:8:ILE:CD1	1:A:8:ILE:HG13	0.93	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:53:ARG:CA	1:A:53:ARG:HG2	0.93	1.75
1:A:40:MET:SD	1:A:40:MET:HE2	0.93	1.56
1:A:8:ILE:CD1	1:A:8:ILE:HG12	0.93	1.48
1:A:38:LEU:HD23	1:A:38:LEU:HD11	0.92	1.00
1:A:40:MET:CG	1:A:40:MET:HB2	0.92	1.47
1:A:40:MET:SD	1:A:40:MET:HE3	0.92	1.56
1:A:31:ILE:CG1	1:A:31:ILE:HD12	0.92	1.47
1:A:5:ARG:HH22	1:A:7:SER:HB3	0.92	0.77
1:A:20:PHE:CD1	1:A:20:PHE:CG	0.92	0.92
1:A:56:GLU:CD	1:A:56:GLU:HG2	0.92	1.41
1:A:20:PHE:CZ	1:A:20:PHE:CE2	0.91	0.92
1:A:8:ILE:CD1	1:A:8:ILE:CG1	0.91	0.91
1:A:40:MET:CG	1:A:40:MET:HB3	0.91	1.47
1:A:54:GLN:CD	1:A:54:GLN:HG2	0.91	1.43
1:A:55:LYS:NZ	1:A:55:LYS:HE2	0.91	1.29
1:A:56:GLU:CD	1:A:56:GLU:CG	0.91	0.87
1:A:29:GLU:CG	1:A:29:GLU:HB2	0.90	1.44
1:A:20:PHE:CG	1:A:20:PHE:CD2	0.90	0.90
1:A:20:PHE:CZ	1:A:20:PHE:CE1	0.90	0.90
1:A:38:LEU:CD1	1:A:38:LEU:HD23	0.90	1.53
1:A:40:MET:SD	1:A:40:MET:HE1	0.90	1.56
1:A:40:MET:CG	1:A:40:MET:CB	0.90	0.90
1:A:53:ARG:CG	1:A:53:ARG:HB2	0.89	1.45
1:A:56:GLU:CD	1:A:56:GLU:HG3	0.89	1.41
1:A:53:ARG:CG	1:A:53:ARG:HB3	0.89	1.45
1:A:29:GLU:CG	1:A:29:GLU:HB3	0.89	1.44
1:A:55:LYS:NZ	1:A:55:LYS:HE3	0.89	1.29
1:A:55:LYS:CG	1:A:55:LYS:HB3	0.89	1.43
1:A:53:ARG:CB	1:A:53:ARG:HD3	0.88	1.92
1:A:55:LYS:CG	1:A:55:LYS:HB2	0.88	1.43
1:A:8:ILE:C	1:A:9:GLU:HA	0.88	1.86
1:A:12:VAL:HG23	1:A:16:LEU:CD2	0.88	1.98
1:A:29:GLU:CB	1:A:29:GLU:HG2	0.88	1.42
1:A:11:ASN:CG	1:A:11:ASN:N	0.87	2.31
1:A:55:LYS:CB	1:A:55:LYS:CG	0.87	0.87
1:A:38:LEU:HB3	1:A:39:HIS:N	0.87	1.63
1:A:38:LEU:CD1	1:A:38:LEU:C	0.87	2.46
1:A:29:GLU:CB	1:A:29:GLU:HG3	0.86	1.42
1:A:41:GLU:CG	1:A:41:GLU:CB	0.86	0.87
1:A:11:ASN:OD1	1:A:11:ASN:CB	0.86	0.76
1:A:20:PHE:CE1	1:A:20:PHE:HZ	0.86	1.69
1:A:12:VAL:CG2	1:A:16:LEU:HD22	0.86	2.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:11:ASN:CA	1:A:11:ASN:OD1	0.86	2.07
1:A:40:MET:CB	1:A:40:MET:HG3	0.85	1.38
1:A:55:LYS:CB	1:A:55:LYS:HG2	0.85	1.40
1:A:29:GLU:CB	1:A:29:GLU:CG	0.85	0.85
1:A:43:GLU:OE2	1:A:43:GLU:CD	0.84	0.61
1:A:36:GLU:CG	1:A:36:GLU:HB2	0.84	1.39
1:A:40:MET:CB	1:A:40:MET:HG2	0.84	1.38
1:A:36:GLU:CG	1:A:36:GLU:HB3	0.84	1.39
1:A:53:ARG:CB	1:A:53:ARG:HG2	0.84	1.37
1:A:54:GLN:CD	1:A:54:GLN:CG	0.84	0.79
1:A:55:LYS:CB	1:A:55:LYS:HG3	0.83	1.40
1:A:11:ASN:ND2	1:A:11:ASN:CB	0.83	0.75
1:A:31:ILE:CD1	1:A:31:ILE:CG1	0.83	0.83
1:A:11:ASN:CA	1:A:11:ASN:HD22	0.83	1.69
1:A:53:ARG:CB	1:A:53:ARG:CG	0.82	0.83
1:A:58:ARG:NH2	1:A:60:ASN:CB	0.82	1.86
1:A:25:LYS:CB	1:A:25:LYS:HD2	0.82	2.05
1:A:5:ARG:HH22	1:A:7:SER:CB	0.81	1.62
1:A:36:GLU:CG	1:A:36:GLU:CB	0.81	0.83
1:A:25:LYS:CB	1:A:25:LYS:HG2	0.81	1.34
1:A:53:ARG:CB	1:A:53:ARG:HG3	0.81	1.37
1:A:25:LYS:CB	1:A:25:LYS:HG3	0.81	1.34
1:A:31:ILE:CD1	1:A:31:ILE:HG13	0.81	1.35
1:A:5:ARG:NH2	1:A:7:SER:HB3	0.81	1.31
1:A:11:ASN:CB	1:A:11:ASN:HD21	0.81	1.57
1:A:54:GLN:CD	1:A:54:GLN:HE22	0.81	1.48
1:A:38:LEU:CD1	1:A:38:LEU:HB3	0.80	1.34
1:A:37:GLN:CD	1:A:37:GLN:HG2	0.80	1.30
1:A:12:VAL:CG2	1:A:16:LEU:CD2	0.80	2.59
1:A:20:PHE:CE2	1:A:20:PHE:HZ	0.80	1.71
1:A:31:ILE:CD1	1:A:31:ILE:HG12	0.79	1.35
1:A:36:GLU:CB	1:A:36:GLU:HG3	0.79	1.36
1:A:38:LEU:CD1	1:A:38:LEU:HD22	0.79	1.34
1:A:25:LYS:CG	1:A:25:LYS:HB2	0.79	1.32
1:A:8:ILE:CD1	1:A:8:ILE:CG2	0.79	2.50
1:A:25:LYS:CG	1:A:25:LYS:HB3	0.79	1.32
1:A:37:GLN:CD	1:A:37:GLN:HG3	0.79	1.30
1:A:54:GLN:CD	1:A:54:GLN:HE21	0.79	1.48
1:A:37:GLN:CD	1:A:37:GLN:CG	0.79	0.78
1:A:53:ARG:HG2	1:A:53:ARG:O	0.79	1.77
1:A:55:LYS:NZ	1:A:55:LYS:CE	0.78	0.81
1:A:5:ARG:NH2	1:A:7:SER:CB	0.78	1.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:20:PHE:CZ	1:A:20:PHE:HE1	0.77	1.53
1:A:25:LYS:CD	1:A:25:LYS:HE3	0.77	1.30
1:A:36:GLU:CB	1:A:36:GLU:HG2	0.77	1.36
1:A:8:ILE:CD1	1:A:8:ILE:CA	0.77	2.61
1:A:41:GLU:CG	1:A:41:GLU:C	0.76	2.57
1:A:20:PHE:CG	1:A:20:PHE:HD2	0.76	1.53
1:A:11:ASN:OD1	1:A:11:ASN:HB2	0.76	1.00
1:A:23:ASN:C	1:A:24:GLN:N	0.76	0.87
1:A:17:GLU:OE1	1:A:17:GLU:CD	0.76	0.58
1:A:8:ILE:O	1:A:9:GLU:CG	0.75	2.23
1:A:38:LEU:HD22	1:A:38:LEU:HD13	0.75	1.01
1:A:52:ARG:CZ	1:A:52:ARG:HH12	0.75	1.45
1:A:20:PHE:CG	1:A:20:PHE:HD1	0.75	1.54
1:A:52:ARG:CZ	1:A:52:ARG:HH11	0.75	1.45
1:A:20:PHE:CZ	1:A:20:PHE:HE2	0.75	1.54
1:A:25:LYS:CD	1:A:25:LYS:HE2	0.75	1.30
1:A:54:GLN:CD	1:A:54:GLN:NE2	0.74	0.85
1:A:36:GLU:HG2	1:A:36:GLU:CD	0.74	1.44
1:A:11:ASN:ND2	1:A:11:ASN:N	0.74	2.34
1:A:25:LYS:CE	1:A:25:LYS:HD2	0.74	1.27
1:A:41:GLU:CD	1:A:41:GLU:OE2	0.73	0.48
1:A:25:LYS:CE	1:A:25:LYS:HD3	0.73	1.28
1:A:25:LYS:CB	1:A:25:LYS:CG	0.73	0.74
1:A:8:ILE:C	1:A:9:GLU:HB2	0.72	2.08
1:A:5:ARG:CZ	1:A:7:SER:CB	0.72	2.02
1:A:37:GLN:O	1:A:38:LEU:HB2	0.72	1.82
1:A:38:LEU:CD1	1:A:39:HIS:N	0.72	2.51
1:A:38:LEU:CG	1:A:39:HIS:N	0.71	2.30
1:A:18:LYS:NZ	1:A:18:LYS:HE2	0.71	1.10
1:A:18:LYS:NZ	1:A:18:LYS:HE3	0.71	1.10
1:A:18:LYS:CB	1:A:18:LYS:HG2	0.71	1.25
1:A:58:ARG:CZ	1:A:60:ASN:HB2	0.71	1.53
1:A:8:ILE:C	1:A:9:GLU:HG3	0.70	2.10
1:A:42:LYS:NZ	1:A:42:LYS:HD3	0.70	1.93
1:A:43:GLU:OE2	1:A:43:GLU:OE1	0.70	0.70
1:A:18:LYS:CB	1:A:18:LYS:HG3	0.70	1.25
1:A:18:LYS:HE2	1:A:18:LYS:CD	0.70	1.46
1:A:16:LEU:HB3	1:A:48:TRP:CZ3	0.69	2.21
1:A:38:LEU:CD1	1:A:38:LEU:CD2	0.69	0.78
1:A:41:GLU:OE2	1:A:41:GLU:OE1	0.69	0.70
1:A:53:ARG:CG	1:A:53:ARG:C	0.69	2.54
1:A:25:LYS:HE2	1:A:25:LYS:NZ	0.69	1.37

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:18:LYS:CG	1:A:18:LYS:HB3	0.69	1.23
1:A:18:LYS:CG	1:A:18:LYS:HB2	0.69	1.23
1:A:36:GLU:HG3	1:A:36:GLU:CD	0.69	1.44
1:A:42:LYS:CE	1:A:42:LYS:HZ1	0.69	1.41
1:A:42:LYS:CE	1:A:42:LYS:HZ3	0.69	1.40
1:A:52:ARG:CZ	1:A:52:ARG:HH21	0.69	1.40
1:A:23:ASN:C	1:A:23:ASN:O	0.68	0.75
1:A:38:LEU:CD1	1:A:38:LEU:CB	0.68	0.77
1:A:55:LYS:CE	1:A:55:LYS:HZ1	0.68	1.39
1:A:55:LYS:CE	1:A:55:LYS:HZ2	0.68	1.39
1:A:38:LEU:HD11	1:A:38:LEU:CD2	0.68	0.40
1:A:52:ARG:CZ	1:A:52:ARG:HH22	0.68	1.40
1:A:42:LYS:CE	1:A:42:LYS:HZ2	0.67	1.41
1:A:1:ARG:HH21	1:A:2:ARG:HH12	0.67	1.16
1:A:38:LEU:CD1	1:A:38:LEU:HB2	0.67	1.21
1:A:55:LYS:CE	1:A:55:LYS:HZ3	0.67	1.39
1:A:11:ASN:ND2	1:A:11:ASN:HB3	0.67	1.06
1:A:25:LYS:CE	1:A:25:LYS:HZ2	0.67	1.37
1:A:25:LYS:CE	1:A:25:LYS:HZ3	0.67	1.37
1:A:38:LEU:HD11	1:A:38:LEU:HD21	0.67	0.67
1:A:8:ILE:C	1:A:9:GLU:N	0.67	0.72
1:A:52:ARG:NH1	1:A:52:ARG:CZ	0.67	0.82
1:A:25:LYS:CE	1:A:25:LYS:HZ1	0.66	1.37
1:A:18:LYS:HE3	1:A:18:LYS:CD	0.66	1.46
1:A:52:ARG:NH1	1:A:52:ARG:CD	0.66	2.56
1:A:18:LYS:CE	1:A:18:LYS:HD2	0.66	1.32
1:A:11:ASN:CG	1:A:11:ASN:HB2	0.64	1.12
1:A:25:LYS:HE3	1:A:25:LYS:NZ	0.64	1.37
1:A:18:LYS:CG	1:A:18:LYS:HD2	0.64	1.28
1:A:11:ASN:CG	1:A:11:ASN:HB3	0.64	1.12
1:A:25:LYS:CD	1:A:25:LYS:CE	0.64	0.69
1:A:25:LYS:CE	1:A:25:LYS:NZ	0.64	0.79
1:A:8:ILE:C	1:A:9:GLU:CB	0.63	2.30
1:A:38:LEU:CB	1:A:39:HIS:N	0.63	2.02
1:A:40:MET:CE	1:A:40:MET:HG2	0.63	2.21
1:A:18:LYS:HG3	1:A:18:LYS:HD3	0.63	1.15
1:A:18:LYS:CG	1:A:18:LYS:HD3	0.62	1.28
1:A:48:TRP:CZ3	1:A:52:ARG:HG2	0.62	2.30
1:A:40:MET:CA	1:A:40:MET:HG2	0.62	2.02
1:A:18:LYS:CE	1:A:18:LYS:HD3	0.61	1.32
1:A:29:GLU:CD	1:A:29:GLU:OE2	0.61	0.68
1:A:40:MET:HG2	1:A:40:MET:N	0.61	2.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:25:LYS:CG	1:A:25:LYS:N	0.61	2.63
1:A:7:SER:C	1:A:8:ILE:HD12	0.61	2.20
1:A:52:ARG:NH2	1:A:52:ARG:CZ	0.60	0.75
1:A:57:LYS:HD2	1:A:58:ARG:N	0.60	1.79
1:A:37:GLN:CD	1:A:37:GLN:HE21	0.59	1.26
1:A:37:GLN:CD	1:A:37:GLN:HE22	0.59	1.26
1:A:25:LYS:CE	1:A:25:LYS:HG3	0.59	2.17
1:A:55:LYS:CB	1:A:55:LYS:HD2	0.58	2.17
1:A:13:ARG:HG2	1:A:14:PHE:N	0.58	2.14
1:A:18:LYS:CG	1:A:18:LYS:CB	0.58	0.60
1:A:18:LYS:HG2	1:A:18:LYS:CD	0.58	1.38
1:A:29:GLU:CD	1:A:29:GLU:OE1	0.58	0.75
1:A:25:LYS:HD2	1:A:25:LYS:HB3	0.57	1.66
1:A:38:LEU:CD1	1:A:38:LEU:HG	0.57	1.20
1:A:5:ARG:CZ	1:A:7:SER:HG	0.57	2.05
1:A:40:MET:CG	1:A:40:MET:N	0.56	2.67
1:A:37:GLN:O	1:A:38:LEU:HD12	0.55	2.02
1:A:18:LYS:HG2	1:A:18:LYS:HD2	0.55	1.13
1:A:8:ILE:CD1	1:A:8:ILE:HB	0.55	2.17
1:A:8:ILE:CD1	1:A:8:ILE:N	0.54	2.70
1:A:38:LEU:HD13	1:A:38:LEU:CG	0.54	1.07
1:A:38:LEU:CG	1:A:38:LEU:HD12	0.54	1.08
1:A:13:ARG:HB2	1:A:48:TRP:HE1	0.54	1.63
1:A:32:LEU:C	1:A:32:LEU:HD12	0.54	2.28
1:A:16:LEU:HG	1:A:49:PHE:CE1	0.54	2.38
1:A:40:MET:HB2	1:A:40:MET:HG3	0.53	1.31
1:A:11:ASN:CG	1:A:11:ASN:H	0.53	2.11
1:A:38:LEU:CD1	1:A:38:LEU:HD21	0.53	1.40
1:A:38:LEU:HB3	1:A:38:LEU:HD13	0.53	1.10
1:A:45:ILE:CG2	1:A:46:ARG:N	0.53	2.72
1:A:18:LYS:CG	1:A:18:LYS:C	0.52	2.75
1:A:31:ILE:CG2	1:A:45:ILE:HG21	0.52	2.34
1:A:38:LEU:HB2	1:A:38:LEU:HD12	0.52	0.96
1:A:55:LYS:HE3	1:A:55:LYS:HZ1	0.52	1.16
1:A:11:ASN:CG	1:A:11:ASN:HD21	0.51	1.16
1:A:11:ASN:CG	1:A:11:ASN:HD22	0.51	1.16
1:A:23:ASN:C	1:A:24:GLN:HA	0.51	2.18
1:A:26:PRO:HB2	1:A:31:ILE:CD1	0.50	2.36
1:A:23:ASN:O	1:A:23:ASN:N	0.50	2.40
1:A:29:GLU:CA	1:A:29:GLU:HG2	0.50	2.04
1:A:45:ILE:O	1:A:49:PHE:CD2	0.50	2.64
1:A:11:ASN:ND2	1:A:11:ASN:H	0.49	2.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:16:LEU:HB3	1:A:48:TRP:CH2	0.49	2.42
1:A:39:HIS:C	1:A:40:MET:HG2	0.49	2.33
1:A:23:ASN:O	1:A:23:ASN:CB	0.48	2.56
1:A:37:GLN:CD	1:A:37:GLN:NE2	0.48	0.59
1:A:38:LEU:CD2	1:A:39:HIS:CD2	0.47	2.86
1:A:10:THR:C	1:A:12:VAL:N	0.47	2.56
1:A:45:ILE:HG13	1:A:49:PHE:CE2	0.47	2.45
1:A:55:LYS:HE2	1:A:55:LYS:HZ3	0.47	1.16
1:A:13:ARG:HB2	1:A:48:TRP:NE1	0.47	2.25
1:A:39:HIS:N	1:A:39:HIS:CG	0.46	2.23
1:A:24:GLN:C	1:A:26:PRO:HD3	0.46	2.34
1:A:26:PRO:HB2	1:A:31:ILE:HD12	0.46	1.87
1:A:48:TRP:CH2	1:A:52:ARG:HG2	0.46	2.46
1:A:10:THR:O	1:A:11:ASN:C	0.45	2.52
1:A:18:LYS:HG3	1:A:18:LYS:CD	0.45	1.38
1:A:55:LYS:CA	1:A:55:LYS:HG3	0.45	2.18
1:A:8:ILE:C	1:A:9:GLU:CG	0.45	2.52
1:A:25:LYS:N	1:A:26:PRO:HD3	0.45	2.25
1:A:11:ASN:HD22	1:A:11:ASN:HB3	0.44	0.90
1:A:38:LEU:HD13	1:A:38:LEU:CB	0.44	1.25
1:A:5:ARG:NH1	1:A:7:SER:HB3	0.44	1.96
1:A:45:ILE:HG23	1:A:49:PHE:HE2	0.44	1.73
1:A:53:ARG:HB2	1:A:53:ARG:HG3	0.44	1.32
1:A:25:LYS:HE3	1:A:25:LYS:HD3	0.44	1.19
1:A:11:ASN:CG	1:A:11:ASN:CB	0.43	0.46
1:A:45:ILE:HG22	1:A:46:ARG:N	0.43	2.27
1:A:29:GLU:CG	1:A:29:GLU:N	0.43	2.76
1:A:17:GLU:OE1	1:A:17:GLU:OE2	0.42	0.47
1:A:25:LYS:HD2	1:A:25:LYS:HE2	0.42	1.20
1:A:44:VAL:HA	1:A:47:VAL:HG13	0.42	1.90
1:A:38:LEU:HD13	1:A:38:LEU:CD2	0.41	1.20
1:A:36:GLU:CG	1:A:36:GLU:CD	0.41	0.93
1:A:45:ILE:HG23	1:A:49:PHE:CE2	0.40	2.52

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	61/63 (97%)	42 (69%)	7 (11%)	12 (20%)	0	2
All	All	61/63 (97%)	42 (69%)	7 (11%)	12 (20%)	0	2

All 12 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	THR
1	A	7	SER
1	A	9	GLU
1	A	38	LEU
1	A	43	GLU
1	A	48	TRP
1	A	49	PHE
1	A	58	ARG
1	A	60	ASN
1	A	61	PRO
1	A	62	CYS

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	60/60 (100%)	31 (52%)	29 (48%)	0	1
All	All	60/60 (100%)	31 (52%)	29 (48%)	0	1

All 29 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	1	ARG
1	A	2	ARG
1	A	3	LYS
1	A	4	LYS
1	A	6	THR
1	A	11	ASN
1	A	12	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	13	ARG
1	A	16	LEU
1	A	17	GLU
1	A	21	LEU
1	A	25	LYS
1	A	27	THR
1	A	33	LEU
1	A	34	ILE
1	A	38	LEU
1	A	40	MET
1	A	41	GLU
1	A	42	LYS
1	A	44	VAL
1	A	45	ILE
1	A	47	VAL
1	A	50	CYS
1	A	53	ARG
1	A	56	GLU
1	A	57	LYS
1	A	59	ILE
1	A	60	ASN
1	A	63	SER

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	16:LEU	C	17:GLU	N	1.20
1	A	24:GLN	C	25:LYS	N	1.19
1	A	21:LEU	C	22:ALA	N	1.17
1	A	22:ALA	C	23:ASN	N	1.17
1	A	20:PHE	C	21:LEU	N	1.13
1	A	56:GLU	C	57:LYS	N	1.13
1	A	11:ASN	C	12:VAL	N	1.08
1	A	40:MET	C	41:GLU	N	1.05
1	A	4:LYS	C	5:ARG	N	0.92
1	A	23:ASN	C	24:GLN	N	0.87
1	A	2:ARG	C	3:LYS	N	0.86
1	A	9:GLU	C	10:THR	N	0.74
1	A	38:LEU	C	39:HIS	N	0.73
1	A	5:ARG	C	6:THR	N	0.72
1	A	8:ILE	C	9:GLU	N	0.72
1	A	57:LYS	C	58:ARG	N	0.71
1	A	60:ASN	C	61:PRO	N	0.63
1	A	1:ARG	C	2:ARG	N	0.56
1	A	3:LYS	C	4:LYS	N	0.56
1	A	6:THR	C	7:SER	N	0.46
1	A	7:SER	C	8:ILE	N	0.37
1	A	59:ILE	C	60:ASN	N	0.37
1	A	58:ARG	C	59:ILE	N	0.34
1	A	61:PRO	C	62:CYS	N	0.26
1	A	62:CYS	C	63:SER	N	0.18

7 Chemical shift validation

No chemical shift data were provided