



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:55 PM BST

PDB ID : 1HDP
Title : SOLUTION STRUCTURE OF A POU-SPECIFIC HOMEODOMAIN: 3D-NMR STUDIES OF HUMAN B-CELL TRANSCRIPTION FACTOR OCT-2
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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
<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

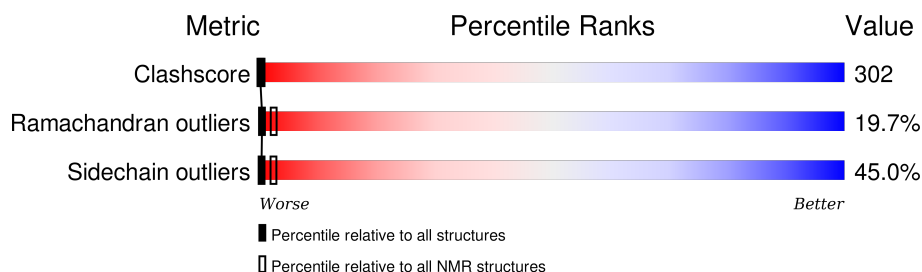
1 Overall quality at a glance

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	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.

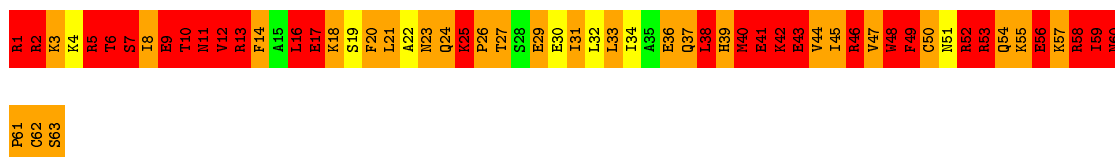
Mol	Chain	Residues	Atoms						Trace
1	A	63	Total	C	H	N	O	S	0
			1097	334	563	104	93	3	

4 Residue-property plots

These plots are provided for all protein, RNA 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: OCT-2 POU HOMEODOMAIN

Chain A: 



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. 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	29.10	313/541 (57.9%)	15.70	259/721 (35.9%)
All	All	29.10	313/541 (57.9%)	15.70	259/721 (35.9%)

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	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	61	PRO	N-CD	-98.07	0.10	1.47
1	A	56	GLU	CD-OE2	-89.77	0.26	1.25
1	A	9	GLU	CD-OE1	-89.46	0.27	1.25
1	A	30	GLU	CD-OE2	-84.24	0.33	1.25
1	A	36	GLU	CD-OE1	-83.84	0.33	1.25
1	A	63	SER	CA-CB	-83.74	0.27	1.52
1	A	2	ARG	NE-CZ	-83.73	0.24	1.33
1	A	62	CYS	CB-SG	-83.39	0.40	1.82
1	A	7	SER	CB-OG	-82.54	0.34	1.42
1	A	2	ARG	CZ-NH2	-81.15	0.27	1.33
1	A	17	GLU	CD-OE2	-79.19	0.38	1.25
1	A	36	GLU	CD-OE2	-78.35	0.39	1.25
1	A	56	GLU	CD-OE1	-76.91	0.41	1.25
1	A	5	ARG	CZ-NH2	-76.68	0.33	1.33
1	A	2	ARG	CD-NE	-73.62	0.21	1.46
1	A	30	GLU	CG-CD	-72.06	0.43	1.51
1	A	30	GLU	CD-OE1	-70.64	0.47	1.25
1	A	63	SER	CB-OG	-70.16	0.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	GLU	CD-OE2	-69.83	0.48	1.25
1	A	1	ARG	CD-NE	-69.31	0.28	1.46
1	A	61	PRO	CA-C	-68.08	0.16	1.52
1	A	58	ARG	CZ-NH1	-68.05	0.44	1.33
1	A	2	ARG	CZ-NH1	-67.09	0.45	1.33
1	A	43	GLU	CD-OE1	-66.57	0.52	1.25
1	A	13	ARG	CZ-NH2	-66.32	0.46	1.33
1	A	7	SER	CA-CB	-65.88	0.54	1.52
1	A	1	ARG	NE-CZ	-64.56	0.49	1.33
1	A	62	CYS	N-CA	-64.11	0.18	1.46
1	A	1	ARG	CZ-NH1	-63.76	0.50	1.33
1	A	17	GLU	CD-OE1	-61.34	0.58	1.25
1	A	9	GLU	CD-OE2	-60.26	0.59	1.25
1	A	58	ARG	CZ-NH2	-59.98	0.55	1.33
1	A	60	ASN	C-O	-59.88	0.09	1.23
1	A	46	ARG	CZ-NH2	-58.38	0.57	1.33
1	A	43	GLU	CD-OE2	-58.12	0.61	1.25
1	A	3	LYS	C-O	-56.78	0.15	1.23
1	A	1	ARG	CZ-NH2	-55.35	0.61	1.33
1	A	61	PRO	C-O	-55.13	0.12	1.23
1	A	13	ARG	CZ-NH1	-54.37	0.62	1.33
1	A	3	LYS	CA-CB	-53.85	0.35	1.53
1	A	63	SER	N-CA	-53.17	0.40	1.46
1	A	5	ARG	NE-CZ	-52.90	0.64	1.33
1	A	9	GLU	CB-CG	-52.06	0.53	1.52
1	A	58	ARG	CD-NE	-52.01	0.58	1.46
1	A	29	GLU	CD-OE2	-51.67	0.68	1.25
1	A	1	ARG	N-CA	-51.26	0.43	1.46
1	A	14	PHE	CG-CD2	-50.82	0.62	1.38
1	A	37	GLN	CD-OE1	-50.62	0.12	1.24
1	A	62	CYS	C-N	-50.38	0.18	1.34
1	A	10	THR	CB-OG1	-50.34	0.42	1.43
1	A	60	ASN	CB-CG	-50.10	0.35	1.51
1	A	58	ARG	C-O	-50.00	0.28	1.23
1	A	60	ASN	CG-ND2	-50.00	0.07	1.32
1	A	8	ILE	C-O	-49.11	0.30	1.23
1	A	54	GLN	CD-OE1	-49.07	0.15	1.24
1	A	61	PRO	CA-CB	-48.73	0.56	1.53
1	A	41	GLU	CD-OE1	-48.37	0.72	1.25
1	A	4	LYS	CA-CB	-48.28	0.47	1.53
1	A	39	HIS	CG-CD2	-48.01	0.54	1.35
1	A	53	ARG	CD-NE	-47.91	0.65	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	LYS	CD-CE	-47.42	0.32	1.51
1	A	61	PRO	C-N	-46.84	0.26	1.34
1	A	18	LYS	CE-NZ	-46.57	0.32	1.49
1	A	57	LYS	CE-NZ	-46.26	0.33	1.49
1	A	63	SER	C-O	-46.08	0.35	1.23
1	A	11	ASN	CB-CG	-45.63	0.46	1.51
1	A	53	ARG	NE-CZ	-45.52	0.73	1.33
1	A	29	GLU	CD-OE1	-45.39	0.75	1.25
1	A	3	LYS	N-CA	-44.97	0.56	1.46
1	A	5	ARG	CD-NE	-44.91	0.70	1.46
1	A	4	LYS	CE-NZ	-44.85	0.36	1.49
1	A	3	LYS	CB-CG	-44.82	0.31	1.52
1	A	3	LYS	CD-CE	-44.53	0.40	1.51
1	A	58	ARG	NE-CZ	-44.47	0.75	1.33
1	A	62	CYS	CA-CB	-44.41	0.56	1.53
1	A	63	SER	CA-C	-44.41	0.37	1.52
1	A	6	THR	C-O	-44.26	0.39	1.23
1	A	52	ARG	CZ-NH2	-44.19	0.75	1.33
1	A	1	ARG	CA-CB	-44.18	0.56	1.53
1	A	58	ARG	CB-CG	-44.09	0.33	1.52
1	A	60	ASN	CG-OD1	-43.38	0.28	1.24
1	A	58	ARG	C-N	-43.27	0.34	1.34
1	A	56	GLU	CG-CD	-42.96	0.87	1.51
1	A	19	SER	CB-OG	-42.81	0.86	1.42
1	A	2	ARG	C-O	-42.77	0.42	1.23
1	A	59	ILE	CA-CB	-42.61	0.56	1.54
1	A	1	ARG	CG-CD	-42.37	0.46	1.51
1	A	59	ILE	C-N	-42.16	0.37	1.34
1	A	5	ARG	CA-CB	-42.06	0.61	1.53
1	A	7	SER	C-N	-42.05	0.37	1.34
1	A	2	ARG	N-CA	-41.83	0.62	1.46
1	A	39	HIS	CB-CG	-41.78	0.74	1.50
1	A	4	LYS	N-CA	-41.71	0.62	1.46
1	A	10	THR	CA-CB	-41.66	0.45	1.53
1	A	1	ARG	C-O	-41.63	0.44	1.23
1	A	6	THR	CB-OG1	-41.53	0.60	1.43
1	A	59	ILE	CB-CG1	-41.47	0.38	1.54
1	A	2	ARG	CA-CB	-40.95	0.63	1.53
1	A	62	CYS	CA-C	-40.80	0.46	1.52
1	A	2	ARG	CG-CD	-40.72	0.50	1.51
1	A	58	ARG	CA-CB	-40.71	0.64	1.53
1	A	61	PRO	N-CA	-40.68	0.78	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	ASN	CA-CB	-40.62	0.47	1.53
1	A	39	HIS	CG-ND1	-40.47	0.49	1.38
1	A	58	ARG	CG-CD	-40.17	0.51	1.51
1	A	24	GLN	CD-NE2	-40.14	0.32	1.32
1	A	5	ARG	CZ-NH1	-39.97	0.81	1.33
1	A	9	GLU	CA-CB	-39.56	0.67	1.53
1	A	7	SER	N-CA	-39.54	0.67	1.46
1	A	39	HIS	CE1-NE2	-39.51	0.41	1.32
1	A	14	PHE	CE1-CZ	-39.33	0.62	1.37
1	A	52	ARG	CZ-NH1	-39.16	0.82	1.33
1	A	2	ARG	CA-C	-39.16	0.51	1.52
1	A	6	THR	CB-CG2	-39.15	0.23	1.52
1	A	62	CYS	C-O	-38.83	0.49	1.23
1	A	36	GLU	CG-CD	-38.79	0.93	1.51
1	A	30	GLU	CB-CG	-38.77	0.78	1.52
1	A	9	GLU	C-O	-38.35	0.50	1.23
1	A	6	THR	C-N	-38.10	0.46	1.34
1	A	53	ARG	CZ-NH2	-38.03	0.83	1.33
1	A	60	ASN	C-N	-37.30	0.63	1.34
1	A	24	GLN	CD-OE1	-37.16	0.42	1.24
1	A	11	ASN	CG-OD1	-36.69	0.43	1.24
1	A	57	LYS	CB-CG	-36.66	0.53	1.52
1	A	5	ARG	CG-CD	-36.48	0.60	1.51
1	A	36	GLU	CB-CG	-36.36	0.83	1.52
1	A	59	ILE	N-CA	-36.28	0.73	1.46
1	A	4	LYS	CB-CG	-36.18	0.54	1.52
1	A	60	ASN	N-CA	-35.55	0.75	1.46
1	A	5	ARG	CB-CG	-35.54	0.56	1.52
1	A	29	GLU	CB-CG	-35.27	0.85	1.52
1	A	39	HIS	CD2-NE2	-35.09	0.60	1.38
1	A	3	LYS	CA-C	-34.70	0.62	1.52
1	A	6	THR	CA-CB	-34.61	0.63	1.53
1	A	11	ASN	CG-ND2	-34.45	0.46	1.32
1	A	38	LEU	CG-CD1	-34.40	0.24	1.51
1	A	18	LYS	CB-CG	-34.28	0.59	1.52
1	A	41	GLU	CB-CG	-34.03	0.87	1.52
1	A	53	ARG	CZ-NH1	-33.97	0.88	1.33
1	A	3	LYS	C-N	-33.95	0.56	1.34
1	A	1	ARG	CA-C	-33.84	0.65	1.52
1	A	1	ARG	C-N	-33.74	0.56	1.34
1	A	9	GLU	CG-CD	-33.47	1.01	1.51
1	A	4	LYS	CG-CD	-33.35	0.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	LYS	CG-CD	-33.24	0.39	1.52
1	A	51	ASN	CG-OD1	-33.08	0.51	1.24
1	A	25	LYS	CD-CE	-32.79	0.69	1.51
1	A	7	SER	C-O	-32.77	0.61	1.23
1	A	46	ARG	CZ-NH1	-32.43	0.90	1.33
1	A	38	LEU	CB-CG	-32.37	0.58	1.52
1	A	20	PHE	CG-CD2	-32.03	0.90	1.38
1	A	6	THR	CA-C	-31.78	0.70	1.52
1	A	5	ARG	N-CA	-31.60	0.83	1.46
1	A	37	GLN	CG-CD	-31.60	0.78	1.51
1	A	46	ARG	NE-CZ	-31.47	0.92	1.33
1	A	3	LYS	CE-NZ	-31.23	0.70	1.49
1	A	54	GLN	CG-CD	-31.07	0.79	1.51
1	A	20	PHE	CG-CD1	-30.88	0.92	1.38
1	A	4	LYS	C-O	-30.69	0.65	1.23
1	A	57	LYS	C-O	-29.56	0.67	1.23
1	A	37	GLN	CD-NE2	-29.55	0.58	1.32
1	A	6	THR	N-CA	-29.37	0.87	1.46
1	A	59	ILE	CB-CG2	-29.28	0.62	1.52
1	A	58	ARG	CA-C	-29.10	0.77	1.52
1	A	60	ASN	CA-C	-28.85	0.78	1.52
1	A	57	LYS	CG-CD	-28.78	0.54	1.52
1	A	25	LYS	CB-CG	-28.74	0.74	1.52
1	A	59	ILE	C-O	-28.72	0.68	1.23
1	A	39	HIS	ND1-CE1	-28.66	0.63	1.34
1	A	46	ARG	CB-CG	-28.50	0.75	1.52
1	A	2	ARG	CB-CG	-28.41	0.75	1.52
1	A	25	LYS	CE-NZ	-27.88	0.79	1.49
1	A	13	ARG	NE-CZ	-27.65	0.97	1.33
1	A	4	LYS	CD-CE	-27.26	0.83	1.51
1	A	57	LYS	C-N	-27.23	0.71	1.34
1	A	55	LYS	CE-NZ	-27.20	0.81	1.49
1	A	8	ILE	C-N	-26.98	0.71	1.34
1	A	5	ARG	C-N	-26.94	0.72	1.34
1	A	59	ILE	CA-C	-26.60	0.83	1.52
1	A	4	LYS	CA-C	-26.52	0.83	1.52
1	A	24	GLN	CG-CD	-26.42	0.90	1.51
1	A	38	LEU	C-N	-26.40	0.73	1.34
1	A	42	LYS	CE-NZ	-26.25	0.83	1.49
1	A	18	LYS	CD-CE	-26.03	0.86	1.51
1	A	10	THR	CB-CG2	-25.81	0.67	1.52
1	A	9	GLU	C-N	-25.77	0.74	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	ARG	CB-CG	-25.73	0.83	1.52
1	A	23	ASN	C-O	-25.17	0.75	1.23
1	A	38	LEU	C-O	-25.10	0.75	1.23
1	A	20	PHE	CE1-CZ	-24.63	0.90	1.37
1	A	33	LEU	CG-CD2	-24.60	0.60	1.51
1	A	55	LYS	CB-CG	-24.11	0.87	1.52
1	A	23	ASN	CG-OD1	-24.05	0.71	1.24
1	A	17	GLU	CG-CD	-23.77	1.16	1.51
1	A	20	PHE	CE2-CZ	-23.71	0.92	1.37
1	A	46	ARG	CD-NE	-23.51	1.06	1.46
1	A	23	ASN	CG-ND2	-23.38	0.74	1.32
1	A	1	ARG	CB-CG	-23.15	0.90	1.52
1	A	5	ARG	C-O	-22.86	0.80	1.23
1	A	13	ARG	CD-NE	-22.73	1.07	1.46
1	A	5	ARG	CA-C	-22.65	0.94	1.52
1	A	14	PHE	CG-CD1	-22.52	1.04	1.38
1	A	55	LYS	CD-CE	-22.38	0.95	1.51
1	A	42	LYS	CD-CE	-22.30	0.95	1.51
1	A	18	LYS	CG-CD	-21.44	0.79	1.52
1	A	43	GLU	CG-CD	-21.00	1.20	1.51
1	A	61	PRO	CB-CG	-20.80	0.46	1.50
1	A	2	ARG	C-N	-20.76	0.86	1.34
1	A	23	ASN	C-N	-20.37	0.87	1.34
1	A	52	ARG	NE-CZ	-20.32	1.06	1.33
1	A	33	LEU	CG-CD1	-20.30	0.76	1.51
1	A	53	ARG	CG-CD	-20.10	1.01	1.51
1	A	33	LEU	CB-CG	-19.69	0.95	1.52
1	A	38	LEU	CA-CB	-19.64	1.08	1.53
1	A	40	MET	C-O	-19.11	0.87	1.23
1	A	21	LEU	CB-CG	-19.03	0.97	1.52
1	A	14	PHE	CB-CG	-19.00	1.19	1.51
1	A	46	ARG	CG-CD	-18.99	1.04	1.51
1	A	54	GLN	CD-NE2	-18.96	0.85	1.32
1	A	40	MET	CB-CG	-18.89	0.90	1.51
1	A	61	PRO	CG-CD	-18.79	0.88	1.50
1	A	39	HIS	CA-CB	-18.12	1.14	1.53
1	A	51	ASN	CG-ND2	-17.99	0.87	1.32
1	A	4	LYS	C-N	-17.98	0.92	1.34
1	A	8	ILE	CB-CG1	-17.45	1.05	1.54
1	A	42	LYS	CB-CG	-17.40	1.05	1.52
1	A	10	THR	N-CA	-17.35	1.11	1.46
1	A	23	ASN	CB-CG	-17.24	1.11	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	PHE	CE2-CZ	-17.08	1.04	1.37
1	A	21	LEU	CG-CD1	-17.06	0.88	1.51
1	A	21	LEU	CG-CD2	-16.69	0.90	1.51
1	A	42	LYS	CG-CD	-16.14	0.97	1.52
1	A	8	ILE	N-CA	-16.01	1.14	1.46
1	A	38	LEU	CG-CD2	-16.00	0.92	1.51
1	A	40	MET	CG-SD	-15.71	1.40	1.81
1	A	29	GLU	CG-CD	-15.42	1.28	1.51
1	A	12	VAL	CA-CB	-15.17	1.22	1.54
1	A	50	CYS	CB-SG	-15.01	1.56	1.82
1	A	58	ARG	N-CA	-14.94	1.16	1.46
1	A	40	MET	SD-CE	-14.84	0.94	1.77
1	A	27	THR	CB-OG1	-14.79	1.13	1.43
1	A	52	ARG	CG-CD	-14.73	1.15	1.51
1	A	59	ILE	CG1-CD1	-14.42	0.51	1.50
1	A	14	PHE	CD1-CE1	-14.38	1.10	1.39
1	A	14	PHE	CD2-CE2	-14.32	1.10	1.39
1	A	9	GLU	CA-C	-13.95	1.16	1.52
1	A	39	HIS	N-CA	-13.89	1.18	1.46
1	A	8	ILE	CB-CG2	-13.44	1.11	1.52
1	A	57	LYS	CA-CB	-13.38	1.24	1.53
1	A	55	LYS	CG-CD	-12.82	1.08	1.52
1	A	40	MET	C-N	-12.59	1.05	1.34
1	A	11	ASN	N-CA	-12.49	1.21	1.46
1	A	9	GLU	N-CA	-11.93	1.22	1.46
1	A	56	GLU	CB-CG	-11.81	1.29	1.52
1	A	7	SER	CA-C	-11.73	1.22	1.52
1	A	24	GLN	CA-CB	-11.69	1.28	1.53
1	A	57	LYS	CA-C	-11.51	1.23	1.52
1	A	11	ASN	C-N	-11.21	1.08	1.34
1	A	24	GLN	C-O	-10.85	1.02	1.23
1	A	38	LEU	CA-C	-10.36	1.26	1.52
1	A	8	ILE	CA-C	-10.22	1.26	1.52
1	A	41	GLU	CG-CD	-10.15	1.36	1.51
1	A	21	LEU	CA-CB	-9.92	1.30	1.53
1	A	8	ILE	CA-CB	-9.74	1.32	1.54
1	A	10	THR	CA-C	-9.74	1.27	1.52
1	A	31	ILE	CG1-CD1	-9.68	0.83	1.50
1	A	23	ASN	CA-CB	-9.20	1.29	1.53
1	A	56	GLU	C-N	-8.98	1.13	1.34
1	A	20	PHE	C-N	-8.97	1.13	1.34
1	A	24	GLN	CB-CG	-8.96	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	ALA	CA-CB	-8.85	1.33	1.52
1	A	26	PRO	N-CD	-8.78	1.35	1.47
1	A	51	ASN	CB-CG	-8.77	1.30	1.51
1	A	26	PRO	N-CA	-8.69	1.32	1.47
1	A	56	GLU	C-O	-8.69	1.06	1.23
1	A	23	ASN	N-CA	-8.68	1.28	1.46
1	A	8	ILE	CG1-CD1	-8.50	0.91	1.50
1	A	13	ARG	CG-CD	-8.46	1.30	1.51
1	A	19	SER	CA-CB	-8.44	1.40	1.52
1	A	24	GLN	N-CA	-8.41	1.29	1.46
1	A	27	THR	CB-CG2	-8.36	1.24	1.52
1	A	25	LYS	CG-CD	-7.42	1.27	1.52
1	A	21	LEU	C-N	-7.38	1.17	1.34
1	A	22	ALA	C-N	-7.38	1.17	1.34
1	A	12	VAL	CB-CG2	-7.13	1.37	1.52
1	A	11	ASN	C-O	-7.04	1.09	1.23
1	A	25	LYS	CA-CB	-6.89	1.38	1.53
1	A	13	ARG	CB-CG	-6.57	1.34	1.52
1	A	20	PHE	C-O	-6.47	1.11	1.23
1	A	23	ASN	CA-C	-6.46	1.36	1.52
1	A	22	ALA	CA-C	-6.42	1.36	1.52
1	A	26	PRO	CA-CB	-6.37	1.40	1.53
1	A	24	GLN	C-N	-6.28	1.19	1.34
1	A	52	ARG	CD-NE	-6.13	1.36	1.46
1	A	49	PHE	CG-CD2	-6.03	1.29	1.38
1	A	26	PRO	C-O	-6.03	1.11	1.23
1	A	16	LEU	C-N	-5.93	1.20	1.34
1	A	41	GLU	CA-CB	-5.90	1.41	1.53
1	A	40	MET	CA-CB	-5.75	1.41	1.53
1	A	37	GLN	C-O	-5.64	1.12	1.23
1	A	49	PHE	CG-CD1	-5.58	1.30	1.38
1	A	25	LYS	N-CA	-5.58	1.35	1.46
1	A	21	LEU	N-CA	-5.55	1.35	1.46
1	A	11	ASN	CA-CB	-5.52	1.38	1.53
1	A	48	TRP	CD2-CE2	-5.52	1.34	1.41
1	A	57	LYS	N-CA	-5.50	1.35	1.46
1	A	18	LYS	C-N	-5.47	1.21	1.34
1	A	12	VAL	N-CA	-5.42	1.35	1.46
1	A	37	GLN	CA-CB	-5.35	1.42	1.53
1	A	52	ARG	CB-CG	-5.33	1.38	1.52
1	A	25	LYS	CA-C	-5.24	1.39	1.52
1	A	13	ARG	N-CA	-5.17	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	GLU	C-N	-5.03	1.22	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ARG	NE-CZ-NH2	-134.60	53.00	120.30
1	A	5	ARG	NE-CZ-NH2	-101.12	69.74	120.30
1	A	56	GLU	OE1-CD-OE2	-76.28	31.76	123.30
1	A	36	GLU	OE1-CD-OE2	-76.14	31.93	123.30
1	A	5	ARG	NE-CZ-NH1	74.08	157.34	120.30
1	A	13	ARG	NE-CZ-NH1	70.53	155.57	120.30
1	A	8	ILE	O-C-N	-67.96	13.97	122.70
1	A	63	SER	N-CA-CB	-66.24	11.14	110.50
1	A	2	ARG	NE-CZ-NH1	61.99	151.29	120.30
1	A	58	ARG	O-C-N	-61.57	24.19	122.70
1	A	17	GLU	OE1-CD-OE2	-57.90	53.82	123.30
1	A	7	SER	O-C-N	-56.03	33.05	122.70
1	A	13	ARG	NH1-CZ-NH2	-55.55	58.30	119.40
1	A	54	GLN	CG-CD-OE1	-53.44	14.73	121.60
1	A	10	THR	CA-CB-CG2	-52.88	38.37	112.40
1	A	13	ARG	NE-CZ-NH2	51.66	146.13	120.30
1	A	9	GLU	OE1-CD-OE2	-51.05	62.04	123.30
1	A	61	PRO	N-CA-CB	50.89	164.37	103.30
1	A	41	GLU	OE1-CD-OE2	-46.29	67.75	123.30
1	A	46	ARG	NE-CZ-NH1	45.69	143.14	120.30
1	A	58	ARG	NE-CZ-NH2	45.43	143.01	120.30
1	A	62	CYS	CA-C-N	-44.46	19.38	117.20
1	A	61	PRO	CA-CB-CG	-42.98	22.33	104.00
1	A	2	ARG	CA-C-O	-42.47	30.91	120.10
1	A	62	CYS	C-N-CA	-40.47	20.54	121.70
1	A	43	GLU	OE1-CD-OE2	-39.09	76.40	123.30
1	A	24	GLN	OE1-CD-NE2	-35.69	39.82	121.90
1	A	14	PHE	CB-CG-CD1	35.45	145.62	120.80
1	A	33	LEU	CB-CG-CD1	34.97	170.45	111.00
1	A	3	LYS	N-CA-CB	34.97	173.54	110.60
1	A	3	LYS	CA-CB-CG	-34.45	37.60	113.40
1	A	1	ARG	NE-CZ-NH1	-33.68	103.46	120.30
1	A	2	ARG	NH1-CZ-NH2	33.01	155.71	119.40
1	A	58	ARG	CD-NE-CZ	32.69	169.36	123.60
1	A	58	ARG	CB-CG-CD	-31.80	28.91	111.60
1	A	58	ARG	NH1-CZ-NH2	-31.70	84.53	119.40
1	A	61	PRO	CA-C-O	-31.70	44.12	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ARG	CG-CD-NE	31.37	177.68	111.80
1	A	38	LEU	CB-CG-CD2	30.48	162.82	111.00
1	A	33	LEU	CB-CG-CD2	30.27	162.46	111.00
1	A	3	LYS	CB-CA-C	-29.75	50.90	110.40
1	A	33	LEU	CD1-CG-CD2	-28.11	26.19	110.50
1	A	52	ARG	NE-CZ-NH1	27.50	134.05	120.30
1	A	62	CYS	O-C-N	27.45	166.61	122.70
1	A	7	SER	N-CA-CB	-27.41	69.38	110.50
1	A	2	ARG	O-C-N	26.61	165.27	122.70
1	A	8	ILE	CA-C-N	26.55	175.61	117.20
1	A	37	GLN	OE1-CD-NE2	-25.96	62.19	121.90
1	A	55	LYS	CD-CE-NZ	25.83	171.12	111.70
1	A	62	CYS	CA-C-O	25.67	174.00	120.10
1	A	13	ARG	CD-NE-CZ	25.13	158.78	123.60
1	A	54	GLN	CG-CD-NE2	25.08	176.88	116.70
1	A	60	ASN	N-CA-CB	-25.00	65.61	110.60
1	A	56	GLU	CG-CD-OE1	24.69	167.68	118.30
1	A	58	ARG	NE-CZ-NH1	24.31	132.46	120.30
1	A	46	ARG	NE-CZ-NH2	-24.17	108.22	120.30
1	A	8	ILE	CA-C-O	23.96	170.41	120.10
1	A	36	GLU	CG-CD-OE2	23.53	165.36	118.30
1	A	5	ARG	CB-CA-C	-23.30	63.79	110.40
1	A	60	ASN	CB-CG-OD1	23.23	168.05	121.60
1	A	7	SER	CA-C-O	23.17	168.76	120.10
1	A	58	ARG	CA-C-N	23.16	168.16	117.20
1	A	60	ASN	O-C-N	-23.05	77.30	121.10
1	A	9	GLU	O-C-N	-22.72	86.35	122.70
1	A	58	ARG	CA-C-O	22.64	167.64	120.10
1	A	14	PHE	CG-CD1-CE1	22.55	145.60	120.80
1	A	61	PRO	O-C-N	22.48	158.67	122.70
1	A	6	THR	CA-CB-OG1	22.33	155.90	109.00
1	A	36	GLU	CG-CD-OE1	22.21	162.72	118.30
1	A	53	ARG	CD-NE-CZ	21.96	154.34	123.60
1	A	37	GLN	CG-CD-NE2	21.80	169.02	116.70
1	A	29	GLU	OE1-CD-OE2	-21.67	97.29	123.30
1	A	8	ILE	C-N-CA	21.67	175.88	121.70
1	A	9	GLU	CG-CD-OE2	21.60	161.50	118.30
1	A	24	GLN	CG-CD-OE1	21.37	164.34	121.60
1	A	20	PHE	CD1-CG-CD2	-21.35	90.55	118.30
1	A	3	LYS	CB-CG-CD	21.22	166.76	111.60
1	A	14	PHE	CZ-CE2-CD2	21.21	145.55	120.10
1	A	2	ARG	CA-C-N	21.19	163.82	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLU	CG-CD-OE2	21.13	160.56	118.30
1	A	60	ASN	CA-CB-CG	-21.10	66.97	113.40
1	A	38	LEU	CD1-CG-CD2	-20.99	47.54	110.50
1	A	62	CYS	CB-CA-C	20.82	152.03	110.40
1	A	63	SER	CB-CA-C	-20.62	70.92	110.10
1	A	20	PHE	CB-CG-CD1	20.61	135.23	120.80
1	A	52	ARG	NH1-CZ-NH2	-20.57	96.78	119.40
1	A	46	ARG	CD-NE-CZ	20.48	152.28	123.60
1	A	30	GLU	CB-CG-CD	20.46	169.45	114.20
1	A	17	GLU	CG-CD-OE1	20.40	159.09	118.30
1	A	3	LYS	CA-C-N	20.34	161.94	117.20
1	A	54	GLN	OE1-CD-NE2	20.21	168.38	121.90
1	A	42	LYS	CG-CD-CE	20.16	172.38	111.90
1	A	62	CYS	N-CA-C	-20.01	56.98	111.00
1	A	40	MET	CG-SD-CE	19.95	132.13	100.20
1	A	18	LYS	CG-CD-CE	19.82	171.35	111.90
1	A	4	LYS	CB-CG-CD	-19.80	60.12	111.60
1	A	57	LYS	CD-CE-NZ	-19.68	66.45	111.70
1	A	39	HIS	CA-CB-CG	19.53	146.80	113.60
1	A	5	ARG	CA-CB-CG	19.41	156.10	113.40
1	A	60	ASN	CA-C-N	19.35	171.29	117.10
1	A	57	LYS	O-C-N	-19.25	91.91	122.70
1	A	20	PHE	CB-CG-CD2	19.16	134.22	120.80
1	A	11	ASN	CA-CB-CG	19.16	155.55	113.40
1	A	58	ARG	C-N-CA	18.96	169.10	121.70
1	A	37	GLN	CB-CG-CD	18.83	160.55	111.60
1	A	7	SER	CA-C-N	18.63	158.19	117.20
1	A	60	ASN	CB-CG-ND2	-18.50	72.31	116.70
1	A	14	PHE	CB-CG-CD2	-18.29	108.00	120.80
1	A	10	THR	CA-CB-OG1	-18.23	70.72	109.00
1	A	61	PRO	CA-C-N	18.17	157.18	117.20
1	A	1	ARG	CD-NE-CZ	18.04	148.85	123.60
1	A	2	ARG	C-N-CA	18.03	166.78	121.70
1	A	39	HIS	ND1-CG-CD2	-17.95	80.87	106.00
1	A	13	ARG	CG-CD-NE	17.77	149.12	111.80
1	A	52	ARG	NE-CZ-NH2	17.74	129.17	120.30
1	A	53	ARG	NE-CZ-NH2	-17.68	111.46	120.30
1	A	41	GLU	CG-CD-OE1	17.64	153.59	118.30
1	A	10	THR	N-CA-C	17.58	158.47	111.00
1	A	46	ARG	CG-CD-NE	17.05	147.60	111.80
1	A	3	LYS	C-N-CA	16.93	164.03	121.70
1	A	60	ASN	N-CA-C	16.86	156.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	MET	CB-CG-SD	16.78	162.75	112.40
1	A	6	THR	OG1-CB-CG2	-16.70	71.60	110.00
1	A	51	ASN	OD1-CG-ND2	-16.56	83.80	121.90
1	A	2	ARG	N-CA-CB	16.35	140.02	110.60
1	A	30	GLU	CG-CD-OE2	-16.33	85.63	118.30
1	A	24	GLN	CG-CD-NE2	16.30	155.83	116.70
1	A	20	PHE	CE1-CZ-CE2	-16.27	90.72	120.00
1	A	3	LYS	CA-C-O	-16.15	86.19	120.10
1	A	5	ARG	N-CA-CB	16.15	139.66	110.60
1	A	61	PRO	C-N-CA	16.07	161.86	121.70
1	A	31	ILE	CB-CG1-CD1	16.05	158.83	113.90
1	A	42	LYS	CD-CE-NZ	16.05	148.61	111.70
1	A	9	GLU	CB-CG-CD	15.98	157.34	114.20
1	A	38	LEU	O-C-N	-15.57	97.78	122.70
1	A	63	SER	CA-CB-OG	15.46	152.93	111.20
1	A	7	SER	CB-CA-C	15.30	139.17	110.10
1	A	61	PRO	CB-CG-CD	15.24	165.95	106.50
1	A	23	ASN	O-C-N	-15.14	98.48	122.70
1	A	59	ILE	CA-C-O	15.02	151.65	120.10
1	A	21	LEU	CB-CG-CD2	14.91	136.35	111.00
1	A	7	SER	C-N-CA	14.84	158.80	121.70
1	A	55	LYS	CB-CG-CD	14.79	150.06	111.60
1	A	1	ARG	CB-CG-CD	-14.69	73.42	111.60
1	A	21	LEU	CB-CG-CD1	14.50	135.65	111.00
1	A	53	ARG	CB-CG-CD	14.48	149.26	111.60
1	A	17	GLU	CG-CD-OE2	14.39	147.08	118.30
1	A	62	CYS	N-CA-CB	14.33	136.40	110.60
1	A	25	LYS	CA-CB-CG	14.32	144.91	113.40
1	A	6	THR	O-C-N	-14.18	100.01	122.70
1	A	36	GLU	CB-CG-CD	13.85	151.59	114.20
1	A	18	LYS	CA-CB-CG	13.70	143.53	113.40
1	A	38	LEU	CA-CB-CG	13.66	146.72	115.30
1	A	60	ASN	C-N-CD	-13.66	90.55	120.60
1	A	46	ARG	CB-CG-CD	13.63	147.03	111.60
1	A	59	ILE	CB-CA-C	13.62	138.84	111.60
1	A	43	GLU	CG-CD-OE2	13.61	145.52	118.30
1	A	36	GLU	CA-CB-CG	13.52	143.15	113.40
1	A	4	LYS	N-CA-CB	-13.34	86.59	110.60
1	A	40	MET	CA-CB-CG	13.32	135.95	113.30
1	A	38	LEU	CB-CG-CD1	13.31	133.63	111.00
1	A	20	PHE	CG-CD1-CE1	13.20	135.31	120.80
1	A	60	ASN	CB-CA-C	12.98	136.35	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ASN	CB-CG-ND2	12.93	147.73	116.70
1	A	1	ARG	NE-CZ-NH2	12.87	126.73	120.30
1	A	21	LEU	CD1-CG-CD2	-12.69	72.44	110.50
1	A	20	PHE	CZ-CE2-CD2	12.60	135.22	120.10
1	A	4	LYS	N-CA-C	12.49	144.72	111.00
1	A	25	LYS	CG-CD-CE	12.42	149.16	111.90
1	A	58	ARG	N-CA-C	12.39	144.46	111.00
1	A	39	HIS	CG-ND1-CE1	12.38	125.53	108.20
1	A	9	GLU	CA-C-N	12.30	144.25	117.20
1	A	5	ARG	NH1-CZ-NH2	12.29	132.92	119.40
1	A	9	GLU	N-CA-C	12.25	144.07	111.00
1	A	20	PHE	CG-CD2-CE2	12.13	134.14	120.80
1	A	25	LYS	CD-CE-NZ	12.03	139.38	111.70
1	A	30	GLU	OE1-CD-OE2	11.87	137.54	123.30
1	A	60	ASN	C-N-CA	11.85	171.77	122.00
1	A	59	ILE	CA-C-N	-11.72	91.41	117.20
1	A	7	SER	N-CA-C	11.66	142.47	111.00
1	A	56	GLU	CB-CG-CD	11.63	145.60	114.20
1	A	20	PHE	CD1-CE1-CZ	11.63	134.05	120.10
1	A	14	PHE	CG-CD2-CE2	-11.59	108.05	120.80
1	A	55	LYS	CA-CB-CG	11.54	138.79	113.40
1	A	4	LYS	CA-CB-CG	-11.27	88.60	113.40
1	A	9	GLU	CB-CA-C	-11.25	87.90	110.40
1	A	39	HIS	CG-CD2-NE2	10.81	129.75	109.20
1	A	63	SER	N-CA-C	-10.80	81.84	111.00
1	A	59	ILE	C-N-CA	-10.79	94.72	121.70
1	A	61	PRO	N-CA-C	-10.59	84.56	112.10
1	A	6	THR	CA-CB-CG2	-10.40	97.84	112.40
1	A	59	ILE	N-CA-CB	-10.33	87.05	110.80
1	A	41	GLU	CG-CD-OE2	10.18	138.66	118.30
1	A	10	THR	N-CA-CB	-10.12	91.08	110.30
1	A	5	ARG	N-CA-C	10.11	138.30	111.00
1	A	9	GLU	C-N-CA	10.07	146.89	121.70
1	A	14	PHE	CD1-CE1-CZ	-10.06	108.03	120.10
1	A	59	ILE	CA-CB-CG2	10.04	130.98	110.90
1	A	53	ARG	NH1-CZ-NH2	9.98	130.38	119.40
1	A	4	LYS	CA-C-O	-9.96	99.17	120.10
1	A	25	LYS	CB-CG-CD	9.89	137.32	111.60
1	A	43	GLU	CG-CD-OE1	9.89	138.08	118.30
1	A	61	PRO	CA-N-CD	-9.88	97.67	111.50
1	A	57	LYS	CA-CB-CG	-9.83	91.78	113.40
1	A	46	ARG	NH1-CZ-NH2	-9.78	108.64	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	PRO	N-CD-CG	-9.74	88.59	103.20
1	A	1	ARG	NH1-CZ-NH2	9.46	129.81	119.40
1	A	33	LEU	CA-CB-CG	9.44	137.01	115.30
1	A	10	THR	OG1-CB-CG2	-9.41	88.35	110.00
1	A	30	GLU	CG-CD-OE1	9.26	136.82	118.30
1	A	46	ARG	CA-CB-CG	9.20	133.63	113.40
1	A	14	PHE	CD1-CG-CD2	-9.17	106.38	118.30
1	A	4	LYS	CB-CA-C	9.14	128.68	110.40
1	A	18	LYS	CB-CG-CD	9.13	135.33	111.60
1	A	9	GLU	CG-CD-OE1	9.08	136.45	118.30
1	A	2	ARG	CG-CD-NE	-8.94	93.04	111.80
1	A	40	MET	O-C-N	-8.93	108.42	122.70
1	A	5	ARG	CD-NE-CZ	8.91	136.07	123.60
1	A	2	ARG	CB-CG-CD	8.78	134.43	111.60
1	A	29	GLU	CG-CD-OE1	8.11	134.51	118.30
1	A	58	ARG	CB-CA-C	-7.94	94.52	110.40
1	A	29	GLU	CB-CG-CD	7.91	135.56	114.20
1	A	7	SER	CA-CB-OG	7.73	132.06	111.20
1	A	57	LYS	CA-C-O	7.69	136.25	120.10
1	A	38	LEU	CA-C-O	7.69	136.25	120.10
1	A	1	ARG	N-CA-C	-7.66	90.33	111.00
1	A	14	PHE	CE1-CZ-CE2	-7.57	106.38	120.00
1	A	8	ILE	CB-CG1-CD1	7.42	134.66	113.90
1	A	42	LYS	CA-CB-CG	7.30	129.45	113.40
1	A	59	ILE	N-CA-C	7.17	130.35	111.00
1	A	29	GLU	CA-CB-CG	7.12	129.07	113.40
1	A	61	PRO	CB-CA-C	-6.89	94.77	112.00
1	A	1	ARG	CG-CD-NE	-6.85	97.42	111.80
1	A	4	LYS	CD-CE-NZ	6.80	127.33	111.70
1	A	3	LYS	O-C-N	-6.77	111.87	122.70
1	A	23	ASN	OD1-CG-ND2	-6.76	106.35	121.90
1	A	57	LYS	CA-C-N	6.65	131.84	117.20
1	A	6	THR	CA-C-N	6.55	131.61	117.20
1	A	55	LYS	CG-CD-CE	6.45	131.25	111.90
1	A	23	ASN	CA-C-N	6.41	131.31	117.20
1	A	58	ARG	CG-CD-NE	-6.38	98.40	111.80
1	A	2	ARG	CA-CB-CG	6.19	127.02	113.40
1	A	13	ARG	CB-CG-CD	6.10	127.46	111.60
1	A	3	LYS	N-CA-C	6.04	127.32	111.00
1	A	4	LYS	O-C-N	5.93	132.18	122.70
1	A	58	ARG	CA-CB-CG	-5.79	100.66	113.40
1	A	8	ILE	CG1-CB-CG2	-5.68	98.91	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	LYS	C-N-CA	5.54	135.55	121.70
1	A	6	THR	C-N-CA	5.38	135.15	121.70
1	A	40	MET	CA-C-N	5.38	129.03	117.20
1	A	21	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	23	ASN	C-N-CA	5.31	134.99	121.70
1	A	4	LYS	C-N-CA	5.27	134.88	121.70
1	A	8	ILE	CA-CB-CG2	5.24	121.38	110.90
1	A	4	LYS	CA-C-N	5.20	128.64	117.20
1	A	10	THR	O-C-N	5.17	130.97	122.70
1	A	18	LYS	CD-CE-NZ	5.17	123.59	111.70
1	A	24	GLN	CB-CG-CD	-5.13	98.25	111.60
1	A	39	HIS	CB-CG-ND1	5.04	135.80	123.20

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	46	ARG	Sidechain
1	A	5	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	13	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	523	319
All	All	534	563	523	319

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 302.

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:CA	1:A:38:LEU:CD1	1.52	1.81
1:A:42:LYS:CD	1:A:42:LYS:NZ	1.50	1.71
1:A:55:LYS:CD	1:A:55:LYS:NZ	1.49	1.75
1:A:25:LYS:CD	1:A:25:LYS:CB	1.49	1.88
1:A:25:LYS:CE	1:A:25:LYS:CG	1.48	1.89
1:A:55:LYS:CB	1:A:55:LYS:CD	1.48	1.89
1:A:11:ASN:CA	1:A:11:ASN:CG	1.47	1.81
1:A:8:ILE:O	1:A:9:GLU:CA	1.45	1.65
1:A:20:PHE:CD1	1:A:20:PHE:CZ	1.42	2.07
1:A:20:PHE:CE2	1:A:20:PHE:CG	1.42	2.07
1:A:18:LYS:CA	1:A:18:LYS:CG	1.42	1.95
1:A:52:ARG:NH2	1:A:52:ARG:NE	1.41	1.64
1:A:20:PHE:CD2	1:A:20:PHE:CZ	1.38	2.09
1:A:20:PHE:CG	1:A:20:PHE:CE1	1.38	2.09
1:A:53:ARG:CA	1:A:53:ARG:CG	1.37	1.99
1:A:41:GLU:CG	1:A:41:GLU:CA	1.37	2.01
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:54:GLN:CD	1:A:54:GLN:CB	1.35	1.95
1:A:25:LYS:CA	1:A:25:LYS:CG	1.33	2.04
1:A:41:GLU:CG	1:A:41:GLU:OE2	1.33	1.76
1:A:52:ARG:NH1	1:A:52:ARG:NE	1.31	1.73
1:A:29:GLU:CB	1:A:29:GLU:CD	1.30	1.98
1:A:29:GLU:OE2	1:A:29:GLU:CG	1.30	1.79
1:A:41:GLU:CD	1:A:41:GLU:CB	1.30	1.96
1:A:11:ASN:ND2	1:A:11:ASN:CA	1.28	1.97

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:23:ASN:C	1:A:24:GLN:CA	1.28	2.00
1:A:8:ILE:CA	1:A:9:GLU:N	1.27	1.97
1:A:20:PHE:CB	1:A:20:PHE:CD2	1.27	2.17
1:A:29:GLU:CG	1:A:29:GLU:CA	1.26	2.13
1:A:40:MET:CE	1:A:40:MET:CG	1.24	2.15
1:A:20:PHE:CB	1:A:20:PHE:CD1	1.23	2.19
1:A:40:MET:CA	1:A:40:MET:CG	1.23	2.15
1:A:36:GLU:CA	1:A:36:GLU:CG	1.22	2.17
1:A:40:MET:CB	1:A:40:MET:SD	1.21	2.28
1:A:56:GLU:CB	1:A:56:GLU:CD	1.20	2.07
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:23:ASN:O	1:A:23:ASN:CA	1.17	1.93
1:A:31:ILE:CD1	1:A:31:ILE:CB	1.15	2.23
1:A:29:GLU:OE1	1:A:29:GLU:CG	1.14	1.89
1:A:37:GLN:CD	1:A:37:GLN:CB	1.13	2.16
1:A:58:ARG:NH2	1:A:60:ASN:HB2	1.12	1.15
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:HD13	1:A:8:ILE:CG1	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:54:GLN:CD	1:A:54:GLN:HG3	0.99	1.43
1:A:42:LYS:HE3	1:A:42:LYS:NZ	0.98	1.37
1:A:53:ARG:CB	1:A:53:ARG:HD2	0.96	1.89
1:A:38:LEU:HD23	1:A:39:HIS:CD2	0.96	1.95
1:A:8:ILE:HD12	1:A:8:ILE:CG1	0.96	1.54
1:A:56:GLU:CG	1:A:56:GLU:CD	0.96	0.87
1:A:56:GLU:HG2	1:A:56:GLU:CD	0.95	1.41
1:A:41:GLU:CB	1:A:41:GLU:HG3	0.95	1.48
1:A:42:LYS:CE	1:A:42:LYS:NZ	0.95	0.83
1:A:54:GLN:CD	1:A:54:GLN:HG2	0.95	1.43
1:A:31:ILE:HD11	1:A:31:ILE:CG1	0.94	1.47
1:A:41:GLU:HB3	1:A:41:GLU:CG	0.94	1.48
1:A:31:ILE:HD13	1:A:31:ILE:CG1	0.94	1.47
1:A:41:GLU:HB2	1:A:41:GLU:CG	0.94	1.48
1:A:56:GLU:HG3	1:A:56:GLU:CD	0.94	1.41
1:A:41:GLU:CB	1:A:41:GLU:HG2	0.94	1.48

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:53:ARG:CA	1:A:53:ARG:HG2	0.93	1.75
1:A:8:ILE:CD1	1:A:8:ILE:HG13	0.93	1.48
1:A:40:MET:SD	1:A:40:MET:HE1	0.93	1.56
1:A:8:ILE:CD1	1:A:8:ILE:HG12	0.93	1.48
1:A:40:MET:HE3	1:A:40:MET:SD	0.93	1.56
1:A:8:ILE:O	1:A:9:GLU:HA	0.93	1.61
1:A:38:LEU:HD11	1:A:38:LEU:HD23	0.92	1.00
1:A:40:MET:HB2	1:A:40:MET:CG	0.92	1.47
1:A:41:GLU:CD	1:A:41:GLU:OE1	0.92	0.72
1:A:31:ILE:HD12	1:A:31:ILE:CG1	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:40:MET:HE2	1:A:40:MET:SD	0.92	1.56
1:A:20:PHE:CE2	1:A:20:PHE:CZ	0.91	0.92
1:A:8:ILE:CD1	1:A:8:ILE:CG1	0.91	0.91
1:A:53:ARG:C	1:A:53:ARG:HG2	0.91	1.85
1:A:40:MET:HB3	1:A:40:MET:CG	0.91	1.47
1:A:55:LYS:HE2	1:A:55:LYS:NZ	0.91	1.29
1:A:29:GLU:CG	1:A:29:GLU:HB2	0.90	1.44
1:A:20:PHE:CD2	1:A:20:PHE:CG	0.90	0.90
1:A:38:LEU:CD1	1:A:38:LEU:HD23	0.90	1.53
1:A:20:PHE:CZ	1:A:20:PHE:CE1	0.90	0.90
1:A:40:MET:CB	1:A:40:MET:CG	0.90	0.90
1:A:53:ARG:HB2	1:A:53:ARG:CG	0.89	1.45
1:A:53:ARG:HB3	1:A:53:ARG:CG	0.89	1.45
1:A:55:LYS:HE3	1:A:55:LYS:NZ	0.89	1.29
1:A:29:GLU:CG	1:A:29:GLU:HB3	0.89	1.44
1:A:55:LYS:CG	1:A:55:LYS:HB3	0.89	1.43
1:A:54:GLN:CD	1:A:54:GLN:CG	0.88	0.79
1:A:53:ARG:CB	1:A:53:ARG:HD3	0.88	1.92
1:A:55:LYS:HB2	1:A:55:LYS:CG	0.88	1.43
1:A:12:VAL:HG23	1:A:16:LEU:CD2	0.88	1.98
1:A:29:GLU:HG2	1:A:29:GLU:CB	0.88	1.42
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:29:GLU:HG3	1:A:29:GLU:CB	0.86	1.42
1:A:41:GLU:CG	1:A:41:GLU:CB	0.86	0.87
1:A:11:ASN:CB	1:A:11:ASN:OD1	0.86	0.76
1:A:20:PHE:HZ	1:A:20:PHE:CE1	0.86	1.69
1:A:12:VAL:CG2	1:A:16:LEU:HD22	0.86	2.01
1:A:54:GLN:HE22	1:A:54:GLN:CD	0.86	1.48
1:A:37:GLN:CG	1:A:37:GLN:CD	0.86	0.78

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:11:ASN:CA	1:A:11:ASN:OD1	0.86	2.07
1:A:37:GLN:CD	1:A:37:GLN:HG2	0.85	1.30
1:A:40:MET:CB	1:A:40:MET:HG3	0.85	1.38
1:A:37:GLN:HG3	1:A:37:GLN:CD	0.85	1.30
1:A:55:LYS:CB	1:A:55:LYS:HG2	0.85	1.40
1:A:29:GLU:CG	1:A:29:GLU:CB	0.85	0.85
1:A:36:GLU:HB2	1:A:36:GLU:CG	0.84	1.39
1:A:40:MET:HG2	1:A:40:MET:CB	0.84	1.38
1:A:36:GLU:HB3	1:A:36:GLU:CG	0.84	1.39
1:A:53:ARG:CB	1:A:53:ARG:HG2	0.84	1.37
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:54:GLN:CD	1:A:54:GLN:HE21	0.83	1.48
1:A:11:ASN:HD22	1:A:11:ASN:CA	0.83	1.69
1:A:11:ASN:N	1:A:11:ASN:CG	0.82	2.31
1:A:53:ARG:CB	1:A:53:ARG:CG	0.82	0.83
1:A:38:LEU:C	1:A:38:LEU:CD1	0.82	2.46
1:A:58:ARG:NH2	1:A:60:ASN:CB	0.82	1.86
1:A:25:LYS:HD2	1:A:25:LYS:CB	0.82	2.05
1:A:5:ARG:HH22	1:A:7:SER:CB	0.81	1.62
1:A:36:GLU:CB	1:A:36:GLU:CG	0.81	0.83
1:A:53:ARG:CB	1:A:53:ARG:HG3	0.81	1.37
1:A:25:LYS:HG2	1:A:25:LYS:CB	0.81	1.34
1:A:25:LYS:HG3	1:A:25:LYS:CB	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:23:ASN:C	1:A:24:GLN:N	0.81	0.87
1:A:38:LEU:HB3	1:A:38:LEU:CD1	0.80	1.34
1:A:43:GLU:OE2	1:A:43:GLU:CD	0.80	0.61
1:A:12:VAL:CG2	1:A:16:LEU:CD2	0.80	2.59
1:A:20:PHE:HZ	1:A:20:PHE:CE2	0.80	1.71
1:A:54:GLN:CD	1:A:54:GLN:NE2	0.80	0.85
1:A:38:LEU:HD22	1:A:38:LEU:CD1	0.79	1.34
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:25:LYS:HB2	1:A:25:LYS:CG	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:53:ARG:HG2	1:A:53:ARG:O	0.79	1.77
1:A:36:GLU:CD	1:A:36:GLU:HG3	0.79	1.44

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:55:LYS:CE	1:A:55:LYS:NZ	0.78	0.81
1:A:5:ARG:NH2	1:A:7:SER:CB	0.78	1.78
1:A:25:LYS:CD	1:A:25:LYS:HE3	0.77	1.30
1:A:20:PHE:CZ	1:A:20:PHE:HE1	0.77	1.53
1:A:36:GLU:HG2	1:A:36:GLU:CB	0.77	1.36
1:A:8:ILE:CD1	1:A:8:ILE:CA	0.77	2.61
1:A:20:PHE:HD2	1:A:20:PHE:CG	0.76	1.53
1:A:36:GLU:CD	1:A:36:GLU:HG2	0.76	1.44
1:A:11:ASN:HB2	1:A:11:ASN:OD1	0.76	1.00
1:A:8:ILE:O	1:A:9:GLU:CG	0.75	2.23
1:A:38:LEU:HD13	1:A:38:LEU:HD22	0.75	1.01
1:A:52:ARG:CZ	1:A:52:ARG:HH12	0.75	1.45
1:A:52:ARG:CZ	1:A:52:ARG:HH11	0.75	1.45
1:A:20:PHE:HD1	1:A:20:PHE:CG	0.75	1.54
1:A:20:PHE:HE2	1:A:20:PHE:CZ	0.75	1.54
1:A:25:LYS:HE2	1:A:25:LYS:CD	0.75	1.30
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:25:LYS:HD3	1:A:25:LYS:CE	0.73	1.28
1:A:25:LYS:CG	1:A:25:LYS:CB	0.73	0.74
1:A:37:GLN:O	1:A:38:LEU:HB2	0.73	1.82
1:A:5:ARG:CZ	1:A:7:SER:CB	0.72	2.02
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:41:GLU:CG	1:A:41:GLU:C	0.71	2.57
1:A:18:LYS:HE2	1:A:18:LYS:NZ	0.71	1.10
1:A:18:LYS:CB	1:A:18:LYS:HG2	0.71	1.25
1:A:18:LYS:HE3	1:A:18:LYS:NZ	0.71	1.10
1:A:17:GLU:OE1	1:A:17:GLU:CD	0.71	0.58
1:A:58:ARG:CZ	1:A:60:ASN:HB2	0.71	1.53
1:A:8:ILE:O	1:A:9:GLU:HG3	0.71	1.86
1:A:42:LYS:HD3	1:A:42:LYS:NZ	0.70	1.93
1:A:43:GLU:OE1	1:A:43:GLU:OE2	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:38:LEU:CD2	1:A:38:LEU:CD1	0.69	0.78
1:A:16:LEU:HB3	1:A:48:TRP:CZ3	0.69	2.21
1:A:41:GLU:OE1	1:A:41:GLU:OE2	0.69	0.70
1:A:25:LYS:HE2	1:A:25:LYS:NZ	0.69	1.37
1:A:11:ASN:CG	1:A:11:ASN:HB2	0.69	1.12
1:A:18:LYS:HB3	1:A:18:LYS:CG	0.69	1.23
1:A:18:LYS:HB2	1:A:18:LYS:CG	0.69	1.23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:8:ILE:O	1:A:9:GLU:HB2	0.68	1.85
1:A:38:LEU:CB	1:A:38:LEU:CD1	0.68	0.77
1:A:55:LYS:CE	1:A:55:LYS:HZ1	0.68	1.39
1:A:11:ASN:HB3	1:A:11:ASN:CG	0.68	1.12
1:A:55:LYS:HZ2	1:A:55:LYS:CE	0.68	1.39
1:A:38:LEU:CD2	1:A:38:LEU:HD11	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:41:GLU:CD	1:A:41:GLU:OE2	0.67	0.48
1:A:38:LEU:HB2	1:A:38:LEU:CD1	0.67	1.21
1:A:55:LYS:CE	1:A:55:LYS:HZ3	0.67	1.39
1:A:1:ARG:HH21	1:A:2:ARG:HH12	0.67	1.16
1:A:11:ASN:ND2	1:A:11:ASN:HB3	0.67	1.06
1:A:38:LEU:HD21	1:A:38:LEU:HD11	0.67	0.67
1:A:25:LYS:HZ2	1:A:25:LYS:CE	0.67	1.37
1:A:25:LYS:CE	1:A:25:LYS:HZ3	0.67	1.37
1:A:52:ARG:CZ	1:A:52:ARG:NH1	0.67	0.82
1:A:25:LYS:HZ1	1:A:25:LYS:CE	0.66	1.37
1:A:18:LYS:HE3	1:A:18:LYS:CD	0.66	1.46
1:A:8:ILE:C	1:A:9:GLU:HA	0.66	1.86
1:A:52:ARG:NH1	1:A:52:ARG:CD	0.66	2.56
1:A:18:LYS:HD2	1:A:18:LYS:CE	0.66	1.32
1:A:53:ARG:C	1:A:53:ARG:CG	0.65	2.54
1:A:8:ILE:C	1:A:9:GLU:CA	0.65	1.93
1:A:25:LYS:NZ	1:A:25:LYS:HE3	0.64	1.37
1:A:18:LYS:HD2	1:A:18:LYS:CG	0.64	1.28
1:A:37:GLN:CD	1:A:37:GLN:HE22	0.64	1.26
1:A:25:LYS:CD	1:A:25:LYS:CE	0.64	0.69
1:A:23:ASN:O	1:A:23:ASN:C	0.64	0.75
1:A:25:LYS:NZ	1:A:25:LYS:CE	0.64	0.79
1:A:37:GLN:HE21	1:A:37:GLN:CD	0.63	1.26
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:HD3	1:A:18:LYS:HG3	0.63	1.15
1:A:8:ILE:C	1:A:9:GLU:HB2	0.62	2.08
1:A:48:TRP:CZ3	1:A:52:ARG:HG2	0.62	2.30
1:A:18:LYS:HD3	1:A:18:LYS:CG	0.62	1.28
1:A:40:MET:HG2	1:A:40:MET:CA	0.62	2.02
1:A:18:LYS:HD3	1:A:18:LYS:CE	0.61	1.32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:40:MET:HG2	1:A:40:MET:N	0.61	2.10
1:A:25:LYS:CG	1:A:25:LYS:N	0.61	2.63
1:A:52:ARG:CZ	1:A:52:ARG:NH2	0.60	0.75
1:A:57:LYS:HD2	1:A:58:ARG:N	0.60	1.79
1:A:25:LYS:HG3	1:A:25:LYS:CE	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:8:ILE:C	1:A:9:GLU:N	0.58	0.72
1:A:18:LYS:CB	1:A:18:LYS:CG	0.58	0.60
1:A:18:LYS:HG2	1:A:18:LYS:CD	0.58	1.38
1:A:25:LYS:HD2	1:A:25:LYS:HB3	0.57	1.66
1:A:38:LEU:HG	1:A:38:LEU:CD1	0.57	1.20
1:A:5:ARG:CZ	1:A:7:SER:HG	0.57	2.05
1:A:40:MET:N	1:A:40:MET:CG	0.56	2.67
1:A:7:SER:C	1:A:8:ILE:HD12	0.56	2.20
1:A:11:ASN:HD22	1:A:11:ASN:CG	0.56	1.16
1:A:37:GLN:O	1:A:38:LEU:HD12	0.55	2.02
1:A:18:LYS:HD2	1:A:18:LYS:HG2	0.55	1.13
1:A:8:ILE:CD1	1:A:8:ILE:HB	0.55	2.17
1:A:11:ASN:HD21	1:A:11:ASN:CG	0.55	1.16
1:A:29:GLU:OE1	1:A:29:GLU:CD	0.55	0.75
1:A:8:ILE:CD1	1:A:8:ILE:N	0.54	2.70
1:A:38:LEU:HD12	1:A:38:LEU:CG	0.54	1.08
1:A:38:LEU:HD13	1:A:38:LEU:CG	0.54	1.07
1:A:13:ARG:HB2	1:A:48:TRP:HE1	0.54	1.63
1:A:16:LEU:HG	1:A:49:PHE:CE1	0.54	2.38
1:A:40:MET:HG3	1:A:40:MET:HB2	0.53	1.31
1:A:37:GLN:NE2	1:A:37:GLN:CD	0.53	0.59
1:A:38:LEU:HD21	1:A:38:LEU:CD1	0.53	1.40
1:A:38:LEU:HD13	1:A:38:LEU:HB3	0.53	1.10
1:A:45:ILE:CG2	1:A:46:ARG:N	0.53	2.72
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:8:ILE:C	1:A:9:GLU:HG3	0.52	2.10
1:A:26:PRO:HB2	1:A:31:ILE:CD1	0.50	2.36
1:A:23:ASN:N	1:A:23:ASN:O	0.50	2.40
1:A:11:ASN:CB	1:A:11:ASN:CG	0.50	0.46
1:A:29:GLU:HG2	1:A:29:GLU:CA	0.50	2.04
1:A:29:GLU:OE2	1:A:29:GLU:CD	0.50	0.68
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:16:LEU:HB3	1:A:48:TRP:CH2	0.49	2.42
1:A:32:LEU:C	1:A:32:LEU:HD12	0.49	2.28
1:A:23:ASN:O	1:A:23:ASN:CB	0.48	2.56
1:A:11:ASN:H	1:A:11:ASN:CG	0.48	2.11
1:A:8:ILE:HD12	1:A:8:ILE:N	0.48	2.18
1:A:18:LYS:C	1:A:18:LYS:CG	0.47	2.75
1:A:38:LEU:CD2	1:A:39:HIS:CD2	0.47	2.86
1:A:55:LYS:HE2	1:A:55:LYS:HZ3	0.47	1.16
1:A:45:ILE:HG13	1:A:49:PHE:CE2	0.47	2.45
1:A:13:ARG:HB2	1:A:48:TRP:NE1	0.47	2.25
1:A:39:HIS:CG	1:A:39:HIS:N	0.46	2.23
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: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:25:LYS:N	1:A:26:PRO:HD3	0.45	2.25
1:A:36:GLU:CD	1:A:36:GLU:CG	0.45	0.93
1:A:11:ASN:HB3	1:A:11:ASN:HD22	0.44	0.90
1:A:17:GLU:OE2	1:A:17:GLU:OE1	0.44	0.47
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:39:HIS:C	1:A:40:MET:HG2	0.44	2.33
1:A:53:ARG:HB2	1:A:53:ARG:HG3	0.44	1.32
1:A:58:ARG:HH21	1:A:60:ASN:HB3	0.44	1.28
1:A:25:LYS:HD3	1:A:25:LYS:HE3	0.44	1.19
1:A:45:ILE:HG22	1:A:46:ARG:N	0.43	2.27
1:A:58:ARG:HH21	1:A:58:ARG:CZ	0.43	1.23
1:A:58:ARG:HH21	1:A:60:ASN:CB	0.43	1.16
1:A:29:GLU:N	1:A:29:GLU:CG	0.43	2.76
1:A:10:THR:C	1:A:12:VAL:N	0.42	2.56
1:A:25:LYS:HE2	1:A:25:LYS:HD2	0.42	1.20
1:A:44:VAL:HA	1:A:47:VAL:HG13	0.42	1.90
1:A:24:GLN:C	1:A:26:PRO:HD3	0.41	2.34
1:A:38:LEU:HD13	1:A:38:LEU:CD2	0.41	1.20
1:A:23:ASN:C	1:A:24:GLN:HA	0.41	2.18
1:A:11:ASN:ND2	1:A:11:ASN:CG	0.41	0.46
1:A:45:ILE:HG23	1:A:49:PHE:CE2	0.40	2.52
1:A:10:THR:O	1:A:11:ASN:C	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	7	SER
1	A	62	CYS
1	A	58	ARG
1	A	43	GLU
1	A	60	ASN
1	A	6	THR
1	A	48	TRP
1	A	38	LEU
1	A	2	ARG
1	A	9	GLU
1	A	49	PHE
1	A	61	PRO

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%)	33 (55%)	27 (45%)	0	2
All	All	60/60 (100%)	33 (55%)	27 (45%)	0	2

All 27 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	21	LEU
1	A	11	ASN
1	A	42	LYS
1	A	1	ARG
1	A	16	LEU
1	A	50	CYS
1	A	45	ILE
1	A	60	ASN
1	A	41	GLU
1	A	53	ARG
1	A	6	THR
1	A	40	MET
1	A	33	LEU
1	A	44	VAL
1	A	34	ILE
1	A	13	ARG
1	A	59	ILE
1	A	56	GLU
1	A	2	ARG
1	A	25	LYS
1	A	63	SER
1	A	12	VAL
1	A	3	LYS
1	A	38	LEU
1	A	17	GLU
1	A	47	VAL
1	A	27	THR

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided