



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:30 AM BST

PDB ID : 3PAT
Title : COMPARISON BETWEEN THE CRYSTAL AND THE SOLUTION
STRUCTURES OF THE EF HAND PARVALBUMIN
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Deposited on : 1994-03-22

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

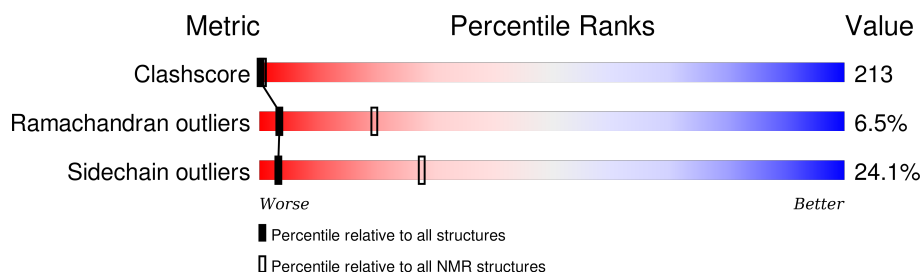
1 Overall quality at a glance

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	110	

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 are 2 unique types of molecules in this entry. The entry contains 836 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PARVALBUMIN.

Mol	Chain	Residues	Atoms					Trace
1	A	110	Total	C	N	O	S	0
			834	532	135	166	1	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

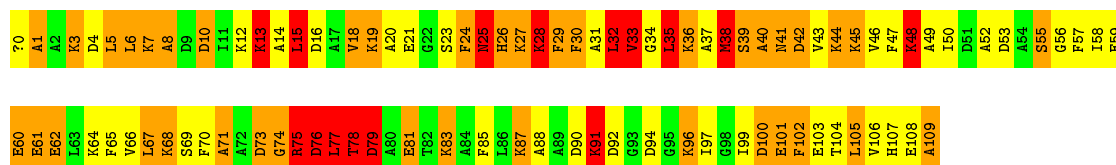
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

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: PARVALBUMIN

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
X-PLOR	refinement	3.2

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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACE

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	14.07	234/842 (27.8%)	8.79	214/1123 (19.1%)
All	All	14.07	234/842 (27.8%)	8.79	214/1123 (19.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	1	1
All	All	1	1

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	GLU	CD-OE2	-92.25	0.24	1.25
1	A	62	GLU	CD-OE2	-82.18	0.35	1.25
1	A	103	GLU	CD-OE1	-74.40	0.43	1.25
1	A	59	GLU	CD-OE1	-73.45	0.44	1.25
1	A	103	GLU	CD-OE2	-71.31	0.47	1.25
1	A	61	GLU	CD-OE1	-69.73	0.48	1.25
1	A	75	ARG	CZ-NH1	-69.13	0.43	1.33
1	A	108	GLU	CD-OE2	-68.65	0.50	1.25
1	A	21	GLU	CG-CD	-56.07	0.67	1.51
1	A	28	LYS	CD-CE	-55.09	0.13	1.51
1	A	7	LYS	CA-CB	-51.94	0.39	1.53
1	A	101	GLU	CD-OE1	-51.25	0.69	1.25
1	A	75	ARG	CZ-NH2	-45.63	0.73	1.33
1	A	61	GLU	CB-CG	-45.42	0.65	1.52
1	A	7	LYS	CD-CE	-44.15	0.40	1.51
1	A	61	GLU	CG-CD	-43.95	0.86	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ASP	CB-CG	-43.82	0.59	1.51
1	A	21	GLU	CD-OE2	-42.10	0.79	1.25
1	A	12	LYS	CE-NZ	-41.98	0.44	1.49
1	A	62	GLU	CG-CD	-41.08	0.90	1.51
1	A	75	ARG	C-O	-41.01	0.45	1.23
1	A	101	GLU	CD-OE2	-40.80	0.80	1.25
1	A	33	VAL	CB-CG1	-40.50	0.67	1.52
1	A	109	ALA	C-OXT	-40.36	0.46	1.23
1	A	25	ASN	C-O	-40.30	0.46	1.23
1	A	33	VAL	CB-CG2	-40.20	0.68	1.52
1	A	60	GLU	CG-CD	-38.36	0.94	1.51
1	A	29	PHE	CG-CD1	-37.72	0.82	1.38
1	A	29	PHE	CG-CD2	-37.71	0.82	1.38
1	A	38	MET	C-O	-37.71	0.51	1.23
1	A	30	PHE	CG-CD1	-37.38	0.82	1.38
1	A	108	GLU	CD-OE1	-36.73	0.85	1.25
1	A	83	LYS	CE-NZ	-36.65	0.57	1.49
1	A	87	LYS	CD-CE	-35.99	0.61	1.51
1	A	55	SER	CB-OG	-35.84	0.95	1.42
1	A	109	ALA	C-O	-35.42	0.56	1.23
1	A	7	LYS	C-N	-35.12	0.53	1.34
1	A	19	LYS	CE-NZ	-33.82	0.64	1.49
1	A	60	GLU	CD-OE2	-33.27	0.89	1.25
1	A	100	ASP	CG-OD1	-33.16	0.49	1.25
1	A	30	PHE	CG-CD2	-33.08	0.89	1.38
1	A	21	GLU	CD-OE1	-32.93	0.89	1.25
1	A	7	LYS	CE-NZ	-32.58	0.67	1.49
1	A	28	LYS	CB-CG	-32.56	0.64	1.52
1	A	81	GLU	CD-OE1	-32.07	0.90	1.25
1	A	3	LYS	CE-NZ	-31.84	0.69	1.49
1	A	27	LYS	CD-CE	-31.36	0.72	1.51
1	A	81	GLU	CD-OE2	-31.20	0.91	1.25
1	A	7	LYS	CB-CG	-31.19	0.68	1.52
1	A	13	LYS	CE-NZ	-31.11	0.71	1.49
1	A	96	LYS	CE-NZ	-29.77	0.74	1.49
1	A	103	GLU	CB-CG	-29.27	0.96	1.52
1	A	62	GLU	CD-OE1	-29.17	0.93	1.25
1	A	29	PHE	CE1-CZ	-29.06	0.82	1.37
1	A	29	PHE	CE2-CZ	-29.02	0.82	1.37
1	A	38	MET	CG-SD	-28.90	1.06	1.81
1	A	30	PHE	CE2-CZ	-28.78	0.82	1.37
1	A	108	GLU	CB-CG	-28.73	0.97	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	PHE	CG-CD1	-28.70	0.95	1.38
1	A	70	PHE	CG-CD2	-28.67	0.95	1.38
1	A	44	LYS	CB-CG	-28.23	0.76	1.52
1	A	75	ARG	CD-NE	-28.11	0.98	1.46
1	A	101	GLU	CG-CD	-28.08	1.09	1.51
1	A	25	ASN	CG-ND2	-27.58	0.64	1.32
1	A	75	ARG	NE-CZ	-27.51	0.97	1.33
1	A	3	LYS	CB-CG	-27.48	0.78	1.52
1	A	0	ACE	C-N	-27.45	0.70	1.34
1	A	45	LYS	CE-NZ	-27.39	0.80	1.49
1	A	7	LYS	CG-CD	-26.69	0.61	1.52
1	A	27	LYS	CE-NZ	-26.60	0.82	1.49
1	A	103	GLU	CG-CD	-26.60	1.12	1.51
1	A	59	GLU	CG-CD	-26.47	1.12	1.51
1	A	64	LYS	CE-NZ	-26.25	0.83	1.49
1	A	91	LYS	CE-NZ	-25.45	0.85	1.49
1	A	30	PHE	CE1-CZ	-25.41	0.89	1.37
1	A	91	LYS	CD-CE	-25.38	0.87	1.51
1	A	19	LYS	CD-CE	-25.36	0.87	1.51
1	A	76	ASP	CG-OD1	-25.35	0.67	1.25
1	A	25	ASN	CG-OD1	-25.14	0.68	1.24
1	A	3	LYS	CD-CE	-25.11	0.88	1.51
1	A	25	ASN	C-N	-24.79	0.77	1.34
1	A	71	ALA	C-O	-24.60	0.76	1.23
1	A	105	LEU	CG-CD2	-24.20	0.62	1.51
1	A	78	THR	CB-OG1	-23.79	0.95	1.43
1	A	59	GLU	CD-OE2	-23.74	0.99	1.25
1	A	75	ARG	C-N	-23.64	0.79	1.34
1	A	73	ASP	CG-OD1	-23.35	0.71	1.25
1	A	87	LYS	CB-CG	-22.92	0.90	1.52
1	A	68	LYS	CE-NZ	-22.90	0.91	1.49
1	A	65	PHE	CG-CD2	-22.62	1.04	1.38
1	A	70	PHE	CE2-CZ	-21.96	0.95	1.37
1	A	70	PHE	CE1-CZ	-21.95	0.95	1.37
1	A	65	PHE	CG-CD1	-21.55	1.06	1.38
1	A	6	LEU	C-O	-21.52	0.82	1.23
1	A	60	GLU	CD-OE1	-21.43	1.02	1.25
1	A	87	LYS	CE-NZ	-21.41	0.95	1.49
1	A	77	LEU	CG-CD1	-21.27	0.73	1.51
1	A	64	LYS	CD-CE	-20.79	0.99	1.51
1	A	6	LEU	CG-CD1	-20.68	0.75	1.51
1	A	15	LEU	CG-CD1	-20.63	0.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	LYS	CB-CG	-20.33	0.97	1.52
1	A	96	LYS	CB-CG	-20.27	0.97	1.52
1	A	45	LYS	CG-CD	-20.27	0.83	1.52
1	A	68	LYS	CD-CE	-20.19	1.00	1.51
1	A	38	MET	C-N	-20.05	0.88	1.34
1	A	67	LEU	CG-CD2	-19.79	0.78	1.51
1	A	100	ASP	CG-OD2	-19.46	0.80	1.25
1	A	68	LYS	CG-CD	-19.44	0.86	1.52
1	A	73	ASP	CG-OD2	-19.14	0.81	1.25
1	A	15	LEU	CG-CD2	-18.96	0.81	1.51
1	A	53	ASP	C-N	-18.91	0.90	1.34
1	A	76	ASP	CG-OD2	-18.68	0.82	1.25
1	A	68	LYS	CB-CG	-18.41	1.02	1.52
1	A	12	LYS	CD-CE	-18.23	1.05	1.51
1	A	90	ASP	C-O	-17.84	0.89	1.23
1	A	108	GLU	CG-CD	-17.37	1.25	1.51
1	A	48	LYS	CD-CE	-17.29	1.08	1.51
1	A	7	LYS	N-CA	-17.16	1.12	1.46
1	A	65	PHE	CE1-CZ	-17.15	1.04	1.37
1	A	83	LYS	CD-CE	-17.11	1.08	1.51
1	A	48	LYS	CG-CD	-17.05	0.94	1.52
1	A	36	LYS	CB-CG	-16.62	1.07	1.52
1	A	44	LYS	CD-CE	-16.52	1.09	1.51
1	A	77	LEU	CG-CD2	-16.50	0.90	1.51
1	A	53	ASP	C-O	-16.44	0.92	1.23
1	A	35	LEU	CG-CD2	-16.43	0.91	1.51
1	A	75	ARG	CG-CD	-16.29	1.11	1.51
1	A	65	PHE	CE2-CZ	-16.27	1.06	1.37
1	A	24	PHE	CG-CD1	-16.25	1.14	1.38
1	A	6	LEU	CG-CD2	-15.67	0.93	1.51
1	A	44	LYS	CE-NZ	-15.56	1.10	1.49
1	A	13	LYS	CD-CE	-15.50	1.12	1.51
1	A	42	ASP	CG-OD2	-15.49	0.89	1.25
1	A	90	ASP	CG-OD2	-15.40	0.90	1.25
1	A	71	ALA	C-N	-15.38	0.98	1.34
1	A	6	LEU	CA-C	-15.32	1.13	1.52
1	A	42	ASP	CG-OD1	-15.21	0.90	1.25
1	A	6	LEU	CA-CB	-14.89	1.19	1.53
1	A	76	ASP	CB-CG	-14.70	1.20	1.51
1	A	83	LYS	CG-CD	-14.67	1.02	1.52
1	A	79	ASP	CG-OD2	-14.45	0.92	1.25
1	A	1	ALA	CA-CB	-14.30	1.22	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	LEU	CG-CD1	-14.28	0.99	1.51
1	A	102	PHE	CG-CD1	-14.27	1.17	1.38
1	A	90	ASP	CG-OD1	-14.25	0.92	1.25
1	A	28	LYS	CG-CD	-14.20	1.04	1.52
1	A	79	ASP	CG-OD1	-14.14	0.92	1.25
1	A	78	THR	C-O	-14.11	0.96	1.23
1	A	19	LYS	CG-CD	-13.92	1.05	1.52
1	A	1	ALA	N-CA	-13.84	1.18	1.46
1	A	13	LYS	CG-CD	-13.81	1.05	1.52
1	A	78	THR	CB-CG2	-13.79	1.06	1.52
1	A	87	LYS	CG-CD	-13.55	1.06	1.52
1	A	12	LYS	CB-CG	-13.37	1.16	1.52
1	A	4	ASP	CG-OD2	-13.35	0.94	1.25
1	A	36	LYS	CD-CE	-13.25	1.18	1.51
1	A	24	PHE	CG-CD2	-13.03	1.19	1.38
1	A	97	ILE	CG1-CD1	-12.98	0.60	1.50
1	A	102	PHE	CG-CD2	-12.97	1.19	1.38
1	A	12	LYS	CG-CD	-12.58	1.09	1.52
1	A	52	ALA	C-O	-12.36	0.99	1.23
1	A	48	LYS	CE-NZ	-12.31	1.18	1.49
1	A	67	LEU	CG-CD1	-12.14	1.06	1.51
1	A	24	PHE	CE2-CZ	-12.06	1.14	1.37
1	A	36	LYS	CE-NZ	-12.06	1.18	1.49
1	A	7	LYS	C-O	-11.76	1.01	1.23
1	A	45	LYS	CD-CE	-11.70	1.22	1.51
1	A	5	LEU	C-O	-11.64	1.01	1.23
1	A	4	ASP	CG-OD1	-11.62	0.98	1.25
1	A	90	ASP	C-N	-11.56	1.07	1.34
1	A	41	ASN	CB-CG	-11.46	1.24	1.51
1	A	74	GLY	N-CA	-11.35	1.29	1.46
1	A	79	ASP	CB-CG	-11.21	1.28	1.51
1	A	38	MET	SD-CE	-11.14	1.15	1.77
1	A	35	LEU	CG-CD1	-10.86	1.11	1.51
1	A	96	LYS	CD-CE	-10.65	1.24	1.51
1	A	35	LEU	CB-CG	-10.65	1.21	1.52
1	A	67	LEU	CB-CG	-10.58	1.21	1.52
1	A	102	PHE	CE2-CZ	-10.53	1.17	1.37
1	A	64	LYS	CG-CD	-10.53	1.16	1.52
1	A	38	MET	CB-CG	-9.99	1.19	1.51
1	A	16	ASP	CG-OD1	-9.75	1.02	1.25
1	A	28	LYS	CE-NZ	-9.65	1.25	1.49
1	A	10	ASP	CG-OD2	-9.55	1.03	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	PHE	CE1-CZ	-9.55	1.19	1.37
1	A	102	PHE	CE1-CZ	-9.47	1.19	1.37
1	A	36	LYS	CG-CD	-9.30	1.20	1.52
1	A	53	ASP	CG-OD2	-9.24	1.04	1.25
1	A	8	ALA	N-CA	-9.21	1.27	1.46
1	A	13	LYS	CB-CG	-9.15	1.27	1.52
1	A	39	SER	CB-OG	-9.05	1.30	1.42
1	A	53	ASP	CG-OD1	-8.99	1.04	1.25
1	A	78	THR	C-N	-8.92	1.13	1.34
1	A	108	GLU	C-O	-8.65	1.06	1.23
1	A	91	LYS	CG-CD	-8.55	1.23	1.52
1	A	81	GLU	CB-CG	-8.22	1.36	1.52
1	A	73	ASP	C-O	-8.11	1.07	1.23
1	A	10	ASP	CG-OD1	-8.06	1.06	1.25
1	A	73	ASP	CA-C	-8.03	1.32	1.52
1	A	32	LEU	CG-CD1	-8.01	1.22	1.51
1	A	16	ASP	CG-OD2	-7.95	1.07	1.25
1	A	107	HIS	CE1-NE2	-7.92	1.14	1.32
1	A	60	GLU	CB-CG	-7.89	1.37	1.52
1	A	69	SER	CB-OG	-7.70	1.32	1.42
1	A	7	LYS	CA-C	-7.68	1.32	1.52
1	A	108	GLU	C-N	-7.63	1.16	1.34
1	A	34	GLY	C-O	-7.63	1.11	1.23
1	A	73	ASP	CA-CB	-7.48	1.37	1.53
1	A	19	LYS	CB-CG	-7.43	1.32	1.52
1	A	32	LEU	CG-CD2	-7.35	1.24	1.51
1	A	5	LEU	C-N	-7.32	1.17	1.34
1	A	8	ALA	CA-CB	-7.31	1.37	1.52
1	A	67	LEU	C-O	-6.94	1.10	1.23
1	A	66	VAL	C-O	-6.81	1.10	1.23
1	A	109	ALA	CA-CB	-6.81	1.38	1.52
1	A	75	ARG	CB-CG	-6.66	1.34	1.52
1	A	109	ALA	CA-C	-6.61	1.35	1.52
1	A	74	GLY	C-N	-6.60	1.18	1.34
1	A	37	ALA	CA-CB	-6.57	1.38	1.52
1	A	107	HIS	CG-CD2	-6.35	1.25	1.35
1	A	107	HIS	CG-ND1	-6.25	1.25	1.38
1	A	62	GLU	CB-CG	-6.14	1.40	1.52
1	A	92	ASP	CG-OD2	-6.10	1.11	1.25
1	A	74	GLY	C-O	-5.77	1.14	1.23
1	A	36	LYS	C-N	-5.61	1.21	1.34
1	A	52	ALA	C-N	-5.52	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	VAL	C-O	-5.50	1.12	1.23
1	A	36	LYS	C-O	-5.47	1.12	1.23
1	A	52	ALA	CA-CB	-5.16	1.41	1.52
1	A	45	LYS	CB-CG	-5.13	1.38	1.52
1	A	94	ASP	C-O	-5.11	1.13	1.23
1	A	6	LEU	CB-CG	-5.09	1.37	1.52
1	A	67	LEU	C-N	-5.08	1.22	1.34
1	A	25	ASN	CB-CG	-5.07	1.39	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	NE-CZ-NH2	70.42	155.51	120.30
1	A	25	ASN	O-C-N	-69.04	12.24	122.70
1	A	103	GLU	OE1-CD-OE2	-66.33	43.70	123.30
1	A	100	ASP	CB-CG-OD1	-63.92	60.77	118.30
1	A	75	ARG	O-C-N	-57.14	31.28	122.70
1	A	61	GLU	OE1-CD-OE2	-53.66	58.91	123.30
1	A	75	ARG	NH1-CZ-NH2	-44.88	70.03	119.40
1	A	29	PHE	CD1-CG-CD2	-42.81	62.64	118.30
1	A	29	PHE	CB-CG-CD1	39.83	148.68	120.80
1	A	29	PHE	CB-CG-CD2	39.82	148.67	120.80
1	A	38	MET	O-C-N	-39.19	60.00	122.70
1	A	30	PHE	CB-CG-CD2	36.74	146.52	120.80
1	A	30	PHE	CD1-CG-CD2	-36.73	70.56	118.30
1	A	38	MET	CG-SD-CE	36.29	158.26	100.20
1	A	33	VAL	CG1-CB-CG2	-33.73	56.92	110.90
1	A	62	GLU	CG-CD-OE2	-33.61	51.08	118.30
1	A	100	ASP	CB-CG-OD2	33.03	148.03	118.30
1	A	29	PHE	CE1-CZ-CE2	-31.87	62.64	120.00
1	A	30	PHE	CB-CG-CD1	31.60	142.92	120.80
1	A	75	ARG	NE-CZ-NH1	28.32	134.46	120.30
1	A	75	ARG	CD-NE-CZ	27.82	162.55	123.60
1	A	30	PHE	CE1-CZ-CE2	-27.48	70.53	120.00
1	A	27	LYS	CD-CE-NZ	27.14	174.12	111.70
1	A	25	ASN	OD1-CG-ND2	-26.79	60.29	121.90
1	A	25	ASN	CA-C-N	26.44	175.36	117.20
1	A	109	ALA	CA-C-O	26.27	175.26	120.10
1	A	29	PHE	CG-CD2-CE2	25.38	148.72	120.80
1	A	29	PHE	CG-CD1-CE1	25.30	148.63	120.80
1	A	25	ASN	CA-C-O	24.75	172.08	120.10
1	A	29	PHE	CD1-CE1-CZ	23.84	148.71	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	VAL	CA-CB-CG1	23.81	146.61	110.90
1	A	29	PHE	CZ-CE2-CD2	23.79	148.65	120.10
1	A	33	VAL	CA-CB-CG2	23.75	146.53	110.90
1	A	75	ARG	CA-C-N	23.41	168.71	117.20
1	A	30	PHE	CG-CD2-CE2	23.09	146.19	120.80
1	A	70	PHE	CD1-CG-CD2	-23.01	88.39	118.30
1	A	108	GLU	OE1-CD-OE2	-22.81	95.92	123.30
1	A	7	LYS	CB-CG-CD	22.55	170.22	111.60
1	A	62	GLU	CG-CD-OE1	22.43	163.16	118.30
1	A	61	GLU	CB-CG-CD	22.13	173.96	114.20
1	A	70	PHE	CB-CG-CD1	21.86	136.10	120.80
1	A	30	PHE	CD1-CE1-CZ	21.79	146.24	120.10
1	A	73	ASP	CB-CG-OD2	21.66	137.79	118.30
1	A	61	GLU	CG-CD-OE1	21.61	161.52	118.30
1	A	25	ASN	C-N-CA	21.59	175.67	121.70
1	A	36	LYS	CB-CG-CD	21.23	166.79	111.60
1	A	70	PHE	CB-CG-CD2	21.02	135.51	120.80
1	A	28	LYS	CA-CB-CG	20.96	159.51	113.40
1	A	30	PHE	CG-CD1-CE1	20.39	143.22	120.80
1	A	103	GLU	CG-CD-OE2	20.32	158.94	118.30
1	A	6	LEU	CB-CG-CD2	20.24	145.40	111.00
1	A	105	LEU	CB-CG-CD1	20.18	145.30	111.00
1	A	38	MET	CB-CG-SD	20.14	172.83	112.40
1	A	28	LYS	CB-CG-CD	19.84	163.18	111.60
1	A	103	GLU	CG-CD-OE1	19.53	157.36	118.30
1	A	30	PHE	CZ-CE2-CD2	19.29	143.25	120.10
1	A	67	LEU	CB-CG-CD1	19.12	143.51	111.00
1	A	75	ARG	CG-CD-NE	19.10	151.91	111.80
1	A	87	LYS	CB-CG-CD	19.02	161.06	111.60
1	A	75	ARG	CA-C-O	18.99	159.97	120.10
1	A	62	GLU	OE1-CD-OE2	18.72	145.76	123.30
1	A	21	GLU	OE1-CD-OE2	18.66	145.69	123.30
1	A	75	ARG	C-N-CA	18.63	168.28	121.70
1	A	62	GLU	CB-CG-CD	18.52	164.19	114.20
1	A	7	LYS	CG-CD-CE	18.47	167.30	111.90
1	A	76	ASP	CB-CG-OD2	18.42	134.88	118.30
1	A	13	LYS	CG-CD-CE	18.18	166.44	111.90
1	A	38	MET	CA-C-N	18.15	157.13	117.20
1	A	7	LYS	N-CA-C	18.06	159.77	111.00
1	A	13	LYS	CB-CG-CD	18.05	158.52	111.60
1	A	77	LEU	CB-CG-CD2	17.79	141.24	111.00
1	A	59	GLU	CG-CD-OE2	17.64	153.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LYS	CD-CE-NZ	17.63	152.24	111.70
1	A	70	PHE	CE1-CZ-CE2	-17.53	88.45	120.00
1	A	71	ALA	O-C-N	-17.37	94.91	122.70
1	A	59	GLU	CG-CD-OE1	-17.36	83.57	118.30
1	A	68	LYS	CD-CE-NZ	-17.16	72.23	111.70
1	A	28	LYS	CD-CE-NZ	17.12	151.09	111.70
1	A	13	LYS	CD-CE-NZ	17.08	150.98	111.70
1	A	83	LYS	CD-CE-NZ	17.05	150.93	111.70
1	A	97	ILE	CB-CG1-CD1	16.91	161.26	113.90
1	A	73	ASP	OD1-CG-OD2	-16.57	91.81	123.30
1	A	81	GLU	OE1-CD-OE2	-16.54	103.46	123.30
1	A	53	ASP	O-C-N	-16.39	96.48	122.70
1	A	91	LYS	CD-CE-NZ	16.38	149.37	111.70
1	A	12	LYS	CD-CE-NZ	16.11	148.75	111.70
1	A	100	ASP	CA-CB-CG	15.86	148.30	113.40
1	A	96	LYS	CD-CE-NZ	15.71	147.84	111.70
1	A	68	LYS	CG-CD-CE	-15.69	64.84	111.90
1	A	7	LYS	CA-C-O	15.55	152.76	120.10
1	A	25	ASN	CB-CG-OD1	15.40	152.41	121.60
1	A	45	LYS	CB-CG-CD	15.40	151.63	111.60
1	A	7	LYS	N-CA-CB	-15.29	83.07	110.60
1	A	19	LYS	CD-CE-NZ	15.28	146.85	111.70
1	A	108	GLU	CG-CD-OE1	14.94	148.19	118.30
1	A	65	PHE	CD1-CG-CD2	-14.68	99.21	118.30
1	A	100	ASP	OD1-CG-OD2	14.68	151.19	123.30
1	A	83	LYS	CB-CG-CD	14.64	149.66	111.60
1	A	83	LYS	CG-CD-CE	14.58	155.64	111.90
1	A	65	PHE	CB-CG-CD1	14.41	130.89	120.80
1	A	38	MET	C-N-CA	14.40	157.69	121.70
1	A	15	LEU	CB-CG-CD2	14.07	134.93	111.00
1	A	67	LEU	CD1-CG-CD2	-13.91	68.76	110.50
1	A	70	PHE	CG-CD1-CE1	13.64	135.81	120.80
1	A	70	PHE	CG-CD2-CE2	13.63	135.79	120.80
1	A	75	ARG	CB-CG-CD	13.48	146.65	111.60
1	A	67	LEU	CB-CG-CD2	13.46	133.88	111.00
1	A	73	ASP	CB-CG-OD1	13.44	130.40	118.30
1	A	61	GLU	CA-CB-CG	13.35	142.78	113.40
1	A	91	LYS	CG-CD-CE	13.19	151.46	111.90
1	A	70	PHE	CD1-CE1-CZ	13.09	135.81	120.10
1	A	70	PHE	CZ-CE2-CD2	13.04	135.75	120.10
1	A	6	LEU	CD1-CG-CD2	-13.03	71.41	110.50
1	A	48	LYS	CG-CD-CE	13.02	150.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	PHE	CB-CG-CD2	13.00	129.90	120.80
1	A	7	LYS	O-C-N	-12.90	102.05	122.70
1	A	3	LYS	CA-CB-CG	12.78	141.51	113.40
1	A	25	ASN	CB-CG-ND2	12.75	147.30	116.70
1	A	90	ASP	CB-CG-OD1	12.63	129.67	118.30
1	A	64	LYS	CG-CD-CE	12.59	149.68	111.90
1	A	42	ASP	CB-CG-OD1	12.58	129.62	118.30
1	A	77	LEU	CD1-CG-CD2	-12.43	73.21	110.50
1	A	42	ASP	CB-CG-OD2	12.23	129.31	118.30
1	A	19	LYS	CG-CD-CE	12.09	148.18	111.90
1	A	68	LYS	CB-CG-CD	12.07	142.97	111.60
1	A	90	ASP	O-C-N	-11.88	103.70	122.70
1	A	77	LEU	CB-CG-CD1	11.79	131.05	111.00
1	A	60	GLU	OE1-CD-OE2	11.71	137.35	123.30
1	A	42	ASP	OD1-CG-OD2	-11.70	101.08	123.30
1	A	65	PHE	CE1-CZ-CE2	-11.55	99.21	120.00
1	A	15	LEU	CB-CG-CD1	11.18	130.01	111.00
1	A	6	LEU	CB-CG-CD1	11.14	129.94	111.00
1	A	12	LYS	CB-CG-CD	11.03	140.27	111.60
1	A	21	GLU	CG-CD-OE2	-11.02	96.27	118.30
1	A	3	LYS	CB-CG-CD	10.93	140.02	111.60
1	A	38	MET	CA-C-O	10.84	142.87	120.10
1	A	90	ASP	OD1-CG-OD2	-10.80	102.78	123.30
1	A	61	GLU	CG-CD-OE2	10.64	139.57	118.30
1	A	24	PHE	CB-CG-CD2	10.46	128.12	120.80
1	A	27	LYS	CG-CD-CE	10.45	143.26	111.90
1	A	15	LEU	CD1-CG-CD2	-10.43	79.22	110.50
1	A	0	ACE	O-C-N	-10.42	106.03	122.70
1	A	44	LYS	CG-CD-CE	10.34	142.91	111.90
1	A	6	LEU	CA-C-O	-10.29	98.49	120.10
1	A	90	ASP	CB-CG-OD2	10.28	127.55	118.30
1	A	87	LYS	CD-CE-NZ	-10.22	88.19	111.70
1	A	3	LYS	CD-CE-NZ	10.21	135.19	111.70
1	A	44	LYS	CD-CE-NZ	10.17	135.09	111.70
1	A	6	LEU	CA-CB-CG	10.05	138.42	115.30
1	A	45	LYS	CG-CD-CE	9.83	141.40	111.90
1	A	78	THR	CA-CB-CG2	9.66	125.92	112.40
1	A	44	LYS	CA-CB-CG	9.56	134.44	113.40
1	A	19	LYS	CB-CG-CD	9.25	135.65	111.60
1	A	71	ALA	CA-C-N	9.20	137.43	117.20
1	A	65	PHE	CG-CD1-CE1	9.14	130.86	120.80
1	A	76	ASP	OD1-CG-OD2	-9.08	106.05	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	PHE	CZ-CE2-CD2	9.00	130.90	120.10
1	A	12	LYS	CG-CD-CE	8.98	138.84	111.90
1	A	87	LYS	CG-CD-CE	-8.73	85.70	111.90
1	A	24	PHE	CD1-CG-CD2	-8.53	107.21	118.30
1	A	102	PHE	CB-CG-CD2	8.50	126.75	120.80
1	A	60	GLU	CG-CD-OE2	-8.48	101.34	118.30
1	A	102	PHE	CD1-CG-CD2	-8.41	107.36	118.30
1	A	78	THR	OG1-CB-CG2	-8.41	90.67	110.00
1	A	65	PHE	CG-CD2-CE2	8.29	129.92	120.80
1	A	45	LYS	CD-CE-NZ	8.24	130.65	111.70
1	A	65	PHE	CD1-CE1-CZ	8.16	129.90	120.10
1	A	64	LYS	CB-CG-CD	7.97	132.32	111.60
1	A	44	LYS	CB-CG-CD	7.91	132.17	111.60
1	A	48	LYS	CB-CG-CD	7.87	132.06	111.60
1	A	4	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	101	GLU	OE1-CD-OE2	-7.66	114.10	123.30
1	A	91	LYS	CA-CB-CG	7.64	130.21	113.40
1	A	53	ASP	CA-C-O	7.37	135.57	120.10
1	A	64	LYS	CD-CE-NZ	7.32	128.53	111.70
1	A	78	THR	O-C-N	-7.32	110.99	122.70
1	A	102	PHE	CB-CG-CD1	7.25	125.87	120.80
1	A	24	PHE	CE1-CZ-CE2	-7.10	107.22	120.00
1	A	16	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	102	PHE	CE1-CZ-CE2	-7.03	107.34	120.00
1	A	91	LYS	CB-CG-CD	6.86	129.45	111.60
1	A	71	ALA	C-N-CA	6.75	138.58	121.70
1	A	6	LEU	CA-C-N	6.73	132.00	117.20
1	A	78	THR	CA-CB-OG1	6.73	123.12	109.00
1	A	24	PHE	CD1-CE1-CZ	6.61	128.03	120.10
1	A	24	PHE	CG-CD2-CE2	6.60	128.06	120.80
1	A	96	LYS	CB-CG-CD	6.55	128.62	111.60
1	A	87	LYS	CA-CB-CG	6.52	127.75	113.40
1	A	6	LEU	CB-CA-C	-6.28	98.27	110.20
1	A	3	LYS	CG-CD-CE	6.26	130.68	111.90
1	A	90	ASP	CA-C-N	6.25	130.94	117.20
1	A	10	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	36	LYS	CG-CD-CE	6.00	129.90	111.90
1	A	7	LYS	C-N-CA	-5.89	106.97	121.70
1	A	107	HIS	ND1-CG-CD2	-5.88	97.77	106.00
1	A	36	LYS	CA-CB-CG	5.84	126.26	113.40
1	A	52	ALA	O-C-N	-5.83	113.37	122.70
1	A	96	LYS	CA-CB-CG	5.81	126.18	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	GLU	O-C-N	-5.76	113.48	122.70
1	A	101	GLU	CG-CD-OE2	5.75	129.81	118.30
1	A	108	GLU	CB-CG-CD	-5.74	98.70	114.20
1	A	102	PHE	CD1-CE1-CZ	5.71	126.95	120.10
1	A	102	PHE	CG-CD2-CE2	5.63	127.00	120.80
1	A	32	LEU	CB-CG-CD2	5.57	120.48	111.00
1	A	24	PHE	CB-CG-CD1	5.50	124.65	120.80
1	A	21	GLU	CB-CG-CD	5.47	128.97	114.20
1	A	7	LYS	CA-C-N	-5.46	105.18	117.20
1	A	6	LEU	C-N-CA	5.40	135.21	121.70
1	A	4	ASP	OD1-CG-OD2	-5.34	113.15	123.30
1	A	59	GLU	CB-CG-CD	5.21	128.25	114.20
1	A	81	GLU	CG-CD-OE2	5.14	128.59	118.30
1	A	105	LEU	CD1-CG-CD2	-5.08	95.27	110.50
1	A	52	ALA	CA-C-N	5.03	128.28	117.20
1	A	53	ASP	CB-CG-OD1	5.01	122.81	118.30

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	7	LYS	CA

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	25	ASN	Mainchain

6.2 Too-close contacts [i](#)

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	834	0	813	352
All	All	836	0	813	352

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 213.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:19:LYS:CE	1:A:19:LYS:CG	1.48	1.85
1:A:13:LYS:NZ	1:A:13:LYS:CD	1.46	1.77
1:A:76:ASP:CB	1:A:76:ASP:OD1	1.45	1.63
1:A:87:LYS:CB	1:A:87:LYS:CD	1.44	1.94
1:A:45:LYS:CG	1:A:45:LYS:CE	1.44	1.94
1:A:6:LEU:CB	1:A:6:LEU:CD1	1.43	1.94
1:A:75:ARG:NH2	1:A:75:ARG:NE	1.41	1.66
1:A:45:LYS:CD	1:A:45:LYS:NZ	1.40	1.84
1:A:44:LYS:CD	1:A:44:LYS:CB	1.39	1.99
1:A:3:LYS:CD	1:A:3:LYS:CB	1.36	2.04
1:A:77:LEU:CB	1:A:77:LEU:CD1	1.36	2.03
1:A:27:LYS:CE	1:A:27:LYS:CG	1.36	2.01
1:A:30:PHE:CE1	1:A:30:PHE:CG	1.35	2.11
1:A:30:PHE:CD2	1:A:30:PHE:CZ	1.35	2.11
1:A:29:PHE:CZ	1:A:29:PHE:CD2	1.34	2.14
1:A:87:LYS:CB	1:A:87:LYS:CE	1.34	2.06
1:A:29:PHE:CG	1:A:29:PHE:CE1	1.34	2.14
1:A:29:PHE:CD1	1:A:29:PHE:CZ	1.34	2.14
1:A:29:PHE:CE2	1:A:29:PHE:CG	1.34	2.14
1:A:91:LYS:CG	1:A:91:LYS:CE	1.34	2.04
1:A:3:LYS:CG	1:A:3:LYS:CE	1.32	2.06
1:A:61:GLU:CG	1:A:61:GLU:CA	1.31	2.08
1:A:96:LYS:CD	1:A:96:LYS:NZ	1.31	1.91
1:A:30:PHE:CG	1:A:30:PHE:CE2	1.29	2.19
1:A:30:PHE:CD1	1:A:30:PHE:CZ	1.29	2.19
1:A:25:ASN:O	1:A:26:HIS:CA	1.28	1.80
1:A:15:LEU:CD1	1:A:15:LEU:CB	1.28	2.08
1:A:109:ALA:OXT	1:A:109:ALA:CA	1.28	1.81
1:A:75:ARG:O	1:A:76:ASP:CA	1.27	1.81
1:A:33:VAL:CG1	1:A:33:VAL:CA	1.26	2.12
1:A:25:ASN:ND2	1:A:25:ASN:CB	1.26	1.95
1:A:44:LYS:CA	1:A:44:LYS:CG	1.26	2.13
1:A:33:VAL:CA	1:A:33:VAL:CG2	1.26	2.12
1:A:62:GLU:OE1	1:A:62:GLU:CG	1.25	1.81
1:A:45:LYS:CD	1:A:45:LYS:CB	1.25	2.15
1:A:3:LYS:CA	1:A:3:LYS:CG	1.24	2.15
1:A:38:MET:SD	1:A:38:MET:CE	1.24	1.15
1:A:100:ASP:CA	1:A:100:ASP:CG	1.24	2.05
1:A:38:MET:SD	1:A:38:MET:CB	1.23	2.24
1:A:38:MET:CG	1:A:38:MET:CE	1.22	2.17
1:A:15:LEU:CB	1:A:15:LEU:CD2	1.22	2.17
1:A:30:PHE:CD1	1:A:30:PHE:CB	1.21	2.22
1:A:87:LYS:CG	1:A:87:LYS:CA	1.21	2.19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:29:PHE:CB	1:A:29:PHE:CD1	1.19	2.25
1:A:29:PHE:CB	1:A:29:PHE:CD2	1.18	2.25
1:A:75:ARG:CA	1:A:75:ARG:O	1.18	1.89
1:A:109:ALA:O	1:A:109:ALA:CA	1.17	1.91
1:A:38:MET:SD	1:A:38:MET:CG	1.15	1.06
1:A:73:ASP:CB	1:A:73:ASP:OD1	1.13	1.95
1:A:25:ASN:O	1:A:25:ASN:CA	1.12	1.97
1:A:30:PHE:CD2	1:A:30:PHE:CB	1.12	2.30
1:A:76:ASP:OD2	1:A:76:ASP:CB	1.12	1.87
1:A:75:ARG:C	1:A:76:ASP:CA	1.08	2.22
1:A:25:ASN:OD1	1:A:25:ASN:CB	1.06	2.02
1:A:25:ASN:C	1:A:26:HIS:CA	1.05	2.25
1:A:38:MET:SD	1:A:38:MET:HE3	1.03	1.73
1:A:38:MET:SD	1:A:38:MET:HE1	1.03	1.73
1:A:77:LEU:CD2	1:A:77:LEU:CB	1.03	2.25
1:A:38:MET:HE2	1:A:38:MET:SD	1.03	1.73
1:A:33:VAL:CG1	1:A:33:VAL:HG23	1.02	1.58
1:A:33:VAL:HB	1:A:33:VAL:CG2	1.02	1.58
1:A:62:GLU:CB	1:A:62:GLU:CD	1.00	2.28
1:A:33:VAL:HB	1:A:33:VAL:CG1	1.00	1.57
1:A:33:VAL:HG12	1:A:33:VAL:CG2	1.00	1.58
1:A:6:LEU:CG	1:A:6:LEU:HD22	0.99	1.56
1:A:62:GLU:CD	1:A:62:GLU:CG	0.99	0.90
1:A:45:LYS:HE2	1:A:45:LYS:NZ	0.99	1.40
1:A:6:LEU:CD2	1:A:6:LEU:HG	0.99	1.70
1:A:73:ASP:CB	1:A:73:ASP:OD2	0.99	2.09
1:A:6:LEU:CG	1:A:6:LEU:HD21	0.98	1.56
1:A:77:LEU:HG	1:A:77:LEU:CD1	0.98	1.59
1:A:75:ARG:CA	1:A:76:ASP:N	0.98	2.25
1:A:6:LEU:CD1	1:A:6:LEU:HG	0.98	1.63
1:A:6:LEU:CD2	1:A:6:LEU:CB	0.98	2.21
1:A:45:LYS:HE3	1:A:45:LYS:NZ	0.98	1.40
1:A:75:ARG:NH2	1:A:75:ARG:HH11	0.98	1.56
1:A:77:LEU:HD23	1:A:77:LEU:CG	0.98	1.53
1:A:77:LEU:HD22	1:A:77:LEU:CG	0.98	1.53
1:A:25:ASN:CA	1:A:26:HIS:N	0.97	2.27
1:A:6:LEU:CG	1:A:6:LEU:HD23	0.97	1.55
1:A:77:LEU:CG	1:A:77:LEU:HD21	0.95	1.53
1:A:45:LYS:NZ	1:A:45:LYS:CE	0.95	0.80
1:A:87:LYS:CG	1:A:87:LYS:HB3	0.94	1.49
1:A:87:LYS:HB2	1:A:87:LYS:CG	0.94	1.49
1:A:62:GLU:OE2	1:A:62:GLU:CG	0.94	0.73

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:6:LEU:CG	1:A:6:LEU:CD2	0.93	0.93
1:A:15:LEU:CD1	1:A:15:LEU:HG	0.92	1.57
1:A:15:LEU:CG	1:A:15:LEU:HD23	0.92	1.46
1:A:62:GLU:CD	1:A:62:GLU:HG2	0.92	1.37
1:A:15:LEU:CG	1:A:15:LEU:HD21	0.92	1.46
1:A:3:LYS:HD2	1:A:3:LYS:CE	0.91	1.46
1:A:30:PHE:HZ	1:A:30:PHE:CE2	0.91	1.67
1:A:96:LYS:HE2	1:A:96:LYS:NZ	0.91	1.31
1:A:96:LYS:NZ	1:A:96:LYS:HE3	0.91	1.31
1:A:15:LEU:HD22	1:A:15:LEU:CG	0.91	1.46
1:A:77:LEU:CG	1:A:77:LEU:CD2	0.90	0.90
1:A:3:LYS:HD3	1:A:3:LYS:CE	0.90	1.46
1:A:87:LYS:CG	1:A:87:LYS:CB	0.90	0.90
1:A:77:LEU:HG	1:A:77:LEU:CD2	0.89	1.68
1:A:13:LYS:NZ	1:A:13:LYS:HE2	0.89	1.28
1:A:29:PHE:HZ	1:A:29:PHE:CE2	0.89	1.68
1:A:15:LEU:CD2	1:A:15:LEU:HG	0.89	1.59
1:A:30:PHE:CE1	1:A:30:PHE:CZ	0.88	0.89
1:A:96:LYS:CE	1:A:96:LYS:NZ	0.88	0.74
1:A:25:ASN:OD1	1:A:25:ASN:CG	0.88	0.68
1:A:13:LYS:NZ	1:A:13:LYS:HE3	0.88	1.28
1:A:3:LYS:CD	1:A:3:LYS:CE	0.88	0.88
1:A:19:LYS:HD2	1:A:19:LYS:CE	0.88	1.41
1:A:30:PHE:CG	1:A:30:PHE:CD2	0.87	0.89
1:A:6:LEU:CG	1:A:6:LEU:HD12	0.87	1.41
1:A:15:LEU:HD12	1:A:15:LEU:CG	0.87	1.41
1:A:15:LEU:HD11	1:A:15:LEU:CG	0.87	1.41
1:A:6:LEU:CG	1:A:6:LEU:HD13	0.87	1.41
1:A:15:LEU:HD13	1:A:15:LEU:CG	0.87	1.41
1:A:45:LYS:HD2	1:A:45:LYS:CG	0.86	1.40
1:A:91:LYS:HD3	1:A:91:LYS:CE	0.86	1.40
1:A:45:LYS:HD3	1:A:45:LYS:CG	0.86	1.40
1:A:3:LYS:HE2	1:A:3:LYS:NZ	0.86	1.31
1:A:91:LYS:HD2	1:A:91:LYS:CE	0.85	1.40
1:A:87:LYS:CB	1:A:87:LYS:HG2	0.85	1.39
1:A:19:LYS:CE	1:A:19:LYS:HD3	0.85	1.41
1:A:77:LEU:CG	1:A:77:LEU:HD13	0.84	1.39
1:A:6:LEU:CG	1:A:6:LEU:HD11	0.84	1.41
1:A:91:LYS:CD	1:A:91:LYS:CE	0.84	0.87
1:A:75:ARG:NH2	1:A:75:ARG:CZ	0.84	0.73
1:A:91:LYS:CD	1:A:91:LYS:HE2	0.84	1.40
1:A:44:LYS:CB	1:A:44:LYS:HG3	0.84	1.37

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:77:LEU:CG	1:A:77:LEU:HD12	0.83	1.39
1:A:87:LYS:CB	1:A:87:LYS:HG3	0.83	1.39
1:A:44:LYS:HB2	1:A:44:LYS:CG	0.83	1.36
1:A:44:LYS:HB3	1:A:44:LYS:CG	0.83	1.36
1:A:45:LYS:HG3	1:A:45:LYS:CD	0.83	1.37
1:A:44:LYS:CB	1:A:44:LYS:HG2	0.83	1.37
1:A:91:LYS:HE2	1:A:91:LYS:NZ	0.83	1.39
1:A:3:LYS:HG3	1:A:3:LYS:CB	0.83	1.36
1:A:33:VAL:CB	1:A:33:VAL:HG23	0.83	1.36
1:A:45:LYS:CD	1:A:45:LYS:HG2	0.82	1.37
1:A:38:MET:SD	1:A:38:MET:HG2	0.82	1.46
1:A:75:ARG:C	1:A:76:ASP:N	0.82	0.79
1:A:91:LYS:HE3	1:A:91:LYS:NZ	0.82	1.39
1:A:29:PHE:HZ	1:A:29:PHE:CE1	0.82	1.68
1:A:19:LYS:CE	1:A:19:LYS:CD	0.82	0.87
1:A:33:VAL:CB	1:A:33:VAL:HG12	0.82	1.35
1:A:33:VAL:HG13	1:A:33:VAL:CB	0.82	1.35
1:A:33:VAL:CB	1:A:33:VAL:HG21	0.82	1.36
1:A:87:LYS:CB	1:A:87:LYS:HE2	0.81	2.05
1:A:77:LEU:HD11	1:A:77:LEU:CG	0.81	1.39
1:A:30:PHE:CD1	1:A:30:PHE:CG	0.81	0.82
1:A:87:LYS:HE3	1:A:87:LYS:CB	0.81	2.04
1:A:3:LYS:HG2	1:A:3:LYS:CB	0.81	1.36
1:A:3:LYS:HB3	1:A:3:LYS:CG	0.81	1.36
1:A:3:LYS:NZ	1:A:3:LYS:HE3	0.81	1.31
1:A:15:LEU:CD2	1:A:15:LEU:CG	0.81	0.81
1:A:45:LYS:CD	1:A:45:LYS:CG	0.81	0.83
1:A:30:PHE:CZ	1:A:30:PHE:CE2	0.81	0.82
1:A:33:VAL:HG22	1:A:33:VAL:CB	0.81	1.36
1:A:38:MET:SD	1:A:38:MET:HG3	0.81	1.46
1:A:33:VAL:CB	1:A:33:VAL:HG11	0.81	1.35
1:A:62:GLU:HG3	1:A:62:GLU:OE2	0.80	1.04
1:A:29:PHE:CZ	1:A:29:PHE:CE1	0.80	0.82
1:A:13:LYS:CE	1:A:13:LYS:NZ	0.80	0.71
1:A:25:ASN:OD1	1:A:25:ASN:ND2	0.80	0.66
1:A:29:PHE:CZ	1:A:29:PHE:CE2	0.80	0.82
1:A:29:PHE:CD1	1:A:29:PHE:CG	0.80	0.82
1:A:3:LYS:HB2	1:A:3:LYS:CG	0.79	1.36
1:A:29:PHE:CD2	1:A:29:PHE:CG	0.79	0.82
1:A:33:VAL:HG11	1:A:33:VAL:HG23	0.79	1.27
1:A:3:LYS:CD	1:A:3:LYS:HE2	0.79	1.45
1:A:19:LYS:HE3	1:A:19:LYS:CD	0.79	1.41

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:100:ASP:HB2	1:A:100:ASP:CG	0.78	1.22
1:A:19:LYS:HE3	1:A:19:LYS:NZ	0.78	1.25
1:A:91:LYS:CD	1:A:91:LYS:HE3	0.78	1.40
1:A:3:LYS:CB	1:A:3:LYS:CG	0.77	0.78
1:A:27:LYS:CE	1:A:27:LYS:HD3	0.77	1.31
1:A:27:LYS:CE	1:A:27:LYS:HD2	0.77	1.31
1:A:100:ASP:HB3	1:A:100:ASP:CG	0.77	1.22
1:A:30:PHE:CE1	1:A:30:PHE:HZ	0.76	1.73
1:A:60:GLU:OE1	1:A:60:GLU:CB	0.76	1.96
1:A:19:LYS:CD	1:A:19:LYS:HE2	0.76	1.41
1:A:44:LYS:CB	1:A:44:LYS:CG	0.76	0.76
1:A:25:ASN:C	1:A:26:HIS:N	0.76	0.77
1:A:50:ILE:HG22	1:A:58:ILE:HG23	0.76	1.58
1:A:3:LYS:CD	1:A:3:LYS:HE3	0.75	1.45
1:A:19:LYS:HE2	1:A:19:LYS:NZ	0.75	1.25
1:A:15:LEU:CD1	1:A:15:LEU:CG	0.75	0.75
1:A:6:LEU:CG	1:A:6:LEU:CD1	0.75	0.75
1:A:73:ASP:OD2	1:A:73:ASP:CG	0.74	0.81
1:A:61:GLU:CG	1:A:61:GLU:HB3	0.73	1.27
1:A:73:ASP:CG	1:A:73:ASP:OD1	0.73	0.71
1:A:39:SER:O	1:A:43:VAL:HG23	0.73	1.84
1:A:19:LYS:HG3	1:A:19:LYS:CE	0.73	2.09
1:A:62:GLU:OE2	1:A:62:GLU:HG2	0.73	1.25
1:A:77:LEU:CG	1:A:77:LEU:CD1	0.72	0.73
1:A:61:GLU:HB2	1:A:61:GLU:CG	0.72	1.27
1:A:91:LYS:HZ3	1:A:91:LYS:CE	0.72	1.42
1:A:33:VAL:HG21	1:A:33:VAL:HG12	0.72	1.28
1:A:27:LYS:CD	1:A:27:LYS:CE	0.71	0.72
1:A:91:LYS:HZ2	1:A:91:LYS:CE	0.71	1.42
1:A:91:LYS:HZ1	1:A:91:LYS:CE	0.71	1.42
1:A:68:LYS:C	1:A:68:LYS:HE2	0.70	2.03
1:A:75:ARG:NH2	1:A:75:ARG:NH1	0.70	0.71
1:A:27:LYS:CE	1:A:27:LYS:HZ1	0.70	1.40
1:A:91:LYS:CE	1:A:91:LYS:NZ	0.70	0.85
1:A:44:LYS:CB	1:A:44:LYS:HD3	0.69	2.14
1:A:102:PHE:O	1:A:106:VAL:HG23	0.69	1.86
1:A:27:LYS:HZ2	1:A:27:LYS:CE	0.69	1.40
1:A:30:PHE:HE1	1:A:30:PHE:CZ	0.69	1.46
1:A:27:LYS:CE	1:A:27:LYS:HZ3	0.69	1.40
1:A:30:PHE:HD2	1:A:30:PHE:CG	0.68	1.46
1:A:100:ASP:CB	1:A:100:ASP:CG	0.68	0.59
1:A:47:PHE:CD1	1:A:99:ILE:CD1	0.68	2.76

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:45:LYS:CE	1:A:45:LYS:HZ3	0.68	1.38
1:A:60:GLU:OE1	1:A:60:GLU:HB2	0.68	1.84
1:A:25:ASN:HD21	1:A:25:ASN:CG	0.68	1.30
1:A:33:VAL:CB	1:A:33:VAL:CG2	0.68	0.68
1:A:25:ASN:HD22	1:A:25:ASN:CG	0.67	1.30
1:A:30:PHE:CG	1:A:30:PHE:HD1	0.67	1.42
1:A:33:VAL:CG1	1:A:33:VAL:CB	0.67	0.67
1:A:75:ARG:HH21	1:A:75:ARG:CZ	0.67	1.38
1:A:45:LYS:HZ2	1:A:45:LYS:CE	0.67	1.38
1:A:27:LYS:NZ	1:A:27:LYS:CE	0.67	0.82
1:A:45:LYS:HZ1	1:A:45:LYS:CE	0.67	1.38
1:A:35:LEU:HG	1:A:106:VAL:HG11	0.67	1.64
1:A:33:VAL:HG13	1:A:33:VAL:CG2	0.66	1.21
1:A:30:PHE:CZ	1:A:30:PHE:HE2	0.66	1.42
1:A:27:LYS:CD	1:A:27:LYS:HE3	0.65	1.23
1:A:76:ASP:OD1	1:A:76:ASP:CA	0.65	2.41
1:A:13:LYS:HD3	1:A:13:LYS:NZ	0.65	2.00
1:A:61:GLU:CB	1:A:61:GLU:HG3	0.65	1.19
1:A:27:LYS:HE2	1:A:27:LYS:CD	0.65	1.23
1:A:33:VAL:HG22	1:A:33:VAL:HG13	0.65	0.82
1:A:61:GLU:CG	1:A:61:GLU:CB	0.65	0.65
1:A:33:VAL:HG22	1:A:33:VAL:CG1	0.65	1.21
1:A:25:ASN:ND2	1:A:25:ASN:CG	0.64	0.63
1:A:33:VAL:CG1	1:A:33:VAL:CG2	0.64	0.65
1:A:87:LYS:CA	1:A:87:LYS:HG3	0.64	2.05
1:A:29:PHE:HD1	1:A:29:PHE:CG	0.63	1.39
1:A:27:LYS:HE2	1:A:27:LYS:NZ	0.63	1.29
1:A:96:LYS:CE	1:A:96:LYS:HZ1	0.63	1.34
1:A:96:LYS:HZ3	1:A:96:LYS:CE	0.63	1.34
1:A:78:THR:O	1:A:79:ASP:CB	0.63	2.40
1:A:29:PHE:CZ	1:A:29:PHE:HE1	0.63	1.39
1:A:45:LYS:HD3	1:A:45:LYS:NZ	0.63	1.99
1:A:109:ALA:O	1:A:109:ALA:C	0.63	0.56
1:A:14:ALA:HB1	1:A:29:PHE:CD1	0.62	2.29
1:A:29:PHE:HE2	1:A:29:PHE:CZ	0.62	1.39
1:A:27:LYS:NZ	1:A:27:LYS:HE3	0.62	1.29
1:A:96:LYS:HZ2	1:A:96:LYS:CE	0.62	1.34
1:A:76:ASP:OD2	1:A:76:ASP:CG	0.61	0.82
1:A:29:PHE:HD2	1:A:29:PHE:CG	0.61	1.39
1:A:47:PHE:CG	1:A:99:ILE:HD13	0.61	2.30
1:A:20:ALA:HB3	1:A:23:SER:OG	0.61	1.94
1:A:61:GLU:HG2	1:A:61:GLU:CB	0.61	1.19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:75:ARG:O	1:A:76:ASP:N	0.60	0.47
1:A:75:ARG:O	1:A:75:ARG:C	0.60	0.45
1:A:45:LYS:HE2	1:A:45:LYS:CG	0.60	2.17
1:A:35:LEU:HG	1:A:106:VAL:CG1	0.60	2.27
1:A:13:LYS:CE	1:A:13:LYS:HZ1	0.60	1.31
1:A:61:GLU:HG2	1:A:61:GLU:CD	0.60	1.31
1:A:13:LYS:HZ3	1:A:13:LYS:CE	0.60	1.31
1:A:61:GLU:CD	1:A:61:GLU:HG3	0.60	1.31
1:A:3:LYS:HG2	1:A:3:LYS:CE	0.60	2.17
1:A:13:LYS:CE	1:A:13:LYS:HZ2	0.60	1.31
1:A:3:LYS:HZ1	1:A:3:LYS:CE	0.59	1.29
1:A:91:LYS:HD2	1:A:91:LYS:HE3	0.59	1.19
1:A:100:ASP:OD2	1:A:100:ASP:CG	0.59	0.80
1:A:3:LYS:HZ2	1:A:3:LYS:CE	0.59	1.30
1:A:3:LYS:HZ3	1:A:3:LYS:CE	0.59	1.30
1:A:61:GLU:CA	1:A:61:GLU:HG3	0.59	2.00
1:A:25:ASN:O	1:A:25:ASN:C	0.58	0.46
1:A:26:HIS:NE2	1:A:27:LYS:HG3	0.58	2.13
1:A:56:GLY:O	1:A:57:PHE:CD1	0.58	2.57
1:A:20:ALA:HB3	1:A:23:SER:CB	0.58	2.29
1:A:27:LYS:HE3	1:A:27:LYS:HD3	0.58	1.13
1:A:27:LYS:CE	1:A:27:LYS:CB	0.57	2.81
1:A:50:ILE:HB	1:A:58:ILE:HD12	0.57	1.76
1:A:55:SER:O	1:A:57:PHE:CD2	0.57	2.57
1:A:78:THR:O	1:A:79:ASP:HB2	0.57	2.00
1:A:47:PHE:C	1:A:47:PHE:CD1	0.56	2.79
1:A:27:LYS:HE2	1:A:27:LYS:HD2	0.56	1.15
1:A:19:LYS:CE	1:A:19:LYS:HZ1	0.56	1.26
1:A:19:LYS:HZ3	1:A:19:LYS:CE	0.55	1.26
1:A:19:LYS:HZ2	1:A:19:LYS:CE	0.55	1.26
1:A:76:ASP:CG	1:A:76:ASP:OD1	0.55	0.67
1:A:47:PHE:CD1	1:A:99:ILE:HD13	0.55	2.35
1:A:75:ARG:NH2	1:A:81:GLU:OE1	0.54	2.39
1:A:3:LYS:NZ	1:A:3:LYS:CE	0.54	0.69
1:A:6:LEU:HB2	1:A:6:LEU:CD1	0.53	2.18
1:A:26:HIS:CE1	1:A:88:ALA:HB1	0.53	2.38
1:A:109:ALA:C	1:A:109:ALA:OXT	0.53	0.46
1:A:50:ILE:CG2	1:A:58:ILE:HD12	0.53	2.33
1:A:19:LYS:HE3	1:A:19:LYS:HG3	0.53	1.75
1:A:77:LEU:CA	1:A:77:LEU:CD2	0.52	2.86
1:A:27:LYS:HE3	1:A:27:LYS:HZ1	0.52	1.15
1:A:99:ILE:O	1:A:102:PHE:N	0.52	2.43

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:19:LYS:HE3	1:A:19:LYS:HZ1	0.52	1.11
1:A:33:VAL:HG11	1:A:33:VAL:CG2	0.52	0.84
1:A:50:ILE:CG2	1:A:58:ILE:HG23	0.52	2.32
1:A:10:ASP:HB3	1:A:33:VAL:O	0.51	2.05
1:A:75:ARG:HH12	1:A:75:ARG:NH2	0.51	0.61
1:A:47:PHE:CE2	1:A:58:ILE:HD11	0.51	2.41
1:A:42:ASP:O	1:A:46:VAL:HG23	0.51	2.04
1:A:27:LYS:HE2	1:A:27:LYS:HZ3	0.51	1.17
1:A:99:ILE:O	1:A:100:ASP:C	0.51	2.50
1:A:71:ALA:O	1:A:73:ASP:N	0.50	2.44
1:A:75:ARG:NH1	1:A:81:GLU:OE1	0.50	2.44
1:A:3:LYS:C	1:A:3:LYS:CG	0.50	2.78
1:A:67:LEU:HD12	1:A:75:ARG:CB	0.50	2.37
1:A:19:LYS:CE	1:A:19:LYS:NZ	0.49	0.64
1:A:33:VAL:CG1	1:A:33:VAL:HG21	0.49	0.84
1:A:47:PHE:CD2	1:A:58:ILE:HD11	0.49	2.43
1:A:50:ILE:CB	1:A:58:ILE:HD12	0.49	2.38
1:A:47:PHE:CE2	1:A:58:ILE:HG12	0.48	2.43
1:A:39:SER:O	1:A:41:ASN:N	0.48	2.46
1:A:67:LEU:HD12	1:A:75:ARG:HB2	0.48	1.85
1:A:30:PHE:CD1	1:A:30:PHE:CA	0.48	2.94
1:A:14:ALA:O	1:A:18:VAL:HG22	0.48	2.09
1:A:71:ALA:HB3	1:A:74:GLY:HA3	0.47	1.86
1:A:33:VAL:CG1	1:A:33:VAL:C	0.47	2.81
1:A:39:SER:O	1:A:40:ALA:C	0.47	2.53
1:A:47:PHE:O	1:A:48:LYS:C	0.47	2.53
1:A:47:PHE:CG	1:A:99:ILE:CD1	0.46	2.97
1:A:47:PHE:CD2	1:A:99:ILE:HD13	0.46	2.46
1:A:19:LYS:HZ3	1:A:19:LYS:HE2	0.46	1.14
1:A:47:PHE:O	1:A:50:ILE:N	0.45	2.49
1:A:47:PHE:CD1	1:A:99:ILE:HD11	0.45	2.47
1:A:28:LYS:O	1:A:32:LEU:HD12	0.45	2.12
1:A:20:ALA:HB3	1:A:23:SER:HB3	0.45	1.87
1:A:13:LYS:HZ3	1:A:13:LYS:HE2	0.44	1.16
1:A:45:LYS:HG3	1:A:45:LYS:CE	0.44	2.03
1:A:50:ILE:CG2	1:A:58:ILE:CG2	0.43	2.96
1:A:47:PHE:CE1	1:A:99:ILE:CD1	0.43	3.01
1:A:100:ASP:O	1:A:104:THR:CB	0.43	2.67
1:A:19:LYS:HD3	1:A:19:LYS:HE2	0.43	1.31
1:A:50:ILE:HG13	1:A:102:PHE:CZ	0.43	2.48
1:A:25:ASN:O	1:A:26:HIS:N	0.43	0.33
1:A:47:PHE:CE2	1:A:58:ILE:CG1	0.43	3.01

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:14:ALA:HB1	1:A:29:PHE:CE1	0.43	2.48
1:A:27:LYS:O	1:A:31:ALA:HB2	0.42	2.13
1:A:3:LYS:HE2	1:A:3:LYS:HZ3	0.42	1.21
1:A:55:SER:O	1:A:56:GLY:C	0.42	2.57
1:A:24:PHE:CD1	1:A:25:ASN:N	0.42	2.88
1:A:18:VAL:CG1	1:A:24:PHE:HA	0.42	2.44
1:A:100:ASP:O	1:A:104:THR:HB	0.42	2.14
1:A:67:LEU:CA	1:A:67:LEU:HD23	0.41	2.33
1:A:3:LYS:HZ1	1:A:3:LYS:HE3	0.41	1.21
1:A:24:PHE:CD1	1:A:24:PHE:C	0.41	2.94
1:A:47:PHE:HA	1:A:50:ILE:HG12	0.41	1.92
1:A:47:PHE:HA	1:A:50:ILE:CG1	0.40	2.46
1:A:47:PHE:C	1:A:49:ALA:N	0.40	2.73
1:A:55:SER:O	1:A:57:PHE:N	0.40	2.55
1:A:6:LEU:HB3	1:A:6:LEU:CD1	0.40	2.23

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	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	3	19
All	All	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	3	19

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

Mol	Chain	Res	Type
1	A	1	ALA
1	A	79	ASP
1	A	76	ASP
1	A	40	ALA
1	A	8	ALA
1	A	26	HIS
1	A	38	MET

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	83/83 (100%)	63 (76%)	20 (24%)	3	28
All	All	83/83 (100%)	63 (76%)	20 (24%)	3	28

All 20 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	75	ARG
1	A	77	LEU
1	A	83	LYS
1	A	5	LEU
1	A	38	MET
1	A	7	LYS
1	A	33	VAL
1	A	105	LEU
1	A	85	PHE
1	A	28	LYS
1	A	36	LYS
1	A	78	THR
1	A	35	LEU
1	A	15	LEU
1	A	32	LEU
1	A	91	LYS
1	A	48	LYS
1	A	76	ASP
1	A	101	GLU
1	A	13	LYS

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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