



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 AM UTC

PDB ID : 3PAT / pdb_00003pat
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

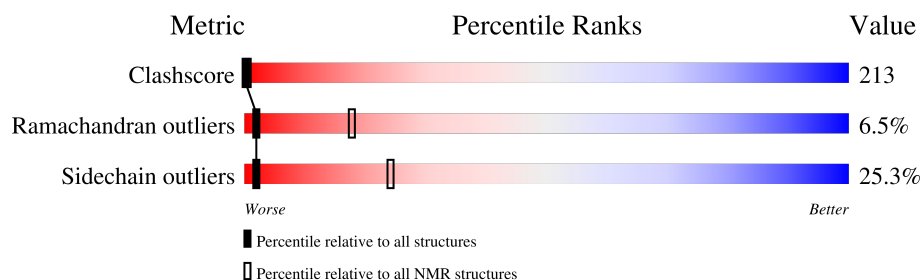
1 Overall quality at a glance

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	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 (CCD ID: CA) (formula: Ca).

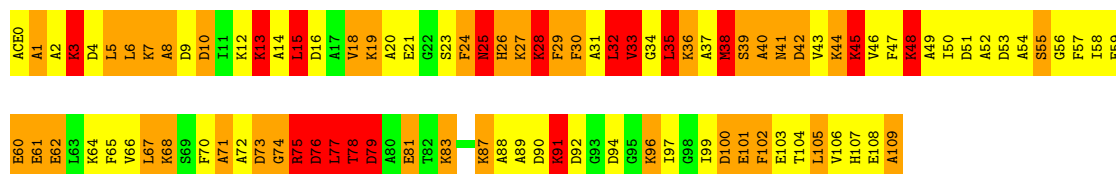
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

4 Residue-property plots

These plots are provided for all protein, RNA, 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: 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.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	12.48	267/842 (31.7%)	8.14	208/1123 (18.5%)
All	All	12.48	267/842 (31.7%)	8.14	208/1123 (18.5%)

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

Mol	Chain	Chirality	Planarity
1	A	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	7	LYS	CA-CB	-71.44	0.39	1.53
1	A	75	ARG	CZ-NH1	-63.98	0.43	1.32
1	A	25	ASN	C-O	-61.27	0.46	1.24
1	A	7	LYS	C-N	-57.43	0.53	1.33
1	A	38	MET	C-O	-57.36	0.51	1.24
1	A	61	GLU	CD-OE2	-53.25	0.24	1.25
1	A	75	ARG	C-O	-48.20	0.45	1.23
1	A	62	GLU	CD-OE2	-47.42	0.35	1.25
1	A	28	LYS	CD-CE	-46.31	0.13	1.52
1	A	75	ARG	CZ-NH2	-45.94	0.73	1.33
1	A	71	ALA	C-O	-44.15	0.76	1.23
1	A	103	GLU	CD-OE1	-42.92	0.43	1.25
1	A	59	GLU	CD-OE1	-42.37	0.44	1.25
1	A	103	GLU	CD-OE2	-41.13	0.47	1.25
1	A	25	ASN	C-N	-40.46	0.77	1.33
1	A	61	GLU	CD-OE1	-40.21	0.48	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ASP	CG-OD1	-40.14	0.49	1.25
1	A	108	GLU	CD-OE2	-39.58	0.50	1.25
1	A	75	ARG	C-N	-38.58	0.79	1.33
1	A	109	ALA	C-OXT	-38.44	0.46	1.23
1	A	7	LYS	CD-CE	-37.19	0.40	1.52
1	A	38	MET	C-N	-37.10	0.88	1.33
1	A	100	ASP	CB-CG	-36.93	0.59	1.52
1	A	12	LYS	CE-NZ	-35.08	0.44	1.49
1	A	75	ARG	CD-NE	-33.99	0.98	1.46
1	A	109	ALA	C-O	-33.75	0.56	1.23
1	A	21	GLU	CG-CD	-33.68	0.67	1.52
1	A	25	ASN	CG-ND2	-33.02	0.64	1.33
1	A	75	ARG	NE-CZ	-32.52	0.97	1.33
1	A	0	ACE	C-N	-31.21	0.70	1.33
1	A	53	ASP	C-N	-30.82	0.90	1.33
1	A	76	ASP	CG-OD1	-30.69	0.67	1.25
1	A	83	LYS	CE-NZ	-30.64	0.57	1.49
1	A	6	LEU	C-O	-30.50	0.82	1.23
1	A	87	LYS	CD-CE	-30.39	0.61	1.52
1	A	7	LYS	CG-CD	-30.25	0.61	1.52
1	A	78	THR	CB-OG1	-30.05	0.95	1.43
1	A	38	MET	CG-SD	-29.89	1.06	1.80
1	A	101	GLU	CD-OE1	-29.51	0.69	1.25
1	A	6	LEU	CA-C	-29.48	1.13	1.52
1	A	28	LYS	CB-CG	-29.27	0.64	1.52
1	A	90	ASP	C-O	-29.06	0.89	1.24
1	A	25	ASN	CG-OD1	-28.90	0.68	1.23
1	A	61	GLU	CB-CG	-28.86	0.65	1.52
1	A	19	LYS	CE-NZ	-28.28	0.64	1.49
1	A	73	ASP	CG-OD1	-28.27	0.71	1.25
1	A	7	LYS	CB-CG	-28.04	0.68	1.52
1	A	7	LYS	N-CA	-27.91	1.12	1.46
1	A	105	LEU	CG-CD2	-27.35	0.62	1.52
1	A	7	LYS	CE-NZ	-27.25	0.67	1.49
1	A	29	PHE	CG-CD1	-26.99	0.82	1.38
1	A	29	PHE	CG-CD2	-26.98	0.82	1.38
1	A	30	PHE	CG-CD1	-26.75	0.82	1.38
1	A	3	LYS	CE-NZ	-26.63	0.69	1.49
1	A	27	LYS	CD-CE	-26.54	0.72	1.52
1	A	61	GLU	CG-CD	-26.41	0.86	1.52
1	A	13	LYS	CE-NZ	-26.03	0.71	1.49
1	A	33	VAL	CB-CG1	-25.68	0.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	MET	SD-CE	-25.63	1.15	1.79
1	A	33	VAL	CB-CG2	-25.49	0.68	1.52
1	A	44	LYS	CB-CG	-25.38	0.76	1.52
1	A	71	ALA	C-N	-25.00	0.98	1.33
1	A	96	LYS	CE-NZ	-24.91	0.74	1.49
1	A	3	LYS	CB-CG	-24.70	0.78	1.52
1	A	62	GLU	CG-CD	-24.69	0.90	1.52
1	A	21	GLU	CD-OE2	-24.22	0.79	1.25
1	A	77	LEU	CG-CD1	-24.06	0.73	1.52
1	A	6	LEU	CA-CB	-23.71	1.19	1.53
1	A	30	PHE	CG-CD2	-23.68	0.89	1.38
1	A	100	ASP	CG-OD2	-23.56	0.80	1.25
1	A	101	GLU	CD-OE2	-23.46	0.80	1.25
1	A	6	LEU	CG-CD1	-23.40	0.75	1.52
1	A	15	LEU	CG-CD1	-23.34	0.75	1.52
1	A	97	ILE	CG1-CD1	-23.31	0.60	1.51
1	A	55	SER	CB-OG	-23.24	0.95	1.42
1	A	73	ASP	CG-OD2	-23.17	0.81	1.25
1	A	60	GLU	CG-CD	-23.06	0.94	1.52
1	A	45	LYS	CG-CD	-22.97	0.83	1.52
1	A	53	ASP	C-O	-22.95	0.92	1.24
1	A	45	LYS	CE-NZ	-22.92	0.80	1.49
1	A	76	ASP	CG-OD2	-22.61	0.82	1.25
1	A	67	LEU	CG-CD2	-22.40	0.78	1.52
1	A	27	LYS	CE-NZ	-22.27	0.82	1.49
1	A	68	LYS	CG-CD	-22.04	0.86	1.52
1	A	64	LYS	CE-NZ	-21.97	0.83	1.49
1	A	91	LYS	CD-CE	-21.55	0.87	1.52
1	A	19	LYS	CD-CE	-21.53	0.87	1.52
1	A	15	LEU	CG-CD2	-21.47	0.81	1.52
1	A	3	LYS	CD-CE	-21.32	0.88	1.52
1	A	91	LYS	CE-NZ	-21.31	0.85	1.49
1	A	108	GLU	CD-OE1	-21.11	0.85	1.25
1	A	87	LYS	CB-CG	-20.59	0.90	1.52
1	A	70	PHE	CG-CD1	-20.55	0.95	1.38
1	A	70	PHE	CG-CD2	-20.53	0.95	1.38
1	A	78	THR	C-O	-20.50	0.96	1.24
1	A	7	LYS	C-O	-19.41	1.01	1.24
1	A	48	LYS	CG-CD	-19.32	0.94	1.52
1	A	68	LYS	CE-NZ	-19.18	0.91	1.49
1	A	60	GLU	CD-OE2	-19.10	0.89	1.25
1	A	21	GLU	CD-OE1	-18.91	0.89	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	ALA	C-O	-18.89	0.99	1.24
1	A	90	ASP	C-N	-18.87	1.07	1.33
1	A	29	PHE	CE1-CZ	-18.84	0.82	1.38
1	A	29	PHE	CE2-CZ	-18.81	0.82	1.38
1	A	42	ASP	CG-OD2	-18.75	0.89	1.25
1	A	77	LEU	CG-CD2	-18.71	0.90	1.52
1	A	30	PHE	CE2-CZ	-18.66	0.82	1.38
1	A	90	ASP	CG-OD2	-18.65	0.90	1.25
1	A	35	LEU	CG-CD2	-18.64	0.91	1.52
1	A	103	GLU	CB-CG	-18.64	0.96	1.52
1	A	42	ASP	CG-OD1	-18.41	0.90	1.25
1	A	81	GLU	CD-OE1	-18.41	0.90	1.25
1	A	108	GLU	CB-CG	-18.29	0.97	1.52
1	A	91	LYS	CB-CG	-18.27	0.97	1.52
1	A	96	LYS	CB-CG	-18.21	0.97	1.52
1	A	107	HIS	CE1-NE2	-18.12	1.14	1.32
1	A	87	LYS	CE-NZ	-17.95	0.95	1.49
1	A	81	GLU	CD-OE2	-17.90	0.91	1.25
1	A	6	LEU	CG-CD2	-17.78	0.93	1.52
1	A	64	LYS	CD-CE	-17.72	0.99	1.52
1	A	79	ASP	CG-OD2	-17.49	0.92	1.25
1	A	5	LEU	C-O	-17.27	1.01	1.24
1	A	90	ASP	CG-OD1	-17.25	0.92	1.25
1	A	68	LYS	CD-CE	-17.22	1.00	1.52
1	A	79	ASP	CG-OD1	-17.11	0.92	1.25
1	A	101	GLU	CG-CD	-16.89	1.09	1.52
1	A	62	GLU	CD-OE1	-16.73	0.93	1.25
1	A	83	LYS	CG-CD	-16.63	1.02	1.52
1	A	68	LYS	CB-CG	-16.53	1.02	1.52
1	A	30	PHE	CE1-CZ	-16.53	0.89	1.38
1	A	105	LEU	CG-CD1	-16.22	0.99	1.52
1	A	65	PHE	CG-CD2	-16.21	1.04	1.38
1	A	4	ASP	CG-OD2	-16.16	0.94	1.25
1	A	28	LYS	CG-CD	-16.09	1.04	1.52
1	A	103	GLU	CG-CD	-16.00	1.12	1.52
1	A	59	GLU	CG-CD	-15.92	1.12	1.52
1	A	35	LEU	CB-CG	-15.89	1.21	1.53
1	A	67	LEU	CB-CG	-15.79	1.21	1.53
1	A	19	LYS	CG-CD	-15.77	1.05	1.52
1	A	13	LYS	CG-CD	-15.65	1.05	1.52
1	A	12	LYS	CD-CE	-15.59	1.05	1.52
1	A	73	ASP	C-O	-15.51	1.07	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	PHE	CG-CD1	-15.44	1.06	1.38
1	A	7	LYS	CA-C	-15.37	1.32	1.52
1	A	87	LYS	CG-CD	-15.35	1.06	1.52
1	A	36	LYS	CB-CG	-14.93	1.07	1.52
1	A	73	ASP	CA-C	-14.92	1.32	1.53
1	A	48	LYS	CD-CE	-14.81	1.08	1.52
1	A	83	LYS	CD-CE	-14.66	1.08	1.52
1	A	1	ALA	N-CA	-14.51	1.18	1.46
1	A	78	THR	C-N	-14.40	1.13	1.33
1	A	70	PHE	CE2-CZ	-14.34	0.95	1.38
1	A	70	PHE	CE1-CZ	-14.33	0.95	1.38
1	A	12	LYS	CG-CD	-14.26	1.09	1.52
1	A	44	LYS	CD-CE	-14.17	1.09	1.52
1	A	8	ALA	N-CA	-14.15	1.27	1.46
1	A	4	ASP	CG-OD1	-14.07	0.98	1.25
1	A	78	THR	CB-CG2	-13.85	1.06	1.52
1	A	67	LEU	CG-CD1	-13.82	1.06	1.52
1	A	75	ARG	CG-CD	-13.74	1.11	1.52
1	A	59	GLU	CD-OE2	-13.59	0.99	1.25
1	A	13	LYS	CD-CE	-13.31	1.12	1.52
1	A	44	LYS	CE-NZ	-13.07	1.10	1.49
1	A	108	GLU	C-O	-12.84	1.06	1.24
1	A	76	ASP	CB-CG	-12.47	1.20	1.52
1	A	35	LEU	CG-CD1	-12.39	1.11	1.52
1	A	60	GLU	CD-OE1	-12.25	1.02	1.25
1	A	107	HIS	CG-ND1	-12.04	1.25	1.38
1	A	108	GLU	C-N	-12.03	1.16	1.33
1	A	12	LYS	CB-CG	-12.00	1.16	1.52
1	A	64	LYS	CG-CD	-11.94	1.16	1.52
1	A	16	ASP	CG-OD1	-11.81	1.02	1.25
1	A	5	LEU	C-N	-11.71	1.17	1.33
1	A	24	PHE	CG-CD1	-11.65	1.14	1.38
1	A	10	ASP	CG-OD2	-11.57	1.03	1.25
1	A	66	VAL	C-O	-11.47	1.10	1.24
1	A	36	LYS	CD-CE	-11.44	1.18	1.52
1	A	65	PHE	CE1-CZ	-11.30	1.04	1.38
1	A	74	GLY	N-CA	-11.27	1.29	1.45
1	A	74	GLY	C-N	-11.25	1.18	1.33
1	A	53	ASP	CG-OD2	-11.19	1.04	1.25
1	A	38	MET	CB-CG	-11.03	1.19	1.52
1	A	41	ASN	CB-CG	-10.95	1.24	1.52
1	A	53	ASP	CG-OD1	-10.88	1.04	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	LEU	C-O	-10.83	1.10	1.24
1	A	65	PHE	CE2-CZ	-10.74	1.06	1.38
1	A	36	LYS	CG-CD	-10.54	1.20	1.52
1	A	73	ASP	CA-CB	-10.54	1.37	1.53
1	A	108	GLU	CG-CD	-10.46	1.25	1.52
1	A	37	ALA	CA-CB	-10.40	1.38	1.53
1	A	48	LYS	CE-NZ	-10.36	1.18	1.49
1	A	102	PHE	CG-CD1	-10.24	1.17	1.38
1	A	36	LYS	CE-NZ	-10.15	1.18	1.49
1	A	45	LYS	CD-CE	-10.15	1.22	1.52
1	A	107	HIS	CG-CD2	-9.90	1.25	1.35
1	A	10	ASP	CG-OD1	-9.76	1.06	1.25
1	A	8	ALA	CA-CB	-9.69	1.37	1.53
1	A	91	LYS	CG-CD	-9.69	1.23	1.52
1	A	16	ASP	CG-OD2	-9.62	1.07	1.25
1	A	79	ASP	CB-CG	-9.54	1.28	1.52
1	A	24	PHE	CG-CD2	-9.35	1.19	1.38
1	A	102	PHE	CG-CD2	-9.31	1.19	1.38
1	A	96	LYS	CD-CE	-9.28	1.24	1.52
1	A	34	GLY	C-O	-9.24	1.11	1.23
1	A	32	LEU	CG-CD1	-9.19	1.22	1.52
1	A	1	ALA	CA-CB	-9.13	1.22	1.52
1	A	36	LYS	C-O	-8.90	1.12	1.24
1	A	52	ALA	C-N	-8.84	1.21	1.33
1	A	36	LYS	C-N	-8.62	1.21	1.33
1	A	32	LEU	CG-CD2	-8.46	1.24	1.52
1	A	6	LEU	C-N	-8.26	1.22	1.33
1	A	13	LYS	CB-CG	-8.20	1.27	1.52
1	A	109	ALA	CA-C	-8.19	1.35	1.52
1	A	28	LYS	CE-NZ	-8.14	1.25	1.49
1	A	24	PHE	CE2-CZ	-8.07	1.14	1.38
1	A	67	LEU	C-N	-7.89	1.22	1.33
1	A	6	LEU	CB-CG	-7.83	1.37	1.53
1	A	51	ASP	C-N	-7.78	1.23	1.33
1	A	94	ASP	C-O	-7.74	1.13	1.24
1	A	18	VAL	C-O	-7.63	1.12	1.24
1	A	89	ALA	C-O	-7.52	1.14	1.23
1	A	92	ASP	CG-OD2	-7.38	1.11	1.25
1	A	105	LEU	CB-CG	-7.19	1.39	1.53
1	A	102	PHE	CE2-CZ	-7.11	1.17	1.38
1	A	72	ALA	C-O	-7.10	1.15	1.24
1	A	74	GLY	C-O	-7.04	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	VAL	C-N	-6.78	1.25	1.33
1	A	35	LEU	C-O	-6.72	1.15	1.24
1	A	19	LYS	CB-CG	-6.66	1.32	1.52
1	A	52	ALA	CA-CB	-6.61	1.41	1.53
1	A	75	ARG	CA-CB	-6.58	1.44	1.52
1	A	71	ALA	CA-C	-6.52	1.46	1.53
1	A	24	PHE	CE1-CZ	-6.48	1.19	1.38
1	A	102	PHE	CE1-CZ	-6.43	1.19	1.38
1	A	5	LEU	CA-C	-6.40	1.44	1.52
1	A	105	LEU	C-O	-6.36	1.16	1.24
1	A	35	LEU	C-N	-6.30	1.25	1.34
1	A	54	ALA	C-N	-6.20	1.24	1.33
1	A	94	ASP	C-N	-6.09	1.25	1.33
1	A	37	ALA	C-O	-6.07	1.15	1.23
1	A	105	LEU	C-N	-5.98	1.26	1.33
1	A	75	ARG	CB-CG	-5.96	1.34	1.52
1	A	34	GLY	C-N	-5.86	1.26	1.33
1	A	18	VAL	C-N	-5.85	1.26	1.33
1	A	3	LYS	C-N	-5.83	1.25	1.33
1	A	39	SER	CB-OG	-5.83	1.30	1.42
1	A	51	ASP	CG-OD2	-5.82	1.14	1.25
1	A	75	ARG	CA-C	-5.81	1.46	1.53
1	A	9	ASP	C-N	-5.78	1.25	1.34
1	A	4	ASP	CA-CB	-5.76	1.43	1.53
1	A	92	ASP	CG-OD1	-5.69	1.14	1.25
1	A	54	ALA	C-O	-5.56	1.17	1.24
1	A	2	ALA	C-N	-5.54	1.25	1.33
1	A	32	LEU	C-O	-5.52	1.17	1.24
1	A	51	ASP	C-O	-5.48	1.17	1.24
1	A	9	ASP	CG-OD2	-5.47	1.15	1.25
1	A	10	ASP	C-N	-5.41	1.27	1.33
1	A	72	ALA	C-N	-5.40	1.26	1.33
1	A	89	ALA	C-N	-5.37	1.25	1.33
1	A	51	ASP	CG-OD1	-5.36	1.15	1.25
1	A	81	GLU	CB-CG	-5.30	1.36	1.52
1	A	32	LEU	CB-CG	-5.14	1.43	1.53
1	A	9	ASP	CG-OD1	-5.12	1.15	1.25
1	A	60	GLU	CB-CG	-5.10	1.37	1.52
1	A	3	LYS	C-O	-5.09	1.17	1.24
1	A	25	ASN	CB-CG	-5.06	1.39	1.52
1	A	4	ASP	C-N	-5.03	1.25	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	25	ASN	O-C-N	-82.97	12.24	122.59
1	A	75	ARG	O-C-N	-66.23	31.28	122.68
1	A	25	ASN	OD1-CG-ND2	-62.31	60.29	122.60
1	A	38	MET	O-C-N	-47.06	60.00	122.59
1	A	7	LYS	N-CA-C	44.41	159.77	111.36
1	A	75	ARG	NE-CZ-NH2	40.34	155.51	119.20
1	A	75	ARG	NH1-CZ-NH2	-37.90	70.03	119.30
1	A	29	PHE	CD1-CG-CD2	-37.30	62.64	118.60
1	A	61	GLU	CB-CG-CD	36.09	173.96	112.60
1	A	25	ASN	CA-C-O	36.07	172.08	120.51
1	A	100	ASP	CA-CB-CG	35.70	148.30	112.60
1	A	103	GLU	OE1-CD-OE2	-33.00	43.70	122.90
1	A	30	PHE	CD1-CG-CD2	-32.03	70.56	118.60
1	A	29	PHE	CE1-CZ-CE2	-31.87	62.64	120.00
1	A	7	LYS	CA-C-O	30.51	152.76	120.42
1	A	62	GLU	CB-CG-CD	30.35	164.19	112.60
1	A	62	GLU	CG-CD-OE2	-29.27	51.08	118.40
1	A	25	ASN	CA-C-N	28.34	175.67	121.54
1	A	25	ASN	C-N-CA	28.34	175.67	121.54
1	A	71	ALA	O-C-N	-28.15	94.91	123.62
1	A	30	PHE	CE1-CZ-CE2	-27.48	70.53	120.00
1	A	75	ARG	CD-NE-CZ	27.25	162.55	124.40
1	A	61	GLU	OE1-CD-OE2	-26.66	58.91	122.90
1	A	38	MET	CG-SD-CE	26.07	158.26	100.90
1	A	7	LYS	CB-CG-CD	25.62	170.22	111.30
1	A	75	ARG	CA-C-O	25.23	159.97	122.38
1	A	100	ASP	CB-CG-OD1	-25.05	60.77	118.40
1	A	33	VAL	CG1-CB-CG2	-24.49	56.92	110.80
1	A	75	ARG	CA-C-N	24.47	168.28	121.54
1	A	75	ARG	C-N-CA	24.47	168.28	121.54
1	A	7	LYS	CG-CD-CE	24.35	167.30	111.30
1	A	36	LYS	CB-CG-CD	24.12	166.79	111.30
1	A	13	LYS	CG-CD-CE	23.97	166.44	111.30
1	A	28	LYS	CA-CB-CG	22.71	159.51	114.10
1	A	97	ILE	CB-CG1-CD1	22.60	161.26	113.80
1	A	28	LYS	CB-CG-CD	22.55	163.18	111.30
1	A	38	MET	CA-C-N	22.29	157.69	121.58
1	A	38	MET	C-N-CA	22.29	157.69	121.58
1	A	87	LYS	CB-CG-CD	21.63	161.06	111.30
1	A	33	VAL	CA-CB-CG1	21.30	146.61	110.40
1	A	53	ASP	O-C-N	-21.29	96.48	122.24
1	A	33	VAL	CA-CB-CG2	21.25	146.53	110.40
1	A	25	ASN	CB-CG-ND2	20.60	147.30	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	LYS	CB-CG-CD	20.53	158.52	111.30
1	A	68	LYS	CG-CD-CE	-20.20	64.84	111.30
1	A	70	PHE	CD1-CG-CD2	-20.14	88.39	118.60
1	A	38	MET	CB-CG-SD	20.04	172.83	112.70
1	A	6	LEU	CA-C-O	-19.83	98.49	121.49
1	A	62	GLU	CG-CD-OE1	19.46	163.16	118.40
1	A	27	LYS	CD-CE-NZ	19.45	174.12	111.90
1	A	83	LYS	CG-CD-CE	19.28	155.64	111.30
1	A	67	LEU	CD1-CG-CD2	-19.11	68.76	110.80
1	A	61	GLU	CG-CD-OE1	18.75	161.52	118.40
1	A	7	LYS	N-CA-CB	-18.30	83.07	110.16
1	A	75	ARG	CG-CD-NE	18.14	151.91	112.00
1	A	109	ALA	CA-C-O	18.09	175.26	121.00
1	A	6	LEU	CD1-CG-CD2	-17.90	71.41	110.80
1	A	7	LYS	O-C-N	-17.63	102.05	122.15
1	A	103	GLU	CG-CD-OE2	17.63	158.94	118.40
1	A	45	LYS	CB-CG-CD	17.54	151.63	111.30
1	A	70	PHE	CE1-CZ-CE2	-17.53	88.45	120.00
1	A	91	LYS	CG-CD-CE	17.46	151.46	111.30
1	A	48	LYS	CG-CD-CE	17.24	150.94	111.30
1	A	77	LEU	CD1-CG-CD2	-17.09	73.21	110.80
1	A	103	GLU	CG-CD-OE1	16.94	157.36	118.40
1	A	64	LYS	CG-CD-CE	16.69	149.68	111.30
1	A	83	LYS	CB-CG-CD	16.68	149.66	111.30
1	A	90	ASP	O-C-N	-16.58	103.70	123.27
1	A	29	PHE	CG-CD2-CE2	16.48	148.72	120.70
1	A	29	PHE	CB-CG-CD1	16.46	148.68	120.70
1	A	29	PHE	CB-CG-CD2	16.45	148.67	120.70
1	A	29	PHE	CG-CD1-CE1	16.43	148.63	120.70
1	A	19	LYS	CG-CD-CE	16.04	148.18	111.30
1	A	29	PHE	CD1-CE1-CZ	15.95	148.71	120.00
1	A	29	PHE	CZ-CE2-CD2	15.92	148.65	120.00
1	A	25	ASN	CB-CG-OD1	15.80	152.41	120.80
1	A	38	MET	CA-C-O	15.64	142.87	120.51
1	A	75	ARG	CB-CG-CD	15.37	146.65	111.30
1	A	59	GLU	CG-CD-OE2	15.30	153.59	118.40
1	A	30	PHE	CB-CG-CD2	15.19	146.52	120.70
1	A	59	GLU	CG-CD-OE1	-15.14	83.57	118.40
1	A	30	PHE	CG-CD2-CE2	15.00	146.19	120.70
1	A	30	PHE	CD1-CE1-CZ	14.58	146.24	120.00
1	A	15	LEU	CD1-CG-CD2	-14.36	79.22	110.80
1	A	61	GLU	CA-CB-CG	14.34	142.78	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	LYS	CG-CD-CE	13.89	143.26	111.30
1	A	68	LYS	CB-CG-CD	13.77	142.97	111.30
1	A	44	LYS	CG-CD-CE	13.74	142.91	111.30
1	A	3	LYS	CA-CB-CG	13.71	141.51	114.10
1	A	53	ASP	CA-C-O	13.66	135.57	119.32
1	A	30	PHE	CG-CD1-CE1	13.25	143.22	120.70
1	A	45	LYS	CG-CD-CE	13.09	141.40	111.30
1	A	30	PHE	CB-CG-CD1	13.07	142.92	120.70
1	A	75	ARG	NE-CZ-NH1	12.96	134.46	121.50
1	A	73	ASP	OD1-CG-OD2	-12.95	91.81	122.90
1	A	108	GLU	CG-CD-OE1	12.95	148.19	118.40
1	A	65	PHE	CD1-CG-CD2	-12.93	99.21	118.60
1	A	30	PHE	CZ-CE2-CD2	12.92	143.25	120.00
1	A	100	ASP	CB-CG-OD2	12.88	148.03	118.40
1	A	7	LYS	CD-CE-NZ	12.61	152.24	111.90
1	A	12	LYS	CB-CG-CD	12.60	140.27	111.30
1	A	3	LYS	CB-CG-CD	12.49	140.02	111.30
1	A	68	LYS	CD-CE-NZ	-12.40	72.23	111.90
1	A	28	LYS	CD-CE-NZ	12.25	151.09	111.90
1	A	13	LYS	CD-CE-NZ	12.21	150.98	111.90
1	A	83	LYS	CD-CE-NZ	12.20	150.93	111.90
1	A	12	LYS	CG-CD-CE	11.98	138.84	111.30
1	A	100	ASP	OD1-CG-OD2	11.79	151.19	122.90
1	A	91	LYS	CD-CE-NZ	11.71	149.37	111.90
1	A	6	LEU	CB-CG-CD2	11.57	145.40	110.70
1	A	65	PHE	CE1-CZ-CE2	-11.55	99.21	120.00
1	A	105	LEU	CB-CG-CD1	11.53	145.30	110.70
1	A	12	LYS	CD-CE-NZ	11.52	148.75	111.90
1	A	108	GLU	OE1-CD-OE2	-11.24	95.92	122.90
1	A	96	LYS	CD-CE-NZ	11.23	147.84	111.90
1	A	87	LYS	CG-CD-CE	-11.13	85.70	111.30
1	A	67	LEU	CB-CG-CD1	10.94	143.51	110.70
1	A	19	LYS	CD-CE-NZ	10.92	146.85	111.90
1	A	19	LYS	CB-CG-CD	10.59	135.65	111.30
1	A	6	LEU	CA-C-N	10.51	135.21	120.29
1	A	6	LEU	C-N-CA	10.51	135.21	120.29
1	A	77	LEU	CB-CG-CD2	10.18	141.24	110.70
1	A	44	LYS	CA-CB-CG	10.17	134.44	114.10
1	A	21	GLU	CB-CG-CD	9.63	128.97	112.60
1	A	21	GLU	CG-CD-OE2	-9.62	96.27	118.40
1	A	62	GLU	OE1-CD-OE2	9.53	145.76	122.90
1	A	21	GLU	OE1-CD-OE2	9.49	145.69	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	THR	OG1-CB-CG2	-9.32	90.67	109.30
1	A	59	GLU	CB-CG-CD	9.21	128.25	112.60
1	A	61	GLU	CG-CD-OE2	9.21	139.57	118.40
1	A	64	LYS	CB-CG-CD	9.14	132.32	111.30
1	A	42	ASP	OD1-CG-OD2	-9.09	101.08	122.90
1	A	44	LYS	CB-CG-CD	9.07	132.17	111.30
1	A	78	THR	CA-CB-CG2	9.07	125.92	110.50
1	A	70	PHE	CB-CG-CD1	9.06	136.10	120.70
1	A	107	HIS	CG-CD2-NE2	9.04	116.24	107.20
1	A	48	LYS	CB-CG-CD	9.03	132.06	111.30
1	A	78	THR	CA-CB-OG1	9.02	123.12	109.60
1	A	71	ALA	CA-C-N	8.92	138.58	121.54
1	A	71	ALA	C-N-CA	8.92	138.58	121.54
1	A	70	PHE	CG-CD1-CE1	8.89	135.81	120.70
1	A	70	PHE	CG-CD2-CE2	8.88	135.79	120.70
1	A	70	PHE	CD1-CE1-CZ	8.78	135.81	120.00
1	A	70	PHE	CZ-CE2-CD2	8.75	135.75	120.00
1	A	78	THR	O-C-N	-8.72	110.99	122.42
1	A	70	PHE	CB-CG-CD2	8.71	135.51	120.70
1	A	73	ASP	CB-CG-OD2	8.43	137.79	118.40
1	A	3	LYS	CG-CD-CE	8.43	130.68	111.30
1	A	90	ASP	OD1-CG-OD2	-8.38	102.78	122.90
1	A	107	HIS	ND1-CG-CD2	-8.33	97.77	106.10
1	A	108	GLU	CB-CG-CD	-8.18	98.70	112.60
1	A	81	GLU	OE1-CD-OE2	-8.10	103.46	122.90
1	A	36	LYS	CG-CD-CE	8.09	129.90	111.30
1	A	15	LEU	CB-CG-CD2	8.08	134.93	110.70
1	A	91	LYS	CA-CB-CG	8.05	130.21	114.10
1	A	91	LYS	CB-CG-CD	7.89	129.45	111.30
1	A	67	LEU	CB-CG-CD2	7.73	133.88	110.70
1	A	103	GLU	CB-CG-CD	7.72	125.72	112.60
1	A	7	LYS	CA-C-N	-7.63	106.97	121.54
1	A	7	LYS	C-N-CA	-7.63	106.97	121.54
1	A	24	PHE	CD1-CG-CD2	-7.59	107.21	118.60
1	A	96	LYS	CB-CG-CD	7.53	128.62	111.30
1	A	76	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	71	ALA	CA-C-O	7.49	127.66	120.09
1	A	102	PHE	CD1-CG-CD2	-7.49	107.36	118.60
1	A	60	GLU	CG-CD-OE2	-7.42	101.34	118.40
1	A	87	LYS	CD-CE-NZ	-7.41	88.19	111.90
1	A	73	ASP	CA-C-O	-7.29	113.61	121.78
1	A	3	LYS	CD-CE-NZ	7.28	135.19	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	LYS	CD-CE-NZ	7.25	135.09	111.90
1	A	76	ASP	CB-CG-OD2	7.16	134.88	118.40
1	A	24	PHE	CE1-CZ-CE2	-7.10	107.22	120.00
1	A	105	LEU	CD1-CG-CD2	-7.06	95.27	110.80
1	A	102	PHE	CE1-CZ-CE2	-7.03	107.34	120.00
1	A	76	ASP	OD1-CG-OD2	-7.02	106.05	122.90
1	A	52	ALA	O-C-N	-6.94	113.37	122.39
1	A	107	HIS	CE1-NE2-CD2	-6.93	102.07	109.00
1	A	87	LYS	CA-CB-CG	6.82	127.75	114.10
1	A	77	LEU	CB-CG-CD1	6.78	131.05	110.70
1	A	41	ASN	OD1-CG-ND2	6.59	129.19	122.60
1	A	108	GLU	O-C-N	-6.44	113.48	122.37
1	A	15	LEU	CB-CG-CD1	6.44	130.01	110.70
1	A	6	LEU	CB-CG-CD1	6.42	129.94	110.70
1	A	32	LEU	CD1-CG-CD2	-6.36	96.81	110.80
1	A	6	LEU	CA-CB-CG	6.32	138.42	116.30
1	A	6	LEU	CB-CA-C	-6.12	98.27	111.11
1	A	36	LYS	CA-CB-CG	6.08	126.26	114.10
1	A	65	PHE	CZ-CE2-CD2	6.06	130.90	120.00
1	A	96	LYS	CA-CB-CG	6.04	126.18	114.10
1	A	60	GLU	OE1-CD-OE2	6.02	137.35	122.90
1	A	65	PHE	CB-CG-CD1	5.99	130.89	120.70
1	A	65	PHE	CG-CD1-CE1	5.97	130.86	120.70
1	A	45	LYS	CD-CE-NZ	5.86	130.65	111.90
1	A	6	LEU	N-CA-C	5.85	117.49	109.18
1	A	73	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	90	ASP	CA-C-N	5.67	132.88	122.79
1	A	90	ASP	C-N-CA	5.67	132.88	122.79
1	A	0	ACE	O-C-N	-5.66	106.03	123.00
1	A	65	PHE	CD1-CE1-CZ	5.50	129.90	120.00
1	A	78	THR	CA-C-N	5.47	131.99	121.54
1	A	78	THR	C-N-CA	5.47	131.99	121.54
1	A	65	PHE	CG-CD2-CE2	5.42	129.92	120.70
1	A	24	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	65	PHE	CB-CG-CD2	5.41	129.90	120.70
1	A	73	ASP	CB-CG-OD1	5.22	130.40	118.40
1	A	64	LYS	CD-CE-NZ	5.20	128.53	111.90
1	A	96	LYS	CG-CD-CE	5.11	123.06	111.30
1	A	30	PHE	CA-CB-CG	-5.05	108.75	113.80

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

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	818	353
All	All	836	0	818	353

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:OD1	1:A:76:ASP:CB	1.45	1.63
1:A:45:LYS:CG	1:A:45:LYS:CE	1.44	1.94
1:A:87:LYS:CB	1:A:87:LYS:CD	1.44	1.94
1:A:6:LEU:CD1	1:A:6:LEU:CB	1.43	1.94
1:A:75:ARG:NH2	1:A:75:ARG:NE	1.41	1.66
1:A:45:LYS:NZ	1:A:45:LYS:CD	1.40	1.84
1:A:44:LYS:CB	1:A:44:LYS:CD	1.39	1.99
1:A:3:LYS:CB	1:A:3:LYS:CD	1.36	2.04
1:A:27:LYS:CE	1:A:27:LYS:CG	1.36	2.01
1:A:77:LEU:CD1	1:A:77:LEU:CB	1.36	2.03
1:A:30:PHE:CG	1:A:30:PHE:CE1	1.35	2.11
1:A:30:PHE:CZ	1:A:30:PHE:CD2	1.35	2.11
1:A:29:PHE:CZ	1:A:29:PHE:CD2	1.34	2.14
1:A:29:PHE:CG	1:A:29:PHE:CE1	1.34	2.14
1:A:87:LYS:CB	1:A:87:LYS:CE	1.34	2.06
1:A:29:PHE:CZ	1:A:29:PHE:CD1	1.34	2.14
1:A:29:PHE:CG	1:A:29:PHE:CE2	1.34	2.14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:91:LYS:CE	1:A:91:LYS:CG	1.34	2.04
1:A:3:LYS:CE	1:A:3:LYS:CG	1.32	2.06
1:A:61:GLU:CG	1:A:61:GLU:CA	1.31	2.08
1:A:96:LYS:NZ	1:A:96:LYS:CD	1.31	1.91
1:A:30:PHE:CG	1:A:30:PHE:CE2	1.29	2.19
1:A:30:PHE:CZ	1:A:30:PHE:CD1	1.29	2.19
1:A:15:LEU:CD1	1:A:15:LEU:CB	1.28	2.08
1:A:25:ASN:O	1:A:26:HIS:CA	1.28	1.80
1:A:100:ASP:CG	1:A:100:ASP:CA	1.28	2.05
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:33:VAL:CA	1:A:33:VAL:CG2	1.26	2.12
1:A:44:LYS:CG	1:A:44:LYS:CA	1.26	2.13
1:A:62:GLU:CG	1:A:62:GLU:OE1	1.25	1.81
1:A:45:LYS:CD	1:A:45:LYS:CB	1.25	2.15
1:A:3:LYS:CG	1:A:3:LYS:CA	1.24	2.15
1:A:38:MET:SD	1:A:38:MET:CE	1.24	1.15
1:A:38:MET:SD	1:A:38:MET:CB	1.23	2.24
1:A:38:MET:CE	1:A:38:MET:CG	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
1:A:29:PHE:CD1	1:A:29:PHE:CB	1.19	2.25
1:A:29:PHE:CD2	1:A:29:PHE:CB	1.18	2.25
1:A:75:ARG:O	1:A:75:ARG:CA	1.18	1.89
1:A:109:ALA:CA	1:A:109:ALA:O	1.17	1.91
1:A:38:MET:SD	1:A:38:MET:CG	1.15	1.06
1:A:73:ASP:OD1	1:A:73:ASP:CB	1.13	1.95
1:A:75:ARG:C	1:A:76:ASP:CA	1.13	2.22
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:CB	1:A:76:ASP:OD2	1.12	1.87
1:A:25:ASN:C	1:A:26:HIS:CA	1.09	2.25
1:A:38:MET:SD	1:A:38:MET:HE3	1.08	1.73
1:A:38:MET:SD	1:A:38:MET:HE2	1.06	1.73
1:A:62:GLU:CD	1:A:62:GLU:CB	1.06	2.28
1:A:25:ASN:CB	1:A:25:ASN:OD1	1.06	2.02
1:A:38:MET:SD	1:A:38:MET:HE1	1.04	1.73
1:A:77:LEU:CB	1:A:77:LEU:CD2	1.03	2.25
1:A:33:VAL:CG1	1:A:33:VAL:HG23	1.02	1.58

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:33:VAL:CG2	1:A:33:VAL:HB	1.02	1.58
1:A:33:VAL:CG1	1:A:33:VAL:HB	1.00	1.57
1:A:33:VAL:CG2	1:A:33:VAL:HG12	1.00	1.58
1:A:6:LEU:CG	1:A:6:LEU:HD22	0.99	1.56
1:A:45:LYS:NZ	1:A:45:LYS:HE2	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:CD1	1:A:77:LEU:HG	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:CB	1:A:6:LEU:CD2	0.98	2.21
1:A:45:LYS:NZ	1:A:45:LYS:HE3	0.98	1.40
1:A:75:ARG:NH2	1:A:75:ARG:HH11	0.98	1.56
1:A:77:LEU:CG	1:A:77:LEU:HD23	0.98	1.53
1:A:77:LEU:CG	1:A:77:LEU:HD22	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:CE	1:A:45:LYS:NZ	0.95	0.80
1:A:87:LYS:CG	1:A:87:LYS:HB3	0.94	1.49
1:A:87:LYS:CG	1:A:87:LYS:HB2	0.94	1.49
1:A:25:ASN:OD1	1:A:25:ASN:CG	0.93	0.68
1:A:62:GLU:CG	1:A:62:GLU:CD	0.93	0.90
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:15:LEU:CG	1:A:15:LEU:HD21	0.92	1.46
1:A:3:LYS:CE	1:A:3:LYS:HD2	0.91	1.46
1:A:30:PHE:CE2	1:A:30:PHE:HZ	0.91	1.67
1:A:96:LYS:NZ	1:A:96:LYS:HE2	0.91	1.31
1:A:96:LYS:NZ	1:A:96:LYS:HE3	0.91	1.31
1:A:15:LEU:CG	1:A:15:LEU:HD22	0.91	1.46
1:A:77:LEU:CD2	1:A:77:LEU:CG	0.90	0.90
1:A:3:LYS:CE	1:A:3:LYS:HD3	0.90	1.46
1:A:87:LYS:CB	1:A:87:LYS:CG	0.90	0.90
1:A:77:LEU:CD2	1:A:77:LEU:HG	0.89	1.68
1:A:13:LYS:NZ	1:A:13:LYS:HE2	0.89	1.28
1:A:29:PHE:CE2	1:A:29:PHE:HZ	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:NZ	1:A:96:LYS:CE	0.88	0.74

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:62:GLU:CD	1:A:62:GLU:HG2	0.88	1.37
1:A:3:LYS:CD	1:A:3:LYS:CE	0.88	0.88
1:A:13:LYS:NZ	1:A:13:LYS:HE3	0.88	1.28
1:A:19:LYS:CE	1:A:19:LYS:HD2	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:75:ARG:C	1:A:76:ASP:N	0.87	0.79
1:A:15:LEU:CG	1:A:15:LEU:HD12	0.87	1.41
1:A:15:LEU:CG	1:A:15:LEU:HD11	0.87	1.41
1:A:6:LEU:CG	1:A:6:LEU:HD13	0.87	1.41
1:A:15:LEU:CG	1:A:15:LEU:HD13	0.87	1.41
1:A:45:LYS:CG	1:A:45:LYS:HD2	0.86	1.40
1:A:91:LYS:CE	1:A:91:LYS:HD3	0.86	1.40
1:A:3:LYS:NZ	1:A:3:LYS:HE2	0.86	1.31
1:A:45:LYS:CG	1:A:45:LYS:HD3	0.86	1.40
1:A:91:LYS:CE	1:A:91:LYS:HD2	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:62:GLU:CG	1:A:62:GLU:OE2	0.85	0.73
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:CE	1:A:91:LYS:CD	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
1:A:77:LEU:CG	1:A:77:LEU:HD12	0.83	1.39
1:A:44:LYS:CG	1:A:44:LYS:HB2	0.83	1.36
1:A:87:LYS:CB	1:A:87:LYS:HG3	0.83	1.39
1:A:44:LYS:CG	1:A:44:LYS:HB3	0.83	1.36
1:A:44:LYS:CB	1:A:44:LYS:HG2	0.83	1.37
1:A:45:LYS:CD	1:A:45:LYS:HG3	0.83	1.37
1:A:91:LYS:HE2	1:A:91:LYS:NZ	0.83	1.39
1:A:3:LYS:CB	1:A:3:LYS:HG3	0.83	1.36
1:A:33:VAL:HG23	1:A:33:VAL:CB	0.83	1.36
1:A:38:MET:SD	1:A:38:MET:HG2	0.82	1.46
1:A:45:LYS:CD	1:A:45:LYS:HG2	0.82	1.37
1:A:91:LYS:NZ	1:A:91:LYS:HE3	0.82	1.39
1:A:29:PHE:CE1	1:A:29:PHE:HZ	0.82	1.68
1:A:19:LYS:CE	1:A:19:LYS:CD	0.82	0.87
1:A:33:VAL:HG12	1:A:33:VAL:CB	0.82	1.35
1:A:33:VAL:CB	1:A:33:VAL:HG13	0.82	1.35
1:A:33:VAL:CB	1:A:33:VAL:HG21	0.82	1.36

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:87:LYS:CB	1:A:87:LYS:HE2	0.81	2.05
1:A:30:PHE:CG	1:A:30:PHE:CD1	0.81	0.82
1:A:77:LEU:CG	1:A:77:LEU:HD11	0.81	1.39
1:A:3:LYS:CB	1:A:3:LYS:HG2	0.81	1.36
1:A:87:LYS:CB	1:A:87:LYS:HE3	0.81	2.04
1:A:3:LYS:CG	1:A:3:LYS:HB3	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:30:PHE:CZ	1:A:30:PHE:CE2	0.81	0.82
1:A:33:VAL:CB	1:A:33:VAL:HG22	0.81	1.36
1:A:45:LYS:CG	1:A:45:LYS:CD	0.81	0.83
1:A:38:MET:SD	1:A:38:MET:HG3	0.81	1.46
1:A:25:ASN:C	1:A:26:HIS:N	0.81	0.77
1:A:33:VAL:CB	1:A:33:VAL:HG11	0.81	1.35
1:A:62:GLU:OE2	1:A:62:GLU:HG3	0.80	1.04
1:A:29:PHE:CZ	1:A:29:PHE:CE1	0.80	0.82
1:A:13:LYS:NZ	1:A:13:LYS:CE	0.80	0.71
1:A:25:ASN:ND2	1:A:25:ASN:OD1	0.80	0.66
1:A:29:PHE:CZ	1:A:29:PHE:CE2	0.80	0.82
1:A:29:PHE:CG	1:A:29:PHE:CD1	0.80	0.82
1:A:3:LYS:CG	1:A:3:LYS:HB2	0.79	1.36
1:A:29:PHE:CD2	1:A:29:PHE:CG	0.79	0.82
1:A:33:VAL:HG23	1:A:33:VAL:HG11	0.79	1.27
1:A:73:ASP:OD2	1:A:73:ASP:CG	0.79	0.81
1:A:3:LYS:CD	1:A:3:LYS:HE2	0.79	1.45
1:A:19:LYS:CD	1:A:19:LYS:HE3	0.79	1.41
1:A:19:LYS:HE3	1:A:19:LYS:NZ	0.78	1.25
1:A:73:ASP:OD1	1:A:73:ASP:CG	0.78	0.71
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:30:PHE:CE1	1:A:30:PHE:HZ	0.76	1.73
1:A:60:GLU:CB	1:A:60:GLU:OE1	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: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:NZ	1:A:19:LYS:HE2	0.75	1.25
1:A:68:LYS:HE2	1:A:68:LYS:C	0.75	2.03
1:A:15:LEU:CD1	1:A:15:LEU:CG	0.75	0.75
1:A:6:LEU:CD1	1:A:6:LEU:CG	0.75	0.75

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:61:GLU:CG	1:A:61:GLU:HB3	0.73	1.27
1:A:39:SER:O	1:A:43:VAL:HG23	0.73	1.84
1:A:100:ASP:CG	1:A:100:ASP:HB2	0.73	1.22
1:A:19:LYS:CE	1:A:19:LYS:HG3	0.73	2.09
1:A:61:GLU:CG	1:A:61:GLU:HB2	0.72	1.27
1:A:77:LEU:CD1	1:A:77:LEU:CG	0.72	0.73
1:A:25:ASN:ND2	1:A:25:ASN:CG	0.72	0.63
1:A:91:LYS:CE	1:A:91:LYS:HZ3	0.72	1.42
1:A:33:VAL:HG12	1:A:33:VAL:HG21	0.72	1.28
1:A:100:ASP:CG	1:A:100:ASP:HB3	0.72	1.22
1:A:27:LYS:CE	1:A:27:LYS:CD	0.71	0.72
1:A:91:LYS:CE	1:A:91:LYS:HZ2	0.71	1.42
1:A:91:LYS:CE	1:A:91:LYS:HZ1	0.71	1.42
1:A:109:ALA:O	1:A:109:ALA:C	0.70	0.56
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:CE	1:A:27:LYS:HZ2	0.69	1.40
1:A:30:PHE:CZ	1:A:30:PHE:HE1	0.69	1.46
1:A:27:LYS:CE	1:A:27:LYS:HZ3	0.69	1.40
1:A:30:PHE:CG	1:A:30:PHE:HD2	0.68	1.46
1:A:47:PHE:CD1	1:A:99:ILE:CD1	0.68	2.76
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:33:VAL:CG2	1:A:33:VAL:CB	0.68	0.68
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:27:LYS:CE	1:A:27:LYS:NZ	0.67	0.82
1:A:45:LYS:CE	1:A:45:LYS:HZ2	0.67	1.38
1:A:75:ARG:CZ	1:A:75:ARG:HH21	0.67	1.38
1:A:35:LEU:HG	1:A:106:VAL:HG11	0.67	1.64
1:A:45:LYS:CE	1:A:45:LYS:HZ1	0.67	1.38
1:A:33:VAL:CG2	1:A:33:VAL:HG13	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:NZ	1:A:13:LYS:HD3	0.65	2.00
1:A:75:ARG:O	1:A:75:ARG:C	0.65	0.45
1:A:27:LYS:CD	1:A:27:LYS:HE2	0.65	1.23
1:A:33:VAL:HG13	1:A:33:VAL:HG22	0.65	0.82

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:61:GLU:CG	1:A:61:GLU:CB	0.65	0.65
1:A:25:ASN:CG	1:A:25:ASN:HD22	0.65	1.30
1:A:33:VAL:CG1	1:A:33:VAL:HG22	0.65	1.21
1:A:33:VAL:CG1	1:A:33:VAL:CG2	0.64	0.65
1:A:25:ASN:CG	1:A:25:ASN:HD21	0.64	1.30
1:A:87:LYS:CA	1:A:87:LYS:HG3	0.64	2.05
1:A:29:PHE:CG	1:A:29:PHE:HD1	0.63	1.39
1:A:27:LYS:NZ	1:A:27:LYS:HE2	0.63	1.29
1:A:25:ASN:O	1:A:25:ASN:C	0.63	0.46
1:A:96:LYS:CE	1:A:96:LYS:HZ1	0.63	1.34
1:A:78:THR:O	1:A:79:ASP:CB	0.63	2.40
1:A:96:LYS:CE	1:A:96:LYS:HZ3	0.63	1.34
1:A:29:PHE:CZ	1:A:29:PHE:HE1	0.63	1.39
1:A:45:LYS:NZ	1:A:45:LYS:HD3	0.63	1.99
1:A:14:ALA:HB1	1:A:29:PHE:CD1	0.62	2.29
1:A:100:ASP:CG	1:A:100:ASP:CB	0.62	0.59
1:A:29:PHE:CZ	1:A:29:PHE:HE2	0.62	1.39
1:A:27:LYS:NZ	1:A:27:LYS:HE3	0.62	1.29
1:A:96:LYS:CE	1:A:96:LYS:HZ2	0.62	1.34
1:A:61:GLU:CB	1:A:61:GLU:HG3	0.62	1.19
1:A:29:PHE:CG	1:A:29:PHE:HD2	0.61	1.39
1:A:76:ASP:OD2	1:A:76:ASP:CG	0.61	0.82
1:A:20:ALA:HB3	1:A:23:SER:OG	0.61	1.94
1:A:47:PHE:CG	1:A:99:ILE:HD13	0.61	2.30
1:A:47:PHE:CD1	1:A:47:PHE:C	0.61	2.79
1:A:61:GLU:CD	1:A:61:GLU:HG2	0.61	1.31
1:A:61:GLU:CB	1:A:61:GLU:HG2	0.61	1.19
1:A:75:ARG:O	1:A:76:ASP:N	0.60	0.47
1:A:45:LYS:CG	1:A:45:LYS:HE2	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:13:LYS:CE	1:A:13:LYS:HZ3	0.60	1.31
1:A:3:LYS:CE	1:A:3:LYS:HG2	0.60	2.17
1:A:13:LYS:CE	1:A:13:LYS:HZ2	0.60	1.31
1:A:76:ASP:OD1	1:A:76:ASP:CG	0.60	0.67
1:A:3:LYS:CE	1:A:3:LYS:HZ1	0.59	1.29
1:A:91:LYS:HD2	1:A:91:LYS:HE3	0.59	1.19
1:A:3:LYS:CE	1:A:3:LYS:HZ2	0.59	1.30
1:A:3:LYS:CE	1:A:3:LYS:HZ3	0.59	1.30
1:A:61:GLU:CA	1:A:61:GLU:HG3	0.59	2.00
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:20:ALA:HB3	1:A:23:SER:CB	0.58	2.29
1:A:109:ALA:OXT	1:A:109:ALA:C	0.58	0.46
1:A:27:LYS:HD3	1:A:27:LYS:HE3	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:61:GLU:HG3	1:A:61:GLU:CD	0.57	1.31
1:A:78:THR:O	1:A:79:ASP:HB2	0.57	2.00
1:A:27:LYS:HD2	1:A:27:LYS:HE2	0.56	1.15
1:A:19:LYS:CE	1:A:19:LYS:HZ1	0.56	1.26
1:A:19:LYS:CE	1:A:19:LYS:HZ3	0.55	1.26
1:A:99:ILE:O	1:A:100:ASP:C	0.55	2.50
1:A:19:LYS:CE	1:A:19:LYS:HZ2	0.55	1.26
1:A:47:PHE:CD1	1:A:99:ILE:HD13	0.55	2.35
1:A:3:LYS:CG	1:A:3:LYS:C	0.54	2.78
1:A:100:ASP:CG	1:A:100:ASP:OD2	0.54	0.80
1:A:75:ARG:NH2	1:A:81:GLU:OE1	0.54	2.39
1:A:3:LYS:CE	1:A:3:LYS:NZ	0.54	0.69
1:A:6:LEU:CD1	1:A:6:LEU:HB2	0.53	2.18
1:A:26:HIS:CE1	1:A:88:ALA:HB1	0.53	2.38
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:CD2	1:A:77:LEU:CA	0.52	2.86
1:A:27:LYS:HZ1	1:A:27:LYS:HE3	0.52	1.15
1:A:99:ILE:O	1:A:102:PHE:N	0.52	2.43
1:A:33:VAL:CG1	1:A:33:VAL:C	0.52	2.81
1:A:19:LYS:HE3	1:A:19:LYS:HZ1	0.52	1.11
1:A:33:VAL:CG2	1:A:33:VAL:HG11	0.52	0.84
1:A:39:SER:O	1:A:40:ALA:C	0.52	2.53
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:47:PHE:O	1:A:48:LYS:C	0.51	2.53
1:A:75:ARG:NH2	1:A:75:ARG:HH12	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:HZ3	1:A:27:LYS:HE2	0.51	1.17
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:50:ILE:CB	1:A:58:ILE:HD12	0.49	2.38
1:A:39:SER:O	1:A:41:ASN:N	0.48	2.46
1:A:47:PHE:CE2	1:A:58:ILE:HG12	0.48	2.43
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:55:SER:O	1:A:56:GLY:C	0.47	2.57
1:A:39:SER:C	1:A:43:VAL:HG23	0.47	2.35
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:HE2	1:A:19:LYS:HZ3	0.46	1.14
1:A:24:PHE:CD1	1:A:24:PHE:C	0.46	2.94
1:A:47:PHE:C	1:A:49:ALA:N	0.45	2.73
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:HE2	1:A:13:LYS:HZ3	0.44	1.16
1:A:45:LYS:CE	1:A:45:LYS:HG3	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
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: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:HD23	1:A:67:LEU:CA	0.41	2.33
1:A:3:LYS:HE3	1:A:3:LYS:HZ1	0.41	1.21
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:55:SER:O	1:A:57:PHE:N	0.40	2.55
1:A:6:LEU:CD1	1:A:6:LEU:HB3	0.40	2.23
1:A:55:SER:C	1:A:57:PHE:N	0.40	2.78

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	2	18
All	All	108/110 (98%)	84 (78%)	17 (16%)	7 (6%)	2	18

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	8	ALA
1	A	26	HIS
1	A	38	MET
1	A	40	ALA
1	A	76	ASP
1	A	79	ASP

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/83 (100%)	62 (75%)	21 (25%)	2	24
All	All	83/83 (100%)	62 (75%)	21 (25%)	2	24

All 21 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	3	LYS
1	A	5	LEU
1	A	7	LYS

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Mol	Chain	Res	Type
1	A	13	LYS
1	A	15	LEU
1	A	28	LYS
1	A	32	LEU
1	A	33	VAL
1	A	35	LEU
1	A	36	LYS
1	A	38	MET
1	A	45	LYS
1	A	48	LYS
1	A	75	ARG
1	A	76	ASP
1	A	77	LEU
1	A	78	THR
1	A	83	LYS
1	A	91	LYS
1	A	101	GLU
1	A	105	LEU

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](#)

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	74:GLY	C	75:ARG	N	1.18
1	A	5:LEU	C	6:LEU	N	1.17
1	A	108:GLU	C	109:ALA	N	1.16
1	A	78:THR	C	79:ASP	N	1.13
1	A	90:ASP	C	91:LYS	N	1.07
1	A	71:ALA	C	72:ALA	N	0.98
1	A	53:ASP	C	54:ALA	N	0.90
1	A	38:MET	C	39:SER	N	0.87
1	A	75:ARG	C	76:ASP	N	0.79
1	A	25:ASN	C	26:HIS	N	0.77
1	A	0:ACE	C	1:ALA	N	0.70
1	A	7:LYS	C	8:ALA	N	0.53

7 Chemical shift validation

No chemical shift data were provided