



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:08 PM BST

PDB ID : 1K8M
Title : Solution Structure of the Lipoic Acid-Bearing Domain of the E2 component of Human, Mitochondrial Branched-Chain alpha-Ketoacid Dehydrogenase
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Deposited on : 2001-10-24

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

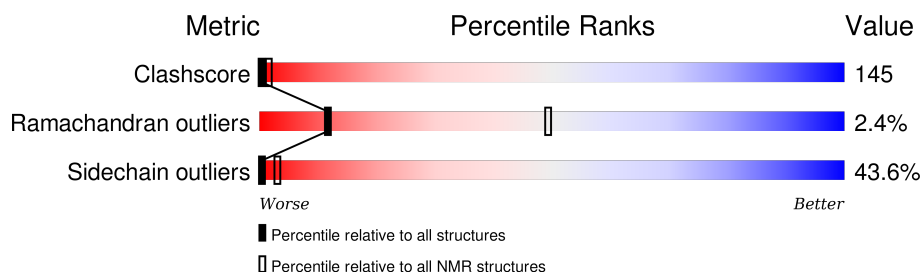
1 Overall quality at a glance

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	93	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1378 atoms, of which 688 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E2 component of Branched-Chain alpha-Ketoacid Dehydrogenase.

Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1378	439	688	107	142	2	

There are 9 discrepancies between the modelled and reference sequences:

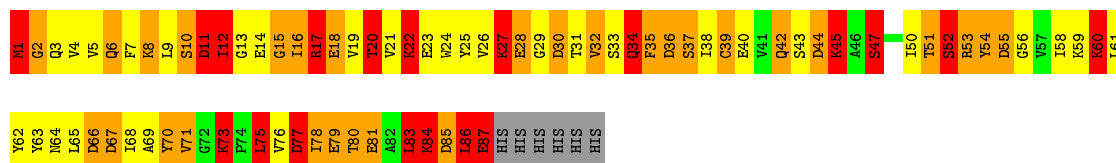
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING MET	UNP P11182
A	86	LEU	-	EXPRESSION TAG	UNP P11182
A	87	GLU	-	EXPRESSION TAG	UNP P11182
A	88	HIS	-	EXPRESSION TAG	UNP P11182
A	89	HIS	-	EXPRESSION TAG	UNP P11182
A	90	HIS	-	EXPRESSION TAG	UNP P11182
A	91	HIS	-	EXPRESSION TAG	UNP P11182
A	92	HIS	-	EXPRESSION TAG	UNP P11182
A	93	HIS	-	EXPRESSION TAG	UNP P11182

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: E2 component of Branched-Chain alpha-Ketoacid Dehydrogenase

Chain A: 



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *distance geometry simulated annealing molecular dynamics torsion angle dynamics*.

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
ARIA	refinement	1.0
ARIA	structure solution	1.0

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	14.79	199/699 (28.5%)	8.53	152/944 (16.1%)
All	All	14.79	199/699 (28.5%)	8.53	152/944 (16.1%)

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	0
All	All	1	0

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	53	ARG	CZ-NH1	-86.75	0.20	1.33
1	A	10	SER	CB-OG	-75.33	0.44	1.42
1	A	40	GLU	CD-OE1	-71.88	0.46	1.25
1	A	17	ARG	CZ-NH1	-71.19	0.40	1.33
1	A	23	GLU	CD-OE1	-66.76	0.52	1.25
1	A	81	GLU	CD-OE1	-63.06	0.56	1.25
1	A	14	GLU	CD-OE2	-58.11	0.61	1.25
1	A	17	ARG	CZ-NH2	-56.80	0.59	1.33
1	A	28	GLU	CD-OE1	-55.51	0.64	1.25
1	A	87	GLU	CD-OE1	-55.13	0.65	1.25
1	A	87	GLU	CG-CD	-50.80	0.75	1.51
1	A	28	GLU	CD-OE2	-47.77	0.73	1.25
1	A	87	GLU	CD-OE2	-47.59	0.73	1.25
1	A	14	GLU	CD-OE1	-47.20	0.73	1.25
1	A	23	GLU	CD-OE2	-46.92	0.74	1.25
1	A	17	ARG	CD-NE	-44.88	0.70	1.46
1	A	18	GLU	CD-OE2	-44.64	0.76	1.25
1	A	39	CYS	CB-SG	-44.02	1.07	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	GLU	CD-OE1	-43.02	0.78	1.25
1	A	53	ARG	CZ-NH2	-42.66	0.77	1.33
1	A	35	PHE	CB-CG	-42.32	0.79	1.51
1	A	81	GLU	CD-OE2	-41.55	0.80	1.25
1	A	14	GLU	CB-CG	-41.24	0.73	1.52
1	A	3	GLN	CD-OE1	-39.75	0.36	1.24
1	A	81	GLU	CG-CD	-39.73	0.92	1.51
1	A	44	ASP	CB-CG	-39.45	0.68	1.51
1	A	1	MET	CG-SD	-38.38	0.81	1.81
1	A	70	TYR	CE2-CZ	-38.33	0.88	1.38
1	A	87	GLU	C-O	-38.22	0.50	1.23
1	A	70	TYR	CG-CD1	-38.19	0.89	1.39
1	A	70	TYR	CE1-CZ	-38.11	0.89	1.38
1	A	70	TYR	CG-CD2	-38.01	0.89	1.39
1	A	43	SER	CB-OG	-37.93	0.93	1.42
1	A	52	SER	CB-OG	-37.55	0.93	1.42
1	A	47	SER	CB-OG	-37.41	0.93	1.42
1	A	11	ASP	CB-CG	-37.33	0.73	1.51
1	A	53	ARG	NE-CZ	-37.32	0.84	1.33
1	A	23	GLU	CG-CD	-36.23	0.97	1.51
1	A	59	LYS	CE-NZ	-35.31	0.60	1.49
1	A	70	TYR	CB-CG	-34.78	0.99	1.51
1	A	1	MET	CA-CB	-34.40	0.78	1.53
1	A	53	ARG	CG-CD	-34.36	0.66	1.51
1	A	11	ASP	CG-OD2	-34.10	0.47	1.25
1	A	53	ARG	CD-NE	-33.90	0.88	1.46
1	A	44	ASP	CG-OD1	-33.79	0.47	1.25
1	A	14	GLU	CG-CD	-33.70	1.01	1.51
1	A	40	GLU	CD-OE2	-33.29	0.89	1.25
1	A	35	PHE	CD1-CE1	-33.17	0.72	1.39
1	A	35	PHE	CD2-CE2	-33.12	0.73	1.39
1	A	70	TYR	CD2-CE2	-32.32	0.90	1.39
1	A	70	TYR	CD1-CE1	-32.31	0.90	1.39
1	A	1	MET	N-CA	-32.23	0.81	1.46
1	A	33	SER	CB-OG	-32.16	1.00	1.42
1	A	35	PHE	CG-CD2	-31.72	0.91	1.38
1	A	35	PHE	CG-CD1	-31.42	0.91	1.38
1	A	34	GLN	CD-NE2	-31.36	0.54	1.32
1	A	84	LYS	CE-NZ	-31.27	0.70	1.49
1	A	84	LYS	CB-CG	-31.01	0.68	1.52
1	A	86	LEU	CG-CD1	-29.57	0.42	1.51
1	A	3	GLN	CD-NE2	-29.36	0.59	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	SER	CB-OG	-29.30	1.04	1.42
1	A	34	GLN	CD-OE1	-29.17	0.59	1.24
1	A	22	LYS	CE-NZ	-28.89	0.76	1.49
1	A	17	ARG	NE-CZ	-28.73	0.95	1.33
1	A	55	ASP	CB-CG	-28.40	0.92	1.51
1	A	85	ASP	CG-OD2	-28.30	0.60	1.25
1	A	85	ASP	CG-OD1	-28.07	0.60	1.25
1	A	70	TYR	CZ-OH	-27.91	0.90	1.37
1	A	73	LYS	CE-NZ	-27.88	0.79	1.49
1	A	79	GLU	CD-OE2	-27.69	0.95	1.25
1	A	28	GLU	CG-CD	-27.36	1.10	1.51
1	A	45	LYS	CE-NZ	-26.59	0.82	1.49
1	A	10	SER	C-O	-26.20	0.73	1.23
1	A	79	GLU	CD-OE1	-25.62	0.97	1.25
1	A	45	LYS	CB-CG	-24.37	0.86	1.52
1	A	35	PHE	CE1-CZ	-24.23	0.91	1.37
1	A	35	PHE	CE2-CZ	-24.15	0.91	1.37
1	A	40	GLU	CG-CD	-23.87	1.16	1.51
1	A	27	LYS	CE-NZ	-23.80	0.89	1.49
1	A	55	ASP	CG-OD2	-22.72	0.73	1.25
1	A	17	ARG	CG-CD	-22.70	0.95	1.51
1	A	1	MET	SD-CE	-22.64	0.51	1.77
1	A	84	LYS	CD-CE	-21.91	0.96	1.51
1	A	87	GLU	CB-CG	-21.77	1.10	1.52
1	A	3	GLN	CG-CD	-21.76	1.01	1.51
1	A	34	GLN	CB-CG	-21.67	0.94	1.52
1	A	1	MET	CB-CG	-21.35	0.83	1.51
1	A	71	VAL	CB-CG2	-21.07	1.08	1.52
1	A	30	ASP	CG-OD2	-20.86	0.77	1.25
1	A	11	ASP	CG-OD1	-20.73	0.77	1.25
1	A	22	LYS	CG-CD	-20.25	0.83	1.52
1	A	75	LEU	CG-CD1	-20.21	0.77	1.51
1	A	71	VAL	CB-CG1	-20.16	1.10	1.52
1	A	66	ASP	CG-OD1	-19.22	0.81	1.25
1	A	6	GLN	CD-OE1	-19.02	0.82	1.24
1	A	59	LYS	CD-CE	-18.79	1.04	1.51
1	A	17	ARG	CB-CG	-18.72	1.02	1.52
1	A	85	ASP	CB-CG	-18.43	1.13	1.51
1	A	86	LEU	CG-CD2	-18.23	0.84	1.51
1	A	18	GLU	CG-CD	-18.17	1.24	1.51
1	A	87	GLU	CA-CB	-18.08	1.14	1.53
1	A	45	LYS	CD-CE	-18.06	1.06	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	ASP	CG-OD1	-17.88	0.84	1.25
1	A	75	LEU	CG-CD2	-17.81	0.85	1.51
1	A	73	LYS	CB-CG	-17.54	1.05	1.52
1	A	22	LYS	CD-CE	-17.43	1.07	1.51
1	A	67	ASP	CG-OD2	-16.81	0.86	1.25
1	A	40	GLU	CB-CG	-16.54	1.20	1.52
1	A	73	LYS	CG-CD	-16.46	0.96	1.52
1	A	8	LYS	CE-NZ	-16.30	1.08	1.49
1	A	53	ARG	CB-CG	-16.09	1.09	1.52
1	A	66	ASP	CG-OD2	-15.77	0.89	1.25
1	A	3	GLN	CB-CG	-15.73	1.10	1.52
1	A	67	ASP	CG-OD1	-15.51	0.89	1.25
1	A	73	LYS	CD-CE	-15.23	1.13	1.51
1	A	12	ILE	CB-CG2	-15.20	1.05	1.52
1	A	44	ASP	CG-OD2	-15.01	0.90	1.25
1	A	84	LYS	CG-CD	-14.97	1.01	1.52
1	A	8	LYS	CB-CG	-14.80	1.12	1.52
1	A	27	LYS	CG-CD	-14.67	1.02	1.52
1	A	10	SER	C-N	-14.63	1.00	1.34
1	A	87	GLU	CA-C	-14.46	1.15	1.52
1	A	79	GLU	CG-CD	-14.15	1.30	1.51
1	A	14	GLU	C-O	-14.14	0.96	1.23
1	A	55	ASP	CG-OD1	-13.93	0.93	1.25
1	A	87	GLU	N-CA	-13.90	1.18	1.46
1	A	63	TYR	CE2-CZ	-13.88	1.20	1.38
1	A	63	TYR	CE1-CZ	-13.81	1.20	1.38
1	A	63	TYR	CG-CD1	-13.39	1.21	1.39
1	A	51	THR	CB-OG1	-13.37	1.16	1.43
1	A	63	TYR	CG-CD2	-13.12	1.22	1.39
1	A	2	GLY	N-CA	-13.05	1.26	1.46
1	A	25	TYR	CE2-CZ	-12.74	1.22	1.38
1	A	2	GLY	C-O	-12.62	1.03	1.23
1	A	25	TYR	CG-CD1	-12.41	1.23	1.39
1	A	62	TYR	CE1-CZ	-12.14	1.22	1.38
1	A	25	TYR	CE1-CZ	-12.10	1.22	1.38
1	A	34	GLN	CG-CD	-12.05	1.23	1.51
1	A	81	GLU	CB-CG	-11.72	1.29	1.52
1	A	67	ASP	CB-CG	-11.59	1.27	1.51
1	A	62	TYR	CG-CD2	-11.58	1.24	1.39
1	A	25	TYR	CG-CD2	-11.54	1.24	1.39
1	A	62	TYR	CE2-CZ	-11.41	1.23	1.38
1	A	12	ILE	CB-CG1	-11.35	1.22	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	LEU	CA-C	-11.33	1.23	1.52
1	A	16	ILE	C-O	-11.30	1.01	1.23
1	A	62	TYR	CG-CD1	-11.09	1.24	1.39
1	A	66	ASP	CB-CG	-11.08	1.28	1.51
1	A	42	GLN	CG-CD	-10.82	1.26	1.51
1	A	6	GLN	CD-NE2	-10.60	1.06	1.32
1	A	75	LEU	CB-CG	-10.58	1.21	1.52
1	A	6	GLN	CB-CG	-10.52	1.24	1.52
1	A	36	ASP	CG-OD1	-10.45	1.01	1.25
1	A	36	ASP	CG-OD2	-10.43	1.01	1.25
1	A	83	LEU	CG-CD2	-10.42	1.13	1.51
1	A	23	GLU	CB-CG	-10.31	1.32	1.52
1	A	86	LEU	C-O	-9.65	1.05	1.23
1	A	83	LEU	CG-CD1	-9.59	1.16	1.51
1	A	60	LYS	CE-NZ	-9.50	1.25	1.49
1	A	42	GLN	CD-OE1	-9.17	1.03	1.24
1	A	13	GLY	C-O	-9.05	1.09	1.23
1	A	54	TYR	CE1-CZ	-8.82	1.27	1.38
1	A	86	LEU	CB-CG	-8.76	1.27	1.52
1	A	45	LYS	CG-CD	-8.57	1.23	1.52
1	A	10	SER	CA-CB	-8.43	1.40	1.52
1	A	30	ASP	CB-CG	-8.43	1.34	1.51
1	A	54	TYR	CG-CD2	-8.42	1.28	1.39
1	A	60	LYS	CD-CE	-8.33	1.30	1.51
1	A	64	ASN	CG-OD1	-8.24	1.05	1.24
1	A	51	THR	CB-CG2	-8.17	1.25	1.52
1	A	77	ASP	CG-OD2	-8.16	1.06	1.25
1	A	85	ASP	CA-CB	-8.05	1.36	1.53
1	A	27	LYS	CD-CE	-8.03	1.31	1.51
1	A	86	LEU	CA-CB	-8.01	1.35	1.53
1	A	1	MET	CA-C	-7.79	1.32	1.52
1	A	60	LYS	CB-CG	-7.77	1.31	1.52
1	A	77	ASP	CG-OD1	-7.65	1.07	1.25
1	A	85	ASP	C-N	-7.55	1.16	1.34
1	A	64	ASN	CG-ND2	-7.51	1.14	1.32
1	A	2	GLY	C-N	-7.40	1.17	1.34
1	A	20	THR	CB-OG1	-7.25	1.28	1.43
1	A	1	MET	C-O	-7.20	1.09	1.23
1	A	59	LYS	CB-CG	-7.08	1.33	1.52
1	A	16	ILE	C-N	-7.07	1.17	1.34
1	A	8	LYS	CG-CD	-6.99	1.28	1.52
1	A	8	LYS	CD-CE	-6.96	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	C-N	-6.88	1.20	1.33
1	A	79	GLU	CB-CG	-6.79	1.39	1.52
1	A	15	GLY	C-O	-6.72	1.12	1.23
1	A	86	LEU	C-N	-6.58	1.19	1.34
1	A	15	GLY	N-CA	-6.55	1.36	1.46
1	A	11	ASP	CA-CB	-6.25	1.40	1.53
1	A	12	ILE	C-O	-6.04	1.11	1.23
1	A	85	ASP	C-O	-5.95	1.12	1.23
1	A	14	GLU	C-N	-5.69	1.22	1.33
1	A	2	GLY	CA-C	-5.38	1.43	1.51
1	A	6	GLN	CG-CD	-5.32	1.38	1.51
1	A	54	TYR	CE2-CZ	-5.18	1.31	1.38
1	A	14	GLU	CA-CB	-5.01	1.43	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ARG	NE-CZ-NH2	94.05	167.32	120.30
1	A	53	ARG	NE-CZ-NH2	93.16	166.88	120.30
1	A	17	ARG	NE-CZ-NH1	81.84	161.22	120.30
1	A	17	ARG	NH1-CZ-NH2	-79.95	31.45	119.40
1	A	44	ASP	CB-CG-OD1	-73.15	52.46	118.30
1	A	44	ASP	CB-CG-OD2	41.34	155.51	118.30
1	A	53	ARG	NH1-CZ-NH2	-40.02	75.38	119.40
1	A	11	ASP	CB-CG-OD2	-38.25	83.87	118.30
1	A	86	LEU	CB-CG-CD2	36.06	172.29	111.00
1	A	17	ARG	CD-NE-CZ	32.12	168.56	123.60
1	A	53	ARG	CD-NE-CZ	31.56	167.78	123.60
1	A	86	LEU	CD1-CG-CD2	-29.81	21.07	110.50
1	A	86	LEU	CB-CG-CD1	28.34	159.18	111.00
1	A	11	ASP	CB-CG-OD1	27.71	143.24	118.30
1	A	34	GLN	OE1-CD-NE2	-27.52	58.61	121.90
1	A	1	MET	CA-CB-CG	26.87	158.97	113.30
1	A	3	GLN	OE1-CD-NE2	-26.77	60.33	121.90
1	A	84	LYS	CA-CB-CG	23.88	165.93	113.40
1	A	53	ARG	CG-CD-NE	22.91	159.92	111.80
1	A	1	MET	CG-SD-CE	22.55	136.28	100.20
1	A	85	ASP	CB-CG-OD1	21.44	137.59	118.30
1	A	22	LYS	CB-CG-CD	21.34	167.09	111.60
1	A	17	ARG	CG-CD-NE	20.91	155.71	111.80
1	A	85	ASP	CB-CG-OD2	20.60	136.84	118.30
1	A	55	ASP	CB-CG-OD2	-20.32	100.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	LYS	CD-CE-NZ	20.19	158.14	111.70
1	A	84	LYS	CB-CG-CD	20.04	163.70	111.60
1	A	45	LYS	CB-CG-CD	20.00	163.60	111.60
1	A	85	ASP	OD1-CG-OD2	-19.86	85.57	123.30
1	A	87	GLU	CA-C-O	19.45	160.94	120.10
1	A	45	LYS	CA-CB-CG	19.39	156.06	113.40
1	A	18	GLU	OE1-CD-OE2	-18.25	101.39	123.30
1	A	75	LEU	CB-CG-CD2	18.18	141.90	111.00
1	A	1	MET	CB-CG-SD	17.99	166.38	112.40
1	A	28	GLU	OE1-CD-OE2	-17.88	101.84	123.30
1	A	22	LYS	CG-CD-CE	17.61	164.72	111.90
1	A	73	LYS	CB-CG-CD	17.60	157.35	111.60
1	A	84	LYS	CD-CE-NZ	17.58	152.14	111.70
1	A	40	GLU	OE1-CD-OE2	-17.32	102.52	123.30
1	A	30	ASP	CB-CG-OD1	16.63	133.27	118.30
1	A	3	GLN	CG-CD-NE2	16.36	155.96	116.70
1	A	34	GLN	CG-CD-OE1	16.22	154.03	121.60
1	A	44	ASP	CA-CB-CG	16.00	148.61	113.40
1	A	40	GLU	CG-CD-OE2	15.94	150.17	118.30
1	A	84	LYS	CG-CD-CE	15.77	159.22	111.90
1	A	39	CYS	CA-CB-SG	15.76	142.37	114.00
1	A	10	SER	O-C-N	-15.64	97.67	122.70
1	A	44	ASP	OD1-CG-OD2	15.12	152.03	123.30
1	A	73	LYS	CD-CE-NZ	15.05	146.32	111.70
1	A	23	GLU	CB-CG-CD	15.02	154.75	114.20
1	A	1	MET	N-CA-CB	-14.52	84.46	110.60
1	A	14	GLU	CA-CB-CG	14.17	144.57	113.40
1	A	75	LEU	CB-CG-CD1	13.77	134.40	111.00
1	A	75	LEU	CD1-CG-CD2	-13.72	69.33	110.50
1	A	66	ASP	CB-CG-OD2	12.99	129.99	118.30
1	A	53	ARG	CB-CG-CD	-12.95	77.94	111.60
1	A	23	GLU	OE1-CD-OE2	-12.92	107.80	123.30
1	A	17	ARG	CB-CG-CD	12.81	144.90	111.60
1	A	30	ASP	OD1-CG-OD2	-12.79	99.01	123.30
1	A	34	GLN	CG-CD-NE2	12.77	147.35	116.70
1	A	3	GLN	CB-CG-CD	12.69	144.59	111.60
1	A	27	LYS	CB-CG-CD	12.65	144.50	111.60
1	A	55	ASP	CB-CG-OD1	12.58	129.62	118.30
1	A	14	GLU	OE1-CD-OE2	-12.10	108.78	123.30
1	A	27	LYS	CG-CD-CE	12.09	148.16	111.90
1	A	70	TYR	CA-CB-CG	12.08	136.36	113.40
1	A	73	LYS	CG-CD-CE	11.84	147.42	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	LYS	CD-CE-NZ	11.82	138.90	111.70
1	A	35	PHE	CA-CB-CG	11.62	141.79	113.90
1	A	59	LYS	CD-CE-NZ	11.24	137.56	111.70
1	A	3	GLN	CG-CD-OE1	11.06	143.71	121.60
1	A	81	GLU	CB-CG-CD	10.95	143.75	114.20
1	A	23	GLU	CG-CD-OE2	10.61	139.51	118.30
1	A	30	ASP	CB-CG-OD2	10.47	127.73	118.30
1	A	35	PHE	CD1-CG-CD2	10.47	131.92	118.30
1	A	10	SER	CA-CB-OG	10.02	138.26	111.20
1	A	35	PHE	CB-CG-CD2	-9.87	113.89	120.80
1	A	45	LYS	CG-CD-CE	9.74	141.13	111.90
1	A	1	MET	CB-CA-C	9.45	129.30	110.40
1	A	35	PHE	CB-CG-CD1	-9.44	114.19	120.80
1	A	81	GLU	CG-CD-OE2	9.40	137.10	118.30
1	A	10	SER	CA-C-N	9.12	137.25	117.20
1	A	3	GLN	CA-CB-CG	9.09	133.40	113.40
1	A	14	GLU	CB-CG-CD	9.06	138.65	114.20
1	A	8	LYS	CG-CD-CE	8.93	138.68	111.90
1	A	12	ILE	CA-CB-CG1	8.91	127.94	111.00
1	A	75	LEU	CA-CB-CG	8.80	135.55	115.30
1	A	34	GLN	CA-CB-CG	8.62	132.37	113.40
1	A	63	TYR	CD1-CG-CD2	-8.53	108.52	117.90
1	A	86	LEU	CA-CB-CG	8.50	134.84	115.30
1	A	53	ARG	CA-CB-CG	8.43	131.94	113.40
1	A	67	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	66	ASP	OD1-CG-OD2	-8.33	107.47	123.30
1	A	1	MET	N-CA-C	8.22	133.19	111.00
1	A	63	TYR	CB-CG-CD2	8.13	125.88	121.00
1	A	83	LEU	CB-CG-CD1	7.79	124.24	111.00
1	A	55	ASP	CA-CB-CG	7.69	130.32	113.40
1	A	10	SER	C-N-CA	7.68	140.90	121.70
1	A	63	TYR	CB-CG-CD1	7.67	125.60	121.00
1	A	12	ILE	CG1-CB-CG2	-7.58	94.71	111.40
1	A	73	LYS	CA-CB-CG	7.54	129.98	113.40
1	A	28	GLU	CG-CD-OE2	7.53	133.36	118.30
1	A	71	VAL	CG1-CB-CG2	-7.53	98.86	110.90
1	A	14	GLU	CG-CD-OE1	7.17	132.64	118.30
1	A	11	ASP	CA-CB-CG	7.09	128.99	113.40
1	A	12	ILE	CB-CG1-CD1	7.08	133.73	113.90
1	A	81	GLU	CG-CD-OE1	-7.07	104.16	118.30
1	A	35	PHE	CE1-CZ-CE2	7.04	132.67	120.00
1	A	71	VAL	CA-CB-CG1	6.96	121.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	GLN	OE1-CD-NE2	-6.75	106.36	121.90
1	A	83	LEU	CB-CG-CD2	6.66	122.32	111.00
1	A	8	LYS	CA-CB-CG	6.57	127.85	113.40
1	A	67	ASP	OD1-CG-OD2	-6.46	111.03	123.30
1	A	6	GLN	CG-CD-NE2	6.43	132.13	116.70
1	A	77	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	17	ARG	CA-CB-CG	6.33	127.32	113.40
1	A	79	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	A	25	TYR	CB-CG-CD2	6.21	124.72	121.00
1	A	36	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	35	PHE	CG-CD2-CE2	-6.11	114.08	120.80
1	A	36	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	25	TYR	CD1-CG-CD2	-6.03	111.26	117.90
1	A	16	ILE	O-C-N	-5.97	113.15	122.70
1	A	18	GLU	CG-CD-OE1	5.91	130.11	118.30
1	A	35	PHE	CG-CD1-CE1	-5.85	114.37	120.80
1	A	63	TYR	CG-CD2-CE2	5.82	125.95	121.30
1	A	43	SER	CA-CB-OG	5.77	126.77	111.20
1	A	36	ASP	OD1-CG-OD2	-5.74	112.39	123.30
1	A	35	PHE	CD1-CE1-CZ	-5.64	113.33	120.10
1	A	83	LEU	CD1-CG-CD2	-5.62	93.63	110.50
1	A	63	TYR	CE1-CZ-CE2	-5.60	110.83	119.80
1	A	63	TYR	CG-CD1-CE1	5.59	125.77	121.30
1	A	71	VAL	CA-CB-CG2	5.51	119.17	110.90
1	A	40	GLU	CG-CD-OE1	-5.50	107.31	118.30
1	A	62	TYR	CB-CG-CD1	5.49	124.30	121.00
1	A	77	ASP	OD1-CG-OD2	-5.49	112.87	123.30
1	A	62	TYR	CD1-CG-CD2	-5.48	111.88	117.90
1	A	14	GLU	CA-C-N	5.41	127.03	116.20
1	A	35	PHE	CZ-CE2-CD2	-5.39	113.64	120.10
1	A	63	TYR	CD1-CE1-CZ	5.36	124.62	119.80
1	A	67	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	77	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	60	LYS	CB-CG-CD	5.29	125.35	111.60
1	A	87	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	87	GLU	CG-CD-OE1	-5.18	107.94	118.30
1	A	53	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	A	18	GLU	CG-CD-OE2	5.10	128.49	118.30
1	A	47	SER	CA-CB-OG	5.09	124.94	111.20
1	A	34	GLN	CB-CG-CD	5.05	124.74	111.60
1	A	11	ASP	OD1-CG-OD2	5.04	132.88	123.30
1	A	25	TYR	CB-CG-CD1	5.02	124.01	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	63	TYR	CZ-CE2-CD2	5.00	124.30	119.80

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	1	MET	CA

There are no planarity outliers.

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	690	688	681	199
All	All	690	688	681	199

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 145.

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

Atom-1	Atom-2	Clash(\AA)	Distance(\AA)
1:A:75:LEU:CB	1:A:75:LEU:CD1	1.51	1.83
1:A:34:GLN:NE2	1:A:34:GLN:CG	1.49	1.71
1:A:53:ARG:NE	1:A:53:ARG:NH2	1.49	1.60
1:A:22:LYS:CG	1:A:22:LYS:CE	1.47	1.89
1:A:87:GLU:CA	1:A:87:GLU:O	1.45	1.63
1:A:75:LEU:CB	1:A:75:LEU:CD2	1.43	1.96
1:A:22:LYS:NZ	1:A:22:LYS:CD	1.42	1.80
1:A:73:LYS:CD	1:A:73:LYS:NZ	1.39	1.84
1:A:1:MET:C	1:A:1:MET:CB	1.38	1.91
1:A:34:GLN:CD	1:A:34:GLN:CB	1.34	1.92
1:A:11:ASP:CA	1:A:11:ASP:CG	1.33	1.94
1:A:10:SER:CA	1:A:10:SER:OG	1.33	1.75
1:A:86:LEU:O	1:A:87:GLU:HG2	1.33	1.20
1:A:45:LYS:CD	1:A:45:LYS:CB	1.33	2.07
1:A:34:GLN:CG	1:A:34:GLN:OE1	1.31	1.78
1:A:86:LEU:CD2	1:A:86:LEU:CB	1.28	2.10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:18:GLU:CG	1:A:18:GLU:OE2	1.26	1.82
1:A:18:GLU:CG	1:A:18:GLU:OE1	1.25	1.84
1:A:81:GLU:CD	1:A:81:GLU:CB	1.18	2.11
1:A:39:CYS:SG	1:A:39:CYS:CB	1.17	1.07
1:A:34:GLN:CG	1:A:34:GLN:CA	1.14	2.27
1:A:75:LEU:HG	1:A:75:LEU:CD2	1.12	1.66
1:A:22:LYS:CD	1:A:22:LYS:CB	1.12	2.26
1:A:86:LEU:O	1:A:87:GLU:CG	1.08	1.97
1:A:45:LYS:CG	1:A:45:LYS:CA	1.08	2.31
1:A:1:MET:C	1:A:1:MET:N	1.06	1.97
1:A:1:MET:CB	1:A:1:MET:HA	1.04	1.58
1:A:39:CYS:CA	1:A:39:CYS:SG	1.03	2.45
1:A:12:ILE:HG22	1:A:16:ILE:HD11	1.03	1.03
1:A:81:GLU:CD	1:A:81:GLU:CG	1.01	0.92
1:A:75:LEU:HG	1:A:75:LEU:CD1	1.00	1.63
1:A:75:LEU:HD12	1:A:75:LEU:CD2	1.00	1.85
1:A:81:GLU:CD	1:A:81:GLU:HG3	1.00	1.45
1:A:81:GLU:CD	1:A:81:GLU:HG2	0.99	1.45
1:A:34:GLN:CB	1:A:34:GLN:HG3	0.98	1.52
1:A:12:ILE:CG2	1:A:16:ILE:HD11	0.98	1.88
1:A:34:GLN:CG	1:A:34:GLN:HB2	0.97	1.50
1:A:34:GLN:CG	1:A:34:GLN:HB3	0.97	1.50
1:A:34:GLN:CB	1:A:34:GLN:HG2	0.96	1.52
1:A:75:LEU:HD23	1:A:75:LEU:CD1	0.96	1.85
1:A:34:GLN:NE2	1:A:34:GLN:CB	0.96	2.27
1:A:75:LEU:HD22	1:A:75:LEU:CG	0.96	1.49
1:A:75:LEU:HD23	1:A:75:LEU:CG	0.95	1.49
1:A:86:LEU:C	1:A:87:GLU:HG2	0.95	1.72
1:A:73:LYS:HE3	1:A:73:LYS:NZ	0.95	1.35
1:A:86:LEU:C	1:A:87:GLU:CG	0.95	2.02
1:A:75:LEU:HD21	1:A:75:LEU:CG	0.95	1.49
1:A:73:LYS:HE2	1:A:73:LYS:NZ	0.94	1.35
1:A:39:CYS:HB3	1:A:39:CYS:SG	0.94	1.58
1:A:1:MET:N	1:A:1:MET:HA	0.93	1.57
1:A:39:CYS:HB2	1:A:39:CYS:SG	0.93	1.58
1:A:34:GLN:CG	1:A:34:GLN:CB	0.93	0.94
1:A:86:LEU:C	1:A:87:GLU:HG3	0.93	1.82
1:A:75:LEU:CD2	1:A:75:LEU:CD1	0.92	0.93
1:A:73:LYS:CE	1:A:73:LYS:NZ	0.91	0.79
1:A:22:LYS:NZ	1:A:22:LYS:HE2	0.90	1.30
1:A:11:ASP:CG	1:A:11:ASP:HB3	0.90	1.35
1:A:22:LYS:NZ	1:A:22:LYS:HE3	0.90	1.30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:10:SER:HB3	1:A:10:SER:OG	0.89	1.15
1:A:11:ASP:CG	1:A:11:ASP:HB2	0.89	1.35
1:A:10:SER:HB2	1:A:10:SER:OG	0.89	1.15
1:A:75:LEU:HD12	1:A:75:LEU:CG	0.89	1.42
1:A:9:LEU:HD21	1:A:19:VAL:CG1	0.88	1.98
1:A:53:ARG:HH11	1:A:53:ARG:NH2	0.87	1.55
1:A:75:LEU:HD13	1:A:75:LEU:CG	0.87	1.42
1:A:75:LEU:HB2	1:A:75:LEU:CD1	0.86	2.01
1:A:45:LYS:CB	1:A:45:LYS:CG	0.85	0.86
1:A:75:LEU:CD2	1:A:75:LEU:CG	0.85	0.86
1:A:4:VAL:HG12	1:A:79:GLU:HG3	0.85	1.45
1:A:75:LEU:HD13	1:A:75:LEU:CD2	0.85	1.39
1:A:22:LYS:NZ	1:A:22:LYS:CE	0.84	0.76
1:A:75:LEU:HD11	1:A:75:LEU:CG	0.83	1.42
1:A:45:LYS:HB3	1:A:45:LYS:CG	0.83	1.38
1:A:39:CYS:HG	1:A:39:CYS:CB	0.83	1.86
1:A:11:ASP:CB	1:A:11:ASP:CG	0.82	0.73
1:A:75:LEU:HD22	1:A:75:LEU:CD1	0.82	1.37
1:A:12:ILE:HG22	1:A:16:ILE:CD1	0.82	1.99
1:A:45:LYS:HB2	1:A:45:LYS:CG	0.81	1.38
1:A:45:LYS:HG2	1:A:45:LYS:CB	0.81	1.35
1:A:53:ARG:CZ	1:A:53:ARG:NH2	0.81	0.77
1:A:45:LYS:HG3	1:A:45:LYS:CB	0.81	1.35
1:A:22:LYS:CG	1:A:22:LYS:HD3	0.79	1.33
1:A:22:LYS:CG	1:A:22:LYS:HD2	0.79	1.33
1:A:22:LYS:CG	1:A:22:LYS:CD	0.78	0.83
1:A:22:LYS:HG3	1:A:22:LYS:CD	0.78	1.32
1:A:22:LYS:HG2	1:A:22:LYS:CD	0.77	1.32
1:A:75:LEU:CD1	1:A:75:LEU:CG	0.76	0.77
1:A:34:GLN:CD	1:A:34:GLN:OE1	0.76	0.59
1:A:75:LEU:HD13	1:A:75:LEU:HD22	0.75	1.05
1:A:75:LEU:CD2	1:A:75:LEU:HD11	0.75	0.96
1:A:20:THR:OG1	1:A:68:ILE:HD13	0.74	1.82
1:A:20:THR:OG1	1:A:68:ILE:CD1	0.74	2.36
1:A:32:VAL:HG11	1:A:38:ILE:HG12	0.74	1.59
1:A:10:SER:CB	1:A:10:SER:OG	0.73	0.44
1:A:4:VAL:HG12	1:A:79:GLU:CG	0.71	2.14
1:A:1:MET:HB3	1:A:1:MET:CA	0.71	1.31
1:A:86:LEU:HD23	1:A:86:LEU:HD11	0.70	0.73
1:A:9:LEU:HD21	1:A:19:VAL:HG12	0.70	1.62
1:A:1:MET:HB3	1:A:1:MET:CG	0.70	1.34
1:A:22:LYS:NZ	1:A:22:LYS:HD3	0.70	1.99

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:1:MET:HB2	1:A:1:MET:CG	0.70	1.34
1:A:86:LEU:CD2	1:A:86:LEU:CG	0.70	0.84
1:A:1:MET:O	1:A:1:MET:CB	0.69	2.37
1:A:1:MET:CA	1:A:1:MET:H2	0.69	1.39
1:A:53:ARG:CZ	1:A:53:ARG:HH21	0.69	1.41
1:A:34:GLN:NE2	1:A:34:GLN:OE1	0.69	0.56
1:A:22:LYS:CG	1:A:22:LYS:HE2	0.69	2.13
1:A:10:SER:HG	1:A:10:SER:CA	0.69	1.77
1:A:18:GLU:CD	1:A:18:GLU:OE2	0.68	0.76
1:A:1:MET:H3	1:A:1:MET:CA	0.68	1.39
1:A:73:LYS:CE	1:A:73:LYS:HZ3	0.67	1.37
1:A:73:LYS:HZ1	1:A:73:LYS:CE	0.67	1.37
1:A:1:MET:HB2	1:A:1:MET:CA	0.67	1.31
1:A:1:MET:N	1:A:1:MET:CA	0.66	0.81
1:A:73:LYS:CE	1:A:73:LYS:HZ2	0.66	1.37
1:A:21:VAL:HG11	1:A:24:TRP:CD1	0.66	2.26
1:A:53:ARG:NH2	1:A:53:ARG:HE	0.65	1.82
1:A:22:LYS:HZ1	1:A:22:LYS:CE	0.65	1.35
1:A:86:LEU:HD21	1:A:86:LEU:CD1	0.64	1.18
1:A:22:LYS:HZ2	1:A:22:LYS:CE	0.64	1.35
1:A:1:MET:SD	1:A:1:MET:HG2	0.63	1.31
1:A:22:LYS:HZ3	1:A:22:LYS:CE	0.63	1.35
1:A:86:LEU:HD12	1:A:86:LEU:CD2	0.63	1.17
1:A:86:LEU:HD23	1:A:86:LEU:CD1	0.63	1.31
1:A:21:VAL:HG11	1:A:24:TRP:NE1	0.63	2.09
1:A:75:LEU:CD2	1:A:75:LEU:HB3	0.63	2.15
1:A:34:GLN:CD	1:A:34:GLN:HE21	0.61	1.22
1:A:75:LEU:HD21	1:A:75:LEU:CD1	0.61	1.10
1:A:53:ARG:HH12	1:A:53:ARG:NH2	0.61	0.43
1:A:34:GLN:CD	1:A:34:GLN:HE22	0.61	1.22
1:A:1:MET:SD	1:A:1:MET:HG3	0.61	1.31
1:A:60:LYS:O	1:A:76:VAL:HG23	0.61	1.95
1:A:1:MET:SD	1:A:1:MET:HE2	0.60	1.23
1:A:1:MET:CB	1:A:1:MET:HG2	0.60	1.32
1:A:1:MET:SD	1:A:1:MET:HE1	0.60	1.23
1:A:86:LEU:HB3	1:A:87:GLU:HG3	0.60	1.73
1:A:87:GLU:O	1:A:87:GLU:C	0.59	0.50
1:A:1:MET:SD	1:A:1:MET:HE3	0.59	1.24
1:A:18:GLU:CD	1:A:18:GLU:OE1	0.59	0.78
1:A:81:GLU:CD	1:A:81:GLU:OE2	0.59	0.79
1:A:12:ILE:O	1:A:71:VAL:HG21	0.59	1.98
1:A:1:MET:CB	1:A:1:MET:HG3	0.58	1.32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:26:VAL:HG21	1:A:38:ILE:HG23	0.57	1.74
1:A:53:ARG:NH2	1:A:53:ARG:NH1	0.57	0.75
1:A:86:LEU:HD21	1:A:86:LEU:HD11	0.57	0.92
1:A:26:VAL:HG11	1:A:32:VAL:HG13	0.57	1.76
1:A:11:ASP:CG	1:A:11:ASP:OD1	0.57	0.77
1:A:86:LEU:HD13	1:A:86:LEU:HD22	0.56	0.66
1:A:86:LEU:HD22	1:A:86:LEU:CD1	0.56	1.12
1:A:34:GLN:NE2	1:A:34:GLN:CD	0.54	0.54
1:A:24:TRP:CZ3	1:A:61:LEU:HD22	0.54	2.38
1:A:76:VAL:HG13	1:A:78:ILE:HD11	0.54	1.80
1:A:19:VAL:C	1:A:68:ILE:HG23	0.53	2.24
1:A:9:LEU:C	1:A:9:LEU:HD13	0.53	2.23
1:A:84:LYS:HA	1:A:87:GLU:O	0.53	2.04
1:A:42:GLN:HG2	1:A:47:SER:HB3	0.53	1.81
1:A:58:ILE:HG12	1:A:78:ILE:HG23	0.52	1.80
1:A:86:LEU:HB3	1:A:87:GLU:CG	0.51	2.34
1:A:34:GLN:NE2	1:A:34:GLN:HB2	0.51	2.19
1:A:1:MET:O	1:A:1:MET:HB3	0.51	2.02
1:A:24:TRP:CH2	1:A:61:LEU:HD22	0.51	2.40
1:A:26:VAL:HG11	1:A:32:VAL:CG1	0.51	2.35
1:A:1:MET:N	1:A:2:GLY:N	0.50	2.56
1:A:1:MET:HB2	1:A:1:MET:HG3	0.49	1.16
1:A:26:VAL:HB	1:A:58:ILE:HD12	0.49	1.84
1:A:28:GLU:HG2	1:A:61:LEU:H	0.48	1.68
1:A:24:TRP:CH2	1:A:39:CYS:HB3	0.48	2.43
1:A:7:PHE:CZ	1:A:50:ILE:HG13	0.47	2.44
1:A:86:LEU:CD2	1:A:86:LEU:HD13	0.46	1.00
1:A:86:LEU:CD2	1:A:86:LEU:CD1	0.46	0.47
1:A:5:VAL:N	1:A:78:ILE:O	0.46	2.47
1:A:20:THR:HG23	1:A:67:ASP:O	0.45	2.11
1:A:86:LEU:HD12	1:A:86:LEU:HD21	0.45	1.09
1:A:73:LYS:HD2	1:A:73:LYS:NZ	0.45	2.08
1:A:56:GLY:CA	1:A:79:GLU:O	0.45	2.64
1:A:9:LEU:HB2	1:A:69:ALA:HB1	0.45	1.87
1:A:53:ARG:HH22	1:A:53:ARG:HH12	0.45	0.46
1:A:86:LEU:CD2	1:A:86:LEU:HD11	0.45	0.64
1:A:1:MET:C	1:A:1:MET:HB3	0.45	1.89
1:A:31:THR:HG23	1:A:56:GLY:O	0.44	2.12
1:A:18:GLU:HB3	1:A:68:ILE:HG22	0.44	1.90
1:A:29:GLY:N	1:A:58:ILE:O	0.43	2.51
1:A:31:THR:CG2	1:A:56:GLY:O	0.43	2.66
1:A:58:ILE:HG12	1:A:78:ILE:CG2	0.43	2.44

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:9:LEU:HD23	1:A:69:ALA:HB3	0.42	1.91
1:A:58:ILE:CG1	1:A:78:ILE:HG23	0.42	2.45
1:A:1:MET:SD	1:A:1:MET:CE	0.42	0.51
1:A:27:LYS:O	1:A:30:ASP:HB2	0.42	2.15
1:A:52:SER:O	1:A:53:ARG:CG	0.42	2.67
1:A:1:MET:SD	1:A:1:MET:CG	0.42	0.81
1:A:26:VAL:CG1	1:A:32:VAL:HG13	0.42	2.44
1:A:12:ILE:HG21	1:A:17:ARG:O	0.41	2.15
1:A:77:ASP:OD1	1:A:77:ASP:N	0.41	2.52
1:A:5:VAL:CG2	1:A:80:THR:OG1	0.41	2.69
1:A:9:LEU:C	1:A:9:LEU:CD1	0.41	2.90
1:A:21:VAL:CG1	1:A:24:TRP:CD1	0.41	3.02
1:A:20:THR:CB	1:A:68:ILE:HD13	0.40	2.46
1:A:60:LYS:N	1:A:60:LYS:HD2	0.40	2.31
1:A:83:LEU:O	1:A:87:GLU:C	0.40	2.59

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	85/93 (91%)	79 (93%)	4 (5%)	2 (2%)	12	49
All	All	85/93 (91%)	79 (93%)	4 (5%)	2 (2%)	12	49

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	15	GLY
1	A	11	ASP

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	78/84 (93%)	44 (56%)	34 (44%)	0	3
All	All	78/84 (93%)	44 (56%)	34 (44%)	0	3

All 34 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	1	MET
1	A	51	THR
1	A	84	LYS
1	A	34	GLN
1	A	47	SER
1	A	86	LEU
1	A	78	ILE
1	A	35	PHE
1	A	37	SER
1	A	36	ASP
1	A	87	GLU
1	A	80	THR
1	A	54	TYR
1	A	45	LYS
1	A	55	ASP
1	A	8	LYS
1	A	44	ASP
1	A	52	SER
1	A	73	LYS
1	A	22	LYS
1	A	65	LEU
1	A	32	VAL
1	A	27	LYS
1	A	17	ARG
1	A	60	LYS
1	A	12	ILE
1	A	6	GLN
1	A	75	LEU
1	A	66	ASP
1	A	83	LEU
1	A	85	ASP
1	A	77	ASP
1	A	20	THR
1	A	70	TYR

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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided