



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:34 AM UTC

PDB ID : 2HX6 / pdb_00002hx6
Title : Solution structure analysis of the phage T4 endoribonuclease RegB
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Deposited on : 2006-08-02

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

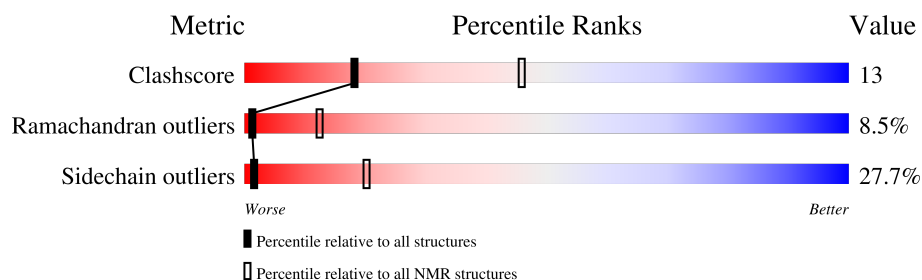
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	153	

2 Ensemble composition and analysis

This entry contains 15 models. Model 8 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:81, A:102-A:141, A:150-A:153 (122)	1.42	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 5, 6, 7, 8, 10, 11, 12
2	2, 4, 13, 14, 15
Single-model clusters	9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2528 atoms, of which 1266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribonuclease.

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2528	798	1266	228	231	5	

There is a discrepancy between the modelled and reference sequences:

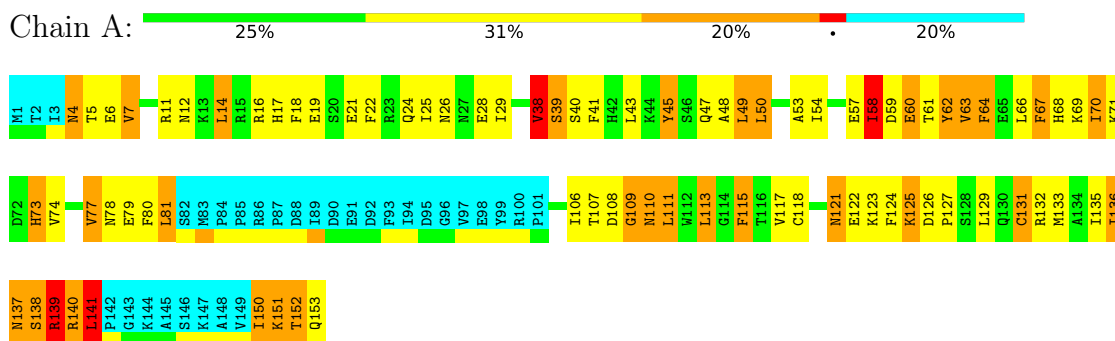
Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ALA	HIS	engineered mutation	UNP P13312

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: Ribonuclease

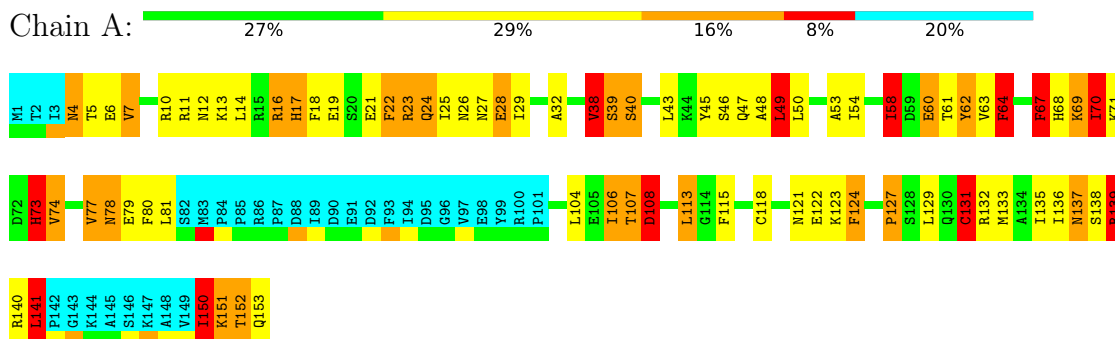


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

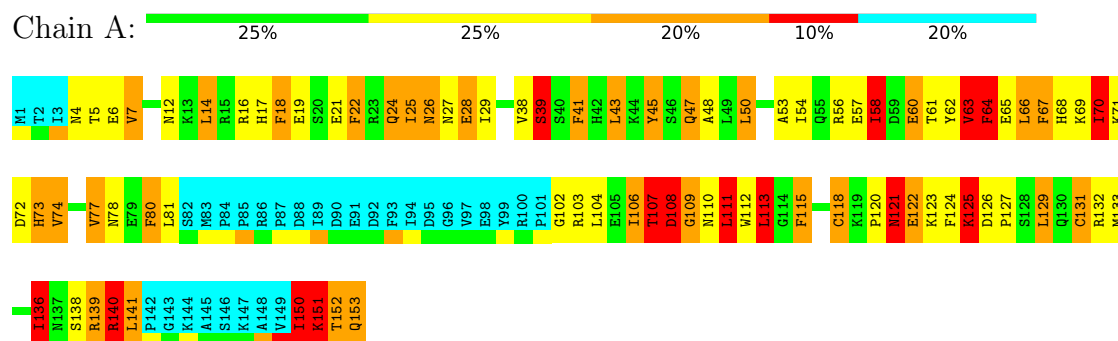
4.2.1 Score per residue for model 1

- Molecule 1: Ribonuclease



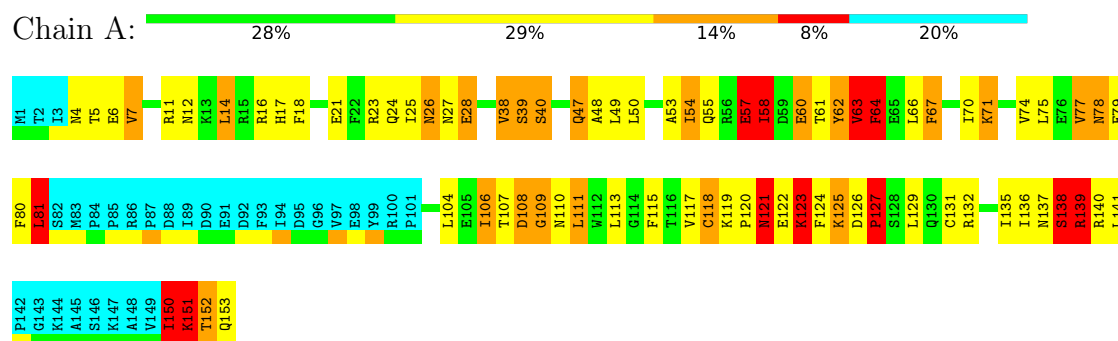
4.2.2 Score per residue for model 2

- Molecule 1: Ribonuclease



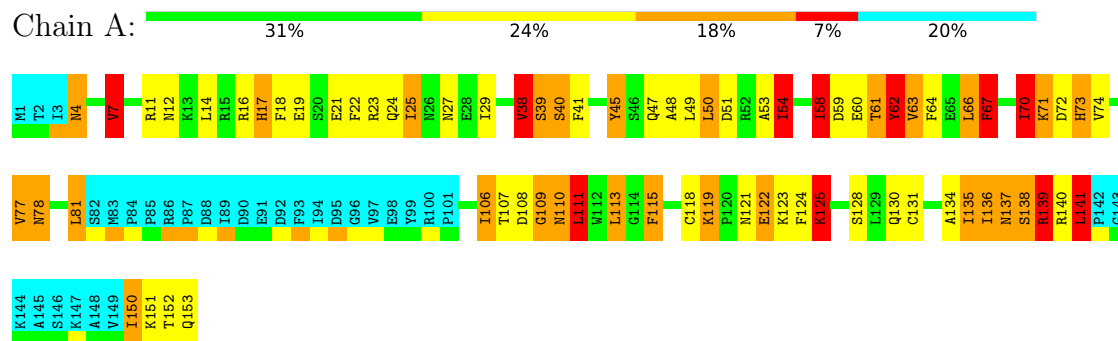
4.2.3 Score per residue for model 3

- Molecule 1: Ribonuclease



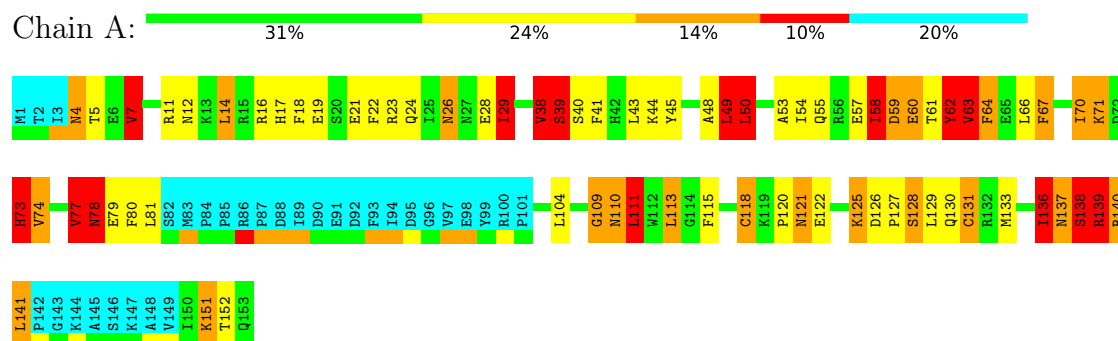
4.2.4 Score per residue for model 4

- Molecule 1: Ribonuclease



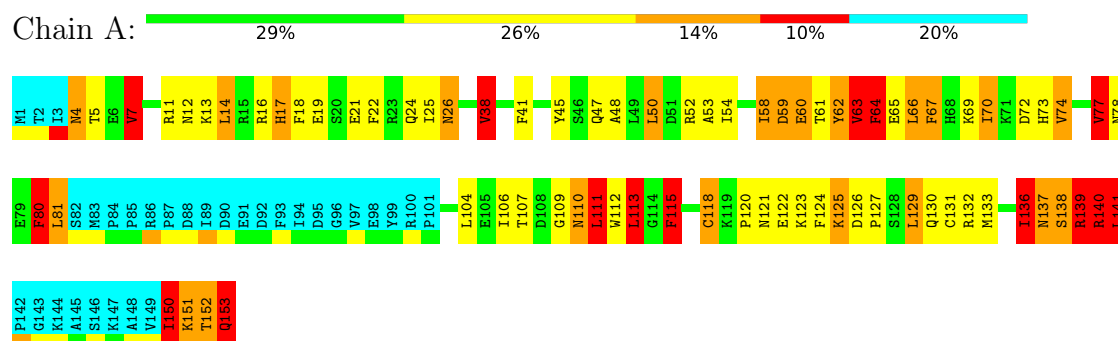
4.2.11 Score per residue for model 11

- Molecule 1: Ribonuclease



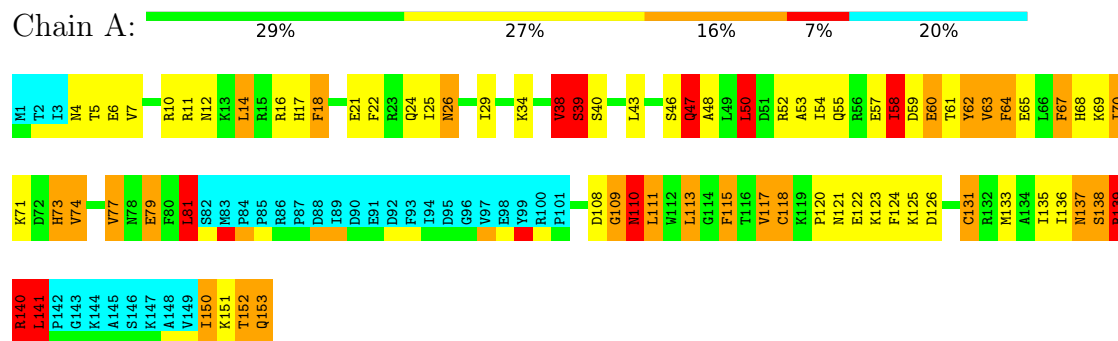
4.2.12 Score per residue for model 12

- Molecule 1: Ribonuclease



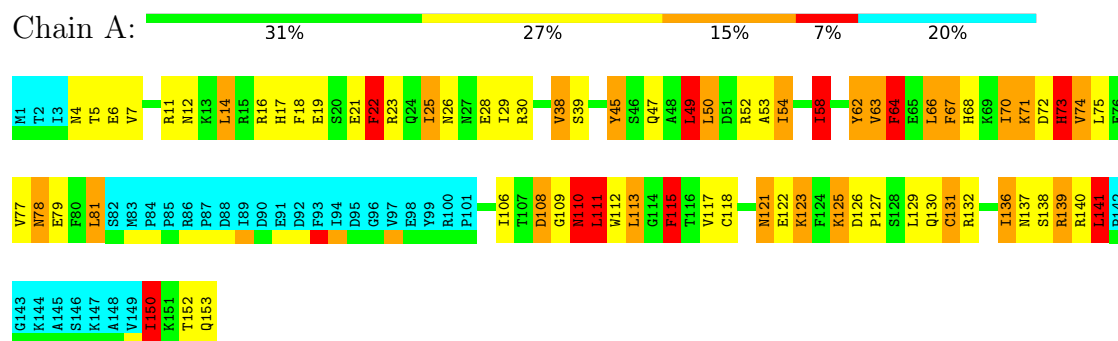
4.2.13 Score per residue for model 13

- Molecule 1: Ribonuclease



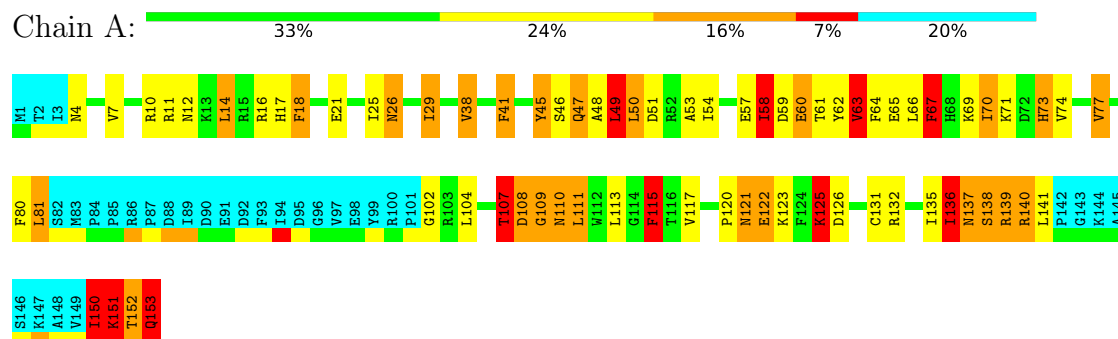
4.2.14 Score per residue for model 14

- Molecule 1: Ribonuclease



4.2.15 Score per residue for model 15

- Molecule 1: Ribonuclease



5 Refinement protocol and experimental data overview

The models were refined using the following method: *mix of manual and automatic NOE assignment procedure*.

Of the 30 calculated structures, 15 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with favorable non-bond energy, structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
INCA	structure solution	1.0
INCA	refinement	1.0

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.54±0.03	2±2/1041 (0.2± 0.1%)	2.63±0.06	97±8/1395 (6.9± 0.6%)
All	All	1.54	30/15615 (0.2%)	2.63	1449/20925 (6.9%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	4.3±1.7
All	All	0	64

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	109	GLY	CA-C	-7.68	1.42	1.52	4	2
1	A	73	HIS	C-N	7.09	1.43	1.33	1	2
1	A	113	LEU	CA-CB	7.08	1.63	1.53	14	3
1	A	17	HIS	CA-CB	6.82	1.64	1.53	10	5
1	A	107	THR	C-N	6.75	1.39	1.33	3	1
1	A	49	LEU	CA-C	-6.18	1.44	1.52	11	1
1	A	57	GLU	C-N	5.68	1.41	1.33	3	1
1	A	108	ASP	CA-C	-5.63	1.45	1.52	2	1
1	A	69	LYS	N-CA	5.49	1.53	1.46	15	1
1	A	126	ASP	CA-C	5.40	1.59	1.52	5	1
1	A	152	THR	CA-C	-5.37	1.46	1.53	7	1
1	A	59	ASP	CA-C	-5.37	1.47	1.52	13	1
1	A	151	LYS	CA-C	-5.37	1.46	1.52	3	1
1	A	60	GLU	CA-C	-5.33	1.47	1.53	2	1
1	A	81	LEU	N-CA	5.30	1.52	1.46	4	1
1	A	60	GLU	CA-CB	5.20	1.59	1.52	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	58	ILE	N-CA	5.19	1.52	1.46	3	1
1	A	74	VAL	CA-C	-5.13	1.46	1.52	14	1
1	A	27	ASN	C-N	5.11	1.41	1.34	3	3
1	A	108	ASP	CA-CB	5.04	1.61	1.53	3	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	150	ILE	CA-C-N	17.66	153.11	120.97	1	9
1	A	150	ILE	C-N-CA	17.66	153.11	120.97	1	9
1	A	110	ASN	CA-CB-CG	17.09	129.69	112.60	14	3
1	A	152	THR	CA-C-N	14.81	148.36	121.70	5	9
1	A	152	THR	C-N-CA	14.81	148.36	121.70	5	9
1	A	78	ASN	CA-CB-CG	14.53	127.13	112.60	14	6
1	A	152	THR	N-CA-C	12.95	129.65	110.48	10	10
1	A	73	HIS	CA-CB-CG	12.66	126.46	113.80	11	2
1	A	141	LEU	N-CA-C	12.26	127.92	110.40	12	5
1	A	139	ARG	CA-C-N	12.20	144.85	121.54	15	7
1	A	139	ARG	C-N-CA	12.20	144.85	121.54	15	7
1	A	60	GLU	CA-C-N	12.19	141.40	120.68	1	3
1	A	60	GLU	C-N-CA	12.19	141.40	120.68	1	3
1	A	111	LEU	N-CA-CB	11.99	128.17	110.06	8	8
1	A	73	HIS	CA-C-N	11.83	135.86	120.60	14	3
1	A	73	HIS	C-N-CA	11.83	135.86	120.60	14	3
1	A	140	ARG	CA-C-N	11.77	150.52	121.80	13	3
1	A	140	ARG	C-N-CA	11.77	150.52	121.80	13	3
1	A	71	LYS	N-CA-C	10.82	124.16	111.71	13	4
1	A	110	ASN	CA-C-N	10.82	138.10	122.09	4	11
1	A	110	ASN	C-N-CA	10.82	138.10	122.09	4	11
1	A	71	LYS	CA-C-N	10.82	139.08	120.58	4	4
1	A	71	LYS	C-N-CA	10.82	139.08	120.58	4	4
1	A	63	VAL	CA-C-N	10.72	134.38	120.44	11	14
1	A	63	VAL	C-N-CA	10.72	134.38	120.44	11	14
1	A	138	SER	N-CA-CB	10.70	128.18	110.42	15	4
1	A	29	ILE	CA-CB-CG1	10.68	128.55	110.40	11	3
1	A	115	PHE	CA-CB-CG	10.67	124.47	113.80	13	10
1	A	80	PHE	CA-CB-CG	10.61	124.41	113.80	12	11
1	A	137	ASN	CA-CB-CG	10.62	123.22	112.60	5	4
1	A	150	ILE	N-CA-C	10.51	125.99	108.86	9	4
1	A	53	ALA	CA-C-N	10.42	133.69	120.56	10	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	ALA	C-N-CA	10.42	133.69	120.56	10	15
1	A	50	LEU	CD1-CG-CD2	10.33	133.53	110.80	13	1
1	A	67	PHE	CA-CB-CG	10.26	124.06	113.80	9	14
1	A	126	ASP	CA-C-N	10.25	132.65	119.84	8	5
1	A	126	ASP	C-N-CA	10.25	132.65	119.84	8	5
1	A	48	ALA	CA-C-N	9.95	134.41	120.29	15	13
1	A	48	ALA	C-N-CA	9.95	134.41	120.29	15	13
1	A	4	ASN	CA-C-N	9.92	133.34	120.44	13	15
1	A	4	ASN	C-N-CA	9.92	133.34	120.44	13	15
1	A	73	HIS	CB-CG-CD2	-9.92	118.31	131.20	11	2
1	A	125	LYS	CB-CA-C	9.82	129.95	110.42	5	1
1	A	77	VAL	CB-CA-C	9.73	128.02	112.26	8	7
1	A	141	LEU	N-CA-CB	9.70	127.97	109.44	5	3
1	A	109	GLY	CA-C-N	9.61	139.90	121.54	9	12
1	A	109	GLY	C-N-CA	9.61	139.90	121.54	9	12
1	A	17	HIS	CA-C-N	9.57	132.88	120.44	9	15
1	A	17	HIS	C-N-CA	9.57	132.88	120.44	9	15
1	A	124	PHE	N-CA-C	9.52	121.21	108.07	4	4
1	A	124	PHE	CA-C-N	9.52	139.72	121.54	4	5
1	A	124	PHE	C-N-CA	9.52	139.72	121.54	4	5
1	A	122	GLU	CA-C-N	9.48	139.65	121.54	4	10
1	A	122	GLU	C-N-CA	9.48	139.65	121.54	4	10
1	A	61	THR	CA-C-N	9.46	133.90	120.28	7	13
1	A	61	THR	C-N-CA	9.46	133.90	120.28	7	13
1	A	151	LYS	N-CA-C	9.43	126.64	107.69	7	7
1	A	27	ASN	CA-CB-CG	9.36	121.96	112.60	8	3
1	A	60	GLU	CB-CA-C	9.36	127.06	112.00	9	8
1	A	72	ASP	CA-C-N	9.35	139.39	121.54	14	5
1	A	72	ASP	C-N-CA	9.35	139.39	121.54	14	5
1	A	152	THR	CA-C-O	9.34	131.76	121.02	5	7
1	A	28	GLU	N-CA-CB	9.26	124.64	110.28	3	4
1	A	74	VAL	CA-C-N	9.15	132.55	120.28	3	9
1	A	74	VAL	C-N-CA	9.15	132.55	120.28	3	9
1	A	121	ASN	CA-CB-CG	9.10	121.70	112.60	5	3
1	A	127	PRO	CB-CA-C	9.06	126.50	111.56	3	2
1	A	152	THR	N-CA-CB	-8.94	97.77	110.46	2	4
1	A	16	ARG	CA-C-N	8.84	131.93	120.44	12	14
1	A	16	ARG	C-N-CA	8.84	131.93	120.44	12	14
1	A	45	TYR	CB-CG-CD1	8.79	133.99	120.80	7	2
1	A	59	ASP	CB-CA-C	8.74	125.32	111.51	10	1
1	A	151	LYS	CB-CA-C	8.74	125.36	109.37	10	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	81	LEU	CA-C-N	8.74	132.69	120.29	13	1
1	A	81	LEU	C-N-CA	8.74	132.69	120.29	13	1
1	A	117	VAL	N-CA-CB	8.66	120.17	110.72	10	2
1	A	121	ASN	N-CA-C	8.65	129.22	110.80	2	7
1	A	136	ILE	CA-C-N	8.61	137.99	121.54	11	7
1	A	136	ILE	C-N-CA	8.61	137.99	121.54	11	7
1	A	7	VAL	CA-C-N	8.61	132.15	120.44	14	13
1	A	7	VAL	C-N-CA	8.61	132.15	120.44	14	13
1	A	38	VAL	CA-C-N	8.60	137.97	121.54	10	12
1	A	38	VAL	C-N-CA	8.60	137.97	121.54	10	12
1	A	126	ASP	CA-C-O	-8.52	112.80	121.06	6	4
1	A	121	ASN	CA-C-N	8.51	137.80	121.54	6	2
1	A	121	ASN	C-N-CA	8.51	137.80	121.54	6	2
1	A	69	LYS	N-CA-CB	8.48	123.37	110.30	5	3
1	A	62	TYR	CA-C-N	8.45	131.37	120.56	7	13
1	A	62	TYR	C-N-CA	8.45	131.37	120.56	7	13
1	A	58	ILE	N-CA-C	8.31	126.62	109.34	2	4
1	A	26	ASN	CA-CB-CG	8.27	120.87	112.60	3	7
1	A	70	ILE	CA-C-N	8.20	137.19	121.54	14	11
1	A	70	ILE	C-N-CA	8.20	137.19	121.54	14	11
1	A	136	ILE	N-CA-C	8.17	118.79	108.82	12	3
1	A	57	GLU	CA-C-N	8.17	136.68	121.97	2	7
1	A	57	GLU	C-N-CA	8.17	136.68	121.97	2	7
1	A	45	TYR	CB-CG-CD2	-8.12	108.61	120.80	7	3
1	A	120	PRO	CA-C-N	8.12	137.05	121.54	2	5
1	A	120	PRO	C-N-CA	8.12	137.05	121.54	2	5
1	A	26	ASN	CB-CA-C	8.11	127.27	110.31	2	3
1	A	139	ARG	CB-CG-CD	8.10	129.93	111.30	5	7
1	A	77	VAL	CA-C-N	8.08	132.59	120.31	3	11
1	A	77	VAL	C-N-CA	8.08	132.59	120.31	3	11
1	A	139	ARG	N-CA-CB	8.03	124.07	110.49	12	3
1	A	107	THR	CA-CB-CG2	8.03	124.15	110.50	2	3
1	A	125	LYS	N-CA-CB	7.97	123.95	110.49	4	3
1	A	47	GLN	N-CA-C	7.94	122.54	113.01	3	4
1	A	132	ARG	CA-C-N	7.92	133.00	122.30	3	3
1	A	132	ARG	C-N-CA	7.92	133.00	122.30	3	3
1	A	13	LYS	CA-C-O	7.92	129.08	119.97	7	1
1	A	19	GLU	N-CA-C	7.90	119.97	111.36	7	10
1	A	18	PHE	CB-CA-C	-7.89	98.81	110.96	13	1
1	A	58	ILE	CB-CA-C	7.83	124.14	111.29	11	6
1	A	123	LYS	CA-C-N	7.81	132.54	120.75	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	123	LYS	C-N-CA	7.81	132.54	120.75	13	4
1	A	6	GLU	CA-C-N	7.79	131.49	120.42	5	8
1	A	6	GLU	C-N-CA	7.79	131.49	120.42	5	8
1	A	45	TYR	CA-CB-CG	7.75	127.84	113.90	7	2
1	A	67	PHE	N-CA-CB	7.74	122.21	110.30	14	12
1	A	53	ALA	N-CA-C	7.73	120.60	111.71	9	5
1	A	64	PHE	CA-CB-CG	-7.72	106.08	113.80	2	8
1	A	111	LEU	N-CA-C	7.70	122.36	110.20	11	7
1	A	151	LYS	CA-CB-CG	7.68	129.46	114.10	2	2
1	A	138	SER	CA-C-N	7.63	136.12	121.54	3	5
1	A	138	SER	C-N-CA	7.63	136.12	121.54	3	5
1	A	118	CYS	CA-C-N	7.62	133.59	121.62	13	5
1	A	118	CYS	C-N-CA	7.62	133.59	121.62	13	5
1	A	43	LEU	CB-CA-C	7.61	123.64	109.71	2	2
1	A	125	LYS	CA-C-N	7.59	140.32	121.80	15	2
1	A	125	LYS	C-N-CA	7.59	140.32	121.80	15	2
1	A	152	THR	CB-CA-C	7.55	123.92	111.23	7	4
1	A	141	LEU	CA-C-N	7.51	127.05	119.24	8	7
1	A	141	LEU	C-N-CA	7.51	127.05	119.24	8	7
1	A	106	ILE	CB-CA-C	7.50	121.28	110.33	7	2
1	A	12	ASN	CA-C-N	7.50	131.07	120.28	5	12
1	A	12	ASN	C-N-CA	7.50	131.07	120.28	5	12
1	A	129	LEU	N-CA-C	-7.45	97.11	109.24	7	7
1	A	9	ILE	CA-C-N	7.43	130.58	120.54	5	1
1	A	9	ILE	C-N-CA	7.43	130.58	120.54	5	1
1	A	49	LEU	CB-CA-C	-7.43	98.22	110.85	11	1
1	A	151	LYS	O-C-N	-7.36	114.17	122.86	12	3
1	A	50	LEU	CA-C-N	7.34	130.86	120.28	8	8
1	A	50	LEU	C-N-CA	7.34	130.86	120.28	8	8
1	A	130	GLN	N-CA-CB	7.32	118.54	110.35	8	2
1	A	24	GLN	N-CA-C	7.26	118.84	111.07	13	10
1	A	153	GLN	CB-CA-C	7.26	123.90	110.10	15	2
1	A	137	ASN	CB-CA-C	7.24	122.81	109.70	1	1
1	A	17	HIS	CA-CB-CG	-7.23	106.57	113.80	7	2
1	A	151	LYS	N-CA-CB	-7.22	98.77	110.69	7	4
1	A	63	VAL	CB-CA-C	7.18	121.43	112.02	7	3
1	A	109	GLY	O-C-N	7.13	130.08	122.52	4	1
1	A	48	ALA	N-CA-C	7.11	119.93	111.33	8	5
1	A	139	ARG	N-CA-C	-7.08	95.72	110.80	4	2
1	A	49	LEU	CA-C-O	7.02	128.03	120.10	9	6
1	A	131	CYS	N-CA-CB	7.01	122.34	110.49	11	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	150	ILE	O-C-N	-7.00	115.92	122.71	3	2
1	A	39	SER	N-CA-C	7.00	125.72	110.80	9	3
1	A	54	ILE	CA-CB-CG1	7.00	122.30	110.40	15	3
1	A	136	ILE	CB-CA-C	-6.98	100.72	110.91	10	1
1	A	69	LYS	CA-C-N	6.96	132.26	121.19	13	6
1	A	69	LYS	C-N-CA	6.96	132.26	121.19	13	6
1	A	58	ILE	CA-C-N	6.94	134.80	121.54	7	10
1	A	58	ILE	C-N-CA	6.94	134.80	121.54	7	10
1	A	65	GLU	CA-C-N	6.89	129.40	120.44	12	3
1	A	65	GLU	C-N-CA	6.89	129.40	120.44	12	3
1	A	23	ARG	N-CA-CB	6.88	120.35	110.16	1	5
1	A	67	PHE	CA-C-N	6.88	130.07	120.29	11	2
1	A	67	PHE	C-N-CA	6.88	130.07	120.29	11	2
1	A	122	GLU	N-CA-C	-6.87	95.53	107.49	13	4
1	A	18	PHE	CA-CB-CG	-6.84	106.96	113.80	15	1
1	A	50	LEU	CB-CA-C	6.79	123.14	110.70	4	6
1	A	77	VAL	CA-C-O	6.79	127.81	120.47	3	4
1	A	25	ILE	CB-CA-C	-6.76	103.16	112.02	9	1
1	A	126	ASP	O-C-N	-6.75	116.50	121.23	6	3
1	A	11	ARG	N-CA-C	6.71	118.60	111.28	5	12
1	A	58	ILE	CA-CB-CG1	6.71	121.81	110.40	11	2
1	A	126	ASP	CA-CB-CG	6.70	119.30	112.60	2	1
1	A	108	ASP	CA-C-N	6.67	134.49	121.41	3	1
1	A	108	ASP	C-N-CA	6.67	134.49	121.41	3	1
1	A	58	ILE	N-CA-CB	6.64	122.19	111.23	3	2
1	A	79	GLU	CA-C-N	6.61	129.14	120.28	13	5
1	A	79	GLU	C-N-CA	6.61	129.14	120.28	13	5
1	A	103	ARG	N-CA-C	-6.61	98.20	109.24	2	2
1	A	49	LEU	CA-C-N	6.61	129.67	120.29	10	7
1	A	49	LEU	C-N-CA	6.61	129.67	120.29	10	7
1	A	59	ASP	CA-CB-CG	6.56	119.16	112.60	4	3
1	A	136	ILE	CA-CB-CG1	6.55	121.54	110.40	12	3
1	A	113	LEU	N-CA-CB	6.55	120.84	110.55	12	7
1	A	150	ILE	CB-CG1-CD1	6.53	127.52	113.80	9	1
1	A	150	ILE	CA-CB-CG1	6.52	121.49	110.40	8	3
1	A	108	ASP	CA-CB-CG	6.52	119.12	112.60	3	1
1	A	150	ILE	N-CA-CB	6.50	118.79	110.99	4	3
1	A	17	HIS	N-CA-CB	6.49	119.66	110.12	10	3
1	A	22	PHE	CA-CB-CG	-6.48	107.32	113.80	8	6
1	A	46	SER	CA-C-N	6.48	134.00	121.18	13	3
1	A	46	SER	C-N-CA	6.48	134.00	121.18	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	151	LYS	CA-C-N	6.47	132.90	123.13	7	2
1	A	151	LYS	C-N-CA	6.47	132.90	123.13	7	2
1	A	70	ILE	CB-CA-C	-6.46	103.61	111.88	7	2
1	A	45	TYR	N-CA-CB	6.45	121.08	110.69	9	1
1	A	78	ASN	CB-CA-C	6.45	123.06	110.67	3	2
1	A	62	TYR	CB-CG-CD1	6.45	130.47	120.80	4	1
1	A	22	PHE	N-CA-CB	6.43	120.25	110.28	1	2
1	A	74	VAL	CB-CA-C	-6.42	100.75	111.29	2	2
1	A	139	ARG	CA-CB-CG	6.42	126.94	114.10	11	7
1	A	21	GLU	CB-CA-C	6.42	123.47	110.38	7	1
1	A	59	ASP	CA-C-N	6.42	133.80	121.54	12	2
1	A	59	ASP	C-N-CA	6.42	133.80	121.54	12	2
1	A	70	ILE	N-CA-CB	6.40	120.18	110.58	2	2
1	A	137	ASN	N-CA-C	-6.36	98.25	109.06	6	4
1	A	152	THR	CA-CB-OG1	6.35	119.12	109.60	8	4
1	A	111	LEU	CB-CA-C	-6.32	99.10	109.53	4	2
1	A	80	PHE	N-CA-CB	6.32	119.17	110.01	3	2
1	A	140	ARG	N-CA-CB	6.32	121.16	110.49	15	2
1	A	113	LEU	CB-CA-C	-6.30	99.14	109.53	6	4
1	A	108	ASP	N-CA-CB	6.29	121.13	110.49	15	4
1	A	140	ARG	N-CA-C	6.28	124.17	110.80	13	3
1	A	39	SER	CA-C-N	6.26	133.49	121.54	8	8
1	A	39	SER	C-N-CA	6.26	133.49	121.54	8	8
1	A	111	LEU	CD1-CG-CD2	-6.21	97.14	110.80	2	2
1	A	123	LYS	N-CA-C	6.21	119.96	111.39	12	1
1	A	18	PHE	N-CA-CB	6.19	118.99	110.01	5	2
1	A	116	THR	N-CA-C	-6.18	99.83	109.72	6	2
1	A	118	CYS	N-CA-CB	6.16	120.91	110.49	1	3
1	A	80	PHE	CA-C-N	6.16	128.81	120.44	15	2
1	A	80	PHE	C-N-CA	6.16	128.81	120.44	15	2
1	A	62	TYR	CB-CG-CD2	-6.12	111.62	120.80	4	1
1	A	132	ARG	N-CA-C	-6.10	97.20	107.99	12	4
1	A	108	ASP	N-CA-C	-6.07	100.09	109.14	14	3
1	A	61	THR	CA-C-O	6.00	126.79	119.11	11	4
1	A	63	VAL	CA-CB-CG1	5.99	120.58	110.40	15	11
1	A	52	ARG	N-CA-C	5.99	117.68	111.03	9	3
1	A	152	THR	O-C-N	5.98	130.61	122.48	5	1
1	A	124	PHE	N-CA-CB	-5.97	101.80	111.24	9	1
1	A	139	ARG	CA-C-O	-5.94	112.02	120.51	13	1
1	A	152	THR	CA-CB-CG2	-5.94	100.41	110.50	3	1
1	A	12	ASN	CB-CA-C	-5.93	100.83	110.79	8	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	127	PRO	N-CA-C	5.92	124.67	112.47	2	3
1	A	10	ARG	CA-C-N	5.91	128.79	120.28	13	3
1	A	10	ARG	C-N-CA	5.91	128.79	120.28	13	3
1	A	49	LEU	CD1-CG-CD2	5.90	123.79	110.80	11	2
1	A	81	LEU	N-CA-CB	5.88	118.60	110.07	13	1
1	A	78	ASN	CA-C-N	5.88	129.25	120.31	3	1
1	A	78	ASN	C-N-CA	5.88	129.25	120.31	3	1
1	A	76	GLU	CA-C-N	5.87	129.93	120.30	6	1
1	A	76	GLU	C-N-CA	5.87	129.93	120.30	6	1
1	A	61	THR	CB-CA-C	5.87	121.63	109.95	7	3
1	A	41	PHE	N-CA-CB	5.86	120.13	110.69	11	1
1	A	107	THR	N-CA-CB	5.86	122.42	111.53	1	1
1	A	14	LEU	N-CA-CB	5.84	118.55	110.07	2	1
1	A	128	SER	N-CA-C	-5.84	100.19	109.59	4	2
1	A	60	GLU	N-CA-CB	5.83	119.69	110.49	15	3
1	A	67	PHE	CB-CA-C	5.83	122.17	109.99	5	2
1	A	12	ASN	CA-CB-CG	5.83	118.42	112.60	6	2
1	A	124	PHE	CB-CA-C	-5.83	99.75	111.17	12	2
1	A	68	HIS	CB-CA-C	5.82	121.37	109.55	7	1
1	A	29	ILE	N-CA-C	5.82	116.56	110.62	15	1
1	A	53	ALA	CB-CA-C	-5.80	101.73	110.90	3	1
1	A	79	GLU	N-CA-CB	5.79	119.26	110.28	10	3
1	A	68	HIS	CA-CB-CG	-5.79	108.01	113.80	7	1
1	A	11	ARG	CA-C-N	5.79	130.38	120.71	13	5
1	A	11	ARG	C-N-CA	5.79	130.38	120.71	13	5
1	A	40	SER	N-CA-CB	5.79	120.27	110.49	4	3
1	A	44	LYS	N-CA-C	-5.78	99.23	109.06	11	2
1	A	70	ILE	CA-CB-CG2	5.76	120.28	110.50	2	2
1	A	129	LEU	N-CA-CB	5.74	119.59	110.57	10	2
1	A	70	ILE	CA-CB-CG1	-5.74	100.64	110.40	9	1
1	A	29	ILE	N-CA-CB	5.74	118.34	110.54	11	1
1	A	116	THR	CA-C-N	5.73	128.87	120.91	7	1
1	A	116	THR	C-N-CA	5.73	128.87	120.91	7	1
1	A	62	TYR	CA-C-O	5.72	126.57	120.10	7	1
1	A	41	PHE	CA-CB-CG	5.72	119.52	113.80	15	1
1	A	123	LYS	CB-CA-C	5.72	120.81	111.26	2	1
1	A	106	ILE	O-C-N	-5.71	117.09	123.26	1	1
1	A	127	PRO	N-CA-CB	-5.71	97.25	103.25	1	2
1	A	52	ARG	CB-CA-C	-5.71	101.88	110.90	5	1
1	A	16	ARG	CB-CG-CD	5.71	124.42	111.30	7	1
1	A	140	ARG	CA-CB-CG	-5.70	102.70	114.10	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	127	PRO	CA-N-CD	-5.69	104.03	112.00	3	2
1	A	115	PHE	N-CA-C	-5.68	99.65	108.90	4	2
1	A	28	GLU	CB-CG-CD	-5.67	102.97	112.60	5	1
1	A	65	GLU	N-CA-CB	-5.66	101.86	110.07	15	1
1	A	133	MET	CG-SD-CE	-5.63	88.51	100.90	2	3
1	A	81	LEU	N-CA-C	5.63	119.76	113.01	14	3
1	A	23	ARG	CA-CB-CG	5.61	125.33	114.10	1	1
1	A	38	VAL	N-CA-C	-5.61	101.72	109.46	5	1
1	A	40	SER	N-CA-C	-5.60	98.86	110.80	1	1
1	A	141	LEU	CA-C-O	-5.60	114.51	120.23	8	1
1	A	70	ILE	N-CA-C	5.60	120.74	113.07	4	1
1	A	66	LEU	N-CA-CB	-5.59	101.85	110.13	2	1
1	A	117	VAL	CB-CA-C	-5.58	105.20	111.45	6	1
1	A	25	ILE	N-CA-CB	5.58	117.71	110.57	5	2
1	A	134	ALA	N-CA-CB	-5.55	102.41	110.84	4	1
1	A	137	ASN	CA-C-N	5.55	132.13	121.54	13	1
1	A	137	ASN	C-N-CA	5.55	132.13	121.54	13	1
1	A	16	ARG	N-CA-C	5.52	116.97	111.07	6	1
1	A	125	LYS	N-CA-C	-5.52	102.63	111.02	10	1
1	A	138	SER	CB-CA-C	-5.51	99.45	110.42	11	1
1	A	153	GLN	N-CA-C	5.50	126.39	111.00	12	1
1	A	66	LEU	O-C-N	-5.50	116.16	122.09	9	1
1	A	47	GLN	CB-CA-C	5.50	121.38	110.17	13	1
1	A	117	VAL	N-CA-C	-5.47	100.70	108.58	10	1
1	A	74	VAL	CA-CB-CG2	-5.44	101.15	110.40	3	1
1	A	119	LYS	N-CA-C	5.42	121.80	109.81	4	1
1	A	38	VAL	CB-CA-C	5.42	119.07	111.70	4	3
1	A	126	ASP	N-CA-C	5.42	121.78	109.81	3	1
1	A	47	GLN	CA-C-O	-5.42	112.76	120.51	8	1
1	A	81	LEU	CB-CG-CD1	5.41	126.94	110.70	15	1
1	A	22	PHE	CA-C-N	5.39	127.77	120.44	14	1
1	A	22	PHE	C-N-CA	5.39	127.77	120.44	14	1
1	A	135	ILE	CA-CB-CG2	5.38	119.64	110.50	4	2
1	A	102	GLY	CA-C-N	5.38	131.44	122.73	9	1
1	A	102	GLY	C-N-CA	5.38	131.44	122.73	9	1
1	A	39	SER	CB-CA-C	5.37	121.11	110.42	2	1
1	A	135	ILE	CA-C-N	5.37	130.81	123.46	5	2
1	A	135	ILE	C-N-CA	5.37	130.81	123.46	5	2
1	A	4	ASN	N-CA-C	5.37	122.23	110.80	8	1
1	A	45	TYR	CB-CA-C	-5.36	100.83	110.36	6	3
1	A	106	ILE	CA-CB-CG1	5.35	119.50	110.40	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	LEU	CB-CA-C	-5.33	102.48	110.90	2	1
1	A	141	LEU	O-C-N	-5.32	115.58	121.53	9	2
1	A	56	ARG	CA-C-N	5.32	132.00	122.38	7	1
1	A	56	ARG	C-N-CA	5.32	132.00	122.38	7	1
1	A	117	VAL	CA-C-N	5.31	131.67	121.54	3	2
1	A	117	VAL	C-N-CA	5.31	131.67	121.54	3	2
1	A	48	ALA	CA-C-O	5.30	126.13	120.24	12	1
1	A	52	ARG	CA-C-O	-5.29	115.24	120.80	12	1
1	A	51	ASP	CA-CB-CG	5.28	117.88	112.60	4	1
1	A	38	VAL	CA-CB-CG2	5.28	119.38	110.40	14	1
1	A	137	ASN	N-CA-CB	5.28	119.06	110.77	12	1
1	A	150	ILE	CB-CA-C	5.28	118.57	110.55	2	1
1	A	151	LYS	CA-C-O	5.27	127.21	120.57	7	1
1	A	30	ARG	N-CA-C	5.27	116.70	111.07	14	1
1	A	26	ASN	N-CA-CB	5.26	119.13	110.39	12	2
1	A	34	LYS	CA-C-N	5.26	127.76	120.29	13	1
1	A	34	LYS	C-N-CA	5.26	127.76	120.29	13	1
1	A	55	GLN	CB-CA-C	-5.26	99.65	110.38	3	1
1	A	121	ASN	N-CA-CB	5.26	119.38	110.49	3	2
1	A	19	GLU	CA-C-N	5.25	127.75	120.29	14	2
1	A	19	GLU	C-N-CA	5.25	127.75	120.29	14	2
1	A	64	PHE	CA-C-N	5.24	127.56	120.44	9	1
1	A	64	PHE	C-N-CA	5.24	127.56	120.44	9	1
1	A	78	ASN	N-CA-C	5.22	116.78	111.14	1	1
1	A	72	ASP	N-CA-C	-5.19	106.80	113.23	2	1
1	A	54	ILE	CA-CB-CG2	5.19	119.32	110.50	4	1
1	A	130	GLN	N-CA-C	-5.16	104.24	110.44	5	1
1	A	77	VAL	CA-CB-CG2	5.16	119.17	110.40	8	2
1	A	72	ASP	CB-CA-C	-5.16	100.36	110.11	12	2
1	A	113	LEU	O-C-N	-5.15	117.30	123.27	1	1
1	A	10	ARG	CB-CA-C	5.15	119.04	110.81	5	1
1	A	16	ARG	CB-CA-C	5.13	119.57	110.85	3	1
1	A	81	LEU	CA-C-O	5.11	125.69	119.05	14	1
1	A	73	HIS	CB-CG-ND1	5.11	130.36	122.70	11	1
1	A	70	ILE	CA-C-O	5.08	126.18	120.64	15	1
1	A	12	ASN	N-CA-CB	5.07	117.75	110.20	7	2
1	A	128	SER	N-CA-CB	5.05	120.92	111.52	11	1
1	A	112	TRP	CB-CG-CD2	-5.05	119.72	126.80	12	1
1	A	47	GLN	CA-C-N	5.05	127.01	120.44	5	1
1	A	47	GLN	C-N-CA	5.05	127.01	120.44	5	1
1	A	4	ASN	N-CA-CB	5.05	118.56	110.73	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	4	ASN	CA-CB-CG	-5.04	107.56	112.60	13	1
1	A	17	HIS	CE1-NE2-CD2	-5.03	103.97	109.00	5	1
1	A	112	TRP	CB-CA-C	5.01	119.84	111.22	2	1
1	A	75	LEU	N-CA-C	5.01	117.47	111.71	14	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	62	TYR	Sidechain	12
1	A	64	PHE	Sidechain	12
1	A	45	TYR	Sidechain	8
1	A	151	LYS	Peptide,Mainchain	7
1	A	115	PHE	Sidechain	5
1	A	139	ARG	Sidechain,Peptide	4
1	A	41	PHE	Sidechain	3
1	A	80	PHE	Sidechain	2
1	A	150	ILE	Peptide	2
1	A	73	HIS	Sidechain	2
1	A	140	ARG	Peptide	1
1	A	18	PHE	Sidechain	1
1	A	56	ARG	Sidechain	1
1	A	126	ASP	Peptide	1
1	A	81	LEU	Peptide	1
1	A	109	GLY	Peptide	1
1	A	138	SER	Peptide	1

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	1023	1031	1031	27±7
All	All	15345	15465	15465	407

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD12	1:A:111:LEU:HD12	1.00	1.32	2	1
1:A:150:ILE:HD13	1:A:151:LYS:HB3	0.88	1.44	2	1
1:A:50:LEU:HD23	1:A:54:ILE:HD11	0.85	1.48	8	4
1:A:66:LEU:HD12	1:A:111:LEU:HD23	0.85	1.49	3	1
1:A:66:LEU:CD1	1:A:111:LEU:HD12	0.82	2.04	2	1
1:A:136:ILE:HD13	1:A:141:LEU:HD11	0.75	1.56	4	1
1:A:73:HIS:CD2	1:A:152:THR:HB	0.74	2.17	7	1
1:A:50:LEU:CD2	1:A:54:ILE:HD11	0.72	2.13	8	4
1:A:150:ILE:HD13	1:A:151:LYS:O	0.70	1.86	1	2
1:A:150:ILE:HD13	1:A:151:LYS:HG2	0.70	1.64	12	1
1:A:73:HIS:CD2	1:A:151:LYS:HG3	0.68	2.24	2	1
1:A:50:LEU:HD23	1:A:54:ILE:CD1	0.68	2.18	8	3
1:A:66:LEU:HD13	1:A:111:LEU:HD13	0.67	1.65	5	1
1:A:62:TYR:CE2	1:A:136:ILE:HG21	0.67	2.24	10	2
1:A:73:HIS:NE2	1:A:151:LYS:HG3	0.66	2.06	2	2
1:A:111:LEU:HA	1:A:136:ILE:HG23	0.66	1.67	10	2
1:A:66:LEU:HD11	1:A:151:LYS:HE3	0.65	1.67	3	1
1:A:49:LEU:HD22	1:A:50:LEU:H	0.65	1.51	9	3
1:A:45:TYR:CZ	1:A:50:LEU:HD12	0.65	2.27	14	2
1:A:45:TYR:CE1	1:A:50:LEU:HD12	0.65	2.27	8	1
1:A:106:ILE:HD13	1:A:153:GLN:HG2	0.65	1.68	12	1
1:A:73:HIS:CD2	1:A:152:THR:HA	0.64	2.28	1	1
1:A:73:HIS:CD2	1:A:153:GLN:HA	0.64	2.27	13	1
1:A:106:ILE:HG23	1:A:150:ILE:HD12	0.64	1.67	2	1
1:A:38:VAL:HG22	1:A:81:LEU:HD23	0.64	1.69	14	1
1:A:106:ILE:HD12	1:A:113:LEU:HD23	0.64	1.70	4	1
1:A:111:LEU:HD13	1:A:136:ILE:HD12	0.63	1.69	12	1
1:A:136:ILE:HD13	1:A:141:LEU:HD12	0.63	1.69	7	1
1:A:38:VAL:HG23	1:A:81:LEU:HD11	0.63	1.71	13	2
1:A:29:ILE:HD13	1:A:41:PHE:CE1	0.62	2.29	10	2
1:A:139:ARG:HD3	1:A:140:ARG:HG2	0.62	1.72	1	4
1:A:66:LEU:CD1	1:A:111:LEU:HD23	0.62	2.21	3	1
1:A:138:SER:CB	1:A:141:LEU:HD21	0.62	2.25	10	1
1:A:111:LEU:HB3	1:A:136:ILE:HG23	0.61	1.72	12	5
1:A:111:LEU:HG	1:A:136:ILE:HG23	0.61	1.71	9	1
1:A:39:SER:HB3	1:A:81:LEU:HD21	0.61	1.72	14	1
1:A:18:PHE:O	1:A:22:PHE:HB2	0.60	1.95	7	1
1:A:49:LEU:H	1:A:49:LEU:HD13	0.60	1.56	9	2
1:A:49:LEU:HD22	1:A:50:LEU:N	0.60	2.11	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:SER:HB3	1:A:141:LEU:HD21	0.60	1.73	10	1
1:A:49:LEU:HD13	1:A:50:LEU:H	0.60	1.55	14	1
1:A:14:LEU:HD12	1:A:54:ILE:HA	0.60	1.74	8	3
1:A:137:ASN:HA	1:A:141:LEU:HB2	0.60	1.73	11	1
1:A:45:TYR:CE2	1:A:50:LEU:HD12	0.60	2.32	14	1
1:A:60:GLU:O	1:A:63:VAL:HG12	0.60	1.97	3	6
1:A:150:ILE:HD13	1:A:152:THR:H	0.59	1.56	7	1
1:A:70:ILE:HD13	1:A:153:GLN:HB2	0.59	1.74	13	1
1:A:73:HIS:CE1	1:A:106:ILE:HD12	0.59	2.33	1	1
1:A:150:ILE:CD1	1:A:152:THR:H	0.58	2.11	3	2
1:A:70:ILE:HD13	1:A:153:GLN:N	0.58	2.14	12	1
1:A:66:LEU:HG	1:A:111:LEU:HD21	0.58	1.75	14	2
1:A:136:ILE:HG22	1:A:137:ASN:H	0.58	1.59	11	5
1:A:139:ARG:CD	1:A:140:ARG:H	0.57	2.11	12	1
1:A:21:GLU:HB3	1:A:64:PHE:CD1	0.57	2.33	14	12
1:A:4:ASN:HA	1:A:7:VAL:HG13	0.57	1.77	12	4
1:A:57:GLU:OE1	1:A:136:ILE:HD12	0.57	1.99	10	1
1:A:18:PHE:CE2	1:A:50:LEU:HD11	0.57	2.33	11	1
1:A:70:ILE:HD12	1:A:151:LYS:HE2	0.57	1.74	2	1
1:A:107:THR:O	1:A:150:ILE:HG22	0.57	2.00	12	1
1:A:66:LEU:CD2	1:A:109:GLY:HA3	0.57	2.30	15	1
1:A:152:THR:HG23	1:A:152:THR:O	0.57	2.00	2	4
1:A:50:LEU:O	1:A:54:ILE:HG22	0.56	1.99	9	1
1:A:50:LEU:HD23	1:A:54:ILE:CG1	0.56	2.30	6	4
1:A:49:LEU:HD22	1:A:49:LEU:H	0.56	1.60	11	1
1:A:45:TYR:CD2	1:A:50:LEU:HD13	0.56	2.35	7	2
1:A:49:LEU:HD11	1:A:133:MET:HA	0.56	1.78	1	1
1:A:39:SER:HB2	1:A:81:LEU:HD11	0.56	1.77	7	1
1:A:106:ILE:HD11	1:A:115:PHE:CE1	0.56	2.36	12	2
1:A:111:LEU:CD2	1:A:136:ILE:HG23	0.55	2.31	4	1
1:A:70:ILE:HG23	1:A:73:HIS:CD2	0.55	2.36	11	1
1:A:70:ILE:HD12	1:A:73:HIS:CE1	0.55	2.35	5	1
1:A:49:LEU:HD13	1:A:50:LEU:N	0.55	2.17	7	3
1:A:108:ASP:HB2	1:A:150:ILE:HG22	0.55	1.79	14	1
1:A:18:PHE:CE1	1:A:50:LEU:HD11	0.55	2.37	3	5
1:A:139:ARG:CD	1:A:140:ARG:HG2	0.55	2.32	8	4
1:A:38:VAL:HG23	1:A:81:LEU:HD23	0.54	1.79	4	1
1:A:73:HIS:HE1	1:A:150:ILE:HD11	0.54	1.62	5	1
1:A:66:LEU:HD22	1:A:153:GLN:C	0.54	2.26	2	1
1:A:63:VAL:HG23	1:A:111:LEU:HD21	0.54	1.77	15	2
1:A:63:VAL:HG13	1:A:67:PHE:CE1	0.54	2.37	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD12	1:A:111:LEU:CD1	0.54	2.21	2	1
1:A:14:LEU:HD23	1:A:54:ILE:HA	0.54	1.79	4	2
1:A:81:LEU:HD12	1:A:126:ASP:HA	0.54	1.80	7	1
1:A:25:ILE:HG12	1:A:68:HIS:CE1	0.54	2.37	2	6
1:A:39:SER:CB	1:A:81:LEU:HD11	0.54	2.33	7	1
1:A:66:LEU:HG	1:A:109:GLY:HA3	0.54	1.80	8	5
1:A:57:GLU:HG2	1:A:136:ILE:HD11	0.53	1.80	7	1
1:A:14:LEU:HG	1:A:59:ASP:HA	0.53	1.80	15	1
1:A:139:ARG:CD	1:A:141:LEU:HD23	0.53	2.33	9	1
1:A:73:HIS:CG	1:A:153:GLN:HG2	0.53	2.38	13	1
1:A:108:ASP:HB3	1:A:151:LYS:H	0.53	1.64	3	1
1:A:57:GLU:CG	1:A:141:LEU:HD23	0.53	2.33	5	1
1:A:110:ASN:O	1:A:136:ILE:HG22	0.53	2.03	2	2
1:A:18:PHE:CZ	1:A:50:LEU:HG	0.52	2.39	13	3
1:A:106:ILE:CD1	1:A:113:LEU:HD23	0.52	2.33	4	1
1:A:50:LEU:HD21	1:A:54:ILE:HD12	0.52	1.81	9	2
1:A:57:GLU:HA	1:A:141:LEU:HD22	0.52	1.79	10	2
1:A:66:LEU:HD13	1:A:111:LEU:CD1	0.52	2.34	5	1
1:A:66:LEU:HD12	1:A:111:LEU:HD21	0.52	1.80	6	3
1:A:18:PHE:CE1	1:A:50:LEU:HD21	0.52	2.39	12	1
1:A:73:HIS:CG	1:A:153:GLN:HA	0.52	2.39	4	1
1:A:66:LEU:CG	1:A:111:LEU:HD21	0.52	2.34	14	2
1:A:22:PHE:CZ	1:A:45:TYR:CE2	0.52	2.98	14	2
1:A:140:ARG:HG3	1:A:141:LEU:HD13	0.51	1.82	12	1
1:A:66:LEU:HD11	1:A:151:LYS:HD3	0.51	1.80	7	1
1:A:150:ILE:HD11	1:A:153:GLN:H	0.51	1.65	8	1
1:A:66:LEU:HD23	1:A:109:GLY:HA3	0.51	1.82	15	1
1:A:66:LEU:HD21	1:A:151:LYS:HD3	0.50	1.84	7	1
1:A:69:LYS:O	1:A:152:THR:HG21	0.50	2.06	1	1
1:A:73:HIS:CE1	1:A:152:THR:N	0.50	2.79	10	1
1:A:104:LEU:HD23	1:A:106:ILE:HD11	0.50	1.84	10	1
1:A:32:ALA:CB	1:A:74:VAL:HG11	0.50	2.37	1	1
1:A:118:CYS:CB	1:A:121:ASN:HD21	0.50	2.20	10	2
1:A:49:LEU:HD22	1:A:49:LEU:C	0.50	2.32	14	1
1:A:106:ILE:HG23	1:A:150:ILE:CD1	0.50	2.36	2	1
1:A:18:PHE:CZ	1:A:50:LEU:HD21	0.49	2.42	12	1
1:A:62:TYR:CD2	1:A:141:LEU:HD13	0.49	2.42	4	1
1:A:38:VAL:HG23	1:A:81:LEU:HD22	0.49	1.83	7	1
1:A:62:TYR:CD2	1:A:136:ILE:HG21	0.49	2.41	10	1
1:A:111:LEU:H	1:A:111:LEU:HD23	0.49	1.67	11	3
1:A:63:VAL:HG21	1:A:136:ILE:HD11	0.49	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ILE:HB	1:A:141:LEU:HD12	0.49	1.83	11	1
1:A:81:LEU:HD22	1:A:125:LYS:HB2	0.49	1.85	11	1
1:A:49:LEU:HD12	1:A:50:LEU:H	0.49	1.68	15	1
1:A:106:ILE:HG21	1:A:153:GLN:HG2	0.49	1.84	7	1
1:A:14:LEU:HD13	1:A:54:ILE:HG23	0.49	1.84	12	1
1:A:106:ILE:HD12	1:A:115:PHE:CE1	0.48	2.42	10	1
1:A:138:SER:HB2	1:A:141:LEU:HB2	0.48	1.84	1	1
1:A:141:LEU:HD23	1:A:141:LEU:N	0.48	2.23	11	1
1:A:70:ILE:HD11	1:A:106:ILE:HD12	0.48	1.84	2	1
1:A:14:LEU:HD13	1:A:54:ILE:HG13	0.48	1.85	3	1
1:A:141:LEU:N	1:A:141:LEU:CD2	0.48	2.76	7	1
1:A:38:VAL:HG21	1:A:78:ASN:ND2	0.48	2.24	8	2
1:A:49:LEU:HD23	1:A:134:ALA:H	0.48	1.68	10	1
1:A:38:VAL:HG22	1:A:39:SER:H	0.48	1.68	3	1
1:A:66:LEU:CD1	1:A:111:LEU:HD21	0.48	2.39	14	3
1:A:150:ILE:CD1	1:A:151:LYS:HB3	0.48	2.28	2	1
1:A:139:ARG:CG	1:A:140:ARG:H	0.48	2.21	6	2
1:A:70:ILE:HD13	1:A:153:GLN:HE21	0.47	1.68	2	1
1:A:18:PHE:CD1	1:A:50:LEU:HD11	0.47	2.44	8	5
1:A:21:GLU:HB3	1:A:64:PHE:CD2	0.47	2.44	10	2
1:A:67:PHE:HA	1:A:70:ILE:HB	0.47	1.87	1	1
1:A:66:LEU:HD11	1:A:113:LEU:HD13	0.47	1.87	12	1
1:A:151:LYS:H	1:A:151:LYS:CD	0.47	2.22	15	1
1:A:81:LEU:HD13	1:A:125:LYS:HB3	0.47	1.87	9	1
1:A:13:LYS:HA	1:A:16:ARG:HG3	0.47	1.87	8	4
1:A:50:LEU:CD2	1:A:54:ILE:HD12	0.47	2.39	14	2
1:A:78:ASN:O	1:A:81:LEU:HD23	0.47	2.09	10	1
1:A:38:VAL:CG2	1:A:81:LEU:HD23	0.47	2.39	14	1
1:A:4:ASN:HA	1:A:7:VAL:CG1	0.47	2.40	8	4
1:A:150:ILE:HD12	1:A:151:LYS:O	0.47	2.10	9	1
1:A:111:LEU:HD13	1:A:136:ILE:CG1	0.47	2.40	10	1
1:A:125:LYS:H	1:A:127:PRO:HD3	0.47	1.69	5	1
1:A:74:VAL:HA	1:A:77:VAL:CG1	0.47	2.39	13	1
1:A:138:SER:CB	1:A:139:ARG:HD2	0.46	2.40	3	1
1:A:24:GLN:HE21	1:A:68:HIS:CE1	0.46	2.28	9	2
1:A:106:ILE:HD12	1:A:115:PHE:CZ	0.46	2.45	10	1
1:A:25:ILE:HD13	1:A:68:HIS:CE1	0.46	2.45	5	1
1:A:139:ARG:O	1:A:141:LEU:N	0.46	2.45	13	1
1:A:66:LEU:HD12	1:A:111:LEU:CD2	0.46	2.32	3	1
1:A:138:SER:HB2	1:A:139:ARG:CD	0.46	2.40	11	1
1:A:45:TYR:CE1	1:A:50:LEU:HD13	0.46	2.46	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:SER:HB2	1:A:139:ARG:HD2	0.46	1.87	3	1
1:A:73:HIS:CE1	1:A:153:GLN:HE22	0.46	2.27	5	1
1:A:32:ALA:HB3	1:A:74:VAL:HG21	0.45	1.87	9	1
1:A:26:ASN:HA	1:A:29:ILE:HG13	0.45	1.87	10	2
1:A:58:ILE:HD13	1:A:59:ASP:N	0.45	2.25	11	1
1:A:64:PHE:HA	1:A:67:PHE:CD2	0.45	2.46	7	1
1:A:38:VAL:HG11	1:A:78:ASN:CG	0.45	2.36	11	1
1:A:47:GLN:HA	1:A:50:LEU:CB	0.45	2.40	13	1
1:A:28:GLU:CD	1:A:71:LYS:HB2	0.45	2.36	5	1
1:A:26:ASN:HA	1:A:29:ILE:CG1	0.45	2.41	10	1
1:A:25:ILE:CD1	1:A:67:PHE:CD1	0.45	3.00	4	2
1:A:66:LEU:C	1:A:66:LEU:HD13	0.45	2.37	3	1
1:A:53:ALA:HB1	1:A:60:GLU:CD	0.45	2.36	5	1
1:A:66:LEU:HD11	1:A:113:LEU:CD1	0.45	2.42	12	1
1:A:18:PHE:CE1	1:A:50:LEU:CD1	0.45	3.00	7	2
1:A:106:ILE:HG23	1:A:150:ILE:O	0.45	2.12	1	1
1:A:14:LEU:HD12	1:A:58:ILE:HA	0.45	1.87	14	2
1:A:45:TYR:CE2	1:A:50:LEU:HD13	0.45	2.47	7	1
1:A:38:VAL:HG21	1:A:78:ASN:HB3	0.44	1.89	2	1
1:A:139:ARG:HD2	1:A:140:ARG:H	0.44	1.72	12	1
1:A:50:LEU:C	1:A:50:LEU:HD23	0.44	2.37	14	1
1:A:111:LEU:HD23	1:A:136:ILE:HG23	0.44	1.89	4	1
1:A:70:ILE:CG1	1:A:153:GLN:HA	0.44	2.42	9	1
1:A:73:HIS:CE1	1:A:152:THR:H	0.44	2.31	10	1
1:A:64:PHE:O	1:A:68:HIS:CD2	0.44	2.70	7	4
1:A:151:LYS:HE3	1:A:153:GLN:N	0.44	2.28	2	1
1:A:139:ARG:HG2	1:A:140:ARG:HG2	0.44	1.89	13	1
1:A:111:LEU:HD13	1:A:113:LEU:HD23	0.44	1.88	2	1
1:A:24:GLN:CG	1:A:68:HIS:CE1	0.44	3.00	6	1
1:A:67:PHE:CE1	1:A:113:LEU:HD11	0.44	2.48	7	1
1:A:66:LEU:O	1:A:70:ILE:HG13	0.44	2.12	4	1
1:A:29:ILE:HD13	1:A:41:PHE:CE2	0.44	2.47	9	1
1:A:73:HIS:CB	1:A:152:THR:O	0.44	2.66	12	1
1:A:106:ILE:HD11	1:A:115:PHE:CZ	0.44	2.47	14	2
1:A:24:GLN:HB3	1:A:68:HIS:CE1	0.44	2.48	1	1
1:A:62:TYR:CZ	1:A:136:ILE:HG21	0.44	2.48	4	1
1:A:38:VAL:HG21	1:A:78:ASN:CG	0.44	2.38	5	1
1:A:49:LEU:HD22	1:A:131:CYS:SG	0.44	2.53	1	1
1:A:50:LEU:O	1:A:50:LEU:HD13	0.44	2.13	13	1
1:A:73:HIS:HB2	1:A:153:GLN:HB3	0.44	1.88	13	1
1:A:139:ARG:HD3	1:A:140:ARG:HG3	0.44	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:TYR:CE2	1:A:141:LEU:HD13	0.43	2.47	4	1
1:A:81:LEU:HD13	1:A:125:LYS:HB2	0.43	1.90	14	1
1:A:106:ILE:HA	1:A:150:ILE:O	0.43	2.13	1	1
1:A:38:VAL:CG2	1:A:39:SER:N	0.43	2.80	5	1
1:A:13:LYS:O	1:A:16:ARG:HD2	0.43	2.12	7	1
1:A:111:LEU:CA	1:A:136:ILE:HG23	0.43	2.43	8	2
1:A:49:LEU:HD21	1:A:132:ARG:O	0.43	2.14	1	1
1:A:71:LYS:O	1:A:74:VAL:HG23	0.43	2.13	2	1
1:A:136:ILE:HB	1:A:141:LEU:HD21	0.43	1.90	4	1
1:A:63:VAL:CG2	1:A:111:LEU:HD21	0.43	2.43	15	1
1:A:151:LYS:CE	1:A:153:GLN:HB3	0.43	2.44	2	1
1:A:138:SER:HB2	1:A:141:LEU:HG	0.43	1.91	6	1
1:A:17:HIS:CD2	1:A:61:THR:HG22	0.43	2.48	9	1
1:A:108:ASP:HB2	1:A:151:LYS:HB2	0.43	1.91	1	1
1:A:74:VAL:HA	1:A:77:VAL:HG13	0.43	1.90	11	2
1:A:10:ARG:HE	1:A:58:ILE:HD11	0.43	1.72	1	1
1:A:73:HIS:HB2	1:A:152:THR:O	0.43	2.13	12	1
1:A:22:PHE:CZ	1:A:45:TYR:CZ	0.43	3.07	14	1
1:A:66:LEU:CG	1:A:111:LEU:HD23	0.43	2.44	15	1
1:A:14:LEU:HD22	1:A:58:ILE:C	0.43	2.39	2	2
1:A:73:HIS:CD2	1:A:153:GLN:HE22	0.43	2.31	5	1
1:A:74:VAL:O	1:A:78:ASN:HB3	0.43	2.14	14	1
1:A:24:GLN:HG2	1:A:68:HIS:CE1	0.43	2.49	2	1
1:A:14:LEU:HD22	1:A:18:PHE:CD2	0.43	2.48	5	1
1:A:66:LEU:HD21	1:A:108:ASP:HB3	0.43	1.90	5	1
1:A:70:ILE:HD13	1:A:153:GLN:OXT	0.43	2.14	15	1
1:A:63:VAL:HA	1:A:111:LEU:HD11	0.42	1.90	4	1
1:A:14:LEU:HD12	1:A:54:ILE:HG13	0.42	1.90	7	1
1:A:49:LEU:O	1:A:52:ARG:HB2	0.42	2.13	14	1
1:A:81:LEU:HD23	1:A:81:LEU:O	0.42	2.13	1	1
1:A:58:ILE:HD12	1:A:58:ILE:C	0.42	2.40	3	1
1:A:133:MET:HE3	1:A:135:ILE:HG12	0.42	1.92	1	1
1:A:62:TYR:CD2	1:A:141:LEU:HD21	0.42	2.49	14	1
1:A:150:ILE:HD11	1:A:152:THR:H	0.42	1.73	3	1
1:A:70:ILE:HG23	1:A:73:HIS:NE2	0.42	2.30	11	1
1:A:150:ILE:HD13	1:A:152:THR:N	0.42	2.29	7	1
1:A:14:LEU:HD22	1:A:59:ASP:N	0.42	2.30	6	1
1:A:49:LEU:H	1:A:49:LEU:CD1	0.42	2.23	9	1
1:A:28:GLU:CG	1:A:71:LYS:HG2	0.42	2.45	11	1
1:A:73:HIS:CD2	1:A:152:THR:CB	0.42	2.98	7	1
1:A:57:GLU:HA	1:A:140:ARG:HG3	0.42	1.92	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLN:O	1:A:51:ASP:N	0.42	2.53	15	2
1:A:45:TYR:CD1	1:A:50:LEU:HD13	0.42	2.50	1	2
1:A:138:SER:HB3	1:A:139:ARG:HG3	0.42	1.92	1	1
1:A:62:TYR:HE2	1:A:136:ILE:HG21	0.42	1.74	8	2
1:A:38:VAL:HG12	1:A:39:SER:H	0.41	1.75	2	1
1:A:73:HIS:CE1	1:A:150:ILE:HD11	0.41	2.48	5	1
1:A:63:VAL:HG13	1:A:67:PHE:CZ	0.41	2.51	8	1
1:A:38:VAL:HG23	1:A:81:LEU:HD21	0.41	1.92	12	1
1:A:110:ASN:HD21	1:A:141:LEU:HD11	0.41	1.75	14	1
1:A:136:ILE:HG22	1:A:137:ASN:O	0.41	2.15	6	1
1:A:60:GLU:OE1	1:A:136:ILE:HD11	0.41	2.16	12	1
1:A:38:VAL:HG21	1:A:78:ASN:CB	0.41	2.45	5	1
1:A:118:CYS:HB2	1:A:121:ASN:HD21	0.41	1.76	11	1
1:A:22:PHE:CE2	1:A:45:TYR:CD2	0.41	3.09	5	1
1:A:4:ASN:HA	1:A:7:VAL:HB	0.41	1.90	10	1
1:A:111:LEU:CB	1:A:136:ILE:HG23	0.41	2.43	12	1
1:A:38:VAL:HG23	1:A:81:LEU:HD13	0.41	1.92	1	1
1:A:73:HIS:CD2	1:A:152:THR:CA	0.41	3.03	1	1
1:A:81:LEU:HA	1:A:125:LYS:HB2	0.41	1.93	3	1
1:A:13:LYS:O	1:A:17:HIS:CG	0.41	2.73	12	2
1:A:70:ILE:HD11	1:A:153:GLN:CB	0.41	2.46	9	1
1:A:28:GLU:HG2	1:A:71:LYS:HG2	0.41	1.93	11	1
1:A:106:ILE:HG13	1:A:113:LEU:HD12	0.41	1.93	2	1
1:A:138:SER:HB3	1:A:139:ARG:HD2	0.41	1.93	6	1
1:A:50:LEU:O	1:A:54:ILE:HG13	0.41	2.16	10	2
1:A:106:ILE:HD13	1:A:153:GLN:OXT	0.40	2.16	4	1
1:A:77:VAL:HG23	1:A:80:PHE:CE1	0.40	2.51	12	1
1:A:49:LEU:CD2	1:A:50:LEU:H	0.40	2.30	8	1
1:A:66:LEU:HD11	1:A:153:GLN:NE2	0.40	2.31	2	1
1:A:45:TYR:CD2	1:A:50:LEU:CD1	0.40	3.04	11	1
1:A:41:PHE:HA	1:A:127:PRO:O	0.40	2.16	12	1
1:A:73:HIS:CD2	1:A:153:GLN:CA	0.40	3.04	13	1
1:A:64:PHE:O	1:A:68:HIS:CG	0.40	2.75	2	1
1:A:66:LEU:CD2	1:A:153:GLN:C	0.40	2.95	2	1
1:A:54:ILE:O	1:A:58:ILE:HG22	0.40	2.16	5	1
1:A:66:LEU:HD12	1:A:113:LEU:HD21	0.40	1.93	9	1
1:A:73:HIS:CE1	1:A:151:LYS:HB2	0.40	2.50	15	1

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	121/153 (79%)	100±3 (82±2%)	11±3 (9±2%)	10±2 (8±2%)	1	12
All	All	1815/2295 (79%)	1496 (82%)	165 (9%)	154 (8%)	1	12

All 30 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	131	CYS	15
1	A	58	ILE	14
1	A	110	ASN	11
1	A	39	SER	9
1	A	138	SER	9
1	A	40	SER	8
1	A	127	PRO	8
1	A	118	CYS	8
1	A	121	ASN	6
1	A	4	ASN	5
1	A	140	ARG	5
1	A	71	LYS	5
1	A	139	ARG	5
1	A	126	ASP	5
1	A	124	PHE	4
1	A	125	LYS	4
1	A	119	LYS	4
1	A	123	LYS	4
1	A	47	GLN	4
1	A	59	ASP	4
1	A	109	GLY	3
1	A	122	GLU	3
1	A	102	GLY	2
1	A	74	VAL	2
1	A	60	GLU	2
1	A	108	ASP	1
1	A	57	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	120	PRO	1
1	A	141	LEU	1
1	A	73	HIS	1

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	112/139 (81%)	81±3 (72±3%)	31±3 (28±3%)	1	20
All	All	1680/2085 (81%)	1215 (72%)	465 (28%)	1	20

All 79 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	58	ILE	15
1	A	136	ILE	15
1	A	141	LEU	15
1	A	67	PHE	14
1	A	5	THR	13
1	A	137	ASN	13
1	A	14	LEU	12
1	A	38	VAL	12
1	A	150	ILE	12
1	A	63	VAL	12
1	A	7	VAL	11
1	A	115	PHE	11
1	A	139	ARG	11
1	A	22	PHE	10
1	A	26	ASN	10
1	A	49	LEU	10
1	A	25	ILE	10
1	A	111	LEU	10
1	A	121	ASN	10
1	A	125	LYS	10
1	A	47	GLN	9
1	A	77	VAL	9

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Mol	Chain	Res	Type	Models (Total)
1	A	113	LEU	9
1	A	153	GLN	9
1	A	29	ILE	8
1	A	70	ILE	8
1	A	28	GLU	7
1	A	43	LEU	7
1	A	81	LEU	7
1	A	151	LYS	7
1	A	50	LEU	7
1	A	54	ILE	6
1	A	73	HIS	6
1	A	104	LEU	6
1	A	106	ILE	6
1	A	39	SER	6
1	A	123	LYS	5
1	A	129	LEU	5
1	A	18	PHE	5
1	A	135	ILE	5
1	A	66	LEU	5
1	A	55	GLN	5
1	A	117	VAL	5
1	A	60	GLU	4
1	A	108	ASP	4
1	A	45	TYR	4
1	A	130	GLN	4
1	A	133	MET	4
1	A	17	HIS	3
1	A	78	ASN	3
1	A	107	THR	3
1	A	75	LEU	3
1	A	80	PHE	3
1	A	110	ASN	3
1	A	10	ARG	3
1	A	126	ASP	3
1	A	23	ARG	2
1	A	46	SER	2
1	A	57	GLU	2
1	A	127	PRO	2
1	A	61	THR	2
1	A	79	GLU	2
1	A	124	PHE	2
1	A	152	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	138	SER	2
1	A	140	ARG	2
1	A	56	ARG	1
1	A	118	CYS	1
1	A	71	LYS	1
1	A	62	TYR	1
1	A	122	GLU	1
1	A	52	ARG	1
1	A	69	LYS	1
1	A	103	ARG	1
1	A	76	GLU	1
1	A	16	ARG	1
1	A	21	GLU	1
1	A	128	SER	1
1	A	112	TRP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided