



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:14 AM UTC

PDB ID : 1SPD / pdb_00001spd
Title : AMYOTROPHIC LATERAL SCLEROSIS AND STRUCTURAL DEFECTS
IN CU,ZN SUPEROXIDE DISMUTASE
Authors : Parge, H.E.; Tainer, J.A.
Deposited on : 1993-07-21
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

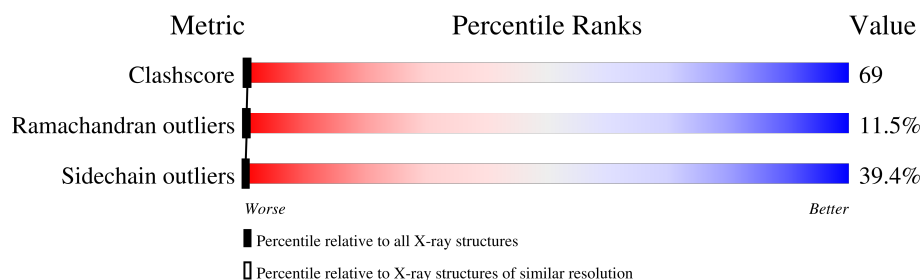
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

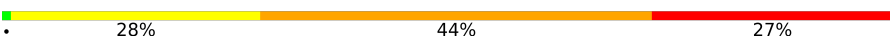
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	154	
1	B	154	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2230 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1113	681	203	225	4			
1	B	154	Total	C	N	O	S	0	0	0
			1113	681	203	225	4			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

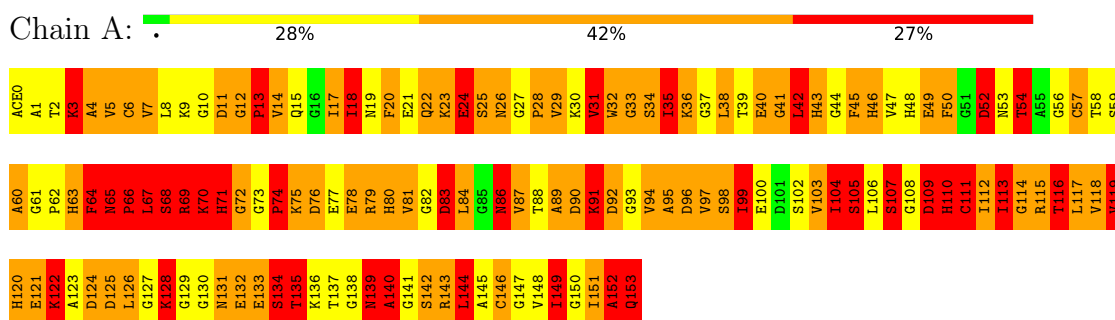
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

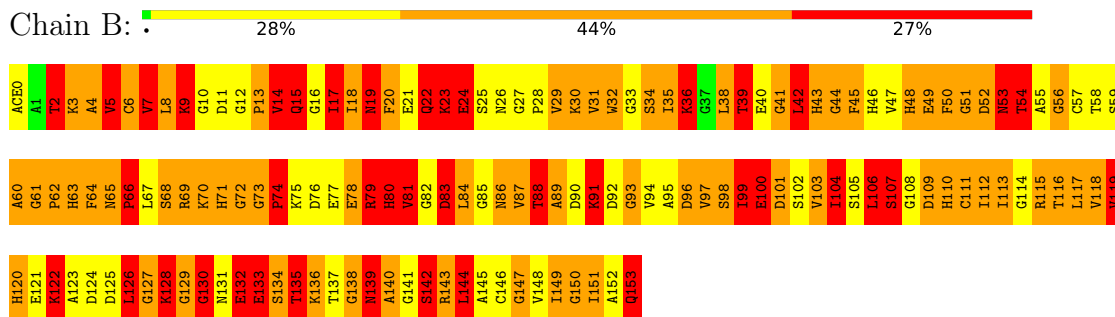
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: SUPEROXIDE DISMUTASE



• Molecule 1: SUPEROXIDE DISMUTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	113.57Å 113.57Å 71.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.224 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2230	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 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	2.81	83/1129 (7.4%)	4.49	352/1522 (23.1%)
1	B	2.86	88/1129 (7.8%)	4.63	372/1522 (24.4%)
All	All	2.83	171/2258 (7.6%)	4.56	724/3044 (23.8%)

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	25.89	1.85	1.33
1	B	0	ACE	C-N	23.63	1.80	1.33
1	B	150	GLY	N-CA	15.24	1.59	1.45
1	B	14	VAL	C-N	-14.73	1.13	1.33
1	B	33	GLY	N-CA	12.72	1.63	1.45
1	B	17	ILE	N-CA	10.47	1.58	1.46
1	A	33	GLY	N-CA	10.32	1.54	1.45
1	B	5	VAL	N-CA	10.19	1.57	1.46
1	A	28	PRO	C-N	10.01	1.45	1.33
1	A	76	ASP	N-CA	9.70	1.56	1.46
1	A	80	HIS	CE1-NE2	-9.69	1.22	1.32
1	A	19	ASN	C-N	9.41	1.45	1.33
1	A	29	VAL	CA-C	9.28	1.62	1.52
1	B	41	GLY	N-CA	9.07	1.58	1.45
1	B	118	VAL	C-O	8.93	1.32	1.24
1	B	120	HIS	CE1-NE2	8.93	1.41	1.32
1	A	18	ILE	C-O	8.90	1.33	1.24
1	B	80	HIS	CE1-NE2	-8.89	1.23	1.32
1	A	47	VAL	C-N	-8.86	1.22	1.33
1	B	4	ALA	C-O	8.61	1.34	1.23
1	A	56	GLY	CA-C	8.39	1.62	1.52
1	B	14	VAL	CA-C	-8.28	1.42	1.52
1	A	76	ASP	C-O	8.27	1.32	1.23
1	A	20	PHE	N-CA	8.18	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	SER	C-O	8.15	1.34	1.23
1	A	17	ILE	C-O	8.14	1.32	1.24
1	B	12	GLY	CA-C	8.06	1.63	1.51
1	A	120	HIS	ND1-CE1	-7.96	1.24	1.32
1	B	10	GLY	CA-C	7.96	1.59	1.52
1	A	80	HIS	CG-CD2	7.95	1.44	1.35
1	B	27	GLY	N-CA	7.93	1.55	1.44
1	A	72	GLY	N-CA	-7.92	1.36	1.45
1	A	99	ILE	C-O	7.86	1.34	1.24
1	A	53	ASN	N-CA	7.84	1.57	1.46
1	A	44	GLY	N-CA	7.77	1.55	1.45
1	B	151	ILE	CA-C	7.75	1.61	1.52
1	B	36	LYS	C-O	7.65	1.33	1.23
1	A	117	LEU	CA-C	7.60	1.61	1.52
1	A	89	ALA	C-O	7.58	1.33	1.24
1	B	21	GLU	N-CA	7.57	1.55	1.45
1	A	41	GLY	CA-C	7.54	1.62	1.52
1	A	2	THR	CB-OG1	7.52	1.55	1.43
1	A	9	LYS	N-CA	7.52	1.55	1.46
1	B	120	HIS	ND1-CE1	-7.44	1.25	1.32
1	B	147	GLY	CA-C	7.37	1.59	1.51
1	B	81	VAL	C-O	-7.36	1.15	1.24
1	A	2	THR	CA-CB	7.32	1.65	1.53
1	B	35	ILE	N-CA	7.23	1.54	1.46
1	B	5	VAL	C-O	7.20	1.31	1.23
1	A	4	ALA	C-N	7.17	1.43	1.33
1	B	120	HIS	N-CA	7.08	1.55	1.46
1	B	63	HIS	CE1-NE2	-7.07	1.25	1.32
1	B	121	GLU	N-CA	7.01	1.54	1.46
1	A	27	GLY	CA-C	6.99	1.61	1.51
1	A	68	SER	C-N	6.94	1.43	1.33
1	A	4	ALA	C-O	6.94	1.33	1.23
1	B	90	ASP	N-CA	6.91	1.55	1.46
1	B	125	ASP	CA-CB	6.81	1.62	1.52
1	B	45	PHE	N-CA	6.78	1.55	1.46
1	A	120	HIS	CE1-NE2	6.70	1.39	1.32
1	A	120	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	93	GLY	C-O	6.68	1.32	1.23
1	B	34	SER	C-O	6.65	1.31	1.23
1	A	112	ILE	CA-CB	6.62	1.62	1.54
1	B	71	HIS	CG-CD2	6.61	1.43	1.35
1	A	150	GLY	C-N	6.60	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	ARG	NE-CZ	6.55	1.40	1.33
1	B	45	PHE	C-O	6.54	1.31	1.23
1	B	97	VAL	N-CA	6.53	1.54	1.46
1	B	80	HIS	C-N	-6.50	1.24	1.33
1	A	146	CYS	N-CA	6.49	1.53	1.46
1	B	26	ASN	N-CA	6.49	1.54	1.46
1	A	73	GLY	N-CA	6.48	1.53	1.44
1	B	65	ASN	N-CA	-6.47	1.37	1.46
1	A	54	THR	CA-CB	6.47	1.64	1.53
1	B	20	PHE	C-O	6.46	1.31	1.23
1	B	7	VAL	N-CA	6.46	1.53	1.46
1	B	51	GLY	CA-C	6.41	1.60	1.51
1	B	87	VAL	C-O	6.37	1.30	1.23
1	B	73	GLY	CA-C	6.37	1.61	1.51
1	A	124	ASP	N-CA	6.34	1.54	1.46
1	A	35	ILE	N-CA	6.33	1.54	1.46
1	A	147	GLY	CA-C	6.32	1.57	1.51
1	B	73	GLY	N-CA	6.32	1.53	1.44
1	A	111	CYS	CA-C	-6.30	1.45	1.52
1	A	67	LEU	N-CA	6.30	1.54	1.46
1	A	12	GLY	N-CA	6.29	1.53	1.44
1	A	86	ASN	C-O	6.28	1.31	1.23
1	A	88	THR	CB-OG1	6.25	1.53	1.43
1	B	55	ALA	CA-C	6.25	1.61	1.53
1	B	80	HIS	N-CA	6.24	1.54	1.46
1	B	117	LEU	C-O	6.24	1.31	1.24
1	B	117	LEU	CA-C	6.24	1.60	1.52
1	B	129	GLY	N-CA	6.21	1.54	1.45
1	A	149	ILE	CA-CB	6.17	1.59	1.53
1	B	15	GLN	N-CA	6.17	1.54	1.46
1	B	80	HIS	ND1-CE1	6.17	1.38	1.32
1	B	144	LEU	C-O	6.16	1.32	1.24
1	B	18	ILE	CA-CB	6.15	1.62	1.54
1	A	62	PRO	CA-C	6.13	1.61	1.52
1	A	34	SER	C-N	6.12	1.42	1.33
1	B	118	VAL	CA-C	6.09	1.60	1.52
1	B	20	PHE	N-CA	6.05	1.54	1.46
1	A	15	GLN	CA-C	-6.04	1.45	1.53
1	B	40	GLU	C-N	6.03	1.42	1.33
1	A	95	ALA	C-O	5.98	1.30	1.23
1	B	88	THR	CA-CB	5.98	1.61	1.53
1	B	12	GLY	N-CA	5.97	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	HIS	CE1-NE2	-5.94	1.26	1.32
1	B	99	ILE	CA-C	5.92	1.59	1.52
1	B	71	HIS	C-O	-5.90	1.16	1.24
1	A	80	HIS	ND1-CE1	5.90	1.38	1.32
1	B	150	GLY	CA-C	5.89	1.58	1.52
1	A	57	CYS	N-CA	-5.89	1.38	1.46
1	B	77	GLU	CA-C	5.88	1.60	1.52
1	B	101	ASP	N-CA	5.88	1.53	1.46
1	B	112	ILE	CA-CB	5.86	1.62	1.54
1	A	65	ASN	CA-CB	5.83	1.62	1.53
1	A	30	LYS	CA-C	5.83	1.60	1.52
1	A	74	PRO	CA-CB	-5.82	1.45	1.53
1	A	15	GLN	N-CA	5.79	1.54	1.46
1	A	86	ASN	C-N	-5.75	1.26	1.33
1	A	14	VAL	C-O	-5.74	1.16	1.23
1	B	3	LYS	C-N	5.74	1.40	1.33
1	B	54	THR	N-CA	5.73	1.53	1.46
1	A	21	GLU	C-O	5.71	1.30	1.24
1	B	119	VAL	C-O	5.66	1.30	1.24
1	A	5	VAL	C-N	5.64	1.41	1.33
1	B	52	ASP	CA-CB	-5.63	1.45	1.53
1	B	67	LEU	C-N	-5.61	1.25	1.33
1	B	43	HIS	C-N	5.59	1.39	1.33
1	A	75	LYS	C-O	5.59	1.31	1.24
1	B	2	THR	CA-CB	5.58	1.62	1.53
1	B	13	PRO	C-O	5.58	1.31	1.24
1	A	5	VAL	C-O	5.57	1.30	1.24
1	A	122	LYS	CA-C	5.54	1.60	1.53
1	A	23	LYS	C-O	5.53	1.30	1.24
1	A	121	GLU	N-CA	5.53	1.53	1.46
1	A	27	GLY	N-CA	5.53	1.52	1.44
1	A	117	LEU	C-O	5.50	1.30	1.24
1	A	15	GLN	C-O	5.49	1.29	1.24
1	A	57	CYS	C-N	-5.47	1.26	1.33
1	A	89	ALA	C-N	-5.46	1.26	1.33
1	A	13	PRO	C-O	-5.40	1.17	1.24
1	A	17	ILE	N-CA	5.38	1.52	1.46
1	B	83	ASP	C-N	-5.32	1.26	1.33
1	B	70	LYS	N-CA	5.29	1.53	1.45
1	B	35	ILE	C-O	5.25	1.31	1.24
1	B	110	HIS	CA-CB	5.25	1.61	1.53
1	B	140	ALA	CA-CB	5.24	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	HIS	C-O	5.24	1.32	1.24
1	A	144	LEU	N-CA	5.23	1.52	1.46
1	B	148	VAL	CA-C	5.20	1.58	1.52
1	A	134	SER	CA-CB	-5.20	1.47	1.53
1	B	8	LEU	N-CA	-5.20	1.40	1.46
1	B	97	VAL	C-O	5.20	1.29	1.23
1	B	19	ASN	C-N	5.18	1.42	1.33
1	B	119	VAL	N-CA	5.18	1.52	1.46
1	A	143	ARG	CZ-NH2	5.18	1.40	1.33
1	A	94	VAL	N-CA	5.15	1.52	1.46
1	B	93	GLY	N-CA	-5.12	1.38	1.45
1	A	138	GLY	N-CA	5.11	1.52	1.44
1	B	138	GLY	C-N	-5.08	1.26	1.33
1	A	29	VAL	CA-CB	-5.07	1.48	1.54
1	A	6	CYS	C-N	-5.06	1.27	1.33
1	B	96	ASP	CA-C	5.06	1.59	1.52
1	A	74	PRO	N-CA	5.06	1.53	1.47
1	B	15	GLN	C-O	5.05	1.30	1.24
1	B	63	HIS	ND1-CE1	5.05	1.37	1.32
1	A	49	GLU	CA-CB	5.03	1.61	1.53
1	A	150	GLY	N-CA	5.02	1.52	1.45

All (724) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	VAL	O-C-N	-21.09	96.21	122.57
1	B	14	VAL	CA-C-N	20.50	160.69	121.54
1	B	14	VAL	C-N-CA	20.50	160.69	121.54
1	B	110	HIS	CA-CB-CG	19.22	133.02	113.80
1	A	38	LEU	CA-C-N	17.54	145.55	120.82
1	A	38	LEU	C-N-CA	17.54	145.55	120.82
1	A	146	CYS	O-C-N	17.40	142.04	123.42
1	A	26	ASN	CA-C-N	-16.68	95.68	121.87
1	A	26	ASN	C-N-CA	-16.68	95.68	121.87
1	B	101	ASP	O-C-N	16.32	142.50	123.41
1	A	52	ASP	CA-CB-CG	15.94	128.54	112.60
1	B	4	ALA	O-C-N	15.90	140.43	123.42
1	B	96	ASP	CA-C-N	-15.36	102.14	123.03
1	B	96	ASP	C-N-CA	-15.36	102.14	123.03
1	B	4	ALA	CA-C-N	-15.31	100.94	122.69
1	B	4	ALA	C-N-CA	-15.31	100.94	122.69
1	A	20	PHE	CA-CB-CG	15.05	128.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	VAL	CA-C-O	14.97	139.49	120.78
1	A	4	ALA	O-C-N	14.90	142.32	122.36
1	B	77	GLU	N-CA-C	-14.47	93.75	111.40
1	B	29	VAL	O-C-N	14.29	138.03	123.03
1	B	151	ILE	N-CA-CB	14.16	125.96	110.53
1	A	109	ASP	CA-CB-CG	13.76	126.36	112.60
1	B	149	ILE	CA-C-N	-13.72	104.47	122.03
1	B	149	ILE	C-N-CA	-13.72	104.47	122.03
1	B	63	HIS	CA-CB-CG	-13.38	100.42	113.80
1	A	4	ALA	CA-C-N	-13.22	98.17	121.97
1	A	4	ALA	C-N-CA	-13.22	98.17	121.97
1	B	149	ILE	N-CA-CB	13.21	125.75	110.95
1	A	80	HIS	CB-CG-CD2	-13.16	114.08	131.20
1	A	122	LYS	CA-C-N	13.14	140.17	121.24
1	A	122	LYS	C-N-CA	13.14	140.17	121.24
1	A	56	GLY	CA-C-N	13.13	143.65	122.65
1	A	56	GLY	C-N-CA	13.13	143.65	122.65
1	A	131	ASN	OD1-CG-ND2	-13.04	109.56	122.60
1	A	131	ASN	CA-CB-CG	12.97	125.57	112.60
1	B	42	LEU	CA-C-O	12.87	134.23	120.33
1	A	78	GLU	N-CA-CB	12.85	131.57	110.37
1	B	19	ASN	O-C-N	12.80	139.78	123.15
1	B	9	LYS	CA-C-N	12.73	132.51	121.82
1	B	9	LYS	C-N-CA	12.73	132.51	121.82
1	B	79	ARG	CB-CG-CD	12.61	140.29	111.30
1	B	42	LEU	N-CA-C	12.46	130.20	108.02
1	B	36	LYS	O-C-N	12.43	137.41	123.25
1	A	8	LEU	O-C-N	12.35	137.49	123.16
1	B	40	GLU	N-CA-C	12.33	127.61	110.35
1	B	40	GLU	CA-C-O	12.33	134.38	121.07
1	A	99	ILE	CA-C-O	-12.31	112.41	120.66
1	B	42	LEU	N-CA-CB	-12.29	92.16	110.84
1	B	135	THR	CA-CB-OG1	-12.25	91.22	109.60
1	B	26	ASN	CA-CB-CG	12.23	124.83	112.60
1	A	43	HIS	CA-CB-CG	-12.16	101.64	113.80
1	A	50	PHE	O-C-N	12.14	137.06	123.22
1	B	100	GLU	N-CA-CB	12.14	129.29	110.71
1	B	4	ALA	CA-C-O	-12.11	108.28	121.23
1	A	80	HIS	CB-CG-ND1	12.10	140.85	122.70
1	B	32	TRP	O-C-N	12.09	138.31	123.44
1	A	77	GLU	N-CA-C	-11.91	95.07	113.89
1	A	28	PRO	N-CA-C	11.89	136.96	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	CA-CB-CG	11.88	125.68	113.80
1	A	107	SER	O-C-N	11.85	138.35	122.59
1	A	19	ASN	CA-C-N	-11.80	104.93	122.39
1	A	19	ASN	C-N-CA	-11.80	104.93	122.39
1	A	131	ASN	CB-CG-ND2	11.76	134.04	116.40
1	A	49	GLU	N-CA-C	11.72	125.52	111.33
1	A	125	ASP	CA-C-N	11.70	143.89	121.54
1	A	125	ASP	C-N-CA	11.70	143.89	121.54
1	A	11	ASP	CA-CB-CG	11.47	124.07	112.60
1	B	71	HIS	CB-CG-CD2	-11.46	116.31	131.20
1	A	33	GLY	CA-C-O	-11.31	110.28	121.48
1	A	76	ASP	N-CA-C	11.29	125.34	109.31
1	A	59	SER	N-CA-C	11.27	126.13	112.38
1	B	45	PHE	O-C-N	11.26	137.56	123.14
1	A	29	VAL	O-C-N	11.22	134.90	122.67
1	A	78	GLU	N-CA-C	-11.18	89.08	108.20
1	B	64	PHE	CA-C-O	11.18	133.56	120.70
1	B	55	ALA	N-CA-C	-11.16	85.26	107.69
1	B	21	GLU	CA-C-O	-11.06	108.08	121.36
1	A	138	GLY	N-CA-C	-11.06	97.87	116.01
1	B	43	HIS	CA-CB-CG	-11.06	102.74	113.80
1	A	65	ASN	CA-C-N	10.98	133.56	119.84
1	A	65	ASN	C-N-CA	10.98	133.56	119.84
1	B	105	SER	CA-C-O	-10.98	109.92	121.55
1	B	107	SER	CA-C-O	-10.88	104.96	120.51
1	B	120	HIS	CA-CB-CG	-10.82	102.98	113.80
1	A	50	PHE	CA-C-O	-10.74	108.87	120.36
1	B	72	GLY	CA-C-N	-10.68	105.10	121.87
1	B	72	GLY	C-N-CA	-10.68	105.10	121.87
1	B	2	THR	CB-CA-C	10.55	128.87	109.46
1	B	149	ILE	CB-CA-C	-10.54	98.75	111.08
1	B	92	ASP	CA-CB-CG	-10.49	102.11	112.60
1	B	149	ILE	CA-CB-CG1	10.45	128.16	110.40
1	A	86	ASN	N-CA-C	-10.41	93.40	109.85
1	B	87	VAL	CA-CB-CG1	10.41	128.10	110.40
1	B	86	ASN	CA-CB-CG	10.39	122.99	112.60
1	A	65	ASN	CA-C-O	-10.34	106.00	120.16
1	A	88	THR	CA-C-O	10.31	131.67	120.43
1	A	46	HIS	CA-CB-CG	-10.31	103.49	113.80
1	B	71	HIS	CB-CG-ND1	10.30	138.15	122.70
1	A	14	VAL	CA-C-N	-10.25	104.28	122.32
1	A	14	VAL	C-N-CA	-10.25	104.28	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	PHE	CA-C-O	10.20	131.34	120.63
1	A	68	SER	N-CA-C	10.19	132.51	110.80
1	A	145	ALA	O-C-N	10.11	135.00	123.27
1	B	143	ARG	CA-C-O	-10.10	109.65	120.46
1	A	9	LYS	O-C-N	-10.10	113.46	123.46
1	B	6	CYS	CA-C-O	10.07	131.77	119.98
1	A	32	TRP	O-C-N	10.02	134.68	123.25
1	B	52	ASP	N-CA-C	-10.01	92.92	109.24
1	A	1	ALA	CA-C-O	9.99	137.78	120.80
1	B	18	ILE	CA-CB-CG2	9.96	127.43	110.50
1	B	143	ARG	NE-CZ-NH1	9.95	131.45	121.50
1	A	8	LEU	CA-C-O	-9.93	109.50	120.92
1	B	110	HIS	N-CA-C	9.92	124.96	112.86
1	A	67	LEU	N-CA-CB	9.92	125.88	110.71
1	A	115	ARG	NE-CZ-NH2	-9.90	110.29	119.20
1	A	149	ILE	CB-CA-C	9.87	122.26	111.80
1	A	64	PHE	CA-CB-CG	9.86	123.66	113.80
1	A	53	ASN	CA-CB-CG	9.78	122.38	112.60
1	B	9	LYS	CA-C-O	9.77	131.07	120.71
1	B	66	PRO	CA-C-N	9.76	140.18	121.54
1	B	66	PRO	C-N-CA	9.76	140.18	121.54
1	B	79	ARG	N-CA-C	9.75	124.87	108.20
1	B	135	THR	OG1-CB-CG2	9.73	128.77	109.30
1	B	61	GLY	CA-C-N	9.72	129.54	120.21
1	B	61	GLY	C-N-CA	9.72	129.54	120.21
1	A	68	SER	CA-C-O	9.72	134.40	120.51
1	B	2	THR	CA-C-N	9.71	140.28	121.63
1	B	2	THR	C-N-CA	9.71	140.28	121.63
1	A	21	GLU	CB-CG-CD	9.70	129.09	112.60
1	B	104	ILE	CA-C-O	9.69	132.89	120.78
1	A	91	LYS	O-C-N	9.66	134.26	122.86
1	B	12	GLY	N-CA-C	-9.66	92.64	112.34
1	B	16	GLY	N-CA-C	9.65	126.04	111.18
1	B	21	GLU	N-CA-CB	9.64	126.12	110.41
1	B	96	ASP	N-CA-C	-9.63	94.98	110.20
1	A	76	ASP	N-CA-CB	-9.61	96.10	109.94
1	B	141	GLY	O-C-N	-9.59	113.79	122.90
1	A	117	LEU	O-C-N	9.55	134.66	123.30
1	A	122	LYS	O-C-N	-9.52	111.99	122.85
1	A	2	THR	N-CA-CB	-9.46	94.50	110.49
1	B	78	GLU	N-CA-C	9.46	123.83	110.68
1	B	104	ILE	N-CA-CB	-9.43	95.67	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	HIS	CA-C-N	9.40	138.90	121.97
1	B	80	HIS	C-N-CA	9.40	138.90	121.97
1	B	10	GLY	O-C-N	9.38	131.76	123.60
1	B	93	GLY	O-C-N	9.35	134.85	122.70
1	B	65	ASN	CA-CB-CG	-9.34	103.26	112.60
1	A	86	ASN	OD1-CG-ND2	9.34	131.94	122.60
1	A	44	GLY	N-CA-C	-9.32	100.61	112.54
1	B	96	ASP	O-C-N	9.31	134.00	123.01
1	B	100	GLU	CB-CA-C	-9.30	97.86	110.79
1	B	35	ILE	CA-C-O	-9.30	108.59	121.51
1	B	32	TRP	CA-C-N	-9.29	103.20	121.41
1	B	32	TRP	C-N-CA	-9.29	103.20	121.41
1	B	71	HIS	O-C-N	9.27	133.89	123.04
1	B	71	HIS	CA-CB-CG	9.26	123.06	113.80
1	B	64	PHE	N-CA-CB	9.26	124.14	109.51
1	B	40	GLU	CA-C-N	-9.25	103.28	121.41
1	B	40	GLU	C-N-CA	-9.25	103.28	121.41
1	B	54	THR	CA-CB-OG1	-9.25	95.72	109.60
1	B	140	ALA	N-CA-C	9.22	122.32	111.71
1	A	71	HIS	CB-CG-CD2	-9.20	119.25	131.20
1	A	86	ASN	CA-CB-CG	9.20	121.80	112.60
1	B	55	ALA	O-C-N	9.18	136.91	122.96
1	A	124	ASP	O-C-N	9.17	134.51	122.96
1	A	50	PHE	CA-CB-CG	-9.15	104.65	113.80
1	A	142	SER	CA-C-N	9.15	137.60	123.23
1	A	142	SER	C-N-CA	9.15	137.60	123.23
1	A	2	THR	CA-CB-OG1	-9.13	95.90	109.60
1	A	17	ILE	CB-CA-C	9.13	122.01	110.96
1	B	116	THR	O-C-N	9.13	133.60	123.10
1	A	124	ASP	N-CA-C	9.12	122.99	109.59
1	B	50	PHE	O-C-N	9.05	133.54	123.13
1	A	34	SER	O-C-N	9.03	134.34	122.96
1	A	99	ILE	O-C-N	9.01	132.40	122.94
1	A	71	HIS	CA-C-N	8.98	135.41	120.86
1	A	71	HIS	C-N-CA	8.98	135.41	120.86
1	A	38	LEU	N-CA-C	8.97	122.19	110.43
1	A	86	ASN	CB-CA-C	8.97	127.06	109.66
1	B	94	VAL	N-CA-C	-8.96	95.54	108.53
1	B	81	VAL	N-CA-CB	8.94	125.97	111.23
1	A	116	THR	CA-CB-CG2	8.91	125.65	110.50
1	A	145	ALA	CA-C-N	-8.90	105.32	121.62
1	A	145	ALA	C-N-CA	-8.90	105.32	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH1	-8.89	112.61	121.50
1	B	53	ASN	O-C-N	8.88	131.44	122.30
1	A	42	LEU	O-C-N	8.84	132.94	122.96
1	B	39	THR	CA-C-O	-8.83	112.12	120.95
1	A	29	VAL	CA-C-N	-8.82	111.03	122.77
1	A	29	VAL	C-N-CA	-8.82	111.03	122.77
1	B	7	VAL	N-CA-C	-8.79	94.02	107.73
1	A	48	HIS	CA-C-N	8.76	132.38	120.38
1	A	48	HIS	C-N-CA	8.76	132.38	120.38
1	A	69	ARG	NH1-CZ-NH2	8.76	130.69	119.30
1	B	131	ASN	CB-CG-ND2	8.76	129.54	116.40
1	A	24	GLU	CA-C-O	8.70	132.96	120.51
1	B	93	GLY	CA-C-N	-8.68	111.91	123.10
1	B	93	GLY	C-N-CA	-8.68	111.91	123.10
1	A	14	VAL	N-CA-CB	-8.67	97.91	112.47
1	B	109	ASP	CA-CB-CG	8.62	121.22	112.60
1	A	66	PRO	N-CA-CB	-8.61	94.21	103.25
1	A	7	VAL	CB-CA-C	8.60	122.03	110.42
1	B	136	LYS	CB-CG-CD	8.60	131.09	111.30
1	A	39	THR	N-CA-C	-8.60	97.28	110.10
1	A	32	TRP	CA-C-N	-8.58	109.74	121.23
1	A	32	TRP	C-N-CA	-8.58	109.74	121.23
1	A	28	PRO	CA-C-O	8.57	136.19	120.60
1	A	98	SER	CA-C-O	-8.56	111.40	120.99
1	B	15	GLN	CA-CB-CG	8.56	131.21	114.10
1	B	94	VAL	CA-C-N	-8.55	110.72	122.86
1	B	94	VAL	C-N-CA	-8.55	110.72	122.86
1	B	28	PRO	CA-C-N	-8.54	108.33	122.67
1	B	28	PRO	C-N-CA	-8.54	108.33	122.67
1	A	77	GLU	N-CA-CB	8.50	123.19	110.95
1	B	73	GLY	N-CA-C	-8.49	95.01	112.34
1	B	77	GLU	CA-CB-CG	8.47	131.03	114.10
1	A	71	HIS	CB-CG-ND1	8.45	135.38	122.70
1	A	65	ASN	N-CA-C	8.44	128.46	109.81
1	A	116	THR	O-C-N	8.44	133.62	123.24
1	B	85	GLY	CA-C-O	8.44	135.25	120.57
1	A	33	GLY	CA-C-N	-8.44	108.86	122.36
1	A	33	GLY	C-N-CA	-8.44	108.86	122.36
1	A	34	SER	CA-C-N	-8.41	106.82	121.97
1	A	34	SER	C-N-CA	-8.41	106.82	121.97
1	B	149	ILE	O-C-N	8.37	132.21	122.83
1	B	72	GLY	O-C-N	8.35	133.37	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	VAL	CA-CB-CG2	8.35	124.59	110.40
1	A	17	ILE	N-CA-C	-8.34	95.48	108.23
1	A	88	THR	N-CA-C	8.33	122.82	109.24
1	A	105	SER	O-C-N	8.32	132.00	122.84
1	B	13	PRO	CA-C-N	-8.32	106.99	121.97
1	B	13	PRO	C-N-CA	-8.32	106.99	121.97
1	B	139	ASN	OD1-CG-ND2	8.31	130.91	122.60
1	A	20	PHE	CA-C-O	-8.31	110.06	120.20
1	B	107	SER	CA-CB-OG	8.30	127.70	111.10
1	B	19	ASN	N-CA-C	8.29	122.38	109.52
1	A	2	THR	N-CA-C	8.28	128.44	110.80
1	A	15	GLN	CA-CB-CG	8.26	130.61	114.10
1	B	24	GLU	CB-CG-CD	8.24	126.61	112.60
1	B	124	ASP	O-C-N	8.24	133.54	122.82
1	B	13	PRO	CA-C-O	-8.23	105.62	120.60
1	A	125	ASP	CA-CB-CG	-8.21	104.39	112.60
1	B	17	ILE	CB-CA-C	8.20	123.12	110.50
1	B	81	VAL	O-C-N	8.18	132.79	122.57
1	A	32	TRP	CA-C-O	-8.16	112.52	121.33
1	A	110	HIS	N-CA-CB	-8.15	96.71	110.49
1	B	143	ARG	N-CA-C	-8.15	93.57	107.99
1	B	55	ALA	N-CA-CB	8.14	124.11	110.69
1	A	14	VAL	CA-CB-CG1	-8.13	96.58	110.40
1	B	121	GLU	N-CA-C	8.12	121.16	111.33
1	B	5	VAL	O-C-N	8.11	132.19	123.02
1	B	54	THR	N-CA-CB	-8.09	98.23	110.12
1	B	131	ASN	OD1-CG-ND2	-8.07	114.53	122.60
1	A	77	GLU	CA-C-O	8.06	128.13	119.03
1	B	77	GLU	CB-CG-CD	8.05	126.29	112.60
1	B	75	LYS	O-C-N	-8.02	111.12	121.95
1	A	146	CYS	CA-C-O	-8.01	112.66	121.23
1	A	137	THR	CA-C-N	-8.00	111.58	122.63
1	A	137	THR	C-N-CA	-8.00	111.58	122.63
1	A	105	SER	CB-CA-C	-8.00	100.49	113.37
1	B	48	HIS	CA-C-O	8.00	129.58	120.54
1	B	112	ILE	N-CA-C	8.00	119.81	112.29
1	A	115	ARG	CD-NE-CZ	7.97	135.56	124.40
1	B	120	HIS	ND1-CE1-NE2	7.96	116.36	108.40
1	B	7	VAL	CA-C-O	7.95	130.45	120.75
1	A	75	LYS	CA-CB-CG	7.94	129.97	114.10
1	A	110	HIS	CA-C-O	7.93	131.85	120.51
1	A	19	ASN	O-C-N	7.91	133.31	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	GLY	N-CA-C	-7.90	96.22	112.34
1	B	132	GLU	N-CA-CB	7.90	121.95	110.58
1	B	104	ILE	CA-C-N	7.89	132.66	120.75
1	B	104	ILE	C-N-CA	7.89	132.66	120.75
1	B	113	ILE	CA-C-O	7.89	129.47	121.58
1	A	2	THR	OG1-CB-CG2	7.85	125.00	109.30
1	A	149	ILE	CA-C-O	7.85	131.49	120.89
1	B	153	GLN	CB-CG-CD	7.85	125.94	112.60
1	A	119	VAL	N-CA-C	-7.84	96.42	107.80
1	B	125	ASP	N-CA-C	7.84	123.39	112.72
1	B	112	ILE	N-CA-CB	-7.84	100.62	112.15
1	B	91	LYS	N-CA-CB	7.84	123.74	110.49
1	A	6	CYS	O-C-N	7.83	133.00	122.59
1	A	67	LEU	N-CA-C	-7.83	93.99	107.61
1	A	98	SER	N-CA-C	-7.82	96.71	108.99
1	A	80	HIS	ND1-CE1-NE2	7.82	116.22	108.40
1	B	101	ASP	CA-C-N	7.82	136.47	121.54
1	B	101	ASP	C-N-CA	7.82	136.47	121.54
1	A	89	ALA	O-C-N	-7.81	113.42	123.02
1	B	131	ASN	CA-CB-CG	7.79	120.39	112.60
1	B	150	GLY	N-CA-C	-7.78	99.52	111.12
1	B	20	PHE	N-CA-C	7.74	122.87	107.62
1	A	134	SER	N-CA-C	-7.73	95.57	110.56
1	B	122	LYS	CA-CB-CG	7.72	129.55	114.10
1	A	48	HIS	CB-CA-C	7.71	122.47	110.14
1	A	74	PRO	N-CD-CG	-7.70	91.65	103.20
1	B	83	ASP	O-C-N	7.70	132.05	123.04
1	B	99	ILE	N-CA-CB	7.69	126.30	111.92
1	A	133	GLU	CA-C-N	-7.69	111.02	121.71
1	A	133	GLU	C-N-CA	-7.69	111.02	121.71
1	B	107	SER	O-C-N	7.69	132.81	122.59
1	B	54	THR	O-C-N	7.68	130.26	122.12
1	B	104	ILE	N-CA-C	7.67	125.29	109.34
1	B	84	LEU	N-CA-C	-7.66	102.13	112.94
1	B	58	THR	CA-CB-OG1	7.65	121.08	109.60
1	A	129	GLY	N-CA-C	7.65	128.12	115.66
1	A	99	ILE	CB-CA-C	-7.64	104.56	111.74
1	B	65	ASN	CB-CG-ND2	-7.64	104.94	116.40
1	A	78	GLU	CA-CB-CG	7.64	129.38	114.10
1	B	144	LEU	CA-CB-CG	7.63	143.01	116.30
1	B	101	ASP	N-CA-C	-7.61	95.74	108.75
1	A	90	ASP	N-CA-C	-7.59	94.63	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	GLU	CB-CG-CD	7.59	125.50	112.60
1	A	111	CYS	O-C-N	7.58	132.03	122.93
1	B	7	VAL	CB-CA-C	7.54	120.83	111.25
1	A	76	ASP	O-C-N	-7.53	111.92	121.78
1	A	129	GLY	CA-C-N	7.51	136.14	121.41
1	A	129	GLY	C-N-CA	7.51	136.14	121.41
1	A	87	VAL	CA-C-N	-7.50	112.37	122.72
1	A	87	VAL	C-N-CA	-7.50	112.37	122.72
1	B	15	GLN	CA-C-O	7.48	131.21	120.51
1	B	44	GLY	CA-C-N	-7.47	111.26	122.47
1	B	44	GLY	C-N-CA	-7.47	111.26	122.47
1	A	98	SER	N-CA-CB	7.45	125.38	111.52
1	B	118	VAL	N-CA-CB	7.44	123.64	111.44
1	B	43	HIS	N-CA-CB	-7.43	99.41	110.85
1	A	143	ARG	N-CA-C	-7.42	92.42	107.41
1	B	134	SER	O-C-N	7.41	130.89	122.22
1	A	111	CYS	CB-CA-C	7.39	123.00	110.81
1	B	54	THR	CB-CA-C	7.38	123.05	110.79
1	A	139	ASN	N-CA-C	7.38	126.52	110.80
1	A	14	VAL	O-C-N	7.38	130.86	122.97
1	A	119	VAL	CA-C-O	-7.38	112.64	120.53
1	B	120	HIS	N-CA-C	7.37	121.85	110.20
1	A	9	LYS	CA-C-N	7.37	129.50	120.51
1	A	9	LYS	C-N-CA	7.37	129.50	120.51
1	A	31	VAL	CA-C-N	-7.36	109.01	121.75
1	A	31	VAL	C-N-CA	-7.36	109.01	121.75
1	A	4	ALA	CA-C-O	-7.36	114.28	122.01
1	B	44	GLY	O-C-N	7.31	130.41	122.96
1	B	83	ASP	N-CA-CB	7.30	121.26	109.95
1	A	125	ASP	CA-C-O	-7.28	109.93	119.10
1	B	102	SER	CA-C-N	7.27	131.96	120.47
1	B	102	SER	C-N-CA	7.27	131.96	120.47
1	B	14	VAL	N-CA-CB	-7.25	99.26	111.23
1	A	61	GLY	CA-C-N	7.25	128.91	119.84
1	A	61	GLY	C-N-CA	7.25	128.91	119.84
1	B	38	LEU	CA-C-N	7.24	132.85	121.56
1	B	38	LEU	C-N-CA	7.24	132.85	121.56
1	A	60	ALA	N-CA-CB	-7.24	98.02	110.32
1	A	77	GLU	CA-C-N	-7.21	113.47	122.84
1	A	77	GLU	C-N-CA	-7.21	113.47	122.84
1	A	74	PRO	CA-C-N	7.20	132.22	120.63
1	A	74	PRO	C-N-CA	7.20	132.22	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	LYS	N-CA-CB	-7.18	98.59	110.65
1	B	20	PHE	O-C-N	7.15	132.31	123.01
1	A	94	VAL	N-CA-C	-7.15	94.47	109.34
1	B	74	PRO	N-CA-C	-7.14	97.76	112.47
1	A	105	SER	CA-C-O	-7.12	113.22	120.77
1	A	19	ASN	N-CA-C	7.12	121.18	110.14
1	B	109	ASP	CA-C-O	-7.11	110.35	120.51
1	B	148	VAL	CA-CB-CG2	7.11	122.48	110.40
1	B	40	GLU	CA-CB-CG	7.09	128.29	114.10
1	B	111	CYS	CA-C-N	-7.08	112.22	122.28
1	B	111	CYS	C-N-CA	-7.08	112.22	122.28
1	B	17	ILE	CA-C-O	-7.08	112.75	120.67
1	A	62	PRO	O-C-N	-7.07	113.09	122.64
1	A	144	LEU	CA-C-N	-7.07	110.62	122.29
1	A	144	LEU	C-N-CA	-7.07	110.62	122.29
1	B	92	ASP	O-C-N	7.07	131.50	122.39
1	B	60	ALA	N-CA-CB	-7.06	99.64	110.44
1	B	120	HIS	CE1-NE2-CD2	-7.06	101.94	109.00
1	B	99	ILE	O-C-N	7.05	131.04	123.00
1	A	52	ASP	CA-C-O	-7.05	113.50	121.39
1	B	20	PHE	CA-C-O	-7.04	112.67	120.70
1	B	58	THR	N-CA-C	7.01	121.42	113.01
1	A	14	VAL	CB-CA-C	7.00	120.98	110.90
1	A	29	VAL	N-CA-CB	7.00	118.92	110.31
1	A	83	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	137	THR	CA-C-O	6.99	127.30	119.41
1	A	5	VAL	O-C-N	6.98	131.30	122.57
1	A	70	LYS	N-CA-C	-6.97	99.55	110.36
1	A	3	LYS	CA-C-O	6.96	130.47	120.51
1	A	134	SER	CA-C-O	-6.95	113.07	120.71
1	B	115	ARG	O-C-N	6.93	132.85	122.94
1	B	35	ILE	O-C-N	6.93	131.27	122.61
1	A	96	ASP	O-C-N	6.91	131.81	122.82
1	B	148	VAL	CA-C-N	6.91	131.47	121.80
1	B	148	VAL	C-N-CA	6.91	131.47	121.80
1	B	3	LYS	CA-C-N	-6.91	108.98	121.62
1	B	3	LYS	C-N-CA	-6.91	108.98	121.62
1	B	71	HIS	N-CA-CB	6.91	120.65	109.95
1	B	3	LYS	N-CA-CB	-6.89	99.33	111.39
1	B	126	LEU	N-CA-CB	-6.89	98.84	110.49
1	B	122	LYS	CA-C-O	6.87	130.05	121.46
1	B	79	ARG	CA-CB-CG	6.87	127.84	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	83	ASP	N-CA-C	6.86	119.03	109.15
1	B	92	ASP	N-CA-C	6.86	121.25	113.02
1	A	92	ASP	O-C-N	6.84	131.12	122.57
1	B	117	LEU	N-CA-C	-6.84	97.75	108.90
1	A	116	THR	OG1-CB-CG2	-6.84	95.63	109.30
1	A	86	ASN	N-CA-CB	-6.81	100.17	111.20
1	A	150	GLY	CA-C-N	-6.79	114.47	123.17
1	A	150	GLY	C-N-CA	-6.79	114.47	123.17
1	B	58	THR	CA-CB-CG2	-6.79	98.95	110.50
1	B	103	VAL	N-CA-C	6.79	119.53	111.05
1	A	133	GLU	O-C-N	6.78	132.33	122.43
1	A	54	THR	N-CA-C	6.75	125.17	110.80
1	B	45	PHE	CB-CA-C	6.74	120.80	111.23
1	B	62	PRO	N-CD-CG	-6.74	93.10	103.20
1	A	5	VAL	CA-C-N	-6.72	108.71	121.54
1	A	5	VAL	C-N-CA	-6.72	108.71	121.54
1	A	110	HIS	CA-CB-CG	6.72	120.52	113.80
1	B	71	HIS	CA-C-O	6.71	128.34	120.69
1	B	86	ASN	N-CA-CB	-6.71	100.44	111.66
1	A	47	VAL	O-C-N	-6.71	115.93	123.18
1	B	117	LEU	CB-CA-C	6.71	121.98	109.71
1	B	6	CYS	CB-CA-C	-6.70	102.36	110.94
1	B	95	ALA	N-CA-CB	6.70	121.02	110.84
1	B	2	THR	N-CA-CB	-6.67	100.15	110.29
1	A	139	ASN	OD1-CG-ND2	6.67	129.27	122.60
1	B	87	VAL	CB-CA-C	6.66	122.63	110.71
1	B	28	PRO	CB-CA-C	6.65	122.54	111.56
1	A	117	LEU	CA-C-N	-6.64	113.90	123.06
1	A	117	LEU	C-N-CA	-6.64	113.90	123.06
1	B	118	VAL	O-C-N	6.64	130.20	123.10
1	B	77	GLU	CA-C-O	6.62	127.63	120.55
1	B	86	ASN	O-C-N	6.61	130.79	123.25
1	B	5	VAL	N-CA-CB	6.61	124.59	112.36
1	B	11	ASP	CB-CA-C	6.60	121.76	111.13
1	B	34	SER	CB-CA-C	-6.59	103.06	111.70
1	B	91	LYS	CB-CA-C	-6.59	97.30	110.42
1	A	54	THR	CA-C-N	6.58	134.12	121.54
1	A	54	THR	C-N-CA	6.58	134.12	121.54
1	B	19	ASN	CA-C-N	-6.58	113.41	123.14
1	B	19	ASN	C-N-CA	-6.58	113.41	123.14
1	A	117	LEU	N-CA-CB	6.57	121.71	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	VAL	CG1-CB-CG2	-6.56	96.36	110.80
1	B	138	GLY	CA-C-N	6.55	134.05	121.54
1	B	138	GLY	C-N-CA	6.55	134.05	121.54
1	B	101	ASP	CA-C-O	-6.53	112.50	120.54
1	A	53	ASN	CA-C-O	6.53	131.17	119.36
1	A	139	ASN	O-C-N	6.53	131.27	122.59
1	B	69	ARG	CA-CB-CG	-6.52	101.05	114.10
1	A	140	ALA	N-CA-C	6.52	124.68	110.80
1	A	11	ASP	N-CA-C	-6.51	104.44	112.38
1	B	104	ILE	CA-CB-CG1	-6.51	99.34	110.40
1	B	103	VAL	CA-C-O	-6.50	113.61	120.57
1	B	124	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	1	ALA	CB-CA-C	-6.49	100.76	110.50
1	A	97	VAL	N-CA-CB	-6.49	101.60	110.56
1	A	5	VAL	N-CA-CB	6.48	121.92	111.23
1	B	153	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	B	149	ILE	N-CA-C	-6.47	98.96	108.54
1	B	144	LEU	CD1-CG-CD2	-6.47	96.56	110.80
1	A	9	LYS	CA-CB-CG	6.47	127.03	114.10
1	A	96	ASP	CA-C-N	-6.46	112.16	122.50
1	A	96	ASP	C-N-CA	-6.46	112.16	122.50
1	B	40	GLU	CB-CA-C	-6.46	99.41	109.61
1	B	136	LYS	CA-C-O	6.45	129.74	120.51
1	B	101	ASP	N-CA-CB	6.45	122.80	111.13
1	B	97	VAL	CA-C-O	-6.44	115.33	121.64
1	B	5	VAL	CG1-CB-CG2	-6.43	96.65	110.80
1	A	22	GLN	CA-C-O	6.42	128.35	120.25
1	B	60	ALA	CA-C-N	6.39	131.91	121.87
1	B	60	ALA	C-N-CA	6.39	131.91	121.87
1	B	34	SER	N-CA-CB	6.39	122.99	111.36
1	A	33	GLY	O-C-N	6.39	130.29	123.96
1	B	11	ASP	CA-C-O	6.39	128.28	120.55
1	A	73	GLY	N-CA-C	-6.39	99.31	112.34
1	A	10	GLY	CA-C-O	-6.38	113.93	121.08
1	A	143	ARG	NE-CZ-NH1	-6.38	115.12	121.50
1	B	13	PRO	N-CA-C	-6.36	99.37	112.47
1	B	64	PHE	N-CA-C	-6.35	100.50	109.96
1	A	28	PRO	N-CA-CB	-6.35	96.59	103.25
1	A	7	VAL	N-CA-CB	-6.31	103.23	111.82
1	B	123	ALA	N-CA-CB	-6.30	99.85	109.94
1	B	67	LEU	N-CA-C	6.30	124.22	110.80
1	A	22	GLN	N-CA-C	6.29	118.67	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	VAL	CA-C-N	6.29	131.63	122.77
1	A	47	VAL	C-N-CA	6.29	131.63	122.77
1	B	147	GLY	O-C-N	-6.28	117.72	123.56
1	B	65	ASN	CB-CG-OD1	6.28	133.36	120.80
1	B	137	THR	N-CA-CB	-6.28	99.89	110.49
1	B	79	ARG	CB-CA-C	-6.27	100.74	110.78
1	B	120	HIS	CA-C-O	6.27	128.20	121.05
1	A	112	ILE	CA-CB-CG2	6.26	121.14	110.50
1	B	29	VAL	CA-C-O	-6.25	113.07	121.32
1	B	107	SER	N-CA-CB	6.24	121.04	110.49
1	B	94	VAL	O-C-N	6.23	129.50	123.14
1	A	31	VAL	CA-C-O	6.23	126.96	120.36
1	A	36	LYS	CA-CB-CG	6.23	126.56	114.10
1	A	3	LYS	CG-CD-CE	6.23	125.62	111.30
1	A	78	GLU	CA-C-O	-6.22	114.07	120.54
1	A	59	SER	N-CA-CB	-6.22	99.75	110.32
1	A	139	ASN	CB-CG-ND2	-6.21	107.08	116.40
1	A	149	ILE	CA-CB-CG2	6.21	121.06	110.50
1	B	26	ASN	CA-C-N	6.21	131.63	121.87
1	B	26	ASN	C-N-CA	6.21	131.63	121.87
1	B	63	HIS	CE1-NE2-CD2	6.21	115.21	109.00
1	B	10	GLY	CA-C-N	-6.20	113.38	122.86
1	B	10	GLY	C-N-CA	-6.20	113.38	122.86
1	A	53	ASN	N-CA-C	-6.18	106.10	113.21
1	B	66	PRO	O-C-N	-6.18	114.29	122.64
1	B	126	LEU	N-CA-C	6.18	123.96	110.80
1	B	150	GLY	O-C-N	-6.17	118.30	123.73
1	B	19	ASN	CB-CG-ND2	-6.16	107.16	116.40
1	B	134	SER	N-CA-C	-6.16	104.62	111.71
1	B	132	GLU	N-CA-C	-6.16	97.80	108.52
1	B	49	GLU	N-CA-C	6.15	123.90	110.80
1	A	87	VAL	O-C-N	6.15	129.71	123.07
1	A	91	LYS	CD-CE-NZ	-6.15	92.23	111.90
1	A	110	HIS	CB-CA-C	6.14	122.64	110.42
1	B	119	VAL	CA-CB-CG1	6.14	120.83	110.40
1	A	104	ILE	CA-CB-CG1	6.14	120.83	110.40
1	B	138	GLY	CA-C-O	-6.13	109.91	120.57
1	B	87	VAL	N-CA-CB	-6.12	100.47	111.92
1	A	31	VAL	O-C-N	6.12	129.81	123.20
1	A	39	THR	N-CA-CB	6.12	119.05	109.69
1	B	30	LYS	N-CA-C	6.12	119.67	109.95
1	A	2	THR	CA-C-N	6.11	133.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	THR	C-N-CA	6.11	133.22	121.54
1	B	96	ASP	N-CA-CB	6.11	119.29	110.06
1	B	96	ASP	CA-C-O	-6.08	114.12	121.05
1	A	35	ILE	CB-CA-C	6.08	121.26	111.29
1	B	35	ILE	N-CA-C	-6.05	99.56	109.12
1	A	62	PRO	N-CA-CB	6.05	109.60	103.25
1	B	130	GLY	CA-C-N	6.05	133.09	121.54
1	B	130	GLY	C-N-CA	6.05	133.09	121.54
1	A	108	GLY	CA-C-O	-6.04	118.30	122.22
1	B	80	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	99	ILE	N-CA-CB	6.03	117.81	109.84
1	A	113	ILE	CB-CG1-CD1	6.03	126.47	113.80
1	A	114	GLY	CA-C-N	6.02	133.29	122.64
1	A	114	GLY	C-N-CA	6.02	133.29	122.64
1	A	115	ARG	N-CA-CB	5.98	120.14	110.51
1	B	38	LEU	CD1-CG-CD2	-5.98	97.64	110.80
1	A	139	ASN	CB-CA-C	-5.98	98.52	110.42
1	A	40	GLU	CA-C-N	-5.97	112.24	122.21
1	A	40	GLU	C-N-CA	-5.97	112.24	122.21
1	B	20	PHE	N-CA-CB	-5.97	100.37	110.46
1	B	100	GLU	N-CA-C	-5.97	97.23	107.61
1	A	143	ARG	CA-CB-CG	5.96	126.03	114.10
1	A	78	GLU	O-C-N	5.96	130.14	123.05
1	A	28	PRO	CA-C-N	-5.96	112.88	120.98
1	A	28	PRO	C-N-CA	-5.96	112.88	120.98
1	A	123	ALA	N-CA-CB	-5.96	100.54	109.71
1	A	6	CYS	N-CA-C	-5.95	98.12	110.80
1	A	151	ILE	CA-C-O	-5.95	114.26	120.51
1	B	40	GLU	CG-CD-OE1	5.95	132.08	118.40
1	A	32	TRP	CA-CB-CG	5.94	124.89	113.60
1	A	139	ASN	CA-C-O	-5.93	112.03	120.51
1	B	106	LEU	CA-C-O	-5.92	114.26	121.89
1	A	121	GLU	CA-C-O	-5.91	114.60	120.80
1	B	32	TRP	CA-CB-CG	5.88	124.78	113.60
1	B	77	GLU	O-C-N	-5.88	115.06	122.17
1	A	87	VAL	CA-C-O	-5.87	114.03	120.43
1	B	123	ALA	CA-C-O	5.86	127.22	120.60
1	B	89	ALA	O-C-N	5.86	129.43	122.46
1	A	48	HIS	N-CA-C	-5.85	98.74	108.34
1	B	135	THR	CB-CA-C	-5.85	98.49	109.72
1	A	127	GLY	CA-C-O	5.84	130.73	120.57
1	A	77	GLU	OE1-CD-OE2	-5.84	108.89	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ASN	CA-C-N	-5.83	112.56	119.84
1	B	65	ASN	C-N-CA	-5.83	112.56	119.84
1	A	135	THR	N-CA-CB	5.82	120.32	110.49
1	B	127	GLY	CA-C-O	5.82	127.92	120.36
1	A	40	GLU	CA-CB-CG	5.80	125.70	114.10
1	B	6	CYS	N-CA-CB	5.79	118.83	110.37
1	A	80	HIS	CA-C-O	-5.78	114.89	121.72
1	A	119	VAL	CB-CA-C	5.78	119.39	110.96
1	A	12	GLY	CA-C-N	5.78	127.06	119.84
1	A	12	GLY	C-N-CA	5.78	127.06	119.84
1	A	96	ASP	N-CA-CB	5.78	119.18	109.94
1	B	62	PRO	CA-C-N	-5.77	110.47	120.97
1	B	62	PRO	C-N-CA	-5.77	110.47	120.97
1	B	140	ALA	CA-C-O	-5.77	113.58	120.10
1	B	133	GLU	CA-C-N	5.76	128.58	120.28
1	B	133	GLU	C-N-CA	5.76	128.58	120.28
1	A	110	HIS	ND1-CE1-NE2	5.75	114.16	108.40
1	A	77	GLU	CB-CA-C	5.74	119.62	109.75
1	B	6	CYS	CA-C-N	5.74	129.66	122.43
1	B	6	CYS	C-N-CA	5.74	129.66	122.43
1	A	19	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	B	26	ASN	CB-CA-C	5.73	121.82	110.42
1	A	66	PRO	CA-N-CD	-5.72	104.00	112.00
1	A	128	LYS	CA-CB-CG	5.72	125.53	114.10
1	A	57	CYS	CA-C-N	5.71	134.13	121.80
1	A	57	CYS	C-N-CA	5.71	134.13	121.80
1	A	74	PRO	O-C-N	-5.69	114.96	122.64
1	B	147	GLY	CA-C-O	5.69	127.57	121.37
1	A	52	ASP	CA-C-N	-5.68	111.01	122.55
1	A	52	ASP	C-N-CA	-5.68	111.01	122.55
1	B	76	ASP	O-C-N	5.68	129.79	122.23
1	A	77	GLU	CG-CD-OE1	5.67	131.45	118.40
1	A	117	LEU	N-CA-C	-5.67	99.66	108.90
1	A	58	THR	N-CA-C	-5.66	103.88	112.04
1	A	60	ALA	O-C-N	5.66	129.75	122.39
1	A	140	ALA	CA-C-N	5.66	132.50	121.41
1	A	140	ALA	C-N-CA	5.66	132.50	121.41
1	B	149	ILE	CB-CG1-CD1	5.65	125.67	113.80
1	A	29	VAL	N-CA-C	-5.65	102.24	109.30
1	A	57	CYS	O-C-N	-5.64	115.57	122.34
1	A	47	VAL	N-CA-C	-5.63	100.37	108.48
1	B	104	ILE	O-C-N	-5.63	115.54	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	THR	O-C-N	5.61	130.37	122.41
1	B	143	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	B	67	LEU	CA-C-N	5.59	132.22	121.54
1	B	67	LEU	C-N-CA	5.59	132.22	121.54
1	A	140	ALA	N-CA-CB	-5.58	101.05	110.49
1	B	52	ASP	N-CA-CB	5.58	119.53	110.43
1	B	31	VAL	N-CA-CB	5.58	119.67	111.52
1	A	120	HIS	CA-CB-CG	5.58	119.38	113.80
1	B	143	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	A	111	CYS	N-CA-CB	-5.55	101.38	110.21
1	B	15	GLN	CB-CA-C	5.55	121.46	110.42
1	A	98	SER	O-C-N	5.54	129.59	123.33
1	B	148	VAL	CA-C-O	5.54	126.50	120.57
1	B	102	SER	CA-C-O	5.53	128.41	120.51
1	A	135	THR	O-C-N	5.52	129.93	122.59
1	A	38	LEU	CA-C-O	5.50	127.92	121.87
1	B	33	GLY	CA-C-N	5.50	131.94	121.87
1	B	33	GLY	C-N-CA	5.50	131.94	121.87
1	A	133	GLU	CA-C-O	-5.50	112.07	119.11
1	B	128	LYS	CA-CB-CG	5.50	125.10	114.10
1	A	24	GLU	O-C-N	-5.47	115.32	122.59
1	B	92	ASP	CA-C-N	5.46	132.12	121.41
1	B	92	ASP	C-N-CA	5.46	132.12	121.41
1	A	137	THR	O-C-N	-5.46	114.61	122.36
1	B	43	HIS	N-CA-C	5.45	118.59	110.14
1	A	94	VAL	CA-C-O	-5.45	113.97	120.78
1	B	38	LEU	CB-CA-C	5.45	118.72	109.84
1	B	85	GLY	N-CA-C	5.45	126.09	113.18
1	A	115	ARG	N-CA-C	-5.44	101.96	110.17
1	A	127	GLY	CA-C-N	5.44	131.92	121.54
1	A	127	GLY	C-N-CA	5.44	131.92	121.54
1	A	66	PRO	CA-C-O	-5.43	110.71	120.60
1	B	62	PRO	CA-N-CD	-5.43	104.39	112.00
1	B	32	TRP	N-CA-C	-5.42	98.72	108.48
1	B	79	ARG	CG-CD-NE	5.42	123.92	112.00
1	B	63	HIS	N-CA-CB	5.42	118.10	110.36
1	B	78	GLU	CA-C-N	5.41	129.88	122.84
1	B	78	GLU	C-N-CA	5.41	129.88	122.84
1	A	133	GLU	N-CA-C	-5.41	106.63	113.18
1	B	21	GLU	CB-CA-C	-5.41	100.27	109.51
1	A	153	GLN	CB-CG-CD	5.40	121.78	112.60
1	B	106	LEU	N-CA-C	5.40	116.92	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	VAL	CA-CB-CG2	5.39	119.57	110.40
1	B	107	SER	CA-C-N	5.38	131.96	121.41
1	B	107	SER	C-N-CA	5.38	131.96	121.41
1	B	113	ILE	O-C-N	-5.38	117.08	122.62
1	A	118	VAL	O-C-N	5.37	128.98	123.18
1	A	92	ASP	CA-C-N	5.36	131.92	121.41
1	A	92	ASP	C-N-CA	5.36	131.92	121.41
1	A	30	LYS	CA-C-N	-5.36	115.54	122.99
1	A	30	LYS	C-N-CA	-5.36	115.54	122.99
1	B	122	LYS	O-C-N	-5.36	115.59	122.72
1	A	125	ASP	N-CA-C	5.36	119.30	112.87
1	B	11	ASP	N-CA-CB	-5.35	102.40	111.17
1	B	69	ARG	CB-CG-CD	5.35	123.60	111.30
1	B	86	ASN	CA-C-O	-5.34	115.56	121.33
1	B	104	ILE	CA-CB-CG2	5.34	119.59	110.50
1	A	15	GLN	N-CA-CB	-5.34	102.64	110.97
1	B	148	VAL	N-CA-CB	5.34	117.40	110.99
1	A	68	SER	N-CA-CB	-5.34	101.47	110.49
1	B	110	HIS	N-CA-CB	-5.33	104.15	112.41
1	B	151	ILE	N-CA-C	-5.33	101.86	108.89
1	A	90	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	24	GLU	CA-C-N	5.32	131.70	121.54
1	B	24	GLU	C-N-CA	5.32	131.70	121.54
1	B	99	ILE	CA-CB-CG2	5.31	119.53	110.50
1	A	115	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	B	136	LYS	O-C-N	5.30	129.65	122.59
1	A	18	ILE	O-C-N	5.30	128.98	123.26
1	A	109	ASP	OD1-CG-OD2	-5.29	110.20	122.90
1	B	45	PHE	CA-CB-CG	5.29	119.08	113.80
1	A	152	ALA	CA-C-O	5.28	128.06	120.51
1	B	100	GLU	CA-C-N	-5.27	112.66	121.94
1	B	100	GLU	C-N-CA	-5.27	112.66	121.94
1	A	118	VAL	CB-CA-C	5.27	118.47	110.62
1	B	123	ALA	CB-CA-C	5.27	119.57	110.77
1	A	69	ARG	CG-CD-NE	-5.27	100.42	112.00
1	B	9	LYS	O-C-N	-5.26	116.53	123.21
1	A	95	ALA	O-C-N	5.23	129.59	122.48
1	A	7	VAL	N-CA-C	-5.22	100.04	107.77
1	A	44	GLY	CA-C-N	5.22	129.04	121.26
1	A	44	GLY	C-N-CA	5.22	129.04	121.26
1	A	81	VAL	CA-CB-CG2	5.21	119.26	110.40
1	B	94	VAL	N-CA-CB	5.21	120.84	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	GLY	CA-C-O	-5.20	111.52	120.57
1	A	91	LYS	N-CA-CB	5.20	117.66	110.17
1	A	75	LYS	CB-CG-CD	5.17	123.20	111.30
1	A	119	VAL	O-C-N	5.17	129.15	123.10
1	B	65	ASN	N-CA-CB	5.15	119.54	110.37
1	A	46	HIS	N-CA-C	5.15	117.36	109.95
1	B	59	SER	CB-CA-C	5.14	119.25	110.56
1	B	63	HIS	CG-CD2-NE2	-5.14	102.06	107.20
1	A	19	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	59	SER	CA-CB-OG	-5.14	100.82	111.10
1	A	120	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
1	B	97	VAL	CB-CA-C	-5.14	102.45	110.52
1	B	142	SER	N-CA-C	5.13	121.74	110.80
1	A	113	ILE	N-CA-C	-5.13	102.88	109.30
1	B	128	LYS	CB-CG-CD	5.11	123.06	111.30
1	A	104	ILE	CB-CA-C	5.11	118.94	111.33
1	A	116	THR	CA-C-O	-5.09	115.15	121.11
1	B	90	ASP	CA-C-O	-5.08	115.87	120.95
1	B	35	ILE	CA-CB-CG2	5.08	119.14	110.50
1	B	72	GLY	CA-C-O	5.08	127.38	121.90
1	B	112	ILE	CB-CA-C	5.08	118.83	111.88
1	B	153	GLN	CA-CB-CG	5.08	124.25	114.10
1	A	86	ASN	CB-CG-ND2	-5.07	108.80	116.40
1	B	23	LYS	CA-C-O	5.07	127.75	120.51
1	A	32	TRP	CB-CG-CD1	5.06	134.49	126.90
1	B	137	THR	CA-C-O	-5.05	113.29	120.51
1	A	83	ASP	O-C-N	5.04	129.57	122.77
1	A	143	ARG	CA-C-O	-5.04	114.92	121.11
1	A	87	VAL	N-CA-CB	-5.03	103.44	111.58
1	B	32	TRP	N-CA-CB	5.03	119.06	110.71
1	A	143	ARG	CA-C-N	-5.02	112.28	121.52
1	A	143	ARG	C-N-CA	-5.02	112.28	121.52
1	B	5	VAL	CA-CB-CG1	5.01	118.92	110.40
1	B	95	ALA	O-C-N	5.01	129.73	123.12
1	B	153	GLN	CG-CD-NE2	5.01	123.91	116.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1113	0	1076	146	0
1	B	1113	0	1076	165	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	2230	0	2152	302	0

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 69.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG21	1:B:143:ARG:HB3	1.33	1.10
1:B:42:LEU:HD22	1:B:86:ASN:OD1	1.59	1.03
1:A:152:ALA:HA	1:B:52:ASP:HB2	1.41	1.02
1:B:18:ILE:HD13	1:B:45:PHE:HZ	1.29	0.97
1:A:35:ILE:HD11	1:A:119:VAL:HG21	1.44	0.97
1:A:66:PRO:HG2	1:A:81:VAL:HG11	1.46	0.96
1:B:72:GLY:HA2	1:B:79:ARG:HA	1.45	0.96
1:B:31:VAL:O	1:B:98:SER:HA	1.70	0.91
1:A:125:ASP:O	1:A:128:LYS:NZ	2.05	0.88
1:A:122:LYS:NZ	1:A:139:ASN:HD22	1.72	0.88
1:B:18:ILE:HD13	1:B:45:PHE:CZ	2.10	0.85
1:B:6:CYS:SG	1:B:147:GLY:HA3	2.17	0.83
1:A:5:VAL:HG22	1:A:6:CYS:H	1.44	0.82
1:A:122:LYS:HZ2	1:A:139:ASN:HD22	1.25	0.81
1:A:52:ASP:HB3	1:A:54:THR:OG1	1.81	0.80
1:A:6:CYS:HB2	1:A:149:ILE:HG13	1.64	0.80
1:B:97:VAL:HG12	1:B:98:SER:H	1.47	0.79
1:B:41:GLY:O	1:B:88:THR:HA	1.82	0.79
1:B:20:PHE:HA	1:B:30:LYS:O	1.82	0.79
1:B:43:HIS:O	1:B:86:ASN:HA	1.82	0.79
1:A:152:ALA:HB1	1:A:153:GLN:NE2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HB1	1:B:93:GLY:HA2	1.65	0.78
1:A:118:VAL:HG22	1:A:146:CYS:HB3	1.64	0.77
1:B:118:VAL:HG21	1:B:143:ARG:CB	2.12	0.77
1:B:31:VAL:HG22	1:B:99:ILE:HB	1.65	0.77
1:A:104:ILE:HD13	1:A:112:ILE:HD13	1.66	0.77
1:B:74:PRO:HD2	1:B:126:LEU:CD2	2.16	0.74
1:B:38:LEU:HD23	1:B:93:GLY:O	1.87	0.74
1:B:50:PHE:O	1:B:60:ALA:HA	1.86	0.74
1:A:64:PHE:CD2	1:A:81:VAL:HG13	2.22	0.74
1:A:122:LYS:NZ	1:A:139:ASN:ND2	2.35	0.74
1:A:112:ILE:O	1:A:115:ARG:HB2	1.89	0.73
1:A:118:VAL:HG11	1:A:143:ARG:HG3	1.69	0.73
1:B:97:VAL:HG12	1:B:98:SER:N	2.05	0.72
1:B:18:ILE:CD1	1:B:45:PHE:HZ	2.00	0.71
1:B:39:THR:O	1:B:43:HIS:NE2	2.21	0.71
1:A:122:LYS:HZ2	1:A:139:ASN:ND2	1.89	0.71
1:A:57:CYS:HB3	1:A:143:ARG:HG2	1.72	0.70
1:B:71:HIS:HA	1:B:80:HIS:CE1	2.26	0.70
1:B:72:GLY:HA2	1:B:79:ARG:CA	2.18	0.70
1:A:109:ASP:O	1:A:111:CYS:HB2	1.92	0.70
1:B:74:PRO:HD2	1:B:126:LEU:HD23	1.74	0.69
1:A:105:SER:OG	1:A:110:HIS:HB2	1.93	0.68
1:A:79:ARG:HH11	1:A:79:ARG:HB2	1.56	0.68
1:B:71:HIS:O	1:B:128:LYS:NZ	2.21	0.67
1:A:22:GLN:OE1	1:A:106:LEU:HB2	1.95	0.67
1:A:14:VAL:HG12	1:A:37:GLY:HA3	1.75	0.67
1:A:117:LEU:HB2	1:A:149:ILE:CD1	2.24	0.67
1:A:52:ASP:C	1:A:54:THR:H	2.02	0.66
1:A:109:ASP:O	1:A:111:CYS:N	2.28	0.66
1:B:80:HIS:HB2	1:B:83:ASP:OD1	1.96	0.66
1:A:118:VAL:CG1	1:A:143:ARG:HG3	2.26	0.66
1:A:4:ALA:HB3	1:A:20:PHE:HB2	1.77	0.65
1:B:18:ILE:CD1	1:B:45:PHE:CZ	2.78	0.65
1:B:71:HIS:HA	1:B:80:HIS:ND1	2.12	0.65
1:A:105:SER:O	1:A:106:LEU:HD23	1.96	0.65
1:B:80:HIS:HB2	1:B:83:ASP:CG	2.21	0.64
1:A:84:LEU:HD21	1:A:104:ILE:HG12	1.79	0.64
1:A:5:VAL:O	1:A:149:ILE:HA	1.98	0.64
1:A:81:VAL:HG23	1:A:103:VAL:HG12	1.79	0.64
1:B:64:PHE:CD2	1:B:112:ILE:HG22	2.32	0.64
1:B:65:ASN:HD21	1:B:68:SER:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG11	1:B:143:ARG:HG2	1.79	0.63
1:A:79:ARG:HH11	1:A:79:ARG:CB	2.12	0.63
1:B:46:HIS:HB3	1:B:63:HIS:CD2	2.33	0.63
1:B:19:ASN:ND2	1:B:32:TRP:NE1	2.46	0.62
1:A:106:LEU:HD22	1:A:113:ILE:HD11	1.81	0.62
1:A:18:ILE:HD12	1:A:45:PHE:CZ	2.34	0.62
1:B:122:LYS:HB3	1:B:140:ALA:O	1.99	0.62
1:B:72:GLY:CA	1:B:79:ARG:HA	2.26	0.62
1:B:46:HIS:HB3	1:B:63:HIS:HD2	1.64	0.62
1:A:74:PRO:HD2	1:A:75:LYS:H	1.65	0.61
1:B:5:VAL:HG13	1:B:6:CYS:N	2.14	0.61
1:B:112:ILE:HA	1:B:115:ARG:HE	1.63	0.61
1:B:65:ASN:HD21	1:B:68:SER:N	1.98	0.61
1:B:9:LYS:HZ2	1:B:9:LYS:HB3	1.65	0.60
1:A:18:ILE:HD12	1:A:45:PHE:HZ	1.66	0.60
1:A:43:HIS:O	1:A:86:ASN:HA	2.01	0.60
1:A:106:LEU:HD22	1:A:113:ILE:CD1	2.32	0.60
1:A:117:LEU:HB2	1:A:149:ILE:HD11	1.82	0.60
1:A:121:GLU:HB2	1:A:144:LEU:HG	1.84	0.60
1:B:64:PHE:O	1:B:81:VAL:HB	2.02	0.60
1:A:124:ASP:OD1	1:A:126:LEU:HD23	2.01	0.60
1:A:50:PHE:O	1:A:60:ALA:HA	2.02	0.60
1:B:45:PHE:HD2	1:B:119:VAL:HG23	1.67	0.59
1:A:122:LYS:HE3	1:A:139:ASN:O	2.01	0.59
1:A:118:VAL:HG11	1:A:143:ARG:CG	2.32	0.59
1:A:125:ASP:HB2	1:A:139:ASN:HB2	1.84	0.59
1:A:31:VAL:HG13	1:A:99:ILE:HB	1.84	0.59
1:B:64:PHE:CE2	1:B:112:ILE:HG22	2.38	0.59
1:B:81:VAL:HG13	1:B:103:VAL:CG1	2.33	0.59
1:B:113:ILE:HG23	1:B:150:GLY:HA2	1.85	0.59
1:A:64:PHE:HB3	1:A:82:GLY:HA3	1.84	0.58
1:B:57:CYS:SG	1:B:145:ALA:C	2.86	0.58
1:A:118:VAL:HG22	1:A:146:CYS:CB	2.32	0.58
1:B:15:GLN:O	1:B:36:LYS:HB2	2.03	0.58
1:A:118:VAL:HG11	1:A:143:ARG:CD	2.33	0.58
1:B:46:HIS:CE1	1:B:71:HIS:HE1	2.21	0.58
1:A:13:PRO:HG2	1:A:14:VAL:HG13	1.84	0.58
1:A:46:HIS:HD1	1:A:120:HIS:CD2	2.11	0.57
1:A:13:PRO:C	1:A:14:VAL:HG13	2.28	0.57
1:B:31:VAL:CG2	1:B:99:ILE:HB	2.34	0.57
1:A:64:PHE:HB3	1:A:82:GLY:CA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD21	1:A:104:ILE:CG1	2.35	0.57
1:B:73:GLY:O	1:B:74:PRO:C	2.48	0.57
1:B:15:GLN:O	1:B:36:LYS:HE2	2.06	0.56
1:B:65:ASN:ND2	1:B:68:SER:H	2.03	0.56
1:A:40:GLU:HA	1:A:89:ALA:HB3	1.85	0.56
1:A:49:GLU:HG3	1:A:115:ARG:HH21	1.70	0.56
1:A:65:ASN:ND2	1:A:68:SER:HA	2.20	0.56
1:B:81:VAL:HG13	1:B:103:VAL:HG12	1.86	0.56
1:B:43:HIS:O	1:B:87:VAL:HG22	2.06	0.56
1:A:6:CYS:SG	1:A:149:ILE:HD12	2.45	0.56
1:A:35:ILE:CD1	1:A:119:VAL:HG21	2.26	0.56
1:A:134:SER:O	1:A:136:LYS:N	2.39	0.56
1:B:32:TRP:HA	1:B:97:VAL:O	2.06	0.55
1:B:14:VAL:O	1:B:36:LYS:O	2.25	0.55
1:B:53:ASN:HA	1:B:56:GLY:O	2.07	0.55
1:B:118:VAL:HG23	1:B:145:ALA:O	2.06	0.55
1:A:65:ASN:ND2	1:A:69:ARG:N	2.54	0.55
1:A:118:VAL:HG11	1:A:143:ARG:HD2	1.88	0.55
1:B:109:ASP:OD1	1:B:110:HIS:N	2.40	0.55
1:A:42:LEU:HB3	1:A:86:ASN:OD1	2.06	0.55
1:B:79:ARG:O	1:B:79:ARG:HD3	2.07	0.54
1:B:19:ASN:HD21	1:B:32:TRP:NE1	2.05	0.54
1:B:127:GLY:C	1:B:129:GLY:N	2.65	0.54
1:B:128:LYS:C	1:B:130:GLY:H	2.15	0.54
1:B:35:ILE:CG2	1:B:38:LEU:HD13	2.39	0.53
1:A:124:ASP:HB3	1:A:126:LEU:CD2	2.38	0.53
1:B:42:LEU:HD13	1:B:86:ASN:OD1	2.08	0.53
1:B:74:PRO:CD	1:B:126:LEU:HD23	2.39	0.53
1:A:113:ILE:HA	1:A:149:ILE:HG22	1.90	0.53
1:A:106:LEU:O	1:A:107:SER:HB2	2.08	0.53
1:A:5:VAL:HG22	1:A:6:CYS:N	2.21	0.53
1:B:4:ALA:HB3	1:B:20:PHE:HB2	1.91	0.53
1:B:29:VAL:HG11	1:B:104:ILE:HG22	1.91	0.52
1:A:98:SER:C	1:A:99:ILE:HG12	2.35	0.52
1:B:46:HIS:O	1:B:117:LEU:HG	2.10	0.52
1:A:124:ASP:CG	1:A:126:LEU:HD23	2.35	0.52
1:B:48:HIS:CD2	1:B:118:VAL:HG12	2.43	0.52
1:B:134:SER:O	1:B:138:GLY:HA2	2.10	0.52
1:A:34:SER:C	1:A:35:ILE:HG22	2.35	0.51
1:B:69:ARG:NH1	1:B:78:GLU:CD	2.68	0.51
1:A:24:GLU:O	1:A:25:SER:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:O	1:A:136:LYS:HG3	2.10	0.51
1:A:46:HIS:ND1	1:A:120:HIS:CD2	2.78	0.51
1:B:111:CYS:SG	1:B:113:ILE:HD13	2.51	0.51
1:B:63:HIS:HB3	1:B:82:GLY:HA3	1.91	0.51
1:A:98:SER:O	1:A:99:ILE:HG12	2.11	0.51
1:A:122:LYS:HZ1	1:A:139:ASN:HD22	1.57	0.50
1:A:79:ARG:HH11	1:A:79:ARG:CG	2.22	0.50
1:A:116:THR:HG22	1:A:118:VAL:HG23	1.93	0.50
1:B:127:GLY:C	1:B:129:GLY:H	2.19	0.50
1:B:19:ASN:O	1:B:31:VAL:HA	2.12	0.50
1:B:97:VAL:CG1	1:B:98:SER:N	2.76	0.49
1:A:104:ILE:HD12	1:A:104:ILE:C	2.38	0.49
1:B:35:ILE:HG21	1:B:38:LEU:HD13	1.93	0.49
1:A:45:PHE:CE2	1:A:117:LEU:HD21	2.47	0.49
1:A:120:HIS:O	1:A:144:LEU:HD11	2.12	0.49
1:B:34:SER:OG	1:B:36:LYS:NZ	2.45	0.49
1:B:128:LYS:C	1:B:130:GLY:N	2.70	0.49
1:B:29:VAL:HG11	1:B:104:ILE:O	2.12	0.48
1:A:104:ILE:HD12	1:A:104:ILE:O	2.12	0.48
1:B:29:VAL:HG11	1:B:104:ILE:C	2.38	0.48
1:B:5:VAL:CG1	1:B:6:CYS:N	2.77	0.48
1:B:23:LYS:HB3	1:B:24:GLU:OE1	2.14	0.48
1:A:66:PRO:HG2	1:A:81:VAL:CG1	2.33	0.48
1:A:124:ASP:HB3	1:A:126:LEU:HD21	1.95	0.48
1:B:38:LEU:HG	1:B:89:ALA:HB2	1.96	0.48
1:B:69:ARG:NH2	1:B:78:GLU:HG2	2.29	0.48
1:A:72:GLY:HA3	1:A:78:GLU:O	2.14	0.47
1:A:99:ILE:HG22	1:A:100:GLU:N	2.29	0.47
1:B:45:PHE:CD2	1:B:119:VAL:HG23	2.47	0.47
1:B:51:GLY:HA2	1:B:116:THR:OG1	2.13	0.47
1:B:71:HIS:HB2	1:B:135:THR:O	2.14	0.47
1:A:153:GLN:NE2	1:A:153:GLN:H	2.12	0.47
1:B:14:VAL:HG11	1:B:144:LEU:O	2.14	0.47
1:A:33:GLY:C	1:A:34:SER:OG	2.58	0.47
1:A:74:PRO:HG3	1:A:84:LEU:O	2.14	0.47
1:A:125:ASP:C	1:A:128:LYS:NZ	2.72	0.47
1:B:48:HIS:HB3	1:B:60:ALA:O	2.15	0.47
1:B:50:PHE:C	1:B:52:ASP:H	2.22	0.47
1:B:74:PRO:HD2	1:B:126:LEU:HD21	1.94	0.47
1:B:14:VAL:HA	1:B:36:LYS:O	2.15	0.47
1:B:42:LEU:CD2	1:B:86:ASN:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ALA:C	1:B:152:ALA:HB2	2.40	0.47
1:A:12:GLY:C	1:A:14:VAL:H	2.21	0.47
1:A:29:VAL:HG22	1:A:106:LEU:HG	1.97	0.47
1:A:5:VAL:HG13	1:A:6:CYS:N	2.30	0.46
1:A:91:LYS:HE3	1:A:91:LYS:HA	1.97	0.46
1:A:65:ASN:OD1	1:A:80:HIS:HB3	2.15	0.46
1:B:112:ILE:HA	1:B:115:ARG:NE	2.29	0.46
1:B:127:GLY:O	1:B:129:GLY:N	2.48	0.46
1:A:70:LYS:HB3	1:A:135:THR:HG22	1.98	0.46
1:A:6:CYS:SG	1:A:148:VAL:C	2.98	0.46
1:A:89:ALA:HA	1:A:95:ALA:HB2	1.98	0.46
1:A:134:SER:O	1:A:135:THR:C	2.59	0.46
1:B:19:ASN:HD21	1:B:32:TRP:HE1	1.63	0.46
1:B:112:ILE:O	1:B:115:ARG:HG3	2.16	0.46
1:B:46:HIS:NE2	1:B:83:ASP:HB3	2.31	0.46
1:B:106:LEU:HD22	1:B:113:ILE:HD11	1.97	0.46
1:A:65:ASN:ND2	1:A:69:ARG:H	2.13	0.46
1:A:52:ASP:C	1:A:54:THR:N	2.73	0.45
1:B:138:GLY:O	1:B:140:ALA:N	2.49	0.45
1:A:151:ILE:N	1:B:114:GLY:O	2.50	0.45
1:B:72:GLY:H	1:B:80:HIS:HD1	1.65	0.45
1:B:99:ILE:CG2	1:B:100:GLU:N	2.80	0.45
1:A:109:ASP:HB2	1:A:110:HIS:H	1.13	0.45
1:A:14:VAL:HG12	1:A:37:GLY:CA	2.44	0.45
1:B:48:HIS:ND1	1:B:61:GLY:O	2.45	0.45
1:A:54:THR:HG22	1:B:17:ILE:HD11	1.98	0.45
1:A:152:ALA:HB1	1:A:153:GLN:HE22	1.77	0.45
1:B:49:GLU:OE2	1:B:50:PHE:CZ	2.70	0.44
1:B:65:ASN:HD21	1:B:68:SER:CA	2.30	0.44
1:B:97:VAL:CG1	1:B:98:SER:H	2.25	0.44
1:A:45:PHE:CE1	1:A:119:VAL:HB	2.52	0.44
1:A:151:ILE:HB	1:B:114:GLY:O	2.17	0.44
1:B:132:GLU:O	1:B:133:GLU:HB2	2.15	0.44
1:A:65:ASN:HD21	1:A:69:ARG:N	2.15	0.44
1:A:151:ILE:O	1:B:51:GLY:N	2.50	0.44
1:B:9:LYS:CD	1:B:15:GLN:HG3	2.46	0.44
1:A:17:ILE:HG23	1:B:54:THR:HG22	1.99	0.44
1:A:13:PRO:HD2	1:A:14:VAL:HG22	1.99	0.44
1:A:46:HIS:HB3	1:A:63:HIS:CD2	2.52	0.44
1:A:79:ARG:NH1	1:A:83:ASP:O	2.49	0.44
1:A:114:GLY:HA3	1:B:150:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:HB2	1:B:83:ASP:OD2	2.17	0.44
1:B:106:LEU:CD2	1:B:113:ILE:HD11	2.48	0.44
1:B:8:LEU:HD11	1:B:119:VAL:HB	2.00	0.44
1:A:133:GLU:CD	1:A:136:LYS:HZ3	2.25	0.43
1:B:39:THR:O	1:B:43:HIS:CD2	2.71	0.43
1:A:57:CYS:HB3	1:A:143:ARG:CG	2.44	0.43
1:A:95:ALA:O	1:A:97:VAL:HG23	2.18	0.43
1:A:109:ASP:C	1:A:111:CYS:N	2.73	0.43
1:B:23:LYS:HB3	1:B:24:GLU:CD	2.42	0.43
1:B:106:LEU:HA	1:B:111:CYS:HA	2.00	0.43
1:A:79:ARG:CG	1:A:79:ARG:NH1	2.74	0.43
1:A:99:ILE:HG22	1:A:100:GLU:H	1.82	0.43
1:A:122:LYS:HZ1	1:A:139:ASN:ND2	2.10	0.43
1:A:151:ILE:O	1:B:50:PHE:HB3	2.18	0.43
1:B:9:LYS:HB3	1:B:9:LYS:NZ	2.31	0.43
1:B:133:GLU:OE1	1:B:139:ASN:ND2	2.52	0.43
1:B:46:HIS:CD2	1:B:83:ASP:HB3	2.53	0.43
1:B:139:ASN:HD22	1:B:139:ASN:HA	1.57	0.43
1:A:106:LEU:CD2	1:A:112:ILE:HD11	2.49	0.43
1:B:48:HIS:CD2	1:B:118:VAL:CG1	3.02	0.43
1:B:127:GLY:HA2	1:B:134:SER:O	2.19	0.43
1:B:44:GLY:HA3	1:B:120:HIS:HB2	2.00	0.43
1:B:38:LEU:CG	1:B:89:ALA:HB2	2.48	0.43
1:B:14:VAL:C	1:B:36:LYS:O	2.62	0.42
1:A:5:VAL:O	1:A:6:CYS:HB2	2.19	0.42
1:B:46:HIS:CD2	1:B:83:ASP:HA	2.55	0.42
1:B:35:ILE:HD11	1:B:45:PHE:HE2	1.84	0.42
1:A:65:ASN:O	1:A:67:LEU:N	2.52	0.42
1:B:65:ASN:CG	1:B:68:SER:H	2.28	0.42
1:B:79:ARG:NH2	1:B:83:ASP:O	2.53	0.42
1:A:118:VAL:HG12	1:A:120:HIS:CD2	2.54	0.42
1:A:131:ASN:ND2	1:A:134:SER:OG	2.53	0.42
1:A:134:SER:C	1:A:136:LYS:N	2.78	0.42
1:B:3:LYS:HD3	1:B:153:GLN:OXT	2.19	0.42
1:A:70:LYS:CB	1:A:135:THR:HG22	2.49	0.42
1:A:133:GLU:OE1	1:A:136:LYS:NZ	2.52	0.42
1:A:36:LYS:HB3	1:A:37:GLY:H	1.57	0.41
1:B:52:ASP:OD1	1:B:54:THR:HG23	2.20	0.41
1:B:66:PRO:HD3	1:B:81:VAL:HG21	2.02	0.41
1:B:78:GLU:O	1:B:128:LYS:NZ	2.53	0.41
1:B:69:ARG:CZ	1:B:78:GLU:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD21	1:B:119:VAL:HG11	2.02	0.41
1:B:22:GLN:HB2	1:B:29:VAL:HG23	2.01	0.41
1:B:61:GLY:HA3	1:B:62:PRO:HD3	1.72	0.41
1:A:52:ASP:HB3	1:A:54:THR:HG1	1.82	0.41
1:A:71:HIS:O	1:A:78:GLU:HG3	2.20	0.41
1:B:65:ASN:HD21	1:B:68:SER:HA	1.85	0.41
1:B:122:LYS:NZ	1:B:122:LYS:HB2	2.35	0.41
1:B:134:SER:HA	1:B:139:ASN:ND2	2.34	0.41
1:A:81:VAL:O	1:A:104:ILE:HG22	2.20	0.41
1:A:120:HIS:C	1:A:144:LEU:HD11	2.46	0.41
1:B:23:LYS:HZ3	1:B:24:GLU:CD	2.27	0.41
1:A:109:ASP:HB2	1:A:110:HIS:CG	2.55	0.41
1:B:23:LYS:HB3	1:B:24:GLU:H	1.71	0.41
1:A:40:GLU:CG	1:A:41:GLY:N	2.84	0.41
1:B:2:THR:C	1:B:3:LYS:HG3	2.46	0.41
1:B:117:LEU:HD23	1:B:117:LEU:C	2.46	0.41
1:A:6:CYS:CB	1:A:149:ILE:HG13	2.44	0.41
1:B:6:CYS:SG	1:B:147:GLY:CA	3.01	0.41
1:B:9:LYS:HD2	1:B:15:GLN:HG3	2.03	0.41
1:B:13:PRO:CG	1:B:13:PRO:O	2.68	0.41
1:B:80:HIS:O	1:B:81:VAL:HG23	2.21	0.41
1:A:6:CYS:SG	1:A:149:ILE:CD1	3.08	0.41
1:A:120:HIS:HB3	1:A:140:ALA:O	2.21	0.41
1:A:40:GLU:HG3	1:A:89:ALA:O	2.21	0.40
1:B:52:ASP:OD1	1:B:54:THR:CG2	2.69	0.40
1:A:36:LYS:HD3	1:A:94:VAL:HG22	2.02	0.40
1:A:151:ILE:H	1:B:51:GLY:C	2.29	0.40
1:B:47:VAL:HG22	1:B:117:LEU:HD12	2.02	0.40
1:B:79:ARG:NH1	1:B:83:ASP:O	2.54	0.40
1:B:7:VAL:HG23	1:B:17:ILE:HD12	2.03	0.40
1:B:45:PHE:CD2	1:B:87:VAL:HG11	2.55	0.40
1:A:124:ASP:CB	1:A:126:LEU:HD23	2.51	0.40
1:B:35:ILE:HD11	1:B:45:PHE:CE2	2.56	0.40
1:B:47:VAL:HA	1:B:117:LEU:HA	2.03	0.40
1:A:124:ASP:HB3	1:A:126:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	152/154 (99%)	96 (63%)	37 (24%)	19 (12%)	0	0
1	B	152/154 (99%)	110 (72%)	26 (17%)	16 (10%)	0	0
All	All	304/308 (99%)	206 (68%)	63 (21%)	35 (12%)	0	0

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	66	PRO
1	A	93	GLY
1	A	107	SER
1	B	56	GLY
1	B	80	HIS
1	B	81	VAL
1	B	91	LYS
1	B	108	GLY
1	B	126	LEU
1	B	139	ASN
1	A	24	GLU
1	A	135	THR
1	A	140	ALA
1	A	141	GLY
1	B	130	GLY
1	B	133	GLU
1	A	3	LYS
1	A	68	SER
1	A	126	LEU
1	B	22	GLN
1	B	24	GLU
1	B	66	PRO
1	B	107	SER
1	B	142	SER

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Mol	Chain	Res	Type
1	A	152	ALA
1	A	64	PHE
1	A	74	PRO
1	A	84	LEU
1	A	110	HIS
1	B	68	SER
1	B	25	SER
1	A	130	GLY
1	A	28	PRO
1	A	65	ASN

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	118/118 (100%)	69 (58%)	49 (42%)	0	0
1	B	118/118 (100%)	74 (63%)	44 (37%)	0	0
All	All	236/236 (100%)	143 (61%)	93 (39%)	0	0

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	7	VAL
1	A	11	ASP
1	A	13	PRO
1	A	18	ILE
1	A	23	LYS
1	A	26	ASN
1	A	31	VAL
1	A	32	TRP
1	A	35	ILE
1	A	38	LEU
1	A	42	LEU
1	A	52	ASP

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Mol	Chain	Res	Type
1	A	54	THR
1	A	65	ASN
1	A	66	PRO
1	A	67	LEU
1	A	69	ARG
1	A	70	LYS
1	A	71	HIS
1	A	76	ASP
1	A	79	ARG
1	A	83	ASP
1	A	86	ASN
1	A	87	VAL
1	A	90	ASP
1	A	91	LYS
1	A	92	ASP
1	A	96	ASP
1	A	99	ILE
1	A	102	SER
1	A	103	VAL
1	A	104	ILE
1	A	105	SER
1	A	109	ASP
1	A	111	CYS
1	A	113	ILE
1	A	116	THR
1	A	119	VAL
1	A	122	LYS
1	A	128	LYS
1	A	132	GLU
1	A	134	SER
1	A	135	THR
1	A	139	ASN
1	A	142	SER
1	A	144	LEU
1	A	149	ILE
1	A	153	GLN
1	B	2	THR
1	B	5	VAL
1	B	7	VAL
1	B	9	LYS
1	B	14	VAL
1	B	15	GLN

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Mol	Chain	Res	Type
1	B	17	ILE
1	B	19	ASN
1	B	22	GLN
1	B	23	LYS
1	B	24	GLU
1	B	36	LYS
1	B	39	THR
1	B	42	LEU
1	B	53	ASN
1	B	54	THR
1	B	70	LYS
1	B	74	PRO
1	B	79	ARG
1	B	83	ASP
1	B	84	LEU
1	B	88	THR
1	B	91	LYS
1	B	96	ASP
1	B	98	SER
1	B	99	ILE
1	B	100	GLU
1	B	101	ASP
1	B	104	ILE
1	B	106	LEU
1	B	107	SER
1	B	119	VAL
1	B	122	LYS
1	B	128	LYS
1	B	132	GLU
1	B	133	GLU
1	B	135	THR
1	B	136	LYS
1	B	142	SER
1	B	144	LEU
1	B	146	CYS
1	B	149	ILE
1	B	151	ILE
1	B	153	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	131	ASN
1	A	139	ASN
1	A	153	GLN
1	B	19	ASN
1	B	53	ASN
1	B	65	ASN
1	B	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	0:ACE	C	1:ALA	N	1.85
1	B	0:ACE	C	1:ALA	N	1.80
1	B	14:VAL	C	15:GLN	N	1.13

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.