



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:30 PM UTC

PDB ID : 1LYZ / pdb_00001lyz
Title : Real-space refinement of the structure of hen egg-white lysozyme
Authors : Diamond, R.; Phillips, D.C.; Blake, C.C.F.; North, A.C.T.
Deposited on : 1975-02-01
Resolution : 2.00 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
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

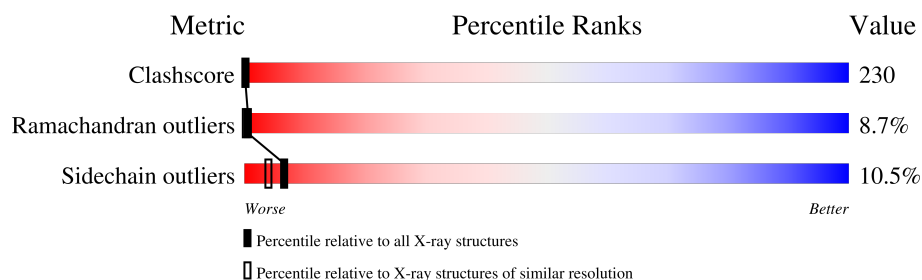
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	129	11% 44% 45%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1102 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 HEN EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 2 is water.

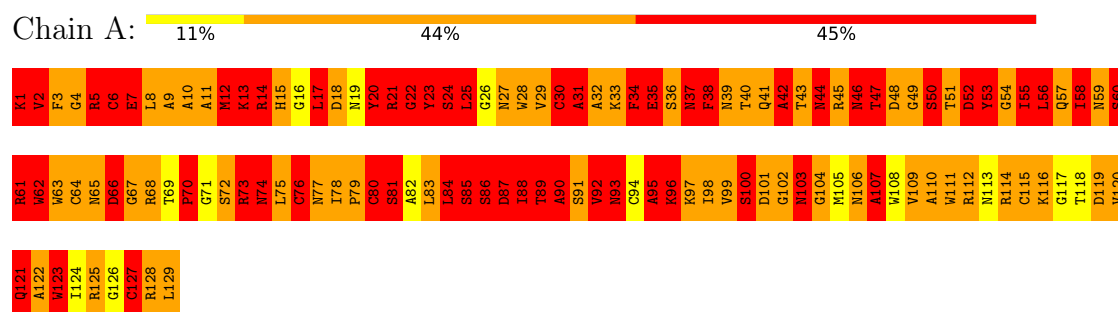
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	101	Total	O	0	0
			101	101		

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: HEN EGG WHITE LYSOZYME



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.10Å 79.10Å 37.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1102	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

5 Model quality i

5.1 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 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	11.71	614/1021 (60.1%)	7.87	599/1379 (43.4%)

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 outliers	#Planarity outliers
1	A	2	58

All (614) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	ALA	CA-C	56.08	2.31	1.52
1	A	50	SER	C-N	-55.43	0.55	1.33
1	A	5	ARG	NE-CZ	-46.33	0.82	1.33
1	A	5	ARG	CZ-NH2	45.30	1.92	1.33
1	A	44	ASN	C-O	-42.72	0.70	1.23
1	A	10	ALA	C-N	-42.46	0.74	1.33
1	A	9	ALA	C-N	37.44	1.82	1.33
1	A	92	VAL	C-O	-37.01	0.80	1.24
1	A	90	ALA	CA-C	-33.60	1.07	1.52
1	A	98	ILE	C-O	-33.42	0.79	1.24
1	A	74	ASN	CA-C	33.24	2.00	1.53
1	A	21	ARG	CZ-NH1	33.02	1.78	1.32
1	A	46	ASN	CG-ND2	-32.36	0.65	1.33
1	A	100	SER	CA-CB	-31.16	1.06	1.53
1	A	67	GLY	C-N	30.89	1.76	1.33
1	A	55	ILE	N-CA	30.56	1.84	1.46
1	A	125	ARG	C-O	-30.28	0.87	1.23
1	A	122	ALA	C-O	-30.20	0.84	1.24
1	A	67	GLY	CA-C	-29.72	1.08	1.51
1	A	12	MET	C-O	29.69	1.61	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	LEU	C-N	29.66	1.70	1.33
1	A	41	GLN	N-CA	29.64	1.84	1.46
1	A	85	SER	CA-C	29.13	1.91	1.52
1	A	31	ALA	CA-CB	29.04	2.00	1.53
1	A	121	GLN	C-O	-28.91	0.87	1.24
1	A	27	ASN	CG-ND2	28.44	1.93	1.33
1	A	23	TYR	N-CA	28.40	1.80	1.46
1	A	80	CYS	N-CA	28.35	1.82	1.46
1	A	89	THR	C-O	-28.08	0.88	1.24
1	A	3	PHE	C-O	-27.86	0.84	1.23
1	A	66	ASP	CA-C	-27.40	1.28	1.52
1	A	8	LEU	CB-CG	-27.19	0.99	1.53
1	A	43	THR	C-O	-26.99	0.89	1.23
1	A	7	GLU	CA-CB	-26.98	1.08	1.53
1	A	59	ASN	C-O	-26.82	0.87	1.23
1	A	90	ALA	C-O	-26.81	0.90	1.24
1	A	21	ARG	N-CA	26.79	1.87	1.46
1	A	40	THR	CA-C	26.75	1.90	1.52
1	A	92	VAL	CA-CB	26.00	1.86	1.54
1	A	126	GLY	C-O	-25.96	0.87	1.24
1	A	17	LEU	CA-CB	-25.75	1.13	1.53
1	A	123	TRP	C-O	25.67	1.53	1.24
1	A	9	ALA	CA-C	-25.63	1.21	1.52
1	A	123	TRP	CA-C	-25.48	1.20	1.52
1	A	119	ASP	CA-C	25.33	1.81	1.53
1	A	3	PHE	CB-CG	-25.22	0.92	1.50
1	A	79	PRO	C-N	-25.19	0.98	1.33
1	A	6	CYS	CA-C	24.80	1.86	1.52
1	A	64	CYS	N-CA	-24.74	1.15	1.45
1	A	88	ILE	C-O	24.57	1.53	1.24
1	A	1	LYS	CA-CB	24.52	2.02	1.53
1	A	64	CYS	C-O	-24.38	0.94	1.23
1	A	40	THR	C-N	-24.34	0.97	1.33
1	A	24	SER	N-CA	-24.12	1.15	1.46
1	A	38	PHE	CA-CB	24.11	1.85	1.54
1	A	23	TYR	C-O	24.08	1.52	1.23
1	A	110	ALA	CA-CB	23.85	1.91	1.53
1	A	116	LYS	C-O	-23.70	0.94	1.24
1	A	60	SER	N-CA	23.61	1.75	1.46
1	A	25	LEU	C-N	-23.59	1.05	1.33
1	A	58	ILE	C-N	23.30	1.65	1.33
1	A	14	ARG	C-O	23.27	1.53	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLY	CA-C	23.22	1.84	1.51
1	A	20	TYR	CG-CD2	23.22	1.88	1.39
1	A	53	TYR	C-O	23.02	1.51	1.23
1	A	15	HIS	C-O	-22.81	0.93	1.24
1	A	26	GLY	CA-C	-22.70	1.26	1.52
1	A	5	ARG	N-CA	-22.63	1.17	1.46
1	A	62	TRP	C-O	-22.59	0.95	1.24
1	A	41	GLN	CA-C	-22.48	1.21	1.52
1	A	49	GLY	C-N	-22.36	1.02	1.33
1	A	3	PHE	CA-C	22.31	1.84	1.53
1	A	119	ASP	CG-OD2	-22.30	0.82	1.25
1	A	82	ALA	C-O	22.18	1.50	1.24
1	A	3	PHE	CG-CD1	22.16	1.85	1.38
1	A	5	ARG	CA-C	-22.11	1.23	1.52
1	A	34	PHE	N-CA	-22.06	1.18	1.46
1	A	74	ASN	N-CA	-21.98	1.15	1.46
1	A	24	SER	C-O	21.93	1.50	1.23
1	A	100	SER	N-CA	21.78	1.69	1.46
1	A	41	GLN	C-N	21.69	1.62	1.33
1	A	20	TYR	N-CA	-21.59	1.18	1.46
1	A	20	TYR	CE1-CZ	21.56	1.90	1.38
1	A	48	ASP	N-CA	21.38	1.74	1.46
1	A	90	ALA	N-CA	21.10	1.73	1.46
1	A	35	GLU	CA-CB	-21.01	1.19	1.53
1	A	77	ASN	CA-C	20.94	1.80	1.53
1	A	67	GLY	N-CA	-20.92	1.12	1.45
1	A	39	ASN	CA-CB	20.91	1.80	1.53
1	A	50	SER	C-O	20.78	1.50	1.24
1	A	1	LYS	C-N	20.65	1.64	1.33
1	A	8	LEU	CA-C	-20.56	1.26	1.52
1	A	58	ILE	CA-C	-20.45	1.30	1.52
1	A	44	ASN	N-CA	-20.34	1.22	1.46
1	A	40	THR	C-O	-20.29	0.98	1.24
1	A	72	SER	CA-C	20.21	1.79	1.52
1	A	91	SER	C-O	-20.17	1.00	1.24
1	A	33	LYS	C-N	20.08	1.60	1.34
1	A	46	ASN	C-O	19.93	1.49	1.24
1	A	5	ARG	C-N	19.85	1.61	1.33
1	A	109	VAL	C-O	19.85	1.47	1.24
1	A	55	ILE	C-O	19.82	1.48	1.24
1	A	9	ALA	N-CA	-19.80	1.23	1.46
1	A	108	TRP	NE1-CE2	-19.61	1.15	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	SER	CA-CB	-19.47	1.23	1.53
1	A	97	LYS	C-O	19.42	1.49	1.24
1	A	74	ASN	C-N	19.38	1.58	1.33
1	A	95	ALA	C-O	-19.37	1.01	1.24
1	A	20	TYR	C-N	-19.31	1.06	1.33
1	A	1	LYS	CB-CG	-19.13	0.95	1.52
1	A	74	ASN	CG-OD1	-19.07	0.87	1.23
1	A	31	ALA	N-CA	-18.91	1.22	1.46
1	A	86	SER	C-O	-18.86	0.98	1.24
1	A	6	CYS	C-O	-18.70	1.00	1.24
1	A	64	CYS	CA-C	18.69	1.75	1.52
1	A	47	THR	CB-OG1	-18.67	1.13	1.43
1	A	28	TRP	NE1-CE2	-18.64	1.17	1.37
1	A	115	CYS	C-O	-18.50	1.00	1.24
1	A	111	TRP	N-CA	18.45	1.67	1.46
1	A	75	LEU	N-CA	-18.40	1.24	1.46
1	A	50	SER	CA-C	18.32	1.77	1.52
1	A	91	SER	N-CA	18.25	1.67	1.46
1	A	81	SER	CB-OG	18.24	1.78	1.42
1	A	99	VAL	CA-CB	18.11	1.79	1.54
1	A	127	CYS	C-N	-18.06	1.07	1.33
1	A	10	ALA	CA-CB	18.01	1.81	1.53
1	A	128	ARG	CA-CB	-18.00	1.30	1.52
1	A	123	TRP	NE1-CE2	-17.97	1.17	1.37
1	A	37	ASN	CA-CB	-17.95	1.26	1.53
1	A	43	THR	CB-OG1	17.88	1.72	1.43
1	A	129	LEU	C-O	-17.86	0.87	1.23
1	A	44	ASN	CG-OD1	-17.74	0.89	1.23
1	A	73	ARG	C-N	17.54	1.56	1.33
1	A	75	LEU	CA-CB	17.52	1.80	1.53
1	A	123	TRP	C-N	17.48	1.56	1.34
1	A	119	ASP	CG-OD1	-17.41	0.92	1.25
1	A	46	ASN	CA-C	17.38	1.76	1.52
1	A	56	LEU	N-CA	17.37	1.63	1.46
1	A	99	VAL	N-CA	-17.33	1.24	1.46
1	A	96	LYS	C-N	-17.32	1.06	1.33
1	A	1	LYS	CA-C	17.31	1.89	1.52
1	A	6	CYS	N-CA	17.31	1.68	1.46
1	A	7	GLU	C-N	-17.29	1.13	1.33
1	A	77	ASN	N-CA	-17.15	1.20	1.46
1	A	55	ILE	CA-C	-17.05	1.28	1.52
1	A	35	GLU	N-CA	17.05	1.67	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	PHE	C-N	17.03	1.58	1.33
1	A	113	ASN	CA-C	17.00	1.74	1.52
1	A	17	LEU	C-O	16.96	1.43	1.24
1	A	22	GLY	C-N	16.78	1.57	1.33
1	A	84	LEU	CB-CG	16.73	1.86	1.53
1	A	51	THR	C-O	-16.65	1.02	1.23
1	A	13	LYS	C-N	16.62	1.56	1.33
1	A	21	ARG	CD-NE	16.57	1.69	1.46
1	A	128	ARG	C-N	-16.55	1.10	1.33
1	A	73	ARG	CG-CD	-16.45	1.03	1.52
1	A	53	TYR	CA-C	-16.38	1.31	1.52
1	A	61	ARG	C-O	-16.38	1.02	1.24
1	A	86	SER	N-CA	-16.26	1.24	1.46
1	A	18	ASP	CG-OD2	16.17	1.56	1.25
1	A	56	LEU	C-O	-16.16	1.01	1.24
1	A	18	ASP	CB-CG	-16.07	1.11	1.52
1	A	21	ARG	CA-CB	16.02	1.79	1.53
1	A	45	ARG	NE-CZ	-16.01	1.15	1.33
1	A	2	VAL	C-N	15.98	1.54	1.33
1	A	122	ALA	CA-C	15.86	1.74	1.52
1	A	88	ILE	C-N	-15.82	1.11	1.33
1	A	13	LYS	C-O	15.76	1.43	1.24
1	A	77	ASN	C-N	-15.73	1.15	1.33
1	A	68	ARG	CA-CB	15.68	1.75	1.53
1	A	45	ARG	CZ-NH1	15.67	1.54	1.32
1	A	22	GLY	CA-C	15.62	1.71	1.51
1	A	65	ASN	CA-C	15.60	1.73	1.52
1	A	27	ASN	C-O	15.57	1.42	1.24
1	A	91	SER	CA-C	-15.44	1.33	1.52
1	A	6	CYS	CA-CB	-15.37	1.27	1.53
1	A	49	GLY	C-O	-15.27	1.03	1.23
1	A	23	TYR	C-N	15.25	1.54	1.33
1	A	35	GLU	CD-OE1	-15.25	0.96	1.25
1	A	46	ASN	CB-CG	-15.21	1.14	1.52
1	A	56	LEU	CB-CG	-15.19	1.23	1.53
1	A	45	ARG	N-CA	-15.18	1.27	1.46
1	A	75	LEU	CB-CG	-15.05	1.23	1.53
1	A	36	SER	CA-CB	-15.01	1.29	1.54
1	A	19	ASN	C-N	-14.80	1.13	1.33
1	A	65	ASN	CG-OD1	-14.80	0.95	1.23
1	A	64	CYS	CB-SG	-14.78	1.32	1.81
1	A	94	CYS	N-CA	14.72	1.64	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	CYS	C-N	14.52	1.55	1.33
1	A	44	ASN	C-N	14.51	1.53	1.33
1	A	63	TRP	CA-CB	14.51	1.76	1.53
1	A	73	ARG	N-CA	-14.47	1.29	1.46
1	A	72	SER	C-O	-14.33	1.06	1.23
1	A	7	GLU	CD-OE1	14.32	1.52	1.25
1	A	100	SER	C-O	-14.30	1.02	1.24
1	A	111	TRP	C-O	14.27	1.41	1.24
1	A	114	ARG	C-O	-14.24	1.04	1.23
1	A	99	VAL	CA-C	14.21	1.73	1.52
1	A	107	ALA	CA-CB	14.16	1.77	1.53
1	A	10	ALA	N-CA	14.12	1.63	1.46
1	A	47	THR	CA-C	14.12	1.72	1.52
1	A	13	LYS	CA-CB	14.10	1.77	1.53
1	A	107	ALA	C-N	-14.02	1.15	1.33
1	A	84	LEU	C-O	-13.94	1.05	1.24
1	A	68	ARG	NE-CZ	-13.92	1.17	1.33
1	A	48	ASP	CA-CB	13.92	1.71	1.52
1	A	23	TYR	CB-CG	-13.91	1.21	1.51
1	A	25	LEU	CA-CB	-13.75	1.30	1.53
1	A	73	ARG	C-O	-13.74	1.08	1.24
1	A	30	CYS	CA-C	-13.74	1.28	1.52
1	A	62	TRP	CD1-NE1	13.73	1.66	1.37
1	A	45	ARG	CA-CB	13.70	1.77	1.53
1	A	58	ILE	C-O	13.62	1.39	1.24
1	A	93	ASN	C-N	-13.60	1.16	1.33
1	A	43	THR	CA-C	13.60	1.69	1.52
1	A	93	ASN	N-CA	13.45	1.64	1.46
1	A	75	LEU	C-O	13.44	1.39	1.24
1	A	20	TYR	CA-CB	13.42	1.73	1.53
1	A	97	LYS	N-CA	13.35	1.63	1.46
1	A	103	ASN	CA-CB	-13.24	1.33	1.54
1	A	30	CYS	CA-CB	13.22	1.75	1.53
1	A	95	ALA	N-CA	13.11	1.62	1.46
1	A	87	ASP	C-N	-13.11	1.15	1.33
1	A	32	ALA	C-O	13.07	1.42	1.23
1	A	13	LYS	N-CA	13.01	1.62	1.46
1	A	68	ARG	CA-C	-12.99	1.36	1.52
1	A	21	ARG	CZ-NH2	-12.97	1.16	1.33
1	A	66	ASP	CG-OD1	-12.92	1.00	1.25
1	A	52	ASP	C-O	-12.83	1.08	1.23
1	A	70	PRO	CA-CB	-12.82	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	SER	C-O	12.77	1.40	1.24
1	A	86	SER	CB-OG	-12.73	1.16	1.42
1	A	107	ALA	C-O	12.73	1.40	1.24
1	A	115	CYS	CA-CB	-12.72	1.31	1.53
1	A	117	GLY	N-CA	-12.72	1.26	1.45
1	A	83	LEU	C-N	-12.64	1.15	1.33
1	A	102	GLY	C-O	-12.57	1.06	1.23
1	A	112	ARG	N-CA	12.57	1.62	1.46
1	A	82	ALA	N-CA	12.57	1.61	1.46
1	A	39	ASN	CG-OD1	12.54	1.47	1.23
1	A	89	THR	CA-CB	-12.50	1.32	1.53
1	A	61	ARG	NE-CZ	-12.46	1.19	1.33
1	A	70	PRO	N-CD	-12.45	1.30	1.47
1	A	116	LYS	C-N	-12.38	1.17	1.33
1	A	62	TRP	CD2-CE2	12.36	1.62	1.41
1	A	25	LEU	C-O	12.35	1.39	1.24
1	A	23	TYR	CA-CB	-12.34	1.34	1.53
1	A	38	PHE	CA-C	-12.30	1.34	1.52
1	A	3	PHE	CG-CD2	-12.28	1.13	1.38
1	A	16	GLY	CA-C	12.28	1.70	1.51
1	A	73	ARG	CB-CG	12.28	1.89	1.52
1	A	40	THR	N-CA	12.27	1.62	1.46
1	A	84	LEU	CA-CB	12.25	1.74	1.53
1	A	17	LEU	N-CA	12.24	1.61	1.46
1	A	32	ALA	N-CA	-12.17	1.29	1.46
1	A	27	ASN	CA-CB	-12.14	1.33	1.53
1	A	15	HIS	CB-CG	-12.12	1.33	1.50
1	A	65	ASN	C-O	12.12	1.38	1.23
1	A	62	TRP	CA-CB	12.11	1.74	1.53
1	A	106	ASN	N-CA	12.11	1.61	1.46
1	A	108	TRP	CD1-NE1	12.06	1.63	1.37
1	A	112	ARG	C-N	-12.05	1.18	1.33
1	A	20	TYR	C-O	12.05	1.38	1.23
1	A	108	TRP	CZ2-CH2	-11.99	1.14	1.37
1	A	10	ALA	CA-C	11.97	1.68	1.52
1	A	87	ASP	CG-OD1	-11.90	1.02	1.25
1	A	3	PHE	N-CA	-11.88	1.29	1.45
1	A	61	ARG	C-N	11.88	1.50	1.33
1	A	37	ASN	CA-C	11.81	1.69	1.52
1	A	93	ASN	CG-OD1	-11.78	1.01	1.23
1	A	51	THR	CA-CB	11.75	1.76	1.53
1	A	76	CYS	CA-CB	11.73	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	VAL	CB-CG1	-11.70	1.14	1.52
1	A	62	TRP	CA-C	-11.67	1.37	1.52
1	A	99	VAL	CB-CG2	-11.66	1.14	1.52
1	A	28	TRP	CD2-CE3	-11.60	1.21	1.40
1	A	49	GLY	N-CA	11.58	1.62	1.45
1	A	111	TRP	CA-CB	11.54	1.72	1.53
1	A	46	ASN	CA-CB	11.46	1.72	1.53
1	A	108	TRP	CA-C	11.46	1.66	1.53
1	A	97	LYS	CD-CE	11.44	1.86	1.52
1	A	103	ASN	CG-ND2	-11.39	1.09	1.33
1	A	28	TRP	N-CA	-11.37	1.32	1.46
1	A	66	ASP	N-CA	11.29	1.56	1.47
1	A	32	ALA	C-N	-11.27	1.19	1.33
1	A	58	ILE	CA-CB	-11.25	1.41	1.54
1	A	62	TRP	CD2-CE3	-11.25	1.22	1.40
1	A	51	THR	N-CA	11.21	1.59	1.45
1	A	90	ALA	CA-CB	11.21	1.72	1.53
1	A	24	SER	CA-CB	11.20	1.71	1.53
1	A	23	TYR	CA-C	11.19	1.66	1.52
1	A	108	TRP	N-CA	-11.13	1.32	1.46
1	A	48	ASP	CG-OD1	-11.12	1.04	1.25
1	A	94	CYS	CA-CB	-11.12	1.36	1.53
1	A	16	GLY	C-N	-11.07	1.20	1.33
1	A	2	VAL	C-O	-10.92	1.11	1.24
1	A	16	GLY	C-O	-10.92	1.08	1.24
1	A	74	ASN	C-O	10.90	1.36	1.23
1	A	97	LYS	C-N	-10.88	1.20	1.33
1	A	3	PHE	CE2-CZ	10.84	1.71	1.38
1	A	87	ASP	CA-C	10.80	1.65	1.52
1	A	47	THR	C-O	-10.76	1.09	1.24
1	A	8	LEU	CG-CD1	10.72	1.88	1.52
1	A	48	ASP	CB-CG	-10.70	1.25	1.52
1	A	114	ARG	N-CA	10.69	1.60	1.46
1	A	38	PHE	CD1-CE1	10.68	1.70	1.38
1	A	38	PHE	CD2-CE2	10.67	1.70	1.38
1	A	123	TRP	N-CA	10.67	1.59	1.46
1	A	111	TRP	CE3-CZ3	-10.63	1.06	1.38
1	A	90	ALA	C-N	-10.61	1.20	1.33
1	A	109	VAL	C-N	-10.54	1.19	1.33
1	A	43	THR	C-N	10.52	1.47	1.33
1	A	79	PRO	CA-C	10.51	1.64	1.52
1	A	61	ARG	CB-CG	10.47	1.83	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	LYS	CA-CB	-10.47	1.36	1.53
1	A	118	THR	C-O	-10.42	1.09	1.23
1	A	11	ALA	CA-C	10.38	1.66	1.52
1	A	111	TRP	CZ2-CH2	-10.37	1.17	1.37
1	A	81	SER	C-N	-10.34	1.20	1.33
1	A	59	ASN	CB-CG	-10.33	1.26	1.52
1	A	115	CYS	N-CA	10.25	1.59	1.46
1	A	31	ALA	C-N	-10.23	1.15	1.33
1	A	25	LEU	CB-CG	-10.22	1.33	1.53
1	A	20	TYR	CA-C	-10.21	1.39	1.52
1	A	51	THR	CB-OG1	-10.18	1.27	1.43
1	A	9	ALA	CA-CB	-10.16	1.37	1.53
1	A	37	ASN	CG-OD1	-10.13	1.04	1.23
1	A	73	ARG	CA-CB	9.98	1.69	1.53
1	A	80	CYS	CA-CB	9.95	1.70	1.53
1	A	69	THR	C-N	-9.88	1.10	1.33
1	A	129	LEU	CG-CD2	9.88	1.85	1.52
1	A	100	SER	CA-C	9.85	1.65	1.52
1	A	81	SER	N-CA	-9.79	1.33	1.46
1	A	96	LYS	C-O	9.79	1.36	1.24
1	A	30	CYS	C-N	-9.76	1.20	1.33
1	A	7	GLU	CB-CG	9.76	1.81	1.52
1	A	36	SER	N-CA	-9.74	1.32	1.46
1	A	68	ARG	N-CA	-9.72	1.35	1.46
1	A	111	TRP	CD2-CE2	9.57	1.57	1.41
1	A	103	ASN	C-O	-9.51	1.11	1.24
1	A	35	GLU	C-N	-9.51	1.17	1.33
1	A	124	ILE	C-N	-9.51	1.20	1.33
1	A	21	ARG	CA-C	-9.50	1.40	1.53
1	A	51	THR	CA-C	-9.47	1.41	1.52
1	A	112	ARG	CD-NE	9.38	1.59	1.46
1	A	111	TRP	CA-C	-9.34	1.40	1.52
1	A	128	ARG	N-CA	9.33	1.58	1.46
1	A	123	TRP	CZ3-CH2	-9.28	1.17	1.40
1	A	84	LEU	CG-CD2	9.27	1.83	1.52
1	A	36	SER	CA-C	9.25	1.65	1.52
1	A	14	ARG	CB-CG	-9.23	1.24	1.52
1	A	53	TYR	N-CA	-9.19	1.33	1.46
1	A	44	ASN	CG-ND2	9.16	1.52	1.33
1	A	20	TYR	CZ-OH	9.15	1.57	1.38
1	A	72	SER	CA-CB	9.14	1.68	1.53
1	A	69	THR	CA-C	9.12	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	SER	C-N	-9.11	1.20	1.33
1	A	20	TYR	CD1-CE1	9.10	1.66	1.38
1	A	104	GLY	C-O	9.10	1.37	1.24
1	A	121	GLN	CA-C	9.07	1.65	1.52
1	A	101	ASP	N-CA	-9.06	1.34	1.46
1	A	38	PHE	C-O	-9.03	1.03	1.24
1	A	67	GLY	C-O	9.01	1.37	1.24
1	A	71	GLY	C-N	-8.98	1.21	1.33
1	A	52	ASP	CB-CG	-8.96	1.29	1.52
1	A	88	ILE	CB-CG1	-8.95	1.35	1.53
1	A	116	LYS	CB-CG	-8.94	1.25	1.52
1	A	34	PHE	CG-CD1	8.92	1.57	1.38
1	A	19	ASN	CB-CG	8.89	1.74	1.52
1	A	116	LYS	CG-CD	-8.78	1.26	1.52
1	A	109	VAL	CA-C	8.77	1.63	1.52
1	A	56	LEU	CG-CD2	8.77	1.81	1.52
1	A	78	ILE	CA-CB	-8.69	1.43	1.54
1	A	114	ARG	CZ-NH1	8.69	1.45	1.32
1	A	63	TRP	CD2-CE2	8.67	1.56	1.41
1	A	8	LEU	CG-CD2	8.64	1.81	1.52
1	A	92	VAL	CB-CG2	8.62	1.80	1.52
1	A	28	TRP	C-O	-8.61	1.13	1.24
1	A	103	ASN	CB-CG	8.61	1.73	1.52
1	A	16	GLY	N-CA	8.55	1.58	1.45
1	A	60	SER	CA-C	-8.53	1.41	1.52
1	A	124	ILE	CA-C	-8.52	1.41	1.52
1	A	28	TRP	C-N	-8.51	1.23	1.33
1	A	63	TRP	C-O	-8.51	1.13	1.24
1	A	14	ARG	C-N	-8.49	1.21	1.33
1	A	45	ARG	C-O	-8.48	1.13	1.24
1	A	95	ALA	CA-C	-8.46	1.40	1.52
1	A	92	VAL	N-CA	-8.46	1.36	1.46
1	A	109	VAL	CA-CB	-8.45	1.43	1.54
1	A	65	ASN	C-N	-8.44	1.19	1.34
1	A	21	ARG	CB-CG	-8.44	1.27	1.52
1	A	113	ASN	CG-OD1	-8.43	1.07	1.23
1	A	103	ASN	CG-OD1	-8.43	1.07	1.23
1	A	84	LEU	N-CA	8.43	1.57	1.46
1	A	66	ASP	CA-CB	8.40	1.70	1.53
1	A	124	ILE	CA-CB	-8.38	1.44	1.54
1	A	63	TRP	CZ2-CH2	8.35	1.53	1.37
1	A	125	ARG	C-N	-8.33	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	GLN	CD-OE1	-8.32	1.07	1.23
1	A	12	MET	CA-C	-8.31	1.41	1.52
1	A	26	GLY	N-CA	-8.24	1.35	1.45
1	A	19	ASN	N-CA	-8.23	1.35	1.46
1	A	112	ARG	CB-CG	8.21	1.77	1.52
1	A	96	LYS	CA-C	8.20	1.63	1.52
1	A	21	ARG	C-N	8.20	1.43	1.33
1	A	68	ARG	CD-NE	8.19	1.57	1.46
1	A	18	ASP	N-CA	-8.16	1.36	1.46
1	A	92	VAL	C-N	8.13	1.46	1.33
1	A	38	PHE	N-CA	-8.12	1.31	1.46
1	A	4	GLY	N-CA	-8.09	1.33	1.45
1	A	81	SER	CA-C	-8.08	1.42	1.52
1	A	45	ARG	CD-NE	-8.07	1.34	1.46
1	A	101	ASP	CA-C	-8.06	1.42	1.52
1	A	125	ARG	N-CA	-8.06	1.35	1.46
1	A	25	LEU	CA-C	-8.02	1.42	1.52
1	A	102	GLY	N-CA	-8.01	1.33	1.45
1	A	107	ALA	N-CA	-7.98	1.35	1.46
1	A	73	ARG	CA-C	7.97	1.61	1.52
1	A	53	TYR	CZ-OH	7.96	1.54	1.38
1	A	44	ASN	CA-C	7.94	1.61	1.52
1	A	74	ASN	CA-CB	7.94	1.79	1.53
1	A	91	SER	CB-OG	7.93	1.58	1.42
1	A	58	ILE	CB-CG1	-7.92	1.37	1.53
1	A	68	ARG	C-N	-7.92	1.23	1.33
1	A	62	TRP	CE2-CZ2	-7.90	1.23	1.39
1	A	76	CYS	C-N	-7.87	1.22	1.33
1	A	91	SER	C-N	7.87	1.43	1.33
1	A	77	ASN	CA-CB	-7.85	1.40	1.53
1	A	111	TRP	CE2-CZ2	-7.80	1.23	1.39
1	A	5	ARG	CG-CD	-7.80	1.29	1.52
1	A	66	ASP	CG-OD2	7.80	1.40	1.25
1	A	56	LEU	CA-CB	-7.76	1.36	1.53
1	A	93	ASN	CA-CB	7.75	1.66	1.53
1	A	123	TRP	CD1-NE1	-7.75	1.21	1.37
1	A	52	ASP	N-CA	-7.74	1.37	1.46
1	A	37	ASN	CG-ND2	-7.71	1.17	1.33
1	A	23	TYR	CD1-CE1	-7.71	1.15	1.38
1	A	5	ARG	CA-CB	-7.66	1.40	1.53
1	A	49	GLY	CA-C	7.65	1.62	1.51
1	A	98	ILE	N-CA	7.60	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ASN	C-O	-7.60	1.13	1.23
1	A	83	LEU	N-CA	-7.58	1.36	1.46
1	A	119	ASP	C-N	7.55	1.43	1.34
1	A	96	LYS	CA-CB	-7.52	1.40	1.53
1	A	42	ALA	C-N	7.50	1.44	1.33
1	A	47	THR	N-CA	7.50	1.56	1.46
1	A	70	PRO	C-N	-7.48	1.24	1.33
1	A	89	THR	CB-OG1	7.45	1.55	1.43
1	A	30	CYS	C-O	7.45	1.35	1.24
1	A	7	GLU	CA-C	-7.37	1.42	1.52
1	A	1	LYS	N-CA	-7.28	1.32	1.46
1	A	50	SER	CA-CB	-7.28	1.41	1.53
1	A	8	LEU	C-O	7.26	1.32	1.24
1	A	79	PRO	N-CD	-7.24	1.37	1.47
1	A	106	ASN	CG-OD1	-7.20	1.09	1.23
1	A	48	ASP	CA-C	-7.19	1.40	1.52
1	A	3	PHE	CD1-CE1	-7.18	1.17	1.38
1	A	75	LEU	C-N	7.18	1.44	1.33
1	A	36	SER	C-O	7.14	1.34	1.23
1	A	100	SER	C-N	-7.14	1.23	1.33
1	A	85	SER	C-O	7.13	1.32	1.23
1	A	93	ASN	C-O	-7.13	1.14	1.24
1	A	61	ARG	CA-CB	-7.13	1.41	1.53
1	A	118	THR	CA-C	7.12	1.62	1.53
1	A	23	TYR	CG-CD1	7.12	1.54	1.39
1	A	48	ASP	CG-OD2	7.12	1.38	1.25
1	A	76	CYS	CA-C	7.11	1.64	1.52
1	A	10	ALA	C-O	-7.09	1.15	1.24
1	A	123	TRP	CG-CD2	-7.09	1.30	1.43
1	A	5	ARG	C-O	-7.08	1.15	1.24
1	A	76	CYS	N-CA	7.08	1.54	1.46
1	A	34	PHE	CG-CD2	7.08	1.53	1.38
1	A	14	ARG	N-CA	7.07	1.55	1.46
1	A	74	ASN	CB-CG	7.07	1.69	1.52
1	A	11	ALA	C-N	-7.05	1.24	1.34
1	A	101	ASP	C-O	-7.04	1.12	1.23
1	A	33	LYS	CE-NZ	-7.01	1.28	1.49
1	A	56	LEU	C-N	7.01	1.42	1.33
1	A	126	GLY	CA-C	7.01	1.62	1.51
1	A	121	GLN	CB-CG	-7.00	1.31	1.52
1	A	36	SER	CB-OG	6.98	1.56	1.42
1	A	123	TRP	CG-CD1	-6.98	1.19	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	CYS	CA-CB	6.96	1.64	1.53
1	A	123	TRP	CA-CB	6.92	1.64	1.53
1	A	4	GLY	C-N	-6.92	1.24	1.33
1	A	9	ALA	C-O	6.92	1.32	1.24
1	A	89	THR	CA-C	6.91	1.62	1.52
1	A	119	ASP	N-CA	-6.91	1.37	1.46
1	A	39	ASN	CG-ND2	-6.89	1.18	1.33
1	A	106	ASN	CB-CG	6.86	1.69	1.52
1	A	127	CYS	CA-C	-6.86	1.43	1.52
1	A	119	ASP	C-O	-6.85	1.13	1.23
1	A	87	ASP	CA-CB	-6.84	1.43	1.53
1	A	14	ARG	CA-CB	-6.82	1.42	1.53
1	A	71	GLY	C-O	-6.79	1.16	1.24
1	A	35	GLU	C-O	6.77	1.32	1.24
1	A	59	ASN	C-N	-6.73	1.25	1.33
1	A	63	TRP	C-N	-6.70	1.25	1.33
1	A	114	ARG	NE-CZ	-6.70	1.25	1.33
1	A	77	ASN	CG-OD1	6.70	1.36	1.23
1	A	63	TRP	CZ3-CH2	-6.67	1.23	1.40
1	A	45	ARG	C-N	6.66	1.43	1.33
1	A	11	ALA	N-CA	6.62	1.54	1.46
1	A	55	ILE	CB-CG2	6.56	1.74	1.52
1	A	40	THR	CB-CG2	-6.54	1.30	1.52
1	A	109	VAL	CB-CG1	6.54	1.74	1.52
1	A	108	TRP	CG-CD2	6.52	1.55	1.43
1	A	124	ILE	C-O	6.50	1.32	1.24
1	A	61	ARG	CA-C	-6.49	1.43	1.52
1	A	14	ARG	CG-CD	6.46	1.71	1.52
1	A	15	HIS	N-CA	6.41	1.54	1.46
1	A	55	ILE	CB-CG1	6.40	1.66	1.53
1	A	116	LYS	CA-CB	6.40	1.64	1.53
1	A	129	LEU	CA-CB	6.39	1.66	1.53
1	A	79	PRO	N-CA	6.38	1.55	1.47
1	A	96	LYS	CG-CD	-6.37	1.33	1.52
1	A	98	ILE	CG1-CD1	6.36	1.76	1.51
1	A	69	THR	C-O	6.35	1.32	1.24
1	A	19	ASN	CG-ND2	-6.33	1.20	1.33
1	A	20	TYR	CG-CD1	-6.32	1.26	1.39
1	A	84	LEU	CG-CD1	-6.32	1.31	1.52
1	A	28	TRP	CG-CD2	6.31	1.55	1.43
1	A	39	ASN	CB-CG	-6.31	1.36	1.52
1	A	15	HIS	C-N	6.31	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	GLN	CG-CD	-6.30	1.36	1.52
1	A	4	GLY	C-O	6.29	1.32	1.23
1	A	3	PHE	CA-CB	-6.28	1.43	1.53
1	A	38	PHE	CB-CG	-6.28	1.36	1.50
1	A	125	ARG	CA-CB	6.26	1.63	1.53
1	A	15	HIS	CE1-NE2	6.26	1.38	1.32
1	A	83	LEU	CA-CB	6.25	1.64	1.53
1	A	105	MET	CA-CB	-6.24	1.43	1.53
1	A	87	ASP	N-CA	6.21	1.53	1.46
1	A	61	ARG	CD-NE	6.16	1.54	1.46
1	A	96	LYS	N-CA	-6.16	1.38	1.46
1	A	14	ARG	CZ-NH1	6.15	1.41	1.32
1	A	111	TRP	CD1-NE1	6.11	1.50	1.37
1	A	79	PRO	C-O	6.11	1.30	1.23
1	A	7	GLU	N-CA	-6.09	1.38	1.46
1	A	38	PHE	CE2-CZ	-6.05	1.20	1.38
1	A	77	ASN	CB-CG	-6.04	1.36	1.52
1	A	111	TRP	CZ3-CH2	6.01	1.55	1.40
1	A	116	LYS	CA-C	6.00	1.60	1.52
1	A	111	TRP	CG-CD1	-5.99	1.22	1.36
1	A	35	GLU	CD-OE2	5.96	1.36	1.25
1	A	69	THR	CB-CG2	5.96	1.72	1.52
1	A	22	GLY	N-CA	-5.95	1.37	1.45
1	A	37	ASN	C-O	-5.92	1.14	1.24
1	A	71	GLY	CA-C	-5.91	1.42	1.51
1	A	117	GLY	C-O	5.91	1.31	1.24
1	A	108	TRP	CD2-CE3	-5.91	1.30	1.40
1	A	17	LEU	CB-CG	-5.90	1.41	1.53
1	A	42	ALA	CA-C	5.89	1.60	1.52
1	A	123	TRP	CB-CG	5.89	1.68	1.50
1	A	42	ALA	C-O	-5.83	1.17	1.23
1	A	27	ASN	CG-OD1	-5.81	1.12	1.23
1	A	28	TRP	CA-C	5.79	1.60	1.52
1	A	53	TYR	CG-CD2	-5.73	1.27	1.39
1	A	78	ILE	CB-CG2	5.72	1.71	1.52
1	A	15	HIS	CD2-NE2	5.72	1.44	1.37
1	A	92	VAL	CA-C	5.71	1.60	1.52
1	A	38	PHE	C-N	5.71	1.43	1.33
1	A	50	SER	N-CA	-5.71	1.38	1.46
1	A	27	ASN	CA-C	5.68	1.60	1.52
1	A	99	VAL	C-N	5.67	1.42	1.34
1	A	114	ARG	CB-CG	-5.66	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	CYS	C-O	-5.63	1.16	1.24
1	A	21	ARG	CG-CD	5.63	1.69	1.52
1	A	31	ALA	CA-C	5.62	1.60	1.52
1	A	44	ASN	CA-CB	5.62	1.62	1.53
1	A	22	GLY	C-O	-5.56	1.16	1.24
1	A	83	LEU	C-O	-5.51	1.17	1.24
1	A	14	ARG	CA-C	5.50	1.60	1.52
1	A	45	ARG	CZ-NH2	5.49	1.40	1.33
1	A	58	ILE	N-CA	-5.48	1.39	1.46
1	A	84	LEU	CA-C	-5.46	1.45	1.52
1	A	19	ASN	CA-C	-5.45	1.45	1.52
1	A	21	ARG	NE-CZ	-5.45	1.27	1.33
1	A	50	SER	CB-OG	-5.45	1.31	1.42
1	A	25	LEU	CG-CD1	5.44	1.70	1.52
1	A	57	GLN	CD-NE2	5.43	1.44	1.33
1	A	88	ILE	CG1-CD1	5.42	1.72	1.51
1	A	15	HIS	CG-CD2	5.41	1.41	1.35
1	A	115	CYS	C-N	5.41	1.41	1.33
1	A	57	GLN	CD-OE1	-5.41	1.13	1.23
1	A	87	ASP	C-O	-5.41	1.17	1.24
1	A	12	MET	N-CA	5.40	1.53	1.46
1	A	124	ILE	CG1-CD1	-5.40	1.30	1.51
1	A	39	ASN	C-N	5.37	1.41	1.33
1	A	93	ASN	CB-CG	-5.36	1.38	1.52
1	A	2	VAL	CA-C	5.35	1.59	1.52
1	A	111	TRP	CG-CD2	-5.34	1.34	1.43
1	A	119	ASP	CB-CG	-5.33	1.38	1.52
1	A	34	PHE	CE1-CZ	5.30	1.54	1.38
1	A	60	SER	C-N	5.29	1.41	1.33
1	A	29	VAL	N-CA	5.28	1.54	1.46
1	A	36	SER	C-N	-5.24	1.26	1.33
1	A	59	ASN	N-CA	-5.23	1.38	1.45
1	A	12	MET	C-N	-5.20	1.26	1.33
1	A	13	LYS	CE-NZ	5.20	1.65	1.49
1	A	25	LEU	CG-CD2	5.18	1.69	1.52
1	A	108	TRP	CD2-CE2	-5.17	1.32	1.41
1	A	46	ASN	CG-OD1	-5.16	1.13	1.23
1	A	70	PRO	N-CA	5.15	1.53	1.47
1	A	46	ASN	C-N	-5.14	1.25	1.33
1	A	7	GLU	CD-OE2	5.11	1.35	1.25
1	A	61	ARG	CZ-NH2	5.09	1.40	1.33
1	A	26	GLY	C-N	5.08	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLU	CB-CG	-5.07	1.37	1.52
1	A	117	GLY	CA-C	5.07	1.58	1.51
1	A	8	LEU	CA-CB	-5.05	1.45	1.53
1	A	1	LYS	CD-CE	-5.03	1.37	1.52
1	A	5	ARG	CB-CG	-5.01	1.37	1.52
1	A	115	CYS	CB-SG	5.01	1.97	1.81

All (599) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ALA	N-CA-C	-40.33	64.03	114.04
1	A	27	ASN	OD1-CG-ND2	-36.67	85.93	122.60
1	A	26	GLY	O-C-N	-35.96	87.31	122.19
1	A	25	LEU	CA-C-N	35.43	158.97	120.00
1	A	25	LEU	C-N-CA	35.43	158.97	120.00
1	A	77	ASN	OD1-CG-ND2	-30.23	92.37	122.60
1	A	24	SER	CA-C-O	-30.12	86.58	120.92
1	A	4	GLY	O-C-N	29.74	161.36	122.70
1	A	5	ARG	NH1-CZ-NH2	-28.16	82.69	119.30
1	A	66	ASP	O-C-N	-27.97	95.84	121.85
1	A	75	LEU	O-C-N	-27.10	94.16	122.07
1	A	24	SER	N-CA-C	26.94	150.24	110.10
1	A	41	GLN	CA-C-O	26.08	150.11	119.60
1	A	1	LYS	N-CA-CB	25.12	153.21	110.50
1	A	108	TRP	O-C-N	24.97	152.17	122.46
1	A	26	GLY	CA-C-O	24.86	147.01	120.66
1	A	2	VAL	N-CA-CB	-24.33	81.80	110.99
1	A	7	GLU	CA-C-N	24.19	154.42	120.79
1	A	7	GLU	C-N-CA	24.19	154.42	120.79
1	A	14	ARG	O-C-N	-24.00	90.68	122.59
1	A	3	PHE	CA-CB-CG	23.61	137.41	113.80
1	A	53	TYR	O-C-N	-23.38	96.04	123.16
1	A	6	CYS	CA-C-O	23.11	153.56	120.51
1	A	114	ARG	NE-CZ-NH2	-22.93	98.57	119.20
1	A	35	GLU	CA-CB-CG	22.71	159.53	114.10
1	A	33	LYS	CA-C-O	22.64	144.22	120.90
1	A	14	ARG	N-CA-CB	22.20	148.01	110.49
1	A	88	ILE	CA-C-O	-21.86	93.46	120.78
1	A	89	THR	O-C-N	21.86	151.66	122.59
1	A	30	CYS	O-C-N	-21.82	87.49	122.41
1	A	5	ARG	O-C-N	-21.72	93.70	122.59
1	A	19	ASN	CA-C-O	-21.59	89.64	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ALA	N-CA-CB	21.43	141.84	110.13
1	A	5	ARG	NE-CZ-NH1	21.39	142.89	121.50
1	A	46	ASN	O-C-N	-21.10	94.53	122.59
1	A	41	GLN	O-C-N	-20.75	92.89	122.36
1	A	6	CYS	O-C-N	-20.44	95.40	122.59
1	A	78	ILE	O-C-N	-19.97	98.33	121.10
1	A	25	LEU	CD1-CG-CD2	-19.68	67.49	110.80
1	A	47	THR	O-C-N	19.49	149.16	122.46
1	A	44	ASN	N-CA-CB	19.19	140.07	110.71
1	A	97	LYS	O-C-N	19.10	148.63	122.46
1	A	33	LYS	O-C-N	-18.96	101.55	122.03
1	A	97	LYS	CA-C-O	-18.74	97.34	119.27
1	A	30	CYS	CA-C-N	18.66	151.87	120.71
1	A	30	CYS	C-N-CA	18.66	151.87	120.71
1	A	71	GLY	O-C-N	18.11	143.85	122.84
1	A	4	GLY	CA-C-O	-17.93	89.37	120.57
1	A	108	TRP	CA-C-O	-17.73	101.98	122.37
1	A	25	LEU	O-C-N	-17.69	99.06	122.59
1	A	64	CYS	O-C-N	17.69	143.32	123.33
1	A	69	THR	O-C-N	17.57	138.26	121.04
1	A	123	TRP	O-C-N	-17.52	103.17	122.09
1	A	66	ASP	CA-C-N	17.29	149.69	122.20
1	A	66	ASP	C-N-CA	17.29	149.69	122.20
1	A	40	THR	O-C-N	17.16	144.69	122.39
1	A	88	ILE	O-C-N	17.10	143.94	122.57
1	A	101	ASP	CA-CB-CG	16.83	129.43	112.60
1	A	62	TRP	CE2-CD2-CE3	16.77	135.57	118.80
1	A	107	ALA	CA-C-N	16.77	147.32	122.16
1	A	107	ALA	C-N-CA	16.77	147.32	122.16
1	A	120	VAL	CA-C-O	-16.34	103.08	120.57
1	A	27	ASN	CB-CG-OD1	16.32	153.44	120.80
1	A	5	ARG	CA-C-O	16.31	143.84	120.51
1	A	19	ASN	O-C-N	16.28	144.24	122.59
1	A	90	ALA	CB-CA-C	16.24	142.73	110.42
1	A	114	ARG	NH1-CZ-NH2	16.20	140.35	119.30
1	A	23	TYR	N-CA-C	-16.07	83.40	109.76
1	A	17	LEU	CA-C-O	-16.02	103.76	120.90
1	A	67	GLY	O-C-N	-15.91	101.58	122.42
1	A	55	ILE	N-CA-C	-15.90	89.23	111.17
1	A	123	TRP	CB-CG-CD2	-15.63	104.92	126.80
1	A	57	GLN	CA-C-O	-15.62	103.76	122.03
1	A	23	TYR	CB-CA-C	15.58	135.66	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASN	O-C-N	15.54	140.97	122.17
1	A	7	GLU	OE1-CD-OE2	-15.43	85.86	122.90
1	A	27	ASN	N-CA-C	-15.38	92.64	111.40
1	A	62	TRP	CG-CD2-CE3	-15.12	118.78	133.90
1	A	59	ASN	CA-CB-CG	15.08	127.68	112.60
1	A	26	GLY	CA-C-N	14.98	145.73	120.71
1	A	26	GLY	C-N-CA	14.98	145.73	120.71
1	A	37	ASN	CA-CB-CG	14.88	127.48	112.60
1	A	55	ILE	O-C-N	-14.77	106.98	121.90
1	A	92	VAL	CA-CB-CG1	14.75	135.47	110.40
1	A	13	LYS	N-CA-C	14.65	142.00	110.80
1	A	27	ASN	N-CA-CB	14.49	131.57	110.13
1	A	57	GLN	CB-CA-C	14.40	133.55	111.95
1	A	111	TRP	CG-CD2-CE3	14.35	148.25	133.90
1	A	57	GLN	CB-CG-CD	-14.34	88.22	112.60
1	A	110	ALA	O-C-N	-14.33	106.62	122.09
1	A	86	SER	N-CA-C	-14.32	95.84	113.02
1	A	100	SER	CA-C-O	-14.31	103.18	119.78
1	A	3	PHE	CB-CG-CD2	14.26	144.94	120.70
1	A	50	SER	CA-C-O	-14.23	100.17	120.51
1	A	32	ALA	CB-CA-C	-14.19	83.90	109.15
1	A	127	CYS	N-CA-C	14.13	131.16	109.96
1	A	39	ASN	CA-C-O	14.08	135.18	120.54
1	A	63	TRP	CD1-CG-CD2	14.04	128.76	106.30
1	A	63	TRP	CG-CD1-NE1	-13.92	92.10	110.20
1	A	24	SER	O-C-N	13.83	140.10	122.95
1	A	107	ALA	O-C-N	-13.80	104.23	122.59
1	A	18	ASP	O-C-N	-13.69	106.19	122.89
1	A	1	LYS	CA-CB-CG	13.68	141.46	114.10
1	A	77	ASN	CB-CG-ND2	13.56	136.74	116.40
1	A	104	GLY	O-C-N	13.54	138.51	122.67
1	A	44	ASN	CA-CB-CG	-13.54	99.06	112.60
1	A	13	LYS	N-CA-CB	-13.54	87.61	110.49
1	A	38	PHE	CE1-CZ-CE2	13.53	144.35	120.00
1	A	1	LYS	CB-CA-C	-13.46	84.52	110.10
1	A	62	TRP	CD2-CE2-CZ2	-13.45	108.95	122.40
1	A	92	VAL	CA-CB-CG2	-13.37	87.66	110.40
1	A	27	ASN	CA-C-O	-13.30	106.32	120.55
1	A	16	GLY	CA-C-O	-13.29	104.95	119.04
1	A	25	LEU	N-CA-C	13.27	139.06	110.80
1	A	5	ARG	NE-CZ-NH2	13.25	131.13	119.20
1	A	28	TRP	CA-C-O	13.24	134.46	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	HIS	O-C-N	-13.23	105.33	122.39
1	A	69	THR	CA-C-O	-13.23	104.53	120.54
1	A	128	ARG	CA-C-O	-13.22	105.82	121.02
1	A	8	LEU	N-CA-CB	13.22	129.91	109.82
1	A	24	SER	CB-CA-C	-13.20	89.31	109.90
1	A	65	ASN	CA-C-O	-13.20	105.52	121.36
1	A	84	LEU	N-CA-CB	13.16	130.13	110.53
1	A	113	ASN	OD1-CG-ND2	13.08	135.68	122.60
1	A	7	GLU	O-C-N	-13.07	104.43	122.46
1	A	21	ARG	O-C-N	-13.07	105.28	122.40
1	A	46	ASN	CB-CA-C	13.06	136.42	110.42
1	A	3	PHE	O-C-N	13.01	138.52	122.65
1	A	23	TYR	CB-CG-CD2	13.01	140.32	120.80
1	A	123	TRP	CA-C-N	13.00	141.89	121.35
1	A	123	TRP	C-N-CA	13.00	141.89	121.35
1	A	108	TRP	CG-CD2-CE3	-12.90	121.00	133.90
1	A	14	ARG	CA-C-N	12.78	144.55	122.56
1	A	14	ARG	C-N-CA	12.78	144.55	122.56
1	A	14	ARG	CA-C-O	12.75	138.74	120.51
1	A	115	CYS	O-C-N	-12.71	105.68	122.59
1	A	76	CYS	CA-C-O	-12.61	102.91	119.80
1	A	19	ASN	CB-CG-ND2	-12.53	97.61	116.40
1	A	120	VAL	N-CA-C	-12.50	95.43	111.05
1	A	51	THR	O-C-N	-12.39	106.50	123.11
1	A	53	TYR	CA-C-N	12.39	140.03	122.06
1	A	53	TYR	C-N-CA	12.39	140.03	122.06
1	A	75	LEU	CA-C-O	12.37	133.80	120.82
1	A	52	ASP	CA-C-N	12.36	140.38	122.09
1	A	52	ASP	C-N-CA	12.36	140.38	122.09
1	A	113	ASN	O-C-N	12.35	134.78	122.07
1	A	54	GLY	CA-C-O	12.34	133.92	122.57
1	A	63	TRP	CE2-CD2-CG	-12.29	92.45	107.20
1	A	111	TRP	CH2-CZ2-CE2	12.26	133.43	117.50
1	A	11	ALA	O-C-N	12.25	138.89	122.59
1	A	80	CYS	CB-CA-C	12.22	134.74	110.42
1	A	15	HIS	CA-C-O	12.21	134.20	119.43
1	A	121	GLN	O-C-N	12.19	138.17	122.33
1	A	3	PHE	CB-CG-CD1	-12.17	100.01	120.70
1	A	94	CYS	CA-C-O	12.14	133.54	120.80
1	A	14	ARG	CB-CG-CD	-12.05	83.59	111.30
1	A	23	TYR	CD1-CE1-CZ	12.04	141.28	119.60
1	A	51	THR	CA-C-N	12.01	140.48	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	THR	C-N-CA	12.01	140.48	122.47
1	A	60	SER	CB-CA-C	-12.00	90.45	110.72
1	A	3	PHE	CB-CA-C	11.98	136.32	110.19
1	A	55	ILE	CA-C-O	-11.95	107.62	120.64
1	A	13	LYS	O-C-N	11.87	138.38	122.59
1	A	72	SER	N-CA-C	11.72	127.57	110.10
1	A	44	ASN	OD1-CG-ND2	-11.70	110.91	122.60
1	A	38	PHE	O-C-N	11.66	134.36	121.88
1	A	76	CYS	CA-C-N	11.64	138.72	122.07
1	A	76	CYS	C-N-CA	11.64	138.72	122.07
1	A	84	LEU	CB-CA-C	-11.63	89.41	109.65
1	A	108	TRP	CB-CG-CD2	11.59	143.03	126.80
1	A	57	GLN	CA-CB-CG	11.57	137.24	114.10
1	A	84	LEU	CA-C-O	11.55	132.31	119.15
1	A	111	TRP	CB-CG-CD1	-11.48	109.68	126.90
1	A	100	SER	N-CA-C	-11.26	96.98	112.30
1	A	17	LEU	CB-CA-C	11.25	128.81	110.81
1	A	20	TYR	O-C-N	-11.23	109.76	123.01
1	A	123	TRP	CG-CD2-CE3	11.21	145.10	133.90
1	A	18	ASP	CB-CG-OD1	11.17	144.10	118.40
1	A	57	GLN	OE1-CD-NE2	-11.14	111.46	122.60
1	A	111	TRP	CB-CA-C	11.03	129.15	110.84
1	A	92	VAL	CB-CA-C	-11.02	97.26	112.14
1	A	128	ARG	CB-CA-C	10.96	128.42	110.88
1	A	90	ALA	N-CA-CB	-10.96	91.97	110.49
1	A	119	ASP	N-CA-CB	10.95	126.59	110.49
1	A	111	TRP	CD2-CE3-CZ3	10.90	132.77	118.60
1	A	39	ASN	CB-CA-C	-10.89	93.36	110.78
1	A	27	ASN	CA-C-N	10.86	135.71	120.29
1	A	27	ASN	C-N-CA	10.86	135.71	120.29
1	A	62	TRP	O-C-N	-10.86	108.15	122.59
1	A	57	GLN	O-C-N	10.84	136.11	122.57
1	A	63	TRP	CA-C-O	-10.83	106.78	120.00
1	A	79	PRO	O-C-N	10.82	135.26	123.03
1	A	103	ASN	CB-CG-ND2	10.79	132.59	116.40
1	A	101	ASP	N-CA-C	-10.78	99.97	113.55
1	A	111	TRP	NE1-CE2-CZ2	10.77	146.26	130.10
1	A	13	LYS	CA-CB-CG	-10.75	92.60	114.10
1	A	79	PRO	CA-C-O	-10.71	108.44	120.97
1	A	19	ASN	CB-CA-C	10.68	131.68	110.42
1	A	123	TRP	CB-CG-CD1	10.67	142.91	126.90
1	A	5	ARG	CG-CD-NE	10.64	135.42	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASP	OD1-CG-OD2	-10.64	97.36	122.90
1	A	67	GLY	CA-C-O	10.63	130.68	119.10
1	A	32	ALA	N-CA-CB	10.62	126.53	110.81
1	A	40	THR	CA-C-O	-10.58	106.68	119.49
1	A	106	ASN	CB-CG-ND2	-10.56	100.56	116.40
1	A	72	SER	CA-CB-OG	-10.53	90.05	111.10
1	A	97	LYS	CA-CB-CG	10.52	135.14	114.10
1	A	21	ARG	NE-CZ-NH2	10.49	128.64	119.20
1	A	64	CYS	CA-C-N	-10.48	104.16	122.07
1	A	64	CYS	C-N-CA	-10.48	104.16	122.07
1	A	111	TRP	CE2-CD2-CE3	-10.47	108.33	118.80
1	A	21	ARG	CD-NE-CZ	-10.46	109.76	124.40
1	A	100	SER	CA-CB-OG	10.36	131.82	111.10
1	A	105	MET	CA-CB-CG	-10.34	93.42	114.10
1	A	119	ASP	CA-CB-CG	10.34	122.94	112.60
1	A	111	TRP	CD1-CG-CD2	10.32	122.82	106.30
1	A	74	ASN	OD1-CG-ND2	10.30	132.90	122.60
1	A	24	SER	CA-C-N	-10.28	101.91	121.54
1	A	24	SER	C-N-CA	-10.28	101.91	121.54
1	A	56	LEU	CD1-CG-CD2	-10.27	88.20	110.80
1	A	123	TRP	CB-CA-C	10.23	127.07	110.90
1	A	77	ASN	N-CA-C	-10.16	97.72	111.54
1	A	68	ARG	CA-CB-CG	-10.16	93.78	114.10
1	A	117	GLY	CA-C-O	-10.15	106.81	119.19
1	A	87	ASP	N-CA-CB	-10.15	94.82	110.65
1	A	7	GLU	CG-CD-OE1	10.14	141.73	118.40
1	A	63	TRP	CB-CG-CD1	-10.13	111.71	126.90
1	A	78	ILE	CA-C-N	10.12	131.57	120.13
1	A	78	ILE	C-N-CA	10.12	131.57	120.13
1	A	73	ARG	O-C-N	-10.12	111.44	123.27
1	A	103	ASN	CA-C-O	10.11	130.45	119.03
1	A	98	ILE	O-C-N	10.10	135.66	121.82
1	A	48	ASP	N-CA-CB	-10.07	93.80	110.22
1	A	47	THR	CA-C-O	-10.07	107.48	119.27
1	A	46	ASN	CA-CB-CG	10.06	122.66	112.60
1	A	2	VAL	CB-CA-C	9.99	124.43	110.84
1	A	107	ALA	N-CA-CB	9.94	127.30	110.49
1	A	43	THR	N-CA-CB	-9.87	94.38	111.55
1	A	22	GLY	CA-C-O	9.79	131.64	119.80
1	A	113	ASN	CA-C-O	-9.77	110.56	120.82
1	A	46	ASN	N-CA-CB	-9.74	94.03	110.49
1	A	14	ARG	NE-CZ-NH2	9.73	127.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	TRP	N-CA-CB	9.73	123.70	110.57
1	A	34	PHE	CA-CB-CG	-9.72	104.08	113.80
1	A	62	TRP	CD2-CE3-CZ3	-9.71	105.98	118.60
1	A	87	ASP	CB-CA-C	-9.70	94.06	110.16
1	A	47	THR	CA-C-N	-9.69	103.81	122.61
1	A	47	THR	C-N-CA	-9.69	103.81	122.61
1	A	101	ASP	O-C-N	-9.68	107.62	122.13
1	A	11	ALA	N-CA-CB	9.62	126.74	110.49
1	A	63	TRP	CG-CD2-CE3	9.61	143.51	133.90
1	A	8	LEU	CD1-CG-CD2	-9.57	89.74	110.80
1	A	124	ILE	O-C-N	-9.52	111.08	122.12
1	A	86	SER	CA-CB-OG	9.49	130.08	111.10
1	A	49	GLY	N-CA-C	-9.46	90.77	113.18
1	A	111	TRP	CD2-CE2-CZ2	-9.45	112.95	122.40
1	A	74	ASN	CB-CA-C	-9.45	95.82	111.51
1	A	103	ASN	OD1-CG-ND2	-9.45	113.15	122.60
1	A	75	LEU	N-CA-CB	9.42	123.67	110.01
1	A	15	HIS	N-CA-C	9.40	124.30	113.02
1	A	27	ASN	CA-CB-CG	-9.38	103.22	112.60
1	A	65	ASN	CB-CA-C	-9.35	93.53	109.51
1	A	114	ARG	CD-NE-CZ	-9.35	111.32	124.40
1	A	53	TYR	N-CA-C	9.31	125.60	109.96
1	A	1	LYS	CA-C-O	-9.24	105.09	120.80
1	A	106	ASN	CA-CB-CG	-9.21	103.39	112.60
1	A	95	ALA	O-C-N	-9.20	111.53	122.11
1	A	96	LYS	CA-C-O	-9.15	107.42	120.51
1	A	28	TRP	CD1-NE1-CE2	9.13	125.34	108.90
1	A	37	ASN	CA-C-O	-9.12	109.63	120.12
1	A	67	GLY	CA-C-N	9.10	136.78	122.49
1	A	67	GLY	C-N-CA	9.10	136.78	122.49
1	A	23	TYR	CE1-CZ-CE2	-9.07	102.15	120.30
1	A	16	GLY	O-C-N	9.06	133.97	122.28
1	A	23	TYR	CA-C-O	-9.05	110.75	120.80
1	A	2	VAL	CA-CB-CG1	-9.04	95.03	110.40
1	A	106	ASN	CA-C-N	9.04	138.80	121.54
1	A	106	ASN	C-N-CA	9.04	138.80	121.54
1	A	72	SER	O-C-N	9.00	134.11	122.95
1	A	29	VAL	CA-CB-CG1	-8.99	95.11	110.40
1	A	87	ASP	OD1-CG-OD2	-8.97	101.37	122.90
1	A	111	TRP	CZ3-CH2-CZ2	-8.97	109.84	121.50
1	A	28	TRP	O-C-N	-8.91	112.00	122.15
1	A	83	LEU	O-C-N	8.85	134.36	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	TYR	CD1-CG-CD2	-8.82	104.87	118.10
1	A	121	GLN	CB-CG-CD	8.81	127.58	112.60
1	A	13	LYS	CD-CE-NZ	-8.80	83.73	111.90
1	A	5	ARG	CB-CA-C	-8.79	92.92	110.42
1	A	21	ARG	CG-CD-NE	-8.75	92.75	112.00
1	A	19	ASN	OD1-CG-ND2	8.75	131.35	122.60
1	A	25	LEU	CA-C-O	8.74	133.01	120.51
1	A	23	TYR	O-C-N	-8.74	112.96	123.19
1	A	108	TRP	CE2-CD2-CE3	8.71	127.51	118.80
1	A	73	ARG	CA-C-N	-8.65	109.14	123.33
1	A	73	ARG	C-N-CA	-8.65	109.14	123.33
1	A	120	VAL	CA-C-N	8.65	134.56	120.63
1	A	120	VAL	C-N-CA	8.65	134.56	120.63
1	A	31	ALA	CB-CA-C	-8.64	96.28	110.79
1	A	55	ILE	N-CA-CB	-8.62	97.01	110.54
1	A	121	GLN	CA-C-O	-8.60	109.46	119.61
1	A	5	ARG	N-CA-C	-8.58	92.53	110.80
1	A	78	ILE	N-CA-CB	8.57	123.21	111.21
1	A	66	ASP	CB-CG-OD1	8.56	138.10	118.40
1	A	108	TRP	CD2-CE2-CZ2	-8.54	113.86	122.40
1	A	51	THR	N-CA-CB	-8.54	97.37	111.20
1	A	9	ALA	CA-C-O	8.53	129.96	121.00
1	A	111	TRP	O-C-N	8.44	132.41	122.20
1	A	70	PRO	CB-CG-CD	8.42	133.05	106.10
1	A	50	SER	N-CA-CB	8.40	124.68	110.49
1	A	97	LYS	CB-CA-C	8.40	126.60	109.55
1	A	95	ALA	CA-C-N	8.38	137.54	121.54
1	A	95	ALA	C-N-CA	8.38	137.54	121.54
1	A	19	ASN	N-CA-CB	-8.38	96.33	110.49
1	A	72	SER	CB-CA-C	-8.37	96.84	109.90
1	A	115	CYS	N-CA-CB	8.37	124.63	110.49
1	A	47	THR	N-CA-CB	-8.35	97.42	110.44
1	A	84	LEU	O-C-N	-8.30	111.55	122.42
1	A	10	ALA	N-CA-C	8.29	120.31	111.28
1	A	74	ASN	O-C-N	8.25	135.08	122.87
1	A	17	LEU	N-CA-C	-8.21	101.26	111.11
1	A	20	TYR	N-CA-C	8.17	123.11	110.20
1	A	10	ALA	CB-CA-C	-8.16	97.24	110.79
1	A	71	GLY	CA-C-O	-8.15	108.41	119.01
1	A	28	TRP	CG-CD1-NE1	-8.11	99.66	110.20
1	A	15	HIS	CE1-NE2-CD2	-8.04	100.96	109.00
1	A	62	TRP	CG-CD1-NE1	8.02	120.62	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	VAL	CA-C-O	8.00	130.59	120.83
1	A	18	ASP	CA-CB-CG	7.99	120.59	112.60
1	A	1	LYS	CG-CD-CE	7.98	129.66	111.30
1	A	70	PRO	N-CA-C	7.98	128.90	112.47
1	A	78	ILE	CA-C-O	7.97	130.63	119.95
1	A	123	TRP	CE2-CD2-CG	-7.96	97.64	107.20
1	A	29	VAL	O-C-N	-7.95	107.30	121.84
1	A	3	PHE	CG-CD2-CE2	7.93	134.18	120.70
1	A	65	ASN	O-C-N	7.86	131.86	123.06
1	A	84	LEU	CB-CG-CD2	-7.84	87.18	110.70
1	A	52	ASP	OD1-CG-OD2	-7.84	104.09	122.90
1	A	122	ALA	N-CA-CB	7.83	123.16	110.40
1	A	19	ASN	CA-C-N	-7.82	110.25	121.42
1	A	19	ASN	C-N-CA	-7.82	110.25	121.42
1	A	82	ALA	O-C-N	7.81	131.10	122.11
1	A	110	ALA	N-CA-C	7.81	119.58	111.14
1	A	63	TRP	CD2-CE2-CZ2	-7.80	114.60	122.40
1	A	110	ALA	CA-C-N	7.79	133.58	121.19
1	A	110	ALA	C-N-CA	7.79	133.58	121.19
1	A	36	SER	CA-C-O	7.79	128.79	119.06
1	A	58	ILE	N-CA-C	7.76	119.00	109.30
1	A	99	VAL	CA-CB-CG2	7.75	123.58	110.40
1	A	20	TYR	CA-C-O	7.74	129.87	121.05
1	A	108	TRP	N-CA-C	7.72	122.00	108.56
1	A	85	SER	CB-CA-C	-7.69	95.31	109.46
1	A	38	PHE	CA-C-O	7.69	131.39	118.94
1	A	36	SER	N-CA-CB	7.66	122.14	110.81
1	A	52	ASP	O-C-N	-7.66	113.34	123.14
1	A	85	SER	O-C-N	-7.65	114.31	122.96
1	A	78	ILE	CA-CB-CG1	7.64	123.39	110.40
1	A	39	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	A	14	ARG	NE-CZ-NH1	-7.59	113.91	121.50
1	A	32	ALA	CA-C-N	-7.56	110.34	120.63
1	A	32	ALA	C-N-CA	-7.56	110.34	120.63
1	A	39	ASN	N-CA-C	7.56	121.13	108.20
1	A	101	ASP	N-CA-CB	7.56	121.36	110.40
1	A	9	ALA	O-C-N	-7.54	114.19	122.03
1	A	77	ASN	N-CA-CB	7.52	123.04	111.84
1	A	56	LEU	CB-CG-CD2	7.52	133.25	110.70
1	A	28	TRP	N-CA-CB	7.51	121.28	110.16
1	A	9	ALA	N-CA-C	-7.51	102.78	110.97
1	A	38	PHE	CZ-CE2-CD2	-7.49	106.52	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLY	N-CA-C	-7.47	101.75	112.81
1	A	106	ASN	N-CA-C	-7.44	102.85	112.23
1	A	20	TYR	CA-CB-CG	-7.42	100.54	113.90
1	A	87	ASP	CA-C-O	-7.42	112.36	120.30
1	A	34	PHE	CD1-CE1-CZ	-7.40	106.68	120.00
1	A	66	ASP	N-CA-CB	-7.39	98.00	110.65
1	A	74	ASN	CA-C-N	-7.39	110.83	120.44
1	A	74	ASN	C-N-CA	-7.39	110.83	120.44
1	A	51	THR	CA-C-O	7.38	130.09	121.46
1	A	51	THR	N-CA-C	7.37	121.49	109.85
1	A	28	TRP	CA-C-N	7.35	132.53	121.65
1	A	28	TRP	C-N-CA	7.35	132.53	121.65
1	A	3	PHE	N-CA-CB	-7.35	100.31	110.38
1	A	3	PHE	CZ-CE2-CD2	-7.35	106.78	120.00
1	A	60	SER	CA-C-O	-7.34	110.92	119.59
1	A	45	ARG	CB-CA-C	-7.34	96.17	109.38
1	A	85	SER	CA-C-O	-7.32	113.05	121.47
1	A	70	PRO	N-CA-CB	7.31	110.92	103.25
1	A	93	ASN	CA-C-N	7.29	132.68	120.88
1	A	93	ASN	C-N-CA	7.29	132.68	120.88
1	A	60	SER	N-CA-C	7.21	122.19	112.88
1	A	73	ARG	N-CA-C	-7.21	96.52	108.34
1	A	66	ASP	N-CA-C	-7.20	103.14	113.21
1	A	33	LYS	N-CA-CB	-7.18	99.57	109.98
1	A	121	GLN	N-CA-C	7.17	121.67	112.34
1	A	126	GLY	N-CA-C	-7.16	104.61	114.64
1	A	70	PRO	N-CD-CG	-7.16	92.46	103.20
1	A	119	ASP	CB-CA-C	-7.14	101.20	112.05
1	A	8	LEU	CB-CG-CD2	7.11	132.02	110.70
1	A	99	VAL	CB-CA-C	-7.09	91.06	111.42
1	A	64	CYS	CA-C-O	-7.08	113.06	120.99
1	A	1	LYS	CD-CE-NZ	7.04	134.44	111.90
1	A	10	ALA	CA-C-N	7.04	134.99	121.54
1	A	10	ALA	C-N-CA	7.04	134.99	121.54
1	A	64	CYS	CB-CA-C	-7.02	94.99	109.94
1	A	124	ILE	CA-CB-CG2	6.99	122.38	110.50
1	A	66	ASP	CA-CB-CG	-6.98	105.62	112.60
1	A	68	ARG	CB-CG-CD	-6.94	95.33	111.30
1	A	22	GLY	CA-C-N	-6.93	112.32	122.65
1	A	22	GLY	C-N-CA	-6.93	112.32	122.65
1	A	13	LYS	CB-CA-C	6.90	124.15	110.42
1	A	89	THR	CA-C-N	-6.89	108.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	THR	C-N-CA	-6.89	108.38	121.54
1	A	3	PHE	CA-C-N	-6.88	107.92	121.41
1	A	3	PHE	C-N-CA	-6.88	107.92	121.41
1	A	103	ASN	O-C-N	6.88	129.73	122.23
1	A	51	THR	CA-CB-CG2	-6.86	98.83	110.50
1	A	80	CYS	CA-C-O	6.86	130.31	120.51
1	A	70	PRO	CA-CB-CG	-6.85	91.49	104.50
1	A	21	ARG	NH1-CZ-NH2	-6.83	110.42	119.30
1	A	116	LYS	N-CA-CB	6.82	122.01	110.49
1	A	90	ALA	CA-C-O	6.81	130.25	120.51
1	A	62	TRP	CD1-NE1-CE2	-6.80	96.65	108.90
1	A	112	ARG	CA-C-N	6.80	129.28	120.44
1	A	112	ARG	C-N-CA	6.80	129.28	120.44
1	A	114	ARG	CA-C-O	-6.79	111.41	119.35
1	A	98	ILE	CA-C-O	-6.76	112.95	120.25
1	A	29	VAL	N-CA-C	-6.76	105.17	111.45
1	A	45	ARG	CG-CD-NE	6.74	126.83	112.00
1	A	20	TYR	CB-CA-C	-6.72	98.17	109.53
1	A	20	TYR	N-CA-CB	-6.71	99.93	110.06
1	A	59	ASN	O-C-N	6.68	130.86	122.65
1	A	92	VAL	O-C-N	6.67	128.34	121.87
1	A	108	TRP	CB-CG-CD1	-6.66	116.91	126.90
1	A	99	VAL	CA-C-N	-6.64	111.06	122.14
1	A	99	VAL	C-N-CA	-6.64	111.06	122.14
1	A	17	LEU	CB-CG-CD1	6.63	130.60	110.70
1	A	106	ASN	CB-CG-OD1	6.63	134.06	120.80
1	A	116	LYS	CA-CB-CG	6.63	127.35	114.10
1	A	31	ALA	CA-C-O	-6.62	113.46	120.55
1	A	44	ASN	CA-C-N	-6.62	113.34	122.93
1	A	44	ASN	C-N-CA	-6.62	113.34	122.93
1	A	68	ARG	N-CA-C	6.60	120.99	112.41
1	A	8	LEU	CA-C-O	6.58	128.31	121.07
1	A	2	VAL	N-CA-C	-6.58	98.96	108.36
1	A	92	VAL	CG1-CB-CG2	6.57	125.26	110.80
1	A	63	TRP	CA-C-N	6.56	133.45	121.85
1	A	63	TRP	C-N-CA	6.56	133.45	121.85
1	A	111	TRP	CG-CD1-NE1	-6.54	101.69	110.20
1	A	128	ARG	CA-CB-CG	6.54	127.18	114.10
1	A	5	ARG	CB-CG-CD	6.54	126.34	111.30
1	A	97	LYS	N-CA-CB	-6.52	100.26	110.44
1	A	45	ARG	NE-CZ-NH2	6.52	125.07	119.20
1	A	103	ASN	CB-CG-OD1	-6.51	107.78	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ILE	CA-C-O	-6.50	113.63	121.04
1	A	34	PHE	CE1-CZ-CE2	6.50	131.69	120.00
1	A	98	ILE	CA-CB-CG2	-6.48	99.49	110.50
1	A	19	ASN	N-CA-C	6.47	124.59	110.80
1	A	14	ARG	CA-CB-CG	6.46	127.02	114.10
1	A	127	CYS	O-C-N	-6.43	115.03	122.93
1	A	33	LYS	CD-CE-NZ	6.39	132.34	111.90
1	A	119	ASP	CB-CG-OD1	-6.33	103.83	118.40
1	A	65	ASN	CB-CG-ND2	-6.32	106.92	116.40
1	A	28	TRP	CB-CA-C	-6.31	100.11	110.85
1	A	119	ASP	O-C-N	6.30	129.66	122.55
1	A	19	ASN	CA-CB-CG	-6.29	106.31	112.60
1	A	43	THR	N-CA-C	-6.29	99.78	109.52
1	A	117	GLY	CA-C-N	6.27	134.88	123.27
1	A	117	GLY	C-N-CA	6.27	134.88	123.27
1	A	112	ARG	CA-CB-CG	-6.27	101.56	114.10
1	A	82	ALA	CA-C-O	-6.25	113.92	120.92
1	A	122	ALA	CB-CA-C	-6.24	96.95	109.99
1	A	120	VAL	O-C-N	-6.23	115.58	121.87
1	A	23	TYR	CE1-CZ-OH	6.23	138.58	119.90
1	A	61	ARG	CA-C-O	-6.22	111.60	119.31
1	A	96	LYS	CG-CD-CE	6.21	125.58	111.30
1	A	51	THR	CA-CB-OG1	6.20	118.90	109.60
1	A	9	ALA	CA-C-N	-6.19	111.99	120.28
1	A	9	ALA	C-N-CA	-6.19	111.99	120.28
1	A	62	TRP	NE1-CE2-CZ2	6.18	139.37	130.10
1	A	36	SER	N-CA-C	6.18	121.70	114.04
1	A	87	ASP	CA-C-N	6.17	133.07	121.97
1	A	87	ASP	C-N-CA	6.17	133.07	121.97
1	A	115	CYS	CA-C-O	6.16	129.32	120.51
1	A	88	ILE	CB-CA-C	6.16	121.38	111.29
1	A	113	ASN	CB-CG-ND2	-6.16	107.17	116.40
1	A	111	TRP	CA-CB-CG	-6.13	101.95	113.60
1	A	14	ARG	CG-CD-NE	-6.11	98.56	112.00
1	A	122	ALA	N-CA-C	-6.10	105.32	112.89
1	A	98	ILE	N-CA-C	6.10	119.62	111.44
1	A	82	ALA	N-CA-CB	6.10	119.72	109.78
1	A	21	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	A	50	SER	N-CA-C	6.09	123.78	110.80
1	A	38	PHE	CD1-CE1-CZ	-6.09	109.04	120.00
1	A	13	LYS	CA-C-O	6.08	129.20	120.51
1	A	108	TRP	CB-CA-C	-6.06	102.57	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	CB-CG-CD	6.06	125.24	111.30
1	A	42	ALA	O-C-N	-6.05	115.43	122.87
1	A	95	ALA	N-CA-CB	-6.04	99.94	109.78
1	A	61	ARG	N-CA-CB	-6.03	100.57	110.40
1	A	47	THR	CA-CB-OG1	-6.03	100.56	109.60
1	A	129	LEU	CD1-CG-CD2	-6.03	97.54	110.80
1	A	90	ALA	N-CA-C	6.02	123.63	110.80
1	A	35	GLU	CA-C-N	6.02	133.07	122.42
1	A	35	GLU	C-N-CA	6.02	133.07	122.42
1	A	34	PHE	CA-C-O	-6.01	113.31	120.10
1	A	119	ASP	OD1-CG-OD2	5.97	137.24	122.90
1	A	59	ASN	OD1-CG-ND2	5.96	128.56	122.60
1	A	59	ASN	N-CA-CB	-5.96	101.92	110.44
1	A	50	SER	O-C-N	5.92	130.47	122.59
1	A	88	ILE	CA-CB-CG1	-5.92	100.34	110.40
1	A	3	PHE	CD1-CE1-CZ	-5.89	109.40	120.00
1	A	57	GLN	CA-C-N	-5.84	113.04	120.98
1	A	57	GLN	C-N-CA	-5.84	113.04	120.98
1	A	59	ASN	CA-C-N	-5.83	113.50	122.60
1	A	59	ASN	C-N-CA	-5.83	113.50	122.60
1	A	56	LEU	N-CA-C	-5.82	103.75	112.54
1	A	63	TRP	CB-CG-CD2	-5.80	118.68	126.80
1	A	96	LYS	CA-C-N	5.80	131.86	121.66
1	A	96	LYS	C-N-CA	5.80	131.86	121.66
1	A	61	ARG	CB-CA-C	5.79	122.09	109.99
1	A	104	GLY	CA-C-O	-5.78	114.33	121.56
1	A	41	GLN	CA-C-N	5.78	128.91	120.71
1	A	41	GLN	C-N-CA	5.78	128.91	120.71
1	A	63	TRP	CZ3-CH2-CZ2	5.77	129.01	121.50
1	A	87	ASP	N-CA-C	5.76	117.79	108.41
1	A	88	ILE	CB-CG1-CD1	5.69	125.75	113.80
1	A	29	VAL	CG1-CB-CG2	5.69	123.31	110.80
1	A	81	SER	N-CA-C	5.64	122.82	110.80
1	A	31	ALA	O-C-N	5.62	128.97	122.17
1	A	38	PHE	N-CA-C	5.62	124.53	113.29
1	A	64	CYS	CA-CB-SG	5.61	127.30	114.40
1	A	118	THR	CA-CB-OG1	5.60	118.00	109.60
1	A	115	CYS	CB-CA-C	-5.59	99.29	110.42
1	A	56	LEU	CA-C-N	5.59	130.34	122.46
1	A	56	LEU	C-N-CA	5.59	130.34	122.46
1	A	92	VAL	CA-C-N	-5.59	111.36	121.14
1	A	92	VAL	C-N-CA	-5.59	111.36	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	MET	CG-SD-CE	5.54	113.08	100.90
1	A	3	PHE	CE1-CZ-CE2	5.53	129.95	120.00
1	A	111	TRP	NE1-CE2-CD2	-5.52	100.22	107.40
1	A	4	GLY	N-CA-C	-5.51	100.12	113.18
1	A	113	ASN	N-CA-C	-5.51	105.17	111.07
1	A	103	ASN	N-CA-CB	5.51	118.88	110.95
1	A	40	THR	CA-CB-CG2	5.49	119.84	110.50
1	A	108	TRP	CD2-CE3-CZ3	-5.48	111.48	118.60
1	A	124	ILE	CA-C-N	5.47	128.53	120.82
1	A	124	ILE	C-N-CA	5.47	128.53	120.82
1	A	15	HIS	ND1-CE1-NE2	5.47	113.87	108.40
1	A	73	ARG	N-CA-CB	5.46	119.34	110.77
1	A	86	SER	O-C-N	-5.46	115.35	122.39
1	A	52	ASP	CB-CA-C	-5.45	103.49	111.23
1	A	28	TRP	CE2-CD2-CE3	5.45	124.25	118.80
1	A	96	LYS	O-C-N	-5.44	115.35	122.59
1	A	9	ALA	N-CA-CB	5.41	117.81	109.91
1	A	12	MET	N-CA-C	5.38	118.06	111.82
1	A	88	ILE	N-CA-CB	5.37	120.09	111.23
1	A	66	ASP	OD1-CG-OD2	-5.37	110.02	122.90
1	A	34	PHE	CG-CD1-CE1	5.36	129.81	120.70
1	A	87	ASP	CB-CG-OD1	5.36	130.72	118.40
1	A	74	ASN	CB-CG-OD1	-5.31	110.18	120.80
1	A	21	ARG	CA-CB-CG	-5.30	103.50	114.10
1	A	45	ARG	NH1-CZ-NH2	-5.30	112.42	119.30
1	A	63	TRP	CA-CB-CG	-5.29	103.55	113.60
1	A	79	PRO	N-CD-CG	5.29	111.13	103.20
1	A	125	ARG	N-CA-C	5.29	117.97	110.10
1	A	17	LEU	CD1-CG-CD2	-5.27	99.22	110.80
1	A	20	TYR	CD1-CE1-CZ	-5.26	110.12	119.60
1	A	91	SER	CA-C-O	5.25	126.52	121.00
1	A	100	SER	CB-CA-C	-5.25	102.24	110.85
1	A	77	ASN	CB-CA-C	-5.24	104.15	111.80
1	A	48	ASP	N-CA-C	5.23	119.83	112.72
1	A	44	ASN	CB-CA-C	-5.22	103.53	110.79
1	A	116	LYS	O-C-N	5.22	129.53	122.59
1	A	23	TYR	CA-CB-CG	5.21	123.27	113.90
1	A	74	ASN	CA-C-O	5.18	129.51	120.85
1	A	43	THR	CA-CB-CG2	5.18	119.31	110.50
1	A	4	GLY	CA-C-N	-5.18	111.65	121.54
1	A	4	GLY	C-N-CA	-5.18	111.65	121.54
1	A	102	GLY	O-C-N	-5.18	115.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	TRP	CE2-CD2-CE3	5.16	123.96	118.80
1	A	81	SER	N-CA-CB	-5.16	101.77	110.49
1	A	115	CYS	CA-C-N	5.16	131.40	121.54
1	A	115	CYS	C-N-CA	5.16	131.40	121.54
1	A	105	MET	CA-C-O	5.16	127.17	119.23
1	A	127	CYS	CA-C-N	5.15	130.82	122.07
1	A	127	CYS	C-N-CA	5.15	130.82	122.07
1	A	71	GLY	CA-C-N	-5.14	113.58	120.82
1	A	71	GLY	C-N-CA	-5.14	113.58	120.82
1	A	98	ILE	CB-CA-C	-5.13	103.80	112.16
1	A	60	SER	O-C-N	5.12	128.35	122.25
1	A	78	ILE	CA-CB-CG2	-5.07	101.88	110.50
1	A	7	GLU	CA-C-O	5.05	125.58	119.31
1	A	93	ASN	CA-C-O	-5.04	113.06	119.31
1	A	19	ASN	CB-CG-OD1	5.03	130.86	120.80
1	A	108	TRP	NE1-CE2-CD2	5.03	113.93	107.40
1	A	60	SER	CA-CB-OG	5.02	121.14	111.10
1	A	53	TYR	CZ-CE2-CD2	-5.02	110.57	119.60
1	A	33	LYS	CG-CD-CE	5.01	122.83	111.30
1	A	105	MET	N-CA-C	-5.01	107.19	113.15
1	A	105	MET	CB-CG-SD	-5.01	97.68	112.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	ARG	CA
1	A	90	ALA	CA

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	LYS	Mainchain
1	A	100	SER	Mainchain
1	A	103	ASN	Sidechain
1	A	114	ARG	Sidechain
1	A	12	MET	Peptide,Mainchain
1	A	121	GLN	Mainchain
1	A	123	TRP	Mainchain
1	A	127	CYS	Mainchain
1	A	13	LYS	Peptide
1	A	14	ARG	Mainchain
1	A	17	LEU	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	A	18	ASP	Mainchain
1	A	2	VAL	Mainchain
1	A	20	TYR	Mainchain,Peptide,Sidechain
1	A	21	ARG	Sidechain
1	A	22	GLY	Mainchain
1	A	23	TYR	Peptide,Mainchain
1	A	24	SER	Mainchain
1	A	30	CYS	Mainchain
1	A	31	ALA	Peptide
1	A	34	PHE	Sidechain
1	A	35	GLU	Sidechain
1	A	37	ASN	Mainchain
1	A	38	PHE	Sidechain
1	A	42	ALA	Mainchain
1	A	44	ASN	Sidechain
1	A	46	ASN	Mainchain
1	A	5	ARG	Mainchain,Sidechain
1	A	50	SER	Mainchain
1	A	52	ASP	Mainchain
1	A	53	TYR	Mainchain,Peptide,Sidechain
1	A	55	ILE	Peptide
1	A	56	LEU	Mainchain
1	A	60	SER	Mainchain
1	A	61	ARG	Sidechain
1	A	66	ASP	Peptide,Mainchain
1	A	7	GLU	Mainchain,Sidechain
1	A	70	PRO	Mainchain
1	A	73	ARG	Mainchain
1	A	76	CYS	Peptide,Mainchain
1	A	85	SER	Peptide,Mainchain
1	A	86	SER	Mainchain
1	A	87	ASP	Mainchain
1	A	93	ASN	Mainchain
1	A	95	ALA	Mainchain
1	A	96	LYS	Mainchain

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	1001	0	939	444	5
2	A	101	0	0	19	6
All	All	1102	0	939	444	8

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 230.

All (444) 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:A:30:CYS:CB	1:A:30:CYS:CA	1.75	1.65
1:A:51:THR:CB	1:A:51:THR:CA	1.76	1.64
1:A:68:ARG:CB	1:A:68:ARG:CA	1.75	1.63
1:A:45:ARG:CB	1:A:45:ARG:CA	1.77	1.62
1:A:13:LYS:CA	1:A:13:LYS:CB	1.77	1.61
1:A:74:ASN:CA	1:A:74:ASN:CB	1.79	1.61
1:A:3:PHE:CD1	1:A:3:PHE:CG	1.85	1.60
1:A:21:ARG:CB	1:A:21:ARG:CA	1.79	1.60
1:A:20:TYR:CZ	1:A:20:TYR:CE1	1.90	1.59
1:A:84:LEU:CB	1:A:84:LEU:CA	1.74	1.59
1:A:112:ARG:CB	1:A:112:ARG:CG	1.77	1.59
1:A:8:LEU:CG	1:A:8:LEU:CD2	1.81	1.58
1:A:7:GLU:CB	1:A:7:GLU:CG	1.81	1.58
1:A:92:VAL:CG2	1:A:92:VAL:CB	1.81	1.58
1:A:99:VAL:CA	1:A:99:VAL:CB	1.79	1.57
1:A:84:LEU:CG	1:A:84:LEU:CD2	1.83	1.57
1:A:20:TYR:CG	1:A:20:TYR:CD2	1.88	1.57
1:A:107:ALA:CA	1:A:107:ALA:CB	1.77	1.57
1:A:98:ILE:CD1	1:A:98:ILE:CG1	1.76	1.56
1:A:61:ARG:CG	1:A:61:ARG:CB	1.83	1.56
1:A:122:ALA:C	1:A:122:ALA:CA	1.74	1.55
1:A:50:SER:C	1:A:50:SER:CA	1.77	1.55
1:A:64:CYS:C	1:A:64:CYS:CA	1.75	1.55
1:A:72:SER:C	1:A:72:SER:CA	1.79	1.55
1:A:63:TRP:CB	1:A:63:TRP:CA	1.76	1.54
1:A:91:SER:N	1:A:91:SER:CA	1.67	1.54
1:A:10:ALA:CB	1:A:10:ALA:CA	1.81	1.54
1:A:38:PHE:CB	1:A:38:PHE:CA	1.85	1.54
1:A:39:ASN:CB	1:A:39:ASN:CA	1.80	1.54
1:A:75:LEU:CB	1:A:75:LEU:CA	1.80	1.53
1:A:92:VAL:CB	1:A:92:VAL:CA	1.87	1.53
1:A:46:ASN:CA	1:A:46:ASN:C	1.76	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:SER:N	1:A:100:SER:CA	1.69	1.53
1:A:56:LEU:CD2	1:A:56:LEU:CG	1.81	1.53
1:A:77:ASN:C	1:A:77:ASN:CA	1.80	1.53
1:A:129:LEU:CD2	1:A:129:LEU:CG	1.85	1.53
1:A:35:GLU:N	1:A:35:GLU:CA	1.67	1.52
1:A:111:TRP:N	1:A:111:TRP:CA	1.67	1.51
1:A:21:ARG:CD	1:A:21:ARG:NE	1.69	1.51
1:A:8:LEU:CG	1:A:8:LEU:CD1	1.87	1.50
1:A:6:CYS:CA	1:A:6:CYS:N	1.68	1.50
1:A:90:ALA:N	1:A:90:ALA:CA	1.73	1.50
1:A:119:ASP:CA	1:A:119:ASP:C	1.81	1.50
1:A:3:PHE:C	1:A:3:PHE:CA	1.84	1.49
1:A:3:PHE:CB	1:A:3:PHE:CD2	1.95	1.49
1:A:6:CYS:CA	1:A:6:CYS:C	1.86	1.49
1:A:73:ARG:CG	1:A:73:ARG:CB	1.89	1.49
1:A:97:LYS:CE	1:A:97:LYS:CD	1.86	1.49
1:A:60:SER:N	1:A:60:SER:CA	1.74	1.48
1:A:122:ALA:HA	1:A:125:ARG:CD	1.43	1.47
1:A:84:LEU:CB	1:A:84:LEU:CG	1.86	1.47
1:A:4:GLY:C	1:A:4:GLY:CA	1.84	1.47
1:A:8:LEU:C	1:A:9:ALA:N	1.70	1.47
1:A:1:LYS:C	1:A:1:LYS:CA	1.89	1.45
1:A:110:ALA:CB	1:A:110:ALA:CA	1.91	1.45
1:A:48:ASP:CA	1:A:48:ASP:N	1.74	1.45
1:A:40:THR:C	1:A:40:THR:CA	1.90	1.44
1:A:85:SER:C	1:A:85:SER:CA	1.91	1.43
1:A:23:TYR:CA	1:A:23:TYR:N	1.80	1.43
1:A:67:GLY:C	1:A:68:ARG:N	1.76	1.43
1:A:80:CYS:CA	1:A:80:CYS:N	1.82	1.43
1:A:21:ARG:CZ	1:A:21:ARG:NH1	1.79	1.41
1:A:31:ALA:CB	1:A:31:ALA:CA	2.00	1.38
1:A:21:ARG:CA	1:A:21:ARG:N	1.87	1.38
1:A:41:GLN:N	1:A:41:GLN:CA	1.84	1.38
1:A:43:THR:CB	1:A:43:THR:OG1	1.72	1.38
1:A:5:ARG:CZ	1:A:5:ARG:CD	2.00	1.38
1:A:9:ALA:C	1:A:10:ALA:N	1.83	1.37
1:A:55:ILE:N	1:A:55:ILE:CA	1.84	1.37
1:A:1:LYS:CA	1:A:1:LYS:CB	2.02	1.35
1:A:74:ASN:CA	1:A:74:ASN:C	2.00	1.34
1:A:5:ARG:CZ	1:A:5:ARG:NH2	1.92	1.33
1:A:50:SER:C	1:A:51:THR:CA	2.00	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:CB	1:A:81:SER:OG	1.78	1.31
1:A:10:ALA:O	1:A:11:ALA:N	1.66	1.28
1:A:27:ASN:CG	1:A:27:ASN:ND2	1.93	1.27
1:A:119:ASP:OD1	1:A:125:ARG:NH2	1.67	1.26
1:A:101:ASP:HB2	2:A:227:HOH:O	1.26	1.25
1:A:3:PHE:CG	1:A:3:PHE:CA	2.20	1.24
1:A:3:PHE:CD1	1:A:3:PHE:CB	2.21	1.23
1:A:3:PHE:CD1	1:A:3:PHE:HB3	1.75	1.22
1:A:10:ALA:C	1:A:11:ALA:CA	2.13	1.21
1:A:101:ASP:OD1	2:A:228:HOH:O	1.58	1.18
1:A:119:ASP:OD2	1:A:119:ASP:CB	1.92	1.18
1:A:97:LYS:O	1:A:101:ASP:OD1	1.60	1.16
1:A:122:ALA:CA	1:A:125:ARG:NE	2.08	1.14
1:A:98:ILE:O	1:A:98:ILE:CA	1.94	1.13
1:A:119:ASP:OD1	1:A:119:ASP:OD2	1.62	1.12
1:A:122:ALA:HA	1:A:125:ARG:NE	1.23	1.12
1:A:32:ALA:C	1:A:32:ALA:N	2.09	1.11
1:A:10:ALA:CA	1:A:11:ALA:N	2.12	1.10
1:A:44:ASN:O	1:A:44:ASN:CA	2.00	1.10
1:A:50:SER:CA	1:A:51:THR:N	2.13	1.10
1:A:122:ALA:CA	1:A:125:ARG:CD	2.32	1.08
1:A:84:LEU:CB	1:A:84:LEU:C	2.26	1.07
1:A:119:ASP:OD2	1:A:119:ASP:CG	0.83	1.07
1:A:68:ARG:CA	1:A:68:ARG:CG	2.34	1.06
1:A:92:VAL:O	1:A:92:VAL:C	0.80	1.05
1:A:13:LYS:CA	1:A:13:LYS:CG	2.36	1.03
1:A:50:SER:O	1:A:51:THR:N	1.90	1.03
1:A:98:ILE:O	1:A:98:ILE:C	0.79	1.03
1:A:73:ARG:CB	1:A:73:ARG:CD	2.37	1.02
1:A:122:ALA:HA	1:A:125:ARG:HD2	1.36	1.02
1:A:32:ALA:C	1:A:32:ALA:CA	2.30	1.02
1:A:56:LEU:CD2	1:A:56:LEU:CD1	2.39	1.01
1:A:5:ARG:NE	1:A:5:ARG:NH1	2.07	1.01
1:A:122:ALA:CA	1:A:125:ARG:HD2	1.91	1.01
1:A:63:TRP:CD1	2:A:206:HOH:O	2.12	1.01
1:A:103:ASN:O	1:A:106:ASN:HB2	1.62	0.98
1:A:51:THR:CA	1:A:51:THR:CG2	2.42	0.97
1:A:21:ARG:CA	1:A:21:ARG:CG	2.42	0.97
1:A:55:ILE:N	1:A:55:ILE:C	2.23	0.96
1:A:5:ARG:CZ	1:A:5:ARG:NE	0.82	0.96
1:A:75:LEU:CA	1:A:75:LEU:CG	2.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:O	1:A:99:VAL:N	1.99	0.96
1:A:3:PHE:CG	1:A:3:PHE:CB	0.92	0.96
1:A:84:LEU:CB	1:A:84:LEU:CD1	2.44	0.96
1:A:21:ARG:CD	1:A:21:ARG:CZ	2.43	0.95
1:A:129:LEU:CD2	1:A:129:LEU:CD1	2.45	0.95
1:A:44:ASN:O	1:A:44:ASN:C	0.70	0.94
1:A:12:MET:HE2	1:A:17:LEU:CD1	1.97	0.94
1:A:92:VAL:CA	1:A:92:VAL:O	2.16	0.94
1:A:3:PHE:CG	1:A:3:PHE:HB3	1.48	0.94
1:A:3:PHE:CG	1:A:3:PHE:HB2	1.48	0.94
1:A:106:ASN:O	1:A:112:ARG:NH2	2.01	0.94
1:A:101:ASP:HB3	2:A:226:HOH:O	1.66	0.92
1:A:122:ALA:C	1:A:122:ALA:CB	2.42	0.92
1:A:44:ASN:O	1:A:45:ARG:N	2.01	0.92
1:A:40:THR:C	1:A:41:GLN:CA	2.43	0.92
1:A:5:ARG:NH1	1:A:123:TRP:O	2.01	0.91
1:A:3:PHE:O	1:A:38:PHE:HB3	1.70	0.91
1:A:64:CYS:C	1:A:64:CYS:CB	2.43	0.90
1:A:77:ASN:C	1:A:77:ASN:N	2.29	0.90
1:A:12:MET:HE2	1:A:17:LEU:HD12	1.51	0.90
1:A:39:ASN:CB	1:A:39:ASN:C	2.43	0.90
1:A:6:CYS:HB2	2:A:140:HOH:O	1.69	0.90
1:A:30:CYS:CB	1:A:30:CYS:C	2.45	0.90
1:A:92:VAL:O	1:A:93:ASN:N	2.05	0.89
1:A:5:ARG:NH2	1:A:5:ARG:NH1	2.21	0.89
1:A:23:TYR:N	1:A:23:TYR:C	2.31	0.89
1:A:41:GLN:HA	1:A:84:LEU:HB3	1.54	0.89
1:A:112:ARG:CG	1:A:112:ARG:CA	2.51	0.88
1:A:12:MET:CE	1:A:17:LEU:HD12	2.03	0.88
1:A:8:LEU:CD1	1:A:8:LEU:CB	2.48	0.88
1:A:13:LYS:CB	1:A:13:LYS:N	2.35	0.88
1:A:12:MET:CE	1:A:17:LEU:CD1	2.51	0.88
1:A:85:SER:HB3	2:A:182:HOH:O	1.73	0.87
1:A:47:THR:C	1:A:48:ASP:CA	2.48	0.86
1:A:45:ARG:CB	1:A:45:ARG:C	2.48	0.86
1:A:72:SER:CA	1:A:73:ARG:N	2.39	0.86
1:A:92:VAL:CG2	1:A:92:VAL:CA	2.54	0.85
1:A:84:LEU:CB	1:A:84:LEU:CD2	2.55	0.85
1:A:89:THR:C	1:A:90:ALA:CA	2.49	0.85
1:A:4:GLY:N	1:A:4:GLY:O	2.10	0.84
1:A:10:ALA:C	1:A:11:ALA:N	0.74	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:CB	1:A:99:VAL:C	2.51	0.83
1:A:59:ASN:C	1:A:60:SER:CA	2.52	0.83
1:A:58:ILE:HG22	1:A:63:TRP:HB2	1.59	0.83
1:A:4:GLY:CA	1:A:4:GLY:O	2.25	0.83
1:A:64:CYS:CA	1:A:65:ASN:N	2.41	0.83
1:A:24:SER:HB3	1:A:27:ASN:HD22	1.43	0.82
1:A:12:MET:HE1	1:A:28:TRP:HB3	1.61	0.82
1:A:75:LEU:HD13	1:A:75:LEU:HA	1.61	0.82
1:A:68:ARG:CB	1:A:68:ARG:C	2.53	0.82
1:A:40:THR:CA	1:A:41:GLN:N	2.39	0.81
1:A:34:PHE:C	1:A:35:GLU:CA	2.54	0.81
1:A:90:ALA:C	1:A:91:SER:CA	2.54	0.80
1:A:77:ASN:C	1:A:77:ASN:CB	2.53	0.79
1:A:50:SER:C	1:A:50:SER:CB	2.53	0.79
1:A:21:ARG:NE	1:A:21:ARG:CG	2.45	0.79
1:A:7:GLU:CG	1:A:7:GLU:C	2.56	0.79
1:A:8:LEU:CD2	1:A:8:LEU:CD1	2.60	0.79
1:A:8:LEU:CA	1:A:9:ALA:N	2.45	0.79
1:A:75:LEU:N	1:A:75:LEU:HD22	1.99	0.78
1:A:27:ASN:ND2	1:A:27:ASN:OD1	2.16	0.78
1:A:122:ALA:CA	1:A:123:TRP:N	2.46	0.78
1:A:85:SER:C	1:A:85:SER:CB	2.57	0.78
1:A:45:ARG:CB	1:A:45:ARG:N	2.44	0.78
1:A:45:ARG:CZ	1:A:68:ARG:NH1	2.47	0.77
1:A:97:LYS:O	1:A:101:ASP:CG	2.27	0.77
1:A:8:LEU:C	1:A:9:ALA:CA	2.56	0.77
1:A:99:VAL:C	1:A:100:SER:CA	2.57	0.77
1:A:119:ASP:C	1:A:119:ASP:CB	2.57	0.77
1:A:107:ALA:CB	1:A:107:ALA:C	2.57	0.77
1:A:63:TRP:CA	1:A:63:TRP:CG	2.67	0.77
1:A:46:ASN:C	1:A:46:ASN:HA	2.04	0.77
1:A:5:ARG:CZ	1:A:5:ARG:HE	1.42	0.77
1:A:100:SER:N	1:A:100:SER:CB	2.39	0.77
1:A:32:ALA:C	1:A:32:ALA:H	1.91	0.76
1:A:75:LEU:CA	1:A:75:LEU:HD22	2.15	0.76
1:A:90:ALA:N	1:A:90:ALA:CB	2.48	0.76
1:A:45:ARG:NH1	1:A:68:ARG:HH12	1.83	0.76
1:A:112:ARG:CB	1:A:112:ARG:CD	2.62	0.76
1:A:3:PHE:C	1:A:3:PHE:HA	2.06	0.76
1:A:75:LEU:CA	1:A:75:LEU:CD2	2.63	0.75
1:A:63:TRP:HD1	2:A:206:HOH:O	1.60	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ASP:CG	1:A:125:ARG:HH22	1.85	0.75
1:A:74:ASN:C	1:A:74:ASN:N	2.43	0.75
1:A:32:ALA:H	1:A:33:LYS:N	1.84	0.74
1:A:92:VAL:CB	1:A:92:VAL:C	2.60	0.74
1:A:4:GLY:C	1:A:4:GLY:N	2.46	0.74
1:A:3:PHE:CG	1:A:3:PHE:N	2.56	0.74
1:A:72:SER:C	1:A:72:SER:CB	2.60	0.74
1:A:84:LEU:CD2	1:A:84:LEU:CD1	2.64	0.73
1:A:51:THR:CB	1:A:51:THR:N	2.52	0.73
1:A:88:ILE:HD12	1:A:92:VAL:HG21	1.70	0.73
1:A:10:ALA:CB	1:A:10:ALA:C	2.62	0.73
1:A:121:GLN:CD	2:A:143:HOH:O	2.31	0.73
1:A:41:GLN:O	1:A:43:THR:HG23	1.88	0.72
1:A:32:ALA:N	1:A:33:LYS:N	2.37	0.71
1:A:48:ASP:N	1:A:48:ASP:CB	2.52	0.71
1:A:1:LYS:C	1:A:1:LYS:CB	2.63	0.71
1:A:6:CYS:C	1:A:6:CYS:CB	2.60	0.71
1:A:55:ILE:N	1:A:55:ILE:CB	2.53	0.71
1:A:7:GLU:CG	1:A:7:GLU:CA	2.54	0.71
1:A:3:PHE:CA	1:A:4:GLY:N	2.53	0.71
1:A:3:PHE:O	1:A:38:PHE:CB	2.39	0.70
1:A:36:SER:OG	1:A:55:ILE:HA	1.91	0.70
1:A:12:MET:HE2	1:A:17:LEU:HD13	1.74	0.70
1:A:21:ARG:CB	1:A:21:ARG:C	2.64	0.70
1:A:47:THR:HA	2:A:203:HOH:O	1.91	0.70
1:A:61:ARG:CG	1:A:61:ARG:CA	2.66	0.70
1:A:99:VAL:CA	1:A:99:VAL:CG1	2.70	0.70
1:A:100:SER:N	1:A:100:SER:C	2.50	0.70
1:A:12:MET:CE	1:A:17:LEU:HD13	2.20	0.70
1:A:64:CYS:CA	1:A:64:CYS:O	2.29	0.70
1:A:111:TRP:N	1:A:111:TRP:C	2.47	0.70
1:A:32:ALA:C	1:A:32:ALA:CB	2.65	0.69
1:A:32:ALA:C	1:A:32:ALA:HB3	2.17	0.69
1:A:6:CYS:N	1:A:6:CYS:CB	2.49	0.69
1:A:99:VAL:CA	1:A:99:VAL:CG2	2.60	0.69
1:A:58:ILE:CG2	1:A:63:TRP:HB2	2.23	0.69
1:A:74:ASN:CB	1:A:74:ASN:N	2.48	0.68
1:A:129:LEU:CD2	1:A:129:LEU:CB	2.69	0.68
1:A:91:SER:N	1:A:91:SER:C	2.49	0.68
1:A:40:THR:C	1:A:40:THR:CB	2.67	0.68
1:A:4:GLY:CA	1:A:5:ARG:N	2.53	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:CYS:C	1:A:64:CYS:N	2.44	0.67
1:A:38:PHE:CA	1:A:38:PHE:CG	2.74	0.67
1:A:101:ASP:CB	2:A:227:HOH:O	2.02	0.67
1:A:110:ALA:CB	1:A:110:ALA:C	2.68	0.67
1:A:20:TYR:CD2	1:A:99:VAL:HG11	2.30	0.66
1:A:51:THR:CG2	1:A:51:THR:C	2.68	0.66
1:A:99:VAL:C	1:A:99:VAL:HG13	2.20	0.66
1:A:111:TRP:O	1:A:116:LYS:N	2.28	0.66
1:A:23:TYR:N	1:A:23:TYR:CB	2.53	0.66
1:A:51:THR:CB	1:A:51:THR:C	2.62	0.66
1:A:35:GLU:N	1:A:35:GLU:CB	2.46	0.66
1:A:75:LEU:HA	1:A:75:LEU:CD1	2.25	0.66
1:A:12:MET:HE3	1:A:17:LEU:CD1	2.26	0.66
1:A:79:PRO:C	1:A:80:CYS:CA	2.55	0.66
1:A:99:VAL:C	1:A:99:VAL:CG1	2.69	0.66
1:A:2:VAL:HA	1:A:38:PHE:O	1.96	0.66
1:A:31:ALA:CB	1:A:31:ALA:C	2.69	0.65
1:A:12:MET:CE	1:A:28:TRP:HB3	2.26	0.65
1:A:50:SER:C	1:A:51:THR:N	0.55	0.65
1:A:66:ASP:HB3	1:A:80:CYS:SG	2.36	0.65
1:A:85:SER:HB2	2:A:181:HOH:O	1.97	0.64
1:A:119:ASP:C	1:A:119:ASP:N	2.50	0.64
1:A:5:ARG:HA	1:A:38:PHE:CE2	2.32	0.64
1:A:60:SER:N	1:A:60:SER:HA	2.04	0.64
1:A:41:GLN:O	1:A:42:ALA:C	2.41	0.64
1:A:97:LYS:CE	1:A:97:LYS:CG	2.75	0.64
1:A:50:SER:C	1:A:50:SER:OG	2.41	0.63
1:A:60:SER:N	1:A:60:SER:CB	2.51	0.63
1:A:21:ARG:NE	2:A:217:HOH:O	2.29	0.63
1:A:13:LYS:NZ	1:A:129:LEU:OXT	2.31	0.63
1:A:30:CYS:CA	1:A:30:CYS:SG	2.85	0.63
1:A:56:LEU:CD2	1:A:56:LEU:HD11	2.28	0.63
1:A:40:THR:CA	1:A:40:THR:O	2.37	0.63
1:A:30:CYS:HB2	1:A:123:TRP:CD1	2.34	0.62
1:A:38:PHE:CB	1:A:38:PHE:C	2.65	0.62
1:A:35:GLU:N	1:A:35:GLU:HB2	2.14	0.62
1:A:68:ARG:C	1:A:68:ARG:HG3	2.24	0.62
1:A:106:ASN:HB3	1:A:112:ARG:HH21	1.64	0.62
1:A:46:ASN:C	1:A:46:ASN:N	2.55	0.62
1:A:30:CYS:CB	1:A:30:CYS:N	2.60	0.62
1:A:51:THR:C	1:A:51:THR:HG22	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG13	1:A:110:ALA:N	2.15	0.62
1:A:65:ASN:O	1:A:79:PRO:HA	2.00	0.61
1:A:3:PHE:C	1:A:38:PHE:HB3	2.20	0.61
1:A:3:PHE:HA	1:A:4:GLY:N	2.16	0.61
1:A:101:ASP:CB	2:A:226:HOH:O	2.33	0.61
1:A:9:ALA:CA	1:A:10:ALA:N	2.56	0.60
1:A:97:LYS:CD	1:A:97:LYS:NZ	2.58	0.60
1:A:68:ARG:CA	1:A:68:ARG:HG3	2.30	0.60
1:A:109:VAL:HG12	2:A:200:HOH:O	2.00	0.60
1:A:20:TYR:CD2	1:A:20:TYR:CD1	2.73	0.60
1:A:74:ASN:CA	1:A:75:LEU:N	2.63	0.60
1:A:85:SER:C	1:A:87:ASP:N	2.50	0.60
1:A:111:TRP:O	1:A:115:CYS:N	2.34	0.60
1:A:20:TYR:C	1:A:21:ARG:CA	2.62	0.60
1:A:63:TRP:CB	1:A:63:TRP:C	2.69	0.60
1:A:75:LEU:CB	1:A:75:LEU:HA	2.16	0.59
1:A:58:ILE:CG2	1:A:63:TRP:CB	2.80	0.59
1:A:37:ASN:C	1:A:39:ASN:H	1.98	0.59
1:A:75:LEU:HA	1:A:75:LEU:HD22	1.85	0.59
1:A:10:ALA:O	1:A:11:ALA:C	2.45	0.59
1:A:5:ARG:NH2	1:A:5:ARG:HH12	1.99	0.59
1:A:68:ARG:CB	1:A:68:ARG:N	2.57	0.58
1:A:68:ARG:CG	1:A:68:ARG:C	2.75	0.58
1:A:77:ASN:CA	1:A:78:ILE:N	2.55	0.58
1:A:15:HIS:HB3	1:A:92:VAL:HG11	1.85	0.58
1:A:84:LEU:C	1:A:84:LEU:HB2	2.25	0.58
1:A:13:LYS:CA	1:A:13:LYS:HG2	2.30	0.58
1:A:7:GLU:CB	1:A:7:GLU:CD	2.74	0.58
1:A:44:ASN:O	1:A:45:ARG:CA	2.51	0.57
1:A:85:SER:C	1:A:87:ASP:H	2.12	0.57
1:A:45:ARG:NH1	1:A:68:ARG:NH1	2.50	0.57
1:A:63:TRP:CE2	1:A:98:ILE:HG12	2.39	0.57
1:A:119:ASP:CA	1:A:120:VAL:N	2.65	0.57
1:A:1:LYS:CA	1:A:1:LYS:O	2.47	0.57
1:A:24:SER:OG	2:A:153:HOH:O	1.95	0.57
1:A:50:SER:CA	1:A:50:SER:O	2.51	0.56
1:A:84:LEU:CB	1:A:84:LEU:O	2.51	0.56
1:A:61:ARG:CB	1:A:61:ARG:CD	2.75	0.56
1:A:64:CYS:HG	1:A:80:CYS:HG	0.60	0.56
1:A:75:LEU:N	1:A:75:LEU:CD2	2.69	0.56
1:A:38:PHE:CA	1:A:38:PHE:CD1	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:N	1:A:123:TRP:N	2.54	0.55
1:A:3:PHE:C	1:A:3:PHE:N	2.53	0.55
1:A:106:ASN:C	1:A:112:ARG:HH21	2.14	0.55
1:A:54:GLY:C	1:A:55:ILE:C	2.75	0.55
1:A:58:ILE:CG2	1:A:63:TRP:CD1	2.88	0.55
1:A:122:ALA:C	1:A:122:ALA:N	2.59	0.55
1:A:76:CYS:C	1:A:77:ASN:C	2.75	0.54
1:A:92:VAL:CG2	1:A:92:VAL:CG1	2.63	0.54
1:A:22:GLY:C	1:A:23:TYR:CA	2.80	0.54
1:A:84:LEU:CA	1:A:84:LEU:CG	2.85	0.54
1:A:7:GLU:C	1:A:7:GLU:HG2	2.31	0.54
1:A:8:LEU:CD1	1:A:8:LEU:CA	2.86	0.54
1:A:106:ASN:C	1:A:112:ARG:NH2	2.65	0.54
1:A:2:VAL:HA	1:A:38:PHE:C	2.32	0.54
1:A:74:ASN:CB	1:A:74:ASN:C	2.82	0.53
1:A:53:TYR:CE2	1:A:80:CYS:HB3	2.43	0.53
1:A:75:LEU:CA	1:A:75:LEU:CD1	2.85	0.53
1:A:59:ASN:C	1:A:60:SER:HA	2.32	0.53
1:A:91:SER:N	1:A:91:SER:CB	2.63	0.53
1:A:80:CYS:O	1:A:83:LEU:HB2	2.09	0.53
1:A:24:SER:HB3	1:A:27:ASN:ND2	2.19	0.53
1:A:75:LEU:CB	1:A:75:LEU:C	2.76	0.52
1:A:8:LEU:C	1:A:9:ALA:C	2.77	0.52
1:A:13:LYS:HG2	1:A:13:LYS:C	2.35	0.52
1:A:98:ILE:O	1:A:99:VAL:CA	2.57	0.52
1:A:5:ARG:CZ	1:A:5:ARG:HD2	2.28	0.52
1:A:52:ASP:HB3	1:A:57:GLN:OE1	2.09	0.52
1:A:63:TRP:HH2	1:A:101:ASP:OD2	1.93	0.52
1:A:41:GLN:O	1:A:42:ALA:O	2.28	0.51
1:A:111:TRP:N	1:A:112:ARG:N	2.57	0.51
1:A:20:TYR:CE2	1:A:99:VAL:HG11	2.46	0.51
1:A:58:ILE:HG23	1:A:63:TRP:CD1	2.46	0.50
1:A:20:TYR:HD2	1:A:99:VAL:HG11	1.75	0.50
1:A:32:ALA:H	1:A:33:LYS:H	1.54	0.50
1:A:68:ARG:CB	1:A:68:ARG:O	2.59	0.50
1:A:12:MET:HE3	1:A:17:LEU:HD12	1.87	0.50
1:A:35:GLU:N	1:A:35:GLU:HA	2.05	0.50
1:A:58:ILE:HD12	1:A:83:LEU:HD13	1.94	0.50
1:A:89:THR:C	1:A:90:ALA:C	2.77	0.50
1:A:106:ASN:CB	1:A:112:ARG:HH21	2.24	0.50
1:A:122:ALA:N	1:A:125:ARG:NE	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:CYS:HB2	1:A:129:LEU:HD11	1.92	0.49
1:A:58:ILE:HG22	1:A:63:TRP:CB	2.37	0.49
1:A:64:CYS:CB	1:A:80:CYS:SG	2.94	0.49
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.94	0.49
1:A:122:ALA:HA	1:A:125:ARG:CG	2.34	0.49
1:A:10:ALA:CB	1:A:10:ALA:N	2.73	0.49
1:A:64:CYS:C	1:A:80:CYS:SG	2.96	0.49
1:A:20:TYR:O	1:A:21:ARG:CA	2.60	0.48
1:A:8:LEU:CD1	1:A:8:LEU:HA	2.42	0.48
1:A:62:TRP:HZ2	2:A:219:HOH:O	1.97	0.48
1:A:122:ALA:N	1:A:123:TRP:H	2.11	0.48
1:A:32:ALA:HB1	1:A:55:ILE:HG13	1.95	0.47
1:A:68:ARG:N	1:A:68:ARG:CG	2.77	0.47
1:A:77:ASN:C	1:A:77:ASN:HB3	2.36	0.47
1:A:20:TYR:CZ	1:A:20:TYR:CD1	2.91	0.47
1:A:109:VAL:CG1	1:A:110:ALA:N	2.78	0.47
1:A:51:THR:HG22	1:A:52:ASP:N	2.30	0.47
1:A:96:LYS:O	1:A:99:VAL:HG12	2.15	0.47
1:A:49:GLY:CA	2:A:214:HOH:O	2.63	0.47
1:A:63:TRP:CH2	1:A:101:ASP:OD2	2.68	0.46
1:A:66:ASP:HB3	1:A:80:CYS:HB2	1.97	0.46
1:A:75:LEU:CG	1:A:75:LEU:HA	2.34	0.46
1:A:13:LYS:CB	1:A:13:LYS:H	2.22	0.46
1:A:20:TYR:CD2	1:A:20:TYR:CB	2.82	0.46
1:A:64:CYS:C	1:A:64:CYS:HB2	2.38	0.46
1:A:98:ILE:O	1:A:98:ILE:HG22	2.14	0.46
1:A:111:TRP:N	1:A:111:TRP:CB	2.71	0.46
1:A:55:ILE:N	1:A:56:LEU:N	2.62	0.45
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.74	0.45
1:A:121:GLN:O	1:A:125:ARG:HG3	2.17	0.45
1:A:67:GLY:O	1:A:68:ARG:N	2.44	0.45
1:A:43:THR:CB	1:A:43:THR:HG1	2.15	0.45
1:A:63:TRP:CB	1:A:63:TRP:N	2.67	0.45
1:A:3:PHE:N	1:A:38:PHE:O	2.40	0.45
1:A:73:ARG:CB	1:A:73:ARG:HD2	2.36	0.45
1:A:84:LEU:CA	1:A:84:LEU:HD23	2.47	0.45
1:A:106:ASN:O	1:A:112:ARG:CZ	2.64	0.45
1:A:21:ARG:NH1	1:A:21:ARG:NH2	2.45	0.45
1:A:88:ILE:HD12	1:A:92:VAL:CG2	2.42	0.45
1:A:66:ASP:HB3	1:A:80:CYS:CB	2.47	0.45
1:A:106:ASN:CA	1:A:112:ARG:HH21	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:N	1:A:10:ALA:N	2.65	0.44
1:A:8:LEU:HD12	1:A:8:LEU:O	2.18	0.44
1:A:100:SER:N	1:A:101:ASP:N	2.65	0.44
1:A:32:ALA:HA	1:A:56:LEU:HD12	1.98	0.44
1:A:77:ASN:HB3	1:A:77:ASN:O	2.17	0.44
1:A:70:PRO:C	1:A:72:SER:H	2.22	0.44
1:A:6:CYS:CA	1:A:7:GLU:N	2.76	0.44
1:A:54:GLY:O	1:A:55:ILE:C	2.61	0.44
1:A:67:GLY:N	1:A:68:ARG:N	2.66	0.44
1:A:92:VAL:O	1:A:95:ALA:HB3	2.18	0.43
1:A:20:TYR:O	1:A:21:ARG:C	2.61	0.43
1:A:54:GLY:C	1:A:56:LEU:N	2.76	0.43
1:A:85:SER:CA	1:A:86:SER:N	2.65	0.43
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.91	0.43
1:A:55:ILE:N	1:A:55:ILE:HB	2.32	0.43
1:A:58:ILE:HG22	1:A:63:TRP:CD1	2.53	0.43
1:A:30:CYS:C	1:A:30:CYS:SG	3.01	0.43
1:A:25:LEU:HD23	1:A:29:VAL:HG23	2.00	0.42
1:A:39:ASN:CA	1:A:39:ASN:CG	2.70	0.42
1:A:58:ILE:HG21	1:A:63:TRP:CB	2.49	0.42
1:A:98:ILE:O	1:A:98:ILE:CG2	2.68	0.42
1:A:59:ASN:O	1:A:60:SER:HA	2.20	0.42
1:A:33:LYS:CG	1:A:34:PHE:N	2.81	0.42
1:A:41:GLN:N	1:A:41:GLN:CB	2.75	0.42
1:A:65:ASN:O	1:A:80:CYS:N	2.53	0.42
1:A:74:ASN:CA	1:A:74:ASN:CG	2.85	0.42
1:A:10:ALA:O	1:A:11:ALA:CA	2.42	0.42
1:A:20:TYR:CG	1:A:20:TYR:CE2	2.90	0.41
1:A:80:CYS:O	1:A:83:LEU:N	2.53	0.41
1:A:121:GLN:CG	2:A:143:HOH:O	2.66	0.41
1:A:10:ALA:C	1:A:11:ALA:C	2.83	0.41
1:A:9:ALA:C	1:A:10:ALA:CA	2.87	0.41
1:A:44:ASN:O	1:A:45:ARG:HA	2.18	0.41
1:A:53:TYR:CD2	1:A:80:CYS:HB3	2.55	0.41
1:A:74:ASN:ND2	1:A:77:ASN:N	2.69	0.41
1:A:77:ASN:CB	1:A:77:ASN:O	2.68	0.41
1:A:49:GLY:HA3	2:A:214:HOH:O	2.21	0.40
1:A:77:ASN:N	1:A:78:ILE:N	2.63	0.40
1:A:80:CYS:O	1:A:83:LEU:CB	2.69	0.40
1:A:14:ARG:HH11	1:A:14:ARG:HD2	1.61	0.40
1:A:53:TYR:CZ	1:A:80:CYS:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:C	1:A:106:ASN:H	2.29	0.40
1:A:78:ILE:HG13	1:A:79:PRO:HD2	2.04	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:193:HOH:O	2:A:213:HOH:O[6_456]	0.06	2.14
2:A:141:HOH:O	2:A:185:HOH:O[8_555]	0.13	2.07
2:A:138(A):HOH:O	2:A:220:HOH:O[4_454]	0.16	2.04
1:A:128:ARG:CD	2:A:186:HOH:O[8_555]	0.89	1.31
1:A:128:ARG:NE	2:A:186:HOH:O[8_555]	1.69	0.51
1:A:47:THR:CG2	1:A:128:ARG:NE[3_555]	2.03	0.17
1:A:47:THR:CG2	1:A:128:ARG:NH2[3_555]	2.19	0.01
1:A:128:ARG:CG	2:A:186:HOH:O[8_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	127/129 (98%)	94 (74%)	22 (17%)	11 (9%)	0 0

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	80	CYS
1	A	90	ALA
1	A	14	ARG
1	A	25	LEU
1	A	102	GLY
1	A	107	ALA

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Mol	Chain	Res	Type
1	A	5	ARG
1	A	89	THR
1	A	13	LYS
1	A	88	ILE

5.3.2 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 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	105/105 (100%)	94 (90%)	11 (10%)	6 4

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	25	LEU
1	A	35	GLU
1	A	47	THR
1	A	50	SER
1	A	58	ILE
1	A	62	TRP
1	A	74	ASN
1	A	81	SER
1	A	84	LEU
1	A	92	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	103	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	37

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	9:ALA	C	10:ALA	N	1.83
1	A	67:GLY	C	68:ARG	N	1.76
1	A	8:LEU	C	9:ALA	N	1.70
1	A	58:ILE	C	59:ASN	N	1.65
1	A	1:LYS	C	2:VAL	N	1.64
1	A	41:GLN	C	42:ALA	N	1.62
1	A	5:ARG	C	6:CYS	N	1.61
1	A	33:LYS	C	34:PHE	N	1.60
1	A	16:GLY	C	17:LEU	N	1.20
1	A	30:CYS	C	31:ALA	N	1.20
1	A	97:LYS	C	98:ILE	N	1.20
1	A	32:ALA	C	33:LYS	N	1.19
1	A	65:ASN	C	66:ASP	N	1.19
1	A	109:VAL	C	110:ALA	N	1.19
1	A	112:ARG	C	113:ASN	N	1.18
1	A	35:GLU	C	36:SER	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	116:LYS	C	117:GLY	N	1.17
1	A	93:ASN	C	94:CYS	N	1.16
1	A	31:ALA	C	32:ALA	N	1.15
1	A	77:ASN	C	78:ILE	N	1.15
1	A	83:LEU	C	84:LEU	N	1.15
1	A	87:ASP	C	88:ILE	N	1.15
1	A	107:ALA	C	108:TRP	N	1.15
1	A	7:GLU	C	8:LEU	N	1.13
1	A	19:ASN	C	20:TYR	N	1.13
1	A	88:ILE	C	89:THR	N	1.11
1	A	69:THR	C	70:PRO	N	1.10
1	A	128:ARG	C	129:LEU	N	1.10
1	A	127:CYS	C	128:ARG	N	1.07
1	A	20:TYR	C	21:ARG	N	1.06
1	A	96:LYS	C	97:LYS	N	1.06
1	A	25:LEU	C	26:GLY	N	1.05
1	A	49:GLY	C	50:SER	N	1.02
1	A	79:PRO	C	80:CYS	N	0.98
1	A	40:THR	C	41:GLN	N	0.97
1	A	10:ALA	C	11:ALA	N	0.74
1	A	50:SER	C	51:THR	N	0.55

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.