



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:45 PM GMT

PDB ID : 1LYZ
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

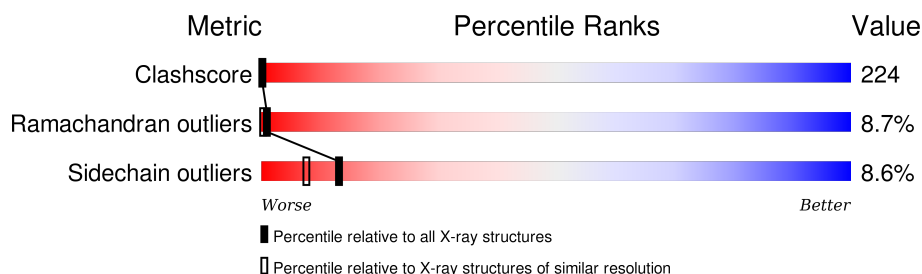
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	129	

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.

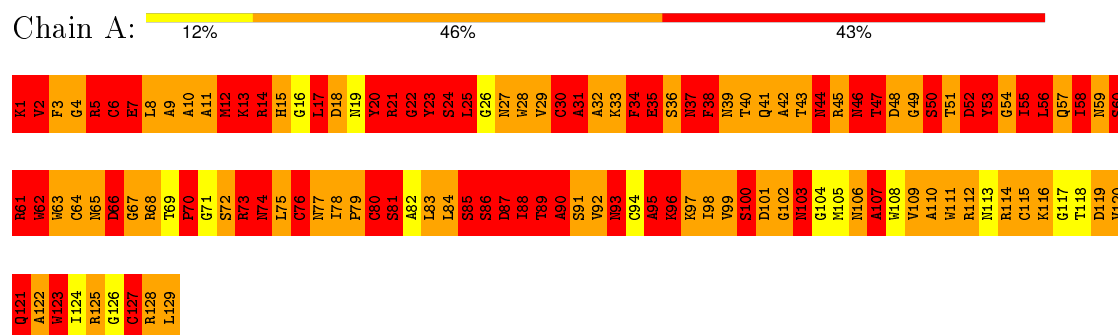
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	101	Total	O	0	0
			101	101		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.10 Å 79.10 Å 37.90 Å 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the 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	9.04	513/1021 (50.2%)	6.88	484/1379 (35.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	58

All (513) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	ARG	CZ-NH2	45.61	1.92	1.33
1	A	20	TYR	CE1-CZ	39.57	1.90	1.38
1	A	5	ARG	NE-CZ	-39.20	0.82	1.33
1	A	20	TYR	CG-CD2	37.66	1.88	1.39
1	A	21	ARG	CZ-NH1	35.33	1.78	1.33
1	A	3	PHE	CB-CG	-34.54	0.92	1.51
1	A	50	SER	C-N	-34.25	0.55	1.34
1	A	3	PHE	CG-CD1	31.09	1.85	1.38
1	A	100	SER	CA-CB	-30.99	1.06	1.52
1	A	32	ALA	CA-C	30.00	2.31	1.52
1	A	64	CYS	CB-SG	-29.29	1.32	1.82
1	A	44	ASN	C-O	-28.03	0.70	1.23
1	A	81	SER	CB-OG	27.99	1.78	1.42
1	A	46	ASN	CG-ND2	-27.02	0.65	1.32
1	A	67	GLY	CA-C	-26.99	1.08	1.51
1	A	35	GLU	CD-OE1	-26.61	0.96	1.25
1	A	10	ALA	C-N	-26.00	0.74	1.34
1	A	7	GLU	CD-OE1	24.46	1.52	1.25
1	A	27	ASN	CG-ND2	24.05	1.93	1.32
1	A	98	ILE	C-O	-23.35	0.79	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ALA	CA-CB	23.00	2.00	1.52
1	A	126	GLY	C-O	-22.51	0.87	1.23
1	A	92	VAL	C-O	-22.36	0.80	1.23
1	A	1	LYS	CA-CB	22.07	2.02	1.53
1	A	67	GLY	N-CA	-22.03	1.12	1.46
1	A	1	LYS	CB-CG	-21.29	0.95	1.52
1	A	9	ALA	C-N	21.27	1.82	1.34
1	A	7	GLU	CA-CB	-20.83	1.08	1.53
1	A	122	ALA	C-O	-20.62	0.84	1.23
1	A	4	GLY	CA-C	20.48	1.84	1.51
1	A	21	ARG	N-CA	20.47	1.87	1.46
1	A	23	TYR	CB-CG	-20.41	1.21	1.51
1	A	3	PHE	C-O	-20.24	0.84	1.23
1	A	12	MET	C-O	20.07	1.61	1.23
1	A	86	SER	CB-OG	-19.67	1.16	1.42
1	A	60	SER	CA-CB	-19.66	1.23	1.52
1	A	73	ARG	CG-CD	-19.54	1.03	1.51
1	A	121	GLN	C-O	-19.09	0.87	1.23
1	A	55	ILE	N-CA	19.04	1.84	1.46
1	A	41	GLN	N-CA	19.02	1.84	1.46
1	A	18	ASP	CB-CG	-18.99	1.11	1.51
1	A	125	ARG	C-O	-18.84	0.87	1.23
1	A	59	ASN	C-O	-18.80	0.87	1.23
1	A	129	LEU	C-O	-18.69	0.87	1.23
1	A	111	TRP	CE3-CZ3	-18.65	1.06	1.38
1	A	67	GLY	C-N	18.60	1.76	1.34
1	A	92	VAL	CB-CG1	-18.53	1.14	1.52
1	A	99	VAL	CB-CG2	-18.47	1.14	1.52
1	A	8	LEU	CB-CG	-18.44	0.99	1.52
1	A	119	ASP	CG-OD2	-18.43	0.82	1.25
1	A	110	ALA	CA-CB	18.37	1.91	1.52
1	A	89	THR	C-O	-18.29	0.88	1.23
1	A	74	ASN	CA-C	18.21	2.00	1.52
1	A	80	CYS	N-CA	18.21	1.82	1.46
1	A	3	PHE	CE2-CZ	17.80	1.71	1.37
1	A	20	TYR	CD1-CE1	17.73	1.66	1.39
1	A	43	THR	C-O	-17.65	0.89	1.23
1	A	17	LEU	CA-CB	-17.61	1.13	1.53
1	A	62	TRP	CD2-CE2	17.50	1.62	1.41
1	A	90	ALA	C-O	-17.45	0.90	1.23
1	A	90	ALA	CA-C	-17.38	1.07	1.52
1	A	23	TYR	N-CA	17.14	1.80	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	PHE	CG-CD2	-17.13	1.13	1.38
1	A	62	TRP	CD1-NE1	16.90	1.66	1.38
1	A	108	TRP	NE1-CE2	-16.67	1.15	1.37
1	A	74	ASN	CG-OD1	-16.65	0.87	1.24
1	A	45	ARG	CZ-NH1	16.64	1.54	1.33
1	A	46	ASN	CB-CG	-16.10	1.14	1.51
1	A	123	TRP	C-O	16.07	1.53	1.23
1	A	40	THR	C-N	-16.02	0.97	1.34
1	A	26	GLY	CA-C	-16.01	1.26	1.51
1	A	36	SER	CA-CB	-15.94	1.29	1.52
1	A	23	TYR	CD1-CE1	-15.89	1.15	1.39
1	A	28	TRP	NE1-CE2	-15.85	1.17	1.37
1	A	8	LEU	C-N	15.77	1.70	1.34
1	A	88	ILE	C-O	15.77	1.53	1.23
1	A	14	ARG	C-O	15.77	1.53	1.23
1	A	35	GLU	CA-CB	-15.75	1.19	1.53
1	A	38	PHE	CD1-CE1	15.71	1.70	1.39
1	A	38	PHE	CD2-CE2	15.71	1.70	1.39
1	A	64	CYS	N-CA	-15.68	1.15	1.46
1	A	15	HIS	C-O	-15.63	0.93	1.23
1	A	24	SER	N-CA	-15.56	1.15	1.46
1	A	7	GLU	CB-CG	15.56	1.81	1.52
1	A	44	ASN	CG-OD1	-15.50	0.89	1.24
1	A	79	PRO	C-N	-15.49	0.98	1.34
1	A	25	LEU	C-N	-15.42	1.05	1.33
1	A	64	CYS	C-O	-15.39	0.94	1.23
1	A	116	LYS	C-O	-15.39	0.94	1.23
1	A	92	VAL	CA-CB	15.34	1.86	1.54
1	A	123	TRP	NE1-CE2	-15.29	1.17	1.37
1	A	23	TYR	C-O	15.25	1.52	1.23
1	A	74	ASN	N-CA	-15.24	1.15	1.46
1	A	53	TYR	C-O	15.07	1.51	1.23
1	A	108	TRP	CD1-NE1	14.84	1.63	1.38
1	A	47	THR	CB-OG1	-14.69	1.13	1.43
1	A	5	ARG	N-CA	-14.68	1.17	1.46
1	A	62	TRP	C-O	-14.65	0.95	1.23
1	A	85	SER	CA-C	14.64	1.91	1.52
1	A	43	THR	CB-OG1	14.55	1.72	1.43
1	A	38	PHE	CA-CB	14.44	1.85	1.53
1	A	40	THR	CA-C	14.39	1.90	1.52
1	A	119	ASP	CG-OD1	-14.38	0.92	1.25
1	A	60	SER	N-CA	14.28	1.75	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	TRP	CZ3-CH2	-14.25	1.17	1.40
1	A	20	TYR	N-CA	-14.22	1.18	1.46
1	A	97	LYS	CD-CE	14.21	1.86	1.51
1	A	48	ASP	N-CA	14.18	1.74	1.46
1	A	24	SER	C-O	14.14	1.50	1.23
1	A	82	ALA	C-O	14.12	1.50	1.23
1	A	50	SER	C-O	14.11	1.50	1.23
1	A	3	PHE	C-N	14.06	1.58	1.33
1	A	1	LYS	CA-C	13.98	1.89	1.52
1	A	97	LYS	C-O	13.88	1.49	1.23
1	A	34	PHE	N-CA	-13.80	1.18	1.46
1	A	10	ALA	CA-CB	13.78	1.81	1.52
1	A	49	GLY	C-N	-13.77	1.02	1.34
1	A	58	ILE	C-N	13.72	1.65	1.34
1	A	73	ARG	CB-CG	13.61	1.89	1.52
1	A	111	TRP	CD2-CE2	13.55	1.57	1.41
1	A	45	ARG	NE-CZ	-13.54	1.15	1.33
1	A	46	ASN	C-O	13.54	1.49	1.23
1	A	21	ARG	CD-NE	13.53	1.69	1.46
1	A	90	ALA	N-CA	13.53	1.73	1.46
1	A	92	VAL	CB-CG2	13.39	1.80	1.52
1	A	18	ASP	CG-OD2	13.36	1.56	1.25
1	A	40	THR	C-O	-13.30	0.98	1.23
1	A	55	ILE	C-O	13.17	1.48	1.23
1	A	1	LYS	C-N	13.04	1.64	1.34
1	A	117	GLY	N-CA	-12.99	1.26	1.46
1	A	65	ASN	CG-OD1	-12.96	0.95	1.24
1	A	77	ASN	N-CA	-12.93	1.20	1.46
1	A	86	SER	C-O	-12.87	0.98	1.23
1	A	109	VAL	C-O	12.81	1.47	1.23
1	A	49	GLY	C-O	-12.71	1.03	1.23
1	A	6	CYS	CA-C	12.71	1.86	1.52
1	A	21	ARG	CZ-NH2	-12.67	1.16	1.33
1	A	48	ASP	CB-CG	-12.60	1.25	1.51
1	A	34	PHE	CG-CD1	12.55	1.57	1.38
1	A	70	PRO	N-CD	-12.52	1.30	1.47
1	A	24	SER	CA-CB	12.50	1.71	1.52
1	A	28	TRP	CD2-CE3	-12.44	1.21	1.40
1	A	123	TRP	CA-C	-12.39	1.20	1.52
1	A	69	THR	C-N	-12.38	1.10	1.34
1	A	123	TRP	CG-CD1	-12.32	1.19	1.36
1	A	41	GLN	C-N	12.32	1.62	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	TRP	CD2-CE2	12.28	1.56	1.41
1	A	9	ALA	CA-C	-12.25	1.21	1.52
1	A	41	GLN	CA-C	-12.24	1.21	1.52
1	A	91	SER	CB-OG	12.12	1.58	1.42
1	A	6	CYS	C-O	-12.07	1.00	1.23
1	A	62	TRP	CD2-CE3	-12.07	1.22	1.40
1	A	108	TRP	CZ2-CH2	-12.04	1.14	1.37
1	A	6	CYS	CA-CB	-12.02	1.27	1.53
1	A	22	GLY	CA-C	12.02	1.71	1.51
1	A	44	ASN	N-CA	-12.00	1.22	1.46
1	A	3	PHE	CA-C	11.97	1.84	1.52
1	A	115	CYS	C-O	-11.94	1.00	1.23
1	A	5	ARG	C-N	11.93	1.61	1.34
1	A	20	TYR	C-N	-11.92	1.06	1.34
1	A	107	ALA	CA-CB	11.88	1.77	1.52
1	A	84	LEU	CB-CG	11.85	1.86	1.52
1	A	91	SER	C-O	-11.82	1.00	1.23
1	A	96	LYS	C-N	-11.81	1.06	1.34
1	A	68	ARG	NE-CZ	-11.78	1.17	1.33
1	A	31	ALA	N-CA	-11.74	1.22	1.46
1	A	99	VAL	CA-CB	11.73	1.79	1.54
1	A	100	SER	N-CA	11.73	1.69	1.46
1	A	95	ALA	C-O	-11.68	1.01	1.23
1	A	33	LYS	C-N	11.66	1.60	1.34
1	A	23	TYR	CG-CD1	11.65	1.54	1.39
1	A	75	LEU	CA-CB	11.63	1.80	1.53
1	A	61	ARG	CB-CG	11.59	1.83	1.52
1	A	9	ALA	N-CA	-11.58	1.23	1.46
1	A	21	ARG	CA-CB	11.53	1.79	1.53
1	A	127	CYS	C-N	-11.48	1.07	1.34
1	A	5	ARG	CA-C	-11.47	1.23	1.52
1	A	20	TYR	CZ-OH	11.42	1.57	1.37
1	A	16	GLY	CA-C	11.31	1.70	1.51
1	A	56	LEU	C-O	-11.31	1.01	1.23
1	A	99	VAL	N-CA	-11.16	1.24	1.46
1	A	6	CYS	N-CA	11.09	1.68	1.46
1	A	3	PHE	CD1-CE1	-11.07	1.17	1.39
1	A	61	ARG	C-O	-11.02	1.02	1.23
1	A	51	THR	C-O	-10.95	1.02	1.23
1	A	75	LEU	N-CA	-10.94	1.24	1.46
1	A	86	SER	N-CA	-10.90	1.24	1.46
1	A	119	ASP	CA-C	10.87	1.81	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	SER	C-O	-10.81	1.02	1.23
1	A	59	ASN	CB-CG	-10.79	1.26	1.51
1	A	13	LYS	C-O	10.78	1.43	1.23
1	A	49	GLY	N-CA	10.74	1.62	1.46
1	A	35	GLU	N-CA	10.72	1.67	1.46
1	A	111	TRP	N-CA	10.71	1.67	1.46
1	A	91	SER	N-CA	10.68	1.67	1.46
1	A	45	ARG	CA-CB	10.68	1.77	1.53
1	A	66	ASP	CG-OD1	-10.68	1.00	1.25
1	A	36	SER	CB-OG	10.67	1.56	1.42
1	A	39	ASN	CG-OD1	10.64	1.47	1.24
1	A	17	LEU	C-O	10.64	1.43	1.23
1	A	74	ASN	C-N	10.63	1.58	1.34
1	A	13	LYS	CA-CB	10.62	1.77	1.53
1	A	111	TRP	CG-CD1	-10.55	1.22	1.36
1	A	61	ARG	NE-CZ	-10.55	1.19	1.33
1	A	52	ASP	CB-CG	-10.52	1.29	1.51
1	A	38	PHE	C-O	-10.46	1.03	1.23
1	A	39	ASN	CA-CB	10.46	1.80	1.53
1	A	128	ARG	CA-CB	-10.46	1.30	1.53
1	A	102	GLY	C-O	-10.44	1.06	1.23
1	A	77	ASN	CA-C	10.43	1.80	1.52
1	A	111	TRP	CZ2-CH2	-10.42	1.17	1.37
1	A	128	ARG	C-N	-10.38	1.10	1.34
1	A	37	ASN	CA-CB	-10.35	1.26	1.53
1	A	93	ASN	CG-OD1	-10.35	1.01	1.24
1	A	63	TRP	CA-CB	10.29	1.76	1.53
1	A	14	ARG	CB-CG	-10.29	1.24	1.52
1	A	72	SER	CA-CB	10.25	1.68	1.52
1	A	32	ALA	C-O	10.25	1.42	1.23
1	A	25	LEU	CA-CB	-10.22	1.30	1.53
1	A	72	SER	CA-C	10.19	1.79	1.52
1	A	63	TRP	CZ3-CH2	-10.16	1.23	1.40
1	A	56	LEU	CB-CG	-10.16	1.23	1.52
1	A	74	ASN	CA-CB	10.16	1.79	1.53
1	A	22	GLY	C-N	10.14	1.57	1.34
1	A	8	LEU	CA-C	-10.14	1.26	1.52
1	A	123	TRP	CB-CG	10.14	1.68	1.50
1	A	109	VAL	CB-CG1	10.13	1.74	1.52
1	A	27	ASN	C-O	10.12	1.42	1.23
1	A	19	ASN	CB-CG	10.10	1.74	1.51
1	A	75	LEU	CB-CG	-10.07	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	TYR	CG-CD1	-10.05	1.26	1.39
1	A	114	ARG	C-O	-10.03	1.04	1.23
1	A	35	GLU	CD-OE2	10.03	1.36	1.25
1	A	115	CYS	CA-CB	-9.99	1.31	1.53
1	A	34	PHE	CG-CD2	9.97	1.53	1.38
1	A	116	LYS	CB-CG	-9.96	1.25	1.52
1	A	13	LYS	C-N	9.96	1.56	1.34
1	A	53	TYR	CZ-OH	9.95	1.54	1.37
1	A	123	TRP	C-N	9.91	1.56	1.34
1	A	30	CYS	CA-CB	9.90	1.75	1.53
1	A	87	ASP	CG-OD1	-9.83	1.02	1.25
1	A	103	ASN	CB-CG	9.79	1.73	1.51
1	A	88	ILE	C-N	-9.79	1.11	1.34
1	A	8	LEU	CG-CD1	9.75	1.88	1.51
1	A	62	TRP	CE2-CZ2	-9.70	1.23	1.39
1	A	68	ARG	CA-CB	9.66	1.75	1.53
1	A	111	TRP	CZ3-CH2	9.65	1.55	1.40
1	A	123	TRP	CD1-NE1	-9.63	1.21	1.38
1	A	73	ARG	C-N	9.60	1.56	1.34
1	A	111	TRP	CE2-CZ2	-9.58	1.23	1.39
1	A	16	GLY	C-O	-9.52	1.08	1.23
1	A	90	ALA	CA-CB	9.51	1.72	1.52
1	A	84	LEU	C-O	-9.48	1.05	1.23
1	A	111	TRP	C-O	9.47	1.41	1.23
1	A	21	ARG	CB-CG	-9.41	1.27	1.52
1	A	103	ASN	CG-ND2	-9.41	1.09	1.32
1	A	45	ARG	N-CA	-9.38	1.27	1.46
1	A	15	HIS	CB-CG	-9.37	1.33	1.50
1	A	50	SER	CA-C	9.37	1.77	1.52
1	A	6	CYS	C-N	9.32	1.55	1.34
1	A	66	ASP	CA-C	-9.31	1.28	1.52
1	A	30	CYS	CA-C	-9.22	1.28	1.52
1	A	55	ILE	CA-C	-9.22	1.28	1.52
1	A	48	ASP	CG-OD1	-9.19	1.04	1.25
1	A	5	ARG	CG-CD	-9.16	1.29	1.51
1	A	84	LEU	CA-CB	9.14	1.74	1.53
1	A	19	ASN	C-N	-9.14	1.13	1.34
1	A	115	CYS	CB-SG	9.14	1.97	1.82
1	A	114	ARG	CZ-NH1	9.12	1.45	1.33
1	A	7	GLU	C-N	-9.10	1.13	1.34
1	A	53	TYR	CG-CD2	-9.10	1.27	1.39
1	A	112	ARG	CB-CG	9.08	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	TRP	CA-CB	9.08	1.74	1.53
1	A	20	TYR	CA-CB	9.06	1.73	1.53
1	A	34	PHE	CE1-CZ	9.05	1.54	1.37
1	A	53	TYR	CE2-CZ	9.00	1.50	1.38
1	A	129	LEU	CG-CD2	9.00	1.85	1.51
1	A	70	PRO	CA-CB	-8.99	1.35	1.53
1	A	51	THR	CA-CB	8.95	1.76	1.53
1	A	116	LYS	C-N	-8.94	1.17	1.33
1	A	37	ASN	CG-OD1	-8.93	1.04	1.24
1	A	23	TYR	CA-CB	-8.91	1.34	1.53
1	A	38	PHE	CB-CG	-8.90	1.36	1.51
1	A	46	ASN	CA-C	8.89	1.76	1.52
1	A	38	PHE	CE2-CZ	-8.88	1.20	1.37
1	A	94	CYS	N-CA	8.84	1.64	1.46
1	A	93	ASN	N-CA	8.84	1.64	1.46
1	A	81	SER	C-O	8.80	1.40	1.23
1	A	23	TYR	C-N	8.80	1.54	1.34
1	A	2	VAL	C-N	8.79	1.54	1.34
1	A	107	ALA	C-O	8.78	1.40	1.23
1	A	72	SER	C-O	-8.76	1.06	1.23
1	A	64	CYS	CA-C	8.76	1.75	1.52
1	A	97	LYS	N-CA	8.73	1.63	1.46
1	A	73	ARG	N-CA	-8.65	1.29	1.46
1	A	56	LEU	N-CA	8.63	1.63	1.46
1	A	104	GLY	C-O	8.63	1.37	1.23
1	A	58	ILE	CA-C	-8.60	1.30	1.52
1	A	7	GLU	CD-OE2	8.56	1.35	1.25
1	A	10	ALA	N-CA	8.55	1.63	1.46
1	A	67	GLY	C-O	8.53	1.37	1.23
1	A	75	LEU	C-O	8.53	1.39	1.23
1	A	25	LEU	C-O	8.52	1.39	1.23
1	A	84	LEU	CG-CD2	8.46	1.83	1.51
1	A	6	CYS	CB-SG	8.46	1.96	1.82
1	A	50	SER	CB-OG	-8.46	1.31	1.42
1	A	32	ALA	N-CA	-8.45	1.29	1.46
1	A	3	PHE	N-CA	-8.44	1.29	1.46
1	A	63	TRP	CG-CD1	8.44	1.48	1.36
1	A	122	ALA	CA-C	8.37	1.74	1.52
1	A	58	ILE	C-O	8.37	1.39	1.23
1	A	16	GLY	N-CA	8.36	1.58	1.46
1	A	13	LYS	N-CA	8.31	1.62	1.46
1	A	44	ASN	C-N	8.30	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	TRP	CB-CG	8.30	1.65	1.50
1	A	63	TRP	CZ2-CH2	8.29	1.53	1.37
1	A	33	LYS	CE-NZ	-8.29	1.28	1.49
1	A	4	GLY	N-CA	-8.27	1.33	1.46
1	A	113	ASN	CA-C	8.26	1.74	1.52
1	A	83	LEU	C-N	-8.22	1.15	1.34
1	A	102	GLY	N-CA	-8.20	1.33	1.46
1	A	111	TRP	CA-CB	8.16	1.72	1.53
1	A	53	TYR	CA-C	-8.15	1.31	1.52
1	A	48	ASP	CA-CB	8.14	1.71	1.53
1	A	74	ASN	CB-CG	8.11	1.69	1.51
1	A	65	ASN	C-O	8.11	1.38	1.23
1	A	94	CYS	CA-CB	-8.11	1.36	1.53
1	A	20	TYR	C-O	8.08	1.38	1.23
1	A	89	THR	CA-CB	-8.08	1.32	1.53
1	A	95	ALA	N-CA	8.04	1.62	1.46
1	A	112	ARG	N-CA	8.03	1.62	1.46
1	A	77	ASN	C-N	-8.03	1.15	1.34
1	A	28	TRP	CG-CD1	-8.01	1.25	1.36
1	A	30	CYS	CB-SG	-8.01	1.68	1.82
1	A	56	LEU	CG-CD2	8.01	1.81	1.51
1	A	97	LYS	CA-CB	-8.00	1.36	1.53
1	A	14	ARG	CG-CD	7.95	1.71	1.51
1	A	107	ALA	C-N	-7.95	1.15	1.34
1	A	65	ASN	CA-C	7.93	1.73	1.52
1	A	87	ASP	C-N	-7.93	1.15	1.34
1	A	31	ALA	C-N	-7.92	1.15	1.34
1	A	40	THR	N-CA	7.91	1.62	1.46
1	A	8	LEU	CG-CD2	7.90	1.81	1.51
1	A	51	THR	CB-OG1	-7.89	1.27	1.43
1	A	106	ASN	CB-CG	7.89	1.69	1.51
1	A	52	ASP	C-O	-7.87	1.08	1.23
1	A	50	SER	CA-CB	-7.86	1.41	1.52
1	A	44	ASN	CG-ND2	7.86	1.52	1.32
1	A	35	GLU	CB-CG	-7.84	1.37	1.52
1	A	63	TRP	CB-CG	7.81	1.64	1.50
1	A	106	ASN	N-CA	7.81	1.61	1.46
1	A	121	GLN	CB-CG	-7.81	1.31	1.52
1	A	93	ASN	C-N	-7.79	1.16	1.34
1	A	63	TRP	CE3-CZ3	7.78	1.51	1.38
1	A	73	ARG	C-O	-7.76	1.08	1.23
1	A	116	LYS	CG-CD	-7.75	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	VAL	CA-C	7.75	1.73	1.52
1	A	82	ALA	N-CA	7.70	1.61	1.46
1	A	103	ASN	CA-CB	-7.69	1.33	1.53
1	A	112	ARG	CD-NE	7.61	1.59	1.46
1	A	46	ASN	CA-CB	7.57	1.72	1.53
1	A	56	LEU	CA-CB	-7.56	1.36	1.53
1	A	27	ASN	CA-CB	-7.51	1.33	1.53
1	A	111	TRP	CD1-NE1	7.49	1.50	1.38
1	A	113	ASN	CG-OD1	-7.47	1.07	1.24
1	A	103	ASN	CG-OD1	-7.46	1.07	1.24
1	A	118	THR	C-O	-7.45	1.09	1.23
1	A	123	TRP	CG-CD2	-7.44	1.30	1.43
1	A	72	SER	CB-OG	-7.44	1.32	1.42
1	A	80	CYS	CA-CB	7.42	1.70	1.53
1	A	91	SER	CA-C	-7.40	1.33	1.52
1	A	35	GLU	C-N	-7.38	1.17	1.34
1	A	66	ASP	CA-CB	7.37	1.70	1.53
1	A	41	GLN	CD-OE1	-7.36	1.07	1.24
1	A	17	LEU	N-CA	7.35	1.61	1.46
1	A	108	TRP	CD2-CE2	-7.32	1.32	1.41
1	A	79	PRO	N-CD	-7.31	1.37	1.47
1	A	47	THR	CA-C	7.31	1.72	1.52
1	A	38	PHE	N-CA	-7.22	1.31	1.46
1	A	9	ALA	CA-CB	-7.13	1.37	1.52
1	A	38	PHE	CA-C	-7.12	1.34	1.52
1	A	47	THR	C-O	-7.09	1.09	1.23
1	A	108	TRP	N-CA	-7.09	1.32	1.46
1	A	61	ARG	C-N	7.08	1.50	1.34
1	A	35	GLU	CG-CD	-7.05	1.41	1.51
1	A	73	ARG	CA-CB	7.03	1.69	1.53
1	A	28	TRP	N-CA	-6.99	1.32	1.46
1	A	26	GLY	N-CA	-6.98	1.35	1.46
1	A	1	LYS	N-CA	-6.97	1.32	1.46
1	A	108	TRP	CG-CD2	6.96	1.55	1.43
1	A	21	ARG	CG-CD	6.96	1.69	1.51
1	A	120	VAL	CB-CG1	6.93	1.67	1.52
1	A	55	ILE	CB-CG2	6.89	1.74	1.52
1	A	114	ARG	N-CA	6.89	1.60	1.46
1	A	76	CYS	CA-CB	6.87	1.69	1.53
1	A	125	ARG	C-N	-6.85	1.20	1.33
1	A	74	ASN	C-O	6.83	1.36	1.23
1	A	96	LYS	C-O	6.83	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	TRP	CE3-CZ3	6.81	1.50	1.38
1	A	34	PHE	CD2-CE2	6.80	1.52	1.39
1	A	36	SER	N-CA	-6.80	1.32	1.46
1	A	23	TYR	CE1-CZ	-6.77	1.29	1.38
1	A	45	ARG	CD-NE	-6.76	1.34	1.46
1	A	49	GLY	CA-C	6.76	1.62	1.51
1	A	28	TRP	CG-CD2	6.74	1.55	1.43
1	A	25	LEU	CB-CG	-6.74	1.33	1.52
1	A	62	TRP	CG-CD1	-6.73	1.27	1.36
1	A	112	ARG	C-N	-6.72	1.18	1.34
1	A	68	ARG	CD-NE	6.62	1.57	1.46
1	A	51	THR	N-CA	6.62	1.59	1.46
1	A	88	ILE	CB-CG1	-6.61	1.35	1.54
1	A	115	CYS	N-CA	6.53	1.59	1.46
1	A	37	ASN	CA-C	6.50	1.69	1.52
1	A	40	THR	CB-CG2	-6.48	1.30	1.52
1	A	65	ASN	C-N	-6.48	1.19	1.34
1	A	68	ARG	CA-C	-6.46	1.36	1.52
1	A	66	ASP	CG-OD2	6.44	1.40	1.25
1	A	20	TYR	CD2-CE2	6.44	1.49	1.39
1	A	39	ASN	CB-CG	-6.42	1.36	1.51
1	A	123	TRP	N-CA	6.41	1.59	1.46
1	A	57	GLN	CG-CD	-6.41	1.36	1.51
1	A	126	GLY	CA-C	6.41	1.62	1.51
1	A	81	SER	N-CA	-6.40	1.33	1.46
1	A	106	ASN	CG-OD1	-6.40	1.09	1.24
1	A	14	ARG	CZ-NH1	6.39	1.41	1.33
1	A	108	TRP	CD2-CE3	-6.37	1.30	1.40
1	A	13	LYS	CE-NZ	6.36	1.65	1.49
1	A	43	THR	CA-C	6.33	1.69	1.52
1	A	114	ARG	CB-CG	-6.32	1.35	1.52
1	A	37	ASN	CG-ND2	-6.32	1.17	1.32
1	A	32	ALA	C-N	-6.32	1.19	1.34
1	A	53	TYR	N-CA	-6.29	1.33	1.46
1	A	2	VAL	C-O	-6.27	1.11	1.23
1	A	89	THR	CB-OG1	6.21	1.55	1.43
1	A	119	ASP	CB-CG	-6.20	1.38	1.51
1	A	128	ARG	N-CA	6.19	1.58	1.46
1	A	109	VAL	C-N	-6.17	1.19	1.34
1	A	30	CYS	C-O	6.14	1.35	1.23
1	A	77	ASN	CB-CG	-6.13	1.36	1.51
1	A	5	ARG	CA-CB	-6.10	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	ASN	C-O	-6.10	1.11	1.23
1	A	62	TRP	CA-C	-6.08	1.37	1.52
1	A	16	GLY	C-N	-6.08	1.20	1.34
1	A	30	CYS	C-N	-6.07	1.20	1.34
1	A	108	TRP	CE3-CZ3	-6.06	1.28	1.38
1	A	2	VAL	CB-CG1	-6.04	1.40	1.52
1	A	58	ILE	CA-CB	-6.02	1.41	1.54
1	A	69	THR	CB-CG2	6.02	1.72	1.52
1	A	78	ILE	CB-CG2	6.00	1.71	1.52
1	A	96	LYS	CA-CB	-5.99	1.40	1.53
1	A	97	LYS	C-N	-5.97	1.20	1.34
1	A	101	ASP	N-CA	-5.94	1.34	1.46
1	A	10	ALA	CA-C	5.92	1.68	1.52
1	A	71	GLY	CA-C	-5.91	1.42	1.51
1	A	22	GLY	N-CA	-5.90	1.37	1.46
1	A	85	SER	C-N	-5.89	1.20	1.34
1	A	48	ASP	CG-OD2	5.88	1.38	1.25
1	A	58	ILE	CB-CG1	-5.88	1.37	1.54
1	A	43	THR	C-N	5.84	1.47	1.34
1	A	124	ILE	C-N	-5.84	1.20	1.34
1	A	45	ARG	CZ-NH2	5.79	1.40	1.33
1	A	81	SER	C-N	-5.77	1.20	1.34
1	A	90	ALA	C-N	-5.77	1.20	1.34
1	A	21	ARG	C-N	5.76	1.43	1.33
1	A	79	PRO	CA-C	5.71	1.64	1.52
1	A	36	SER	C-O	5.70	1.34	1.23
1	A	114	ARG	NE-CZ	-5.67	1.25	1.33
1	A	61	ARG	CA-CB	-5.67	1.41	1.53
1	A	39	ASN	CG-ND2	-5.63	1.18	1.32
1	A	96	LYS	CG-CD	-5.62	1.33	1.52
1	A	109	VAL	CA-CB	-5.61	1.43	1.54
1	A	5	ARG	CB-CG	-5.61	1.37	1.52
1	A	77	ASN	CG-OD1	5.60	1.36	1.24
1	A	111	TRP	CG-CD2	-5.59	1.34	1.43
1	A	68	ARG	N-CA	-5.58	1.35	1.46
1	A	96	LYS	CE-NZ	5.55	1.62	1.49
1	A	1	LYS	CD-CE	-5.55	1.37	1.51
1	A	71	GLY	C-N	-5.53	1.21	1.34
1	A	84	LEU	N-CA	5.52	1.57	1.46
1	A	14	ARG	C-N	-5.50	1.21	1.34
1	A	20	TYR	CB-CG	-5.49	1.43	1.51
1	A	4	GLY	C-O	5.48	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ASP	C-O	-5.46	1.12	1.23
1	A	14	ARG	CA-CB	-5.46	1.42	1.53
1	A	84	LEU	CG-CD1	-5.44	1.31	1.51
1	A	53	TYR	CD1-CE1	-5.43	1.31	1.39
1	A	129	LEU	CA-CB	5.43	1.66	1.53
1	A	61	ARG	CZ-NH2	5.40	1.40	1.33
1	A	15	HIS	C-N	5.39	1.42	1.33
1	A	19	ASN	N-CA	-5.39	1.35	1.46
1	A	93	ASN	CB-CG	-5.38	1.38	1.51
1	A	63	TRP	C-O	-5.38	1.13	1.23
1	A	108	TRP	CA-C	5.33	1.66	1.52
1	A	66	ASP	N-CA	5.29	1.56	1.46
1	A	125	ARG	N-CA	-5.28	1.35	1.46
1	A	11	ALA	CA-C	5.28	1.66	1.52
1	A	23	TYR	CA-C	5.25	1.66	1.52
1	A	111	TRP	CD2-CE3	-5.23	1.32	1.40
1	A	125	ARG	CB-CG	5.23	1.66	1.52
1	A	107	ALA	N-CA	-5.23	1.35	1.46
1	A	62	TRP	CG-CD2	5.21	1.52	1.43
1	A	27	ASN	CG-OD1	-5.20	1.12	1.24
1	A	92	VAL	C-N	5.19	1.46	1.34
1	A	20	TYR	CA-C	-5.18	1.39	1.52
1	A	78	ILE	CA-CB	-5.17	1.43	1.54
1	A	45	ARG	C-O	-5.16	1.13	1.23
1	A	19	ASN	CG-ND2	-5.16	1.20	1.32
1	A	18	ASP	N-CA	-5.14	1.36	1.46
1	A	93	ASN	CA-CB	5.12	1.66	1.53
1	A	98	ILE	N-CA	5.09	1.56	1.46
1	A	70	PRO	C-N	-5.06	1.24	1.33
1	A	85	SER	C-O	5.05	1.32	1.23
1	A	25	LEU	CG-CD1	5.04	1.70	1.51

All (484) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ARG	NE-CZ-NH1	45.17	142.89	120.30
1	A	114	ARG	NE-CZ-NH2	-43.47	98.57	120.30
1	A	3	PHE	CB-CG-CD2	34.48	144.94	120.80
1	A	5	ARG	NH1-CZ-NH2	-33.37	82.69	119.40
1	A	23	TYR	CB-CG-CD2	32.19	140.32	121.00
1	A	7	GLU	OE1-CD-OE2	-31.20	85.86	123.30
1	A	3	PHE	CB-CG-CD1	-29.70	100.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASP	CB-CG-OD1	28.66	144.10	118.30
1	A	63	TRP	CD1-CG-CD2	28.08	128.76	106.30
1	A	4	GLY	O-C-N	24.16	161.36	122.70
1	A	23	TYR	CD1-CE1-CZ	23.87	141.28	119.80
1	A	1	LYS	N-CA-CB	23.67	153.21	110.60
1	A	31	ALA	N-CA-CB	22.67	141.84	110.10
1	A	26	GLY	O-C-N	-22.12	87.31	122.70
1	A	30	CYS	O-C-N	-22.00	87.49	122.70
1	A	66	ASP	CB-CG-OD1	22.00	138.10	118.30
1	A	90	ALA	CB-CA-C	21.75	142.73	110.10
1	A	5	ARG	NE-CZ-NH2	21.66	131.13	120.30
1	A	35	GLU	CA-CB-CG	20.97	159.53	113.40
1	A	14	ARG	N-CA-CB	20.78	148.01	110.60
1	A	111	TRP	CD1-CG-CD2	20.65	122.82	106.30
1	A	14	ARG	O-C-N	-20.02	90.68	122.70
1	A	114	ARG	NH1-CZ-NH2	19.05	140.35	119.40
1	A	41	GLN	O-C-N	-18.63	92.89	122.70
1	A	63	TRP	CE2-CD2-CG	-18.56	92.45	107.30
1	A	108	TRP	O-C-N	18.42	152.17	122.70
1	A	28	TRP	CD1-NE1-CE2	18.15	125.34	109.00
1	A	5	ARG	O-C-N	-18.12	93.70	122.70
1	A	89	THR	O-C-N	18.10	151.66	122.70
1	A	63	TRP	CG-CD1-NE1	-18.00	92.10	110.10
1	A	75	LEU	O-C-N	-17.84	94.16	122.70
1	A	46	ASN	O-C-N	-17.61	94.53	122.70
1	A	32	ALA	CB-CA-C	-17.47	83.90	110.10
1	A	25	LEU	C-N-CA	17.46	158.97	122.30
1	A	32	ALA	N-CA-C	-17.40	64.03	111.00
1	A	4	GLY	CA-C-O	-17.35	89.37	120.60
1	A	6	CYS	O-C-N	-17.06	95.40	122.70
1	A	62	TRP	CG-CD2-CE3	-16.80	118.78	133.90
1	A	21	ARG	NE-CZ-NH2	16.68	128.64	120.30
1	A	123	TRP	CB-CG-CD2	-16.68	104.92	126.60
1	A	47	THR	O-C-N	16.54	149.16	122.70
1	A	92	VAL	CA-CB-CG1	16.38	135.47	110.90
1	A	44	ASN	N-CA-CB	16.37	140.07	110.60
1	A	97	LYS	O-C-N	16.21	148.63	122.70
1	A	66	ASP	O-C-N	-16.09	95.84	123.20
1	A	119	ASP	CB-CG-OD1	-16.08	103.83	118.30
1	A	111	TRP	CH2-CZ2-CE2	16.03	133.43	117.40
1	A	53	TYR	O-C-N	-15.97	96.04	123.20
1	A	24	SER	CA-C-O	-15.96	86.58	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TRP	CG-CD2-CE3	15.95	148.25	133.90
1	A	6	CYS	CA-C-O	15.94	153.56	120.10
1	A	27	ASN	CB-CG-OD1	15.92	153.44	121.60
1	A	27	ASN	OD1-CG-ND2	-15.64	85.93	121.90
1	A	92	VAL	CA-CB-CG2	-15.49	87.66	110.90
1	A	14	ARG	NE-CZ-NH2	15.31	127.95	120.30
1	A	26	GLY	CA-C-O	14.67	147.01	120.60
1	A	24	SER	N-CA-C	14.53	150.24	111.00
1	A	19	ASN	CA-C-O	-14.51	89.64	120.10
1	A	111	TRP	NE1-CE2-CZ2	14.41	146.26	130.40
1	A	25	LEU	CD1-CG-CD2	-14.34	67.49	110.50
1	A	108	TRP	CG-CD2-CE3	-14.34	121.00	133.90
1	A	41	GLN	CA-C-O	14.29	150.11	120.10
1	A	25	LEU	O-C-N	-14.20	99.06	123.20
1	A	62	TRP	CE2-CD2-CE3	14.06	135.57	118.70
1	A	84	LEU	CB-CG-CD2	-14.01	87.18	111.00
1	A	87	ASP	CB-CG-OD1	13.80	130.72	118.30
1	A	40	THR	O-C-N	13.74	144.69	122.70
1	A	62	TRP	CD1-NE1-CE2	-13.72	96.65	109.00
1	A	18	ASP	OD1-CG-OD2	-13.65	97.36	123.30
1	A	38	PHE	CE1-CZ-CE2	13.53	144.35	120.00
1	A	2	VAL	N-CA-CB	-13.50	81.80	111.50
1	A	19	ASN	O-C-N	13.46	144.24	122.70
1	A	111	TRP	CB-CG-CD1	-13.33	109.68	127.00
1	A	88	ILE	O-C-N	13.28	143.94	122.70
1	A	71	GLY	O-C-N	13.22	143.85	122.70
1	A	33	LYS	O-C-N	-13.22	101.55	122.70
1	A	67	GLY	O-C-N	-13.20	101.58	122.70
1	A	56	LEU	CB-CG-CD2	13.09	133.25	111.00
1	A	7	GLU	C-N-CA	13.09	154.42	121.70
1	A	66	ASP	C-N-CA	13.04	149.69	122.30
1	A	46	ASN	CB-CA-C	13.01	136.42	110.40
1	A	3	PHE	CB-CA-C	12.96	136.32	110.40
1	A	90	ALA	N-CA-CB	-12.95	91.97	110.10
1	A	1	LYS	CB-CA-C	-12.94	84.52	110.40
1	A	64	CYS	O-C-N	12.88	143.32	122.70
1	A	77	ASN	OD1-CG-ND2	-12.84	92.37	121.90
1	A	13	LYS	N-CA-CB	-12.77	87.61	110.60
1	A	14	ARG	NE-CZ-NH1	-12.77	113.91	120.30
1	A	1	LYS	CA-CB-CG	12.75	141.46	113.40
1	A	88	ILE	CA-C-O	-12.69	93.46	120.10
1	A	108	TRP	CB-CG-CD2	12.64	143.03	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	TYR	CB-CA-C	12.63	135.66	110.40
1	A	55	ILE	CA-C-N	12.57	144.84	117.20
1	A	123	TRP	CG-CD2-CE3	12.45	145.10	133.90
1	A	52	ASP	CB-CG-OD1	12.39	129.45	118.30
1	A	8	LEU	CB-CG-CD2	12.36	132.02	111.00
1	A	107	ALA	N-CA-CB	12.28	127.30	110.10
1	A	123	TRP	CB-CG-CD1	12.23	142.91	127.00
1	A	123	TRP	O-C-N	-12.21	103.17	122.70
1	A	53	TYR	CA-C-N	12.17	140.55	116.20
1	A	80	CYS	CB-CA-C	12.17	134.74	110.40
1	A	89	THR	CA-C-N	-12.17	90.43	117.20
1	A	3	PHE	CG-CD2-CE2	12.16	134.18	120.80
1	A	13	LYS	CD-CE-NZ	-12.16	83.73	111.70
1	A	101	ASP	CB-CG-OD2	12.14	129.23	118.30
1	A	13	LYS	CA-C-N	-12.10	90.58	117.20
1	A	123	TRP	CE2-CD2-CG	-12.07	97.64	107.30
1	A	30	CYS	C-N-CA	12.07	151.87	121.70
1	A	78	ILE	O-C-N	-11.98	98.33	121.10
1	A	11	ALA	N-CA-CB	11.89	126.74	110.10
1	A	23	TYR	CD1-CG-CD2	-11.84	104.87	117.90
1	A	63	TRP	CB-CG-CD1	-11.76	111.71	127.00
1	A	32	ALA	N-CA-CB	11.73	126.53	110.10
1	A	7	GLU	CG-CD-OE1	11.72	141.73	118.30
1	A	105	MET	CA-CB-CG	-11.70	93.42	113.30
1	A	27	ASN	N-CA-CB	11.65	131.57	110.60
1	A	57	GLN	CB-CA-C	11.58	133.55	110.40
1	A	107	ALA	O-C-N	-11.54	104.23	122.70
1	A	87	ASP	OD1-CG-OD2	-11.54	101.37	123.30
1	A	17	LEU	CB-CG-CD1	11.53	130.60	111.00
1	A	38	PHE	CA-C-N	-11.49	91.92	117.20
1	A	33	LYS	CA-C-O	11.49	144.22	120.10
1	A	13	LYS	N-CA-C	11.48	142.00	111.00
1	A	7	GLU	O-C-N	-11.42	104.43	122.70
1	A	27	ASN	O-C-N	11.42	140.97	122.70
1	A	38	PHE	CZ-CE2-CD2	-11.32	106.52	120.10
1	A	5	ARG	CA-C-O	11.30	143.84	120.10
1	A	5	ARG	CG-CD-NE	11.25	135.42	111.80
1	A	34	PHE	CD1-CE1-CZ	-11.19	106.68	120.10
1	A	62	TRP	CD2-CE2-CZ2	-11.13	108.95	122.30
1	A	46	ASN	CA-C-N	11.12	141.67	117.20
1	A	3	PHE	CZ-CE2-CD2	-11.10	106.78	120.10
1	A	23	TYR	CE1-CZ-CE2	-11.03	102.15	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	VAL	CA-C-N	10.97	141.34	117.20
1	A	66	ASP	CA-C-N	10.95	138.09	116.20
1	A	24	SER	CB-CA-C	-10.94	89.31	110.10
1	A	84	LEU	CB-CA-C	-10.94	89.41	110.20
1	A	24	SER	O-C-N	10.87	140.10	122.70
1	A	97	LYS	CA-C-O	-10.84	97.34	120.10
1	A	57	GLN	CA-CB-CG	10.83	137.24	113.40
1	A	14	ARG	CB-CG-CD	-10.77	83.59	111.60
1	A	20	TYR	CD1-CE1-CZ	-10.75	110.12	119.80
1	A	111	TRP	CD2-CE3-CZ3	10.75	132.77	118.80
1	A	99	VAL	CB-CA-C	-10.71	91.06	111.40
1	A	63	TRP	CG-CD2-CE3	10.68	143.51	133.90
1	A	19	ASN	CB-CA-C	10.64	131.68	110.40
1	A	115	CYS	O-C-N	-10.64	105.68	122.70
1	A	74	ASN	CA-C-N	-10.60	93.89	117.20
1	A	2	VAL	CA-CB-CG1	-10.58	95.03	110.90
1	A	3	PHE	CA-C-N	-10.55	95.11	116.20
1	A	21	ARG	O-C-N	-10.54	105.28	123.20
1	A	29	VAL	CA-CB-CG1	-10.53	95.11	110.90
1	A	62	TRP	CG-CD1-NE1	10.52	120.62	110.10
1	A	15	HIS	O-C-N	-10.51	105.33	123.20
1	A	28	TRP	CG-CD1-NE1	-10.44	99.66	110.10
1	A	25	LEU	N-CA-C	10.39	139.06	111.00
1	A	60	SER	CB-CA-C	-10.34	90.45	110.10
1	A	23	TYR	CB-CG-CD1	-10.33	114.80	121.00
1	A	18	ASP	O-C-N	-10.32	106.19	122.70
1	A	53	TYR	CZ-CE2-CD2	-10.25	110.57	119.80
1	A	107	ALA	C-N-CA	10.25	147.32	121.70
1	A	23	TYR	N-CA-C	-10.22	83.40	111.00
1	A	51	THR	O-C-N	-10.12	106.50	122.70
1	A	11	ALA	O-C-N	10.12	138.89	122.70
1	A	52	ASP	OD1-CG-OD2	-10.11	104.09	123.30
1	A	110	ALA	O-C-N	-10.05	106.62	122.70
1	A	1	LYS	CD-CE-NZ	9.89	134.44	111.70
1	A	21	ARG	CD-NE-CZ	-9.88	109.76	123.60
1	A	104	GLY	O-C-N	9.88	138.51	122.70
1	A	97	LYS	CA-CB-CG	9.88	135.14	113.40
1	A	84	LEU	N-CA-CB	9.87	130.13	110.40
1	A	62	TRP	CD2-CE3-CZ3	-9.86	105.98	118.80
1	A	55	ILE	O-C-N	-9.82	106.98	122.70
1	A	111	TRP	CZ3-CH2-CZ2	-9.80	109.84	121.60
1	A	13	LYS	O-C-N	9.80	138.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PHE	CA-CB-CG	9.79	137.41	113.90
1	A	17	LEU	CB-CA-C	9.79	128.81	110.20
1	A	21	ARG	NE-CZ-NH1	-9.79	115.41	120.30
1	A	8	LEU	N-CA-CB	9.75	129.91	110.40
1	A	51	THR	CA-CB-CG2	-9.69	98.83	112.40
1	A	121	GLN	O-C-N	9.67	138.17	122.70
1	A	61	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	29	VAL	O-C-N	-9.62	107.30	122.70
1	A	26	GLY	C-N-CA	9.61	145.73	121.70
1	A	87	ASP	CB-CG-OD2	9.56	126.90	118.30
1	A	45	ARG	NE-CZ-NH2	9.53	125.07	120.30
1	A	50	SER	CA-C-O	-9.49	100.17	120.10
1	A	13	LYS	CA-CB-CG	-9.46	92.60	113.40
1	A	50	SER	N-CA-CB	9.46	124.68	110.50
1	A	111	TRP	CB-CA-C	9.37	129.15	110.40
1	A	48	ASP	N-CA-CB	-9.33	93.80	110.60
1	A	122	ALA	N-CA-CB	9.33	123.16	110.10
1	A	31	ALA	CB-CA-C	-9.21	96.28	110.10
1	A	38	PHE	CD1-CE1-CZ	-9.21	109.04	120.10
1	A	46	ASN	N-CA-CB	-9.21	94.03	110.60
1	A	101	ASP	O-C-N	-9.17	107.62	123.20
1	A	14	ARG	C-N-CA	9.14	144.55	121.70
1	A	62	TRP	O-C-N	-9.09	108.15	122.70
1	A	21	ARG	CG-CD-NE	-9.07	92.75	111.80
1	A	69	THR	O-C-N	9.03	138.26	121.10
1	A	3	PHE	O-C-N	9.01	138.52	123.20
1	A	39	ASN	CA-C-N	-9.01	97.37	117.20
1	A	128	ARG	CB-CA-C	9.01	128.42	110.40
1	A	57	GLN	CB-CG-CD	-8.99	88.22	111.60
1	A	33	LYS	CD-CE-NZ	8.97	132.34	111.70
1	A	92	VAL	CG1-CB-CG2	8.97	125.26	110.90
1	A	49	GLY	N-CA-C	-8.93	90.77	113.10
1	A	68	ARG	CA-CB-CG	-8.92	93.78	113.40
1	A	3	PHE	CD1-CE1-CZ	-8.91	109.40	120.10
1	A	30	CYS	CA-C-N	8.90	136.78	117.20
1	A	119	ASP	N-CA-CB	8.88	126.59	110.60
1	A	14	ARG	CA-C-O	8.88	138.74	120.10
1	A	114	ARG	CD-NE-CZ	-8.77	111.32	123.60
1	A	122	ALA	CB-CA-C	-8.77	96.95	110.10
1	A	87	ASP	N-CA-CB	-8.77	94.82	110.60
1	A	5	ARG	CB-CA-C	-8.74	92.92	110.40
1	A	16	GLY	CA-C-O	-8.69	104.95	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TRP	CE2-CD2-CE3	-8.64	108.33	118.70
1	A	108	TRP	CA-C-O	-8.63	101.98	120.10
1	A	10	ALA	CB-CA-C	-8.57	97.24	110.10
1	A	39	ASN	CB-CA-C	-8.52	93.36	110.40
1	A	99	VAL	CA-CB-CG2	8.45	123.58	110.90
1	A	53	TYR	C-N-CA	8.44	140.03	122.30
1	A	65	ASN	CB-CA-C	-8.44	93.53	110.40
1	A	103	ASN	CA-C-N	-8.43	99.34	116.20
1	A	66	ASP	CB-CG-OD2	-8.42	110.72	118.30
1	A	111	TRP	CG-CD1-NE1	-8.41	101.69	110.10
1	A	57	GLN	O-C-N	8.38	136.11	122.70
1	A	43	THR	N-CA-CB	-8.38	94.38	110.30
1	A	112	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	1	LYS	CA-C-N	8.36	135.60	117.20
1	A	77	ASN	CB-CG-ND2	8.35	136.74	116.70
1	A	123	TRP	CB-CA-C	8.34	127.07	110.40
1	A	34	PHE	CG-CD1-CE1	8.19	129.81	120.80
1	A	76	CYS	CA-C-O	-8.19	102.91	120.10
1	A	87	ASP	CB-CA-C	-8.17	94.06	110.40
1	A	21	ARG	NH1-CZ-NH2	-8.17	110.42	119.40
1	A	62	TRP	NE1-CE2-CZ2	8.15	139.37	130.40
1	A	120	VAL	CA-C-O	-8.10	103.08	120.10
1	A	97	LYS	CB-CA-C	8.10	126.60	110.40
1	A	98	ILE	O-C-N	8.10	135.66	122.70
1	A	20	TYR	O-C-N	-8.09	109.76	122.70
1	A	123	TRP	C-N-CA	8.07	141.89	121.70
1	A	55	ILE	N-CA-C	-8.06	89.23	111.00
1	A	100	SER	CA-C-O	-8.06	103.18	120.10
1	A	52	ASP	CB-CG-OD2	8.06	125.55	118.30
1	A	105	MET	CG-SD-CE	8.05	113.08	100.20
1	A	19	ASN	CB-CG-ND2	-7.96	97.61	116.70
1	A	20	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	A	19	ASN	N-CA-CB	-7.92	96.33	110.60
1	A	24	SER	C-N-CA	-7.92	101.91	121.70
1	A	101	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	A	79	PRO	O-C-N	7.85	135.26	122.70
1	A	108	TRP	CD1-CG-CD2	-7.84	100.03	106.30
1	A	72	SER	CA-CB-OG	-7.83	90.05	111.20
1	A	72	SER	CA-C-N	-7.83	99.98	117.20
1	A	111	TRP	CD2-CE2-CZ2	-7.79	112.95	122.30
1	A	115	CYS	N-CA-CB	7.79	124.63	110.60
1	A	85	SER	CB-CA-C	-7.79	95.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	GLN	CA-C-O	-7.78	103.76	120.10
1	A	17	LEU	CA-C-O	-7.78	103.76	120.10
1	A	108	TRP	CB-CG-CD1	-7.76	116.91	127.00
1	A	36	SER	N-CA-CB	7.76	122.14	110.50
1	A	29	VAL	CG1-CB-CG2	7.76	123.31	110.90
1	A	74	ASN	O-C-N	7.74	135.08	122.70
1	A	64	CYS	CB-CA-C	-7.71	94.99	110.40
1	A	63	TRP	CA-C-N	7.70	134.15	117.20
1	A	117	GLY	CA-C-O	-7.66	106.81	120.60
1	A	100	SER	CA-CB-OG	7.64	131.82	111.20
1	A	113	ASN	O-C-N	7.55	134.78	122.70
1	A	64	CYS	CA-C-N	-7.51	100.67	117.20
1	A	51	THR	C-N-CA	7.51	140.48	121.70
1	A	52	ASP	C-N-CA	7.47	140.38	121.70
1	A	127	CYS	N-CA-C	7.47	131.16	111.00
1	A	53	TYR	CG-CD2-CE2	7.45	127.26	121.30
1	A	92	VAL	CB-CA-C	-7.44	97.26	111.40
1	A	56	LEU	CD1-CG-CD2	-7.43	88.20	110.50
1	A	69	THR	CA-C-O	-7.41	104.53	120.10
1	A	54	GLY	CA-C-O	7.40	133.92	120.60
1	A	64	CYS	CA-CB-SG	7.39	127.30	114.00
1	A	108	TRP	CE2-CD2-CE3	7.34	127.51	118.70
1	A	123	TRP	CD1-CG-CD2	7.34	112.17	106.30
1	A	119	ASP	OD1-CG-OD2	7.33	137.24	123.30
1	A	96	LYS	CA-C-N	7.30	133.25	117.20
1	A	80	CYS	CA-C-N	-7.29	101.16	117.20
1	A	74	ASN	CB-CA-C	-7.29	95.82	110.40
1	A	38	PHE	O-C-N	7.29	134.36	122.70
1	A	83	LEU	O-C-N	7.29	134.36	122.70
1	A	101	ASP	CA-CB-CG	7.28	129.43	113.40
1	A	108	TRP	N-CA-CB	7.28	123.70	110.60
1	A	84	LEU	CB-CG-CD1	-7.26	98.65	111.00
1	A	124	ILE	O-C-N	-7.26	111.08	122.70
1	A	95	ALA	N-CA-CB	-7.26	99.94	110.10
1	A	101	ASP	CA-C-N	7.19	130.58	116.20
1	A	39	ASN	CA-C-O	7.18	135.18	120.10
1	A	70	PRO	N-CD-CG	-7.16	92.46	103.20
1	A	45	ARG	CG-CD-NE	7.16	126.83	111.80
1	A	47	THR	C-N-CA	-7.16	103.81	121.70
1	A	1	LYS	CA-C-O	-7.15	105.09	120.10
1	A	63	TRP	CD1-NE1-CE2	7.14	115.42	109.00
1	A	72	SER	O-C-N	7.13	134.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	CB-CA-C	-7.12	96.17	110.40
1	A	107	ALA	CA-C-N	7.10	132.83	117.20
1	A	28	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	111	TRP	NE1-CE2-CD2	-7.08	100.22	107.30
1	A	16	GLY	O-C-N	7.04	133.97	122.70
1	A	73	ARG	O-C-N	-7.04	111.44	122.70
1	A	108	TRP	CD2-CE2-CZ2	-7.04	113.86	122.30
1	A	64	CYS	C-N-CA	-7.02	104.16	121.70
1	A	66	ASP	N-CA-CB	-7.00	98.00	110.60
1	A	86	SER	CA-CB-OG	6.99	130.08	111.20
1	A	66	ASP	OD1-CG-OD2	-6.99	110.02	123.30
1	A	95	ALA	O-C-N	-6.98	111.53	122.70
1	A	72	SER	CB-CA-C	-6.98	96.84	110.10
1	A	84	LEU	O-C-N	-6.97	111.55	122.70
1	A	47	THR	CA-CB-CG2	-6.95	102.67	112.40
1	A	65	ASN	CA-C-O	-6.94	105.52	120.10
1	A	8	LEU	CD1-CG-CD2	-6.92	89.74	110.50
1	A	77	ASN	N-CA-CB	6.91	123.04	110.60
1	A	103	ASN	CB-CG-OD1	-6.91	107.78	121.60
1	A	13	LYS	CB-CA-C	6.88	124.15	110.40
1	A	82	ALA	N-CA-CB	6.88	119.72	110.10
1	A	25	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	2	VAL	CB-CA-C	6.86	124.43	111.40
1	A	3	PHE	C-N-CA	-6.85	107.92	122.30
1	A	23	TYR	CE1-CZ-OH	6.85	138.58	120.10
1	A	5	ARG	N-CA-C	-6.84	92.53	111.00
1	A	106	ASN	C-N-CA	6.84	138.80	121.70
1	A	28	TRP	CA-C-O	6.84	134.46	120.10
1	A	112	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	21	ARG	CA-C-N	6.82	129.83	116.20
1	A	51	THR	N-CA-CB	-6.81	97.37	110.30
1	A	70	PRO	CB-CG-CD	6.81	133.05	106.50
1	A	76	CYS	C-N-CA	6.81	138.72	121.70
1	A	128	ARG	CA-C-O	-6.80	105.82	120.10
1	A	27	ASN	N-CA-C	-6.80	92.64	111.00
1	A	34	PHE	CG-CD2-CE2	-6.78	113.34	120.80
1	A	47	THR	N-CA-CB	-6.78	97.42	110.30
1	A	20	TYR	CA-CB-CG	-6.77	100.54	113.40
1	A	71	GLY	CA-C-O	-6.77	108.41	120.60
1	A	35	GLU	OE1-CD-OE2	-6.75	115.20	123.30
1	A	62	TRP	CA-C-N	6.73	132.01	117.20
1	A	129	LEU	CB-CG-CD1	6.73	122.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ASN	CB-CG-ND2	-6.73	100.56	116.70
1	A	15	HIS	CA-C-O	6.71	134.20	120.10
1	A	28	TRP	O-C-N	-6.69	112.00	122.70
1	A	89	THR	CA-CB-CG2	-6.67	103.06	112.40
1	A	108	TRP	NE1-CE2-CD2	6.63	113.93	107.30
1	A	75	LEU	N-CA-CB	6.63	123.67	110.40
1	A	2	VAL	CA-C-N	-6.63	102.61	117.20
1	A	75	LEU	CA-C-N	6.63	131.78	117.20
1	A	124	ILE	CA-C-N	6.62	131.77	117.20
1	A	103	ASN	CB-CG-ND2	6.62	132.59	116.70
1	A	111	TRP	CA-C-N	-6.61	102.67	117.20
1	A	70	PRO	CA-CB-CG	-6.58	91.49	104.00
1	A	27	ASN	CA-C-O	-6.56	106.32	120.10
1	A	75	LEU	CA-C-O	6.53	133.80	120.10
1	A	78	ILE	CA-CB-CG1	6.52	123.39	111.00
1	A	44	ASN	CA-CB-CG	-6.52	99.06	113.40
1	A	34	PHE	CE1-CZ-CE2	6.50	131.69	120.00
1	A	59	ASN	CA-CB-CG	6.49	127.68	113.40
1	A	70	PRO	N-CA-C	6.46	128.90	112.10
1	A	124	ILE	CB-CA-C	6.45	124.49	111.60
1	A	47	THR	CA-C-N	-6.44	103.02	117.20
1	A	83	LEU	CA-CB-CG	-6.44	100.48	115.30
1	A	63	TRP	CD2-CE2-CZ2	-6.42	114.60	122.30
1	A	94	CYS	CA-C-O	6.40	133.54	120.10
1	A	37	ASN	CA-CB-CG	6.40	127.48	113.40
1	A	40	THR	CA-C-O	-6.39	106.68	120.10
1	A	70	PRO	N-CA-CB	6.35	110.92	103.30
1	A	45	ARG	NH1-CZ-NH2	-6.35	112.42	119.40
1	A	110	ALA	CA-C-N	6.35	131.16	117.20
1	A	63	TRP	CA-C-O	-6.34	106.78	120.10
1	A	116	LYS	CA-CB-CG	6.34	127.35	113.40
1	A	116	LYS	N-CA-CB	6.34	122.01	110.60
1	A	95	ALA	C-N-CA	6.34	137.54	121.70
1	A	53	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	14	ARG	CG-CD-NE	-6.30	98.56	111.80
1	A	128	ARG	CA-CB-CG	6.26	127.18	113.40
1	A	68	ARG	CB-CG-CD	-6.26	95.33	111.60
1	A	106	ASN	CB-CG-OD1	6.23	134.06	121.60
1	A	14	ARG	CA-CB-CG	6.19	127.02	113.40
1	A	111	TRP	CA-CB-CG	-6.18	101.95	113.70
1	A	63	TRP	CZ3-CH2-CZ2	6.17	129.01	121.60
1	A	25	LEU	CA-C-O	6.15	133.01	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLN	CB-CG-CD	6.14	127.58	111.60
1	A	72	SER	N-CA-C	6.14	127.57	111.00
1	A	22	GLY	CA-C-O	6.13	131.64	120.60
1	A	33	LYS	N-CA-CB	-6.13	99.57	110.60
1	A	20	TYR	CB-CA-C	-6.11	98.17	110.40
1	A	63	TRP	CB-CG-CD2	-6.09	118.68	126.60
1	A	23	TYR	O-C-N	-6.09	112.96	122.70
1	A	11	ALA	CA-C-N	-6.08	103.82	117.20
1	A	111	TRP	O-C-N	6.07	132.41	122.70
1	A	96	LYS	CA-C-O	-6.04	107.42	120.10
1	A	67	GLY	C-N-CA	6.03	136.78	121.70
1	A	6	CYS	CA-CB-SG	-6.01	103.19	114.00
1	A	22	GLY	CA-C-N	-6.01	103.99	117.20
1	A	47	THR	CA-C-O	-6.01	107.48	120.10
1	A	55	ILE	N-CA-CB	-6.00	97.01	110.80
1	A	113	ASN	OD1-CG-ND2	5.99	135.68	121.90
1	A	101	ASP	N-CA-CB	5.98	121.36	110.60
1	A	55	ILE	CA-C-O	-5.94	107.62	120.10
1	A	28	TRP	N-CA-CB	5.93	121.28	110.60
1	A	20	TYR	N-CA-CB	-5.93	99.93	110.60
1	A	1	LYS	CG-CD-CE	5.92	129.66	111.90
1	A	23	TYR	CG-CD2-CE2	5.88	126.01	121.30
1	A	38	PHE	CG-CD1-CE1	-5.87	114.34	120.80
1	A	52	ASP	O-C-N	-5.85	113.34	122.70
1	A	61	ARG	CB-CA-C	5.85	122.09	110.40
1	A	81	SER	N-CA-CB	-5.82	101.77	110.50
1	A	84	LEU	CA-C-O	5.82	132.31	120.10
1	A	120	VAL	N-CA-C	-5.77	95.43	111.00
1	A	97	LYS	N-CA-CB	-5.74	100.26	110.60
1	A	124	ILE	CA-CB-CG2	5.74	122.38	110.90
1	A	90	ALA	CA-C-N	-5.73	104.59	117.20
1	A	62	TRP	CH2-CZ2-CE2	5.73	123.13	117.40
1	A	65	ASN	O-C-N	5.73	131.86	122.70
1	A	3	PHE	N-CA-CB	-5.71	100.31	110.60
1	A	74	ASN	CB-CG-OD1	-5.71	110.18	121.60
1	A	98	ILE	CA-CB-CG2	-5.71	99.49	110.90
1	A	117	GLY	CA-C-N	5.68	129.70	117.20
1	A	5	ARG	CB-CG-CD	5.67	126.34	111.60
1	A	108	TRP	CD2-CE3-CZ3	-5.63	111.48	118.80
1	A	69	THR	CA-CB-CG2	-5.63	104.52	112.40
1	A	59	ASN	CA-C-N	-5.62	104.84	117.20
1	A	56	LEU	CA-CB-CG	5.62	128.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLY	CA-C-N	-5.62	104.84	117.20
1	A	86	SER	N-CA-C	-5.62	95.84	111.00
1	A	88	ILE	CA-CB-CG1	-5.61	100.34	111.00
1	A	27	ASN	C-N-CA	5.60	135.71	121.70
1	A	67	GLY	CA-C-O	5.60	130.68	120.60
1	A	25	LEU	CA-C-N	5.59	127.38	116.20
1	A	48	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	111	TRP	CE2-CD2-CG	-5.58	102.83	107.30
1	A	92	VAL	CA-C-N	-5.57	104.94	117.20
1	A	61	ARG	N-CA-CB	-5.57	100.57	110.60
1	A	115	CYS	CB-CA-C	-5.56	99.29	110.40
1	A	108	TRP	CA-C-N	-5.55	104.99	117.20
1	A	3	PHE	CE1-CZ-CE2	5.53	129.95	120.00
1	A	100	SER	N-CA-CB	5.52	118.78	110.50
1	A	9	ALA	N-CA-CB	5.50	117.81	110.10
1	A	28	TRP	NE1-CE2-CD2	-5.48	101.82	107.30
1	A	128	ARG	CA-C-N	5.47	129.24	117.20
1	A	53	TYR	N-CA-C	5.41	125.60	111.00
1	A	78	ILE	N-CA-CB	5.40	123.21	110.80
1	A	112	ARG	CA-C-N	5.39	129.07	117.20
1	A	112	ARG	CA-CB-CG	-5.38	101.56	113.40
1	A	38	PHE	CA-C-O	5.38	131.39	120.10
1	A	115	CYS	CA-CB-SG	5.37	123.67	114.00
1	A	73	ARG	N-CA-C	-5.36	96.52	111.00
1	A	63	TRP	CA-CB-CG	-5.34	103.55	113.70
1	A	89	THR	C-N-CA	-5.33	108.38	121.70
1	A	9	ALA	O-C-N	-5.32	114.19	122.70
1	A	10	ALA	C-N-CA	5.32	134.99	121.70
1	A	40	THR	CA-CB-CG2	5.31	119.84	112.40
1	A	79	PRO	N-CD-CG	5.29	111.13	103.20
1	A	117	GLY	C-N-CA	5.27	134.88	121.70
1	A	45	ARG	CB-CG-CD	5.25	125.24	111.60
1	A	82	ALA	O-C-N	5.25	131.10	122.70
1	A	85	SER	O-C-N	-5.24	114.31	122.70
1	A	24	SER	CA-C-N	5.22	128.68	117.20
1	A	23	TYR	CA-CB-CG	5.20	123.27	113.40
1	A	4	GLY	N-CA-C	-5.19	100.12	113.10
1	A	100	SER	N-CA-C	-5.19	96.98	111.00
1	A	61	ARG	CA-C-N	5.17	128.59	117.20
1	A	122	ALA	CA-C-N	-5.16	105.85	117.20
1	A	120	VAL	C-N-CA	5.14	134.56	121.70
1	A	28	TRP	CH2-CZ2-CE2	-5.14	112.26	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	TRP	CB-CA-C	-5.14	100.11	110.40
1	A	116	LYS	CD-CE-NZ	5.14	123.52	111.70
1	A	68	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	34	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	59	ASN	O-C-N	5.10	130.86	122.70
1	A	108	TRP	CE2-CD2-CG	5.08	111.36	107.30
1	A	121	GLN	CA-C-O	-5.07	109.46	120.10
1	A	109	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	A	107	ALA	CB-CA-C	-5.04	102.53	110.10
1	A	121	GLN	CA-C-N	-5.04	106.11	117.20
1	A	19	ASN	N-CA-C	5.03	124.59	111.00
1	A	73	ARG	C-N-CA	-5.02	109.14	121.70
1	A	78	ILE	CA-C-O	5.02	130.63	120.10
1	A	74	ASN	N-CA-C	-5.01	97.46	111.00
1	A	38	PHE	N-CA-C	5.01	124.53	111.00

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	Mainchain,Peptide
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	Mainchain,Peptide
1	A	18	ASP	Mainchain
1	A	2	VAL	Mainchain
1	A	20	TYR	Sidechain,Mainchain,Peptide
1	A	21	ARG	Sidechain
1	A	22	GLY	Mainchain
1	A	23	TYR	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
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	Sidechain,Mainchain
1	A	50	SER	Mainchain
1	A	52	ASP	Mainchain
1	A	53	TYR	Sidechain,Mainchain,Peptide
1	A	55	ILE	Peptide
1	A	56	LEU	Mainchain
1	A	60	SER	Mainchain
1	A	61	ARG	Sidechain
1	A	66	ASP	Mainchain,Peptide
1	A	7	GLU	Sidechain,Mainchain
1	A	70	PRO	Mainchain
1	A	73	ARG	Mainchain
1	A	76	CYS	Mainchain,Peptide
1	A	85	SER	Mainchain,Peptide
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	925	430	5
2	A	101	0	0	19	6
All	All	1102	0	925	430	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 224.

All (430) 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:CA	1:A:30:CYS:CB	1.75	1.65
1:A:51:THR:CA	1:A:51:THR:CB	1.76	1.64
1:A:68:ARG:CA	1:A:68:ARG:CB	1.75	1.63
1:A:45:ARG:CA	1:A:45:ARG:CB	1.77	1.62
1:A:13:LYS:CB	1:A:13:LYS:CA	1.77	1.61
1:A:74:ASN:CB	1:A:74:ASN:CA	1.79	1.61
1:A:3:PHE:CG	1:A:3:PHE:CD1	1.85	1.60
1:A:21:ARG:CA	1:A:21:ARG:CB	1.79	1.60
1:A:20:TYR:CZ	1:A:20:TYR:CE1	1.90	1.59
1:A:112:ARG:CB	1:A:112:ARG:CG	1.77	1.59
1:A:84:LEU:CB	1:A:84:LEU:CA	1.74	1.59
1:A:8:LEU:CD2	1:A:8:LEU:CG	1.81	1.58
1:A:7:GLU:CB	1:A:7:GLU:CG	1.81	1.58
1:A:92:VAL:CB	1:A:92:VAL:CG2	1.81	1.58
1:A:99:VAL:CB	1:A:99:VAL:CA	1.79	1.57
1:A:84:LEU:CG	1:A:84:LEU:CD2	1.83	1.57
1:A:20:TYR:CD2	1:A:20:TYR:CG	1.88	1.57
1:A:107:ALA:CA	1:A:107:ALA:CB	1.77	1.57
1:A:98:ILE:CG1	1:A:98:ILE:CD1	1.76	1.56
1:A:61:ARG:CB	1:A:61:ARG:CG	1.83	1.56
1:A:122:ALA:C	1:A:122:ALA:CA	1.74	1.55
1:A:63:TRP:CA	1:A:63:TRP:CB	1.76	1.54
1:A:91:SER:N	1:A:91:SER:CA	1.67	1.54
1:A:38:PHE:CB	1:A:38:PHE:CA	1.85	1.54
1:A:10:ALA:CB	1:A:10:ALA:CA	1.81	1.54
1:A:39:ASN:CA	1:A:39:ASN:CB	1.80	1.54
1:A:75:LEU:CB	1:A:75:LEU:CA	1.80	1.53
1:A:92:VAL:CA	1:A:92:VAL:CB	1.87	1.53
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:129:LEU:CD2	1:A:129:LEU:CG	1.85	1.53
1:A:35:GLU:CA	1:A:35:GLU:N	1.67	1.52
1:A:46:ASN:CA	1:A:46:ASN:C	1.76	1.52
1:A:111:TRP:N	1:A:111:TRP:CA	1.67	1.51
1:A:50:SER:C	1:A:50:SER:CA	1.77	1.51
1:A:21:ARG:CD	1:A:21:ARG:NE	1.69	1.51
1:A:64:CYS:C	1:A:64:CYS:CA	1.75	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:C	1:A:72:SER:CA	1.79	1.50
1:A:8:LEU:CD1	1:A:8:LEU:CG	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:3:PHE:CB	1:A:3:PHE:CD2	1.95	1.49
1:A:77:ASN:C	1:A:77:ASN:CA	1.80	1.49
1:A:73:ARG:CB	1:A:73:ARG:CG	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:CG	1:A:84:LEU:CB	1.86	1.47
1:A:3:PHE:C	1:A:3:PHE:CA	1.84	1.45
1:A:110:ALA:CB	1:A:110:ALA:CA	1.91	1.45
1:A:48:ASP:N	1:A:48:ASP:CA	1.74	1.45
1:A:6:CYS:CA	1:A:6:CYS:C	1.86	1.44
1:A:119:ASP:CA	1:A:119:ASP:C	1.81	1.44
1:A:4:GLY:CA	1:A:4:GLY:C	1.84	1.44
1:A:23:TYR:CA	1:A:23:TYR:N	1.80	1.43
1:A:80:CYS:N	1:A:80:CYS:CA	1.82	1.43
1:A:8:LEU:C	1:A:9:ALA:N	1.70	1.41
1:A:21:ARG:CZ	1:A:21:ARG:NH1	1.79	1.41
1:A:1:LYS:C	1:A:1:LYS:CA	1.89	1.40
1:A:40:THR:CA	1:A:40:THR:C	1.90	1.39
1:A:85:SER:CA	1:A:85:SER:C	1.91	1.39
1:A:67:GLY:C	1:A:68:ARG:N	1.76	1.38
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:CA	1:A:41:GLN:N	1.84	1.38
1:A:43:THR:OG1	1:A:43:THR:CB	1.72	1.38
1:A:5:ARG:CZ	1:A:5:ARG:CD	2.00	1.38
1:A:55:ILE:CA	1:A:55:ILE:N	1.84	1.37
1:A:1:LYS:CA	1:A:1:LYS:CB	2.02	1.35
1:A:5:ARG:NH2	1:A:5:ARG:CZ	1.92	1.33
1:A:9:ALA:C	1:A:10:ALA:N	1.83	1.32
1:A:81:SER:OG	1:A:81:SER:CB	1.78	1.31
1:A:50:SER:C	1:A:51:THR:CA	2.00	1.31
1:A:74:ASN:CA	1:A:74:ASN:C	2.00	1.29
1:A:10:ALA:O	1:A:11:ALA:N	1.66	1.28
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:CB	1:A:3:PHE:CD1	2.21	1.23
1:A:3:PHE:HB3	1:A:3:PHE:CD1	1.75	1.22
1:A:27:ASN:CG	1:A:27:ASN:ND2	1.93	1.22
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:10:ALA:C	1:A:11:ALA:CA	2.13	1.16
1:A:122:ALA:CA	1:A:125:ARG:NE	2.08	1.14
1:A:98:ILE:CA	1:A:98:ILE:O	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:10:ALA:CA	1:A:11:ALA:N	2.12	1.10
1:A:50:SER:CA	1:A:51:THR:N	2.13	1.10
1:A:44:ASN:O	1:A:44:ASN:CA	2.00	1.10
1:A:122:ALA:CA	1:A:125:ARG:CD	2.32	1.08
1:A:32:ALA:C	1:A:32:ALA:N	2.09	1.06
1:A:68:ARG:CA	1:A:68:ARG:CG	2.34	1.06
1:A:13:LYS:CG	1:A:13:LYS:CA	2.36	1.03
1:A:50:SER:O	1:A:51:THR:N	1.90	1.03
1:A:84:LEU:CB	1:A:84:LEU:C	2.26	1.02
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:119:ASP:OD2	1:A:119:ASP:CG	0.83	1.02
1:A:56:LEU:CD2	1:A:56:LEU:CD1	2.39	1.01
1:A:5:ARG:NH1	1:A:5:ARG:NE	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:92:VAL:O	1:A:92:VAL:C	0.80	1.00
1:A:32:ALA:C	1:A:32:ALA:CA	2.30	0.98
1:A:103:ASN:O	1:A:106:ASN:HB2	1.62	0.98
1:A:98:ILE:C	1:A:98:ILE:O	0.79	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:5:ARG:CZ	1:A:5:ARG:NE	0.82	0.96
1:A:75:LEU:CG	1:A:75:LEU:CA	2.43	0.96
1:A:98:ILE:O	1:A:99:VAL:N	1.99	0.96
1:A:3:PHE:CB	1:A:3:PHE:CG	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:92:VAL:O	1:A:92:VAL:CA	2.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:HB3	1:A:3:PHE:CG	1.48	0.94
1:A:3:PHE:HB2	1:A:3:PHE:CG	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:44:ASN:O	1:A:45:ARG:N	2.01	0.92
1:A:55:ILE:N	1:A:55:ILE:C	2.23	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:6:CYS:HB2	2:A:140:HOH:O	1.69	0.90
1:A:44:ASN:C	1:A:44:ASN:O	0.70	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:41:GLN:HA	1:A:84:LEU:HB3	1.54	0.89
1:A:112:ARG:CA	1:A:112:ARG:CG	2.51	0.88
1:A:12:MET:HE3	1:A:17:LEU:CD1	2.04	0.88
1:A:122:ALA:C	1:A:122:ALA:CB	2.42	0.88
1:A:12:MET:CE	1:A:17:LEU:HD12	2.03	0.88
1:A:8:LEU:CB	1:A:8:LEU:CD1	2.48	0.88
1:A:13:LYS:N	1:A:13:LYS:CB	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:40:THR:C	1:A:41:GLN:CA	2.43	0.87
1:A:12:MET:HE3	1:A:17:LEU:HD12	1.57	0.86
1:A:64:CYS:CB	1:A:64:CYS:C	2.43	0.86
1:A:77:ASN:C	1:A:77:ASN:N	2.29	0.86
1:A:72:SER:CA	1:A:73:ARG:N	2.39	0.86
1:A:39:ASN:CB	1:A:39:ASN:C	2.43	0.85
1:A:92:VAL:CA	1:A:92:VAL:CG2	2.54	0.85
1:A:30:CYS:C	1:A:30:CYS:CB	2.45	0.85
1:A:84:LEU:CB	1:A:84:LEU:CD2	2.55	0.85
1:A:23:TYR:C	1:A:23:TYR:N	2.31	0.84
1:A:4:GLY:O	1:A:4:GLY:N	2.10	0.84
1:A:58:ILE:HG22	1:A:63:TRP:HB2	1.59	0.83
1:A:4:GLY:O	1:A:4:GLY:CA	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:75:LEU:HA	1:A:75:LEU:HD13	1.61	0.82
1:A:47:THR:C	1:A:48:ASP:CA	2.48	0.82
1:A:40:THR:CA	1:A:41:GLN:N	2.39	0.81
1:A:45:ARG:CB	1:A:45:ARG:C	2.48	0.81
1:A:89:THR:C	1:A:90:ALA:CA	2.49	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:NE	1:A:21:ARG:CG	2.45	0.79
1:A:99:VAL:C	1:A:99:VAL:CB	2.51	0.79
1:A:10:ALA:C	1:A:11:ALA:N	0.74	0.79
1:A:8:LEU:CD1	1:A:8:LEU:CD2	2.60	0.79
1:A:8:LEU:CA	1:A:9:ALA:N	2.45	0.79
1:A:59:ASN:C	1:A:60:SER:CA	2.52	0.79
1:A:75:LEU:N	1:A:75:LEU:HD22	1.99	0.78
1:A:27:ASN:OD1	1:A:27:ASN:ND2	2.16	0.78
1:A:122:ALA:CA	1:A:123:TRP:N	2.46	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:63:TRP:CA	1:A:63:TRP:CG	2.67	0.77
1:A:68:ARG:C	1:A:68:ARG:CB	2.53	0.77
1:A:5:ARG:HE	1:A:5:ARG:CZ	1.42	0.77
1:A:100:SER:CB	1:A:100:SER:N	2.39	0.77
1:A:75:LEU:HD22	1:A:75:LEU:CA	2.15	0.76
1:A:90:ALA:CB	1:A:90:ALA:N	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:75:LEU:CD2	1:A:75:LEU:CA	2.63	0.75
1:A:63:TRP:HD1	2:A:206:HOH:O	1.60	0.75
1:A:77:ASN:CB	1:A:77:ASN:C	2.53	0.75
1:A:50:SER:C	1:A:50:SER:CB	2.53	0.75
1:A:7:GLU:C	1:A:7:GLU:CG	2.56	0.74
1:A:3:PHE:N	1:A:3:PHE:CG	2.56	0.74
1:A:85:SER:C	1:A:85:SER:CB	2.57	0.73
1:A:84:LEU:CD1	1:A:84:LEU:CD2	2.64	0.73
1:A:119:ASP:C	1:A:119:ASP:CB	2.57	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:12:MET:HE2	1:A:17:LEU:CD1	2.19	0.73
1:A:97:LYS:O	1:A:101:ASP:CG	2.27	0.73
1:A:99:VAL:C	1:A:100:SER:CA	2.57	0.72
1:A:107:ALA:C	1:A:107:ALA:CB	2.57	0.72
1:A:41:GLN:O	1:A:43:THR:HG23	1.88	0.72
1:A:3:PHE:C	1:A:3:PHE:HA	2.06	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:34:PHE:C	1:A:35:GLU:CA	2.54	0.71
1:A:55:ILE:N	1:A:55:ILE:CB	2.53	0.71
1:A:7:GLU:CA	1:A:7:GLU:CG	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:CA	1:A:4:GLY:N	2.53	0.71
1:A:119:ASP:CG	1:A:125:ARG:HH22	1.85	0.70
1:A:3:PHE:O	1:A:38:PHE:CB	2.39	0.70
1:A:74:ASN:N	1:A:74:ASN:C	2.43	0.70
1:A:36:SER:OG	1:A:55:ILE:HA	1.91	0.70
1:A:99:VAL:CA	1:A:99:VAL:CG1	2.70	0.70
1:A:61:ARG:CG	1:A:61:ARG:CA	2.66	0.70
1:A:47:THR:HA	2:A:203:HOH:O	1.91	0.70
1:A:64:CYS:O	1:A:64:CYS:CA	2.29	0.70
1:A:92:VAL:CB	1:A:92:VAL:C	2.60	0.70
1:A:12:MET:CE	1:A:17:LEU:HD13	2.20	0.70
1:A:72:SER:C	1:A:72:SER:CB	2.60	0.69
1:A:99:VAL:CA	1:A:99:VAL:CG2	2.60	0.69
1:A:6:CYS:N	1:A:6:CYS:CB	2.49	0.69
1:A:58:ILE:CG2	1:A:63:TRP:HB2	2.23	0.69
1:A:90:ALA:C	1:A:91:SER:CA	2.54	0.68
1:A:46:ASN:C	1:A:46:ASN:HA	2.04	0.68
1:A:129:LEU:CB	1:A:129:LEU:CD2	2.69	0.68
1:A:74:ASN:N	1:A:74:ASN:CB	2.48	0.68
1:A:10:ALA:CB	1:A:10:ALA:C	2.62	0.68
1:A:121:GLN:CD	2:A:143:HOH:O	2.31	0.68
1:A:4:GLY:CA	1:A:5:ARG:N	2.53	0.68
1:A:6:CYS:CB	1:A:6:CYS:C	2.60	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:1:LYS:C	1:A:1:LYS:CB	2.63	0.67
1:A:20:TYR:CD2	1:A:99:VAL:HG11	2.30	0.66
1:A:40:THR:O	1:A:40:THR:CA	2.37	0.66
1:A:111:TRP:O	1:A:116:LYS:N	2.28	0.66
1:A:23:TYR:CB	1:A:23:TYR:N	2.53	0.66
1:A:75:LEU:CD1	1:A:75:LEU:HA	2.25	0.66
1:A:35:GLU:CB	1:A:35:GLU:N	2.46	0.66
1:A:2:VAL:HA	1:A:38:PHE:O	1.96	0.66
1:A:100:SER:C	1:A:100:SER:N	2.50	0.65
1:A:111:TRP:N	1:A:111:TRP:C	2.47	0.65
1:A:12:MET:CE	1:A:28:TRP:HB3	2.26	0.65
1:A:66:ASP:HB3	1:A:80:CYS:SG	2.36	0.65
1:A:8:LEU:C	1:A:9:ALA:CA	2.56	0.64
1:A:85:SER:HB2	2:A:181:HOH:O	1.97	0.64
1:A:32:ALA:HB3	1:A:32:ALA:C	2.17	0.64
1:A:5:ARG:HA	1:A:38:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:C	1:A:87:ASP:N	2.50	0.64
1:A:60:SER:HA	1:A:60:SER:N	2.04	0.64
1:A:97:LYS:CG	1:A:97:LYS:CE	2.75	0.64
1:A:32:ALA:C	1:A:32:ALA:CB	2.65	0.63
1:A:60:SER:CB	1:A:60:SER:N	2.51	0.63
1:A:21:ARG:NE	2:A:217:HOH:O	2.29	0.63
1:A:40:THR:CB	1:A:40:THR:C	2.67	0.63
1:A:30:CYS:CA	1:A:30:CYS:SG	2.85	0.63
1:A:13:LYS:NZ	1:A:129:LEU:OXT	2.31	0.63
1:A:56:LEU:CD2	1:A:56:LEU:HD11	2.28	0.63
1:A:30:CYS:HB2	1:A:123:TRP:CD1	2.34	0.62
1:A:106:ASN:HB3	1:A:112:ARG:HH21	1.64	0.62
1:A:35:GLU:HB2	1:A:35:GLU:N	2.14	0.62
1:A:30:CYS:N	1:A:30:CYS:CB	2.60	0.62
1:A:109:VAL:HG13	1:A:110:ALA:N	2.15	0.62
1:A:51:THR:C	1:A:51:THR:CG2	2.68	0.61
1:A:65:ASN:O	1:A:79:PRO:HA	2.00	0.61
1:A:51:THR:C	1:A:51:THR:CB	2.62	0.61
1:A:79:PRO:C	1:A:80:CYS:CA	2.55	0.61
1:A:99:VAL:C	1:A:99:VAL:CG1	2.69	0.61
1:A:3:PHE:HA	1:A:4:GLY:N	2.16	0.61
1:A:99:VAL:C	1:A:99:VAL:HG13	2.20	0.61
1:A:101:ASP:CB	2:A:226:HOH:O	2.33	0.61
1:A:97:LYS:NZ	1:A:97:LYS:CD	2.58	0.60
1:A:9:ALA:CA	1:A:10:ALA:N	2.56	0.60
1:A:31:ALA:C	1:A:31:ALA:CB	2.69	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:110:ALA:C	1:A:110:ALA:CB	2.68	0.60
1:A:119:ASP:N	1:A:119:ASP:C	2.50	0.60
1:A:111:TRP:O	1:A:115:CYS:N	2.34	0.60
1:A:50:SER:C	1:A:51:THR:N	0.55	0.60
1:A:75:LEU:HA	1:A:75:LEU:CB	2.16	0.59
1:A:58:ILE:CG2	1:A:63:TRP:CB	2.80	0.59
1:A:75:LEU:HD22	1:A:75:LEU:HA	1.85	0.59
1:A:41:GLN:O	1:A:42:ALA:C	2.41	0.59
1:A:37:ASN:C	1:A:39:ASN:H	1.98	0.59
1:A:50:SER:C	1:A:50:SER:OG	2.41	0.59
1:A:5:ARG:NH2	1:A:5:ARG:HH12	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:N	1:A:68:ARG:CB	2.57	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:13:LYS:HG2	1:A:13:LYS:CA	2.30	0.58
1:A:44:ASN:O	1:A:45:ARG:CA	2.51	0.57
1:A:46:ASN:N	1:A:46:ASN:C	2.55	0.57
1:A:68:ARG:C	1:A:68:ARG:HG3	2.24	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:O	1:A:1:LYS:CA	2.47	0.57
1:A:51:THR:C	1:A:51:THR:HG22	2.25	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:3:PHE:C	1:A:38:PHE:HB3	2.20	0.56
1:A:61:ARG:CB	1:A:61:ARG:CD	2.75	0.56
1:A:38:PHE:C	1:A:38:PHE:CB	2.65	0.56
1:A:21:ARG:C	1:A:21:ARG:CB	2.64	0.56
1:A:75:LEU:CD2	1:A:75:LEU:N	2.69	0.56
1:A:64:CYS:N	1:A:64:CYS:C	2.44	0.56
1:A:38:PHE:CD1	1:A:38:PHE:CA	2.88	0.56
1:A:122:ALA:N	1:A:123:TRP:N	2.54	0.55
1:A:58:ILE:CG2	1:A:63:TRP:CD1	2.88	0.55
1:A:20:TYR:C	1:A:21:ARG:CA	2.62	0.55
1:A:63:TRP:CB	1:A:63:TRP:C	2.69	0.55
1:A:92:VAL:CG2	1:A:92:VAL:CG1	2.63	0.54
1:A:84:LEU:CG	1:A:84:LEU:CA	2.85	0.54
1:A:12:MET:HE1	1:A:28:TRP:HB3	1.89	0.54
1:A:10:ALA:O	1:A:11:ALA:C	2.45	0.54
1:A:8:LEU:CD1	1:A:8:LEU:CA	2.86	0.54
1:A:68:ARG:CG	1:A:68:ARG:C	2.75	0.54
1:A:12:MET:HE2	1:A:17:LEU:HD12	1.80	0.54
1:A:53:TYR:CE2	1:A:80:CYS:HB3	2.43	0.53
1:A:75:LEU:CD1	1:A:75:LEU:CA	2.85	0.53
1:A:84:LEU:HB2	1:A:84:LEU:C	2.25	0.53
1:A:91:SER:N	1:A:91:SER:CB	2.63	0.53
1:A:3:PHE:C	1:A:3:PHE:N	2.53	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:85:SER:C	1:A:87:ASP:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:12:MET:HE2	1:A:17:LEU:HD13	1.84	0.51
1:A:111:TRP:N	1:A:112:ARG:N	2.57	0.51
1:A:91:SER:N	1:A:91:SER:C	2.49	0.51
1:A:106:ASN:C	1:A:112:ARG:HH21	2.14	0.51
1:A:10:ALA:O	1:A:11:ALA:CA	2.42	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:7:GLU:C	1:A:7:GLU:HG2	2.31	0.50
1:A:68:ARG:O	1:A:68:ARG:CB	2.59	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
1:A:58:ILE:HD12	1:A:83:LEU:HD13	1.94	0.50
1:A:35:GLU:HA	1:A:35:GLU:N	2.05	0.50
1:A:127:CYS:HB2	1:A:129:LEU:HD11	1.92	0.49
1:A:106:ASN:C	1:A:112:ARG:NH2	2.65	0.49
1:A:2:VAL:HA	1:A:38:PHE:C	2.32	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:HA	1:A:84:LEU:HD23	1.94	0.49
1:A:122:ALA:HA	1:A:125:ARG:CG	2.34	0.49
1:A:74:ASN:CB	1:A:74:ASN:C	2.82	0.49
1:A:10:ALA:CB	1:A:10:ALA:N	2.73	0.49
1:A:20:TYR:O	1:A:21:ARG:CA	2.60	0.48
1:A:8:LEU:HA	1:A:8:LEU:CD1	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:4:GLY:C	1:A:4:GLY:N	2.46	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:13:LYS:C	1:A:13:LYS:HG2	2.35	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:7:GLU:CB	1:A:7:GLU:CD	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:77:ASN:N	1:A:78:ILE:N	2.63	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:H	1:A:13:LYS:CB	2.22	0.46
1:A:20:TYR:CD2	1:A:20:TYR:CB	2.82	0.46
1:A:122:ALA:C	1:A:122:ALA:N	2.59	0.46
1:A:54:GLY:C	1:A:55:ILE:C	2.75	0.46
1:A:98:ILE:O	1:A:98:ILE:HG22	2.14	0.46
1:A:111:TRP:CB	1:A:111:TRP:N	2.71	0.46
1:A:121:GLN:O	1:A:125:ARG:HG3	2.17	0.45
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.74	0.45
1:A:55:ILE:N	1:A:56:LEU:N	2.62	0.45
1:A:67:GLY:O	1:A:68:ARG:N	2.44	0.45
1:A:63:TRP:N	1:A:63:TRP:CB	2.67	0.45
1:A:106:ASN:O	1:A:112:ARG:CZ	2.64	0.45
1:A:3:PHE:N	1:A:38:PHE:O	2.40	0.45
1:A:84:LEU:CA	1:A:84:LEU:HD23	2.47	0.45
1:A:73:ARG:CB	1:A:73:ARG:HD2	2.36	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:106:ASN:CA	1:A:112:ARG:HH21	2.30	0.45
1:A:66:ASP:HB3	1:A:80:CYS:CB	2.47	0.45
1:A:9:ALA:N	1:A:10:ALA:N	2.65	0.44
1:A:100:SER:N	1:A:101:ASP:N	2.65	0.44
1:A:8:LEU:HD12	1:A:8:LEU:O	2.18	0.44
1:A:77:ASN:O	1:A:77:ASN:HB3	2.17	0.44
1:A:32:ALA:HA	1:A:56:LEU:HD12	1.98	0.44
1:A:64:CYS:C	1:A:80:CYS:SG	2.96	0.44
1:A:67:GLY:N	1:A:68:ARG:N	2.66	0.44
1:A:75:LEU:C	1:A:75:LEU:CB	2.76	0.44
1:A:6:CYS:CA	1:A:7:GLU:N	2.76	0.44
1:A:92:VAL:O	1:A:95:ALA:HB3	2.18	0.43
1:A:67:GLY:CA	1:A:68:ARG:N	2.57	0.43
1:A:8:LEU:C	1:A:9:ALA:C	2.77	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:22:GLY:C	1:A:23:TYR:CA	2.80	0.43
1:A:58:ILE:HG22	1:A:63:TRP:CD1	2.53	0.43
1:A:55:ILE:HB	1:A:55:ILE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD23	1:A:29:VAL:HG23	2.00	0.42
1:A:121:GLN:CG	2:A:143:HOH:O	2.66	0.42
1:A:43:THR:HG1	1:A:43:THR:CB	2.15	0.42
1:A:58:ILE:HG21	1:A:63:TRP:CB	2.49	0.42
1:A:98:ILE:CG2	1:A:98:ILE:O	2.68	0.42
1:A:77:ASN:C	1:A:77:ASN:HB3	2.36	0.42
1:A:59:ASN:O	1:A:60:SER:HA	2.20	0.42
1:A:76:CYS:C	1:A:77:ASN:C	2.75	0.42
1:A:65:ASN:O	1:A:80:CYS:N	2.53	0.42
1:A:41:GLN:CB	1:A:41:GLN:N	2.75	0.42
1:A:33:LYS:CG	1:A:34:PHE:N	2.81	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:70:PRO:C	1:A:72:SER:H	2.22	0.41
1:A:44:ASN:O	1:A:45:ARG:HA	2.18	0.41
1:A:74:ASN:ND2	1:A:77:ASN:N	2.69	0.41
1:A:53:TYR:CD2	1:A:80:CYS:HB3	2.55	0.41
1:A:12:MET:HE2	1:A:28:TRP:HB3	2.03	0.41
1:A:77:ASN:CB	1:A:77:ASN:O	2.68	0.41
1:A:80:CYS:O	1:A:83:LEU:CB	2.69	0.40
1:A:49:GLY:HA3	2:A:214:HOH:O	2.21	0.40
1:A:53:TYR:CZ	1:A:80:CYS:HB3	2.56	0.40
1:A:14:ARG:HH11	1:A:14:ARG:HD2	1.61	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%)	1 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
1	A	5	ARG
1	A	89	THR
1	A	13	LYS
1	A	88	ILE

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	105/105 (100%)	96 (91%)	9 (9%)	13 7

All (9) 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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	46	ASN
1	A	74	ASN

5.3.3 RNA [i](#)

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 carbohydrates 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.