



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:04 AM UTC

PDB ID : 1LZT / pdb_00001lzt
Title : REFINEMENT OF TRICLINIC LYSOZYME
Authors : Hodsdon, J.M.; Brown, G.M.; Sieker, L.C.; Jensen, L.H.
Deposited on : 1985-04-01
Resolution : 1.97 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

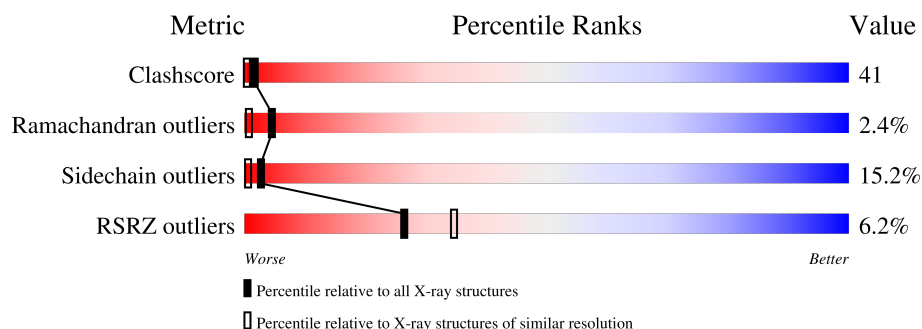
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	129	6% 47% 40% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1221 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			

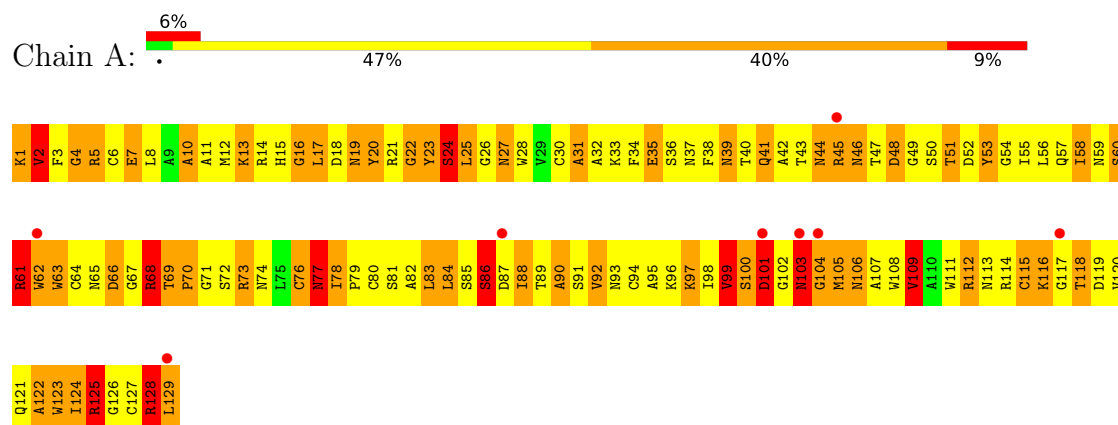
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	220	Total	O	0	0
			220	220		

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 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.

• Molecule 1: HEN EGG WHITE LYSOZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	27.28Å 31.98Å 34.29Å 88.53° 108.57° 111.85°	Depositor
Resolution (Å)	10.00 – 1.97 10.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.97) 99.0 (10.00-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.61 (at 1.98Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.254 , (Not available) 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1221	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	2.21	35/1021 (3.4%)	6.63	471/1379 (34.2%)

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	0	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ASN	CA-C	-18.77	1.32	1.52
1	A	70	PRO	CA-C	8.67	1.62	1.52
1	A	21	ARG	CZ-NH2	7.85	1.43	1.33
1	A	43	THR	CA-C	7.75	1.61	1.52
1	A	125	ARG	NE-CZ	-7.67	1.24	1.33
1	A	25	LEU	N-CA	7.26	1.55	1.46
1	A	43	THR	N-CA	7.20	1.54	1.45
1	A	117	GLY	N-CA	6.74	1.54	1.45
1	A	69	THR	CA-C	6.66	1.59	1.52
1	A	84	LEU	N-CA	6.62	1.53	1.46
1	A	70	PRO	C-N	6.54	1.40	1.33
1	A	2	VAL	CA-CB	-6.41	1.46	1.54
1	A	66	ASP	CA-C	6.34	1.60	1.52
1	A	17	LEU	N-CA	6.21	1.54	1.46
1	A	82	ALA	N-CA	6.17	1.53	1.46
1	A	99	VAL	CA-C	6.07	1.61	1.52
1	A	39	ASN	N-CA	6.06	1.53	1.46
1	A	19	ASN	CA-C	6.02	1.60	1.52
1	A	68	ARG	CZ-NH2	5.95	1.41	1.33
1	A	106	ASN	N-CA	5.90	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ASN	CA-C	5.84	1.60	1.52
1	A	87	ASP	CG-OD2	5.80	1.36	1.25
1	A	69	THR	C-N	-5.59	1.26	1.33
1	A	22	GLY	N-CA	5.55	1.53	1.45
1	A	117	GLY	C-O	5.54	1.30	1.23
1	A	61	ARG	NE-CZ	5.49	1.39	1.33
1	A	21	ARG	CA-CB	5.44	1.61	1.53
1	A	7	GLU	CD-OE1	5.42	1.35	1.25
1	A	103	ASN	N-CA	5.37	1.53	1.46
1	A	102	GLY	CA-C	5.32	1.59	1.51
1	A	105	MET	CA-C	5.30	1.60	1.52
1	A	61	ARG	CA-C	5.23	1.59	1.52
1	A	112	ARG	CA-C	5.16	1.59	1.52
1	A	68	ARG	NE-CZ	5.07	1.38	1.33
1	A	17	LEU	CA-C	5.05	1.59	1.52

All (471) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NH1-CZ-NH2	-40.25	66.98	119.30
1	A	44	ASN	OD1-CG-ND2	38.20	160.81	122.60
1	A	21	ARG	NE-CZ-NH2	34.33	150.09	119.20
1	A	125	ARG	CD-NE-CZ	-32.20	79.33	124.40
1	A	73	ARG	NE-CZ-NH2	-31.86	90.53	119.20
1	A	26	GLY	O-C-N	-31.02	90.24	122.19
1	A	73	ARG	NH1-CZ-NH2	31.00	159.60	119.30
1	A	68	ARG	NE-CZ-NH2	29.26	145.54	119.20
1	A	5	ARG	NH1-CZ-NH2	-27.46	83.60	119.30
1	A	59	ASN	OD1-CG-ND2	-25.45	97.16	122.60
1	A	45	ARG	CA-CB-CG	-23.88	66.35	114.10
1	A	128	ARG	NE-CZ-NH1	-23.70	97.80	121.50
1	A	44	ASN	CA-CB-CG	-23.43	89.17	112.60
1	A	98	ILE	O-C-N	22.53	143.99	121.91
1	A	103	ASN	CA-C-N	-22.17	82.02	121.48
1	A	103	ASN	C-N-CA	-22.17	82.02	121.48
1	A	5	ARG	NE-CZ-NH1	21.90	143.40	121.50
1	A	44	ASN	CB-CG-ND2	-21.90	83.56	116.40
1	A	21	ARG	NE-CZ-NH1	21.42	142.92	121.50
1	A	45	ARG	CD-NE-CZ	-20.84	95.23	124.40
1	A	90	ALA	O-C-N	-20.82	100.63	122.07
1	A	27	ASN	OD1-CG-ND2	-20.81	101.79	122.60
1	A	14	ARG	NH1-CZ-NH2	-20.48	92.67	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	CA-C-O	-19.79	98.13	120.69
1	A	14	ARG	NE-CZ-NH1	19.65	141.15	121.50
1	A	72	SER	CA-C-O	-19.15	98.79	120.81
1	A	26	GLY	CA-C-O	19.13	139.96	120.45
1	A	125	ARG	NE-CZ-NH1	-18.79	102.71	121.50
1	A	65	ASN	CA-C-O	18.63	140.74	120.43
1	A	123	TRP	CG-CD2-CE3	18.14	152.04	133.90
1	A	34	PHE	O-C-N	-18.13	97.62	122.46
1	A	99	VAL	O-C-N	-17.98	103.71	121.87
1	A	103	ASN	CB-CA-C	-17.89	74.81	110.42
1	A	125	ARG	NH1-CZ-NH2	17.66	142.26	119.30
1	A	47	THR	O-C-N	17.40	144.95	122.33
1	A	86	SER	CA-C-O	17.16	139.71	119.97
1	A	119	ASP	CA-CB-CG	-17.00	95.60	112.60
1	A	43	THR	CA-C-O	-16.82	101.54	121.06
1	A	69	THR	CA-C-N	16.74	137.91	119.83
1	A	69	THR	C-N-CA	16.74	137.91	119.83
1	A	61	ARG	CD-NE-CZ	16.69	147.76	124.40
1	A	116	LYS	CA-C-O	-16.59	101.61	121.02
1	A	86	SER	O-C-N	-16.43	102.06	122.27
1	A	71	GLY	O-C-N	-16.13	103.47	122.34
1	A	57	GLN	OE1-CD-NE2	-16.08	106.52	122.60
1	A	1	LYS	O-C-N	-16.00	97.39	123.00
1	A	97	LYS	O-C-N	-15.85	105.75	122.07
1	A	122	ALA	CA-C-O	15.51	136.86	120.42
1	A	117	GLY	O-C-N	15.28	137.02	122.19
1	A	87	ASP	OD1-CG-OD2	-15.23	86.34	122.90
1	A	122	ALA	O-C-N	-15.21	104.81	122.15
1	A	5	ARG	NE-CZ-NH2	15.11	132.79	119.20
1	A	59	ASN	N-CA-CB	-15.09	88.78	110.36
1	A	89	THR	O-C-N	14.94	137.56	122.03
1	A	77	ASN	CA-CB-CG	-14.93	97.67	112.60
1	A	22	GLY	O-C-N	14.83	138.96	122.50
1	A	89	THR	CA-C-O	-14.49	105.79	121.00
1	A	73	ARG	NE-CZ-NH1	-14.27	107.23	121.50
1	A	105	MET	N-CA-C	-14.13	96.10	113.20
1	A	127	CYS	O-C-N	14.06	138.88	122.85
1	A	61	ARG	NE-CZ-NH2	-13.90	106.69	119.20
1	A	68	ARG	NH1-CZ-NH2	-13.90	101.23	119.30
1	A	65	ASN	O-C-N	-13.80	107.67	123.27
1	A	46	ASN	N-CA-CB	-13.75	90.21	110.70
1	A	123	TRP	NE1-CE2-CZ2	-13.61	109.68	130.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASP	O-C-N	-13.40	107.36	123.04
1	A	47	THR	N-CA-CB	-13.30	86.24	110.18
1	A	67	GLY	CA-C-O	13.27	135.31	119.13
1	A	90	ALA	CA-C-O	13.15	134.62	120.82
1	A	34	PHE	N-CA-C	-13.01	97.10	113.23
1	A	21	ARG	CB-CA-C	12.89	135.43	111.06
1	A	68	ARG	O-C-N	12.85	136.23	122.23
1	A	19	ASN	CB-CG-ND2	-12.79	97.22	116.40
1	A	65	ASN	CA-CB-CG	-12.77	99.83	112.60
1	A	65	ASN	CB-CG-ND2	12.66	135.39	116.40
1	A	103	ASN	OD1-CG-ND2	12.61	135.21	122.60
1	A	46	ASN	CA-C-O	-12.58	105.68	121.78
1	A	77	ASN	OD1-CG-ND2	-12.57	110.03	122.60
1	A	65	ASN	OD1-CG-ND2	-12.39	110.21	122.60
1	A	124	ILE	O-C-N	12.39	135.59	122.09
1	A	98	ILE	CA-C-O	-12.32	108.11	121.17
1	A	44	ASN	O-C-N	12.31	139.49	123.24
1	A	94	CYS	CA-C-O	-12.30	108.03	120.70
1	A	16	GLY	O-C-N	-12.26	106.76	122.70
1	A	97	LYS	CA-C-O	12.03	133.45	120.82
1	A	91	SER	O-C-N	12.01	136.27	122.22
1	A	60	SER	CA-C-O	-11.98	104.78	119.28
1	A	3	PHE	O-C-N	11.98	136.74	122.84
1	A	91	SER	CA-C-O	-11.96	106.58	120.10
1	A	27	ASN	CB-CG-ND2	11.80	134.10	116.40
1	A	124	ILE	CA-C-O	-11.77	109.26	119.97
1	A	24	SER	CA-C-O	11.76	134.12	121.19
1	A	52	ASP	O-C-N	-11.72	109.48	123.19
1	A	70	PRO	O-C-N	-11.72	109.53	123.01
1	A	76	CYS	CA-C-O	-11.71	105.97	119.79
1	A	100	SER	CA-C-O	11.71	133.77	120.54
1	A	82	ALA	N-CA-C	-11.69	98.53	111.28
1	A	102	GLY	CA-C-O	11.66	140.86	120.57
1	A	32	ALA	O-C-N	-11.66	106.71	122.33
1	A	118	THR	O-C-N	11.65	138.08	122.59
1	A	123	TRP	CD2-CE2-CZ2	11.63	134.03	122.40
1	A	61	ARG	CG-CD-NE	-11.62	86.44	112.00
1	A	103	ASN	O-C-N	-11.62	107.14	122.59
1	A	74	ASN	O-C-N	11.49	136.65	122.86
1	A	23	TYR	O-C-N	11.47	137.59	123.13
1	A	41	GLN	CB-CA-C	-11.46	89.38	110.01
1	A	97	LYS	N-CA-CB	11.41	126.56	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	LEU	CA-C-O	-11.31	106.44	119.79
1	A	101	ASP	CA-CB-CG	11.22	123.82	112.60
1	A	117	GLY	CA-C-O	-11.20	108.79	120.66
1	A	80	CYS	N-CA-C	11.19	126.03	112.38
1	A	109	VAL	O-C-N	-11.15	109.19	121.80
1	A	70	PRO	CB-CA-C	11.13	125.67	111.64
1	A	123	TRP	CE2-CD2-CG	-11.07	93.91	107.20
1	A	10	ALA	O-C-N	-11.06	109.54	122.15
1	A	103	ASN	N-CA-CB	11.05	129.16	110.49
1	A	128	ARG	NE-CZ-NH2	10.89	129.00	119.20
1	A	15	HIS	CA-C-N	10.85	142.68	121.41
1	A	15	HIS	C-N-CA	10.85	142.68	121.41
1	A	28	TRP	CG-CD2-CE3	10.84	144.74	133.90
1	A	86	SER	CA-C-N	10.81	136.96	121.50
1	A	86	SER	C-N-CA	10.81	136.96	121.50
1	A	87	ASP	CA-CB-CG	-10.77	101.83	112.60
1	A	128	ARG	NH1-CZ-NH2	10.69	133.19	119.30
1	A	7	GLU	N-CA-C	-10.44	99.98	111.36
1	A	41	GLN	N-CA-CB	10.43	126.40	110.44
1	A	41	GLN	CG-CD-OE1	-10.42	99.95	120.80
1	A	83	LEU	N-CA-C	10.38	125.76	113.20
1	A	51	THR	O-C-N	10.36	135.29	123.27
1	A	100	SER	N-CA-CB	-10.34	93.09	110.16
1	A	49	GLY	N-CA-C	-10.32	101.71	113.79
1	A	19	ASN	CA-CB-CG	-10.32	102.28	112.60
1	A	2	VAL	CB-CA-C	-10.31	95.46	110.83
1	A	56	LEU	CA-C-O	10.20	131.62	119.59
1	A	72	SER	CB-CA-C	-10.20	93.58	109.89
1	A	47	THR	CA-CB-CG2	-10.16	93.23	110.50
1	A	81	SER	CA-C-N	10.14	133.87	120.28
1	A	81	SER	C-N-CA	10.14	133.87	120.28
1	A	48	ASP	N-CA-C	10.13	125.21	113.15
1	A	87	ASP	CB-CG-OD2	10.13	141.69	118.40
1	A	105	MET	CA-C-N	10.13	136.93	120.63
1	A	105	MET	C-N-CA	10.13	136.93	120.63
1	A	35	GLU	OE1-CD-OE2	-10.12	98.61	122.90
1	A	20	TYR	N-CA-CB	-10.12	94.13	109.71
1	A	63	TRP	CA-C-O	10.08	130.63	119.24
1	A	30	CYS	O-C-N	10.08	133.64	122.15
1	A	44	ASN	CB-CA-C	-10.08	96.78	110.79
1	A	50	SER	N-CA-C	10.03	125.13	110.59
1	A	99	VAL	N-CA-C	-10.02	98.53	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	TRP	CB-CG-CD2	-10.00	112.80	126.80
1	A	66	ASP	CA-C-O	9.95	130.19	119.34
1	A	125	ARG	CB-CG-CD	9.90	134.07	111.30
1	A	57	GLN	CB-CA-C	-9.87	97.88	111.89
1	A	66	ASP	OD1-CG-OD2	-9.85	99.26	122.90
1	A	41	GLN	CG-CD-NE2	9.75	131.02	116.40
1	A	35	GLU	N-CA-C	-9.69	98.98	112.45
1	A	76	CYS	N-CA-C	-9.59	100.15	112.23
1	A	59	ASN	CA-CB-CG	-9.57	103.03	112.60
1	A	121	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	A	85	SER	O-C-N	9.38	133.54	122.85
1	A	59	ASN	N-CA-C	9.30	122.81	110.53
1	A	34	PHE	CB-CG-CD2	-9.27	104.94	120.70
1	A	118	THR	N-CA-CB	-9.27	94.83	110.49
1	A	116	LYS	CA-C-N	-9.24	109.84	120.00
1	A	116	LYS	C-N-CA	-9.24	109.84	120.00
1	A	106	ASN	O-C-N	9.22	134.32	122.33
1	A	39	ASN	O-C-N	9.18	134.31	123.02
1	A	115	CYS	N-CA-C	-9.15	102.02	113.55
1	A	43	THR	O-C-N	9.12	133.85	123.27
1	A	59	ASN	O-C-N	9.11	133.18	122.79
1	A	60	SER	O-C-N	9.11	134.94	122.37
1	A	13	LYS	O-C-N	9.08	131.75	122.12
1	A	127	CYS	CA-C-O	-9.06	111.12	121.81
1	A	128	ARG	N-CA-CB	-9.05	96.87	110.35
1	A	115	CYS	O-C-N	-9.04	108.56	122.13
1	A	24	SER	CB-CA-C	9.02	124.70	109.72
1	A	59	ASN	CB-CG-ND2	8.98	129.87	116.40
1	A	22	GLY	N-CA-C	8.95	128.71	115.64
1	A	24	SER	CA-C-N	8.94	132.61	120.54
1	A	24	SER	C-N-CA	8.94	132.61	120.54
1	A	127	CYS	CA-C-N	8.91	135.51	122.41
1	A	127	CYS	C-N-CA	8.91	135.51	122.41
1	A	86	SER	CB-CA-C	-8.84	93.70	110.67
1	A	92	VAL	CA-C-O	-8.84	110.71	120.25
1	A	58	ILE	CA-CB-CG1	-8.82	95.40	110.40
1	A	5	ARG	N-CA-CB	-8.76	96.12	110.40
1	A	108	TRP	CE3-CZ3-CH2	8.75	132.47	121.10
1	A	102	GLY	CA-C-N	8.70	138.16	121.54
1	A	102	GLY	C-N-CA	8.70	138.16	121.54
1	A	77	ASN	O-C-N	8.68	133.93	122.47
1	A	38	PHE	O-C-N	8.66	132.88	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	N-CA-CB	8.65	123.41	110.95
1	A	44	ASN	N-CA-CB	-8.65	97.48	110.71
1	A	66	ASP	N-CA-C	8.65	125.90	113.02
1	A	18	ASP	CA-CB-CG	-8.63	103.97	112.60
1	A	44	ASN	N-CA-C	-8.63	92.59	107.61
1	A	103	ASN	CA-CB-CG	-8.54	104.06	112.60
1	A	119	ASP	CA-C-N	-8.51	106.51	120.64
1	A	119	ASP	C-N-CA	-8.51	106.51	120.64
1	A	70	PRO	CA-C-N	8.48	135.42	121.00
1	A	70	PRO	C-N-CA	8.48	135.42	121.00
1	A	77	ASN	CB-CG-ND2	8.45	129.07	116.40
1	A	68	ARG	NE-CZ-NH1	-8.45	113.05	121.50
1	A	5	ARG	CA-CB-CG	8.43	130.97	114.10
1	A	94	CYS	CB-CA-C	8.38	124.14	110.90
1	A	27	ASN	N-CA-CB	-8.37	97.42	110.30
1	A	62	TRP	CA-C-N	-8.33	108.03	122.36
1	A	62	TRP	C-N-CA	-8.33	108.03	122.36
1	A	35	GLU	CB-CG-CD	-8.33	98.44	112.60
1	A	99	VAL	CB-CA-C	8.32	125.05	112.16
1	A	48	ASP	CB-CA-C	-8.30	95.00	110.36
1	A	34	PHE	CA-CB-CG	-8.25	105.55	113.80
1	A	63	TRP	O-C-N	-8.21	111.36	122.36
1	A	92	VAL	N-CA-CB	-8.19	95.47	110.95
1	A	14	ARG	CB-CA-C	-8.16	95.01	110.67
1	A	52	ASP	N-CA-C	-8.13	96.43	109.76
1	A	90	ALA	N-CA-C	-8.13	102.37	111.07
1	A	120	VAL	O-C-N	-8.13	111.41	122.05
1	A	100	SER	O-C-N	-8.11	113.97	123.22
1	A	120	VAL	CA-CB-CG1	-8.11	96.62	110.40
1	A	28	TRP	CD2-CE2-CZ2	8.08	130.48	122.40
1	A	12	MET	O-C-N	8.08	130.69	122.12
1	A	73	ARG	CD-NE-CZ	8.03	135.65	124.40
1	A	114	ARG	CB-CA-C	-8.01	96.13	109.27
1	A	71	GLY	N-CA-C	-8.00	99.97	114.46
1	A	91	SER	N-CA-C	7.95	120.85	111.71
1	A	48	ASP	N-CA-CB	7.92	122.66	110.46
1	A	7	GLU	CA-C-O	-7.90	112.05	120.42
1	A	93	ASN	OD1-CG-ND2	7.89	130.49	122.60
1	A	62	TRP	CG-CD1-NE1	-7.81	100.04	110.20
1	A	57	GLN	CG-CD-NE2	7.76	128.03	116.40
1	A	14	ARG	NE-CZ-NH2	7.75	126.18	119.20
1	A	66	ASP	CB-CA-C	-7.74	97.43	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	VAL	N-CA-CB	-7.74	100.72	111.25
1	A	34	PHE	CD1-CG-CD2	7.71	130.17	118.60
1	A	5	ARG	CD-NE-CZ	-7.70	113.61	124.40
1	A	18	ASP	O-C-N	-7.68	112.38	122.59
1	A	43	THR	CA-CB-OG1	-7.68	98.08	109.60
1	A	47	THR	CA-C-N	-7.67	106.98	122.31
1	A	47	THR	C-N-CA	-7.67	106.98	122.31
1	A	17	LEU	CA-C-O	7.63	128.77	119.31
1	A	51	THR	CA-C-O	-7.62	112.22	121.06
1	A	124	ILE	CA-C-N	-7.62	110.52	121.42
1	A	124	ILE	C-N-CA	-7.62	110.52	121.42
1	A	60	SER	CA-C-N	-7.61	107.74	120.68
1	A	60	SER	C-N-CA	-7.61	107.74	120.68
1	A	8	LEU	N-CA-C	-7.61	102.64	112.23
1	A	91	SER	CA-C-N	-7.60	107.21	120.29
1	A	91	SER	C-N-CA	-7.60	107.21	120.29
1	A	80	CYS	CA-C-N	7.59	131.21	120.28
1	A	80	CYS	C-N-CA	7.59	131.21	120.28
1	A	21	ARG	N-CA-C	-7.58	103.02	113.56
1	A	66	ASP	O-C-N	7.58	131.75	122.20
1	A	72	SER	N-CA-C	7.57	121.31	109.96
1	A	2	VAL	CA-C-O	-7.55	112.48	120.48
1	A	15	HIS	CA-C-O	7.53	128.85	119.59
1	A	1	LYS	CA-C-O	7.52	133.58	120.80
1	A	125	ARG	O-C-N	7.52	131.88	123.01
1	A	126	GLY	CA-C-O	-7.50	111.24	119.27
1	A	58	ILE	O-C-N	7.50	131.28	122.66
1	A	127	CYS	CB-CA-C	7.46	124.61	109.76
1	A	78	ILE	O-C-N	7.45	129.59	121.10
1	A	102	GLY	N-CA-C	-7.43	95.58	113.18
1	A	2	VAL	O-C-N	7.42	130.98	123.18
1	A	78	ILE	CA-CB-CG2	-7.42	97.88	110.50
1	A	45	ARG	NE-CZ-NH2	-7.42	112.53	119.20
1	A	71	GLY	CA-C-O	7.41	128.55	119.88
1	A	84	LEU	O-C-N	7.41	131.37	122.26
1	A	48	ASP	O-C-N	-7.39	110.52	122.42
1	A	23	TYR	CB-CG-CD2	7.38	131.88	120.80
1	A	105	MET	CB-CA-C	7.38	124.13	110.11
1	A	39	ASN	CA-C-O	-7.37	111.94	120.49
1	A	27	ASN	O-C-N	7.37	132.20	122.33
1	A	67	GLY	O-C-N	-7.36	113.21	122.41
1	A	66	ASP	CB-CG-OD1	7.36	135.32	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ALA	CA-C-O	-7.35	113.11	121.19
1	A	25	LEU	N-CA-C	-7.31	102.33	111.11
1	A	41	GLN	N-CA-C	7.29	122.20	113.16
1	A	19	ASN	CB-CG-OD1	7.27	135.34	120.80
1	A	45	ARG	CB-CG-CD	-7.24	94.65	111.30
1	A	36	SER	CA-C-N	-7.20	111.96	122.40
1	A	36	SER	C-N-CA	-7.20	111.96	122.40
1	A	30	CYS	CA-C-O	-7.18	112.81	120.42
1	A	50	SER	CA-C-O	-7.18	113.48	121.89
1	A	16	GLY	CA-C-N	7.14	133.64	121.14
1	A	16	GLY	C-N-CA	7.14	133.64	121.14
1	A	24	SER	N-CA-C	-7.14	99.88	110.23
1	A	31	ALA	N-CA-CB	7.07	120.52	110.12
1	A	57	GLN	CA-CB-CG	-7.07	99.96	114.10
1	A	47	THR	CA-C-O	-7.05	111.29	119.61
1	A	3	PHE	CA-C-O	-7.04	112.95	121.89
1	A	88	ILE	N-CA-C	7.03	123.95	109.34
1	A	10	ALA	CA-C-O	7.02	127.86	120.42
1	A	4	GLY	CA-C-N	-6.99	108.90	121.14
1	A	4	GLY	C-N-CA	-6.99	108.90	121.14
1	A	59	ASN	CA-C-O	-6.97	113.79	121.87
1	A	127	CYS	N-CA-CB	-6.96	99.87	110.45
1	A	32	ALA	CA-C-N	6.93	129.80	120.65
1	A	32	ALA	C-N-CA	6.93	129.80	120.65
1	A	63	TRP	CA-CB-CG	-6.93	100.43	113.60
1	A	1	LYS	CA-CB-CG	-6.92	100.26	114.10
1	A	68	ARG	CB-CG-CD	6.90	127.18	111.30
1	A	52	ASP	CB-CA-C	6.88	121.03	109.48
1	A	36	SER	O-C-N	6.87	131.31	122.04
1	A	37	ASN	O-C-N	6.85	134.05	122.21
1	A	14	ARG	CA-C-O	6.84	127.83	119.97
1	A	123	TRP	NE1-CE2-CD2	6.84	116.29	107.40
1	A	61	ARG	NH1-CZ-NH2	6.79	128.12	119.30
1	A	11	ALA	O-C-N	6.78	129.31	122.12
1	A	123	TRP	CD1-CG-CD2	6.75	117.10	106.30
1	A	10	ALA	CB-CA-C	-6.75	99.38	110.85
1	A	112	ARG	NE-CZ-NH2	6.67	125.21	119.20
1	A	68	ARG	CA-C-O	-6.65	111.52	119.03
1	A	53	TYR	CE1-CZ-OH	-6.65	99.96	119.90
1	A	56	LEU	O-C-N	-6.64	114.35	122.25
1	A	107	ALA	CA-C-O	6.64	127.60	119.97
1	A	23	TYR	N-CA-CB	-6.63	99.46	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	A	21	ARG	CD-NE-CZ	-6.60	115.16	124.40
1	A	12	MET	CA-C-O	-6.59	113.56	120.55
1	A	96	LYS	N-CA-C	-6.59	104.09	111.28
1	A	108	TRP	CD2-CE3-CZ3	-6.56	110.08	118.60
1	A	115	CYS	CA-C-O	6.54	127.19	119.67
1	A	74	ASN	CB-CG-ND2	6.52	126.18	116.40
1	A	32	ALA	CA-C-O	6.51	127.47	119.79
1	A	39	ASN	OD1-CG-ND2	6.49	129.09	122.60
1	A	60	SER	N-CA-CB	-6.47	100.55	110.44
1	A	79	PRO	O-C-N	-6.43	115.25	123.03
1	A	28	TRP	NE1-CE2-CZ2	-6.43	120.46	130.10
1	A	14	ARG	N-CA-C	6.41	119.25	111.82
1	A	57	GLN	CA-C-N	6.38	130.75	121.18
1	A	57	GLN	C-N-CA	6.38	130.75	121.18
1	A	101	ASP	N-CA-CB	6.38	121.27	110.49
1	A	104	GLY	N-CA-C	-6.38	101.58	111.98
1	A	114	ARG	CA-CB-CG	-6.37	101.35	114.10
1	A	6	CYS	CA-C-O	6.37	127.31	120.24
1	A	7	GLU	CG-CD-OE1	6.36	133.03	118.40
1	A	119	ASP	CA-C-O	-6.34	114.69	122.36
1	A	27	ASN	CB-CA-C	-6.34	97.44	110.38
1	A	83	LEU	CB-CA-C	-6.33	98.07	110.11
1	A	77	ASN	N-CA-CB	-6.32	102.54	112.46
1	A	69	THR	CA-C-O	6.31	126.39	119.32
1	A	7	GLU	O-C-N	-6.31	114.96	122.15
1	A	34	PHE	CG-CD1-CE1	-6.29	110.00	120.70
1	A	8	LEU	CA-C-N	-6.25	111.91	120.28
1	A	8	LEU	C-N-CA	-6.25	111.91	120.28
1	A	57	GLN	N-CA-C	6.23	119.99	111.39
1	A	108	TRP	CA-C-O	6.23	127.02	120.54
1	A	41	GLN	OE1-CD-NE2	6.21	128.81	122.60
1	A	97	LYS	CA-CB-CG	-6.20	101.70	114.10
1	A	86	SER	N-CA-CB	6.17	119.84	110.28
1	A	2	VAL	CA-CB-CG1	6.15	120.86	110.40
1	A	20	TYR	CA-C-O	-6.15	113.45	120.58
1	A	8	LEU	O-C-N	6.14	130.56	122.33
1	A	93	ASN	N-CA-C	-6.13	104.71	111.82
1	A	116	LYS	CG-CD-CE	-6.12	97.23	111.30
1	A	117	GLY	N-CA-C	6.10	120.57	112.77
1	A	24	SER	O-C-N	-6.04	115.44	122.87
1	A	108	TRP	CD2-CE2-CZ2	6.00	128.40	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASN	CB-CG-OD1	6.00	132.80	120.80
1	A	52	ASP	OD1-CG-OD2	6.00	137.29	122.90
1	A	41	GLN	CB-CG-CD	-5.97	102.45	112.60
1	A	123	TRP	CG-CD1-NE1	-5.97	102.44	110.20
1	A	55	ILE	CA-C-O	-5.93	114.06	120.47
1	A	62	TRP	CA-CB-CG	-5.93	102.33	113.60
1	A	18	ASP	CA-C-O	5.92	128.98	120.51
1	A	28	TRP	CE2-CD2-CE3	-5.92	112.88	118.80
1	A	15	HIS	O-C-N	-5.92	114.79	122.37
1	A	31	ALA	O-C-N	-5.91	115.85	122.12
1	A	95	ALA	CA-C-N	5.91	128.20	120.28
1	A	95	ALA	C-N-CA	5.91	128.20	120.28
1	A	70	PRO	N-CA-C	-5.90	101.94	111.03
1	A	87	ASP	CB-CG-OD1	5.89	131.94	118.40
1	A	84	LEU	CA-C-O	-5.84	113.06	119.95
1	A	23	TYR	CA-C-O	5.83	126.70	120.46
1	A	14	ARG	N-CA-CB	5.82	119.31	110.28
1	A	49	GLY	O-C-N	-5.82	117.30	122.77
1	A	59	ASN	CB-CA-C	5.82	121.61	109.68
1	A	81	SER	O-C-N	5.81	129.02	122.22
1	A	56	LEU	N-CA-C	-5.80	105.40	112.88
1	A	2	VAL	CA-CB-CG2	5.78	120.22	110.40
1	A	88	ILE	CB-CA-C	-5.78	101.82	111.29
1	A	28	TRP	CA-C-N	5.76	128.35	120.46
1	A	28	TRP	C-N-CA	5.76	128.35	120.46
1	A	64	CYS	O-C-N	5.76	130.14	123.17
1	A	123	TRP	CB-CG-CD1	-5.76	118.27	126.90
1	A	41	GLN	CA-CB-CG	-5.73	102.63	114.10
1	A	68	ARG	CB-CA-C	-5.73	99.89	109.75
1	A	60	SER	CB-CA-C	5.71	120.30	110.01
1	A	114	ARG	N-CA-C	5.71	122.67	114.39
1	A	30	CYS	N-CA-CB	-5.70	101.72	110.16
1	A	14	ARG	CA-CB-CG	-5.70	102.70	114.10
1	A	84	LEU	N-CA-C	-5.70	105.64	112.59
1	A	4	GLY	CA-C-O	-5.68	112.14	122.14
1	A	97	LYS	CB-CA-C	-5.68	101.96	110.88
1	A	43	THR	CA-CB-CG2	5.67	120.14	110.50
1	A	64	CYS	CA-C-N	-5.67	114.90	122.72
1	A	64	CYS	C-N-CA	-5.67	114.90	122.72
1	A	74	ASN	CA-C-N	-5.65	111.25	121.14
1	A	74	ASN	C-N-CA	-5.65	111.25	121.14
1	A	35	GLU	CA-C-O	-5.65	113.11	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	25	LEU	CD1-CG-CD2	-5.64	98.39	110.80
1	A	118	THR	CB-CA-C	5.62	121.61	110.42
1	A	40	THR	CA-C-O	5.62	126.30	119.38
1	A	62	TRP	CD1-CG-CD2	5.62	115.29	106.30
1	A	14	ARG	CA-C-N	5.61	131.97	122.65
1	A	14	ARG	C-N-CA	5.61	131.97	122.65
1	A	79	PRO	CA-C-N	-5.58	111.66	120.60
1	A	79	PRO	C-N-CA	-5.58	111.66	120.60
1	A	45	ARG	N-CA-C	5.57	118.62	109.76
1	A	35	GLU	CG-CD-OE1	5.56	131.19	118.40
1	A	47	THR	OG1-CB-CG2	5.54	120.39	109.30
1	A	101	ASP	N-CA-C	-5.54	99.00	110.80
1	A	113	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	39	ASN	N-CA-C	5.50	117.67	109.25
1	A	127	CYS	N-CA-C	-5.50	103.12	110.55
1	A	51	THR	N-CA-C	-5.49	100.72	109.23
1	A	14	ARG	CG-CD-NE	-5.49	99.93	112.00
1	A	97	LYS	CA-C-N	5.48	127.46	120.56
1	A	97	LYS	C-N-CA	5.48	127.46	120.56
1	A	128	ARG	CA-C-O	5.47	126.61	120.92
1	A	101	ASP	CA-C-O	-5.47	112.69	120.51
1	A	61	ARG	O-C-N	5.46	129.65	122.33
1	A	119	ASP	O-C-N	5.43	129.90	122.29
1	A	128	ARG	O-C-N	-5.42	115.79	122.68
1	A	68	ARG	CG-CD-NE	5.41	123.90	112.00
1	A	112	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	A	73	ARG	CG-CD-NE	-5.40	100.13	112.00
1	A	129	LEU	CB-CG-CD1	-5.39	94.53	110.70
1	A	51	THR	CA-CB-OG1	5.39	117.68	109.60
1	A	46	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	68	ARG	CA-CB-CG	5.35	124.79	114.10
1	A	119	ASP	CB-CA-C	5.34	120.27	111.50
1	A	123	TRP	CA-CB-CG	-5.31	103.51	113.60
1	A	47	THR	CB-CA-C	5.30	122.05	110.18
1	A	37	ASN	CA-C-O	-5.27	114.27	120.81
1	A	37	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	44	ASN	CA-C-N	-5.24	114.01	121.50
1	A	44	ASN	C-N-CA	-5.24	114.01	121.50
1	A	27	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	37	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	1	LYS	CA-C-N	5.23	129.67	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	LYS	C-N-CA	5.23	129.67	123.19
1	A	53	TYR	CB-CG-CD2	-5.23	112.96	120.80
1	A	93	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	116	LYS	CD-CE-NZ	-5.21	95.23	111.90
1	A	123	TRP	CE3-CZ3-CH2	5.17	127.82	121.10
1	A	106	ASN	CB-CG-ND2	5.17	124.15	116.40
1	A	57	GLN	CA-C-O	-5.15	115.87	121.84
1	A	7	GLU	CB-CG-CD	-5.14	103.86	112.60
1	A	35	GLU	CG-CD-OE2	5.13	130.20	118.40
1	A	11	ALA	CA-C-N	-5.13	113.41	120.28
1	A	11	ALA	C-N-CA	-5.13	113.41	120.28
1	A	61	ARG	N-CA-C	-5.12	105.78	112.23
1	A	20	TYR	OH-CZ-CE2	5.12	135.27	119.90
1	A	105	MET	CA-C-O	5.12	125.82	119.12
1	A	85	SER	CA-C-N	-5.10	112.56	120.31
1	A	85	SER	C-N-CA	-5.10	112.56	120.31
1	A	88	ILE	CA-CB-CG1	5.08	119.04	110.40
1	A	113	ASN	O-C-N	5.08	129.42	122.46
1	A	52	ASP	CB-CG-OD2	-5.06	106.76	118.40
1	A	111	TRP	N-CA-C	-5.06	105.84	111.36
1	A	2	VAL	CA-C-N	-5.06	113.92	122.67
1	A	2	VAL	C-N-CA	-5.06	113.92	122.67
1	A	23	TYR	CB-CG-CD1	-5.05	113.23	120.80
1	A	27	ASN	N-CA-C	5.05	118.59	112.23
1	A	89	THR	CA-C-N	-5.04	113.89	120.44
1	A	89	THR	C-N-CA	-5.04	113.89	120.44
1	A	84	LEU	CB-CA-C	5.04	119.13	111.02
1	A	53	TYR	OH-CZ-CE2	5.02	134.96	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ARG	Sidechain

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	959	81	2
2	A	220	0	0	16	0
All	All	1221	0	959	81	2

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 41.

All (81) 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:13:LYS:HE3	1:A:129:LEU:OXT	1.36	1.19
1:A:45:ARG:NH1	2:A:222:HOH:O	1.93	1.00
1:A:128:ARG:NH2	2:A:276:HOH:O	1.96	0.97
1:A:16:GLY:HA2	2:A:140:HOH:O	1.65	0.94
1:A:66:ASP:O	2:A:142:HOH:O	1.86	0.93
1:A:13:LYS:CE	1:A:129:LEU:OXT	2.19	0.90
1:A:66:ASP:HB2	2:A:142:HOH:O	1.74	0.85
1:A:100:SER:O	1:A:101:ASP:CG	2.21	0.84
1:A:62:TRP:HB2	1:A:63:TRP:CD1	2.13	0.82
1:A:99:VAL:O	1:A:103:ASN:OD1	2.07	0.72
1:A:45:ARG:HE	1:A:51:THR:CG2	2.04	0.71
1:A:69:THR:CG2	1:A:70:PRO:HD2	2.22	0.70
1:A:88:ILE:HD12	1:A:92:VAL:HG21	1.73	0.69
1:A:103:ASN:C	1:A:104:GLY:O	2.31	0.69
1:A:10:ALA:HA	1:A:129:LEU:CD2	2.24	0.68
1:A:20:TYR:HE2	1:A:99:VAL:CG1	2.09	0.66
1:A:20:TYR:HE2	1:A:99:VAL:HG12	1.61	0.66
1:A:69:THR:HG23	1:A:70:PRO:HD2	1.78	0.65
1:A:104:GLY:HA3	1:A:106:ASN:HB2	1.77	0.65
1:A:122:ALA:O	1:A:125:ARG:NE	2.30	0.65
1:A:78:ILE:CD1	1:A:83:LEU:HD21	2.26	0.65
1:A:45:ARG:CZ	2:A:145:HOH:O	2.45	0.65
1:A:62:TRP:CH2	1:A:73:ARG:CZ	2.82	0.63
1:A:45:ARG:HE	1:A:51:THR:HG21	1.63	0.61
1:A:2:VAL:HG22	2:A:324:HOH:O	2.00	0.61
1:A:1:LYS:HB2	1:A:86:SER:OG	2.01	0.60
1:A:53:TYR:HE2	1:A:60:SER:HB3	1.67	0.59
1:A:45:ARG:NH2	2:A:145:HOH:O	2.37	0.58
1:A:20:TYR:CE2	1:A:99:VAL:CG1	2.87	0.57
1:A:88:ILE:HD12	1:A:92:VAL:CG2	2.33	0.57
1:A:104:GLY:C	1:A:106:ASN:H	2.15	0.55
1:A:45:ARG:NE	1:A:51:THR:CG2	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HB3	1:A:62:TRP:CD1	2.42	0.54
1:A:13:LYS:CD	1:A:129:LEU:HB3	2.38	0.54
1:A:45:ARG:NE	1:A:51:THR:OG1	2.41	0.54
1:A:39:ASN:ND2	2:A:326:HOH:O	2.40	0.54
1:A:13:LYS:HD2	1:A:129:LEU:HB3	1.89	0.53
1:A:78:ILE:HD11	1:A:83:LEU:HD21	1.89	0.53
1:A:20:TYR:CE2	1:A:99:VAL:HG11	2.43	0.53
1:A:24:SER:O	1:A:27:ASN:HB2	2.09	0.53
1:A:100:SER:O	1:A:101:ASP:CB	2.56	0.52
1:A:45:ARG:CG	1:A:51:THR:HG23	2.41	0.51
1:A:54:GLY:H	1:A:84:LEU:CD2	2.24	0.51
1:A:63:TRP:HH2	1:A:101:ASP:OD2	1.94	0.51
1:A:45:ARG:NE	1:A:51:THR:HG21	2.24	0.51
1:A:100:SER:O	1:A:101:ASP:OD1	2.29	0.51
1:A:2:VAL:HG13	2:A:324:HOH:O	2.11	0.51
1:A:45:ARG:HG3	1:A:51:THR:HG23	1.92	0.50
1:A:31:ALA:O	1:A:35:GLU:HG2	2.11	0.50
1:A:54:GLY:N	1:A:84:LEU:HD23	2.26	0.50
1:A:25:LEU:HD23	1:A:129:LEU:HD13	1.93	0.50
1:A:62:TRP:HB2	1:A:63:TRP:NE1	2.25	0.50
1:A:115:CYS:O	1:A:116:LYS:C	2.55	0.49
1:A:20:TYR:CE2	1:A:99:VAL:HG12	2.45	0.48
1:A:10:ALA:HA	1:A:129:LEU:HD21	1.93	0.48
1:A:46:ASN:C	1:A:48:ASP:N	2.72	0.47
1:A:61:ARG:HB3	1:A:62:TRP:NE1	2.30	0.47
1:A:104:GLY:C	1:A:106:ASN:N	2.70	0.47
1:A:2:VAL:CG2	2:A:324:HOH:O	2.60	0.46
1:A:109:VAL:HG12	1:A:112:ARG:HH11	1.79	0.46
1:A:105:MET:HE2	1:A:105:MET:HB3	1.44	0.46
1:A:104:GLY:CA	1:A:106:ASN:HB2	2.46	0.46
1:A:4:GLY:HA3	1:A:7:GLU:OE1	2.16	0.45
1:A:31:ALA:O	1:A:35:GLU:CG	2.64	0.45
1:A:20:TYR:C	1:A:22:GLY:H	2.25	0.45
1:A:16:GLY:CA	2:A:140:HOH:O	2.43	0.45
1:A:45:ARG:NH1	2:A:145:HOH:O	2.49	0.45
1:A:53:TYR:OH	1:A:66:ASP:OD2	2.24	0.43
1:A:109:VAL:HG12	1:A:112:ARG:NH1	2.33	0.43
1:A:33:LYS:HG2	1:A:123:TRP:CZ3	2.53	0.43
1:A:54:GLY:H	1:A:84:LEU:HD23	1.83	0.43
1:A:76:CYS:O	1:A:77:ASN:CB	2.64	0.43
1:A:54:GLY:N	1:A:84:LEU:CD2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:CZ	1:A:68:ARG:NH1	2.82	0.42
1:A:58:ILE:CG2	1:A:63:TRP:HB2	2.49	0.42
1:A:2:VAL:CG1	2:A:324:HOH:O	2.68	0.42
1:A:125:ARG:H	1:A:125:ARG:HG3	1.55	0.41
1:A:90:ALA:HA	2:A:195:HOH:O	2.20	0.41
1:A:124:ILE:HD13	1:A:124:ILE:HG21	1.57	0.41
1:A:16:GLY:C	2:A:140:HOH:O	2.63	0.41
1:A:1:LYS:HG2	1:A:2:VAL:N	2.35	0.41

All (2) 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)
1:A:109:VAL:CG2	1:A:128:ARG:NH1[1_656]	1.95	0.25
1:A:23:TYR:OH	1:A:68:ARG:NH2[1_565]	2.08	0.12

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%)	119 (94%)	5 (4%)	3 (2%)	4 1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ASP
1	A	103	ASN
1	A	118	THR

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%)	89 (85%)	16 (15%)	3 0

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	17	LEU
1	A	19	ASN
1	A	24	SER
1	A	41	GLN
1	A	44	ASN
1	A	61	ARG
1	A	68	ARG
1	A	77	ASN
1	A	86	SER
1	A	97	LYS
1	A	99	VAL
1	A	103	ASN
1	A	109	VAL
1	A	125	ARG
1	A	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	44	ASN
1	A	46	ASN
1	A	77	ASN
1	A	113	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 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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	129/129 (100%)	0.59	8 (6%) 26 35	5, 10, 15, 16	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	4.8
1	A	104	GLY	4.6
1	A	62	TRP	3.1
1	A	101	ASP	2.3
1	A	129	LEU	2.3
1	A	117	GLY	2.2
1	A	45	ARG	2.1
1	A	87	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.