



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:16 PM UTC

PDB ID : 2LZ2 / pdb_00002lz2
Title : THE THREE DIMENSIONAL STRUCTURE OF TURKEY EGG WHITE
LYSOZYME AT 2.2 ANGSTROMS RESOLUTION
Authors : Parsons, M.R.; Phillips, S.E.V.
Deposited on : 1988-10-20
Resolution : 2.20 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

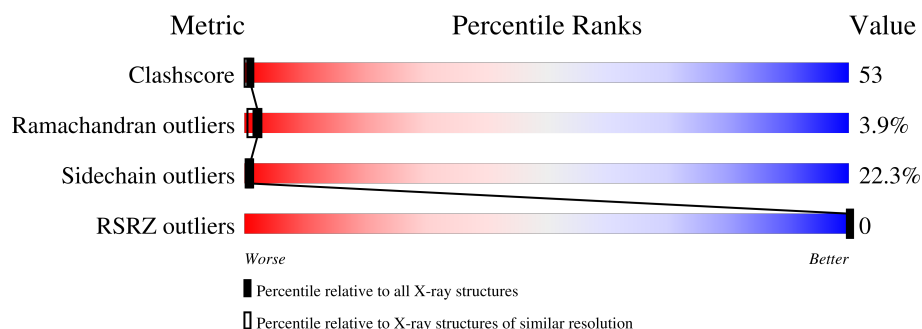
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1105 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.

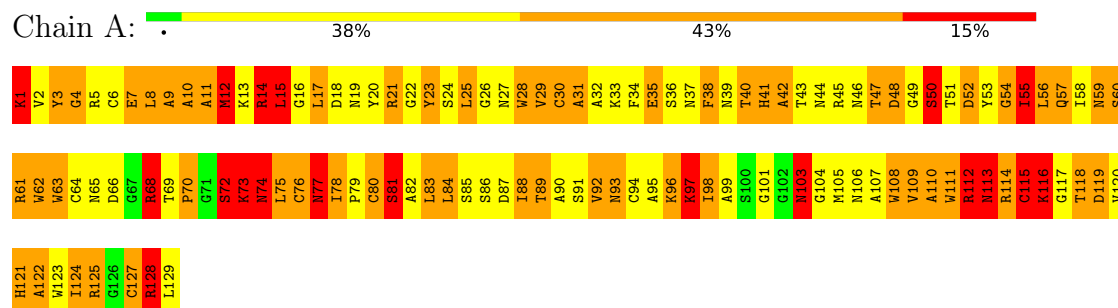
- Molecule 1 is a protein called TURKEY EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			994	611	191	182	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		

• Molecule 1: TURKEY EGG WHITE LYSOZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	71.00Å 71.00Å 84.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 88.2 (10.00-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.21Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.192 , (Not available) 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 176.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1105	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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	1.87	12/1015 (1.2%)	5.00	357/1371 (26.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	THR	CA-CB	7.19	1.63	1.53
1	A	108	TRP	C-N	-6.40	1.25	1.33
1	A	76	CYS	C-O	6.02	1.31	1.24
1	A	128	ARG	NE-CZ	5.48	1.39	1.33
1	A	42	ALA	CA-CB	5.41	1.62	1.53
1	A	25	LEU	C-O	5.30	1.30	1.24
1	A	53	TYR	CA-C	-5.27	1.46	1.52
1	A	50	SER	CB-OG	5.24	1.52	1.42
1	A	26	GLY	N-CA	5.21	1.53	1.45
1	A	111	TRP	C-N	-5.17	1.27	1.33
1	A	118	THR	N-CA	-5.08	1.39	1.45
1	A	64	CYS	N-CA	5.03	1.52	1.45

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASN	CA-CB-CG	32.39	144.99	112.60
1	A	112	ARG	CD-NE-CZ	23.51	157.31	124.40
1	A	119	ASP	CA-CB-CG	21.51	134.11	112.60
1	A	41	HIS	CA-CB-CG	20.30	134.10	113.80
1	A	39	ASN	CA-C-O	-18.68	99.43	120.54
1	A	117	GLY	CA-C-N	18.67	157.30	122.02
1	A	117	GLY	C-N-CA	18.67	157.30	122.02
1	A	77	ASN	CA-C-O	18.33	143.53	120.81
1	A	3	TYR	CA-C-O	17.89	142.83	121.36
1	A	85	SER	CA-C-N	17.06	146.41	120.82
1	A	85	SER	C-N-CA	17.06	146.41	120.82
1	A	58	ILE	CA-C-N	16.71	144.34	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ILE	C-N-CA	16.71	144.34	120.95
1	A	108	TRP	CA-C-N	16.45	151.58	121.97
1	A	108	TRP	C-N-CA	16.45	151.58	121.97
1	A	76	CYS	CA-C-N	15.21	144.46	122.40
1	A	76	CYS	C-N-CA	15.21	144.46	122.40
1	A	11	ALA	N-CA-CB	-14.68	88.72	110.01
1	A	34	PHE	CA-C-O	-14.58	104.97	120.42
1	A	112	ARG	CA-C-N	14.16	148.59	121.54
1	A	112	ARG	C-N-CA	14.16	148.59	121.54
1	A	114	ARG	N-CA-C	13.98	129.78	113.01
1	A	56	LEU	CA-C-O	13.87	133.94	119.51
1	A	17	LEU	N-CA-C	13.55	129.69	112.89
1	A	4	GLY	N-CA-C	-13.52	94.16	112.82
1	A	28	TRP	CB-CG-CD2	13.38	145.53	126.80
1	A	114	ARG	CA-C-N	13.14	142.40	122.17
1	A	114	ARG	C-N-CA	13.14	142.40	122.17
1	A	52	ASP	CA-C-O	-12.80	106.60	120.80
1	A	84	LEU	N-CA-C	12.66	128.50	113.18
1	A	68	ARG	O-C-N	-12.39	108.90	123.28
1	A	121	HIS	CA-C-O	12.36	134.13	120.90
1	A	121	HIS	CA-CB-CG	-12.36	101.44	113.80
1	A	114	ARG	NE-CZ-NH1	12.15	133.65	121.50
1	A	103	ASN	OD1-CG-ND2	12.13	134.73	122.60
1	A	117	GLY	N-CA-C	12.01	132.59	115.30
1	A	77	ASN	CA-CB-CG	11.94	124.54	112.60
1	A	15	LEU	CD1-CG-CD2	-11.87	84.69	110.80
1	A	6	CYS	N-CA-CB	11.73	129.52	110.40
1	A	6	CYS	O-C-N	11.63	138.51	122.46
1	A	65	ASN	CA-CB-CG	-11.60	101.00	112.60
1	A	28	TRP	CA-C-O	11.59	132.64	120.70
1	A	53	TYR	CA-C-O	-11.49	107.67	121.11
1	A	50	SER	CA-CB-OG	-11.49	88.13	111.10
1	A	128	ARG	CA-C-N	11.44	142.29	121.70
1	A	128	ARG	C-N-CA	11.44	142.29	121.70
1	A	53	TYR	O-C-N	11.38	137.24	123.24
1	A	83	LEU	CA-C-O	11.22	133.03	119.79
1	A	38	PHE	CA-C-N	11.20	137.98	122.19
1	A	38	PHE	C-N-CA	11.20	137.98	122.19
1	A	10	ALA	CA-C-N	11.15	134.93	120.44
1	A	10	ALA	C-N-CA	11.15	134.93	120.44
1	A	114	ARG	CD-NE-CZ	11.06	139.88	124.40
1	A	10	ALA	CA-C-O	11.02	132.23	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ILE	N-CA-CB	-10.93	95.92	111.21
1	A	114	ARG	NH1-CZ-NH2	-10.89	105.14	119.30
1	A	49	GLY	CA-C-O	10.84	131.21	119.07
1	A	112	ARG	O-C-N	-10.73	109.22	122.20
1	A	91	SER	CA-C-N	10.48	138.04	120.64
1	A	91	SER	C-N-CA	10.48	138.04	120.64
1	A	76	CYS	CA-C-O	-10.46	107.54	119.05
1	A	28	TRP	CB-CG-CD1	-10.43	111.25	126.90
1	A	77	ASN	N-CA-CB	10.42	128.15	112.30
1	A	24	SER	CA-C-O	-10.34	108.95	121.36
1	A	86	SER	CA-C-N	10.33	136.76	122.19
1	A	86	SER	C-N-CA	10.33	136.76	122.19
1	A	35	GLU	CA-C-O	-10.17	110.22	120.70
1	A	57	GLN	OE1-CD-NE2	10.03	132.63	122.60
1	A	90	ALA	CA-C-N	10.01	134.06	120.44
1	A	90	ALA	C-N-CA	10.01	134.06	120.44
1	A	42	ALA	N-CA-CB	10.00	124.67	109.97
1	A	93	ASN	O-C-N	9.98	135.77	122.30
1	A	8	LEU	CA-C-O	-9.89	110.51	120.70
1	A	60	SER	N-CA-CB	-9.79	94.44	110.40
1	A	84	LEU	CA-C-N	9.76	141.82	121.32
1	A	84	LEU	C-N-CA	9.76	141.82	121.32
1	A	5	ARG	N-CA-C	-9.73	100.63	111.14
1	A	45	ARG	NE-CZ-NH2	-9.71	110.46	119.20
1	A	73	LYS	N-CA-C	9.71	131.49	110.80
1	A	55	ILE	CA-C-O	-9.68	107.85	119.85
1	A	115	CYS	CA-C-O	-9.62	107.68	119.61
1	A	81	SER	CB-CA-C	9.62	129.09	109.95
1	A	128	ARG	CA-CB-CG	9.59	133.27	114.10
1	A	39	ASN	OD1-CG-ND2	9.50	132.10	122.60
1	A	40	THR	CA-CB-CG2	9.46	126.58	110.50
1	A	111	TRP	N-CA-C	-9.45	99.06	111.24
1	A	65	ASN	N-CA-CB	9.44	126.14	110.47
1	A	58	ILE	O-C-N	-9.41	112.42	122.67
1	A	78	ILE	O-C-N	9.40	131.81	121.10
1	A	61	ARG	CA-C-O	-9.39	107.91	119.28
1	A	21	ARG	CA-C-N	9.35	138.34	120.66
1	A	21	ARG	C-N-CA	9.35	138.34	120.66
1	A	64	CYS	N-CA-C	9.25	123.13	109.07
1	A	8	LEU	CA-C-N	9.23	132.64	120.28
1	A	8	LEU	C-N-CA	9.23	132.64	120.28
1	A	52	ASP	CA-CB-CG	9.18	121.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ALA	N-CA-C	-9.16	96.72	110.28
1	A	2	VAL	CB-CA-C	9.15	123.51	110.98
1	A	84	LEU	N-CA-CB	-9.10	95.12	110.41
1	A	128	ARG	NH1-CZ-NH2	-9.08	107.50	119.30
1	A	14	ARG	CB-CA-C	9.04	127.25	110.70
1	A	35	GLU	N-CA-CB	9.04	123.17	110.07
1	A	75	LEU	CA-C-O	-9.02	107.74	119.10
1	A	124	ILE	CA-CB-CG2	8.95	125.71	110.50
1	A	122	ALA	CA-C-O	-8.84	111.08	120.63
1	A	78	ILE	CB-CA-C	8.84	127.44	111.36
1	A	66	ASP	CB-CG-OD2	8.80	138.64	118.40
1	A	54	GLY	CA-C-N	8.79	135.24	120.64
1	A	54	GLY	C-N-CA	8.79	135.24	120.64
1	A	128	ARG	CG-CD-NE	8.73	131.20	112.00
1	A	15	LEU	CA-C-N	8.68	134.70	121.51
1	A	15	LEU	C-N-CA	8.68	134.70	121.51
1	A	125	ARG	O-C-N	-8.59	111.17	122.59
1	A	93	ASN	CA-C-N	-8.56	109.31	120.44
1	A	93	ASN	C-N-CA	-8.56	109.31	120.44
1	A	117	GLY	O-C-N	-8.52	111.02	122.35
1	A	75	LEU	O-C-N	8.51	133.75	122.43
1	A	93	ASN	N-CA-CB	8.51	123.38	110.19
1	A	68	ARG	N-CA-C	8.45	121.26	107.32
1	A	93	ASN	N-CA-C	-8.41	99.93	112.04
1	A	92	VAL	CA-C-O	-8.40	109.43	119.85
1	A	85	SER	CA-C-O	8.39	131.71	121.81
1	A	14	ARG	CA-CB-CG	8.38	130.86	114.10
1	A	32	ALA	CA-C-O	8.38	129.30	120.42
1	A	50	SER	CB-CA-C	8.36	126.83	109.68
1	A	46	ASN	N-CA-CB	-8.33	95.81	110.14
1	A	90	ALA	N-CA-C	8.31	121.46	111.82
1	A	77	ASN	CA-C-N	-8.28	106.80	122.13
1	A	77	ASN	C-N-CA	-8.28	106.80	122.13
1	A	127	CYS	N-CA-C	8.28	122.92	109.59
1	A	108	TRP	CA-C-O	8.24	129.23	120.33
1	A	74	ASN	OD1-CG-ND2	-8.19	114.41	122.60
1	A	2	VAL	CA-C-N	8.17	136.04	122.07
1	A	2	VAL	C-N-CA	8.17	136.04	122.07
1	A	81	SER	O-C-N	-8.16	110.52	122.43
1	A	118	THR	CA-C-N	8.15	136.69	123.33
1	A	118	THR	C-N-CA	8.15	136.69	123.33
1	A	8	LEU	CB-CA-C	8.08	123.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	A	39	ASN	CA-C-N	8.03	135.79	121.66
1	A	39	ASN	C-N-CA	8.03	135.79	121.66
1	A	28	TRP	CB-CA-C	7.98	123.50	110.90
1	A	74	ASN	CA-CB-CG	7.97	120.57	112.60
1	A	125	ARG	NH1-CZ-NH2	7.91	129.59	119.30
1	A	112	ARG	CB-CA-C	7.90	123.96	110.84
1	A	57	GLN	CB-CG-CD	-7.83	99.29	112.60
1	A	27	ASN	N-CA-CB	-7.81	98.64	110.12
1	A	43	THR	N-CA-CB	7.80	125.10	111.13
1	A	104	GLY	CA-C-O	-7.80	110.48	121.40
1	A	14	ARG	CB-CG-CD	7.79	129.21	111.30
1	A	66	ASP	OD1-CG-OD2	-7.78	104.22	122.90
1	A	113	ASN	OD1-CG-ND2	-7.75	114.85	122.60
1	A	45	ARG	NH1-CZ-NH2	7.74	129.36	119.30
1	A	99	ALA	CA-C-O	-7.74	108.98	119.12
1	A	29	VAL	N-CA-CB	-7.72	102.21	110.62
1	A	36	SER	CA-CB-OG	-7.72	95.67	111.10
1	A	112	ARG	CA-CB-CG	7.71	129.51	114.10
1	A	34	PHE	CB-CA-C	7.70	123.94	110.85
1	A	121	HIS	CB-CG-CD2	-7.70	121.19	131.20
1	A	5	ARG	O-C-N	7.68	130.39	122.09
1	A	7	GLU	N-CA-C	-7.65	102.88	111.14
1	A	77	ASN	CB-CA-C	-7.61	99.48	111.51
1	A	117	GLY	CA-C-O	7.57	128.94	119.25
1	A	1	LYS	CA-C-O	-7.55	107.96	120.80
1	A	42	ALA	CB-CA-C	-7.45	96.91	109.65
1	A	52	ASP	N-CA-CB	-7.44	98.24	110.52
1	A	116	LYS	N-CA-CB	-7.42	97.90	109.69
1	A	40	THR	CA-C-N	7.41	133.97	122.49
1	A	40	THR	C-N-CA	7.41	133.97	122.49
1	A	33	LYS	CA-C-O	7.41	131.10	120.51
1	A	9	ALA	N-CA-CB	7.39	120.99	110.12
1	A	35	GLU	CB-CA-C	-7.37	99.25	110.90
1	A	87	ASP	CA-C-N	-7.35	110.94	121.52
1	A	87	ASP	C-N-CA	-7.35	110.94	121.52
1	A	75	LEU	N-CA-CB	7.34	123.68	110.32
1	A	101	GLY	CA-C-N	7.34	135.80	121.41
1	A	101	GLY	C-N-CA	7.34	135.80	121.41
1	A	128	ARG	NE-CZ-NH1	7.33	128.83	121.50
1	A	113	ASN	CB-CG-OD1	7.31	135.41	120.80
1	A	17	LEU	N-CA-CB	-7.29	98.53	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	CYS	N-CA-C	7.28	123.18	113.72
1	A	122	ALA	N-CA-C	-7.25	102.56	111.33
1	A	98	ILE	N-CA-C	-7.19	103.46	110.72
1	A	85	SER	O-C-N	-7.16	114.69	122.85
1	A	121	HIS	CA-C-N	7.14	130.16	120.38
1	A	121	HIS	C-N-CA	7.14	130.16	120.38
1	A	16	GLY	O-C-N	-7.13	113.90	122.38
1	A	121	HIS	CB-CG-ND1	7.13	133.39	122.70
1	A	61	ARG	CA-CB-CG	7.12	128.33	114.10
1	A	59	ASN	N-CA-CB	7.11	120.45	109.85
1	A	79	PRO	N-CA-C	-7.04	99.08	110.55
1	A	86	SER	CB-CA-C	-7.03	99.07	110.74
1	A	110	ALA	O-C-N	7.01	130.19	122.20
1	A	125	ARG	CA-C-O	6.99	130.51	120.51
1	A	77	ASN	OD1-CG-ND2	-6.97	115.62	122.60
1	A	43	THR	OG1-CB-CG2	6.95	123.19	109.30
1	A	6	CYS	CA-C-O	-6.89	110.77	119.31
1	A	61	ARG	NH1-CZ-NH2	-6.89	110.34	119.30
1	A	108	TRP	N-CA-C	-6.85	95.82	108.02
1	A	24	SER	O-C-N	6.85	130.73	123.06
1	A	86	SER	O-C-N	6.84	129.98	122.11
1	A	68	ARG	N-CA-CB	-6.83	98.93	111.36
1	A	83	LEU	O-C-N	6.83	131.48	122.33
1	A	39	ASN	O-C-N	6.79	130.96	123.22
1	A	74	ASN	CA-C-O	-6.78	110.81	120.51
1	A	34	PHE	O-C-N	6.76	129.86	122.15
1	A	34	PHE	CA-CB-CG	-6.76	107.04	113.80
1	A	60	SER	CA-CB-OG	6.75	124.60	111.10
1	A	112	ARG	CA-C-O	6.74	128.90	121.02
1	A	49	GLY	N-CA-C	-6.68	106.23	114.92
1	A	62	TRP	O-C-N	6.68	130.36	121.67
1	A	81	SER	CA-C-O	6.65	127.62	119.11
1	A	107	ALA	CB-CA-C	6.63	123.15	109.95
1	A	37	ASN	CA-CB-CG	-6.63	105.97	112.60
1	A	25	LEU	O-C-N	-6.62	113.78	122.59
1	A	120	VAL	CG1-CB-CG2	-6.62	96.24	110.80
1	A	70	PRO	N-CA-CB	6.60	110.18	103.25
1	A	61	ARG	CD-NE-CZ	6.56	133.59	124.40
1	A	113	ASN	CB-CA-C	6.55	123.46	110.42
1	A	125	ARG	CB-CA-C	6.52	123.39	110.42
1	A	30	CYS	CA-C-O	-6.47	113.69	120.55
1	A	86	SER	CA-C-O	6.46	128.16	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	N-CA-CB	-6.46	99.56	110.49
1	A	13	LYS	N-CA-CB	6.46	119.89	110.26
1	A	53	TYR	CB-CA-C	-6.45	95.91	109.38
1	A	120	VAL	N-CA-C	-6.45	103.54	112.50
1	A	45	ARG	CD-NE-CZ	-6.44	115.39	124.40
1	A	111	TRP	CA-CB-CG	-6.44	101.37	113.60
1	A	88	ILE	CA-C-O	6.42	127.57	119.48
1	A	63	TRP	N-CA-CB	-6.38	102.08	110.88
1	A	124	ILE	CA-C-O	6.36	124.91	119.38
1	A	2	VAL	N-CA-C	-6.34	98.74	107.99
1	A	23	TYR	N-CA-C	-6.33	98.87	109.07
1	A	47	THR	N-CA-CB	6.31	119.62	110.47
1	A	120	VAL	CA-C-O	6.27	127.17	119.58
1	A	66	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	85	SER	N-CA-CB	-6.22	101.00	110.45
1	A	52	ASP	O-C-N	6.21	130.46	123.19
1	A	87	ASP	O-C-N	6.21	130.30	123.22
1	A	14	ARG	CA-C-N	6.21	130.53	120.60
1	A	14	ARG	C-N-CA	6.21	130.53	120.60
1	A	53	TYR	N-CA-C	6.20	119.29	109.50
1	A	103	ASN	CA-C-O	-6.18	112.01	119.49
1	A	40	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	82	ALA	CA-C-O	6.17	126.96	119.31
1	A	50	SER	O-C-N	-6.17	115.76	122.79
1	A	127	CYS	CA-C-N	6.17	133.32	121.54
1	A	127	CYS	C-N-CA	6.17	133.32	121.54
1	A	58	ILE	CB-CA-C	6.14	120.48	111.33
1	A	3	TYR	CB-CG-CD2	6.14	130.01	120.80
1	A	13	LYS	N-CA-C	-6.12	103.94	112.45
1	A	95	ALA	N-CA-CB	6.12	119.24	110.06
1	A	11	ALA	N-CA-C	6.12	117.61	111.07
1	A	119	ASP	CA-C-N	6.09	130.63	120.64
1	A	119	ASP	C-N-CA	6.09	130.63	120.64
1	A	12	MET	O-C-N	-6.08	114.54	122.39
1	A	3	TYR	CB-CA-C	-6.08	99.11	109.51
1	A	11	ALA	CB-CA-C	6.01	120.32	110.88
1	A	54	GLY	O-C-N	6.01	129.28	122.67
1	A	120	VAL	CA-C-N	6.00	128.64	120.54
1	A	120	VAL	C-N-CA	6.00	128.64	120.54
1	A	25	LEU	N-CA-C	5.97	123.52	110.80
1	A	9	ALA	CA-C-O	-5.97	114.22	120.55
1	A	30	CYS	CB-CA-C	5.97	120.70	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	LYS	CA-C-N	5.96	130.53	122.90
1	A	1	LYS	C-N-CA	5.96	130.53	122.90
1	A	46	ASN	OD1-CG-ND2	5.96	128.56	122.60
1	A	116	LYS	CA-C-N	5.94	134.19	121.18
1	A	116	LYS	C-N-CA	5.94	134.19	121.18
1	A	97	LYS	CA-CB-CG	5.90	125.90	114.10
1	A	31	ALA	O-C-N	-5.88	115.33	122.22
1	A	29	VAL	CB-CA-C	5.88	119.16	111.81
1	A	10	ALA	N-CA-C	5.85	117.66	111.28
1	A	128	ARG	CB-CG-CD	5.82	124.69	111.30
1	A	89	THR	OG1-CB-CG2	-5.81	97.68	109.30
1	A	109	VAL	CA-C-N	5.80	128.84	120.38
1	A	109	VAL	C-N-CA	5.80	128.84	120.38
1	A	69	THR	CA-C-N	5.79	127.08	119.84
1	A	69	THR	C-N-CA	5.79	127.08	119.84
1	A	18	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	48	ASP	CB-CA-C	5.77	120.03	109.99
1	A	80	CYS	CB-CA-C	-5.76	98.95	110.42
1	A	61	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	A	34	PHE	N-CA-C	-5.74	105.11	111.36
1	A	81	SER	N-CA-CB	-5.73	100.78	110.41
1	A	69	THR	CB-CA-C	5.73	120.06	110.55
1	A	68	ARG	CB-CG-CD	5.72	124.45	111.30
1	A	94	CYS	O-C-N	-5.68	116.22	122.07
1	A	91	SER	CB-CA-C	5.67	119.86	110.90
1	A	112	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	A	96	LYS	CA-C-O	5.64	126.32	119.38
1	A	87	ASP	CB-CA-C	5.62	119.03	109.80
1	A	112	ARG	N-CA-C	-5.62	102.16	111.37
1	A	16	GLY	CA-C-O	-5.61	112.35	119.19
1	A	1	LYS	CA-CB-CG	5.59	125.29	114.10
1	A	81	SER	CA-C-N	5.58	130.90	121.14
1	A	81	SER	C-N-CA	5.58	130.90	121.14
1	A	15	LEU	CB-CA-C	5.58	122.08	110.32
1	A	55	ILE	N-CA-C	5.58	119.84	112.04
1	A	3	TYR	O-C-N	-5.57	116.82	123.06
1	A	116	LYS	CA-CB-CG	5.56	125.22	114.10
1	A	45	ARG	N-CA-CB	5.54	119.44	110.41
1	A	90	ALA	N-CA-CB	-5.53	101.71	110.28
1	A	27	ASN	CB-CA-C	5.50	119.92	110.79
1	A	80	CYS	CA-CB-SG	-5.47	101.82	114.40
1	A	112	ARG	CG-CD-NE	5.47	124.03	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ALA	O-C-N	5.47	130.48	122.39
1	A	111	TRP	CB-CG-CD2	-5.45	119.17	126.80
1	A	43	THR	CA-CB-CG2	5.42	119.72	110.50
1	A	65	ASN	CA-C-N	5.42	131.30	121.92
1	A	65	ASN	C-N-CA	5.42	131.30	121.92
1	A	80	CYS	N-CA-C	5.42	122.34	110.80
1	A	37	ASN	CB-CA-C	5.41	121.19	110.42
1	A	43	THR	CA-C-N	5.40	130.39	122.77
1	A	43	THR	C-N-CA	5.40	130.39	122.77
1	A	109	VAL	O-C-N	5.40	129.32	122.57
1	A	2	VAL	N-CA-CB	5.40	117.53	111.21
1	A	91	SER	O-C-N	5.39	127.91	122.09
1	A	125	ARG	CA-C-N	5.37	131.93	121.41
1	A	125	ARG	C-N-CA	5.37	131.93	121.41
1	A	99	ALA	CA-C-N	5.35	129.78	120.68
1	A	99	ALA	C-N-CA	5.35	129.78	120.68
1	A	121	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	A	96	LYS	N-CA-CB	-5.34	101.53	110.39
1	A	39	ASN	CB-CG-OD1	-5.33	110.13	120.80
1	A	5	ARG	CA-C-O	-5.32	115.22	120.70
1	A	59	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	111	TRP	CB-CG-CD1	5.31	134.86	126.90
1	A	63	TRP	CH2-CZ2-CE2	-5.28	110.63	117.50
1	A	56	LEU	CA-C-N	5.28	131.62	121.54
1	A	56	LEU	C-N-CA	5.28	131.62	121.54
1	A	98	ILE	CB-CG1-CD1	-5.27	102.73	113.80
1	A	76	CYS	O-C-N	-5.26	115.88	122.35
1	A	68	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	A	90	ALA	CB-CA-C	-5.24	100.61	110.67
1	A	60	SER	CB-CA-C	-5.18	99.17	109.99
1	A	76	CYS	N-CA-CB	-5.16	103.07	110.65
1	A	92	VAL	N-CA-CB	5.15	121.87	111.05
1	A	18	ASP	CA-C-N	-5.14	115.68	124.82
1	A	18	ASP	C-N-CA	-5.14	115.68	124.82
1	A	35	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	10	ALA	CB-CA-C	-5.12	102.30	110.79
1	A	109	VAL	N-CA-CB	-5.11	102.80	111.23
1	A	29	VAL	CA-CB-CG2	-5.09	101.75	110.40
1	A	66	ASP	CA-C-N	5.07	131.35	121.41
1	A	66	ASP	C-N-CA	5.07	131.35	121.41
1	A	84	LEU	O-C-N	-5.07	115.03	122.43
1	A	22	GLY	CA-C-N	5.06	129.99	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLY	C-N-CA	5.06	129.99	123.00
1	A	27	ASN	CA-C-N	5.06	127.32	120.44
1	A	27	ASN	C-N-CA	5.06	127.32	120.44
1	A	47	THR	CB-CA-C	-5.06	101.37	110.37
1	A	107	ALA	N-CA-C	-5.04	107.08	113.18
1	A	28	TRP	CA-C-N	5.03	126.99	120.70
1	A	28	TRP	C-N-CA	5.03	126.99	120.70
1	A	33	LYS	CD-CE-NZ	-5.01	95.86	111.90
1	A	116	LYS	CG-CD-CE	-5.00	99.79	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	994	0	954	103	2
2	A	111	0	0	19	5
All	All	1105	0	954	103	5

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 53.

All (103) 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:11:ALA:HB1	2:A:225:HOH:O	1.46	1.14
1:A:109:VAL:HG13	1:A:110:ALA:H	1.25	0.97
1:A:84:LEU:HB3	2:A:204:HOH:O	1.71	0.90
1:A:128:ARG:C	2:A:238:HOH:O	2.17	0.88
1:A:8:LEU:O	1:A:11:ALA:HB3	1.76	0.84
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.43	0.83
1:A:109:VAL:HA	1:A:112:ARG:HH21	1.46	0.80
1:A:109:VAL:HG23	1:A:112:ARG:NH2	2.00	0.77
1:A:8:LEU:HD22	1:A:55:ILE:HD11	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:CG1	1:A:110:ALA:H	1.94	0.75
1:A:11:ALA:O	1:A:15:LEU:HB2	1.89	0.71
1:A:109:VAL:HG13	1:A:110:ALA:N	2.03	0.70
1:A:88:ILE:HD11	2:A:225:HOH:O	1.94	0.68
1:A:30:CYS:HB2	1:A:123:TRP:CD1	2.28	0.68
1:A:42:ALA:HA	2:A:187:HOH:O	1.93	0.68
1:A:17:LEU:HD13	1:A:28:TRP:CG	2.30	0.67
1:A:109:VAL:HA	1:A:112:ARG:NH2	2.08	0.67
1:A:50:SER:OG	1:A:60:SER:HB3	1.95	0.66
1:A:59:ASN:OD1	1:A:61:ARG:HB3	1.96	0.66
1:A:81:SER:OG	2:A:203:HOH:O	2.13	0.65
1:A:109:VAL:HG23	1:A:112:ARG:HH22	1.61	0.65
1:A:88:ILE:CD1	2:A:225:HOH:O	2.45	0.65
1:A:124:ILE:HD11	2:A:133:HOH:O	1.94	0.65
1:A:111:TRP:CD1	1:A:115:CYS:HB2	2.34	0.62
1:A:109:VAL:O	1:A:112:ARG:HB3	2.00	0.62
1:A:111:TRP:O	1:A:112:ARG:C	2.41	0.62
1:A:115:CYS:O	1:A:118:THR:OG1	2.11	0.62
1:A:121:HIS:CD2	2:A:223:HOH:O	2.52	0.62
1:A:40:THR:O	1:A:54:GLY:HA2	2.00	0.61
1:A:103:ASN:HD22	1:A:103:ASN:N	1.98	0.61
1:A:8:LEU:CD2	1:A:55:ILE:HD11	2.32	0.60
1:A:72:SER:HB3	2:A:220:HOH:O	2.00	0.60
1:A:56:LEU:O	1:A:108:TRP:NE1	2.33	0.60
1:A:31:ALA:O	1:A:35:GLU:N	2.28	0.60
1:A:19:ASN:N	1:A:23:TYR:O	2.35	0.59
1:A:10:ALA:HA	1:A:129:LEU:CD2	2.32	0.59
1:A:14:ARG:HG2	1:A:14:ARG:NH1	2.11	0.58
1:A:3:TYR:CD1	1:A:8:LEU:HB2	2.38	0.58
1:A:121:HIS:NE2	1:A:125:ARG:HB2	2.19	0.58
1:A:8:LEU:HD22	1:A:55:ILE:CD1	2.35	0.57
1:A:10:ALA:HA	1:A:129:LEU:HD21	1.87	0.56
1:A:128:ARG:CA	2:A:238:HOH:O	2.51	0.56
1:A:12:MET:O	1:A:17:LEU:HB2	2.05	0.56
1:A:109:VAL:O	1:A:113:ASN:HB2	2.06	0.56
1:A:125:ARG:HG3	2:A:223:HOH:O	2.06	0.56
1:A:103:ASN:N	1:A:103:ASN:ND2	2.54	0.56
1:A:51:THR:O	1:A:60:SER:HB2	2.05	0.55
1:A:128:ARG:HA	2:A:238:HOH:O	2.05	0.55
1:A:25:LEU:O	1:A:29:VAL:HG23	2.07	0.55
1:A:127:CYS:HB3	1:A:129:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:HB2	2:A:189:HOH:O	2.08	0.52
1:A:63:TRP:O	1:A:76:CYS:HB2	2.10	0.52
1:A:9:ALA:CB	1:A:124:ILE:HG22	2.40	0.52
1:A:106:ASN:OD1	1:A:112:ARG:HG3	2.09	0.51
1:A:21:ARG:NH2	2:A:130:HOH:O	2.44	0.51
1:A:92:VAL:CG1	1:A:92:VAL:O	2.59	0.51
1:A:77:ASN:O	1:A:77:ASN:CG	2.54	0.50
1:A:3:TYR:HB3	1:A:4:GLY:O	2.12	0.50
1:A:125:ARG:O	1:A:125:ARG:HD2	2.11	0.50
1:A:8:LEU:CD1	1:A:88:ILE:HD13	2.42	0.49
1:A:109:VAL:CA	1:A:112:ARG:HH21	2.22	0.49
1:A:8:LEU:O	1:A:8:LEU:HD12	2.14	0.47
1:A:68:ARG:N	1:A:68:ARG:HD3	2.29	0.47
1:A:115:CYS:O	1:A:116:LYS:C	2.58	0.46
1:A:68:ARG:HD2	2:A:151:HOH:O	2.15	0.46
1:A:23:TYR:CE1	1:A:105:MET:HB2	2.50	0.46
1:A:50:SER:HG	1:A:60:SER:HB3	1.81	0.45
1:A:20:TYR:C	1:A:20:TYR:CD2	2.95	0.45
1:A:9:ALA:HB1	1:A:124:ILE:HG22	1.99	0.45
1:A:8:LEU:CD2	1:A:55:ILE:CD1	2.95	0.44
1:A:52:ASP:CG	2:A:147:HOH:O	2.60	0.44
1:A:92:VAL:O	1:A:96:LYS:HG3	2.17	0.44
1:A:29:VAL:CG1	1:A:123:TRP:HB3	2.46	0.44
1:A:61:ARG:O	1:A:61:ARG:CG	2.65	0.44
1:A:97:LYS:NZ	2:A:211:HOH:O	2.50	0.44
1:A:3:TYR:HB3	1:A:8:LEU:HB2	2.00	0.44
1:A:119:ASP:OD1	1:A:121:HIS:HB3	2.18	0.44
1:A:103:ASN:ND2	1:A:103:ASN:H	2.16	0.44
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.70	0.44
1:A:15:LEU:HD22	1:A:15:LEU:HA	1.83	0.43
1:A:52:ASP:HB3	1:A:57:GLN:HB3	2.00	0.43
1:A:4:GLY:O	1:A:8:LEU:HB3	2.19	0.43
1:A:88:ILE:O	1:A:89:THR:C	2.60	0.43
1:A:20:TYR:CE1	1:A:96:LYS:HD3	2.53	0.43
1:A:19:ASN:CA	1:A:23:TYR:O	2.67	0.43
1:A:29:VAL:HG23	1:A:29:VAL:H	1.58	0.43
1:A:108:TRP:O	1:A:112:ARG:HB2	2.19	0.42
1:A:122:ALA:HB1	1:A:125:ARG:HH21	1.85	0.42
1:A:15:LEU:HD21	1:A:89:THR:OG1	2.19	0.42
1:A:1:LYS:O	1:A:40:THR:HG23	2.19	0.42
1:A:93:ASN:ND2	2:A:209:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:CG2	1:A:112:ARG:NH2	2.77	0.42
1:A:121:HIS:CD2	1:A:121:HIS:C	2.96	0.42
1:A:7:GLU:O	1:A:11:ALA:HB2	2.19	0.42
1:A:80:CYS:O	1:A:83:LEU:HB2	2.19	0.42
1:A:3:TYR:CG	1:A:8:LEU:HB2	2.55	0.41
1:A:29:VAL:HG12	1:A:123:TRP:HB3	2.01	0.41
1:A:17:LEU:HD13	1:A:28:TRP:CD2	2.55	0.41
1:A:63:TRP:CD2	1:A:98:ILE:HG12	2.56	0.41
1:A:3:TYR:CB	1:A:8:LEU:HB2	2.50	0.41
1:A:73:LYS:HB2	1:A:74:ASN:H	1.64	0.41
1:A:108:TRP:O	1:A:111:TRP:HB3	2.20	0.41
1:A:3:TYR:HB2	1:A:38:PHE:HB3	2.03	0.40

All (5) 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:229:HOH:O	2:A:229:HOH:O[7_555]	1.15	1.05
2:A:232:HOH:O	2:A:235:HOH:O[3_564]	1.30	0.90
2:A:148:HOH:O	2:A:153:HOH:O[3_564]	1.70	0.50
1:A:77:ASN:CB	2:A:150:HOH:O[11_554]	1.86	0.34
1:A:48:ASP:O	2:A:195:HOH:O[3_564]	2.13	0.07

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%)	104 (82%)	18 (14%)	5 (4%)	2 1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	113	ASN
1	A	128	ARG
1	A	70	PRO
1	A	72	SER

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	103/103 (100%)	80 (78%)	23 (22%)	1 1

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	12	MET
1	A	14	ARG
1	A	15	LEU
1	A	44	ASN
1	A	47	THR
1	A	50	SER
1	A	55	ILE
1	A	62	TRP
1	A	68	ARG
1	A	72	SER
1	A	73	LYS
1	A	75	LEU
1	A	77	ASN
1	A	78	ILE
1	A	81	SER
1	A	97	LYS
1	A	103	ASN
1	A	112	ARG
1	A	114	ARG
1	A	115	CYS
1	A	116	LYS

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Mol	Chain	Res	Type
1	A	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	74	ASN
1	A	93	ASN
1	A	103	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%)	-0.78	0 100 100	16, 38, 74, 100	0

There are no RSRZ outliers to report.

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.