W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 11:50 AM EDT

PDB ID	:	1LZT
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)

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

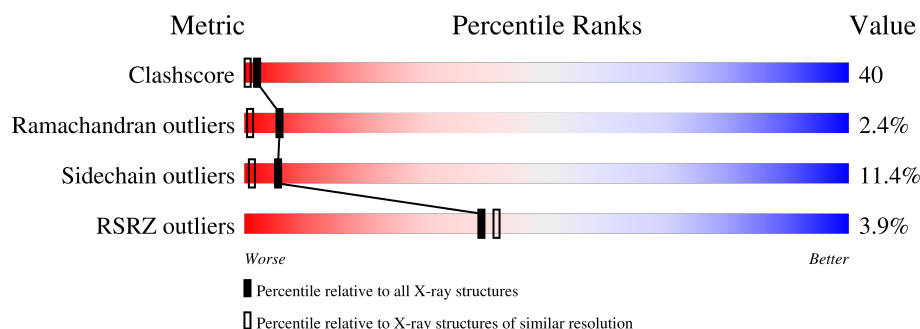|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	Percentile Ranks	Value
Clashscore		40
Ramachandran outliers		2.4%
Sidechain outliers		11.4%
RSRZ outliers		3.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures
◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	4% / 15% / 39% / 40% / 7%

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
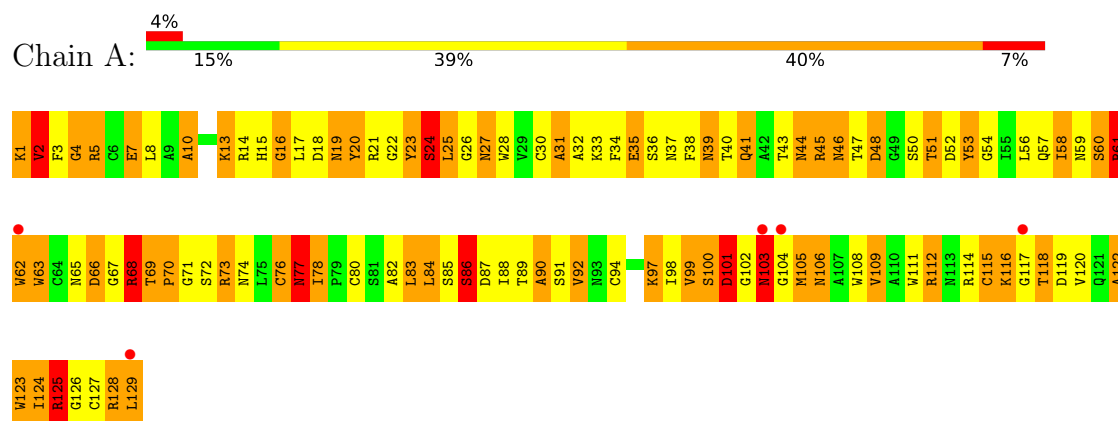
4 Data and refinement statistics (i)

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 32.32 – 1.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.97) 99.8 (32.32-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.25 , 32.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.63	8/1021 (0.8%)	6.68	349/1379 (25.3%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	GLU	CD-OE1	9.10	1.35	1.25
1	A	21	ARG	CZ-NH2	8.16	1.43	1.33
1	A	44	ASN	CA-C	-7.92	1.32	1.52
1	A	125	ARG	NE-CZ	-6.49	1.24	1.33
1	A	68	ARG	CZ-NH2	6.26	1.41	1.33
1	A	35	GLU	CD-OE1	5.69	1.31	1.25
1	A	117	GLY	N-CA	5.40	1.54	1.46
1	A	70	PRO	CA-C	5.04	1.62	1.52

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	A	21	ARG	NE-CZ-NH2	59.59	150.09	120.30
1	A	73	ARG	NE-CZ-NH2	-59.55	90.53	120.30
1	A	68	ARG	NE-CZ-NH2	50.47	145.54	120.30
1	A	21	ARG	NH1-CZ-NH2	-47.66	66.98	119.40
1	A	5	ARG	NE-CZ-NH1	46.20	143.40	120.30
1	A	21	ARG	NE-CZ-NH1	45.24	142.92	120.30
1	A	128	ARG	NE-CZ-NH1	-45.00	97.80	120.30
1	A	14	ARG	NE-CZ-NH1	41.70	141.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	ARG	NH1-CZ-NH2	36.55	159.60	119.40
1	A	125	ARG	NE-CZ-NH1	-35.19	102.71	120.30
1	A	5	ARG	NH1-CZ-NH2	-32.55	83.60	119.40
1	A	125	ARG	CD-NE-CZ	-31.62	79.33	123.60
1	A	61	ARG	NE-CZ-NH2	-27.22	106.69	120.30
1	A	73	ARG	NE-CZ-NH1	-26.13	107.23	120.30
1	A	87	ASP	CB-CG-OD2	25.99	141.69	118.30
1	A	5	ARG	NE-CZ-NH2	24.99	132.79	120.30
1	A	14	ARG	NH1-CZ-NH2	-24.30	92.67	119.40
1	A	34	PHE	CB-CG-CD2	-22.66	104.94	120.80
1	A	45	ARG	CA-CB-CG	-21.39	66.35	113.40
1	A	125	ARG	NH1-CZ-NH2	20.78	142.26	119.40
1	A	35	GLU	OE1-CD-OE2	-20.58	98.61	123.30
1	A	26	GLY	O-C-N	-20.29	90.24	122.70
1	A	45	ARG	CD-NE-CZ	-20.27	95.23	123.60
1	A	123	TRP	CG-CD2-CE3	20.16	152.04	133.90
1	A	87	ASP	OD1-CG-OD2	-19.45	86.34	123.30
1	A	103	ASN	C-N-CA	-19.18	82.02	122.30
1	A	66	ASP	CB-CG-OD1	18.91	135.32	118.30
1	A	123	TRP	NE1-CE2-CZ2	-18.84	109.68	130.40
1	A	23	TYR	CB-CG-CD2	18.13	131.88	121.00
1	A	103	ASN	CB-CA-C	-17.79	74.81	110.40
1	A	128	ARG	NE-CZ-NH2	17.40	129.00	120.30
1	A	61	ARG	CD-NE-CZ	17.26	147.76	123.60
1	A	44	ASN	OD1-CG-ND2	16.91	160.81	121.90
1	A	123	TRP	CE2-CD2-CG	-16.73	93.91	107.30
1	A	68	ARG	NH1-CZ-NH2	-16.52	101.23	119.40
1	A	1	LYS	O-C-N	-15.82	97.39	122.70
1	A	34	PHE	O-C-N	-15.67	97.62	122.70
1	A	45	ARG	NE-CZ-NH2	-15.55	112.53	120.30
1	A	87	ASP	CB-CG-OD1	15.16	131.94	118.30
1	A	68	ARG	NE-CZ-NH1	-14.49	113.05	120.30
1	A	47	THR	O-C-N	13.91	144.95	122.70
1	A	44	ASN	CB-CG-ND2	-13.81	83.56	116.70
1	A	90	ALA	O-C-N	-13.79	100.63	122.70
1	A	47	THR	CA-CB-CG2	-13.70	93.23	112.40
1	A	123	TRP	CD1-CG-CD2	13.50	117.10	106.30
1	A	53	TYR	CB-CG-CD2	-13.40	112.96	121.00
1	A	98	ILE	O-C-N	13.31	143.99	122.70
1	A	23	TYR	CB-CG-CD1	-12.96	113.23	121.00
1	A	86	SER	O-C-N	-12.90	102.06	122.70
1	A	52	ASP	CB-CG-OD2	-12.82	106.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	THR	N-CA-CB	-12.66	86.24	110.30
1	A	66	ASP	OD1-CG-OD2	-12.65	99.26	123.30
1	A	128	ARG	NH1-CZ-NH2	12.54	133.19	119.40
1	A	21	ARG	CB-CA-C	12.52	135.43	110.40
1	A	59	ASN	N-CA-CB	-12.12	88.78	110.60
1	A	61	ARG	CG-CD-NE	-12.08	86.44	111.80
1	A	28	TRP	CG-CD2-CE3	12.04	144.74	133.90
1	A	71	GLY	O-C-N	-12.02	103.47	122.70
1	A	99	VAL	O-C-N	-11.87	103.71	122.70
1	A	14	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	A	100	SER	N-CA-CB	-11.61	93.09	110.50
1	A	116	LYS	CA-C-N	11.47	139.14	116.20
1	A	46	ASN	N-CA-CB	-11.33	90.21	110.60
1	A	18	ASP	CB-CG-OD2	-11.32	108.11	118.30
1	A	102	GLY	CA-C-O	11.26	140.86	120.60
1	A	20	TYR	CB-CG-CD1	-11.24	114.25	121.00
1	A	62	TRP	CD1-CG-CD2	11.24	115.29	106.30
1	A	122	ALA	O-C-N	-11.18	104.81	122.70
1	A	34	PHE	CA-C-N	11.15	141.72	117.20
1	A	44	ASN	CA-CB-CG	-11.01	89.17	113.40
1	A	38	PHE	CB-CG-CD1	10.98	128.49	120.80
1	A	41	GLN	CG-CD-OE1	-10.82	99.95	121.60
1	A	59	ASN	OD1-CG-ND2	-10.76	97.16	121.90
1	A	26	GLY	CA-C-O	10.76	139.96	120.60
1	A	119	ASP	CB-CG-OD2	10.76	127.98	118.30
1	A	125	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	62	TRP	CB-CG-CD2	-10.61	112.80	126.60
1	A	97	LYS	O-C-N	-10.60	105.75	122.70
1	A	41	GLN	CB-CA-C	-10.51	89.38	110.40
1	A	44	ASN	O-C-N	10.49	139.49	122.70
1	A	45	ARG	CA-C-O	-10.46	98.13	120.10
1	A	103	ASN	N-CA-CB	10.31	129.16	110.60
1	A	108	TRP	CE3-CZ3-CH2	10.25	132.47	121.20
1	A	22	GLY	O-C-N	10.16	138.96	122.70
1	A	72	SER	CA-C-O	-10.15	98.79	120.10
1	A	127	CYS	O-C-N	10.11	138.88	122.70
1	A	62	TRP	CG-CD1-NE1	-10.06	100.04	110.10
1	A	32	ALA	O-C-N	-9.99	106.71	122.70
1	A	16	GLY	O-C-N	-9.96	106.76	122.70
1	A	65	ASN	CA-C-O	9.83	140.74	120.10
1	A	34	PHE	CG-CD1-CE1	-9.82	110.00	120.80
1	A	112	ARG	NE-CZ-NH2	9.81	125.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	TRP	CD2-CE2-CZ2	9.78	134.03	122.30
1	A	23	TYR	CA-C-N	-9.77	95.72	117.20
1	A	45	ARG	CA-C-N	9.71	138.56	117.20
1	A	15	HIS	C-N-CA	9.70	142.68	122.30
1	A	129	LEU	CB-CG-CD1	-9.69	94.53	111.00
1	A	118	THR	O-C-N	9.61	138.08	122.70
1	A	87	ASP	O-C-N	-9.59	107.36	122.70
1	A	120	VAL	CA-CB-CG1	-9.52	96.62	110.90
1	A	103	ASN	O-C-N	-9.45	107.14	123.20
1	A	65	ASN	O-C-N	-9.39	107.67	122.70
1	A	86	SER	CA-C-O	9.34	139.71	120.10
1	A	23	TYR	O-C-N	9.30	137.59	122.70
1	A	89	THR	O-C-N	9.29	137.56	122.70
1	A	114	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	20	TYR	CG-CD1-CE1	-9.15	113.98	121.30
1	A	20	TYR	N-CA-CB	-9.15	94.13	110.60
1	A	66	ASP	CA-C-N	-9.14	97.91	116.20
1	A	34	PHE	CD1-CG-CD2	9.13	130.17	118.30
1	A	28	TRP	NE1-CE2-CZ2	-9.04	120.46	130.40
1	A	123	TRP	NE1-CE2-CD2	8.99	116.29	107.30
1	A	117	GLY	O-C-N	8.95	137.02	122.70
1	A	53	TYR	CZ-CE2-CD2	-8.92	111.78	119.80
1	A	97	LYS	N-CA-CB	8.87	126.56	110.60
1	A	17	LEU	CB-CG-CD2	-8.86	95.93	111.00
1	A	43	THR	CA-C-O	-8.84	101.54	120.10
1	A	115	CYS	O-C-N	-8.84	108.56	122.70
1	A	116	LYS	CA-C-O	-8.80	101.61	120.10
1	A	101	ASP	CB-CG-OD1	8.80	126.22	118.30
1	A	53	TYR	CB-CG-CD1	8.79	126.28	121.00
1	A	41	GLN	N-CA-CB	8.78	126.40	110.60
1	A	103	ASN	CA-C-N	8.77	133.73	116.20
1	A	27	ASN	OD1-CG-ND2	-8.74	101.79	121.90
1	A	74	ASN	O-C-N	8.72	136.65	122.70
1	A	72	SER	CB-CA-C	-8.70	93.58	110.10
1	A	125	ARG	CB-CG-CD	8.64	134.07	111.60
1	A	86	SER	CB-CA-C	-8.63	93.70	110.10
1	A	73	ARG	CD-NE-CZ	8.60	135.65	123.60
1	A	74	ASN	CA-C-N	-8.49	98.53	117.20
1	A	91	SER	O-C-N	8.48	136.27	122.70
1	A	68	ARG	O-C-N	8.46	136.23	122.70
1	A	109	VAL	O-C-N	-8.44	109.19	122.70
1	A	99	VAL	CA-C-N	8.44	135.76	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	A	2	VAL	CB-CA-C	-8.39	95.46	111.40
1	A	7	GLU	OE1-CD-OE2	-8.38	113.25	123.30
1	A	52	ASP	O-C-N	-8.26	109.48	122.70
1	A	10	ALA	O-C-N	-8.22	109.54	122.70
1	A	58	ILE	CA-CB-CG1	-8.21	95.40	111.00
1	A	67	GLY	CA-C-O	8.18	135.31	120.60
1	A	118	THR	N-CA-CB	-8.14	94.83	110.30
1	A	19	ASN	CB-CG-ND2	-8.12	97.22	116.70
1	A	119	ASP	CA-CB-CG	-8.09	95.60	113.40
1	A	124	ILE	O-C-N	8.06	135.59	122.70
1	A	5	ARG	N-CA-CB	-8.04	96.12	110.60
1	A	70	PRO	O-C-N	-8.04	109.53	123.20
1	A	5	ARG	CA-CB-CG	7.99	130.97	113.40
1	A	122	ALA	CA-C-O	7.98	136.86	120.10
1	A	3	PHE	O-C-N	7.96	136.74	123.20
1	A	72	SER	CA-C-N	7.94	134.66	117.20
1	A	61	ARG	NH1-CZ-NH2	7.93	128.12	119.40
1	A	61	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	20	TYR	CD1-CE1-CZ	7.90	126.91	119.80
1	A	51	THR	O-C-N	7.87	135.29	122.70
1	A	66	ASP	CB-CG-OD2	7.83	125.34	118.30
1	A	65	ASN	CB-CG-ND2	7.79	135.39	116.70
1	A	53	TYR	CG-CD1-CE1	-7.71	115.13	121.30
1	A	48	ASP	CB-CA-C	-7.70	95.00	110.40
1	A	14	ARG	CB-CA-C	-7.70	95.01	110.40
1	A	24	SER	CB-CA-C	7.68	124.70	110.10
1	A	76	CYS	CA-C-N	7.68	134.10	117.20
1	A	123	TRP	CG-CD1-NE1	-7.66	102.44	110.10
1	A	60	SER	O-C-N	7.65	134.94	122.70
1	A	128	ARG	N-CA-CB	-7.63	96.87	110.60
1	A	118	THR	CA-C-N	-7.58	100.53	117.20
1	A	53	TYR	CE1-CZ-OH	-7.46	99.96	120.10
1	A	48	ASP	O-C-N	-7.46	110.52	123.20
1	A	31	ALA	N-CA-CB	7.44	120.52	110.10
1	A	7	GLU	CG-CD-OE1	7.37	133.03	118.30
1	A	52	ASP	OD1-CG-OD2	7.36	137.29	123.30
1	A	27	ASN	N-CA-CB	-7.32	97.42	110.60
1	A	60	SER	CA-C-O	-7.30	104.78	120.10
1	A	44	ASN	N-CA-CB	-7.29	97.48	110.60
1	A	92	VAL	N-CA-CB	-7.29	95.47	111.50
1	A	106	ASN	O-C-N	7.26	134.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ASN	O-C-N	7.26	134.31	122.70
1	A	27	ASN	CB-CG-ND2	7.25	134.10	116.70
1	A	99	VAL	CB-CA-C	7.19	125.05	111.40
1	A	116	LYS	CD-CE-NZ	-7.16	95.23	111.70
1	A	77	ASN	CA-CB-CG	-7.15	97.67	113.40
1	A	10	ALA	CB-CA-C	-7.15	99.38	110.10
1	A	102	GLY	CA-C-N	-7.15	101.47	117.20
1	A	44	ASN	CA-C-N	-7.14	101.50	117.20
1	A	7	GLU	CA-C-N	7.13	132.90	117.20
1	A	114	ARG	CB-CA-C	-7.13	96.13	110.40
1	A	5	ARG	CD-NE-CZ	-7.13	113.61	123.60
1	A	68	ARG	N-CA-CB	7.12	123.41	110.60
1	A	127	CYS	CB-CA-C	7.10	124.61	110.40
1	A	37	ASN	O-C-N	7.10	134.05	122.70
1	A	63	TRP	O-C-N	-7.09	111.36	122.70
1	A	120	VAL	O-C-N	-7.06	111.41	122.70
1	A	22	GLY	CA-C-N	-7.03	101.73	117.20
1	A	77	ASN	O-C-N	7.02	133.93	122.70
1	A	102	GLY	N-CA-C	-7.01	95.58	113.10
1	A	63	TRP	CA-CB-CG	-6.98	100.43	113.70
1	A	43	THR	O-C-N	6.97	133.85	122.70
1	A	90	ALA	CA-C-O	6.92	134.62	120.10
1	A	19	ASN	CB-CG-OD1	6.87	135.34	121.60
1	A	94	CYS	CB-CA-C	6.87	124.14	110.40
1	A	46	ASN	CA-C-O	-6.87	105.68	120.10
1	A	105	MET	CB-CA-C	6.87	124.13	110.40
1	A	30	CYS	O-C-N	6.84	133.64	122.70
1	A	28	TRP	CD2-CE2-CZ2	6.82	130.48	122.30
1	A	44	ASN	N-CA-C	-6.82	92.59	111.00
1	A	89	THR	CA-C-O	-6.82	105.79	120.10
1	A	44	ASN	CB-CA-C	-6.81	96.78	110.40
1	A	18	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	85	SER	O-C-N	6.77	133.54	122.70
1	A	25	LEU	CB-CG-CD2	6.76	122.50	111.00
1	A	76	CYS	CA-C-O	-6.73	105.97	120.10
1	A	123	TRP	CB-CG-CD1	-6.72	118.27	127.00
1	A	69	THR	C-N-CD	-6.71	105.83	120.60
1	A	108	TRP	CD2-CE3-CZ3	-6.71	110.08	118.80
1	A	48	ASP	N-CA-CB	6.70	122.66	110.60
1	A	57	GLN	OE1-CD-NE2	-6.69	106.52	121.90
1	A	48	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	24	SER	CA-C-O	6.68	134.12	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	VAL	CA-CB-CG1	6.64	120.86	110.90
1	A	60	SER	N-CA-CB	-6.64	100.55	110.50
1	A	102	GLY	C-N-CA	6.58	138.16	121.70
1	A	117	GLY	CA-C-O	-6.56	108.79	120.60
1	A	59	ASN	O-C-N	6.55	133.18	122.70
1	A	45	ARG	CB-CG-CD	-6.52	94.65	111.60
1	A	78	ILE	CA-CB-CG2	-6.51	97.88	110.90
1	A	100	SER	CA-C-O	6.51	133.77	120.10
1	A	8	LEU	CA-C-O	-6.50	106.44	120.10
1	A	17	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	66	ASP	CB-CA-C	-6.49	97.43	110.40
1	A	27	ASN	CB-CA-C	-6.48	97.44	110.40
1	A	38	PHE	CB-CG-CD2	-6.46	116.28	120.80
1	A	18	ASP	O-C-N	-6.45	112.38	122.70
1	A	35	GLU	CG-CD-OE1	6.44	131.19	118.30
1	A	91	SER	CA-C-O	-6.44	106.58	120.10
1	A	1	LYS	CA-C-O	6.42	133.58	120.10
1	A	35	GLU	CA-C-N	6.39	131.25	117.20
1	A	83	LEU	CB-CA-C	-6.38	98.07	110.20
1	A	38	PHE	O-C-N	6.36	132.88	122.70
1	A	97	LYS	CA-C-O	6.36	133.45	120.10
1	A	57	GLN	CB-CA-C	-6.26	97.88	110.40
1	A	70	PRO	C-N-CA	6.25	135.42	122.30
1	A	22	GLY	N-CA-C	6.25	128.71	113.10
1	A	86	SER	N-CA-CB	6.23	119.84	110.50
1	A	120	VAL	CA-C-N	6.22	130.89	117.20
1	A	2	VAL	CA-CB-CG2	6.21	120.22	110.90
1	A	47	THR	CA-C-N	-6.21	103.53	117.20
1	A	85	SER	CA-C-N	-6.21	103.54	117.20
1	A	23	TYR	N-CA-CB	-6.19	99.46	110.60
1	A	65	ASN	CA-CB-CG	-6.17	99.83	113.40
1	A	119	ASP	OD1-CG-OD2	-6.17	111.59	123.30
1	A	28	TRP	CE2-CD2-CG	-6.14	102.39	107.30
1	A	27	ASN	CA-C-N	-6.14	103.69	117.20
1	A	3	PHE	CB-CG-CD1	6.14	125.10	120.80
1	A	28	TRP	CD1-CG-CD2	6.11	111.19	106.30
1	A	57	GLN	CA-CB-CG	-6.11	99.96	113.40
1	A	86	SER	C-N-CA	6.10	136.96	121.70
1	A	105	MET	C-N-CA	6.09	136.93	121.70
1	A	119	ASP	C-N-CA	-6.07	106.51	121.70
1	A	21	ARG	CD-NE-CZ	-6.03	115.16	123.60
1	A	123	TRP	CE3-CZ3-CH2	6.02	127.82	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	ARG	CB-CG-CD	5.99	127.18	111.60
1	A	62	TRP	CA-CB-CG	-5.98	102.33	113.70
1	A	1	LYS	CA-CB-CG	-5.97	100.26	113.40
1	A	41	GLN	CG-CD-NE2	5.97	131.02	116.70
1	A	127	CYS	N-CA-CB	-5.96	99.87	110.60
1	A	35	GLU	CG-CD-OE2	5.95	130.20	118.30
1	A	27	ASN	O-C-N	5.94	132.20	122.70
1	A	67	GLY	O-C-N	-5.93	113.21	122.70
1	A	116	LYS	C-N-CA	-5.93	109.84	122.30
1	A	101	ASP	N-CA-CB	5.93	121.27	110.60
1	A	47	THR	C-N-CA	-5.89	106.98	121.70
1	A	35	GLU	CB-CG-CD	-5.84	98.44	114.20
1	A	34	PHE	CB-CG-CD1	5.82	124.88	120.80
1	A	91	SER	C-N-CA	-5.79	107.21	121.70
1	A	103	ASN	OD1-CG-ND2	5.79	135.21	121.90
1	A	125	ARG	CA-C-N	-5.78	104.64	116.20
1	A	108	TRP	CD1-NE1-CE2	5.78	114.20	109.00
1	A	68	ARG	CG-CD-NE	5.76	123.90	111.80
1	A	129	LEU	CB-CG-CD2	-5.76	101.21	111.00
1	A	94	CYS	CA-C-O	-5.75	108.03	120.10
1	A	92	VAL	CA-C-N	5.74	129.82	117.20
1	A	101	ASP	OD1-CG-OD2	-5.71	112.44	123.30
1	A	62	TRP	CD1-NE1-CE2	5.71	114.14	109.00
1	A	98	ILE	CA-C-O	-5.71	108.11	120.10
1	A	26	GLY	CA-C-N	5.71	129.76	117.20
1	A	82	ALA	CB-CA-C	5.66	118.59	110.10
1	A	13	LYS	O-C-N	5.65	131.75	122.70
1	A	14	ARG	CG-CD-NE	-5.65	99.93	111.80
1	A	20	TYR	OH-CZ-CE2	5.62	135.27	120.10
1	A	59	ASN	CB-CA-C	5.60	121.61	110.40
1	A	59	ASN	CB-CG-OD1	5.60	132.80	121.60
1	A	109	VAL	CA-C-N	5.59	129.50	117.20
1	A	45	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	A	60	SER	C-N-CA	-5.58	107.74	121.70
1	A	80	CYS	N-CA-C	5.57	126.03	111.00
1	A	77	ASN	CA-C-N	-5.56	104.96	117.20
1	A	73	ARG	CG-CD-NE	-5.56	100.13	111.80
1	A	43	THR	CA-CB-CG2	5.53	120.14	112.40
1	A	127	CYS	C-N-CA	5.52	135.51	121.70
1	A	66	ASP	N-CA-C	5.52	125.90	111.00
1	A	105	MET	N-CA-C	-5.52	96.10	111.00
1	A	40	THR	CA-C-N	-5.50	105.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	TYR	OH-CZ-CE2	5.50	134.96	120.10
1	A	40	THR	CA-CB-CG2	-5.49	104.72	112.40
1	A	56	LEU	CA-C-O	5.49	131.62	120.10
1	A	59	ASN	CB-CG-ND2	5.49	129.87	116.70
1	A	114	ARG	CA-CB-CG	-5.47	101.35	113.40
1	A	62	TRP	C-N-CA	-5.47	108.03	121.70
1	A	70	PRO	CB-CA-C	5.47	125.67	112.00
1	A	83	LEU	N-CA-C	5.47	125.76	111.00
1	A	92	VAL	CA-CB-CG1	-5.47	102.70	110.90
1	A	100	SER	O-C-N	-5.46	113.97	122.70
1	A	84	LEU	O-C-N	5.42	131.37	122.70
1	A	52	ASP	N-CA-C	-5.40	96.43	111.00
1	A	20	TYR	CE1-CZ-OH	-5.38	105.56	120.10
1	A	36	SER	O-C-N	5.38	131.31	122.70
1	A	60	SER	CB-CA-C	5.37	120.30	110.10
1	A	123	TRP	CA-CB-CG	-5.37	103.51	113.70
1	A	58	ILE	O-C-N	5.36	131.28	122.70
1	A	1	LYS	CA-C-N	5.33	128.93	117.20
1	A	52	ASP	CB-CA-C	5.32	121.03	110.40
1	A	97	LYS	CA-CB-CG	-5.32	101.70	113.40
1	A	87	ASP	CA-C-N	5.30	128.87	117.20
1	A	48	ASP	N-CA-C	5.26	125.21	111.00
1	A	87	ASP	CA-CB-CG	-5.26	101.83	113.40
1	A	68	ARG	CB-CA-C	-5.25	99.89	110.40
1	A	71	GLY	N-CA-C	-5.25	99.97	113.10
1	A	50	SER	N-CA-C	5.23	125.13	111.00
1	A	56	LEU	O-C-N	-5.22	114.35	122.70
1	A	43	THR	CA-CB-OG1	-5.20	98.08	109.00
1	A	126	GLY	CA-C-O	-5.20	111.24	120.60
1	A	68	ARG	CA-CB-CG	5.18	124.79	113.40
1	A	2	VAL	O-C-N	5.17	130.98	122.70
1	A	77	ASN	OD1-CG-ND2	-5.16	110.03	121.90
1	A	124	ILE	CA-C-O	-5.16	109.26	120.10
1	A	77	ASN	CB-CG-ND2	5.16	129.07	116.70
1	A	34	PHE	N-CA-C	-5.15	97.10	111.00
1	A	122	ALA	N-CA-CB	5.13	117.28	110.10
1	A	4	GLY	C-N-CA	-5.12	108.90	121.70
1	A	125	ARG	O-C-N	5.11	131.88	123.20
1	A	101	ASP	C-N-CA	-5.09	111.61	122.30
1	A	97	LYS	CD-CE-NZ	5.09	123.40	111.70
1	A	108	TRP	CD2-CE2-CZ2	5.09	128.40	122.30
1	A	65	ASN	OD1-CG-ND2	-5.08	110.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	19	ASN	CA-CB-CG	-5.05	102.28	113.40
1	A	38	PHE	CG-CD1-CE1	5.05	126.36	120.80
1	A	66	ASP	O-C-N	5.03	131.75	123.20
1	A	63	TRP	CA-C-O	5.02	130.63	120.10

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	79	2
2	A	220	0	0	15	0
All	All	1221	0	959	79	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 40.

All (79) 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:62:TRP:HB2	1:A:63:TRP:CD1	2.13	0.82
1:A:100:SER:O	1:A:101:ASP:CG	2.21	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:103:ASN:C	1:A:104:GLY:O	2.31	0.64
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:105:MET:HE2	1:A:111:TRP:CD1	2.38	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:45:ARG:NE	1:A:51:THR:CG2	2.70	0.54
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:100:SER:O	1:A:101:ASP:CB	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:C	1:A:106:ASN:H	2.15	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: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:61:ARG:HB3	1:A:62:TRP:NE1	2.30	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: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: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:115:CYS:O	1:A:116:LYS:C	2.55	0.45
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
1:A:46:ASN:C	1:A:48:ASP:N	2.72	0.43
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:104:GLY:C	1:A:106:ASN:N	2.70	0.42
1:A:105:MET:HE2	1:A:105:MET:HB3	1.85	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: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%)	6	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 (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%)	93 (89%)	12 (11%)	5	1

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
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

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Mol	Chain	Res	Type
1	A	86	SER
1	A	97	LYS
1	A	103	ASN
1	A	125	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

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	5 (3%)	39	42	5, 10, 15, 16	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	4.2
1	A	129	LEU	3.5
1	A	104	GLY	3.5
1	A	62	TRP	3.3
1	A	117	GLY	2.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.

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