



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:46 PM GMT

PDB ID : 2LZ2  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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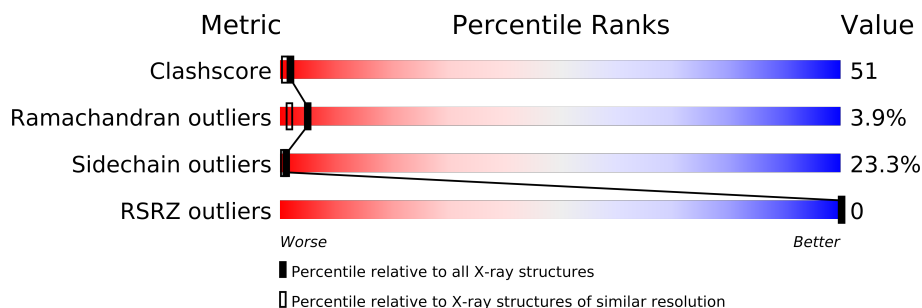
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.00Å 71.00Å 84.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.01 – 2.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 89.6 (10.01-2.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.21Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.192 , (Not available) 0.192 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 144.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 5887 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	1.51	3/1015 (0.3%)	3.99	232/1371 (16.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	SER	CB-OG	7.99	1.52	1.42
1	A	81	SER	CB-OG	6.19	1.50	1.42
1	A	100	SER	CB-OG	5.73	1.49	1.42

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH1	26.70	133.65	120.30
1	A	112	ARG	CD-NE-CZ	24.08	157.31	123.60
1	A	66	ASP	CB-CG-OD2	22.60	138.64	118.30
1	A	45	ARG	NE-CZ-NH2	-19.69	110.46	120.30
1	A	128	ARG	NE-CZ-NH1	17.07	128.83	120.30
1	A	11	ALA	N-CA-CB	-15.27	88.72	110.10
1	A	3	TYR	CB-CG-CD2	15.01	130.01	121.00
1	A	28	TRP	CB-CG-CD2	14.56	145.53	126.60
1	A	113	ASN	CA-CB-CG	14.36	144.99	113.40
1	A	117	GLY	C-N-CA	14.24	157.30	121.70
1	A	125	ARG	NE-CZ-NH1	-13.67	113.47	120.30
1	A	114	ARG	NH1-CZ-NH2	-12.96	105.14	119.40
1	A	28	TRP	CB-CG-CD1	-12.11	111.25	127.00
1	A	41	HIS	CA-CB-CG	12.06	134.10	113.60
1	A	108	TRP	C-N-CA	11.95	151.58	121.70
1	A	114	ARG	CD-NE-CZ	11.63	139.88	123.60
1	A	23	TYR	CB-CG-CD2	-11.21	114.27	121.00
1	A	77	ASN	CA-C-O	11.16	143.53	120.10
1	A	38	PHE	CB-CG-CD1	11.13	128.59	120.80
1	A	3	TYR	CA-C-O	10.82	142.83	120.10
1	A	128	ARG	NH1-CZ-NH2	-10.82	107.50	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	C-N-CA	10.76	148.59	121.70
1	A	60	SER	N-CA-CB	-10.70	94.44	110.50
1	A	6	CYS	N-CA-CB	10.51	129.52	110.60
1	A	42	ALA	N-CA-CB	10.41	124.67	110.10
1	A	20	TYR	CB-CG-CD1	-10.40	114.76	121.00
1	A	23	TYR	CB-CG-CD1	10.39	127.23	121.00
1	A	3	TYR	CB-CG-CD1	-10.30	114.82	121.00
1	A	40	THR	CA-CB-CG2	10.13	126.58	112.40
1	A	66	ASP	OD1-CG-OD2	-10.04	104.22	123.30
1	A	81	SER	CB-CA-C	9.99	129.09	110.10
1	A	83	LEU	CA-C-N	-9.91	95.41	117.20
1	A	85	SER	C-N-CA	9.89	146.41	121.70
1	A	6	CYS	O-C-N	9.88	138.51	122.70
1	A	39	ASN	CA-C-O	-9.84	99.43	120.10
1	A	77	ASN	N-CA-CB	9.75	128.15	110.60
1	A	52	ASP	CB-CG-OD2	-9.54	109.71	118.30
1	A	119	ASP	CA-CB-CG	9.41	134.11	113.40
1	A	125	ARG	NH1-CZ-NH2	9.26	129.59	119.40
1	A	128	ARG	CG-CD-NE	9.24	131.20	111.80
1	A	120	VAL	CG1-CB-CG2	-9.16	96.24	110.90
1	A	76	CYS	C-N-CA	9.10	144.46	121.70
1	A	45	ARG	NH1-CZ-NH2	9.06	129.36	119.40
1	A	58	ILE	C-N-CA	9.06	144.34	121.70
1	A	128	ARG	CA-CB-CG	9.03	133.27	113.40
1	A	76	CYS	CA-C-N	8.81	136.58	117.20
1	A	50	SER	CB-CA-C	8.80	126.83	110.10
1	A	42	ALA	CB-CA-C	-8.79	96.91	110.10
1	A	107	ALA	CB-CA-C	8.70	123.15	110.10
1	A	52	ASP	CB-CG-OD1	8.64	126.08	118.30
1	A	65	ASN	N-CA-CB	8.64	126.14	110.60
1	A	68	ARG	O-C-N	-8.62	108.90	122.70
1	A	15	LEU	CD1-CG-CD2	-8.61	84.69	110.50
1	A	50	SER	CA-CB-OG	-8.54	88.13	111.20
1	A	14	ARG	CB-CA-C	8.43	127.25	110.40
1	A	112	ARG	O-C-N	-8.42	109.22	122.70
1	A	14	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	115	CYS	CA-C-N	8.32	135.50	117.20
1	A	114	ARG	C-N-CA	8.28	142.40	121.70
1	A	53	TYR	O-C-N	8.26	137.24	123.20
1	A	128	ARG	C-N-CA	8.24	142.29	121.70
1	A	61	ARG	NH1-CZ-NH2	-8.23	110.34	119.40
1	A	46	ASN	N-CA-CB	-8.22	95.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ASN	O-C-N	8.17	135.77	122.70
1	A	61	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	61	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	84	LEU	C-N-CA	8.05	141.82	121.70
1	A	20	TYR	CB-CG-CD2	8.01	125.80	121.00
1	A	112	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	A	3	TYR	CA-C-N	-7.95	100.30	116.20
1	A	14	ARG	CA-CB-CG	7.94	130.86	113.40
1	A	78	ILE	CB-CA-C	7.92	127.44	111.60
1	A	48	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	18	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	117	GLY	N-CA-C	7.79	132.59	113.10
1	A	43	THR	N-CA-CB	7.79	125.10	110.30
1	A	9	ALA	N-CA-CB	7.78	120.99	110.10
1	A	84	LEU	N-CA-CB	-7.64	95.12	110.40
1	A	21	ARG	C-N-CA	7.64	138.34	122.30
1	A	119	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	81	SER	O-C-N	-7.62	110.52	122.70
1	A	73	LYS	N-CA-C	7.59	131.49	111.00
1	A	4	GLY	N-CA-C	-7.58	94.16	113.10
1	A	124	ILE	CA-CB-CG2	7.41	125.71	110.90
1	A	112	ARG	CA-CB-CG	7.32	129.51	113.40
1	A	16	GLY	CA-C-N	7.31	133.28	117.20
1	A	117	GLY	O-C-N	-7.30	111.02	122.70
1	A	38	PHE	CB-CG-CD2	-7.28	115.70	120.80
1	A	83	LEU	CB-CG-CD1	7.27	123.36	111.00
1	A	68	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	53	TYR	CB-CA-C	-7.25	95.91	110.40
1	A	34	PHE	CA-C-O	-7.21	104.97	120.10
1	A	56	LEU	CB-CG-CD2	-7.18	98.80	111.00
1	A	121	HIS	CA-CB-CG	-7.15	101.44	113.60
1	A	61	ARG	CD-NE-CZ	7.13	133.59	123.60
1	A	93	ASN	N-CA-CB	7.10	123.38	110.60
1	A	8	LEU	CB-CA-C	7.08	123.66	110.20
1	A	125	ARG	O-C-N	-7.08	111.17	123.20
1	A	116	LYS	N-CA-CB	-7.06	97.90	110.60
1	A	86	SER	CA-C-N	-7.01	101.77	117.20
1	A	35	GLU	N-CA-CB	6.98	123.17	110.60
1	A	114	ARG	N-CA-C	6.96	129.78	111.00
1	A	17	LEU	N-CA-C	6.92	129.69	111.00
1	A	113	ASN	CB-CG-OD1	6.91	135.41	121.60
1	A	75	LEU	O-C-N	6.91	133.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LYS	CD-CE-NZ	-6.89	95.86	111.70
1	A	52	ASP	N-CA-CB	-6.87	98.24	110.60
1	A	11	ALA	CB-CA-C	6.81	120.32	110.10
1	A	77	ASN	CA-C-N	-6.80	102.25	117.20
1	A	61	ARG	CA-CB-CG	6.79	128.33	113.40
1	A	112	ARG	CB-CA-C	6.78	123.96	110.40
1	A	14	ARG	CB-CG-CD	6.77	129.21	111.60
1	A	34	PHE	CB-CA-C	6.77	123.94	110.40
1	A	63	TRP	CH2-CZ2-CE2	-6.77	110.63	117.40
1	A	80	CYS	CA-CB-SG	-6.77	101.82	114.00
1	A	125	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	121	HIS	CA-C-O	6.68	134.13	120.10
1	A	27	ASN	N-CA-CB	-6.65	98.64	110.60
1	A	75	LEU	N-CA-CB	6.64	123.68	110.40
1	A	56	LEU	CA-C-O	6.59	133.94	120.10
1	A	28	TRP	CB-CA-C	6.55	123.50	110.40
1	A	91	SER	C-N-CA	6.54	138.04	121.70
1	A	95	ALA	N-CA-CB	6.53	119.24	110.10
1	A	113	ASN	CB-CA-C	6.53	123.46	110.40
1	A	38	PHE	C-N-CA	6.51	137.98	121.70
1	A	125	ARG	CB-CA-C	6.50	123.39	110.40
1	A	111	TRP	CA-CB-CG	-6.49	101.37	113.70
1	A	68	ARG	N-CA-CB	-6.49	98.93	110.60
1	A	81	SER	N-CA-CB	-6.48	100.78	110.50
1	A	84	LEU	N-CA-C	6.48	128.50	111.00
1	A	78	ILE	N-CA-CB	-6.47	95.92	110.80
1	A	25	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	52	ASP	CA-C-O	-6.43	106.60	120.10
1	A	58	ILE	O-C-N	-6.43	112.42	122.70
1	A	101	GLY	C-N-CA	6.43	135.80	122.30
1	A	2	VAL	CB-CA-C	6.38	123.51	111.40
1	A	8	LEU	CA-C-N	6.36	131.20	117.20
1	A	85	SER	N-CA-CB	-6.33	101.00	110.50
1	A	90	ALA	CB-CA-C	-6.32	100.61	110.10
1	A	15	LEU	CB-CA-C	6.25	122.08	110.20
1	A	35	GLU	CA-C-N	6.22	130.88	117.20
1	A	76	CYS	CA-CB-SG	6.19	125.14	114.00
1	A	83	LEU	CA-C-O	6.16	133.03	120.10
1	A	125	ARG	N-CA-CB	-6.13	99.56	110.60
1	A	17	LEU	CB-CG-CD1	-6.10	100.63	111.00
1	A	29	VAL	CA-CB-CG2	-6.10	101.75	110.90
1	A	111	TRP	CB-CG-CD1	6.04	134.86	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	SER	C-N-CA	6.02	136.76	121.70
1	A	118	THR	C-N-CA	6.00	136.69	121.70
1	A	90	ALA	N-CA-CB	-5.99	101.71	110.10
1	A	76	CYS	CA-C-O	-5.98	107.54	120.10
1	A	28	TRP	CA-C-O	5.97	132.64	120.10
1	A	56	LEU	CA-C-N	-5.97	104.06	117.20
1	A	77	ASN	C-N-CA	-5.96	106.80	121.70
1	A	17	LEU	N-CA-CB	-5.94	98.53	110.40
1	A	53	TYR	CA-C-O	-5.92	107.67	120.10
1	A	4	GLY	CA-C-N	-5.91	104.19	117.20
1	A	115	CYS	CA-C-O	-5.91	107.68	120.10
1	A	15	LEU	C-N-CA	5.91	134.70	122.30
1	A	112	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
1	A	49	GLY	CA-C-O	5.90	131.21	120.60
1	A	75	LEU	CA-C-O	-5.89	107.74	120.10
1	A	45	ARG	CD-NE-CZ	-5.87	115.39	123.60
1	A	128	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	108	TRP	CH2-CZ2-CE2	-5.83	111.57	117.40
1	A	55	ILE	CA-C-O	-5.83	107.85	120.10
1	A	112	ARG	CG-CD-NE	5.82	124.03	111.80
1	A	86	SER	CB-CA-C	-5.81	99.07	110.10
1	A	61	ARG	CA-C-O	-5.80	107.91	120.10
1	A	1	LYS	CA-C-O	-5.78	107.96	120.10
1	A	10	ALA	CA-C-O	5.78	132.23	120.10
1	A	36	SER	CA-CB-OG	-5.75	95.67	111.20
1	A	60	SER	CB-CA-C	-5.75	99.17	110.10
1	A	2	VAL	C-N-CA	5.74	136.04	121.70
1	A	43	THR	OG1-CB-CG2	5.74	123.19	110.00
1	A	39	ASN	CB-CG-OD1	-5.73	110.13	121.60
1	A	70	PRO	N-CA-CB	5.73	110.18	103.30
1	A	80	CYS	CB-CA-C	-5.72	98.95	110.40
1	A	111	TRP	CB-CG-CD2	-5.71	119.17	126.60
1	A	97	LYS	CA-CB-CG	5.68	125.90	113.40
1	A	127	CYS	CA-C-N	-5.67	104.73	117.20
1	A	116	LYS	C-N-CA	5.66	134.19	122.30
1	A	111	TRP	CD1-NE1-CE2	-5.65	103.92	109.00
1	A	3	TYR	CB-CA-C	-5.64	99.11	110.40
1	A	39	ASN	CA-C-N	5.64	129.61	117.20
1	A	78	ILE	O-C-N	5.64	131.81	121.10
1	A	39	ASN	C-N-CA	5.64	135.79	121.70
1	A	65	ASN	CA-CB-CG	-5.64	101.00	113.40
1	A	104	GLY	CA-C-O	-5.62	110.48	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	TRP	N-CA-C	-5.62	95.82	111.00
1	A	97	LYS	CD-CE-NZ	5.61	124.61	111.70
1	A	103	ASN	OD1-CG-ND2	5.58	134.73	121.90
1	A	35	GLU	CB-CA-C	-5.57	99.25	110.40
1	A	72	SER	N-CA-CB	5.57	118.86	110.50
1	A	25	LEU	O-C-N	-5.54	113.78	123.20
1	A	85	SER	CA-C-O	5.53	131.71	120.10
1	A	16	GLY	O-C-N	-5.50	113.90	122.70
1	A	83	LEU	O-C-N	5.49	131.48	122.70
1	A	7	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	A	59	ASN	N-CA-CB	5.47	120.45	110.60
1	A	77	ASN	CB-CA-C	-5.46	99.48	110.40
1	A	54	GLY	C-N-CA	5.42	135.24	121.70
1	A	1	LYS	CA-CB-CG	5.40	125.29	113.40
1	A	119	ASP	N-CA-CB	5.40	120.33	110.60
1	A	37	ASN	CB-CA-C	5.40	121.19	110.40
1	A	116	LYS	CA-CB-CG	5.37	125.22	113.40
1	A	25	LEU	CA-C-N	5.36	126.92	116.20
1	A	89	THR	OG1-CB-CG2	-5.36	97.68	110.00
1	A	24	SER	CA-C-O	-5.31	108.95	120.10
1	A	77	ASN	O-C-N	-5.31	114.21	122.70
1	A	99	ALA	CA-C-O	-5.29	108.98	120.10
1	A	10	ALA	C-N-CA	5.29	134.93	121.70
1	A	42	ALA	N-CA-C	-5.29	96.72	111.00
1	A	34	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	A	33	LYS	CA-C-O	5.24	131.10	120.10
1	A	43	THR	CA-CB-CG2	5.23	119.72	112.40
1	A	10	ALA	CB-CA-C	-5.20	102.30	110.10
1	A	39	ASN	O-C-N	5.16	130.96	122.70
1	A	13	LYS	N-CA-CB	5.16	119.89	110.60
1	A	30	CYS	CB-CA-C	5.15	120.70	110.40
1	A	91	SER	CB-CA-C	5.13	119.86	110.10
1	A	12	MET	O-C-N	-5.10	114.54	122.70
1	A	23	TYR	CZ-CE2-CD2	-5.09	115.22	119.80
1	A	92	VAL	CA-C-O	-5.08	109.43	120.10
1	A	77	ASN	CA-CB-CG	5.06	124.54	113.40
1	A	96	LYS	N-CA-CB	-5.04	101.53	110.60
1	A	128	ARG	CB-CG-CD	5.03	124.69	111.60
1	A	24	SER	O-C-N	5.02	130.73	122.70
1	A	38	PHE	CA-C-N	5.01	128.23	117.20
1	A	63	TRP	CB-CG-CD2	5.01	133.11	126.60
1	A	79	PRO	N-CA-C	-5.01	99.08	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	SER	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	994	0	948	99	2
2	A	111	0	0	17	5
All	All	1105	0	948	99	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 51.

All (99) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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: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:128:ARG:C	2:A:238:HOH:O	2.17	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
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:42:ALA:HA	2:A:187:HOH:O	1.93	0.68
1:A:30:CYS:HB2	1:A:123:TRP:CD1	2.28	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:115:CYS:O	1:A:118:THR:OG1	2.11	0.63
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: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:111:TRP:O	1:A:112:ARG:C	2.41	0.57
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:128:ARG:HA	2:A:238:HOH:O	2.05	0.55
1:A:51:THR:O	1:A:60:SER:HB2	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
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:3:TYR:HB3	1:A:4:GLY:O	2.12	0.50
1:A:125:ARG:HD2	1:A:125:ARG:O	2.11	0.50
1:A:8:LEU:CD1	1:A:88:ILE:HD13	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:VAL:CA	1:A:112:ARG:HH21	2.22	0.49
1:A:109:VAL:CG1	1:A:110:ALA:N	2.68	0.48
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: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:77:ASN:CG	1:A:77:ASN:O	2.54	0.46
1:A:50:SER:HG	1:A:60:SER:HB3	1.81	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: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: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:HA	1:A:83:LEU:HD23	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: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:H	1:A:29:VAL:HG23	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:109:VAL:CG2	1:A:112:ARG:NH2	2.77	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
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:115:CYS:O	1:A:116:LYS:C	2.58	0.41
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:108:TRP:O	1:A:111:TRP:HB3	2.20	0.41
1:A:73:LYS:HB2	1:A:74:ASN:H	1.64	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	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

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%)	<b>5</b> <b>2</b>

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 ⓘ

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%)	79 (77%)	24 (23%)	<b>1</b> <b>1</b>

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU

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Mol	Chain	Res	Type
1	A	12	MET
1	A	14	ARG
1	A	15	LEU
1	A	21	ARG
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	116	LYS
1	A	125	ARG
1	A	128	ARG

Some 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	46	ASN
1	A	93	ASN
1	A	103	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	129/129 (100%)	-0.91	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 ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.