



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:43 PM GMT

PDB ID : 1LSP  
Title : THE CRYSTAL STRUCTURE OF A BULGECIN-INHIBITED G-TYPE  
LYSOZYME FROM THE EGG-WHITE OF THE AUSTRALIAN BLACK  
SWAN. A COMPARISON OF THE BINDING OF BULGECIN TO THREE  
MURAMIDASES  
Authors : Karlsen, S.; Rao, Z.H.; Hough, E.; Isaacs, N.W.  
Deposited on : 1995-02-09  
Resolution : 2.45 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

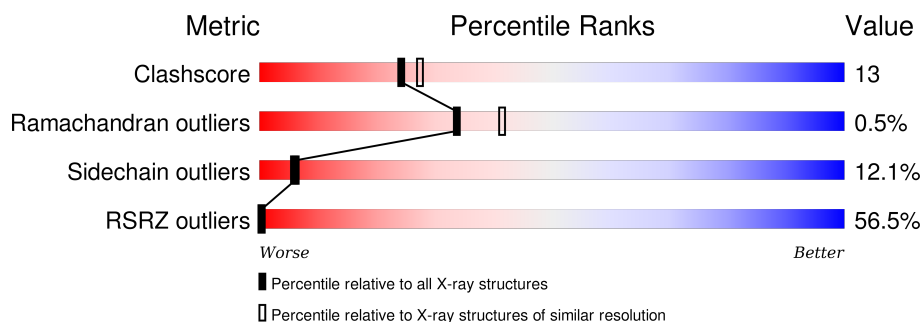
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. 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	185	<div> <div>40%</div> <div>56%</div> <div>33%</div> <div>8%</div> <div>.</div> </div>

## 2 Entry composition (i)

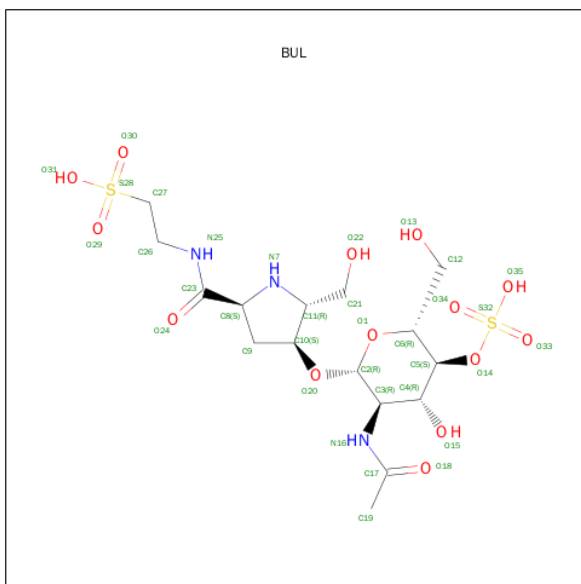
There are 3 unique types of molecules in this entry. The entry contains 1578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 **LYSOZYME**.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1434	892	265	270	7			

- Molecule 2 is BULGECIN A (three-letter code: BUL) (formula:  $\text{C}_{16}\text{H}_{29}\text{N}_3\text{O}_{14}\text{S}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	16	3	14	2		

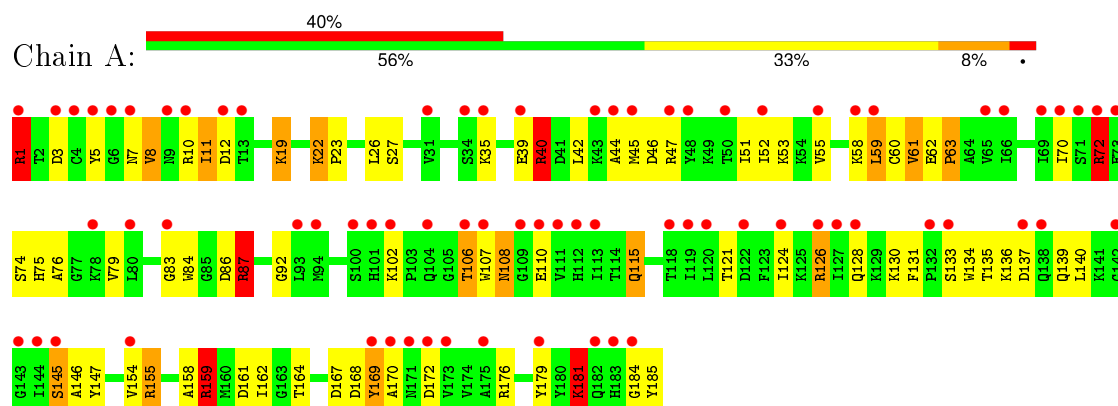
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: LYSOZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.69Å 65.33Å 38.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.45 32.94 – 2.46	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.45) 78.9 (32.94-2.46)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.45Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.175 , (Not available) 0.353 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 88.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 6959 reflections (0.029%)	Xtriage
$F_o, F_c$ correlation	0.66	EDS
Total number of atoms	1578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BUL

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	0.90	0/1461	2.23	56/1965 (2.8%)

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	6

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	-21.15	109.72	120.30
1	A	40	ARG	NE-CZ-NH2	-21.06	109.77	120.30
1	A	176	ARG	NE-CZ-NH2	18.34	129.47	120.30
1	A	155	ARG	NE-CZ-NH2	-12.54	114.03	120.30
1	A	72	ARG	NE-CZ-NH2	-12.41	114.09	120.30
1	A	168	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	159	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	A	167	ASP	CB-CG-OD1	8.09	125.58	118.30
1	A	161	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	A	40	ARG	NH1-CZ-NH2	7.99	128.19	119.40
1	A	72	ARG	NH1-CZ-NH2	7.82	128.00	119.40
1	A	3	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	A	11	ILE	CA-C-O	7.74	136.35	120.10
1	A	42	LEU	CB-CG-CD2	-7.64	98.00	111.00
1	A	181	LYS	CB-CA-C	-7.48	95.44	110.40
1	A	155	ARG	CD-NE-CZ	-7.41	113.22	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	TYR	CB-CG-CD2	-7.40	116.56	121.00
1	A	181	LYS	N-CA-CB	7.39	123.90	110.60
1	A	79	VAL	N-CA-CB	-7.34	95.36	111.50
1	A	87	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	42	LEU	CB-CG-CD1	7.29	123.39	111.00
1	A	126	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	12	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	86	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	A	137	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	172	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	A	146	ALA	CB-CA-C	6.32	119.58	110.10
1	A	161	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	76	ALA	CB-CA-C	6.09	119.23	110.10
1	A	145	SER	O-C-N	-6.07	112.99	122.70
1	A	136	LYS	CB-CA-C	6.04	122.48	110.40
1	A	158	ALA	CB-CA-C	-6.03	101.06	110.10
1	A	168	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	147	TYR	CB-CG-CD1	5.98	124.59	121.00
1	A	11	ILE	O-C-N	-5.86	113.32	122.70
1	A	115	GLN	CA-C-N	5.84	127.89	116.20
1	A	106	THR	N-CA-CB	-5.75	99.38	110.30
1	A	134	TRP	CA-CB-CG	5.63	124.41	113.70
1	A	79	VAL	CB-CA-C	5.60	122.04	111.40
1	A	44	ALA	N-CA-CB	-5.44	102.48	110.10
1	A	110	GLU	CG-CD-OE1	-5.42	107.45	118.30
1	A	135	THR	CA-CB-OG1	-5.42	97.61	109.00
1	A	184	GLY	N-CA-C	5.39	126.58	113.10
1	A	55	VAL	CA-CB-CG2	5.38	118.96	110.90
1	A	169	TYR	CB-CG-CD1	5.37	124.22	121.00
1	A	10	ARG	CD-NE-CZ	-5.31	116.16	123.60
1	A	155	ARG	NH1-CZ-NH2	5.24	125.16	119.40
1	A	39	GLU	OE1-CD-OE2	5.18	129.52	123.30
1	A	46	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	84	TRP	CA-CB-CG	-5.15	103.91	113.70
1	A	46	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	53	LYS	CA-CB-CG	-5.14	102.10	113.40
1	A	59	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	72	ARG	CA-CB-CG	5.06	124.54	113.40
1	A	61	VAL	CB-CA-C	5.03	120.95	111.40
1	A	86	ASP	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ARG	Sidechain
1	A	126	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	87	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	1434	0	1426	37	0
2	A	35	0	26	2	0
3	A	109	0	0	6	0
All	All	1578	0	1452	37	0

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 13.

All (37) 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:7:ASN:HB2	3:A:203:HOH:O	1.27	1.24
1:A:19:LYS:HB3	3:A:218:HOH:O	1.77	0.84
1:A:87:ARG:HB2	2:A:295:BUL:O29	1.93	0.68
1:A:159:ARG:HB3	1:A:162:ILE:HD12	1.76	0.65
1:A:130:LYS:HG2	1:A:131:PHE:CE2	2.33	0.64
1:A:130:LYS:HG2	1:A:131:PHE:CD2	2.32	0.64
1:A:35:LYS:HG2	1:A:179:TYR:HB2	1.80	0.63
1:A:5:TYR:O	1:A:140:LEU:HB2	1.98	0.63
1:A:145:SER:HB2	1:A:170:ALA:HB2	1.80	0.62
1:A:22:LYS:N	1:A:22:LYS:HD2	2.14	0.62
1:A:62:GLU:HG3	3:A:229:HOH:O	2.00	0.61
1:A:22:LYS:HE2	1:A:26:LEU:O	2.02	0.59
1:A:74:SER:O	1:A:75:HIS:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:NE	3:A:209:HOH:O	2.35	0.58
1:A:145:SER:HB2	1:A:170:ALA:CB	2.36	0.54
1:A:19:LYS:HD2	1:A:19:LYS:N	2.22	0.53
1:A:63:PRO:HB2	1:A:185:TYR:O	2.07	0.53
1:A:164:THR:HB	1:A:169:TYR:HB2	1.93	0.51
1:A:155:ARG:HB2	3:A:198:HOH:O	2.11	0.49
1:A:52:ILE:HD11	1:A:70:ILE:HD12	1.94	0.49
1:A:130:LYS:HE2	1:A:154:VAL:O	2.13	0.48
1:A:22:LYS:H	1:A:22:LYS:HD2	1.80	0.47
1:A:19:LYS:HD3	3:A:265:HOH:O	2.14	0.47
1:A:128:GLN:HG2	1:A:139:GLN:OE1	2.16	0.46
1:A:124:ILE:O	1:A:128:GLN:HG3	2.16	0.46
1:A:8:VAL:HG12	1:A:181:LYS:HD3	1.97	0.45
1:A:61:VAL:O	1:A:63:PRO:HD3	2.18	0.44
1:A:108:ASN:H	1:A:108:ASN:HD22	1.65	0.44
1:A:1:ARG:O	1:A:60:CYS:HA	2.18	0.43
1:A:1:ARG:HG2	1:A:1:ARG:HH11	1.84	0.43
1:A:52:ILE:CD1	1:A:70:ILE:HD12	2.49	0.42
1:A:45:MET:HB2	1:A:45:MET:HE2	1.90	0.42
1:A:87:ARG:NH1	2:A:295:BUL:O29	2.53	0.41
1:A:11:ILE:HD11	1:A:140:LEU:HD23	2.01	0.41
1:A:83:GLY:HA3	1:A:107:TRP:HB2	2.02	0.41
1:A:92:GLY:HA2	1:A:107:TRP:O	2.21	0.41
1:A:145:SER:CB	1:A:170:ALA:HB2	2.49	0.40

There are no symmetry-related clashes.

## 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	183/185 (99%)	174 (95%)	8 (4%)	1 (0%)	34 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO

### 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	149/149 (100%)	131 (88%)	18 (12%)	<b>6</b> <b>6</b>

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	8	VAL
1	A	19	LYS
1	A	22	LYS
1	A	23	PRO
1	A	27	SER
1	A	47	ARG
1	A	51	ILE
1	A	58	LYS
1	A	59	LEU
1	A	72	ARG
1	A	102	LYS
1	A	106	THR
1	A	108	ASN
1	A	115	GLN
1	A	121	THR
1	A	133	SER
1	A	181	LYS

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

Mol	Chain	Res	Type
1	A	108	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	BUL	A	295	-	35,36,36	1.44	7 (20%)	40,53,53	3.41	21 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BUL	A	295	-	-	0/28/60/60	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	BUL	O1-C6	-3.07	1.36	1.44
2	A	295	BUL	C2-C3	-2.54	1.48	1.53
2	A	295	BUL	O20-C2	-2.44	1.35	1.41
2	A	295	BUL	O20-C10	-2.41	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	BUL	C11-N7	2.58	1.52	1.48
2	A	295	BUL	C10-C11	3.08	1.59	1.54
2	A	295	BUL	C8-N7	3.51	1.55	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	BUL	O15-C4-C3	-8.91	91.49	109.66
2	A	295	BUL	C5-O14-S32	-6.62	106.15	118.77
2	A	295	BUL	C23-C8-N7	-5.32	101.75	111.73
2	A	295	BUL	O20-C2-O1	-4.04	100.45	110.68
2	A	295	BUL	O15-C4-C5	-3.78	100.92	109.87
2	A	295	BUL	O34-S32-O33	-3.64	96.61	112.46
2	A	295	BUL	O30-S28-C27	-3.46	103.96	106.91
2	A	295	BUL	O29-S28-C27	-3.28	104.10	106.91
2	A	295	BUL	O14-C5-C4	-2.88	102.02	108.43
2	A	295	BUL	O22-C21-C11	-2.60	104.17	111.12
2	A	295	BUL	C26-C27-S28	-2.44	107.15	113.73
2	A	295	BUL	O30-S28-O29	-2.28	105.17	113.48
2	A	295	BUL	O1-C2-C3	2.25	115.68	110.78
2	A	295	BUL	C12-C6-C5	2.55	120.66	113.25
2	A	295	BUL	C2-O1-C6	3.61	120.75	113.75
2	A	295	BUL	O31-S28-O29	3.71	120.24	111.61
2	A	295	BUL	C4-C3-N16	4.51	120.01	110.66
2	A	295	BUL	O35-S32-O33	4.68	126.16	108.56
2	A	295	BUL	C2-O20-C10	5.50	122.98	115.27
2	A	295	BUL	O1-C6-C5	6.47	123.41	109.75
2	A	295	BUL	C9-C8-C23	6.90	121.70	111.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	295	BUL	2	0

## 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	131/185 (70%)	3.15	74 (56%) 0 0	4, 11, 25, 39	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	GLN	71.2
1	A	127	ILE	16.7
1	A	100	SER	16.5
1	A	73	GLU	9.9
1	A	154	VAL	8.7
1	A	80	LEU	6.9
1	A	138	GLN	6.9
1	A	182	GLN	6.3
1	A	44	ALA	6.2
1	A	52	ILE	5.4
1	A	59	LEU	5.2
1	A	43	LYS	4.8
1	A	132	PRO	4.8
1	A	7	ASN	4.7
1	A	169	TYR	4.6
1	A	172	ASP	4.5
1	A	55	VAL	4.4
1	A	83	GLY	4.1
1	A	184	GLY	4.0
1	A	175	ALA	4.0
1	A	143	GLY	4.0
1	A	170	ALA	3.9
1	A	107	TRP	3.9
1	A	78	LYS	3.7
1	A	145	SER	3.7
1	A	118	THR	3.6
1	A	110	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	3.5
1	A	112	HIS	3.5
1	A	6	GLY	3.4
1	A	119	ILE	3.3
1	A	31	VAL	3.3
1	A	34	SER	3.2
1	A	144	ILE	3.1
1	A	12	ASP	3.1
1	A	101	HIS	3.1
1	A	50	THR	3.1
1	A	1	ARG	3.1
1	A	102	LYS	3.1
1	A	13	THR	3.1
1	A	47	ARG	3.0
1	A	137	ASP	3.0
1	A	133	SER	3.0
1	A	45	MET	2.9
1	A	70	ILE	2.9
1	A	111	VAL	2.9
1	A	69	ILE	2.9
1	A	10	ARG	2.8
1	A	58	LYS	2.8
1	A	124	ILE	2.7
1	A	93	LEU	2.7
1	A	126	ARG	2.6
1	A	94	MET	2.6
1	A	173	VAL	2.5
1	A	5	TYR	2.5
1	A	65	VAL	2.4
1	A	109	GLY	2.4
1	A	171	ASN	2.4
1	A	71	SER	2.4
1	A	35	LYS	2.4
1	A	106	THR	2.3
1	A	122	ASP	2.3
1	A	72	ARG	2.3
1	A	9	ASN	2.2
1	A	4	CYS	2.2
1	A	66	ILE	2.1
1	A	39	GLU	2.1
1	A	3	ASP	2.1
1	A	104	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	113	ILE	2.1
1	A	120	LEU	2.0
1	A	183	HIS	2.0
1	A	179	TYR	2.0
1	A	48	TYR	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	BUL	A	295	35/35	0.85	0.33	-0.35	1,16,37,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.