



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:57 PM GMT

PDB ID : 1LMC
Title : THE CRYSTAL STRUCTURE OF A COMPLEX BETWEEN BULGECIN,
A BACTERIAL METABOLITE, AND LYSOZYME FROM THE RAINBOW
TROUT
Authors : Karlsen, S.; Hough, E.
Deposited on : 1994-11-14
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

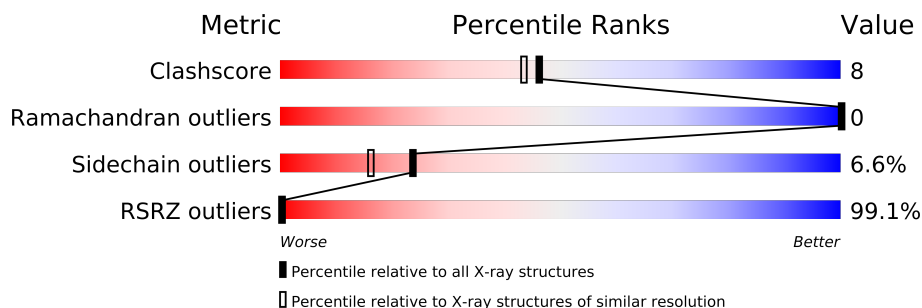
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 ≥ 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 i

There are 3 unique types of molecules in this entry. The entry contains 1144 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.

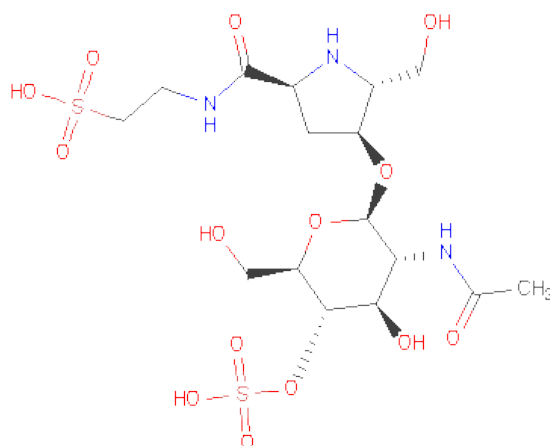
- Molecule 1 is a protein called LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	999	616	185	189	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ASP	ALA	CONFLICT	UNP P11941

- Molecule 2 is BULGECIN A (three-letter code: BUL) (formula: $C_{16}H_{29}N_3O_{14}S_2$).



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

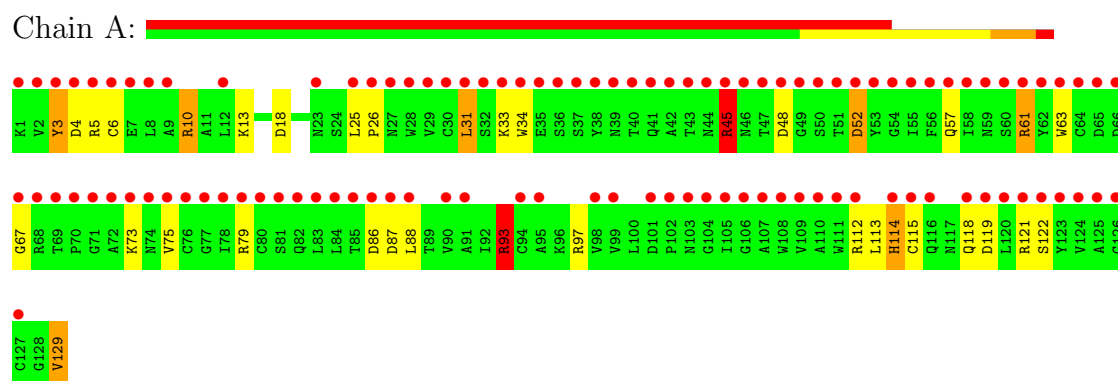
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	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 ($RSRZ > 2$). 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 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.57Å 76.57Å 54.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00 14.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 86.1 (14.69-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.00Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.163 , (Not available) 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.77 , 224.0	EDS
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 10895 reflections	Xtriage
F_o, F_c correlation	0.45	EDS
Total number of atoms	1144	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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	0.85	0/1019	1.95	28/1383 (2.0%)

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	3

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	NE-CZ-NH1	15.67	128.14	120.30
1	A	61	ARG	NE-CZ-NH2	-13.12	113.74	120.30
1	A	79	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	A	61	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	112	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	97	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	A	112	ARG	CD-NE-CZ	7.95	134.73	123.60
1	A	18	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	31	LEU	CA-CB-CG	7.45	132.43	115.30
1	A	52	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	52	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	48	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	4	ASP	CB-CG-OD1	-7.08	111.93	118.30
1	A	48	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	87	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	A	13	LYS	CB-CG-CD	6.75	129.14	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	A	93	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	A	4	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	34	TRP	CA-CB-CG	-5.65	102.96	113.70
1	A	129	VAL	CA-C-O	-5.50	108.55	120.10
1	A	13	LYS	CA-CB-CG	5.42	125.33	113.40
1	A	86	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	112	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	A	119	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	114	HIS	CA-CB-CG	-5.11	104.91	113.60
1	A	3	TYR	CB-CG-CD1	5.09	124.05	121.00
1	A	115	CYS	O-C-N	5.04	130.77	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	93	ARG	Sidechain

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	999	0	956	16	1
2	A	35	0	25	0	0
3	A	110	0	0	4	2
All	All	1144	0	981	16	3

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 8.

All (16) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:ARG:HH11	1:A:45:ARG:HB2	1.54	0.73
1:A:67:GLY:HA2	3:A:164:HOH:O	1.92	0.68
1:A:3:TYR:CE1	1:A:88:LEU:HD11	2.38	0.58
1:A:3:TYR:OH	1:A:88:LEU:HD13	2.06	0.56
1:A:25:LEU:HB3	1:A:26:PRO:HD3	1.87	0.56
1:A:3:TYR:CZ	1:A:88:LEU:HD11	2.41	0.55
1:A:3:TYR:OH	1:A:88:LEU:CD1	2.56	0.54
1:A:52:ASP:HB3	1:A:57:GLN:HB3	1.93	0.50
1:A:3:TYR:CZ	1:A:88:LEU:CD1	2.96	0.49
1:A:93:ARG:HD2	3:A:184:HOH:O	2.12	0.49
1:A:10:ARG:HG2	1:A:129:VAL:HG11	1.95	0.48
1:A:10:ARG:NH1	3:A:160:HOH:O	2.12	0.46
1:A:63:TRP:CZ3	1:A:75:VAL:HG11	2.53	0.44
1:A:114:HIS:HD2	3:A:212:HOH:O	2.01	0.43
1:A:6:CYS:O	1:A:10:ARG:HG3	2.18	0.43
1:A:114:HIS:O	1:A:118:GLN:HG3	2.19	0.42

All (3) 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)
3:A:169:HOH:O	3:A:169:HOH:O[4_556]	0.95	1.25
3:A:143:HOH:O	3:A:143:HOH:O[4_556]	1.25	0.95
1:A:113:LEU:CD1	1:A:113:LEU:CD1[5_675]	2.11	0.09

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%)	127 (100%)	0	0	100 100

There are no Ramachandran outliers to report.

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	106/106 (100%)	99 (93%)	7 (7%)	24 16

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	33	LYS
1	A	45	ARG
1	A	61	ARG
1	A	73	LYS
1	A	121	ARG
1	A	122	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	130	-	36,36,36	1.89	8 (22%)	53,53,53	3.17	24 (45%)

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	130	-	1/1/12/15	0/28/60/60	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	130	BUL	O14-S32	-5.34	1.51	1.60
2	A	130	BUL	C11-N7	4.76	1.55	1.48
2	A	130	BUL	C27-S28	4.35	1.84	1.77
2	A	130	BUL	C8-N7	3.18	1.55	1.46
2	A	130	BUL	O20-C10	-3.14	1.39	1.44
2	A	130	BUL	O1-C6	-2.59	1.37	1.44
2	A	130	BUL	C5-C6	-2.47	1.46	1.52
2	A	130	BUL	C26-N25	2.16	1.51	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	130	BUL	O15-C4-C3	-8.76	91.63	109.61
2	A	130	BUL	O29-S28-C27	-8.13	99.84	106.81
2	A	130	BUL	O24-C23-C8	-6.58	105.85	120.31
2	A	130	BUL	O35-S32-O34	-5.78	86.77	108.82
2	A	130	BUL	O1-C6-C5	5.64	121.48	109.70
2	A	130	BUL	O30-S28-O29	5.21	131.84	113.26
2	A	130	BUL	O14-C5-C6	5.08	119.39	108.59
2	A	130	BUL	O34-S32-O33	4.80	132.54	112.89
2	A	130	BUL	O30-S28-C27	-4.72	102.76	106.81
2	A	130	BUL	O14-C5-C4	-4.59	97.02	107.51
2	A	130	BUL	C8-C23-N25	-3.90	109.11	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	130	BUL	C10-C9-C8	-3.86	95.72	103.33
2	A	130	BUL	O1-C6-C12	3.84	115.77	106.34
2	A	130	BUL	O31-S28-O30	-3.62	103.95	111.78
2	A	130	BUL	C9-C10-C11	3.48	108.84	103.59
2	A	130	BUL	O20-C2-O1	-3.37	102.28	110.69
2	A	130	BUL	O15-C4-C5	-3.22	102.33	109.85
2	A	130	BUL	C9-C8-C23	-2.79	106.96	111.20
2	A	130	BUL	C12-C6-C5	2.78	121.08	113.25
2	A	130	BUL	C4-C3-N16	2.52	115.89	110.56
2	A	130	BUL	O24-C23-N25	2.46	128.04	123.05
2	A	130	BUL	C21-C11-N7	-2.42	106.70	111.69
2	A	130	BUL	O31-S28-C27	-2.33	102.97	105.93
2	A	130	BUL	O20-C10-C9	2.03	120.11	111.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	130	BUL	C6

There are no torsion outliers.

There are no ring outliers.

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	107/129 (82%)	11.59	106 (99%) 0 0	15, 21, 47, 67	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	CYS	38.4
1	A	110	ALA	25.0
1	A	127	CYS	23.7
1	A	47	THR	23.2
1	A	25	LEU	21.9
1	A	36	SER	20.9
1	A	27	ASN	20.2
1	A	109	VAL	19.5
1	A	6	CYS	19.3
1	A	29	VAL	19.2
1	A	124	VAL	18.9
1	A	90	VAL	18.9
1	A	115	CYS	18.2
1	A	3	TYR	18.0
1	A	120	LEU	17.8
1	A	123	TYR	17.7
1	A	87	ASP	17.4
1	A	34	TRP	17.4
1	A	38	TYR	17.2
1	A	42	ALA	17.0
1	A	46	ASN	16.9
1	A	112	ARG	16.9
1	A	30	CYS	16.5
1	A	77	GLY	16.3
1	A	91	ALA	16.1
1	A	88	LEU	16.0
1	A	37	SER	15.8

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Mol	Chain	Res	Type	RSRZ
1	A	1	LYS	15.4
1	A	12	LEU	15.4
1	A	85	THR	15.0
1	A	111	TRP	14.9
1	A	26	PRO	14.6
1	A	28	TRP	14.5
1	A	7	GLU	14.1
1	A	107	ALA	13.9
1	A	121	ARG	13.7
1	A	5	ARG	13.6
1	A	122	SER	13.5
1	A	86	ASP	13.3
1	A	83	LEU	13.1
1	A	8	LEU	13.1
1	A	114	HIS	12.9
1	A	43	THR	12.9
1	A	40	THR	12.6
1	A	99	VAL	12.4
1	A	126	GLY	12.3
1	A	4	ASP	12.3
1	A	119	ASP	12.2
1	A	44	ASN	12.2
1	A	125	ALA	12.0
1	A	33	LYS	12.0
1	A	55	ILE	12.0
1	A	2	VAL	11.8
1	A	102	PRO	11.3
1	A	118	GLN	10.6
1	A	32	SER	10.1
1	A	71	GLY	10.0
1	A	57	GLN	9.9
1	A	63	TRP	9.6
1	A	48	ASP	9.5
1	A	54	GLY	9.4
1	A	41	GLN	9.2
1	A	105	ILE	8.9
1	A	35	GLU	8.8
1	A	39	ASN	8.8
1	A	84	LEU	8.7
1	A	62	TYR	8.6
1	A	67	GLY	8.4
1	A	45	ARG	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	94	CYS	8.2
1	A	9	ALA	8.2
1	A	60	SER	8.2
1	A	64	CYS	7.9
1	A	70	PRO	7.9
1	A	49	GLY	7.8
1	A	81	SER	7.6
1	A	95	ALA	7.6
1	A	68	ARG	7.4
1	A	51	THR	7.3
1	A	108	TRP	7.2
1	A	69	THR	7.1
1	A	31	LEU	6.7
1	A	56	PHE	6.7
1	A	80	CYS	6.7
1	A	72	ALA	6.5
1	A	79	ARG	6.5
1	A	58	ILE	6.4
1	A	66	ASP	6.2
1	A	98	VAL	6.1
1	A	78	ILE	6.0
1	A	65	ASP	5.7
1	A	50	SER	5.7
1	A	61	ARG	5.7
1	A	53	TYR	5.3
1	A	74	ASN	5.2
1	A	101	ASP	4.9
1	A	82	GLN	4.8
1	A	23	ASN	4.7
1	A	75	VAL	4.4
1	A	52	ASP	4.4
1	A	103	ASN	4.2
1	A	104	GLY	4.1
1	A	59	ASN	3.9
1	A	73	LYS	3.1
1	A	106	GLY	2.8
1	A	116	GLN	2.8

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

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BUL	A	130	35/35	-	-	22,28,37,37	35

6.5 Other polymers

There are no such residues in this entry.