



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 05:35 AM EDT

PDB ID : 2LIS
Title : HIGH RESOLUTION STRUCTURE OF THE RED ABALONE LYSIN MONOMER
Authors : Kresge, N.; Vacquier, V.D.; Stout, C.D.
Deposited on : unknown
Resolution : 1.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

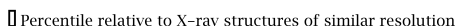
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

i

X-RAY DIFFRACTION

A.



Similar resolution
(#Entries, resolution range(Å))

Quality of chain

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1398 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 SPERM LYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	2	0
			1114	729	198	180	7			

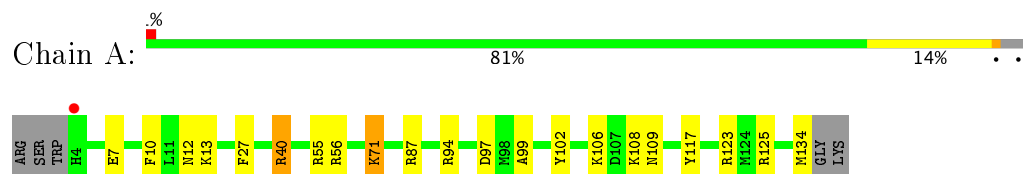
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	284	Total	O	0	0
			284	284		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: SPERM LYSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.41Å 45.31Å 81.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 1.35 20.09 – 1.35	Depositor EDS
% Data completeness (in resolution range)	97.4 (100.00-1.35) 97.4 (20.09-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	4.50	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.07 (at 1.35Å)	Xtriage
Refinement program	SHELXL	Depositor
R, R_{free}	0.137 , 0.179 0.145 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1398	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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

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	0.66	0/1154	1.36	22/1554 (1.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CD-NE-CZ	9.78	137.29	123.60
1	A	123	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	A	123	ARG	CD-NE-CZ	9.05	136.26	123.60
1	A	56	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	40	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	87	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	94	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	A	125	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	40	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	A	10	PHE	CB-CG-CD1	5.99	124.99	120.80
1	A	94	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	10	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	A	27	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	A	40	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	117	TYR	CB-CG-CD2	5.34	124.20	121.00
1	A	71	LYS	CB-CG-CD	5.31	125.40	111.60
1	A	12	ASN	CA-CB-CG	5.24	124.92	113.40
1	A	55[A]	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	55[B]	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	87	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	97	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	56	ARG	CG-CD-NE	5.08	122.46	111.80

There are no chirality outliers.

There are no planarity outliers.

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	1114	0	1144	6	0
2	A	284	0	0	5	0
All	All	1398	0	1144	6	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 3.

All (6) 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:109:ASN:HB3	2:A:2268:HOH:O	2.05	0.56
1:A:7:GLU:HG3	2:A:2146:HOH:O	2.07	0.55
1:A:99:ALA:HA	1:A:102:TYR:CD2	2.50	0.46
1:A:40:ARG:HB2	2:A:2161:HOH:O	2.16	0.46
1:A:40:ARG:NH1	2:A:2271:HOH:O	2.50	0.44
1:A:106:LYS:HE2	2:A:2253:HOH:O	2.20	0.42

There are no symmetry-related clashes.

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	131/136 (96%)	131 (100%)	0	0	100 100

There are no Ramachandran outliers to report.

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	117/119 (98%)	113 (97%)	4 (3%)	42 9

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	71	LYS
1	A	108	LYS
1	A	134	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	61	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [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	131/136 (96%)	-0.19	1 (0%) 86 88	8, 13, 27, 38	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	HIS	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.