



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2R76
Title : Crystal structure of the rare lipoprotein B (SO_1173) from Shewanella oneidensis, Northeast Structural Genomics Consortium Target SoR91A
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Deposited on : 2007-09-07
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

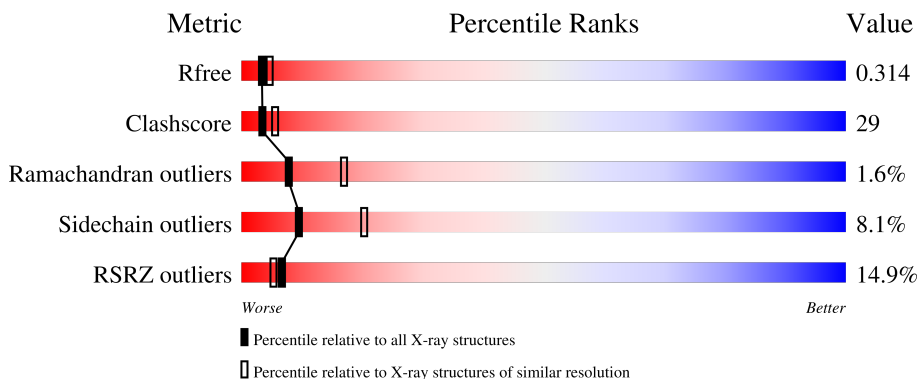
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.60 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))
R_{free}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 $\leq 5\%$. 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	152	
1	B	152	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2141 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 Rare lipoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	Se	0	0	0
			1065	669	186	207	3			
1	B	129	Total	C	N	O	Se	0	0	0
			1038	652	181	202	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	-	expression tag	UNP Q8EHP5
A	47	LYS	SER	SEE REMARK 999	UNP Q8EHP5
A	165	LEU	-	expression tag	UNP Q8EHP5
A	166	GLU	-	expression tag	UNP Q8EHP5
A	167	HIS	-	expression tag	UNP Q8EHP5
A	168	HIS	-	expression tag	UNP Q8EHP5
A	169	HIS	-	expression tag	UNP Q8EHP5
A	170	HIS	-	expression tag	UNP Q8EHP5
A	171	HIS	-	expression tag	UNP Q8EHP5
A	172	HIS	-	expression tag	UNP Q8EHP5
B	21	MSE	-	expression tag	UNP Q8EHP5
B	47	LYS	SER	SEE REMARK 999	UNP Q8EHP5
B	165	LEU	-	expression tag	UNP Q8EHP5
B	166	GLU	-	expression tag	UNP Q8EHP5
B	167	HIS	-	expression tag	UNP Q8EHP5
B	168	HIS	-	expression tag	UNP Q8EHP5
B	169	HIS	-	expression tag	UNP Q8EHP5
B	170	HIS	-	expression tag	UNP Q8EHP5
B	171	HIS	-	expression tag	UNP Q8EHP5
B	172	HIS	-	expression tag	UNP Q8EHP5

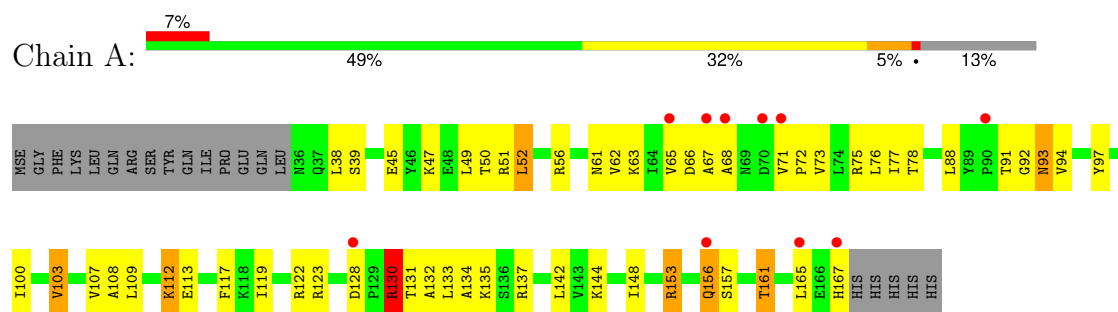
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total 25	O 25	0	0
2	B	13	Total 13	O 13	0	0

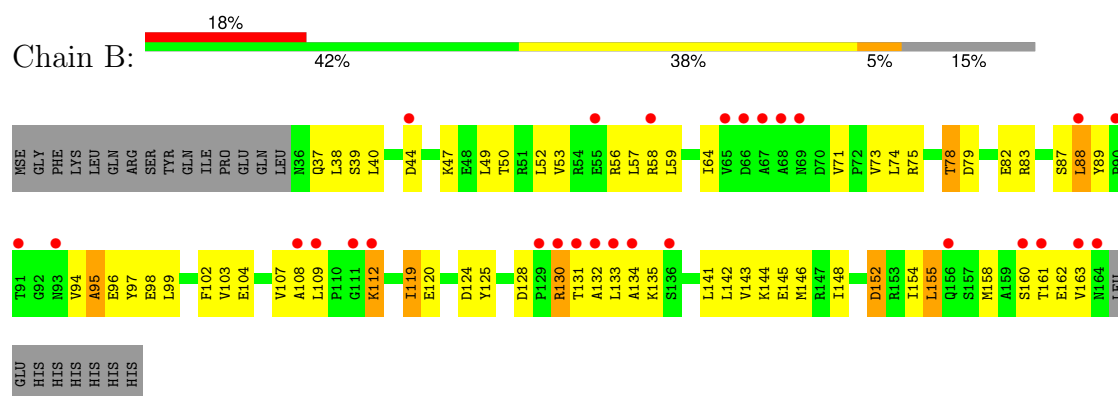
3 Residue-property plots [i](#)

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: Rare lipoprotein B



• Molecule 1: Rare lipoprotein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.09Å 88.09Å 112.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	91.1 (30.00-2.60) 96.7 (30.00-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.25 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.247 , 0.293 0.266 , 0.314	Depositor DCC
R_{free} test set	1307 reflections (9.35%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2141	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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	0.42	0/1075	0.63	0/1448
1	B	0.46	0/1047	0.61	0/1410
All	All	0.44	0/2122	0.62	0/2858

There are no bond length outliers.

There are no bond angle outliers.

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	1065	0	1087	70	0
1	B	1038	0	1063	56	0
2	A	25	0	0	0	0
2	B	13	0	0	0	0
All	All	2141	0	2150	124	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 29.

The worst 5 of 124 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:153:ARG:HH21	1:A:156:GLN:HG2	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:HB3	1:A:73:VAL:HG12	1.53	0.91
1:A:103:VAL:HG13	1:A:119:ILE:HB	1.55	0.85
1:A:130:ARG:HB3	1:A:130:ARG:HH11	1.42	0.84
1:A:109:LEU:HD13	1:A:112:LYS:HD3	1.59	0.83

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	130/152 (86%)	119 (92%)	10 (8%)	1 (1%)	16	34
1	B	127/152 (84%)	116 (91%)	8 (6%)	3 (2%)	5	9
All	All	257/304 (84%)	235 (91%)	18 (7%)	4 (2%)	8	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ARG
1	B	130	ARG
1	B	95	ALA
1	B	132	ALA

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	119/134 (89%)	107 (90%)	12 (10%)	6	12
1	B	116/134 (87%)	109 (94%)	7 (6%)	16	35
All	All	235/268 (88%)	216 (92%)	19 (8%)	9	20

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	GLU
1	B	152	ASP
1	B	155	LEU
1	B	119	ILE
1	A	142	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	ASN
1	B	61	ASN
1	A	149	GLN
1	A	156	GLN
1	A	164	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	129/152 (84%)	0.65	10 (7%) 20 17	20, 49, 84, 104	0
1	B	126/152 (82%)	0.96	28 (22%) 3 2	21, 56, 94, 100	0
All	All	255/304 (83%)	0.80	38 (14%) 7 5	20, 53, 91, 104	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	PRO	4.3
1	A	68	ALA	4.1
1	A	65	VAL	3.9
1	B	132	ALA	3.8
1	A	128	ASP	3.6

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 monosaccharides 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.