

wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 11:40 PM EDT

PDB ID : 6VZE

Title: C-terminal domain of mouse surfactant protein B crystallized at low pH

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Deposited on : 2020-02-28

Resolution : 1.90 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9277 atoms, of which 4415 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 Pulmonary surfactant-associated protein B.

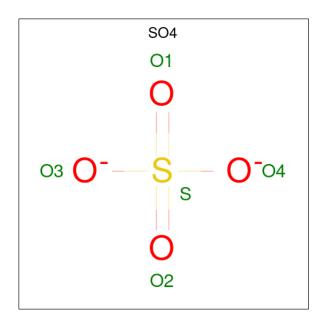
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace				
1	В	73	Total	С	Н	N	О	S	0	0	0			
1		10	1135	361	551	106	108	9						
1	Е	73	Total	С	Н	N	О	S	0	0	0			
1	שנ	75	1134	362	552	106	105	9	0					
1	Н	72	Total	С	Η	N	O	S	0	0	0			
1	11	12	1122	358	544	105	106	9	0	U				
1	D	72	Total	С	Η	N	O	S	0	0	0			
1	D		1123	358	545	105	106	9						
1	F	72	Total	С	Η	N	O	S	0	0	0			
1	I.		1122	358	544	105	106	9	0	U				
1	G	76	Total	С	Η	N	O	S	0	0	0			
1	<u> </u>	9	G	G	10	1169	372	568	109	111	9		0	
1	С	74	Total	С	Н	N	О	S	0	0	0			
1			1145	366	555	107	108	9						
1	A	74	Total	С	Н	N	О	S	0	0	0			
1			1145	364	556	107	109	9		U				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	1	SER	-	expression tag	UNP P50405
E	1	SER	-	expression tag	UNP P50405
Н	1	SER	-	expression tag	UNP P50405
D	1	SER	-	expression tag	UNP P50405
F	1	SER	-	expression tag	UNP P50405
G	1	SER	-	expression tag	UNP P50405
С	1	SER	-	expression tag	UNP P50405
A	1	SER	-	expression tag	UNP P50405

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	18	Total O 18 18	0	0
3	E	24	Total O 24 24	0	0
3	Н	21	Total O 21 21	0	0
3	D	25	Total O 25 25	0	0
3	F	14	Total O 14 14	0	0
3	G	25	Total O 25 25	0	0
3	С	18	Total O 18 18	0	0
3	A	22	Total O 22 22	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	52.19Å 79.01Å 71.92Å	Depositor	
a, b, c, α , β , γ	90.00° 106.43° 90.00°	Depositor	
Resolution (Å)	68.98 - 1.90	Depositor	
% Data completeness	97.2 (68.98-1.90)	Depositor	
(in resolution range)	,		
R_{merge}	0.11	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.40 (at 1.90Å)	Xtriage	
Refinement program	PHENIX 1.17.1_3660	Depositor	
R, R_{free}	0.210 , 0.240	Depositor	
Wilson B-factor (A^2)	36.2	Xtriage	
Anisotropy	0.276	Xtriage	
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	9277	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 15.25% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

3 ligands are 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	Tuno	Chain	Res	Link	B	ond leng	gths	Bond angles		
MIOI	Type	Chain			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	G	101	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	В	101	-	4,4,4	0.40	0	6,6,6	0.05	0
2	SO4	D	101	-	4,4,4	0.15	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

