



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:23 am BST

PDB ID : 6JBO  
Title : Crystal structure of EfeO-like protein Algp7 containing samarium ion  
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Deposited on : 2019-01-26  
Resolution : 1.88 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

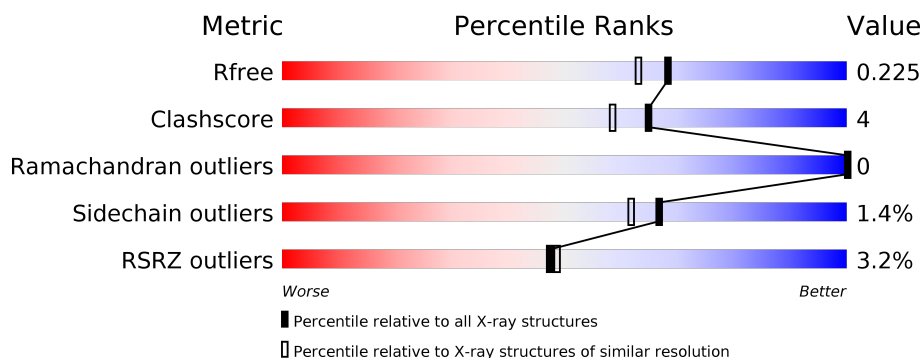
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	283	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	283	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4417 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 Alginate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	1	0
			1984	1261	340	378	5			
1	B	251	Total	C	N	O	S	0	3	0
			1998	1269	342	381	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	VAL	-	expression tag	UNP Q25C86
A	275	LEU	-	expression tag	UNP Q25C86
A	276	GLU	-	expression tag	UNP Q25C86
A	277	HIS	-	expression tag	UNP Q25C86
A	278	HIS	-	expression tag	UNP Q25C86
A	279	HIS	-	expression tag	UNP Q25C86
A	280	HIS	-	expression tag	UNP Q25C86
A	281	HIS	-	expression tag	UNP Q25C86
A	282	HIS	-	expression tag	UNP Q25C86
B	0	VAL	-	expression tag	UNP Q25C86
B	275	LEU	-	expression tag	UNP Q25C86
B	276	GLU	-	expression tag	UNP Q25C86
B	277	HIS	-	expression tag	UNP Q25C86
B	278	HIS	-	expression tag	UNP Q25C86
B	279	HIS	-	expression tag	UNP Q25C86
B	280	HIS	-	expression tag	UNP Q25C86
B	281	HIS	-	expression tag	UNP Q25C86
B	282	HIS	-	expression tag	UNP Q25C86

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			8	4	4		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	1
			8	4	4		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Sm	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		

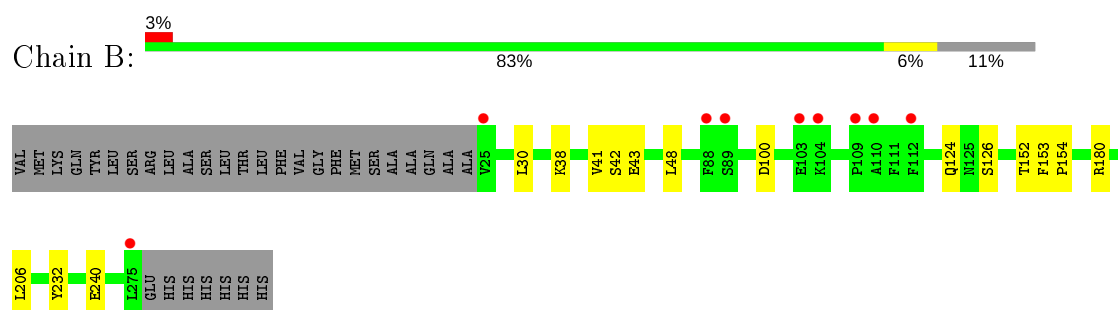
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	197	Total	O	0	0
			197	197		



- Molecule 1: Alginate-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.83Å 97.51Å 104.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 1.88 46.45 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.45-1.88) 99.8 (46.45-1.88)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.22 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.185 , 0.225 0.185 , 0.225	Depositor DCC
$R_{free}$ test set	2218 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: EDO, SM

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	0.38	0/2018	0.51	0/2719
1	B	0.36	0/2038	0.51	0/2745
All	All	0.37	0/4056	0.51	0/5464

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	1984	0	1989	20	0
1	B	1998	0	1999	12	0
2	A	16	0	24	2	0
2	B	20	0	30	3	0
3	B	1	0	0	0	0
4	A	201	0	0	1	0
4	B	197	0	0	2	0
All	All	4417	0	4042	33	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 4.



All (33) 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:B:41:VAL:C	1:B:42[C]:SER:CA	2.43	0.86
1:A:146:LYS:HA	1:A:149:ARG:HH21	1.44	0.81
1:B:42[C]:SER:CA	1:B:43:GLU:N	2.45	0.80
1:A:204:ARG:HE	2:A:302:EDO:H22	1.48	0.76
1:A:233:ARG:HG3	2:B:305:EDO:H12	1.68	0.75
1:B:42[C]:SER:O	1:B:43:GLU:N	2.25	0.70
1:B:42[C]:SER:O	1:B:42[C]:SER:CA	2.40	0.69
1:B:42[B]:SER:N	1:B:42[B]:SER:C	2.47	0.68
1:B:100:ASP:H	1:B:180:ARG:NH2	1.93	0.66
1:A:53:ARG:HA	1:A:138:MET:HE1	1.79	0.64
1:A:149:ARG:HG3	4:A:515:HOH:O	1.99	0.62
1:A:52:THR:HG22	1:A:138:MET:HE2	1.84	0.60
1:A:146:LYS:CA	1:A:149:ARG:HH21	2.14	0.59
1:A:173:LYS:HG3	2:A:301[A]:EDO:H21	1.83	0.58
1:B:152:THR:O	1:B:154:PRO:HD3	2.04	0.56
1:A:53:ARG:CA	1:A:138:MET:HE1	2.37	0.55
1:B:100:ASP:H	1:B:180:ARG:HH22	1.55	0.53
1:A:53:ARG:N	1:A:138:MET:HE1	2.25	0.52
1:A:78:TYR:OH	1:A:92:ASP:OD1	2.23	0.50
1:A:233:ARG:CG	2:B:305:EDO:H12	2.40	0.50
1:B:124:GLN:NE2	4:B:404:HOH:O	2.42	0.49
1:A:146:LYS:HA	1:A:149:ARG:NH2	2.21	0.49
2:B:305:EDO:H21	4:B:407:HOH:O	2.12	0.49
1:A:102:HIS:HB3	1:A:108:ASP:OD2	2.13	0.48
1:B:232:TYR:O	1:B:240:GLU:HG3	2.15	0.46
1:B:38:LYS:HD2	1:B:153:PHE:CE1	2.51	0.46
1:A:53:ARG:HA	1:A:138:MET:CE	2.46	0.45
1:A:152:THR:O	1:A:154:PRO:HD3	2.17	0.43
1:A:72:ALA:O	1:A:76[A]:MET:HG3	2.19	0.43
1:B:30:LEU:HD23	1:B:206:LEU:HD22	2.00	0.42
1:A:148:ILE:HA	1:A:151:LEU:HD12	2.02	0.42
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.81	0.42
1:A:136:LYS:HB2	1:A:136:LYS:HE2	1.72	0.41

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	250/283 (88%)	246 (98%)	4 (2%)	0	100	100
1	B	253/283 (89%)	249 (98%)	4 (2%)	0	100	100
All	All	503/566 (89%)	495 (98%)	8 (2%)	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	208/233 (89%)	204 (98%)	4 (2%)	57	49
1	B	211/233 (91%)	209 (99%)	2 (1%)	78	76
All	All	419/466 (90%)	413 (99%)	6 (1%)	67	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	69	LYS
1	A	86	GLU
1	A	91	LEU
1	B	48	LEU
1	B	126	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 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 ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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	EDO	B	305	-	3,3,3	0.53	0	2,2,2	0.33	0
2	EDO	B	304	-	3,3,3	0.54	0	2,2,2	0.30	0
2	EDO	B	302[B]	-	3,3,3	0.49	0	2,2,2	0.10	0
2	EDO	B	302[A]	-	3,3,3	0.41	0	2,2,2	0.44	0
2	EDO	A	301[B]	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	B	303	-	3,3,3	0.43	0	2,2,2	0.48	0
2	EDO	A	301[A]	-	3,3,3	0.40	0	2,2,2	0.39	0
2	EDO	A	302	-	3,3,3	0.50	0	2,2,2	0.35	0
2	EDO	A	303	-	3,3,3	0.51	0	2,2,2	0.28	0

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	EDO	B	305	-	-	0/1/1/1	-
2	EDO	B	304	-	-	1/1/1/1	-
2	EDO	B	302[B]	-	-	0/1/1/1	-
2	EDO	B	302[A]	-	-	0/1/1/1	-
2	EDO	A	301[B]	-	-	0/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	A	301[A]	-	-	0/1/1/1	-
2	EDO	A	302	-	-	0/1/1/1	-
2	EDO	A	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	304	EDO	O1-C1-C2-O2
2	A	303	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	305	EDO	3	0
2	A	301[A]	EDO	1	0
2	A	302	EDO	1	0

## 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, 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	251/283 (88%)	0.02	7 (2%) 53 54	11, 20, 42, 58	0
1	B	251/283 (88%)	0.14	9 (3%) 42 44	12, 23, 42, 62	0
All	All	502/566 (88%)	0.08	16 (3%) 47 49	11, 21, 42, 62	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	GLU	4.4
1	A	109	PRO	3.6
1	B	109	PRO	3.3
1	A	104	LYS	3.0
1	B	104	LYS	3.0
1	B	112	PHE	2.8
1	B	110	ALA	2.7
1	B	275	LEU	2.5
1	A	88	PHE	2.5
1	A	112	PHE	2.5
1	A	107	LYS	2.4
1	B	103	GLU	2.4
1	B	88	PHE	2.3
1	B	25	VAL	2.2
1	B	89	SER	2.1
1	A	164	VAL	2.1

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	305	4/4	0.75	0.37	37,38,40,41	0
2	EDO	A	302	4/4	0.80	0.16	34,37,45,47	0
2	EDO	B	304	4/4	0.83	0.30	28,32,36,42	0
2	EDO	A	303	4/4	0.83	0.30	32,38,43,44	0
2	EDO	B	302[B]	4/4	0.86	0.35	20,21,28,30	4
2	EDO	B	302[A]	4/4	0.86	0.35	24,24,27,27	4
2	EDO	A	301[B]	4/4	0.90	0.27	18,19,20,20	4
2	EDO	A	301[A]	4/4	0.90	0.27	15,18,19,20	4
2	EDO	B	303	4/4	0.93	0.13	23,26,28,32	0
3	SM	B	301	1/1	0.98	0.03	35,35,35,35	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.