wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:02 PM GMT

PDB ID	:	4H0F
Title	:	Mutant Structure of laminin-binding adhesin (Lmb) from Streptococcus agalactiae
Authors	:	Karthe, P.; Preethi, R.
Deposited on	:	2012-09-08
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

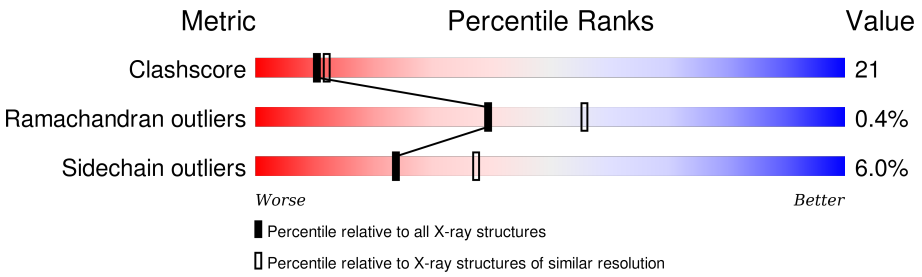
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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. 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 <=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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	264	68% 28% •
1	B	264	62% 34% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4242 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 Laminin-binding surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2084	1331	352	397	4	0	0	0
1	B	264	2080	1328	351	397	4	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	DELETION	UNP Q8DZ80
A	?	-	LEU	DELETION	UNP Q8DZ80
A	?	-	GLU	DELETION	UNP Q8DZ80
A	?	-	ASP	DELETION	UNP Q8DZ80
A	?	-	MET	DELETION	UNP Q8DZ80
A	?	-	GLU	DELETION	UNP Q8DZ80
A	?	-	VAL	DELETION	UNP Q8DZ80
A	?	-	THR	DELETION	UNP Q8DZ80
A	?	-	GLN	DELETION	UNP Q8DZ80
A	?	-	GLY	DELETION	UNP Q8DZ80
A	?	-	ILE	DELETION	UNP Q8DZ80
A	?	-	ASP	DELETION	UNP Q8DZ80
A	124	GLY	-	EXPRESSION TAG	UNP Q8DZ80
A	138	VAL	LEU	CONFLICT	UNP Q8DZ80
B	?	-	GLY	DELETION	UNP Q8DZ80
B	?	-	LEU	DELETION	UNP Q8DZ80
B	?	-	GLU	DELETION	UNP Q8DZ80
B	?	-	ASP	DELETION	UNP Q8DZ80
B	?	-	MET	DELETION	UNP Q8DZ80
B	?	-	GLU	DELETION	UNP Q8DZ80
B	?	-	VAL	DELETION	UNP Q8DZ80
B	?	-	THR	DELETION	UNP Q8DZ80
B	?	-	GLN	DELETION	UNP Q8DZ80
B	?	-	GLY	DELETION	UNP Q8DZ80
B	?	-	ILE	DELETION	UNP Q8DZ80

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	DELETION	UNP Q8DZ80
B	124	GLY	-	EXPRESSION TAG	UNP Q8DZ80
B	138	VAL	LEU	CONFLICT	UNP Q8DZ80

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	40	Total O 40 40	0	0
3	A	36	Total O 36 36	0	0

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 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.

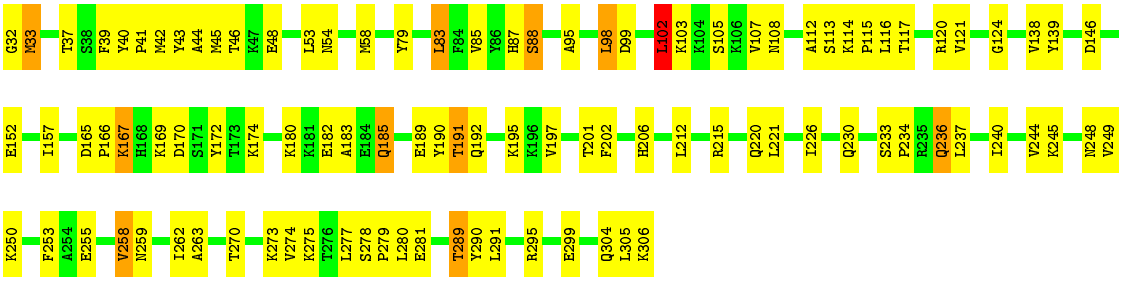
Note EDS failed to run properly.

- Molecule 1: Laminin-binding surface protein

Chain A:

- Molecule 1: Laminin-binding surface protein

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.40Å 93.99Å 66.88Å 90.00° 105.42° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	92.3 (20.00-2.40)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.281	Depositor
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.296	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 18293 reflections	Xtriage
Total number of atoms	4242	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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: ZN

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	0.48	1/2131 (0.0%)	0.69	1/2882 (0.0%)
1	B	0.43	0/2127	0.67	1/2878 (0.0%)
All	All	0.46	1/4258 (0.0%)	0.68	2/5760 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLU	CG-CD	-5.32	1.44	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	LEU	CA-CB-CG	7.79	133.22	115.30
1	B	102	LEU	CA-CB-CG	7.37	132.26	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Sidechain

5.2 Too-close contacts (i)

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	2084	0	2089	85	0
1	B	2080	0	2078	103	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	0	1	0
3	B	40	0	0	4	0
All	All	4242	0	4167	179	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 21.

The worst 5 of 179 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:273:LYS:HE2	1:B:304:GLN:HE22	1.18	1.05
1:A:273:LYS:HE2	1:A:304:GLN:HE22	1.21	1.03
1:B:33:MET:HB3	1:B:54:ASN:HD22	1.29	0.94
1:A:289:THR:HG22	1:A:292:GLU:H	1.31	0.93
1:B:37:THR:HG23	1:B:42:MET:HB2	1.53	0.90

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	262/264 (99%)	245 (94%)	17 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	262/264 (99%)	246 (94%)	14 (5%)	2 (1%)	24	35
All	All	524/528 (99%)	491 (94%)	31 (6%)	2 (0%)	39	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	GLN
1	B	33	MET

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	226/227 (100%)	214 (95%)	12 (5%)	28	44
1	B	225/227 (99%)	210 (93%)	15 (7%)	20	31
All	All	451/454 (99%)	424 (94%)	27 (6%)	24	37

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	MET
1	B	88	SER
1	B	258	VAL
1	B	58	MET
1	A	184	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	GLN
1	B	54	ASN
1	B	236	GLN
1	A	287	ASN
1	B	156	ASN

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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)

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands (i)

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers (i)

EDS failed to run properly - this section will therefore be empty.