Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 10:04 AM EDT

PDB ID	:	6ROC
Title	:	Crystal structure of Borrelia burgdorferi outer surface protein BBA69, mutant Leu214Met (Se-Met data)
Authors	:	Brangulis, K.; Akopjana, I.; Petrovskis, I.; Kazaks, A.; Tars, K.
Deposited on	:	2019-05-11
Resolution	:	2.90 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
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 (1)) were used in the production of this report:

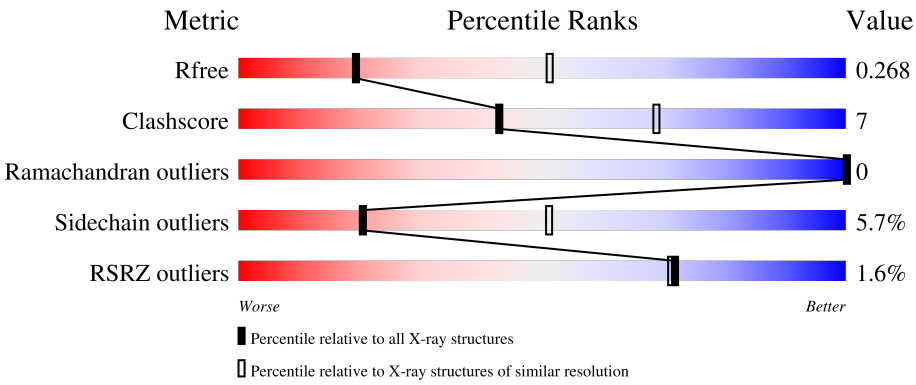
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	192	2% 77% 18% • •
1	B	192	2% 74% 17% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2998 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 Putative surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	184	1510	950	253	305	2	0	0	0
			Total	C	N	O	S			
1	B	181	1488	939	250	297	2	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

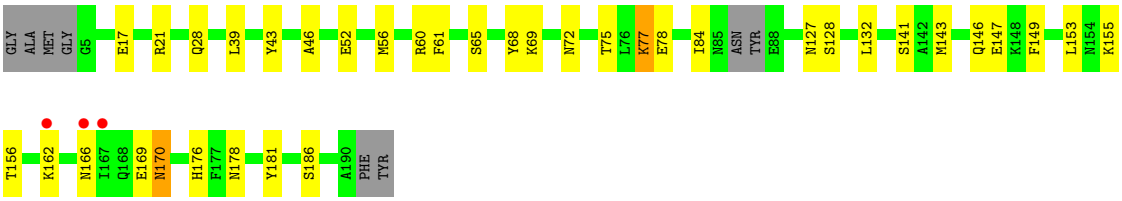
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O50958
A	2	ALA	-	expression tag	UNP O50958
A	3	MET	-	expression tag	UNP O50958
A	4	GLY	-	expression tag	UNP O50958
A	143	MET	LEU	engineered mutation	UNP O50958
B	1	GLY	-	expression tag	UNP O50958
B	2	ALA	-	expression tag	UNP O50958
B	3	MET	-	expression tag	UNP O50958
B	4	GLY	-	expression tag	UNP O50958
B	143	MET	LEU	engineered mutation	UNP O50958

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.

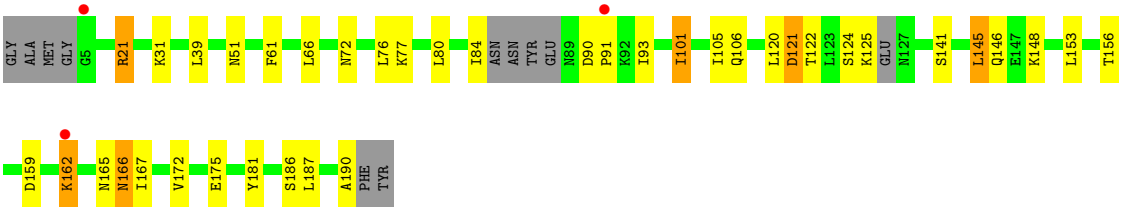
• Molecule 1: Putative surface protein

Chain A:



• Molecule 1: Putative surface protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	73.97Å 110.55Å 61.70Å 90.00° 126.83° 90.00°	Depositor
Resolution (Å)	52.19 – 2.90 52.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (52.19-2.90) 99.5 (52.19-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.199 , 0.267 0.220 , 0.268	Depositor DCC
R_{free} test set	439 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.289 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.574 for H, K, L 0.426 for -H, -K, H+L	Depositor
Outliers	0 of 8797 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2998	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.79	0/1523	0.91	3/2039 (0.1%)
1	B	0.75	0/1500	0.90	4/2005 (0.2%)
All	All	0.77	0/3023	0.91	7/4044 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	120	LEU	CB-CA-C	-8.86	93.37	110.20
1	A	162	LYS	CB-CA-C	-8.68	93.05	110.40
1	B	166	ASN	CB-CA-C	-7.71	94.97	110.40
1	B	162	LYS	CB-CA-C	-7.69	95.02	110.40
1	A	127	ASN	CB-CA-C	7.07	124.53	110.40
1	A	128	SER	N-CA-C	-5.97	94.89	111.00
1	B	121	ASP	N-CA-C	-5.68	95.66	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1510	0	1538	17	0
1	B	1488	0	1530	25	0
All	All	2998	0	3068	41	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 7.

All (41) 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:61:PHE:CE1	1:B:146:GLN:HG3	2.18	0.79
1:B:61:PHE:HE1	1:B:146:GLN:HG3	1.58	0.67
1:A:170:ASN:HD22	1:A:170:ASN:N	1.96	0.63
1:B:106:GLN:HA	1:B:106:GLN:OE1	2.02	0.60
1:A:84:ILE:O	1:A:84:ILE:HG22	2.00	0.60
1:B:80:LEU:O	1:B:84:ILE:HG12	2.03	0.58
1:B:21:ARG:NH1	1:B:146:GLN:HE22	2.03	0.57
1:A:56:MET:HG3	1:A:60:ARG:NH1	2.21	0.56
1:B:61:PHE:HB2	1:B:106:GLN:HE21	1.72	0.54
1:B:51:ASN:OD1	1:B:51:ASN:C	2.46	0.54
1:B:153:LEU:O	1:B:156:THR:HB	2.08	0.53
1:A:61:PHE:HE2	1:A:149:PHE:CE2	2.27	0.53
1:B:121:ASP:O	1:B:122:THR:CG2	2.57	0.52
1:B:61:PHE:CZ	1:B:146:GLN:HG3	2.45	0.52
1:B:145:LEU:CD2	1:B:187:LEU:HD23	2.41	0.50
1:B:101:ILE:O	1:B:105:ILE:HG13	2.11	0.50
1:A:153:LEU:HA	1:A:181:TYR:OH	2.12	0.50
1:A:69:LYS:O	1:A:72:ASN:HB2	2.12	0.50
1:A:43:TYR:O	1:A:46:ALA:HB3	2.12	0.49
1:A:155:LYS:HG2	1:A:155:LYS:O	2.14	0.47
1:B:39:LEU:HD22	1:B:77:LYS:HD3	1.96	0.47
1:B:90:ASP:N	1:B:91:PRO:CD	2.77	0.47
1:B:125:LYS:HA	1:B:125:LYS:HD3	1.75	0.47
1:B:121:ASP:O	1:B:122:THR:HG22	2.16	0.46
1:A:39:LEU:HD22	1:A:77:LYS:HD3	1.98	0.46
1:A:21:ARG:NH1	1:A:146:GLN:OE1	2.43	0.45
1:A:132:LEU:N	1:A:132:LEU:HD23	2.31	0.45
1:B:66:LEU:HD22	1:B:72:ASN:HB3	1.99	0.45
1:A:156:THR:OG1	1:A:176:HIS:HE1	2.00	0.45
1:B:159:ASP:O	1:B:162:LYS:N	2.51	0.44
1:A:61:PHE:HE2	1:A:149:PHE:CD2	2.37	0.42
1:A:17:GLU:OE1	1:B:31:LYS:NZ	2.47	0.42
1:A:21:ARG:NH1	1:A:146:GLN:HE22	2.17	0.42
1:A:75:THR:O	1:A:78:GLU:HB2	2.19	0.42
1:B:153:LEU:HA	1:B:181:TYR:OH	2.19	0.42
1:B:165:ASN:O	1:B:166:ASN:HB2	2.20	0.42
1:B:66:LEU:HD11	1:B:76:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASP:C	1:B:122:THR:HG23	2.41	0.41
1:B:167:ILE:HA	1:B:172:VAL:HG12	2.02	0.41
1:A:28:GLN:HG3	1:A:68:TYR:CE1	2.55	0.41
1:B:148:LYS:HE3	1:B:190:ALA:HB2	2.04	0.40

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	180/192 (94%)	159 (88%)	21 (12%)	0	100	100
1	B	175/192 (91%)	157 (90%)	18 (10%)	0	100	100
All	All	355/384 (92%)	316 (89%)	39 (11%)	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	169/175 (97%)	158 (94%)	11 (6%)	17	45
1	B	167/175 (95%)	159 (95%)	8 (5%)	25	58
All	All	336/350 (96%)	317 (94%)	19 (6%)	20	51

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	65	SER
1	A	77	LYS
1	A	141	SER
1	A	143	MET
1	A	147	GLU
1	A	166	ASN
1	A	169	GLU
1	A	170	ASN
1	A	178	ASN
1	A	186	SER
1	B	21	ARG
1	B	93	ILE
1	B	101	ILE
1	B	124	SER
1	B	141	SER
1	B	145	LEU
1	B	175	GLU
1	B	186	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	165	ASN
1	A	168	GLN
1	A	170	ASN
1	A	176	HIS
1	B	28	GLN
1	B	127	ASN
1	B	138	GLN
1	B	154	ASN
1	B	165	ASN
1	B	168	GLN
1	B	170	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	184/192 (95%)	-0.43	3 (1%)	72	71	30, 73, 120, 142	0
1	B	181/192 (94%)	-0.37	3 (1%)	70	69	42, 73, 115, 136	0
All	All	365/384 (95%)	-0.40	6 (1%)	72	71	30, 73, 118, 142	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	ILE	3.0
1	A	166	ASN	2.9
1	B	91	PRO	2.8
1	B	5	GLY	2.3
1	A	162	LYS	2.0
1	B	162	LYS	2.0

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.