



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2025 – 03:08 pm GMT

PDB ID : 8S2F
Title : Crystal structure of Borrelia burgdorferi paralogous family 12 outer surface protein BBH37
Authors : Brangulis, K.
Deposited on : 2024-02-17
Resolution : 2.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
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)
Validation Pipeline (wwPDB-VP)	:	2.41

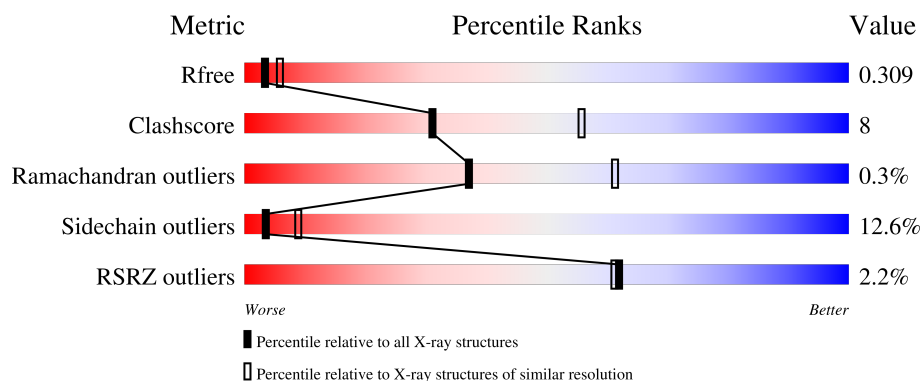
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	AAA	186	 3% 75% 18% . .
1	BBB	186	 2% 80% 13% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2917 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 Lipoprotein, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	180	Total	C	N	O	S	0	0	0
			1441	897	257	282	5			
1	BBB	181	Total	C	N	O	S	0	0	0
			1447	902	257	283	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	127	GLY	-	expression tag	UNP O50692
AAA	128	ALA	-	expression tag	UNP O50692
AAA	129	MET	-	expression tag	UNP O50692
AAA	130	GLY	-	expression tag	UNP O50692
BBB	127	GLY	-	expression tag	UNP O50692
BBB	128	ALA	-	expression tag	UNP O50692
BBB	129	MET	-	expression tag	UNP O50692
BBB	130	GLY	-	expression tag	UNP O50692

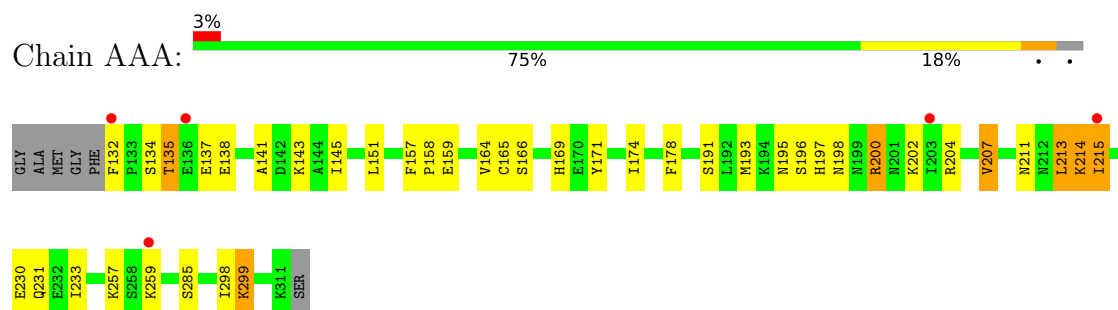
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	14	Total	O	0	0
			14	14		
2	BBB	15	Total	O	0	0
			15	15		

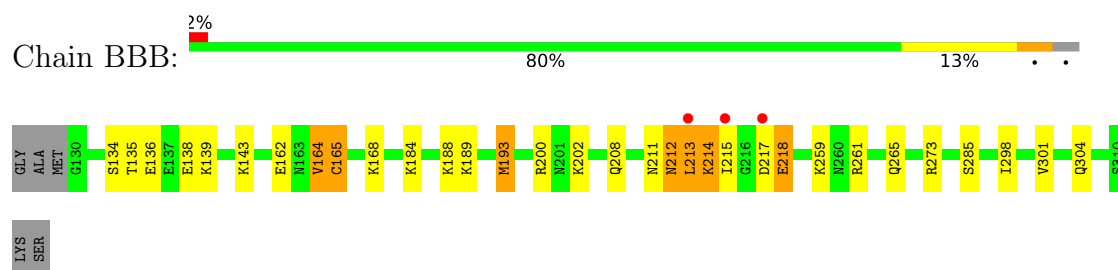
3 Residue-property plots [i](#)

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: Lipoprotein, putative



- Molecule 1: Lipoprotein, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	37.71Å 90.92Å 115.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.38 – 2.70 71.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (71.38-2.70) 99.9 (71.38-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.310 0.224 , 0.309	Depositor DCC
R_{free} test set	596 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2917	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.98% 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	AAA	0.66	0/1454	0.79	0/1938
1	BBB	0.68	0/1461	0.79	0/1948
All	All	0.67	0/2915	0.79	0/3886

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	AAA	1441	0	1477	26	0
1	BBB	1447	0	1476	25	0
2	AAA	14	0	0	0	0
2	BBB	15	0	0	2	0
All	All	2917	0	2953	46	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 8.

All (46) 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:BBB:211:ASN:O	1:BBB:213:LEU:N	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:213:LEU:HD22	1:AAA:215:ILE:HD11	1.71	0.71
1:AAA:165:CYS:HG	1:BBB:165:CYS:HG	0.74	0.71
1:AAA:230:GLU:OE1	1:BBB:168:LYS:NZ	2.27	0.68
1:AAA:215:ILE:HD13	1:AAA:298:ILE:HD11	1.75	0.68
1:BBB:135:THR:HG22	1:BBB:138:GLU:H	1.61	0.65
1:BBB:135:THR:HG21	2:BBB:412:HOH:O	1.98	0.62
1:AAA:178:PHE:HE2	1:AAA:215:ILE:HD12	1.69	0.56
1:AAA:211:ASN:O	1:AAA:214:LYS:HB2	2.05	0.56
1:AAA:174:ILE:HD11	1:AAA:299:LYS:HA	1.88	0.55
1:AAA:135:THR:HG23	1:AAA:137:GLU:OE2	2.06	0.55
1:BBB:213:LEU:O	1:BBB:215:ILE:HD12	2.07	0.55
1:BBB:214:LYS:O	1:BBB:217:ASP:HB2	2.08	0.53
1:AAA:204:ARG:O	1:AAA:207:VAL:HG12	2.09	0.53
1:BBB:218:GLU:CG	1:BBB:298:ILE:HD11	2.42	0.50
1:BBB:218:GLU:CB	1:BBB:298:ILE:HD11	2.42	0.49
1:BBB:214:LYS:N	1:BBB:214:LYS:HD2	2.27	0.49
1:AAA:157:PHE:N	1:AAA:158:PRO:CD	2.77	0.47
1:BBB:164:VAL:HG23	2:BBB:404:HOH:O	2.15	0.46
1:BBB:213:LEU:HD12	1:BBB:215:ILE:HD13	1.96	0.46
1:AAA:135:THR:HG22	1:AAA:138:GLU:H	1.79	0.46
1:AAA:178:PHE:CE2	1:AAA:215:ILE:HD12	2.49	0.46
1:AAA:141:ALA:O	1:AAA:145:ILE:HG12	2.15	0.46
1:BBB:213:LEU:C	1:BBB:215:ILE:H	2.18	0.45
1:BBB:218:GLU:HG3	1:BBB:298:ILE:HD11	1.99	0.45
1:AAA:165:CYS:CB	1:BBB:165:CYS:HG	2.25	0.44
1:BBB:134:SER:O	1:BBB:139:LYS:HD2	2.17	0.44
1:BBB:215:ILE:CG1	1:BBB:301:VAL:HG11	2.47	0.44
1:AAA:215:ILE:HD13	1:AAA:298:ILE:CD1	2.44	0.43
1:BBB:189:LYS:O	1:BBB:193:MET:HG2	2.18	0.43
1:AAA:135:THR:O	1:AAA:138:GLU:HB2	2.19	0.43
1:AAA:165:CYS:HA	1:BBB:165:CYS:SG	2.59	0.43
1:BBB:213:LEU:C	1:BBB:215:ILE:N	2.71	0.43
1:AAA:165:CYS:CB	1:BBB:165:CYS:SG	3.07	0.42
1:AAA:171:TYR:O	1:AAA:174:ILE:HG22	2.19	0.42
1:AAA:164:VAL:HG11	1:AAA:230:GLU:HB3	2.01	0.42
1:AAA:134:SER:O	1:AAA:135:THR:C	2.59	0.41
1:AAA:213:LEU:HD22	1:AAA:213:LEU:HA	1.91	0.41
1:BBB:215:ILE:HG13	1:BBB:301:VAL:HG11	2.01	0.41
1:AAA:174:ILE:HD12	1:AAA:174:ILE:HA	1.88	0.41
1:AAA:197:HIS:O	1:AAA:200:ARG:HB2	2.21	0.41
1:AAA:202:LYS:HA	1:AAA:202:LYS:HD2	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:166:SER:O	1:AAA:169:HIS:HB3	2.20	0.41
1:BBB:213:LEU:HD12	1:BBB:213:LEU:HA	1.74	0.41
1:BBB:215:ILE:HG23	1:BBB:298:ILE:HG23	2.03	0.41
1:BBB:208:GLN:O	1:BBB:212:ASN:N	2.48	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	AAA	178/186 (96%)	166 (93%)	12 (7%)	0	100	100
1	BBB	179/186 (96%)	166 (93%)	12 (7%)	1 (1%)	22	45
All	All	357/372 (96%)	332 (93%)	24 (7%)	1 (0%)	37	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	212	ASN

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	AAA	159/162 (98%)	138 (87%)	21 (13%)	3	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	BBB	159/162 (98%)	140 (88%)	19 (12%)	4 10
All	All	318/324 (98%)	278 (87%)	40 (13%)	3 9

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	132	PHE
1	AAA	135	THR
1	AAA	143	LYS
1	AAA	151	LEU
1	AAA	159	GLU
1	AAA	191	SER
1	AAA	193	MET
1	AAA	195	ASN
1	AAA	196	SER
1	AAA	198	ASN
1	AAA	200	ARG
1	AAA	207	VAL
1	AAA	213	LEU
1	AAA	214	LYS
1	AAA	215	ILE
1	AAA	231	GLN
1	AAA	233	ILE
1	AAA	257	LYS
1	AAA	259	LYS
1	AAA	285	SER
1	AAA	299	LYS
1	BBB	136	GLU
1	BBB	143	LYS
1	BBB	162	GLU
1	BBB	164	VAL
1	BBB	165	CYS
1	BBB	184	LYS
1	BBB	188	LYS
1	BBB	193	MET
1	BBB	200	ARG
1	BBB	202	LYS
1	BBB	213	LEU
1	BBB	214	LYS
1	BBB	218	GLU
1	BBB	259	LYS
1	BBB	261	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BBB	265	GLN
1	BBB	273	ARG
1	BBB	285	SER
1	BBB	304	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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	AAA	180/186 (96%)	0.31	5 (2%) 55 53	28, 47, 86, 121	0
1	BBB	181/186 (97%)	0.11	3 (1%) 69 68	25, 41, 71, 82	0
All	All	361/372 (97%)	0.21	8 (2%) 62 61	25, 44, 78, 121	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	215	ILE	4.9
1	BBB	215	ILE	3.2
1	AAA	203	ILE	3.1
1	AAA	132	PHE	3.1
1	BBB	217	ASP	2.6
1	AAA	136	GLU	2.3
1	AAA	259	LYS	2.3
1	BBB	213	LEU	2.2

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.