



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 04:05 PM EDT

PDB ID : 8Q4K / pdb_00008q4k
Title : Crystal structure of Borrelia burgdorferi BB0158
Authors : Brangulis, K.; Tars, K.
Deposited on : 2023-08-07
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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

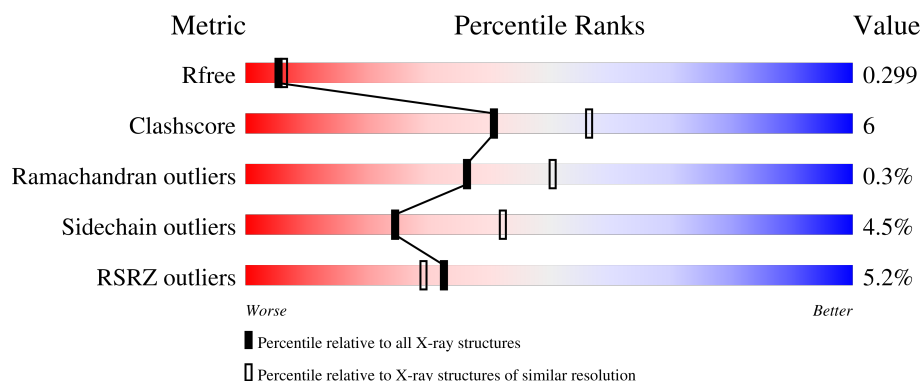
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

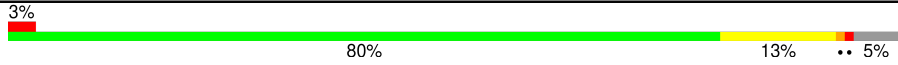
The reported resolution of this entry is 2.40 Å.

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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	214	
1	BBB	214	
1	CCC	214	
1	DDD	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6736 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 S2 lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	203	Total	C	N	O	S	0	0	0
			1628	1055	252	317	4			
1	BBB	198	Total	C	N	O	S	0	0	0
			1586	1027	246	309	4			
1	CCC	205	Total	C	N	O	S	0	0	0
			1642	1062	255	321	4			
1	DDD	201	Total	C	N	O	S	0	0	0
			1617	1049	250	314	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	GLY	-	expression tag	UNP O51180
AAA	2	ALA	-	expression tag	UNP O51180
AAA	3	MET	-	expression tag	UNP O51180
AAA	4	GLY	-	expression tag	UNP O51180
BBB	1	GLY	-	expression tag	UNP O51180
BBB	2	ALA	-	expression tag	UNP O51180
BBB	3	MET	-	expression tag	UNP O51180
BBB	4	GLY	-	expression tag	UNP O51180
CCC	1	GLY	-	expression tag	UNP O51180
CCC	2	ALA	-	expression tag	UNP O51180
CCC	3	MET	-	expression tag	UNP O51180
CCC	4	GLY	-	expression tag	UNP O51180
DDD	1	GLY	-	expression tag	UNP O51180
DDD	2	ALA	-	expression tag	UNP O51180
DDD	3	MET	-	expression tag	UNP O51180
DDD	4	GLY	-	expression tag	UNP O51180

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	DDD	1	Total	O	S	0	0
			5	4	1		

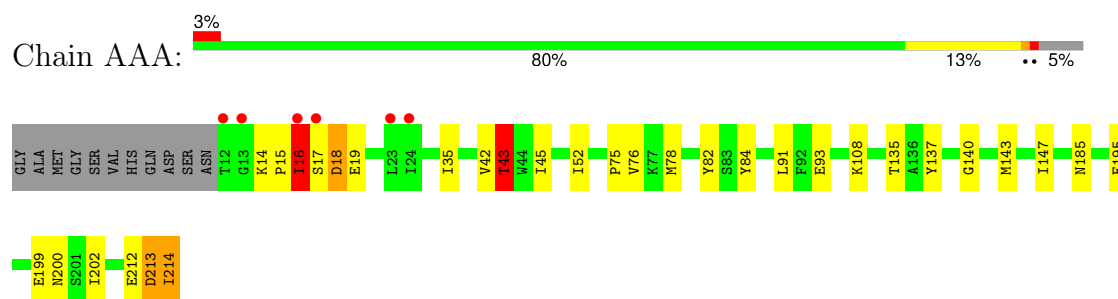
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	74	Total	O	0	0
			74	74		
3	BBB	46	Total	O	0	0
			46	46		
3	CCC	43	Total	O	0	0
			43	43		
3	DDD	85	Total	O	0	0
			85	85		

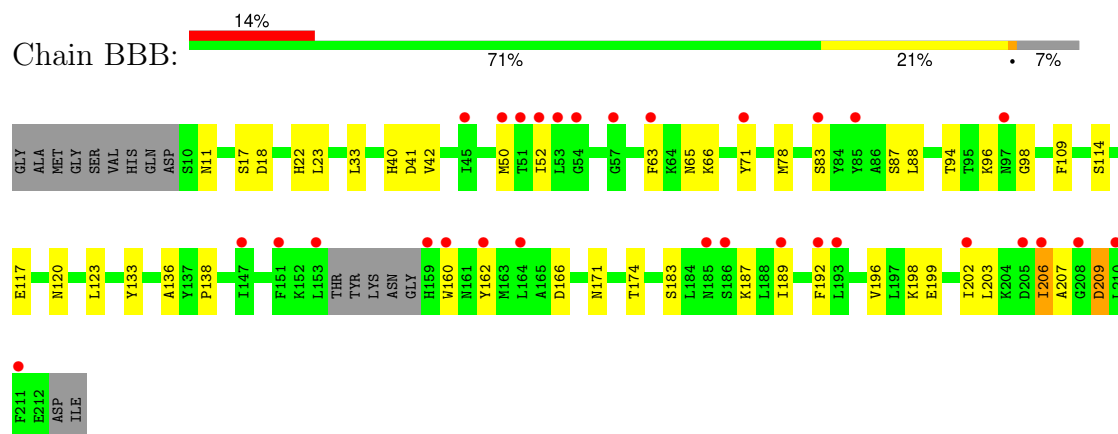
3 Residue-property plots [i](#)

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.

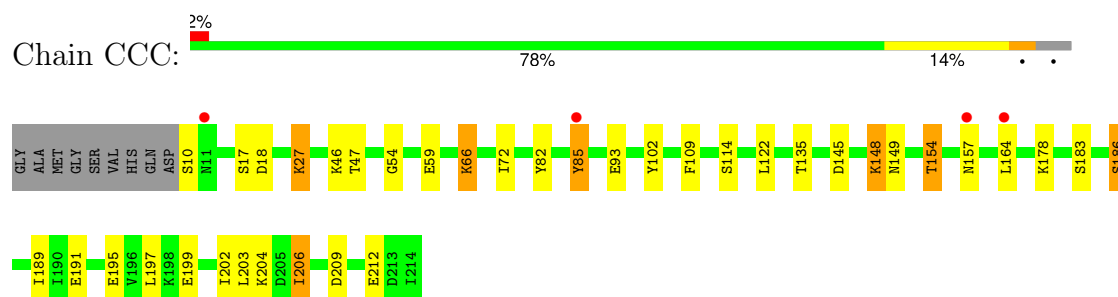
- Molecule 1: S2 lipoprotein



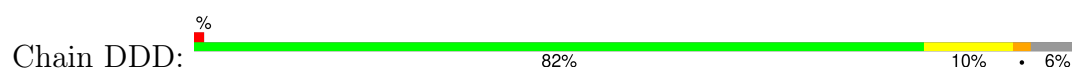
- Molecule 1: S2 lipoprotein

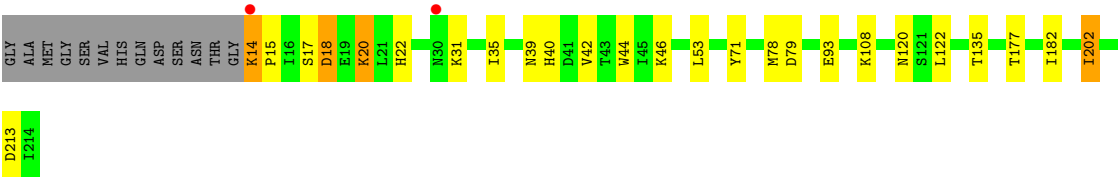


- Molecule 1: S2 lipoprotein



- Molecule 1: S2 lipoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.06Å 81.77Å 80.80Å 90.00° 109.38° 90.00°	Depositor
Resolution (Å)	44.97 – 2.40 44.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.97-2.40) 99.3 (44.97-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.213 , 0.297 0.217 , 0.299	Depositor DCC
R_{free} test set	1821 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6736	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.06	2/1658 (0.1%)	1.38	12/2234 (0.5%)
1	BBB	1.07	0/1614	1.45	4/2173 (0.2%)
1	CCC	1.06	0/1672	1.40	4/2253 (0.2%)
1	DDD	1.08	0/1647	1.36	4/2219 (0.2%)
All	All	1.07	2/6591 (0.0%)	1.40	24/8879 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	91	LEU	C-O	5.85	1.31	1.23
1	AAA	52	ILE	C-O	5.25	1.30	1.24

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	212	GLU	CA-C-N	7.75	133.85	120.68
1	AAA	212	GLU	C-N-CA	7.75	133.85	120.68
1	AAA	43	THR	CB-CA-C	7.28	121.71	109.48
1	CCC	18	ASP	CA-CB-CG	6.99	119.59	112.60
1	DDD	71	TYR	CA-C-O	-6.51	113.81	120.71

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	AAA	1628	0	1657	22	0
1	BBB	1586	0	1614	27	0
1	CCC	1642	0	1668	29	0
1	DDD	1617	0	1647	20	0
2	AAA	10	0	0	0	0
2	DDD	5	0	0	0	0
3	AAA	74	0	0	1	0
3	BBB	46	0	0	2	0
3	CCC	43	0	0	2	0
3	DDD	85	0	0	3	0
All	All	6736	0	6586	85	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 6.

The worst 5 of 85 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:AAA:15:PRO:HD2	1:BBB:65:ASN:HD22	1.33	0.92
1:DDD:14:LYS:HB3	1:DDD:15:PRO:HD3	1.53	0.88
1:AAA:16:ILE:HG22	1:AAA:18:ASP:H	1.45	0.81
1:AAA:15:PRO:HD2	1:BBB:65:ASN:ND2	1.99	0.77
1:CCC:154:THR:HG21	1:CCC:186:SER:CB	2.17	0.75

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	201/214 (94%)	195 (97%)	5 (2%)	1 (0%)	24 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	194/214 (91%)	181 (93%)	13 (7%)	0	100	100
1	CCC	203/214 (95%)	191 (94%)	12 (6%)	0	100	100
1	DDD	199/214 (93%)	194 (98%)	4 (2%)	1 (0%)	24	37
All	All	797/856 (93%)	761 (96%)	34 (4%)	2 (0%)	36	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	16	ILE
1	DDD	18	ASP

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	AAA	183/191 (96%)	177 (97%)	6 (3%)	33	55
1	BBB	179/191 (94%)	167 (93%)	12 (7%)	15	26
1	CCC	185/191 (97%)	174 (94%)	11 (6%)	18	31
1	DDD	182/191 (95%)	178 (98%)	4 (2%)	45	67
All	All	729/764 (95%)	696 (96%)	33 (4%)	24	42

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	206	ILE
1	DDD	14	LYS
1	DDD	202	ILE
1	BBB	166	ASP
1	BBB	160	TRP

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](#)

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	AAA	301	-	4,4,4	0.34	0	6,6,6	0.26	0
2	SO4	AAA	302	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	DDD	301	-	4,4,4	0.26	0	6,6,6	0.12	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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	203/214 (94%)	-0.17	6 (2%) 52 48	23, 35, 79, 116	0
1	BBB	198/214 (92%)	0.92	30 (15%) 5 4	32, 67, 98, 121	0
1	CCC	205/214 (95%)	0.34	4 (1%) 65 60	36, 54, 82, 108	0
1	DDD	201/214 (93%)	-0.18	2 (0%) 79 76	28, 37, 64, 83	0
All	All	807/856 (94%)	0.22	42 (5%) 33 29	23, 48, 90, 121	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	71	TYR	4.1
1	AAA	16	ILE	4.0
1	BBB	211	PHE	4.0
1	BBB	192	PHE	3.6
1	BBB	202	ILE	3.2

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 oligosaccharides 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, 95th 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	SO4	AAA	302	5/5	0.83	0.13	79,79,87,98	0
2	SO4	AAA	301	5/5	0.88	0.19	61,66,68,69	0
2	SO4	DDD	301	5/5	0.90	0.17	65,69,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.