



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:38 PM UTC

PDB ID : 7KWB / pdb_00007kwb
Title : Surface glycan-binding protein B from Bacteroides thetaiotaomicron
Authors : Tamura, K.; Brumer, H.; Van Petegem, F.
Deposited on : 2020-11-30
Resolution : 2.60 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	:	4-5-2 with Phenix2.0
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

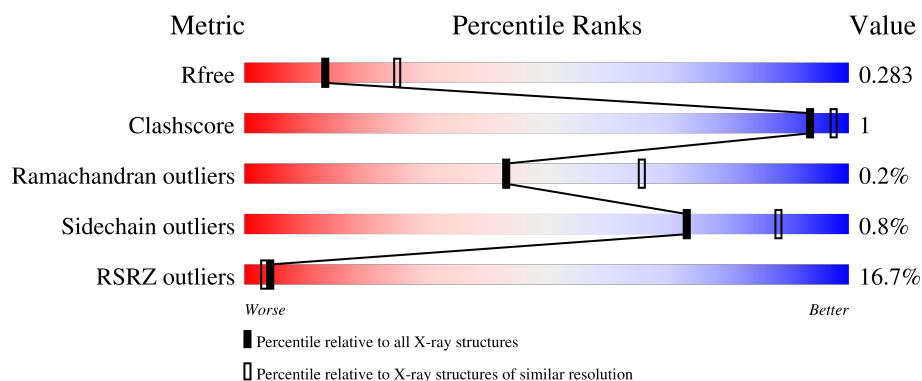
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	A	459	17% 87% 5% 8%
1	B	459	12% 81% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6208 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 BtSGBP-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3171	2023	513	627	8			
1	B	390	Total	C	N	O	S	0	0	0
			2950	1885	472	587	6			

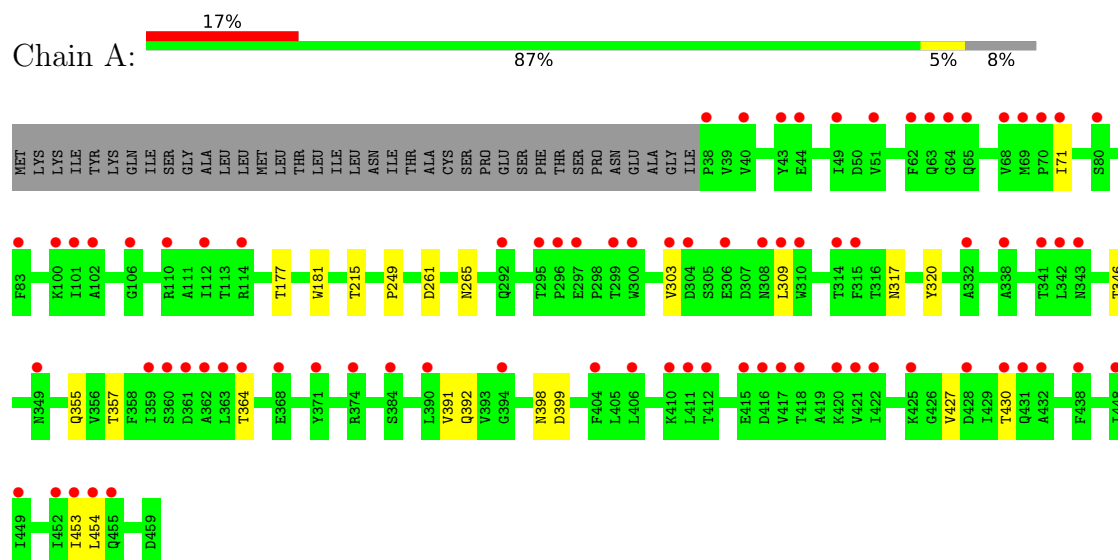
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	50	Total	O	0	0
			50	50		

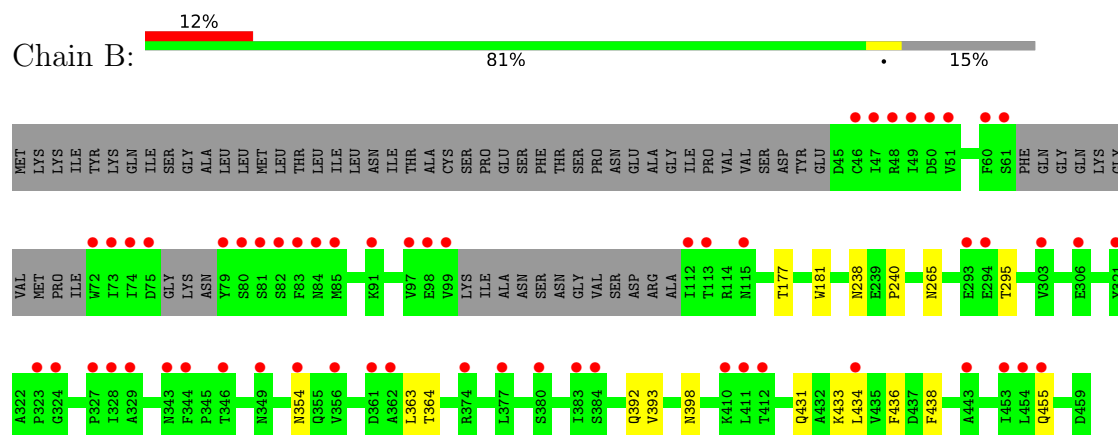
3 Residue-property plots

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: BtSGBP-B



• Molecule 1: BtSGBP-B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.10Å 182.14Å 92.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.40 – 2.60 39.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.40-2.60) 99.8 (39.40-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.286 0.239 , 0.283	Depositor DCC
R_{free} test set	2199 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6208	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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](#)

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	1.04	0/3251	1.31	2/4459 (0.0%)
1	B	1.03	0/3023	1.28	0/4148
All	All	1.04	0/6274	1.30	2/8607 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	249	PRO	CA-C-N	5.03	124.75	119.92
1	A	249	PRO	C-N-CA	5.03	124.75	119.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	455	GLN	Peptide

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	3171	0	2917	9	0
1	B	2950	0	2705	7	0
2	A	37	0	0	0	0
2	B	50	0	0	0	0
All	All	6208	0	5622	16	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 1.

All (16) 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:A:303:VAL:HA	1:A:453:ILE:HD13	1.90	0.53
1:B:238:ASN:O	1:B:240:PRO:HD3	2.10	0.51
1:A:391:VAL:CG2	1:A:399:ASP:HA	2.43	0.48
1:B:392:GLN:HG2	1:B:398:ASN:HD22	1.78	0.48
1:B:434:LEU:HD22	1:B:436:PHE:CE1	2.50	0.47
1:A:177:THR:OG1	1:A:265:ASN:ND2	2.48	0.46
1:B:177:THR:OG1	1:B:265:ASN:ND2	2.50	0.44
1:A:309:LEU:HB2	1:A:454:LEU:O	2.17	0.44
1:A:320:TYR:HB3	1:A:355:GLN:HB2	2.00	0.44
1:A:364:THR:HG22	1:A:430:THR:O	2.17	0.44
1:A:392:GLN:HG2	1:A:398:ASN:HD22	1.82	0.44
1:A:317:ASN:HA	1:A:357:THR:O	2.18	0.43
1:B:363:LEU:O	1:B:431:GLN:HA	2.19	0.42
1:B:393:VAL:HG22	1:B:433:LYS:HB3	2.00	0.42
1:A:215:THR:HB	1:A:261:ASP:HB3	2.02	0.42
1:B:354:ASN:HD21	1:B:438:PHE:HB2	1.86	0.41

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	420/459 (92%)	396 (94%)	23 (6%)	1 (0%)	43	66
1	B	382/459 (83%)	359 (94%)	22 (6%)	1 (0%)	36	58
All	All	802/918 (87%)	755 (94%)	45 (6%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	TRP
1	A	181	TRP

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	325/395 (82%)	322 (99%)	3 (1%)	70	87
1	B	304/395 (77%)	302 (99%)	2 (1%)	76	89
All	All	629/790 (80%)	624 (99%)	5 (1%)	73	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	346	THR
1	A	427	VAL
1	B	295	THR
1	B	364	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	283	ASN
1	A	355	GLN
1	A	378	ASN

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Mol	Chain	Res	Type
1	A	398	ASN
1	A	400	ASN
1	B	198	ASN
1	B	265	ASN
1	B	283	ASN
1	B	317	ASN
1	B	330	ASN
1	B	355	GLN
1	B	381	ASN
1	B	398	ASN
1	B	423	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 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

6.1 Protein, DNA and RNA chains

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	422/459 (91%)	0.92	79 (18%) 3 2	38, 82, 133, 161	0
1	B	390/459 (84%)	0.76	57 (14%) 6 4	39, 74, 124, 144	0
All	All	812/918 (88%)	0.84	136 (16%) 4 3	38, 79, 130, 161	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	TYR	6.8
1	B	361	ASP	6.6
1	B	349	ASN	5.6
1	B	46	CYS	5.3
1	A	412	THR	5.1
1	A	361	ASP	5.1
1	A	63	GLN	5.0
1	A	43	TYR	5.0
1	B	75	ASP	5.0
1	A	304	ASP	4.8
1	B	82	SER	4.7
1	A	38	PRO	4.7
1	A	415	GLU	4.4
1	B	84	ASN	4.2
1	A	303	VAL	4.2
1	B	83	PHE	4.1
1	B	81	SER	4.0
1	B	412	THR	4.0
1	A	292	GLN	4.0
1	A	416	ASP	4.0
1	A	430	THR	3.9
1	A	411	LEU	3.9
1	B	411	LEU	3.8
1	A	349	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	72	TRP	3.7
1	B	99	VAL	3.7
1	B	74	ILE	3.6
1	A	384	SER	3.6
1	A	309	LEU	3.6
1	B	362	ALA	3.5
1	B	48	ARG	3.5
1	A	453	ILE	3.3
1	A	83	PHE	3.3
1	A	362	ALA	3.3
1	A	448	ILE	3.3
1	A	314	THR	3.3
1	A	420	LYS	3.3
1	B	346	THR	3.2
1	A	417	VAL	3.2
1	A	295	THR	3.1
1	B	343	ASN	3.1
1	A	299	THR	3.1
1	B	453	ILE	3.1
1	B	60	PHE	3.1
1	A	360	SER	3.0
1	A	454	LEU	3.0
1	A	112	ILE	3.0
1	A	432	ALA	2.9
1	A	363	LEU	2.9
1	A	364	THR	2.9
1	B	303	VAL	2.9
1	B	356	VAL	2.9
1	A	438	PHE	2.9
1	B	294	GLU	2.9
1	B	61	SER	2.9
1	B	47	ILE	2.8
1	B	454	LEU	2.8
1	B	112	ILE	2.8
1	A	315	PHE	2.8
1	A	40	VAL	2.8
1	A	80	SER	2.8
1	B	80	SER	2.8
1	A	338	ALA	2.8
1	B	85	MET	2.8
1	A	394	GLY	2.7
1	A	110	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	297	GLU	2.7
1	A	69	MET	2.7
1	B	306	GLU	2.7
1	A	341	THR	2.7
1	B	410	LYS	2.7
1	A	49	ILE	2.6
1	A	71	ILE	2.6
1	A	368	GLU	2.6
1	A	308	ASN	2.6
1	A	422	ILE	2.6
1	A	64	GLY	2.5
1	A	100	LYS	2.5
1	A	332	ALA	2.5
1	B	443	ALA	2.5
1	A	306	GLU	2.5
1	B	327	PRO	2.5
1	A	65	GLN	2.5
1	A	114	ARG	2.4
1	A	452	ILE	2.4
1	B	91	LYS	2.4
1	B	115	ASN	2.4
1	A	70	PRO	2.4
1	B	97	VAL	2.4
1	B	383	ILE	2.4
1	A	428	ASP	2.4
1	A	106	GLY	2.3
1	A	406	LEU	2.3
1	A	371	TYR	2.3
1	A	410	LYS	2.3
1	A	425	LYS	2.3
1	B	49	ILE	2.3
1	A	418	THR	2.3
1	A	421	VAL	2.3
1	A	343	ASN	2.3
1	B	50	ASP	2.3
1	A	310	TRP	2.3
1	B	324	GLY	2.3
1	A	62	PHE	2.2
1	B	354	ASN	2.2
1	A	431	GLN	2.2
1	B	434	LEU	2.2
1	A	44	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	2.2
1	A	101	ILE	2.2
1	A	102	ALA	2.2
1	A	449	ILE	2.2
1	B	73	ILE	2.2
1	A	296	PRO	2.1
1	B	455	GLN	2.1
1	A	342	LEU	2.1
1	A	390	LEU	2.1
1	B	377	LEU	2.1
1	B	51	VAL	2.1
1	A	404	PHE	2.1
1	B	98	GLU	2.1
1	B	293	GLU	2.1
1	A	455	GLN	2.1
1	B	328	ILE	2.1
1	B	329	ALA	2.0
1	A	300	TRP	2.0
1	B	323	PRO	2.0
1	A	68	VAL	2.0
1	B	344	PHE	2.0
1	B	380	SER	2.0
1	B	384	SER	2.0
1	B	113	THR	2.0
1	A	359	ILE	2.0
1	A	374	ARG	2.0
1	B	374	ARG	2.0
1	B	321	TYR	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 oligosaccharides 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.