



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 04:55 pm GMT

PDB ID : 3V8U
Title : The crystal structure of transferrin binding protein B (TbpB) from *Neisseria meningitidis* serogroup B
Authors : Noinaj, N.; Easley, N.; Buchanan, S.K.
Deposited on : 2011-12-23
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 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	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

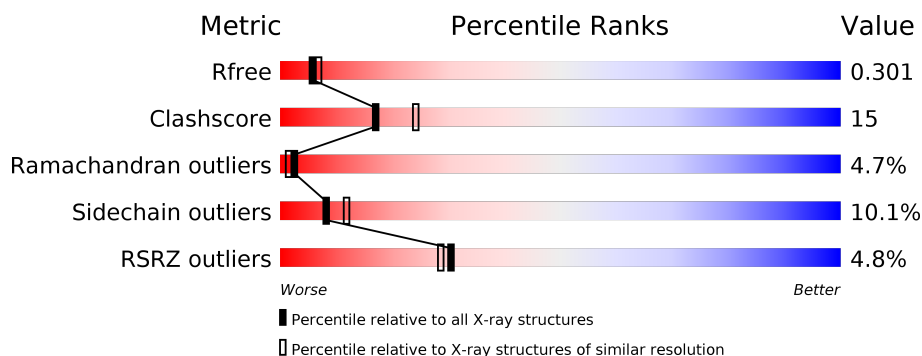
1 Overall quality at a glance

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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (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 $\leq 5\%$. 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	717	
1	B	717	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8366 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 Transferrin binding-protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4113	2586	707	814	6			
1	B	532	Total	C	N	O	S	0	0	0
			4106	2581	708	811	6			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	EXPRESSION TAG	UNP Q9JPI9
A	-24	SER	-	EXPRESSION TAG	UNP Q9JPI9
A	-23	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-22	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-21	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-20	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-19	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-18	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-17	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-16	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-15	ASP	-	EXPRESSION TAG	UNP Q9JPI9
A	-14	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-13	ASP	-	EXPRESSION TAG	UNP Q9JPI9
A	-12	ILE	-	EXPRESSION TAG	UNP Q9JPI9
A	-11	PRO	-	EXPRESSION TAG	UNP Q9JPI9
A	-10	THR	-	EXPRESSION TAG	UNP Q9JPI9
A	-9	THR	-	EXPRESSION TAG	UNP Q9JPI9
A	-8	GLU	-	EXPRESSION TAG	UNP Q9JPI9
A	-7	ASN	-	EXPRESSION TAG	UNP Q9JPI9
A	-6	LEU	-	EXPRESSION TAG	UNP Q9JPI9
A	-5	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-4	PHE	-	EXPRESSION TAG	UNP Q9JPI9
A	-3	GLN	-	EXPRESSION TAG	UNP Q9JPI9
A	-2	GLY	-	EXPRESSION TAG	UNP Q9JPI9
A	-1	ALA	-	EXPRESSION TAG	UNP Q9JPI9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q9JPI9
B	-25	MET	-	EXPRESSION TAG	UNP Q9JPI9
B	-24	SER	-	EXPRESSION TAG	UNP Q9JPI9
B	-23	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-22	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-21	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-20	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-19	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-18	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-17	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-16	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-15	ASP	-	EXPRESSION TAG	UNP Q9JPI9
B	-14	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-13	ASP	-	EXPRESSION TAG	UNP Q9JPI9
B	-12	ILE	-	EXPRESSION TAG	UNP Q9JPI9
B	-11	PRO	-	EXPRESSION TAG	UNP Q9JPI9
B	-10	THR	-	EXPRESSION TAG	UNP Q9JPI9
B	-9	THR	-	EXPRESSION TAG	UNP Q9JPI9
B	-8	GLU	-	EXPRESSION TAG	UNP Q9JPI9
B	-7	ASN	-	EXPRESSION TAG	UNP Q9JPI9
B	-6	LEU	-	EXPRESSION TAG	UNP Q9JPI9
B	-5	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-4	PHE	-	EXPRESSION TAG	UNP Q9JPI9
B	-3	GLN	-	EXPRESSION TAG	UNP Q9JPI9
B	-2	GLY	-	EXPRESSION TAG	UNP Q9JPI9
B	-1	ALA	-	EXPRESSION TAG	UNP Q9JPI9
B	0	MET	-	EXPRESSION TAG	UNP Q9JPI9

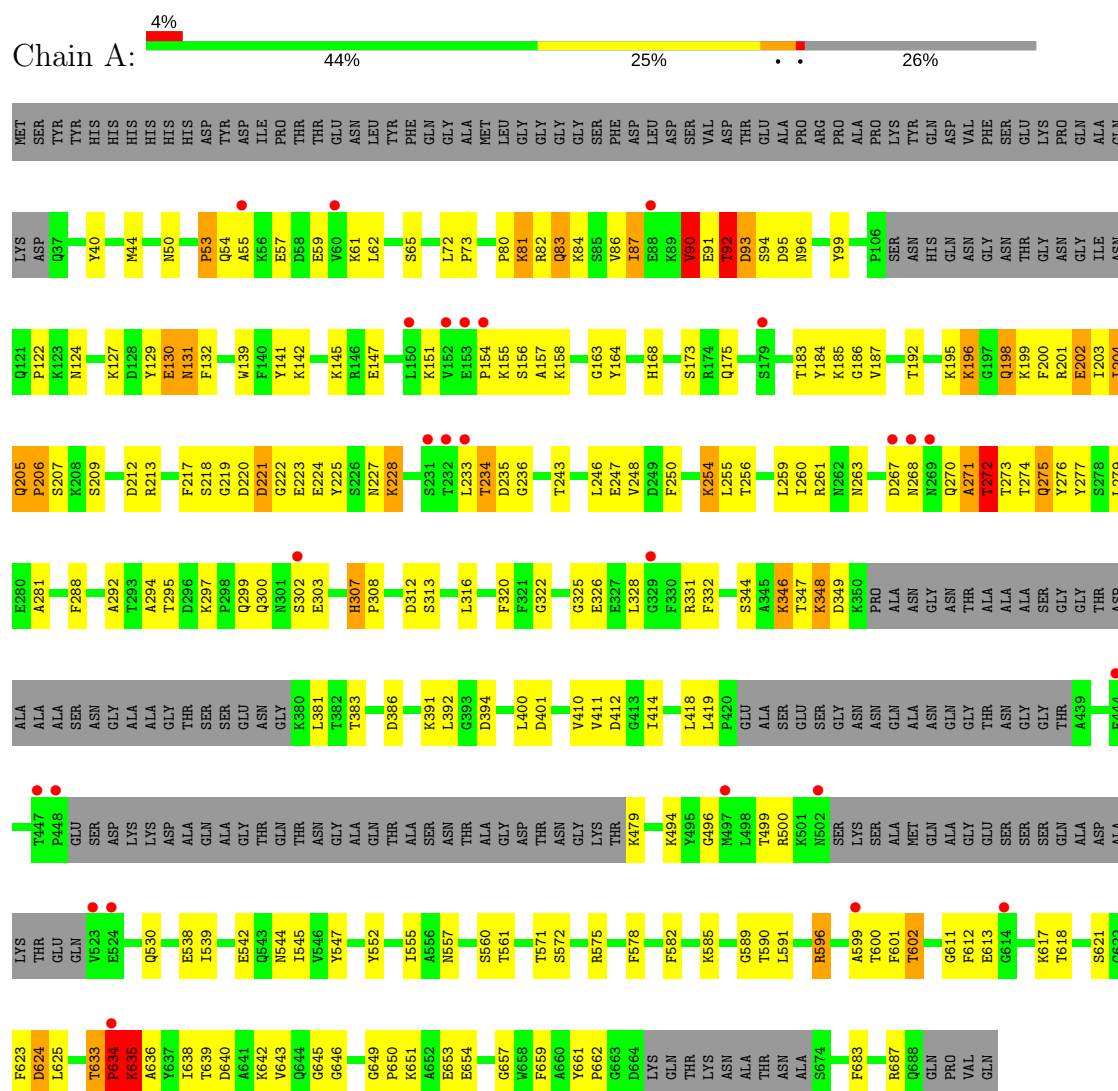
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	78	Total O 78 78	0	0
2	B	69	Total O 69 69	0	0

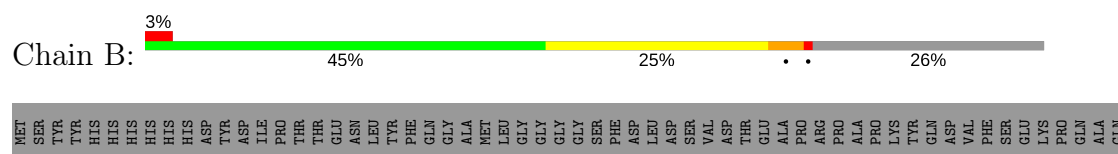
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Transferrin binding-protein B



• Molecule 1: Transferrin binding-protein B



P634	K635	A636	T637	T639	D640	A641	K642	V643	Q644	G645	G646	G649	E653	E654	G657	W658	F659	D664	LYS	GLN	THR	LYS	ASN	ALA	ALA	THR	ASN	S674	S675	V681	V682	F683	R687	G688	GLN	PRO	VAL	GLN	LYS	ASP	Q37	Y40	A43	M44	N50	P53	Q54	A55	K56	E57	D58	E59	V60	K61	L62	S65	L72	P73	P80	K81	R82	Q83	K84	S85	V86	I87	E88	K89	V90	E91	T92	D93	S94	D95	N96	Y99	P106	SER	ASN	HIS	GLN	ASN	GLY	ASN	THR	GLY	ASN	GLY	ILE	ASN	Q121	P122	K123	N124	K127	D128	Y129	E130	F131	F132	W139	F140	Y141	K142	H143	E147	L150	K151	V152	E153	P154	K155	S156	A157	K158	T243	E247	V248	F250	K254	L255	T256	L259	L260	R261	N262	N263	T266	D267	N268	N269	Q270	A271	T272	T273	T274	Q275	Y276	Y277	I203																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.03Å 82.13Å 111.31Å 90.00° 106.07° 90.00°	Depositor
Resolution (Å)	29.50 – 2.40 38.19 – 2.38	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.50-2.40) 94.4 (38.19-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.253 , 0.308 0.246 , 0.301	Depositor DCC
R_{free} test set	2001 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8366	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8259e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.50	0/4200	0.70	0/5667
1	B	0.50	0/4192	0.70	1/5655 (0.0%)
All	All	0.50	0/8392	0.70	1/11322 (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	6
1	B	0	6
All	All	0	12

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	625	LEU	N-CA-C	-7.55	90.61	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	ASP	Peptide
1	A	633	THR	Peptide
1	A	634	PRO	Peptide
1	A	90	VAL	Peptide
1	A	92	THR	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	4113	0	3871	122	0
1	B	4106	0	3871	117	0
2	A	78	0	0	4	0
2	B	69	0	0	4	0
All	All	8366	0	7742	239	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 15.

The worst 5 of 239 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:261:ARG:NH1	1:A:263:ASN:OD1	2.11	0.84
1:B:611:GLY:HA2	1:B:646:GLY:HA2	1.58	0.83
1:B:202:GLU:HB3	1:B:261:ARG:HH21	1.44	0.83
1:A:611:GLY:HA2	1:A:646:GLY:HA2	1.60	0.82
1:A:87:ILE:HD11	1:A:163:GLY:HA2	1.62	0.81

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	518/717 (72%)	446 (86%)	47 (9%)	25 (5%)	2 1
1	B	518/717 (72%)	449 (87%)	45 (9%)	24 (5%)	2 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1036/1434 (72%)	895 (86%)	92 (9%)	49 (5%)	2 1

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	93	ASP
1	A	94	SER
1	A	130	GLU
1	A	155	LYS

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	423/586 (72%)	381 (90%)	42 (10%)	8 12
1	B	422/586 (72%)	379 (90%)	43 (10%)	8 11
All	All	845/1172 (72%)	760 (90%)	85 (10%)	8 12

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	THR
1	B	87	ILE
1	B	585	LYS
1	A	625	LEU
1	B	65	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	HIS
1	B	124	ASN
1	B	307	HIS

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](#)

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	532/717 (74%)	0.28	26 (4%) 29 28	28, 62, 101, 140	0
1	B	532/717 (74%)	0.24	25 (4%) 31 29	30, 61, 101, 141	0
All	All	1064/1434 (74%)	0.26	51 (4%) 30 28	28, 62, 101, 141	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	ASN	6.3
1	A	232	THR	5.0
1	B	302	SER	4.9
1	B	674	SER	4.8
1	B	154	PRO	4.3

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 carbohydrates 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.