



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:54 PM GMT

PDB ID : 4U9C
Title : STRUCTURE OF THE LBPB N-LOBE FROM NEISSERIA MENINGITIDIS
Authors : Brooks, C.L.; Arutyunova, E.; Lemieux, M.J.
Deposited on : 2014-08-05
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

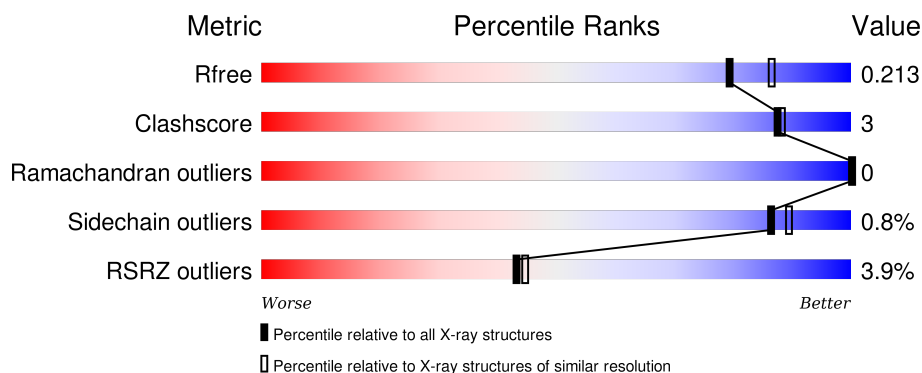
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	346	<div> <div>4%</div> <div>76%</div> <div>6%</div> <div>17%</div> </div>
1	B	346	<div> <div>3%</div> <div>82%</div> <div>5%</div> <div>13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9625 atoms, of which 4529 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 Lactoferrin-binding protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	H	N	O	S	0	0	0
			4525	1448	2216	404	455	2			
1	B	300	Total	C	H	N	O	S	0	0	0
			4726	1507	2313	423	481	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	208	Total	O	0	0
			208	208		
2	B	166	Total	O	0	0
			166	166		

- Molecule 1: Lactoferrin-binding protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.87Å 65.02Å 83.39Å 90.00° 105.87° 90.00°	Depositor
Resolution (Å)	35.09 – 2.00 35.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.09-2.00) 99.2 (35.10-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.173 , 0.213 0.173 , 0.213	Depositor DCC
R_{free} test set	2108 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41764 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9625	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	0/2356	0.60	0/3165
1	B	0.40	0/2463	0.56	0/3313
All	All	0.41	0/4819	0.58	0/6478

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 [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	2309	2216	2215	15	1
1	B	2413	2313	2313	9	1
2	A	208	0	0	8	3
2	B	166	0	0	2	1
All	All	5096	4529	4528	24	5

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 3.

All (24) 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:61:TYR:O	2:A:535:HOH:O	1.93	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LYS:NZ	2:B:401:HOH:O	2.13	0.80
1:A:148:SER:O	2:A:572:HOH:O	1.99	0.80
1:B:119:GLU:O	1:B:122:LYS:NZ	2.13	0.80
1:A:144:LYS:NZ	2:A:401:HOH:O	2.18	0.75
1:A:198:GLY:O	2:A:590:HOH:O	2.08	0.71
1:B:258:LYS:NZ	2:B:499:HOH:O	2.26	0.67
1:A:123:TYR:O	1:A:342:LYS:NZ	2.24	0.67
1:A:103:LYS:NZ	2:A:489:HOH:O	2.35	0.57
1:A:181:GLN:NE2	2:A:479:HOH:O	2.35	0.53
1:B:159:TYR:HD2	1:B:216:ILE:HD13	1.79	0.48
1:A:136:ARG:NE	2:A:537:HOH:O	2.44	0.48
1:A:319:ASP:O	1:A:320:ASN:HB2	2.15	0.47
1:B:147:THR:OG1	1:B:149:ASP:OD1	2.34	0.44
1:A:173:SER:O	1:A:320:ASN:HA	2.18	0.44
1:B:43:VAL:HG11	1:B:311:ARG:HG2	1.99	0.44
1:B:212:TYR:CE1	1:B:216:ILE:CD1	3.01	0.43
1:B:99:LYS:HA	1:B:102:LYS:HE2	2.00	0.43
1:A:260:ASN:N	1:A:261:PRO:CD	2.82	0.42
1:A:308:ALA:HB2	1:A:330:SER:HA	2.01	0.42
1:A:108:TYR:HB3	1:A:111:VAL:HG13	2.02	0.41
1:B:69:ILE:HG23	1:B:70:PRO:HD2	2.03	0.41
1:A:320:ASN:N	2:A:548:HOH:O	2.48	0.40
1:A:189:MET:SD	1:A:219:THR:HG22	2.61	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:459:HOH:O	2:A:595:HOH:O[1_565]	1.94	0.26
2:A:441:HOH:O	2:A:451:HOH:O[2_454]	2.08	0.12
2:A:421:HOH:O	2:B:438:HOH:O[1_554]	2.11	0.09
1:A:61:TYR:OH	1:A:319:ASP:OD2[1_545]	2.16	0.04
1:B:121:GLU:OE2	1:B:211:TYR:OH[2_445]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	276/346 (80%)	269 (98%)	7 (2%)	0	100	100
1	B	296/346 (86%)	290 (98%)	6 (2%)	0	100	100
All	All	572/692 (83%)	559 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	244/295 (83%)	242 (99%)	2 (1%)	86	89
1	B	256/295 (87%)	254 (99%)	2 (1%)	86	89
All	All	500/590 (85%)	496 (99%)	4 (1%)	86	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	ILE
1	A	236	TYR
1	B	149	ASP
1	B	236	TYR

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

5.3.3 RNA ⓘ

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

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	286/346 (82%)	0.18	14 (4%) 33 35	21, 32, 60, 99	0
1	B	300/346 (86%)	0.05	9 (3%) 54 55	24, 35, 59, 77	0
All	All	586/692 (84%)	0.12	23 (3%) 43 45	21, 34, 60, 99	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	ASN	5.9
1	A	72	LYS	4.0
1	A	319	ASP	3.9
1	A	255	VAL	3.6
1	A	147	THR	3.5
1	B	202	SER	3.4
1	B	204	THR	3.2
1	B	205	ASP	3.0
1	A	262	ASN	3.0
1	A	61	TYR	2.9
1	A	169	ARG	2.9
1	A	146	LYS	2.8
1	B	102	LYS	2.6
1	A	264	PRO	2.6
1	B	101	LYS	2.5
1	B	72	LYS	2.4
1	A	203	SER	2.3
1	A	141	ASP	2.3
1	B	44	ASN	2.2
1	B	149	ASP	2.2
1	B	139	GLY	2.2
1	A	197	THR	2.1
1	A	198	GLY	2.1

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.