



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2025 – 08:05 AM EDT

PDB ID : 9B0A  
Title : GA10 nanobody bound to 2C7 peptide mimitope of *Neisseria gonorrhoeae* lipooligosaccharide  
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Deposited on : 2024-03-11  
Resolution : 1.87 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

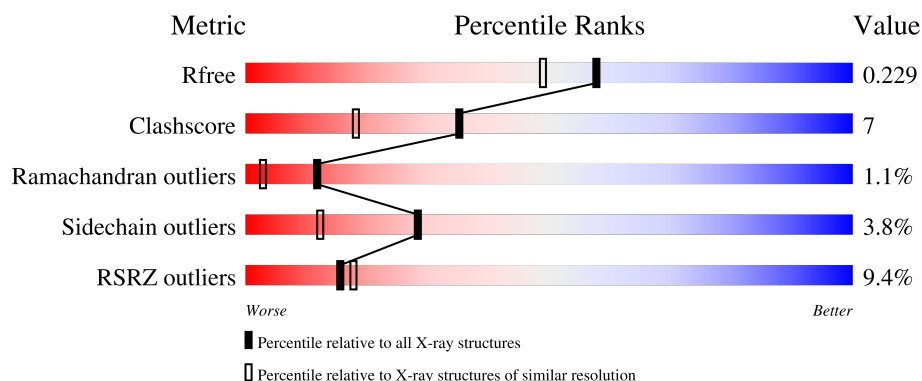
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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  $\geq 3$ , 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	167	<div> <div>5%</div> <div>61%</div> <div>10%</div> <div>•</div> <div>28%</div> </div>
1	B	167	<div> <div>7%</div> <div>63%</div> <div>7%</div> <div>••</div> <div>28%</div> </div>
2	C	18	<div> <div>17%</div> <div>83%</div> <div>17%</div> </div>
2	D	18	<div> <div>22%</div> <div>78%</div> <div>22%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4028 atoms, of which 1860 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 GA10 nanobody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	120	Total	C	H	N	O	S	0	2	0
			1715	553	827	156	175	4			
1	B	120	Total	C	H	N	O	S	0	2	0
			1705	555	812	156	178	4			

- Molecule 2 is a protein called Cyclized peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	18	Total	C	H	N	O	S	0	0	0
			231	79	110	19	21	2			
2	D	18	Total	C	H	N	O	S	0	0	0
			235	80	111	19	23	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	63	Total	O	0	0
			63	63		
3	C	10	Total	O	0	0
			10	10		
3	D	7	Total	O	0	0
			7	7		



- Molecule 1: GA10 nanobody



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	26.88Å 31.63Å 69.78Å 88.86° 87.08° 89.24°	Depositor
Resolution (Å)	34.84 – 1.87 34.84 – 1.87	Depositor EDS
% Data completeness (in resolution range)	69.1 (34.84-1.87) 69.2 (34.84-1.87)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.198 , 0.229 0.198 , 0.229	Depositor DCC
$R_{free}$ test set	1005 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.030 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.30	0/906	0.57	0/1229
1	B	0.77	5/911 (0.5%)	0.80	2/1236 (0.2%)
2	C	0.34	0/125	0.48	0/172
2	D	0.36	0/128	0.54	0/176
All	All	0.56	5/2070 (0.2%)	0.67	2/2813 (0.1%)

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	1
1	B	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	GLU	CD-OE1	11.48	1.38	1.25
1	B	89	GLU	CD-OE2	8.19	1.34	1.25
1	B	89	GLU	CB-CG	7.51	1.66	1.52
1	B	12	VAL	CB-CG1	-6.07	1.40	1.52
1	B	89	GLU	CG-CD	6.01	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	PRO	N-CD-CG	-7.58	91.84	103.20
1	B	12	VAL	CA-CB-CG2	-5.20	103.10	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	ARG	Sidechain
1	B	12	VAL	Peptide
1	B	88	PRO	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	888	827	836	13	0
1	B	893	812	843	15	1
2	C	121	110	117	1	1
2	D	124	111	119	5	0
3	A	62	0	0	0	0
3	B	63	0	0	0	0
3	C	10	0	0	1	0
3	D	7	0	0	0	0
All	All	2168	1860	1915	29	1

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 7.

The worst 5 of 29 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:B:87:LYS:HB2	1:B:88:PRO:HD3	1.31	1.09
1:B:87:LYS:HB2	1:B:88:PRO:CD	2.02	0.90
1:A:-2:SER:N	2:D:9:GLU:HG2	2.01	0.76
1:A:-2:SER:H1	2:D:9:GLU:HG2	1.54	0.70
1:B:11:LEU:O	1:B:12:VAL:HG13	1.93	0.68

All (1) 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)
1:B:74:ASN:HD21	2:C:9:GLU:OE2[1_455]	1.50	0.10

## 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	118/167 (71%)	114 (97%)	4 (3%)	0	100	100
1	B	118/167 (71%)	107 (91%)	8 (7%)	3 (2%)	4	0
2	C	16/18 (89%)	14 (88%)	2 (12%)	0	100	100
2	D	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
All	All	268/370 (72%)	250 (93%)	15 (6%)	3 (1%)	12	3

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	GLN
1	B	89	GLU
1	B	88	PRO

### 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	A	90/129 (70%)	88 (98%)	2 (2%)	47	32
1	B	92/129 (71%)	89 (97%)	3 (3%)	33	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	13/14 (93%)	11 (85%)	2 (15%)	2	0
2	D	14/14 (100%)	13 (93%)	1 (7%)	12	3
All	All	209/286 (73%)	201 (96%)	8 (4%)	28	12

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	18	CYS
2	C	18	CYS
1	B	85	SER
1	B	59	GLU
2	C	1	CYS

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

Mol	Chain	Res	Type
1	A	82	GLN
1	A	84	ASN
1	B	82	GLN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	120/167 (71%)	0.45	8 (6%) 25 27	19, 34, 59, 84	1 (0%)
1	B	120/167 (71%)	0.41	11 (9%) 16 18	17, 32, 61, 79	1 (0%)
2	C	18/18 (100%)	0.89	3 (16%) 5 5	23, 34, 66, 67	0
2	D	18/18 (100%)	1.24	4 (22%) 3 2	27, 38, 64, 84	0
All	All	276/370 (74%)	0.51	26 (9%) 15 18	17, 34, 62, 84	2 (0%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-3	GLY	7.9
2	D	2	GLY	5.7
1	A	117	ARG	5.2
1	B	100	VAL	4.3
1	A	100	VAL	4.1

### 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 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.