



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6CUJ / pdb\_00006cuj  
Title : Crystal structure of the C-terminal domain of neisserial heparin binding antigen (NHBA)  
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Deposited on : 2018-03-26  
Resolution : 1.80 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 : 4-5-2 with Phenix2.0  
Xtrriage (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

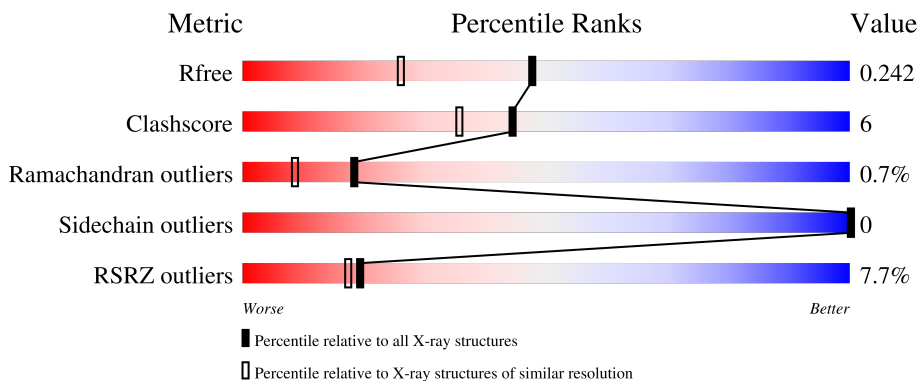
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	161	 7% 88% 6% • 6%
1	B	161	 7% 80% 11% • 9%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2367 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 Gna2132.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1144	720	200	222	2	0	0	0
1	B	146	1102	696	192	212	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	LEU	-	expression tag	UNP Q9JPP1
A	429	GLU	-	expression tag	UNP Q9JPP1
A	430	HIS	-	expression tag	UNP Q9JPP1
A	431	HIS	-	expression tag	UNP Q9JPP1
A	432	HIS	-	expression tag	UNP Q9JPP1
A	433	HIS	-	expression tag	UNP Q9JPP1
A	434	HIS	-	expression tag	UNP Q9JPP1
A	435	HIS	-	expression tag	UNP Q9JPP1
B	428	LEU	-	expression tag	UNP Q9JPP1
B	429	GLU	-	expression tag	UNP Q9JPP1
B	430	HIS	-	expression tag	UNP Q9JPP1
B	431	HIS	-	expression tag	UNP Q9JPP1
B	432	HIS	-	expression tag	UNP Q9JPP1
B	433	HIS	-	expression tag	UNP Q9JPP1
B	434	HIS	-	expression tag	UNP Q9JPP1
B	435	HIS	-	expression tag	UNP Q9JPP1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	53	Total	O	0	0
			53	53		



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.03Å 77.03Å 57.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 1.80 46.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.00-1.80) 99.9 (46.00-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 1.81Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.191 , 0.238 0.199 , 0.242	Depositor DCC
$R_{free}$ test set	1556 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.088 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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 [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	0.34	0/1173	0.61	2/1577 (0.1%)
1	B	0.30	0/1130	0.54	0/1518
All	All	0.32	0/2303	0.58	2/3095 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	GLU	CA-C-N	5.78	132.58	121.54
1	A	329	GLU	C-N-CA	5.78	132.58	121.54

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	1144	0	1076	10	0
1	B	1102	0	1035	19	0
2	A	68	0	0	3	1
2	B	53	0	0	8	1
All	All	2367	0	2111	26	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 6.

The worst 5 of 26 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:329:GLU:O	2:B:501:HOH:O	1.72	1.05
1:B:383:GLU:OE2	2:B:502:HOH:O	1.90	0.89
1:B:277:ILE:HG23	1:B:335:PRO:HG3	1.60	0.81
1:B:332:ARG:NH1	2:B:501:HOH:O	2.20	0.75
1:A:302:ARG:NH1	1:A:304:GLN:HE21	1.94	0.65

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)
2:A:540:HOH:O	2:B:539:HOH:O[4_564]	2.13	0.07

## 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	150/161 (93%)	144 (96%)	5 (3%)	1 (1%)	18	8
1	B	142/161 (88%)	137 (96%)	4 (3%)	1 (1%)	18	8
All	All	292/322 (91%)	281 (96%)	9 (3%)	2 (1%)	18	8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ASN
1	B	278	PHE

### 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	109/118 (92%)	109 (100%)	0	100	100
1	B	105/118 (89%)	105 (100%)	0	100	100
All	All	214/236 (91%)	214 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	GLN
1	A	330	ASN
1	A	426	GLN
1	B	384	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

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	152/161 (94%)	0.15	11 (7%) 21 20	18, 25, 53, 68	0
1	B	146/161 (90%)	0.51	12 (8%) 17 15	19, 31, 52, 84	0
All	All	298/322 (92%)	0.33	23 (7%) 19 17	18, 28, 54, 84	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	ILE	7.7
1	B	278	PHE	5.4
1	B	385	GLY	4.5
1	A	295	PRO	3.5
1	B	397	ALA	3.4

### 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.