



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6QN9 / pdb_00006qn9
Title : Structure of bovine anti-RSV Fab B4
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Deposited on : 2019-02-10
Resolution : 1.89 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

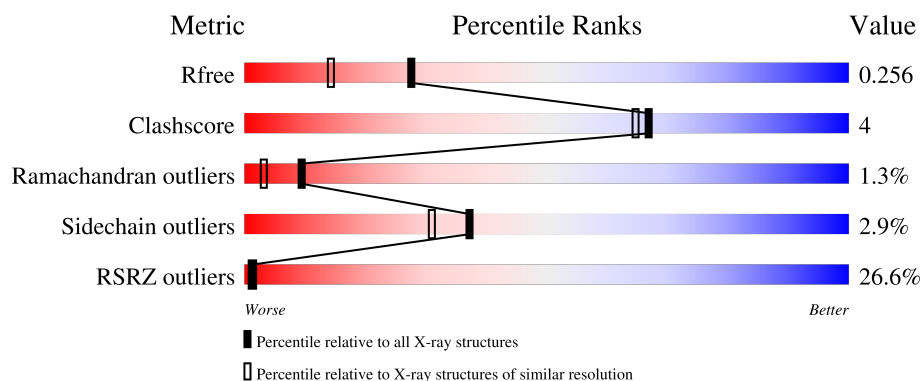
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	H	239	16% 72% 9% 19%
2	L	214	32% 86% 12% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3072 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 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	193	Total	C	N	O	S	0	0	0
			1418	886	234	288	10			

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1565	973	262	325	5			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	S	0	0
			5	4	1		

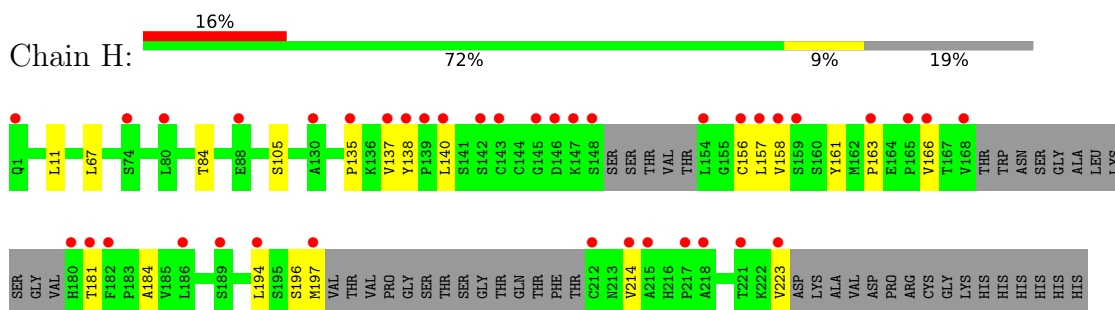
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	48	Total	O	0	0
			48	48		
5	L	24	Total	O	0	0
			24	24		

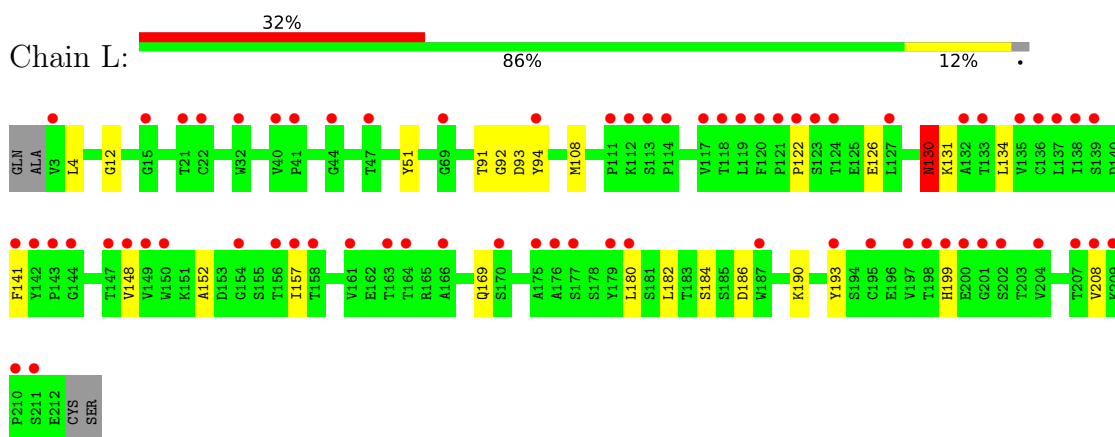
3 Residue-property plots [i](#)

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: Heavy chain



- Molecule 2: light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.33Å 134.87Å 42.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.70 – 1.89 67.70 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (67.70-1.89) 100.0 (67.70-1.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.88Å)	Xtriage
Refinement program	PHENIX (dev_3386: ???)	Depositor
R, R_{free}	0.228 , 0.254 0.231 , 0.256	Depositor DCC
R_{free} test set	1828 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	1.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3072	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	H	0.18	0/1445	0.39	0/1966
2	L	0.15	0/1599	0.37	0/2179
All	All	0.16	0/3044	0.38	0/4145

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

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	H	1418	0	1393	12	0
2	L	1565	0	1518	11	0
3	L	12	0	16	0	0
4	L	5	0	0	0	0
5	H	48	0	0	0	0
5	L	24	0	0	0	0
All	All	3072	0	2927	22	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 4.

All (22) 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)
2:L:186:ASP:O	2:L:193:TYR:OH	2.05	0.75
1:H:135:PRO:HB3	1:H:161:TYR:HB3	1.77	0.66
1:H:184:ALA:HB2	1:H:194:LEU:HD23	1.84	0.60
1:H:184:ALA:HA	1:H:194:LEU:HB3	1.87	0.56
1:H:137:VAL:HG11	1:H:223:VAL:HG11	1.88	0.55
2:L:134:LEU:HB2	2:L:180:LEU:HB3	1.89	0.54
1:H:140:LEU:HD21	1:H:157:LEU:HD22	1.91	0.53
2:L:130:ASN:HA	2:L:184:SER:HB2	1.90	0.53
1:H:214:VAL:HG22	1:H:223:VAL:HB	1.91	0.53
1:H:11:LEU:HB2	1:H:163:PRO:HG3	1.90	0.52
1:H:138:TYR:HB2	1:H:157:LEU:HD23	1.92	0.51
2:L:180:LEU:HG	2:L:182:LEU:HD23	1.92	0.51
2:L:4:LEU:HD11	2:L:91:THR:HG22	1.95	0.47
2:L:152:ALA:HB2	2:L:157:ILE:HD11	1.97	0.47
2:L:12:GLY:HA2	2:L:108:MET:HE2	1.95	0.47
2:L:190:LYS:HB2	2:L:193:TYR:CZ	2.50	0.46
1:H:166:VAL:HG12	1:H:194:LEU:HD21	1.98	0.45
1:H:105:SER:OG	2:L:92:GLY:HA3	2.19	0.43
1:H:137:VAL:HA	1:H:157:LEU:O	2.19	0.42
1:H:181:THR:HA	1:H:196:SER:HA	2.01	0.41
2:L:131:LYS:HD2	2:L:131:LYS:HA	1.95	0.41
2:L:141:PHE:HB2	2:L:199:HIS:NE2	2.36	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	H	185/239 (77%)	176 (95%)	9 (5%)	0	100	100
2	L	208/214 (97%)	191 (92%)	12 (6%)	5 (2%)	4	1
All	All	393/453 (87%)	367 (93%)	21 (5%)	5 (1%)	9	3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	122	PRO
2	L	51	TYR
2	L	94	TYR
2	L	169	GLN
2	L	130	ASN

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	H	165/204 (81%)	160 (97%)	5 (3%)	36	30
2	L	181/184 (98%)	176 (97%)	5 (3%)	38	32
All	All	346/388 (89%)	336 (97%)	10 (3%)	37	31

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	67	LEU
1	H	84	THR
1	H	156	CYS
1	H	158	VAL
1	H	197	MET
2	L	93	ASP
2	L	126	GLU
2	L	130	ASN
2	L	148	VAL
2	L	208	VAL

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	L	303	-	4,4,4	0.24	0	6,6,6	0.10	0
3	GOL	L	302	-	5,5,5	0.96	0	5,5,5	1.03	0
3	GOL	L	301	-	5,5,5	0.95	0	5,5,5	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	L	302	-	-	0/4/4/4	-
3	GOL	L	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	L	301	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	H	193/239 (80%)	1.31	39 (20%) 3 2	38, 56, 135, 155	0
2	L	210/214 (98%)	1.61	68 (32%) 1 1	38, 101, 155, 180	0
All	All	403/453 (88%)	1.46	107 (26%) 1 1	38, 65, 152, 180	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	137	LEU	4.7
1	H	154	LEU	4.5
1	H	223	VAL	4.4
2	L	208	VAL	4.3
2	L	204	VAL	4.3
1	H	138	TYR	4.1
2	L	193	TYR	4.0
1	H	157	LEU	4.0
1	H	212	CYS	3.8
2	L	3	VAL	3.6
2	L	187	TRP	3.6
1	H	215	ALA	3.5
2	L	120	PHE	3.5
1	H	168	VAL	3.5
1	H	197	MET	3.4
1	H	140	LEU	3.4
2	L	118	THR	3.4
2	L	94	TYR	3.4
1	H	218	ALA	3.4
2	L	197	VAL	3.3
2	L	119	LEU	3.3
2	L	40	VAL	3.3
1	H	181	THR	3.3
1	H	135	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	135	VAL	3.2
2	L	176	ALA	3.2
2	L	158	THR	3.2
2	L	117	VAL	3.2
1	H	166	VAL	3.1
2	L	123	SER	3.1
2	L	111	PRO	3.1
1	H	214	VAL	3.1
2	L	166	ALA	3.1
1	H	186	LEU	3.0
2	L	148	VAL	3.0
1	H	156	CYS	3.0
1	H	158	VAL	2.9
2	L	179	TYR	2.9
1	H	1	GLN	2.9
2	L	121	PRO	2.9
2	L	41	PRO	2.8
2	L	147	THR	2.8
1	H	182	PHE	2.8
2	L	144	GLY	2.8
2	L	195	CYS	2.8
2	L	15	GLY	2.8
1	H	194	LEU	2.8
2	L	138	ILE	2.7
1	H	180	HIS	2.7
2	L	143	PRO	2.7
1	H	143	CYS	2.6
2	L	163	THR	2.6
2	L	202	SER	2.6
2	L	122	PRO	2.6
2	L	164	THR	2.6
1	H	80	LEU	2.6
2	L	180	LEU	2.6
1	H	130	ALA	2.6
2	L	149	VAL	2.6
2	L	150	TRP	2.5
2	L	127	LEU	2.5
2	L	124	THR	2.5
1	H	139	PRO	2.5
1	H	217	PRO	2.5
2	L	113	SER	2.4
2	L	198	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	154	GLY	2.4
1	H	148	SER	2.4
2	L	132	ALA	2.4
1	H	142	SER	2.4
2	L	112	LYS	2.4
2	L	133	THR	2.4
2	L	175	ALA	2.4
2	L	141	PHE	2.3
2	L	201	GLY	2.3
2	L	21	THR	2.3
2	L	210	PRO	2.3
1	H	221	THR	2.3
2	L	142	TYR	2.3
2	L	157	ILE	2.3
1	H	137	VAL	2.3
2	L	136	CYS	2.3
1	H	74	SER	2.2
1	H	88	GLU	2.2
2	L	177	SER	2.2
2	L	161	VAL	2.2
1	H	163	PRO	2.2
2	L	114	PRO	2.2
2	L	200	GLU	2.2
2	L	47	THR	2.2
2	L	156	THR	2.1
1	H	159	SER	2.1
2	L	211	SER	2.1
1	H	145	GLY	2.1
2	L	69	GLY	2.1
1	H	165	PRO	2.1
1	H	146	ASP	2.1
1	H	189	SER	2.1
2	L	207	THR	2.1
1	H	147	LYS	2.1
2	L	139	SER	2.1
2	L	44	GLY	2.1
2	L	32	TRP	2.1
2	L	199	HIS	2.1
2	L	22	CYS	2.1
2	L	170	SER	2.0
2	L	209	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	L	302	6/6	0.76	0.18	97,98,98,98	0
3	GOL	L	301	6/6	0.79	0.15	79,80,80,80	0
4	SO4	L	303	5/5	0.84	0.14	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.