wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 10:50 am BST

PDB ID	:	6QN8
Title	:	Structure of bovine anti-RSV Fab B13
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Deposited on	:	2019-02-10
Resolution	:	2.12 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

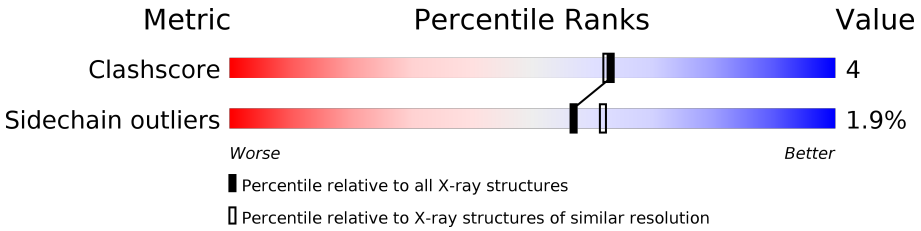
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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))
Clashscore	141614	6778 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	243	86% 7% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20946 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 of bovine anti-RSV B13 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	227	Total	C	N	O	S	0	0	0
			1687	1060	276	340	11			
1	A	235	Total	C	N	O	S	0	0	0
			1750	1097	293	349	11			
1	C	226	Total	C	N	O	S	0	0	0
			1679	1056	275	337	11			
1	E	226	Total	C	N	O	S	0	0	0
			1676	1054	274	337	11			
1	G	224	Total	C	N	O	S	0	0	0
			1663	1046	272	334	11			
1	J	227	Total	C	N	O	S	0	0	0
			1685	1059	276	339	11			

- Molecule 2 is a protein called Light chain of bovine anti-RSV Fab B13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	B	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	D	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	F	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	I	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			
2	K	213	Total	C	N	O	S	0	0	0
			1567	973	263	325	6			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	120	Total O 120 120	0	0
4	L	114	Total O 114 114	0	0
4	A	136	Total O 136 136	0	0
4	B	163	Total O 163 163	0	0
4	C	83	Total O 83 83	0	0
4	D	85	Total O 85 85	0	0
4	E	160	Total O 160 160	0	0
4	F	156	Total O 156 156	0	0
4	G	66	Total O 66 66	0	0
4	I	86	Total O 86 86	0	0
4	J	119	Total O 119 119	0	0
4	K	114	Total O 114 114	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.91Å 132.46Å 118.18Å 90.00° 102.93° 90.00°	Depositor
Resolution (Å)	87.07 – 2.12	Depositor
% Data completeness (in resolution range)	99.0 (87.07-2.12)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.235 , 0.267	Depositor
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.251	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20946	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 32.14 % 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 9.8613e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

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	0.74	1/1790 (0.1%)	0.81	0/2442
1	C	0.70	1/1715 (0.1%)	0.79	0/2342
1	E	0.70	0/1712	0.77	0/2338
1	G	0.69	0/1699	0.78	0/2320
1	H	0.72	0/1723	0.80	0/2353
1	J	0.70	0/1721	0.77	0/2350
2	B	0.74	0/1599	0.76	1/2178 (0.0%)
2	D	0.70	0/1599	0.80	0/2178
2	F	0.75	1/1599 (0.1%)	0.76	0/2178
2	I	0.70	0/1599	0.77	0/2178
2	K	0.72	0/1599	0.76	0/2178
2	L	0.70	0/1599	0.74	0/2178
All	All	0.71	3/19954 (0.0%)	0.78	1/27213 (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	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	GLU	CD-OE1	6.27	1.32	1.25
1	A	168	GLU	CD-OE1	5.62	1.31	1.25
2	F	127	GLU	CD-OE2	5.48	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	167	ARG	CB-CA-C	-5.51	99.38	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	63	LEU	Peptide

4.2 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	1750	0	1704	13	0
1	C	1679	0	1645	27	0
1	E	1676	0	1639	14	0
1	G	1663	0	1625	23	0
1	H	1687	0	1652	24	0
1	J	1685	0	1650	7	0
2	B	1567	0	1533	9	0
2	D	1567	0	1533	14	0
2	F	1567	0	1533	9	0
2	I	1567	0	1533	22	0
2	K	1567	0	1533	12	0
2	L	1567	0	1533	9	0
3	B	1	0	0	0	0
3	J	1	0	0	0	0
4	A	136	0	0	4	0
4	B	163	0	0	5	1
4	C	83	0	0	2	0
4	D	85	0	0	3	0
4	E	160	0	0	2	0
4	F	156	0	0	2	1
4	G	66	0	0	2	0
4	H	120	0	0	3	0
4	I	86	0	0	2	0
4	J	119	0	0	3	0
4	K	114	0	0	2	0
4	L	114	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20946	0	19113	167	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 4.

The worst 5 of 167 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:28:SER:OG	4:A:301:HOH:O	1.70	1.08
1:E:2:VAL:N	1:G:192:SER:O	1.93	1.01
1:H:141:VAL:O	1:H:229:LYS:NZ	1.97	0.97
1:G:41:PRO:O	4:G:301:HOH:O	1.87	0.92
1:H:2:VAL:HG13	1:H:27:LEU:HD11	1.50	0.91

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)
4:B:434:HOH:O	4:F:426:HOH:O[2_454]	2.00	0.20

4.3 Torsion angles

4.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

4.3.2 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	203/210 (97%)	202 (100%)	1 (0%)	88 92
1	C	195/210 (93%)	188 (96%)	7 (4%)	35 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	195/210 (93%)	193 (99%)	2 (1%)	76 81
1	G	193/210 (92%)	191 (99%)	2 (1%)	76 81
1	H	197/210 (94%)	192 (98%)	5 (2%)	47 50
1	J	196/210 (93%)	193 (98%)	3 (2%)	65 70
2	B	182/184 (99%)	177 (97%)	5 (3%)	44 47
2	D	182/184 (99%)	176 (97%)	6 (3%)	38 39
2	F	182/184 (99%)	180 (99%)	2 (1%)	73 79
2	I	182/184 (99%)	176 (97%)	6 (3%)	38 39
2	K	182/184 (99%)	181 (100%)	1 (0%)	88 92
2	L	182/184 (99%)	179 (98%)	3 (2%)	62 68
All	All	2271/2364 (96%)	2228 (98%)	43 (2%)	57 61

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	190	LEU
2	D	183	SER
1	J	43	LYS
1	C	234	ARG
2	D	68	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	191	GLN
2	F	201	HIS
1	J	191	GLN
2	F	70	ASN
2	F	80	GLN

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no carbohydrates in this entry.

4.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.