wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2023 – 07:33 AM EDT

PDB ID	:	3GJE
Title	:	Rational development of high-affinity T-cell receptor-like antibodies
Authors	:	Stewart-Jones, G.; Wadle, A.; Hombach, A.; Shenderov, E.; Held, G.; Fischer, E.; Kleber, S.; Stenner-Liewen, F.; Bauer, S.; McMichael, A.; Knuth, A.; Abken, H.; Hombach, A.A.; Cerundolo, V.; Jones, E.Y.; Renner, C.
Deposited on	:	2009-03-08
Resolution	:	2.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

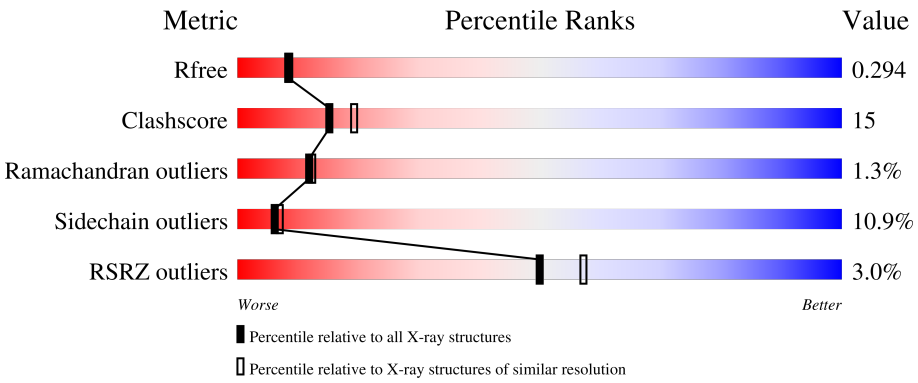
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	212	.% 73% 20% 7%
1	L	212	.% 75% 21% .
2	B	220	5% 65% 29% 5% .
2	H	220	5% 70% 25% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6813 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 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	212	1600	1001	269	326	4	0	0	0
1	A	212	1600	1001	269	326	4	0	0	0

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	220	1621	1020	269	325	7	0	0	0
2	B	220	1621	1020	269	325	7	0	0	0

- Molecule 3 is water.

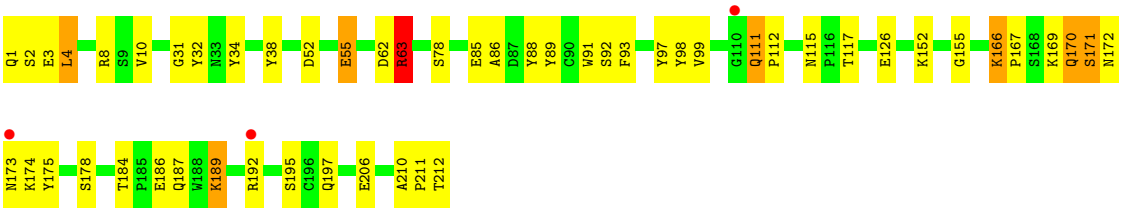
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	L	82	82	82	0	0
3	H	95	95	95	0	0
3	A	94	94	94	0	0
3	B	100	100	100	0	0

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.

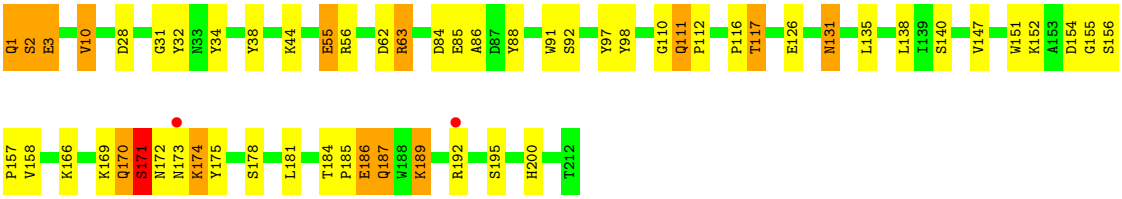
• Molecule 1: Fab Light Chain

Chain L:



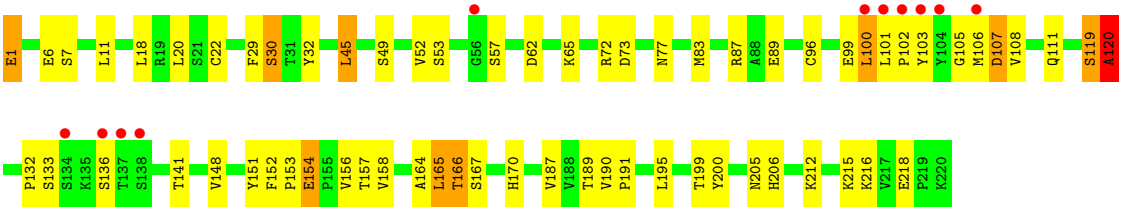
• Molecule 1: Fab Light Chain

Chain A:



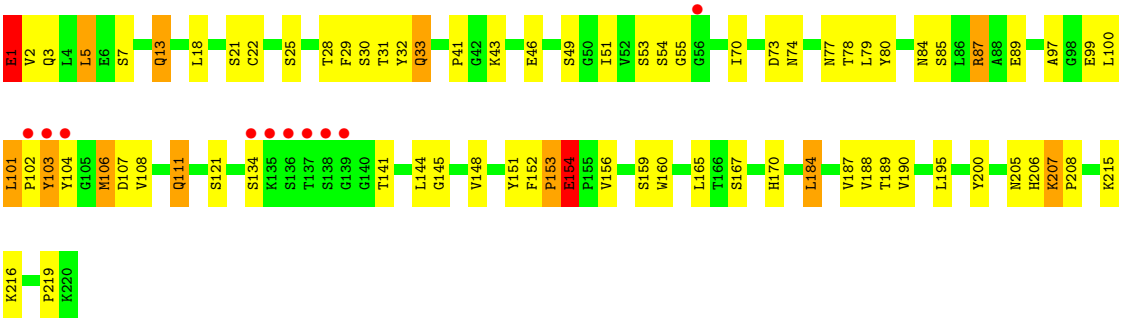
• Molecule 2: Fab Heavy Chain

Chain H:



• Molecule 2: Fab Heavy Chain

Chain B:


E1
V2
Q3
L4
L5
E6
S7
Q13
L18
S21
C22
S25
T28
F29
S30
T31
Y32
Q33
P41
G42
K43
E46
S49
G50
I51
V52
S53
S54
G55
G56
I70
D73
N74
N77
T78
L79
Y80
N84
S85
L86
R87
A88
E89
A97
G98
E99
L100
L101
P102
Y103
Y104
G105
M106
D107
V108
Q111
S121
S134
K135
S136
T137
S138
G139
G140
T141
L144
G145
V148
Y151
F152
P153
E154
P155
V156
S159
W160
L165
T166
S167
H170
L184
V187
V188
T189
V190
L195
Y200
N205
H206
K207
P208
K215
K216
P219
K220

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	117.06Å 117.06Å 78.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 30.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.00-2.30) 99.0 (30.02-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.85 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.302 0.215 , 0.294	Depositor DCC
R_{free} test set	2363 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 26.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

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	0.97	1/1641 (0.1%)	0.96	3/2240 (0.1%)
1	L	0.97	1/1641 (0.1%)	0.90	1/2240 (0.0%)
2	B	1.04	2/1658 (0.1%)	0.93	4/2257 (0.2%)
2	H	1.08	5/1658 (0.3%)	1.05	7/2257 (0.3%)
All	All	1.02	9/6598 (0.1%)	0.96	15/8994 (0.2%)

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	L	0	1
2	B	0	2
2	H	0	5
All	All	0	9

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	96	CYS	CB-SG	-9.50	1.66	1.82
2	H	1	GLU	CD-OE2	9.32	1.35	1.25
2	B	1	GLU	CD-OE2	8.79	1.35	1.25
2	H	120	ALA	N-CA	6.05	1.58	1.46
1	L	10	VAL	CA-CB	5.61	1.66	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	120	ALA	N-CA-C	-12.88	76.22	111.00
1	A	63	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	63	ARG	NE-CZ-NH1	7.54	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	119	SER	C-N-CA	6.56	138.09	121.70
2	B	152	PHE	N-CA-CB	-6.28	99.29	110.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	107	ASP	Peptide
2	H	119	SER	Peptide
2	H	151	TYR	Peptide
2	H	72	ARG	Peptide
1	L	155	GLY	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	1600	0	1534	46	0
1	L	1600	0	1534	49	0
2	B	1621	0	1592	60	0
2	H	1621	0	1592	49	0
3	A	94	0	0	7	0
3	B	100	0	0	12	0
3	H	95	0	0	6	0
3	L	82	0	0	3	0
All	All	6813	0	6252	190	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 15.

The worst 5 of 190 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:126:GLU:HB2	3:A:351:HOH:O	1.41	1.20
1:L:63:ARG:HG2	1:L:63:ARG:HH11	1.12	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:ARG:HD3	1:L:78:SER:O	1.51	1.06
1:L:211:PRO:O	1:L:212:THR:HG23	1.59	1.02
2:H:20:LEU:HG	2:H:83:MET:HE2	1.45	0.95

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	A	210/212 (99%)	188 (90%)	17 (8%)	5 (2%)	6	4
1	L	210/212 (99%)	187 (89%)	21 (10%)	2 (1%)	15	17
2	B	218/220 (99%)	194 (89%)	23 (11%)	1 (0%)	29	35
2	H	218/220 (99%)	203 (93%)	12 (6%)	3 (1%)	11	11
All	All	856/864 (99%)	772 (90%)	73 (8%)	11 (1%)	12	12

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	120	ALA
1	A	2	SER
1	A	111	GLN
1	A	156	SER
1	L	4	LEU

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	179/179 (100%)	161 (90%)	18 (10%)	7 9
1	L	179/179 (100%)	167 (93%)	12 (7%)	16 21
2	B	182/182 (100%)	152 (84%)	30 (16%)	2 2
2	H	182/182 (100%)	163 (90%)	19 (10%)	7 8
All	All	722/722 (100%)	643 (89%)	79 (11%)	6 7

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	49	SER
2	B	167	SER
2	B	87	ARG
2	B	121	SER
2	B	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
2	B	77	ASN
1	A	131	ASN
2	B	111	GLN
2	B	13	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 monosaccharides 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, 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	212/212 (100%)	-0.03	2 (0%)	84	88	24, 43, 66, 75	0
1	L	212/212 (100%)	-0.06	3 (1%)	75	80	23, 44, 66, 75	0
2	B	220/220 (100%)	0.05	10 (4%)	33	40	27, 41, 66, 81	0
2	H	220/220 (100%)	0.09	11 (5%)	28	35	28, 41, 66, 81	0
All	All	864/864 (100%)	0.01	26 (3%)	50	57	23, 42, 66, 81	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	SER	7.0
2	B	56	GLY	6.4
2	H	136	SER	6.0
2	H	56	GLY	5.9
2	B	137	THR	5.2

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.