wwPDB X-ray Structure Validation Summary Report (i)

Jul 26, 2023 – 03:01 AM EDT

PDB ID	:	1AE6
Title	:	IGG-FAB FRAGMENT OF MOUSE MONOCLONAL ANTIBODY CTM01
Authors	:	Banfield, M.J.; Brady, R.L.
Deposited on	:	1997-03-06
Resolution	:	3.00 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:

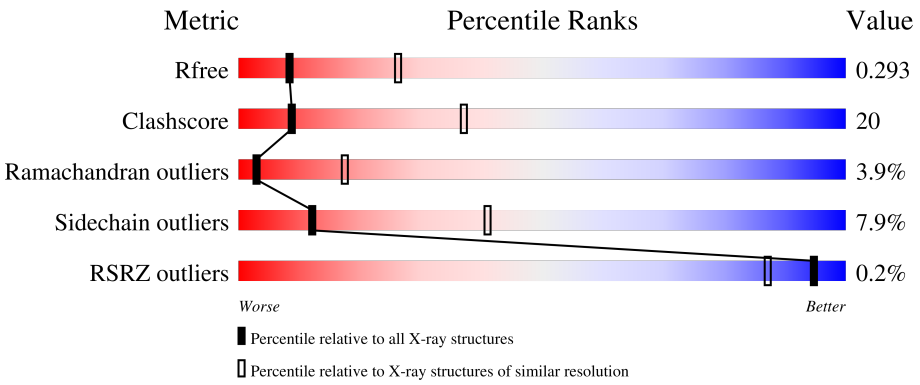
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	L	219	62% 33% 5%
2	H	218	58% 34% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3349 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 IGG CTM01 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1699	1062	288	340	9	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	ALA	SER	conflict	UNP Q8VCI6
L	8	ALA	PRO	conflict	UNP Q8VCI6
L	9	PRO	LEU	conflict	UNP Q8VCI6
L	11	VAL	LEU	conflict	UNP Q8VCI6
L	14	THR	SER	conflict	UNP Q8VCI6
L	15	PRO	LEU	conflict	UNP Q8VCI6
L	17	GLU	ASP	conflict	UNP Q8VCI6
L	18	SER	GLN	conflict	UNP Q8VCI6
L	19	LEU	ALA	conflict	UNP Q8VCI6
L	27	LYS	GLN	conflict	UNP Q8VCI6
L	27B	LEU	VAL	conflict	UNP Q8VCI6
L	27C	LEU	VAL	conflict	UNP Q8VCI6
L	30	ASP	ASN	conflict	UNP Q8VCI6
L	32	PHE	TYR	conflict	UNP Q8VCI6
L	34	TYR	GLU	conflict	UNP Q8VCI6
L	39	ARG	LYS	conflict	UNP Q8VCI6
L	45	GLN	LYS	conflict	UNP Q8VCI6
L	50	ARG	LYS	conflict	UNP Q8VCI6
L	51	MET	VAL	conflict	UNP Q8VCI6
L	54	LEU	ARG	conflict	UNP Q8VCI6
L	55	ALA	PHE	conflict	UNP Q8VCI6
L	70	ALA	ASP	conflict	UNP Q8VCI6
L	74	ARG	LYS	conflict	UNP Q8VCI6
L	75	VAL	ILE	conflict	UNP Q8VCI6
L	83	VAL	LEU	conflict	UNP Q8VCI6
L	89	MET	PHE	conflict	UNP Q8VCI6
L	91	HIS	ALA	conflict	UNP Q8VCI6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	92	LEU	SER	conflict	UNP Q8VCI6
L	93	GLU	HIS	conflict	UNP Q8VCI6
L	94	TYR	VAL	conflict	UNP Q8VCI6
L	96	PHE	TRP	conflict	UNP Q8VCI6
L	100	ALA	GLY	conflict	UNP Q8VCI6
L	106	LEU	ILE	conflict	UNP Q8VCI6
L	211	ASN	GLY	conflict	UNP Q8VCI6

- Molecule 2 is a protein called IGG CTM01 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1650	1048	264	330	8	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	LYS	ARG	conflict	UNP P01869
H	35	ASN	HIS	conflict	UNP P01869
H	37	MET	VAL	conflict	UNP P01869
H	40	LYS	ARG	conflict	UNP P01869
H	43	GLN	GLU	conflict	UNP P01869
H	52	ASP	TYR	conflict	UNP P01869
H	87	THR	SER	conflict	UNP P01869
H	?	-	GLY	deletion	UNP P01869
H	95	GLU	GLY	conflict	UNP P01869
H	97	THR	-	insertion	UNP P01869
H	98	THR	-	insertion	UNP P01869
H	99	TYR	-	insertion	UNP P01869
H	100	TYR	-	insertion	UNP P01869
H	100A	TYR	PHE	conflict	UNP P01869
H	113	ALA	SER	conflict	UNP P01869
H	118	PRO	ALA	conflict	UNP P01869
H	127	GLY	VAL	conflict	UNP P01869
H	128	SER	CYS	conflict	UNP P01869
H	129	ALA	GLY	conflict	UNP P01869
H	130	ALA	ASP	conflict	UNP P01869
H	131	GLN	THR	conflict	UNP P01869
H	133	ASN	GLY	conflict	UNP P01869
H	135	MET	SER	conflict	UNP P01869
H	152	VAL	LEU	conflict	UNP P01869
H	184	PRO	THR	conflict	UNP P01869

Continued on next page...

Continued from previous page...

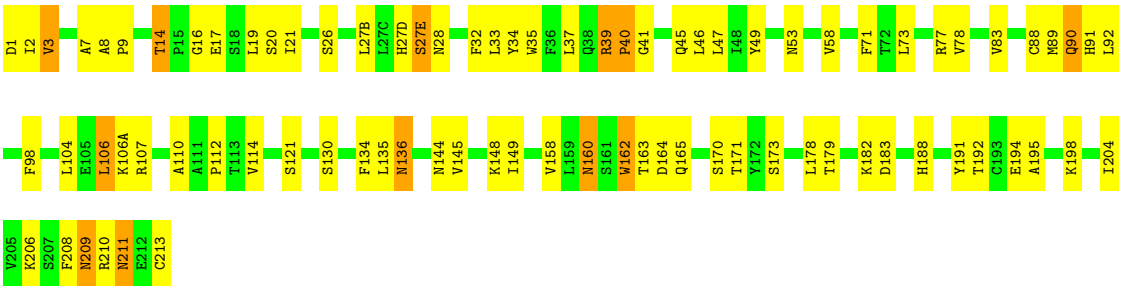
Chain	Residue	Modelled	Actual	Comment	Reference
H	187	PRO	THR	conflict	UNP P01869
H	188	ARG	TRP	conflict	UNP P01869
H	191	GLU	GLN	conflict	UNP P01869
H	192	THR	SER	conflict	UNP P01869
H	193	VAL	ILE	conflict	UNP P01869

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.

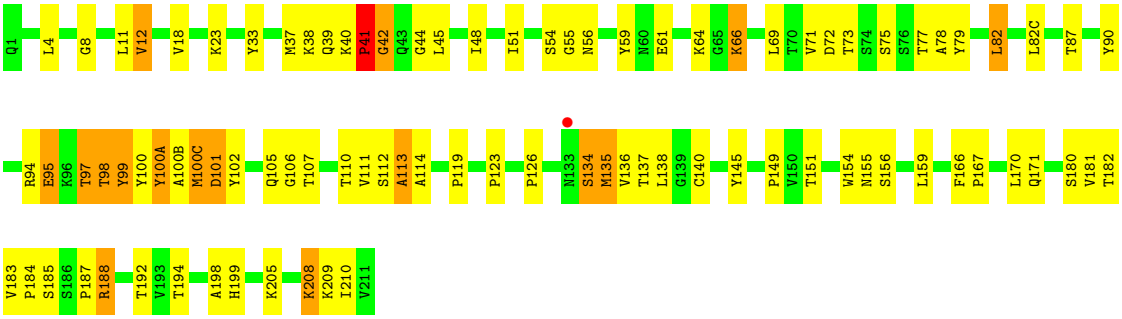
- Molecule 1: IGG CTM01 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG CTM01 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.30Å 66.55Å 61.35Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 19.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.2 (15.00-3.00) 91.1 (19.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.98Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.210 , 0.311 0.206 , 0.293	Depositor DCC
R_{free} test set	542 reflections (6.90%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 65.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3349	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 7.48% 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	L	0.33	0/1739	0.66	1/2360 (0.0%)
2	H	0.34	0/1694	0.69	0/2314
All	All	0.33	0/3433	0.67	1/4674 (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
2	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	39	ARG	C-N-CD	-5.51	108.47	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	99	TYR	Sidechain

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	L	1699	0	1634	66	0
2	H	1650	0	1615	76	0
All	All	3349	0	3249	135	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 20.

The worst 5 of 135 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:H:40:LYS:HD3	2:H:41:PRO:HD2	1.46	0.95
2:H:11:LEU:H	2:H:11:LEU:HD23	1.34	0.91
1:L:27(B):LEU:HD21	1:L:90:GLN:HB2	1.65	0.79
1:L:160:ASN:N	1:L:160:ASN:HD22	1.81	0.78
2:H:188:ARG:HH11	2:H:188:ARG:HG2	1.52	0.75

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	L	217/219 (99%)	191 (88%)	21 (10%)	5 (2%)	6 30
2	H	216/218 (99%)	179 (83%)	25 (12%)	12 (6%)	2 10
All	All	433/437 (99%)	370 (86%)	46 (11%)	17 (4%)	3 17

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	136	ASN
2	H	55	GLY
2	H	98	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	101	ASP
1	L	27(E)	SER

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	L	194/194 (100%)	180 (93%)	14 (7%)	14	45
2	H	187/187 (100%)	171 (91%)	16 (9%)	10	37
All	All	381/381 (100%)	351 (92%)	30 (8%)	12	41

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	12	VAL
2	H	170	LEU
2	H	66	LYS
2	H	208	LYS
2	H	135	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	133	ASN
2	H	164	HIS
2	H	199	HIS
2	H	171	GLN
1	L	160	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 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	L	219/219 (100%)	-0.69	0	100	100	6, 37, 82, 100	0
2	H	218/218 (100%)	-0.55	1 (0%)	91	75	9, 43, 92, 100	0
All	All	437/437 (100%)	-0.62	1 (0%)	95	87	6, 41, 88, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	ASN	2.8

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.