wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 03:50 PM EDT

PDB ID	:	1GIG
Title	:	REFINED THREE-DIMENSIONAL STRUCTURE OF THE FAB FRAGMENT OF A MURINE IGG1, LAMBDA ANTIBODY
Authors	:	Bizebard, T.; Knossow, M.
Deposited on	:	1993-01-20
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 (i)) were used in the production of this report:

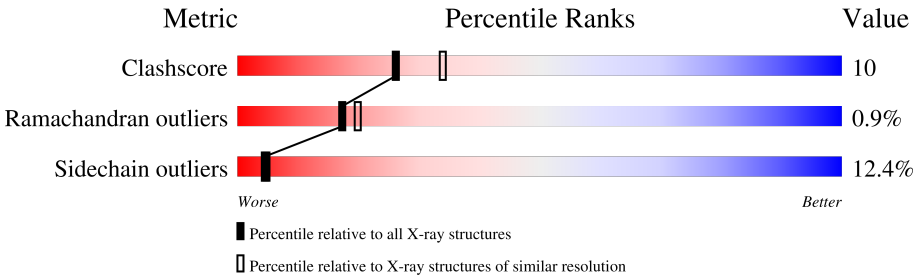
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	210	67% 26% 6% •
2	H	221	62% 32% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3352 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 IGG1-KAPPA HC19 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1589	994	266	323	6			

- Molecule 2 is a protein called IGG1-KAPPA HC19 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1672	1065	270	328	9			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	LYS	conflict	GB 4096752
H	5	LYS	GLN	conflict	GB 4096752
H	28	LEU	SER	conflict	GB 4096752
H	30	ILE	THR	conflict	GB 4096752
H	32	ASN	TYR	conflict	GB 4096752
H	63	LEU	HIS	conflict	GB 4096752
H	69	ILE	PHE	conflict	GB 4096752
H	83	LYS	ASN	conflict	GB 4096752
H	92	MET	LEU	conflict	GB 4096752
H	98	ASP	-	insertion	GB 4096752
H	99	PHE	-	insertion	GB 4096752
H	100	TYR	-	insertion	GB 4096752
H	102	TYR	HIS	conflict	GB 4096752
H	103	ASP	GLY	conflict	GB 4096752
H	105	PHE	-	insertion	GB 4096752
H	106	TYR	-	insertion	GB 4096752
H	107	TYR	-	insertion	GB 4096752
H	108	ALA	-	insertion	GB 4096752
H	109	MET	-	insertion	GB 4096752
H	110	ASP	-	insertion	GB 4096752

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Chain	Residue	Modelled	Actual	Comment	Reference
H	117	SER	LEU	conflict	GB 4096752
H	122	SER	ALA	conflict	GB 4096752
H	135	PRO	SER	conflict	GB 4096752

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	46	Total O 46 46	0	0
3	H	45	Total O 45 45	0	0

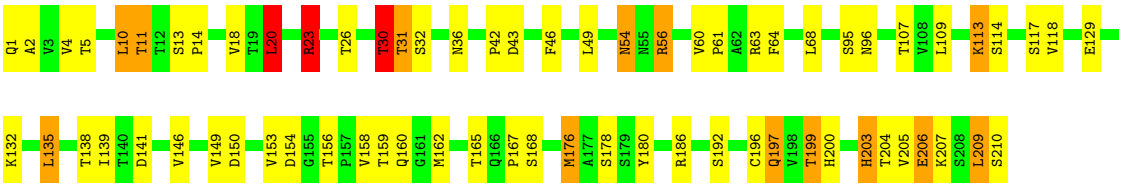
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

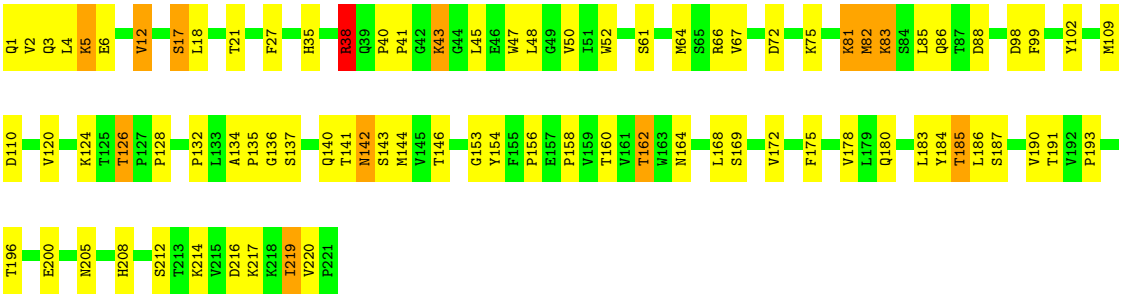
- Molecule 1: IGG1-KAPPA HC19 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG1-KAPPA HC19 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	98.90Å 98.90Å 89.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3352	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.80	0/1627	1.74	31/2224 (1.4%)
2	H	0.81	0/1718	1.67	23/2351 (1.0%)
All	All	0.80	0/3345	1.71	54/4575 (1.2%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	56	ARG	NE-CZ-NH1	13.25	126.93	120.30
2	H	66	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	L	23	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	L	23	ARG	NE-CZ-NH2	-9.36	115.62	120.30
2	H	110	ASP	CB-CG-OD1	9.24	126.62	118.30

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	L	1589	0	1532	32	0
2	H	1672	0	1635	38	0
3	H	45	0	0	0	0
3	L	46	0	0	0	0
All	All	3352	0	3167	67	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 10.

The worst 5 of 67 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:142:ASN:HD22	2:H:143:SER:H	1.13	0.97
2:H:162:THR:HG22	2:H:205:ASN:HB2	1.49	0.93
2:H:142:ASN:ND2	2:H:143:SER:H	1.70	0.89
2:H:40:PRO:HB2	2:H:43:LYS:HE2	1.56	0.87
1:L:165:THR:HG22	2:H:178:VAL:HG13	1.65	0.79

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	208/210 (99%)	198 (95%)	9 (4%)	1 (0%)	29	35
2	H	219/221 (99%)	209 (95%)	7 (3%)	3 (1%)	11	11
All	All	427/431 (99%)	407 (95%)	16 (4%)	4 (1%)	17	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	64	MET
2	H	137	SER
1	L	95	SER
2	H	142	ASN

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	178/178 (100%)	156 (88%)	22 (12%)	4 5
2	H	192/192 (100%)	168 (88%)	24 (12%)	4 5
All	All	370/370 (100%)	324 (88%)	46 (12%)	4 5

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	81	LYS
2	H	146	THR
2	H	82	MET
2	H	126	THR
2	H	160	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	208	HIS
2	H	180	GLN
2	H	35	HIS
1	L	197	GLN
2	H	142	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.