



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 02:42 AM GMT

PDB ID : 1MRC  
Title : PREPARATION, CHARACTERIZATION AND CRYSTALLIZATION OF AN ANTIBODY FAB FRAGMENT THAT RECOGNIZES RNA. CRYSTAL STRUCTURES OF NATIVE FAB AND THREE FAB-MONONUCLEOTIDE COMPLEXES  
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Deposited on : 1994-06-13  
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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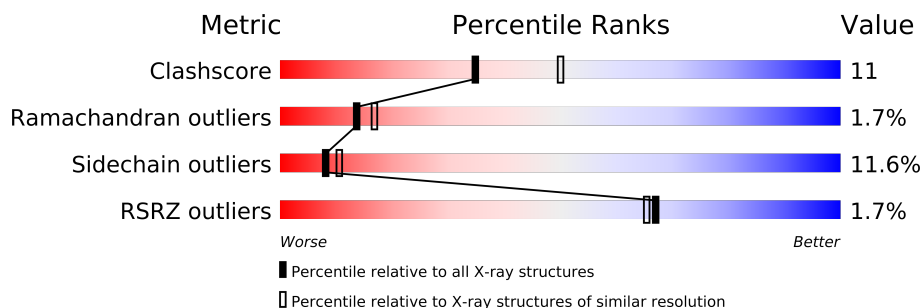
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	219	
2	H	215	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3218 atoms, of which 0 are hydrogen and 0 are deuterium.

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 IGG2B-KAPPA JEL103 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1627	1020	274	327	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	VAL	LEU	CONFLICT	PIR PC4203
L	27B	LEU	ILE	CONFLICT	PIR PC4203
L	27A	SER	THR	CONFLICT	PIR PC4203
L	34	HIS	GLU	CONFLICT	PIR PC4203
L	87	PHE	TYR	CONFLICT	PIR PC4203
L	89	SER	PHE	CONFLICT	PIR PC4203
L	91	SER	GLY	CONFLICT	PIR PC4203
L	92	THR	SER	CONFLICT	PIR PC4203
L	153	LYS	SER	CONFLICT	PIR PC4203
L	167	ASN	ASP	CONFLICT	PIR PC4203

- Molecule 2 is a protein called IGG2B-KAPPA JEL103 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	204	Total	C	N	O	S	0	0	0
			1508	960	240	301	7			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	LYS	ARG	CONFLICT	GB 387221
H	16	ALA	THR	CONFLICT	GB 387221
H	20	LEU	MET	CONFLICT	GB 387221
H	25	SER	ALA	CONFLICT	GB 387221
H	31	SER	ASN	CONFLICT	GB 387221
H	34	MET	ILE	CONFLICT	GB 387221

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Chain	Residue	Modelled	Actual	Comment	Reference
H	35	GLN	GLY	CONFLICT	GB 387221
H	39	GLN	GLU	CONFLICT	GB 387221
H	43	GLN	HIS	CONFLICT	GB 387221
H	50	GLU	ASP	CONFLICT	GB 387221
H	51A	ASP	TYR	CONFLICT	GB 387221
H	53	SER	GLY	CONFLICT	GB 387221
H	54	ASP	GLY	CONFLICT	GB 387221
H	55	SER	GLY	CONFLICT	GB 387221
H	56	TYR	PHE	CONFLICT	GB 387221
H	61	GLN	GLU	CONFLICT	GB 387221
H	62	LYS	ASN	CONFLICT	GB 387221
H	71	VAL	ALA	CONFLICT	GB 387221
H	89	VAL	ILE	CONFLICT	GB 387221
H	91	TYR	HIS	CONFLICT	GB 387221
H	?	-	ARG	DELETION	GB 387221
H	?	-	GLY	DELETION	GB 387221
H	?	-	ILE	DELETION	GB 387221
H	?	-	TYR	DELETION	GB 387221
H	?	-	TYR	DELETION	GB 387221
H	95	LEU	SER	CONFLICT	GB 387221
H	96	ARG	SER	CONFLICT	GB 387221
H	97	GLY	PRO	CONFLICT	GB 387221
H	102	TYR	SER	CONFLICT	GB 387221
H	140	LEU	SER	CONFLICT	GB 387221
H	151	SER	PRO	CONFLICT	GB 387221

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

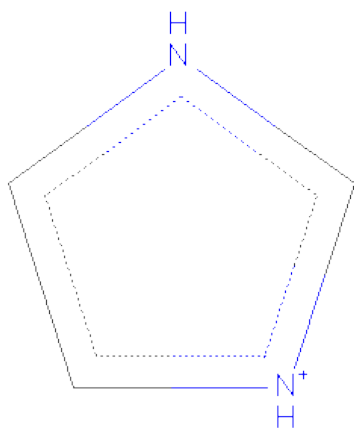
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	N	0	0
			5	3	2		

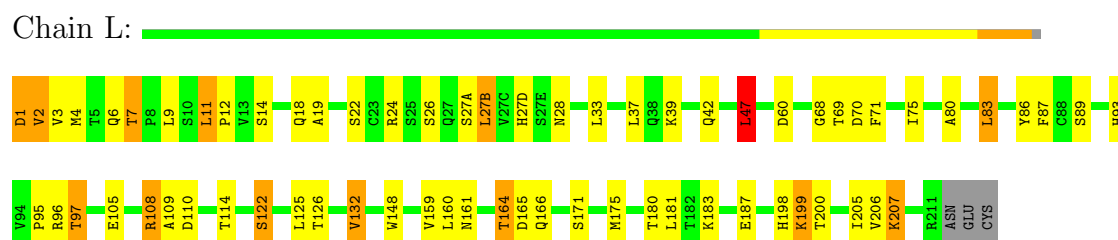
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	36	Total 36	O 36	0	0
6	L	36	Total 36	O 36	0	0

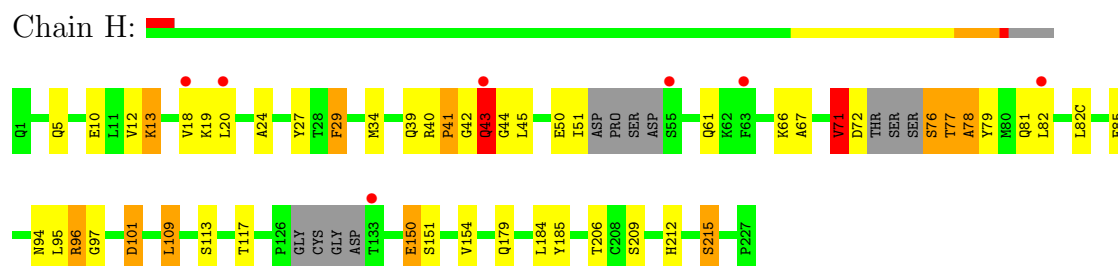
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: IGG2B-KAPPA JEL103 FAB (LIGHT CHAIN)



- Molecule 2: IGG2B-KAPPA JEL103 FAB (HEAVY CHAIN)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.40Å 75.70Å 106.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 49.92 – 2.04	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 75.4 (49.92-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.03Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.191 , (Not available) 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26473 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IMD, 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	L	0.52	0/1665	0.83	2/2269 (0.1%)
2	H	0.51	0/1546	0.84	2/2112 (0.1%)
All	All	0.52	0/3211	0.84	4/4381 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	215	SER	N-CA-C	-7.42	90.96	111.00
1	L	11	LEU	CA-CB-CG	6.18	129.50	115.30
1	L	47	LEU	CA-CB-CG	5.21	127.29	115.30
2	H	78	ALA	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1627	0	1524	36	0
2	H	1508	0	1428	31	0
3	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	5	0	0	0	0
5	L	5	0	4	0	0
6	H	36	0	0	0	0
6	L	36	0	0	1	0
All	All	3218	0	2956	65	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 65 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:2:VAL:O	1:L:97:THR:HG21	1.94	0.67
1:L:80:ALA:O	1:L:83:LEU:HD22	1.97	0.65
2:H:150:GLU:HG3	2:H:185:TYR:CZ	2.32	0.64
2:H:10:GLU:HB3	2:H:109:LEU:HD23	1.79	0.63
2:H:13:LYS:HE2	2:H:113:SER:HA	1.80	0.62

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	214/219 (98%)	206 (96%)	6 (3%)	2 (1%)	25	35
2	H	196/215 (91%)	184 (94%)	7 (4%)	5 (3%)	8	8
All	All	410/434 (94%)	390 (95%)	13 (3%)	7 (2%)	14	17

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	2	VAL
2	H	41	PRO
2	H	150	GLU
1	L	68	GLY

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Mol	Chain	Res	Type
2	H	43	GLN

### 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	L	180/197 (91%)	156 (87%)	24 (13%)	6	7
2	H	165/186 (89%)	149 (90%)	16 (10%)	12	17
All	All	345/383 (90%)	305 (88%)	40 (12%)	8	10

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	180	THR
1	L	199	LYS
2	H	96	ARG
1	L	183	LYS
1	L	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	93	HIS
1	L	157	ASN
2	H	3	GLN
2	H	5	GLN
2	H	81	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
5	IMD	L	902	3	5,5,5	0.77	0	5,5,5	1.20	0
4	SO4	L	903	-	4,4,4	0.30	0	6,6,6	0.55	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
5	IMD	L	902	3	-	0/0/0/0	0/1/1/1
4	SO4	L	903	-	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	216/219 (98%)	-0.46	0 <span>100</span> <span>100</span>	14, 32, 52, 67	0
2	H	204/215 (94%)	-0.11	7 (3%) <span>43</span> <span>41</span>	11, 41, 73, 92	0
All	All	420/434 (96%)	-0.29	7 (1%) <span>67</span> <span>65</span>	11, 35, 69, 92	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	55	SER	3.8
2	H	43	GLN	2.7
2	H	133	THR	2.7
2	H	18	VAL	2.6
2	H	82	LEU	2.4

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	L	903	5/5	0.17	-	79,80,80,81	0
5	IMD	L	902	5/5	0.17	-	38,39,41,41	0
3	ZN	L	600	1/1	0.11	-	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.