



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:32 PM GMT

PDB ID : 1BBD  
Title : THREE DIMENSIONAL STRUCTURE OF THE FAB FRAGMENT OF A  
NEUTRALIZING ANTIBODY TO HUMAN RHINOVIRUS SEROTYPE 2  
Authors : Tormo, J.; Blaas, D.; Fita, I.  
Deposited on : 1992-05-05  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

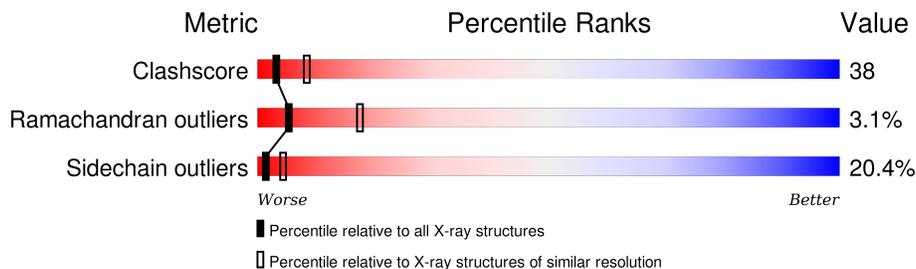
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	220	 27% 44% 23% 5%
2	H	218	 36% 39% 18% 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3342 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 IGG2A-KAPPA 8F5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1707	1063	286	351	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	12	THR	SER	CONFLICT	GB 208622
L	14	THR	SER	CONFLICT	GB 208622
L	15	THR	ALA	CONFLICT	GB 208622
L	18	LYS	ARG	CONFLICT	GB 208622
L	22	THR	SER	CONFLICT	GB 208622
L	33	ARG	GLY	CONFLICT	GB 208622
L	34	THR	ASN	CONFLICT	GB 208622
L	38	TYR	PHE	CONFLICT	GB 208622
L	40	THR	ALA	CONFLICT	GB 208622
L	49	SER	PRO	CONFLICT	GB 208622
L	56	TRP	GLY	CONFLICT	GB 208622
L	80	SER	THR	CONFLICT	GB 208622
L	83	GLY	SER	CONFLICT	GB 208622
L	97	ASN	ASP	CONFLICT	GB 208622
L	98	TYR	HIS	CONFLICT	GB 208622
L	99	ASN	SER	CONFLICT	GB 208622

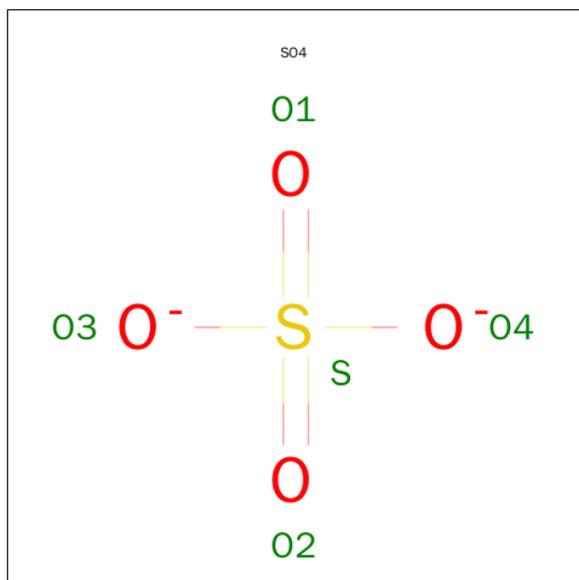
- Molecule 2 is a protein called IGG2A-KAPPA 8F5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	213	1625	1032	259	328	6	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	ARG	LYS	CONFLICT	GB 2072133
H	16	ALA	THR	CONFLICT	GB 2072133
H	24	THR	ALA	CONFLICT	GB 2072133
H	32	ILE	THR	CONFLICT	GB 2072133
H	35	HIS	TYR	CONFLICT	GB 2072133
H	51	LEU	ILE	CONFLICT	GB 2072133
H	57	TYR	ASN	CONFLICT	GB 2072133
H	59	LYS	GLU	CONFLICT	GB 2072133
H	60	TYR	PHE	CONFLICT	GB 2072133
H	63	LYS	ARG	CONFLICT	GB 2072133
H	65	GLN	LEU	CONFLICT	GB 2072133
H	72	VAL	ALA	CONFLICT	GB 2072133
H	82	HIS	GLN	CONFLICT	GB 2072133
H	83	LEU	VAL	CONFLICT	GB 2072133
H	97	ASP	-	INSERTION	GB 2072133
H	98	GLY	-	INSERTION	GB 2072133
H	99	TYR	-	INSERTION	GB 2072133
H	100	TYR	-	INSERTION	GB 2072133
H	101	SER	-	INSERTION	GB 2072133
H	102	TYR	HIS	CONFLICT	GB 2072133
H	103	TYR	LEU	CONFLICT	GB 2072133
H	104	ASP	HIS	CONFLICT	GB 2072133
H	105	MET	GLY	CONFLICT	GB 2072133
H	106	ASP	PRO	CONFLICT	GB 2072133
H	110	PRO	GLN	CONFLICT	GB 2072133
H	113	SER	LEU	CONFLICT	GB 2072133
H	118	SER	ALA	CONFLICT	GB 2072133

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

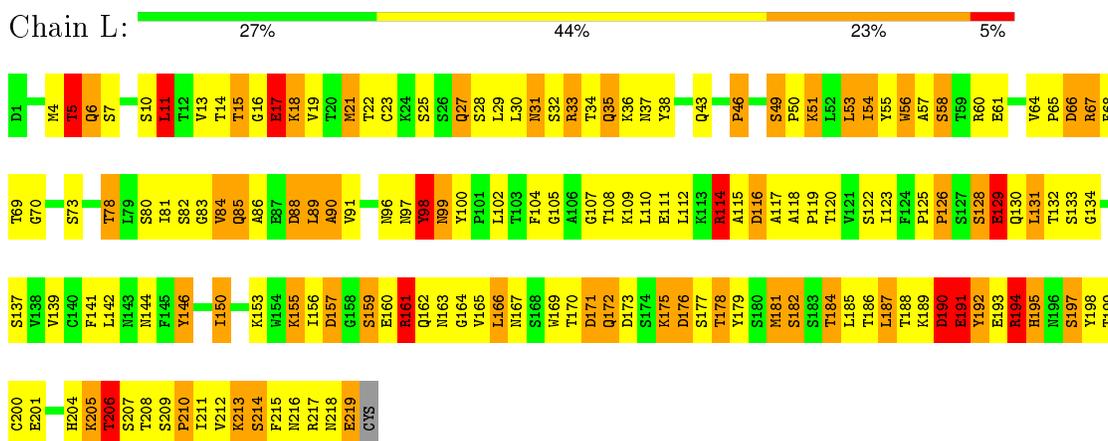
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	5	Total	O	0	0
			5	5		

### 3 Residue-property plots [i](#)

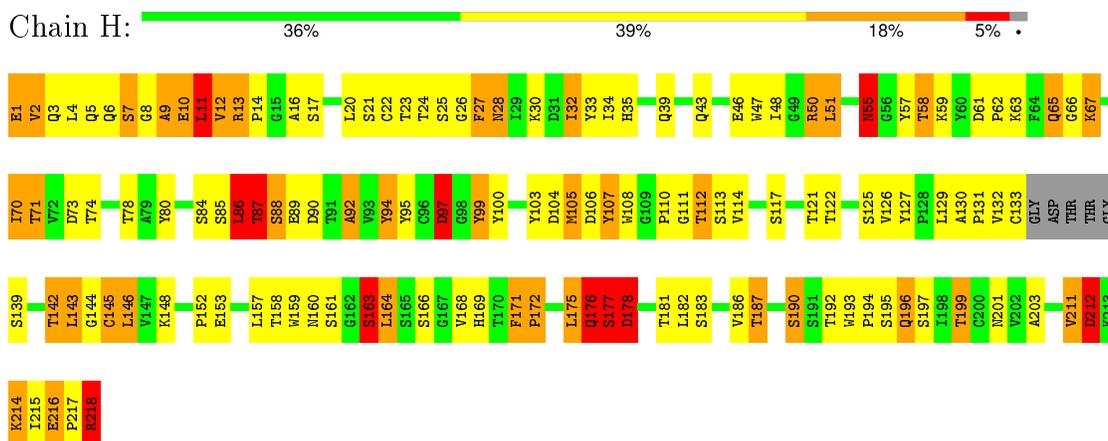
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: IGG2A-KAPPA 8F5 FAB (LIGHT CHAIN)



- Molecule 2: IGG2A-KAPPA 8F5 FAB (HEAVY CHAIN)



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.70Å 86.80Å 128.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.23	1/1744 (0.1%)	2.40	76/2370 (3.2%)
2	H	1.31	4/1669 (0.2%)	2.23	86/2285 (3.8%)
All	All	1.27	5/3413 (0.1%)	2.32	162/4655 (3.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8	GLY	N-CA	8.30	1.58	1.46
2	H	88	SER	CB-OG	6.26	1.50	1.42
2	H	22	CYS	CB-SG	-5.59	1.72	1.81
2	H	125	SER	N-CA	5.04	1.56	1.46
1	L	114	ARG	CD-NE	-5.03	1.38	1.46

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	114	ARG	CD-NE-CZ	26.00	160.01	123.60
1	L	33	ARG	CD-NE-CZ	21.83	154.16	123.60
1	L	60	ARG	NE-CZ-NH1	20.09	130.35	120.30
1	L	60	ARG	NE-CZ-NH2	-18.52	111.04	120.30
1	L	33	ARG	NE-CZ-NH1	17.65	129.12	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1707	0	1644	155	0
2	H	1625	0	1565	100	0
3	H	5	0	0	0	0
4	H	5	0	0	1	0
All	All	3342	0	3209	246	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 38.

The worst 5 of 246 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:L:204:HIS:CD2	1:L:206:THR:HB	1.72	1.25
1:L:118:ALA:HB2	1:L:206:THR:CG2	1.76	1.16
2:H:176:GLN:O	2:H:177:SER:HB3	1.52	1.09
1:L:118:ALA:CB	1:L:206:THR:HG21	1.83	1.08
2:H:192:THR:HG23	2:H:196:GLN:NE2	1.68	1.07

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	217/220 (99%)	194 (89%)	14 (6%)	9 (4%)	<b>3</b> <b>11</b>
2	H	209/218 (96%)	187 (90%)	18 (9%)	4 (2%)	<b>10</b> <b>32</b>
All	All	426/438 (97%)	381 (89%)	32 (8%)	13 (3%)	<b>5</b> <b>17</b>

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	17	GLU
1	L	33	ARG
1	L	191	GLU
1	L	190	ASP
1	L	205	LYS

### 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	197/198 (100%)	152 (77%)	45 (23%)	<b>1</b> <b>3</b>
2	H	186/190 (98%)	153 (82%)	33 (18%)	<b>2</b> <b>7</b>
All	All	383/388 (99%)	305 (80%)	78 (20%)	<b>1</b> <b>4</b>

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	181	MET
1	L	208	THR
2	H	197	SER
1	L	182	SER
1	L	194	ARG

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

Mol	Chain	Res	Type
1	L	143	ASN
2	H	196	GLN
1	L	162	GLN
1	L	48	GLN
1	L	144	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z  > 2$
3	SO4	H	720	-	4,4,4	0.92	0	6,6,6	0.42	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
3	SO4	H	720	-	-	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.

No monomer is involved in short contacts.

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.