



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1IAI
Title : IDIOTYPE-ANTI-IDIOTYPE FAB COMPLEX
Authors : Ban, N.; Escobar, C.; Garcia, R.; Hasel, K.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on : 1993-12-28
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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)
Xtriage (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

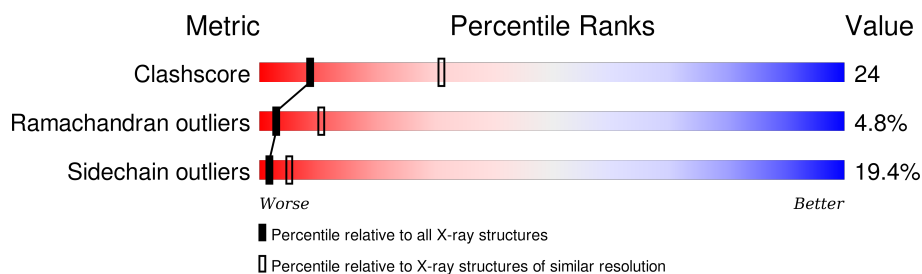
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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 ≥ 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	214	
2	H	219	
3	M	215	
4	I	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6672 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 IDIOTYPIC FAB 730.1.4 (IGG1) OF VIRUS NEUTRALIZING ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1675	1045	281	341	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	8	HIS	GLN	CONFLICT	GB 10121892
L	21	ILE	VAL	CONFLICT	GB 10121892
L	28	ASP	ASN	CONFLICT	GB 10121892
L	30	SER	GLY	CONFLICT	GB 10121892
L	32	ALA	ASN	CONFLICT	GB 10121892
L	46	LEU	ALA	CONFLICT	GB 10121892
L	54	GLN	ARG	CONFLICT	GB 10121892
L	56	THR	SER	CONFLICT	GB 10121892
L	68	ARG	GLY	CONFLICT	GB 10121892
L	73	PHE	LEU	CONFLICT	GB 10121892
L	76	ASN	SER	CONFLICT	GB 10121892
L	77	SER	ASN	CONFLICT	GB 10121892
L	80	ALA	SER	CONFLICT	GB 10121892
L	85	VAL	GLU	CONFLICT	GB 10121892
L	87	TYR	PHE	CONFLICT	GB 10121892
L	89	HIS	GLN	CONFLICT	GB 10121892
L	91	HIS	TYR	CONFLICT	GB 10121892
L	92	TYR	ASN	CONFLICT	GB 10121892
L	94	THR	TYR	CONFLICT	GB 10121892
L	96	PHE	LEU	CONFLICT	GB 10121892
L	100	SER	ALA	CONFLICT	GB 10121892
L	106	ILE	LEU	CONFLICT	GB 10121892

- Molecule 2 is a protein called IDIOTYPIC FAB 730.1.4 (IGG1) OF VIRUS NEUTRALIZING ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1666	1057	265	336	8			

- Molecule 3 is a protein called ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	215	Total	C	N	O	S	0	0	0
			1655	1029	273	345	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	3	GLN	VAL	CONFLICT	GB 1042224
M	10	PHE	ILE	CONFLICT	GB 1042224
M	12	ALA	SER	CONFLICT	GB 1042224
M	18	LYS	ARG	CONFLICT	GB 1042224
M	21	ILE	MET	CONFLICT	GB 1042224
M	25	VAL	ALA	CONFLICT	GB 1042224
M	26	SER	ASN	CONFLICT	GB 1042224
M	28	SER	-	INSERTION	GB 1042224
M	29	ILE	-	INSERTION	GB 1042224
M	31	SER	VAL	CONFLICT	GB 1042224
M	33	ASN	TYR	CONFLICT	GB 1042224
M	34	LEU	MET	CONFLICT	GB 1042224
M	42	GLU	GLY	CONFLICT	GB 1042224
M	47	PRO	ARG	CONFLICT	GB 1042224
M	51	GLY	ASP	CONFLICT	GB 1042224
M	54	ASN	LYS	CONFLICT	GB 1042224
M	61	VAL	ALA	CONFLICT	GB 1042224
M	93	ASN	SER	CONFLICT	GB 1042224
M	95	TYR	HIS	CONFLICT	GB 1042224
M	114	PRO	GLN	CONFLICT	GB 1042224

- Molecule 4 is a protein called ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	218	Total	C	N	O	S	0	0	0
			1676	1066	277	325	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	5	GLN	GLU	CONFLICT	GB 1042226

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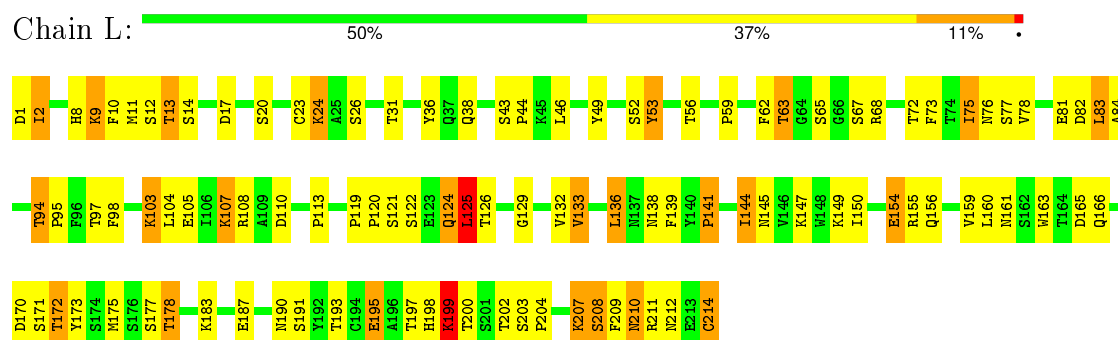
Chain	Residue	Modelled	Actual	Comment	Reference
I	20	LEU	VAL	CONFLICT	GB 1042226
I	28	THR	ALA	CONFLICT	GB 1042226
I	30	ASN	SER	CONFLICT	GB 1042226
I	31	ASN	TYR	CONFLICT	GB 1042226
I	35	SER	ASN	CONFLICT	GB 1042226
I	43	LYS	ARG	CONFLICT	GB 1042226
I	48	VAL	ILE	CONFLICT	GB 1042226
I	53	LEU	PHE	CONFLICT	GB 1042226
I	54	ASN	LYS	CONFLICT	GB 1042226
I	56	ASP	-	INSERTION	GB 1042226
I	58	PHE	ASN	CONFLICT	GB 1042226
I	59	ALA	TYR	CONFLICT	GB 1042226
I	69	LYS	ARG	CONFLICT	GB 1042226
I	71	ILE	THR	CONFLICT	GB 1042226
I	80	ARG	SER	CONFLICT	GB 1042226
I	81	LEU	VAL	CONFLICT	GB 1042226
I	87	SER	ASN	CONFLICT	GB 1042226
I	99	VAL	-	INSERTION	GB 1042226
I	100	LEU	THR	CONFLICT	GB 1042226
I	102	PRO	GLU	CONFLICT	GB 1042226
I	103	LEU	GLY	CONFLICT	GB 1042226
I	104	PHE	ILE	CONFLICT	GB 1042226
I	107	ALA	PRO	CONFLICT	GB 1042226
I	108	VAL	PHE	CONFLICT	GB 1042226
I	109	ASP	ALA	CONFLICT	GB 1042226
I	116	SER	LEU	CONFLICT	GB 1042226
I	121	SER	ALA	CONFLICT	GB 1042226
I	?	-	SER	DELETION	GB 1042226
I	196	ARG	-	INSERTION	GB 1042226

3 Residue-property plots

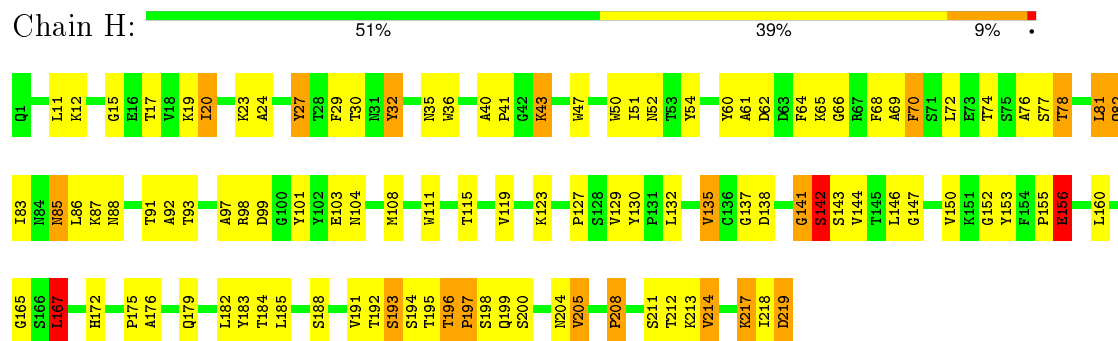
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

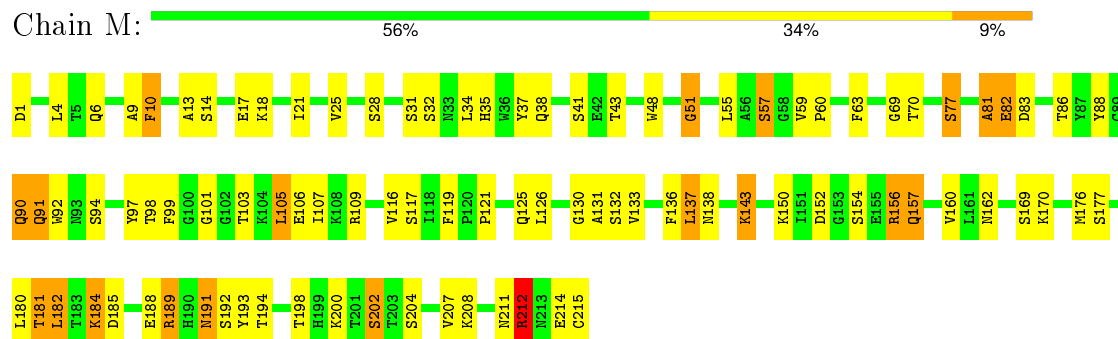
• Molecule 1: IDIOTYPIC FAB 730.1.4 (IGG1) OF VIRUS NEUTRALIZING ANTIBODY



• Molecule 2: IDIOTYPIC FAB 730.1.4 (IGG1) OF VIRUS NEUTRALIZING ANTIBODY

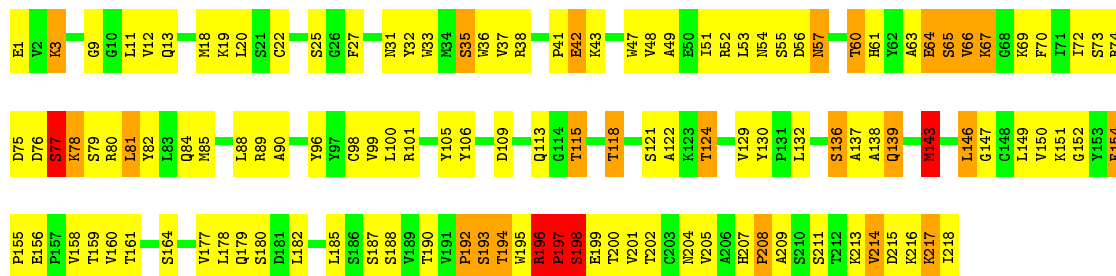


• Molecule 3: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A)



● Molecule 4: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A)

Chain I:  43% 44% 11% •



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	187.58 Å 80.60 Å 75.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.0 (40.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

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	0.73	0/1715	0.95	3/2328 (0.1%)
2	H	0.72	0/1710	0.97	4/2335 (0.2%)
3	M	0.66	0/1696	0.92	3/2306 (0.1%)
4	I	0.78	0/1721	1.06	5/2347 (0.2%)
All	All	0.73	0/6842	0.98	15/9316 (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	L	0	2
3	M	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	76	ASP	N-CA-C	-10.30	83.20	111.00
4	I	77	SER	N-CA-C	-8.74	87.41	111.00
2	H	141	GLY	N-CA-C	-7.22	95.05	113.10
2	H	194	SER	N-CA-CB	-6.90	100.15	110.50
4	I	198	SER	N-CA-C	6.84	129.48	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	173	TYR	Sidechain
1	L	53	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	M	193	TYR	Sidechain

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	1675	0	1591	70	1
2	H	1666	0	1604	82	1
3	M	1655	0	1562	67	0
4	I	1676	0	1637	99	0
All	All	6672	0	6394	309	1

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 24.

The worst 5 of 309 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:143:SER:HA	2:H:193:SER:HA	1.21	1.18
2:H:217:LYS:NZ	2:H:217:LYS:HB2	1.76	0.98
4:I:196:ARG:HB3	4:I:196:ARG:NH1	1.85	0.91
4:I:27:PHE:CZ	4:I:100:LEU:HD11	2.05	0.91
2:H:143:SER:CA	2:H:193:SER:HA	2.03	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:31:THR:OG1	2:H:199:GLN:OE1[4_665]	2.11	0.09

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	212/214 (99%)	180 (85%)	27 (13%)	5 (2%)	7	29
2	H	217/219 (99%)	182 (84%)	24 (11%)	11 (5%)	2	9
3	M	213/215 (99%)	186 (87%)	19 (9%)	8 (4%)	4	16
4	I	216/218 (99%)	173 (80%)	26 (12%)	17 (8%)	1	3
All	All	858/866 (99%)	721 (84%)	96 (11%)	41 (5%)	3	10

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	199	LYS
2	H	142	SER
2	H	193	SER
3	M	41	SER
3	M	82	GLU

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	192/192 (100%)	153 (80%)	39 (20%)	1	4
2	H	186/186 (100%)	152 (82%)	34 (18%)	2	6
3	M	190/190 (100%)	155 (82%)	35 (18%)	2	6
4	I	189/189 (100%)	150 (79%)	39 (21%)	1	4
All	All	757/757 (100%)	610 (81%)	147 (19%)	2	5

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	205	VAL
3	M	91	GLN
4	I	159	THR
2	H	211	SER
3	M	14	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	38	GLN
3	M	93	ASN
4	I	39	GLN
3	M	33	ASN
4	I	139	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 carbohydrates 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 ⓘ

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.