



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:41 AM GMT

PDB ID : 1VFA
Title : BOUND WATER MOLECULES AND CONFORMATIONAL STABILIZATION HELP MEDiate AN ANTIGEN-ANTIBODY ASSOCIATION
Authors : Bhat, T.N.; Poljak, R.J.
Deposited on : 1993-12-03
Resolution : 1.80 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

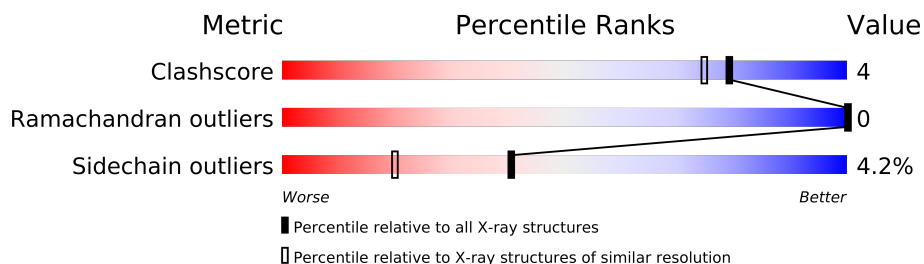
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 1.80 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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	108	
2	B	116	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1764 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 IGG1-KAPPA D1.3 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			837	529	142	164	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	VAL	GLU	CONFLICT	GB 545862
A	50	TYR	LYS	CONFLICT	GB 545862
A	51	THR	ALA	CONFLICT	GB 545862
A	52	THR	GLN	CONFLICT	GB 545862
A	?	-	PRO	DELETION	GB 545862
A	96	ARG	TRP	CONFLICT	GB 545862

- Molecule 2 is a protein called IGG1-KAPPA D1.3 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			904	564	157	179	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	LEU	VAL	CONFLICT	GB 896294

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	13	Total	O	0	0
			13	13		

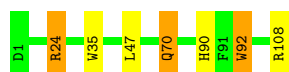
3 Residue-property plots

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.

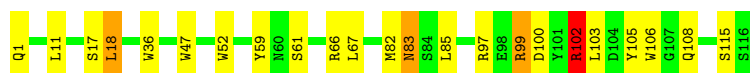
- Molecule 1: IGG1-KAPPA D1.3 FV (LIGHT CHAIN)

Chain A: 



- Molecule 2: IGG1-KAPPA D1.3 FV (HEAVY CHAIN)

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.60 Å 90.60 Å 56.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1764	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	A	0.72	0/858	1.35	7/1164 (0.6%)
2	B	0.78	0/924	1.55	19/1252 (1.5%)
All	All	0.75	0/1782	1.46	26/2416 (1.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	35	TRP	CD1-CG-CD2	8.02	112.72	106.30
2	B	52	TRP	CD1-CG-CD2	7.98	112.68	106.30
2	B	47	TRP	CD1-CG-CD2	7.82	112.55	106.30
2	B	36	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	A	92	TRP	CD1-CG-CD2	7.08	111.97	106.30
2	B	52	TRP	CE2-CD2-CG	-7.06	101.65	107.30
2	B	47	TRP	CE2-CD2-CG	-6.81	101.85	107.30
2	B	106	TRP	CD1-CG-CD2	6.78	111.72	106.30
1	A	92	TRP	CE2-CD2-CG	-6.70	101.94	107.30
2	B	36	TRP	CE2-CD2-CG	-6.67	101.96	107.30
2	B	106	TRP	CE2-CD2-CG	-6.66	101.97	107.30
2	B	66	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	35	TRP	CE2-CD2-CG	-6.38	102.20	107.30
2	B	102	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	35	TRP	CG-CD1-NE1	-5.86	104.24	110.10
2	B	105	TYR	CB-CG-CD1	-5.85	117.49	121.00
2	B	47	TRP	CG-CD1-NE1	-5.82	104.28	110.10
2	B	102	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	24	ARG	NE-CZ-NH1	5.51	123.05	120.30
2	B	36	TRP	CG-CD1-NE1	-5.45	104.65	110.10
2	B	59	TYR	CB-CG-CD1	-5.44	117.74	121.00
2	B	52	TRP	CG-CD1-NE1	-5.27	104.83	110.10
2	B	36	TRP	CG-CD2-CE3	5.23	138.60	133.90
1	A	108	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	A	837	0	811	4	0
2	B	904	0	872	8	0
3	A	10	0	0	0	0
3	B	13	0	0	0	0
All	All	1764	0	1683	12	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 4.

All (12) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:HIS:HD2	1:A:92:TRP:H	1.34	0.75
2:B:18:LEU:HD23	2:B:82:MET:HB2	1.80	0.63
1:A:24:ARG:HH11	1:A:70:GLN:HE21	1.55	0.52
2:B:11:LEU:HD11	2:B:115:SER:HB3	1.94	0.49
2:B:67:LEU:HD12	2:B:82:MET:HG2	1.95	0.48
2:B:99:ARG:HH12	2:B:102:ARG:NH2	2.14	0.46
1:A:24:ARG:HD3	1:A:70:GLN:HE21	1.82	0.45
1:A:24:ARG:HH11	1:A:70:GLN:NE2	2.15	0.44
2:B:100:ASP:HB2	2:B:102:ARG:NH1	2.35	0.42
2:B:17:SER:OG	2:B:83:ASN:HA	2.20	0.42
2:B:97:ARG:O	2:B:103:LEU:HA	2.21	0.41
2:B:18:LEU:HB3	2:B:85:LEU:HD11	2.03	0.40

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	A	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
2	B	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
All	All	220/224 (98%)	212 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	92/92 (100%)	90 (98%)	2 (2%)	64	48
2	B	100/100 (100%)	94 (94%)	6 (6%)	27	10
All	All	192/192 (100%)	184 (96%)	8 (4%)	40	20

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	70	GLN
2	B	1	GLN
2	B	18	LEU
2	B	61	SER
2	B	83	ASN
2	B	102	ARG
2	B	108	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	70	GLN
1	A	90	HIS
2	B	108	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 ⓘ

There are no ligands in this entry.

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 ⓘ

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.