



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:59 AM GMT

PDB ID : 2VIT
Title : INFLUENZA VIRUS HEMAGGLUTININ, MUTANT WITH THR 155 REPLACED BY ILE, COMPLEXED WITH A NEUTRALIZING ANTIBODY
Authors : Bizebard, T.; Fleury, D.; Gigant, B.; Wharton, S.A.; Skehel, J.J.; Knossow, M.
Deposited on : 1997-12-22
Resolution : 3.25 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

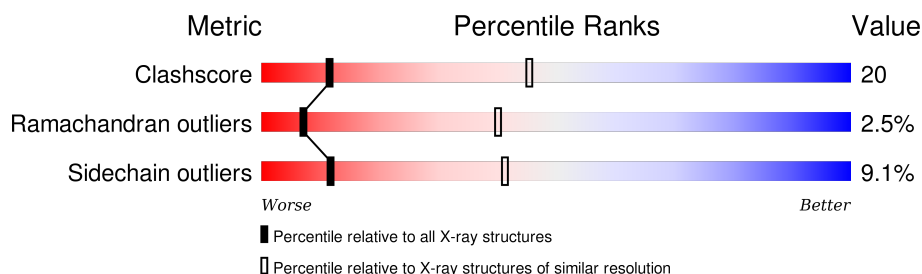
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)

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	A	210	
2	B	221	
3	C	282	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5340 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 IMMUNOGLOBULIN (IGG1, LAMBDA).

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

- Molecule 2 is a protein called IMMUNOGLOBULIN (IGG1, LAMBDA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	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
B	3	GLN	LYS	CONFLICT	GB 4096752
B	5	LYS	GLN	CONFLICT	GB 4096752
B	28	LEU	SER	CONFLICT	GB 4096752
B	30	ILE	THR	CONFLICT	GB 4096752
B	32	ASN	TYR	CONFLICT	GB 4096752
B	63	LEU	HIS	CONFLICT	GB 4096752
B	69	ILE	PHE	CONFLICT	GB 4096752
B	83	LYS	ASN	CONFLICT	GB 4096752
B	92	MET	LEU	CONFLICT	GB 4096752
B	98	ASP	-	INSERTION	GB 4096752
B	99	PHE	-	INSERTION	GB 4096752
B	100	TYR	-	INSERTION	GB 4096752
B	102	TYR	HIS	CONFLICT	GB 4096752
B	103	ASP	GLY	CONFLICT	GB 4096752
B	105	PHE	-	INSERTION	GB 4096752
B	106	TYR	-	INSERTION	GB 4096752
B	107	TYR	-	INSERTION	GB 4096752
B	108	ALA	-	INSERTION	GB 4096752
B	109	MET	-	INSERTION	GB 4096752
B	110	ASP	-	INSERTION	GB 4096752

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Chain	Residue	Modelled	Actual	Comment	Reference
B	117	SER	LEU	CONFLICT	GB 4096752
B	122	SER	ALA	CONFLICT	GB 4096752
B	135	PRO	SER	CONFLICT	GB 4096752

- Molecule 3 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2076	1306	360	399	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	81	ASP	ASN	MODIFIED RESIDUE	UNP P03437
C	155	ILE	THR	ENGINEERED	UNP P03437
C	165	ASP	ASN	MODIFIED RESIDUE	UNP P03437
C	285	ASP	ASN	MODIFIED RESIDUE	UNP P03437

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

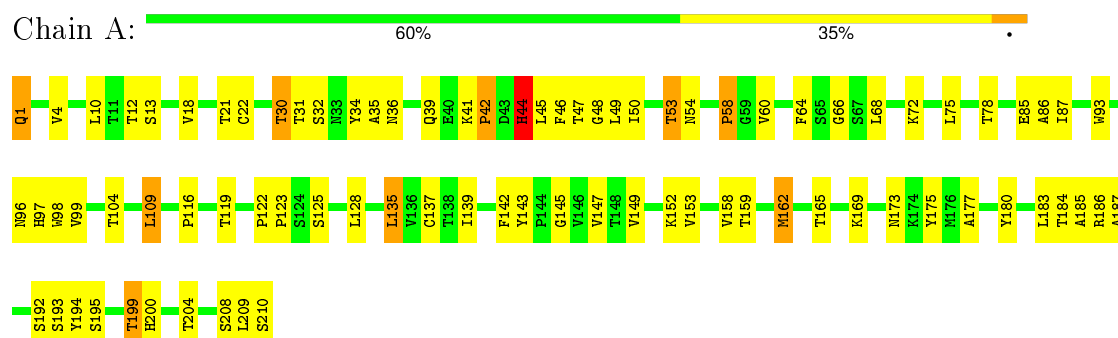
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	C	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

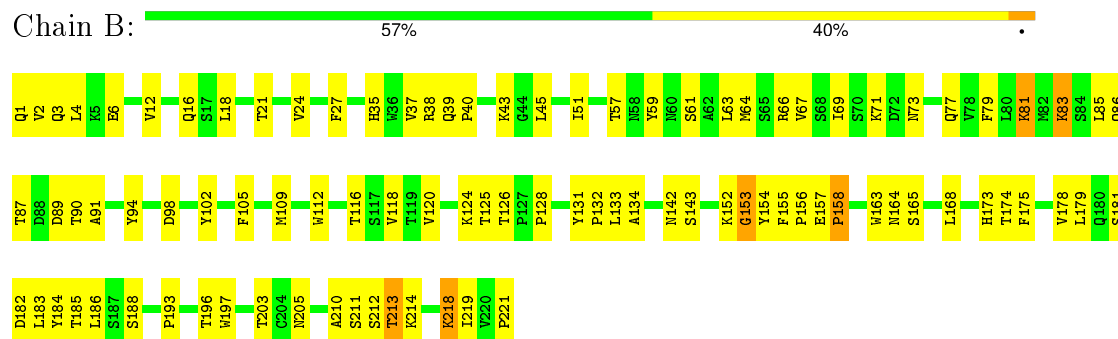
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

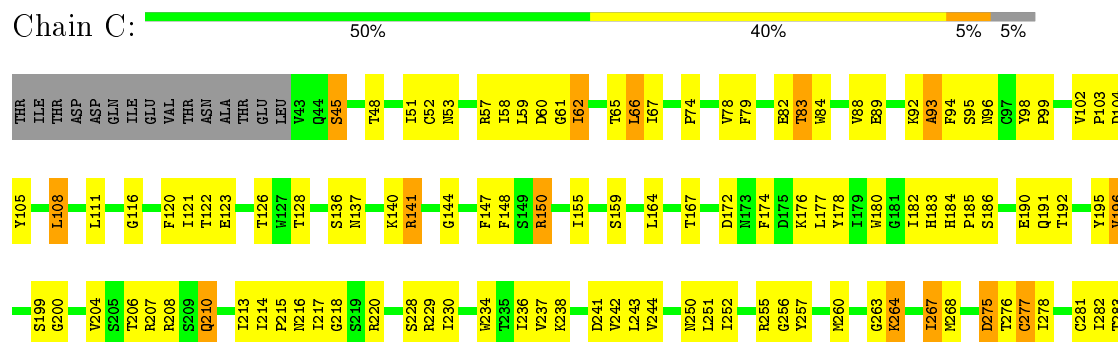
• Molecule 1: IMMUNOGLOBULIN (IGG1, LAMBDA)



• Molecule 2: IMMUNOGLOBULIN (IGG1, LAMBDA)



• Molecule 3: HEMAGGLUTININ



P284	D285	G286	S287	I288
D291	K292	Q295	I296	V297
I298	K299	I300	A304	C305
P306	K307	Y308	V309	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.50 Å 85.50 Å 515.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 3.25	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.25)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.188 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5340	wwPDB-VP
Average B, all atoms (Å ²)	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: ZN

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	0.59	0/1627	0.84	3/2224 (0.1%)
2	B	0.59	0/1718	0.82	2/2351 (0.1%)
3	C	0.58	0/2128	0.82	0/2897
All	All	0.59	0/5473	0.83	5/7472 (0.1%)

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	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	GLY	N-CA-C	5.71	127.38	113.10
1	A	45	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	135	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	45	LEU	N-CA-C	-5.17	97.05	111.00
2	B	16	GLN	N-CA-C	-5.14	97.11	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Sidechain

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	A	1589	0	1532	54	0
2	B	1672	0	1635	72	0
3	C	2076	0	2015	96	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
All	All	5340	0	5182	215	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 20.

The worst 5 of 215 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:B:134:ALA:HB2	2:B:219:ILE:HD11	1.37	1.06
1:A:147:VAL:HG12	1:A:200:HIS:HB2	1.51	0.93
2:B:40:PRO:HG2	2:B:43:LYS:HB2	1.55	0.87
3:C:45:SER:HB3	3:C:296:ASN:OD1	1.77	0.85
2:B:1:GLN:HE21	2:B:3:GLN:HB2	1.44	0.83

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	A	208/210 (99%)	183 (88%)	20 (10%)	5 (2%)	7 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	219/221 (99%)	189 (86%)	25 (11%)	5 (2%)	8	42
3	C	265/282 (94%)	230 (87%)	28 (11%)	7 (3%)	7	39
All	All	692/713 (97%)	602 (87%)	73 (10%)	17 (2%)	7	40

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	173	HIS
2	B	212	SER
3	C	210	GLN
3	C	304	ALA
1	A	58	PRO

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	178/178 (100%)	162 (91%)	16 (9%)	12	42
2	B	192/192 (100%)	180 (94%)	12 (6%)	22	62
3	C	236/250 (94%)	209 (89%)	27 (11%)	7	30
All	All	606/620 (98%)	551 (91%)	55 (9%)	12	41

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	186	LEU
3	C	57	ARG
3	C	264	LYS
2	B	205	ASN
2	B	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	32	ASN
2	B	142	ASN
3	C	210	GLN
2	B	3	GLN
3	C	189	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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