



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:59 PM GMT

PDB ID : 1EO8
Title : INFLUENZA VIRUS HEMAGGLUTININ COMPLEXED WITH A NEUTRALIZING ANTIBODY
Authors : Fleury, D.; Gigant, B.; Daniels, R.S.; Skehel, J.J.; Knossow, M.; Bizebard, T.
Deposited on : 2000-03-22
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

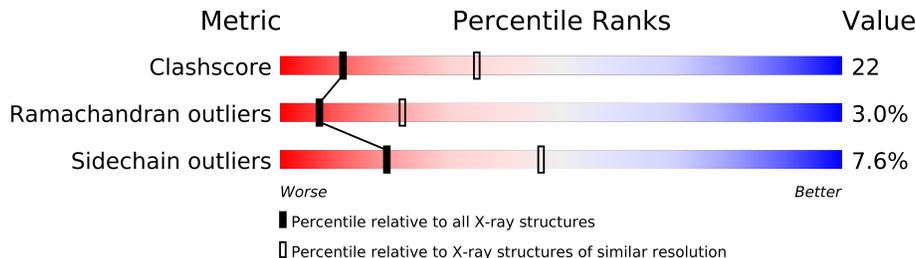
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (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 ≥ 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	328	
2	B	175	
3	L	210	
4	H	217	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7357 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 HEMAGGLUTININ (HA1 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2464	1543	433	475	13	0	0	0

- Molecule 2 is a protein called HEMAGGLUTININ (HA2 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	175	1421	882	250	283	6	0	0	0

- Molecule 3 is a protein called ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	210	1620	1009	270	332	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	40	SER	PRO	CONFLICT	GB 7159941

- Molecule 4 is a protein called ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	217	1648	1046	272	323	7	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

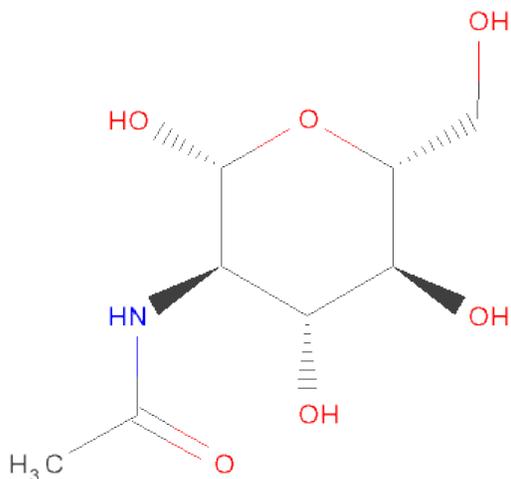
Chain	Residue	Modelled	Actual	Comment	Reference
H	64	LYS	ARG	CONFLICT	GB 7159939
H	187	PRO	THR	CONFLICT	GB 7159939

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Chain	Residue	Modelled	Actual	Comment	Reference
H	188	ARG	TRP	CONFLICT	GB 7159939

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (NAG-NAG-MAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	3	39	22	2	15	0	0

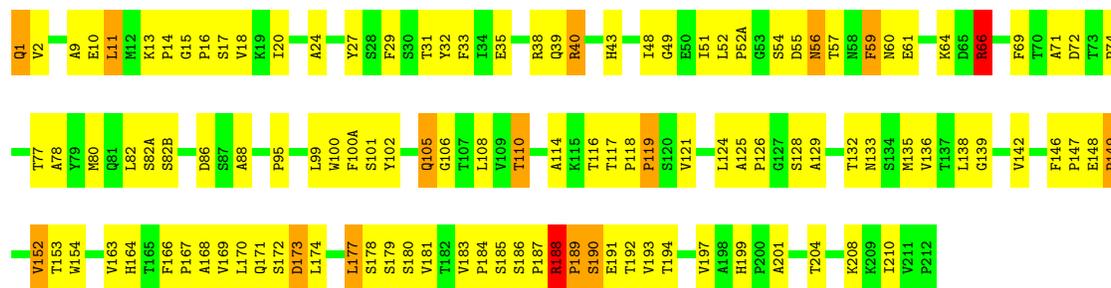
- Molecule 7 is a polymer of unknown type called SUGAR (NAG-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	2	28	16	2	10	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	43	Total O 43 43	0	0
8	B	44	Total O 44 44	0	0
8	H	17	Total O 17 17	0	0
8	L	5	Total O 5 5	0	0

Chain H:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.15Å 138.15Å 129.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.196 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7357	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: NAG, MAN

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	0.60	0/2520	0.86	2/3433 (0.1%)
2	B	0.67	0/1445	0.84	2/1939 (0.1%)
3	L	0.59	0/1658	0.94	5/2249 (0.2%)
4	H	0.60	0/1695	0.87	3/2319 (0.1%)
All	All	0.61	0/7318	0.88	12/9940 (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
6	A	1	0

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	7	SER	N-CA-C	9.20	135.84	111.00
3	L	91	ARG	NE-CZ-NH2	7.17	123.89	120.30
3	L	8	PRO	N-CA-C	-7.07	93.73	112.10
2	B	110	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	321	ARG	NE-CZ-NH1	5.78	123.19	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	452	MAN	C1

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	2464	0	2415	93	0
2	B	1421	0	1344	32	0
3	L	1620	0	1557	109	0
4	H	1648	0	1608	105	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	39	0	34	1	0
7	A	28	0	25	0	0
8	A	43	0	0	3	0
8	B	44	0	0	2	0
8	H	17	0	0	0	0
8	L	5	0	0	0	0
All	All	7357	0	7009	319	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 22.

The worst 5 of 319 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:184:GLU:HA	3:L:187:ARG:HD2	1.34	1.06
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.23	1.02
3:L:6:GLN:HB2	3:L:88:CYS:SG	2.09	0.93
3:L:148:LYS:HB3	3:L:153:GLU:HA	1.52	0.89
4:H:17:SER:HB3	4:H:82(A):SER:HA	1.53	0.88

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	317/328 (97%)	292 (92%)	23 (7%)	2 (1%)	33	72
2	B	173/175 (99%)	159 (92%)	13 (8%)	1 (1%)	33	72
3	L	208/210 (99%)	178 (86%)	17 (8%)	13 (6%)	2	5
4	H	215/217 (99%)	181 (84%)	23 (11%)	11 (5%)	3	9
All	All	913/930 (98%)	810 (89%)	76 (8%)	27 (3%)	7	22

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	27	SER
3	L	93	SER
3	L	148	LYS
3	L	153	GLU
3	L	182	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	A	281/289 (97%)	265 (94%)	16 (6%)	29	64
2	B	149/149 (100%)	144 (97%)	5 (3%)	49	84
3	L	185/185 (100%)	161 (87%)	24 (13%)	6	17
4	H	187/187 (100%)	171 (91%)	16 (9%)	15	40
All	All	802/810 (99%)	741 (92%)	61 (8%)	19	46

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	81	GLU
3	L	148	LYS
4	H	152	VAL
3	L	91	ARG
3	L	106(A)	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	ASN
3	L	38	GLN
4	H	105	GLN
2	B	53	ASN
4	H	56	ASN

5.3.3 RNA [i](#)

There are no RNA chains 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](#)

5 carbohydrates are 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$
6	NAG	A	450	1,6	12,14,15	1.76	4 (33%)	15,19,21	2.08	3 (20%)
6	NAG	A	451	6	12,14,15	1.40	2 (16%)	15,19,21	2.19	5 (33%)
6	MAN	A	452	6	10,11,12	1.21	2 (20%)	11,15,17	2.32	2 (18%)
7	NAG	A	460	1,7	12,14,15	1.30	2 (16%)	15,19,21	2.10	6 (40%)
7	NAG	A	461	7	12,14,15	2.18	3 (25%)	15,19,21	1.83	3 (20%)

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
6	NAG	A	450	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	451	6	-	0/6/23/26	0/1/1/1
6	MAN	A	452	6	1/1/4/5	0/2/19/22	0/1/1/1
7	NAG	A	460	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	461	7	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	461	NAG	C4-C5	5.84	1.65	1.53
6	A	451	NAG	O5-C5	-2.99	1.39	1.45
6	A	450	NAG	C4-C5	-2.82	1.46	1.53
6	A	452	MAN	C3-C2	2.78	1.59	1.52
6	A	451	NAG	C4-C5	-2.75	1.47	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	452	MAN	C4-C3-C2	6.17	118.79	110.50
6	A	450	NAG	C2-N2-C7	-5.43	113.97	123.09
6	A	451	NAG	C2-N2-C7	-5.06	114.59	123.09
7	A	461	NAG	O5-C5-C6	-4.49	102.27	106.98
6	A	450	NAG	O3-C3-C2	-3.88	100.94	109.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	452	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry (i)

2 ligands are 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
5	NAG	A	440	1	12,14,15	1.43	2 (16%)	15,19,21	2.69	5 (33%)
5	NAG	B	410	2	12,14,15	1.97	4 (33%)	15,19,21	3.54	6 (40%)

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	NAG	A	440	1	-	0/6/23/26	0/1/1/1
5	NAG	B	410	2	1/1/5/7	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	410	NAG	O5-C5	4.51	1.53	1.45
5	B	410	NAG	C8-C7	2.91	1.56	1.50
5	A	440	NAG	C6-C5	2.85	1.62	1.52
5	A	440	NAG	O5-C5	2.81	1.50	1.45
5	B	410	NAG	C4-C5	2.25	1.58	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	410	NAG	C3-C2-N2	-9.80	96.84	111.76
5	A	440	NAG	O5-C5-C6	5.86	113.13	106.98
5	B	410	NAG	O3-C3-C2	5.54	120.73	109.09
5	A	440	NAG	O5-C5-C4	-5.21	104.04	110.65
5	A	440	NAG	C3-C2-N2	3.90	117.70	111.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	410	NAG	C1

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

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.