wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 05:50 AM EDT

PDB ID	:	5DUP
Title	:	Influenza A virus H5 hemagglutinin globular head in complex with antibody AVFluIgG03
Authors	:	Zuo, T.; Sun, J.; Wang, G.; Zhou, P.; Wang, X.; Zhang, L.
Deposited on	:	2015-09-20
Resolution	:	3.05 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

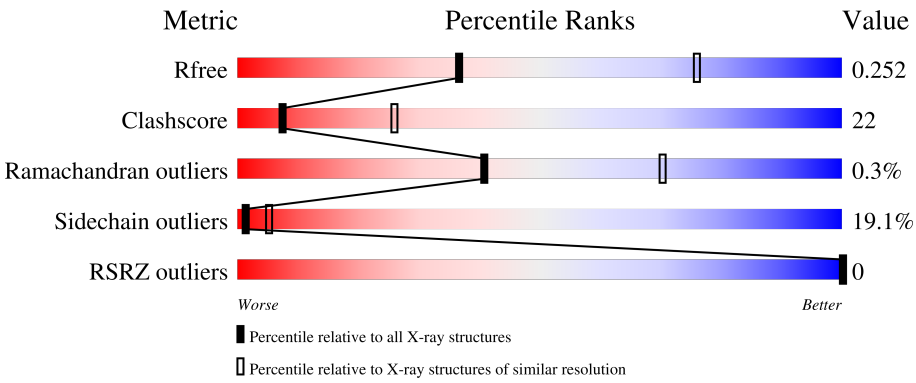
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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.

Mol	Chain	Length	Quality of chain
1	A	233	39% 37% 8% 16%
2	H	234	45% 37% 7% 11%
3	L	215	52% 38% 7% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4703 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1566	993	272	295	6	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	-	expression tag	UNP Q1WDM0
A	43	ASP	-	expression tag	UNP Q1WDM0
A	44	PRO	-	expression tag	UNP Q1WDM0
A	269	HIS	-	expression tag	UNP Q1WDM0
A	270	HIS	-	expression tag	UNP Q1WDM0
A	271	HIS	-	expression tag	UNP Q1WDM0
A	272	HIS	-	expression tag	UNP Q1WDM0
A	273	HIS	-	expression tag	UNP Q1WDM0
A	274	HIS	-	expression tag	UNP Q1WDM0

- Molecule 2 is a protein called AVFluIgG03 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	208	1576	995	264	310	7	0	0	0

- Molecule 3 is a protein called AVFluIgG03 Light Chain.

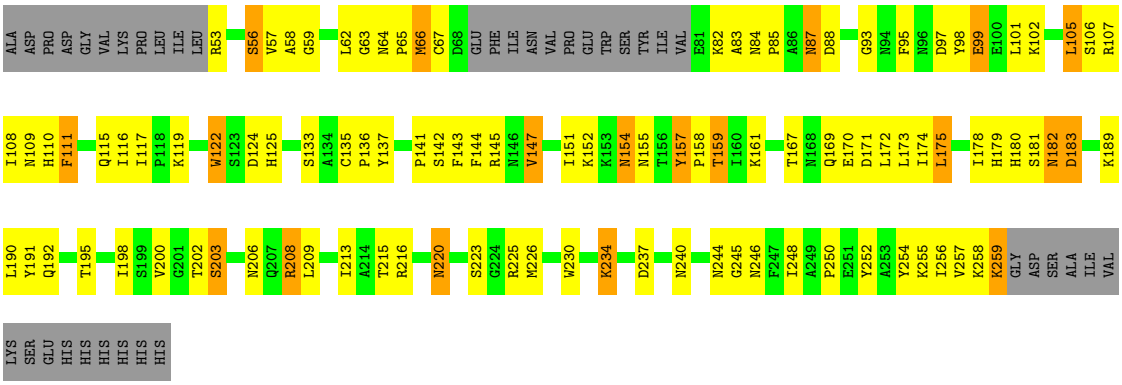
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	209	1561	971	263	323	4	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

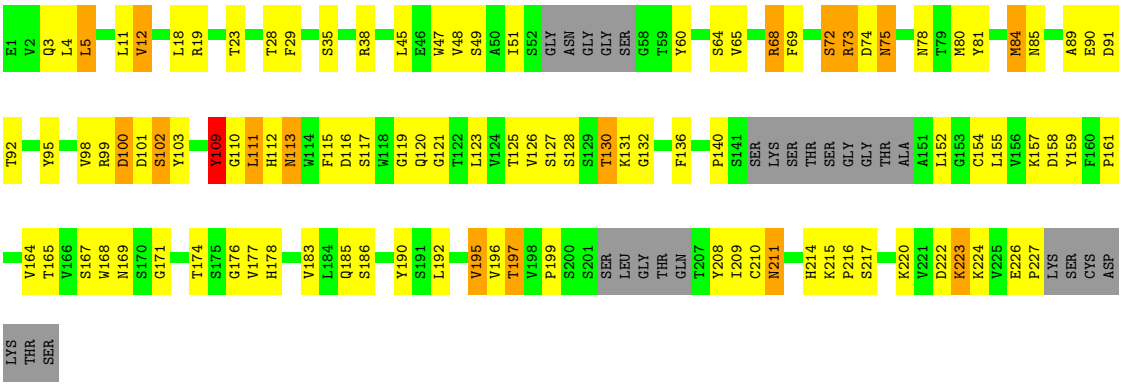
- Molecule 1: Hemagglutinin

Chain A: 39% 37% 8% 16%



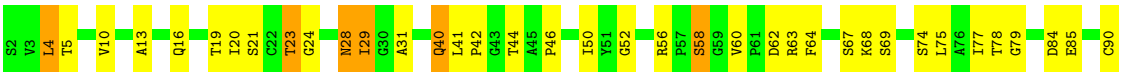
- Molecule 2: AVFluIgG03 Heavy Chain

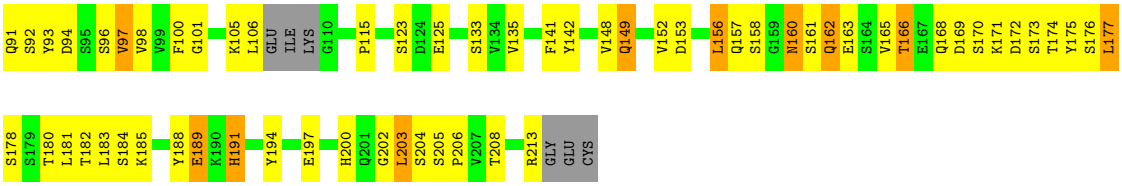
Chain H: 45% 37% 7% 11%



- Molecule 3: AVFluIgG03 Light Chain

Chain L: 52% 38% 7%




Q91
S92
Y93
D94
S95
S96
V97
V98
V99
F100
G101
K105
L106
GLU
ILE
LYS
G110
P115
S123
D124
E125
S133
V134
V135
F141
Y142
V148
Q149
V152
D153
L156
Q157
S158
G159
N160
S161
Q162
E163
S164
V165
T166
E167
Q168
D169
S170
K171
D172
S173
T174
Y175
S176
L177
S178
S179
T180
L181
T182
L183
S184
K185
Y188
E189
K190
H191
Y194
E197
H200
Q201
G202
L203
S204
S205
P206
V207
T208
R213
GLY
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	132.66Å 132.66Å 87.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.94 – 3.05 38.94 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.94-3.05) 99.7 (38.94-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.257 0.195 , 0.252	Depositor DCC
R_{free} test set	837 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4703	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.40	0/1607	0.61	0/2182
2	H	0.50	0/1615	0.67	0/2197
3	L	0.44	0/1594	0.63	0/2168
All	All	0.45	0/4816	0.64	0/6547

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
2	H	0	3
3	L	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	109	TYR	Peptide
2	H	110	GLY	Peptide
2	H	216	PRO	Peptide
3	L	4	LEU	Peptide

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	1566	0	1513	89	0
2	H	1576	0	1509	66	0
3	L	1561	0	1499	62	0
All	All	4703	0	4521	205	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 22.

The worst 5 of 205 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:A:141:PRO:HD2	2:H:111:LEU:HG	1.56	0.88
3:L:5:THR:HB	3:L:23:THR:HG23	1.61	0.83
1:A:133:SER:HB3	2:H:109:TYR:HB3	1.61	0.83
2:H:113:ASN:O	3:L:93:TYR:OH	1.96	0.82
3:L:20:ILE:HB	3:L:75:LEU:HB3	1.63	0.81

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	191/233 (82%)	169 (88%)	21 (11%)	1 (0%)	29 60
2	H	200/234 (86%)	181 (90%)	19 (10%)	0	100 100
3	L	205/215 (95%)	186 (91%)	18 (9%)	1 (0%)	29 60
All	All	596/682 (87%)	536 (90%)	58 (10%)	2 (0%)	41 70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	97	VAL
1	A	83	ALA

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	174/208 (84%)	148 (85%)	26 (15%)	3 11
2	H	177/196 (90%)	133 (75%)	44 (25%)	0 2
3	L	177/182 (97%)	146 (82%)	31 (18%)	2 7
All	All	528/586 (90%)	427 (81%)	101 (19%)	1 5

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	174	THR
3	L	21	SER
3	L	191	HIS
2	H	192	LEU
2	H	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	13	GLN
2	H	24	ASN
2	H	78	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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	195/233 (83%)	-0.28	0	100	100	57, 72, 96, 107	0
2	H	208/234 (88%)	-0.35	0	100	100	45, 55, 65, 70	0
3	L	209/215 (97%)	-0.34	0	100	100	49, 60, 72, 74	0
All	All	612/682 (89%)	-0.32	0	100	100	45, 62, 85, 107	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.