



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 3, 2020 – 04:04 PM EST

PDB ID : 6OCB
Title : Crystal structure of FluA-20 Fab in complex with the head domain of H3
(A/Hong Kong/1/1968)
Authors : Wilson, I.A.; Lang, S.
Deposited on : 2019-03-22
Resolution : 2.10 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

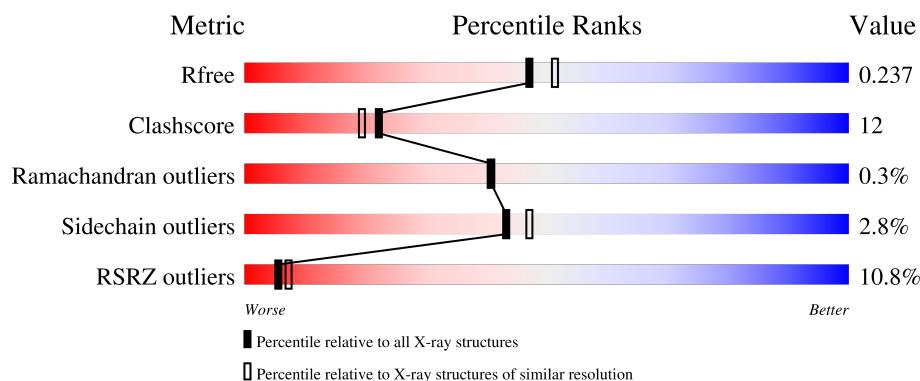
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	H	235	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>6%</div> </div> </div>
2	L	214	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
3	A	274	<div> <div>14%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5746 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 Heavy chain of FluA-20 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	222	Total	C	N	O	S	0	0	0
			1662	1050	273	332	7			

- Molecule 2 is a protein called Light chain of FluA-20 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1646	1031	281	329	5			

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	267	Total	C	N	O	S	0	1	0
			2079	1306	364	398	11			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	expression tag	UNP Q91MA7
A	311	HIS	-	expression tag	UNP Q91MA7
A	312	HIS	-	expression tag	UNP Q91MA7
A	313	HIS	-	expression tag	UNP Q91MA7
A	314	HIS	-	expression tag	UNP Q91MA7
A	315	HIS	-	expression tag	UNP Q91MA7
A	316	HIS	-	expression tag	UNP Q91MA7

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

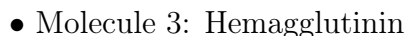
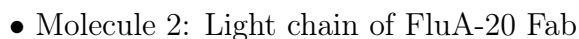


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	76	Total	O	0	0
			76	76		
5	L	114	Total	O	0	0
			114	114		
5	A	155	Total	O	0	0
			155	155		

- Molecule 1: Heavy chain of FluA-20 Fab



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.55Å 84.55Å 271.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.81 – 2.10 44.88 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.81-2.10) 99.4 (44.88-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.202 , 0.239 0.203 , 0.237	Depositor DCC
R_{free} test set	2965 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5746	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	H	0.70	1/1704 (0.1%)	0.91	3/2330 (0.1%)
2	L	0.76	3/1683 (0.2%)	0.96	7/2285 (0.3%)
3	A	0.69	0/2131	0.81	2/2903 (0.1%)
All	All	0.71	4/5518 (0.1%)	0.89	12/7518 (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	H	0	1
2	L	0	1
3	A	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	143	GLU	CB-CG	-12.88	1.27	1.52
2	L	143	GLU	CG-CD	-8.96	1.38	1.51
1	H	140	CYS	CB-SG	-6.65	1.71	1.82
2	L	93	ASN	C-N	-5.49	1.21	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	24	ARG	NE-CZ-NH1	9.11	124.86	120.30
2	L	144	ALA	N-CA-C	-7.71	90.18	111.00
1	H	140	CYS	CA-CB-SG	6.99	126.58	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	143	GLU	CB-CA-C	-6.72	96.95	110.40
3	A	141	ARG	CG-CD-NE	-6.16	98.86	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	219	SER	Mainchain
1	H	154	TRP	Mainchain
2	L	143	GLU	Mainchain

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	H	1662	0	1618	49	0
2	L	1646	0	1608	47	0
3	A	2079	0	2018	31	0
4	A	14	0	13	0	0
5	A	155	0	0	3	0
5	H	76	0	0	5	0
5	L	114	0	0	5	0
All	All	5746	0	5257	125	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 12.

The worst 5 of 125 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:L:125:LEU:HB3	2:L:183:LYS:NZ	1.14	1.43
2:L:125:LEU:CB	2:L:183:LYS:HZ1	1.60	1.15
1:H:212:GLU:HG3	1:H:213:PRO:HD2	1.29	1.14
2:L:125:LEU:CB	2:L:183:LYS:NZ	2.09	1.13
3:A:43:VAL:N	3:A:292:LYS:HZ2	1.58	1.01

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	H	218/235 (93%)	209 (96%)	8 (4%)	1 (0%)	29	26
2	L	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
3	A	266/274 (97%)	258 (97%)	7 (3%)	1 (0%)	34	32
All	All	695/723 (96%)	674 (97%)	19 (3%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	62	ILE
1	H	213	PRO

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	H	192/205 (94%)	182 (95%)	10 (5%)	23	21
2	L	189/190 (100%)	185 (98%)	4 (2%)	53	59
3	A	237/242 (98%)	234 (99%)	3 (1%)	69	75
All	All	618/637 (97%)	601 (97%)	17 (3%)	43	47

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	209	LYS
1	H	211	VAL
2	L	183	LYS
1	H	195	ILE
3	A	152	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	152	ASN
3	A	250	ASN
3	A	189	GLN
3	A	132	GLN
3	A	170	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](#)

1 ligand is 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
4	NAG	A	701	3	14,14,15	0.77	0	17,19,21	1.28	2 (11%)

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
4	NAG	A	701	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	NAG	C1-O5-C5	2.39	115.43	112.19
4	A	701	NAG	C3-C4-C5	2.19	114.15	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	NAG	C3-C2-N2-C7
4	A	701	NAG	C1-C2-N2-C7

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](#)

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	H	222/235 (94%)	0.91	27 (12%) 4 5	24, 50, 100, 126	0
2	L	213/214 (99%)	0.18	12 (5%) 24 29	22, 39, 78, 98	0
3	A	267/274 (97%)	0.53	37 (13%) 2 3	21, 36, 83, 101	0
All	All	702/723 (97%)	0.55	76 (10%) 5 7	21, 41, 93, 126	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	190	GLY	14.1
1	H	189	LEU	13.7
1	H	133	GLY	13.6
1	H	214	LYS	9.1
1	H	191	THR	8.8

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	701	14/15	0.76	0.29	70,77,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.