wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 08:10 PM EDT

PDB ID	:	1RHH
Title	:	Crystal Structure of the Broadly HIV-1 Neutralizing Fab X5 at 1.90 Angstrom Resolution
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Deposited on	:	2003-11-14
Resolution	:	1.90 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:

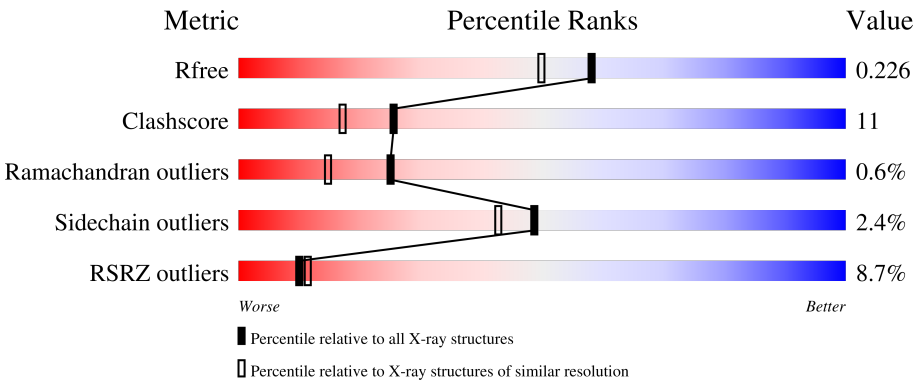
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	215	2%, 82%, 17%, •
1	C	215	5%, 79%, 21%
2	B	239	9%, 81%, 15%, • •
2	D	239	17%, 78%, 16%, • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7366 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 Fab X5, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1636	1018	280	333	5	0	0	0
1	C	215	1636	1018	280	333	5	0	0	0

- Molecule 2 is a protein called Fab X5, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	233	1742	1098	290	346	8	0	0	0
2	D	232	1733	1093	288	344	8	0	0	0

- Molecule 3 is water.

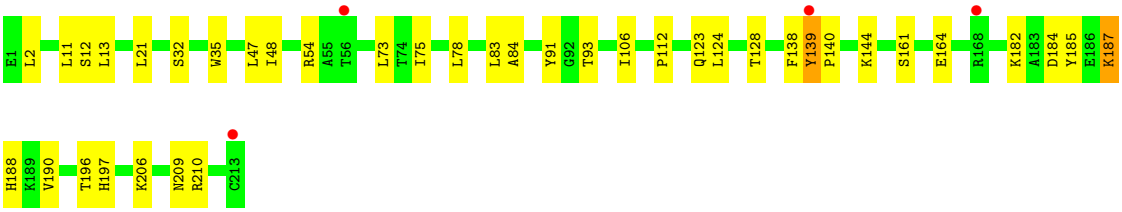
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	217	217	217	0	0
3	B	171	171	171	0	0
3	C	138	138	138	0	0
3	D	93	93	93	0	0

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.

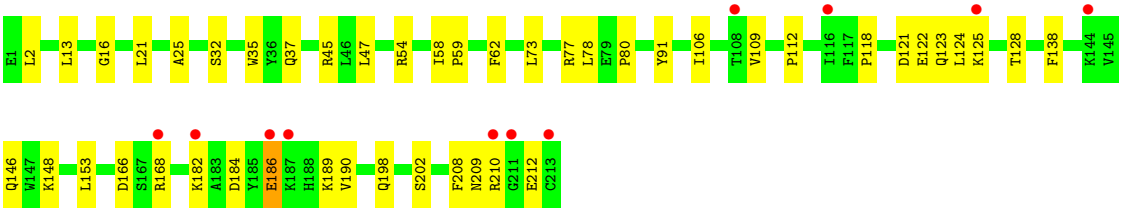
• Molecule 1: Fab X5, light chain

Chain A:



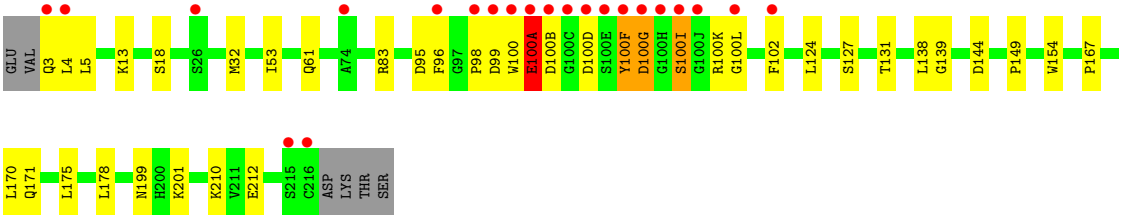
• Molecule 1: Fab X5, light chain

Chain C:



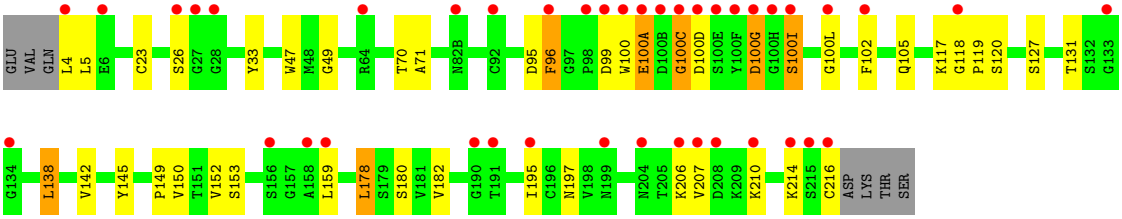
• Molecule 2: Fab X5, heavy chain

Chain B:



• Molecule 2: Fab X5, heavy chain

Chain D:


GLU
VAL
GLN
L4
L5
E6
C23
S26
G27
G28
Y33
W47
M48
G49
R64
T70
A71
N82B
C92
D95
F96
G97
P98
D99
W100
E100A
D100B
G100C
D100D
S100E
Y100F
D100G
G100H
S100I
G100L
F102
Q105
K117
G118
P119
S120
S127
T131
S132
G133
G134
L138
V142
Y145
P149
V150
T151
V152
S153
S156
G157
A158
L159
L178
S179
S180
V181
V182
G190
T191
I195
C196
N197
V198
N199
N204
T205
K206
V207
D208
K209
K210
K214
S215
C216
ASP
LYS
THR
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.60Å 139.60Å 120.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 1.90 29.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.41-1.90) 100.0 (29.41-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 1.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.227 0.224 , 0.226	Depositor DCC
R_{free} test set	4699 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7366	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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	0.34	0/1669	0.67	0/2264
1	C	0.31	0/1669	0.64	0/2264
2	B	0.36	0/1788	0.70	1/2432 (0.0%)
2	D	0.33	0/1779	0.66	0/2420
All	All	0.33	0/6905	0.67	1/9380 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	124	LEU	N-CA-C	-5.62	95.82	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1636	0	1591	34	0
1	C	1636	0	1591	40	0
2	B	1742	0	1662	33	0
2	D	1733	0	1654	42	0
3	A	217	0	0	1	0
3	B	171	0	0	1	0
3	C	138	0	0	2	0
3	D	93	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7366	0	6498	140	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 11.

The worst 5 of 140 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:C:2:LEU:HD21	1:C:25:ALA:HB1	1.42	1.00
1:A:210:ARG:HH11	1:A:210:ARG:HB3	1.28	0.99
2:D:159:LEU:HD11	2:D:182:VAL:HG21	1.42	0.97
2:D:214:LYS:HE3	2:D:216:CYS:SG	2.12	0.89
2:B:99:ASP:CG	2:B:100(D):ASP:HA	1.93	0.88

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	213/215 (99%)	208 (98%)	4 (2%)	1 (0%)	29 18
1	C	213/215 (99%)	208 (98%)	5 (2%)	0	100 100
2	B	231/239 (97%)	216 (94%)	13 (6%)	2 (1%)	17 7
2	D	230/239 (96%)	212 (92%)	16 (7%)	2 (1%)	17 7
All	All	887/908 (98%)	844 (95%)	38 (4%)	5 (1%)	25 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	100(A)	GLU

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Mol	Chain	Res	Type
2	B	100(G)	ASP
2	D	100(C)	GLY
2	D	100(G)	ASP
1	A	139	TYR

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	182/182 (100%)	180 (99%)	2 (1%)	73	73
1	C	182/182 (100%)	180 (99%)	2 (1%)	73	73
2	B	192/198 (97%)	186 (97%)	6 (3%)	40	32
2	D	191/198 (96%)	183 (96%)	8 (4%)	30	20
All	All	747/760 (98%)	729 (98%)	18 (2%)	49	43

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	149	PRO
2	D	207	VAL
2	D	206	LYS
1	C	184	ASP
2	D	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3	GLN
2	B	82(B)	ASN
2	B	105	GLN
1	C	198	GLN
2	D	199	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	215/215 (100%)	0.13	4 (1%)	66	69	17, 25, 36, 50	0
1	C	215/215 (100%)	0.41	11 (5%)	28	31	22, 32, 55, 71	0
2	B	233/239 (97%)	0.66	22 (9%)	8	9	16, 25, 63, 78	0
2	D	232/239 (97%)	1.30	41 (17%)	1	1	22, 37, 71, 80	0
All	All	895/908 (98%)	0.64	78 (8%)	10	11	16, 30, 58, 80	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	100	TRP	19.2
2	D	100(F)	TYR	13.5
2	B	100	TRP	13.5
2	D	99	ASP	12.1
2	B	100(H)	GLY	11.6

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.