



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2017 – 09:09 pm GMT

PDB ID : 1A6U
Title : B1-8 FV FRAGMENT
Authors : Simon, T.; Henrick, K.; Hirshberg, M.; Winter, G.
Deposited on : 1998-03-03
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

<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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

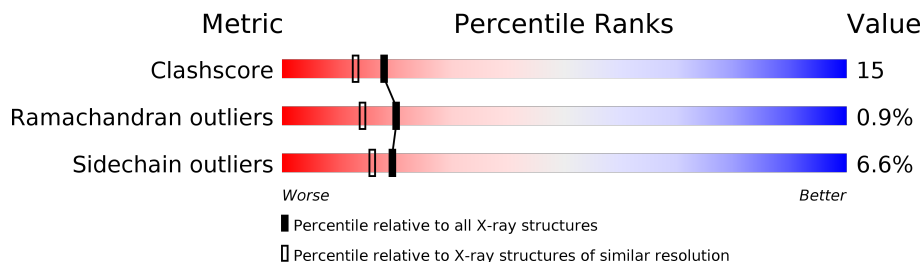
1 Overall quality at a glance

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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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. 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	L	108	
2	H	120	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1892 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 B1-8 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	108	Total	C	N	O	S	0	1	0
			804	506	137	159	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	40	GLU	GLN	VARIANT	UNP P01724

- Molecule 2 is a protein called B1-8 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	120	Total	C	N	O	S	0	0	0
			932	593	153	182	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	416	VAL	LEU	VARIANT	UNP P01751

- Molecule 3 is water.

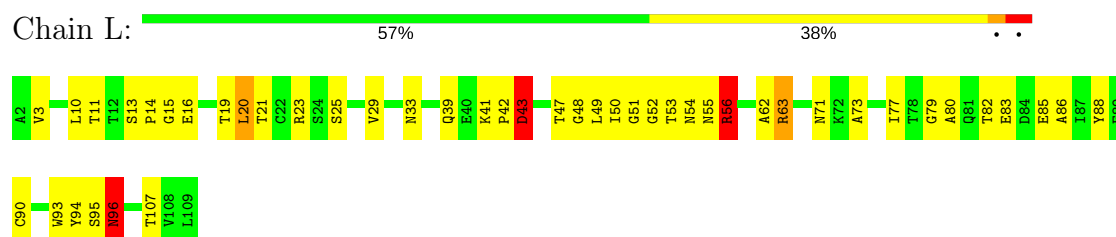
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	84	Total	O	0	0
			84	84		
3	L	72	Total	O	0	0
			72	72		

3 Residue-property plots [i](#)

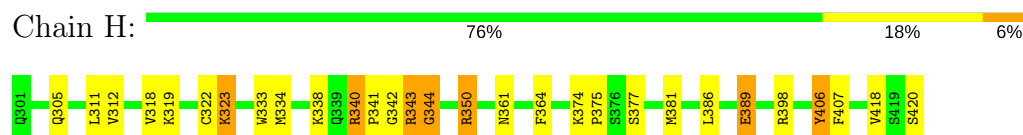
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: B1-8 FV (LIGHT CHAIN)



- Molecule 2: B1-8 FV (HEAVY CHAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.03Å 85.78Å 37.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1892	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	L	1.10	4/827 (0.5%)	1.48	14/1132 (1.2%)
2	H	1.01	1/959 (0.1%)	1.32	7/1303 (0.5%)
All	All	1.05	5/1786 (0.3%)	1.40	21/2435 (0.9%)

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	L	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	96	ASN	CA-C	6.98	1.71	1.52
1	L	96	ASN	C-O	6.71	1.36	1.23
2	H	420	SER	C-OXT	6.18	1.35	1.23
1	L	96	ASN	N-CA	5.29	1.56	1.46
1	L	43	ASP	CA-CB	-5.15	1.42	1.53

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	42	PRO	O-C-N	10.55	139.58	122.70
1	L	43	ASP	CA-C-N	-9.64	96.00	117.20
1	L	43	ASP	CA-C-O	8.27	137.47	120.10
1	L	43	ASP	CA-CB-CG	-8.24	95.27	113.40
2	H	343	ARG	NE-CZ-NH2	7.70	124.15	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	43	ASP	Peptide

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	L	804	0	768	33	0
2	H	932	0	873	19	0
3	H	84	0	0	2	0
3	L	72	0	0	5	0
All	All	1892	0	1641	50	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 15.

The worst 5 of 50 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:L:96:ASN:N	1:L:96:ASN:HD22	1.58	0.94
1:L:83:GLU:OE1	3:L:140:HOH:O	1.87	0.92
1:L:96:ASN:HD22	1:L:96:ASN:H	1.11	0.92
2:H:343:ARG:HG2	2:H:344:GLY:H	1.35	0.88
1:L:96:ASN:ND2	1:L:96:ASN:H	1.68	0.85

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	L	107/108 (99%)	98 (92%)	8 (8%)	1 (1%)	20	14
2	H	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	22	17
All	All	225/228 (99%)	207 (92%)	16 (7%)	2 (1%)	20	14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	53	THR
2	H	342	GLY

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	L	85/85 (100%)	79 (93%)	6 (7%)	17	13
2	H	98/102 (96%)	92 (94%)	6 (6%)	22	18
All	All	183/187 (98%)	171 (93%)	12 (7%)	19	16

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	96	ASN
2	H	305	GLN
2	H	323	LYS
1	L	56	ARG
2	H	322	CYS

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

Mol	Chain	Res	Type
1	L	54	ASN
1	L	96	ASN
1	L	97	HIS
2	H	303	GLN

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Mol	Chain	Res	Type
2	H	354	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 carbohydrates 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.