



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:52 PM GMT

PDB ID : 1VLK
Title : STRUCTURE OF VIRAL INTERLEUKIN-10
Authors : Zdanov, A.; Schalk-Hihi, C.; Wlodawer, A.
Deposited on : 1997-02-14
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

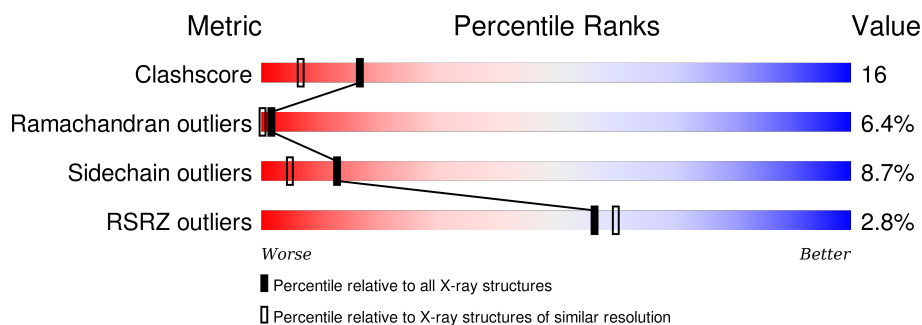
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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.

Mol	Chain	Length	Quality of chain
1	A	145	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1193 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 VIRAL INTERLEUKIN-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1118	711	193	206	8			

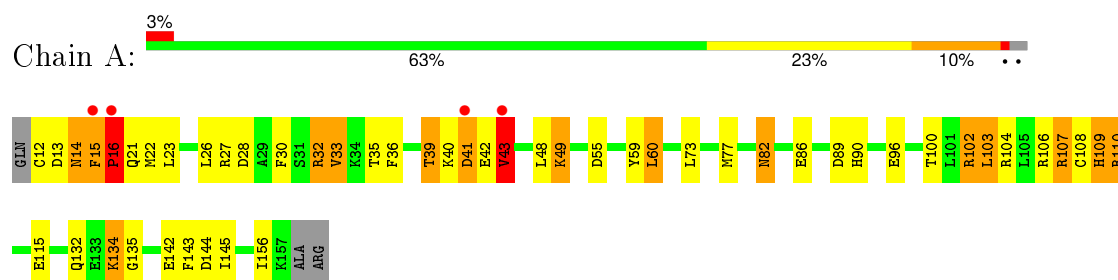
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: VIRAL INTERLEUKIN-10



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	36.27Å 36.27Å 219.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 9.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 79.6 (9.95-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.191 , (Not available) 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 75.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 9860 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1193	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.93	0/1138	2.23	37/1526 (2.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ARG	CD-NE-CZ	23.01	155.81	123.60
1	A	102	ARG	NE-CZ-NH2	-18.42	111.09	120.30
1	A	102	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	A	32	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	A	55	ASP	CB-CG-OD2	10.59	127.83	118.30
1	A	144	ASP	CB-CG-OD1	10.11	127.40	118.30
1	A	39	THR	N-CA-CB	7.83	125.17	110.30
1	A	32	ARG	CG-CD-NE	7.78	128.14	111.80
1	A	100	THR	O-C-N	-6.58	112.18	122.70
1	A	102	ARG	CB-CG-CD	6.57	128.67	111.60
1	A	27	ARG	CD-NE-CZ	6.53	132.74	123.60
1	A	39	THR	C-N-CA	6.43	137.78	121.70
1	A	77	MET	CA-CB-CG	-6.42	102.39	113.30
1	A	43	VAL	N-CA-C	6.18	127.70	111.00
1	A	32	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	A	35	THR	CA-CB-CG2	-6.01	103.98	112.40
1	A	106	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	39	THR	CA-C-O	5.82	132.33	120.10
1	A	36	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	A	82	ASN	OD1-CG-ND2	5.62	134.82	121.90
1	A	16	PRO	CA-N-CD	-5.59	103.68	111.50
1	A	28	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	100	THR	CA-C-N	5.52	129.35	117.20
1	A	30	PHE	CD1-CE1-CZ	-5.50	113.51	120.10
1	A	48	LEU	CB-CA-C	-5.45	99.85	110.20
1	A	142	GLU	N-CA-CB	-5.42	100.85	110.60
1	A	73	LEU	O-C-N	-5.41	114.04	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ASP	OD1-CG-OD2	-5.38	113.08	123.30
1	A	102	ARG	CG-CD-NE	5.31	122.96	111.80
1	A	12	CYS	CB-CA-C	-5.28	99.85	110.40
1	A	107	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	104	ARG	CD-NE-CZ	5.19	130.87	123.60
1	A	55	ASP	O-C-N	-5.17	114.42	122.70
1	A	110	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	143	PHE	CZ-CE2-CD2	-5.15	113.92	120.10
1	A	82	ASN	CA-CB-CG	-5.09	102.21	113.40
1	A	107	ARG	CB-CG-CD	5.08	124.81	111.60

There are no chirality outliers.

There are no planarity outliers.

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	A	1118	0	1070	36	0
2	A	75	0	0	9	0
All	All	1193	0	1070	36	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 16.

All (36) 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:15:PHE:HA	1:A:21:GLN:N	1.55	1.19
1:A:15:PHE:HB3	1:A:22:MET:H	1.21	1.06
1:A:15:PHE:HB3	1:A:22:MET:N	1.70	1.06
1:A:59:TYR:CE2	1:A:60:LEU:HD13	1.98	0.97
1:A:15:PHE:CB	1:A:22:MET:H	1.92	0.82
1:A:15:PHE:CA	1:A:21:GLN:N	2.43	0.80
1:A:15:PHE:HD1	1:A:15:PHE:H	1.32	0.77
1:A:15:PHE:HA	1:A:21:GLN:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:HA	1:A:16:PRO:C	2.04	0.74
1:A:134:LYS:HA	1:A:134:LYS:HE2	1.75	0.67
1:A:22:MET:O	2:A:239:HOH:O	2.12	0.67
1:A:109:HIS:HA	2:A:233:HOH:O	1.95	0.65
1:A:14:ASN:O	1:A:15:PHE:C	2.39	0.60
1:A:15:PHE:N	1:A:15:PHE:CD1	2.67	0.56
1:A:39:THR:HG22	2:A:225:HOH:O	2.04	0.56
1:A:41:ASP:O	1:A:43:VAL:N	2.41	0.53
1:A:15:PHE:CA	1:A:21:GLN:H	2.14	0.52
1:A:102:ARG:NE	2:A:212:HOH:O	2.26	0.52
1:A:108:CYS:O	1:A:110:ARG:N	2.43	0.52
1:A:102:ARG:HD2	1:A:115:GLU:OE1	2.11	0.49
1:A:15:PHE:HA	1:A:21:GLN:CA	2.40	0.48
1:A:15:PHE:HB3	1:A:22:MET:CA	2.44	0.48
1:A:102:ARG:NH2	2:A:212:HOH:O	2.31	0.48
1:A:49:LYS:HB3	1:A:49:LYS:HE3	1.26	0.46
1:A:89:ASP:HB3	2:A:249:HOH:O	2.16	0.46
1:A:108:CYS:O	1:A:109:HIS:C	2.54	0.46
1:A:59:TYR:CD2	1:A:60:LEU:HD13	2.48	0.45
1:A:59:TYR:CE2	1:A:60:LEU:CD1	2.86	0.45
1:A:132:GLN:O	1:A:135:GLY:N	2.47	0.44
1:A:26:LEU:HB2	2:A:239:HOH:O	2.18	0.43
1:A:145:ILE:HG21	1:A:145:ILE:HD13	1.49	0.42
1:A:60:LEU:HB2	2:A:201:HOH:O	2.20	0.42
1:A:102:ARG:O	1:A:103:LEU:C	2.58	0.41
1:A:33:VAL:HG23	1:A:90:HIS:HB2	2.03	0.41
1:A:15:PHE:HB3	1:A:23:LEU:H	1.86	0.40
1:A:86:GLU:HG3	2:A:238:HOH:O	2.21	0.40

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	140/145 (97%)	123 (88%)	8 (6%)	9 (6%)	2 0

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	14	ASN
1	A	16	PRO
1	A	40	LYS
1	A	41	ASP
1	A	43	VAL
1	A	42	GLU
1	A	109	HIS
1	A	156	ILE

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	A	115/132 (87%)	105 (91%)	10 (9%)	13 5

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	32	ARG
1	A	33	VAL
1	A	49	LYS
1	A	60	LEU
1	A	82	ASN
1	A	96	GLU
1	A	103	LEU
1	A	107	ARG
1	A	134	LYS

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

Mol	Chain	Res	Type
1	A	63	GLN
1	A	90	HIS
1	A	97	ASN
1	A	116	ASN
1	A	129	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 [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	142/145 (97%)	-0.37	4 (2%) 56 60	20, 35, 84, 93	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	5.6
1	A	15	PHE	3.9
1	A	16	PRO	2.8
1	A	41	ASP	2.5

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 carbohydrates 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.