



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:33 AM GMT

PDB ID : 2R02
Title : Crystal Structure of ALIX/AIP1 in complex with the HIV-1 YPLTSL Late Domain
Authors : Hill, C.P.; Zhai, Q.; Fisher, R.D.
Deposited on : 2007-08-17
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

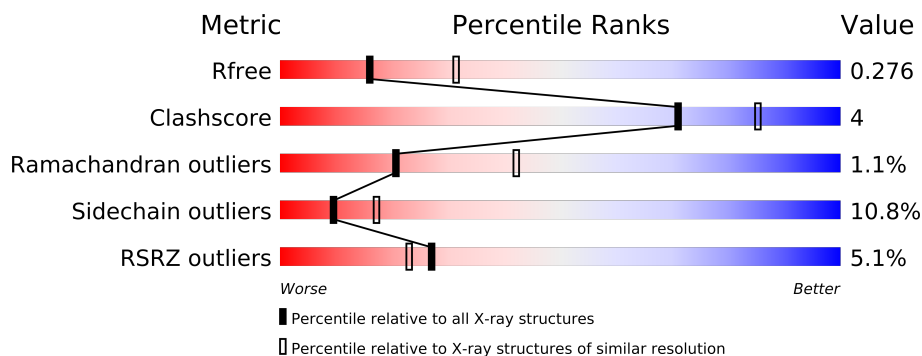
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	697	
2	B	11	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5593 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5486	3461	938	1069	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	TYR	LYS	ENGINEERED	UNP Q8WUM4
A	269	TYR	LYS	ENGINEERED	UNP Q8WUM4

- Molecule 2 is a protein called p6-gag.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			90	59	14	17			

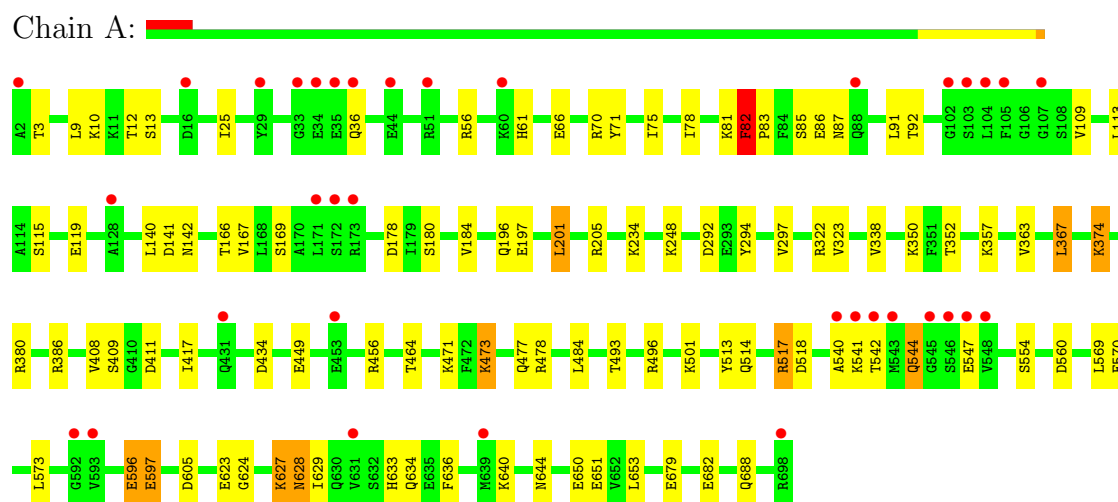
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		

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: Programmed cell death 6-interacting protein



- Molecule 2: p6-gag



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.92Å 99.08Å 73.23Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 35.70 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.60) 98.2 (35.70-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.224 , 0.285 0.221 , 0.276	Depositor DCC
R_{free} test set	1501 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 29832 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	A	0.83	10/5570 (0.2%)	0.73	5/7523 (0.1%)
2	B	3.11	1/91 (1.1%)	0.85	1/123 (0.8%)
All	All	0.92	11/5661 (0.2%)	0.73	6/7646 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	44	LEU	C-O	29.25	1.78	1.23
1	A	547	GLU	CD-OE2	24.27	1.52	1.25
1	A	547	GLU	CD-OE1	16.65	1.44	1.25
1	A	627	LYS	CD-CE	13.71	1.85	1.51
1	A	627	LYS	CE-NZ	13.03	1.81	1.49
1	A	554	SER	CB-OG	12.40	1.58	1.42
1	A	374	LYS	CE-NZ	9.79	1.73	1.49
1	A	544	GLN	CD-OE1	6.59	1.38	1.24
1	A	374	LYS	CD-CE	6.31	1.67	1.51
1	A	544	GLN	CD-NE2	5.87	1.47	1.32
1	A	541	LYS	CD-CE	5.55	1.65	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	LYS	CD-CE-NZ	-9.46	89.94	111.70
1	A	547	GLU	OE1-CD-OE2	7.97	132.87	123.30
1	A	374	LYS	CD-CE-NZ	-6.66	96.39	111.70
2	B	44	LEU	CA-C-O	-5.75	108.03	120.10
1	A	201	LEU	CB-CG-CD1	5.44	120.24	111.00
1	A	547	GLU	CG-CD-OE2	-5.14	108.02	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5486	0	0	24	0
2	B	90	0	0	1	0
3	A	17	0	0	0	0
All	All	5593	0	0	25	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (25) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:627:LYS:CE	1:A:627:LYS:CD	1.85	1.51
1:A:374:LYS:NZ	1:A:374:LYS:CE	1.73	1.48
1:A:627:LYS:NZ	1:A:627:LYS:CE	1.81	1.40
2:B:44:LEU:C	2:B:44:LEU:O	1.78	1.19
1:A:627:LYS:CG	1:A:627:LYS:CE	2.66	0.73
1:A:374:LYS:NZ	1:A:374:LYS:CD	2.53	0.70
1:A:141:ASP:O	1:A:205:ARG:CZ	2.43	0.67
1:A:627:LYS:NZ	1:A:627:LYS:CD	2.59	0.65
1:A:197:GLU:OE2	1:A:248:LYS:NZ	2.34	0.61
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.66	0.58
1:A:71:TYR:OH	1:A:119:GLU:OE2	2.22	0.57
1:A:196:GLN:O	1:A:197:GLU:C	2.42	0.57
1:A:3:THR:CG2	1:A:294:TYR:O	2.55	0.55
1:A:10:LYS:NZ	1:A:178:ASP:OD2	2.43	0.52
1:A:409:SER:OG	1:A:411:ASP:CB	2.60	0.50
1:A:624:GLY:O	1:A:628:ASN:ND2	2.47	0.48
1:A:81:LYS:O	1:A:82:PHE:C	2.53	0.46
1:A:322:ARG:NH1	1:A:323:VAL:O	2.48	0.46
1:A:540:ALA:CB	1:A:640:LYS:CG	2.94	0.45
1:A:66:GLU:O	1:A:70:ARG:N	2.51	0.44
1:A:434:ASP:OD1	1:A:513:TYR:OH	2.37	0.42
1:A:363:VAL:O	1:A:367:LEU:N	2.53	0.42
1:A:386:ARG:NH2	1:A:570:GLU:OE2	2.52	0.42
1:A:596:GLU:O	1:A:597:GLU:C	2.58	0.41
1:A:633:HIS:O	1:A:636:PHE:N	2.54	0.41

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	A	695/697 (100%)	638 (92%)	49 (7%)	8 (1%)	19	39
2	B	9/11 (82%)	7 (78%)	2 (22%)	0	100	100
All	All	704/708 (99%)	645 (92%)	51 (7%)	8 (1%)	21	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	87	ASN
1	A	544	GLN
1	A	85	SER
1	A	82	PHE
1	A	473	LYS
1	A	83	PRO
1	A	25	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	600/600 (100%)	535 (89%)	65 (11%)	9	17
2	B	11/11 (100%)	10 (91%)	1 (9%)	14	25
All	All	611/611 (100%)	545 (89%)	66 (11%)	9	17

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	THR
1	A	13	SER
1	A	56	ARG
1	A	61	HIS
1	A	75	ILE
1	A	78	ILE
1	A	82	PHE
1	A	86	GLU
1	A	91	LEU
1	A	92	THR
1	A	109	VAL
1	A	113	LEU
1	A	115	SER
1	A	140	LEU
1	A	142	ASN
1	A	166	THR
1	A	167	VAL
1	A	169	SER
1	A	180	SER
1	A	184	VAL
1	A	201	LEU
1	A	234	LYS
1	A	292	ASP
1	A	297	VAL
1	A	338	VAL
1	A	350	LYS
1	A	352	THR
1	A	357	LYS
1	A	367	LEU
1	A	380	ARG
1	A	408	VAL
1	A	417	ILE
1	A	449	GLU
1	A	456	ARG
1	A	464	THR
1	A	471	LYS
1	A	473	LYS
1	A	477	GLN
1	A	478	ARG
1	A	484	LEU
1	A	493	THR
1	A	496	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	501	LYS
1	A	514	GLN
1	A	517	ARG
1	A	518	ASP
1	A	542	THR
1	A	560	ASP
1	A	569	LEU
1	A	573	LEU
1	A	596	GLU
1	A	597	GLU
1	A	605	ASP
1	A	623	GLU
1	A	628	ASN
1	A	629	ILE
1	A	634	GLN
1	A	644	ASN
1	A	650	GLU
1	A	651	GLU
1	A	653	LEU
1	A	679	GLU
1	A	682	GLU
1	A	688	GLN
2	B	34	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	697/697 (100%)	0.30	35 (5%) 28 24	40, 85, 140, 181	2 (0%)
2	B	11/11 (100%)	0.61	1 (9%) 9 7	86, 109, 165, 166	0
All	All	708/708 (100%)	0.30	36 (5%) 27 23	40, 86, 141, 181	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	LEU	4.9
1	A	105	PHE	4.9
1	A	103	SER	4.7
1	A	102	GLY	4.4
1	A	88	GLN	3.8
1	A	542	THR	3.7
1	A	29	TYR	3.5
1	A	33	GLY	3.1
1	A	593	VAL	3.1
2	B	41	LEU	3.1
1	A	546	SER	3.0
1	A	543	MET	3.0
1	A	540	ALA	2.9
1	A	541	LYS	2.8
1	A	60	LYS	2.8
1	A	172	SER	2.7
1	A	34	GLU	2.7
1	A	547	GLU	2.7
1	A	431	GLN	2.5
1	A	545	GLY	2.5
1	A	16	ASP	2.5
1	A	2	ALA	2.3
1	A	592	GLY	2.3
1	A	171	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	128	ALA	2.2
1	A	173	ARG	2.2
1	A	36	GLN	2.2
1	A	631	VAL	2.2
1	A	44	GLU	2.1
1	A	107	GLY	2.1
1	A	51	ARG	2.1
1	A	698	ARG	2.1
1	A	35	GLU	2.1
1	A	639	MET	2.0
1	A	453	GLU	2.0
1	A	548	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.