



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:00 PM UTC

PDB ID : 5YS4 / pdb_00005ys4
Title : Crystal structure of retroviral protease-like domain of Ddi1 from Leishmania major
Authors : Suguna, K.; Kumar, S.
Deposited on : 2017-11-13
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

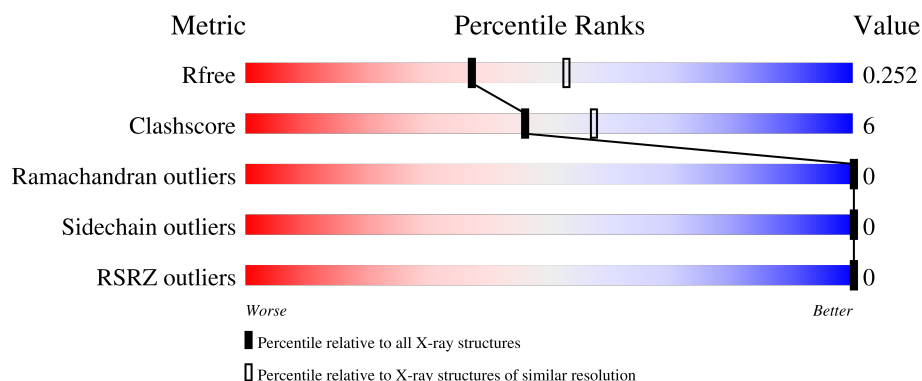
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	130	 83% 9% 8%
1	B	130	 87% 5% 8%
1	C	130	 73% 17% 10%
1	D	130	 79% 9% 12%
1	E	130	 77% 9% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	130	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 72%, a yellow segment representing 16%, and a grey segment representing 12%.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5694 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 DNA-damage inducible protein DDI1-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			930	596	159	162	13			
1	B	119	Total	C	N	O	S	0	3	0
			929	598	154	165	12			
1	C	117	Total	C	N	O	S	0	1	0
			910	583	153	162	12			
1	D	115	Total	C	N	O	S	0	0	0
			875	561	149	153	12			
1	E	112	Total	C	N	O	S	0	0	0
			807	520	137	139	11			
1	F	115	Total	C	N	O	S	0	0	0
			862	549	148	152	13			

- Molecule 2 is water.

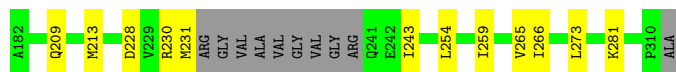
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	99	Total	O	0	0
			99	99		
2	C	89	Total	O	0	0
			89	89		
2	D	75	Total	O	0	0
			75	75		
2	E	15	Total	O	0	0
			15	15		
2	F	19	Total	O	0	0
			19	19		

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.

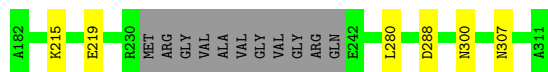
- Molecule 1: DNA-damage inducible protein DDI1-like protein

Chain A: 



- Molecule 1: DNA-damage inducible protein DDI1-like protein

Chain B: 



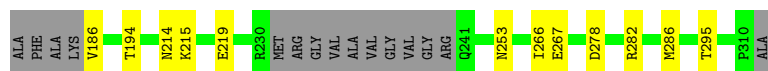
- Molecule 1: DNA-damage inducible protein DDI1-like protein

Chain C: 



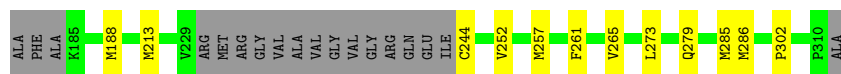
- Molecule 1: DNA-damage inducible protein DDI1-like protein

Chain D: 



- Molecule 1: DNA-damage inducible protein DDI1-like protein

Chain E: 



- Molecule 1: DNA-damage inducible protein DDI1-like protein

Chain F: 

ALA	PHE	ALA	LYS	V186	D205	A208	Q209	M213	M214	A218	L223	M224	V227	G233	VAL	ALA	VAL	GLY	VAL	GLY	ARG	Q241	M249	I259	F263	L266	Q269	D272	L273	L277	K281	R282	H283	D288	N307	ASP	LEU	PRO	ALA
-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.79Å 56.78Å 91.40Å 76.56° 84.48° 89.99°	Depositor
Resolution (Å)	26.34 – 2.30 26.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (26.34-2.30) 97.7 (26.34-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575	Depositor
R, R_{free}	0.236 , 0.259 0.227 , 0.252	Depositor DCC
R_{free} test set	1912 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5694	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% 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 [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	0.12	0/944	0.32	0/1277
1	B	0.11	0/944	0.31	0/1281
1	C	0.12	0/927	0.31	0/1257
1	D	0.12	0/889	0.33	0/1206
1	E	0.15	0/821	0.36	0/1119
1	F	0.20	0/875	0.47	0/1187
All	All	0.14	0/5400	0.35	0/7327

There are no bond length outliers.

There are no bond angle outliers.

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	930	0	945	8	0
1	B	929	0	930	6	0
1	C	910	0	928	16	0
1	D	875	0	878	10	0
1	E	807	0	773	14	0
1	F	862	0	845	16	0
2	A	84	0	0	0	0
2	B	99	0	0	2	0
2	C	89	0	0	1	0
2	D	75	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	15	0	0	2	0
2	F	19	0	0	1	0
All	All	5694	0	5299	61	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 6.

All (61) 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:255:ALA:HB2	1:C:301:VAL:HG22	1.64	0.78
1:D:215:LYS:NZ	1:D:219:GLU:OE2	2.33	0.61
1:D:282:ARG:NH1	2:D:403:HOH:O	2.34	0.59
1:F:259:ILE:HD11	1:F:283:HIS:CG	2.38	0.59
1:C:212:ILE:HG23	1:C:266:ILE:HD13	1.84	0.58
1:B:307:ASN:ND2	2:B:405:HOH:O	2.37	0.56
1:C:243:ILE:HG22	1:C:266:ILE:HA	1.87	0.56
1:C:215:LYS:NZ	1:C:219:GLU:OE2	2.38	0.55
1:B:215:LYS:NZ	1:B:219:GLU:OE2	2.40	0.55
1:E:244:CYS:N	2:E:401:HOH:O	2.41	0.54
1:C:257:MET:HE2	1:C:259[A]:ILE:HD11	1.88	0.54
1:A:231:MET:HE3	1:A:243:ILE:HB	1.88	0.54
1:F:213:MET:HE3	1:F:218:ALA:HB2	1.90	0.54
1:A:209:GLN:NE2	1:D:186:VAL:O	2.41	0.53
1:E:188:MET:HE2	1:E:188:MET:HA	1.90	0.53
1:F:241:GLN:N	2:F:403:HOH:O	2.41	0.53
1:E:261:PHE:HE1	1:E:279:GLN:HB3	1.74	0.53
1:B:288:ASP:HA	1:C:286:MET:HG2	1.92	0.52
1:C:185:LYS:HE2	1:E:302:PRO:HG3	1.92	0.51
1:F:213:MET:HB2	1:F:273:LEU:HD13	1.91	0.51
1:F:213:MET:HE2	1:F:263:PHE:CE1	2.46	0.51
1:E:286:MET:HG2	1:F:288:ASP:HA	1.94	0.50
1:E:261:PHE:CE1	1:E:279:GLN:HB3	2.47	0.50
1:D:286:MET:HB2	1:D:295:THR:HB	1.94	0.49
1:F:205:ASP:OD2	1:F:208:ALA:HB2	2.12	0.49
1:F:224:MET:HA	1:F:227:VAL:HG23	1.93	0.49
1:F:214:ASN:HB3	1:F:269:GLN:HB3	1.95	0.49
1:E:261:PHE:HZ	1:E:285:MET:HE1	1.77	0.49
1:F:277:LEU:HD21	1:F:281:LYS:HE3	1.95	0.49
1:E:244:CYS:HB3	1:E:265:VAL:O	2.13	0.48
1:C:194:THR:HB	1:C:253:ASN:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:THR:HB	1:D:253:ASN:HB3	1.96	0.48
1:A:254:LEU:HB3	1:A:259:ILE:HD12	1.96	0.47
1:D:267:GLU:O	2:D:401:HOH:O	2.20	0.47
1:E:257:MET:SD	2:E:404:HOH:O	2.61	0.47
1:A:228:ASP:OD1	1:A:230:ARG:HG2	2.15	0.47
1:A:243:ILE:HG13	1:A:266:ILE:HD12	1.97	0.46
1:B:280:LEU:HB3	1:C:289:LEU:HD13	1.97	0.46
1:B:300:ASN:ND2	2:B:401:HOH:O	2.34	0.46
1:C:269:GLN:HG2	1:C:271:MET:O	2.17	0.45
1:C:293:CYS:SG	1:C:300:ASN:HB3	2.56	0.45
1:D:278:ASP:O	1:D:282:ARG:HG3	2.16	0.45
1:C:307:ASN:HB3	1:E:286:MET:HE1	1.98	0.44
1:F:224:MET:HE3	1:F:224:MET:HB3	1.80	0.44
1:E:188:MET:HE3	1:F:209:GLN:OE1	2.17	0.44
1:E:213:MET:O	1:E:265:VAL:HA	2.18	0.44
1:F:213:MET:HE1	1:F:223:LEU:HD12	1.98	0.44
1:E:252:VAL:HB	1:E:261:PHE:HD2	1.84	0.43
1:B:307:ASN:O	1:D:286:MET:HE1	2.17	0.43
1:F:266:ILE:CG2	1:F:269:GLN:HB2	2.49	0.43
1:D:214:ASN:HA	1:D:266:ILE:O	2.19	0.42
1:A:281:LYS:HD2	1:D:186:VAL:HG21	2.01	0.42
1:C:253:ASN:ND2	2:C:403:HOH:O	2.31	0.41
1:F:249:MET:HE3	1:F:249:MET:HB2	1.91	0.41
1:A:213:MET:O	1:A:265:VAL:HA	2.21	0.41
1:C:214:ASN:HA	1:C:266:ILE:O	2.21	0.41
1:C:230:ARG:HH11	1:C:230:ARG:HG3	1.85	0.41
1:A:213:MET:HB2	1:A:273:LEU:HD13	2.02	0.40
1:E:213:MET:HB2	1:E:273:LEU:HD13	2.02	0.40
1:F:213:MET:HG3	1:F:272:ASP:O	2.21	0.40
1:C:265:VAL:C	1:C:266:ILE:HD12	2.47	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	116/130 (89%)	115 (99%)	1 (1%)	0	100	100
1	B	118/130 (91%)	114 (97%)	4 (3%)	0	100	100
1	C	114/130 (88%)	112 (98%)	2 (2%)	0	100	100
1	D	111/130 (85%)	109 (98%)	2 (2%)	0	100	100
1	E	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
1	F	111/130 (85%)	106 (96%)	5 (4%)	0	100	100
All	All	678/780 (87%)	662 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	102/112 (91%)	102 (100%)	0	100	100
1	B	100/112 (89%)	100 (100%)	0	100	100
1	C	102/112 (91%)	102 (100%)	0	100	100
1	D	95/112 (85%)	95 (100%)	0	100	100
1	E	80/112 (71%)	80 (100%)	0	100	100
1	F	91/112 (81%)	91 (100%)	0	100	100
All	All	570/672 (85%)	570 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	B	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	307	ASN
1	C	284	GLN
1	D	248	HIS
1	D	253	ASN
1	D	292	ASN
1	D	300	ASN
1	E	253	ASN
1	F	253	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 oligosaccharides 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	120/130 (92%)	-1.53	0 100 100	11, 25, 53, 65	0
1	B	119/130 (91%)	-1.59	0 100 100	10, 24, 44, 56	3 (2%)
1	C	117/130 (90%)	-1.53	0 100 100	11, 26, 50, 60	1 (0%)
1	D	115/130 (88%)	-1.54	0 100 100	12, 26, 51, 59	0
1	E	112/130 (86%)	-1.21	0 100 100	38, 61, 79, 90	0
1	F	115/130 (88%)	-1.38	0 100 100	36, 47, 65, 85	0
All	All	698/780 (89%)	-1.46	0 100 100	10, 32, 68, 90	4 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.