



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:07 AM GMT

PDB ID : 2PUS
Title : Unprecedented activation mechanism of a non-canonical RNA-dependent RNA polymerase
Authors : Garriga, D.; Navarro, A.; Querol-Audi, J.; Abaitua, F.; Rodriguez, J.F.; Verdaguier, N.
Deposited on : 2007-05-09
Resolution : 2.40 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>

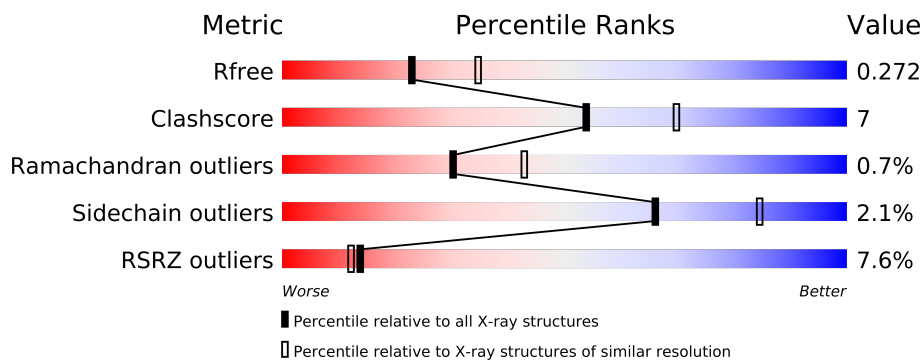
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	852	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6185 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 IBDV VP1 RNA-dependant RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			5917	3786	1008	1101	22			

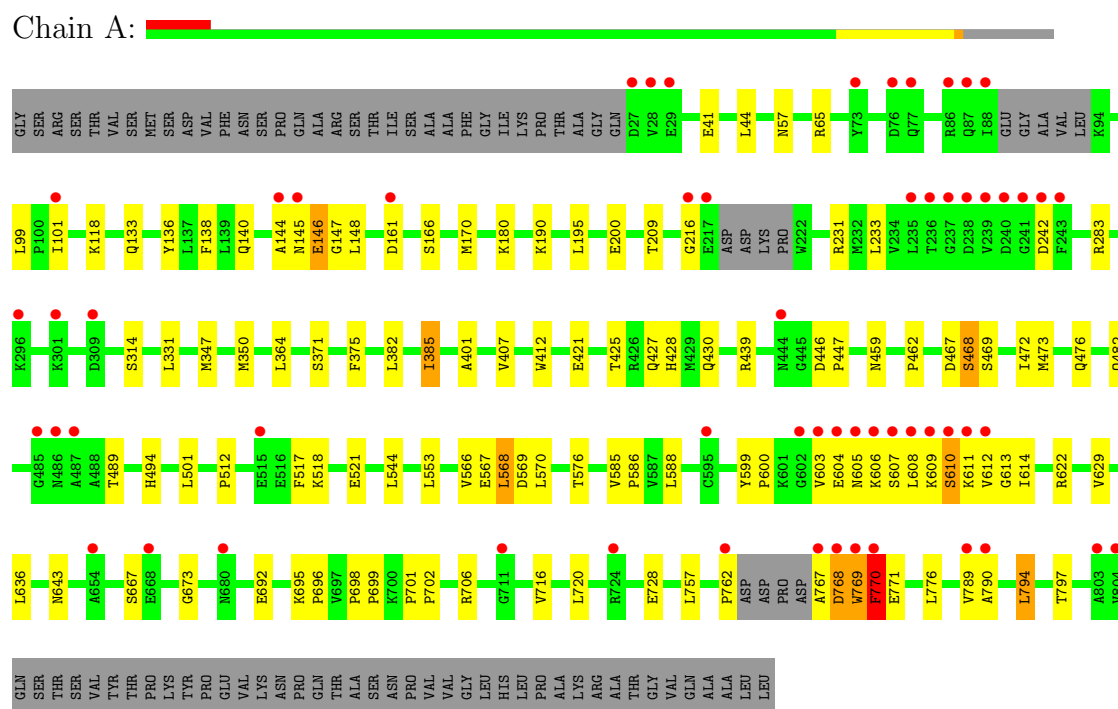
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	268	Total	O	0	0
			268	268		

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: IBDV VP1 RNA-dependant RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.17Å 123.17Å 362.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.40 19.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.89-2.40) 95.4 (19.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.263 0.247 , 0.272	Depositor DCC
R_{free} test set	3094 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 61373 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6185	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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	0.34	1/6055 (0.0%)	0.69	16/8233 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	ALA	N-CA	-8.52	1.29	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	SER	N-CA-CB	-18.96	82.06	110.50
1	A	607	SER	CB-CA-C	-16.00	79.70	110.10
1	A	606	LYS	CB-CA-C	-15.14	80.12	110.40
1	A	604	GLU	CB-CA-C	11.88	134.16	110.40
1	A	603	VAL	N-CA-C	-11.81	79.11	111.00
1	A	604	GLU	N-CA-CB	-9.25	93.95	110.60
1	A	767	ALA	N-CA-CB	8.66	122.22	110.10
1	A	605	ASN	N-CA-C	-8.45	88.19	111.00
1	A	567	GLU	N-CA-C	8.38	133.63	111.00
1	A	769	TRP	N-CA-C	-7.49	90.78	111.00
1	A	469	SER	N-CA-CB	-6.78	100.33	110.50
1	A	770	PHE	N-CA-CB	6.52	122.33	110.60
1	A	608	LEU	N-CA-C	6.29	127.99	111.00
1	A	762	PRO	N-CA-CB	6.10	110.62	103.30
1	A	567	GLU	CB-CA-C	-6.02	98.36	110.40
1	A	468	SER	N-CA-C	-5.14	97.12	111.00

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	5917	0	5868	81	0
2	A	268	0	0	6	0
All	All	6185	0	5868	81	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 7.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:PHE:CE1	1:A:144:ALA:HB1	1.80	1.16
1:A:138:PHE:CZ	1:A:144:ALA:HB1	1.95	1.01
1:A:138:PHE:CZ	1:A:144:ALA:CB	2.55	0.89
1:A:544:LEU:HD21	1:A:566:VAL:HG23	1.62	0.81
1:A:347:MET:HA	1:A:350:MET:HE2	1.63	0.80
1:A:609:LYS:CB	1:A:614:ILE:HG13	2.10	0.80
1:A:401:ALA:H	1:A:494:HIS:HD2	1.34	0.75
1:A:459:ASN:O	1:A:797:THR:HG21	1.86	0.74
1:A:145:ASN:ND2	1:A:146:GLU:OE2	2.21	0.73
1:A:576:THR:HG22	1:A:585:VAL:HG23	1.75	0.69
1:A:576:THR:CG2	1:A:585:VAL:HG23	2.22	0.68
1:A:145:ASN:O	1:A:147:GLY:N	2.27	0.68
1:A:364:LEU:HD21	1:A:385:ILE:HD12	1.77	0.67
1:A:144:ALA:HB3	2:A:988:HOH:O	1.94	0.66
1:A:412:TRP:CE2	1:A:568:LEU:HB3	2.30	0.66
1:A:769:TRP:O	1:A:771:GLU:N	2.28	0.66
1:A:553:LEU:HD13	1:A:585:VAL:HG11	1.77	0.65
1:A:401:ALA:H	1:A:494:HIS:CD2	2.14	0.64
1:A:768:ASP:O	2:A:931:HOH:O	2.15	0.63
1:A:144:ALA:CB	2:A:988:HOH:O	2.45	0.63
1:A:146:GLU:N	1:A:146:GLU:OE2	2.31	0.62
1:A:144:ALA:N	2:A:988:HOH:O	2.32	0.62
1:A:425:THR:H	1:A:428:HIS:HD2	1.49	0.61
1:A:412:TRP:NE1	1:A:568:LEU:HB3	2.16	0.60
1:A:65:ARG:H	1:A:476:GLN:HE22	1.50	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:610:SER:HB3	1:A:613:GLY:H	1.66	0.59
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.85	0.59
1:A:138:PHE:HB2	1:A:636:LEU:HD11	1.85	0.57
1:A:200:GLU:HB2	1:A:769:TRP:NE1	2.21	0.55
1:A:421:GLU:HG2	1:A:489:THR:HG21	1.88	0.55
1:A:145:ASN:O	1:A:146:GLU:C	2.45	0.54
1:A:462:PRO:HB2	1:A:794:LEU:HD21	1.91	0.53
1:A:136:TYR:O	1:A:140:GLN:HG2	2.09	0.52
1:A:190:LYS:HD3	1:A:195:LEU:HD21	1.91	0.52
1:A:472:ILE:O	1:A:472:ILE:HG23	2.09	0.52
1:A:427:GLN:HA	1:A:430:GLN:HG2	1.92	0.51
1:A:41:GLU:HG3	1:A:118:LYS:HD2	1.92	0.51
1:A:99:LEU:HB3	1:A:101:ILE:HD13	1.93	0.50
1:A:145:ASN:O	1:A:148:LEU:N	2.44	0.50
1:A:200:GLU:HG2	1:A:769:TRP:CD1	2.46	0.50
1:A:769:TRP:HE3	1:A:770:PHE:H	1.59	0.49
1:A:576:THR:HG23	1:A:585:VAL:HG23	1.94	0.48
1:A:209:THR:O	1:A:371:SER:HB2	2.14	0.48
1:A:706:ARG:HH12	1:A:728:GLU:HB3	1.78	0.48
1:A:200:GLU:CB	1:A:769:TRP:NE1	2.77	0.48
1:A:385:ILE:HG21	1:A:570:LEU:HD22	1.95	0.47
1:A:314:SER:O	1:A:468:SER:HB2	2.14	0.47
1:A:472:ILE:O	1:A:473:MET:HB2	2.15	0.47
1:A:692:GLU:HA	1:A:695:LYS:HD2	1.95	0.47
1:A:200:GLU:HB2	1:A:769:TRP:HE1	1.79	0.47
1:A:588:LEU:HD22	1:A:629:VAL:CG2	2.45	0.46
1:A:145:ASN:C	1:A:147:GLY:N	2.69	0.46
1:A:576:THR:HG23	1:A:585:VAL:CG2	2.46	0.45
1:A:133:GLN:HE21	1:A:643:ASN:HD22	1.63	0.45
1:A:768:ASP:CG	1:A:768:ASP:O	2.54	0.45
1:A:512:PRO:HA	1:A:517:PHE:CG	2.52	0.45
1:A:698:PRO:HA	1:A:699:PRO:HD3	1.91	0.45
1:A:44:LEU:HG	1:A:170:MET:SD	2.57	0.45
1:A:425:THR:H	1:A:428:HIS:CD2	2.31	0.44
1:A:609:LYS:C	1:A:611:LYS:N	2.68	0.44
1:A:716:VAL:O	1:A:720:LEU:HB2	2.17	0.44
1:A:170:MET:HG3	1:A:331:LEU:O	2.18	0.44
1:A:789:VAL:O	1:A:790:ALA:HB3	2.18	0.43
1:A:568:LEU:H	1:A:568:LEU:HG	1.38	0.43
1:A:609:LYS:O	1:A:611:LYS:N	2.52	0.43
1:A:382:LEU:HD13	1:A:586:PRO:HA	2.01	0.43
1:A:599:TYR:HA	1:A:600:PRO:HD2	1.93	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:695:LYS:HA	1:A:696:PRO:HD3	1.94	0.42
1:A:231:ARG:HH12	1:A:283:ARG:HH21	1.67	0.42
1:A:568:LEU:O	1:A:569:ASP:C	2.58	0.42
1:A:146:GLU:HG2	2:A:1081:HOH:O	2.20	0.41
1:A:421:GLU:HB3	1:A:482:GLN:O	2.20	0.41
1:A:518:LYS:O	1:A:521:GLU:HG2	2.20	0.41
1:A:701:PRO:HA	1:A:702:PRO:HD3	1.97	0.41
1:A:375:PHE:CE1	1:A:385:ILE:HD13	2.55	0.41
1:A:446:ASP:HA	1:A:447:PRO:HD3	1.90	0.41
1:A:41:GLU:CG	1:A:118:LYS:HD2	2.50	0.41
1:A:57:ASN:O	1:A:180:LYS:NZ	2.53	0.41
1:A:467:ASP:OD2	2:A:879:HOH:O	2.22	0.40
1:A:667:SER:O	1:A:673:GLY:HA3	2.22	0.40
1:A:588:LEU:HD22	1:A:629:VAL:HG21	2.02	0.40

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	757/852 (89%)	721 (95%)	31 (4%)	5 (1%)	30	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	770	PHE
1	A	216	GLY
1	A	242	ASP
1	A	612	VAL

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	627/730 (86%)	614 (98%)	13 (2%)	66 84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ASP
1	A	166	SER
1	A	233	LEU
1	A	385	ILE
1	A	407	VAL
1	A	439	ARG
1	A	501	LEU
1	A	568	LEU
1	A	610	SER
1	A	757	LEU
1	A	768	ASP
1	A	776	LEU
1	A	794	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	145	ASN
1	A	172	GLN
1	A	299	ASN
1	A	336	ASN
1	A	376	ASN
1	A	428	HIS
1	A	430	GLN
1	A	451	GLN
1	A	476	GLN
1	A	482	GLN
1	A	494	HIS

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	765/852 (89%)	0.30	58 (7%) 14 12	20, 38, 53, 59	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	LEU	8.6
1	A	607	SER	8.0
1	A	242	ASP	7.7
1	A	216	GLY	7.2
1	A	144	ALA	6.1
1	A	73	TYR	5.9
1	A	28	VAL	5.8
1	A	611	LYS	5.7
1	A	236	THR	5.6
1	A	605	ASN	5.6
1	A	609	LYS	5.3
1	A	767	ALA	5.3
1	A	604	GLU	5.2
1	A	238	ASP	5.2
1	A	87	GLN	5.0
1	A	239	VAL	4.8
1	A	612	VAL	4.7
1	A	27	ASP	4.6
1	A	241	GLY	4.5
1	A	217	GLU	4.5
1	A	790	ALA	4.5
1	A	606	LYS	4.4
1	A	240	ASP	4.1
1	A	237	GLY	4.0
1	A	603	VAL	3.8
1	A	789	VAL	3.7
1	A	602	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	3.5
1	A	76	ASP	3.5
1	A	486	ASN	3.5
1	A	610	SER	3.5
1	A	86	ARG	3.4
1	A	243	PHE	3.2
1	A	762	PRO	3.2
1	A	595	CYS	3.1
1	A	770	PHE	3.1
1	A	29	GLU	3.1
1	A	145	ASN	3.1
1	A	161	ASP	3.0
1	A	804	VAL	3.0
1	A	485	GLY	2.9
1	A	768	ASP	2.9
1	A	235	LEU	2.8
1	A	296	LYS	2.7
1	A	301	LYS	2.6
1	A	654	ALA	2.6
1	A	77	GLN	2.5
1	A	101	ILE	2.5
1	A	487	ALA	2.4
1	A	680	ASN	2.4
1	A	515	GLU	2.3
1	A	769	TRP	2.3
1	A	724	ARG	2.3
1	A	668	GLU	2.3
1	A	711	GLY	2.3
1	A	444	ASN	2.2
1	A	803	ALA	2.1
1	A	309	ASP	2.1

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.