



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 08:09 pm GMT

PDB ID : 1XR6
Title : Crystal Structure of RNA-dependent RNA Polymerase 3D from human rhinovirus serotype 1B
Authors : Love, R.A.; Maegley, K.A.; Yu, X.; Ferre, R.A.; Lingardo, L.K.; Diehl, W.; Parge, H.E.; Dragovich, P.S.; Fuhrman, S.A.
Deposited on : 2004-10-13
Resolution : 2.50 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 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	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

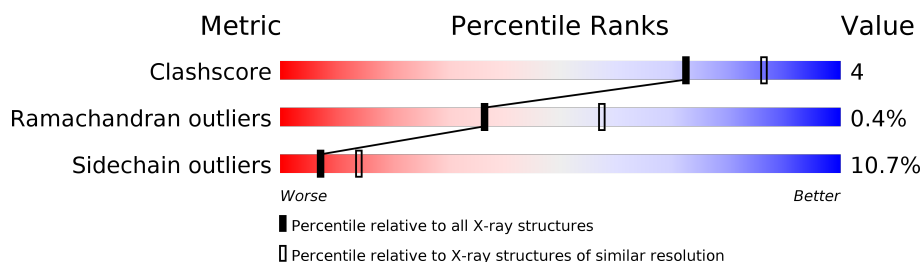
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	122078	4826 (2.50-2.50)
Ramachandran outliers	120005	4734 (2.50-2.50)
Sidechain outliers	119972	4736 (2.50-2.50)

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	A	460	 81% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3940 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3688	2378	606	688	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	LEU	SER	SEE REMARK 999	UNP P12916
A	44	THR	ARG	SEE REMARK 999	UNP P12916

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is water.

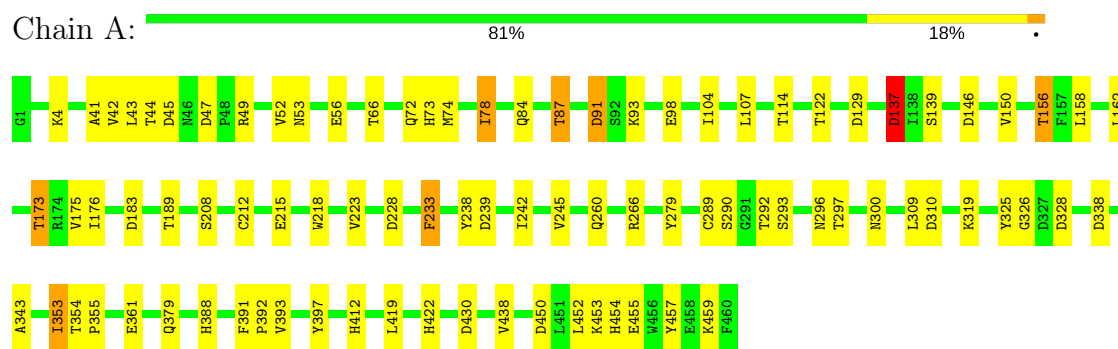
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	251	Total	O	0	0
			251	251		

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: Genome polypeptide



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.39Å 88.39Å 186.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.9 (20.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.229 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3940	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	0.41	0/3776	0.72	11/5103 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	338	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	239	ASP	CB-CG-OD2	6.48	124.14	118.30
1	A	45	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	91	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	137	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	450	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	183	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	129	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	228	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	146	ASP	CB-CG-OD2	5.03	122.82	118.30

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	3688	0	3699	27	0
2	A	1	0	0	0	0
3	A	251	0	0	2	0
All	All	3940	0	3699	27	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 4.

All (27) 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:388:HIS:HD2	1:A:422:HIS:HD2	1.41	0.67
1:A:388:HIS:CD2	1:A:422:HIS:HD2	2.12	0.66
1:A:156:THR:HG21	1:A:279:TYR:OH	1.99	0.62
1:A:84:GLN:O	1:A:87:THR:HB	2.03	0.58
1:A:208:SER:HB3	1:A:297:THR:HG21	1.84	0.58
1:A:74:MET:O	1:A:78:ILE:HG23	2.06	0.56
1:A:393:VAL:HG13	1:A:397:TYR:CE2	2.40	0.56
1:A:215:GLU:OE2	1:A:422:HIS:HE1	1.89	0.55
1:A:41:ALA:HB1	1:A:173:THR:HB	1.89	0.55
1:A:208:SER:CB	1:A:297:THR:HG21	2.38	0.54
1:A:42:VAL:O	1:A:173:THR:HG21	2.08	0.54
1:A:296:ASN:HB3	1:A:326:GLY:HA2	1.91	0.53
1:A:53:ASN:HD22	1:A:56:GLU:H	1.57	0.52
1:A:453:LYS:NZ	3:A:669:HOH:O	2.43	0.51
1:A:238:TYR:CE2	1:A:242:ILE:HD11	2.47	0.49
1:A:137:ASP:OD2	1:A:139:SER:OG	2.29	0.47
1:A:343:ALA:HB1	1:A:353:ILE:HG12	1.97	0.47
1:A:91:ASP:OD2	1:A:93:LYS:HB2	2.15	0.46
1:A:354:THR:HB	1:A:355:PRO:HD2	1.99	0.44
1:A:391:PHE:CG	1:A:392:PRO:HD2	2.52	0.44
1:A:457:TYR:C	1:A:459:LYS:H	2.21	0.44
1:A:73:HIS:HD2	1:A:310:ASP:OD1	2.01	0.44
1:A:104:ILE:HG22	1:A:107:LEU:HB3	1.99	0.44
1:A:52:VAL:HG12	1:A:53:ASN:N	2.34	0.43
1:A:78:ILE:HD11	3:A:636:HOH:O	2.18	0.42
1:A:354:THR:HB	1:A:355:PRO:CD	2.49	0.42
1:A:233:PHE:CE1	1:A:353:ILE:HD12	2.57	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	458/460 (100%)	441 (96%)	15 (3%)	2 (0%)	36 57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	SER
1	A	289	CYS

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	411/411 (100%)	367 (89%)	44 (11%)	7 14

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	43	LEU
1	A	44	THR
1	A	49	ARG
1	A	66	THR
1	A	72	GLN
1	A	78	ILE
1	A	87	THR
1	A	98	GLU

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Mol	Chain	Res	Type
1	A	114	THR
1	A	122	THR
1	A	137	ASP
1	A	150	VAL
1	A	156	THR
1	A	158	LEU
1	A	162	LEU
1	A	173	THR
1	A	175	VAL
1	A	176	ILE
1	A	189	THR
1	A	212	CYS
1	A	218	TRP
1	A	223	VAL
1	A	233	PHE
1	A	245	VAL
1	A	260	GLN
1	A	266	ARG
1	A	292	THR
1	A	293	SER
1	A	300	ASN
1	A	309	LEU
1	A	319	LYS
1	A	325	TYR
1	A	328	ASP
1	A	353	ILE
1	A	361	GLU
1	A	379	GLN
1	A	412	HIS
1	A	419	LEU
1	A	430	ASP
1	A	438	VAL
1	A	452	LEU
1	A	454	HIS
1	A	455	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	8	HIS
1	A	53	ASN

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Mol	Chain	Res	Type
1	A	73	HIS
1	A	84	GLN
1	A	237	ASN
1	A	256	ASN
1	A	260	GLN
1	A	300	ASN
1	A	368	ASN
1	A	388	HIS
1	A	412	HIS
1	A	422	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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

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.