



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 07:06 pm GMT

PDB ID : 1XR7
Title : Crystal structure of RNA-dependent RNA Polymerase 3D from human rhinovirus serotype 16
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 : 2.30 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 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

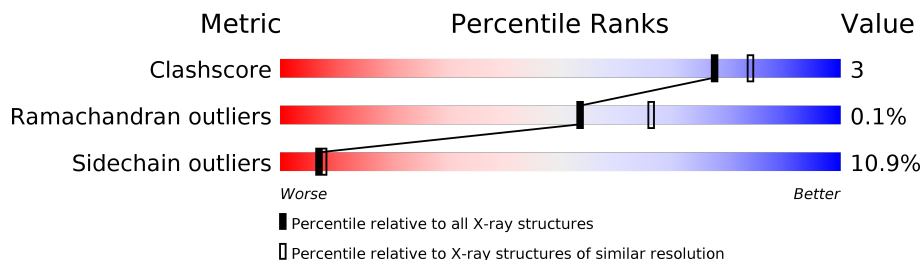
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	122078	5071 (2.30-2.30)
Ramachandran outliers	120005	5021 (2.30-2.30)
Sidechain outliers	119972	5020 (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 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	
1	B	460	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7569 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
			3682	2381	599	685	17			
1	B	460	Total	C	N	O	S	0	0	0
			3682	2381	599	685	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	GLY	ASP	SEE REMARK 999	UNP Q82122
B	149	GLY	ASP	SEE REMARK 999	UNP Q82122

- Molecule 2 is water.

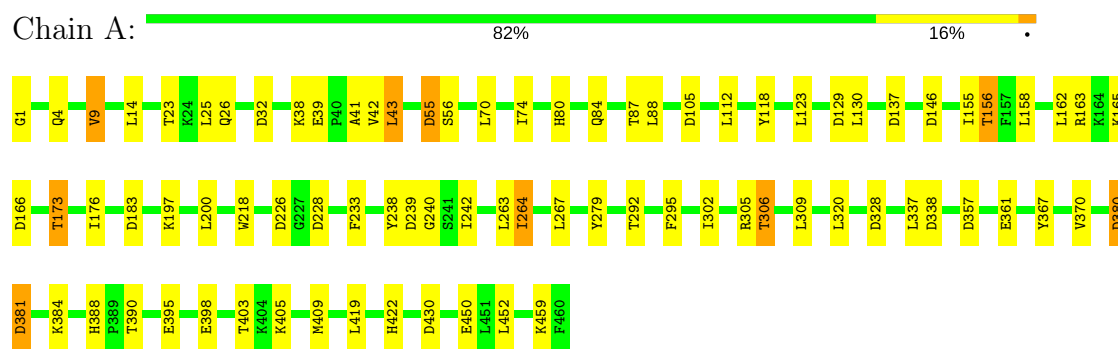
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		
2	B	94	Total	O	0	0
			94	94		

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 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 polyprotein



• Molecule 1: Genome polyprotein



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.98Å 100.95Å 116.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	99.3 (20.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.254 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7569	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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	0.39	0/3773	0.73	15/5104 (0.3%)
1	B	0.41	0/3773	0.76	18/5104 (0.4%)
All	All	0.40	0/7546	0.75	33/10208 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ASP	CB-CG-OD2	6.74	124.37	118.30
1	B	55	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	166	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	430	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	226	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	226	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	380	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	328	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	430	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	327	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	357	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	381	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	55	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	381	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	146	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	183	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	366	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	53	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	239	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	89	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	129	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	166	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	380	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	137	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	239	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	32	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	11	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	129	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	137	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	228	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	338	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	357	ASP	CB-CG-OD2	5.02	122.81	118.30

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	3682	0	3693	22	0
1	B	3682	0	3693	25	0
2	A	111	0	0	1	0
2	B	94	0	0	1	0
All	All	7569	0	7386	47	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 3.

All (47) 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:B:118:TYR:HB2	1:B:155:ILE:HD11	1.63	0.79
1:B:80:HIS:HD2	1:B:305:ARG:HE	1.33	0.76
1:B:42:VAL:O	1:B:173:THR:HG21	1.91	0.71
1:A:302:ILE:O	1:A:306:THR:HG23	1.95	0.67
1:A:118:TYR:HB2	1:A:155:ILE:HD11	1.77	0.67
1:B:302:ILE:O	1:B:306:THR:HG23	1.96	0.66
1:A:80:HIS:HD2	1:A:305:ARG:HE	1.44	0.65
1:B:41:ALA:HB2	1:B:163:ARG:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:THR:HG23	1:B:423:ASN:OD1	2.00	0.62
1:B:156:THR:HG21	1:B:279:TYR:OH	2.01	0.59
1:B:67:GLU:HA	1:B:67:GLU:OE2	2.03	0.58
1:A:388:HIS:HD2	1:A:422:HIS:ND1	2.03	0.56
1:B:181:ILE:HA	1:B:184:THR:CG2	2.35	0.55
1:B:181:ILE:HA	1:B:184:THR:HG22	1.88	0.55
1:B:41:ALA:HB1	1:B:173:THR:HB	1.89	0.54
1:B:434:LYS:NZ	2:B:620:HOH:O	2.40	0.54
1:A:41:ALA:HB1	1:A:173:THR:HB	1.90	0.54
1:B:238:TYR:CE2	1:B:242:ILE:HD11	2.43	0.54
1:A:380:ASP:OD1	1:A:388:HIS:HE1	1.93	0.51
1:A:238:TYR:CE2	1:A:242:ILE:HD11	2.47	0.50
1:B:388:HIS:HD2	1:B:422:HIS:ND1	2.10	0.49
1:A:367:TYR:HA	1:A:370:VAL:HG12	1.94	0.49
1:B:23:THR:HG21	1:B:40:PRO:HB3	1.93	0.49
1:B:74:ILE:HA	1:B:306:THR:CG2	2.43	0.48
1:A:41:ALA:HB2	1:A:163:ARG:HG3	1.96	0.47
1:B:38:LYS:HB2	1:B:398:GLU:HG2	1.97	0.46
1:B:72:GLU:O	1:B:76:VAL:HG13	2.17	0.45
1:A:84:GLN:O	1:A:87:THR:HB	2.15	0.45
1:A:42:VAL:O	1:A:173:THR:HG21	2.16	0.45
1:A:118:TYR:HB2	1:A:155:ILE:CD1	2.44	0.45
1:A:156:THR:HG21	1:A:279:TYR:OH	2.17	0.44
1:A:1:GLY:N	1:A:240:GLY:O	2.45	0.44
1:B:161:GLU:OE1	1:B:174:ARG:HD3	2.18	0.43
1:A:4:GLN:HB3	2:A:625:HOH:O	2.18	0.43
1:B:274:PHE:CE2	1:B:275:LYS:HE2	2.54	0.43
1:A:9:VAL:HG13	1:A:14:LEU:O	2.18	0.42
1:A:74:ILE:HG12	1:A:306:THR:HG21	2.00	0.42
1:B:63:LYS:HA	1:B:63:LYS:HD3	1.92	0.42
1:A:39:GLU:OE2	1:A:165:LYS:HE2	2.20	0.42
1:B:75:GLN:HB2	1:B:75:GLN:HE21	1.66	0.41
1:B:84:GLN:O	1:B:87:THR:HB	2.20	0.41
1:A:38:LYS:NZ	1:A:395:GLU:OE2	2.50	0.41
1:A:23:THR:HG22	1:A:43:LEU:HD22	2.02	0.41
1:B:23:THR:HG21	1:B:40:PRO:CB	2.51	0.41
1:B:80:HIS:HE1	1:B:318:ASP:OD1	2.03	0.41
1:A:264:ILE:HD11	1:A:295:PHE:CZ	2.57	0.40
1:A:88:LEU:HB3	1:A:197:LYS:HD3	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	458/460 (100%)	447 (98%)	11 (2%)	0	100	100
1	B	458/460 (100%)	446 (97%)	11 (2%)	1 (0%)	49	61
All	All	916/920 (100%)	893 (98%)	22 (2%)	1 (0%)	53	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	GLY

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	409/409 (100%)	369 (90%)	40 (10%)	9	10
1	B	409/409 (100%)	360 (88%)	49 (12%)	5	6
All	All	818/818 (100%)	729 (89%)	89 (11%)	7	8

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	25	LEU
1	A	26	GLN
1	A	43	LEU
1	A	55	ASP

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Mol	Chain	Res	Type
1	A	56	SER
1	A	70	LEU
1	A	105	ASP
1	A	112	LEU
1	A	123	LEU
1	A	130	LEU
1	A	156	THR
1	A	158	LEU
1	A	162	LEU
1	A	173	THR
1	A	176	ILE
1	A	200	LEU
1	A	218	TRP
1	A	228	ASP
1	A	233	PHE
1	A	263	LEU
1	A	264	ILE
1	A	267	LEU
1	A	292	THR
1	A	306	THR
1	A	309	LEU
1	A	320	LEU
1	A	337	LEU
1	A	361	GLU
1	A	381	ASP
1	A	384	LYS
1	A	390	THR
1	A	398	GLU
1	A	403	THR
1	A	405	LYS
1	A	409	MET
1	A	419	LEU
1	A	450	GLU
1	A	452	LEU
1	A	459	LYS
1	B	9	VAL
1	B	19	THR
1	B	21	THR
1	B	25	LEU
1	B	26	GLN
1	B	42	VAL
1	B	43	LEU

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Mol	Chain	Res	Type
1	B	56	SER
1	B	62	TYR
1	B	70	LEU
1	B	75	GLN
1	B	89	ASP
1	B	115	SER
1	B	123	LEU
1	B	130	LEU
1	B	145	LEU
1	B	156	THR
1	B	158	LEU
1	B	165	LYS
1	B	173	THR
1	B	176	ILE
1	B	184	THR
1	B	200	LEU
1	B	218	TRP
1	B	228	ASP
1	B	233	PHE
1	B	253	VAL
1	B	262	THR
1	B	263	LEU
1	B	264	ILE
1	B	271	LYS
1	B	293	SER
1	B	309	LEU
1	B	313	LYS
1	B	320	LEU
1	B	337	LEU
1	B	344	LYS
1	B	351	LEU
1	B	361	GLU
1	B	381	ASP
1	B	384	LYS
1	B	398	GLU
1	B	403	THR
1	B	419	LEU
1	B	426	GLU
1	B	450	GLU
1	B	451	LEU
1	B	452	LEU
1	B	459	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	133	ASN
1	A	193	ASN
1	A	237	ASN
1	A	347	GLN
1	A	379	GLN
1	A	388	HIS
1	A	418	HIS
1	B	26	GLN
1	B	75	GLN
1	B	80	HIS
1	B	133	ASN
1	B	193	ASN
1	B	201	ASN
1	B	237	ASN
1	B	379	GLN
1	B	388	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](#)

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 ⓘ

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.