WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 06:03 AM EST

PDB ID	:	1XR5
Title	:	Crystal Structure of the RNA-dependent RNA Polymerase 3D from human rhinovirus serotype 14
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	:	2.80 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	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		1.7%
Sidechain outliers		17.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
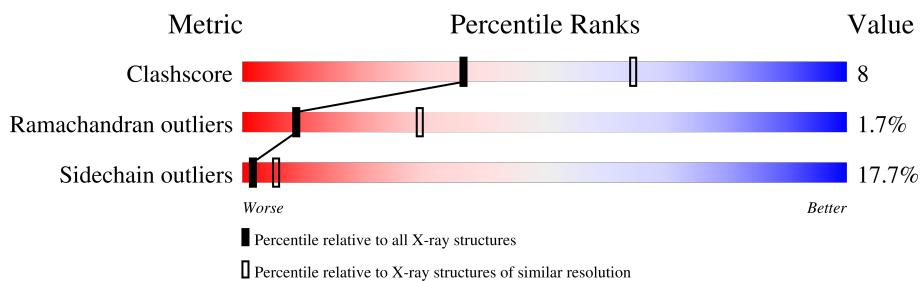
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	466	66% 27% 5% ••

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3681 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 3678	C 2368	N 605	O 686	S 19	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	HIS	-	expression tag	UNP P03303
A	462	HIS	-	expression tag	UNP P03303
A	463	HIS	-	expression tag	UNP P03303
A	464	HIS	-	expression tag	UNP P03303
A	465	HIS	-	expression tag	UNP P03303
A	466	HIS	-	expression tag	UNP P03303

- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

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

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

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. 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. 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

Chain A:
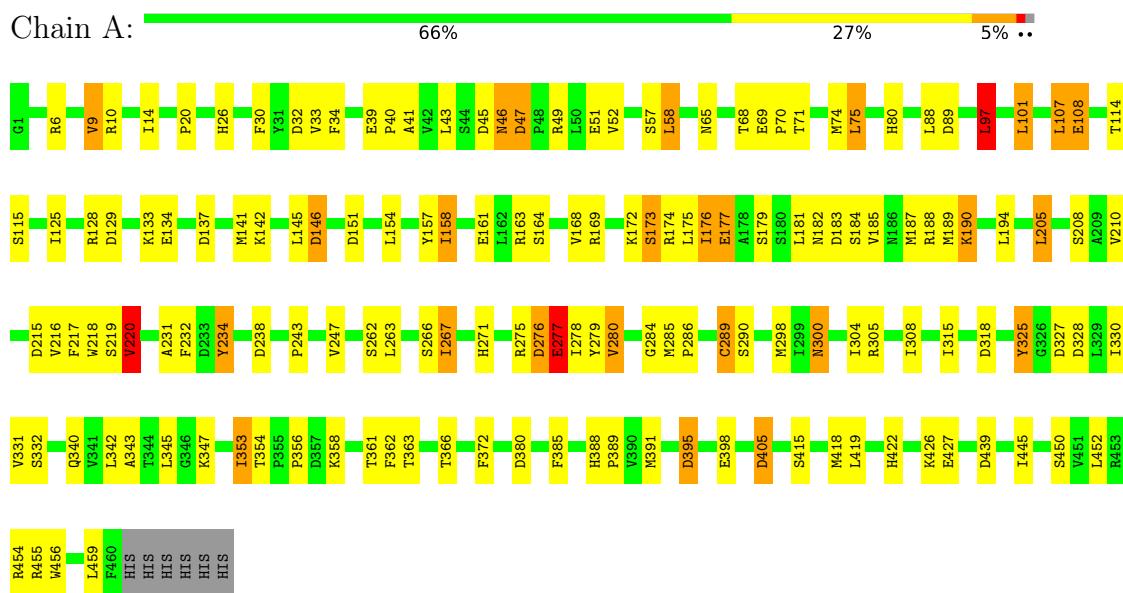
4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.33Å 97.33Å 153.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	92.7 (20.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.265 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3681	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.44	0/3766	0.79	14/5108 (0.3%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	327	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	238	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	318	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	380	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	129	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	439	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	146	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	405	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	328	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	137	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	45	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	151	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	32	ASP	CB-CG-OD2	5.15	122.93	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	3678	0	3695	58	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
All	All	3681	0	3695	58	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 8.

All (58) 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:389:PRO:HD2	1:A:422:HIS:CD2	2.25	0.71
1:A:184:SER:O	1:A:188:ARG:HB2	1.93	0.68
1:A:6:ARG:HD2	1:A:279:TYR:CE2	2.29	0.67
1:A:194:LEU:HD11	1:A:298:MET:HE1	1.78	0.65
1:A:289:CYS:SG	1:A:290:SER:N	2.71	0.64
1:A:41:ALA:HB1	1:A:173:SER:HB3	1.79	0.64
1:A:107:LEU:HD12	1:A:188:ARG:NH2	2.17	0.60
1:A:58:LEU:HD12	1:A:175:LEU:HD21	1.84	0.59
1:A:232:PHE:CD2	1:A:353:ILE:HD11	2.36	0.59
1:A:88:LEU:HD13	1:A:205:LEU:HD13	1.88	0.56
1:A:210:VAL:HA	1:A:325:TYR:CE2	2.41	0.56
1:A:217:PHE:O	1:A:220:VAL:HG13	2.06	0.55
1:A:164:SER:O	1:A:168:VAL:HG23	2.07	0.55
1:A:154:LEU:HD23	1:A:179:SER:HA	1.89	0.55
1:A:80:HIS:HD2	1:A:305:ARG:HE	1.54	0.54
1:A:145:LEU:HA	1:A:182:ASN:HD21	1.73	0.54
1:A:194:LEU:HD11	1:A:298:MET:CE	2.38	0.54
1:A:388:HIS:CD2	1:A:456:TRP:CH2	2.97	0.53
1:A:65:ASN:HD21	1:A:243:PRO:CD	2.22	0.53
1:A:157:TYR:HB2	1:A:176:ILE:HG12	1.91	0.52
1:A:330:ILE:HD11	1:A:372:PHE:HB2	1.92	0.52
1:A:43:LEU:HG	1:A:158:ILE:HD12	1.93	0.51
1:A:108:GLU:O	1:A:188:ARG:NH2	2.45	0.49
1:A:185:VAL:O	1:A:189:MET:HB2	2.12	0.49
1:A:51:GLU:O	1:A:52:VAL:HG23	2.13	0.49
1:A:231:ALA:HB3	1:A:356:PRO:HG3	1.92	0.49
1:A:276:ASP:O	1:A:277:GLU:C	2.51	0.49
1:A:161:GLU:OE2	1:A:163:ARG:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:HD2	1:A:456:TRP:CH2	2.31	0.48
1:A:267:ILE:HG22	1:A:286:PRO:HG2	1.95	0.48
1:A:358:LYS:NZ	1:A:395:ASP:OD1	2.45	0.48
1:A:80:HIS:CD2	1:A:305:ARG:HE	2.33	0.47
1:A:308:ILE:HG22	1:A:315:ILE:HD13	1.98	0.46
1:A:33:VAL:HG23	1:A:34:PHE:CD1	2.51	0.46
1:A:181:LEU:O	1:A:185:VAL:HG13	2.17	0.45
1:A:70:PRO:HB2	1:A:75:LEU:CD2	2.47	0.45
1:A:101:LEU:HD21	1:A:141:MET:HG2	1.99	0.45
1:A:145:LEU:HA	1:A:182:ASN:ND2	2.32	0.44
1:A:271:HIS:ND1	1:A:280:VAL:HB	2.32	0.44
1:A:46:ASN:O	1:A:47:ASP:C	2.56	0.44
1:A:9:VAL:HB	1:A:14:ILE:O	2.18	0.43
1:A:194:LEU:HD21	1:A:298:MET:HE1	2.00	0.43
1:A:71:THR:HB	1:A:74:MET:HB2	1.99	0.43
1:A:415:SER:O	1:A:419:LEU:HD13	2.18	0.43
1:A:97:LEU:O	1:A:101:LEU:HB2	2.19	0.42
1:A:234:TYR:OH	1:A:300:ASN:ND2	2.53	0.42
1:A:177:GLU:H	1:A:177:GLU:HG2	1.76	0.42
1:A:343:ALA:HA	1:A:353:ILE:HG23	2.01	0.42
1:A:39:GLU:HB3	1:A:40:PRO:HD2	2.01	0.42
1:A:177:GLU:HG3	1:A:286:PRO:HA	2.01	0.42
1:A:158:ILE:HD11	1:A:173:SER:HB2	2.02	0.42
1:A:172:LYS:O	1:A:173:SER:C	2.58	0.41
1:A:49:ARG:HD2	1:A:168:VAL:HG11	2.02	0.41
1:A:187:MET:HA	1:A:190:LYS:HG2	2.01	0.41
1:A:231:ALA:O	1:A:356:PRO:HD3	2.21	0.41
1:A:455:ARG:O	1:A:459:LEU:HD13	2.21	0.41
1:A:210:VAL:HA	1:A:325:TYR:CZ	2.56	0.41
1:A:30:PHE:HA	1:A:33:VAL:HG22	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	458/466 (98%)	409 (89%)	41 (9%)	8 (2%)	9 29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	VAL
1	A	277	GLU
1	A	362	PHE
1	A	97	LEU
1	A	275	ARG
1	A	47	ASP
1	A	20	PRO
1	A	284	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	417/423 (99%)	343 (82%)	74 (18%)	2 5

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	10	ARG
1	A	26	HIS
1	A	46	ASN
1	A	57	SER
1	A	58	LEU
1	A	68	THR
1	A	69	GLU
1	A	75	LEU
1	A	89	ASP
1	A	97	LEU

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Mol	Chain	Res	Type
1	A	101	LEU
1	A	107	LEU
1	A	108	GLU
1	A	114	THR
1	A	115	SER
1	A	125	ILE
1	A	128	ARG
1	A	133	LYS
1	A	134	GLU
1	A	142	LYS
1	A	146	ASP
1	A	158	ILE
1	A	169	ARG
1	A	173	SER
1	A	174	ARG
1	A	176	ILE
1	A	177	GLU
1	A	183	ASP
1	A	190	LYS
1	A	205	LEU
1	A	208	SER
1	A	216	VAL
1	A	218	TRP
1	A	219	SER
1	A	220	VAL
1	A	234	TYR
1	A	247	VAL
1	A	262	SER
1	A	263	LEU
1	A	266	SER
1	A	267	ILE
1	A	276	ASP
1	A	277	GLU
1	A	278	ILE
1	A	280	VAL
1	A	285	MET
1	A	289	CYS
1	A	300	ASN
1	A	304	ILE
1	A	325	TYR
1	A	331	VAL
1	A	332	SER

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	342	LEU
1	A	345	LEU
1	A	347	LYS
1	A	353	ILE
1	A	354	THR
1	A	361	THR
1	A	363	THR
1	A	366	THR
1	A	385	PHE
1	A	391	MET
1	A	395	ASP
1	A	398	GLU
1	A	405	ASP
1	A	418	MET
1	A	426	LYS
1	A	427	GLU
1	A	445	ILE
1	A	450	SER
1	A	452	LEU
1	A	454	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	46	ASN
1	A	80	HIS
1	A	186	ASN
1	A	300	ASN
1	A	369	ASN
1	A	388	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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.