



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:10 PM GMT

PDB ID : 1SH0
Title : Crystal Structure of Norwalk Virus Polymerase (Triclinic)
Authors : Ng, K.K.; Pendas-Franco, N.; Rojo, J.; Boga, J.A.; Machin, A.; Alonso, J.M.; Parra, F.
Deposited on : 2004-02-24
Resolution : 2.17 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

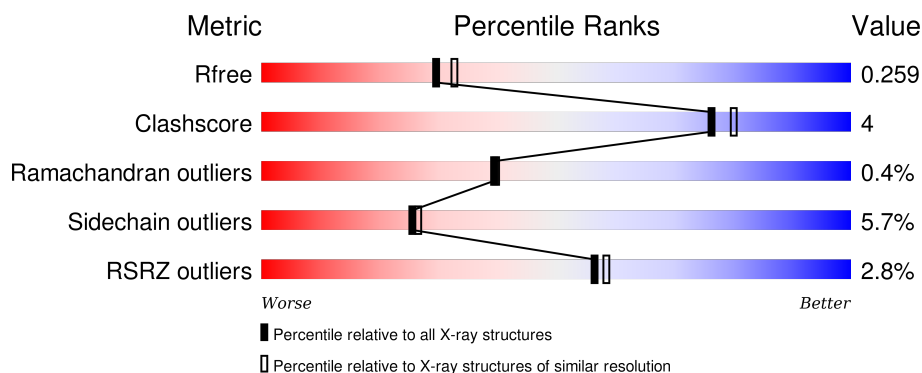
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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.

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	510	<div> <div>3%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8321 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 RNA Polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			3939	2501	675	741	22			
1	B	503	Total	C	N	O	S	0	0	0
			3948	2507	677	742	22			

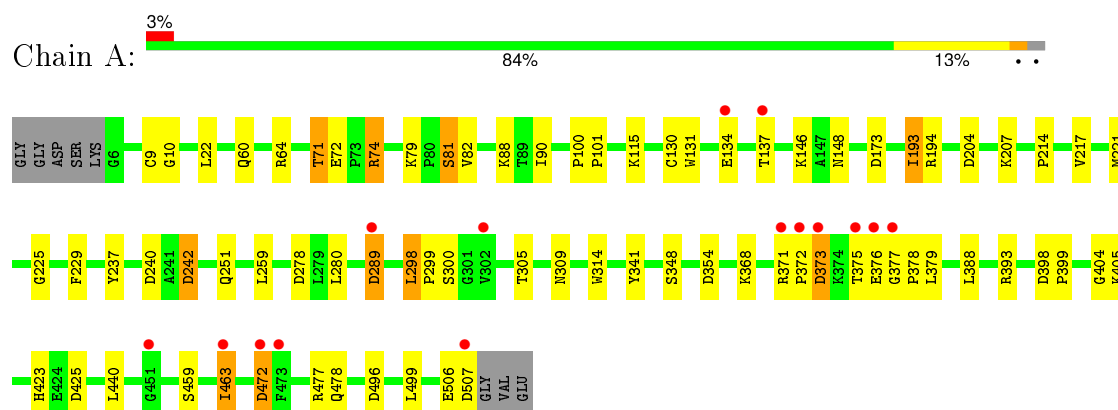
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	218	Total	O	0	0
			218	218		
2	B	216	Total	O	0	0
			216	216		

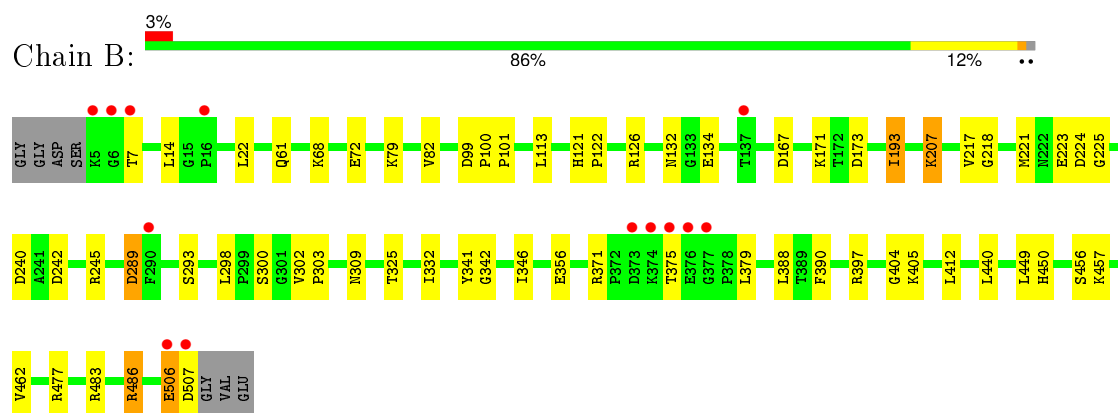
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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: RNA Polymerase



• Molecule 1: RNA Polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.14Å 59.91Å 100.09Å 104.36° 92.49° 111.91°	Depositor
Resolution (Å)	35.58 – 2.17 32.42 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.1 (35.58-2.17) 85.3 (32.42-2.17)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.256 0.198 , 0.259	Depositor DCC
R_{free} test set	2892 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57276 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8321	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.38	0/4041	0.69	7/5483 (0.1%)
1	B	0.38	0/4050	0.69	6/5494 (0.1%)
All	All	0.38	0/8091	0.69	13/10977 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	289	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	507	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	354	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	173	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	173	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	167	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	224	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	425	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	472	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	373	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	242	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	242	ASP	CB-CG-OD2	5.03	122.83	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	3939	0	3906	37	0
1	B	3948	0	3919	24	0
2	A	218	0	0	1	0
2	B	216	0	0	0	0
All	All	8321	0	7825	60	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 (60) 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:486:ARG:HH11	1:B:486:ARG:HG2	1.25	0.99
1:B:486:ARG:NH1	1:B:486:ARG:HG2	1.99	0.76
1:B:486:ARG:CG	1:B:486:ARG:HH11	1.99	0.75
1:B:325:THR:HG21	1:B:332:ILE:HD11	1.70	0.73
1:A:74:ARG:HG2	1:A:251:GLN:HG2	1.72	0.69
1:A:221:MET:HE1	1:A:229:PHE:HE2	1.58	0.68
1:A:459:SER:O	1:A:463:ILE:HG22	1.98	0.63
1:B:221:MET:HE1	1:B:404:GLY:HA3	1.81	0.63
1:B:207:LYS:HG3	1:B:218:GLY:HA3	1.81	0.61
1:A:79:LYS:HB3	1:A:82:VAL:HG22	1.84	0.58
1:A:398:ASP:HB2	1:A:399:PRO:CD	2.34	0.57
1:B:412:LEU:HD21	1:B:457:LYS:HE3	1.87	0.56
1:A:60:GLN:NE2	2:A:655:HOH:O	2.39	0.54
1:A:9:CYS:SG	1:A:64:ARG:HG2	2.48	0.54
1:A:194:ARG:NH2	1:A:278:ASP:OD2	2.42	0.53
1:A:204:ASP:O	1:A:207:LYS:HG3	2.10	0.52
1:A:240:ASP:HB3	1:A:388:LEU:HD23	1.92	0.51
1:B:14:LEU:HD11	1:B:293:SER:HB2	1.93	0.51
1:B:405:LYS:HG2	1:B:450:HIS:CE1	2.46	0.51
1:B:346:ILE:HD11	1:B:390:PHE:HB2	1.94	0.50
1:A:221:MET:HE1	1:A:229:PHE:CE2	2.43	0.48
1:A:221:MET:CE	1:A:229:PHE:HE2	2.25	0.48
1:A:221:MET:HE3	1:A:225:GLY:HA3	1.96	0.48
1:A:74:ARG:CG	1:A:251:GLN:HG2	2.44	0.47
1:B:221:MET:HE3	1:B:225:GLY:HA3	1.95	0.47
1:A:398:ASP:HB2	1:A:399:PRO:HD2	1.96	0.47
1:A:221:MET:CE	1:A:229:PHE:CE2	2.99	0.46
1:A:81:SER:HB2	1:B:99:ASP:OD2	2.14	0.46
1:B:240:ASP:HB3	1:B:388:LEU:HD23	1.97	0.46
1:B:79:LYS:O	1:B:82:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:CYS:HB3	1:A:137:THR:HG22	1.99	0.45
1:A:217:VAL:HA	1:A:341:TYR:CE2	2.52	0.45
1:B:405:LYS:HD2	1:B:449:LEU:O	2.18	0.44
1:A:305:THR:O	1:A:309:ASN:HB2	2.18	0.44
1:B:207:LYS:HB2	1:B:207:LYS:HE2	1.59	0.44
1:A:393:ARG:NH1	1:A:507:ASP:HB3	2.33	0.44
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.86	0.44
1:A:398:ASP:CB	1:A:399:PRO:CD	2.96	0.44
1:A:115:LYS:HE2	1:A:131:TRP:CE2	2.52	0.44
1:B:309:ASN:HB3	1:B:342:GLY:HA2	1.99	0.44
1:A:377:GLY:HA3	1:A:378:PRO:HD3	1.83	0.44
1:A:100:PRO:HA	1:A:101:PRO:HD3	1.88	0.43
1:B:113:LEU:HD11	1:B:193:ILE:HG22	2.00	0.43
1:A:242:ASP:N	1:A:242:ASP:OD1	2.51	0.43
1:B:217:VAL:HA	1:B:341:TYR:CE2	2.54	0.43
1:A:496:ASP:HB3	1:A:499:LEU:HD12	2.01	0.43
1:A:298:LEU:HA	1:A:299:PRO:HD3	1.88	0.42
1:A:214:PRO:HG2	1:A:314:TRP:CE2	2.53	0.42
1:A:10:GLY:HA3	1:A:71:THR:HG21	2.01	0.42
1:A:393:ARG:HH12	1:A:507:ASP:HB3	1.85	0.42
1:A:148:ASN:HA	1:A:193:ILE:HD11	2.02	0.42
1:B:302:VAL:HG22	1:B:303:PRO:HD2	2.01	0.42
1:B:440:LEU:HD22	1:B:462:VAL:HG22	2.01	0.41
1:B:341:TYR:OH	1:B:506:GLU:HB2	2.20	0.41
1:A:115:LYS:HE2	1:A:131:TRP:CD2	2.56	0.41
1:A:221:MET:HE1	1:A:404:GLY:HA3	2.02	0.41
1:B:121:HIS:HA	1:B:122:PRO:HA	1.78	0.41
1:A:259:LEU:HD12	1:A:280:LEU:HG	2.02	0.40
1:A:90:ILE:HG12	1:A:314:TRP:CE2	2.57	0.40
1:A:237:TYR:O	1:A:348:SER:HA	2.21	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	500/510 (98%)	483 (97%)	14 (3%)	3 (1%)	30	27
1	B	501/510 (98%)	486 (97%)	14 (3%)	1 (0%)	52	57
All	All	1001/1020 (98%)	969 (97%)	28 (3%)	4 (0%)	39	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	ASP
1	B	375	THR
1	A	372	PRO
1	A	376	GLU

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	433/438 (99%)	409 (94%)	24 (6%)	27	28
1	B	434/438 (99%)	409 (94%)	25 (6%)	25	26
All	All	867/876 (99%)	818 (94%)	49 (6%)	25	26

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	71	THR
1	A	72	GLU
1	A	74	ARG
1	A	81	SER
1	A	88	LYS
1	A	134	GLU
1	A	146	LYS
1	A	193	ILE

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Mol	Chain	Res	Type
1	A	289	ASP
1	A	298	LEU
1	A	300	SER
1	A	368	LYS
1	A	371	ARG
1	A	375	THR
1	A	379	LEU
1	A	405	LYS
1	A	423	HIS
1	A	440	LEU
1	A	463	ILE
1	A	472	ASP
1	A	477	ARG
1	A	478	GLN
1	A	506	GLU
1	B	7	THR
1	B	22	LEU
1	B	61	GLN
1	B	68	LYS
1	B	72	GLU
1	B	126	ARG
1	B	132	ASN
1	B	134	GLU
1	B	171	LYS
1	B	193	ILE
1	B	207	LYS
1	B	223	GLU
1	B	245	ARG
1	B	289	ASP
1	B	298	LEU
1	B	300	SER
1	B	356	GLU
1	B	371	ARG
1	B	379	LEU
1	B	397	ARG
1	B	456	SER
1	B	477	ARG
1	B	483	ARG
1	B	486	ARG
1	B	506	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	92	ASN
1	A	478	GLN
1	B	92	ASN
1	B	124	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 [i](#)

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	502/510 (98%)	0.04	15 (2%) 54 56	9, 19, 31, 43	0
1	B	503/510 (98%)	0.08	13 (2%) 59 61	11, 19, 31, 46	0
All	All	1005/1020 (98%)	0.06	28 (2%) 56 58	9, 19, 31, 46	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	GLY	6.3
1	A	375	THR	6.2
1	A	373	ASP	6.2
1	A	377	GLY	5.2
1	A	376	GLU	4.9
1	B	373	ASP	4.3
1	B	375	THR	3.9
1	A	472	ASP	3.2
1	A	473	PHE	3.1
1	A	371	ARG	3.0
1	B	376	GLU	3.0
1	B	374	LYS	3.0
1	B	7	THR	2.8
1	B	507	ASP	2.8
1	B	16	PRO	2.7
1	A	463	ILE	2.6
1	A	137	THR	2.6
1	B	5	LYS	2.5
1	B	6	GLY	2.5
1	A	289	ASP	2.5
1	B	290	PHE	2.4
1	A	451	GLY	2.4
1	A	134	GLU	2.3
1	B	506	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	372	PRO	2.2
1	A	507	ASP	2.2
1	A	302	VAL	2.2
1	B	137	THR	2.1

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 carbohydrates 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.