

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 11:36 pm BST

PDB ID : 4NLX

Title : Poliovirus Polymerase - G289A/C290V Loop Mutant

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Deposited on : 2013-11-14

Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

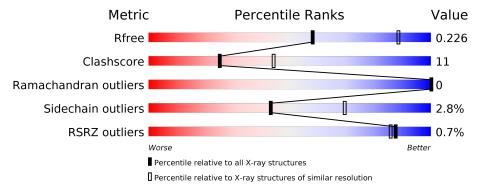
Validation Pipeline (wwPDB-VP) : 2.11

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 2.60 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.



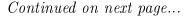
Metric	$egin{aligned} ext{Whole archive} \ (\# ext{Entries}) \end{aligned}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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% 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		
			<mark>%</mark>		
1	A	461	82%	16%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CAS	A	212	-	-	X	-
3	1PE	A	906	-	-	-	X





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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	A	907	_	-	_	X



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3891 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.

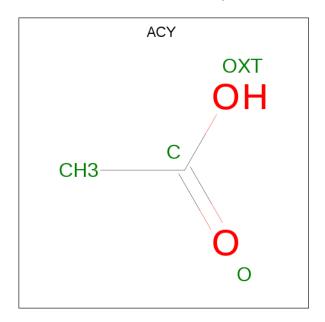
• Molecule 1 is a protein called RNA-directed RNA polymerase 3D-POL.

Mol	Chain	Residues		Atoms				ZeroOcc	$\mathbf{AltConf}$	Trace	
1	A	461	Total 3706	$\frac{As}{3}$	C 2377	N 607	O 698	S 21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
A	289	ALA	GLY	ENGINEERED MUTATION	UNP P03300
A	290	VAL	CYS	ENGINEERED MUTATION	UNP P03300
A	446	ASP	LEU	ENGINEERED MUTATION	UNP P03300
A	455	ASP	ARG	ENGINEERED MUTATION	UNP P03300

• Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total C	O 2	0	0

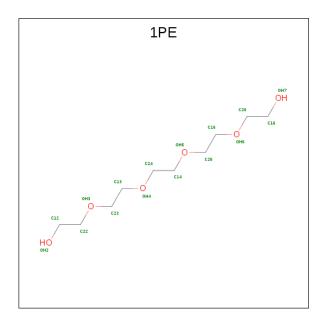
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$\alpha \cdots \tau$	r	•	
Continued	trom	nromanne	naae
\circ	110116	picolous	puyc

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

 \bullet Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\mathrm{C_{10}H_{22}O_6}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

• Molecule 5 is water.



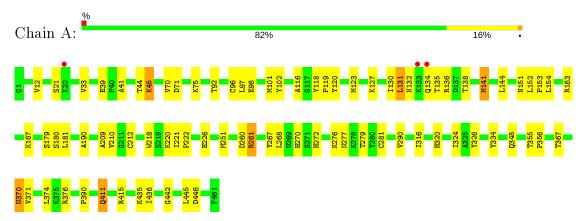
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	132	Total O 132 132	0	0



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.

• Molecule 1: RNA-directed RNA polymerase 3D-POL





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	129.18Å 129.18Å 111.61Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 - 2.60	Depositor
Resolution (A)	29.89 - 2.60	EDS
% Data completeness	96.7 (30.00-2.60)	Depositor
(in resolution range)	99.0 (29.89-2.60)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.93 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
υ .	0.208 , 0.236	Depositor
R, R_{free}	0.203 , 0.226	DCC
R_{free} test set	6055 reflections $(9.73%)$	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 33.5	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3891	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: CAS, NA, ACY, 1PE

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).

Mal	Chain	Bond	lengths	Bond	angles
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/3766	0.60	0/5090

There are no bond length outliers.

There are no bond angle outliers.

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	3706	0	3652	80	0
2	A	20	0	15	0	0
3	A	32	0	44	2	0
4	A	1	0	0	0	0
5	A	132	0	0	2	0
All	All	3891	0	3711	80	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 11.

The worst 5 of 80 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:281:CAS:CE2	1:A:281:CAS:AS	2.21	1.47
1:A:212:CAS:CE2	1:A:212:CAS:AS	2.22	1.47
1:A:96:CAS:AS	1:A:96:CAS:CE2	2.23	1.46
1:A:212:CAS:CE1	1:A:212:CAS:AS	2.23	1.45
1:A:281:CAS:AS	1:A:281:CAS:CE1	2.24	1.44

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	456/461 (99%)	439 (96%)	17 (4%)	0	100 100	

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	400/400 (100%)	389 (97%)	11 (3%)	43 69	

5 of 11 residues with a non-rotameric sidechain are listed below:

Mo	1	Chain	Res	Type
1		Α	151	ASN
1		A	218	TRP

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Mol	Chain	Res	Type
1	A	345	GLN
1	A	141	MET
1	A	270	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	A	411	GLN
1	A	370	ASN
1	A	134	GLN
1	A	409	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Tuno	Chain	Res Link		В	ond leng	$_{ m gths}$	E	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	CAS	A	281	1	5,8,9	6.56	2 (40%)	1,9,11	0.73	0
1	CAS	A	96	1	5,8,9	6.82	2 (40%)	1,9,11	0.03	0
1	CAS	A	212	1	5,8,9	6.56	2 (40%)	1,9,11	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	A	281	1	-	0/0/7/9	-
1	CAS	A	96	1	-	0/0/7/9	-
1	CAS	A	212	1	-	0/0/7/9	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	A	96	CAS	AS-CE1	11.23	2.25	1.96
1	A	281	CAS	AS-CE1	10.94	2.24	1.96
1	A	212	CAS	AS-CE1	10.55	2.23	1.96
1	A	96	CAS	AS-CE2	10.25	2.23	1.96
1	A	212	CAS	AS-CE2	10.09	2.22	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	281	CAS	2	0
1	A	96	CAS	2	0
1	A	212	CAS	8	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Mol Type Chain		Res	Link	В	ond leng	gths	Bond angles		
10101	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1PE	A	907	-	15,15,15	1.18	1 (6%)	14,14,14	0.86	0
2	ACY	A	904	-	1,3,3	2.82	1 (100%)	0,3,3	0.00	-
3	1PE	A	906	-	15,15,15	1.18	0	14,14,14	0.85	0
2	ACY	A	901	-	1,3,3	3.05	1 (100%)	0,3,3	0.00	-
2	ACY	A	905	-	1,3,3	3.41	1 (100%)	0,3,3	0.00	-
2	ACY	A	902	-	1,3,3	3.22	1 (100%)	0,3,3	0.00	-
2	ACY	A	903	-	1,3,3	2.62	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	906	_	-	3/13/13/13	-
3	1PE	A	907	-	-	5/13/13/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${f Observed(\AA)}$	$\operatorname{Ideal}(ext{\AA})$
2	A	905	ACY	СН3-С	3.41	1.53	1.48
2	A	902	ACY	СН3-С	3.22	1.52	1.48
2	A	901	ACY	СН3-С	3.05	1.52	1.48
2	A	904	ACY	СН3-С	2.82	1.52	1.48
2	A	903	ACY	СН3-С	2.62	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	906	1PE	OH2-C12-C22-OH3
3	A	907	1PE	OH4-C13-C23-OH3
3	A	907	1PE	OH2-C12-C22-OH3
3	A	907	1PE	ОН7-С16-С26-ОН6
3	A	906	1PE	ОН7-С16-С26-ОН6

There are no ring outliers.

1 monomer is involved in 2 short contacts:



\mathbf{Mol}	Chain	Res	Type	Clashes	Symm-Clashes
3	Α	906	1PE	2	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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 $>$ $#$ RSRZ $>$ 2		$OWAB(Å^2)$	Q<0.9
1	A	458/461 (99%)	-0.62	3 (0%) 87	86	13, 26, 51, 67	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	LYS	2.3
1	A	134	GLN	2.1
1	A	22	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	${f B-factors(A^2)}$	Q<0.9
1	CAS	A	212	9/10	0.93	0.17	22,25,56,59	0
1	CAS	A	96	9/10	0.97	0.12	38,40,54,57	0
1	CAS	A	281	9/10	0.99	0.12	21,23,25,26	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-}factors}({f A}^2)$	Q < 0.9
3	1PE	A	907	16/16	0.49	0.47	148,155,169,169	0
3	1PE	A	906	16/16	0.58	0.62	138,140,145,146	0
2	ACY	A	905	4/4	0.69	0.27	60,62,62,62	0
2	ACY	A	902	4/4	0.75	0.19	66,67,67,67	0
2	ACY	A	904	4/4	0.93	0.15	43,43,43,44	0
4	NA	A	908	1/1	0.94	0.25	32,32,32,32	0
2	ACY	A	901	4/4	0.97	0.11	25,29,29,29	0
2	ACY	A	903	4/4	0.99	0.14	23,25,25,27	0

6.5 Other polymers (i)

There are no such residues in this entry.

