W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 03:44 pm GMT

PDB ID	:	4Z92
Title	:	crystal structure of parechovirus-1 virion
Authors	:	Kalynych, S.; Palkova, L.; Plevka, P.
Deposited on	:	2015-04-09
Resolution	:	3.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 3.10 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.
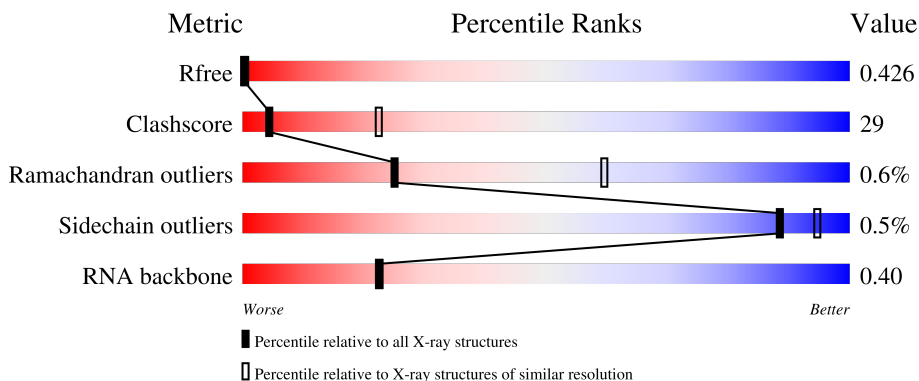
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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%

Mol	Chain	Length	Quality of chain
1	A	234	47% 34% · 18%
2	B	253	51% 42% · 6%
3	C	289	51% 37% · 11%
4	D	6	33% 17% 50%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5404 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 capsid subunit VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1471	946	248	270	7			

- Molecule 2 is a protein called Capsid subunit VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1845	1167	318	350	10			

- Molecule 3 is a protein called capsid subunit VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	257	Total	C	N	O	S	0	0	0
			1969	1252	326	385	6			

- Molecule 4 is a RNA chain called RNA (5'-R(*AP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	P	0	0	0
			119	55	15	44	5			

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.
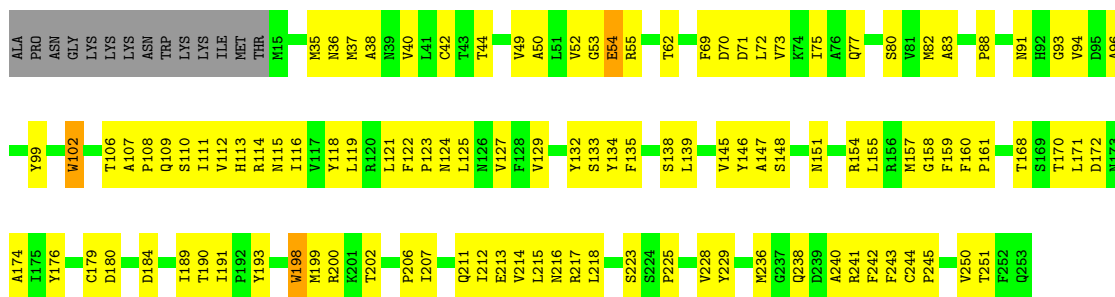
• Molecule 1: capsid subunit VP1

Chain A:
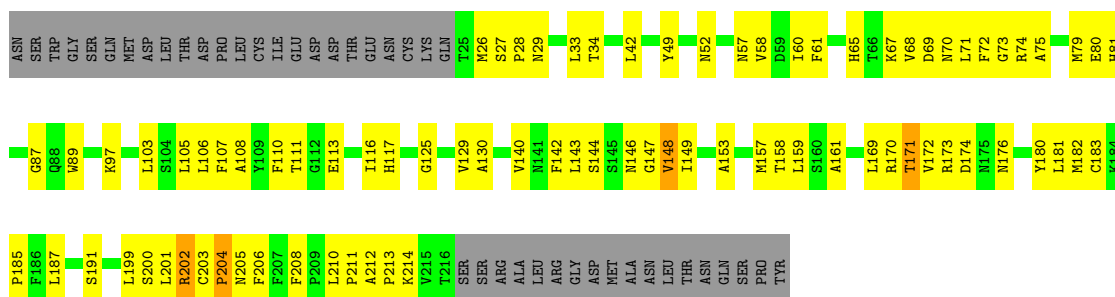
• Molecule 2: Capsid subunit VP3

Chain B:

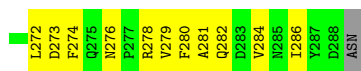• Molecule 3: capsid subunit VP0

Chain C:

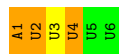L272 D273 F274 Q275 N276 P277 R278 V279 F280 A281 Q282 D283 V284 N285 I286 Y287 D288 ASN
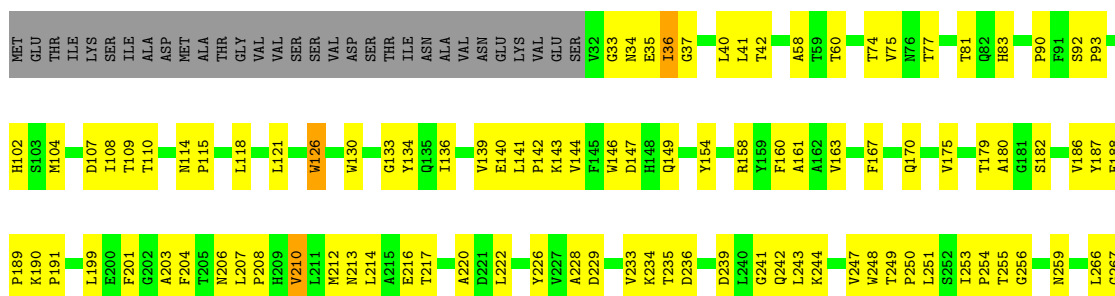
• Molecule 4: RNA (5'-R(*AP*UP*UP*UP*UP*U)-3')

Chain D:

	33%	17%	50%

A1 U2 U3 U4 U5 U6

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	399.50Å 399.50Å 332.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.00 – 3.10 63.93 – 3.09	Depositor EDS
% Data completeness (in resolution range)	78.2 (65.00-3.10) 82.8 (63.93-3.09)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.07Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.290 , (Not available) 0.426 , 0.426	Depositor DCC
R_{free} test set	11563 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	77.56 , -7.7	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.09	EDS
Total number of atoms	5404	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

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	0.36	0/1513	0.65	4/2064 (0.2%)
2	B	0.35	1/1888 (0.1%)	0.54	0/2567
3	C	0.28	0/2021	0.55	0/2774
4	D	0.29	0/131	0.91	0/201
All	All	0.33	1/5553 (0.0%)	0.59	4/7606 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	GLU	CG-CD	-6.53	1.42	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	CYS	N-CA-C	-6.71	92.89	111.00
1	A	173	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	202	ARG	N-CA-C	5.89	126.91	111.00
1	A	171	THR	N-CA-C	-5.11	97.21	111.00

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	1471	0	1394	107	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1845	0	1781	123	0
3	C	1969	0	1862	108	2
4	D	119	0	63	8	0
All	All	5404	0	5100	304	2

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 29.

The worst 5 of 304 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)
4:D:1:A:H4'	4:D:2:U:H5'	1.19	1.11
1:A:57:ASN:HB3	2:B:241:ARG:HH21	1.30	0.93
1:A:201:LEU:HD13	1:A:204:PRO:HB3	1.54	0.88
4:D:1:A:H4'	4:D:2:U:C5'	2.05	0.87
3:C:158:ARG:HD2	3:C:281:ALA:HB2	1.57	0.86

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASN:OD1	3:C:107:ASP:CB[2_655]	1.39	0.81
1:A:52:ASN:ND2	3:C:110:THR:OG1[2_655]	2.02	0.18

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	190/234 (81%)	172 (90%)	16 (8%)	2 (1%)	14	46
2	B	237/253 (94%)	217 (92%)	20 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	255/289 (88%)	224 (88%)	29 (11%)	2 (1%)	19	54
All	All	682/776 (88%)	613 (90%)	65 (10%)	4 (1%)	25	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	36	ILE
1	A	148	VAL
3	C	210	VAL
1	A	204	PRO

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	158/209 (76%)	158 (100%)	0	100	100
2	B	201/220 (91%)	199 (99%)	2 (1%)	76	90
3	C	215/252 (85%)	214 (100%)	1 (0%)	88	94
All	All	574/681 (84%)	571 (100%)	3 (0%)	88	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	102	TRP
2	B	198	TRP
3	C	126	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	242	GLN
3	C	213	ASN
2	B	216	ASN

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Mol	Chain	Res	Type
3	C	206	ASN
2	B	151	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	6/6 (100%)	3 (50%)	3 (50%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	2	U
4	D	3	U
4	D	4	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	1	A
4	D	2	U
4	D	3	U

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.