Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2016 – 02:09 PM EST

PDB ID	:	5M74
Title	:	Rebuild and re-refined model for Human Parechovirus 1
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Deposited on	:	2016-10-26
Resolution	:	3.09 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 (i) symbol.

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

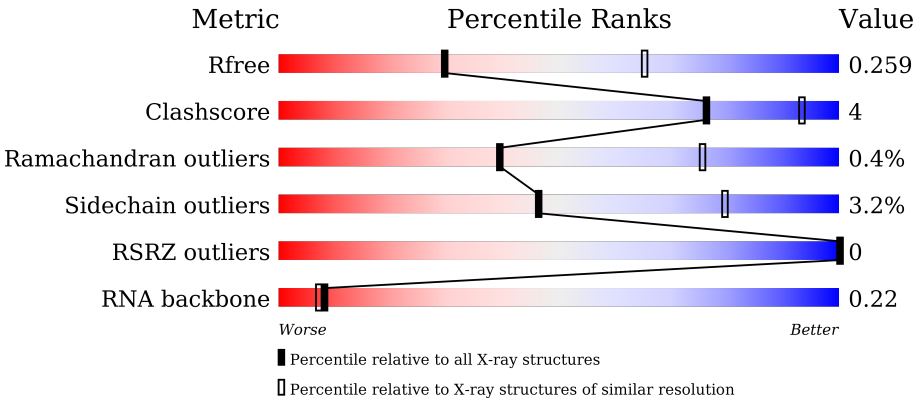
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 3.09 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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 <=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	234	70% 12% 18%
2	B	253	85% 9% • 6%
3	C	289	80% 9% • 11%
4	D	6	33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5485 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 protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1507	971	250	279	7			

- Molecule 2 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1864	1185	320	349	10			

- Molecule 3 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	257	Total	C	N	O	S	0	0	0
			1994	1264	332	392	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	35	ASP	GLU	conflict	UNP Q66578

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

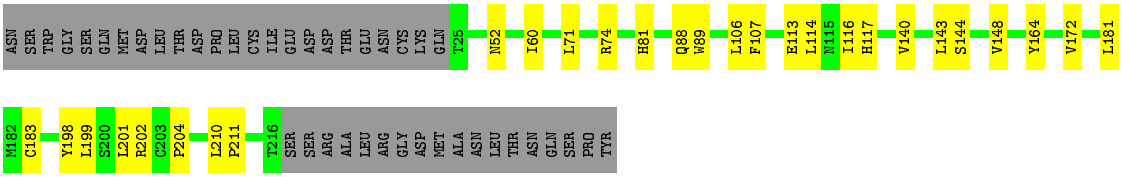
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	P	0	0	0
			120	55	15	45	5			

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 (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.

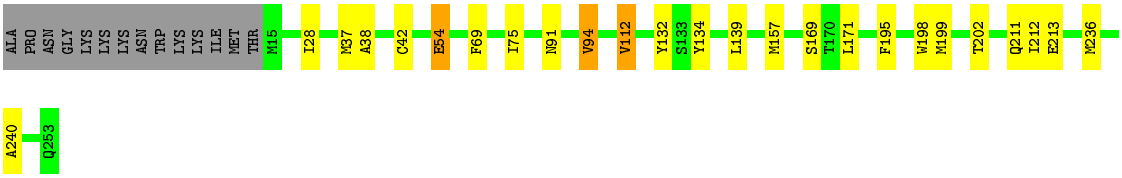
- Molecule 1: Capsid protein VP1

Chain A:



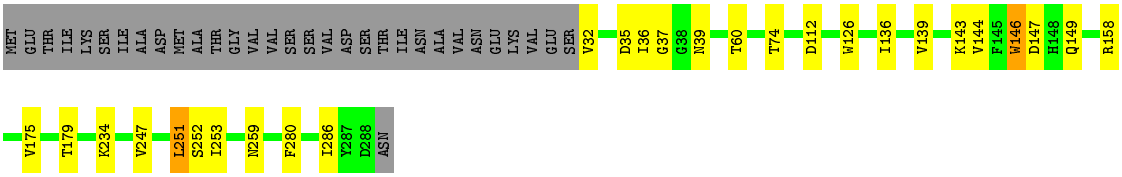
- Molecule 2: Capsid protein VP3

Chain B:



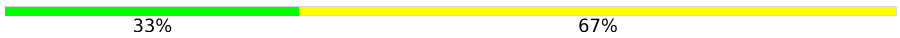
- Molecule 3: Capsid protein VP0

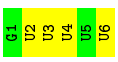
Chain C:



- Molecule 4: RNA (5'-R(*GP*UP*UP*UP*UP*U)-3')

Chain D:





4 Data and refinement statistics (i)

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 – 3.09 63.93 – 3.09	Depositor EDS
% Data completeness (in resolution range)	82.7 (65.00-3.09) 82.8 (63.93-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.258 , 0.261 0.257 , 0.259	Depositor DCC
R_{free} test set	11563 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 5.5	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	0.84	EDS
Total number of atoms	5485	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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.*

[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	0.41	0/1551	0.63	0/2113
2	B	0.39	0/1909	0.66	0/2592
3	C	0.38	0/2047	0.61	0/2809
4	D	0.35	0/132	0.70	0/203
All	All	0.39	0/5639	0.63	0/7717

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

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	1507	0	1444	18	0
2	B	1864	0	1814	16	0
3	C	1994	0	1899	13	0
4	D	120	0	63	1	0
All	All	5485	0	5220	41	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 (41) 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:116:ILE:HG21	1:A:181:LEU:HD12	1.78	0.66
1:A:116:ILE:HG21	1:A:181:LEU:CD1	2.31	0.60
1:A:201:LEU:HD13	1:A:204:PRO:HB3	1.83	0.60
2:B:171:LEU:HD11	2:B:211:GLN:NE2	2.21	0.55
3:C:35:ASP:O	3:C:60:THR:HG21	2.07	0.55
2:B:91:ASN:O	2:B:94:VAL:HG22	2.08	0.54
1:A:106:LEU:HD13	2:B:75:ILE:HG21	1.88	0.54
2:B:157:MET:HB2	2:B:212:ILE:HG12	1.90	0.52
3:C:136:ILE:HD11	3:C:247:VAL:HG22	1.93	0.51
1:A:88:GLN:HE22	1:A:143:LEU:HD13	1.76	0.50
1:A:210:LEU:HB2	1:A:211:PRO:HD2	1.94	0.49
1:A:74:ARG:HG3	2:B:38:ALA:HA	1.95	0.48
1:A:107:PHE:O	1:A:172:VAL:HG11	2.14	0.47
1:A:71:LEU:HD13	2:B:132:TYR:CZ	2.49	0.47
1:A:114:LEU:HD11	1:A:199:LEU:HD23	1.97	0.46
1:A:181:LEU:HD21	1:A:183:CYS:SG	2.56	0.46
3:C:139:VAL:CG2	3:C:144:VAL:HG21	2.45	0.46
2:B:139:LEU:HD12	2:B:139:LEU:N	2.31	0.45
3:C:234:LYS:HA	3:C:286:ILE:HD12	1.98	0.45
1:A:60:ILE:HD13	2:B:199:MET:HG3	1.98	0.45
3:C:143:LYS:HA	3:C:146:TRP:CE3	2.51	0.45
3:C:32:VAL:HA	3:C:36:ILE:HD12	1.99	0.45
3:C:253:ILE:HD13	3:C:259:ASN:HA	1.99	0.45
3:C:144:VAL:O	3:C:147:ASP:HB2	2.16	0.45
1:A:164:TYR:OH	2:B:54:GLU:OE2	2.32	0.44
2:B:134:TYR:HB2	2:B:199:MET:HE3	2.00	0.44
3:C:126:TRP:CE2	3:C:251:LEU:HD13	2.52	0.44
1:A:117:HIS:HB2	1:A:198:TYR:HB2	1.99	0.44
2:B:171:LEU:N	2:B:171:LEU:HD12	2.34	0.43
1:A:198:TYR:HB2	2:B:37:MET:HE3	2.01	0.43
3:C:126:TRP:CZ2	3:C:251:LEU:HD13	2.54	0.43
1:A:113:GLU:HB2	1:A:202:ARG:HB3	2.02	0.42
2:B:236:MET:HB3	2:B:240:ALA:HB2	2.01	0.42
2:B:171:LEU:HD13	2:B:213:GLU:CD	2.41	0.41
3:C:175:VAL:HG22	3:C:179:THR:HB	2.03	0.41
1:A:81:HIS:HB2	1:A:89:TRP:CZ2	2.56	0.40
3:C:139:VAL:HG22	3:C:144:VAL:HG11	2.02	0.40
3:C:158:ARG:HG3	3:C:280:PHE:CZ	2.56	0.40
1:A:71:LEU:HD13	2:B:132:TYR:OH	2.21	0.40
4:D:4:U:O2	4:D:4:U:O4'	2.40	0.40
2:B:112:VAL:HG12	2:B:212:ILE:O	2.22	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	190/234 (81%)	179 (94%)	10 (5%)	1 (0%)	34	72
2	B	237/253 (94%)	225 (95%)	11 (5%)	1 (0%)	39	75
3	C	255/289 (88%)	236 (92%)	18 (7%)	1 (0%)	39	75
All	All	682/776 (88%)	640 (94%)	39 (6%)	3 (0%)	39	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	VAL
3	C	37	GLY
2	B	94	VAL

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	166/209 (79%)	163 (98%)	3 (2%)	66	88
2	B	204/220 (93%)	195 (96%)	9 (4%)	35	71
3	C	222/252 (88%)	215 (97%)	7 (3%)	46	79
All	All	592/681 (87%)	573 (97%)	19 (3%)	46	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	140	VAL
1	A	144	SER
2	B	28	ILE
2	B	42	CYS
2	B	54	GLU
2	B	69	PHE
2	B	112	VAL
2	B	169	SER
2	B	195	PHE
2	B	198	TRP
2	B	202	THR
3	C	39	ASN
3	C	74	THR
3	C	112	ASP
3	C	146	TRP
3	C	149	GLN
3	C	251	LEU
3	C	252	SER

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

Mol	Chain	Res	Type
1	A	88	GLN
1	A	115	ASN
1	A	131	HIS
2	B	151	ASN
2	B	216	ASN
3	C	39	ASN
3	C	172	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	5/6 (83%)	3 (60%)	0

All (3) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
4	D	6	U

There are no RNA pucker outliers to report.

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 carbohydrates 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

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, 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>2			OWAB(Å^2)	Q<0.9
1	A	192/234 (82%)	-0.31	0	100	100	33, 48, 72, 99	0
2	B	239/253 (94%)	-0.41	0	100	100	32, 41, 57, 71	0
3	C	257/289 (88%)	-0.35	0	100	100	30, 43, 70, 79	0
4	D	6/6 (100%)	0.63	0	100	100	54, 58, 65, 71	0
All	All	694/782 (88%)	-0.35	0	100	100	30, 44, 66, 99	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.