



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:18 pm BST

PDB ID : 4N43
Title : Human enterovirus 71 uncoating intermediate captured at atomic resolution
Authors : Chen, R.; Lyu, K.
Deposited on : 2013-10-08
Resolution : 3.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

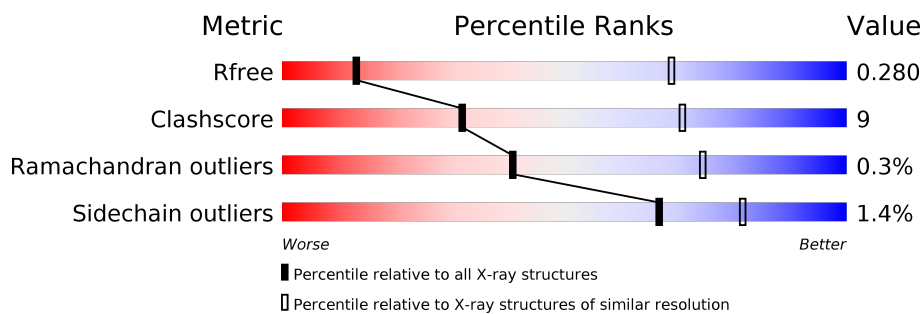
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	297	
2	B	254	
3	C	242	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5259 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	225	Total	C	N	O	S	0	0	0
			1780	1139	300	330	11			

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1777	1143	292	334	8			

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	223	Total	C	N	O	S	0	0	0
			1702	1097	278	316	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	227	GLN	LYS	CONFLICT	UNP Q9WPJ0

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 2	Depositor
Cell constants a, b, c, α , β , γ	352.42Å 352.42Å 352.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.80 49.84 – 3.80	Depositor EDS
% Data completeness (in resolution range)	68.0 (49.84-3.80) 59.4 (49.84-3.80)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.245 , 0.274 0.277 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	5259	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.22	0/1835	0.40	0/2501
2	B	0.22	0/1830	0.41	0/2509
3	C	0.22	0/1748	0.42	0/2393
All	All	0.22	0/5413	0.41	0/7403

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	1780	0	1724	31	0
2	B	1777	0	1712	39	0
3	C	1702	0	1692	41	0
All	All	5259	0	5128	92	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 9.

All (92) 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:149:GLN:HG2	1:A:247:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:H	3:C:235:ILE:HG12	1.49	0.78
2:B:151:THR:HG22	2:B:152:GLN:HG3	1.74	0.70
2:B:122:LEU:HB2	2:B:183:ILE:HB	1.74	0.68
2:B:186:ARG:NH1	3:C:124:SER:O	2.27	0.67
1:A:268:ASN:HB2	2:B:171:PRO:HD3	1.79	0.65
2:B:134:THR:HG23	2:B:146:PRO:HG3	1.78	0.64
3:C:85:VAL:HB	3:C:194:VAL:HG13	1.80	0.64
3:C:59:PRO:HD2	3:C:68:ARG:HD3	1.80	0.63
3:C:142:LEU:HD12	3:C:143:PRO:HD2	1.81	0.62
1:A:262:ILE:HG21	2:B:128:PRO:HG2	1.83	0.61
3:C:146:ARG:NH1	3:C:199:GLN:OE1	2.34	0.61
1:A:181:VAL:HG11	1:A:188:ALA:HB2	1.83	0.61
3:C:115:LEU:HB2	3:C:169:ILE:HD11	1.83	0.60
2:B:85:VAL:HG23	2:B:86:LEU:HG	1.85	0.59
2:B:80:TRP:HB3	2:B:85:VAL:HG11	1.85	0.59
1:A:265:PRO:HB3	2:B:174:GLN:HB2	1.85	0.59
2:B:177:VAL:HG11	3:C:100:LEU:HD22	1.85	0.58
2:B:71:TRP:HD1	2:B:232:ILE:HB	1.68	0.58
1:A:287:THR:HG21	3:C:94:GLY:H	1.68	0.58
1:A:291:ARG:H	1:A:291:ARG:HH11	1.51	0.58
2:B:23:ILE:HG21	2:B:237:THR:HG21	1.87	0.57
2:B:71:TRP:NE1	2:B:222:LEU:HB2	2.20	0.56
1:A:155:PHE:HB3	1:A:177:PRO:HG2	1.87	0.56
2:B:87:THR:O	2:B:97:GLN:NE2	2.36	0.56
1:A:127:THR:HG22	1:A:264:ARG:HE	1.70	0.56
2:B:186:ARG:NH2	3:C:159:PHE:O	2.39	0.56
1:A:93:ILE:HD11	1:A:109:TRP:HB2	1.88	0.56
1:A:278:ASN:OD1	2:B:134:THR:N	2.38	0.55
2:B:71:TRP:CD1	2:B:232:ILE:HB	2.41	0.54
2:B:184:ASN:O	2:B:188:ASN:N	2.41	0.54
1:A:210:THR:O	2:B:208:ASN:ND2	2.40	0.54
3:C:57:ASN:HA	3:C:68:ARG:HD2	1.89	0.53
2:B:71:TRP:CZ3	2:B:218:PRO:HB3	2.43	0.53
3:C:59:PRO:HG2	3:C:67:GLU:HB2	1.92	0.52
1:A:276:ASN:OD1	1:A:278:ASN:ND2	2.43	0.51
1:A:106:TYR:OH	1:A:164:ASP:O	2.23	0.51
2:B:174:GLN:HE22	3:C:103:GLN:HG3	1.74	0.51
1:A:128:TYR:HB2	1:A:261:TRP:HB2	1.93	0.51
1:A:156:VAL:HB	1:A:232:THR:HG23	1.94	0.50
2:B:97:GLN:HA	2:B:207:LEU:HD11	1.92	0.50
3:C:130:LYS:HB2	3:C:200:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:HB3	1:A:258:VAL:HG12	1.94	0.49
3:C:121:PHE:HA	3:C:214:ILE:HG22	1.95	0.49
2:B:32:ILE:HD11	2:B:193:ILE:HG12	1.95	0.49
3:C:109:THR:OG1	3:C:228:LEU:HB3	2.13	0.48
1:A:116:TYR:HD2	1:A:119:MET:HB2	1.79	0.48
2:B:177:VAL:HG12	3:C:49:VAL:HG21	1.96	0.48
2:B:186:ARG:HG3	3:C:125:PHE:HA	1.96	0.48
1:A:166:ARG:NH2	1:A:237:THR:O	2.46	0.48
3:C:135:TYR:HB2	3:C:167:LEU:HD21	1.95	0.48
1:A:192:VAL:HG22	3:C:24:ILE:HG21	1.96	0.47
3:C:72:PRO:HB3	3:C:213:TYR:CE1	2.49	0.47
3:C:235:ILE:HA	3:C:236:LEU:HA	1.55	0.47
2:B:126:VAL:HG13	2:B:212:PHE:CD1	2.50	0.46
2:B:97:GLN:HG2	2:B:207:LEU:HD21	1.99	0.45
1:A:126:PHE:CG	1:A:260:ALA:HB1	2.52	0.45
1:A:164:ASP:OD1	1:A:164:ASP:N	2.47	0.45
1:A:284:ILE:HG22	1:A:285:LYS:H	1.81	0.45
1:A:191:SER:OG	3:C:21:SER:OG	2.35	0.44
3:C:46:LEU:O	3:C:49:VAL:HG22	2.17	0.44
2:B:71:TRP:CH2	2:B:218:PRO:HB3	2.53	0.44
3:C:78:GLY:O	3:C:79:LYS:HG2	2.18	0.44
1:A:211:PHE:HA	2:B:208:ASN:ND2	2.33	0.44
2:B:136:ALA:HB2	2:B:143:ASP:HB3	1.98	0.44
2:B:122:LEU:HD22	2:B:216:VAL:HG12	2.00	0.43
2:B:186:ARG:HE	3:C:162:GLN:HG3	1.82	0.43
3:C:91:GLY:HA3	3:C:111:TRP:CH2	2.53	0.43
1:A:261:TRP:HA	3:C:39:GLU:HA	2.00	0.43
2:B:89:THR:HG21	2:B:155:ALA:HB2	2.00	0.43
2:B:95:ASN:O	2:B:99:HIS:ND1	2.41	0.43
3:C:115:LEU:HG	3:C:172:ILE:HD13	1.99	0.43
1:A:268:ASN:HB2	2:B:171:PRO:CD	2.48	0.43
3:C:96:TRP:O	3:C:102:GLY:HA3	2.19	0.43
2:B:71:TRP:HB3	2:B:232:ILE:O	2.19	0.42
3:C:134:ALA:HA	3:C:154:HIS:HA	2.01	0.42
3:C:109:THR:HG22	3:C:230:LYS:HE3	2.00	0.42
3:C:29:HIS:HA	3:C:30:PRO:HD2	1.93	0.42
1:A:282:ASN:O	1:A:282:ASN:ND2	2.52	0.42
3:C:128:THR:OG1	3:C:129:GLY:N	2.53	0.42
1:A:196:SER:HB2	1:A:201:TYR:CE1	2.55	0.42
3:C:132:LEU:HB2	3:C:199:GLN:HB2	2.02	0.41
3:C:133:ILE:HG12	3:C:196:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LYS:HE2	2:B:130:TYR:HB3	2.01	0.41
2:B:249:ARG:H	2:B:249:ARG:HD2	1.84	0.41
3:C:113:GLY:HA3	3:C:224:PHE:HA	2.02	0.41
3:C:104:LEU:HD13	3:C:104:LEU:HA	1.92	0.41
3:C:132:LEU:HD23	3:C:156:ILE:HD13	2.02	0.41
3:C:50:GLU:HA	3:C:219:ALA:HB2	2.03	0.41
1:A:291:ARG:H	1:A:291:ARG:HD2	1.86	0.40
2:B:81:LYS:O	2:B:85:VAL:HG13	2.20	0.40
3:C:58:VAL:HB	3:C:59:PRO:HD3	2.03	0.40

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	223/297 (75%)	202 (91%)	21 (9%)	0	100	100
2	B	225/254 (89%)	209 (93%)	16 (7%)	0	100	100
3	C	219/242 (90%)	201 (92%)	16 (7%)	2 (1%)	17	54
All	All	667/793 (84%)	612 (92%)	53 (8%)	2 (0%)	41	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	82	LEU
3	C	58	VAL

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	193/251 (77%)	189 (98%)	4 (2%)	53	74
2	B	195/214 (91%)	194 (100%)	1 (0%)	88	94
3	C	187/202 (93%)	184 (98%)	3 (2%)	62	79
All	All	575/667 (86%)	567 (99%)	8 (1%)	67	81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	TYR
1	A	284	ILE
1	A	285	LYS
1	A	291	ARG
2	B	100	TYR
3	C	86	PHE
3	C	200	THR
3	C	236	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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.