



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 10:40 AM EDT

PDB ID : 4GMP
Title : Crystal structure of enterovirus 71 strain 1095 procapsid
Authors : Yoder, J.D.; Hafenstein, S.
Deposited on : 2012-08-16
Resolution : 3.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

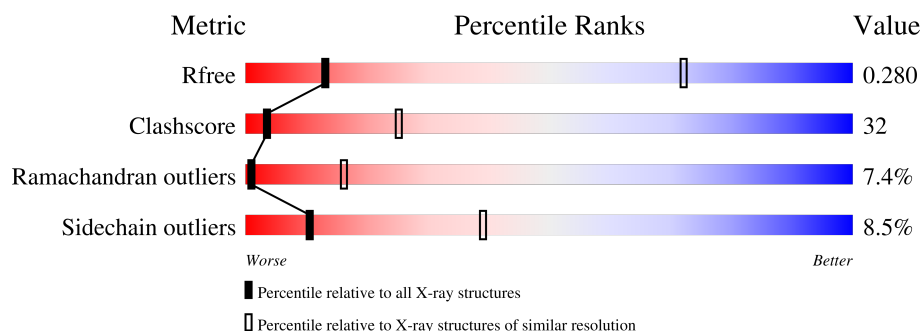
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	323	
2	1	297	
3	3	242	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5395 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 VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	237	Total	C	N	O	S	0	0	0
			1833	1179	301	345	8			

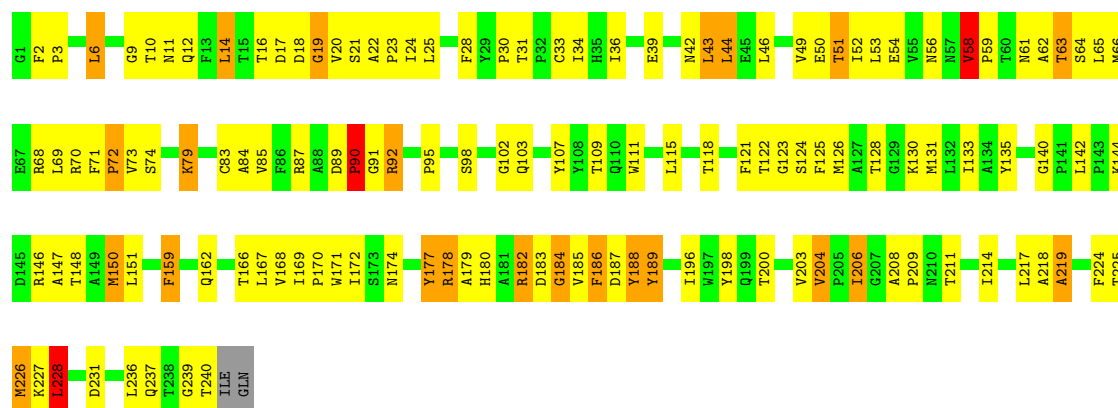
- Molecule 2 is a protein called capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	218	Total	C	N	O	S	0	0	0
			1717	1101	289	316	11			

- Molecule 3 is a protein called capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	240	Total	C	N	O	S	0	0	0
			1845	1188	304	342	11			

Chain 3:



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 ₂	Depositor
Cell constants a, b, c, α , β , γ	350.25Å 350.25Å 350.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.53 – 3.90 49.53 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.53-3.90) 99.9 (49.53-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.88Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.285 0.262 , 0.280	Depositor DCC
R_{free} test set	3398 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	109.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	5395	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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

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	0	0.44	0/1888	0.67	0/2591
2	1	0.46	0/1769	0.68	0/2411
3	3	0.49	0/1897	0.71	0/2596
All	All	0.47	0/5554	0.69	0/7598

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	0	1833	0	1774	124	3
2	1	1717	0	1674	125	8
3	3	1845	0	1822	134	1
All	All	5395	0	5270	341	9

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 32.

The worst 5 of 341 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)
3:3:20:VAL:HG22	3:3:21:SER:H	1.17	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:229:MET:HE2	2:1:231:GLY:H	1.24	1.02
3:3:206:ILE:HD12	3:3:206:ILE:H	1.23	1.01
3:3:109:THR:HB	3:3:228:LEU:HB3	1.52	0.91
3:3:58:VAL:HG23	3:3:59:PRO:HD3	1.50	0.90

The worst 5 of 9 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)
1:0:208:THR:CG2	2:1:283:SER:OG[13_454]	1.16	1.04
1:0:208:THR:CG2	2:1:283:SER:CB[13_454]	1.57	0.63
2:1:282:ASN:ND2	2:1:283:SER:N[13_454]	1.68	0.52
3:3:63:THR:CG2	3:3:63:THR:CG2[13_454]	1.71	0.49
2:1:282:ASN:O	2:1:282:ASN:CB[13_454]	1.75	0.45

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	0	235/323 (73%)	175 (74%)	42 (18%)	18 (8%)	1	16
2	1	214/297 (72%)	171 (80%)	27 (13%)	16 (8%)	1	16
3	3	238/242 (98%)	187 (79%)	34 (14%)	17 (7%)	1	17
All	All	687/862 (80%)	533 (78%)	103 (15%)	51 (7%)	1	16

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	97	ALA
1	0	112	SER
1	0	127	VAL
2	1	169	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	196	SER

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	0	201/272 (74%)	188 (94%)	13 (6%)	17	46
2	1	186/250 (74%)	168 (90%)	18 (10%)	8	32
3	3	200/202 (99%)	181 (90%)	19 (10%)	8	33
All	All	587/724 (81%)	537 (92%)	50 (8%)	10	39

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	237	THR
3	3	53	LEU
3	3	228	LEU
2	1	245	TYR
3	3	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	1	278	ASN
3	3	48	GLN
3	3	176	HIS
3	3	110	GLN
2	1	152	GLN

5.3.3 RNA ⓘ

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 monosaccharides 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.