



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 01:08 pm GMT

PDB ID : 2WZR
Title : The Structure of Foot and Mouth Disease Virus Serotype SAT1
Authors : Adams, P.; Lea, S.; Newman, J.; Blakemore, W.; King, A.; Stuart, D.; Fry, E.
Deposited on : 2009-12-02
Resolution : 3.00 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 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 : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

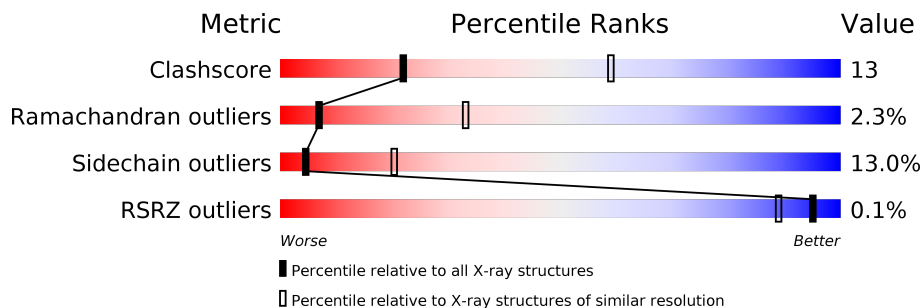
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

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 $\leq 5\%$. 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	1	219	 63% 20% 5% • 11%
2	2	219	 69% 21% • 5%
3	3	221	 70% 22% 6% •
4	4	85	 42% 11% •• 45%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5210 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 POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	194	Total	C	N	O	S	0	0	2
			1501	947	266	283	5			

- Molecule 2 is a protein called POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	207	Total	C	N	O	S	0	0	0
			1639	1041	282	312	4			

- Molecule 3 is a protein called POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	221	Total	C	N	O	S	0	0	0
			1717	1099	276	333	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	163	PHE	ILE	conflict	UNP Q6PMU1

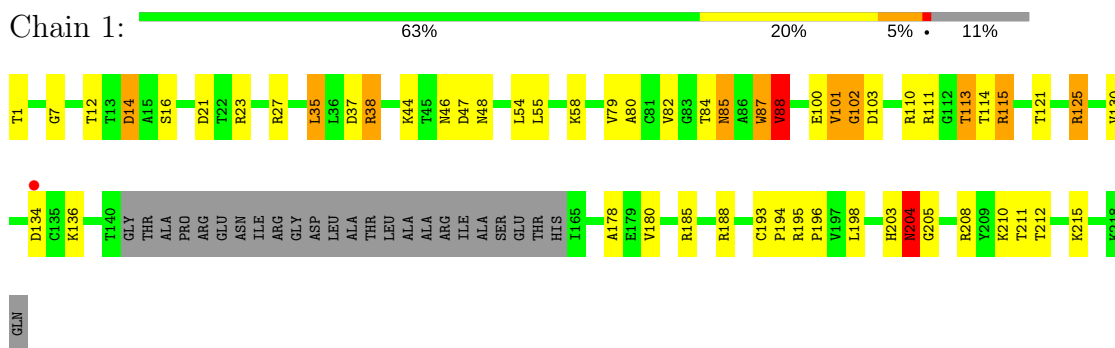
- Molecule 4 is a protein called POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	47	Total	C	N	O	S	0	0	1
			353	220	59	72	2			

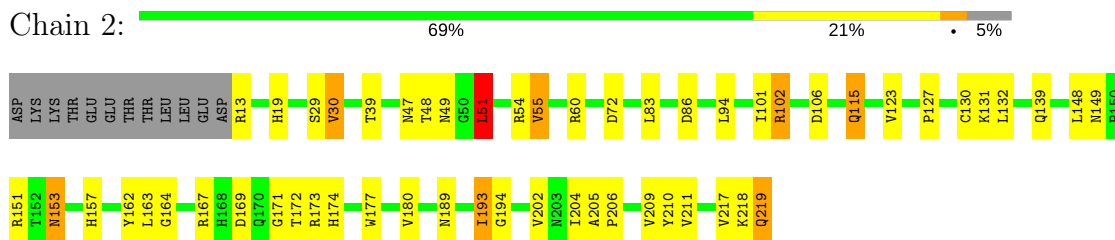
3 Residue-property plots [i](#)

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.

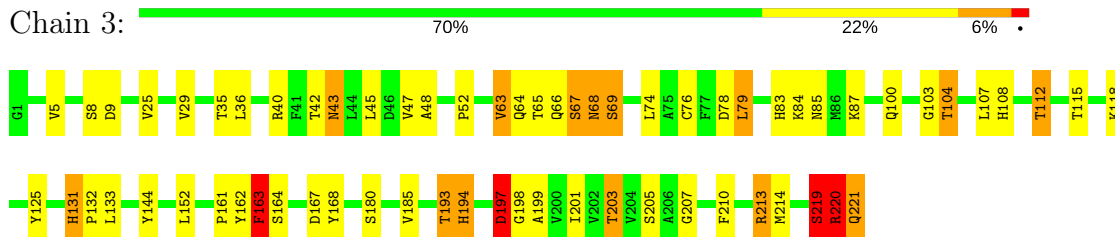
• Molecule 1: POLYPROTEIN



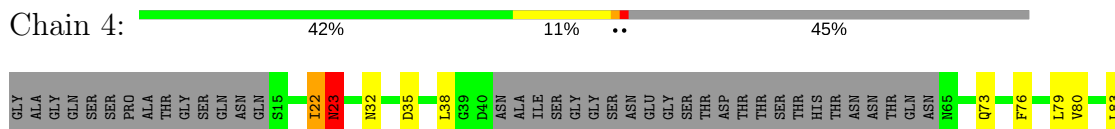
• Molecule 2: POLYPROTEIN



• Molecule 3: POLYPROTEIN



• Molecule 4: POLYPROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	305.14Å 305.14Å 723.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.00 – 3.00 16.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	60.1 (17.00-3.00) 58.7 (16.99-3.00)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.27 (at 3.02Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , (Not available) 0.359 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.247 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.246 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.248 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.248 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.248 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.247 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.329 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.49	EDS
Total number of atoms	5210	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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	1	0.64	0/1536	0.99	4/2097 (0.2%)
2	2	0.63	0/1680	0.88	1/2293 (0.0%)
3	3	0.68	1/1774 (0.1%)	0.98	3/2427 (0.1%)
4	4	0.69	0/358	0.80	0/481
All	All	0.66	1/5348 (0.0%)	0.94	8/7298 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	163	PHE	CB-CG	-6.08	1.41	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	87	TRP	N-CA-C	8.27	133.33	111.00
3	3	220	ARG	N-CA-C	7.47	131.16	111.00
3	3	198	GLY	N-CA-C	-6.12	97.80	113.10
1	1	14	ASP	CB-CA-C	-5.74	98.93	110.40
2	2	51	LEU	CA-CB-CG	5.66	128.32	115.30

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	1	1501	0	1482	36	0
2	2	1639	0	1601	41	0
3	3	1717	0	1601	67	0
4	4	353	0	327	7	0
All	All	5210	0	5011	129	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 13.

The worst 5 of 129 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)
1:1:100:GLU:HB2	3:3:220:ARG:HH22	1.26	1.00
1:1:100:GLU:HB2	3:3:220:ARG:NH2	1.92	0.83
3:3:108:HIS:HB2	3:3:203:THR:HG22	1.62	0.82
2:2:172:THR:HG22	2:2:173:ARG:H	1.46	0.81
1:1:35:LEU:O	1:1:38:ARG:HD2	1.80	0.80

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	1	190/219 (87%)	173 (91%)	12 (6%)	5 (3%)	6	30
2	2	205/219 (94%)	192 (94%)	12 (6%)	1 (0%)	31	71
3	3	219/221 (99%)	204 (93%)	8 (4%)	7 (3%)	4	24
4	4	43/85 (51%)	37 (86%)	4 (9%)	2 (5%)	2	15
All	All	657/744 (88%)	606 (92%)	36 (6%)	15 (2%)	7	33

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	88	VAL
1	1	102	GLY
3	3	69	SER
3	3	131	HIS
3	3	197	ASP

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	1	162/182 (89%)	142 (88%)	20 (12%)	5	22
2	2	180/192 (94%)	159 (88%)	21 (12%)	6	24
3	3	184/184 (100%)	156 (85%)	28 (15%)	3	15
4	4	37/67 (55%)	33 (89%)	4 (11%)	7	28
All	All	563/625 (90%)	490 (87%)	73 (13%)	4	20

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	149	ASN
2	2	219	GLN
3	3	219	SER
2	2	180	VAL
3	3	8	SER

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

Mol	Chain	Res	Type
2	2	219	GLN
3	3	43	ASN
3	3	153	ASN
2	2	189	ASN
3	3	194	HIS

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 [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, 95th 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	1	194/219 (88%)	-0.57	1 (0%) 90 74	4, 15, 71, 101	0
2	2	207/219 (94%)	-0.62	0 100 100	5, 14, 40, 93	0
3	3	221/221 (100%)	-0.54	0 100 100	5, 14, 76, 131	0
4	4	47/85 (55%)	-0.10	0 100 100	8, 39, 112, 119	0
All	All	669/744 (89%)	-0.54	1 (0%) 95 89	4, 15, 77, 131	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	134	ASP	2.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.