



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 06:49 PM BST

PDB ID : 6VSO
Title : DengueV-2 Capsid Structure
Authors : White, M.; Xia, H.; Shi, P.
Deposited on : 2020-02-11
Resolution : 3.00 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

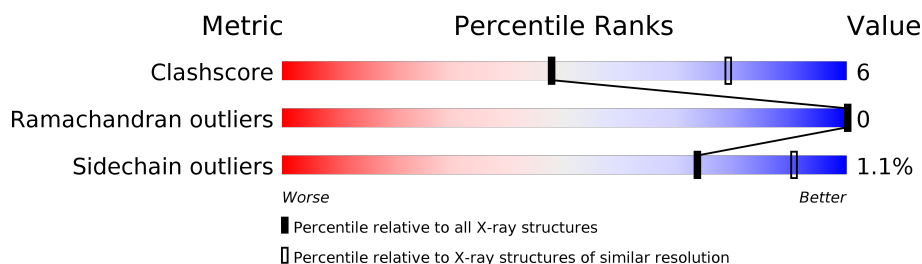
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	81	85% 10% 5%
1	B	81	74% 21% . .
1	C	81	84% 10% 6%
1	D	81	81% 15% .
1	E	81	80% 14% 6%
1	F	81	85% 12% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3701 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.

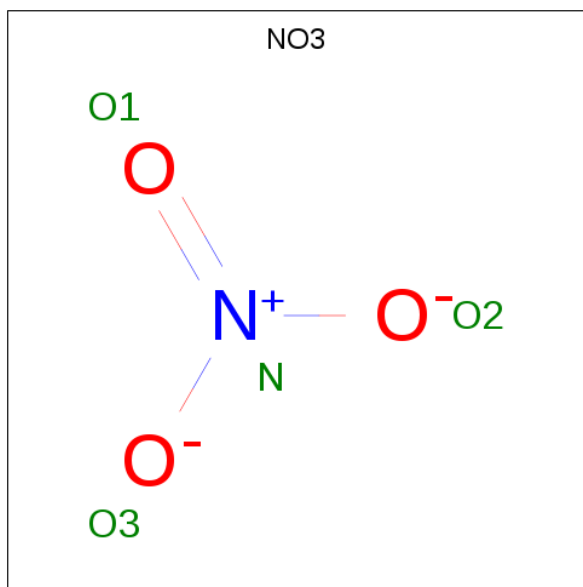
- Molecule 1 is a protein called Capsid premembrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	77	Total	C	N	O	S	0	0	0
			585	383	106	93	3			
1	B	78	Total	C	N	O	S	0	0	0
			615	400	117	95	3			
1	C	76	Total	C	N	O	S	0	0	0
			582	380	108	91	3			
1	D	78	Total	C	N	O	S	0	0	0
			596	390	110	93	3			
1	E	76	Total	C	N	O	S	0	0	0
			594	387	112	92	3			
1	F	79	Total	C	N	O	S	0	0	0
			620	403	118	96	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP A0A2D2BF61
B	20	MET	-	initiating methionine	UNP A0A2D2BF61
C	20	MET	-	initiating methionine	UNP A0A2D2BF61
D	20	MET	-	initiating methionine	UNP A0A2D2BF61
E	20	MET	-	initiating methionine	UNP A0A2D2BF61
F	20	MET	-	initiating methionine	UNP A0A2D2BF61

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	F	1	Total	N	O	0	0
			4	1	3		
2	F	1	Total	N	O	0	0
			4	1	3		
2	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	C	5	Total 5	O 5	0	0
4	E	2	Total 2	O 2	0	0
4	F	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

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.

Note EDS failed to run properly.

- Molecule 1: Capsid premembrane protein

Chain A: 




- Molecule 1: Capsid premembrane protein

Chain B: 




- Molecule 1: Capsid premembrane protein

Chain C: 



- Molecule 1: Capsid premembrane protein

Chain D: 



- Molecule 1: Capsid premembrane protein

Chain E: 



- Molecule 1: Capsid premembrane protein

Chain F:

85%

12%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.00Å 142.00Å 67.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.30 – 3.00	Depositor
% Data completeness (in resolution range)	90.8 (45.30-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.186 , 0.225	Depositor
Wilson B-factor (Å ²)	-84.1	Xtriage
Anisotropy	-0.385	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.396 for -h,-k,l	Xtriage
Total number of atoms	3701	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5956e-03.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NO3

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	0.28	0/594	0.45	0/800
1	B	0.27	0/624	0.42	0/836
1	C	0.28	0/591	0.46	0/796
1	D	0.26	0/605	0.43	0/814
1	E	0.28	0/603	0.51	0/810
1	F	0.30	0/629	0.47	0/843
All	All	0.28	0/3646	0.46	0/4899

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	585	0	618	9	0
1	B	615	0	668	13	0
1	C	582	0	617	9	0
1	D	596	0	629	9	0
1	E	594	0	638	10	0
1	F	620	0	670	7	0
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	0	0	0
2	C	12	0	0	0	0
2	D	8	0	0	0	0
2	E	20	0	0	1	0
2	F	12	0	0	0	0
3	E	12	0	16	1	0
3	F	6	0	8	3	0
4	A	2	0	0	0	0
4	C	5	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
All	All	3701	0	3864	46	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 6.

All (46) 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:24:SER:OG	1:C:27:GLN:NE2	2.05	0.89
1:F:89:GLY:HA3	3:F:204:GOL:H11	1.69	0.74
1:F:40:GLY:O	1:F:68:ARG:HD3	1.99	0.63
1:A:32:ARG:HD3	1:A:46:LEU:HD13	1.84	0.60
1:E:41:ARG:HG3	1:E:41:ARG:HH11	1.66	0.59
1:C:32:ARG:HD3	1:C:46:LEU:HD11	1.87	0.56
1:B:27:GLN:HG2	1:B:31:LYS:HE3	1.90	0.54
1:A:24:SER:CB	1:C:27:GLN:HE22	2.23	0.51
1:A:57:LEU:HD23	1:B:45:LYS:HE3	1.92	0.51
1:C:39:GLN:OE1	1:C:41:ARG:NH2	2.44	0.49
1:C:25:THR:HB	1:D:62:THR:HG22	1.94	0.49
1:D:33:PHE:HA	1:D:37:MET:SD	2.52	0.49
1:F:61:PRO:HG2	1:F:66:LEU:HD11	1.93	0.48
1:C:46:LEU:HD12	1:D:57:LEU:HD22	1.96	0.48
1:E:45:LYS:NZ	3:E:207:GOL:O3	2.43	0.47
1:A:91:MET:SD	1:B:55:ARG:HD3	2.56	0.46
1:E:82:ARG:NE	2:E:201:NO3:O3	2.45	0.45
1:B:40:GLY:O	1:B:68:ARG:HD3	2.16	0.45
1:D:44:LEU:HD23	1:D:76:LYS:HG3	1.98	0.45
1:E:61:PRO:HG2	1:E:66:LEU:HD13	1.99	0.45
1:E:41:ARG:NH1	1:E:41:ARG:HG3	2.32	0.44
1:B:27:GLN:O	1:B:31:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:PHE:HB3	1:D:84:PHE:CE1	2.52	0.44
1:D:68:ARG:O	1:D:72:ILE:HG23	2.18	0.44
1:A:57:LEU:HD21	1:B:46:LEU:HA	2.00	0.43
1:A:90:ARG:HH21	1:E:97:ARG:HG3	1.84	0.43
1:E:93:ASN:O	1:E:97:ARG:HG2	2.19	0.43
1:F:35:LEU:HA	1:F:35:LEU:HD23	1.76	0.42
1:A:96:ASN:HA	1:A:96:ASN:HD22	1.66	0.42
1:B:34:SER:O	1:B:37:MET:HG2	2.19	0.42
1:B:81:LEU:HA	1:B:81:LEU:HD23	1.77	0.42
1:C:39:GLN:HG3	1:D:26:VAL:HG21	2.01	0.42
1:F:67:LYS:HE3	1:F:67:LYS:HB2	1.69	0.42
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.92	0.42
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.86	0.41
1:E:85:ARG:HD3	3:F:204:GOL:O3	2.20	0.41
1:A:38:LEU:HA	1:A:38:LEU:HD23	1.84	0.41
1:B:44:LEU:O	1:B:48:MET:HG2	2.20	0.41
1:F:89:GLY:HA3	3:F:204:GOL:C1	2.47	0.41
1:B:47:PHE:CE2	1:B:68:ARG:HG2	2.55	0.41
1:B:74:LYS:O	1:B:78:ILE:HG13	2.20	0.40
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.92	0.40
1:B:35:LEU:HD11	1:D:38:LEU:HD11	2.02	0.40
1:E:60:PRO:HA	1:E:61:PRO:HD3	2.01	0.40
1:F:42:GLY:O	1:F:68:ARG:NH1	2.42	0.40
1:E:68:ARG:O	1:E:72:ILE:HG23	2.21	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	75/81 (93%)	74 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	76/81 (94%)	76 (100%)	0	0	100	100
1	C	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
1	D	76/81 (94%)	76 (100%)	0	0	100	100
1	E	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
1	F	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
All	All	452/486 (93%)	448 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	58/70 (83%)	58 (100%)	0	100	100
1	B	63/70 (90%)	61 (97%)	2 (3%)	39	74
1	C	58/70 (83%)	58 (100%)	0	100	100
1	D	58/70 (83%)	58 (100%)	0	100	100
1	E	60/70 (86%)	60 (100%)	0	100	100
1	F	63/70 (90%)	61 (97%)	2 (3%)	39	74
All	All	360/420 (86%)	356 (99%)	4 (1%)	73	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	ARG
1	B	68	ARG
1	F	37	MET
1	F	79	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	96	ASN
1	C	27	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NO3	E	201	-	1,3,3	0.64	0	0,3,3	0.00	-
2	NO3	F	203	-	1,3,3	0.68	0	0,3,3	0.00	-
3	GOL	F	204	-	5,5,5	1.01	0	5,5,5	1.12	0
3	GOL	E	206	-	5,5,5	0.79	0	5,5,5	1.03	0
2	NO3	B	201	-	1,3,3	0.76	0	0,3,3	0.00	-
2	NO3	E	203	-	1,3,3	0.72	0	0,3,3	0.00	-
2	NO3	E	204	-	1,3,3	0.71	0	0,3,3	0.00	-
2	NO3	A	205	-	1,3,3	0.74	0	0,3,3	0.00	-
2	NO3	C	202	-	1,3,3	0.73	0	0,3,3	0.00	-
2	NO3	E	202	-	1,3,3	0.69	0	0,3,3	0.00	-
2	NO3	A	204	-	1,3,3	0.66	0	0,3,3	0.00	-
2	NO3	E	205	-	1,3,3	0.66	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NO3	B	202	-	1,3,3	0.70	0	0,3,3	0.00	-
2	NO3	A	202	-	1,3,3	0.74	0	0,3,3	0.00	-
2	NO3	D	202	-	1,3,3	0.73	0	0,3,3	0.00	-
2	NO3	C	203	-	1,3,3	0.68	0	0,3,3	0.00	-
3	GOL	E	207	-	5,5,5	0.93	0	5,5,5	0.96	0
2	NO3	D	201	-	1,3,3	0.69	0	0,3,3	0.00	-
2	NO3	A	201	-	1,3,3	0.70	0	0,3,3	0.00	-
2	NO3	C	201	-	1,3,3	0.68	0	0,3,3	0.00	-
2	NO3	F	202	-	1,3,3	0.65	0	0,3,3	0.00	-
2	NO3	A	203	-	1,3,3	0.68	0	0,3,3	0.00	-
2	NO3	F	201	-	1,3,3	0.66	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	206	-	-	0/4/4/4	-
3	GOL	F	204	-	-	1/4/4/4	-
3	GOL	E	207	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	207	GOL	O1-C1-C2-C3
3	E	207	GOL	O1-C1-C2-O2
3	F	204	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	NO3	1	0
3	F	204	GOL	3	0
3	E	207	GOL	1	0

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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.