wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 07:45 PM JST

PDB ID	:	7XD8
Title	:	Crystal Structure of Dengue Virus Serotype 2 (DENV2) Polymerase Elongation Complex (Native Form)
Authors	:	Wu, J.; Wang, X.; Gong, P.
Deposited on	:	2022-03-26
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

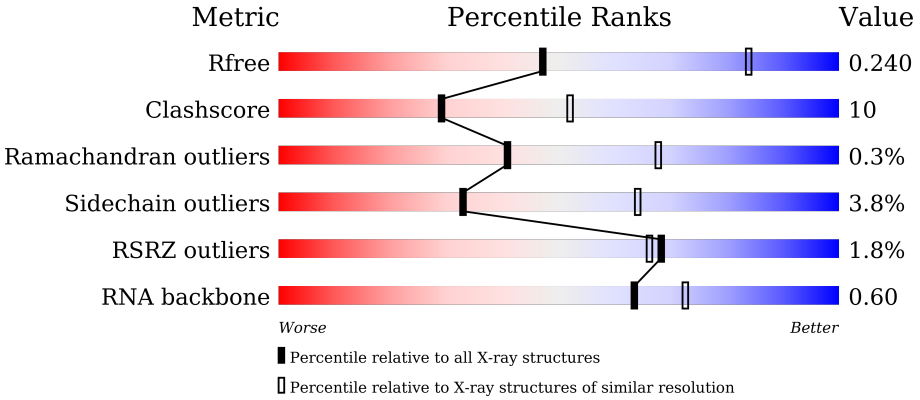
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

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 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 <=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	647	74% 20% • •
1	D	647	% 77% 19% • •
1	G	647	% 74% 21% • •
1	J	647	74% 21% • •

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Mol	Chain	Length	Quality of chain
1	M	647	77% 18%
1	P	647	9% 72% 21% 6%
2	B	30	10% 20% 10% 60%
2	E	30	20% 17% 63%
2	H	30	27% 7% 63%
2	K	30	27% 10% 60%
2	N	30	23% 17% 60%
2	Q	30	17% 17% 63%
3	C	9	67% 33%
3	F	9	44% 44% 11%
3	I	9	33% 44% 22%
3	L	9	78% 22%
3	O	9	78% 22%
3	R	9	44% 33% 22%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31489 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 NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	620	4900	3082	871	914	33	0	0	0
1	D	621	4917	3095	873	915	34	0	0	0
1	G	623	4874	3067	867	906	34	0	0	0
1	J	623	4901	3086	871	910	34	0	0	0
1	M	624	4909	3086	873	916	34	0	0	0
1	P	611	4160	2587	753	790	30	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	901	GLY	-	expression tag	UNP Q91H74
A	902	SER	-	expression tag	UNP Q91H74
A	903	SER	-	expression tag	UNP Q91H74
A	904	SER	-	expression tag	UNP Q91H74
A	905	HIS	-	expression tag	UNP Q91H74
A	906	HIS	-	expression tag	UNP Q91H74
A	907	HIS	-	expression tag	UNP Q91H74
A	908	HIS	-	expression tag	UNP Q91H74
A	909	HIS	-	expression tag	UNP Q91H74
A	910	HIS	-	expression tag	UNP Q91H74
D	901	GLY	-	expression tag	UNP Q91H74
D	902	SER	-	expression tag	UNP Q91H74
D	903	SER	-	expression tag	UNP Q91H74
D	904	SER	-	expression tag	UNP Q91H74
D	905	HIS	-	expression tag	UNP Q91H74
D	906	HIS	-	expression tag	UNP Q91H74
D	907	HIS	-	expression tag	UNP Q91H74

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Chain	Residue	Modelled	Actual	Comment	Reference
D	908	HIS	-	expression tag	UNP Q91H74
D	909	HIS	-	expression tag	UNP Q91H74
D	910	HIS	-	expression tag	UNP Q91H74
G	901	GLY	-	expression tag	UNP Q91H74
G	902	SER	-	expression tag	UNP Q91H74
G	903	SER	-	expression tag	UNP Q91H74
G	904	SER	-	expression tag	UNP Q91H74
G	905	HIS	-	expression tag	UNP Q91H74
G	906	HIS	-	expression tag	UNP Q91H74
G	907	HIS	-	expression tag	UNP Q91H74
G	908	HIS	-	expression tag	UNP Q91H74
G	909	HIS	-	expression tag	UNP Q91H74
G	910	HIS	-	expression tag	UNP Q91H74
J	901	GLY	-	expression tag	UNP Q91H74
J	902	SER	-	expression tag	UNP Q91H74
J	903	SER	-	expression tag	UNP Q91H74
J	904	SER	-	expression tag	UNP Q91H74
J	905	HIS	-	expression tag	UNP Q91H74
J	906	HIS	-	expression tag	UNP Q91H74
J	907	HIS	-	expression tag	UNP Q91H74
J	908	HIS	-	expression tag	UNP Q91H74
J	909	HIS	-	expression tag	UNP Q91H74
J	910	HIS	-	expression tag	UNP Q91H74
M	901	GLY	-	expression tag	UNP Q91H74
M	902	SER	-	expression tag	UNP Q91H74
M	903	SER	-	expression tag	UNP Q91H74
M	904	SER	-	expression tag	UNP Q91H74
M	905	HIS	-	expression tag	UNP Q91H74
M	906	HIS	-	expression tag	UNP Q91H74
M	907	HIS	-	expression tag	UNP Q91H74
M	908	HIS	-	expression tag	UNP Q91H74
M	909	HIS	-	expression tag	UNP Q91H74
M	910	HIS	-	expression tag	UNP Q91H74
P	901	GLY	-	expression tag	UNP Q91H74
P	902	SER	-	expression tag	UNP Q91H74
P	903	SER	-	expression tag	UNP Q91H74
P	904	SER	-	expression tag	UNP Q91H74
P	905	HIS	-	expression tag	UNP Q91H74
P	906	HIS	-	expression tag	UNP Q91H74
P	907	HIS	-	expression tag	UNP Q91H74
P	908	HIS	-	expression tag	UNP Q91H74
P	909	HIS	-	expression tag	UNP Q91H74

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Chain	Residue	Modelled	Actual	Comment	Reference
P	910	HIS	-	expression tag	UNP Q91H74

- Molecule 2 is a RNA chain called RNA (30-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	12	251	113	42	84	12	0	0	0
2	E	11	229	103	37	78	11	0	0	0
2	H	11	229	103	37	78	11	0	0	0
2	K	12	251	113	42	84	12	0	0	0
2	N	12	251	113	42	84	12	0	0	0
2	Q	11	229	103	37	78	11	0	0	0

- Molecule 3 is a RNA chain called RNA (9-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	9	195	87	36	63	9	0	0	0
3	F	9	195	87	36	63	9	0	0	0
3	I	9	195	87	36	63	9	0	0	0
3	L	9	194	87	36	62	9	0	0	0
3	O	9	195	87	36	63	9	0	0	0
3	R	9	195	87	36	63	9	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	2	2	2	0	0
4	D	2	2	2	0	0

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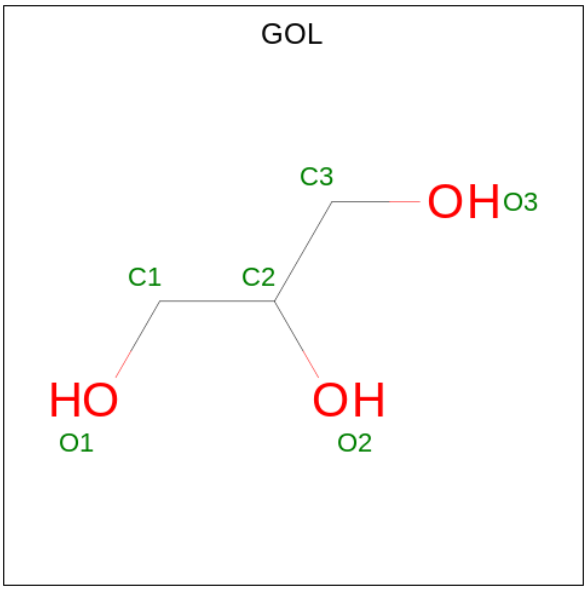
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total Zn 2 2	0	0
4	J	2	Total Zn 2 2	0	0
4	M	2	Total Zn 2 2	0	0
4	P	2	Total Zn 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	M	1	Total C O 6 3 3	0	0
5	P	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

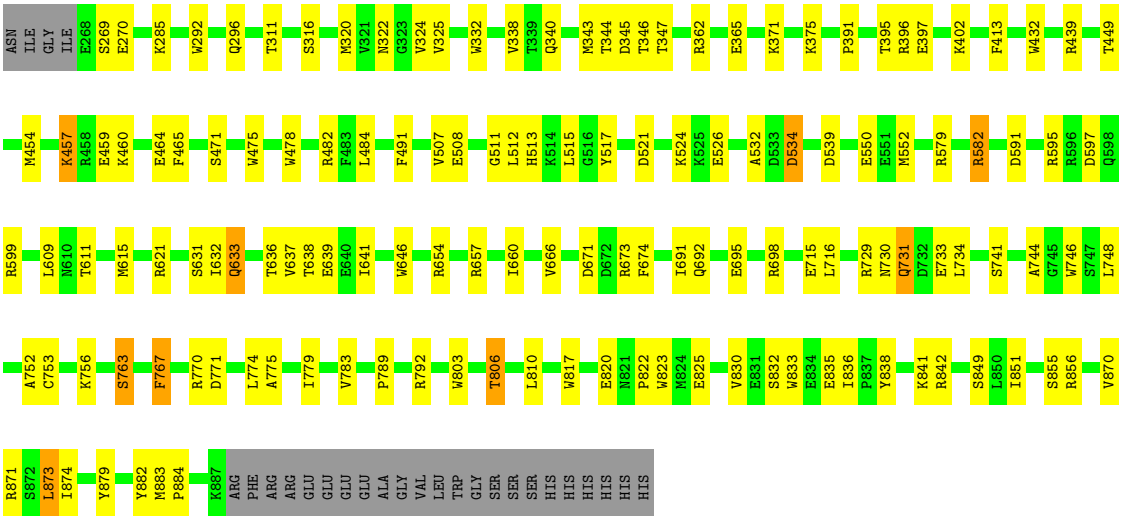
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	29	29	29	0	0
			Total	O		
6	B	8	8	8	0	0
			Total	O		
6	C	2	2	2	0	0
			Total	O		
6	D	26	26	26	0	0
			Total	O		
6	E	6	6	6	0	0
			Total	O		
6	F	6	6	6	0	0
			Total	O		
6	G	33	33	33	0	0
			Total	O		
6	H	2	2	2	0	0
			Total	O		
6	I	2	2	2	0	0
			Total	O		
6	J	29	29	29	0	0
			Total	O		
6	K	5	5	5	0	0
			Total	O		
6	L	1	1	1	0	0
			Total	O		
6	M	23	23	23	0	0
			Total	O		
6	N	3	3	3	0	0
			Total	O		
6	P	1	1	1	0	0
			Total	O		
6	R	1	1	1	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 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.

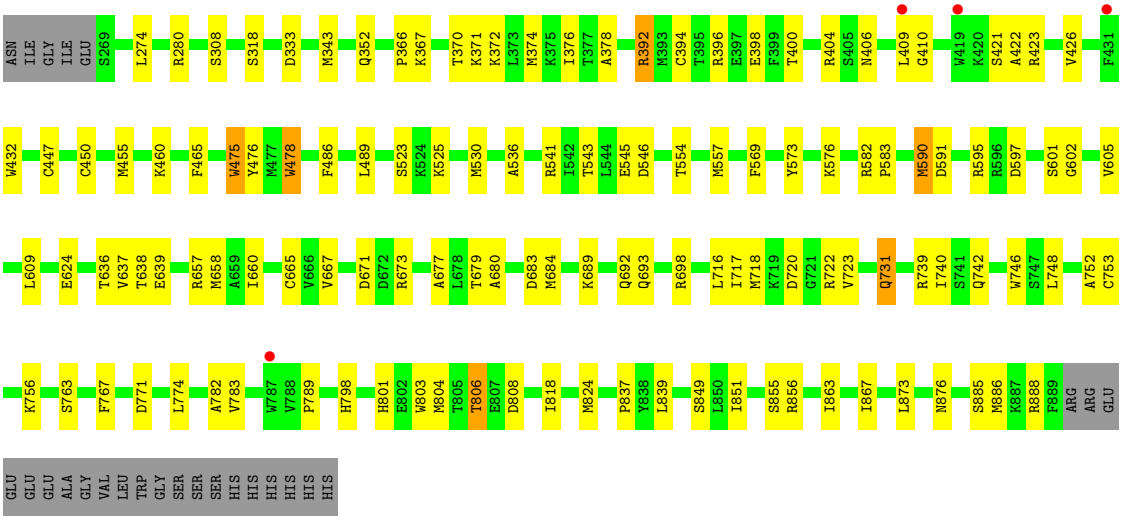
- Molecule 1: NS5

Chain A:



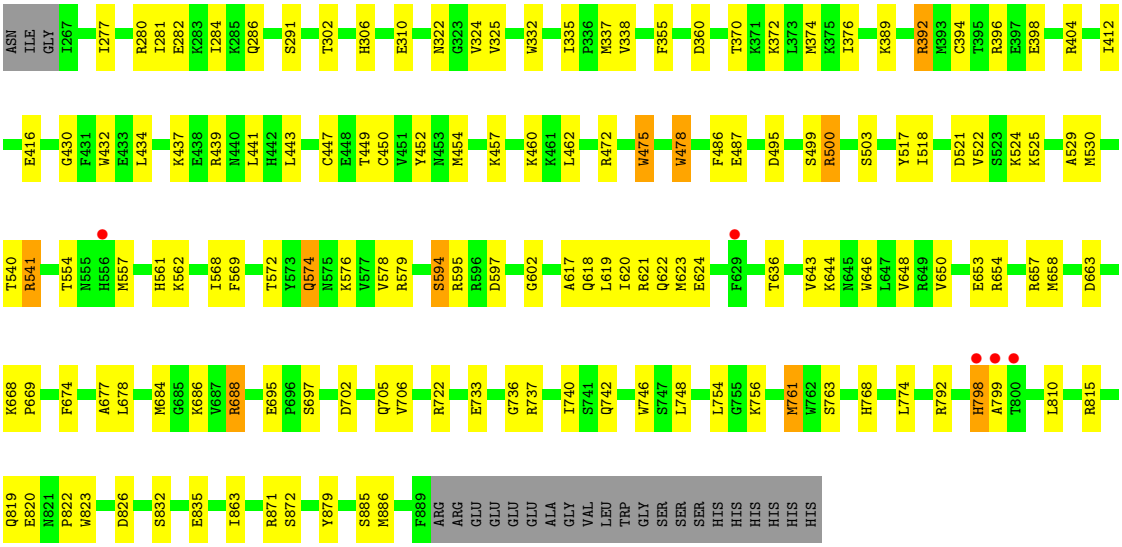
- Molecule 1: NS5

Chain D:



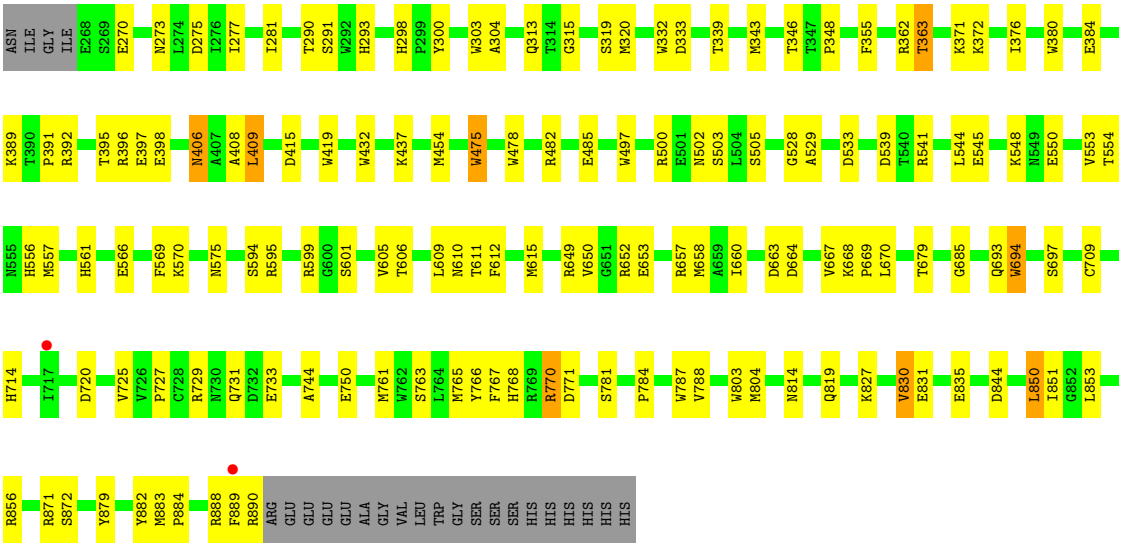
- Molecule 1: NS5

Chain G:



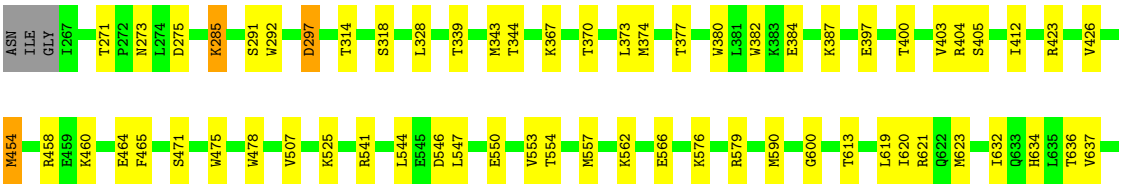
- Molecule 1: NS5

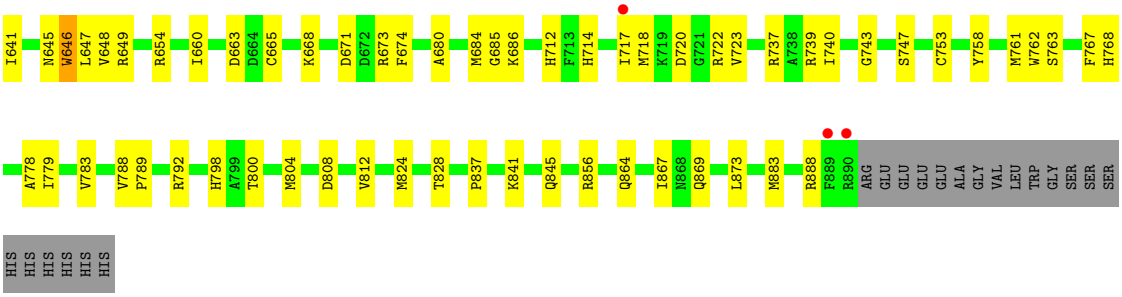
Chain J:



- Molecule 1: NS5

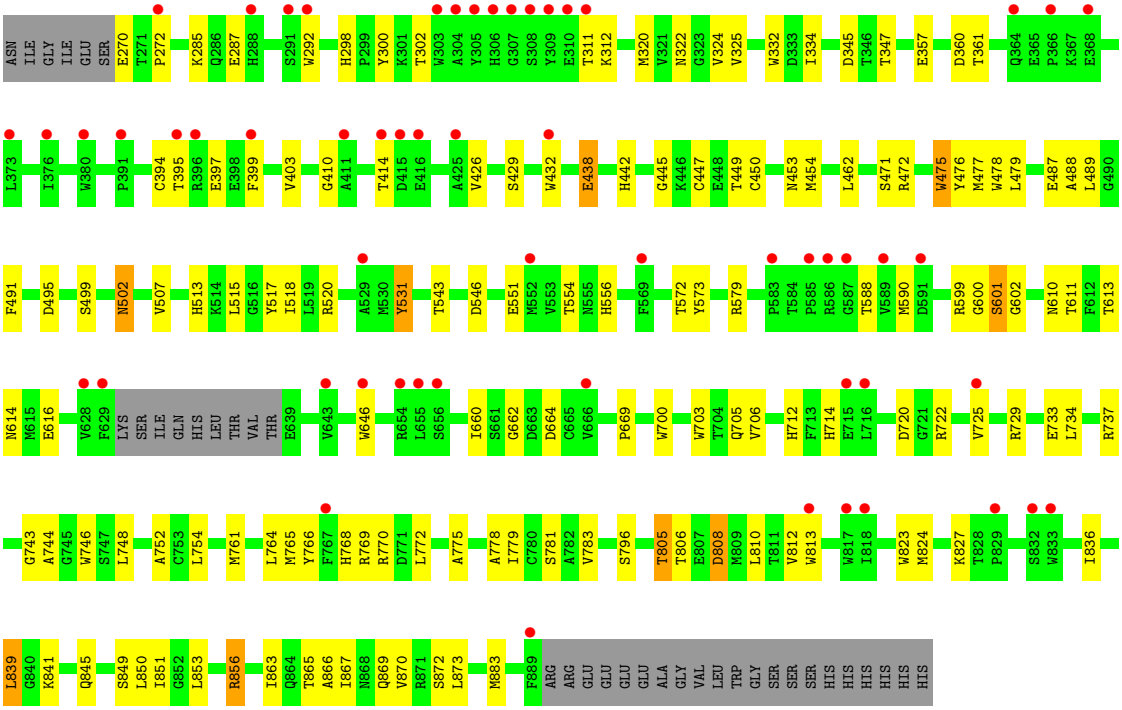
Chain M:





- Molecule 1: NS5

Chain P:



- Molecule 2: RNA (30-mer)

Chain B:

- Molecule 2: RNA (30-mer)

Chain E:

- Molecule 2: RNA (30-mer)

Chain H: 27% 7% • 63%

• Molecule 2: RNA (30-mer)

Chain K: 27% 10% • 60%

• Molecule 2: RNA (30-mer)

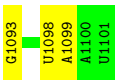
Chain N: 23% 17% 60%

• Molecule 2: RNA (30-mer)

Chain Q: 17% 17% • 63%

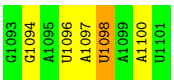
• Molecule 3: RNA (9-mer)

Chain C: 67% 33%



• Molecule 3: RNA (9-mer)

Chain F: 44% 44% 11%



• Molecule 3: RNA (9-mer)

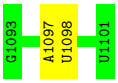
Chain I: 33% 44% 22%

• Molecule 3: RNA (9-mer)

Chain L:

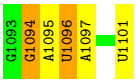
• Molecule 3: RNA (9-mer)

Chain O:



• Molecule 3: RNA (9-mer)

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	141.73Å 156.32Å 174.42Å 90.00° 94.22° 90.00°	Depositor
Resolution (Å)	49.92 – 2.85 49.92 – 2.85	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.92-2.85) 87.3 (49.92-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.199 , 0.243 0.196 , 0.240	Depositor DCC
R_{free} test set	7872 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	67.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31489	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 (i)

5.1 Standard geometry (i)

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

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	0.48	0/5018	0.67	1/6812 (0.0%)
1	D	0.46	0/5036	0.66	0/6833
1	G	0.42	0/4994	0.63	0/6789
1	J	0.45	1/5021 (0.0%)	0.65	1/6819 (0.0%)
1	M	0.45	0/5027	0.66	0/6826
1	P	0.41	2/4259 (0.0%)	0.58	0/5848
2	B	0.87	0/279	1.61	7/431 (1.6%)
2	E	0.68	0/254	1.42	2/392 (0.5%)
2	H	0.70	0/254	1.33	3/392 (0.8%)
2	K	0.69	0/279	1.26	0/431
2	N	0.68	0/279	1.13	0/431
2	Q	0.59	0/254	1.18	2/392 (0.5%)
3	C	0.89	0/218	1.41	4/336 (1.2%)
3	F	0.76	0/218	1.39	3/336 (0.9%)
3	I	0.77	0/218	1.58	4/336 (1.2%)
3	L	0.80	0/217	1.31	1/334 (0.3%)
3	O	0.67	0/218	1.25	0/336
3	R	0.71	0/218	1.35	1/336 (0.3%)
All	All	0.48	3/32261 (0.0%)	0.75	29/44410 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	438	GLU	CD-OE1	8.08	1.34	1.25
1	P	531	TYR	CE1-CZ	-5.08	1.31	1.38
1	J	709	CYS	CB-SG	-5.05	1.73	1.81

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1007	U	N3-C2-O2	-8.71	116.10	122.20
3	C	1093	G	C8-N9-C4	6.61	109.04	106.40
3	C	1099	A	N1-C6-N6	-6.34	114.80	118.60
3	C	1093	G	N3-C4-C5	6.06	131.63	128.60
3	I	1097	A	O5'-P-OP2	-5.96	100.33	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	770	ARG	Sidechain

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	4900	0	4643	92	0
1	D	4917	0	4668	83	0
1	G	4874	0	4560	92	0
1	J	4901	0	4624	93	0
1	M	4909	0	4631	85	0
1	P	4160	0	3302	102	0
2	B	251	0	129	13	0
2	E	229	0	118	2	0
2	H	229	0	118	3	0
2	K	251	0	129	5	0
2	N	251	0	129	4	0
2	Q	229	0	118	5	0
3	C	195	0	97	2	0
3	F	195	0	97	1	0
3	I	195	0	97	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	194	0	97	2	0
3	O	195	0	97	2	0
3	R	195	0	97	4	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	M	2	0	0	0	0
4	P	2	0	0	0	0
5	C	6	0	8	3	0
5	D	6	0	8	2	0
5	E	6	0	8	0	0
5	M	6	0	8	3	0
5	P	6	0	8	0	0
6	A	29	0	0	3	0
6	B	8	0	0	1	0
6	C	2	0	0	0	0
6	D	26	0	0	0	0
6	E	6	0	0	1	0
6	F	6	0	0	0	0
6	G	33	0	0	4	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
6	J	29	0	0	0	0
6	K	5	0	0	0	0
6	L	1	0	0	0	0
6	M	23	0	0	1	0
6	N	3	0	0	0	0
6	P	1	0	0	0	0
6	R	1	0	0	0	0
All	All	31489	0	27791	566	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 10.

The worst 5 of 566 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:P:447:CYS:SG	1:P:450:CYS:HB2	1.93	1.06
1:P:475:TRP:CE3	1:P:600:GLY:HA2	2.04	0.93
1:M:475:TRP:HZ3	1:M:576:LYS:HD2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:CYS:HB3	1:A:789:PRO:HG3	1.60	0.84
1:J:781:SER:HB3	1:J:882:TYR:H	1.42	0.83

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	618/647 (96%)	586 (95%)	30 (5%)	2 (0%)	41	68
1	D	619/647 (96%)	592 (96%)	26 (4%)	1 (0%)	47	75
1	G	621/647 (96%)	605 (97%)	16 (3%)	0	100	100
1	J	621/647 (96%)	595 (96%)	26 (4%)	0	100	100
1	M	622/647 (96%)	593 (95%)	27 (4%)	2 (0%)	41	68
1	P	607/647 (94%)	559 (92%)	42 (7%)	6 (1%)	15	40
All	All	3708/3882 (96%)	3530 (95%)	167 (4%)	11 (0%)	41	68

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	601	SER
1	M	646	TRP
1	A	767	PHE
1	D	601	SER
1	P	488	ALA

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	505/564 (90%)	485 (96%)	20 (4%)	31	62
1	D	508/564 (90%)	494 (97%)	14 (3%)	43	73
1	G	494/564 (88%)	475 (96%)	19 (4%)	33	64
1	J	502/564 (89%)	481 (96%)	21 (4%)	30	60
1	M	504/564 (89%)	487 (97%)	17 (3%)	37	67
1	P	318/564 (56%)	302 (95%)	16 (5%)	24	53
All	All	2831/3384 (84%)	2724 (96%)	107 (4%)	33	64

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	409	LEU
1	J	830	VAL
1	P	646	TRP
1	J	475	TRP
1	J	663	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	801	HIS
1	M	731	GLN
1	J	814	ASN
1	M	440	ASN
1	M	798	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	11/30 (36%)	0	0
2	E	10/30 (33%)	0	0
2	H	10/30 (33%)	0	0
2	K	11/30 (36%)	1 (9%)	0
2	N	11/30 (36%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Q	10/30 (33%)	1 (10%)	0
3	C	8/9 (88%)	0	0
3	F	8/9 (88%)	1 (12%)	0
3	I	8/9 (88%)	1 (12%)	0
3	L	8/9 (88%)	0	0
3	O	8/9 (88%)	0	0
3	R	8/9 (88%)	3 (37%)	0
All	All	111/234 (47%)	7 (6%)	0

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	F	1094	G
3	I	1094	G
2	K	1007	U
2	Q	1000	G
3	R	1094	G

There are no RNA pucker outliers to report.

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)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
5	GOL	C	1201	-	5,5,5	1.11	0	5,5,5	0.74	0
5	GOL	M	2003	-	5,5,5	1.42	2 (40%)	5,5,5	0.77	0
5	GOL	D	2003	-	5,5,5	1.28	0	5,5,5	1.36	1 (20%)
5	GOL	P	2003	-	5,5,5	1.32	1 (20%)	5,5,5	0.76	0
5	GOL	E	1101	-	5,5,5	1.48	2 (40%)	5,5,5	1.04	0

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
5	GOL	C	1201	-	-	4/4/4/4	-
5	GOL	M	2003	-	-	0/4/4/4	-
5	GOL	D	2003	-	-	2/4/4/4	-
5	GOL	P	2003	-	-	2/4/4/4	-
5	GOL	E	1101	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1101	GOL	C3-C2	2.36	1.61	1.51
5	M	2003	GOL	C1-C2	2.30	1.61	1.51
5	P	2003	GOL	C1-C2	2.26	1.61	1.51
5	E	1101	GOL	C1-C2	2.22	1.60	1.51
5	M	2003	GOL	C3-C2	2.12	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	2003	GOL	C3-C2-C1	-2.31	102.74	111.70

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1201	GOL	O1-C1-C2-C3
5	C	1201	GOL	C1-C2-C3-O3
5	C	1201	GOL	O2-C2-C3-O3
5	D	2003	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	P	2003	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1201	GOL	3	0
5	M	2003	GOL	3	0
5	D	2003	GOL	2	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)

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	A	620/647 (95%)	-0.33	0	100	100	42, 61, 81, 119	0
1	D	621/647 (95%)	-0.24	4 (0%)	89	89	44, 65, 91, 110	0
1	G	623/647 (96%)	-0.18	5 (0%)	86	85	48, 70, 97, 133	0
1	J	623/647 (96%)	-0.31	2 (0%)	94	94	50, 68, 90, 135	0
1	M	624/647 (96%)	-0.29	3 (0%)	91	90	46, 63, 84, 115	0
1	P	611/647 (94%)	0.36	57 (9%)	8	5	54, 116, 154, 177	0
2	B	12/30 (40%)	-0.02	0	100	100	46, 51, 96, 129	2 (16%)
2	E	11/30 (36%)	-0.14	0	100	100	55, 59, 72, 104	0
2	H	11/30 (36%)	-0.04	0	100	100	56, 65, 80, 88	1 (9%)
2	K	12/30 (40%)	0.11	0	100	100	55, 65, 102, 128	2 (16%)
2	N	12/30 (40%)	-0.02	0	100	100	53, 58, 91, 111	2 (16%)
2	Q	11/30 (36%)	-0.31	0	100	100	85, 96, 108, 112	0
3	C	9/9 (100%)	-0.26	0	100	100	47, 53, 54, 57	0
3	F	9/9 (100%)	-0.15	0	100	100	52, 56, 70, 79	0
3	I	9/9 (100%)	0.03	0	100	100	58, 63, 68, 79	0
3	L	9/9 (100%)	0.14	0	100	100	60, 64, 77, 79	0
3	O	9/9 (100%)	0.17	0	100	100	56, 59, 83, 88	0
3	R	9/9 (100%)	0.14	0	100	100	85, 92, 108, 109	0
All	All	3845/4116 (93%)	-0.16	71 (1%)	68	66	42, 67, 129, 177	7 (0%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	817	TRP	4.9
1	P	307	GLY	4.4
1	P	415	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	P	292	TRP	4.3
1	P	818	ILE	4.1

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	P	2002	1/1	0.80	0.05	142,142,142,142	1
5	GOL	P	2003	6/6	0.83	0.16	59,61,70,72	0
5	GOL	M	2003	6/6	0.92	0.16	53,56,60,63	0
5	GOL	D	2003	6/6	0.92	0.47	66,67,68,72	0
5	GOL	C	1201	6/6	0.95	0.22	46,53,59,63	6
5	GOL	E	1101	6/6	0.96	0.37	57,61,64,66	0
4	ZN	A	2001	1/1	0.97	0.14	51,51,51,51	1
4	ZN	G	2002	1/1	0.97	0.11	68,68,68,68	1
4	ZN	P	2001	1/1	0.97	0.06	90,90,90,90	0
4	ZN	J	2002	1/1	0.98	0.14	65,65,65,65	0
4	ZN	J	2001	1/1	0.98	0.13	55,55,55,55	1
4	ZN	A	2002	1/1	0.99	0.12	51,51,51,51	1
4	ZN	D	2001	1/1	0.99	0.18	47,47,47,47	1
4	ZN	D	2002	1/1	0.99	0.08	74,74,74,74	0
4	ZN	M	2001	1/1	0.99	0.12	68,68,68,68	0
4	ZN	M	2002	1/1	0.99	0.16	52,52,52,52	1
4	ZN	G	2001	1/1	0.99	0.14	51,51,51,51	1

6.5 Other polymers (i)

There are no such residues in this entry.