Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2022 – 10:44 AM EST

PDB ID	:	7LW0
Title	:	Structural and Biochemical Insight into Assembly of Molecular Motors Involved in Viral DNA Packaging
Authors	:	Ortega, M.E.
Deposited on	:	2021-02-26
Resolution	:	2.32 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

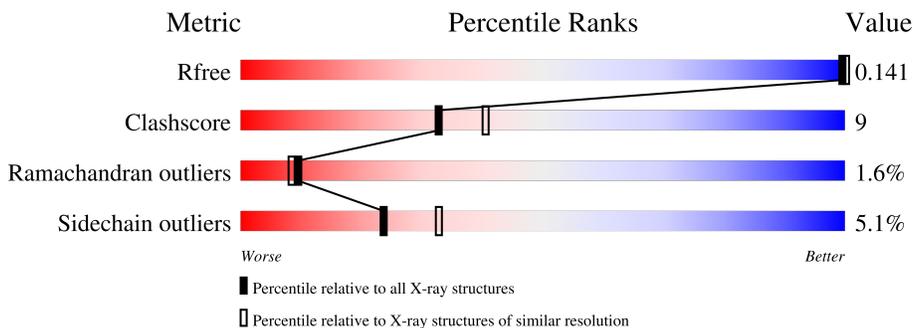|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.32 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	Percentile Ranks	Value
Rfree		0.141
Clashscore		9
Ramachandran outliers		1.6%
Sidechain outliers		5.1%

Worse — Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

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%

Mol	Chain	Length	Quality of chain
1	A	56	88% 12%
1	B	56	80% 20%
1	C	56	77% 23%
1	D	56	79% 21%
1	E	56	82% 18%
1	F	56	71% 27% •
1	G	56	73% 27%

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Mol	Chain	Length	Quality of chain
1	H	56	77% 20% ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3504 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 Terminase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			
1	B	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			
1	C	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			
1	D	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			
1	E	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			
1	F	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			
1	G	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			
1	H	56	Total	C	N	O	S	0	0	0
			438	275	78	82	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	CYS	GLU	conflict	UNP P03707
B	56	CYS	GLU	conflict	UNP P03707
C	56	CYS	GLU	conflict	UNP P03707
D	56	CYS	GLU	conflict	UNP P03707
E	56	CYS	GLU	conflict	UNP P03707
F	56	CYS	GLU	conflict	UNP P03707
G	56	CYS	GLU	conflict	UNP P03707
H	56	CYS	GLU	conflict	UNP P03707

3 Residue-property plots ⓘ

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.

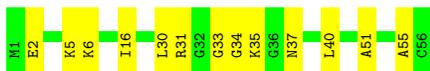- Molecule 1: Terminase small subunit

Chain A:

88%　　12%

M1 K6 L30 R31 K35 L40 K48 D54 A55 C56

- Molecule 1: Terminase small subunit

Chain B:

80%　　20%

M1 K5 A14 S15 I16 R17 W22 M27 R31 G32 G33 N37 E38 V39 L40 C56

- Molecule 1: Terminase small subunit

Chain C:

77%　　23%

M1 E2 K5 K6 I16 L30 R31 G32 G33 G34 K35 G36 N37 L40 A51 A55 C56

- Molecule 1: Terminase small subunit

Chain D:

79%　　21%

M1 K5 I16 N21 W22 Q23 V29 L30 R31 G34 L40 K48 E52 R53 C56

- Molecule 1: Terminase small subunit

Chain E:

82%　　18%

M1 S15 I16 R17 N21 Q25 L30 R31 G34 E38 D42 D54 A55 C56
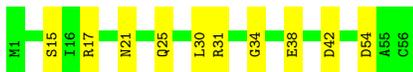
- Molecule 1: Terminase small subunit

Chain F:

71%　　27%　　•

M1 E2 K6 D10 R17 N21 W22 Q23 V29 L30 R31 G32 G33 G34 K35 G36 Y41 E52 A55 C56

• Molecule 1: Terminase small subunit

Chain G:

73%   27%

M1 K5 K6 A9 A14 S15 I16 Q20 Q23 L30 R31 G36 N37 E38 D42 S43 A44 A45 K48 C56

• Molecule 1: Terminase small subunit

Chain H:

77%   20%   •

M1 E2 K5 I16 R17 Q20 Q23 L30 R31 G32 G33 G34 N37 E38 V39 L40 C56
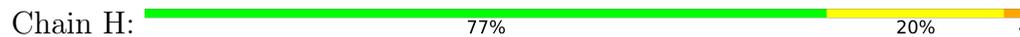
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.75Å 42.77Å 57.22Å 89.98° 89.98° 89.88°	Depositor
Resolution (Å)	34.26 – 2.32 34.26 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.1 (34.26-2.32) 92.6 (34.26-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.119 , 0.152 0.120 , 0.141	Depositor DCC
R_{free} test set	1673 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 0.4	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,-h,l 0.000 for -k,h,l 0.430 for h,-k,-l 0.448 for -h,k,-l 0.447 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3504	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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	A	0.72	0/445	0.84	0/598
1	B	0.73	0/445	0.85	0/598
1	C	0.74	0/445	0.82	0/598
1	D	0.73	0/445	0.88	0/598
1	E	0.68	0/445	0.84	0/598
1	F	0.70	0/445	0.92	0/598
1	G	0.69	0/445	0.85	0/598
1	H	0.76	0/445	0.81	0/598
All	All	0.72	0/3560	0.85	0/4784

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	438	0	434	2	0
1	B	438	0	434	8	0
1	C	438	0	434	14	0
1	D	438	0	434	11	0
1	E	438	0	434	5	0
1	F	438	0	434	8	0
1	G	438	0	434	14	0
1	H	438	0	434	14	0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3504	0	3472	61	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 (61) 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:G:45:ALA:HA	1:G:48:LYS:HD2	1.63	0.80
1:B:5:LYS:HD2	1:B:16:ILE:HG23	1.69	0.73
1:C:40:LEU:HD21	1:H:23:GLN:NE2	2.05	0.72
1:C:5:LYS:HG2	1:C:16:ILE:HG23	1.72	0.68
1:C:33:GLY:HA2	1:H:38:GLU:HA	1.74	0.68
1:C:31:ARG:HH11	1:H:37:ASN:HD21	1.42	0.68
1:C:34:GLY:C	1:C:35:LYS:HE2	2.18	0.64
1:G:5:LYS:NZ	1:G:20:GLN:HE21	1.98	0.61
1:H:33:GLY:H	1:H:37:ASN:ND2	2.00	0.60
1:B:31:ARG:HB2	1:B:40:LEU:HB2	1.85	0.59
1:H:5:LYS:HE3	1:H:20:GLN:HE21	1.68	0.59
1:B:5:LYS:HD2	1:B:16:ILE:CG2	2.33	0.59
1:D:23:GLN:NE2	1:D:29:VAL:HG21	2.20	0.56
1:E:30:LEU:HD11	1:E:42:ASP:HB2	1.86	0.56
1:B:40:LEU:HD21	1:G:23:GLN:NE2	2.22	0.55
1:C:31:ARG:HH11	1:H:37:ASN:ND2	2.03	0.55
1:D:40:LEU:HD21	1:F:23:GLN:NE2	2.21	0.54
1:H:31:ARG:HE	1:H:31:ARG:HA	1.74	0.53
1:F:52:GLU:HA	1:F:55:ALA:HB3	1.90	0.53
1:B:33:GLY:HA2	1:G:38:GLU:HA	1.92	0.52
1:B:37:ASN:HA	1:G:5:LYS:HZ2	1.76	0.51
1:C:40:LEU:HD21	1:H:23:GLN:HE22	1.75	0.51
1:D:5:LYS:HD2	1:D:16:ILE:HG23	1.92	0.51
1:D:23:GLN:HE21	1:D:29:VAL:HG21	1.75	0.51
1:H:2:GLU:OE2	1:H:40:LEU:HD13	2.11	0.50
1:E:38:GLU:OE1	1:E:38:GLU:N	2.42	0.49
1:C:33:GLY:HA3	1:C:37:ASN:HB3	1.93	0.49
1:C:31:ARG:HB2	1:C:40:LEU:HB2	1.95	0.48
1:F:17:ARG:H	1:F:17:ARG:HD2	1.78	0.48
1:G:44:ALA:O	1:G:48:LYS:HG3	2.13	0.48
1:D:31:ARG:HA	1:F:34:GLY:O	2.14	0.48
1:G:5:LYS:CD	1:G:16:ILE:HG23	2.43	0.48
1:E:30:LEU:HD13	1:E:42:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:LEU:HB3	1:H:31:ARG:H	1.51	0.47
1:E:31:ARG:HD2	1:E:31:ARG:N	2.30	0.47
1:G:5:LYS:HZ3	1:G:20:GLN:HE21	1.62	0.46
1:C:2:GLU:OE1	1:H:31:ARG:NH2	2.49	0.46
1:A:31:ARG:HB2	1:A:40:LEU:HB2	1.97	0.45
1:G:30:LEU:HD21	1:G:42:ASP:HB2	1.99	0.44
1:D:31:ARG:CZ	1:F:31:ARG:HA	2.48	0.44
1:G:5:LYS:HD2	1:G:16:ILE:HG23	2.00	0.43
1:E:21:ASN:O	1:E:25:GLN:HG3	2.20	0.42
1:C:2:GLU:HG2	1:C:30:LEU:CD2	2.50	0.42
1:D:30:LEU:O	1:D:31:ARG:C	2.58	0.42
1:D:48:LYS:O	1:D:52:GLU:HG3	2.18	0.42
1:F:6:LYS:HB2	1:F:6:LYS:HE3	1.80	0.41
1:H:34:GLY:H	1:H:37:ASN:ND2	2.18	0.41
1:G:6:LYS:HA	1:G:16:ILE:HD11	2.02	0.41
1:C:40:LEU:HD21	1:H:23:GLN:HE21	1.83	0.41
1:G:9:ALA:HB1	1:G:14:ALA:O	2.20	0.41
1:C:35:LYS:HD3	1:C:35:LYS:HA	1.76	0.41
1:C:51:ALA:O	1:C:55:ALA:HB2	2.21	0.41
1:F:29:VAL:HG22	1:F:41:TYR:CE2	2.56	0.41
1:B:14:ALA:HA	1:D:31:ARG:NH2	2.35	0.40
1:D:48:LYS:HD3	1:D:48:LYS:HA	1.93	0.40
1:G:5:LYS:HZ1	1:G:20:GLN:HE21	1.66	0.40
1:B:22:TRP:O	1:B:27:MET:HB2	2.21	0.40
1:A:54:ASP:OD1	1:G:36:GLY:HA2	2.21	0.40
1:D:40:LEU:HD23	1:D:40:LEU:HA	1.92	0.40
1:F:6:LYS:O	1:F:10:ASP:HB2	2.21	0.40
1:H:5:LYS:HD2	1:H:16:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	54/56 (96%)	52 (96%)	1 (2%)	1 (2%)	8	6
1	B	54/56 (96%)	50 (93%)	3 (6%)	1 (2%)	8	6
1	C	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
1	D	54/56 (96%)	52 (96%)	1 (2%)	1 (2%)	8	6
1	E	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8	6
1	F	54/56 (96%)	49 (91%)	3 (6%)	2 (4%)	3	1
1	G	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
1	H	54/56 (96%)	48 (89%)	5 (9%)	1 (2%)	8	6
All	All	432/448 (96%)	396 (92%)	29 (7%)	7 (2%)	9	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	34	GLY
1	B	38	GLU
1	A	30	LEU
1	F	36	GLY
1	H	30	LEU
1	D	34	GLY
1	F	33	GLY

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	44/44 (100%)	41 (93%)	3 (7%)	16	20
1	B	44/44 (100%)	43 (98%)	1 (2%)	50	66
1	C	44/44 (100%)	43 (98%)	1 (2%)	50	66
1	D	44/44 (100%)	42 (96%)	2 (4%)	27	38
1	E	44/44 (100%)	41 (93%)	3 (7%)	16	20
1	F	44/44 (100%)	39 (89%)	5 (11%)	5	6
1	G	44/44 (100%)	43 (98%)	1 (2%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	44/44 (100%)	42 (96%)	2 (4%)	27 38
All	All	352/352 (100%)	334 (95%)	18 (5%)	24 33

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	35	LYS
1	A	48	LYS
1	B	17	ARG
1	C	6	LYS
1	D	21	ASN
1	D	53	ARG
1	E	15	SER
1	E	17	ARG
1	E	54	ASP
1	F	2	GLU
1	F	17	ARG
1	F	21	ASN
1	F	35	LYS
1	F	56	CYS
1	G	31	ARG
1	H	2	GLU
1	H	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	GLN
1	D	20	GLN
1	D	25	GLN
1	D	37	ASN
1	G	20	GLN
1	H	20	GLN
1	H	21	ASN
1	H	37	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

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.