Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:26 AM EDT

PDB ID	:	2F5U
Title	:	Structural Characterization of the UL25 DNA Packaging Protein from Herpes Simplex Virus Type 1
Authors	:	Bowman, B.R.
Deposited on	:	2005-11-27
Resolution	:	2.10 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 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:

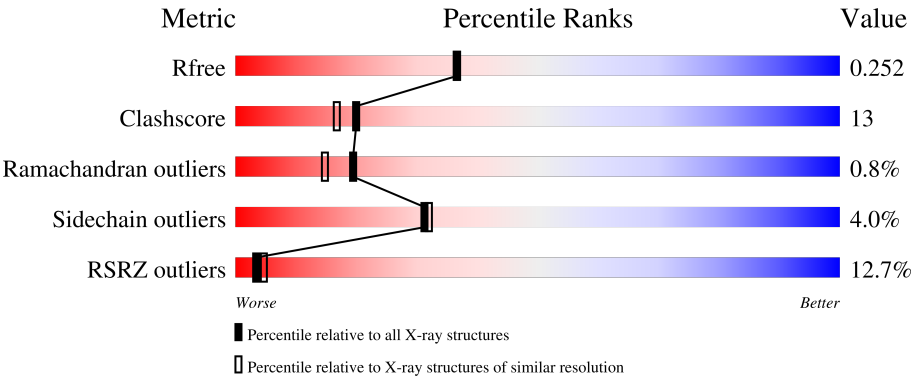
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	447	12% 69% 21% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3337 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 Virion protein UL25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3149	1990	573	571	15	0	0	0

- Molecule 2 is water.

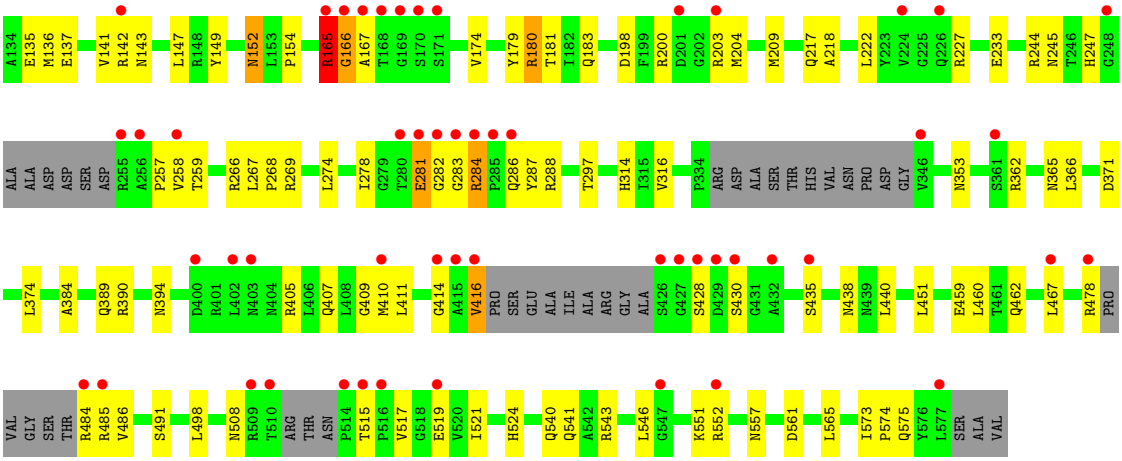
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	188	188	188	0	0

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: Virion protein UL25

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.60Å 67.60Å 119.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.10 – 2.10 34.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.10-2.10) 100.0 (34.10-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.13 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.251 0.227 , 0.252	Depositor DCC
R_{free} test set	2527 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3337	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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

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	0.35	0/3209	0.58	0/4353

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	3149	0	3144	79	0
2	A	188	0	0	4	0
All	All	3337	0	3144	79	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.

All (79) 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:142:ARG:HH22	1:A:438:ASN:HB3	1.22	0.98
1:A:281:GLU:HG2	1:A:282:GLY:N	1.94	0.81
1:A:258:VAL:HG23	1:A:259:THR:HG23	1.63	0.79
1:A:152:ASN:HD21	1:A:217:GLN:HE22	1.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASN:HD22	1:A:366:LEU:H	1.33	0.76
1:A:353:ASN:ND2	1:A:366:LEU:H	1.84	0.75
1:A:165:ARG:HE	1:A:166:GLY:H	1.34	0.75
1:A:198:ASP:OD1	1:A:200:ARG:HD3	1.92	0.69
1:A:459:GLU:H	1:A:462:GLN:NE2	1.90	0.69
1:A:180:ARG:CZ	1:A:204:MET:HE3	2.23	0.69
1:A:459:GLU:H	1:A:462:GLN:HE21	1.39	0.68
1:A:200:ARG:O	1:A:203:ARG:HG2	1.94	0.68
1:A:142:ARG:NH2	1:A:438:ASN:HB3	2.03	0.67
1:A:484:ARG:O	1:A:484:ARG:HG2	1.97	0.65
1:A:394:ASN:HA	1:A:435:SER:O	1.96	0.64
1:A:165:ARG:HE	1:A:166:GLY:N	1.96	0.64
1:A:314:HIS:HD2	1:A:316:VAL:H	1.47	0.63
1:A:407:GLN:HB2	1:A:410:MET:HE2	1.79	0.63
1:A:515:THR:HG23	1:A:519:GLU:OE1	1.99	0.61
1:A:281:GLU:HG2	1:A:282:GLY:H	1.66	0.60
1:A:384:ALA:HB1	1:A:467:LEU:HD21	1.82	0.60
1:A:181:THR:HG21	1:A:491:SER:HB3	1.84	0.59
1:A:297:THR:HG22	1:A:478:ARG:HH12	1.68	0.59
1:A:287:TYR:H	1:A:540:GLN:HE21	1.49	0.59
1:A:267:LEU:N	1:A:268:PRO:HD2	2.18	0.58
1:A:136:MET:CE	1:A:451:LEU:HD23	2.35	0.57
1:A:218:ALA:O	1:A:524:HIS:HE1	1.88	0.57
1:A:384:ALA:HB3	1:A:460:LEU:HD23	1.87	0.57
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.71	0.55
1:A:281:GLU:CG	1:A:282:GLY:N	2.67	0.55
1:A:274:LEU:O	1:A:278:ILE:HG12	2.08	0.54
1:A:409:GLY:HA2	1:A:416:VAL:HG21	1.90	0.54
1:A:551:LYS:HG3	1:A:552:ARG:N	2.22	0.54
1:A:508:ASN:HD21	1:A:515:THR:CB	2.22	0.53
1:A:394:ASN:OD1	1:A:435:SER:O	2.26	0.53
1:A:180:ARG:NE	1:A:204:MET:HE3	2.24	0.53
1:A:142:ARG:HH22	1:A:438:ASN:CB	2.10	0.52
1:A:541:GLN:HE22	1:A:552:ARG:HH22	1.58	0.52
1:A:141:VAL:HG12	1:A:143:ASN:OD1	2.10	0.51
1:A:414:GLY:C	1:A:416:VAL:H	2.12	0.51
1:A:286:GLN:HG3	1:A:288:ARG:HG2	1.92	0.51
1:A:561:ASP:O	1:A:565:LEU:HD23	2.10	0.51
1:A:174:VAL:HG23	1:A:575:GLN:HG2	1.93	0.51
1:A:183:GLN:NE2	1:A:204:MET:HE1	2.26	0.50
1:A:384:ALA:HB1	1:A:467:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:HD13	1:A:574:PRO:HG2	1.94	0.50
1:A:353:ASN:HD21	1:A:365:ASN:HA	1.77	0.49
1:A:561:ASP:HB3	2:A:718:HOH:O	2.11	0.49
1:A:136:MET:HE3	1:A:451:LEU:HD23	1.95	0.49
1:A:268:PRO:HG2	2:A:641:HOH:O	2.13	0.49
1:A:517:VAL:O	1:A:521:ILE:HG13	2.14	0.48
1:A:244:ARG:HH21	1:A:245:ASN:HD21	1.61	0.48
1:A:283:GLY:O	1:A:284:ARG:HB2	2.14	0.48
1:A:180:ARG:NH2	1:A:204:MET:HE3	2.28	0.47
1:A:411:LEU:CD1	1:A:574:PRO:HG2	2.45	0.47
1:A:227:ARG:HD3	1:A:374:LEU:HB2	1.95	0.47
1:A:179:TYR:CD2	1:A:209:MET:SD	3.08	0.47
1:A:543:ARG:HH11	1:A:543:ARG:HG2	1.79	0.47
1:A:405:ARG:HH11	1:A:405:ARG:HG3	1.79	0.46
1:A:227:ARG:HD3	1:A:371:ASP:OD2	2.15	0.46
1:A:136:MET:HE1	1:A:451:LEU:HD23	1.97	0.45
1:A:149:TYR:OH	1:A:451:LEU:HD21	2.16	0.45
1:A:557:ASN:HB3	1:A:573:ILE:HB	1.98	0.45
1:A:180:ARG:CZ	1:A:204:MET:CE	2.94	0.45
1:A:543:ARG:HG2	2:A:761:HOH:O	2.17	0.44
1:A:137:GLU:HA	1:A:147:LEU:O	2.18	0.44
1:A:266:ARG:O	1:A:269:ARG:HG2	2.17	0.44
1:A:136:MET:HE3	1:A:451:LEU:CD2	2.48	0.43
1:A:165:ARG:NE	1:A:166:GLY:H	2.10	0.43
1:A:180:ARG:NH2	1:A:204:MET:CE	2.81	0.43
1:A:428:SER:O	1:A:430:SER:N	2.42	0.43
1:A:152:ASN:ND2	1:A:154:PRO:HD2	2.33	0.42
1:A:521:ILE:HG23	2:A:670:HOH:O	2.19	0.42
1:A:233:GLU:OE2	1:A:362:ARG:NH2	2.48	0.42
1:A:257:PRO:HG3	1:A:266:ARG:NH1	2.35	0.42
1:A:281:GLU:C	1:A:283:GLY:H	2.21	0.41
1:A:165:ARG:O	1:A:167:ALA:N	2.54	0.41
1:A:459:GLU:N	1:A:462:GLN:HE21	2.13	0.41
1:A:485:ARG:O	1:A:486:VAL:CG2	2.68	0.41

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	398/447 (89%)	371 (93%)	24 (6%)	3 (1%)	19 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	GLY
1	A	165	ARG
1	A	247	HIS

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	324/351 (92%)	311 (96%)	13 (4%)	31 32

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	GLU
1	A	152	ASN
1	A	165	ARG
1	A	180	ARG
1	A	222	LEU
1	A	281	GLU
1	A	284	ARG
1	A	389	GLN

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Mol	Chain	Res	Type
1	A	390	ARG
1	A	416	VAL
1	A	440	LEU
1	A	498	LEU
1	A	546	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	226	GLN
1	A	245	ASN
1	A	298	GLN
1	A	314	HIS
1	A	323	HIS
1	A	353	ASN
1	A	389	GLN
1	A	394	ASN
1	A	403	ASN
1	A	462	GLN
1	A	508	ASN
1	A	524	HIS
1	A	549	ASN
1	A	575	GLN

5.3.3 RNA

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

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, 95^{th} 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	410/447 (91%)	0.68	52 (12%) 3 5	10, 26, 73, 104	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	GLY	13.1
1	A	255	ARG	10.8
1	A	426	SER	10.2
1	A	283	GLY	8.0
1	A	280	THR	7.8
1	A	346	VAL	7.6
1	A	430	SER	7.4
1	A	165	ARG	7.2
1	A	402	LEU	6.5
1	A	415	ALA	6.4
1	A	170	SER	6.3
1	A	416	VAL	5.7
1	A	428	SER	5.7
1	A	429	ASP	5.4
1	A	577	LEU	5.0
1	A	509	ARG	4.9
1	A	403	ASN	4.4
1	A	410	MET	4.4
1	A	281	GLU	4.4
1	A	427	GLY	4.1
1	A	224	VAL	4.0
1	A	166	GLY	3.7
1	A	284	ARG	3.5
1	A	484	ARG	3.5
1	A	285	PRO	3.4
1	A	258	VAL	3.4
1	A	171	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	ARG	3.2
1	A	167	ALA	3.2
1	A	515	THR	3.2
1	A	552	ARG	3.2
1	A	201	ASP	3.1
1	A	168	THR	3.0
1	A	514	PRO	2.9
1	A	414	GLY	2.8
1	A	400	ASP	2.8
1	A	226	GLN	2.8
1	A	478	ARG	2.8
1	A	169	GLY	2.7
1	A	435	SER	2.7
1	A	256	ALA	2.6
1	A	361	SER	2.4
1	A	203	ARG	2.3
1	A	432	ALA	2.3
1	A	547	GLY	2.3
1	A	516	PRO	2.2
1	A	485	ARG	2.2
1	A	519	GLU	2.1
1	A	248	GLY	2.1
1	A	467	LEU	2.0
1	A	510	THR	2.0
1	A	286	GLN	2.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.