



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:33 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

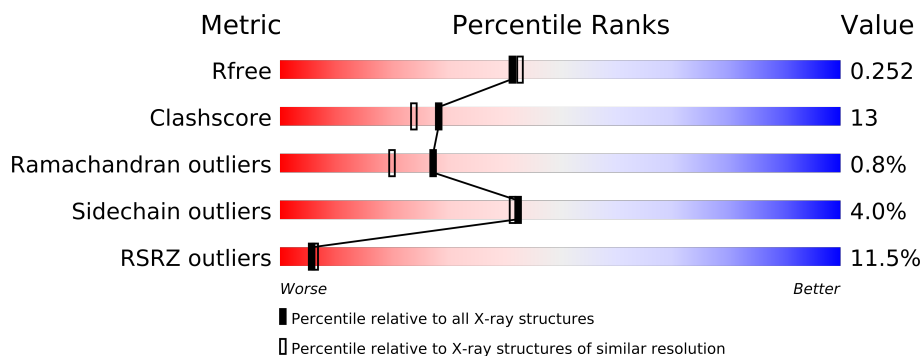
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	447	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3337 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	410	Total	C	N	O	S	0	0	0
			3149	1990	573	571	15			

- Molecule 2 is water.

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

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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%)	DCC
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 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25583 reflections	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (79) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:459:GLU:H	1:A:462:GLN:NE2	1.90	0.69
1:A:198:ASP:OD1	1:A:200:ARG:HD3	1.92	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:407:GLN:HB2	1:A:410:MET:HE2	1.79	0.63
1:A:314:HIS:HD2	1:A:316:VAL:H	1.47	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
1:A:411:LEU:HD13	1:A:574:PRO:HG2	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:543:ARG:HH11	1:A:543:ARG:HG2	1.79	0.47
1:A:179:TYR:CD2	1:A:209:MET:SD	3.08	0.47
1:A:405:ARG:HG3	1:A:405:ARG:HH11	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:266:ARG:O	1:A:269:ARG:HG2	2.17	0.44
1:A:137:GLU:HA	1:A:147:LEU:O	2.18	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

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	398/447 (89%)	371 (93%)	24 (6%)	3 (1%)	27	20

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 ⓘ

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%)	42	41

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
1	A	390	ARG
1	A	416	VAL
1	A	440	LEU
1	A	498	LEU
1	A	546	LEU

Some 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 chains 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 carbohydrates 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, 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	410/447 (91%)	0.62	47 (11%) 5 6	10, 26, 73, 104	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	GLY	13.0
1	A	255	ARG	9.5
1	A	426	SER	9.0
1	A	283	GLY	7.6
1	A	165	ARG	7.0
1	A	415	ALA	6.8
1	A	430	SER	6.8
1	A	346	VAL	6.7
1	A	170	SER	6.3
1	A	402	LEU	6.0
1	A	280	THR	5.7
1	A	416	VAL	5.6
1	A	428	SER	5.6
1	A	429	ASP	5.2
1	A	281	GLU	4.9
1	A	427	GLY	4.9
1	A	403	ASN	4.6
1	A	509	ARG	4.1
1	A	410	MET	3.8
1	A	577	LEU	3.7
1	A	224	VAL	3.6
1	A	284	ARG	3.4
1	A	285	PRO	3.3
1	A	166	GLY	3.3
1	A	514	PRO	3.3
1	A	142	ARG	3.1
1	A	258	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	484	ARG	3.0
1	A	256	ALA	3.0
1	A	515	THR	2.9
1	A	431	GLY	2.8
1	A	167	ALA	2.8
1	A	171	SER	2.8
1	A	552	ARG	2.8
1	A	201	ASP	2.7
1	A	248	GLY	2.6
1	A	478	ARG	2.6
1	A	226	GLN	2.4
1	A	400	ASP	2.3
1	A	432	ALA	2.2
1	A	414	GLY	2.2
1	A	168	THR	2.2
1	A	203	ARG	2.1
1	A	519	GLU	2.1
1	A	361	SER	2.1
1	A	516	PRO	2.1
1	A	433	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.