



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:19 AM UTC

PDB ID : 2F5U / pdb_00002f5u
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

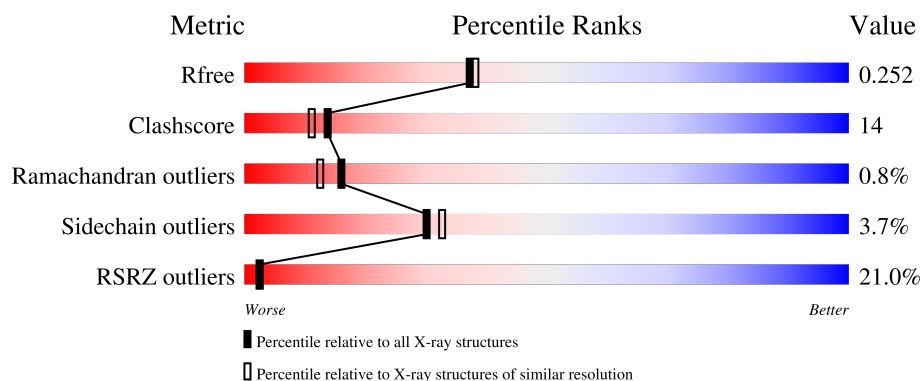
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	19% 65% 24% 8%

2 Entry composition

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

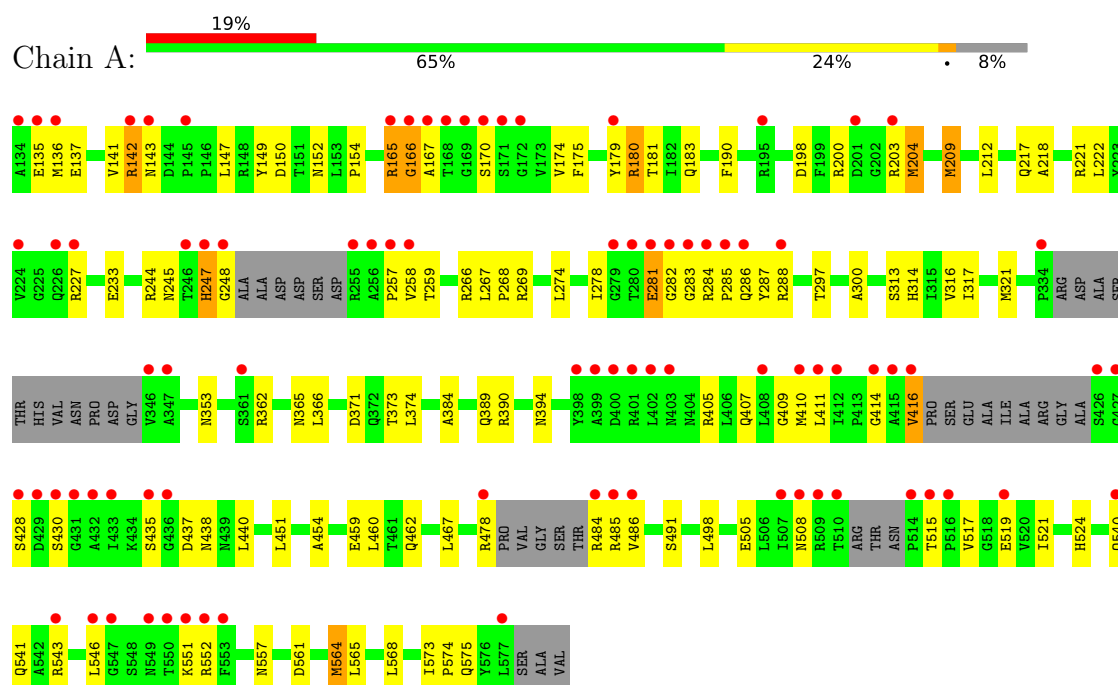
- Molecule 2 is water.

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

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 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



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) 99.9 (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%)	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 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.

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 [i](#)

5.1 Standard geometry [i](#)

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	3/3209 (0.1%)	0.88	10/4353 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	MET	SD-CE	-8.69	1.57	1.79
1	A	564	MET	SD-CE	-7.54	1.60	1.79
1	A	209	MET	SD-CE	-7.53	1.60	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	THR	N-CA-C	-6.75	104.00	111.36
1	A	437	ASP	N-CA-C	-5.89	104.48	112.26
1	A	150	ASP	N-CA-C	5.65	119.80	111.04
1	A	142	ARG	N-CA-C	5.49	117.97	111.33
1	A	285	PRO	N-CA-C	-5.28	102.40	110.95
1	A	190	PHE	CA-C-N	5.24	125.55	119.47
1	A	190	PHE	C-N-CA	5.24	125.55	119.47
1	A	313	SER	N-CA-C	5.14	119.56	113.28
1	A	300	ALA	N-CA-C	5.08	117.67	110.50
1	A	170	SER	N-CA-C	-5.06	106.94	113.02

There are no chirality outliers.

There are no planarity outliers.

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	3149	0	3144	91	0
2	A	188	0	0	4	0
All	All	3337	0	3144	91	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 14.

All (91) 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:180:ARG:CZ	1:A:204:MET:HE3	1.98	0.93
1:A:136:MET:HE3	1:A:451:LEU:HD23	1.57	0.85
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
1:A:353:ASN:HD22	1:A:366:LEU:H	1.33	0.76
1:A:180:ARG:NH2	1:A:204:MET:HE3	2.01	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:564:MET:HE3	1:A:568:LEU:HG	1.72	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:136:MET:HE3	1:A:451:LEU:CD2	2.28	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:407:GLN:HG3	1:A:410:MET:HE2	1.83	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:175:PHE:CE1	1:A:209:MET:HE3	2.37	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:218:ALA:O	1:A:524:HIS:HE1	1.88	0.57
1:A:183:GLN:NE2	1:A:204:MET:HE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ALA:HB3	1:A:460:LEU:HD23	1.87	0.57
1:A:407:GLN:HB2	1:A:410:MET:HE2	1.88	0.56
1:A:175:PHE:CD1	1:A:209:MET:HE3	2.41	0.56
1:A:414:GLY:C	1:A:416:VAL:H	2.12	0.56
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:407:GLN:CG	1:A:410:MET:HE2	2.38	0.53
1:A:407:GLN:CB	1:A:410:MET:HE2	2.39	0.52
1:A:142:ARG:HH22	1:A:438:ASN:CB	2.10	0.52
1:A:204:MET:HE2	1:A:204:MET:HA	1.92	0.52
1:A:136:MET:CE	1:A:451:LEU:HD23	2.35	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:136:MET:HE1	1:A:454:ALA:HB3	1.91	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: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
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: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: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:281:GLU:C	1:A:283:GLY:H	2.21	0.46
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:O	1:A:269:ARG:HG2	2.17	0.44
1:A:485:ARG:C	1:A:486:VAL:HG23	2.43	0.44
1:A:212:LEU:C	1:A:212:LEU:HD23	2.43	0.43
1:A:428:SER:C	1:A:430:SER:H	2.25	0.43
1:A:165:ARG:NE	1:A:166:GLY:H	2.10	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:317:ILE:HG22	1:A:321:MET:HE2	2.00	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: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:165:ARG:C	1:A:167:ALA:H	2.28	0.41
1:A:485:ARG:O	1:A:486:VAL:CG2	2.68	0.41
1:A:136:MET:HE1	1:A:454:ALA:CB	2.51	0.40
1:A:414:GLY:C	1:A:416:VAL:N	2.76	0.40
1:A:247:HIS:O	1:A:248:GLY:C	2.63	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	398/447 (89%)	371 (93%)	24 (6%)	3 (1%)	16 12

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%)	312 (96%)	12 (4%)	30	33

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	GLU
1	A	180	ARG
1	A	221	ARG
1	A	222	LEU
1	A	281	GLU
1	A	389	GLN
1	A	390	ARG
1	A	416	VAL
1	A	440	LEU
1	A	498	LEU
1	A	505	GLU
1	A	546	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	159	HIS
1	A	226	GLN
1	A	245	ASN
1	A	286	GLN
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	462	GLN
1	A	508	ASN

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Mol	Chain	Res	Type
1	A	524	HIS
1	A	549	ASN
1	A	575	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

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%)	0.94	86 (20%) 2 2	10, 26, 73, 104	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	SER	7.5
1	A	283	GLY	6.4
1	A	346	VAL	5.8
1	A	514	PRO	5.8
1	A	285	PRO	5.7
1	A	416	VAL	5.5
1	A	509	ARG	5.5
1	A	415	ALA	5.5
1	A	427	GLY	5.4
1	A	280	THR	5.3
1	A	428	SER	5.3
1	A	510	THR	5.2
1	A	282	GLY	5.0
1	A	547	GLY	4.8
1	A	552	ARG	4.7
1	A	402	LEU	4.7
1	A	284	ARG	4.6
1	A	165	ARG	4.5
1	A	248	GLY	4.2
1	A	170	SER	4.1
1	A	167	ALA	4.0
1	A	435	SER	4.0
1	A	410	MET	3.9
1	A	430	SER	3.9
1	A	478	ARG	3.8
1	A	168	THR	3.8
1	A	224	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	400	ASP	3.7
1	A	255	ARG	3.6
1	A	281	GLU	3.5
1	A	484	ARG	3.5
1	A	429	ASP	3.4
1	A	433	ILE	3.4
1	A	247	HIS	3.3
1	A	577	LEU	3.3
1	A	286	GLN	3.3
1	A	203	ARG	3.2
1	A	486	VAL	3.2
1	A	142	ARG	3.1
1	A	432	ALA	3.1
1	A	549	ASN	3.0
1	A	551	LYS	3.0
1	A	399	ALA	3.0
1	A	515	THR	3.0
1	A	519	GLU	3.0
1	A	169	GLY	2.9
1	A	550	THR	2.9
1	A	403	ASN	2.9
1	A	136	MET	2.8
1	A	227	ARG	2.8
1	A	485	ARG	2.7
1	A	414	GLY	2.7
1	A	401	ARG	2.7
1	A	279	GLY	2.7
1	A	134	ALA	2.6
1	A	516	PRO	2.6
1	A	431	GLY	2.6
1	A	553	PHE	2.6
1	A	398	TYR	2.6
1	A	412	ILE	2.5
1	A	546	LEU	2.5
1	A	258	VAL	2.5
1	A	195	ARG	2.5
1	A	226	GLN	2.5
1	A	288	ARG	2.4
1	A	166	GLY	2.4
1	A	143	ASN	2.4
1	A	246	THR	2.4
1	A	201	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	543	ARG	2.3
1	A	145	PRO	2.2
1	A	347	ALA	2.2
1	A	257	PRO	2.2
1	A	172	GLY	2.2
1	A	411	LEU	2.2
1	A	135	GLU	2.1
1	A	408	LEU	2.1
1	A	171	SER	2.1
1	A	436	GLY	2.1
1	A	540	GLN	2.1
1	A	334	PRO	2.1
1	A	507	ILE	2.1
1	A	256	ALA	2.1
1	A	179	TYR	2.0
1	A	361	SER	2.0
1	A	508	ASN	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 oligosaccharides 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.