



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:05 am GMT

PDB ID : 2PUS
Title : Unprecedented activation mechanism of a non-canonical RNA-dependent RNA polymerase
Authors : Garriga, D.; Navarro, A.; Querol-Audi, J.; Abaitua, F.; Rodriguez, J.F.; Verdaguier, N.
Deposited on : 2007-05-09
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

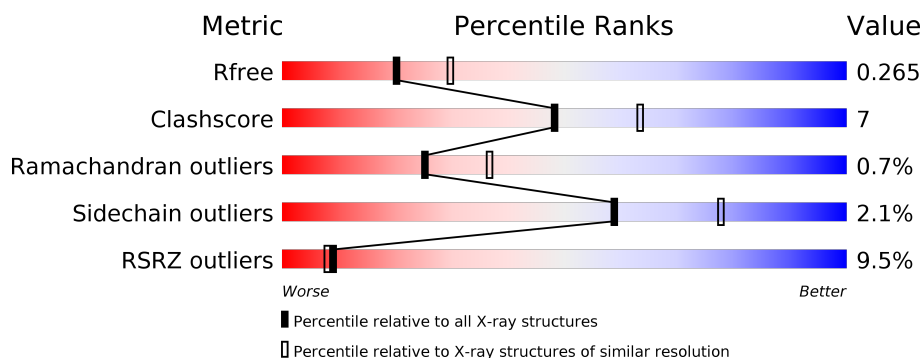
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	852	<div> <div>9%</div> <div>76%</div> <div>13%</div> <div>10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6185 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 IBDV VP1 RNA-dependant RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			5917	3786	1008	1101	22			

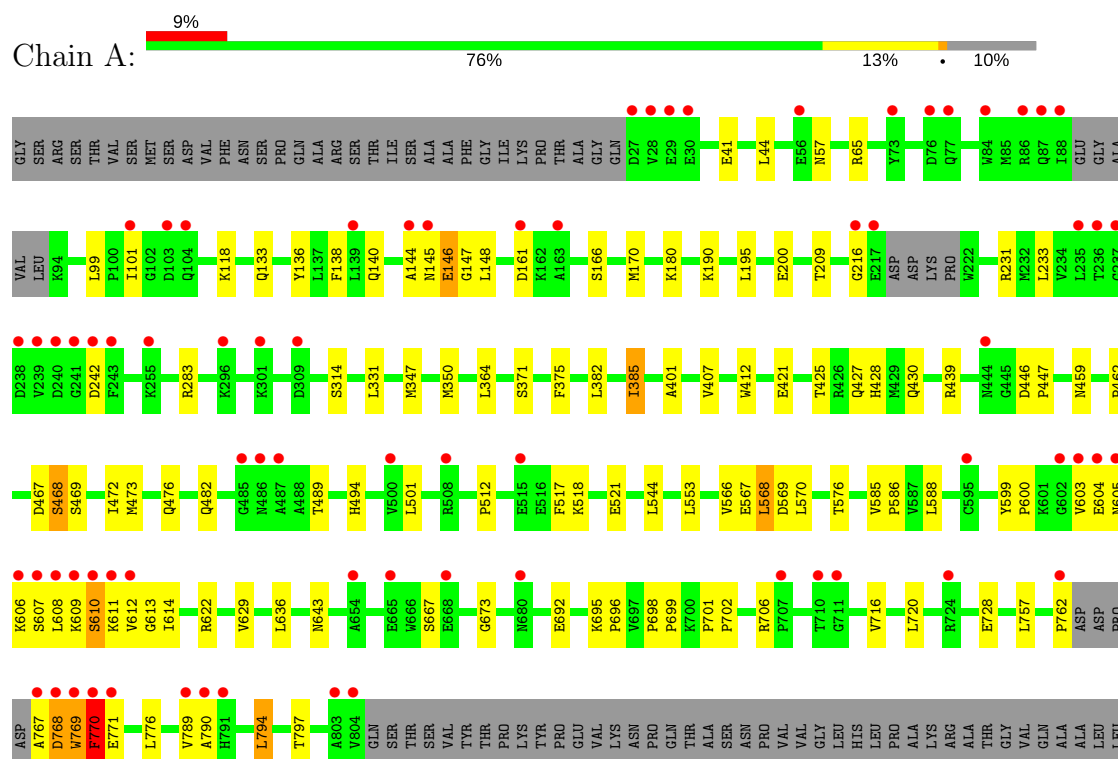
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	268	Total	O	0	0
			268	268		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: IBDV VP1 RNA-dependant RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.17Å 123.17Å 362.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.40 19.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.89-2.40) 95.4 (19.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.263 0.239 , 0.265	Depositor DCC
R_{free} test set	3094 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6185	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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

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	0.34	1/6055 (0.0%)	0.69	16/8233 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	ALA	N-CA	-8.52	1.29	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	SER	N-CA-CB	-18.96	82.06	110.50
1	A	607	SER	CB-CA-C	-16.00	79.70	110.10
1	A	606	LYS	CB-CA-C	-15.14	80.12	110.40
1	A	604	GLU	CB-CA-C	11.88	134.16	110.40
1	A	603	VAL	N-CA-C	-11.81	79.11	111.00
1	A	604	GLU	N-CA-CB	-9.25	93.95	110.60
1	A	767	ALA	N-CA-CB	8.66	122.22	110.10
1	A	605	ASN	N-CA-C	-8.45	88.19	111.00
1	A	567	GLU	N-CA-C	8.38	133.63	111.00
1	A	769	TRP	N-CA-C	-7.49	90.78	111.00
1	A	469	SER	N-CA-CB	-6.78	100.33	110.50
1	A	770	PHE	N-CA-CB	6.52	122.33	110.60
1	A	608	LEU	N-CA-C	6.29	127.99	111.00
1	A	762	PRO	N-CA-CB	6.10	110.62	103.30
1	A	567	GLU	CB-CA-C	-6.02	98.36	110.40
1	A	468	SER	N-CA-C	-5.14	97.12	111.00

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	5917	0	5868	81	0
2	A	268	0	0	6	0
All	All	6185	0	5868	81	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 7.

All (81) 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:138:PHE:CE1	1:A:144:ALA:HB1	1.80	1.16
1:A:138:PHE:CZ	1:A:144:ALA:HB1	1.95	1.01
1:A:138:PHE:CZ	1:A:144:ALA:CB	2.55	0.89
1:A:544:LEU:HD21	1:A:566:VAL:HG23	1.62	0.81
1:A:347:MET:HA	1:A:350:MET:HE2	1.63	0.80
1:A:609:LYS:CB	1:A:614:ILE:HG13	2.10	0.80
1:A:401:ALA:H	1:A:494:HIS:HD2	1.34	0.75
1:A:459:ASN:O	1:A:797:THR:HG21	1.86	0.74
1:A:145:ASN:ND2	1:A:146:GLU:OE2	2.21	0.73
1:A:576:THR:HG22	1:A:585:VAL:HG23	1.75	0.69
1:A:576:THR:CG2	1:A:585:VAL:HG23	2.22	0.68
1:A:145:ASN:O	1:A:147:GLY:N	2.27	0.68
1:A:364:LEU:HD21	1:A:385:ILE:HD12	1.77	0.67
1:A:144:ALA:HB3	2:A:988:HOH:O	1.94	0.66
1:A:412:TRP:CE2	1:A:568:LEU:HB3	2.30	0.66
1:A:769:TRP:O	1:A:771:GLU:N	2.28	0.66
1:A:553:LEU:HD13	1:A:585:VAL:HG11	1.77	0.65
1:A:401:ALA:H	1:A:494:HIS:CD2	2.14	0.64
1:A:768:ASP:O	2:A:931:HOH:O	2.15	0.63
1:A:144:ALA:CB	2:A:988:HOH:O	2.45	0.63
1:A:146:GLU:N	1:A:146:GLU:OE2	2.31	0.62
1:A:144:ALA:N	2:A:988:HOH:O	2.32	0.62
1:A:425:THR:H	1:A:428:HIS:HD2	1.49	0.61
1:A:412:TRP:NE1	1:A:568:LEU:HB3	2.16	0.60
1:A:65:ARG:H	1:A:476:GLN:HE22	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:SER:HB3	1:A:613:GLY:H	1.66	0.59
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.85	0.59
1:A:138:PHE:HB2	1:A:636:LEU:HD11	1.85	0.57
1:A:200:GLU:HB2	1:A:769:TRP:NE1	2.21	0.55
1:A:421:GLU:HG2	1:A:489:THR:HG21	1.88	0.55
1:A:145:ASN:O	1:A:146:GLU:C	2.45	0.54
1:A:462:PRO:HB2	1:A:794:LEU:HD21	1.91	0.53
1:A:136:TYR:O	1:A:140:GLN:HG2	2.09	0.52
1:A:190:LYS:HD3	1:A:195:LEU:HD21	1.91	0.52
1:A:472:ILE:O	1:A:472:ILE:HG23	2.09	0.52
1:A:427:GLN:HA	1:A:430:GLN:HG2	1.92	0.51
1:A:41:GLU:HG3	1:A:118:LYS:HD2	1.92	0.51
1:A:99:LEU:HB3	1:A:101:ILE:HD13	1.93	0.50
1:A:145:ASN:O	1:A:148:LEU:N	2.44	0.50
1:A:200:GLU:HG2	1:A:769:TRP:CD1	2.46	0.50
1:A:769:TRP:HE3	1:A:770:PHE:H	1.59	0.49
1:A:209:THR:O	1:A:371:SER:HB2	2.14	0.48
1:A:576:THR:HG23	1:A:585:VAL:HG23	1.94	0.48
1:A:706:ARG:HH12	1:A:728:GLU:HB3	1.78	0.48
1:A:200:GLU:CB	1:A:769:TRP:NE1	2.77	0.48
1:A:385:ILE:HG21	1:A:570:LEU:HD22	1.95	0.47
1:A:314:SER:O	1:A:468:SER:HB2	2.14	0.47
1:A:472:ILE:O	1:A:473:MET:HB2	2.15	0.47
1:A:692:GLU:HA	1:A:695:LYS:HD2	1.95	0.47
1:A:200:GLU:HB2	1:A:769:TRP:HE1	1.79	0.47
1:A:588:LEU:HD22	1:A:629:VAL:CG2	2.45	0.46
1:A:145:ASN:C	1:A:147:GLY:N	2.69	0.46
1:A:576:THR:HG23	1:A:585:VAL:CG2	2.46	0.45
1:A:133:GLN:HE21	1:A:643:ASN:HD22	1.63	0.45
1:A:512:PRO:HA	1:A:517:PHE:CG	2.52	0.45
1:A:698:PRO:HA	1:A:699:PRO:HD3	1.91	0.45
1:A:768:ASP:CG	1:A:768:ASP:O	2.54	0.45
1:A:44:LEU:HG	1:A:170:MET:SD	2.57	0.45
1:A:425:THR:H	1:A:428:HIS:CD2	2.31	0.44
1:A:609:LYS:C	1:A:611:LYS:N	2.68	0.44
1:A:716:VAL:O	1:A:720:LEU:HB2	2.17	0.44
1:A:170:MET:HG3	1:A:331:LEU:O	2.18	0.44
1:A:789:VAL:O	1:A:790:ALA:HB3	2.18	0.43
1:A:568:LEU:H	1:A:568:LEU:HG	1.38	0.43
1:A:609:LYS:O	1:A:611:LYS:N	2.52	0.43
1:A:382:LEU:HD13	1:A:586:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HH12	1:A:283:ARG:HH21	1.67	0.42
1:A:599:TYR:HA	1:A:600:PRO:HD2	1.93	0.42
1:A:695:LYS:HA	1:A:696:PRO:HD3	1.94	0.42
1:A:568:LEU:O	1:A:569:ASP:C	2.58	0.42
1:A:146:GLU:HG2	2:A:1081:HOH:O	2.20	0.41
1:A:421:GLU:HB3	1:A:482:GLN:O	2.20	0.41
1:A:518:LYS:O	1:A:521:GLU:HG2	2.20	0.41
1:A:701:PRO:HA	1:A:702:PRO:HD3	1.97	0.41
1:A:375:PHE:CE1	1:A:385:ILE:HD13	2.55	0.41
1:A:446:ASP:HA	1:A:447:PRO:HD3	1.90	0.41
1:A:41:GLU:CG	1:A:118:LYS:HD2	2.50	0.41
1:A:57:ASN:O	1:A:180:LYS:NZ	2.53	0.41
1:A:467:ASP:OD2	2:A:879:HOH:O	2.22	0.40
1:A:667:SER:O	1:A:673:GLY:HA3	2.22	0.40
1:A:588:LEU:HD22	1:A:629:VAL:HG21	2.02	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	757/852 (89%)	721 (95%)	31 (4%)	5 (1%)	25	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	770	PHE
1	A	216	GLY
1	A	242	ASP
1	A	612	VAL

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	627/730 (86%)	614 (98%)	13 (2%)	59 78

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

Mol	Chain	Res	Type
1	A	161	ASP
1	A	166	SER
1	A	233	LEU
1	A	385	ILE
1	A	407	VAL
1	A	439	ARG
1	A	501	LEU
1	A	568	LEU
1	A	610	SER
1	A	757	LEU
1	A	768	ASP
1	A	776	LEU
1	A	794	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	145	ASN
1	A	172	GLN
1	A	299	ASN
1	A	336	ASN
1	A	376	ASN
1	A	428	HIS
1	A	430	GLN
1	A	451	GLN
1	A	476	GLN
1	A	482	GLN
1	A	494	HIS

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 carbohydrates 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	765/852 (89%)	0.44	73 (9%) 9 8	20, 38, 53, 59	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	607	SER	9.6
1	A	608	LEU	9.2
1	A	216	GLY	7.7
1	A	242	ASP	7.4
1	A	73	TYR	6.5
1	A	144	ALA	6.4
1	A	609	LYS	6.4
1	A	604	GLU	6.2
1	A	611	LYS	6.0
1	A	612	VAL	5.7
1	A	238	ASP	5.5
1	A	236	THR	5.4
1	A	241	GLY	5.4
1	A	28	VAL	5.3
1	A	767	ALA	5.3
1	A	87	GLN	5.3
1	A	239	VAL	5.2
1	A	217	GLU	5.0
1	A	610	SER	5.0
1	A	790	ALA	4.9
1	A	603	VAL	4.9
1	A	605	ASN	4.8
1	A	240	ASP	4.7
1	A	27	ASP	4.4
1	A	237	GLY	4.3
1	A	606	LYS	4.3
1	A	789	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	486	ASN	4.2
1	A	243	PHE	4.1
1	A	602	GLY	4.0
1	A	88	ILE	3.7
1	A	86	ARG	3.6
1	A	485	GLY	3.5
1	A	235	LEU	3.5
1	A	161	ASP	3.5
1	A	770	PHE	3.3
1	A	724	ARG	3.3
1	A	762	PRO	3.2
1	A	804	VAL	3.2
1	A	76	ASP	3.2
1	A	29	GLU	3.2
1	A	487	ALA	3.1
1	A	145	ASN	3.1
1	A	711	GLY	3.0
1	A	768	ASP	2.9
1	A	595	CYS	2.8
1	A	791	HIS	2.7
1	A	77	GLN	2.7
1	A	680	ASN	2.7
1	A	444	ASN	2.6
1	A	515	GLU	2.5
1	A	668	GLU	2.5
1	A	301	LYS	2.4
1	A	654	ALA	2.4
1	A	104	GLN	2.4
1	A	101	ILE	2.4
1	A	769	TRP	2.4
1	A	771	GLU	2.3
1	A	296	LYS	2.3
1	A	30	GLU	2.3
1	A	255	LYS	2.2
1	A	803	ALA	2.2
1	A	707	PRO	2.2
1	A	103	ASP	2.2
1	A	56	GLU	2.2
1	A	163	ALA	2.2
1	A	84	TRP	2.2
1	A	500	VAL	2.1
1	A	139	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	710	THR	2.1
1	A	508	ARG	2.1
1	A	665	GLU	2.0
1	A	309	ASP	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 carbohydrates 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.