



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:01 AM GMT

PDB ID : 2Z83
Title : Crystal Structure of Catalytic Domain of Japanese Encephalitis Virus NS3
Helicase/Nucleoside Triphosphatase at a Resolution 1.8
Authors : Yamashita, T.
Deposited on : 2007-08-30
Resolution : 1.80 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

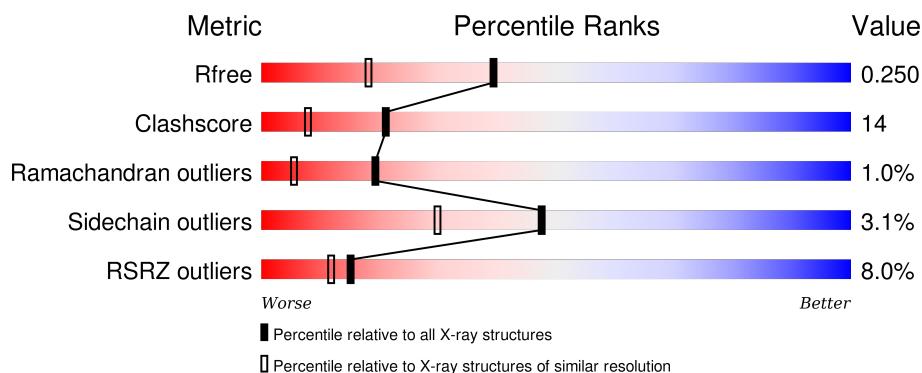
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	459	<div> <div>7%</div> <div>72%</div> <div>19%</div> <div>• 7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3775 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 Helicase/Nucleoside Triphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3364	2120	601	625	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MET	-	EXPRESSION TAG	UNP Q5NT71
A	168	ALA	-	EXPRESSION TAG	UNP Q5NT71
A	169	SER	-	EXPRESSION TAG	UNP Q5NT71
A	170	MET	-	EXPRESSION TAG	UNP Q5NT71
A	171	THR	-	EXPRESSION TAG	UNP Q5NT71
A	172	GLY	-	EXPRESSION TAG	UNP Q5NT71
A	173	GLY	-	EXPRESSION TAG	UNP Q5NT71
A	174	GLN	-	EXPRESSION TAG	UNP Q5NT71
A	175	GLN	-	EXPRESSION TAG	UNP Q5NT71
A	176	MET	-	EXPRESSION TAG	UNP Q5NT71
A	177	GLY	-	EXPRESSION TAG	UNP Q5NT71
A	178	ARG	-	EXPRESSION TAG	UNP Q5NT71
A	179	GLY	-	EXPRESSION TAG	UNP Q5NT71
A	180	SER	-	EXPRESSION TAG	UNP Q5NT71
A	620	HIS	-	EXPRESSION TAG	UNP Q5NT71
A	621	HIS	-	EXPRESSION TAG	UNP Q5NT71
A	622	HIS	-	EXPRESSION TAG	UNP Q5NT71
A	623	HIS	-	EXPRESSION TAG	UNP Q5NT71
A	624	HIS	-	EXPRESSION TAG	UNP Q5NT71
A	625	HIS	-	EXPRESSION TAG	UNP Q5NT71

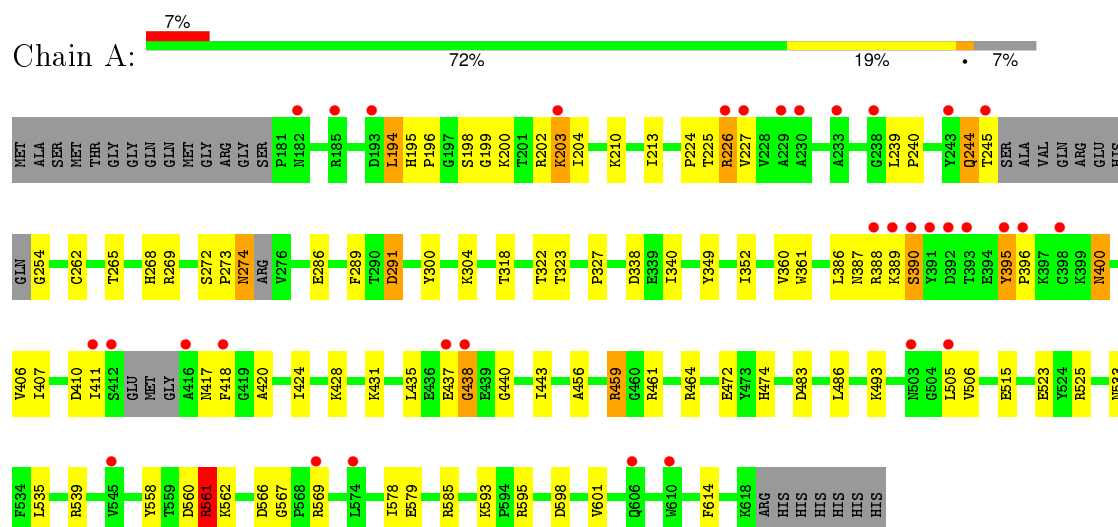
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	411	Total	O	0	0
			411	411		

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 errors 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 ($\text{RSRZ} > 2$). 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: Helicase/Nucleoside Triphosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.06 Å 68.02 Å 65.22 Å 90.00° 116.87° 90.00°	Depositor
Resolution (Å)	32.41 – 1.80 32.41 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.41-1.80) 99.9 (32.41-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 1.80 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.249 0.198 , 0.250	Depositor DCC
R_{free} test set	2154 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.1	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42729 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3775	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.72	0/3437	0.86	5/4655 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ARG	NE-CZ-NH2	-17.19	111.70	120.30
1	A	459	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	A	561	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	561	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	459	ARG	CD-NE-CZ	5.65	131.51	123.60

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	3364	0	3332	96	0
2	A	411	0	0	27	0
All	All	3775	0	3332	96	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 (96) 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:225:THR:O	2:A:1034:HOH:O	1.62	1.17
1:A:561:ARG:HH11	1:A:561:ARG:CG	1.57	1.16
1:A:561:ARG:HH11	1:A:561:ARG:HG3	1.13	1.10
1:A:274:ASN:HB3	2:A:648:HOH:O	1.49	1.09
1:A:226:ARG:H	1:A:226:ARG:HD2	1.26	0.97
1:A:569:ARG:HA	1:A:593:LYS:HD2	1.44	0.96
1:A:566:ASP:OD1	1:A:595:ARG:HD2	1.73	0.89
1:A:561:ARG:HG3	1:A:561:ARG:NH1	1.88	0.87
1:A:561:ARG:CG	1:A:561:ARG:NH1	2.34	0.86
1:A:338:ASP:OD2	1:A:474:HIS:HD2	1.61	0.83
1:A:268:HIS:HE1	2:A:707:HOH:O	1.63	0.82
1:A:226:ARG:HD2	1:A:226:ARG:N	1.95	0.81
1:A:561:ARG:HD3	1:A:614:PHE:O	1.81	0.81
1:A:194:LEU:HD21	1:A:204:ILE:HD12	1.64	0.79
1:A:327:PRO:O	1:A:459:ARG:NH2	2.16	0.79
1:A:400:ASN:HB2	2:A:743:HOH:O	1.83	0.78
1:A:291:ASP:OD2	2:A:1027:HOH:O	2.03	0.77
1:A:506:VAL:HG22	1:A:525:ARG:NH2	2.01	0.75
1:A:486:LEU:HD11	2:A:972:HOH:O	1.87	0.74
1:A:322:THR:HA	2:A:987:HOH:O	1.90	0.70
1:A:244:GLN:O	1:A:245:THR:HG22	1.90	0.70
1:A:561:ARG:HH11	1:A:561:ARG:HG2	1.50	0.69
1:A:274:ASN:CB	2:A:648:HOH:O	2.20	0.67
1:A:533:ASN:ND2	1:A:558:TYR:H	1.92	0.67
1:A:198:SER:HB2	2:A:1028:HOH:O	1.96	0.66
1:A:515:GLU:HG3	2:A:967:HOH:O	1.94	0.65
1:A:323:THR:OG1	2:A:731:HOH:O	2.14	0.65
1:A:386:LEU:HD12	1:A:406:VAL:CG1	2.28	0.63
1:A:523:GLU:HG3	2:A:891:HOH:O	1.99	0.62
1:A:578:ILE:HD12	1:A:579:GLU:H	1.64	0.62
1:A:428:LYS:CE	2:A:966:HOH:O	2.47	0.61
1:A:268:HIS:CE1	2:A:707:HOH:O	2.46	0.61
1:A:417:ASN:HA	1:A:461:ARG:HH21	1.67	0.60
1:A:213:ILE:HD13	1:A:240:PRO:HD2	1.82	0.59
1:A:566:ASP:OD1	1:A:595:ARG:CD	2.49	0.59
1:A:272:SER:HB3	1:A:539:ARG:NH2	2.18	0.58
1:A:431:LYS:HB3	1:A:486:LEU:HD22	1.85	0.57
1:A:338:ASP:OD2	1:A:474:HIS:CD2	2.51	0.57
1:A:505:LEU:O	2:A:992:HOH:O	2.17	0.56
1:A:386:LEU:HD12	1:A:406:VAL:HG11	1.87	0.55
1:A:210:LYS:HG2	1:A:239:LEU:HD21	1.88	0.55
1:A:428:LYS:HE3	2:A:966:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:HIS:HD2	1:A:196:PRO:O	1.91	0.54
1:A:210:LYS:CG	1:A:239:LEU:HD21	2.38	0.53
1:A:388:ARG:NH1	1:A:390:SER:HB3	2.24	0.53
1:A:506:VAL:HG22	1:A:525:ARG:HH22	1.71	0.52
1:A:472:GLU:OE1	1:A:474:HIS:HE1	1.93	0.52
1:A:289:PHE:HB3	2:A:780:HOH:O	2.08	0.52
1:A:567:GLY:O	1:A:593:LYS:HE2	2.10	0.52
1:A:387:ASN:HD21	1:A:389:LYS:HE3	1.75	0.52
1:A:349:TYR:HB3	1:A:352:ILE:HD12	1.92	0.51
1:A:202:ARG:HB3	1:A:202:ARG:NH1	2.25	0.51
1:A:417:ASN:O	1:A:418:PHE:CD1	2.63	0.51
1:A:387:ASN:O	1:A:390:SER:HB2	2.10	0.51
1:A:386:LEU:HD12	1:A:406:VAL:HG13	1.93	0.51
1:A:395:TYR:HB3	1:A:396:PRO:HD3	1.92	0.51
1:A:340:ILE:HD12	1:A:424:ILE:HG23	1.93	0.51
1:A:387:ASN:HD22	1:A:388:ARG:H	1.59	0.50
1:A:199:GLY:O	1:A:203:LYS:HG2	2.11	0.50
1:A:200:LYS:NZ	1:A:286:GLU:OE2	2.42	0.48
1:A:535:LEU:HD13	1:A:539:ARG:HH22	1.78	0.48
1:A:483:ASP:HB2	1:A:486:LEU:HG	1.96	0.48
1:A:289:PHE:CB	2:A:780:HOH:O	2.62	0.47
1:A:386:LEU:HD21	1:A:395:TYR:HA	1.95	0.47
1:A:224:PRO:HG3	1:A:286:GLU:HB2	1.95	0.47
1:A:598:ASP:O	1:A:601:VAL:HG22	2.15	0.47
1:A:194:LEU:HB2	2:A:1018:HOH:O	2.14	0.46
1:A:245:THR:CG2	1:A:262:CYS:H	2.29	0.46
1:A:272:SER:HB2	1:A:273:PRO:HD2	1.96	0.46
1:A:265:THR:O	1:A:269:ARG:HG3	2.15	0.46
1:A:390:SER:O	1:A:395:TYR:HB2	2.16	0.46
1:A:396:PRO:HD3	2:A:1026:HOH:O	2.14	0.46
1:A:388:ARG:HA	1:A:388:ARG:HD3	1.64	0.46
1:A:300:TYR:OH	1:A:304:LYS:HE3	2.16	0.45
1:A:561:ARG:CD	1:A:614:PHE:O	2.61	0.45
1:A:226:ARG:CD	1:A:226:ARG:N	2.73	0.45
1:A:464:ARG:HB2	2:A:936:HOH:O	2.17	0.45
1:A:361:TRP:HB3	1:A:407:ILE:HD13	1.99	0.45
1:A:417:ASN:HA	1:A:461:ARG:NH2	2.32	0.44
1:A:585:ARG:NE	2:A:1005:HOH:O	2.50	0.44
1:A:506:VAL:CG2	1:A:525:ARG:HH22	2.32	0.43
1:A:400:ASN:HB3	2:A:748:HOH:O	2.18	0.42
1:A:318:THR:HG21	1:A:456:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:SER:OG	1:A:274:ASN:ND2	2.52	0.42
1:A:505:LEU:HD23	2:A:954:HOH:O	2.18	0.42
1:A:360:VAL:HG23	1:A:420:ALA:HB2	2.01	0.42
1:A:387:ASN:ND2	1:A:388:ARG:H	2.18	0.42
1:A:254:GLY:N	2:A:806:HOH:O	2.53	0.42
1:A:194:LEU:HD23	1:A:200:LYS:HB3	2.02	0.41
1:A:435:LEU:HD11	1:A:443:ILE:HD13	2.02	0.41
1:A:389:LYS:HB2	2:A:751:HOH:O	2.21	0.41
1:A:493:LYS:HG3	2:A:1004:HOH:O	2.19	0.41
1:A:431:LYS:HB3	1:A:486:LEU:CD2	2.49	0.40
1:A:560:ASP:OD1	1:A:562:LYS:HG3	2.22	0.40
1:A:202:ARG:HB3	1:A:202:ARG:HH11	1.86	0.40
1:A:438:GLY:C	1:A:440:GLY:H	2.23	0.40

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	418/459 (91%)	398 (95%)	16 (4%)	4 (1%)	19 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	SER
1	A	411	ILE
1	A	437	GLU
1	A	438	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	355/381 (93%)	344 (97%)	11 (3%)	47 30

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	LEU
1	A	203	LYS
1	A	226	ARG
1	A	227	VAL
1	A	244	GLN
1	A	274	ASN
1	A	291	ASP
1	A	395	TYR
1	A	400	ASN
1	A	410	ASP
1	A	561	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	274	ASN
1	A	288	HIS
1	A	400	ASN
1	A	474	HIS
1	A	533	ASN

5.3.3 RNA ⓘ

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	426/459 (92%)	0.42	34 (7%) 15 12	23, 36, 60, 81	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	TYR	8.3
1	A	393	THR	7.8
1	A	392	ASP	7.0
1	A	503	ASN	5.0
1	A	412	SER	4.8
1	A	229	ALA	4.6
1	A	245	THR	4.5
1	A	418	PHE	4.4
1	A	390	SER	3.9
1	A	395	TYR	3.9
1	A	226	ARG	3.8
1	A	437	GLU	3.8
1	A	610	TRP	3.5
1	A	505	LEU	3.5
1	A	238	GLY	3.2
1	A	389	LYS	3.2
1	A	227	VAL	3.2
1	A	569	ARG	3.1
1	A	230	ALA	3.1
1	A	396	PRO	3.0
1	A	398	CYS	2.9
1	A	438	GLY	2.8
1	A	388	ARG	2.7
1	A	185	ARG	2.6
1	A	193	ASP	2.5
1	A	182	ASN	2.5
1	A	574	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	416	ALA	2.1
1	A	545	VAL	2.1
1	A	243	TYR	2.1
1	A	203	LYS	2.1
1	A	411	ILE	2.1
1	A	606	GLN	2.1
1	A	233	ALA	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.