



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:08 AM UTC

PDB ID : 4UV6 / pdb_00004uv6
Title : Crystal structure of apical membrane antigen 1 from Plasmodium knowlesi
Authors : Vulliez-Le Normand, B.; Saul, F.A.; Bentley, G.A.
Deposited on : 2014-08-04
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

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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

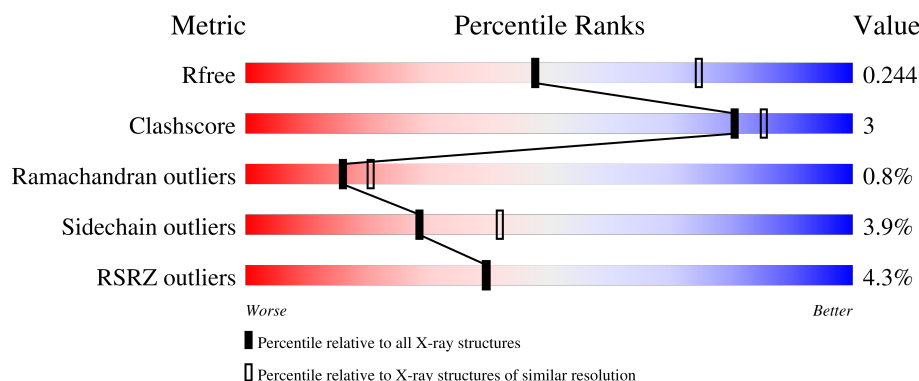
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	370	2% 79% 11% 9%
1	B	370	5% 78% 12% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5809 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 APICAL MEROZOITE ANTIGEN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2704	1700	467	521	16			
1	B	336	Total	C	N	O	S	0	2	0
			2719	1709	473	522	15			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLU	-	cloning artifact	UNP B3L5E1
A	42	PHE	-	cloning artifact	UNP B3L5E1
A	388	GLY	-	cloning artifact	UNP B3L5E1
A	389	LEU	-	expression tag	UNP B3L5E1
A	390	GLU	-	expression tag	UNP B3L5E1
A	391	GLN	-	expression tag	UNP B3L5E1
A	392	LYS	-	expression tag	UNP B3L5E1
A	393	LEU	-	expression tag	UNP B3L5E1
A	394	ILE	-	expression tag	UNP B3L5E1
A	395	SER	-	expression tag	UNP B3L5E1
A	396	GLU	-	expression tag	UNP B3L5E1
A	397	GLU	-	expression tag	UNP B3L5E1
A	398	ASP	-	expression tag	UNP B3L5E1
A	399	LEU	-	expression tag	UNP B3L5E1
A	400	ASN	-	expression tag	UNP B3L5E1
A	401	SER	-	expression tag	UNP B3L5E1
A	402	ALA	-	expression tag	UNP B3L5E1
A	403	VAL	-	expression tag	UNP B3L5E1
A	404	ASP	-	expression tag	UNP B3L5E1
A	405	HIS	-	expression tag	UNP B3L5E1
A	406	HIS	-	expression tag	UNP B3L5E1
A	407	HIS	-	expression tag	UNP B3L5E1
A	408	HIS	-	expression tag	UNP B3L5E1
A	409	HIS	-	expression tag	UNP B3L5E1
A	410	HIS	-	expression tag	UNP B3L5E1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	107	LYS	ASN	engineered mutation	UNP B3L5E1
A	178	ASN	SER	engineered mutation	UNP B3L5E1
A	189	GLU	ASN	engineered mutation	UNP B3L5E1
A	240	ARG	SER	engineered mutation	UNP B3L5E1
B	41	GLU	-	cloning artifact	UNP B3L5E1
B	42	PHE	-	cloning artifact	UNP B3L5E1
B	388	GLY	-	cloning artifact	UNP B3L5E1
B	389	LEU	-	expression tag	UNP B3L5E1
B	390	GLU	-	expression tag	UNP B3L5E1
B	391	GLN	-	expression tag	UNP B3L5E1
B	392	LYS	-	expression tag	UNP B3L5E1
B	393	LEU	-	expression tag	UNP B3L5E1
B	394	ILE	-	expression tag	UNP B3L5E1
B	395	SER	-	expression tag	UNP B3L5E1
B	396	GLU	-	expression tag	UNP B3L5E1
B	397	GLU	-	expression tag	UNP B3L5E1
B	398	ASP	-	expression tag	UNP B3L5E1
B	399	LEU	-	expression tag	UNP B3L5E1
B	400	ASN	-	expression tag	UNP B3L5E1
B	401	SER	-	expression tag	UNP B3L5E1
B	402	ALA	-	expression tag	UNP B3L5E1
B	403	VAL	-	expression tag	UNP B3L5E1
B	404	ASP	-	expression tag	UNP B3L5E1
B	405	HIS	-	expression tag	UNP B3L5E1
B	406	HIS	-	expression tag	UNP B3L5E1
B	407	HIS	-	expression tag	UNP B3L5E1
B	408	HIS	-	expression tag	UNP B3L5E1
B	409	HIS	-	expression tag	UNP B3L5E1
B	410	HIS	-	expression tag	UNP B3L5E1
B	107	LYS	ASN	engineered mutation	UNP B3L5E1
B	178	ASN	SER	engineered mutation	UNP B3L5E1
B	189	GLU	ASN	engineered mutation	UNP B3L5E1
B	240	ARG	SER	engineered mutation	UNP B3L5E1

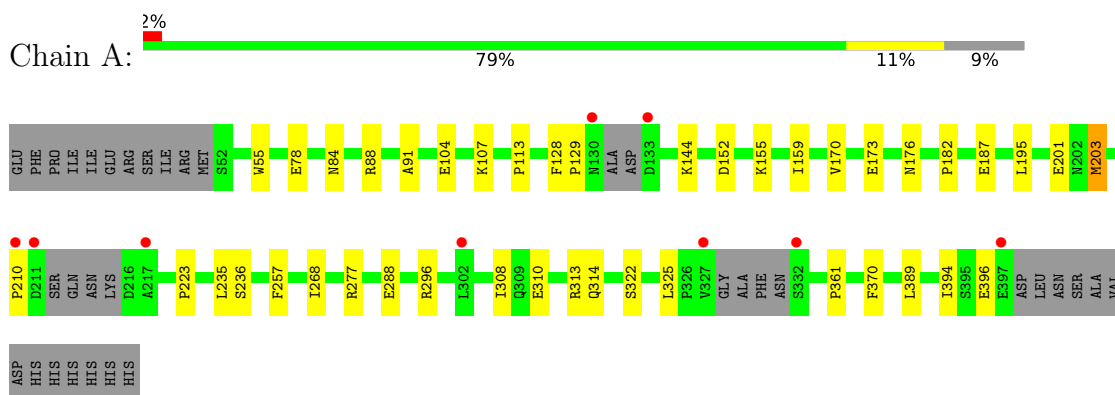
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	213	Total O 213 213	0	0
2	B	173	Total O 173 173	0	0

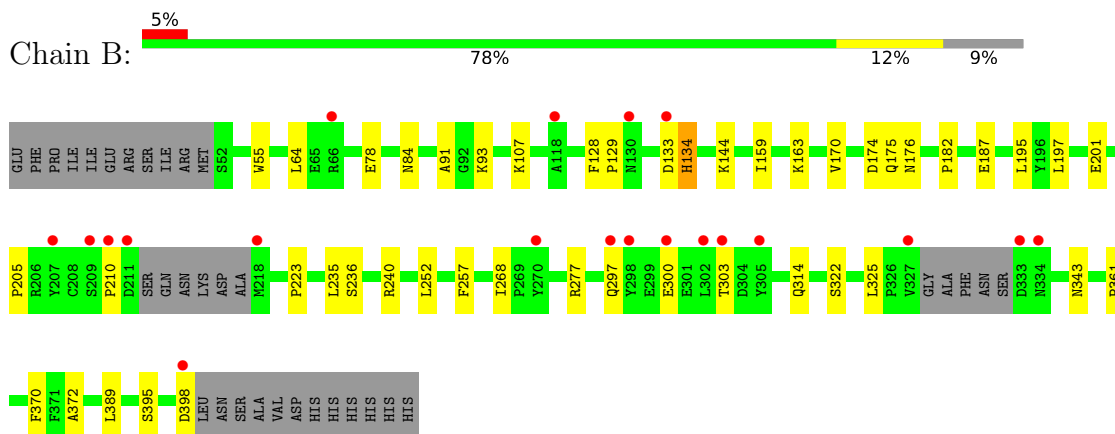
3 Residue-property plots [i](#)

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: APICAL MEROZOITE ANTIGEN 1



• Molecule 1: APICAL MEROZOITE ANTIGEN 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.32Å 105.70Å 104.75Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	47.09 – 2.45 47.09 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.09-2.45) 97.1 (47.09-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.171 , 0.227 0.188 , 0.244	Depositor DCC
R_{free} test set	843 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5809	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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	0.85	1/2763 (0.0%)	1.27	10/3726 (0.3%)
1	B	0.82	0/2785	1.26	8/3757 (0.2%)
All	All	0.84	1/5548 (0.0%)	1.27	18/7483 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	ARG	CA-C	-5.10	1.46	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	GLU	N-CA-C	-7.22	103.44	112.90
1	B	174	ASP	CA-CB-CG	5.75	118.36	112.60
1	B	129	PRO	CA-C-N	-5.53	113.70	121.72
1	B	129	PRO	C-N-CA	-5.53	113.70	121.72
1	B	268	ILE	N-CA-C	-5.45	103.61	108.95
1	B	84	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	308	ILE	CA-C-N	5.31	127.39	120.28
1	A	308	ILE	C-N-CA	5.31	127.39	120.28
1	A	396	GLU	CA-C-N	5.28	131.21	121.70
1	A	396	GLU	C-N-CA	5.28	131.21	121.70
1	A	84	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	268	ILE	N-CA-C	-5.16	103.89	108.95
1	B	144	LYS	CA-C-N	5.09	127.37	120.65
1	B	144	LYS	C-N-CA	5.09	127.37	120.65
1	B	370	PHE	N-CA-C	5.08	117.61	110.14
1	A	370	PHE	N-CA-C	5.01	117.51	110.14
1	A	144	LYS	CA-C-N	5.00	127.26	120.65
1	A	144	LYS	C-N-CA	5.00	127.26	120.65

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	2704	0	2582	15	0
1	B	2719	0	2601	13	0
2	A	213	0	0	0	0
2	B	173	0	0	1	0
All	All	5809	0	5183	28	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 3.

All (28) 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:288:GLU:HG3	1:A:296:ARG:HH22	1.62	0.65
1:A:78:GLU:HB2	1:A:91:ALA:HB2	1.78	0.64
1:A:201:GLU:HB2	1:A:223:PRO:HD3	1.80	0.63
1:B:78:GLU:HB2	1:B:91:ALA:HB2	1.80	0.63
1:B:322:SER:HA	1:B:325:LEU:HD12	1.82	0.61
1:A:322:SER:HA	1:A:325:LEU:HD12	1.82	0.61
1:B:201:GLU:HB2	1:B:223:PRO:HD3	1.83	0.60
1:A:55:TRP:CD2	1:A:389:LEU:HD11	2.46	0.50
1:B:182:PRO:HG2	1:B:195:LEU:HB2	1.94	0.49
1:B:55:TRP:CD2	1:B:389:LEU:HD11	2.48	0.47
1:A:104:GLU:HG3	1:A:203:MET:HE1	1.96	0.47
1:A:182:PRO:HG2	1:A:195:LEU:HB2	1.95	0.47
1:A:113:PRO:HB3	1:A:129:PRO:HA	1.97	0.46
1:A:257:PHE:HB3	1:A:361:PRO:HB3	1.98	0.46
1:B:257:PHE:HB3	1:B:361:PRO:HB3	1.99	0.44
1:B:300:GLU:HB2	1:B:303:THR:HG23	1.99	0.44
1:B:252:LEU:HB2	1:B:372:ALA:HB3	2.00	0.43
1:A:288:GLU:HG3	1:A:296:ARG:NH2	2.30	0.43
1:A:159:ILE:HG23	1:A:235:LEU:HD21	2.01	0.43
1:A:310:GLU:OE1	1:A:313:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD12	1:B:343:ASN:HB3	2.03	0.41
1:A:152:ASP:O	1:A:155:LYS:HG2	2.21	0.41
1:B:93:LYS:HB3	1:B:240:ARG:HG3	2.03	0.41
1:B:159:ILE:HG23	1:B:235:LEU:HD21	2.01	0.41
1:B:134:HIS:HB3	2:B:2055:HOH:O	2.19	0.41
1:B:205:PRO:HD3	1:B:297:GLN:HB3	2.01	0.41
1:A:152:ASP:HA	1:A:155:LYS:HE3	2.03	0.40
1:A:104:GLU:CG	1:A:203:MET:HE1	2.51	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	328/370 (89%)	311 (95%)	15 (5%)	2 (1%)	21	27
1	B	332/370 (90%)	314 (95%)	15 (4%)	3 (1%)	14	17
All	All	660/740 (89%)	625 (95%)	30 (4%)	5 (1%)	16	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	B	176	ASN
1	A	210	PRO
1	B	134	HIS
1	B	210	PRO

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	294/325 (90%)	284 (97%)	10 (3%)	32	47
1	B	295/325 (91%)	282 (96%)	13 (4%)	25	37
All	All	589/650 (91%)	566 (96%)	23 (4%)	28	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LYS
1	A	128	PHE
1	A	170	VAL
1	A	173	GLU
1	A	187	GLU
1	A	203	MET
1	A	236	SER
1	A	277	ARG
1	A	314	GLN
1	A	394	ILE
1	B	107	LYS
1	B	128	PHE
1	B	133	ASP
1	B	163	LYS
1	B	170	VAL
1	B	175	GLN
1	B	187	GLU
1	B	197	LEU
1	B	236	SER
1	B	277	ARG
1	B	314	GLN
1	B	395	SER
1	B	398	ASP

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	142	ASN
1	A	150	ASN
1	A	231	ASN
1	A	283	ASN
1	A	294	GLN
1	A	297	GLN
1	A	315	ASN
1	A	316	ASN
1	A	366	ASN
1	B	142	ASN
1	B	150	ASN
1	B	231	ASN
1	B	283	ASN
1	B	294	GLN
1	B	297	GLN
1	B	316	ASN

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 oligosaccharides 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	336/370 (90%)	-0.17	9 (2%) 56 57	18, 36, 76, 106	0
1	B	336/370 (90%)	0.13	20 (5%) 27 24	22, 42, 90, 118	2 (0%)
All	All	672/740 (90%)	-0.02	29 (4%) 40 39	18, 40, 82, 118	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	VAL	4.8
1	B	327	VAL	4.6
1	B	302	LEU	4.4
1	A	397	GLU	4.2
1	A	302	LEU	3.7
1	B	210	PRO	3.6
1	B	207	TYR	3.5
1	B	305	TYR	3.3
1	B	218	MET	2.9
1	B	66[A]	ARG	2.9
1	A	130	ASN	2.9
1	B	297	GLN	2.9
1	B	303	THR	2.8
1	A	210	PRO	2.7
1	B	398	ASP	2.6
1	B	300	GLU	2.5
1	B	118	ALA	2.5
1	A	217	ALA	2.5
1	B	334	ASN	2.4
1	A	332	SER	2.3
1	A	211	ASP	2.3
1	B	333	ASP	2.3
1	B	211	ASP	2.3
1	B	130	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	209	SER	2.2
1	A	133	ASP	2.2
1	B	133	ASP	2.2
1	B	298	TYR	2.2
1	B	270	TYR	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.