



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:12 AM GMT

PDB ID : 4F6C
Title : Crystal structure of Aureusimine biosynthetic cluster reductase domain
Authors : Mok, M.; Junop, M.
Deposited on : 2012-05-14
Resolution : 2.81 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>

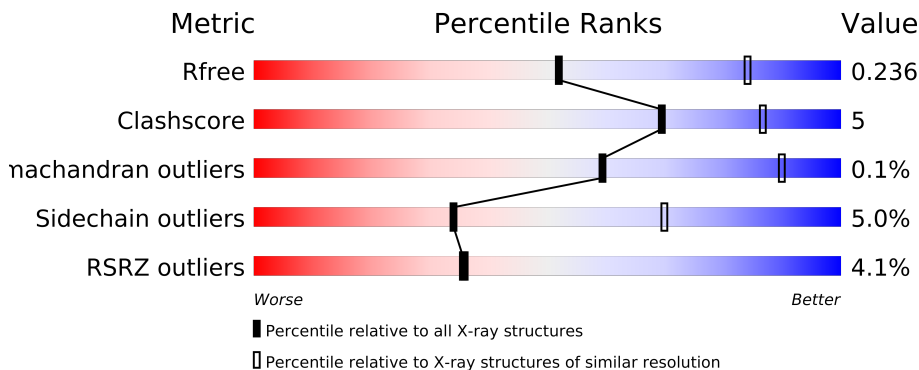
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.81 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	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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. 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	427	
1	B	427	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5545 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 AusA reductase domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	Se	0	0	0
			2740	1748	461	514	3	14			
1	B	368	Total	C	N	O	S	Se	0	0	0
			2801	1790	473	520	3	15			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1976	MSE	-	EXPRESSION TAG	UNP Q99X42
A	1977	GLY	-	EXPRESSION TAG	UNP Q99X42
A	1978	SER	-	EXPRESSION TAG	UNP Q99X42
A	1979	SER	-	EXPRESSION TAG	UNP Q99X42
A	1980	HIS	-	EXPRESSION TAG	UNP Q99X42
A	1981	HIS	-	EXPRESSION TAG	UNP Q99X42
A	1982	HIS	-	EXPRESSION TAG	UNP Q99X42
A	1983	HIS	-	EXPRESSION TAG	UNP Q99X42
A	1984	HIS	-	EXPRESSION TAG	UNP Q99X42
A	1985	HIS	-	EXPRESSION TAG	UNP Q99X42
A	1986	SER	-	EXPRESSION TAG	UNP Q99X42
A	1987	SER	-	EXPRESSION TAG	UNP Q99X42
A	1988	GLY	-	EXPRESSION TAG	UNP Q99X42
A	1989	LEU	-	EXPRESSION TAG	UNP Q99X42
A	1990	VAL	-	EXPRESSION TAG	UNP Q99X42
A	1991	PRO	-	EXPRESSION TAG	UNP Q99X42
A	1992	ARG	-	EXPRESSION TAG	UNP Q99X42
A	1993	GLY	-	EXPRESSION TAG	UNP Q99X42
A	1994	SER	-	EXPRESSION TAG	UNP Q99X42
A	1995	HIS	-	EXPRESSION TAG	UNP Q99X42
A	1996	MSE	-	EXPRESSION TAG	UNP Q99X42
A	1997	ALA	-	EXPRESSION TAG	UNP Q99X42
A	1998	SER	-	EXPRESSION TAG	UNP Q99X42
A	1999	MSE	-	EXPRESSION TAG	UNP Q99X42
A	2000	THR	-	EXPRESSION TAG	UNP Q99X42

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2001	GLY	-	EXPRESSION TAG	UNP Q99X42
A	2002	GLY	-	EXPRESSION TAG	UNP Q99X42
A	2003	GLN	-	EXPRESSION TAG	UNP Q99X42
A	2004	GLN	-	EXPRESSION TAG	UNP Q99X42
A	2005	MSE	-	EXPRESSION TAG	UNP Q99X42
A	2006	GLY	-	EXPRESSION TAG	UNP Q99X42
A	2007	ARG	-	EXPRESSION TAG	UNP Q99X42
A	2008	ASP	-	EXPRESSION TAG	UNP Q99X42
A	2009	PRO	-	EXPRESSION TAG	UNP Q99X42
A	2392	ALA	-	EXPRESSION TAG	UNP Q99X42
A	2393	ALA	-	EXPRESSION TAG	UNP Q99X42
A	2394	ALA	-	EXPRESSION TAG	UNP Q99X42
A	2395	LEU	-	EXPRESSION TAG	UNP Q99X42
A	2396	GLU	-	EXPRESSION TAG	UNP Q99X42
A	2397	HIS	-	EXPRESSION TAG	UNP Q99X42
A	2398	HIS	-	EXPRESSION TAG	UNP Q99X42
A	2399	HIS	-	EXPRESSION TAG	UNP Q99X42
A	2400	HIS	-	EXPRESSION TAG	UNP Q99X42
A	2401	HIS	-	EXPRESSION TAG	UNP Q99X42
A	2402	HIS	-	EXPRESSION TAG	UNP Q99X42
B	1976	MSE	-	EXPRESSION TAG	UNP Q99X42
B	1977	GLY	-	EXPRESSION TAG	UNP Q99X42
B	1978	SER	-	EXPRESSION TAG	UNP Q99X42
B	1979	SER	-	EXPRESSION TAG	UNP Q99X42
B	1980	HIS	-	EXPRESSION TAG	UNP Q99X42
B	1981	HIS	-	EXPRESSION TAG	UNP Q99X42
B	1982	HIS	-	EXPRESSION TAG	UNP Q99X42
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B	1986	SER	-	EXPRESSION TAG	UNP Q99X42
B	1987	SER	-	EXPRESSION TAG	UNP Q99X42
B	1988	GLY	-	EXPRESSION TAG	UNP Q99X42
B	1989	LEU	-	EXPRESSION TAG	UNP Q99X42
B	1990	VAL	-	EXPRESSION TAG	UNP Q99X42
B	1991	PRO	-	EXPRESSION TAG	UNP Q99X42
B	1992	ARG	-	EXPRESSION TAG	UNP Q99X42
B	1993	GLY	-	EXPRESSION TAG	UNP Q99X42
B	1994	SER	-	EXPRESSION TAG	UNP Q99X42
B	1995	HIS	-	EXPRESSION TAG	UNP Q99X42
B	1996	MSE	-	EXPRESSION TAG	UNP Q99X42
B	1997	ALA	-	EXPRESSION TAG	UNP Q99X42

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1998	SER	-	EXPRESSION TAG	UNP Q99X42
B	1999	MSE	-	EXPRESSION TAG	UNP Q99X42
B	2000	THR	-	EXPRESSION TAG	UNP Q99X42
B	2001	GLY	-	EXPRESSION TAG	UNP Q99X42
B	2002	GLY	-	EXPRESSION TAG	UNP Q99X42
B	2003	GLN	-	EXPRESSION TAG	UNP Q99X42
B	2004	GLN	-	EXPRESSION TAG	UNP Q99X42
B	2005	MSE	-	EXPRESSION TAG	UNP Q99X42
B	2006	GLY	-	EXPRESSION TAG	UNP Q99X42
B	2007	ARG	-	EXPRESSION TAG	UNP Q99X42
B	2008	ASP	-	EXPRESSION TAG	UNP Q99X42
B	2009	PRO	-	EXPRESSION TAG	UNP Q99X42
B	2392	ALA	-	EXPRESSION TAG	UNP Q99X42
B	2393	ALA	-	EXPRESSION TAG	UNP Q99X42
B	2394	ALA	-	EXPRESSION TAG	UNP Q99X42
B	2395	LEU	-	EXPRESSION TAG	UNP Q99X42
B	2396	GLU	-	EXPRESSION TAG	UNP Q99X42
B	2397	HIS	-	EXPRESSION TAG	UNP Q99X42
B	2398	HIS	-	EXPRESSION TAG	UNP Q99X42
B	2399	HIS	-	EXPRESSION TAG	UNP Q99X42
B	2400	HIS	-	EXPRESSION TAG	UNP Q99X42
B	2401	HIS	-	EXPRESSION TAG	UNP Q99X42
B	2402	HIS	-	EXPRESSION TAG	UNP Q99X42

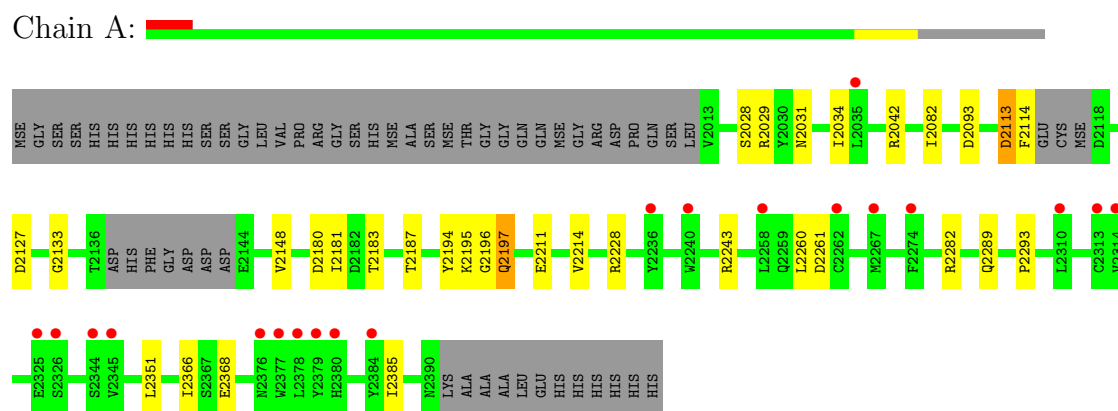
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	B	3	Total O 3 3	0	0

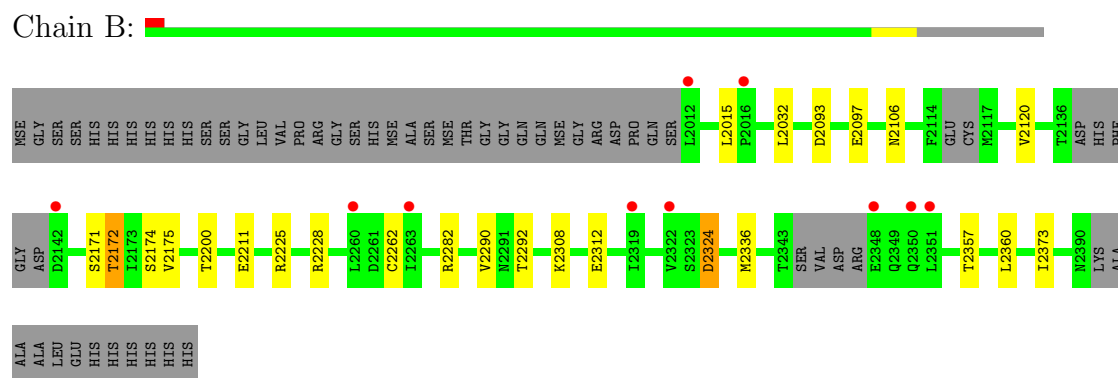
3 Residue-property plots

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 ($RSRZ > 2$). 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: AusA reductase domain protein



- Molecule 1: AusA reductase domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.70Å 106.45Å 124.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.43 – 2.81 44.43 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.43-2.81) 94.9 (44.43-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.206 , 0.243 0.200 , 0.236	Depositor DCC
R_{free} test set	1919 reflections (5.79%)	DCC
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 75.7	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34704 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5545	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.41	0/2778	0.56	0/3771
1	B	0.45	0/2837	0.62	0/3841
All	All	0.43	0/5615	0.59	0/7612

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	2740	0	0	15	0
1	B	2801	0	0	12	0
2	A	1	0	0	1	0
2	B	3	0	0	1	0
All	All	5545	0	0	26	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 5.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2172:THR:CG2	1:B:2174:SER:N	2.36	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2282:ARG:NH2	1:A:2368:GLU:CG	2.37	0.87
1:B:2172:THR:CG2	1:B:2174:SER:OG	2.24	0.85
1:A:2031:ASN:ND2	2:A:2501:HOH:O	2.25	0.69
1:B:2324:ASP:OD2	1:B:2324:ASP:N	2.26	0.69
1:A:2366:ILE:CG2	1:A:2366:ILE:O	2.41	0.68
1:A:2093:ASP:OD2	1:A:2243:ARG:NH1	2.27	0.68
1:B:2225:ARG:NH2	1:B:2292:THR:O	2.31	0.64
1:A:2113:ASP:N	1:A:2113:ASP:OD1	2.29	0.62
1:B:2171:SER:O	1:B:2228:ARG:CA	2.53	0.57
1:B:2172:THR:CG2	1:B:2174:SER:CB	2.83	0.56
1:B:2282:ARG:NH1	2:B:2503:HOH:O	2.39	0.54
1:A:2243:ARG:NH2	1:B:2097:GLU:OE1	2.43	0.51
1:A:2211:GLU:OE2	1:A:2228:ARG:NH2	2.45	0.49
1:A:2195:LYS:N	1:A:2197:GLN:OE1	2.46	0.49
1:A:2282:ARG:CD	1:A:2368:GLU:OE2	2.61	0.48
1:A:2194:TYR:CE1	1:A:2196:GLY:N	2.81	0.48
1:B:2172:THR:CG2	1:B:2174:SER:CA	2.94	0.45
1:A:2029:ARG:NH1	1:A:2293:PRO:O	2.50	0.44
1:A:2042:ARG:N	1:A:2289:GLN:O	2.52	0.43
1:B:2211:GLU:OE2	1:B:2228:ARG:NE	2.53	0.42
1:A:2180:ASP:OD1	1:A:2181:ILE:N	2.52	0.42
1:A:2042:ARG:NH2	1:A:2127:ASP:O	2.53	0.41
1:B:2211:GLU:OE2	1:B:2228:ARG:NH2	2.53	0.41
1:B:2308:LYS:NZ	1:B:2312:GLU:OE2	2.54	0.41
1:A:2187:THR:O	1:A:2195:LYS:CE	2.69	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	362/427 (85%)	351 (97%)	10 (3%)	1 (0%)	50	83
1	B	360/427 (84%)	336 (93%)	24 (7%)	0	100	100
All	All	722/854 (84%)	687 (95%)	34 (5%)	1 (0%)	59	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2133	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	271/362 (75%)	258 (95%)	13 (5%)	35	71
1	B	291/362 (80%)	276 (95%)	15 (5%)	32	68
All	All	562/724 (78%)	534 (95%)	28 (5%)	34	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2028	SER
1	A	2034	ILE
1	A	2082	ILE
1	A	2113	ASP
1	A	2114	PHE
1	A	2148	VAL
1	A	2183	THR
1	A	2197	GLN
1	A	2214	VAL
1	A	2260	LEU
1	A	2261	ASP
1	A	2351	LEU
1	A	2385	ILE
1	B	2015	LEU
1	B	2032	LEU
1	B	2093	ASP
1	B	2106	ASN
1	B	2120	VAL
1	B	2172	THR
1	B	2175	VAL
1	B	2200	THR
1	B	2262	CYS
1	B	2290	VAL

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Mol	Chain	Res	Type
1	B	2324	ASP
1	B	2336	MSE
1	B	2357	THR
1	B	2360	LEU
1	B	2373	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	368/427 (86%)	0.19	20 (5%)	25 25	60, 97, 150, 164	0
1	B	368/427 (86%)	0.06	10 (2%)	52 53	54, 86, 140, 164	0
All	All	736/854 (86%)	0.13	30 (4%)	35 36	54, 91, 145, 164	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2142	ASP	5.8
1	A	2262	CYS	4.9
1	A	2345	VAL	4.4
1	A	2310	LEU	3.9
1	A	2379	TYR	3.8
1	B	2322	VAL	3.5
1	A	2267	MSE	3.4
1	A	2258	LEU	3.0
1	A	2376	ASN	2.9
1	A	2236	TYR	2.8
1	A	2344	SER	2.7
1	B	2012	LEU	2.6
1	A	2314	VAL	2.6
1	A	2325	GLU	2.6
1	B	2351	LEU	2.5
1	B	2263	ILE	2.4
1	B	2319	ILE	2.4
1	A	2035	LEU	2.3
1	A	2380	HIS	2.3
1	B	2348	GLU	2.2
1	B	2350	GLN	2.2
1	B	2260	LEU	2.2
1	A	2384	TYR	2.2
1	A	2240	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2016	PRO	2.1
1	A	2377	TRP	2.1
1	A	2274	PHE	2.1
1	A	2326	SER	2.0
1	A	2313	CYS	2.0
1	A	2378	LEU	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.