



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 08:18 PM EDT

PDB ID : 3L6D
Title : Crystal structure of putative oxidoreductase from *Pseudomonas putida* KT2440
Authors : Malashkevich, V.N.; Patskovsky, Y.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYS-GXRC)
Deposited on : unknown
Resolution : 1.90 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	:	rb-20030345
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)	:	rb-20030345

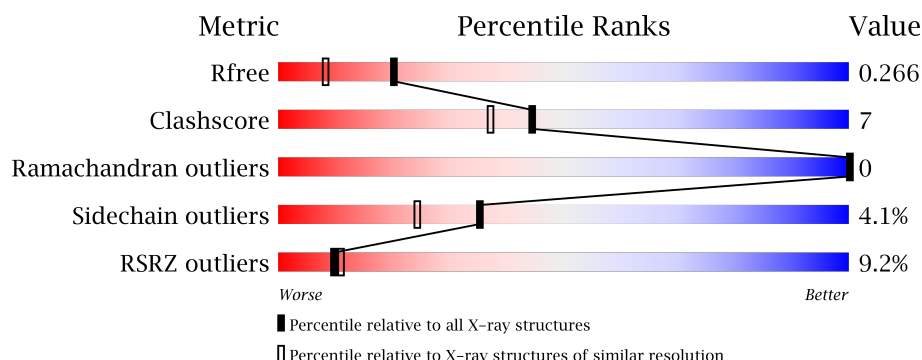
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	306	<div> <div>8%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
1	B	306	<div> <div>9%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4780 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	Se	0	3	0
			2229	1412	402	407	2	6			
1	B	295	Total	C	N	O	S	Se	0	1	0
			2237	1413	403	412	2	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q88J51
A	2	SER	-	EXPRESSION TAG	UNP Q88J51
A	3	LEU	-	EXPRESSION TAG	UNP Q88J51
A	299	GLU	PRO	CONFLICT	UNP Q88J51
A	302	HIS	-	EXPRESSION TAG	UNP Q88J51
A	303	HIS	-	EXPRESSION TAG	UNP Q88J51
A	304	HIS	-	EXPRESSION TAG	UNP Q88J51
A	305	HIS	-	EXPRESSION TAG	UNP Q88J51
A	306	HIS	-	EXPRESSION TAG	UNP Q88J51
B	1	MSE	-	EXPRESSION TAG	UNP Q88J51
B	2	SER	-	EXPRESSION TAG	UNP Q88J51
B	3	LEU	-	EXPRESSION TAG	UNP Q88J51
B	299	GLU	PRO	CONFLICT	UNP Q88J51
B	302	HIS	-	EXPRESSION TAG	UNP Q88J51
B	303	HIS	-	EXPRESSION TAG	UNP Q88J51
B	304	HIS	-	EXPRESSION TAG	UNP Q88J51
B	305	HIS	-	EXPRESSION TAG	UNP Q88J51
B	306	HIS	-	EXPRESSION TAG	UNP Q88J51

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		

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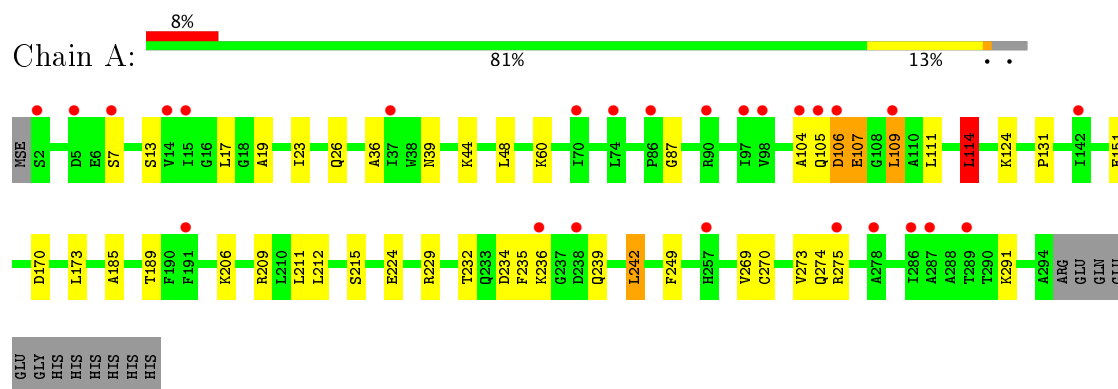
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	175	Total	O	0	0
			175	175		

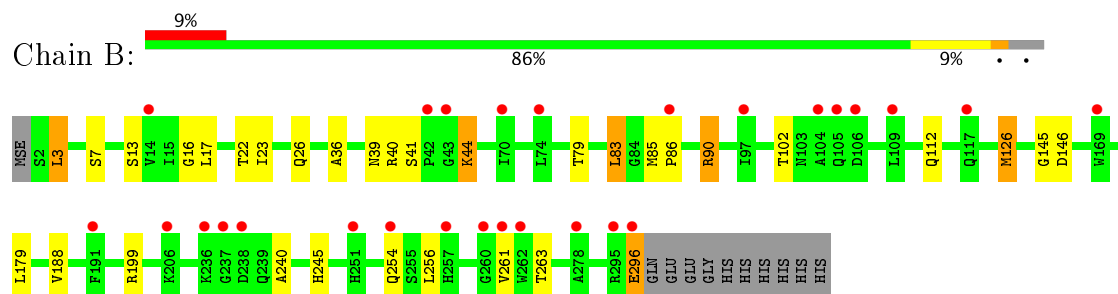
3 Residue-property plots [i](#)

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: Putative oxidoreductase



• Molecule 1: Putative oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.34Å 37.65Å 104.25Å 90.00° 93.35° 90.00°	Depositor
Resolution (Å)	19.94 – 1.90 19.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-1.90) 98.5 (19.92-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.260 0.214 , 0.266	Depositor DCC
R_{free} test set	2610 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4780	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% 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	0.75	0/2280	0.73	4/3085 (0.1%)
1	B	0.79	0/2278	0.72	1/3081 (0.0%)
All	All	0.77	0/4558	0.73	5/6166 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	114	LEU	CA-CB-CG	6.73	130.79	115.30
1	A	242	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	3	LEU	CA-CB-CG	6.53	130.33	115.30
1	A	170	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	209	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	THR	Peptide

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	2229	0	2199	39	0
1	B	2237	0	2195	30	1
2	A	139	0	0	5	0
2	B	175	0	0	1	0
All	All	4780	0	4394	66	1

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 (66) 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:104:ALA:O	1:A:107:GLU:HG3	1.58	1.02
1:A:17:LEU:O	1:A:44:LYS:HG2	1.72	0.88
1:A:19:ALA:O	1:A:23:ILE:HG12	1.74	0.86
1:A:270:CYS:O	1:A:274:GLN:HG2	1.75	0.86
1:A:60:LYS:HE2	1:A:87:GLY:HA3	1.66	0.78
1:A:124:LYS:HE2	1:A:173:LEU:HD21	1.69	0.75
1:B:17:LEU:HG	1:B:39:ASN:HB2	1.69	0.74
1:A:212:LEU:HD12	2:A:347:HOH:O	1.91	0.70
1:B:39:ASN:HD22	1:B:41:SER:N	1.90	0.70
1:A:17:LEU:HD12	1:A:39:ASN:HB2	1.79	0.64
1:A:151:GLU:HG3	2:A:364:HOH:O	1.98	0.63
1:B:39:ASN:ND2	1:B:40:ARG:H	2.00	0.59
1:A:109:LEU:HD12	1:A:109:LEU:N	2.19	0.57
1:A:206:LYS:HE2	2:A:441:HOH:O	2.03	0.57
1:B:23:ILE:HD12	1:B:26:GLN:HE21	1.70	0.57
1:A:109:LEU:CD1	1:A:109:LEU:N	2.68	0.57
1:B:23:ILE:HD12	1:B:26:GLN:NE2	2.20	0.56
1:A:109:LEU:CD1	1:A:109:LEU:H	2.18	0.56
1:A:104:ALA:O	1:A:107:GLU:CG	2.46	0.55
1:A:212:LEU:CD1	2:A:347:HOH:O	2.54	0.55
1:B:256:LEU:HD13	1:B:263:THR:HG21	1.88	0.54
1:A:106:ASP:H	1:A:109:LEU:HD13	1.73	0.54
1:B:261:VAL:HG23	1:B:263:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:HD22	1:B:41:SER:H	1.55	0.53
1:A:211[A]:LEU:HD11	1:B:179:LEU:HA	1.92	0.52
1:A:106:ASP:HA	1:A:109:LEU:HD13	1.92	0.52
1:A:224:GLU:HG2	2:A:382:HOH:O	2.10	0.51
1:A:106:ASP:CA	1:A:109:LEU:HD13	2.40	0.51
1:A:60:LYS:HE2	1:A:87:GLY:CA	2.41	0.49
1:A:105:GLN:O	1:A:106:ASP:OD1	2.29	0.49
1:A:23:ILE:HG13	1:A:131:PRO:HB3	1.95	0.47
1:B:85:MSE:HB3	1:B:86:PRO:HD2	1.97	0.47
1:A:106:ASP:HA	1:A:109:LEU:HD22	1.96	0.47
1:A:17:LEU:O	1:A:44:LYS:CG	2.54	0.47
1:B:16:GLY:O	1:B:17:LEU:HD23	2.16	0.46
1:B:39:ASN:CG	1:B:40:ARG:H	2.19	0.45
1:A:26:GLN:HG3	1:A:48:LEU:HD21	1.97	0.45
1:B:240:ALA:HB1	1:B:245:HIS:CE1	2.51	0.45
1:B:39:ASN:ND2	1:B:40:ARG:N	2.65	0.45
1:A:114:LEU:HD12	1:A:114:LEU:C	2.36	0.45
1:A:232:THR:HG23	1:A:234:ASP:HB3	1.98	0.45
1:B:16:GLY:HA2	1:B:39:ASN:OD1	2.17	0.45
1:B:112:GLN:NE2	1:B:145:GLY:HA2	2.32	0.44
1:B:17:LEU:CD1	1:B:39:ASN:HB2	2.48	0.44
1:A:269:VAL:HG13	1:B:188:VAL:HG21	1.99	0.44
1:B:17:LEU:CG	1:B:39:ASN:HB2	2.44	0.44
1:A:215:SER:HB3	1:B:179:LEU:HD11	2.00	0.44
1:B:126[B]:MSE:HB2	1:B:126[B]:MSE:HE3	1.81	0.44
1:B:79:THR:O	1:B:83:LEU:CD2	2.67	0.43
1:A:232:THR:HG23	1:A:234:ASP:CB	2.49	0.43
1:B:79:THR:O	1:B:83:LEU:HD22	2.19	0.43
1:B:13:SER:HA	1:B:36:ALA:O	2.19	0.42
1:B:146:ASP:HB2	2:B:365:HOH:O	2.18	0.42
1:A:13:SER:HA	1:A:36:ALA:O	2.19	0.42
1:B:240:ALA:HB1	1:B:245:HIS:HE1	1.82	0.42
1:A:105:GLN:O	1:A:106:ASP:CB	2.68	0.42
1:A:106:ASP:N	1:A:109:LEU:HD13	2.34	0.42
1:A:185:ALA:O	1:A:189:THR:HG23	2.19	0.42
1:A:235:PHE:CZ	1:A:291:LYS:HD2	2.55	0.42
1:B:199:ARG:HD2	1:B:261:VAL:HG12	2.01	0.41
1:B:22:THR:OG1	1:B:44:LYS:HG2	2.20	0.41
1:A:249:PHE:CE2	1:A:273:VAL:HG21	2.56	0.41
1:B:16:GLY:C	1:B:17:LEU:HD23	2.41	0.40
1:A:229:ARG:HA	1:A:232:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:CG2	1:A:234:ASP:HB3	2.51	0.40
1:B:296:GLU:H	1:B:296:GLU:HG3	1.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:NH2	1:B:296:GLU:OE1[2_555]	2.18	0.02

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	294/306 (96%)	287 (98%)	7 (2%)	0	100	100
1	B	294/306 (96%)	286 (97%)	8 (3%)	0	100	100
All	All	588/612 (96%)	573 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	222/224 (99%)	212 (96%)	10 (4%)	32	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	222/224 (99%)	213 (96%)	9 (4%)	35	24
All	All	444/448 (99%)	425 (96%)	19 (4%)	35	22

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	106	ASP
1	A	107	GLU
1	A	109	LEU
1	A	111	LEU
1	A	114	LEU
1	A	236	LYS
1	A	239	GLN
1	A	242	LEU
1	A	275	ARG
1	B	3	LEU
1	B	7	SER
1	B	44	LYS
1	B	83	LEU
1	B	90	ARG
1	B	126[A]	MSE
1	B	126[B]	MSE
1	B	254	GLN
1	B	296	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	80	HIS
1	A	140	HIS
1	B	26	GLN
1	B	39	ASN
1	B	112	GLN
1	B	116	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	287/306 (93%)	0.48	26 (9%) 10 11	19, 30, 48, 66	0
1	B	289/306 (94%)	0.47	27 (9%) 9 10	16, 27, 45, 68	0
All	All	576/612 (94%)	0.48	53 (9%) 10 11	16, 28, 48, 68	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ASP	6.0
1	B	257	HIS	5.1
1	B	105	GLN	5.1
1	B	43	GLY	4.4
1	B	296	GLU	4.4
1	B	74	LEU	3.8
1	B	104	ALA	3.7
1	A	15	ILE	3.7
1	A	74	LEU	3.6
1	B	42	PRO	3.5
1	A	286	ILE	3.2
1	A	105	GLN	3.1
1	A	106	ASP	3.0
1	A	70	ILE	3.0
1	B	278	ALA	3.0
1	A	191	PHE	2.9
1	B	261	VAL	2.9
1	A	97	ILE	2.9
1	A	2	SER	2.8
1	B	191	PHE	2.8
1	A	257	HIS	2.8
1	B	14	VAL	2.7
1	B	117	GLN	2.7
1	B	251	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	7	SER	2.6
1	B	106	ASP	2.6
1	A	236	LYS	2.5
1	A	90	ARG	2.5
1	B	97	ILE	2.5
1	B	295	ARG	2.5
1	B	70	ILE	2.5
1	A	14	VAL	2.4
1	B	236	LYS	2.4
1	B	238	ASP	2.4
1	B	254	GLN	2.3
1	A	86	PRO	2.3
1	B	206	LYS	2.3
1	A	275	ARG	2.3
1	A	278	ALA	2.3
1	A	287	ALA	2.3
1	A	238	ASP	2.3
1	A	109	LEU	2.2
1	B	109	LEU	2.2
1	A	289	THR	2.2
1	A	104	ALA	2.2
1	A	142	ILE	2.2
1	B	86	PRO	2.2
1	A	98	VAL	2.1
1	B	237	GLY	2.1
1	B	260	GLY	2.1
1	A	37	ILE	2.1
1	B	262	TRP	2.1
1	B	169	TRP	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 [i](#)

There are no such residues in this entry.