



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:36 PM UTC

PDB ID : 8HWO / pdb_00008hwo
Title : Crystal Structure of mutant GDSE Esterase of Photobacterium sp. J15
Authors : Rahman, N.N.A.; Leow, T.C.; Jonet, M.A.
Deposited on : 2023-01-01
Resolution : 1.96 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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

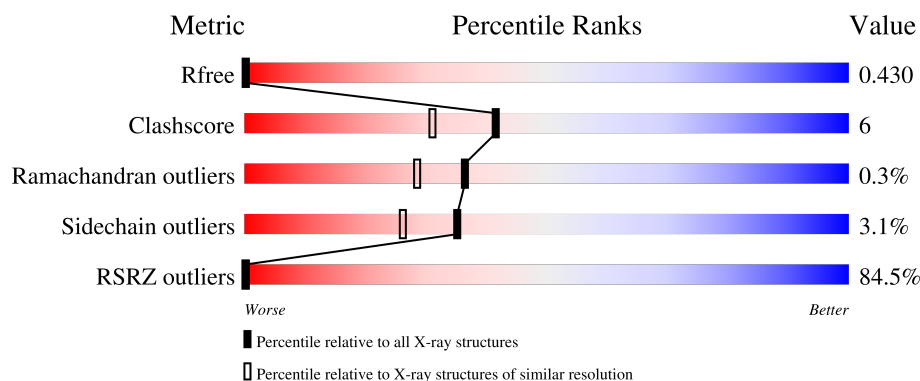
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	328	84% 88%11%.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2515 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 GDSL-family esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2515	1595	435	479	6			

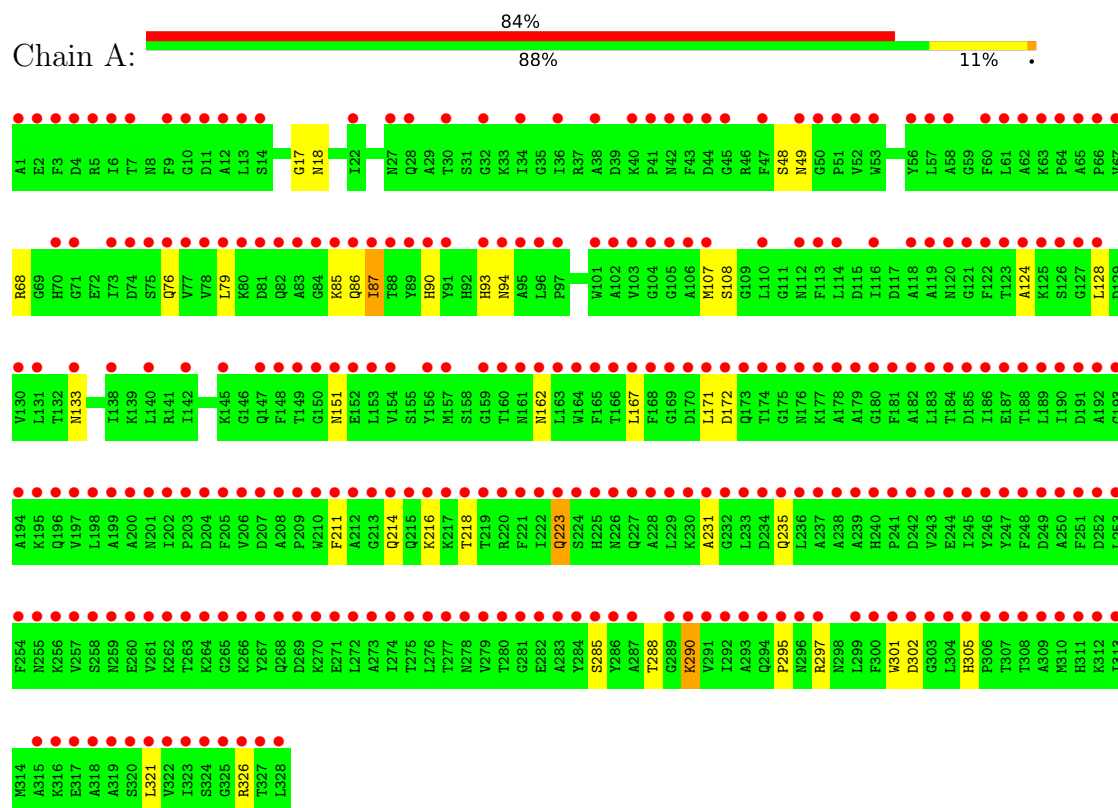
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	SER	engineered mutation	UNP A0A0K0PV22

3 Residue-property plots

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: GDSL-family esterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.12Å 55.82Å 120.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.96 40.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.00-1.96) 99.5 (40.00-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.244 , 0.299 0.439 , 0.430	Depositor DCC
R_{free} test set	2037 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	2515	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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 [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	1.05	1/2570 (0.0%)	1.38	1/3484 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	PRO	C-O	-5.29	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	LEU	N-CA-C	-5.96	102.49	110.24

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	2515	0	2460	32	0
All	All	2515	0	2460	32	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 6.

All (32) 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:108:SER:H	1:A:162:ASN:HD21	1.22	0.86
1:A:290:LYS:HD2	1:A:290:LYS:C	2.08	0.79
1:A:302:ASP:OD2	1:A:305:HIS:HD2	1.69	0.75
1:A:297:ARG:HA	1:A:297:ARG:HE	1.59	0.68
1:A:214:GLN:O	1:A:218:THR:HG23	1.97	0.65
1:A:290:LYS:C	1:A:290:LYS:CD	2.72	0.61
1:A:18:ASN:HD22	1:A:68:ARG:HH11	1.48	0.60
1:A:107:MET:H	1:A:133:ASN:HD22	1.51	0.59
1:A:107:MET:H	1:A:133:ASN:ND2	2.02	0.58
1:A:18:ASN:ND2	1:A:68:ARG:HH11	2.04	0.56
1:A:297:ARG:HA	1:A:297:ARG:NE	2.21	0.56
1:A:107:MET:HE3	1:A:133:ASN:HD21	1.72	0.55
1:A:290:LYS:O	1:A:290:LYS:CE	2.56	0.54
1:A:167:LEU:HD11	1:A:218:THR:HG22	1.90	0.53
1:A:231:ALA:O	1:A:235:GLN:HG3	2.11	0.51
1:A:93:HIS:HD2	1:A:94:ASN:O	1.92	0.51
1:A:211:PHE:HB3	1:A:218:THR:HG21	1.93	0.51
1:A:290:LYS:O	1:A:290:LYS:HE3	2.10	0.51
1:A:79:LEU:HB2	1:A:87:ILE:HD11	1.93	0.49
1:A:76:GLN:HE22	1:A:90:HIS:HB2	1.78	0.48
1:A:223:GLN:HE21	1:A:223:GLN:C	2.21	0.48
1:A:285:SER:HB3	1:A:290:LYS:HE3	1.97	0.46
1:A:151:ASN:OD1	1:A:151:ASN:C	2.59	0.45
1:A:49:ASN:HB3	1:A:301:TRP:CZ3	2.51	0.45
1:A:124:ALA:CB	1:A:128:LEU:HD12	2.47	0.45
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.84	0.44
1:A:18:ASN:HD22	1:A:18:ASN:HA	1.73	0.43
1:A:288:THR:OG1	1:A:290:LYS:HG3	2.19	0.42
1:A:79:LEU:HB2	1:A:87:ILE:CD1	2.50	0.42
1:A:108:SER:N	1:A:162:ASN:HD21	2.03	0.41
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.95	0.41
1:A:48:SER:HA	1:A:301:TRP:CD1	2.56	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	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	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	258/258 (100%)	250 (97%)	8 (3%)	35	26

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
1	A	86	GLN
1	A	87	ILE
1	A	172	ASP
1	A	216	LYS
1	A	223	GLN
1	A	290	LYS
1	A	326	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	76	GLN
1	A	90	HIS
1	A	93	HIS
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	147	GLN
1	A	161	ASN
1	A	162	ASN
1	A	173	GLN
1	A	223	GLN
1	A	240	HIS
1	A	305	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 oligosaccharides 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	328/328 (100%)	3.67	277 (84%) 0 0	8, 16, 35, 77	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	16.6
1	A	97	PRO	8.5
1	A	171	LEU	8.1
1	A	250	ALA	8.1
1	A	3	PHE	8.0
1	A	2	GLU	7.9
1	A	243	VAL	7.8
1	A	167	LEU	7.8
1	A	231	ALA	7.7
1	A	221	PHE	7.7
1	A	220	ARG	7.6
1	A	176	ASN	7.6
1	A	213	GLY	7.5
1	A	229	LEU	7.4
1	A	272	LEU	7.4
1	A	223	GLN	7.4
1	A	239	ALA	7.3
1	A	265	GLY	7.3
1	A	290	LYS	7.2
1	A	280	THR	6.9
1	A	321	LEU	6.7
1	A	323	ILE	6.7
1	A	149	THR	6.6
1	A	85	LYS	6.6
1	A	328	LEU	6.4
1	A	165	PHE	6.3
1	A	322	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASN	6.2
1	A	172	ASP	6.2
1	A	168	PHE	6.1
1	A	210	TRP	6.1
1	A	84	GLY	6.0
1	A	200	ALA	6.0
1	A	263	THR	6.0
1	A	246	TYR	6.0
1	A	13	LEU	6.0
1	A	170	ASP	6.0
1	A	211	PHE	6.0
1	A	279	VAL	5.9
1	A	205	PHE	5.9
1	A	268	GLN	5.8
1	A	87	ILE	5.8
1	A	238	ALA	5.8
1	A	261	VAL	5.8
1	A	208	ALA	5.8
1	A	326	ARG	5.7
1	A	198	LEU	5.7
1	A	228	ALA	5.7
1	A	197	VAL	5.6
1	A	247	TYR	5.6
1	A	219	THR	5.6
1	A	181	PHE	5.6
1	A	216	LYS	5.6
1	A	81	ASP	5.5
1	A	233	LEU	5.5
1	A	199	ALA	5.4
1	A	257	VAL	5.4
1	A	82	GLN	5.4
1	A	83	ALA	5.3
1	A	236	LEU	5.3
1	A	206	VAL	5.3
1	A	159	GLY	5.3
1	A	258	SER	5.2
1	A	183	LEU	5.2
1	A	248	PHE	5.2
1	A	237	ALA	5.2
1	A	218	THR	5.2
1	A	119	ALA	5.2
1	A	166	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	318	ALA	5.0
1	A	4	ASP	5.0
1	A	60	PHE	5.0
1	A	178	ALA	4.9
1	A	88	THR	4.9
1	A	267	TYR	4.8
1	A	297	ARG	4.8
1	A	217	LYS	4.8
1	A	304	LEU	4.8
1	A	270	LYS	4.8
1	A	254	PHE	4.8
1	A	324	SER	4.8
1	A	255	ASN	4.8
1	A	325	GLY	4.8
1	A	214	GLN	4.7
1	A	53	TRP	4.7
1	A	232	GLY	4.7
1	A	241	PRO	4.7
1	A	203	PRO	4.6
1	A	174	THR	4.6
1	A	327	THR	4.6
1	A	269	ASP	4.6
1	A	283	ALA	4.6
1	A	274	ILE	4.6
1	A	224	SER	4.5
1	A	266	LYS	4.5
1	A	121	GLY	4.5
1	A	163	LEU	4.5
1	A	5	ARG	4.5
1	A	120	ASN	4.4
1	A	169	GLY	4.4
1	A	164	TRP	4.4
1	A	313	ILE	4.4
1	A	154	VAL	4.3
1	A	96	LEU	4.3
1	A	152	GLU	4.3
1	A	194	ALA	4.3
1	A	293	ALA	4.2
1	A	227	GLN	4.2
1	A	153	LEU	4.2
1	A	235	GLN	4.2
1	A	173	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	319	ALA	4.1
1	A	196	GLN	4.1
1	A	192	ALA	4.1
1	A	271	GLU	4.1
1	A	122	PHE	4.0
1	A	230	LYS	4.0
1	A	162	ASN	4.0
1	A	123	THR	4.0
1	A	275	THR	4.0
1	A	161	ASN	4.0
1	A	180	GLY	3.9
1	A	56	TYR	3.9
1	A	264	LYS	3.9
1	A	320	SER	3.9
1	A	114	LEU	3.9
1	A	222	ILE	3.9
1	A	259	ASN	3.8
1	A	276	LEU	3.8
1	A	179	ALA	3.8
1	A	182	ALA	3.8
1	A	6	ILE	3.8
1	A	78	VAL	3.8
1	A	195	LYS	3.8
1	A	273	ALA	3.8
1	A	294	GLN	3.8
1	A	252	ASP	3.7
1	A	86	GLN	3.7
1	A	188	THR	3.7
1	A	177	LYS	3.7
1	A	105	GLY	3.7
1	A	124	ALA	3.7
1	A	126	SER	3.7
1	A	303	GLY	3.7
1	A	299	LEU	3.7
1	A	309	ALA	3.7
1	A	186	ILE	3.7
1	A	251	PHE	3.6
1	A	295	PRO	3.6
1	A	93	HIS	3.6
1	A	212	ALA	3.6
1	A	193	GLY	3.6
1	A	187	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	226	ASN	3.5
1	A	240	HIS	3.5
1	A	160	THR	3.5
1	A	292	ILE	3.5
1	A	300	PHE	3.5
1	A	95	ALA	3.5
1	A	189	LEU	3.5
1	A	147	GLN	3.4
1	A	80	LYS	3.4
1	A	38	ALA	3.4
1	A	215	GLN	3.4
1	A	253	LEU	3.4
1	A	116	ILE	3.4
1	A	28	GLN	3.4
1	A	291	VAL	3.4
1	A	43	PHE	3.4
1	A	244	GLU	3.3
1	A	202	ILE	3.3
1	A	204	ASP	3.3
1	A	191	ASP	3.3
1	A	316	LYS	3.2
1	A	125	LYS	3.2
1	A	301	TRP	3.2
1	A	245	ILE	3.2
1	A	130	VAL	3.2
1	A	175	GLY	3.2
1	A	289	GLY	3.2
1	A	249	ASP	3.2
1	A	190	ILE	3.1
1	A	148	PHE	3.1
1	A	74	ASP	3.1
1	A	79	LEU	3.1
1	A	296	ASN	3.1
1	A	71	GLY	3.1
1	A	110	LEU	3.1
1	A	260	GLU	3.1
1	A	150	GLY	3.1
1	A	287	ALA	3.1
1	A	207	ASP	3.0
1	A	281	GLY	3.0
1	A	256	LYS	3.0
1	A	282	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	89	TYR	2.9
1	A	113	PHE	2.9
1	A	76	GLN	2.9
1	A	40	LYS	2.9
1	A	44	ASP	2.9
1	A	103	VAL	2.9
1	A	90	HIS	2.9
1	A	317	GLU	2.9
1	A	52	VAL	2.8
1	A	286	TYR	2.8
1	A	128	LEU	2.8
1	A	32	GLY	2.8
1	A	67	VAL	2.8
1	A	225	HIS	2.8
1	A	27	ASN	2.8
1	A	36	ILE	2.8
1	A	201	ASN	2.7
1	A	22	ILE	2.7
1	A	101	TRP	2.7
1	A	209	PRO	2.6
1	A	242	ASP	2.6
1	A	285	SER	2.6
1	A	112	ASN	2.6
1	A	49	ASN	2.6
1	A	157	MET	2.6
1	A	142	ILE	2.6
1	A	278	ASN	2.6
1	A	184	THR	2.6
1	A	62	ALA	2.5
1	A	75	SER	2.5
1	A	51	PRO	2.5
1	A	102	ALA	2.5
1	A	106	ALA	2.5
1	A	277	THR	2.5
1	A	61	LEU	2.5
1	A	118	ALA	2.5
1	A	47	PHE	2.4
1	A	57	LEU	2.4
1	A	107	MET	2.4
1	A	311	HIS	2.4
1	A	156	TYR	2.4
1	A	138	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	30	THR	2.4
1	A	307	THR	2.4
1	A	308	THR	2.4
1	A	58	ALA	2.4
1	A	77	VAL	2.4
1	A	94	ASN	2.4
1	A	9	PHE	2.4
1	A	34	ILE	2.4
1	A	66	PRO	2.4
1	A	50	GLY	2.4
1	A	310	MET	2.4
1	A	185	ASP	2.3
1	A	42	ASN	2.3
1	A	145	LYS	2.3
1	A	234	ASP	2.3
1	A	14	SER	2.3
1	A	11	ASP	2.3
1	A	302	ASP	2.3
1	A	63	LYS	2.3
1	A	12	ALA	2.2
1	A	73	ILE	2.2
1	A	70	HIS	2.2
1	A	131	LEU	2.2
1	A	10	GLY	2.2
1	A	262	LYS	2.2
1	A	315	ALA	2.2
1	A	45	GLY	2.2
1	A	127	GLY	2.2
1	A	65	ALA	2.2
1	A	305	HIS	2.1
1	A	284	TYR	2.1
1	A	41	PRO	2.1
1	A	64	PRO	2.1
1	A	133	ASN	2.1
1	A	312	LYS	2.1
1	A	104	GLY	2.1
1	A	306	PRO	2.1
1	A	7	THR	2.0
1	A	140	LEU	2.0
1	A	91	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.