



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:21 AM UTC

PDB ID : 5AID / pdb_00005aid
Title : Crystal structure of the Mep2 mutant delta442 from *Candida albicans*
Authors : van den Berg, B.; Chembath, A.; Rutherford, J.
Deposited on : 2015-02-12
Resolution : 3.40 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

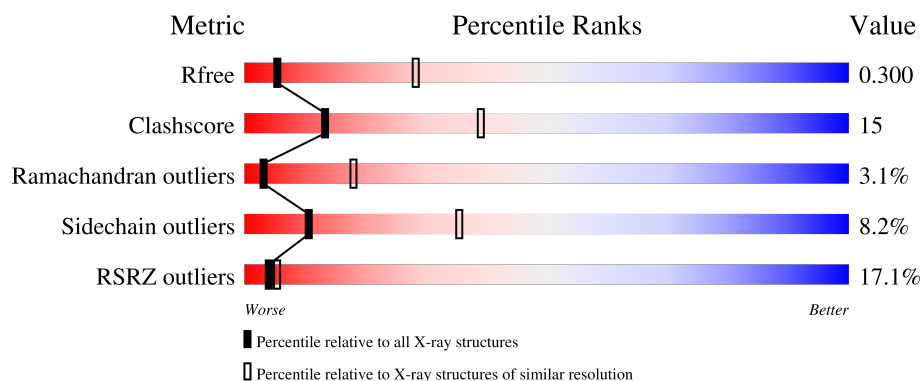
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	448	15% 54% 31% • 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3041 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 MEP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	7	3	0
			3041	2008	488	517	28			

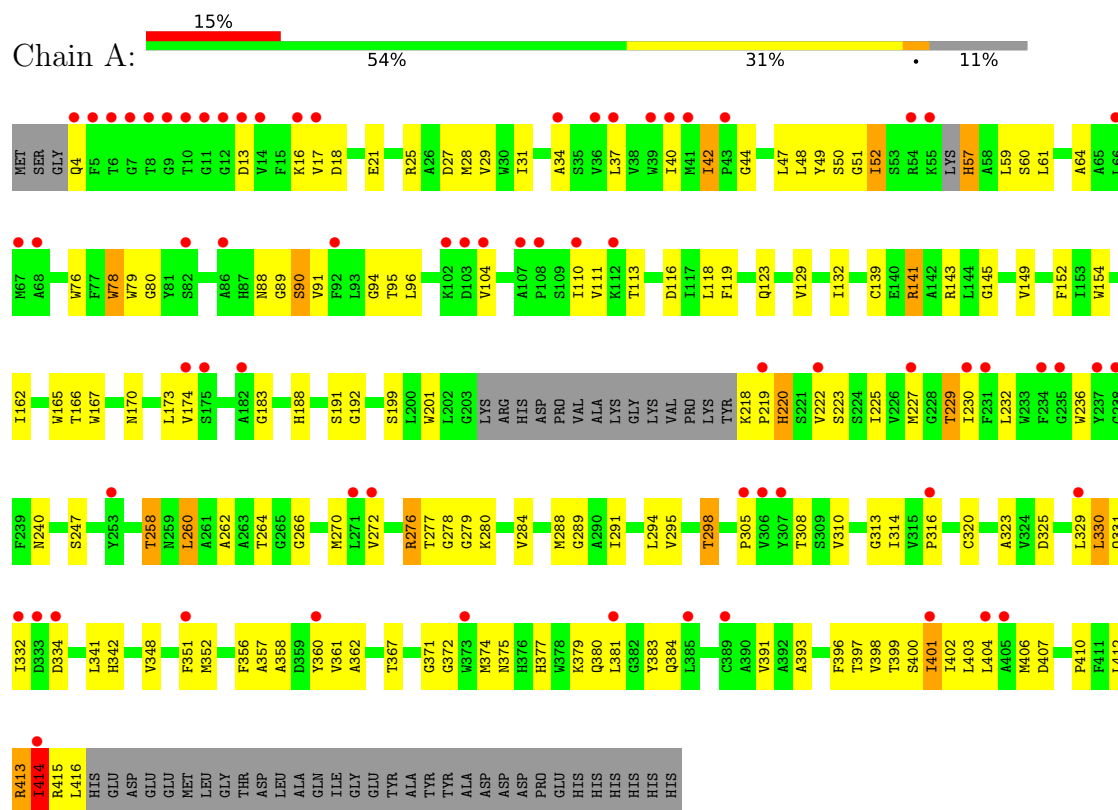
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	ASN	conflict	UNP Q59UP8
A	443	HIS	-	expression tag	UNP Q59UP8
A	444	HIS	-	expression tag	UNP Q59UP8
A	445	HIS	-	expression tag	UNP Q59UP8
A	446	HIS	-	expression tag	UNP Q59UP8
A	447	HIS	-	expression tag	UNP Q59UP8
A	448	HIS	-	expression tag	UNP Q59UP8

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: MEP2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	114.73Å 114.73Å 289.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	96.66 – 3.40 96.66 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (96.66-3.40) 92.3 (96.66-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.236 , 0.289 0.251 , 0.300	Depositor DCC
R_{free} test set	1055 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	124.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 124.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.029 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.024 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3041	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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	0.58	0/3144	0.97	6/4287 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	VAL	N-CA-C	-6.32	104.89	111.58
1	A	42	ILE	CA-C-N	-5.87	112.51	119.84
1	A	42	ILE	C-N-CA	-5.87	112.51	119.84
1	A	260	LEU	CA-CB-CG	5.48	135.48	116.30
1	A	298	THR	CA-C-N	-5.01	114.88	120.45
1	A	298	THR	C-N-CA	-5.01	114.88	120.45

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	3041	0	2992	89	0
All	All	3041	0	2992	89	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 15.

All (89) 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:13:ASP:HB3	1:A:16:LYS:HB3	1.67	0.77
1:A:288:MET:HE3	1:A:341:LEU:HD11	1.70	0.73
1:A:264:THR:HG21	1:A:310:VAL:HG13	1.74	0.69
1:A:232:LEU:O	1:A:236:TRP:HD1	1.74	0.69
1:A:143:ARG:HD3	1:A:413:ARG:HB2	1.75	0.69
1:A:4:GLN:HA	1:A:17:VAL:HG11	1.77	0.66
1:A:34:ALA:HA	1:A:37:LEU:HD12	1.79	0.65
1:A:57:HIS:HE2	1:A:139[A]:CYS:HG	1.25	0.64
1:A:380:GLN:HA	1:A:383:TYR:HD2	1.62	0.63
1:A:356:PHE:HA	1:A:374:MET:HG2	1.80	0.63
1:A:167:TRP:HZ2	1:A:183:GLY:HA3	1.64	0.62
1:A:348:VAL:HG12	1:A:352:MET:HE2	1.81	0.61
1:A:89:GLY:HA2	1:A:95:THR:HG23	1.84	0.59
1:A:27:ASP:OD1	1:A:247:SER:OG	2.17	0.58
1:A:396:PHE:O	1:A:400:SER:OG	2.14	0.57
1:A:295:VAL:HG11	1:A:342:HIS:HA	1.87	0.57
1:A:276:ARG:NH1	1:A:325:ASP:OD2	2.38	0.56
1:A:104:VAL:HG13	1:A:116:ASP:HB3	1.88	0.56
1:A:141:ARG:HH21	1:A:416:LEU:HD12	1.69	0.56
1:A:219:PRO:O	1:A:220:HIS:ND1	2.37	0.55
1:A:201:TRP:HB3	1:A:404:LEU:HD21	1.89	0.55
1:A:407:ASP:HB2	1:A:414:ILE:HD11	1.87	0.55
1:A:61:LEU:HA	1:A:64:ALA:HB3	1.88	0.54
1:A:399:THR:O	1:A:403:LEU:HG	2.09	0.53
1:A:236:TRP:CD1	1:A:294:LEU:HD13	2.44	0.52
1:A:89:GLY:HA3	1:A:94:GLY:HA2	1.92	0.51
1:A:57:HIS:NE2	1:A:139[A]:CYS:SG	2.65	0.51
1:A:236:TRP:HZ3	1:A:298:THR:HG1	1.57	0.50
1:A:351:PHE:CE1	1:A:381:LEU:HD11	2.46	0.50
1:A:199:SER:O	1:A:332:ILE:HD13	2.11	0.50
1:A:50:SER:N	1:A:61:LEU:HD11	2.27	0.49
1:A:277:THR:O	1:A:279:GLY:N	2.45	0.49
1:A:262:ALA:HB2	1:A:294:LEU:HD21	1.94	0.49
1:A:357:ALA:O	1:A:372:GLY:N	2.46	0.49
1:A:48:LEU:HD23	1:A:49:TYR:CE1	2.49	0.48
1:A:380:GLN:NE2	1:A:384:GLN:OE1	2.45	0.48
1:A:223:SER:O	1:A:227:MET:N	2.41	0.48
1:A:240:ASN:ND2	1:A:258:THR:OG1	2.46	0.48
1:A:225:ILE:O	1:A:229:THR:N	2.41	0.47
1:A:362:ALA:O	1:A:367:THR:HB	2.15	0.47
1:A:52:ILE:HA	1:A:225:ILE:HD11	1.97	0.47
1:A:305:PRO:HB2	1:A:308:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ALA:HB2	1:A:294:LEU:CD2	2.45	0.46
1:A:398:VAL:HA	1:A:401:ILE:HG22	1.98	0.46
1:A:90:SER:O	1:A:170:ASN:HB2	2.15	0.46
1:A:266:GLY:HA2	1:A:289:GLY:HA3	1.96	0.46
1:A:407:ASP:CB	1:A:414:ILE:HD11	2.46	0.46
1:A:377:HIS:ND1	1:A:380:GLN:HB2	2.31	0.45
1:A:398:VAL:O	1:A:402:ILE:HG12	2.15	0.45
1:A:165:TRP:O	1:A:173:LEU:HB2	2.16	0.45
1:A:88:ASN:ND2	1:A:95:THR:HG21	2.31	0.45
1:A:316:PRO:HD3	1:A:352:MET:HE1	2.00	0.44
1:A:188:HIS:O	1:A:192:GLY:N	2.51	0.44
1:A:404:LEU:C	1:A:406:MET:H	2.26	0.44
1:A:76:TRP:HA	1:A:80:GLY:HA3	1.99	0.43
1:A:141:ARG:NH2	1:A:416:LEU:HD12	2.34	0.43
1:A:288:MET:HE2	1:A:288:MET:HB3	1.78	0.43
1:A:4:GLN:HG2	1:A:16:LYS:NZ	2.33	0.43
1:A:119:PHE:O	1:A:123:GLN:HB2	2.18	0.43
1:A:358:ALA:HB1	1:A:360:TYR:CE2	2.54	0.43
1:A:79:TRP:CZ2	1:A:152:PHE:HE1	2.36	0.43
1:A:371:GLY:HA3	1:A:375:ASN:HD21	1.84	0.43
1:A:91:VAL:HA	1:A:170:ASN:O	2.19	0.43
1:A:232:LEU:O	1:A:236:TRP:CD1	2.64	0.42
1:A:154:TRP:HD1	1:A:402:ILE:HD11	1.84	0.42
1:A:167:TRP:CZ2	1:A:183:GLY:HA3	2.50	0.42
1:A:320:CYS:HA	1:A:323:ALA:HB3	2.02	0.42
1:A:31:ILE:HB	1:A:118:LEU:HD21	2.02	0.42
1:A:264:THR:OG1	1:A:313:GLY:HA3	2.20	0.42
1:A:47:LEU:HD13	1:A:227:MET:HG3	2.02	0.42
1:A:393:ALA:O	1:A:397:THR:HG23	2.19	0.42
1:A:25:ARG:HD3	1:A:28:MET:CE	2.50	0.41
1:A:78:TRP:CD1	1:A:79:TRP:CE3	3.08	0.41
1:A:162:ILE:HG23	1:A:391:VAL:HG22	2.02	0.41
1:A:145:GLY:O	1:A:149:VAL:HG23	2.21	0.41
1:A:277:THR:O	1:A:280:LYS:N	2.52	0.41
1:A:291:ILE:O	1:A:295:VAL:HG23	2.21	0.41
1:A:414:ILE:CD1	1:A:415:ARG:H	2.34	0.41
1:A:42:ILE:C	1:A:44:GLY:H	2.29	0.41
1:A:48:LEU:O	1:A:52:ILE:HB	2.21	0.41
1:A:50:SER:H	1:A:61:LEU:HD11	1.85	0.41
1:A:18:ASP:O	1:A:21:GLU:HG3	2.21	0.41
1:A:51:GLY:C	1:A:225:ILE:HG13	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG12	1:A:113:THR:HG22	2.02	0.40
1:A:225:ILE:HD13	1:A:284:VAL:HG13	2.04	0.40
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.78	0.40
1:A:375:ASN:OD1	1:A:375:ASN:N	2.53	0.40
1:A:330:LEU:O	1:A:331:GLN:HB3	2.22	0.40
1:A:402:ILE:O	1:A:406:MET:HB2	2.22	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	395/448 (88%)	334 (85%)	49 (12%)	12 (3%)	3	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	278	GLY
1	A	413	ARG
1	A	220	HIS
1	A	414	ILE
1	A	78	TRP
1	A	334	ASP
1	A	141	ARG
1	A	60	SER
1	A	330	LEU
1	A	410	PRO
1	A	314	ILE

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	307/346 (89%)	282 (92%)	25 (8%)	11	36

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	40	ILE
1	A	52	ILE
1	A	57	HIS
1	A	59	LEU
1	A	110	ILE
1	A	129	VAL
1	A	132	ILE
1	A	166	THR
1	A	174	VAL
1	A	191	SER
1	A	218	LYS
1	A	222	VAL
1	A	229	THR
1	A	230	ILE
1	A	258	THR
1	A	260	LEU
1	A	270	MET
1	A	272	VAL
1	A	276	ARG
1	A	329	LEU
1	A	379	LYS
1	A	401	ILE
1	A	412	LEU
1	A	414	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	259	ASN

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	398/448 (88%)	0.87	68 (17%) 4 5	77, 126, 186, 228	5 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	PHE	11.6
1	A	40	ILE	10.1
1	A	231	PHE	9.7
1	A	7	GLY	9.2
1	A	333	ASP	8.5
1	A	36	VAL	7.9
1	A	37	LEU	7.6
1	A	6	THR	7.3
1	A	8	THR	7.3
1	A	4	GLN	6.1
1	A	103	ASP	5.8
1	A	227	MET	5.6
1	A	385	LEU	5.1
1	A	13	ASP	5.0
1	A	12	GLY	5.0
1	A	9	GLY	4.8
1	A	5	PHE	4.7
1	A	39	TRP	4.5
1	A	404	LEU	4.5
1	A	175	SER	4.4
1	A	10	THR	4.4
1	A	66	LEU	4.1
1	A	238	GLY	4.1
1	A	92	PHE	4.0
1	A	230	ILE	4.0
1	A	237	TYR	4.0
1	A	14	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	11	GLY	3.8
1	A	54	ARG	3.8
1	A	16	LYS	3.7
1	A	41	MET	3.4
1	A	55	LYS	3.4
1	A	271	LEU	3.4
1	A	351	PHE	3.4
1	A	329	LEU	3.4
1	A	182	ALA	3.4
1	A	67	MET	3.2
1	A	405	ALA	3.2
1	A	381	LEU	3.2
1	A	17	VAL	3.0
1	A	414	ILE	2.9
1	A	43	PRO	2.9
1	A	389	CYS	2.9
1	A	174	VAL	2.9
1	A	86	ALA	2.8
1	A	334	ASP	2.7
1	A	110	ILE	2.7
1	A	373	TRP	2.6
1	A	272	VAL	2.6
1	A	219	PRO	2.6
1	A	360	TYR	2.6
1	A	107	ALA	2.6
1	A	253	TYR	2.5
1	A	305	PRO	2.5
1	A	102	LYS	2.5
1	A	235	GLY	2.5
1	A	332	ILE	2.4
1	A	108	PRO	2.4
1	A	34	ALA	2.4
1	A	307	TYR	2.4
1	A	104	VAL	2.3
1	A	222	VAL	2.3
1	A	112	LYS	2.3
1	A	401	ILE	2.3
1	A	316	PRO	2.2
1	A	82	SER	2.2
1	A	306	VAL	2.1
1	A	68	ALA	2.1

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.