



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 PM UTC

PDB ID : 1VRD / pdb_00001vrd
Title : Crystal structure of Inosine-5'-monophosphate dehydrogenase (TM1347) from THERMOTOGA MARITIMA at 2.18 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-02-22
Resolution : 2.18 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

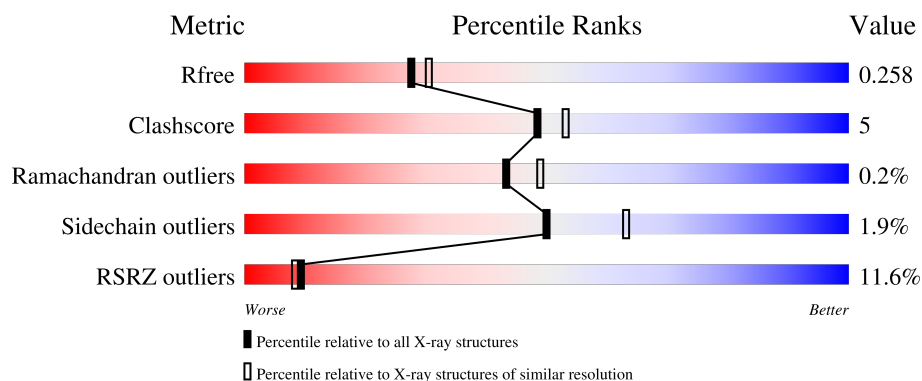
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	494	6% 56% 9% 35%
1	B	494	9% 54% 10% 36%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4876 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 inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2363	1490	414	448	11			
1	B	317	Total	C	N	O	S	0	0	0
			2307	1455	404	438	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9X168
A	-10	GLY	-	expression tag	UNP Q9X168
A	-9	SER	-	expression tag	UNP Q9X168
A	-8	ASP	-	expression tag	UNP Q9X168
A	-7	LYS	-	expression tag	UNP Q9X168
A	-6	ILE	-	expression tag	UNP Q9X168
A	-5	HIS	-	expression tag	UNP Q9X168
A	-4	HIS	-	expression tag	UNP Q9X168
A	-3	HIS	-	expression tag	UNP Q9X168
A	-2	HIS	-	expression tag	UNP Q9X168
A	-1	HIS	-	expression tag	UNP Q9X168
A	0	HIS	-	expression tag	UNP Q9X168
B	-11	MET	-	expression tag	UNP Q9X168
B	-10	GLY	-	expression tag	UNP Q9X168
B	-9	SER	-	expression tag	UNP Q9X168
B	-8	ASP	-	expression tag	UNP Q9X168
B	-7	LYS	-	expression tag	UNP Q9X168
B	-6	ILE	-	expression tag	UNP Q9X168
B	-5	HIS	-	expression tag	UNP Q9X168
B	-4	HIS	-	expression tag	UNP Q9X168
B	-3	HIS	-	expression tag	UNP Q9X168
B	-2	HIS	-	expression tag	UNP Q9X168
B	-1	HIS	-	expression tag	UNP Q9X168
B	0	HIS	-	expression tag	UNP Q9X168

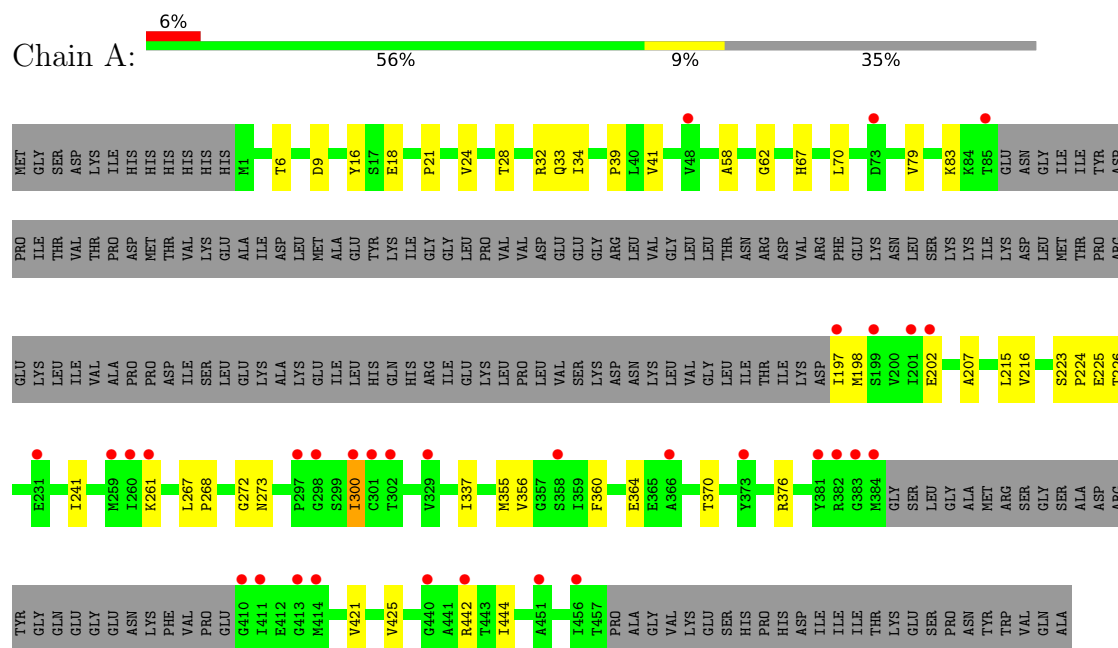
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	107	Total 107	O 107	0	0
2	B	99	Total 99	O 99	0	0

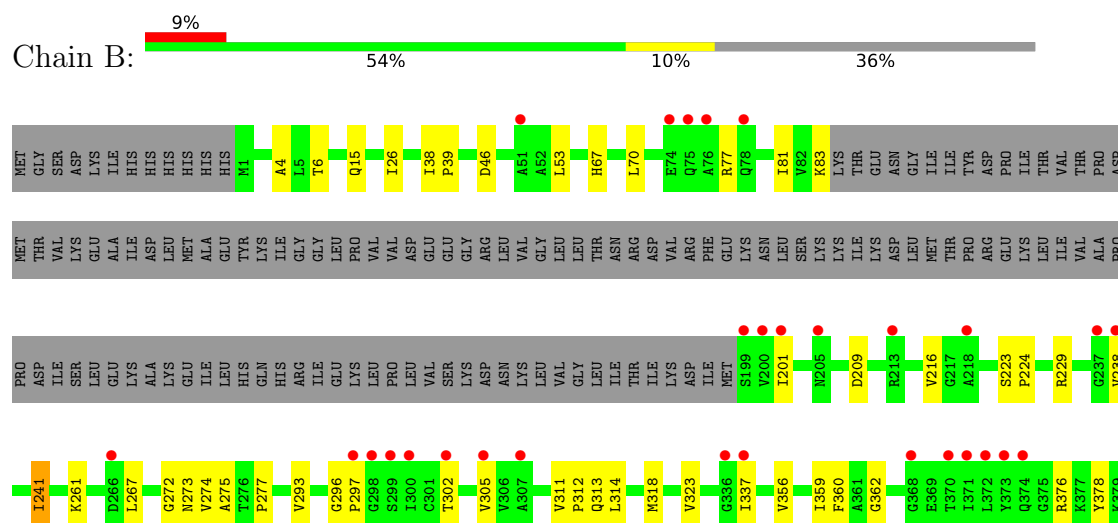
3 Residue-property plots

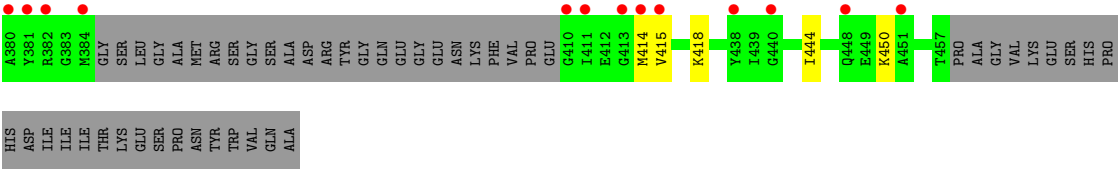
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: inosine-5'-monophosphate dehydrogenase



- Molecule 1: inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	120.08Å 120.08Å 144.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.18 46.12 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.2 (46.12-2.18) 94.2 (46.12-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.258 0.218 , 0.258	Depositor DCC
R_{free} test set	2553 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4876	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	0.93	1/2390 (0.0%)	1.03	0/3233
1	B	0.87	2/2335 (0.1%)	0.99	3/3164 (0.1%)
All	All	0.90	3/4725 (0.1%)	1.01	3/6397 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	ILE	CA-CB	6.00	1.61	1.54
1	A	216	VAL	CA-CB	5.40	1.61	1.55
1	B	305	VAL	CA-CB	5.02	1.60	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	GLN	N-CA-C	5.50	118.20	111.82
1	B	38	ILE	N-CA-C	-5.46	104.72	109.19
1	B	302	THR	N-CA-C	5.22	116.66	111.07

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	2363	0	2454	27	0
1	B	2307	0	2361	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	107	0	0	3	0
2	B	99	0	0	2	0
All	All	4876	0	4815	52	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 5.

All (52) 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:B:15:GLN:NE2	1:B:450:LYS:O	2.01	0.93
1:A:198:MET:O	1:A:202:GLU:HG2	1.80	0.81
1:A:442:ARG:HD2	2:A:576:HOH:O	1.80	0.80
1:B:70:LEU:O	1:B:229:ARG:NH2	2.18	0.75
1:B:241:ILE:HD12	1:B:267:LEU:HD21	1.70	0.73
1:B:6:THR:HB	2:B:556:HOH:O	1.95	0.66
1:A:79:VAL:O	1:A:83:LYS:HG2	1.98	0.64
1:B:362:GLY:HA3	1:B:418:LYS:HE2	1.83	0.60
1:A:300:ILE:O	1:A:300:ILE:CG2	2.52	0.58
1:A:356:VAL:HG23	1:A:360:PHE:CE2	2.39	0.57
1:A:33:GLN:HG2	2:A:562:HOH:O	2.05	0.56
1:B:356:VAL:HG23	1:B:360:PHE:CE2	2.42	0.54
1:A:364:GLU:HG3	2:A:584:HOH:O	2.08	0.54
1:B:223:SER:HB2	1:B:224:PRO:HD2	1.90	0.53
1:A:39:PRO:HG3	1:A:444:ILE:HD11	1.89	0.53
1:B:77:ARG:NH1	1:B:81:ILE:HD11	2.25	0.52
1:B:83:LYS:HD3	1:B:216:VAL:HG12	1.93	0.51
1:B:241:ILE:CD1	1:B:267:LEU:HD21	2.41	0.50
1:A:207:ALA:HB1	1:A:215:LEU:HD12	1.93	0.50
1:B:337:ILE:HG22	1:B:359:ILE:HD12	1.95	0.48
1:B:46:ASP:HA	1:B:67:HIS:CD2	2.48	0.48
1:A:21:PRO:O	1:A:24:VAL:HG22	2.14	0.47
1:A:376:ARG:NH2	1:B:376:ARG:HH12	2.13	0.46
1:B:277:PRO:CB	1:B:323:VAL:HG21	2.46	0.46
1:A:223:SER:HB2	1:A:224:PRO:CD	2.46	0.46
1:A:6:THR:HG22	1:A:9:ASP:OD2	2.16	0.46
1:B:53:LEU:HD11	1:B:360:PHE:HB3	1.98	0.45
1:A:241:ILE:HG13	1:A:267:LEU:HD21	1.99	0.45
1:A:58:ALA:HA	1:A:62:GLY:O	2.17	0.45
1:B:296:GLY:N	1:B:297:PRO:HD3	2.32	0.44
1:A:356:VAL:HG23	1:A:360:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:NZ	1:B:267:LEU:O	2.50	0.44
1:B:314:LEU:HG	1:B:318:MET:HE2	2.00	0.43
1:A:241:ILE:CG1	1:A:267:LEU:HD21	2.49	0.43
1:B:275:ALA:HB1	1:B:311:VAL:HB	2.00	0.43
1:A:356:VAL:CG2	1:A:360:PHE:CE2	3.02	0.43
1:A:34:ILE:HD11	1:A:268:PRO:HG2	1.99	0.43
1:B:39:PRO:HG3	1:B:444:ILE:HD11	2.01	0.43
1:B:67:HIS:CE1	1:B:70:LEU:HG	2.54	0.43
1:A:67:HIS:CE1	1:A:70:LEU:HG	2.54	0.42
1:A:225:GLU:O	1:A:226:THR:C	2.63	0.42
1:B:209:ASP:HB2	2:B:563:HOH:O	2.19	0.42
1:A:272:GLY:HA3	1:A:273:ASN:HA	1.92	0.42
1:B:272:GLY:HA3	1:B:273:ASN:HA	1.97	0.41
1:A:421:VAL:O	1:A:425:VAL:HG23	2.20	0.41
1:B:274:VAL:O	1:B:293:VAL:HA	2.21	0.41
1:A:41:VAL:O	1:A:355:MET:HA	2.21	0.41
1:A:300:ILE:O	1:A:300:ILE:HG22	2.20	0.41
1:B:378:TYR:HB3	1:B:414:MET:HG2	2.03	0.41
1:A:28:THR:HB	1:A:444:ILE:HD12	2.03	0.41
1:B:4:ALA:CB	1:B:312:PRO:HD2	2.51	0.41
1:A:16:TYR:CE2	1:A:18:GLU:HG3	2.56	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	315/494 (64%)	304 (96%)	11 (4%)	0	100	100
1	B	311/494 (63%)	304 (98%)	6 (2%)	1 (0%)	36	39
All	All	626/988 (63%)	608 (97%)	17 (3%)	1 (0%)	43	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	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	246/405 (61%)	240 (98%)	6 (2%)	43	55
1	B	235/405 (58%)	232 (99%)	3 (1%)	61	74
All	All	481/810 (59%)	472 (98%)	9 (2%)	50	63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	197	ILE
1	A	261	LYS
1	A	300	ILE
1	A	337	ILE
1	A	370	THR
1	B	238	VAL
1	B	241	ILE
1	B	415	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	249	HIS

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 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	321/494 (64%)	0.74	32 (9%) 12 11	27, 37, 57, 76	0
1	B	317/494 (64%)	1.01	42 (13%) 7 6	27, 37, 61, 80	0
All	All	638/988 (64%)	0.87	74 (11%) 9 8	27, 37, 60, 80	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	SER	6.3
1	A	85	THR	5.5
1	A	298	GLY	5.3
1	B	299	SER	5.2
1	A	197	ILE	4.8
1	B	438	TYR	4.5
1	A	413	GLY	4.5
1	A	410	GLY	4.4
1	B	413	GLY	4.4
1	B	382	ARG	4.3
1	B	300	ILE	4.3
1	A	411	ILE	4.0
1	A	381	TYR	4.0
1	B	237	GLY	3.9
1	B	298	GLY	3.8
1	B	337	ILE	3.8
1	B	414	MET	3.7
1	B	384	MET	3.7
1	A	440	GLY	3.7
1	A	300	ILE	3.6
1	B	51	ALA	3.6
1	B	373	TYR	3.6
1	B	410	GLY	3.5
1	A	442	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	384	MET	3.4
1	B	218	ALA	3.4
1	B	201	ILE	3.4
1	B	374	GLN	3.3
1	B	200	VAL	3.3
1	A	48	VAL	3.2
1	B	371	ILE	3.2
1	A	302	THR	3.2
1	B	411	ILE	3.2
1	A	382	ARG	3.1
1	B	297	PRO	3.0
1	B	78	GLN	2.9
1	B	380	ALA	2.8
1	B	372	LEU	2.8
1	A	231	GLU	2.8
1	A	260	ILE	2.8
1	B	205	ASN	2.7
1	A	329	VAL	2.6
1	B	415	VAL	2.6
1	A	383	GLY	2.6
1	B	368	GLY	2.6
1	A	202	GLU	2.6
1	B	266	ASP	2.5
1	A	261	LYS	2.5
1	B	75	GLN	2.5
1	A	73	ASP	2.4
1	A	301	CYS	2.4
1	A	414	MET	2.3
1	B	76	ALA	2.3
1	A	201	ILE	2.3
1	A	297	PRO	2.3
1	B	440	GLY	2.3
1	B	381	TYR	2.3
1	A	199	SER	2.2
1	B	307	ALA	2.2
1	B	451	ALA	2.2
1	A	358	SER	2.2
1	B	305	VAL	2.1
1	B	448	GLN	2.1
1	A	366	ALA	2.1
1	B	74	GLU	2.1
1	B	302	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	213	ARG	2.1
1	B	238	VAL	2.1
1	A	451	ALA	2.1
1	A	259	MET	2.1
1	B	336	GLY	2.1
1	A	456	ILE	2.1
1	B	370	THR	2.0
1	A	373	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.