



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:04 PM UTC

PDB ID : 1ZUP / pdb_00001zup
Title : CRYSTAL STRUCTURE OF A PUTATIVE NUCLEASE WITH A RIBONUCLEASE H-LIKE MOTIF FOLD (TM1739) FROM THERMOTOGA MARITIMA AT 2.20 Å RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-05-31
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

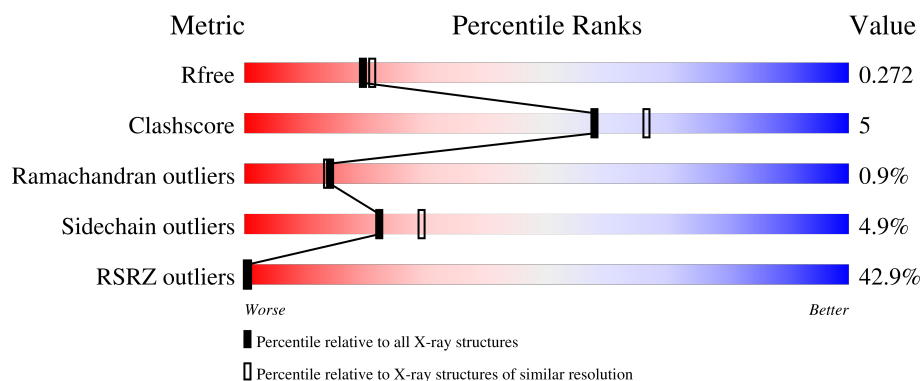
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	315	13% 80% 12% 7%
1	B	315	64% 75% 15% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4471 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 hypothetical protein TM1739.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	Se	0	5	0
			2336	1500	394	435	1	6			
1	B	287	Total	C	N	O	S	Se	0	1	0
			2065	1317	347	395	1	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q9X261
A	-10	GLY	-	expression tag	UNP Q9X261
A	-9	SER	-	expression tag	UNP Q9X261
A	-8	ASP	-	expression tag	UNP Q9X261
A	-7	LYS	-	expression tag	UNP Q9X261
A	-6	ILE	-	expression tag	UNP Q9X261
A	-5	HIS	-	expression tag	UNP Q9X261
A	-4	HIS	-	expression tag	UNP Q9X261
A	-3	HIS	-	expression tag	UNP Q9X261
A	-2	HIS	-	expression tag	UNP Q9X261
A	-1	HIS	-	expression tag	UNP Q9X261
A	0	HIS	-	expression tag	UNP Q9X261
A	1	MSE	MET	modified residue	UNP Q9X261
A	129	MSE	MET	modified residue	UNP Q9X261
A	136	MSE	MET	modified residue	UNP Q9X261
A	148	MSE	MET	modified residue	UNP Q9X261
A	203	MSE	MET	modified residue	UNP Q9X261
A	293	MSE	MET	modified residue	UNP Q9X261
B	-11	MSE	-	expression tag	UNP Q9X261
B	-10	GLY	-	expression tag	UNP Q9X261
B	-9	SER	-	expression tag	UNP Q9X261
B	-8	ASP	-	expression tag	UNP Q9X261
B	-7	LYS	-	expression tag	UNP Q9X261
B	-6	ILE	-	expression tag	UNP Q9X261
B	-5	HIS	-	expression tag	UNP Q9X261

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q9X261
B	-3	HIS	-	expression tag	UNP Q9X261
B	-2	HIS	-	expression tag	UNP Q9X261
B	-1	HIS	-	expression tag	UNP Q9X261
B	0	HIS	-	expression tag	UNP Q9X261
B	1	MSE	MET	modified residue	UNP Q9X261
B	129	MSE	MET	modified residue	UNP Q9X261
B	136	MSE	MET	modified residue	UNP Q9X261
B	148	MSE	MET	modified residue	UNP Q9X261
B	203	MSE	MET	modified residue	UNP Q9X261
B	293	MSE	MET	modified residue	UNP Q9X261

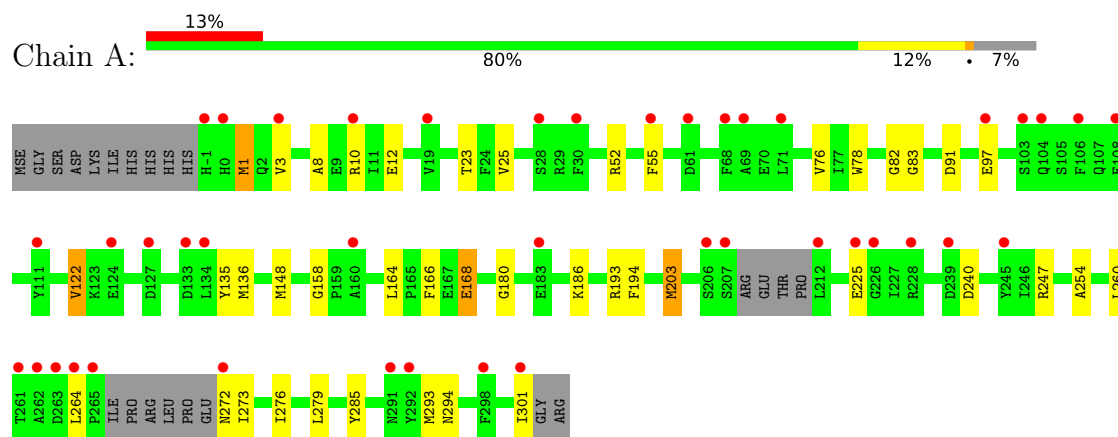
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	13	Total O 13 13	0	0

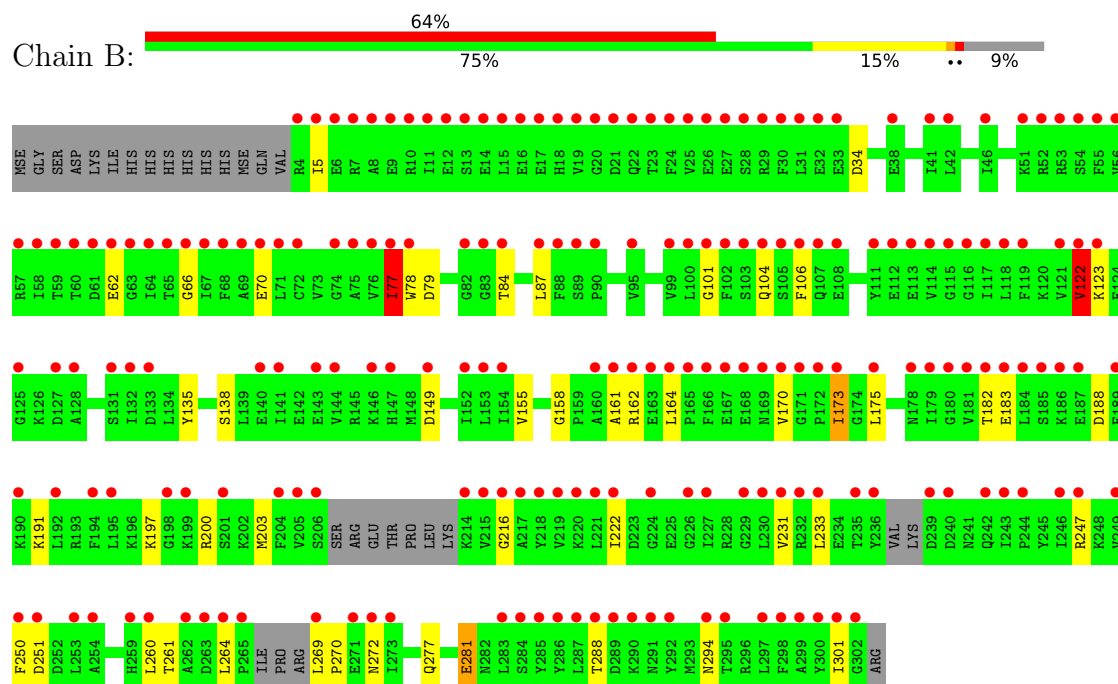
3 Residue-property plots [i](#)

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: hypothetical protein TM1739



- Molecule 1: hypothetical protein TM1739



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.43Å 82.43Å 234.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.7 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.228 , 0.266 0.239 , 0.272	Depositor DCC
R_{free} test set	2114 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4471	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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	1.09	6/2369 (0.3%)	1.03	6/3177 (0.2%)
1	B	0.97	5/2092 (0.2%)	1.03	8/2810 (0.3%)
All	All	1.04	11/4461 (0.2%)	1.03	14/5987 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	ASP	CA-C	10.64	1.66	1.52
1	A	1	MSE	SE-CE	-8.45	1.70	1.95
1	B	34	ASP	C-N	8.34	1.44	1.33
1	B	251	ASP	C-O	7.76	1.33	1.24
1	A	203	MSE	SE-CE	-6.60	1.75	1.95
1	A	136	MSE	CB-CG	6.46	1.71	1.52
1	A	25	VAL	CA-C	-5.59	1.45	1.53
1	A	293	MSE	SE-CE	5.37	2.11	1.95
1	B	216	GLY	C-O	5.26	1.30	1.23
1	B	138	SER	C-O	-5.25	1.18	1.24
1	A	254	ALA	CA-CB	-5.22	1.45	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	ASP	O-C-N	8.71	134.18	122.59
1	B	251	ASP	CA-C-O	8.19	129.10	120.42
1	B	77	ILE	CB-CA-C	-7.77	100.28	110.84
1	A	122	VAL	CB-CA-C	7.07	119.73	110.12
1	A	180	GLY	N-CA-C	6.97	121.08	112.64
1	B	122	VAL	CB-CA-C	6.25	118.86	110.42
1	A	158	GLY	CA-C-N	6.06	126.07	119.89
1	A	158	GLY	C-N-CA	6.06	126.07	119.89
1	A	168	GLU	N-CA-C	6.02	118.61	111.33
1	A	225	GLU	N-CA-C	5.58	119.83	112.25
1	B	158	GLY	CA-C-N	5.52	125.52	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	GLY	C-N-CA	5.52	125.52	119.89
1	B	123	LYS	N-CA-C	5.42	117.39	110.61
1	B	77	ILE	N-CA-CB	5.36	117.43	110.99

There are no chirality outliers.

There are no planarity outliers.

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	2336	0	2302	25	0
1	B	2065	0	1915	20	0
2	A	57	0	0	0	0
2	B	13	0	0	0	0
All	All	4471	0	4217	39	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 (39) 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:203:MSE:HE1	1:A:247:ARG:HG3	1.67	0.76
1:A:1:MSE:HE2	1:A:3:VAL:CG2	2.14	0.76
1:A:203:MSE:HE1	1:A:247:ARG:CG	2.30	0.62
1:A:1:MSE:HE3	1:B:106:PHE:CZ	2.37	0.60
1:A:1:MSE:HE3	1:B:106:PHE:HZ	1.68	0.58
1:B:203:MSE:HE3	1:B:250:PHE:CD2	2.40	0.57
1:A:1:MSE:HE2	1:A:3:VAL:HG21	1.86	0.56
1:A:148:MSE:CE	1:A:164:LEU:HD22	2.37	0.55
1:B:277:GLN:O	1:B:281:GLU:HG3	2.10	0.52
1:A:193:ARG:NH1	1:A:194:PHE:CZ	2.79	0.51
1:B:161:ALA:O	1:B:162:ARG:C	2.54	0.51
1:A:76:VAL:HG13	1:A:279:LEU:HD13	1.93	0.50
1:A:203:MSE:HE1	1:A:247:ARG:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:VAL:HG21	1:B:135:TYR:CG	2.47	0.49
1:A:273:ILE:HG12	1:A:276:ILE:HD12	1.94	0.48
1:A:301:ILE:HG23	1:B:5:ILE:HD13	1.96	0.47
1:A:10:ARG:HG3	1:B:294:ASN:ND2	2.30	0.47
1:A:148:MSE:HE1	1:A:164:LEU:HD22	1.96	0.47
1:A:10:ARG:HD3	1:A:12:GLU:OE2	2.16	0.45
1:A:78:TRP:CZ2	1:A:260:LEU:HD21	2.52	0.45
1:A:55:PHE:HB3	1:A:294:ASN:OD1	2.15	0.45
1:B:188:ASP:O	1:B:191:LYS:HB2	2.17	0.45
1:B:70:GLU:OE2	1:B:288:THR:OG1	2.34	0.44
1:A:8:ALA:HB2	1:B:301:ILE:HG21	1.99	0.44
1:A:82:GLY:O	1:A:83:GLY:C	2.61	0.44
1:B:78:TRP:CZ2	1:B:260:LEU:HD21	2.52	0.43
1:B:272[A]:ASN:N	1:B:272[A]:ASN:HD22	2.16	0.43
1:B:155:VAL:HG22	1:B:173:ILE:HG23	1.99	0.43
1:A:285[B]:TYR:O	1:A:285[B]:TYR:CG	2.71	0.43
1:B:66:GLY:HA2	1:B:101:GLY:O	2.19	0.43
1:B:182:THR:O	1:B:183:GLU:HB2	2.19	0.43
1:A:1:MSE:HE2	1:A:3:VAL:HG23	2.00	0.42
1:A:166:PHE:CE2	1:A:168:GLU:HA	2.54	0.42
1:B:277:GLN:O	1:B:281:GLU:CG	2.67	0.42
1:A:97:GLU:OE1	1:A:135:TYR:OH	2.32	0.42
1:A:203:MSE:CE	1:A:247:ARG:HA	2.49	0.42
1:B:77:ILE:CD1	1:B:87:LEU:HG	2.49	0.42
1:A:186:LYS:NZ	1:B:62:GLU:OE1	2.41	0.41
1:B:200:ARG:NH2	1:B:247:ARG:HD2	2.35	0.41

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	292/315 (93%)	282 (97%)	9 (3%)	1 (0%)	36	42
1	B	280/315 (89%)	252 (90%)	24 (9%)	4 (1%)	9	7
All	All	572/630 (91%)	534 (93%)	33 (6%)	5 (1%)	14	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	PRO
1	B	264	LEU
1	A	264	LEU
1	B	197	LYS
1	B	170	VAL

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	241/274 (88%)	235 (98%)	6 (2%)	42	56
1	B	195/274 (71%)	180 (92%)	15 (8%)	12	13
All	All	436/548 (80%)	415 (95%)	21 (5%)	22	30

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	52	ARG
1	A	91	ASP
1	A	122	VAL
1	A	240	ASP
1	A	272	ASN
1	B	77	ILE
1	B	79	ASP
1	B	84	THR
1	B	104	GLN
1	B	122	VAL

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Mol	Chain	Res	Type
1	B	149	ASP
1	B	164	LEU
1	B	173	ILE
1	B	175	LEU
1	B	222	ILE
1	B	231	VAL
1	B	233	LEU
1	B	261	THR
1	B	269	LEU
1	B	281	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	259	HIS
1	A	277	GLN
1	B	147	HIS
1	B	242	GLN

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

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	287/315 (91%)	1.06	42 (14%) 6 4	28, 65, 82, 121	5 (1%)
1	B	282/315 (89%)	2.97	202 (71%) 0 0	41, 63, 80, 119	1 (0%)
All	All	569/630 (90%)	2.01	244 (42%) 0 0	28, 64, 81, 121	6 (1%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	PRO	7.8
1	B	64	ILE	6.7
1	B	297	LEU	6.6
1	B	301	ILE	6.6
1	B	66	GLY	6.5
1	B	67	ILE	6.4
1	B	56	VAL	6.2
1	B	68	PHE	6.2
1	B	65	THR	6.1
1	B	220	LYS	6.0
1	B	17	GLU	5.9
1	B	58	ILE	5.9
1	B	19	VAL	5.9
1	B	59	THR	5.9
1	B	302	GLY	5.8
1	B	262	ALA	5.6
1	B	229	GLY	5.6
1	B	264	LEU	5.5
1	B	69	ALA	5.5
1	B	55	PHE	5.5
1	B	15	LEU	5.4
1	B	11	ILE	5.4
1	B	63	GLY	5.3
1	B	171	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	57	ARG	5.3
1	B	184	LEU	5.2
1	B	122	VAL	5.2
1	B	298	PHE	5.2
1	B	265	PRO	5.2
1	B	100	LEU	5.1
1	B	132	ILE	5.1
1	B	179	ILE	5.0
1	B	83	GLY	4.9
1	B	246	ILE	4.9
1	A	0	HIS	4.9
1	B	41	ILE	4.7
1	B	259	HIS	4.7
1	B	14	GLU	4.7
1	B	218	TYR	4.7
1	B	60	THR	4.6
1	B	13	SER	4.6
1	B	101	GLY	4.5
1	B	105	SER	4.5
1	B	149	ASP	4.5
1	B	251	ASP	4.5
1	B	114	VAL	4.4
1	B	230	LEU	4.4
1	B	117	ILE	4.4
1	B	128	ALA	4.4
1	B	30	PHE	4.4
1	B	18	HIS	4.3
1	B	102	PHE	4.3
1	B	299	ALA	4.3
1	B	131	SER	4.3
1	B	295	THR	4.3
1	B	84	THR	4.2
1	A	263	ASP	4.2
1	B	219	VAL	4.2
1	B	24	PHE	4.2
1	B	121	VAL	4.1
1	B	5	ILE	4.1
1	B	169	ASN	4.1
1	B	95	VAL	4.1
1	B	90	PRO	4.1
1	B	254	ALA	4.1
1	B	192	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	221	LEU	4.1
1	B	180	GLY	4.1
1	B	291	ASN	4.0
1	B	106	PHE	4.0
1	B	292	TYR	4.0
1	B	99	VAL	3.9
1	B	28	SER	3.9
1	B	21	ASP	3.9
1	B	165	PRO	3.9
1	B	42	LEU	3.9
1	B	115	GLY	3.8
1	B	116	GLY	3.8
1	B	119	PHE	3.8
1	B	140	GLU	3.8
1	B	222	ILE	3.8
1	B	289	ASP	3.7
1	B	232	ARG	3.7
1	B	166	PHE	3.7
1	B	4	ARG	3.6
1	B	205	VAL	3.6
1	B	108	GLU	3.6
1	B	249	VAL	3.6
1	B	104	GLN	3.6
1	B	61	ASP	3.6
1	A	262	ALA	3.6
1	B	46	ILE	3.5
1	B	286	TYR	3.5
1	B	125	GLY	3.5
1	B	54	SER	3.5
1	B	236	TYR	3.5
1	B	204	PHE	3.5
1	B	8	ALA	3.5
1	B	269	LEU	3.5
1	A	61	ASP	3.4
1	B	152	ILE	3.4
1	B	300	TYR	3.4
1	B	52	ARG	3.4
1	B	22	GLN	3.4
1	B	153	LEU	3.3
1	B	53	ARG	3.3
1	B	147	HIS	3.3
1	B	23	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	250	PHE	3.3
1	B	31	LEU	3.3
1	B	82	GLY	3.2
1	B	216	GLY	3.2
1	B	10	ARG	3.2
1	B	77	ILE	3.2
1	B	103	SER	3.2
1	B	195	LEU	3.2
1	B	172	PRO	3.2
1	B	288	THR	3.2
1	B	71	LEU	3.2
1	B	7	ARG	3.1
1	B	206	SER	3.1
1	B	183	GLU	3.1
1	B	27	GLU	3.1
1	B	294	ASN	3.1
1	B	231	VAL	3.1
1	A	265	PRO	3.1
1	B	29	ARG	3.1
1	B	227	ILE	3.1
1	A	239	ASP	3.1
1	B	75	ALA	3.1
1	B	170	VAL	3.1
1	A	291	ASN	3.0
1	A	301	ILE	3.0
1	B	141	ILE	3.0
1	B	271	GLU	3.0
1	B	201	SER	3.0
1	B	235	THR	3.0
1	B	78	TRP	3.0
1	B	185	SER	2.9
1	B	284	SER	2.9
1	B	253	LEU	2.9
1	B	215	VAL	2.9
1	B	189	PHE	2.9
1	A	207	SER	2.8
1	B	290	LYS	2.8
1	A	228	ARG	2.8
1	B	162	ARG	2.8
1	B	178	ASN	2.8
1	A	-1	HIS	2.8
1	B	113	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	104[A]	GLN	2.8
1	B	107	GLN	2.8
1	B	182	THR	2.7
1	B	164	LEU	2.7
1	A	19	VAL	2.7
1	B	51	LYS	2.7
1	A	111	TYR	2.7
1	A	106	PHE	2.7
1	B	272[A]	ASN	2.7
1	B	16	GLU	2.7
1	B	112	GLU	2.7
1	B	168	GLU	2.7
1	B	118	LEU	2.7
1	A	272	ASN	2.6
1	B	123	LYS	2.6
1	B	6	GLU	2.6
1	B	243	ILE	2.6
1	A	183	GLU	2.6
1	B	263	ASP	2.6
1	B	186	LYS	2.6
1	A	264	LEU	2.6
1	B	74	GLY	2.5
1	B	154	ILE	2.5
1	B	127	ASP	2.5
1	B	224	GLY	2.5
1	B	12	GLU	2.5
1	B	70	GLU	2.5
1	B	26	GLU	2.5
1	B	173	ILE	2.4
1	A	245	TYR	2.4
1	B	89	SER	2.4
1	A	298	PHE	2.4
1	B	190	LYS	2.4
1	B	133	ASP	2.4
1	B	163	GLU	2.4
1	A	206	SER	2.4
1	B	273	ILE	2.4
1	B	260	LEU	2.4
1	B	285	TYR	2.4
1	B	143	GLU	2.4
1	B	199	LYS	2.4
1	B	214	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	72	CYS	2.4
1	A	134	LEU	2.4
1	B	160	ALA	2.3
1	A	3	VAL	2.3
1	B	181	VAL	2.3
1	B	20	GLY	2.3
1	A	160	ALA	2.3
1	B	283	LEU	2.3
1	B	25	VAL	2.3
1	A	225	GLU	2.3
1	A	69	ALA	2.2
1	A	28	SER	2.2
1	A	71	LEU	2.2
1	A	30	PHE	2.2
1	B	194	PHE	2.2
1	A	97	GLU	2.2
1	A	124	GLU	2.2
1	B	242	GLN	2.2
1	A	261	THR	2.2
1	A	55	PHE	2.2
1	B	88	PHE	2.2
1	B	187	GLU	2.2
1	A	292	TYR	2.2
1	B	287	LEU	2.2
1	B	76	VAL	2.2
1	A	68	PHE	2.2
1	B	239	ASP	2.2
1	A	226	GLY	2.2
1	A	103	SER	2.2
1	B	217	ALA	2.2
1	A	212	LEU	2.1
1	B	87	LEU	2.1
1	B	233	LEU	2.1
1	B	240	ASP	2.1
1	B	146	LYS	2.1
1	A	127	ASP	2.1
1	A	133	ASP	2.1
1	B	167	GLU	2.1
1	B	144	VAL	2.1
1	B	198	GLY	2.1
1	A	10	ARG	2.1
1	B	247	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	108	GLU	2.1
1	B	33	GLU	2.1
1	B	175	LEU	2.1
1	B	32	GLU	2.0
1	B	62	GLU	2.0
1	B	111	TYR	2.0
1	B	226	GLY	2.0
1	B	9	GLU	2.0
1	B	38	GLU	2.0
1	B	161	ALA	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.