



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 11:44 AM EDT

PDB ID : 3NI7
Title : Crystal structure of the TetR transcriptional regulator from *Nitrosomonas europaea* ATCC 19718
Authors : Knapik, A.; Chruszcz, M.; Cymborowski, M.; Xu, X.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Minor, W.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-06-15
Resolution : 2.78 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

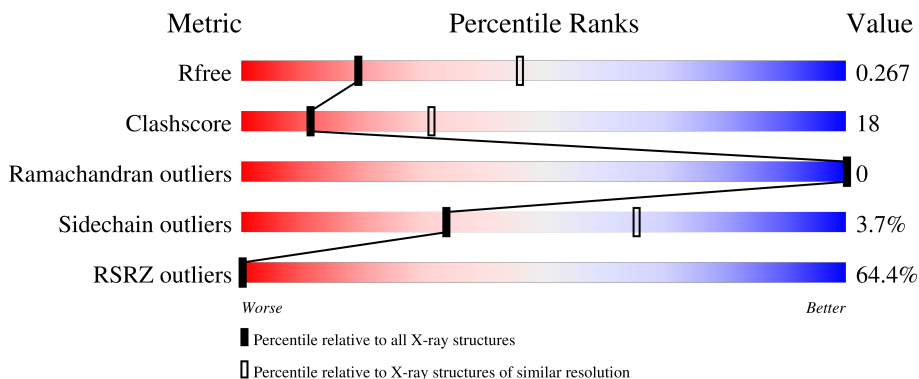
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	213	
1	B	213	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2735 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 Bacterial regulatory proteins, TetR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	174	1383	880	241	252	10	0	1	0
1	B	173	1352	869	233	241	9	0	0	0

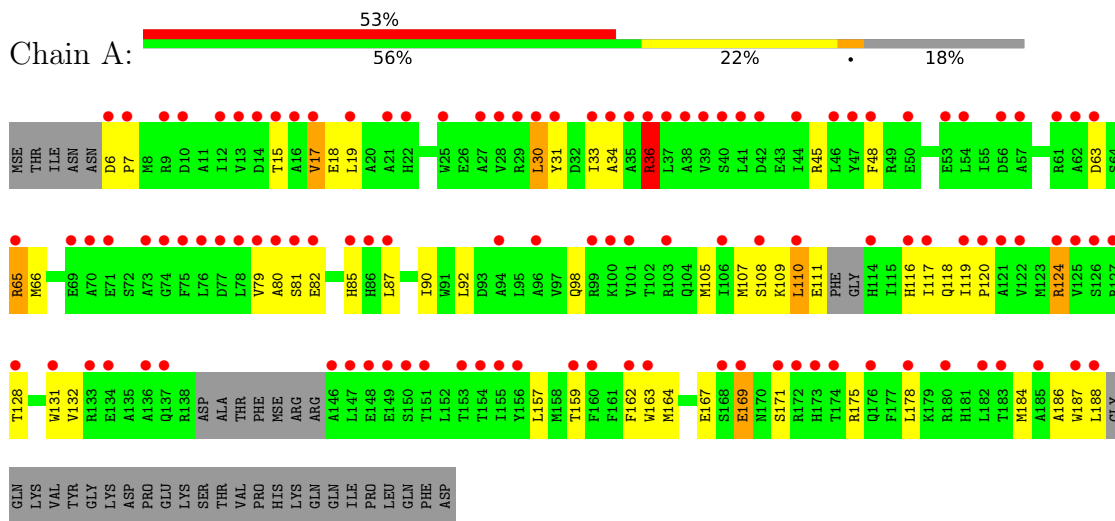
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q82XH4
B	1	MSE	-	initiating methionine	UNP Q82XH4

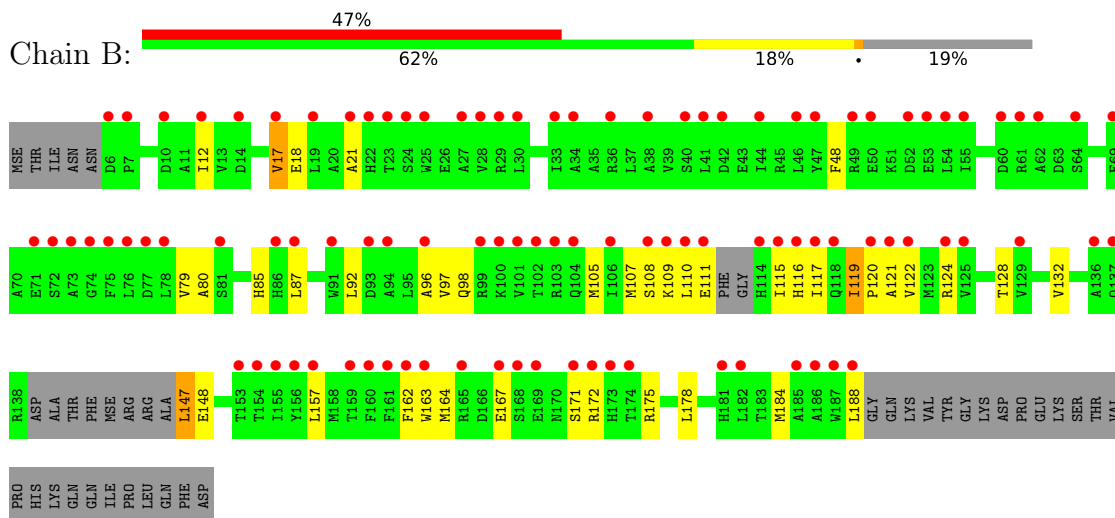
3 Residue-property plots

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: Bacterial regulatory proteins, TetR family



- Molecule 1: Bacterial regulatory proteins, TetR family



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.22Å 75.38Å 98.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.78 34.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.78) 99.7 (34.62-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.249 , 0.279 0.255 , 0.267	Depositor DCC
R_{free} test set	583 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtrriage
Anisotropy	0.991	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 138.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2735	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% 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	0.96	2/1399 (0.1%)	0.90	2/1881 (0.1%)
1	B	0.91	2/1369 (0.1%)	0.85	1/1843 (0.1%)
All	All	0.94	4/2768 (0.1%)	0.88	3/3724 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	GLU	CB-CG	-5.84	1.41	1.52
1	B	148	GLU	CG-CD	5.71	1.60	1.51
1	B	167	GLU	CB-CG	-5.67	1.41	1.52
1	A	167	GLU	CB-CG	-5.36	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	65	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	36	ARG	NE-CZ-NH2	-5.39	117.60	120.30

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	1383	0	1325	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1352	0	1297	39	0
All	All	2735	0	2622	95	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 18.

All (95) 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:110:LEU:HD23	1:A:111:GLU:N	1.52	1.25
1:A:110:LEU:HD23	1:A:110:LEU:C	1.76	1.06
1:A:116:HIS:O	1:A:120:PRO:HD3	1.54	1.06
1:A:110:LEU:C	1:A:110:LEU:CD2	2.30	0.98
1:B:115:ILE:O	1:B:119:ILE:HG22	1.63	0.98
1:A:117:ILE:O	1:A:120:PRO:HG2	1.69	0.93
1:A:119:ILE:HG23	1:A:120:PRO:HD3	1.52	0.89
1:A:85:HIS:CD2	1:A:178:LEU:HD23	2.16	0.80
1:A:119:ILE:N	1:A:120:PRO:HD2	1.97	0.79
1:A:116:HIS:O	1:A:120:PRO:CD	2.30	0.78
1:A:117:ILE:O	1:A:120:PRO:CG	2.30	0.78
1:A:19:LEU:HD21	1:A:36:ARG:HG3	1.68	0.75
1:B:119:ILE:HG23	1:B:120:PRO:HD3	1.67	0.75
1:A:107:MSE:O	1:A:110:LEU:HB3	1.88	0.73
1:B:119:ILE:HG23	1:B:120:PRO:CD	2.19	0.73
1:A:117:ILE:C	1:A:120:PRO:HD2	2.11	0.71
1:B:105:MSE:O	1:B:108:SER:HB3	1.90	0.71
1:A:110:LEU:HD23	1:A:111:GLU:CB	2.20	0.70
1:A:110:LEU:HD23	1:A:111:GLU:CA	2.20	0.69
1:A:157:LEU:HD12	1:B:157:LEU:HD12	1.72	0.69
1:A:119:ILE:CG2	1:A:120:PRO:HD3	2.21	0.69
1:A:117:ILE:O	1:A:120:PRO:HD2	1.94	0.67
1:A:110:LEU:CD2	1:A:111:GLU:CB	2.73	0.67
1:A:17:VAL:HG13	1:A:98:GLN:HG3	1.77	0.66
1:A:162:PHE:CE1	1:B:111:GLU:HA	2.31	0.65
1:A:119:ILE:N	1:A:120:PRO:CD	2.59	0.65
1:A:119:ILE:HG23	1:A:120:PRO:CD	2.27	0.64
1:B:110:LEU:HG	1:B:111:GLU:N	2.12	0.63
1:B:92:LEU:HD22	1:B:163:TRP:CD2	2.33	0.62
1:A:105:MSE:O	1:A:108:SER:HB3	1.99	0.62
1:B:17:VAL:HG13	1:B:98:GLN:HG3	1.81	0.62
1:A:117:ILE:O	1:A:120:PRO:CD	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HB	1:B:184:MSE:CE	2.32	0.60
1:A:162:PHE:HE1	1:B:111:GLU:HA	1.67	0.59
1:A:107:MSE:CE	1:A:164:MSE:HE1	2.32	0.59
1:B:119:ILE:N	1:B:120:PRO:HD2	2.17	0.59
1:B:171:SER:O	1:B:175:ARG:HG3	2.03	0.59
1:A:92:LEU:HD22	1:A:163:TRP:CD2	2.38	0.58
1:B:128:THR:O	1:B:132:VAL:HG23	2.03	0.58
1:A:171:SER:O	1:A:175:ARG:HG3	2.03	0.58
1:B:117:ILE:O	1:B:120:PRO:HG2	2.04	0.57
1:A:63:ASP:OD2	1:A:124:ARG:NH2	2.37	0.57
1:A:119:ILE:HD12	1:A:119:ILE:O	2.05	0.56
1:B:116:HIS:O	1:B:120:PRO:HG3	2.05	0.56
1:A:110:LEU:C	1:A:110:LEU:HD22	2.22	0.55
1:B:85:HIS:CD2	1:B:178:LEU:HD23	2.41	0.55
1:A:116:HIS:O	1:A:119:ILE:CG2	2.55	0.55
1:A:118:GLN:C	1:A:120:PRO:HD2	2.26	0.55
1:B:110:LEU:O	1:B:111:GLU:C	2.43	0.55
1:A:107:MSE:HE2	1:A:164:MSE:HE1	1.89	0.54
1:A:128:THR:O	1:A:132:VAL:HG23	2.09	0.53
1:A:116:HIS:O	1:A:119:ILE:HG22	2.10	0.52
1:A:111:GLU:HA	1:B:162:PHE:CE1	2.46	0.51
1:B:87:LEU:HD12	1:B:132:VAL:HG13	1.92	0.51
1:B:116:HIS:O	1:B:120:PRO:CG	2.59	0.51
1:A:119:ILE:HB	1:B:184:MSE:HE3	1.94	0.50
1:A:117:ILE:C	1:A:120:PRO:CD	2.80	0.49
1:A:45:ARG:HA	1:A:48:PHE:O	2.13	0.48
1:B:124:ARG:O	1:B:128:THR:OG1	2.26	0.47
1:A:30:LEU:HD12	1:A:33:ILE:HD12	1.97	0.47
1:A:6:ASP:N	1:A:7:PRO:CD	2.78	0.47
1:B:12:ILE:HG21	1:B:48:PHE:CD1	2.50	0.47
1:A:66:MSE:HE3	1:A:131:TRP:CE3	2.49	0.46
1:B:107:MSE:O	1:B:110:LEU:HB2	2.16	0.46
1:A:79:VAL:HG12	1:A:80:ALA:N	2.31	0.46
1:B:116:HIS:O	1:B:120:PRO:CD	2.64	0.46
1:B:119:ILE:O	1:B:119:ILE:HD12	2.16	0.45
1:B:171:SER:O	1:B:172:ARG:C	2.56	0.44
1:A:111:GLU:HA	1:B:162:PHE:HE1	1.83	0.44
1:B:92:LEU:HD22	1:B:163:TRP:CG	2.53	0.44
1:A:119:ILE:CG2	1:A:120:PRO:CD	2.91	0.43
1:A:15:THR:HG23	1:A:36:ARG:HD2	2.00	0.43
1:B:119:ILE:HG23	1:B:120:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:NH1	1:A:90:ILE:HD12	2.33	0.43
1:B:147:LEU:HA	1:B:147:LEU:HD12	1.75	0.43
1:B:188:LEU:N	1:B:188:LEU:HD12	2.33	0.43
1:A:31:TYR:O	1:A:34:ALA:HB3	2.19	0.43
1:B:18:GLU:O	1:B:21:ALA:HB3	2.19	0.43
1:A:92:LEU:HD22	1:A:163:TRP:CG	2.54	0.43
1:A:18:GLU:HB3	1:A:36:ARG:HH22	1.85	0.42
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.70	0.42
1:A:169:GLU:O	1:A:169:GLU:HG2	2.18	0.42
1:B:119:ILE:N	1:B:120:PRO:CD	2.82	0.42
1:A:110:LEU:HD22	1:A:110:LEU:O	2.19	0.42
1:B:79:VAL:HG12	1:B:80:ALA:N	2.34	0.41
1:A:159:THR:HG21	1:A:178:LEU:HD13	2.02	0.41
1:A:15:THR:CG2	1:A:33:ILE:HG23	2.50	0.41
1:A:110:LEU:CD2	1:A:111:GLU:N	2.44	0.41
1:A:188:LEU:N	1:A:188:LEU:HD12	2.35	0.41
1:B:121:ALA:O	1:B:122:VAL:C	2.56	0.41
1:A:87:LEU:HD12	1:A:132:VAL:HG13	2.03	0.41
1:A:186:ALA:O	1:A:187:TRP:C	2.59	0.41
1:B:96:ALA:O	1:B:97:VAL:C	2.59	0.40
1:B:107:MSE:CE	1:B:164:MSE:HE1	2.51	0.40
1:A:81:SER:OG	1:A:82:GLU:N	2.53	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	169/213 (79%)	165 (98%)	4 (2%)	0	100	100
1	B	167/213 (78%)	159 (95%)	8 (5%)	0	100	100
All	All	336/426 (79%)	324 (96%)	12 (4%)	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	137/176 (78%)	129 (94%)	8 (6%)	20	47
1	B	131/176 (74%)	128 (98%)	3 (2%)	50	79
All	All	268/352 (76%)	257 (96%)	11 (4%)	34	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	30	LEU
1	A	36	ARG
1	A	109	LYS
1	A	110	LEU
1	A	124	ARG
1	A	184[A]	MSE
1	A	184[B]	MSE
1	B	17	VAL
1	B	109	LYS
1	B	119	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	165/213 (77%)	2.69	112 (67%) 0 0	75, 95, 126, 159	0
1	B	164/213 (76%)	2.87	100 (60%) 0 0	78, 99, 133, 172	0
All	All	329/426 (77%)	2.78	212 (64%) 0 0	75, 97, 133, 172	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	HIS	10.9
1	B	77	ASP	8.5
1	B	94	ALA	7.8
1	A	74	GLY	7.8
1	A	136	ALA	7.8
1	B	117	ILE	7.6
1	B	50	GLU	7.5
1	A	117	ILE	7.2
1	B	7	PRO	7.2
1	B	73	ALA	7.1
1	A	73	ALA	7.0
1	B	38	ALA	6.9
1	B	108	SER	6.7
1	B	21	ALA	6.7
1	A	7	PRO	6.5
1	A	162	PHE	6.4
1	B	19	LEU	6.4
1	A	76	LEU	6.3
1	B	12	ILE	6.3
1	A	69	GLU	6.0
1	A	34	ALA	5.7
1	A	101	VAL	5.7
1	B	93	ASP	5.5
1	A	30	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	169	GLU	5.3
1	B	168	SER	5.2
1	B	17	VAL	5.2
1	A	16	ALA	5.2
1	B	162	PHE	5.1
1	B	27	ALA	5.1
1	B	28	VAL	5.1
1	A	40	SER	5.0
1	B	125	VAL	5.0
1	B	81	SER	4.9
1	A	81	SER	4.8
1	B	153	THR	4.8
1	B	122	VAL	4.8
1	A	108	SER	4.7
1	B	100	LYS	4.7
1	A	27	ALA	4.7
1	B	101	VAL	4.7
1	A	173	HIS	4.7
1	B	172	ARG	4.7
1	A	114	HIS	4.6
1	B	121	ALA	4.6
1	B	186	ALA	4.6
1	B	76	LEU	4.5
1	A	42	ASP	4.5
1	B	174	THR	4.4
1	B	120	PRO	4.4
1	A	168	SER	4.4
1	A	6	ASP	4.2
1	A	82	GLU	4.2
1	B	110	LEU	4.2
1	A	171	SER	4.2
1	B	62	ALA	4.1
1	A	120	PRO	4.1
1	B	74	GLY	4.1
1	B	87	LEU	4.1
1	A	96	ALA	4.1
1	B	188	LEU	4.0
1	B	165	ARG	4.0
1	A	87	LEU	4.0
1	A	176	GLN	3.9
1	A	131	TRP	3.9
1	B	96	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	100	LYS	3.9
1	A	28	VAL	3.9
1	A	94	ALA	3.8
1	B	167	GLU	3.8
1	B	137	GLN	3.8
1	A	148	GLU	3.8
1	A	103	ARG	3.8
1	A	174	THR	3.7
1	A	99	ARG	3.7
1	B	136	ALA	3.7
1	B	46	LEU	3.7
1	B	36	ARG	3.7
1	A	172	ARG	3.6
1	B	109	LYS	3.6
1	B	10	ASP	3.6
1	A	163	TRP	3.6
1	A	75	PHE	3.6
1	A	10	ASP	3.5
1	B	154	THR	3.5
1	A	17	VAL	3.5
1	B	23	THR	3.5
1	B	115	ILE	3.5
1	A	38	ALA	3.5
1	A	44	ILE	3.4
1	B	14	ASP	3.4
1	B	54	LEU	3.3
1	B	71	GLU	3.3
1	B	44	ILE	3.3
1	A	48	PHE	3.3
1	A	116	HIS	3.3
1	B	53	GLU	3.3
1	A	29	ARG	3.3
1	B	6	ASP	3.3
1	B	47	TYR	3.3
1	A	57	ALA	3.3
1	A	77	ASP	3.3
1	A	106	ILE	3.2
1	B	163	TRP	3.2
1	A	159	THR	3.2
1	B	157	LEU	3.2
1	B	106	ILE	3.2
1	A	122	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	55	ILE	3.2
1	A	133	ARG	3.2
1	A	110	LEU	3.1
1	B	78	LEU	3.1
1	A	169	GLU	3.1
1	A	62	ALA	3.1
1	A	25	TRP	3.1
1	A	54	LEU	3.1
1	B	156	TYR	3.0
1	A	124	ARG	3.0
1	B	182	LEU	3.0
1	B	185	ALA	3.0
1	B	160	PHE	2.9
1	A	187	TRP	2.9
1	A	71	GLU	2.9
1	B	111	GLU	2.9
1	A	188	LEU	2.9
1	B	60	ASP	2.9
1	B	114	HIS	2.8
1	B	72	SER	2.8
1	A	36	ARG	2.8
1	A	33	ILE	2.8
1	A	137	GLN	2.8
1	B	171	SER	2.8
1	A	19	LEU	2.8
1	A	119	ILE	2.8
1	A	183	THR	2.8
1	A	147	LEU	2.7
1	A	185	ALA	2.7
1	B	91	TRP	2.7
1	B	103	ARG	2.7
1	A	155	ILE	2.7
1	A	78	LEU	2.7
1	A	37	LEU	2.7
1	B	159	THR	2.7
1	A	61	ARG	2.7
1	A	65	ARG	2.7
1	A	13	VAL	2.6
1	A	39	VAL	2.6
1	A	156	TYR	2.6
1	A	153	THR	2.6
1	A	21	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	2.6
1	B	161	PHE	2.6
1	B	29	ARG	2.6
1	B	99	ARG	2.6
1	B	42	ASP	2.6
1	B	49	ARG	2.6
1	B	173	HIS	2.5
1	A	160	PHE	2.5
1	A	47	TYR	2.5
1	A	146	ALA	2.5
1	A	121	ALA	2.5
1	A	128	THR	2.5
1	A	41	LEU	2.4
1	B	69	GLU	2.4
1	A	35	ALA	2.4
1	B	187	TRP	2.4
1	B	22	HIS	2.4
1	B	86	HIS	2.4
1	B	64	SER	2.3
1	B	155	ILE	2.3
1	B	129	VAL	2.3
1	B	118	GLN	2.3
1	B	52	ASP	2.3
1	B	40	SER	2.3
1	A	125	VAL	2.3
1	A	80	ALA	2.3
1	B	33	ILE	2.3
1	B	61	ARG	2.3
1	A	22	HIS	2.2
1	B	30	LEU	2.2
1	A	15	THR	2.2
1	B	124	ARG	2.2
1	B	24	SER	2.2
1	A	85	HIS	2.2
1	B	41	LEU	2.2
1	B	25	TRP	2.2
1	A	56	ASP	2.2
1	B	75	PHE	2.2
1	A	126	SER	2.2
1	A	154	THR	2.2
1	A	182	LEU	2.2
1	A	180	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	79	VAL	2.2
1	A	46	LEU	2.2
1	A	151	THR	2.2
1	A	9	ARG	2.1
1	A	134	GLU	2.1
1	A	50	GLU	2.1
1	A	149	GLU	2.1
1	A	14	ASP	2.1
1	A	70	ALA	2.1
1	A	63	ASP	2.1
1	A	12	ILE	2.1
1	A	127	ARG	2.1
1	A	53	GLU	2.1
1	B	104	GLN	2.0
1	A	31	TYR	2.0
1	A	150	SER	2.0
1	B	102	THR	2.0
1	B	181	HIS	2.0
1	B	34	ALA	2.0
1	A	86	HIS	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 monosaccharides 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.