



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:33 AM EDT

PDB ID : 5R12 / pdb_00005r12
Title : PanDDA analysis group deposition – Auto-refined data of Aar2/RNaseH for ground state model 16, DMSO-free
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Deposited on : 2020-02-12
Resolution : 1.70 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

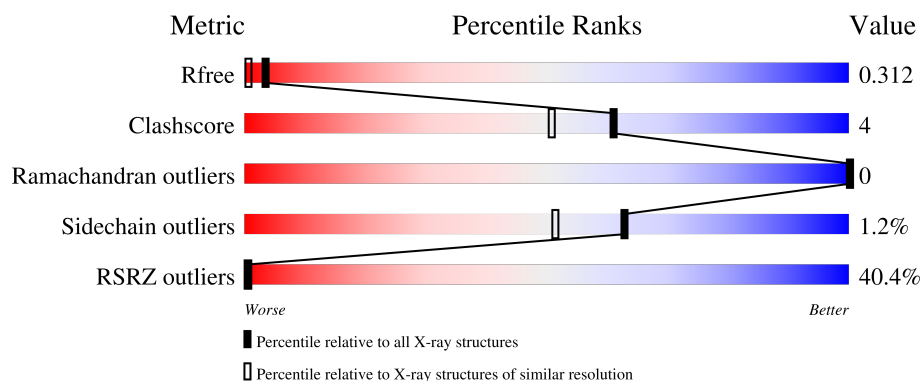
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	258	36% 83% 8% 8%
2	B	308	41% 85% 12% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4676 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1994	1278	334	371	11	0	12	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	expression tag	UNP P33334
A	1834	ALA	-	expression tag	UNP P33334
A	1835	MET	-	expression tag	UNP P33334

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	300	2580	1654	421	485	20	0	9	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	170	SER	LEU	conflict	UNP P32357
B	?	-	GLN	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	GLY	deletion	UNP P32357
B	?	-	SER	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ASN	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ASP	deletion	UNP P32357

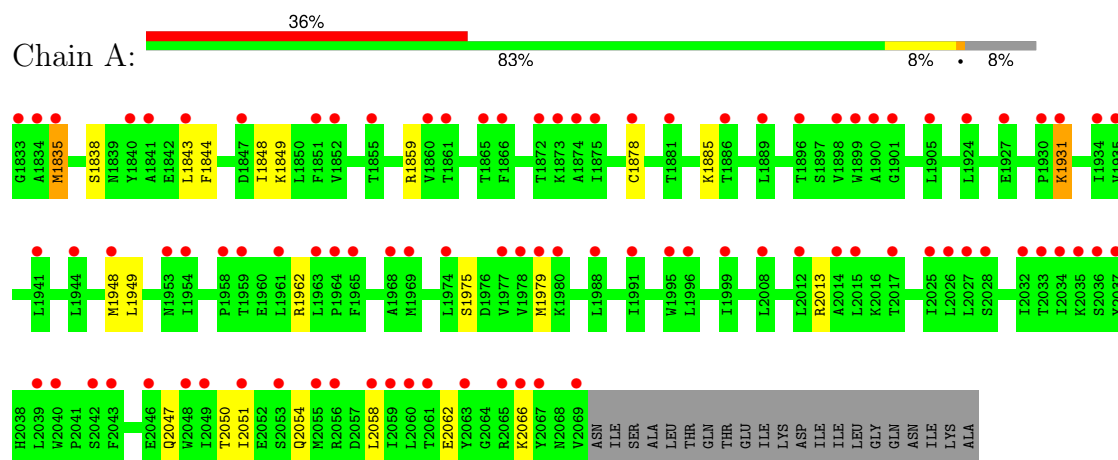
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	33	Total O 33 33	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: Pre-mRNA-splicing factor 8



• Molecule 2: A1 cistron-splicing factor AAR2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.48Å 82.61Å 92.85Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	22.32 – 1.70 22.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (22.32-1.70) 99.2 (22.32-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.266 , 0.298 0.276 , 0.312	Depositor DCC
R_{free} test set	2101 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4676	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	0.75	1/2041 (0.0%)	0.92	0/2765
2	B	0.63	0/2651	0.78	0/3581
All	All	0.69	1/4692 (0.0%)	0.84	0/6346

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1878	CYS	C-N	9.78	1.48	1.33

There are no bond angle outliers.

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	1994	0	2020	13	0
2	B	2580	0	2450	25	0
3	A	69	0	0	0	0
3	B	33	0	0	1	0
All	All	4676	0	4470	38	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 4.

All (38) 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)
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.71	0.71
1:A:2062:GLU:O	1:A:2066:LYS:HG2	1.93	0.68
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.75	0.68
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.29	0.66
2:B:1:MET:N	3:B:401:HOH:O	2.33	0.61
2:B:96:PHE:CB	2:B:102:MET:HE3	2.31	0.61
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	1.85	0.59
1:A:1844:PHE:O	1:A:1885:LYS:NZ	2.23	0.55
2:B:287:ARG:O	2:B:291:ILE:HD13	2.07	0.55
1:A:2062:GLU:HB3	1:A:2066:LYS:HE3	1.88	0.54
2:B:258:LYS:HD2	2:B:258:LYS:H	1.74	0.53
2:B:69:ILE:HD13	2:B:80:MET:HA	1.92	0.51
2:B:6:PHE:HZ	2:B:44[A]:ILE:HD11	1.75	0.50
2:B:1:MET:HB3	2:B:35:ASP:HA	1.94	0.49
2:B:275:LEU:HD22	2:B:283:LEU:HD13	1.96	0.48
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.49	0.48
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.39	0.47
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.62	0.47
1:A:2047:GLN:O	1:A:2051:ILE:HG12	2.15	0.46
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.97	0.46
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.52	0.45
1:A:1859:ARG:HH22	1:A:1979[A]:MET:HE1	1.82	0.45
2:B:64[A]:MET:SD	2:B:123:MET:HG2	2.56	0.44
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	2.00	0.44
2:B:242:GLN:O	2:B:246:MET:HG3	2.18	0.43
2:B:17:ILE:O	2:B:18:ASP:C	2.59	0.43
2:B:54[B]:MET:HE1	2:B:143:SER:CB	2.48	0.43
2:B:6:PHE:CZ	2:B:44[A]:ILE:HD11	2.52	0.42
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.54	0.42
2:B:210:LEU:O	2:B:215:LYS:N	2.52	0.42
2:B:301:SER:O	2:B:302:LEU:HD23	2.20	0.42
1:A:2050:THR:HG22	1:A:2054:GLN:NE2	2.36	0.41
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.96	0.41
1:A:1948:MET:O	1:A:1949:LEU:C	2.63	0.41
2:B:237:TYR:CE2	2:B:241:LEU:HD11	2.56	0.41
2:B:268:LEU:HA	2:B:268:LEU:HD23	1.82	0.40
1:A:1975:SER:O	1:A:1979[A]:MET:SD	2.80	0.40
2:B:228:PHE:HB2	2:B:243:TRP:CD1	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	247/258 (96%)	242 (98%)	5 (2%)	0	100	100
2	B	306/308 (99%)	293 (96%)	13 (4%)	0	100	100
All	All	553/566 (98%)	535 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	225/233 (97%)	221 (98%)	4 (2%)	51	36
2	B	287/284 (101%)	284 (99%)	3 (1%)	68	58
All	All	512/517 (99%)	505 (99%)	7 (1%)	63	46

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1838	SER
1	A	1931[A]	LYS
1	A	1931[B]	LYS
2	B	282	ILE
2	B	301	SER
2	B	315	GLU

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	1907	GLN
2	B	47	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 [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	237/258 (91%)	1.94	92 (38%) 1 0	23, 66, 104, 139	12 (5%)
2	B	300/308 (97%)	1.95	125 (41%) 0 0	22, 77, 117, 204	9 (3%)
All	All	537/566 (94%)	1.95	217 (40%) 0 0	22, 70, 113, 204	21 (3%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1979[A]	MET	10.8
1	A	1878	CYS	8.2
1	A	2034	ILE	6.5
2	B	203[A]	TYR	6.1
2	B	146	THR	6.0
1	A	2039	LEU	5.9
2	B	22	PHE	5.3
2	B	189	ILE	5.2
1	A	2048	TRP	5.2
2	B	73	PRO	5.0
1	A	1996	LEU	5.0
2	B	126	ILE	5.0
1	A	2060	LEU	4.9
2	B	54[A]	MET	4.9
2	B	275	LEU	4.8
1	A	1934	ILE	4.8
1	A	2036	SER	4.7
2	B	288	VAL	4.7
2	B	210	LEU	4.6
1	A	2059	ILE	4.5
2	B	291	ILE	4.5
2	B	256	VAL	4.4
2	B	316	LEU	4.4
2	B	53	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1861	THR	4.3
2	B	103	VAL	4.3
1	A	1900	ALA	4.3
1	A	2069	VAL	4.3
1	A	1843	LEU	4.2
2	B	96	PHE	4.2
2	B	108	ILE	4.2
1	A	1931[A]	LYS	4.2
1	A	2063	TYR	4.2
2	B	179	THR	4.2
2	B	283	LEU	4.1
2	B	208	VAL	4.1
2	B	267	ILE	4.1
2	B	1	MET	4.0
1	A	1866	PHE	4.0
1	A	1924	LEU	4.0
2	B	124	ASP	4.0
2	B	6	PHE	3.9
2	B	71	TYR	3.9
2	B	120	PHE	3.9
2	B	246	MET	3.9
2	B	77	LEU	3.8
1	A	1840	TYR	3.8
1	A	1896	THR	3.8
2	B	279	TYR	3.8
1	A	2015	LEU	3.7
2	B	174	HIS	3.7
1	A	2043	PHE	3.7
1	A	1969	MET	3.7
2	B	281	ASP	3.6
2	B	52	SER	3.6
2	B	228	PHE	3.6
2	B	294	TYR	3.6
1	A	1988	LEU	3.5
1	A	1860	VAL	3.5
1	A	2051	ILE	3.5
2	B	92	ILE	3.5
1	A	2035	LYS	3.5
2	B	317	LEU	3.5
1	A	1999	ILE	3.4
2	B	129	ILE	3.4
2	B	170	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	2012	LEU	3.4
1	A	1963	LEU	3.3
1	A	2025	ILE	3.3
2	B	233	PHE	3.3
2	B	68	TYR	3.3
1	A	1961	LEU	3.3
2	B	101	MET	3.2
1	A	2026	LEU	3.2
1	A	1965	PHE	3.2
1	A	1980	LYS	3.2
1	A	2053[A]	SER	3.2
2	B	76	GLY	3.2
1	A	1958	PRO	3.2
2	B	33	ILE	3.2
1	A	1873	LYS	3.2
2	B	313	TYR	3.1
2	B	175	SER	3.1
2	B	89	PHE	3.1
1	A	1964	PRO	3.1
1	A	1834	ALA	3.1
2	B	67	PHE	3.1
1	A	2014	ALA	3.1
2	B	214	PHE	3.1
2	B	20	TYR	3.0
1	A	1875	ILE	3.0
1	A	1889	LEU	3.0
1	A	2065	ARG	3.0
2	B	198	PHE	3.0
2	B	177[A]	ASN	3.0
1	A	2067	TYR	3.0
1	A	2017[A]	THR	3.0
1	A	2061	THR	3.0
1	A	2055	MET	2.9
1	A	1881	THR	2.9
1	A	2049	ILE	2.9
2	B	137	PHE	2.9
2	B	299	LYS	2.9
1	A	2027	LEU	2.9
2	B	282	ILE	2.9
2	B	59	TRP	2.9
1	A	1835	MET	2.9
1	A	2066	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	55	ARG	2.9
1	A	1852	VAL	2.8
2	B	87	ALA	2.8
2	B	80	MET	2.8
2	B	213	ILE	2.8
1	A	2040	TRP	2.8
2	B	47	GLN	2.8
1	A	1865	THR	2.8
1	A	2056[A]	ARG	2.7
1	A	1954	ILE	2.7
2	B	122[A]	GLN	2.7
2	B	125	LYS	2.7
2	B	142	SER	2.7
2	B	176	LEU	2.7
2	B	191	PRO	2.6
2	B	14	THR	2.6
2	B	145	THR	2.6
1	A	2037	TYR	2.6
2	B	40	HIS	2.6
2	B	41[A]	VAL	2.6
1	A	1899	TRP	2.6
1	A	1872	THR	2.6
1	A	2058	LEU	2.6
1	A	1930	PRO	2.6
2	B	305	THR	2.5
2	B	30	PHE	2.5
2	B	29	PRO	2.5
1	A	1959	THR	2.5
1	A	1905	LEU	2.5
1	A	2008	LEU	2.5
2	B	17	ILE	2.5
2	B	139	TYR	2.5
2	B	172	PRO	2.5
2	B	270	TYR	2.5
2	B	186	ARG	2.5
2	B	287	ARG	2.5
2	B	217	SER	2.5
1	A	1927	GLU	2.4
1	A	1833	GLY	2.4
1	A	1874	ALA	2.4
2	B	173	ALA	2.4
1	A	1855[A]	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	13	VAL	2.4
2	B	216	ASN	2.4
2	B	303	HIS	2.4
2	B	241	LEU	2.4
2	B	257	PRO	2.4
1	A	1851	PHE	2.4
2	B	183	PHE	2.4
1	A	1953	ASN	2.4
2	B	252	SER	2.4
2	B	304	ASN	2.4
2	B	78	TYR	2.4
1	A	1898[A]	VAL	2.4
2	B	2	ASN	2.4
2	B	135	ASN	2.4
2	B	276	PRO	2.4
1	A	1941	LEU	2.4
1	A	1841	ALA	2.4
2	B	113	THR	2.4
2	B	19	GLN	2.3
1	A	1886	THR	2.3
1	A	2033	THR	2.3
2	B	284	LEU	2.3
2	B	114	TRP	2.3
2	B	204	TYR	2.3
2	B	130	VAL	2.3
2	B	150	ASN	2.3
1	A	1901	GLY	2.3
2	B	106	PRO	2.3
1	A	1968	ALA	2.3
2	B	188	ALA	2.3
1	A	2042	SER	2.3
2	B	263	LYS	2.3
2	B	220	TYR	2.3
2	B	192	GLY	2.3
1	A	1977	VAL	2.3
2	B	23	ASN	2.2
2	B	109	ASP	2.2
1	A	1944	LEU	2.2
1	A	1974	LEU	2.2
1	A	2032	ILE	2.2
2	B	123	MET	2.2
2	B	100	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	128	LYS	2.2
2	B	258	LYS	2.2
2	B	64[A]	MET	2.1
2	B	24	VAL	2.1
1	A	1847	ASP	2.1
1	A	1948	MET	2.1
1	A	1978	VAL	2.1
2	B	308	ILE	2.1
2	B	147	VAL	2.1
1	A	2028	SER	2.1
2	B	253	SER	2.1
2	B	152	LEU	2.1
2	B	190	ARG	2.1
2	B	224	LEU	2.1
2	B	293	LEU	2.1
1	A	1995	TRP	2.1
2	B	97	LYS	2.1
1	A	1991	ILE	2.1
2	B	235	GLY	2.0
1	A	2046	GLU	2.0
2	B	111	ASP	2.0
2	B	102	MET	2.0
1	A	1935	VAL	2.0
2	B	121	VAL	2.0
2	B	74	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.