



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:51 PM UTC

PDB ID : 5R1N / pdb_00005r1n
Title : PanDDA analysis group deposition – Auto-refined data of Aar2/RNaseH for ground state model 38, DMSO-free
Authors : Wollenhaupt, J.; Metz, A.; Barthel, T.; Lima, G.M.A.; Heine, A.; Mueller, U.; Klebe, G.; Weiss, M.S.
Deposited on : 2020-02-12
Resolution : 1.94 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

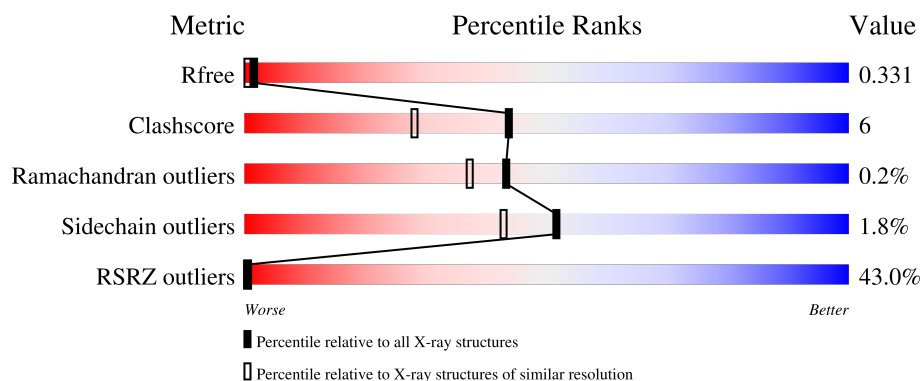
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	39% 77% 14% 8%
2	B	308	42% 79% 18% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4624 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	2575	1651	420	484	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

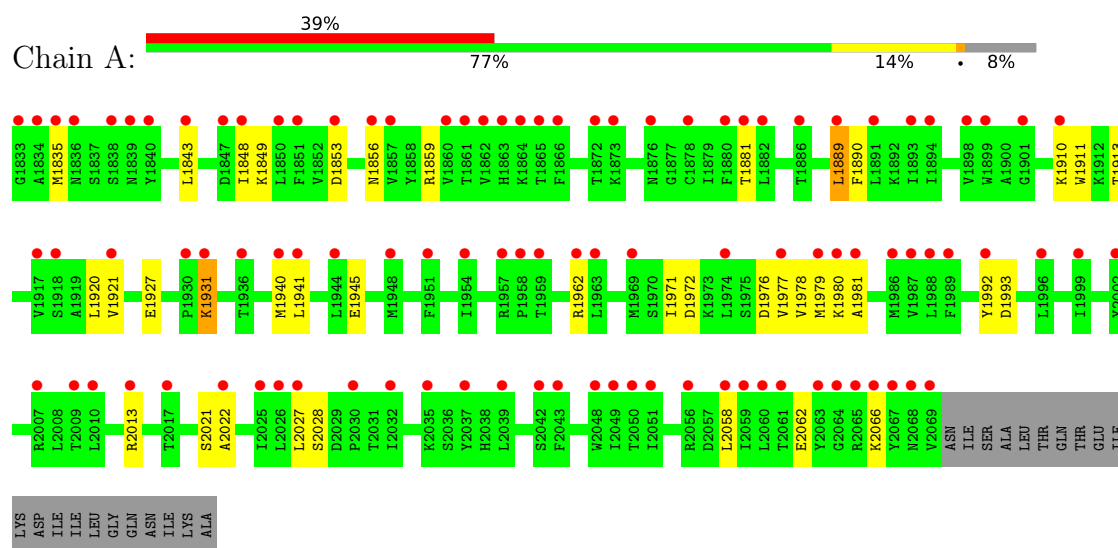
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	21	Total O 21 21	0	0

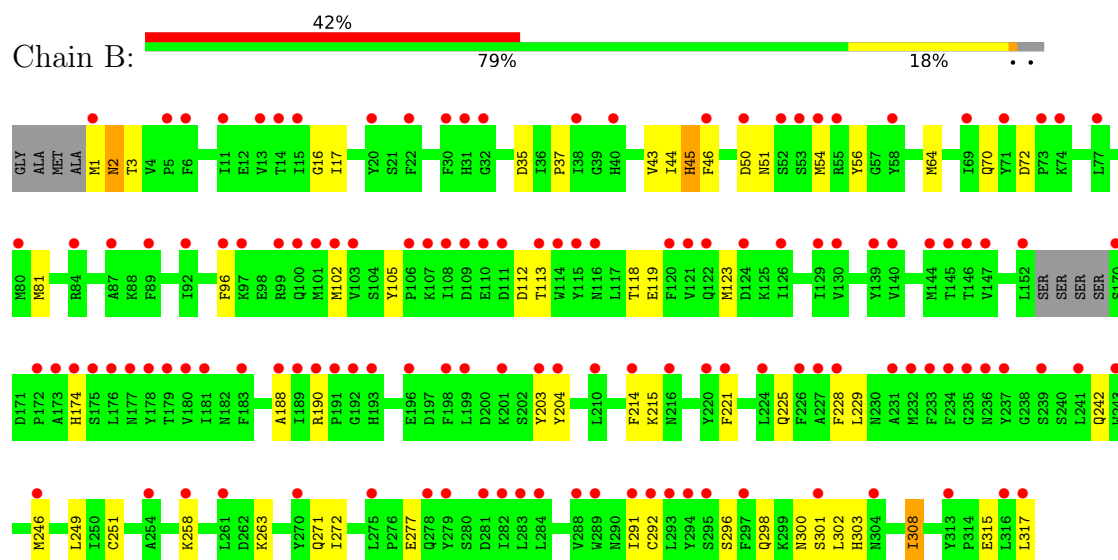
3 Residue-property plots

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	88.36Å 82.58Å 92.57Å 90.00° 107.67° 90.00°	Depositor
Resolution (Å)	22.04 – 1.94 22.04 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (22.04-1.94) 99.6 (22.04-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.281 , 0.330 0.290 , 0.331	Depositor DCC
R_{free} test set	2095 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.7	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	0.93	EDS
Total number of atoms	4624	wwPDB-VP
Average B, all atoms (Å ²)	87.0	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

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	0.84	1/2041 (0.0%)	1.09	5/2765 (0.2%)
2	B	0.74	0/2643	0.91	3/3570 (0.1%)
All	All	0.79	1/4684 (0.0%)	0.99	8/6335 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1911	TRP	CA-CB	5.47	1.61	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1881	THR	OG1-CB-CG2	6.98	123.26	109.30
2	B	249	LEU	CA-C-N	-5.90	113.01	120.56
2	B	249	LEU	C-N-CA	-5.90	113.01	120.56
1	A	1889	LEU	CB-CG-CD2	5.34	126.72	110.70
2	B	308	ILE	CA-CB-CG1	-5.34	101.32	110.40
1	A	1856	ASN	CA-C-N	5.22	127.24	120.56
1	A	1856	ASN	C-N-CA	5.22	127.24	120.56
1	A	1890	PHE	N-CA-C	-5.07	98.09	107.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1853	ASP	Sidechain

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	1994	0	2020	22	0
2	B	2575	0	2444	33	0
3	A	34	0	0	1	0
3	B	21	0	0	1	0
All	All	4624	0	4464	55	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 6.

All (55) 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:1962:ARG:O	1:A:2013:ARG:NH1	2.17	0.77
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.32	0.76
1:A:1993:ASP:OD1	3:A:2101:HOH:O	2.08	0.72
1:A:2062:GLU:O	1:A:2066:LYS:HG2	1.90	0.71
2:B:258:LYS:HD2	2:B:258:LYS:H	1.57	0.69
1:A:1910:LYS:O	1:A:1940:MET:HE1	1.94	0.66
2:B:251:CYS:O	2:B:296:SER:HB2	1.99	0.62
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.36	0.61
2:B:1:MET:N	3:B:402:HOH:O	2.34	0.59
1:A:1848:ILE:H	1:A:1931[A]:LYS:NZ	2.01	0.59
2:B:44[A]:ILE:O	2:B:44[A]:ILE:HG23	2.02	0.58
2:B:251:CYS:SG	2:B:292:CYS:SG	3.02	0.57
2:B:298:GLN:HA	2:B:298:GLN:OE1	2.05	0.57
2:B:50:ASP:OD1	2:B:51:ASN:N	2.37	0.56
1:A:2062:GLU:HB3	1:A:2066:LYS:HE3	1.88	0.55
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.91	0.52
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.34	0.52
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.93	0.50
2:B:1:MET:HB3	2:B:35:ASP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:PHE:CD2	2:B:271:GLN:HG2	2.48	0.49
1:A:1848:ILE:N	1:A:1931[A]:LYS:HZ2	2.07	0.48
2:B:301:SER:O	2:B:302:LEU:HD23	2.14	0.48
2:B:300:ASN:O	2:B:303:HIS:NE2	2.48	0.47
1:A:1941:LEU:O	1:A:1945:GLU:HB2	2.15	0.47
2:B:46:PHE:N	2:B:56:TYR:O	2.46	0.47
2:B:43:VAL:HG13	2:B:43:VAL:O	2.15	0.46
2:B:221:PHE:O	2:B:225:GLN:HG3	2.17	0.45
1:A:1976:ASP:O	1:A:1980:LYS:HG3	2.16	0.45
2:B:214:PHE:O	2:B:215:LYS:HB2	2.16	0.45
1:A:2021:SER:O	1:A:2022:ALA:C	2.58	0.44
1:A:2027:LEU:O	1:A:2028:SER:C	2.61	0.44
2:B:16:GLY:HA3	2:B:45:HIS:CE1	2.53	0.44
2:B:225:GLN:O	2:B:229:LEU:HG	2.18	0.44
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	2.00	0.43
1:A:1971:ILE:O	1:A:1972:ASP:C	2.61	0.43
1:A:1927:GLU:OE2	1:A:1927:GLU:N	2.42	0.43
2:B:112:ASP:O	2:B:113:THR:C	2.60	0.43
2:B:70:GLN:HB3	2:B:81:MET:CE	2.49	0.42
2:B:2:ASN:HD22	2:B:3:THR:H	1.68	0.42
2:B:118:THR:O	2:B:119:GLU:C	2.61	0.42
2:B:64[A]:MET:SD	2:B:123:MET:HG2	2.60	0.42
1:A:1913:THR:HB	1:A:1940:MET:HE1	2.00	0.42
2:B:272:ILE:HG21	2:B:308:ILE:HG23	2.02	0.42
1:A:1977:VAL:HG13	1:A:1978:VAL:N	2.34	0.41
2:B:17:ILE:O	2:B:17:ILE:HG23	2.19	0.41
2:B:277:GLU:H	2:B:277:GLU:CD	2.28	0.41
2:B:242:GLN:O	2:B:246:MET:HG3	2.20	0.41
1:A:1920:LEU:O	1:A:1921:VAL:C	2.60	0.41
2:B:72:ASP:C	2:B:72:ASP:OD1	2.62	0.41
2:B:263:LYS:HD3	2:B:263:LYS:HA	1.93	0.41
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.56	0.40
2:B:188:ALA:HA	2:B:204:TYR:CD1	2.57	0.40
1:A:1992:TYR:O	1:A:1993:ASP:C	2.63	0.40
1:A:1859:ARG:NH1	1:A:1979[A]:MET:SD	2.89	0.40
1:A:1980:LYS:O	1:A:1981:ALA:C	2.64	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%)	239 (97%)	8 (3%)	0	100	100
2	B	305/308 (99%)	290 (95%)	13 (4%)	2 (1%)	18	9
All	All	552/566 (98%)	529 (96%)	21 (4%)	2 (0%)	43	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54[A]	MET
2	B	54[B]	MET

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	43
2	B	286/284 (101%)	280 (98%)	6 (2%)	47	37
All	All	511/517 (99%)	501 (98%)	10 (2%)	51	39

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1889	LEU
1	A	1931[A]	LYS
1	A	1931[B]	LYS

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Mol	Chain	Res	Type
2	B	2	ASN
2	B	45	HIS
2	B	174	HIS
2	B	291	ILE
2	B	315	GLU
2	B	317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1907	GLN
1	A	2038	HIS
2	B	66	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	237/258 (91%)	2.01	101 (42%) 0 0	24, 75, 127, 206	12 (5%)
2	B	300/308 (97%)	1.93	130 (43%) 0 0	26, 83, 141, 239	8 (2%)
All	All	537/566 (94%)	1.97	231 (43%) 0 0	24, 80, 139, 239	20 (3%)

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1940	MET	10.0
2	B	80	MET	8.5
1	A	2051	ILE	8.2
1	A	1979[A]	MET	6.8
2	B	54[A]	MET	6.6
2	B	316	LEU	6.4
2	B	129	ILE	6.0
1	A	2048	TRP	5.9
2	B	246	MET	5.6
1	A	1860	VAL	5.5
2	B	22	PHE	5.5
1	A	2060	LEU	5.5
2	B	283	LEU	5.4
1	A	1977	VAL	4.9
1	A	1988	LEU	4.8
2	B	77	LEU	4.8
1	A	1936	THR	4.7
2	B	199	LEU	4.6
1	A	1980	LYS	4.4
1	A	1850	LEU	4.4
2	B	38	ILE	4.4
2	B	203[A]	TYR	4.4
1	A	2061	THR	4.3
2	B	189	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1878	CYS	4.3
2	B	74	LYS	4.3
1	A	1857	VAL	4.2
1	A	1987	VAL	4.2
2	B	101	MET	4.2
2	B	103	VAL	4.2
1	A	1834	ALA	4.1
2	B	114	TRP	4.0
2	B	52	SER	4.0
1	A	1851	PHE	4.0
1	A	2043	PHE	4.0
2	B	176	LEU	4.0
2	B	102	MET	3.9
1	A	2027	LEU	3.8
2	B	120	PHE	3.8
1	A	1986	MET	3.8
2	B	108	ILE	3.8
2	B	53	SER	3.7
1	A	1969	MET	3.7
2	B	96	PHE	3.7
2	B	198	PHE	3.6
2	B	317	LEU	3.6
1	A	1992	TYR	3.6
1	A	1872	THR	3.5
1	A	2017[A]	THR	3.5
1	A	1893	ILE	3.5
1	A	1996	LEU	3.5
1	A	1989	PHE	3.4
1	A	1889	LEU	3.4
2	B	224	LEU	3.4
2	B	97	LYS	3.3
2	B	220	TYR	3.3
1	A	1891	LEU	3.3
2	B	261	LEU	3.3
2	B	191	PRO	3.3
1	A	2030	PRO	3.3
1	A	2037	TYR	3.2
2	B	126	ILE	3.2
2	B	233	PHE	3.2
2	B	55	ARG	3.2
2	B	99	ARG	3.2
1	A	2010	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	275	LEU	3.2
1	A	2063	TYR	3.1
2	B	152	LEU	3.1
1	A	2032	ILE	3.1
2	B	73	PRO	3.1
2	B	121	VAL	3.1
2	B	284	LEU	3.1
1	A	2064	GLY	3.1
2	B	181	ILE	3.1
1	A	1866	PHE	3.1
2	B	210	LEU	3.0
2	B	139	TYR	3.0
1	A	1948	MET	3.0
2	B	58	TYR	3.0
2	B	31	HIS	3.0
2	B	124	ASP	3.0
1	A	1836	ASN	3.0
2	B	282	ILE	3.0
2	B	122[A]	GLN	3.0
2	B	190	ARG	3.0
2	B	69	ILE	3.0
2	B	279	TYR	2.9
2	B	231	ALA	2.9
2	B	100	GLN	2.9
1	A	2042	SER	2.9
1	A	2035	LYS	2.9
1	A	2059	ILE	2.9
1	A	2039	LEU	2.9
1	A	1881	THR	2.9
2	B	30	PHE	2.8
2	B	295	SER	2.8
1	A	1835	MET	2.8
1	A	1894	ILE	2.8
2	B	196	GLU	2.8
2	B	46	PHE	2.8
2	B	89	PHE	2.8
2	B	92	ILE	2.8
1	A	2007	ARG	2.7
2	B	6	PHE	2.7
2	B	111	ASP	2.7
2	B	288	VAL	2.7
2	B	294	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1861	THR	2.7
2	B	172	PRO	2.7
1	A	2049	ILE	2.7
1	A	1838	SER	2.7
1	A	1856	ASN	2.7
2	B	140	VAL	2.7
1	A	2002	TYR	2.7
2	B	71	TYR	2.7
2	B	214	PHE	2.7
2	B	146	THR	2.7
1	A	1921	VAL	2.7
1	A	1833	GLY	2.6
2	B	188	ALA	2.6
2	B	115	TYR	2.6
1	A	1880	PHE	2.6
1	A	1873	LYS	2.6
1	A	1941	LEU	2.6
2	B	278	GLN	2.6
2	B	313	TYR	2.6
1	A	1865	THR	2.6
2	B	183	PHE	2.6
1	A	1843	LEU	2.6
1	A	1999	ILE	2.6
1	A	2013	ARG	2.6
2	B	221	PHE	2.6
1	A	2058	LEU	2.6
2	B	1	MET	2.6
1	A	1901	GLY	2.6
2	B	235	GLY	2.6
2	B	232	MET	2.5
2	B	297	PHE	2.5
2	B	243	TRP	2.5
2	B	289	TRP	2.5
1	A	2068	ASN	2.5
2	B	170	SER	2.5
1	A	2069	VAL	2.5
2	B	281	ASP	2.5
1	A	1954	ILE	2.5
2	B	11	ILE	2.5
1	A	1957	ARG	2.5
2	B	173	ALA	2.5
2	B	13	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	147	VAL	2.5
1	A	2066	LYS	2.5
2	B	192	GLY	2.5
2	B	304	ASN	2.5
2	B	40	HIS	2.5
1	A	1862	VAL	2.5
1	A	1931[A]	LYS	2.5
1	A	1882	LEU	2.4
1	A	1963	LEU	2.4
1	A	2026	LEU	2.4
2	B	291	ILE	2.4
2	B	177[A]	ASN	2.4
2	B	193	HIS	2.4
2	B	178	TYR	2.4
1	A	1848	ILE	2.4
2	B	179	THR	2.4
1	A	2065	ARG	2.4
1	A	1930	PRO	2.4
2	B	106	PRO	2.4
1	A	1918[A]	SER	2.4
2	B	201	LYS	2.4
1	A	1853	ASP	2.4
1	A	1951	PHE	2.4
1	A	2067	TYR	2.3
1	A	2050	THR	2.3
2	B	87	ALA	2.3
1	A	1974	LEU	2.3
1	A	2009	THR	2.3
2	B	14	THR	2.3
2	B	15	ILE	2.3
2	B	109	ASP	2.3
1	A	1898[A]	VAL	2.3
2	B	180	VAL	2.3
1	A	1886	THR	2.3
2	B	227	ALA	2.2
2	B	228	PHE	2.2
2	B	270	TYR	2.2
2	B	175	SER	2.2
2	B	84	ARG	2.2
1	A	1944	LEU	2.2
2	B	5	PRO	2.2
2	B	239	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1981	ALA	2.2
1	A	1899	TRP	2.2
1	A	1839	ASN	2.2
2	B	174	HIS	2.2
2	B	258	LYS	2.2
1	A	1959	THR	2.2
1	A	1840	TYR	2.2
2	B	20	TYR	2.2
1	A	2025	ILE	2.2
1	A	1864	LYS	2.2
2	B	116	ASN	2.2
2	B	216	ASN	2.2
2	B	236	ASN	2.2
1	A	1917	VAL	2.2
2	B	32	GLY	2.2
2	B	293	LEU	2.2
2	B	107	LYS	2.2
2	B	204	TYR	2.1
2	B	237	TYR	2.1
2	B	50	ASP	2.1
2	B	113	THR	2.1
1	A	1863	HIS	2.1
1	A	2022	ALA	2.1
1	A	1962	ARG	2.1
1	A	2056[A]	ARG	2.1
2	B	110	GLU	2.1
2	B	234	PHE	2.1
2	B	301	SER	2.1
1	A	1958	PRO	2.1
2	B	241	LEU	2.1
1	A	1847	ASP	2.1
2	B	144	MET	2.0
2	B	130	VAL	2.0
2	B	292	CYS	2.0
2	B	254	ALA	2.0
1	A	1910	LYS	2.0
2	B	226	PHE	2.0
2	B	145	THR	2.0
1	A	1876	ASN	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.