



Full wwPDB X-ray Structure Validation Report i

Mar 2, 2021 – 11:35 AM EST

PDB ID : 5R1K
Title : PanDDA analysis group deposition – Auto-refined data of Aar2/RNaseH for ground state model 35, 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 : 1.99 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 i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.17.1
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) : 2.17.1

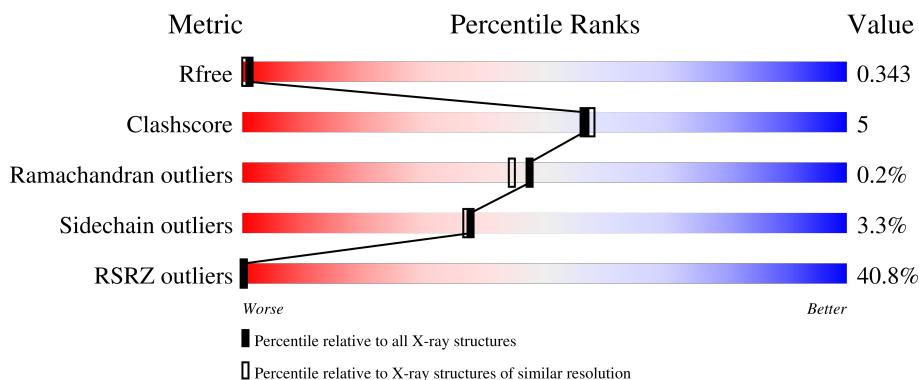
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

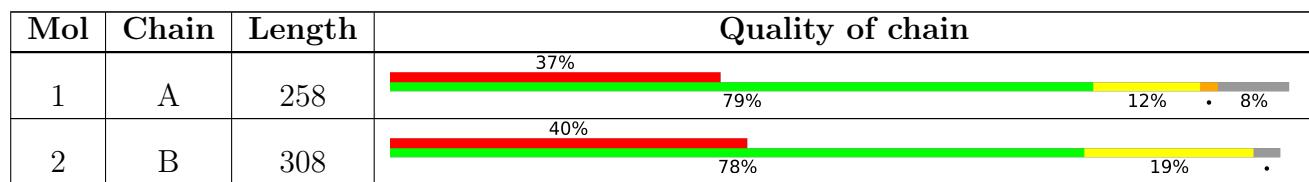
The reported resolution of this entry is 1.99 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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.



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4605 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	
1	A	237	Total	C 2002	N 1283	O 335	S 372	12	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	
2	B	300	Total	C 2568	N 1645	O 420	S 483	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

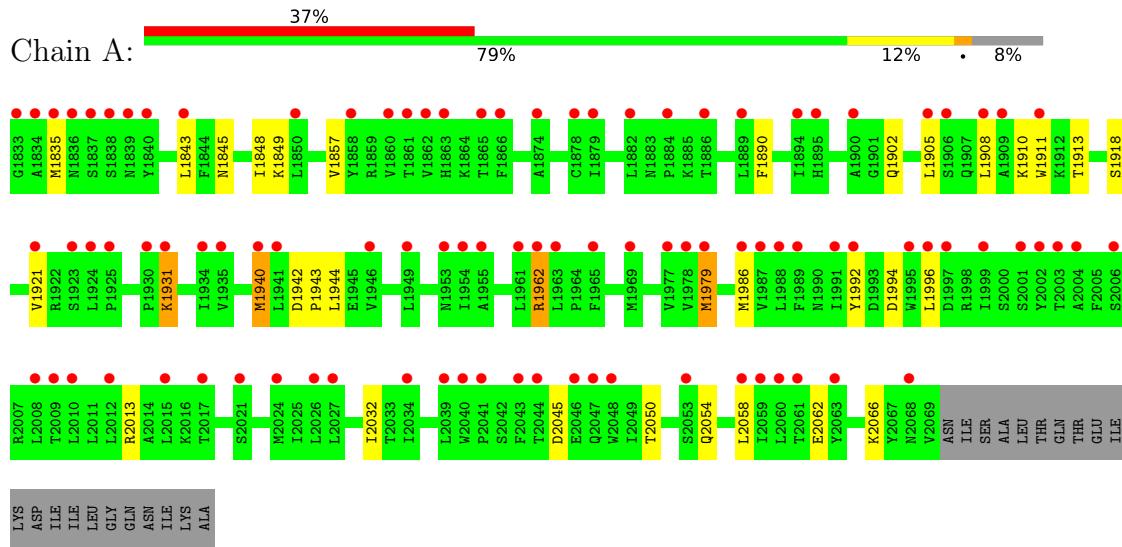
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O 25 25	0	0
3	B	10	Total O 10 10	0	0

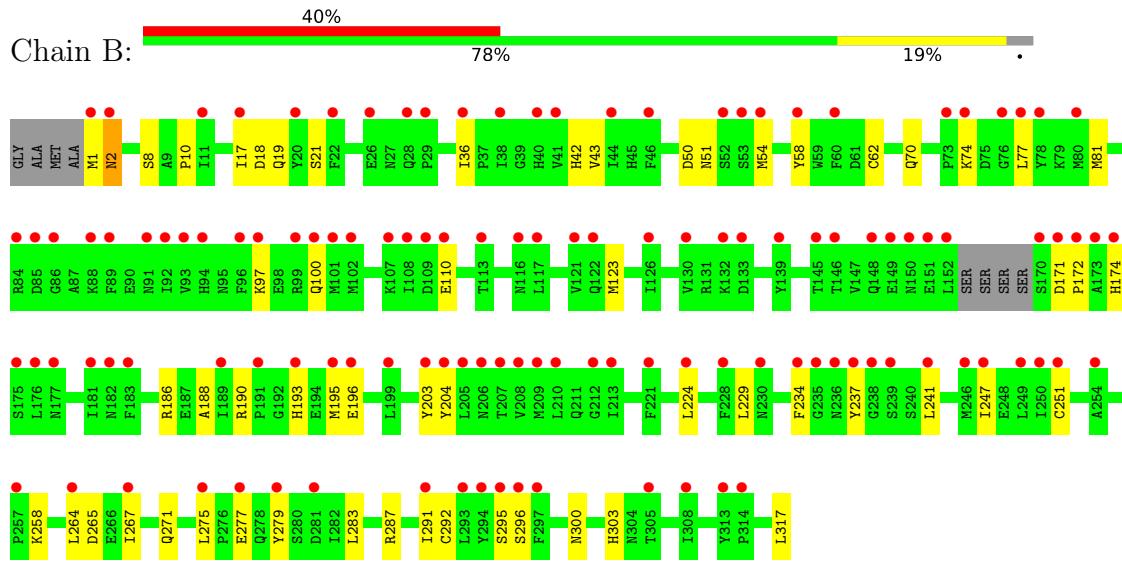
3 Residue-property plots [\(i\)](#)

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: Pre-mRNA-splicing factor 8



- Molecule 2: A1 cistron-splicing factor AAR2



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.89 Å 82.66 Å 91.95 Å 90.00° 107.58° 90.00°	Depositor
Resolution (Å)	21.24 – 1.99 44.85 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.24-1.99) 99.4 (44.85-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	0.98 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R , R_{free}	0.272 , 0.326 0.286 , 0.343	Depositor DCC
R_{free} test set	2100 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.9	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4605	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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	0.90	4/2049 (0.2%)	0.99	6/2775 (0.2%)
2	B	0.79	2/2638 (0.1%)	0.86	3/3563 (0.1%)
All	All	0.84	6/4687 (0.1%)	0.92	9/6338 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1992	TYR	CE2-CZ	-7.21	1.29	1.38
1	A	1921	VAL	CB-CG1	6.26	1.66	1.52
1	A	1992	TYR	CZ-OH	-6.05	1.27	1.37
2	B	58	TYR	CD1-CE1	5.86	1.48	1.39
1	A	1890	PHE	CA-CB	-5.75	1.41	1.53
2	B	234	PHE	CD2-CE2	5.54	1.50	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	LEU	CB-CG-CD1	7.41	123.59	111.00
1	A	1944	LEU	CB-CG-CD1	7.11	123.09	111.00
1	A	1908	LEU	CB-CG-CD1	-6.72	99.57	111.00
1	A	1994	ASP	CB-CG-OD1	5.98	123.68	118.30
2	B	265	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	1940	MET	CG-SD-CE	-5.55	91.32	100.20
1	A	1996	LEU	CB-CG-CD1	5.51	120.37	111.00
2	B	264	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	A	1986	MET	CG-SD-CE	-5.05	92.12	100.20

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	2002	0	2029	16	0
2	B	2568	0	2439	31	0
3	A	25	0	0	0	0
3	B	10	0	0	2	0
All	All	4605	0	4468	45	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 (45) 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:74:LYS:NZ	3:B:401:HOH:O	2.00	0.93
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.13	0.81
1:A:2062:GLU:O	1:A:2066:LYS:HG2	1.84	0.77
2:B:50:ASP:OD1	2:B:51:ASN:N	2.24	0.70
2:B:287:ARG:O	2:B:291:ILE:HD13	1.92	0.68
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.43	0.64
2:B:70:GLN:HB3	2:B:81:MET:HE1	1.79	0.64
2:B:1:MET:N	3:B:402:HOH:O	2.35	0.58
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.86	0.57
1:A:1857:VAL:HG21	1:A:1913:THR:OG1	2.06	0.56
1:A:1848:ILE:H	1:A:1931[A]:LYS:NZ	2.04	0.55
2:B:70:GLN:HB3	2:B:81:MET:CE	2.38	0.53
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.43	0.53
2:B:193:HIS:ND1	2:B:196:GLU:OE1	2.32	0.53
2:B:97:LYS:O	2:B:100:GLN:N	2.40	0.53
2:B:300:ASN:O	2:B:303:HIS:NE2	2.43	0.52
2:B:291:ILE:HA	2:B:295:SER:HB2	1.93	0.50
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.32	0.50
1:A:2050:THR:HG22	1:A:2054:GLN:NE2	2.27	0.50
1:A:1910:LYS:HA	1:A:1940:MET:SD	2.53	0.49
2:B:224:LEU:C	2:B:224:LEU:HD23	2.34	0.48
2:B:2:ASN:CG	2:B:62:CYS:HB3	2.35	0.47
2:B:277:GLU:OE1	2:B:277:GLU:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:VAL:HG13	2:B:43:VAL:O	2.14	0.47
2:B:275:LEU:HD22	2:B:283:LEU:HD13	1.97	0.47
1:A:1911:TRP:CD2	2:B:195:MET:HB2	2.51	0.46
2:B:186:ARG:HA	2:B:186:ARG:HD3	1.75	0.46
1:A:2062:GLU:HB3	1:A:2066:LYS:HE3	1.98	0.45
2:B:237:TYR:CE2	2:B:241:LEU:HD11	2.52	0.45
2:B:251:CYS:O	2:B:296:SER:HB2	2.16	0.45
1:A:1902:GLN:HB2	1:A:1905:LEU:HD21	1.98	0.45
2:B:8:SER:OG	2:B:10:PRO:HD3	2.17	0.44
2:B:171:ASP:HA	2:B:172:PRO:HD3	1.89	0.43
2:B:19:GLN:OE1	2:B:19:GLN:N	2.46	0.42
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	2.00	0.42
1:A:1845:ASN:OD1	1:A:1849:LYS:NZ	2.53	0.42
2:B:190:ARG:HD3	2:B:203[B]:TYR:CE1	2.55	0.42
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	2.02	0.41
2:B:18:ASP:OD2	2:B:42:HIS:ND1	2.53	0.41
2:B:188:ALA:HA	2:B:204:TYR:CD1	2.56	0.41
1:A:1911:TRP:CE3	2:B:195:MET:HB2	2.55	0.41
2:B:2:ASN:O	2:B:36:ILE:HB	2.21	0.41
2:B:110:GLU:O	2:B:110:GLU:HG2	2.21	0.41
2:B:247:ILE:HG22	2:B:292:CYS:SG	2.61	0.41
2:B:267:ILE:O	2:B:271:GLN:HG3	2.21	0.41

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	248/258 (96%)	240 (97%)	8 (3%)	0	100 100
2	B	305/308 (99%)	285 (93%)	18 (6%)	2 (1%)	22 16
All	All	553/566 (98%)	525 (95%)	26 (5%)	2 (0%)	47 30

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 [\(i\)](#)

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	226/233 (97%)	215 (95%)	11 (5%)	25 21
2	B	286/284 (101%)	277 (97%)	9 (3%)	40 40
All	All	512/517 (99%)	492 (96%)	20 (4%)	38 30

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1918[A]	SER
1	A	1918[B]	SER
1	A	1931[A]	LYS
1	A	1931[B]	LYS
1	A	1962	ARG
1	A	1979[A]	MET
1	A	1979[B]	MET
1	A	1979[C]	MET
1	A	2032	ILE
1	A	2045	ASP
2	B	2	ASN
2	B	17	ILE
2	B	21	SER
2	B	77	LEU
2	B	123	MET
2	B	174	HIS
2	B	258	LYS
2	B	279	TYR
2	B	317	LEU

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
1	A	2038	HIS

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 i

6.1 Protein, DNA and RNA chains i

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%)	1.86	96 (40%) 0 0	51, 84, 121, 138	0
2	B	300/308 (97%)	2.02	123 (41%) 0 0	60, 96, 137, 191	0
All	All	537/566 (94%)	1.95	219 (40%) 0 0	51, 92, 132, 191	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	53	SER	9.3
2	B	175	SER	9.2
1	A	1833	GLY	8.9
2	B	109	ASP	8.7
2	B	1	MET	7.0
2	B	172	PRO	6.5
2	B	277	GLU	6.0
2	B	89	PHE	6.0
2	B	88	LYS	5.8
2	B	150	ASN	5.8
2	B	52	SER	5.8
2	B	100	GLN	5.7
2	B	181	ILE	5.5
1	A	1878	CYS	5.2
2	B	92	ILE	5.2
2	B	99	ARG	5.2
1	A	2027	LEU	5.1
2	B	96	PHE	5.1
2	B	171	ASP	5.0
2	B	193	HIS	5.0
1	A	1940	MET	4.8
1	A	1988	LEU	4.6
2	B	97	LYS	4.5
1	A	1838	SER	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	17	ILE	4.2
2	B	291	ILE	4.2
2	B	208	VAL	4.2
2	B	173	ALA	4.1
1	A	1866	PHE	4.1
1	A	2060	LEU	4.1
2	B	36	ILE	4.1
1	A	1963	LEU	4.0
2	B	94	HIS	4.0
2	B	174	HIS	4.0
2	B	237	TYR	3.9
2	B	54[A]	MET	3.9
2	B	86	GLY	3.9
2	B	189	ILE	3.9
2	B	22	PHE	3.8
1	A	2039	LEU	3.8
2	B	281	ASP	3.7
1	A	2044	THR	3.7
2	B	170	SER	3.7
1	A	1836	ASN	3.7
1	A	1996	LEU	3.6
1	A	1905	LEU	3.6
1	A	1977	VAL	3.6
1	A	1979[A]	MET	3.5
1	A	1921	VAL	3.5
2	B	77	LEU	3.4
2	B	107	LYS	3.4
1	A	2026	LEU	3.4
2	B	296	SER	3.4
2	B	126	ILE	3.4
1	A	1834	ALA	3.3
1	A	1955	ALA	3.3
1	A	1969	MET	3.3
1	A	2034	ILE	3.3
2	B	108	ILE	3.3
2	B	293	LEU	3.3
2	B	213	ILE	3.3
2	B	239	SER	3.3
2	B	84	ARG	3.3
1	A	2040	TRP	3.3
1	A	2015	LEU	3.3
2	B	249	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1865	THR	3.2
1	A	1840	TYR	3.2
1	A	1889	LEU	3.2
1	A	2004	ALA	3.2
2	B	176	LEU	3.2
2	B	122[A]	GLN	3.2
2	B	133	ASP	3.2
1	A	1962	ARG	3.1
2	B	149	GLU	3.1
1	A	2003	THR	3.1
1	A	2009	THR	3.1
2	B	177[A]	ASN	3.1
1	A	1900	ALA	3.1
1	A	1987	VAL	3.1
1	A	1935	VAL	3.1
2	B	41[A]	VAL	3.1
2	B	20	TYR	3.1
2	B	60	PHE	3.0
2	B	117	LEU	3.0
2	B	73	PRO	3.0
1	A	2048	TRP	3.0
1	A	2017[A]	THR	3.0
1	A	1997	ASP	3.0
2	B	275	LEU	3.0
1	A	1989	PHE	3.0
2	B	250	ILE	3.0
2	B	110	GLU	3.0
1	A	2046	GLU	2.9
2	B	241	LEU	2.9
2	B	264	LEU	2.9
1	A	1946	VAL	2.9
1	A	2012	LEU	2.9
2	B	228	PHE	2.9
1	A	1886	THR	2.8
2	B	246	MET	2.8
2	B	152	LEU	2.8
2	B	85	ASP	2.8
1	A	1861	THR	2.8
1	A	2061	THR	2.8
1	A	1894	ILE	2.8
2	B	251	CYS	2.8
1	A	1837	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	254	ALA	2.8
2	B	38	ILE	2.8
2	B	294	TYR	2.8
1	A	2010	LEU	2.7
2	B	139	TYR	2.7
1	A	1961	LEU	2.7
1	A	1879	ILE	2.7
2	B	207	THR	2.7
1	A	2002	TYR	2.7
2	B	132	LYS	2.7
1	A	1906	SER	2.7
2	B	295	SER	2.7
1	A	1930	PRO	2.7
2	B	93	VAL	2.7
2	B	191	PRO	2.7
2	B	40	HIS	2.7
1	A	1909	ALA	2.6
1	A	1999	ILE	2.6
2	B	308	ILE	2.6
2	B	196	GLU	2.6
2	B	210	LEU	2.6
2	B	238	GLY	2.6
2	B	151	GLU	2.6
2	B	102	MET	2.6
1	A	2008	LEU	2.6
1	A	1839	ASN	2.6
1	A	2043	PHE	2.5
2	B	203[A]	TYR	2.5
2	B	205	LEU	2.5
1	A	2021	SER	2.5
1	A	2047	GLN	2.5
2	B	116	ASN	2.5
1	A	1991	ILE	2.5
2	B	148	GLN	2.5
1	A	1860	VAL	2.5
2	B	236	ASN	2.5
2	B	29	PRO	2.5
2	B	305	THR	2.5
2	B	28	GLN	2.5
1	A	1934	ILE	2.5
2	B	183	PHE	2.5
1	A	2068	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	230[A]	ASN	2.5
2	B	26	GLU	2.5
1	A	1858	TYR	2.4
1	A	1965	PHE	2.4
1	A	1992	TYR	2.4
2	B	313	TYR	2.4
2	B	91	ASN	2.4
2	B	221	PHE	2.4
1	A	1978	VAL	2.4
2	B	146	THR	2.4
1	A	1862	VAL	2.4
1	A	1835	MET	2.4
2	B	121	VAL	2.4
2	B	76	GLY	2.3
1	A	1954	ILE	2.3
1	A	2001[A]	SER	2.3
1	A	2053[A]	SER	2.3
2	B	44[A]	ILE	2.3
2	B	130	VAL	2.3
2	B	195	MET	2.3
2	B	46	PHE	2.3
2	B	78	TYR	2.3
1	A	2024[A]	MET	2.3
2	B	58	TYR	2.3
2	B	279	TYR	2.3
1	A	1995	TRP	2.3
1	A	1863	HIS	2.3
2	B	113	THR	2.3
1	A	1895	HIS	2.3
2	B	235	GLY	2.3
1	A	1884	PRO	2.3
1	A	1941	LEU	2.3
1	A	2058	LEU	2.3
1	A	1986	MET	2.2
2	B	182	ASN	2.2
1	A	1843	LEU	2.2
1	A	1949	LEU	2.2
2	B	74	LYS	2.2
1	A	1908	LEU	2.2
1	A	2006	SER	2.2
1	A	2041	PRO	2.2
2	B	209	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	224	LEU	2.1
2	B	257	PRO	2.1
1	A	2059	ILE	2.1
2	B	212	GLY	2.1
2	B	247	ILE	2.1
1	A	1882	LEU	2.1
2	B	199	LEU	2.1
2	B	101	MET	2.1
2	B	145	THR	2.1
1	A	1925	PRO	2.1
2	B	204	TYR	2.1
1	A	1911	TRP	2.1
2	B	11	ILE	2.1
2	B	267	ILE	2.1
2	B	314	PRO	2.1
1	A	1931[A]	LYS	2.1
1	A	1874	ALA	2.1
2	B	2	ASN	2.1
1	A	1924	LEU	2.1
1	A	2063	TYR	2.0
1	A	1953	ASN	2.0
2	B	206	ASN	2.0
2	B	234	PHE	2.0
2	B	80	MET	2.0
1	A	1923	SER	2.0
2	B	297	PHE	2.0
1	A	1850	LEU	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.