Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2021 – 11:40 AM EST

PDB ID	:	5R1H
Title	:	PanDDA analysis group deposition – Auto-refined data of Aar2/RNaseH for ground state model 32, 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	:	2.06 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:

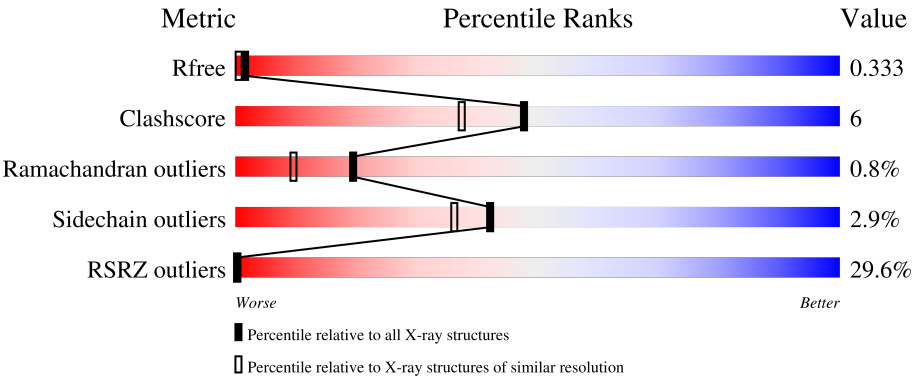
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	25% 71% 19% • 8%
2	B	308	31% 79% 17% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4607 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	2002	1283	335	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
			Total	C	N	O	S			
2	B	300	2563	1642	419	482	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.

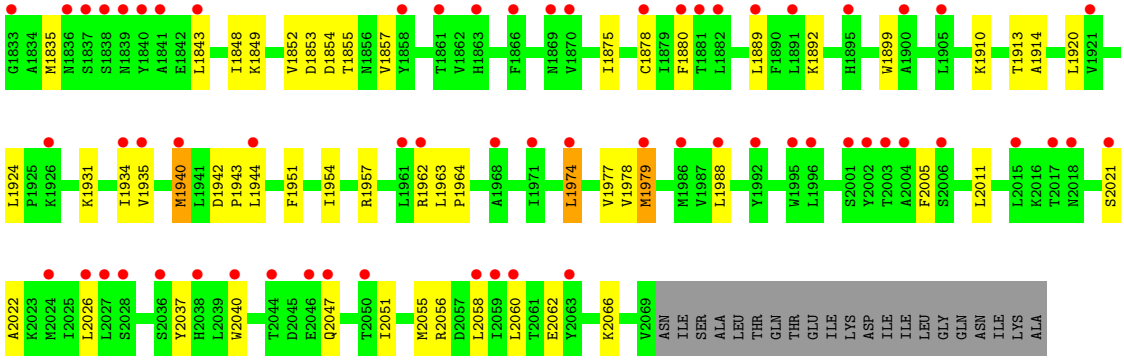
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	15	Total O 15 15	0	0

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.

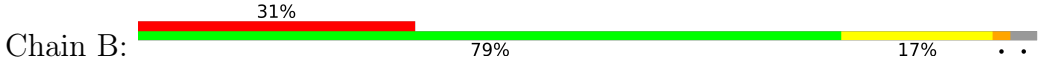
• Molecule 1: Pre-mRNA-splicing factor 8

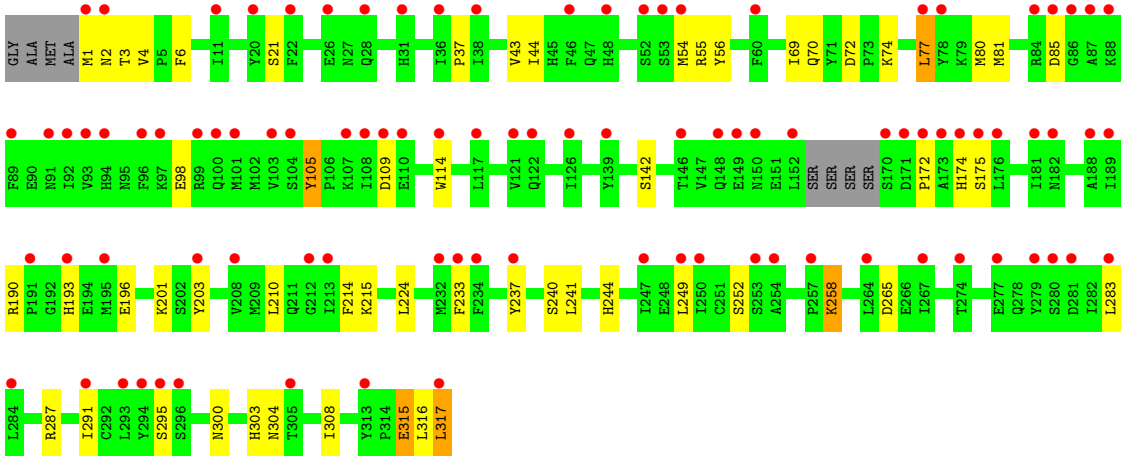
Chain A:



• Molecule 2: A1 cistron-splicing factor AAR2

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.00Å 82.99Å 92.17Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	20.55 – 2.06 44.96 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.55-2.06) 98.9 (44.96-2.06)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.268 , 0.320 0.283 , 0.333	Depositor DCC
R_{free} test set	1965 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4607	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

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	0.92	8/2049 (0.4%)	1.02	7/2775 (0.3%)
2	B	0.76	2/2630 (0.1%)	0.84	2/3552 (0.1%)
All	All	0.83	10/4679 (0.2%)	0.93	9/6327 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2005	PHE	CE2-CZ	7.44	1.51	1.37
1	A	1935	VAL	CB-CG1	-6.17	1.39	1.52
1	A	1880	PHE	CB-CG	6.05	1.61	1.51
2	B	114	TRP	CB-CG	5.90	1.60	1.50
1	A	2037	TYR	CD2-CE2	-5.57	1.30	1.39
2	B	105	TYR	CD1-CE1	-5.42	1.31	1.39
1	A	1899	TRP	CB-CG	5.36	1.59	1.50
1	A	2037	TYR	CD1-CE1	-5.35	1.31	1.39
1	A	2040	TRP	CB-CG	-5.22	1.40	1.50
1	A	1852	VAL	CB-CG1	5.12	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1889	LEU	CB-CG-CD1	8.48	125.42	111.00
1	A	1974	LEU	CB-CG-CD2	8.26	125.04	111.00
2	B	249	LEU	CB-CG-CD2	-7.15	98.85	111.00
1	A	1963	LEU	CB-CG-CD2	6.93	122.79	111.00
1	A	1940	MET	CG-SD-CE	-6.66	89.55	100.20
1	A	1988	LEU	CB-CG-CD2	6.14	121.44	111.00
2	B	308	ILE	CA-CB-CG1	-5.45	100.65	111.00
1	A	2011	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	A	1963	LEU	CB-CG-CD1	-5.37	101.87	111.00

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	25	0
2	B	2563	0	2433	30	0
3	A	27	0	0	0	0
3	B	15	0	0	2	0
All	All	4607	0	4462	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:2062:GLU:O	1:A:2066:LYS:HG2	1.77	0.84
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.34	0.75
2:B:224:LEU:HD23	2:B:224:LEU:O	1.88	0.73
2:B:224:LEU:HD23	2:B:224:LEU:C	2.11	0.71
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.72	0.70
2:B:70:GLN:HB3	2:B:81:MET:HE1	1.75	0.68
2:B:1:MET:N	3:B:402:HOH:O	2.26	0.68
1:A:1875:ILE:HD12	1:A:1979[B]:MET:HE3	1.82	0.61
2:B:300:ASN:O	2:B:303:HIS:NE2	2.35	0.60
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.26	0.57
1:A:1951:PHE:HB3	1:A:1954:ILE:HD12	1.86	0.56
2:B:55:ARG:HD2	2:B:233:PHE:O	2.06	0.55
1:A:1910:LYS:HG2	1:A:1940:MET:SD	2.47	0.55
2:B:74:LYS:NZ	3:B:401:HOH:O	2.13	0.55
2:B:265:ASP:OD2	2:B:304:ASN:HB2	2.07	0.54
1:A:1848:ILE:H	1:A:1931[A]:LYS:NZ	2.05	0.52
1:A:2047:GLN:O	1:A:2051:ILE:HG12	2.10	0.51
2:B:287:ARG:O	2:B:291:ILE:HD13	2.10	0.51
1:A:2021:SER:O	1:A:2022:ALA:C	2.48	0.51
2:B:237:TYR:CE2	2:B:241:LEU:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:GLN:HB3	2:B:81:MET:CE	2.42	0.49
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.13	0.49
2:B:77:LEU:O	2:B:77:LEU:HD23	2.13	0.49
1:A:1853:ASP:OD2	1:A:1855[B]:THR:HG23	2.12	0.48
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.48	0.48
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.48	0.48
2:B:6:PHE:HZ	2:B:44[A]:ILE:HD11	1.79	0.47
2:B:291:ILE:HA	2:B:295:SER:HB2	1.96	0.47
2:B:193:HIS:ND1	2:B:196:GLU:OE1	2.33	0.47
2:B:172:PRO:HA	2:B:175:SER:OG	2.15	0.47
2:B:201:LYS:HG3	2:B:252:SER:O	2.15	0.46
2:B:43:VAL:HG13	2:B:43:VAL:O	2.14	0.46
2:B:224:LEU:C	2:B:224:LEU:CD2	2.83	0.46
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	1.98	0.46
1:A:1974:LEU:O	1:A:1977:VAL:HG12	2.16	0.46
1:A:1857:VAL:HG21	1:A:1913:THR:OG1	2.16	0.45
1:A:2062:GLU:HB3	1:A:2066:LYS:HE3	1.99	0.45
1:A:1934:ILE:HA	1:A:1957:ARG:O	2.16	0.44
1:A:1914:ALA:HB1	1:A:1944:LEU:HA	1.98	0.44
1:A:1977:VAL:CG1	1:A:1978:VAL:N	2.80	0.44
1:A:1854:ASP:OD2	1:A:1940:MET:SD	2.77	0.43
2:B:72:ASP:OD1	2:B:72:ASP:C	2.55	0.42
2:B:244:HIS:HE1	2:B:283:LEU:O	2.02	0.42
2:B:56:TYR:CZ	2:B:77:LEU:HB2	2.55	0.41
2:B:85:ASP:C	2:B:85:ASP:OD1	2.58	0.41
1:A:1920:LEU:O	1:A:1924:LEU:HG	2.20	0.41
1:A:2056[B]:ARG:O	1:A:2060:LEU:HG	2.21	0.41
1:A:1940:MET:HE2	1:A:1940:MET:HB3	1.83	0.41
2:B:258:LYS:HD2	2:B:258:LYS:H	1.86	0.41
1:A:1940:MET:HA	1:A:1940:MET:HE3	2.03	0.41
2:B:315:GLU:C	2:B:317:LEU:N	2.74	0.41
2:B:214:PHE:O	2:B:215:LYS:HB2	2.21	0.41
1:A:2026:LEU:HG	1:A:2055:MET:CE	2.51	0.41
2:B:3:THR:HG22	2:B:4:VAL:N	2.37	0.40
2:B:69:ILE:HD13	2:B:80:MET:HA	2.03	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	248/258 (96%)	236 (95%)	11 (4%)	1 (0%)	34 25
2	B	304/308 (99%)	280 (92%)	20 (7%)	4 (1%)	12 4
All	All	552/566 (98%)	516 (94%)	31 (6%)	5 (1%)	19 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54[A]	MET
2	B	54[B]	MET
2	B	210	LEU
2	B	316	LEU
1	A	1964	PRO

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%)	221 (98%)	5 (2%)	52 46
2	B	285/284 (100%)	274 (96%)	11 (4%)	32 25
All	All	511/517 (99%)	495 (97%)	16 (3%)	42 34

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET

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Mol	Chain	Res	Type
1	A	1962	ARG
1	A	1979[A]	MET
1	A	1979[B]	MET
1	A	1979[C]	MET
2	B	2	ASN
2	B	21	SER
2	B	77	LEU
2	B	98	GLU
2	B	109	ASP
2	B	142	SER
2	B	174	HIS
2	B	240	SER
2	B	258	LYS
2	B	315	GLU
2	B	317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1869	ASN
1	A	1907	GLN
2	B	47	GLN
2	B	174	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

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, 95^{th} 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%)	1.48	64 (27%) 0 0	50, 89, 140, 286	0
2	B	300/308 (97%)	1.82	95 (31%) 0 0	56, 105, 160, 218	0
All	All	537/566 (94%)	1.67	159 (29%) 0 0	50, 98, 154, 286	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	53	SER	12.4
2	B	109	ASP	9.2
2	B	175	SER	8.4
1	A	1878	CYS	8.3
1	A	1833	GLY	6.7
2	B	92	ILE	6.7
2	B	193	HIS	6.5
1	A	2027	LEU	6.4
2	B	52	SER	6.3
2	B	172	PRO	5.8
2	B	176	LEU	5.3
2	B	96	PHE	5.2
2	B	99	ARG	5.2
2	B	89	PHE	5.1
1	A	1838	SER	5.0
2	B	1	MET	4.8
1	A	1840	TYR	4.7
2	B	171	ASP	4.6
2	B	100	GLN	4.6
1	A	1882	LEU	4.5
2	B	174	HIS	4.5
2	B	108	ILE	4.5
2	B	149	GLU	4.3
2	B	101	MET	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	317	LEU	4.3
2	B	281	ASP	4.3
2	B	85	ASP	4.2
2	B	181	ILE	4.2
2	B	88	LYS	4.2
1	A	2063	TYR	4.2
1	A	2040	TRP	4.1
1	A	1866	PHE	4.1
2	B	212	GLY	4.0
2	B	208	VAL	4.0
2	B	237	TYR	3.9
2	B	122[A]	GLN	3.9
2	B	87	ALA	3.8
2	B	78	TYR	3.8
1	A	2060	LEU	3.8
1	A	1940	MET	3.8
1	A	1979[A]	MET	3.8
2	B	189	ILE	3.7
2	B	277	GLU	3.7
2	B	173	ALA	3.7
1	A	1880	PHE	3.7
2	B	107	LYS	3.6
2	B	150	ASN	3.5
2	B	22	PHE	3.5
1	A	2017[A]	THR	3.5
2	B	257	PRO	3.5
1	A	2046	GLU	3.5
2	B	296	SER	3.5
1	A	2002	TYR	3.4
1	A	1839	ASN	3.4
2	B	38	ILE	3.3
2	B	254	ALA	3.3
2	B	203[A]	TYR	3.2
1	A	1996	LEU	3.2
2	B	264	LEU	3.2
2	B	110	GLU	3.2
2	B	279	TYR	3.2
2	B	36	ILE	3.2
1	A	2003	THR	3.1
2	B	280	SER	3.1
2	B	117	LEU	3.1
1	A	1881	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	97	LYS	3.0
1	A	2006	SER	3.0
2	B	295	SER	3.0
1	A	1986	MET	2.9
1	A	2026	LEU	2.9
2	B	146	THR	2.9
2	B	84	ARG	2.9
2	B	234	PHE	2.9
2	B	284	LEU	2.9
1	A	1934	ILE	2.8
1	A	2044	THR	2.8
2	B	54[A]	MET	2.8
1	A	1995	TRP	2.8
2	B	91	ASN	2.8
2	B	104	SER	2.8
2	B	126	ILE	2.8
1	A	1905	LEU	2.8
2	B	191	PRO	2.8
2	B	152	LEU	2.8
1	A	2021	SER	2.8
1	A	2036	SER	2.7
1	A	1861	THR	2.7
1	A	2001[A]	SER	2.7
2	B	232	MET	2.7
2	B	148	GLN	2.6
2	B	283	LEU	2.6
1	A	1863	HIS	2.6
1	A	1988	LEU	2.6
1	A	2015	LEU	2.6
2	B	2	ASN	2.6
1	A	1935	VAL	2.6
2	B	20	TYR	2.6
1	A	1961	LEU	2.6
2	B	77	LEU	2.6
1	A	2038	HIS	2.5
2	B	313	TYR	2.5
2	B	11	ILE	2.5
2	B	247	ILE	2.5
2	B	86	GLY	2.5
1	A	1921	VAL	2.5
1	A	2024[A]	MET	2.5
2	B	26	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1837	SER	2.5
1	A	1870	VAL	2.5
2	B	31	HIS	2.5
2	B	267	ILE	2.5
2	B	291	ILE	2.5
1	A	2047	GLN	2.5
1	A	1836	ASN	2.4
1	A	2018	ASN	2.4
2	B	46	PHE	2.4
2	B	60	PHE	2.4
2	B	182	ASN	2.4
1	A	2004	ALA	2.4
2	B	139	TYR	2.4
2	B	170	SER	2.3
2	B	294	TYR	2.3
2	B	93	VAL	2.3
2	B	94	HIS	2.3
2	B	249	LEU	2.3
2	B	48	HIS	2.3
1	A	2028	SER	2.3
1	A	1858	TYR	2.2
2	B	121	VAL	2.2
1	A	1971	ILE	2.2
1	A	1944	LEU	2.2
1	A	2058	LEU	2.2
2	B	253	SER	2.2
1	A	1891	LEU	2.2
2	B	188	ALA	2.2
1	A	2050	THR	2.2
2	B	195	MET	2.2
1	A	1992	TYR	2.2
1	A	1900	ALA	2.2
1	A	1926	LYS	2.2
1	A	1889	LEU	2.1
1	A	1841	ALA	2.1
1	A	1962	ARG	2.1
2	B	213	ILE	2.1
1	A	1869	ASN	2.1
2	B	103	VAL	2.1
1	A	1895	HIS	2.1
1	A	1968	ALA	2.1
1	A	1843	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	28	GLN	2.1
1	A	2059	ILE	2.1
2	B	250	ILE	2.1
2	B	293	LEU	2.1
2	B	233	PHE	2.1
2	B	305	THR	2.0
1	A	1974	LEU	2.0
2	B	114	TRP	2.0
2	B	274	THR	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.