



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:37 AM GMT

PDB ID : 2RH5
Title : Structure of Apo Adenylate Kinase from Aquifex Aeolicus
Authors : Thai, V.; Wolf-Watz, M.; Fenn, T; Pozharski, E.; Wilson, M.A.; Petsko, G.A.; Kern, D.
Deposited on : 2007-10-05
Resolution : 2.48 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

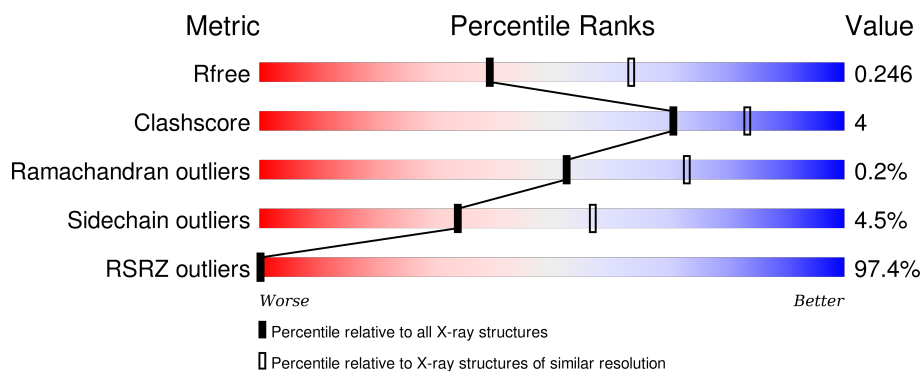
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	206	<div> <div>96%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	206	<div> <div>95%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
1	C	206	<div> <div>96%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4867 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 Adenylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1614	1041	277	293	3			
1	C	202	Total	C	N	O	S	0	0	0
			1614	1041	277	293	3			
1	B	202	Total	C	N	O	S	0	0	0
			1614	1041	277	293	3			

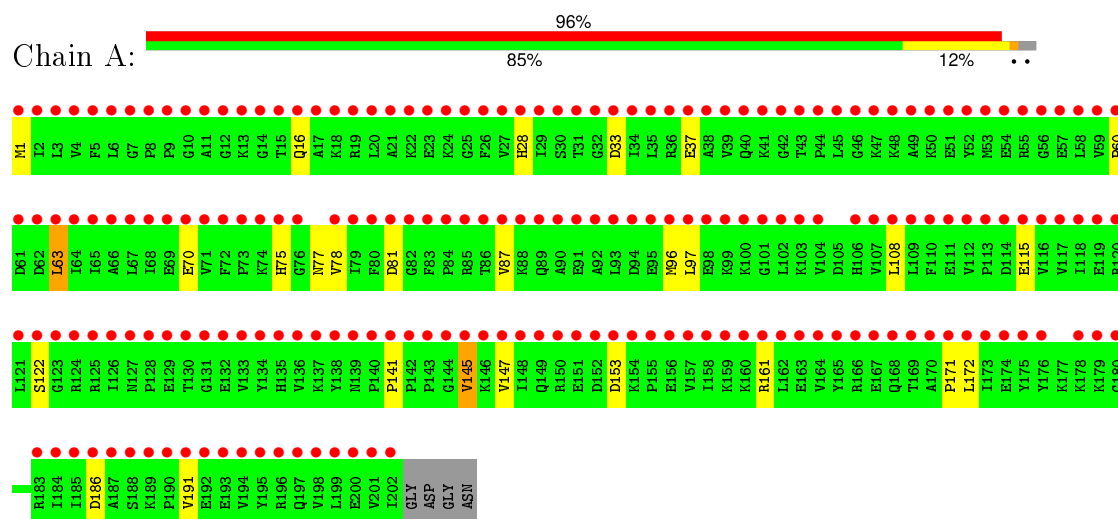
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	3	Total	O	0	0
			3	3		
2	C	3	Total	O	0	0
			3	3		

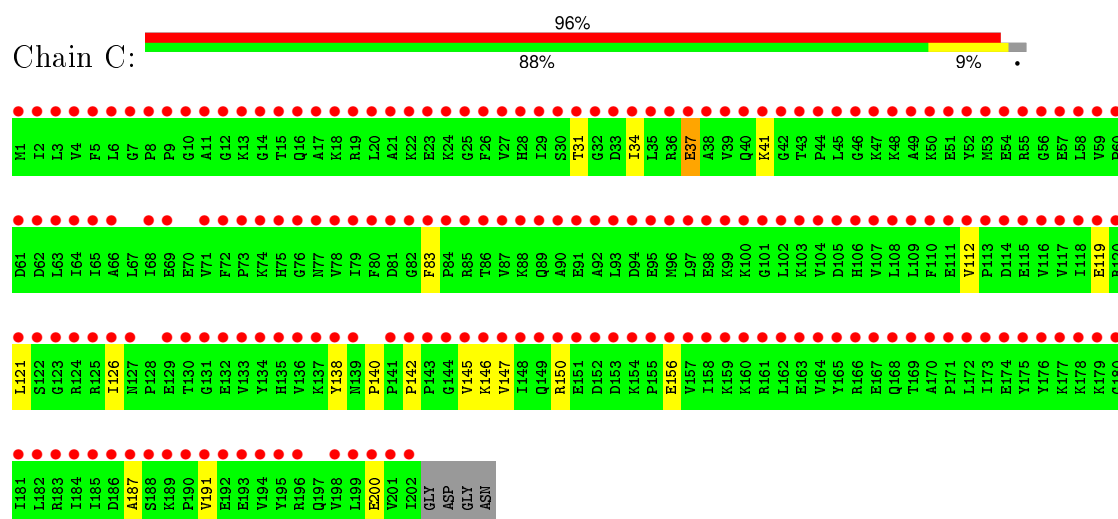
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

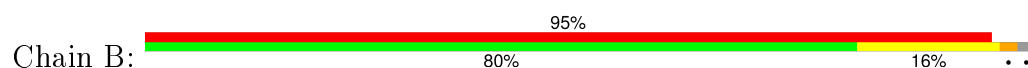
• Molecule 1: Adenylate kinase



• Molecule 1: Adenylate kinase



• Molecule 1: Adenylate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.68 Å 157.60 Å 84.71 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.14 – 2.48 47.13 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.3 (47.14-2.48) 89.5 (47.13-2.48)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.08 (at 2.48 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.255 0.188 , 0.246	Depositor DCC
R_{free} test set	1110 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	2.840	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 24554 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4867	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	0/1645	0.64	0/2218
1	B	0.43	0/1645	0.56	0/2218
1	C	0.49	0/1645	0.61	0/2218
All	All	0.48	0/4935	0.60	0/6654

There are no bond length outliers.

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	1614	0	1692	14	0
1	B	1614	0	1692	24	0
1	C	1614	0	1692	6	0
2	A	19	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
All	All	4867	0	5076	44	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 (44) 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:75:HIS:HD2	1:A:77:ASN:H	1.32	0.77
1:B:118:ILE:O	1:B:122:SER:HB2	1.87	0.73
1:B:43:THR:HB	1:B:44:PRO:HD2	1.72	0.71
1:B:186:ASP:H	1:B:197:GLN:HE22	1.38	0.70
1:C:126:ILE:HG13	1:C:150:ARG:HE	1.60	0.65
1:B:3:LEU:HD11	1:B:202:ILE:HD12	1.82	0.61
1:B:178:LYS:O	1:B:179:LYS:HG3	2.03	0.59
1:B:128:PRO:HG3	1:B:148:ILE:HG23	1.86	0.56
1:A:115:GLU:H	1:A:115:GLU:CD	2.11	0.54
1:B:127:ASN:C	1:B:127:ASN:HD22	2.11	0.53
1:A:60:PRO:HD2	1:A:63:LEU:HD22	1.89	0.52
1:C:37:GLU:O	1:C:41:LYS:HG3	2.11	0.49
1:B:83:PHE:CD1	1:B:84:PRO:HA	2.47	0.49
1:A:122:SER:HA	1:A:153:ASP:O	2.13	0.49
1:C:142:PRO:O	1:C:145:VAL:HG12	2.12	0.49
1:A:75:HIS:CD2	1:A:77:ASN:H	2.20	0.49
1:C:31:THR:HG21	1:C:83:PHE:CD1	2.48	0.48
1:B:170:ALA:HB3	1:B:171:PRO:HD3	1.97	0.47
1:B:29:ILE:HG23	1:B:34:ILE:HD11	1.97	0.47
1:B:190:PRO:HG2	1:B:193:GLU:HG3	1.95	0.47
1:B:127:ASN:HD22	1:B:129:GLU:H	1.64	0.46
1:B:152:ASP:N	1:B:152:ASP:OD2	2.47	0.45
1:B:185:ILE:HD12	1:B:197:GLN:HB3	2.00	0.44
1:A:87:VAL:CG2	1:A:171:PRO:HB2	2.48	0.44
1:B:115:GLU:H	1:B:115:GLU:CD	2.20	0.44
1:B:154:LYS:HD3	1:B:156:GLU:OE2	2.17	0.44
1:C:112:VAL:HG23	1:C:187:ALA:HB3	2.00	0.43
1:B:156:GLU:H	1:B:156:GLU:HG3	1.49	0.43
1:B:186:ASP:H	1:B:197:GLN:NE2	2.12	0.43
1:A:141:PRO:HB2	1:A:145:VAL:HG12	2.02	0.42
1:B:157:VAL:O	1:B:161:ARG:HB2	2.19	0.42
1:B:127:ASN:ND2	1:B:129:GLU:H	2.18	0.42
1:C:138:TYR:O	1:C:140:PRO:HD3	2.19	0.42
1:A:108:LEU:HD12	1:A:108:LEU:N	2.35	0.42
1:B:191:VAL:O	1:B:194:VAL:HG22	2.19	0.41
1:A:1:MET:N	1:A:77:ASN:OD1	2.53	0.41
1:B:36:ARG:O	1:B:40:GLN:HG3	2.21	0.41
1:B:94:ASP:OD2	1:B:179:LYS:NZ	2.53	0.41
1:A:16:GLN:HE22	1:A:191:VAL:HG13	1.85	0.41
1:A:28:HIS:HE1	1:A:81:ASP:OD2	2.03	0.41
1:A:33:ASP:O	1:A:37:GLU:HG3	2.20	0.40
1:B:118:ILE:O	1:B:122:SER:CB	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:OD1	1:A:186:ASP:C	2.59	0.40
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.88	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	200/206 (97%)	196 (98%)	4 (2%)	0	100	100
1	B	200/206 (97%)	196 (98%)	3 (2%)	1 (0%)	34	53
1	C	200/206 (97%)	193 (96%)	7 (4%)	0	100	100
All	All	600/618 (97%)	585 (98%)	14 (2%)	1 (0%)	52	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	LYS

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	176/178 (99%)	168 (96%)	8 (4%)	34	57
1	B	176/178 (99%)	169 (96%)	7 (4%)	38	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	176/178 (99%)	167 (95%)	9 (5%)	29 51
All	All	528/534 (99%)	504 (96%)	24 (4%)	34 57

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	70	GLU
1	A	78	VAL
1	A	96	MET
1	A	145	VAL
1	A	147	VAL
1	A	161	ARG
1	A	172	LEU
1	C	34	ILE
1	C	37	GLU
1	C	119	GLU
1	C	121	LEU
1	C	146	LYS
1	C	147	VAL
1	C	156	GLU
1	C	191	VAL
1	C	200	GLU
1	B	1	MET
1	B	63	LEU
1	B	122	SER
1	B	127	ASN
1	B	133	VAL
1	B	148	ILE
1	B	156	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	75	HIS
1	B	75	HIS
1	B	127	ASN
1	B	197	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 carbohydrates 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	202/206 (98%)	20.69	197 (97%) 0 0	39, 46, 53, 58	0
1	B	202/206 (98%)	19.68	196 (97%) 0 0	37, 47, 52, 57	0
1	C	202/206 (98%)	20.46	197 (97%) 0 0	36, 46, 54, 57	0
All	All	606/618 (98%)	20.27	590 (97%) 0 0	36, 46, 53, 58	0

All (590) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	SER	90.2
1	B	157	VAL	74.5
1	A	15	THR	74.0
1	C	155	PRO	73.5
1	B	156	GLU	70.5
1	A	69	GLU	69.3
1	A	26	PHE	65.4
1	B	60	PRO	64.4
1	C	143	PRO	64.4
1	C	117	VAL	63.9
1	C	118	ILE	63.2
1	B	83	PHE	63.0
1	C	16	GLN	62.9
1	B	66	ALA	62.9
1	B	67	LEU	62.3
1	A	49	ALA	62.1
1	A	158	ILE	61.6
1	B	102	LEU	60.1
1	A	46	GLY	59.4
1	C	59	VAL	59.2
1	B	105	ASP	59.0
1	C	187	ALA	57.5
1	C	76	GLY	56.8

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Mol	Chain	Res	Type	RSRZ
1	C	84	PRO	56.6
1	B	38	ALA	55.3
1	A	72	PHE	55.0
1	C	45	LEU	54.5
1	B	155	PRO	54.4
1	C	85	ARG	53.5
1	B	92	ALA	53.3
1	B	172	LEU	52.7
1	A	32	GLY	52.5
1	A	140	PRO	52.4
1	B	35	LEU	52.4
1	B	84	PRO	52.4
1	C	202	ILE	52.3
1	A	14	GLY	51.4
1	A	66	ALA	51.3
1	B	98	GLU	50.3
1	A	154	LYS	49.9
1	C	138	TYR	49.4
1	A	165	TYR	49.2
1	C	65	ILE	49.1
1	C	86	THR	48.9
1	B	130	THR	48.8
1	A	201	VAL	48.5
1	A	2	ILE	48.2
1	C	186	ASP	47.1
1	C	87	VAL	47.1
1	C	32	GLY	47.0
1	C	142	PRO	46.9
1	A	141	PRO	46.8
1	B	36	ARG	46.8
1	C	96	MET	46.3
1	B	139	ASN	46.0
1	A	117	VAL	46.0
1	B	104	VAL	45.9
1	B	181	ILE	45.9
1	C	136	VAL	45.8
1	A	133	VAL	45.6
1	A	53	MET	45.5
1	C	101	GLY	45.4
1	B	109	LEU	44.9
1	A	170	ALA	44.9
1	B	185	ILE	44.4

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Mol	Chain	Res	Type	RSRZ
1	A	90	ALA	44.2
1	C	77	ASN	44.1
1	C	183	ARG	44.1
1	A	185	ILE	44.0
1	B	25	GLY	43.7
1	B	51	GLU	43.6
1	C	31	THR	43.5
1	C	10	GLY	43.2
1	A	43	THR	42.8
1	B	125	ARG	42.7
1	A	20	LEU	42.7
1	A	122	SER	42.3
1	C	15	THR	42.3
1	C	62	ASP	42.3
1	C	14	GLY	41.7
1	B	202	ILE	41.2
1	B	144	GLY	41.1
1	C	7	GLY	40.9
1	C	164	VAL	40.8
1	A	64	ILE	40.7
1	A	62	ASP	40.7
1	A	196	ARG	40.6
1	B	9	PRO	40.6
1	C	60	PRO	40.6
1	C	81	ASP	40.4
1	A	12	GLY	40.1
1	A	173	ILE	40.0
1	C	131	GLY	39.9
1	A	67	LEU	39.8
1	A	192	GLU	39.3
1	B	20	LEU	39.3
1	B	131	GLY	39.0
1	B	197	GLN	38.9
1	A	171	PRO	38.6
1	B	59	VAL	38.5
1	C	95	GLU	38.4
1	B	145	VAL	38.2
1	A	184	ILE	37.6
1	C	63	LEU	37.6
1	A	4	VAL	37.1
1	B	46	GLY	36.9
1	B	154	LYS	36.6

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Mol	Chain	Res	Type	RSRZ
1	C	182	LEU	36.5
1	A	71	VAL	36.3
1	B	81	ASP	36.2
1	C	42	GLY	35.7
1	B	137	LYS	35.6
1	A	55	ARG	35.5
1	C	88	LYS	35.5
1	C	100	LYS	35.4
1	B	64	ILE	35.2
1	B	132	GLU	35.0
1	A	176	TYR	34.2
1	A	174	GLU	34.2
1	B	27	VAL	34.0
1	C	144	GLY	33.5
1	A	116	VAL	33.1
1	A	25	GLY	33.0
1	C	82	GLY	32.9
1	A	202	ILE	32.8
1	A	172	LEU	32.7
1	C	23	GLU	32.6
1	A	161	ARG	32.5
1	B	188	SER	32.5
1	C	173	ILE	32.4
1	C	137	LYS	32.4
1	C	69	GLU	32.2
1	A	47	LYS	32.2
1	C	174	GLU	32.0
1	C	75	HIS	31.9
1	B	180	GLY	31.4
1	A	195	TYR	31.4
1	B	68	ILE	31.3
1	A	68	ILE	30.8
1	A	130	THR	30.6
1	C	123	GLY	30.6
1	A	112	VAL	30.5
1	A	197	GLN	30.4
1	C	17	ALA	30.2
1	B	142	PRO	30.0
1	B	15	THR	29.9
1	A	118	ILE	29.9
1	B	24	LYS	29.9
1	C	120	ARG	29.5

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Mol	Chain	Res	Type	RSRZ
1	B	186	ASP	29.4
1	B	97	LEU	29.2
1	A	86	THR	29.0
1	A	94	ASP	29.0
1	B	103	LYS	28.6
1	C	147	VAL	28.4
1	B	166	ARG	28.3
1	B	191	VAL	28.2
1	B	2	ILE	28.1
1	C	198	VAL	28.0
1	B	82	GLY	27.9
1	A	114	ASP	27.8
1	C	94	ASP	27.7
1	A	159	LYS	27.5
1	A	63	LEU	27.2
1	B	58	LEU	27.2
1	B	91	GLU	27.2
1	B	55	ARG	27.0
1	A	178	LYS	26.9
1	C	21	ALA	26.8
1	A	74	LYS	26.7
1	C	38	ALA	26.7
1	C	43	THR	26.6
1	C	157	VAL	26.6
1	C	168	GLN	26.6
1	B	10	GLY	26.6
1	A	128	PRO	26.5
1	C	20	LEU	26.3
1	C	181	ILE	26.3
1	C	108	LEU	26.2
1	C	188	SER	26.1
1	B	175	TYR	26.0
1	C	130	THR	25.9
1	B	49	ALA	25.6
1	C	24	LYS	25.6
1	C	159	LYS	25.5
1	A	24	LYS	25.3
1	A	186	ASP	25.2
1	A	147	VAL	25.1
1	B	110	PHE	24.9
1	B	14	GLY	24.8
1	A	79	ILE	24.8

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Mol	Chain	Res	Type	RSRZ
1	C	74	LYS	24.8
1	B	111	GLU	24.7
1	B	54	GLU	24.5
1	A	5	PHE	24.4
1	A	61	ASP	24.4
1	B	85	ARG	24.4
1	A	168	GLN	24.2
1	C	162	LEU	24.2
1	A	123	GLY	24.2
1	B	198	VAL	24.0
1	A	134	TYR	23.9
1	C	29	ILE	23.9
1	C	58	LEU	23.8
1	B	78	VAL	23.8
1	C	160	LYS	23.8
1	C	80	PHE	23.7
1	A	115	GLU	23.7
1	B	99	LYS	23.6
1	A	109	LEU	23.5
1	C	152	ASP	23.2
1	B	87	VAL	23.2
1	B	22	LYS	22.9
1	A	135	HIS	22.8
1	B	153	ASP	22.6
1	A	157	VAL	22.3
1	A	87	VAL	22.2
1	C	44	PRO	22.2
1	B	107	VAL	22.0
1	C	83	PHE	22.0
1	C	105	ASP	21.9
1	B	143	PRO	21.9
1	B	26	PHE	21.9
1	A	6	LEU	21.8
1	C	148	ILE	21.8
1	A	108	LEU	21.5
1	B	88	LYS	21.5
1	A	113	PRO	21.4
1	B	135	HIS	21.3
1	A	155	PRO	21.3
1	A	21	ALA	21.3
1	A	89	GLN	21.2
1	C	53	MET	21.1

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Mol	Chain	Res	Type	RSRZ
1	C	161	ARG	21.0
1	A	13	LYS	21.0
1	B	19	ARG	20.7
1	A	136	VAL	20.4
1	C	110	PHE	20.4
1	A	139	ASN	20.3
1	C	107	VAL	20.1
1	C	179	LYS	20.1
1	A	22	LYS	19.9
1	B	101	GLY	19.8
1	A	83	PHE	19.7
1	A	153	ASP	19.6
1	A	91	GLU	19.6
1	B	17	ALA	19.5
1	B	95	GLU	19.4
1	A	29	ILE	19.3
1	A	102	LEU	19.3
1	A	85	ARG	19.2
1	C	163	GLU	18.8
1	B	16	GLN	18.8
1	B	159	LYS	18.7
1	A	169	THR	18.7
1	A	180	GLY	18.6
1	A	3	LEU	18.6
1	C	78	VAL	18.5
1	B	33	ASP	18.5
1	B	70	GLU	18.5
1	B	126	ILE	18.5
1	A	121	LEU	18.3
1	A	80	PHE	18.3
1	A	160	LYS	18.3
1	B	21	ALA	18.2
1	C	90	ALA	18.1
1	B	113	PRO	18.1
1	C	92	ALA	18.0
1	A	40	GLN	18.0
1	A	48	LYS	18.0
1	A	78	VAL	17.9
1	C	46	GLY	17.9
1	A	103	LYS	17.8
1	A	30	SER	17.8
1	B	149	GLN	17.8

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Mol	Chain	Res	Type	RSRZ
1	C	61	ASP	17.7
1	A	167	GLU	17.7
1	A	190	PRO	17.6
1	A	194	VAL	17.5
1	B	158	ILE	17.3
1	C	165	TYR	17.3
1	A	138	TYR	17.3
1	C	71	VAL	17.1
1	B	165	TYR	17.0
1	C	66	ALA	16.9
1	A	107	VAL	16.8
1	A	38	ALA	16.8
1	B	45	LEU	16.8
1	A	88	LYS	16.6
1	B	12	GLY	16.6
1	A	16	GLN	16.6
1	A	143	PRO	16.4
1	C	171	PRO	16.3
1	C	8	PRO	16.1
1	C	151	GLU	16.1
1	B	93	LEU	16.1
1	B	136	VAL	15.9
1	A	51	GLU	15.8
1	B	100	LYS	15.7
1	B	52	TYR	15.7
1	A	50	LYS	15.6
1	A	44	PRO	15.4
1	C	99	LYS	15.3
1	C	56	GLY	15.3
1	A	33	ASP	15.3
1	C	127	ASN	15.3
1	C	9	PRO	15.3
1	B	170	ALA	15.3
1	C	129	GLU	15.2
1	B	173	ILE	15.1
1	B	4	VAL	15.1
1	A	60	PRO	15.1
1	A	52	TYR	15.0
1	C	26	PHE	14.8
1	C	192	GLU	14.8
1	A	193	GLU	14.7
1	B	77	ASN	14.7

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Mol	Chain	Res	Type	RSRZ
1	C	33	ASP	14.6
1	B	164	VAL	14.6
1	C	102	LEU	14.6
1	C	25	GLY	14.6
1	B	76	GLY	14.6
1	C	79	ILE	14.5
1	B	50	LYS	14.4
1	B	47	LYS	14.3
1	A	164	VAL	14.2
1	A	75	HIS	14.2
1	C	115	GLU	14.2
1	C	64	ILE	14.1
1	A	127	ASN	14.1
1	A	129	GLU	14.0
1	B	73	PRO	14.0
1	A	70	GLU	14.0
1	C	103	LYS	13.9
1	C	185	ILE	13.8
1	C	93	LEU	13.7
1	C	132	GLU	13.7
1	B	167	GLU	13.6
1	C	55	ARG	13.5
1	B	178	LYS	13.3
1	A	152	ASP	13.3
1	A	95	GLU	13.2
1	B	37	GLU	13.2
1	A	36	ARG	13.1
1	C	172	LEU	13.1
1	B	115	GLU	12.9
1	A	150	ARG	12.7
1	A	17	ALA	12.7
1	C	177	LYS	12.5
1	B	11	ALA	12.4
1	A	126	ILE	12.4
1	B	39	VAL	12.1
1	A	151	GLU	12.0
1	B	63	LEU	12.0
1	A	200	GLU	12.0
1	C	158	ILE	12.0
1	B	8	PRO	12.0
1	B	123	GLY	11.9
1	A	191	VAL	11.8

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Mol	Chain	Res	Type	RSRZ
1	A	31	THR	11.7
1	B	124	ARG	11.6
1	B	134	TYR	11.6
1	A	101	GLY	11.5
1	C	57	GLU	11.5
1	A	56	GLY	11.5
1	A	175	TYR	11.5
1	C	135	HIS	11.3
1	C	124	ARG	11.3
1	A	179	LYS	11.3
1	A	166	ARG	11.2
1	A	93	LEU	11.1
1	A	73	PRO	11.0
1	C	54	GLU	11.0
1	A	19	ARG	10.9
1	B	65	ILE	10.8
1	B	43	THR	10.6
1	B	1	MET	10.6
1	C	189	LYS	10.6
1	A	92	ALA	10.6
1	C	39	VAL	10.6
1	B	6	LEU	10.5
1	B	182	LEU	10.5
1	C	19	ARG	10.5
1	C	97	LEU	10.5
1	A	84	PRO	10.4
1	A	111	GLU	10.4
1	C	109	LEU	10.3
1	C	47	LYS	10.3
1	C	156	GLU	10.3
1	B	23	GLU	10.2
1	B	96	MET	10.2
1	C	41	LYS	10.2
1	C	18	LYS	10.1
1	B	30	SER	10.1
1	C	72	PHE	10.0
1	C	125	ARG	10.0
1	B	28	HIS	10.0
1	B	169	THR	9.8
1	B	69	GLU	9.7
1	C	40	GLN	9.7
1	C	73	PRO	9.5

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Mol	Chain	Res	Type	RSRZ
1	C	175	TYR	9.5
1	C	141	PRO	9.5
1	A	65	ILE	9.5
1	A	9	PRO	9.5
1	C	176	TYR	9.4
1	B	196	ARG	9.4
1	C	116	VAL	9.4
1	C	196	ARG	9.3
1	A	98	GLU	9.3
1	A	10	GLY	9.2
1	A	11	ALA	9.2
1	B	162	LEU	9.1
1	C	145	VAL	9.1
1	A	45	LEU	8.9
1	A	131	GLY	8.8
1	A	142	PRO	8.7
1	B	138	TYR	8.7
1	A	27	VAL	8.7
1	B	114	ASP	8.6
1	C	106	HIS	8.6
1	B	190	PRO	8.6
1	B	72	PHE	8.5
1	C	111	GLU	8.5
1	B	133	VAL	8.5
1	C	201	VAL	8.4
1	C	190	PRO	8.4
1	C	154	LYS	8.4
1	A	59	VAL	8.4
1	B	201	VAL	8.2
1	B	168	GLN	8.2
1	B	199	LEU	8.2
1	A	58	LEU	8.2
1	B	121	LEU	8.1
1	C	52	TYR	8.1
1	B	3	LEU	8.1
1	B	183	ARG	8.0
1	A	137	LYS	7.8
1	B	18	LYS	7.8
1	A	183	ARG	7.6
1	B	71	VAL	7.6
1	B	62	ASP	7.5
1	B	189	LYS	7.5

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Mol	Chain	Res	Type	RSRZ
1	C	199	LEU	7.5
1	B	106	HIS	7.5
1	B	192	GLU	7.5
1	B	61	ASP	7.4
1	C	126	ILE	7.4
1	C	114	ASP	7.2
1	B	120	ARG	7.2
1	B	171	PRO	7.2
1	B	187	ALA	7.2
1	B	34	ILE	7.2
1	B	13	LYS	7.1
1	C	180	GLY	7.0
1	C	169	THR	7.0
1	A	41	LYS	6.9
1	A	96	MET	6.9
1	B	42	GLY	6.9
1	A	18	LYS	6.9
1	C	1	MET	6.8
1	B	161	ARG	6.6
1	C	170	ALA	6.6
1	C	89	GLN	6.5
1	B	32	GLY	6.5
1	B	200	GLU	6.4
1	B	89	GLN	6.3
1	C	68	ILE	6.3
1	A	34	ILE	6.3
1	A	188	SER	6.3
1	B	112	VAL	6.2
1	B	140	PRO	6.2
1	B	141	PRO	6.2
1	B	148	ILE	6.1
1	C	139	ASN	6.1
1	C	121	LEU	6.1
1	A	146	LYS	6.0
1	B	41	LYS	6.0
1	A	76	GLY	6.0
1	B	146	LYS	5.9
1	C	4	VAL	5.9
1	A	1	MET	5.8
1	B	29	ILE	5.8
1	C	11	ALA	5.8
1	B	152	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	150	ARG	5.7
1	B	177	LYS	5.7
1	A	110	PHE	5.7
1	B	75	HIS	5.7
1	A	163	GLU	5.5
1	C	191	VAL	5.4
1	A	7	GLY	5.4
1	C	104	VAL	5.4
1	B	184	ILE	5.4
1	B	176	TYR	5.4
1	C	6	LEU	5.4
1	B	90	ALA	5.3
1	A	104	VAL	5.2
1	A	37	GLU	5.2
1	C	178	LYS	5.2
1	A	54	GLU	5.1
1	B	57	GLU	5.1
1	C	27	VAL	5.0
1	A	23	GLU	5.0
1	A	119	GLU	4.9
1	C	12	GLY	4.9
1	A	42	GLY	4.8
1	A	198	VAL	4.8
1	A	120	ARG	4.8
1	A	162	LEU	4.7
1	A	156	GLU	4.7
1	A	187	ALA	4.7
1	B	193	GLU	4.6
1	C	91	GLU	4.6
1	C	167	GLU	4.5
1	C	149	GLN	4.3
1	A	199	LEU	4.3
1	A	39	VAL	4.3
1	B	129	GLU	4.3
1	B	122	SER	4.2
1	B	127	ASN	4.2
1	B	194	VAL	4.2
1	C	28	HIS	4.1
1	B	179	LYS	4.1
1	C	119	GLU	4.1
1	C	153	ASP	4.0
1	B	56	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	4.0
1	A	35	LEU	4.0
1	B	119	GLU	4.0
1	A	82	GLY	4.0
1	A	99	LYS	3.9
1	C	133	VAL	3.8
1	C	200	GLU	3.8
1	B	48	LYS	3.8
1	A	97	LEU	3.8
1	A	8	PRO	3.7
1	C	194	VAL	3.6
1	C	184	ILE	3.6
1	A	100	LYS	3.6
1	A	148	ILE	3.6
1	B	80	PHE	3.6
1	A	149	GLN	3.6
1	C	150	ARG	3.5
1	C	98	GLU	3.5
1	B	116	VAL	3.4
1	B	108	LEU	3.3
1	B	94	ASP	3.3
1	B	53	MET	3.3
1	B	195	TYR	3.2
1	C	49	ALA	3.2
1	A	57	GLU	3.1
1	C	50	LYS	3.1
1	B	163	GLU	3.1
1	A	132	GLU	3.1
1	A	81	ASP	3.0
1	A	28	HIS	3.0
1	C	122	SER	2.9
1	C	13	LYS	2.9
1	C	146	LYS	2.9
1	C	51	GLU	2.8
1	B	86	THR	2.8
1	A	106	HIS	2.8
1	A	189	LYS	2.8
1	B	40	GLN	2.8
1	C	112	VAL	2.7
1	C	2	ILE	2.7
1	B	174	GLU	2.6
1	C	5	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	22	LYS	2.6
1	C	193	GLU	2.6
1	A	144	GLY	2.6
1	C	166	ARG	2.5
1	C	195	TYR	2.5
1	C	48	LYS	2.5
1	B	44	PRO	2.5
1	B	74	LYS	2.4
1	C	34	ILE	2.4
1	B	147	VAL	2.4
1	C	35	LEU	2.4
1	C	36	ARG	2.4
1	C	3	LEU	2.4
1	A	145	VAL	2.4
1	C	113	PRO	2.3
1	B	7	GLY	2.3
1	C	134	TYR	2.3
1	B	160	LYS	2.3
1	A	125	ARG	2.2
1	A	124	ARG	2.0
1	C	37	GLU	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.