



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 03:26 AM EST

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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

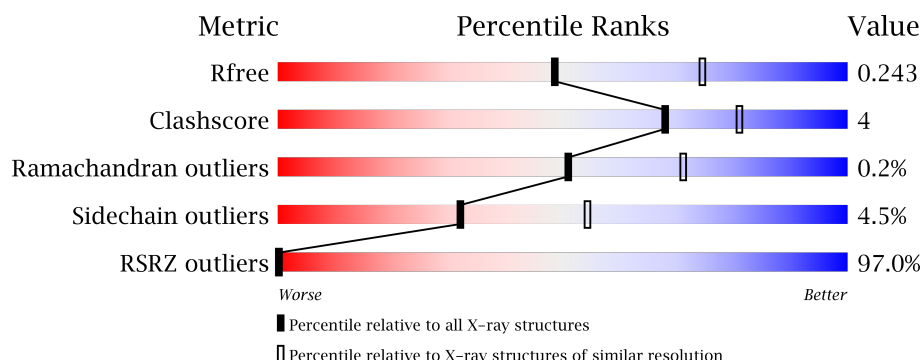
1 Overall quality at a glance

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}	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (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>95%</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>95%</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			

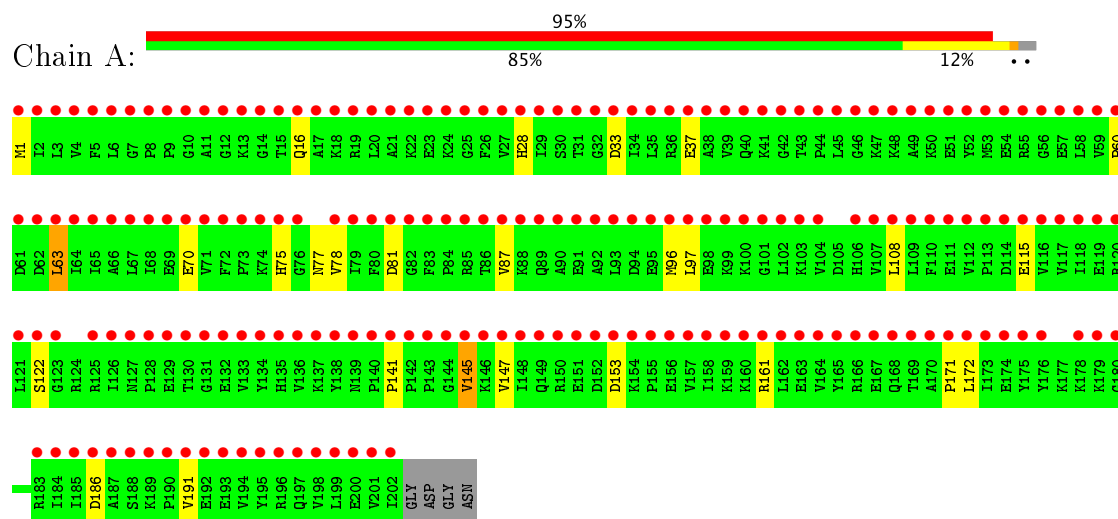
- Molecule 2 is water.

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

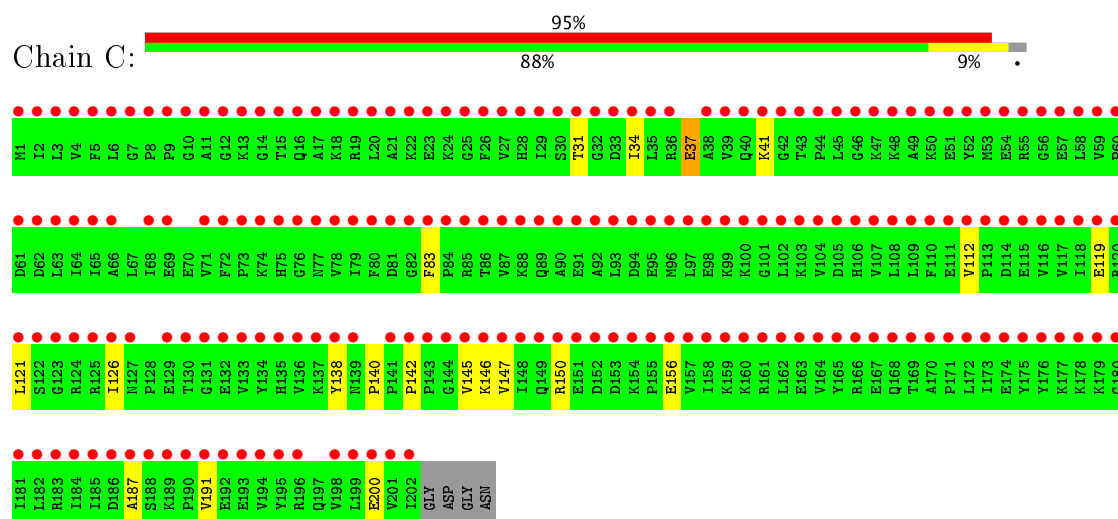
3 Residue-property plots

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

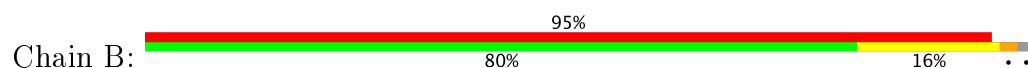
• Molecule 1: Adenylate kinase



• 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 0.185 , 0.243	Depositor DCC
R_{free} test set	1094 reflections (4.78%)	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
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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	0.53	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%)	32	51
1	C	200/206 (97%)	193 (96%)	7 (4%)	0	100	100
All	All	600/618 (97%)	585 (98%)	14 (2%)	1 (0%)	51	71

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%)	32	54
1	B	176/178 (99%)	169 (96%)	7 (4%)	36	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	176/178 (99%)	167 (95%)	9 (5%)	28	48
All	All	528/534 (99%)	504 (96%)	24 (4%)	32	54

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%)	19.99	196 (97%) 0 0	39, 46, 53, 58	0
1	B	202/206 (98%)	19.01	196 (97%) 0 0	37, 47, 52, 57	0
1	C	202/206 (98%)	19.75	196 (97%) 0 0	36, 46, 54, 57	0
All	All	606/618 (98%)	19.58	588 (97%) 0 0	36, 46, 53, 58	0

All (588) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	SER	87.9
1	B	157	VAL	71.7
1	A	15	THR	71.5
1	C	155	PRO	70.4
1	B	156	GLU	68.6
1	A	69	GLU	67.4
1	A	26	PHE	63.9
1	B	60	PRO	61.8
1	C	143	PRO	61.7
1	B	83	PHE	61.5
1	C	117	VAL	61.5
1	C	118	ILE	61.2
1	C	16	GLN	61.2
1	B	66	ALA	60.5
1	B	67	LEU	60.4
1	A	158	ILE	59.7
1	A	49	ALA	59.7
1	B	102	LEU	58.3
1	A	46	GLY	57.1
1	C	59	VAL	57.0
1	B	105	ASP	56.9
1	C	187	ALA	55.3
1	C	76	GLY	54.5

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Mol	Chain	Res	Type	RSRZ
1	C	84	PRO	54.2
1	A	72	PHE	53.7
1	B	38	ALA	53.2
1	C	45	LEU	52.8
1	B	155	PRO	52.2
1	C	85	ARG	52.1
1	B	92	ALA	51.3
1	B	172	LEU	51.1
1	B	35	LEU	50.8
1	C	202	ILE	50.7
1	A	32	GLY	50.4
1	A	140	PRO	50.2
1	B	84	PRO	50.2
1	A	14	GLY	49.4
1	A	66	ALA	49.4
1	B	98	GLU	48.9
1	A	154	LYS	48.7
1	C	138	TYR	48.3
1	A	165	TYR	48.0
1	C	65	ILE	47.6
1	C	86	THR	47.3
1	B	130	THR	47.2
1	A	2	ILE	46.7
1	A	201	VAL	46.7
1	B	36	ARG	45.6
1	C	186	ASP	45.4
1	C	87	VAL	45.3
1	C	32	GLY	45.1
1	C	142	PRO	44.9
1	A	141	PRO	44.9
1	B	139	ASN	44.7
1	B	181	ILE	44.4
1	C	96	MET	44.4
1	A	117	VAL	44.2
1	B	104	VAL	44.2
1	C	136	VAL	44.0
1	A	133	VAL	43.8
1	C	101	GLY	43.6
1	B	109	LEU	43.6
1	A	53	MET	43.6
1	A	170	ALA	43.2
1	B	185	ILE	43.0

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Mol	Chain	Res	Type	RSRZ
1	C	183	ARG	42.9
1	C	77	ASN	42.9
1	A	185	ILE	42.6
1	A	90	ALA	42.5
1	B	51	GLU	42.3
1	C	31	THR	42.0
1	B	25	GLY	42.0
1	B	125	ARG	41.6
1	C	10	GLY	41.5
1	A	43	THR	41.4
1	A	20	LEU	41.4
1	A	122	SER	41.2
1	C	15	THR	40.8
1	C	62	ASP	40.7
1	C	14	GLY	40.0
1	B	202	ILE	40.0
1	A	196	ARG	39.5
1	B	144	GLY	39.5
1	A	64	ILE	39.4
1	C	7	GLY	39.3
1	C	164	VAL	39.3
1	A	62	ASP	39.2
1	C	81	ASP	38.9
1	B	9	PRO	38.9
1	C	60	PRO	38.9
1	A	173	ILE	38.7
1	A	67	LEU	38.6
1	A	12	GLY	38.5
1	C	131	GLY	38.3
1	A	192	GLU	38.2
1	B	20	LEU	38.1
1	B	197	GLN	37.8
1	B	131	GLY	37.5
1	C	95	GLU	37.3
1	B	59	VAL	37.0
1	A	171	PRO	37.0
1	B	145	VAL	36.7
1	C	63	LEU	36.4
1	A	184	ILE	36.4
1	B	154	LYS	35.7
1	A	4	VAL	35.6
1	B	46	GLY	35.5

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Mol	Chain	Res	Type	RSRZ
1	C	182	LEU	35.3
1	A	71	VAL	34.9
1	B	81	ASP	34.9
1	B	137	LYS	34.8
1	C	88	LYS	34.6
1	A	55	ARG	34.6
1	C	100	LYS	34.6
1	C	42	GLY	34.3
1	B	64	ILE	34.1
1	B	132	GLU	34.0
1	A	176	TYR	33.4
1	A	174	GLU	33.2
1	B	27	VAL	32.6
1	C	144	GLY	32.2
1	A	116	VAL	31.8
1	A	202	ILE	31.8
1	A	172	LEU	31.7
1	C	23	GLU	31.7
1	A	25	GLY	31.7
1	A	161	ARG	31.7
1	B	188	SER	31.6
1	C	137	LYS	31.6
1	C	82	GLY	31.6
1	A	47	LYS	31.4
1	C	173	ILE	31.4
1	C	69	GLU	31.3
1	C	174	GLU	31.1
1	C	75	HIS	31.0
1	A	195	TYR	30.6
1	B	68	ILE	30.3
1	B	180	GLY	30.2
1	A	68	ILE	29.8
1	A	130	THR	29.6
1	A	197	GLN	29.5
1	C	123	GLY	29.4
1	A	112	VAL	29.3
1	B	24	LYS	29.1
1	C	17	ALA	29.0
1	A	118	ILE	28.9
1	B	15	THR	28.9
1	B	142	PRO	28.7
1	C	120	ARG	28.7

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Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	28.3
1	B	186	ASP	28.3
1	A	86	THR	28.0
1	A	94	ASP	27.9
1	B	103	LYS	27.9
1	B	166	ARG	27.6
1	C	147	VAL	27.3
1	B	2	ILE	27.2
1	B	191	VAL	27.1
1	C	198	VAL	27.0
1	A	114	ASP	26.8
1	B	82	GLY	26.8
1	A	159	LYS	26.8
1	C	94	ASP	26.7
1	B	91	GLU	26.4
1	A	63	LEU	26.3
1	B	58	LEU	26.3
1	B	55	ARG	26.3
1	A	178	LYS	26.2
1	A	74	LYS	26.1
1	C	168	GLN	25.8
1	C	21	ALA	25.8
1	C	43	THR	25.7
1	C	38	ALA	25.6
1	C	157	VAL	25.5
1	C	20	LEU	25.5
1	B	10	GLY	25.5
1	C	181	ILE	25.4
1	C	188	SER	25.4
1	B	175	TYR	25.4
1	A	128	PRO	25.3
1	C	108	LEU	25.3
1	C	130	THR	25.0
1	C	24	LYS	25.0
1	C	159	LYS	24.9
1	A	24	LYS	24.7
1	B	49	ALA	24.6
1	B	110	PHE	24.3
1	A	186	ASP	24.3
1	C	74	LYS	24.1
1	A	147	VAL	24.1
1	A	79	ILE	24.0

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Mol	Chain	Res	Type	RSRZ
1	B	111	GLU	23.9
1	A	5	PHE	23.8
1	B	14	GLY	23.8
1	B	54	GLU	23.8
1	B	85	ARG	23.8
1	A	168	GLN	23.5
1	A	61	ASP	23.5
1	C	162	LEU	23.5
1	A	134	TYR	23.3
1	A	123	GLY	23.2
1	C	160	LYS	23.2
1	C	80	PHE	23.1
1	C	29	ILE	23.1
1	C	58	LEU	23.1
1	B	198	VAL	23.1
1	B	99	LYS	23.0
1	A	115	GLU	23.0
1	B	78	VAL	22.9
1	A	109	LEU	22.7
1	C	152	ASP	22.4
1	B	87	VAL	22.3
1	B	22	LYS	22.3
1	A	135	HIS	22.2
1	B	153	ASP	21.8
1	C	83	PHE	21.4
1	A	157	VAL	21.4
1	B	26	PHE	21.4
1	A	87	VAL	21.3
1	C	44	PRO	21.2
1	A	6	LEU	21.1
1	B	107	VAL	21.1
1	C	105	ASP	21.1
1	C	148	ILE	21.1
1	B	143	PRO	21.0
1	B	88	LYS	20.9
1	A	108	LEU	20.8
1	B	135	HIS	20.8
1	A	89	GLN	20.5
1	A	113	PRO	20.5
1	C	161	ARG	20.4
1	A	21	ALA	20.4
1	A	13	LYS	20.4

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Mol	Chain	Res	Type	RSRZ
1	A	155	PRO	20.4
1	C	53	MET	20.2
1	B	19	ARG	20.2
1	C	110	PHE	19.9
1	A	139	ASN	19.7
1	A	136	VAL	19.6
1	C	179	LYS	19.6
1	A	22	LYS	19.4
1	C	107	VAL	19.3
1	A	83	PHE	19.2
1	A	91	GLU	19.0
1	B	101	GLY	19.0
1	A	153	ASP	18.9
1	B	95	GLU	18.8
1	B	17	ALA	18.7
1	A	29	ILE	18.7
1	A	102	LEU	18.7
1	A	85	ARG	18.6
1	C	163	GLU	18.2
1	B	159	LYS	18.2
1	B	16	GLN	18.2
1	A	169	THR	18.0
1	A	3	LEU	18.0
1	B	70	GLU	18.0
1	B	126	ILE	17.9
1	A	80	PHE	17.9
1	A	180	GLY	17.8
1	B	33	ASP	17.8
1	C	78	VAL	17.8
1	A	160	LYS	17.8
1	A	121	LEU	17.7
1	A	48	LYS	17.5
1	B	21	ALA	17.5
1	A	40	GLN	17.5
1	C	90	ALA	17.4
1	B	113	PRO	17.3
1	A	103	LYS	17.3
1	C	92	ALA	17.3
1	A	30	SER	17.3
1	B	149	GLN	17.2
1	A	167	GLU	17.2
1	A	78	VAL	17.1

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Mol	Chain	Res	Type	RSRZ
1	C	46	GLY	17.1
1	C	61	ASP	17.0
1	A	190	PRO	16.9
1	C	165	TYR	16.8
1	A	138	TYR	16.8
1	A	194	VAL	16.8
1	B	158	ILE	16.7
1	B	165	TYR	16.6
1	C	71	VAL	16.4
1	C	66	ALA	16.2
1	B	45	LEU	16.2
1	A	107	VAL	16.2
1	A	88	LYS	16.2
1	A	16	GLN	16.1
1	A	38	ALA	16.1
1	B	12	GLY	15.9
1	A	143	PRO	15.7
1	C	151	GLU	15.7
1	C	171	PRO	15.6
1	B	93	LEU	15.5
1	C	8	PRO	15.4
1	B	136	VAL	15.3
1	A	51	GLU	15.3
1	B	100	LYS	15.2
1	B	52	TYR	15.2
1	A	50	LYS	15.2
1	C	99	LYS	14.9
1	C	127	ASN	14.8
1	C	129	GLU	14.8
1	A	33	ASP	14.7
1	A	44	PRO	14.7
1	C	56	GLY	14.7
1	A	52	TYR	14.6
1	B	170	ALA	14.6
1	C	9	PRO	14.6
1	B	173	ILE	14.6
1	B	4	VAL	14.5
1	C	26	PHE	14.5
1	A	60	PRO	14.4
1	C	192	GLU	14.3
1	A	193	GLU	14.3
1	B	77	ASN	14.3

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Mol	Chain	Res	Type	RSRZ
1	C	102	LEU	14.1
1	C	33	ASP	14.1
1	B	164	VAL	14.0
1	C	25	GLY	14.0
1	B	76	GLY	14.0
1	B	50	LYS	14.0
1	C	79	ILE	14.0
1	B	47	LYS	13.9
1	A	75	HIS	13.8
1	C	115	GLU	13.7
1	A	164	VAL	13.6
1	C	64	ILE	13.6
1	A	127	ASN	13.6
1	A	129	GLU	13.6
1	A	70	GLU	13.5
1	C	103	LYS	13.5
1	B	73	PRO	13.4
1	C	185	ILE	13.3
1	C	93	LEU	13.3
1	C	132	GLU	13.3
1	B	167	GLU	13.2
1	C	55	ARG	13.2
1	B	178	LYS	12.9
1	A	95	GLU	12.8
1	B	37	GLU	12.8
1	A	36	ARG	12.8
1	A	152	ASP	12.7
1	C	172	LEU	12.7
1	B	115	GLU	12.5
1	A	150	ARG	12.3
1	C	177	LYS	12.2
1	A	17	ALA	12.2
1	A	126	ILE	12.0
1	B	11	ALA	11.9
1	A	151	GLU	11.7
1	A	200	GLU	11.7
1	B	63	LEU	11.6
1	C	158	ILE	11.6
1	B	39	VAL	11.6
1	B	8	PRO	11.4
1	B	123	GLY	11.4
1	A	191	VAL	11.3

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Mol	Chain	Res	Type	RSRZ
1	B	124	ARG	11.3
1	B	134	TYR	11.2
1	A	31	THR	11.2
1	A	175	TYR	11.1
1	C	57	GLU	11.1
1	A	101	GLY	11.0
1	C	135	HIS	11.0
1	C	124	ARG	11.0
1	A	56	GLY	11.0
1	A	179	LYS	11.0
1	A	166	ARG	10.9
1	A	93	LEU	10.8
1	C	54	GLU	10.6
1	A	19	ARG	10.6
1	A	73	PRO	10.5
1	B	65	ILE	10.4
1	C	189	LYS	10.3
1	B	43	THR	10.2
1	C	19	ARG	10.2
1	B	1	MET	10.1
1	A	92	ALA	10.1
1	B	6	LEU	10.1
1	B	182	LEU	10.1
1	C	39	VAL	10.1
1	C	97	LEU	10.1
1	A	111	GLU	10.0
1	C	47	LYS	10.0
1	A	84	PRO	10.0
1	C	109	LEU	10.0
1	C	156	GLU	10.0
1	C	41	LYS	9.9
1	B	23	GLU	9.9
1	C	18	LYS	9.8
1	B	30	SER	9.8
1	C	72	PHE	9.7
1	B	96	MET	9.7
1	C	125	ARG	9.7
1	B	28	HIS	9.7
1	B	169	THR	9.5
1	B	69	GLU	9.4
1	C	40	GLN	9.4
1	C	175	TYR	9.2

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Mol	Chain	Res	Type	RSRZ
1	C	176	TYR	9.2
1	A	65	ILE	9.1
1	B	196	ARG	9.1
1	C	73	PRO	9.1
1	C	196	ARG	9.1
1	C	141	PRO	9.0
1	A	9	PRO	9.0
1	A	98	GLU	9.0
1	C	116	VAL	9.0
1	B	162	LEU	8.8
1	A	10	GLY	8.8
1	A	11	ALA	8.8
1	C	145	VAL	8.7
1	A	45	LEU	8.6
1	B	138	TYR	8.5
1	A	131	GLY	8.4
1	A	142	PRO	8.3
1	C	106	HIS	8.3
1	B	72	PHE	8.3
1	A	27	VAL	8.3
1	B	114	ASP	8.3
1	C	111	GLU	8.2
1	B	190	PRO	8.2
1	C	154	LYS	8.1
1	B	133	VAL	8.1
1	C	201	VAL	8.0
1	C	190	PRO	8.0
1	A	59	VAL	8.0
1	B	168	GLN	7.9
1	B	199	LEU	7.9
1	A	58	LEU	7.9
1	B	201	VAL	7.9
1	C	52	TYR	7.8
1	B	121	LEU	7.8
1	B	3	LEU	7.8
1	B	183	ARG	7.7
1	A	137	LYS	7.6
1	B	18	LYS	7.5
1	A	183	ARG	7.4
1	B	189	LYS	7.3
1	B	71	VAL	7.2
1	B	106	HIS	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	199	LEU	7.2
1	B	192	GLU	7.2
1	B	62	ASP	7.2
1	C	126	ILE	7.1
1	B	61	ASP	7.1
1	B	120	ARG	7.0
1	C	114	ASP	6.9
1	B	34	ILE	6.9
1	B	13	LYS	6.9
1	B	171	PRO	6.8
1	B	187	ALA	6.8
1	A	41	LYS	6.7
1	C	180	GLY	6.7
1	A	18	LYS	6.7
1	C	169	THR	6.7
1	B	42	GLY	6.6
1	A	96	MET	6.6
1	C	1	MET	6.4
1	B	161	ARG	6.4
1	C	89	GLN	6.3
1	C	170	ALA	6.3
1	B	200	GLU	6.2
1	B	32	GLY	6.2
1	B	89	GLN	6.1
1	C	68	ILE	6.1
1	A	188	SER	6.1
1	A	34	ILE	6.1
1	B	112	VAL	5.9
1	B	140	PRO	5.9
1	C	139	ASN	5.9
1	B	141	PRO	5.9
1	B	148	ILE	5.9
1	A	146	LYS	5.8
1	C	121	LEU	5.8
1	B	41	LYS	5.8
1	B	146	LYS	5.7
1	A	76	GLY	5.7
1	C	4	VAL	5.6
1	B	29	ILE	5.6
1	B	177	LYS	5.6
1	B	150	ARG	5.6
1	A	110	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	11	ALA	5.5
1	A	1	MET	5.5
1	B	152	ASP	5.5
1	B	75	HIS	5.5
1	A	163	GLU	5.3
1	B	176	TYR	5.2
1	C	191	VAL	5.2
1	B	184	ILE	5.2
1	A	7	GLY	5.2
1	C	6	LEU	5.2
1	C	104	VAL	5.1
1	B	90	ALA	5.1
1	C	178	LYS	5.0
1	A	37	GLU	5.0
1	A	104	VAL	5.0
1	A	54	GLU	4.9
1	B	57	GLU	4.9
1	C	27	VAL	4.8
1	A	23	GLU	4.8
1	A	119	GLU	4.7
1	C	12	GLY	4.7
1	A	120	ARG	4.6
1	A	42	GLY	4.6
1	A	198	VAL	4.6
1	A	162	LEU	4.5
1	A	156	GLU	4.5
1	B	193	GLU	4.5
1	C	91	GLU	4.5
1	A	187	ALA	4.4
1	C	167	GLU	4.4
1	C	149	GLN	4.2
1	A	199	LEU	4.1
1	B	122	SER	4.1
1	B	129	GLU	4.1
1	B	127	ASN	4.1
1	A	39	VAL	4.1
1	B	194	VAL	4.0
1	B	179	LYS	4.0
1	C	28	HIS	4.0
1	C	119	GLU	3.9
1	C	153	ASP	3.8
1	A	35	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	119	GLU	3.8
1	B	56	GLY	3.8
1	A	99	LYS	3.8
1	B	117	VAL	3.8
1	A	82	GLY	3.8
1	B	48	LYS	3.7
1	C	200	GLU	3.7
1	C	133	VAL	3.6
1	A	97	LEU	3.6
1	A	8	PRO	3.5
1	A	100	LYS	3.5
1	C	184	ILE	3.5
1	C	194	VAL	3.5
1	B	80	PHE	3.4
1	A	148	ILE	3.4
1	A	149	GLN	3.4
1	C	150	ARG	3.4
1	C	98	GLU	3.4
1	B	116	VAL	3.3
1	B	108	LEU	3.2
1	B	94	ASP	3.1
1	B	195	TYR	3.1
1	B	53	MET	3.1
1	C	49	ALA	3.0
1	C	50	LYS	3.0
1	A	57	GLU	3.0
1	B	163	GLU	3.0
1	A	132	GLU	3.0
1	A	81	ASP	2.9
1	A	28	HIS	2.8
1	C	122	SER	2.8
1	C	13	LYS	2.8
1	C	146	LYS	2.7
1	C	51	GLU	2.7
1	B	86	THR	2.7
1	A	189	LYS	2.7
1	A	106	HIS	2.6
1	B	40	GLN	2.6
1	C	2	ILE	2.5
1	C	112	VAL	2.5
1	C	5	PHE	2.5
1	B	174	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	22	LYS	2.5
1	C	193	GLU	2.5
1	A	144	GLY	2.4
1	C	166	ARG	2.4
1	C	195	TYR	2.4
1	C	48	LYS	2.4
1	B	74	LYS	2.3
1	B	44	PRO	2.3
1	C	34	ILE	2.3
1	C	35	LEU	2.3
1	C	36	ARG	2.3
1	B	147	VAL	2.3
1	C	3	LEU	2.3
1	A	145	VAL	2.2
1	C	113	PRO	2.2
1	B	7	GLY	2.2
1	C	134	TYR	2.2
1	B	160	LYS	2.2
1	A	125	ARG	2.1

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 carbohydrates 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.