Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:47 pm BST

PDB ID	:	1SB2
Title	:	High resolution Structure determination of rhodocetin
Authors	:	Paaventhan, P.; Kong, C.G.; Joseph, J.S.; Chung, M.C.M.; Kolatkar, P.R.
Deposited on	:	2004-02-10
Resolution	:	1.90 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:

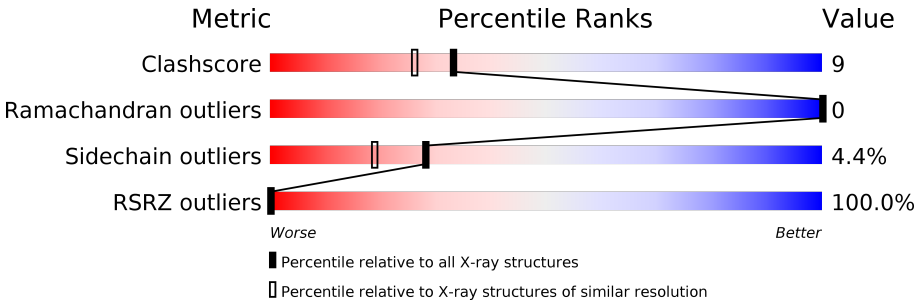
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	133	99% 80% 16%
2	B	129	96% 82% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2271 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 Rhodocetin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1103	698	182	211	12			

- Molecule 2 is a protein called Rhodocetin beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	S	0	0	0
			1001	650	167	178	6			

- Molecule 3 is water.

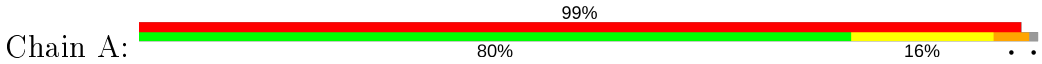
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	70	Total	O	0	0
			70	70		

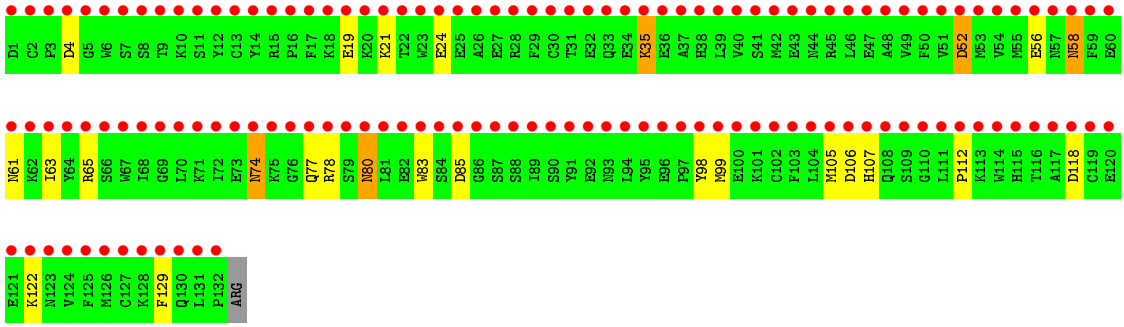
3 Residue-property plots (i)

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 (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: Rhodocetin alpha subunit

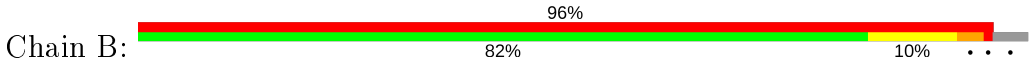
Chain A:

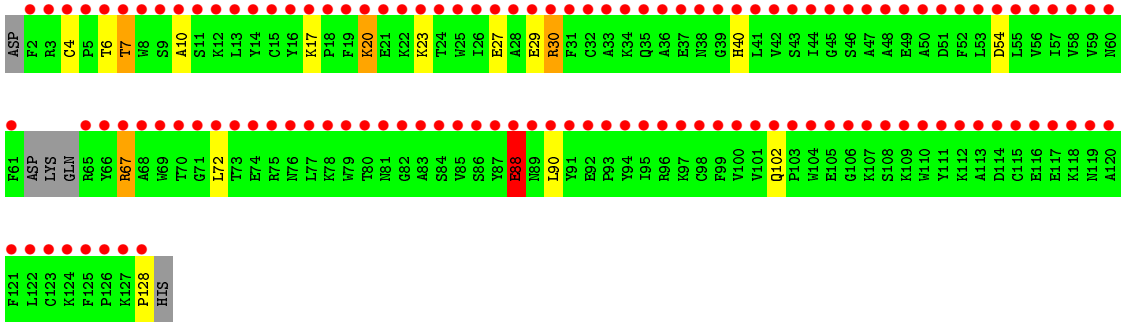




- Molecule 2: Rhodocetin beta subunit

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.88Å 65.94Å 118.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.87 – 1.90 28.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (28.87-1.90) 97.2 (28.83-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.63 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.189 , 0.231 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2271	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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	0.99	3/1133 (0.3%)	0.92	5/1524 (0.3%)
2	B	0.91	2/1030 (0.2%)	0.93	6/1391 (0.4%)
All	All	0.96	5/2163 (0.2%)	0.93	11/2915 (0.4%)

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
2	B	1	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	GLU	CD-OE2	10.44	1.37	1.25
2	B	88	GLU	CD-OE1	8.36	1.34	1.25
2	B	88	GLU	CB-CG	6.34	1.64	1.52
1	A	24	GLU	CD-OE1	6.06	1.32	1.25
1	A	65	ARG	CB-CG	-5.30	1.38	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	128	PRO	N-CA-CB	9.81	115.07	103.30
1	A	106	ASP	CB-CG-OD2	7.86	125.38	118.30
2	B	30	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	A	4	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	118	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	85	ASP	CB-CG-OD2	5.98	123.68	118.30
2	B	67	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	B	88	GLU	CG-CD-OE2	-5.77	106.77	118.30
2	B	54	ASP	CB-CG-OD2	5.67	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	88	GLU	OE1-CD-OE2	5.25	129.59	123.30
1	A	52	ASP	CB-CG-OD2	5.08	122.87	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	PHE	CA

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	1103	0	1029	19	0
2	B	1001	0	957	16	0
3	A	97	0	0	6	0
3	B	70	0	0	2	0
All	All	2271	0	1986	34	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 9.

All (34) 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:67:ARG:HD2	2:B:102:GLN:OE1	1.65	0.95
1:A:63:ILE:HD11	3:A:191:HOH:O	1.85	0.77
2:B:6:THR:O	2:B:7:THR:HG22	1.86	0.76
1:A:19:GLU:HG3	3:A:154:HOH:O	1.92	0.69
2:B:29:GLU:OE1	2:B:40:HIS:HD2	1.78	0.67
1:A:63:ILE:CD1	3:A:191:HOH:O	2.42	0.66
1:A:74:ASN:HD21	1:A:99:MET:H	1.47	0.63
1:A:74:ASN:HD21	1:A:98:TYR:HA	1.64	0.62
2:B:88:GLU:HG3	2:B:90:LEU:H	1.66	0.60
1:A:35:LYS:HD2	1:A:129:PHE:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:CG	3:A:154:HOH:O	2.51	0.55
2:B:23:LYS:HB3	2:B:27:GLU:HG3	1.88	0.54
1:A:80:ASN:HD22	1:A:80:ASN:H	1.58	0.52
1:A:63:ILE:HG23	1:A:107:HIS:O	2.08	0.52
2:B:7:THR:CG2	2:B:17:LYS:HE2	2.40	0.52
1:A:74:ASN:ND2	1:A:99:MET:H	2.07	0.51
2:B:7:THR:HG23	2:B:17:LYS:HD2	1.92	0.50
2:B:6:THR:O	2:B:7:THR:CG2	2.58	0.50
2:B:40:HIS:HE1	3:B:142:HOH:O	1.95	0.49
2:B:7:THR:HG23	2:B:17:LYS:HE2	1.95	0.48
1:A:105:MET:HB2	1:A:112:PRO:HB2	1.95	0.48
1:A:58:ASN:HB2	3:A:159:HOH:O	2.13	0.48
1:A:52:ASP:OD1	1:A:107:HIS:HD2	1.96	0.48
2:B:88:GLU:CG	2:B:90:LEU:H	2.28	0.46
1:A:80:ASN:HD22	1:A:80:ASN:N	2.15	0.45
1:A:83:TRP:CZ3	2:B:72:LEU:HB2	2.52	0.44
2:B:6:THR:O	2:B:7:THR:CB	2.66	0.44
1:A:56:GLU:HB3	1:A:61:ASN:HD22	1.82	0.44
2:B:67:ARG:CD	2:B:102:GLN:OE1	2.52	0.44
1:A:21:LYS:HA	1:A:122:LYS:HE3	2.00	0.43
2:B:4:CYS:SG	2:B:10:ALA:HB2	2.60	0.42
1:A:74:ASN:H	1:A:74:ASN:HD22	1.66	0.41
1:A:19:GLU:CD	3:A:154:HOH:O	2.58	0.41
2:B:20:LYS:NZ	3:B:184:HOH:O	2.53	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	130/133 (98%)	124 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	120/129 (93%)	115 (96%)	5 (4%)	0	100 100
All	All	250/262 (95%)	239 (96%)	11 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	122/124 (98%)	116 (95%)	6 (5%)	25 15
2	B	103/113 (91%)	99 (96%)	4 (4%)	32 23
All	All	225/237 (95%)	215 (96%)	10 (4%)	28 19

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

Mol	Chain	Res	Type
1	A	35	LYS
1	A	58	ASN
1	A	74	ASN
1	A	77	GLN
1	A	78	ARG
1	A	80	ASN
2	B	7	THR
2	B	20	LYS
2	B	30	ARG
2	B	88	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	74	ASN
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	107	HIS
1	A	123	ASN
2	B	40	HIS
2	B	60	ASN
2	B	89	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	132/133 (99%)	15.86	132 (100%)	0	0	18, 25, 42, 54	0
2	B	124/129 (96%)	16.62	124 (100%)	0	0	19, 26, 38, 47	0
All	All	256/262 (97%)	16.23	256 (100%)	0	0	18, 25, 41, 54	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	CYS	73.1
2	B	6	THR	72.0
2	B	111	TYR	63.4
1	A	97	PRO	46.8
2	B	123	CYS	44.9
2	B	84	SER	42.1
1	A	77	GLN	39.6
1	A	86	GLY	38.6
2	B	115	CYS	38.1
1	A	39	LEU	36.5
1	A	9	THR	36.3
2	B	66	TYR	36.1
2	B	91	TYR	35.5
1	A	85	ASP	35.2
2	B	92	GLU	35.1
1	A	132	PRO	34.8
2	B	85	VAL	34.7
1	A	98	TYR	32.7
1	A	76	GLY	32.4
2	B	19	PHE	32.4
1	A	46	LEU	32.2
1	A	27	GLU	31.2
2	B	121	PHE	31.0
2	B	102	GLN	30.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	ASN	30.4
1	A	10	LYS	29.0
1	A	127	CYS	28.8
2	B	122	LEU	28.0
1	A	79	SER	28.0
1	A	78	ARG	27.4
1	A	108	GLN	26.9
2	B	82	GLY	26.2
2	B	69	TRP	25.7
1	A	120	GLU	25.7
2	B	106	GLY	25.7
2	B	93	PRO	25.4
2	B	90	LEU	25.3
1	A	118	ASP	25.1
1	A	126	MET	25.0
1	A	47	GLU	24.9
2	B	120	ALA	24.8
2	B	59	VAL	24.0
1	A	124	VAL	23.9
2	B	107	LYS	23.4
2	B	14	TYR	23.0
1	A	109	SER	23.0
1	A	57	ASN	22.8
2	B	108	SER	22.7
2	B	13	LEU	22.2
2	B	25	TRP	22.2
2	B	126	PRO	22.1
1	A	88	SER	21.6
2	B	89	ASN	21.4
2	B	27	GLU	21.2
2	B	4	CYS	21.1
2	B	83	ALA	20.8
2	B	32	CYS	20.7
1	A	105	MET	20.6
2	B	71	GLY	20.5
1	A	94	LEU	20.2
2	B	36	ALA	20.0
2	B	79	TRP	20.0
1	A	8	SER	19.7
2	B	70	THR	19.7
2	B	96	ARG	19.7
1	A	115	HIS	19.5

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Mol	Chain	Res	Type	RSRZ
1	A	4	ASP	19.5
2	B	10	ALA	19.4
1	A	83	TRP	19.4
2	B	18	PRO	19.3
1	A	92	GLU	19.0
1	A	72	ILE	18.7
2	B	55	LEU	18.6
1	A	41	SER	18.6
2	B	103	PRO	18.6
1	A	6	TRP	18.5
2	B	98	CYS	18.4
2	B	56	VAL	18.4
2	B	67	ARG	18.3
2	B	81	ASN	18.3
2	B	101	VAL	18.2
1	A	114	TRP	18.1
2	B	8	TRP	17.9
1	A	14	TYR	17.6
1	A	11	SER	17.5
1	A	31	THR	17.5
2	B	28	ALA	17.4
2	B	30	ARG	17.3
1	A	30	CYS	17.2
2	B	119	ASN	17.1
2	B	26	ILE	17.1
1	A	130	GLN	16.9
1	A	2	CYS	16.7
1	A	112	PRO	16.6
2	B	15	CYS	16.5
1	A	110	GLY	16.5
1	A	131	LEU	16.4
1	A	40	VAL	16.2
1	A	17	PHE	16.2
2	B	65	ARG	16.1
1	A	125	PHE	16.1
2	B	57	ILE	15.9
2	B	125	PHE	15.9
2	B	48	ALA	15.8
2	B	94	TYR	15.8
1	A	84	SER	15.8
2	B	21	GLU	15.5
1	A	24	GLU	15.4

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Mol	Chain	Res	Type	RSRZ
1	A	28	ARG	15.3
1	A	95	TYR	15.2
2	B	17	LYS	15.1
1	A	49	VAL	15.0
2	B	12	LYS	14.8
1	A	19	GLU	14.7
2	B	86	SER	14.6
2	B	75	ARG	14.6
1	A	60	GLU	14.5
1	A	68	ILE	14.4
2	B	5	PRO	14.2
1	A	50	PHE	14.2
1	A	38	HIS	14.1
1	A	82	GLU	14.0
1	A	44	ASN	14.0
2	B	49	GLU	14.0
2	B	24	THR	13.9
2	B	110	TRP	13.8
1	A	16	PRO	13.8
1	A	96	GLU	13.8
2	B	95	ILE	13.7
1	A	64	TYR	13.6
2	B	99	PHE	13.6
2	B	3	ARG	13.5
2	B	72	LEU	13.5
1	A	80	ASN	13.4
1	A	58	ASN	13.4
1	A	89	ILE	13.4
2	B	51	ASP	13.3
2	B	112	LYS	12.9
2	B	46	SER	12.9
1	A	59	PHE	12.8
1	A	91	TYR	12.6
2	B	2	PHE	12.6
1	A	100	GLU	12.6
2	B	16	TYR	12.5
1	A	13	CYS	12.5
1	A	90	SER	12.5
2	B	113	ALA	12.4
2	B	77	LEU	12.4
2	B	45	GLY	12.4
1	A	51	VAL	12.4

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Mol	Chain	Res	Type	RSRZ
1	A	129	PHE	12.4
1	A	102	CYS	12.4
1	A	87	SER	12.3
1	A	43	GLU	12.2
2	B	38	ASN	12.2
2	B	29	GLU	12.0
1	A	15	ARG	12.0
1	A	20	LYS	11.8
1	A	22	THR	11.7
2	B	114	ASP	11.7
2	B	7	THR	11.7
2	B	42	VAL	11.6
1	A	23	TRP	11.5
2	B	116	GLU	11.4
2	B	88	GLU	11.4
1	A	55	MET	11.4
1	A	53	MET	11.3
1	A	66	SER	11.1
1	A	69	GLY	11.1
1	A	128	LYS	11.0
1	A	62	LYS	11.0
1	A	5	GLY	10.9
1	A	106	ASP	10.8
2	B	41	LEU	10.8
2	B	76	ASN	10.7
2	B	87	TYR	10.6
1	A	12	TYR	10.5
1	A	33	GLN	10.4
2	B	124	LYS	10.3
2	B	52	PHE	10.2
1	A	117	ALA	10.1
2	B	20	LYS	10.1
1	A	116	THR	9.8
1	A	75	LYS	9.6
1	A	56	GLU	9.5
2	B	37	GLU	9.5
2	B	100	VAL	9.5
1	A	65	ARG	9.4
2	B	11	SER	9.4
1	A	67	TRP	9.4
1	A	42	MET	9.4
1	A	26	ALA	9.3

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Mol	Chain	Res	Type	RSRZ
1	A	107	HIS	9.3
2	B	34	LYS	9.2
1	A	34	GLU	9.2
2	B	50	ALA	9.1
2	B	53	LEU	9.0
1	A	61	ASN	9.0
1	A	104	LEU	9.0
2	B	128	PRO	9.0
2	B	74	GLU	8.8
2	B	73	THR	8.6
2	B	31	PHE	8.5
2	B	23	LYS	8.5
2	B	22	LYS	8.5
1	A	21	LYS	8.5
2	B	44	ILE	8.4
1	A	113	LYS	8.4
1	A	70	LEU	8.4
1	A	36	GLU	8.2
1	A	37	ALA	8.1
1	A	54	VAL	8.1
1	A	35	LYS	8.1
2	B	58	VAL	8.0
1	A	103	PHE	8.0
1	A	48	ALA	7.8
1	A	73	GLU	7.8
1	A	121	GLU	7.8
1	A	18	LYS	7.8
2	B	61	PHE	7.6
1	A	99	MET	7.5
1	A	101	LYS	7.5
2	B	54	ASP	7.4
2	B	35	GLN	7.3
1	A	81	LEU	7.2
1	A	63	ILE	7.0
2	B	127	LYS	7.0
2	B	43	SER	7.0
2	B	9	SER	7.0
2	B	97	LYS	6.8
1	A	29	PHE	6.7
1	A	52	ASP	6.7
2	B	78	LYS	6.4
1	A	122	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
2	B	47	ALA	6.0
1	A	111	LEU	6.0
1	A	123	ASN	5.9
2	B	33	ALA	5.9
2	B	68	ALA	5.8
2	B	109	LYS	5.7
1	A	3	PRO	5.6
1	A	1	ASP	5.5
1	A	74	ASN	5.5
2	B	80	THR	5.4
2	B	60	ASN	5.4
1	A	71	LYS	5.3
2	B	40	HIS	5.3
1	A	7	SER	5.2
2	B	39	GLY	4.4
1	A	45	ARG	4.3
1	A	25	GLU	4.1
2	B	105	GLU	3.6
1	A	32	GLU	3.6
2	B	104	TRP	3.5
2	B	117	GLU	3.4
2	B	118	LYS	2.8

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.