



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 06:35 PM EDT

PDB ID : 1SB2
Title : High resolution Structure determination of rhodocetin
Authors : Paaventhana, 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

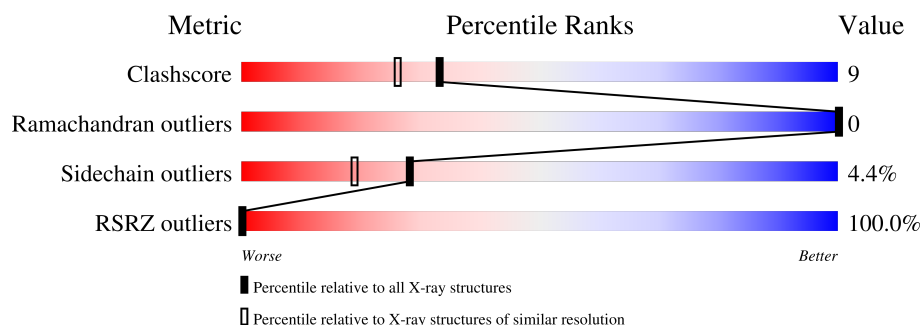
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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 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.

Mol	Chain	Length	Quality of chain
1	A	133	<div> <div>99%</div> <div>80%16%...</div> </div>
2	B	129	<div> <div>96%</div> <div>82%10%...</div> </div>

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			

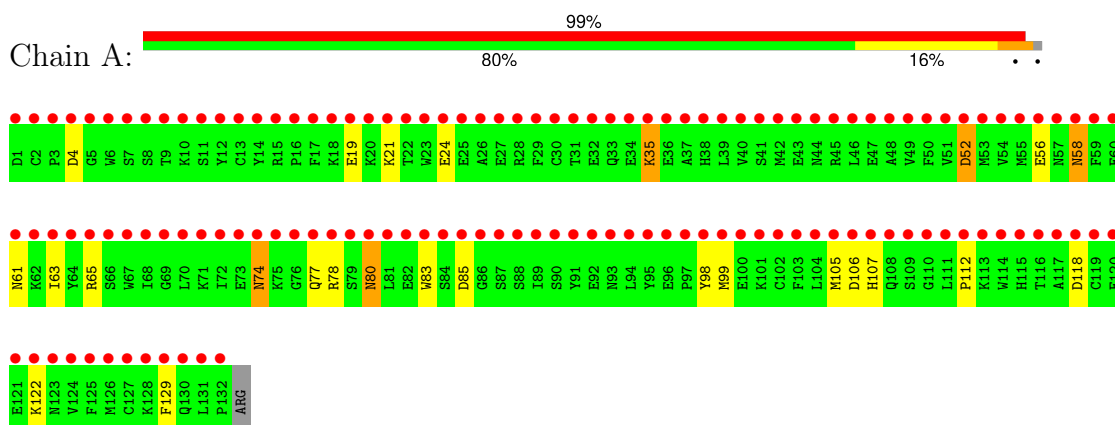
- Molecule 3 is water.

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

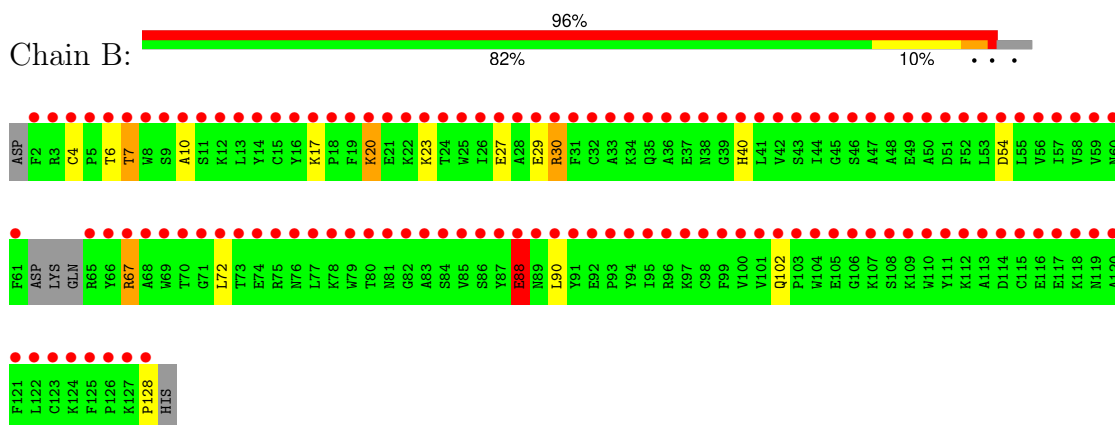
3 Residue-property plots

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: Rhodocetin alpha subunit



• Molecule 2: Rhodocetin beta subunit



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

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

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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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:H	1:A:80:ASN:HD22	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:HD22	1:A:74:ASN:H	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 ⓘ

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

Sometimes 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 [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, 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	132/133 (99%)	15.74	132 (100%) 0 0	18, 25, 42, 54	0
2	B	124/129 (96%)	16.50	124 (100%) 0 0	19, 26, 38, 47	0
All	All	256/262 (97%)	16.11	256 (100%) 0 0	18, 25, 41, 54	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	6	THR	70.2
1	A	119	CYS	69.5
2	B	111	TYR	60.6
1	A	97	PRO	44.5
2	B	84	SER	43.9
2	B	123	CYS	41.6
1	A	77	GLN	38.5
2	B	115	CYS	38.4
1	A	86	GLY	37.3
1	A	9	THR	36.5
1	A	85	ASP	36.4
1	A	39	LEU	36.0
2	B	91	TYR	35.4
2	B	66	TYR	34.7
1	A	46	LEU	33.4
2	B	92	GLU	33.4
2	B	85	VAL	33.3
1	A	132	PRO	32.9
2	B	102	GLN	32.4
1	A	98	TYR	32.1
2	B	19	PHE	31.3
1	A	27	GLU	30.4
1	A	10	LYS	30.3
2	B	121	PHE	30.1

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Mol	Chain	Res	Type	RSRZ
1	A	127	CYS	29.9
1	A	93	ASN	29.7
1	A	76	GLY	29.5
1	A	79	SER	28.5
1	A	108	GLN	27.4
2	B	122	LEU	26.9
2	B	82	GLY	26.7
1	A	78	ARG	26.6
2	B	90	LEU	25.8
2	B	69	TRP	25.8
2	B	107	LYS	25.8
2	B	93	PRO	25.4
1	A	120	GLU	25.2
1	A	47	GLU	24.7
1	A	118	ASP	24.6
1	A	124	VAL	24.5
2	B	106	GLY	24.2
2	B	14	TYR	23.8
1	A	126	MET	23.7
2	B	120	ALA	23.6
2	B	59	VAL	23.0
2	B	71	GLY	22.8
2	B	126	PRO	22.6
2	B	25	TRP	22.5
1	A	57	ASN	22.3
1	A	109	SER	22.1
2	B	13	LEU	22.1
2	B	32	CYS	21.9
2	B	89	ASN	21.8
2	B	108	SER	21.6
2	B	27	GLU	21.4
1	A	88	SER	21.4
2	B	18	PRO	20.6
1	A	8	SER	20.4
2	B	83	ALA	20.3
1	A	105	MET	20.2
2	B	4	CYS	20.2
2	B	79	TRP	20.0
1	A	83	TRP	19.6
2	B	70	THR	19.6
1	A	4	ASP	19.5
1	A	41	SER	19.4

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Mol	Chain	Res	Type	RSRZ
2	B	96	ARG	19.2
2	B	10	ALA	19.2
1	A	94	LEU	19.1
1	A	92	GLU	19.1
1	A	115	HIS	19.0
1	A	72	ILE	18.9
1	A	6	TRP	18.8
2	B	103	PRO	18.4
2	B	98	CYS	18.4
2	B	56	VAL	18.4
2	B	81	ASN	18.3
1	A	114	TRP	18.3
2	B	36	ALA	18.2
1	A	11	SER	18.1
2	B	8	TRP	17.9
2	B	101	VAL	17.8
2	B	67	ARG	17.8
2	B	26	ILE	17.6
2	B	55	LEU	17.3
2	B	119	ASN	17.1
2	B	30	ARG	17.0
1	A	110	GLY	17.0
1	A	2	CYS	17.0
1	A	130	GLN	16.8
1	A	14	TYR	16.8
2	B	28	ALA	16.8
1	A	31	THR	16.7
2	B	48	ALA	16.7
1	A	84	SER	16.5
1	A	30	CYS	16.4
1	A	40	VAL	16.2
1	A	131	LEU	16.1
2	B	15	CYS	16.1
1	A	112	PRO	16.0
2	B	125	PHE	15.9
2	B	65	ARG	15.9
2	B	94	TYR	15.7
1	A	17	PHE	15.7
2	B	57	ILE	15.6
1	A	95	TYR	15.6
2	B	17	LYS	15.6
1	A	125	PHE	15.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	ILE	15.5
1	A	49	VAL	15.4
2	B	21	GLU	15.4
1	A	19	GLU	15.4
2	B	86	SER	15.2
1	A	24	GLU	15.2
1	A	28	ARG	15.1
2	B	12	LYS	15.1
2	B	95	ILE	14.9
1	A	82	GLU	14.6
2	B	75	ARG	14.3
2	B	5	PRO	14.3
1	A	60	GLU	14.2
1	A	38	HIS	14.1
1	A	16	PRO	14.1
2	B	24	THR	13.8
1	A	96	GLU	13.8
2	B	3	ARG	13.8
1	A	44	ASN	13.7
1	A	89	ILE	13.7
2	B	72	LEU	13.6
2	B	99	PHE	13.6
1	A	64	TYR	13.5
1	A	51	VAL	13.4
1	A	50	PHE	13.4
1	A	58	ASN	13.3
2	B	2	PHE	13.3
2	B	51	ASP	13.3
2	B	49	GLU	13.2
2	B	112	LYS	13.2
2	B	110	TRP	13.1
1	A	80	ASN	13.0
1	A	100	GLU	13.0
1	A	59	PHE	12.9
2	B	42	VAL	12.6
1	A	13	CYS	12.6
2	B	29	GLU	12.5
1	A	43	GLU	12.5
2	B	46	SER	12.5
2	B	7	THR	12.3
1	A	90	SER	12.2
1	A	102	CYS	12.2

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Mol	Chain	Res	Type	RSRZ
2	B	45	GLY	12.2
2	B	77	LEU	12.2
1	A	23	TRP	12.1
2	B	16	TYR	12.1
2	B	116	GLU	12.1
1	A	91	TYR	12.0
1	A	87	SER	11.9
1	A	129	PHE	11.9
2	B	38	ASN	11.8
1	A	20	LYS	11.7
1	A	22	THR	11.6
1	A	53	MET	11.5
2	B	41	LEU	11.4
1	A	15	ARG	11.3
1	A	55	MET	11.3
2	B	88	GLU	11.2
1	A	69	GLY	11.1
1	A	106	ASP	11.0
1	A	66	SER	11.0
2	B	114	ASP	10.9
2	B	113	ALA	10.9
1	A	62	LYS	10.8
1	A	33	GLN	10.7
1	A	5	GLY	10.6
1	A	128	LYS	10.6
1	A	12	TYR	10.4
2	B	87	TYR	10.4
2	B	76	ASN	10.2
2	B	124	LYS	10.1
1	A	75	LYS	9.9
2	B	52	PHE	9.8
2	B	20	LYS	9.7
2	B	100	VAL	9.5
1	A	56	GLU	9.5
1	A	116	THR	9.5
2	B	128	PRO	9.4
1	A	117	ALA	9.4
1	A	65	ARG	9.4
2	B	37	GLU	9.3
1	A	34	GLU	9.3
1	A	104	LEU	9.2
2	B	34	LYS	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	21	LYS	9.1
1	A	26	ALA	9.0
1	A	42	MET	9.0
1	A	107	HIS	9.0
1	A	61	ASN	8.9
2	B	53	LEU	8.9
2	B	11	SER	8.9
2	B	50	ALA	8.8
1	A	67	TRP	8.8
1	A	37	ALA	8.7
2	B	74	GLU	8.6
2	B	22	LYS	8.5
2	B	23	LYS	8.5
1	A	113	LYS	8.3
2	B	31	PHE	8.3
1	A	70	LEU	8.3
2	B	44	ILE	8.2
2	B	73	THR	8.2
1	A	54	VAL	8.2
1	A	121	GLU	8.0
1	A	103	PHE	8.0
1	A	36	GLU	8.0
2	B	58	VAL	7.9
1	A	73	GLU	7.9
1	A	48	ALA	7.8
1	A	35	LYS	7.8
2	B	35	GLN	7.7
1	A	18	LYS	7.7
1	A	99	MET	7.6
2	B	43	SER	7.5
1	A	81	LEU	7.5
2	B	61	PHE	7.4
2	B	54	ASP	7.4
1	A	101	LYS	7.3
2	B	9	SER	7.1
1	A	29	PHE	7.1
2	B	97	LYS	7.0
1	A	63	ILE	6.9
1	A	111	LEU	6.9
2	B	127	LYS	6.8
1	A	52	ASP	6.6
1	A	123	ASN	6.4

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Mol	Chain	Res	Type	RSRZ
2	B	78	LYS	6.2
1	A	122	LYS	6.1
2	B	33	ALA	6.1
2	B	68	ALA	5.9
2	B	109	LYS	5.8
1	A	1	ASP	5.7
2	B	60	ASN	5.7
2	B	47	ALA	5.7
2	B	80	THR	5.6
1	A	3	PRO	5.6
1	A	71	LYS	5.2
1	A	7	SER	5.1
2	B	40	HIS	5.0
1	A	74	ASN	4.8
2	B	39	GLY	4.6
1	A	45	ARG	4.2
1	A	25	GLU	4.1
1	A	32	GLU	3.6
2	B	105	GLU	3.6
2	B	117	GLU	3.4
2	B	104	TRP	3.4
2	B	118	LYS	2.8

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.