



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2021 – 12:20 PM JST

PDB ID : 7EK8
Title : Crystal structure of apo streptavidin at ambient temperature
Authors : DeMirici, H.; Ertem, F.B.; Destan, E.; Ayan, E.
Deposited on : 2021-04-04
Resolution : 1.70 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 : 2.23.1
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) : 2.23.1

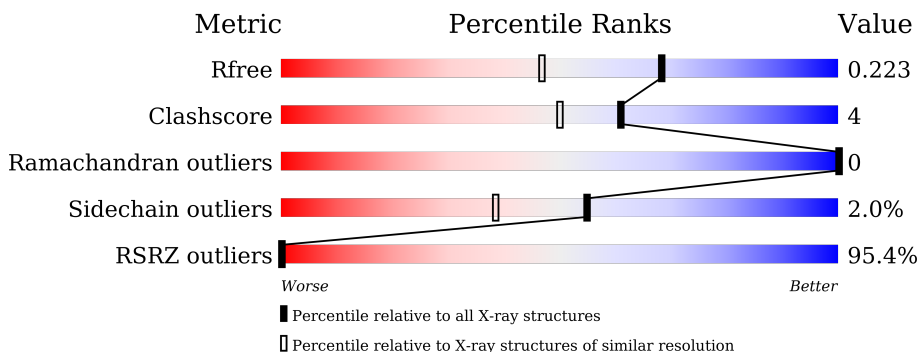
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	123	<div style="display: flex; justify-content: space-between;"> <div style="width: 93%; height: 10px; background-color: red;"></div> <div style="width: 89%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">93% 89% 10% .</p>
1	B	123	<div style="display: flex; justify-content: space-between;"> <div style="width: 93%; height: 10px; background-color: red;"></div> <div style="width: 85%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">93% 85% 13% ..</p>
1	C	123	<div style="display: flex; justify-content: space-between;"> <div style="width: 94%; height: 10px; background-color: red;"></div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">94% 92% 5% ..</p>
1	D	123	<div style="display: flex; justify-content: space-between;"> <div style="width: 94%; height: 10px; background-color: red;"></div> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">94% 91% 7% .</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4166 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 Streptavidin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
1	A	121	942	594	159	189	0	8	0
1	B	121	937	588	163	186	0	8	0
1	C	120	950	597	161	192	0	10	0
1	D	120	940	591	160	189	0	10	0

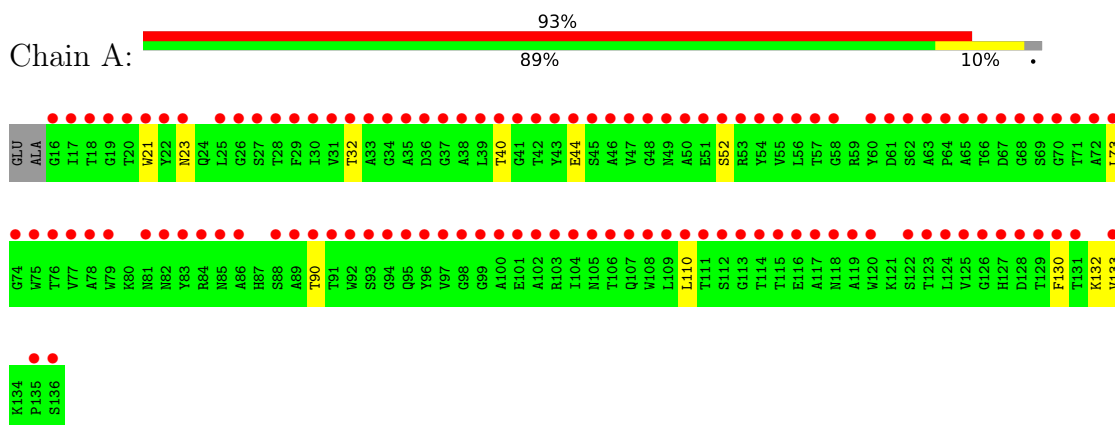
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	100	101	101	0	1
2	B	94	95	95	0	1
2	C	111	115	115	0	4
2	D	85	86	86	0	1

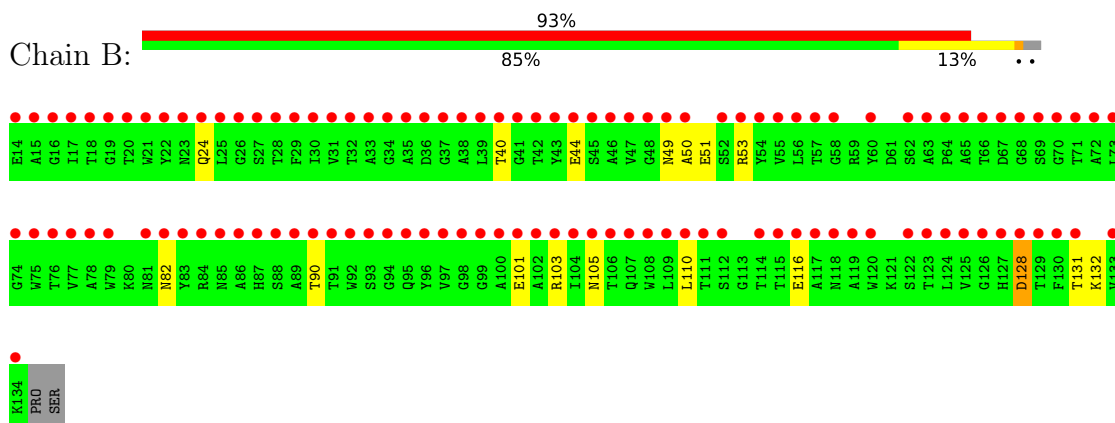
3 Residue-property plots [i](#)

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.

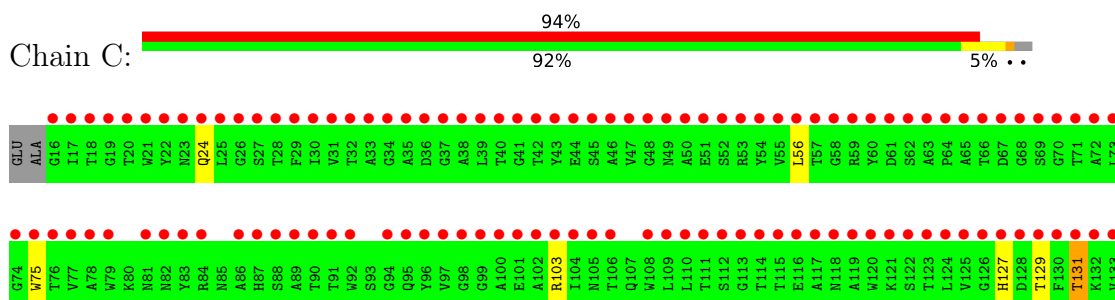
- Molecule 1: Streptavidin



- Molecule 1: Streptavidin



- Molecule 1: Streptavidin



K134
P135
SER

● Molecule 1: Streptavidin

Chain D: 94%
91% 7%

GLU
ALA
G16
I17
T18
G19
T20
W21
Y22
N23
Q24
L25
G26
S27
T28
F29
I30
V31
T32
A33
G34
A35
D36
G37
A38
L39
T40
G41
T42
Y43
E44
S45
A46
V47
G48
N49
A50
E51
S52
R53
Y54
V55
L56
T57
G58
R59
Y60
D61
S62
A63
F64
A65
T66
D67
G68
S69
G70
T71
A72
L73

G74
W75
T76
V77
A78
W79
K80
N81
N82
Y83
R84
N85
A86
H87
S88
A89
T90
T91
R92
S93
G94
D95
Y96
W97
G98
G99
A100
E101
A102
R103
I104
N105
T106
Q107
W108
L109
L110
T111
S112
G113
T114
T115
E116
A117
N118
A119
W120
K121
S122
T123
L124
V125
G126
H127
D128
T129
F130
T131
K132
V133

K134
P135
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.40Å 87.70Å 58.90Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	48.49 – 1.70 48.49 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.49-1.70) 100.0 (48.49-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.70Å)	Xtrriage
Refinement program	PHENIX dev_3318	Depositor
R, R_{free}	0.190 , 0.224 0.190 , 0.223	Depositor DCC
R_{free} test set	1932 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtrriage
Anisotropy	0.560	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 87.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4166	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.71	2/982 (0.2%)	0.75	0/1346
1	B	0.53	0/975	0.69	0/1334
1	C	0.56	0/994	0.68	0/1362
1	D	0.57	0/984	0.64	0/1349
All	All	0.60	2/3935 (0.1%)	0.69	0/5391

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52[A]	SER	C-O	8.61	1.39	1.23
1	A	52[B]	SER	C-O	8.61	1.39	1.23

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	942	0	890	6	0
1	B	937	0	891	17	0
1	C	950	0	903	5	0
1	D	940	0	896	5	0
2	A	101	0	0	3	1
2	B	95	0	0	13	0
2	C	115	0	0	3	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	86	0	0	2	1
All	All	4166	0	3580	33	3

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 (33) 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:B:128:ASP:OD1	2:B:201:HOH:O	1.94	0.85
1:B:116:GLU:OE1	2:B:202:HOH:O	2.01	0.77
1:B:103[B]:ARG:NH2	2:B:204:HOH:O	2.13	0.76
1:D:36[A]:ASP:OD2	2:D:201:HOH:O	2.08	0.71
1:C:129[A]:THR:OG1	2:C:201[A]:HOH:O	2.11	0.68
1:B:103[A]:ARG:HD3	1:B:131:THR:HG22	1.74	0.68
1:B:132:LYS:O	2:B:205:HOH:O	2.14	0.66
1:D:103:ARG:HH21	1:D:129[A]:THR:HG21	1.61	0.65
1:B:51:GLU:OE1	2:B:203:HOH:O	2.13	0.65
1:C:127[B]:HIS:ND1	2:C:206:HOH:O	2.29	0.64
1:B:82:ASN:ND2	2:B:207:HOH:O	2.35	0.59
1:B:105:ASN:ND2	2:B:208:HOH:O	2.36	0.58
1:D:16:GLY:N	2:D:205:HOH:O	2.37	0.57
1:C:103:ARG:HD3	1:C:131[B]:THR:HG22	1.88	0.55
1:B:116:GLU:HG3	2:B:282:HOH:O	2.07	0.54
1:A:44:GLU:OE1	2:A:201:HOH:O	2.18	0.53
1:D:21:TRP:CZ2	1:D:132:LYS:HE3	2.44	0.52
1:B:103[A]:ARG:NH2	2:B:212:HOH:O	2.44	0.51
1:C:24:GLN:OE1	2:C:202:HOH:O	2.20	0.49
1:A:40:THR:OG1	2:A:202:HOH:O	2.20	0.47
1:B:44:GLU:HB3	1:B:53:ARG:HG2	1.97	0.47
1:C:56[B]:LEU:HG	1:C:75:TRP:CD1	2.49	0.47
1:A:23:ASN:HB3	1:A:130:PHE:CE2	2.50	0.46
1:B:103[B]:ARG:HE	1:B:105:ASN:HD21	1.63	0.46
1:B:40[B]:THR:HG23	2:B:215:HOH:O	2.17	0.44
1:A:21:TRP:CZ2	1:A:132:LYS:HE3	2.53	0.43
1:A:32:THR:HB	2:A:202:HOH:O	2.18	0.43
1:A:90:THR:OG1	1:A:110:LEU:HD13	2.18	0.42
1:D:49:ASN:OD1	1:D:49:ASN:N	2.49	0.42
1:B:50:ALA:N	2:B:203:HOH:O	2.42	0.42
1:B:49:ASN:HB2	2:B:203:HOH:O	2.20	0.41
1:B:128:ASP:HA	2:B:201:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:OG1	1:B:110[A]:LEU:HD13	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:HOH:O	2:C:282:HOH:O[1_655]	2.09	0.11
2:C:293:HOH:O	2:C:299:HOH:O[1_655]	2.13	0.07
2:A:292:HOH:O	2:D:209:HOH:O[2_846]	2.17	0.03

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	126/123 (102%)	124 (98%)	2 (2%)	0	100	100
1	B	126/123 (102%)	125 (99%)	1 (1%)	0	100	100
1	C	128/123 (104%)	125 (98%)	3 (2%)	0	100	100
1	D	128/123 (104%)	127 (99%)	1 (1%)	0	100	100
All	All	508/492 (103%)	501 (99%)	7 (1%)	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	96/91 (106%)	94 (98%)	2 (2%)	53	36
1	B	94/91 (103%)	91 (97%)	3 (3%)	39	20
1	C	98/91 (108%)	96 (98%)	2 (2%)	55	38
1	D	96/91 (106%)	94 (98%)	2 (2%)	53	36
All	All	384/364 (106%)	375 (98%)	9 (2%)	55	33

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	133	VAL
1	B	24	GLN
1	B	101	GLU
1	B	128	ASP
1	C	131[A]	THR
1	C	131[B]	THR
1	D	107[A]	GLN
1	D	107[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	121/123 (98%)	3.64	114 (94%)	0 0	6, 14, 31, 41 2 (1%)
1	B	121/123 (98%)	3.85	114 (94%)	0 0	5, 14, 38, 65 1 (0%)
1	C	120/123 (97%)	4.17	116 (96%)	0 0	5, 12, 60, 90 1 (0%)
1	D	120/123 (97%)	4.39	116 (96%)	0 0	6, 16, 56, 101 1 (0%)
All	All	482/492 (97%)	4.01	460 (95%)	0 0	5, 14, 42, 101 5 (1%)

All (460) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	ALA	19.7
1	D	47	VAL	18.9
1	C	47	VAL	17.5
1	D	45	SER	16.4
1	C	48	GLY	15.3
1	D	100	ALA	14.1
1	C	50	ALA	14.0
1	C	135	PRO	11.6
1	A	136	SER	10.6
1	D	48	GLY	10.3
1	D	135	PRO	10.2
1	B	47	VAL	9.2
1	C	49	ASN	9.0
1	A	135	PRO	8.6
1	A	100	ALA	8.3
1	B	46	ALA	7.8
1	D	99	GLY	7.8
1	C	46	ALA	7.7
1	D	50	ALA	7.6
1	B	24	GLN	7.4
1	C	100	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
1	D	25	LEU	7.3
1	A	35	ALA	7.3
1	B	120	TRP	7.3
1	B	14	GLU	7.1
1	A	83[A]	TYR	7.0
1	D	83	TYR	6.9
1	C	134	LYS	6.9
1	A	66	THR	6.9
1	D	97	VAL	6.9
1	D	26	GLY	6.8
1	B	15	ALA	6.7
1	D	49	ASN	6.7
1	D	133	VAL	6.6
1	C	25	LEU	6.3
1	A	99	GLY	6.3
1	B	48	GLY	6.2
1	D	35[A]	ALA	6.2
1	C	83	TYR	6.2
1	B	25	LEU	6.2
1	B	66	THR	6.1
1	C	120	TRP	6.1
1	D	102	ALA	6.0
1	C	77	VAL	5.9
1	D	36[A]	ASP	5.8
1	B	100	ALA	5.8
1	C	29	PHE	5.8
1	A	22[A]	TYR	5.7
1	C	24	GLN	5.6
1	C	117	ALA	5.6
1	D	29	PHE	5.6
1	B	55	VAL	5.6
1	A	52[A]	SER	5.6
1	D	73[A]	LEU	5.5
1	A	97[A]	VAL	5.4
1	B	43	TYR	5.4
1	B	97	VAL	5.4
1	C	56[A]	LEU	5.3
1	A	133	VAL	5.3
1	C	79	TRP	5.3
1	D	79	TRP	5.2
1	A	73	LEU	5.2
1	C	102	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	35[A]	ALA	5.1
1	B	29	PHE	5.1
1	B	79	TRP	5.1
1	C	92	TRP	5.1
1	C	45	SER	5.1
1	D	17	ILE	5.0
1	C	73[A]	LEU	5.0
1	C	31	VAL	5.0
1	C	30	ILE	5.0
1	B	75	TRP	5.0
1	D	117	ALA	4.9
1	B	117	ALA	4.9
1	C	42[A]	THR	4.9
1	A	21	TRP	4.8
1	B	45	SER	4.8
1	C	133	VAL	4.8
1	D	44	GLU	4.8
1	B	30	ILE	4.8
1	B	21	TRP	4.8
1	D	108	TRP	4.8
1	B	42	THR	4.7
1	B	72	ALA	4.7
1	B	110[A]	LEU	4.7
1	A	79	TRP	4.7
1	B	77	VAL	4.7
1	D	96	TYR	4.7
1	A	120	TRP	4.7
1	B	92	TRP	4.7
1	A	31	VAL	4.6
1	A	46	ALA	4.6
1	D	110	LEU	4.6
1	B	83	TYR	4.6
1	D	134	LYS	4.6
1	C	51	GLU	4.6
1	A	77	VAL	4.6
1	D	31	VAL	4.6
1	D	22	TYR	4.6
1	B	89	ALA	4.5
1	C	104	ILE	4.5
1	B	134	LYS	4.5
1	A	102	ALA	4.5
1	A	129[A]	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	43	TYR	4.5
1	A	17	ILE	4.5
1	A	108	TRP	4.5
1	D	84	ARG	4.4
1	A	47	VAL	4.4
1	D	125	VAL	4.4
1	C	21	TRP	4.4
1	A	60	TYR	4.4
1	A	96	TYR	4.4
1	B	129[A]	THR	4.4
1	B	17	ILE	4.4
1	A	75	TRP	4.4
1	C	43	TYR	4.4
1	D	92	TRP	4.4
1	B	56	LEU	4.4
1	D	51	GLU	4.4
1	A	92	TRP	4.4
1	B	26	GLY	4.4
1	B	73[A]	LEU	4.4
1	A	33	ALA	4.4
1	B	133	VAL	4.4
1	C	40[A]	THR	4.4
1	C	26	GLY	4.3
1	B	108	TRP	4.3
1	C	38	ALA	4.3
1	D	77	VAL	4.3
1	A	104	ILE	4.3
1	C	54	TYR	4.3
1	B	109	LEU	4.3
1	A	55	VAL	4.3
1	C	97	VAL	4.3
1	B	99	GLY	4.3
1	A	54	TYR	4.3
1	D	40[A]	THR	4.3
1	C	75	TRP	4.3
1	D	30	ILE	4.3
1	B	54	TYR	4.3
1	D	39	LEU	4.3
1	C	55	VAL	4.2
1	C	108	TRP	4.2
1	D	129[A]	THR	4.2
1	D	21	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	75	TRP	4.2
1	B	119	ALA	4.2
1	D	66	THR	4.2
1	D	56	LEU	4.2
1	A	29	PHE	4.1
1	C	63	ALA	4.1
1	C	129[A]	THR	4.1
1	D	109	LEU	4.1
1	D	55	VAL	4.1
1	B	20	THR	4.1
1	B	76	THR	4.1
1	B	123	THR	4.1
1	A	130	PHE	4.1
1	A	56	LEU	4.1
1	D	54	TYR	4.1
1	B	125	VAL	4.1
1	D	120	TRP	4.1
1	D	111	THR	4.1
1	B	104	ILE	4.1
1	B	36	ASP	4.1
1	B	111	THR	4.1
1	C	123	THR	4.1
1	D	33	ALA	4.1
1	D	130	PHE	4.1
1	B	31[A]	VAL	4.0
1	D	76	THR	4.0
1	D	115	THR	4.0
1	C	53	ARG	4.0
1	B	50	ALA	4.0
1	C	35	ALA	4.0
1	A	131	THR	4.0
1	A	124	LEU	4.0
1	A	72	ALA	4.0
1	B	102	ALA	4.0
1	C	20	THR	4.0
1	D	20	THR	4.0
1	D	57[A]	THR	4.0
1	B	101	GLU	4.0
1	B	78	ALA	4.0
1	A	25	LEU	4.0
1	C	89	ALA	4.0
1	B	64	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	130	PHE	4.0
1	A	71[A]	THR	4.0
1	C	101	GLU	4.0
1	D	24	GLN	4.0
1	A	76	THR	3.9
1	C	115	THR	3.9
1	D	98	GLY	3.9
1	B	63	ALA	3.9
1	A	32	THR	3.9
1	A	57[A]	THR	3.9
1	B	40[A]	THR	3.9
1	A	103	ARG	3.9
1	A	43	TYR	3.9
1	A	30	ILE	3.9
1	B	98	GLY	3.9
1	C	84	ARG	3.9
1	C	78	ALA	3.9
1	D	78	ALA	3.9
1	B	60	TYR	3.9
1	C	103	ARG	3.9
1	A	125	VAL	3.9
1	D	65	ALA	3.9
1	D	72	ALA	3.9
1	C	52	SER	3.9
1	B	96	TYR	3.9
1	A	20	THR	3.9
1	B	91	THR	3.9
1	C	17	ILE	3.8
1	D	124	LEU	3.8
1	C	116	GLU	3.8
1	A	90	THR	3.8
1	A	110	LEU	3.8
1	C	90	THR	3.8
1	D	131	THR	3.8
1	A	36	ASP	3.8
1	C	33	ALA	3.8
1	C	106	THR	3.8
1	C	72	ALA	3.8
1	C	96	TYR	3.7
1	B	131	THR	3.7
1	D	28	THR	3.7
1	C	28	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	90	THR	3.7
1	A	67	ASP	3.7
1	C	110	LEU	3.7
1	B	106	THR	3.7
1	C	91	THR	3.7
1	D	60	TYR	3.7
1	D	38	ALA	3.7
1	A	39	LEU	3.7
1	B	39	LEU	3.7
1	D	37	GLY	3.7
1	A	123	THR	3.7
1	B	115	THR	3.7
1	A	109	LEU	3.7
1	B	57	THR	3.7
1	C	66	THR	3.7
1	C	114	THR	3.7
1	B	22	TYR	3.6
1	C	60	TYR	3.6
1	D	32	THR	3.6
1	D	91	THR	3.6
1	C	130	PHE	3.6
1	D	103	ARG	3.6
1	B	116	GLU	3.6
1	B	124	LEU	3.6
1	D	104	ILE	3.6
1	C	119	ALA	3.6
1	A	115	THR	3.6
1	B	90	THR	3.6
1	C	131[A]	THR	3.6
1	D	114	THR	3.6
1	C	68	GLY	3.6
1	D	53	ARG	3.6
1	C	111	THR	3.6
1	D	16	GLY	3.6
1	C	39	LEU	3.6
1	C	109	LEU	3.6
1	C	44	GLU	3.5
1	C	88[A]	SER	3.5
1	B	33	ALA	3.5
1	D	86	ALA	3.5
1	C	118	ASN	3.5
1	C	99	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	127[A]	HIS	3.5
1	A	68	GLY	3.5
1	D	89	ALA	3.5
1	B	18	THR	3.5
1	A	34	GLY	3.4
1	B	49	ASN	3.4
1	C	128[A]	ASP	3.4
1	B	44	GLU	3.4
1	B	114	THR	3.4
1	D	123	THR	3.4
1	A	38	ALA	3.4
1	B	53	ARG	3.4
1	C	22	TYR	3.4
1	B	71	THR	3.4
1	A	91	THR	3.4
1	D	42	THR	3.4
1	D	106	THR	3.4
1	A	94	GLY	3.4
1	C	86	ALA	3.4
1	A	42	THR	3.4
1	C	57	THR	3.4
1	D	71	THR	3.4
1	A	78	ALA	3.3
1	B	86	ALA	3.3
1	A	82	ASN	3.3
1	C	125	VAL	3.3
1	A	89	ALA	3.3
1	C	71	THR	3.3
1	A	26	GLY	3.3
1	B	58	GLY	3.3
1	B	28	THR	3.3
1	D	23	ASN	3.3
1	A	62	SER	3.3
1	C	27	SER	3.3
1	D	64	PRO	3.3
1	C	65	ALA	3.3
1	B	68	GLY	3.3
1	C	124	LEU	3.3
1	A	50	ALA	3.3
1	A	98	GLY	3.3
1	C	98	GLY	3.3
1	B	32	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	32	THR	3.2
1	B	82	ASN	3.2
1	A	111	THR	3.2
1	C	74	GLY	3.2
1	D	34	GLY	3.2
1	D	67	ASP	3.2
1	A	65	ALA	3.2
1	D	27	SER	3.2
1	C	76	THR	3.2
1	A	122	SER	3.2
1	A	106	THR	3.2
1	A	37	GLY	3.2
1	C	70	GLY	3.2
1	A	27	SER	3.2
1	D	119	ALA	3.2
1	A	64	PRO	3.2
1	B	52	SER	3.1
1	B	103[A]	ARG	3.1
1	D	69[A]	SER	3.1
1	D	88[A]	SER	3.1
1	B	38	ALA	3.1
1	A	18	THR	3.1
1	C	62	SER	3.1
1	A	88[A]	SER	3.1
1	B	88[A]	SER	3.1
1	C	81	ASN	3.1
1	D	63	ALA	3.1
1	C	69[A]	SER	3.1
1	D	52	SER	3.1
1	A	63	ALA	3.1
1	A	84	ARG	3.0
1	B	67	ASP	3.0
1	A	126	GLY	3.0
1	B	74	GLY	3.0
1	B	93	SER	3.0
1	A	40	THR	3.0
1	A	119	ALA	3.0
1	B	65	ALA	3.0
1	C	18	THR	3.0
1	A	112	SER	2.9
1	C	64	PRO	2.9
1	B	84	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	34	GLY	2.9
1	D	74	GLY	2.9
1	D	128[A]	ASP	2.9
1	B	128	ASP	2.9
1	C	82	ASN	2.9
1	D	82	ASN	2.9
1	B	70	GLY	2.9
1	B	87	HIS	2.9
1	C	112	SER	2.8
1	C	23	ASN	2.8
1	A	41	GLY	2.8
1	B	19	GLY	2.8
1	B	27	SER	2.8
1	C	126	GLY	2.8
1	D	107[A]	GLN	2.8
1	A	28	THR	2.8
1	A	45	SER	2.8
1	D	93	SER	2.8
1	C	58	GLY	2.8
1	D	94	GLY	2.8
1	D	122	SER	2.7
1	C	36	ASP	2.7
1	A	85	ASN	2.7
1	A	93	SER	2.7
1	A	19	GLY	2.7
1	B	94	GLY	2.7
1	D	18	THR	2.7
1	B	112	SER	2.7
1	C	113	GLY	2.7
1	A	114	THR	2.7
1	A	113	GLY	2.7
1	D	68	GLY	2.7
1	B	81	ASN	2.7
1	D	118	ASN	2.7
1	A	16	GLY	2.7
1	C	19	GLY	2.6
1	A	53	ARG	2.6
1	A	101	GLU	2.6
1	B	23	ASN	2.6
1	D	81	ASN	2.6
1	A	74	GLY	2.6
1	D	95	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	62	SER	2.6
1	B	69	SER	2.6
1	B	37	GLY	2.6
1	D	58	GLY	2.6
1	A	48	GLY	2.5
1	B	126	GLY	2.5
1	C	94	GLY	2.5
1	D	41	GLY	2.5
1	D	127	HIS	2.5
1	A	70	GLY	2.5
1	B	16	GLY	2.5
1	D	116	GLU	2.5
1	A	105	ASN	2.5
1	B	95	GLN	2.5
1	C	122	SER	2.5
1	A	86	ALA	2.5
1	B	105	ASN	2.5
1	D	105	ASN	2.5
1	C	121	LYS	2.5
1	A	51	GLU	2.5
1	D	70	GLY	2.5
1	A	23	ASN	2.5
1	D	62	SER	2.5
1	B	34	GLY	2.5
1	B	127	HIS	2.5
1	D	19	GLY	2.5
1	A	95	GLN	2.4
1	B	122	SER	2.4
1	A	107	GLN	2.4
1	C	95	GLN	2.4
1	C	105	ASN	2.4
1	A	58	GLY	2.4
1	A	69	SER	2.4
1	D	101	GLU	2.4
1	D	85	ASN	2.4
1	B	41	GLY	2.4
1	D	126	GLY	2.4
1	B	107	GLN	2.3
1	A	116	GLU	2.3
1	D	87	HIS	2.3
1	D	113	GLY	2.3
1	A	128	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	44	GLU	2.3
1	A	61	ASP	2.3
1	A	127	HIS	2.3
1	B	85	ASN	2.3
1	A	117	ALA	2.2
1	C	67	ASP	2.2
1	C	37	GLY	2.2
1	C	41	GLY	2.2
1	C	61	ASP	2.2
1	A	118	ASN	2.2
1	B	118	ASN	2.2
1	C	132	LYS	2.2
1	D	112	SER	2.1
1	C	87	HIS	2.1
1	D	61	ASP	2.1
1	A	81	ASN	2.1
1	C	16	GLY	2.0
1	C	59	ARG	2.0
1	A	49	ASN	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.