



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:24 PM GMT

PDB ID : 1AO3
Title : A3 DOMAIN OF VON WILLEBRAND FACTOR
Authors : Bienkowski, J.; Cruz, M.; Handin, R.; Liddington, R.
Deposited on : 1997-07-16
Resolution : 2.20 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

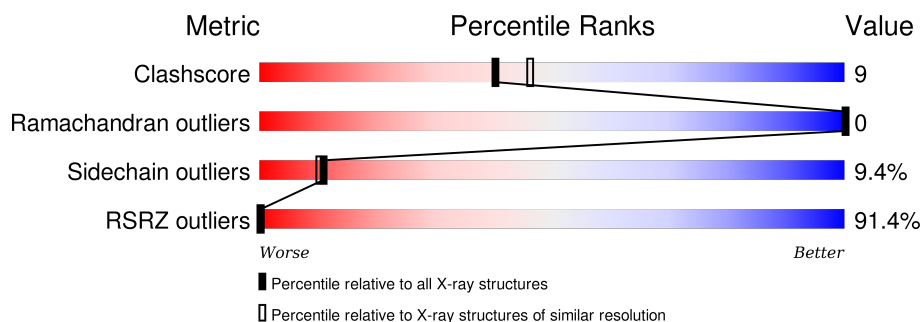
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	187	<div> <div>91%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>5%</div> </div> </div>
1	B	187	<div> <div>91%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2971 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 VON WILLEBRAND FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	0
			1401	887	240	268	6			
1	B	187	Total	C	N	O	S	0	0	0
			1401	887	240	268	6			

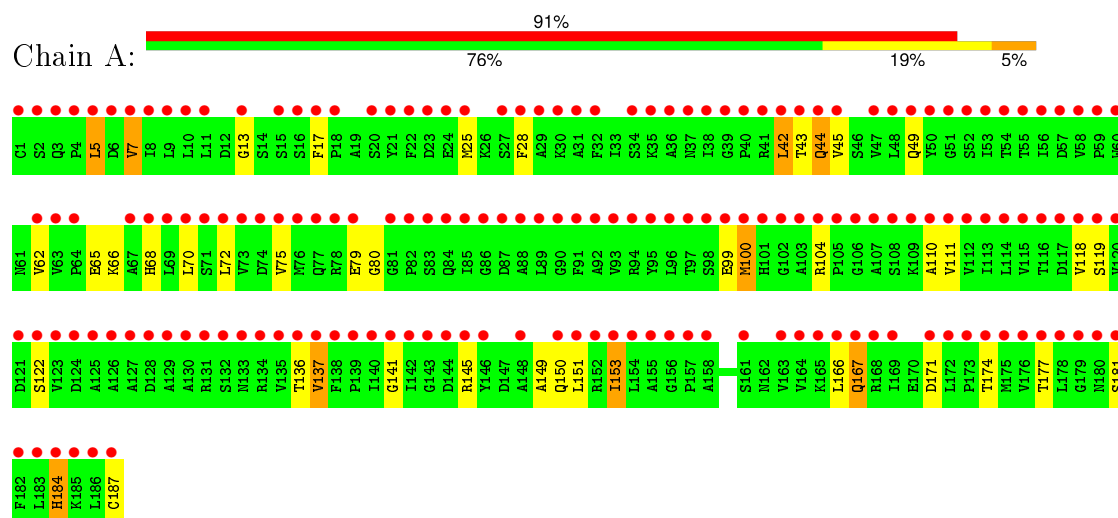
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	85	Total	O	0	0
			85	85		

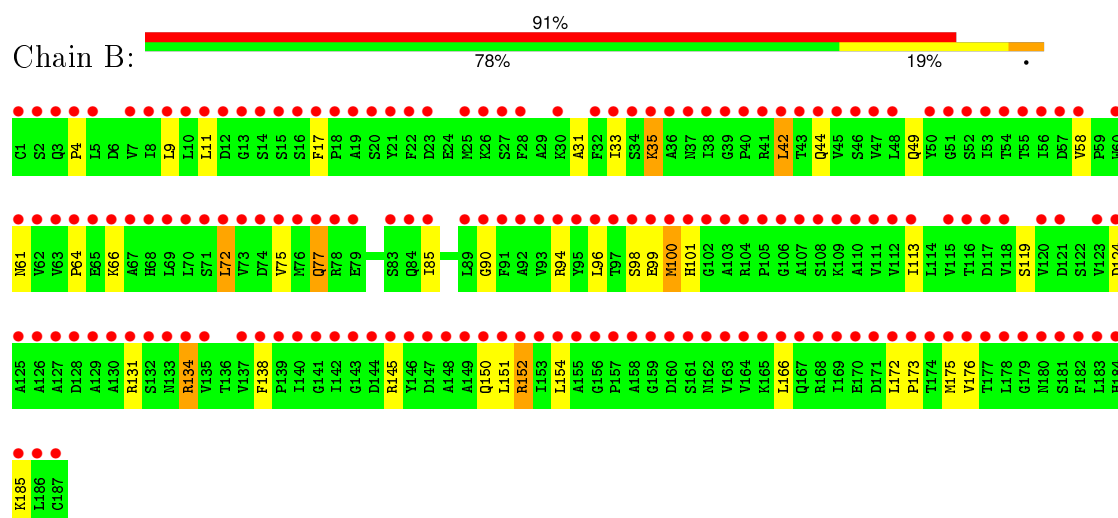
3 Residue-property plots

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 ($RSRZ > 2$). 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: VON WILLEBRAND FACTOR



• Molecule 1: VON WILLEBRAND FACTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.00 Å 65.10 Å 57.80 Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 14.48 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.5 (8.00-2.20) 63.6 (14.48-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.18 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.158 , 0.215 0.473 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 301.2	EDS
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14054 reflections	Xtriage
F_o, F_c correlation	0.47	EDS
Total number of atoms	2971	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.06% 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	0.50	0/1426	0.78	2/1938 (0.1%)
1	B	0.47	0/1426	0.71	1/1938 (0.1%)
All	All	0.49	0/2852	0.75	3/3876 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	7	VAL	CB-CA-C	-5.67	100.62	111.40
1	B	96	LEU	CA-CB-CG	5.26	127.41	115.30

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	1401	0	1419	24	6
1	B	1401	0	1419	25	5
2	A	84	0	0	2	1
2	B	85	0	0	4	0
All	All	2971	0	2838	49	6

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 (49) 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:119:SER:H	1:A:150:GLN:HE22	1.28	0.79
1:A:149:ALA:O	1:A:153:ILE:HG23	1.88	0.73
1:B:119:SER:H	1:B:150:GLN:HE22	1.37	0.72
1:A:171:ASP:O	1:A:174:THR:HG22	1.95	0.65
1:A:17:PHE:CZ	1:A:145:ARG:HD3	2.32	0.65
1:A:167:GLN:NE2	1:A:167:GLN:H	1.97	0.63
1:A:181:SER:HB2	2:A:3100:HOH:O	2.00	0.61
1:A:111:VAL:HG13	1:A:137:VAL:HB	1.83	0.61
1:A:181:SER:O	1:A:184:HIS:HB2	2.03	0.58
1:B:98:SER:OG	1:B:101:HIS:HD2	1.87	0.58
1:B:90:GLY:O	1:B:94:ARG:HD2	2.09	0.53
1:B:172:LEU:HB3	1:B:173:PRO:HD3	1.91	0.52
1:A:25:MET:O	1:A:28:PHE:HB3	2.09	0.52
1:A:99:GLU:HG3	1:A:100:MET:SD	2.49	0.52
1:B:138:PHE:HE2	1:B:185:LYS:HE2	1.74	0.52
1:A:44:GLN:NE2	1:A:104:ARG:HD2	2.25	0.51
1:B:33:ILE:O	1:B:66:LYS:HE2	2.12	0.50
1:B:124:ASP:HB2	2:B:2251:HOH:O	2.11	0.50
1:B:58:VAL:HG22	1:B:72:LEU:HB3	1.94	0.49
1:B:152:ARG:HD3	2:B:244:HOH:O	2.11	0.49
1:A:141:GLY:HA3	1:A:151:LEU:HD11	1.95	0.49
1:A:13:GLY:HA3	1:A:49:GLN:HE21	1.78	0.49
1:B:85:ILE:HD12	1:B:119:SER:HB2	1.96	0.47
1:B:138:PHE:CE2	1:B:185:LYS:HE2	2.50	0.47
1:B:35:LYS:HD2	1:B:176:VAL:HG12	1.96	0.47
1:B:4:PRO:HA	1:B:42:LEU:O	2.14	0.46
1:B:31:ALA:O	1:B:35:LYS:HG3	2.15	0.46
1:A:110:ALA:HA	1:A:136:THR:O	2.15	0.46
1:B:44:GLN:HE22	1:B:64:PRO:HG3	1.81	0.46
1:A:66:LYS:O	1:A:70:LEU:HG	2.16	0.46
1:B:94:ARG:O	1:B:98:SER:HB2	2.17	0.45
1:A:42:LEU:HB3	1:A:43:THR:H	1.58	0.45
1:B:77:GLN:HE21	1:B:77:GLN:HA	1.81	0.45
1:A:174:THR:HA	1:A:177:THR:OG1	2.16	0.45
1:A:167:GLN:H	1:A:167:GLN:CD	2.19	0.45
1:B:77:GLN:NE2	2:B:2262:HOH:O	2.51	0.44
1:A:150:GLN:NE2	2:A:221:HOH:O	2.50	0.44
1:A:62:VAL:CG1	1:A:68:HIS:CD2	3.01	0.44
1:B:11:LEU:O	1:B:49:GLN:HA	2.17	0.43
1:B:172:LEU:O	1:B:175:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG12	1:A:145:ARG:O	2.19	0.42
1:A:79:GLU:HG3	1:A:80:GLY:O	2.20	0.42
1:B:85:ILE:HG23	1:B:113:ILE:HD11	2.01	0.42
1:A:49:GLN:NE2	1:A:79:GLU:H	2.18	0.42
1:B:17:PHE:CZ	1:B:145:ARG:HD3	2.55	0.41
1:A:49:GLN:HE22	1:A:79:GLU:H	1.67	0.41
1:B:72:LEU:O	1:B:75:VAL:HG12	2.20	0.41
1:B:94:ARG:NH2	2:B:3131:HOH:O	2.54	0.41
1:B:134:ARG:HB3	1:B:134:ARG:HH11	1.85	0.41

All (6) 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)
1:A:100:MET:SD	1:B:100:MET:CE[1_454]	1.52	0.68
1:A:100:MET:CE	1:B:100:MET:CE[1_454]	1.65	0.55
1:A:100:MET:CG	1:B:100:MET:CE[1_454]	1.82	0.38
1:A:100:MET:CB	1:B:100:MET:CE[1_454]	1.89	0.31
1:A:122:SER:N	2:A:224:HOH:O[2_555]	2.10	0.10
1:A:100:MET:CB	1:B:100:MET:CB[1_454]	2.16	0.04

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	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
1	B	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
All	All	370/374 (99%)	358 (97%)	12 (3%)	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	154/154 (100%)	139 (90%)	15 (10%)	10	9
1	B	154/154 (100%)	140 (91%)	14 (9%)	12	11
All	All	308/308 (100%)	279 (91%)	29 (9%)	11	10

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	VAL
1	A	42	LEU
1	A	44	GLN
1	A	45	VAL
1	A	65	GLU
1	A	72	LEU
1	A	75	VAL
1	A	100	MET
1	A	137	VAL
1	A	153	ILE
1	A	166	LEU
1	A	167	GLN
1	A	184	HIS
1	A	187	CYS
1	B	9	LEU
1	B	35	LYS
1	B	42	LEU
1	B	61	ASN
1	B	72	LEU
1	B	77	GLN
1	B	99	GLU
1	B	100	MET
1	B	131	ARG
1	B	134	ARG
1	B	151	LEU
1	B	152	ARG

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Mol	Chain	Res	Type
1	B	154	LEU
1	B	166	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	49	GLN
1	A	101	HIS
1	A	150	GLN
1	A	167	GLN
1	B	37	ASN
1	B	44	GLN
1	B	61	ASN
1	B	77	GLN
1	B	101	HIS
1	B	150	GLN

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, 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	187/187 (100%)	4.88	171 (91%) 0 0	5, 16, 68, 89	0
1	B	187/187 (100%)	4.72	171 (91%) 0 0	4, 15, 53, 76	0
All	All	374/374 (100%)	4.80	342 (91%) 0 0	4, 16, 59, 89	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	PRO	19.3
1	A	17	PHE	18.2
1	A	40	PRO	17.7
1	A	175	MET	17.3
1	B	1	CYS	16.6
1	A	2	SER	16.1
1	B	115	VAL	14.5
1	A	181	SER	14.5
1	A	186	LEU	14.3
1	B	62	VAL	12.6
1	A	135	VAL	12.4
1	B	179	GLY	12.1
1	A	4	PRO	11.3
1	B	45	VAL	11.0
1	B	180	ASN	11.0
1	B	9	LEU	10.8
1	B	36	ALA	10.6
1	B	182	PHE	10.2
1	A	64	PRO	10.1
1	A	103	ALA	10.0
1	A	1	CYS	9.7
1	B	67	ALA	9.5
1	A	47	VAL	9.2
1	B	93	VAL	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	9.1
1	A	5	LEU	8.7
1	B	50	TYR	8.6
1	B	35	LYS	8.5
1	B	91	PHE	8.5
1	B	96	LEU	8.5
1	A	77	GLN	8.4
1	A	155	ALA	8.4
1	B	95	TYR	8.3
1	B	185	LYS	8.2
1	B	3	GLN	8.1
1	B	159	GLY	8.1
1	A	157	PRO	8.0
1	B	175	MET	8.0
1	A	62	VAL	8.0
1	B	124	ASP	7.9
1	A	63	VAL	7.8
1	B	176	VAL	7.8
1	A	32	PHE	7.8
1	B	89	LEU	7.7
1	B	14	SER	7.7
1	B	126	ALA	7.7
1	A	185	LYS	7.6
1	A	42	LEU	7.6
1	A	3	GLN	7.5
1	B	100	MET	7.5
1	A	113	ILE	7.3
1	B	2	SER	7.2
1	B	135	VAL	7.2
1	B	61	ASN	7.2
1	A	88	ALA	7.1
1	A	91	PHE	7.1
1	B	110	ALA	7.1
1	A	25	MET	7.0
1	B	112	VAL	7.0
1	B	63	VAL	7.0
1	B	47	VAL	6.9
1	B	151	LEU	6.9
1	B	186	LEU	6.9
1	A	83	SER	6.8
1	A	73	VAL	6.8
1	A	50	TYR	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	163	VAL	6.8
1	B	43	THR	6.8
1	A	37	ASN	6.8
1	B	137	VAL	6.7
1	A	187	CYS	6.7
1	B	70	LEU	6.7
1	B	52	SER	6.7
1	A	139	PRO	6.5
1	B	15	SER	6.5
1	A	137	VAL	6.5
1	A	178	LEU	6.4
1	B	177	THR	6.4
1	B	65	GLU	6.3
1	B	53	ILE	6.3
1	A	28	PHE	6.3
1	B	21	TYR	6.3
1	B	66	LYS	6.3
1	B	143	GLY	6.3
1	A	70	LEU	6.2
1	A	154	LEU	6.2
1	B	139	PRO	6.2
1	B	103	ALA	6.2
1	A	105	PRO	6.1
1	A	96	LEU	6.0
1	A	92	ALA	6.0
1	B	172	LEU	6.0
1	B	4	PRO	6.0
1	B	154	LEU	6.0
1	A	58	VAL	5.9
1	A	151	LEU	5.8
1	A	34	SER	5.8
1	A	183	LEU	5.8
1	A	133	ASN	5.8
1	A	60	TRP	5.7
1	A	43	THR	5.7
1	B	56	ILE	5.7
1	A	45	VAL	5.6
1	A	134	ARG	5.6
1	A	95	TYR	5.6
1	B	23	ASP	5.5
1	A	81	GLY	5.5
1	B	90	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	74	ASP	5.5
1	A	118	VAL	5.5
1	A	71	SER	5.5
1	B	178	LEU	5.5
1	A	94	ARG	5.4
1	A	146	TYR	5.4
1	A	180	ASN	5.4
1	A	177	THR	5.4
1	B	169	ILE	5.4
1	B	42	LEU	5.3
1	B	117	ASP	5.3
1	A	9	LEU	5.3
1	B	101	HIS	5.3
1	A	123	VAL	5.3
1	B	108	SER	5.2
1	A	182	PHE	5.2
1	A	142	ILE	5.2
1	B	146	TYR	5.2
1	A	98	SER	5.2
1	B	16	SER	5.2
1	A	49	GLN	5.2
1	B	17	PHE	5.2
1	A	55	THR	5.2
1	A	27	SER	5.2
1	A	39	GLY	5.1
1	B	64	PRO	5.1
1	A	119	SER	5.0
1	A	48	LEU	5.0
1	A	125	ALA	5.0
1	A	16	SER	5.0
1	B	155	ALA	5.0
1	A	126	ALA	5.0
1	B	68	HIS	5.0
1	A	153	ILE	4.9
1	A	107	ALA	4.9
1	B	77	GLN	4.9
1	B	58	VAL	4.8
1	A	120	VAL	4.8
1	B	76	MET	4.8
1	A	23	ASP	4.8
1	B	134	ARG	4.7
1	B	104	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	28	PHE	4.7
1	B	51	GLY	4.7
1	B	158	ALA	4.7
1	A	167	GLN	4.6
1	A	102	GLY	4.6
1	B	165	LYS	4.6
1	A	7	VAL	4.6
1	A	100	MET	4.5
1	B	133	ASN	4.5
1	A	110	ALA	4.5
1	A	161	SER	4.5
1	B	113	ILE	4.5
1	B	145	ARG	4.5
1	B	144	ASP	4.5
1	A	184	HIS	4.4
1	B	25	MET	4.4
1	B	187	CYS	4.4
1	B	33	ILE	4.4
1	A	68	HIS	4.4
1	B	19	ALA	4.4
1	B	48	LEU	4.4
1	B	73	VAL	4.4
1	B	98	SER	4.4
1	B	174	THR	4.3
1	A	11	LEU	4.3
1	B	94	ARG	4.3
1	B	22	PHE	4.3
1	B	13	GLY	4.3
1	B	160	ASP	4.3
1	B	181	SER	4.3
1	B	148	ALA	4.3
1	A	106	GLY	4.2
1	B	107	ALA	4.2
1	A	13	GLY	4.2
1	B	149	ALA	4.2
1	A	127	ALA	4.2
1	A	173	PRO	4.1
1	A	131	ARG	4.1
1	B	11	LEU	4.1
1	B	72	LEU	4.1
1	A	53	ILE	4.0
1	A	89	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	83	SER	4.0
1	A	79	GLU	4.0
1	A	54	THR	4.0
1	A	78	ARG	4.0
1	B	32	PHE	4.0
1	A	158	ALA	4.0
1	A	75	VAL	3.9
1	A	140	ILE	3.9
1	A	122	SER	3.9
1	A	172	LEU	3.9
1	A	90	GLY	3.9
1	B	39	GLY	3.8
1	A	128	ASP	3.8
1	A	114	LEU	3.8
1	A	108	SER	3.8
1	A	176	VAL	3.8
1	B	102	GLY	3.8
1	B	173	PRO	3.8
1	A	76	MET	3.8
1	B	74	ASP	3.8
1	B	161	SER	3.7
1	A	36	ALA	3.7
1	A	41	ARG	3.7
1	B	84	GLN	3.7
1	B	99	GLU	3.7
1	B	184	HIS	3.7
1	B	162	ASN	3.6
1	B	8	ILE	3.6
1	B	78	ARG	3.6
1	B	123	VAL	3.6
1	A	84	GLN	3.5
1	B	109	LYS	3.5
1	A	67	ALA	3.5
1	A	101	HIS	3.5
1	B	164	VAL	3.5
1	B	44	GLN	3.5
1	B	140	ILE	3.5
1	B	7	VAL	3.5
1	A	121	ASP	3.5
1	A	174	THR	3.5
1	B	54	THR	3.5
1	A	93	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	118	VAL	3.4
1	B	69	LEU	3.4
1	A	52	SER	3.4
1	B	105	PRO	3.4
1	B	30	LYS	3.4
1	A	109	LYS	3.4
1	B	55	THR	3.4
1	A	104	ARG	3.4
1	A	179	GLY	3.4
1	B	71	SER	3.4
1	B	37	ASN	3.3
1	A	144	ASP	3.3
1	A	171	ASP	3.3
1	A	138	PHE	3.3
1	B	130	ALA	3.3
1	A	18	PRO	3.3
1	A	169	ILE	3.3
1	B	156	GLY	3.3
1	A	152	ARG	3.3
1	B	60	TRP	3.3
1	B	57	ASP	3.3
1	B	5	LEU	3.3
1	A	130	ALA	3.2
1	B	92	ALA	3.2
1	B	40	PRO	3.2
1	A	51	GLY	3.2
1	B	131	ARG	3.2
1	A	21	TYR	3.2
1	B	34	SER	3.2
1	B	168	ARG	3.2
1	A	143	GLY	3.2
1	B	20	SER	3.1
1	A	99	GLU	3.1
1	B	38	ILE	3.1
1	A	124	ASP	3.1
1	B	12	ASP	3.1
1	B	41	ARG	3.1
1	B	152	ARG	3.1
1	B	166	LEU	3.1
1	A	87	ASP	3.1
1	A	44	GLN	3.0
1	A	117	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	79	GLU	3.0
1	A	10	LEU	3.0
1	A	156	GLY	3.0
1	B	125	ALA	3.0
1	A	116	THR	3.0
1	A	29	ALA	2.9
1	A	129	ALA	2.9
1	A	136	THR	2.9
1	B	127	ALA	2.9
1	A	112	VAL	2.9
1	A	30	LYS	2.9
1	A	145	ARG	2.8
1	A	164	VAL	2.8
1	A	148	ALA	2.8
1	A	85	ILE	2.8
1	A	165	LYS	2.8
1	A	115	VAL	2.8
1	B	111	VAL	2.7
1	B	85	ILE	2.7
1	B	171	ASP	2.7
1	B	120	VAL	2.7
1	B	97	THR	2.7
1	B	121	ASP	2.7
1	B	147	ASP	2.7
1	B	157	PRO	2.7
1	A	38	ILE	2.7
1	A	111	VAL	2.7
1	A	166	LEU	2.6
1	A	24	GLU	2.6
1	A	20	SER	2.6
1	A	35	LYS	2.6
1	B	153	ILE	2.6
1	A	97	THR	2.5
1	B	10	LEU	2.5
1	B	26	LYS	2.5
1	A	8	ILE	2.5
1	B	129	ALA	2.5
1	A	132	SER	2.5
1	B	18	PRO	2.4
1	B	183	LEU	2.4
1	A	163	VAL	2.4
1	B	106	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	128	ASP	2.3
1	A	72	LEU	2.3
1	B	138	PHE	2.3
1	A	168	ARG	2.3
1	A	15	SER	2.3
1	B	132	SER	2.3
1	A	59	PRO	2.3
1	B	150	GLN	2.3
1	A	86	GLY	2.3
1	A	31	ALA	2.2
1	A	56	ILE	2.2
1	B	75	VAL	2.2
1	A	150	GLN	2.2
1	B	170	GLU	2.2
1	A	57	ASP	2.2
1	A	6	ASP	2.2
1	B	27	SER	2.2
1	A	22	PHE	2.2
1	B	142	ILE	2.2
1	B	46	SER	2.1
1	B	116	THR	2.1
1	B	141	GLY	2.1
1	B	167	GLN	2.1
1	A	141	GLY	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 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.