



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:51 am GMT

PDB ID : 2GZ4
Title : 1.5 Å Crystal Structure of a Protein of Unknown Function ATU1052 from *Agrobacterium tumefaciens*
Authors : Zhang, R.; Xu, X.; Zheng, H.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-05-10
Resolution : 1.50 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	:	trunk28620
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)	:	recalc28949

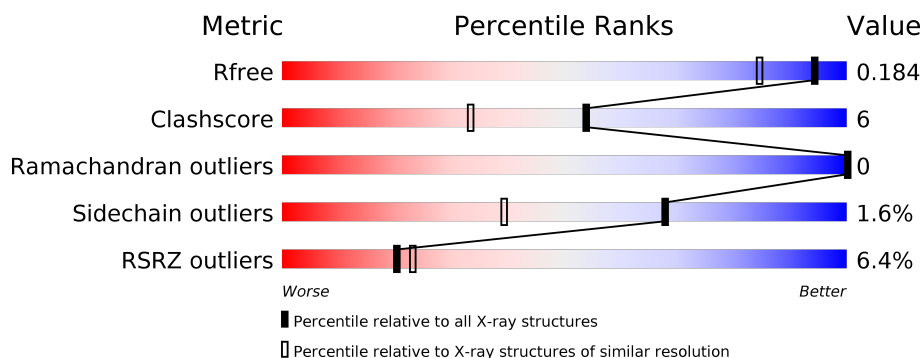
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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	207	<div> <div>7%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
1	B	207	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>•</div> </div>
1	C	207	<div> <div>5%</div> <div>85%</div> <div>8%</div> <div>• 5%</div> </div>
1	D	207	<div> <div>8%</div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7422 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 Hypothetical protein Atu1052.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1561	990	282	280	9			
1	B	198	Total	C	N	O	S	0	0	0
			1553	986	280	278	9			
1	C	196	Total	C	N	O	S	0	0	0
			1535	976	275	275	9			
1	D	197	Total	C	N	O	S	0	0	0
			1544	980	279	276	9			

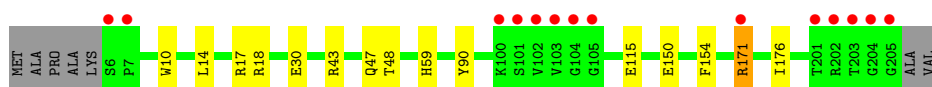
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	313	Total	O	0	0
			313	313		
2	B	350	Total	O	0	0
			350	350		
2	C	286	Total	O	0	0
			286	286		
2	D	280	Total	O	0	0
			280	280		

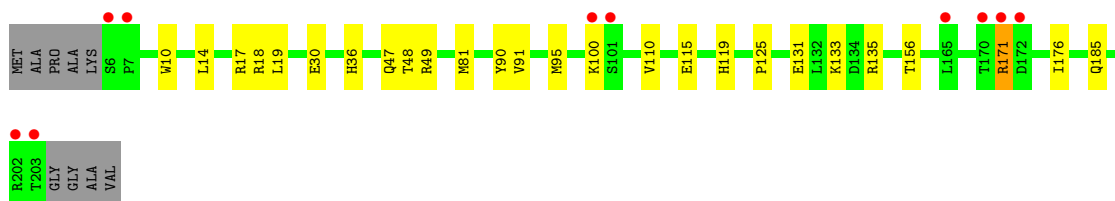
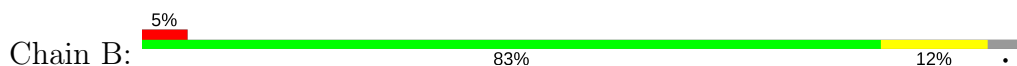
3 Residue-property plots [i](#)

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.

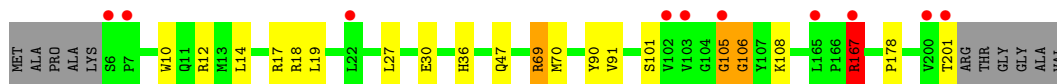
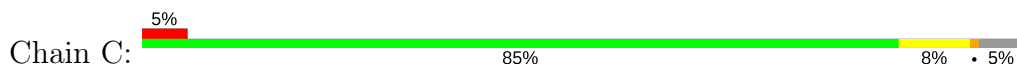
- Molecule 1: Hypothetical protein Atu1052



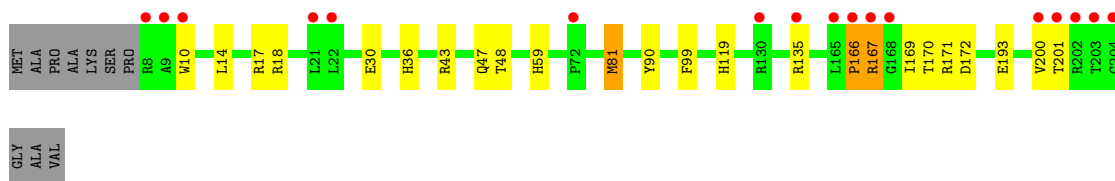
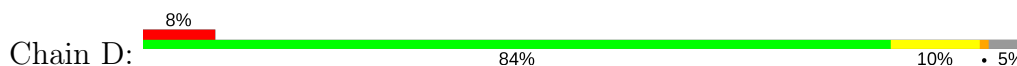
- Molecule 1: Hypothetical protein Atu1052



- Molecule 1: Hypothetical protein Atu1052



- Molecule 1: Hypothetical protein Atu1052



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.99Å 108.65Å 80.95Å 90.00° 93.74° 90.00°	Depositor
Resolution (Å)	24.13 – 1.50 24.13 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (24.13-1.50) 96.9 (24.13-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.152 , 0.183 0.153 , 0.184	Depositor DCC
R_{free} test set	6318 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7422	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.97 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6668e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.43	0/1596	0.61	0/2159
1	B	0.44	0/1588	0.65	2/2149 (0.1%)
1	C	0.44	0/1570	0.69	4/2125 (0.2%)
1	D	0.45	0/1578	0.63	1/2134 (0.0%)
All	All	0.44	0/6332	0.64	7/8567 (0.1%)

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
1	D	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	105	GLY	N-CA-C	6.40	129.09	113.10
1	B	49	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	D	81	MET	CG-SD-CE	5.76	109.42	100.20
1	C	106	GLY	N-CA-C	-5.57	99.17	113.10
1	C	69	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	49	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	166	PRO	Peptide

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	1561	0	1565	12	0
1	B	1553	0	1559	23	0
1	C	1535	0	1539	18	0
1	D	1544	0	1550	30	0
2	A	313	0	0	4	0
2	B	350	0	0	4	0
2	C	286	0	0	8	0
2	D	280	0	0	9	0
All	All	7422	0	6213	75	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 6.

All (75) 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:D:200:VAL:HG12	2:D:485:HOH:O	1.06	1.24
1:B:81:MET:SD	2:B:542:HOH:O	2.21	0.96
1:B:95:MET:SD	1:B:100:LYS:NZ	2.43	0.91
1:C:167:ARG:NH1	2:C:280:HOH:O	1.99	0.85
1:B:47:GLN:HE21	1:D:14:LEU:H	1.32	0.78
1:B:14:LEU:H	1:D:47:GLN:HE21	1.34	0.76
1:A:14:LEU:H	1:C:47:GLN:HE21	1.32	0.75
1:A:47:GLN:HE21	1:C:14:LEU:H	1.33	0.75
1:B:115:GLU:CD	2:B:302:HOH:O	2.25	0.75
1:D:81:MET:HE3	1:D:119:HIS:ND1	2.04	0.72
1:C:167:ARG:HG2	1:C:167:ARG:O	1.91	0.70
1:D:193:GLU:HG2	2:D:484:HOH:O	1.92	0.68
1:D:166:PRO:HA	1:D:167:ARG:HB2	1.77	0.65
1:A:154:PHE:CZ	2:C:492:HOH:O	2.50	0.64
1:B:48:THR:O	1:D:36:HIS:HE1	1.84	0.60
1:D:200:VAL:CG1	2:D:485:HOH:O	1.89	0.60
1:D:81:MET:CE	1:D:119:HIS:CE1	2.86	0.59
1:A:150:GLU:HG3	2:A:518:HOH:O	2.02	0.58
1:D:166:PRO:HB3	2:D:441:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:TRP:CG	1:D:18:ARG:HD2	2.39	0.57
1:B:131:GLU:OE2	1:B:135:ARG:NE	2.37	0.57
1:D:81:MET:HE3	1:D:119:HIS:CE1	2.39	0.57
1:D:81:MET:HE3	1:D:119:HIS:HD1	1.70	0.57
1:A:48:THR:O	1:C:36:HIS:HE1	1.89	0.56
1:C:27:LEU:HD23	2:C:493:HOH:O	2.08	0.54
1:B:36:HIS:HE1	1:D:48:THR:O	1.91	0.54
1:B:100:LYS:N	1:B:100:LYS:HD2	2.23	0.54
1:C:105:GLY:O	1:C:108:LYS:HB2	2.08	0.53
1:D:167:ARG:HB2	2:D:441:HOH:O	2.09	0.53
1:B:81:MET:CE	1:B:119:HIS:ND1	2.71	0.53
1:A:10:TRP:CG	1:A:18:ARG:HD2	2.44	0.52
1:B:156:THR:HG22	2:B:548:HOH:O	2.10	0.52
1:C:10:TRP:CG	1:C:18:ARG:HD2	2.45	0.51
1:B:81:MET:HE3	1:B:125:PRO:HD2	1.93	0.49
1:C:178:PRO:HG2	2:C:392:HOH:O	2.12	0.49
1:C:69:ARG:NH1	2:C:319:HOH:O	2.46	0.49
1:D:166:PRO:CA	1:D:167:ARG:HB2	2.43	0.49
1:C:12:ARG:N	2:C:492:HOH:O	2.45	0.49
1:B:185:GLN:NE2	2:B:248:HOH:O	2.46	0.48
1:D:167:ARG:CB	2:D:441:HOH:O	2.62	0.48
1:B:81:MET:HE2	1:B:119:HIS:ND1	2.29	0.48
1:B:81:MET:HE3	1:B:125:PRO:CD	2.44	0.47
1:D:81:MET:HE2	1:D:119:HIS:CE1	2.48	0.47
1:D:167:ARG:HA	1:D:167:ARG:HD3	1.61	0.47
1:B:81:MET:HE1	1:B:119:HIS:ND1	2.30	0.47
1:B:171:ARG:CZ	1:B:176:ILE:HG22	2.45	0.47
1:D:169:ILE:HB	2:D:441:HOH:O	2.15	0.46
1:B:10:TRP:CG	1:B:18:ARG:HD2	2.50	0.46
1:D:166:PRO:HA	1:D:167:ARG:CB	2.46	0.46
1:D:135:ARG:HE	1:D:135:ARG:HA	1.79	0.46
1:A:176:ILE:HG21	2:A:517:HOH:O	2.16	0.45
1:A:17:ARG:CZ	1:A:30:GLU:HG3	2.47	0.45
1:D:17:ARG:CZ	1:D:30:GLU:HG3	2.46	0.45
1:D:135:ARG:HA	1:D:135:ARG:NE	2.32	0.44
1:D:201:THR:HB	2:D:482:HOH:O	2.16	0.43
1:A:43:ARG:HD3	1:A:59:HIS:HB2	1.99	0.43
1:B:17:ARG:CZ	1:B:30:GLU:HG3	2.48	0.43
1:B:110:VAL:HG11	1:D:99:PHE:CE1	2.54	0.43
1:C:167:ARG:NH2	2:C:491:HOH:O	2.50	0.43
1:B:81:MET:CE	1:B:119:HIS:CE1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:MET:CE	1:C:167:ARG:HD3	2.49	0.42
1:A:171:ARG:CZ	1:A:176:ILE:HG22	2.50	0.42
1:D:170:THR:OG1	1:D:172:ASP:OD1	2.34	0.42
1:C:201:THR:O	1:C:201:THR:HG22	2.20	0.42
1:A:115:GLU:CD	2:A:484:HOH:O	2.58	0.41
1:C:19:LEU:HD23	1:C:91:VAL:HG21	2.01	0.41
1:C:17:ARG:CZ	1:C:30:GLU:HG3	2.50	0.41
1:A:150:GLU:HG3	2:A:517:HOH:O	2.21	0.41
1:B:19:LEU:HD23	1:B:91:VAL:HG21	2.03	0.41
1:D:10:TRP:CD2	1:D:18:ARG:HD2	2.56	0.41
1:C:201:THR:HG21	2:C:316:HOH:O	2.21	0.40
1:B:81:MET:HE1	1:B:119:HIS:HD1	1.85	0.40
1:D:43:ARG:HD3	1:D:59:HIS:HB2	2.03	0.40
1:C:105:GLY:N	1:C:106:GLY:HA3	2.36	0.40
1:D:171:ARG:CZ	2:D:438:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	198/207 (96%)	197 (100%)	1 (0%)	0	100	100
1	B	196/207 (95%)	195 (100%)	1 (0%)	0	100	100
1	C	194/207 (94%)	193 (100%)	1 (0%)	0	100	100
1	D	195/207 (94%)	194 (100%)	1 (0%)	0	100	100
All	All	783/828 (95%)	779 (100%)	4 (0%)	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	162/166 (98%)	160 (99%)	2 (1%)	75	52
1	B	162/166 (98%)	159 (98%)	3 (2%)	62	30
1	C	160/166 (96%)	157 (98%)	3 (2%)	62	30
1	D	160/166 (96%)	158 (99%)	2 (1%)	73	48
All	All	644/664 (97%)	634 (98%)	10 (2%)	68	39

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

Mol	Chain	Res	Type
1	A	90	TYR
1	A	171	ARG
1	B	90	TYR
1	B	133	LYS
1	B	171	ARG
1	C	90	TYR
1	C	101	SER
1	C	167	ARG
1	D	90	TYR
1	D	167	ARG

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	47	GLN
1	B	36	HIS
1	B	47	GLN
1	B	127	HIS
1	C	36	HIS
1	C	47	GLN
1	D	36	HIS
1	D	47	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	200/207 (96%)	0.25	14 (7%) 17 19	8, 13, 28, 35	0
1	B	198/207 (95%)	0.19	10 (5%) 29 32	9, 13, 27, 35	0
1	C	196/207 (94%)	0.30	10 (5%) 29 32	9, 14, 29, 32	0
1	D	197/207 (95%)	0.30	17 (8%) 11 12	8, 15, 27, 41	0
All	All	791/828 (95%)	0.26	51 (6%) 20 23	8, 14, 28, 41	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	GLY	10.4
1	C	167	ARG	9.5
1	D	201	THR	9.1
1	D	203	THR	8.1
1	C	201	THR	8.0
1	C	6	SER	7.7
1	C	7	PRO	6.4
1	D	167	ARG	6.1
1	A	205	GLY	6.0
1	C	200	VAL	5.6
1	A	204	GLY	5.4
1	B	6	SER	5.3
1	D	202	ARG	5.2
1	A	103	VAL	5.2
1	A	7	PRO	5.1
1	C	165	LEU	5.1
1	B	101	SER	5.0
1	A	101	SER	4.5
1	A	6	SER	4.3
1	D	200	VAL	4.2
1	B	171	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	100	LYS	4.1
1	C	102	VAL	4.0
1	B	7	PRO	3.6
1	D	10	TRP	3.3
1	D	9	ALA	3.2
1	A	203	THR	3.2
1	B	203	THR	3.2
1	D	165	LEU	3.2
1	A	201	THR	2.8
1	B	170	THR	2.8
1	B	202	ARG	2.8
1	A	171	ARG	2.8
1	A	104	GLY	2.7
1	D	168	GLY	2.7
1	A	202	ARG	2.7
1	D	130	ARG	2.5
1	D	166	PRO	2.5
1	B	165	LEU	2.4
1	C	105	GLY	2.4
1	C	103	VAL	2.4
1	D	22	LEU	2.4
1	C	22	LEU	2.3
1	D	21	LEU	2.2
1	A	100	LYS	2.2
1	A	102	VAL	2.2
1	B	172	ASP	2.2
1	A	105	GLY	2.1
1	D	72	PRO	2.1
1	D	135	ARG	2.0
1	D	8	ARG	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.