Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:44 AM GMT

PDB ID	:	2Y7O
Title	:	STRUCTURE OF N-TERMINAL DOMAIN OF CANDIDA ALBICANS ALS9-2 - G299W MUTANT
Authors	:	Salgado, P.S.; Burchell, L.; Cota, E.
Deposited on	:	2011-01-31
Resolution	:	1.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

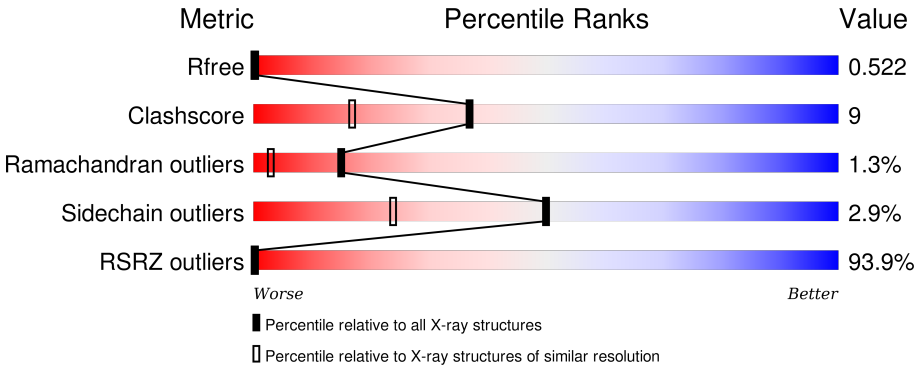
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 <=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	312	94% 88% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2637 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 AGGLUTININ-LIKE ALS9 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	1	0	0
			2362	1497	365	490	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q5A8T1
A	51	THR	ASN	CONFLICT	UNP Q5A8T1
A	212	VAL	ILE	CONFLICT	UNP Q5A8T1
A	296	TRP	GLY	ENGINEERED MUTATION	UNP Q5A8T1

- Molecule 2 is water.

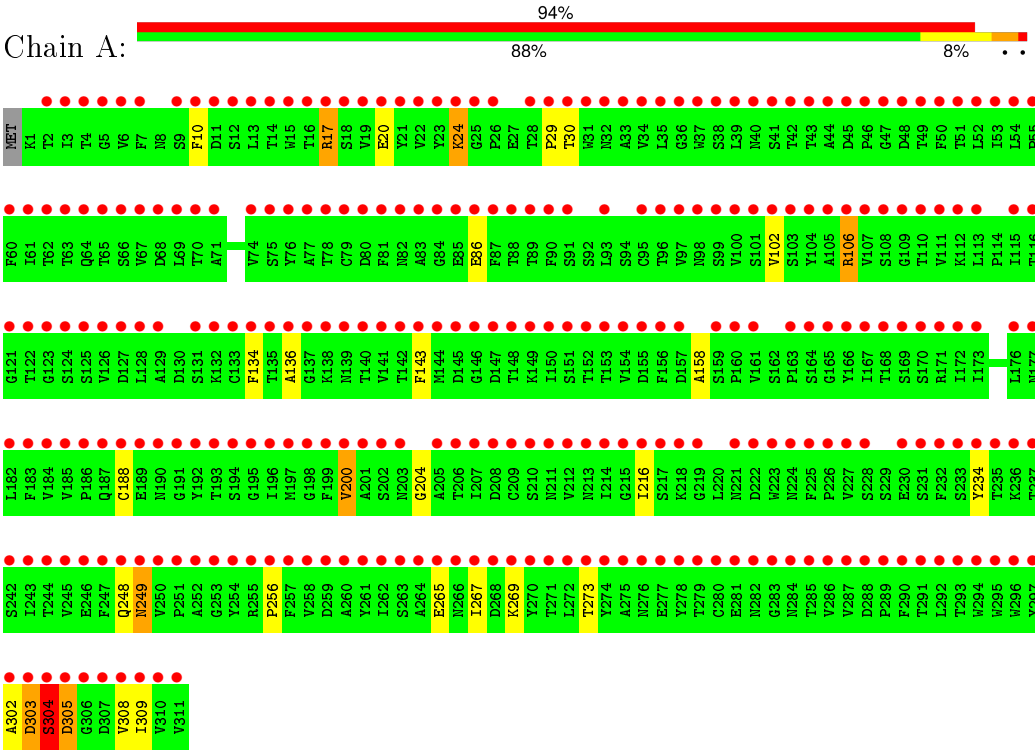
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	275	Total	O	0	0
			275	275		

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 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: AGGLUTININ-LIKE ALS9 PROTEIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.37Å 68.31Å 89.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.51 – 1.75 46.46 – 1.26	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.51-1.75) 30.7 (46.46-1.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.39 (at 1.26Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.223 0.549 , 0.522	Depositor DCC
R_{free} test set	1289 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	4.4	Xtriage
Anisotropy	2.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 215.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 32766 reflections	Xtriage
F_o,F_c correlation	0.42	EDS
Total number of atoms	2637	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.74	14/2420 (0.6%)	1.19	4/3314 (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	A	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	ARG	CZ-NH1	53.99	2.03	1.33
1	A	106	ARG	CZ-NH2	11.09	1.47	1.33
1	A	106	ARG	NE-CZ	9.77	1.45	1.33
1	A	301	GLU	CD-OE2	8.36	1.34	1.25
1	A	86	GLU	CD-OE1	6.43	1.32	1.25
1	A	234	TYR	CE1-CZ	-6.27	1.30	1.38
1	A	304	SER	C-O	6.18	1.35	1.23
1	A	24	LYS	CE-NZ	6.07	1.64	1.49
1	A	301	GLU	CD-OE1	5.94	1.32	1.25
1	A	265	GLU	CD-OE1	5.88	1.32	1.25
1	A	134	PHE	CE1-CZ	5.82	1.48	1.37
1	A	304	SER	CB-OG	5.76	1.49	1.42
1	A	143	PHE	CE2-CZ	5.58	1.48	1.37
1	A	188	CYS	CB-SG	-5.37	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ARG	NE-CZ-NH2	-27.27	106.67	120.30
1	A	265	GLU	C-N-CA	-7.58	102.76	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	308	VAL	CG1-CB-CG2	-5.14	102.68	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain

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	2362	0	2231	43	0
2	A	275	0	0	1	0
All	All	2637	0	2231	43	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 (43) 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:298:LYS:HA	1:A:299:ASN:CB	1.47	1.31
1:A:299:ASN:N	1:A:301:GLU:OE1	1.79	1.16
1:A:298:LYS:HA	1:A:299:ASN:HB2	1.18	1.14
1:A:301:GLU:O	1:A:302:ALA:HB3	1.39	1.10
1:A:298:LYS:HA	1:A:299:ASN:HB3	1.30	1.08
1:A:299:ASN:H	1:A:301:GLU:CD	1.61	1.02
1:A:298:LYS:CA	1:A:299:ASN:CB	2.38	1.02
1:A:303:ASP:CG	1:A:304:SER:H	1.66	0.97
1:A:298:LYS:NZ	1:A:300:SER:HB2	1.81	0.96
1:A:301:GLU:O	1:A:302:ALA:CB	2.12	0.93
1:A:298:LYS:CA	1:A:299:ASN:HB2	2.00	0.90
1:A:298:LYS:HG2	1:A:300:SER:N	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:ND2	1:A:299:ASN:O	2.07	0.88
1:A:298:LYS:HZ3	1:A:300:SER:HB2	1.39	0.83
1:A:298:LYS:HZ3	1:A:300:SER:CB	1.94	0.81
1:A:17:ARG:HB3	2:A:2019:HOH:O	1.80	0.80
1:A:298:LYS:HG2	1:A:300:SER:H	1.45	0.79
1:A:303:ASP:CG	1:A:304:SER:N	2.40	0.75
1:A:300:SER:H	1:A:301:GLU:HA	1.52	0.74
1:A:298:LYS:NZ	1:A:300:SER:CB	2.50	0.74
1:A:298:LYS:C	1:A:301:GLU:OE1	2.28	0.71
1:A:298:LYS:CA	1:A:299:ASN:HB3	2.14	0.71
1:A:298:LYS:HD2	1:A:309:ILE:HD11	1.76	0.66
1:A:300:SER:N	1:A:301:GLU:HA	2.17	0.59
1:A:299:ASN:C	1:A:299:ASN:HD22	1.98	0.56
1:A:298:LYS:O	1:A:301:GLU:OE1	2.25	0.55
1:A:299:ASN:N	1:A:301:GLU:CD	2.44	0.55
1:A:303:ASP:OD2	1:A:304:SER:N	2.28	0.53
1:A:204:GLY:HA3	1:A:267:ILE:HD13	1.89	0.53
1:A:200:VAL:HG13	1:A:273:THR:HB	1.91	0.52
1:A:136:ALA:HB2	1:A:158:ALA:HB2	1.96	0.48
1:A:248:GLN:O	1:A:249:ASN:O	2.32	0.47
1:A:216:ILE:HG22	1:A:256:PRO:HA	1.99	0.44
1:A:24:LYS:HB3	1:A:24:LYS:HE3	1.85	0.44
1:A:298:LYS:HZ1	1:A:303:ASP:CB	2.31	0.44
1:A:298:LYS:HZ1	1:A:303:ASP:HB3	1.83	0.43
1:A:136:ALA:CB	1:A:158:ALA:HB2	2.47	0.43
1:A:298:LYS:CG	1:A:299:ASN:HB3	2.48	0.43
1:A:267:ILE:HD12	1:A:269:LYS:O	2.19	0.43
1:A:298:LYS:HZ2	1:A:300:SER:HB2	1.74	0.42
1:A:29:PRO:HA	1:A:30:THR:HA	1.88	0.41
1:A:298:LYS:NZ	1:A:303:ASP:HB2	2.36	0.41
1:A:248:GLN:O	1:A:249:ASN:C	2.57	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	309/312 (99%)	295 (96%)	10 (3%)	4 (1%)	15 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
1	A	299	ASN
1	A	305	ASP
1	A	303	ASP

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	272/274 (99%)	264 (97%)	8 (3%)	50 24

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	17	ARG
1	A	20	GLU
1	A	102	VAL
1	A	200	VAL
1	A	299	ASN
1	A	304	SER
1	A	305	ASP

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

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	311/312 (99%)	4.87	292 (93%)	0	0	12, 22, 39, 63	4 (1%)

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	TRP	14.6
1	A	10	PHE	13.5
1	A	24	LYS	13.3
1	A	56	CYS	12.0
1	A	137	GLY	11.9
1	A	22	VAL	11.1
1	A	274	TYR	11.0
1	A	223	TRP	11.0
1	A	37	TRP	10.8
1	A	21	TYR	10.2
1	A	298	LYS	10.1
1	A	39	LEU	10.0
1	A	109	GLY	9.7
1	A	254	TYR	9.6
1	A	248	GLN	9.5
1	A	100	VAL	9.4
1	A	161	VAL	9.3
1	A	63	THR	9.2
1	A	289	PRO	9.2
1	A	14	THR	9.1
1	A	206	THR	8.9
1	A	207	ILE	8.9
1	A	16	THR	8.9
1	A	96	THR	8.7
1	A	264	ALA	8.5
1	A	35	LEU	8.1
1	A	272	LEU	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	297	TYR	8.1
1	A	203	ASN	8.0
1	A	138	LYS	7.9
1	A	30	THR	7.9
1	A	143	PHE	7.9
1	A	185	VAL	7.9
1	A	282	ASN	7.7
1	A	78	THR	7.7
1	A	156	PHE	7.6
1	A	280	CYS	7.6
1	A	148	THR	7.5
1	A	208	ASP	7.5
1	A	261	TYR	7.5
1	A	159	SER	7.3
1	A	36	GLY	7.3
1	A	309	ILE	7.3
1	A	136	ALA	7.2
1	A	58	PHE	7.2
1	A	183	PHE	7.2
1	A	50	PHE	7.2
1	A	182	LEU	7.1
1	A	192	TYR	7.0
1	A	104	TYR	7.0
1	A	273	THR	7.0
1	A	13	LEU	7.0
1	A	216	ILE	6.9
1	A	267	ILE	6.9
1	A	168	THR	6.8
1	A	290	PHE	6.8
1	A	122	THR	6.7
1	A	5	GLY	6.7
1	A	244	THR	6.6
1	A	129	ALA	6.6
1	A	9	SER	6.6
1	A	278	TYR	6.6
1	A	119	VAL	6.6
1	A	88	THR	6.6
1	A	135	THR	6.5
1	A	271	THR	6.5
1	A	221	ASN	6.4
1	A	296	TRP	6.3
1	A	225	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	19	VAL	6.3
1	A	28	THR	6.2
1	A	23	TYR	6.2
1	A	311	VAL	6.2
1	A	170	SER	6.2
1	A	49	THR	6.2
1	A	95	CYS	6.1
1	A	245	VAL	6.1
1	A	15	TRP	6.1
1	A	151	SER	6.0
1	A	188	CYS	6.0
1	A	184	VAL	6.0
1	A	232	PHE	5.9
1	A	77	ALA	5.9
1	A	107	VAL	5.9
1	A	293	THR	5.9
1	A	117	PHE	5.9
1	A	270	TYR	5.8
1	A	197	MET	5.8
1	A	17	ARG	5.8
1	A	166	TYR	5.8
1	A	291	THR	5.7
1	A	152	THR	5.7
1	A	256	PRO	5.7
1	A	61	ILE	5.6
1	A	26	PRO	5.5
1	A	292	LEU	5.5
1	A	93	LEU	5.5
1	A	305	ASP	5.5
1	A	250	VAL	5.5
1	A	147	ASP	5.4
1	A	201	ALA	5.4
1	A	69	LEU	5.4
1	A	55	PRO	5.4
1	A	51	THR	5.4
1	A	60	PHE	5.3
1	A	90	PHE	5.3
1	A	173	ILE	5.3
1	A	199	PHE	5.3
1	A	79	CYS	5.3
1	A	81	PHE	5.3
1	A	302	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	124	SER	5.3
1	A	54	LEU	5.2
1	A	83	ALA	5.2
1	A	97	VAL	5.2
1	A	53	ILE	5.2
1	A	31	TRP	5.1
1	A	67	VAL	5.1
1	A	205	ALA	5.1
1	A	257	PHE	5.1
1	A	212	VAL	5.1
1	A	165	GLY	5.1
1	A	285	THR	5.1
1	A	42	THR	5.1
1	A	71	ALA	5.1
1	A	87	PHE	5.0
1	A	102	VAL	5.0
1	A	266	ASN	5.0
1	A	6	VAL	5.0
1	A	20	GLU	5.0
1	A	259	ASP	4.9
1	A	74	VAL	4.9
1	A	179	LEU	4.9
1	A	99	SER	4.9
1	A	230	GLU	4.8
1	A	252	ALA	4.8
1	A	76	TYR	4.8
1	A	283	GLY	4.7
1	A	106	ARG	4.7
1	A	308	VAL	4.7
1	A	62	THR	4.7
1	A	193	THR	4.7
1	A	176	LEU	4.7
1	A	3	ILE	4.7
1	A	253	GLY	4.6
1	A	45	ASP	4.6
1	A	306	GLY	4.6
1	A	186	PRO	4.6
1	A	286	VAL	4.6
1	A	310	VAL	4.6
1	A	187	GLN	4.6
1	A	251	PRO	4.5
1	A	150	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	12	SER	4.5
1	A	7	PHE	4.5
1	A	247	PHE	4.5
1	A	120	GLY	4.4
1	A	40	ASN	4.4
1	A	209	CYS	4.4
1	A	279	THR	4.4
1	A	34	VAL	4.4
1	A	146	GLY	4.4
1	A	133	CYS	4.3
1	A	284	ASN	4.3
1	A	227	VAL	4.3
1	A	294	TRP	4.3
1	A	115	ILE	4.3
1	A	52	LEU	4.3
1	A	191	GLY	4.3
1	A	47	GLY	4.2
1	A	153	THR	4.2
1	A	164	SER	4.2
1	A	142	THR	4.2
1	A	217	SER	4.2
1	A	128	LEU	4.2
1	A	18	SER	4.2
1	A	123	GLY	4.1
1	A	234	TYR	4.1
1	A	139	ASN	4.1
1	A	144	MET	4.1
1	A	263	SER	4.1
1	A	46	PRO	4.1
1	A	84	GLY	4.0
1	A	127	ASP	4.0
1	A	157	ASP	4.0
1	A	110	THR	4.0
1	A	125	SER	4.0
1	A	167	ILE	4.0
1	A	68	ASP	3.9
1	A	126	VAL	3.9
1	A	75	SER	3.9
1	A	237	THR	3.9
1	A	160	PRO	3.9
1	A	105	ALA	3.9
1	A	172	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	111	VAL	3.9
1	A	198	GLY	3.9
1	A	154	VAL	3.8
1	A	243	ILE	3.8
1	A	287	VAL	3.8
1	A	218	LYS	3.8
1	A	228	SER	3.8
1	A	196	ILE	3.7
1	A	224	ASN	3.7
1	A	181	SER	3.7
1	A	155	ASP	3.7
1	A	276	ASN	3.7
1	A	214	ILE	3.7
1	A	43	THR	3.7
1	A	241	THR	3.6
1	A	33	ALA	3.6
1	A	238	CYS	3.6
1	A	215	GLY	3.6
1	A	258	VAL	3.5
1	A	4	THR	3.5
1	A	268	ASP	3.5
1	A	57	VAL	3.4
1	A	265	GLU	3.4
1	A	307	ASP	3.4
1	A	275	ALA	3.4
1	A	38	SER	3.4
1	A	222	ASP	3.4
1	A	140	THR	3.4
1	A	178	LYS	3.3
1	A	288	ASP	3.3
1	A	141	VAL	3.3
1	A	235	THR	3.3
1	A	118	ASN	3.2
1	A	189	GLU	3.2
1	A	213	ASN	3.2
1	A	101	SER	3.1
1	A	194	SER	3.1
1	A	202	SER	3.1
1	A	32	ASN	3.1
1	A	98	ASN	3.1
1	A	211	ASN	3.1
1	A	103	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	ILE	3.0
1	A	260	ALA	3.0
1	A	2	THR	3.0
1	A	246	GLU	3.0
1	A	177	ASN	3.0
1	A	44	ALA	3.0
1	A	29	PRO	2.9
1	A	303	ASP	2.9
1	A	64	GLN	2.9
1	A	91	SER	2.9
1	A	231	SER	2.9
1	A	82	ASN	2.9
1	A	180	SER	2.9
1	A	149	LYS	2.9
1	A	131	SER	2.9
1	A	113	LEU	2.9
1	A	190	ASN	2.9
1	A	11	ASP	2.8
1	A	226	PRO	2.8
1	A	86	GLU	2.8
1	A	132	LYS	2.8
1	A	80	ASP	2.7
1	A	163	PRO	2.7
1	A	89	THR	2.7
1	A	145	ASP	2.6
1	A	85	GLU	2.6
1	A	134	PHE	2.6
1	A	108	SER	2.6
1	A	304	SER	2.6
1	A	70	THR	2.6
1	A	66	SER	2.6
1	A	233	SER	2.5
1	A	300	SER	2.5
1	A	41	SER	2.5
1	A	169	SER	2.5
1	A	112	LYS	2.5
1	A	195	GLY	2.5
1	A	240	SER	2.5
1	A	121	GLY	2.4
1	A	65	THR	2.4
1	A	281	GLU	2.4
1	A	239	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASP	2.4
1	A	116	THR	2.4
1	A	200	VAL	2.4
1	A	242	SER	2.3
1	A	269	LYS	2.3
1	A	171	ARG	2.3
1	A	255	ARG	2.3
1	A	236	LYS	2.3
1	A	277	GLU	2.2
1	A	210	SER	2.2
1	A	25	GLY	2.1
1	A	219	GLY	2.1
1	A	249	ASN	2.1

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.