Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:39 pm BST

PDB ID	:	2OF3
Title	:	TOG domain structure from C.elegans Zyg9
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Deposited on	:	2007-01-02
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 following versions of software and data (see references ①) were used in the production of this report:

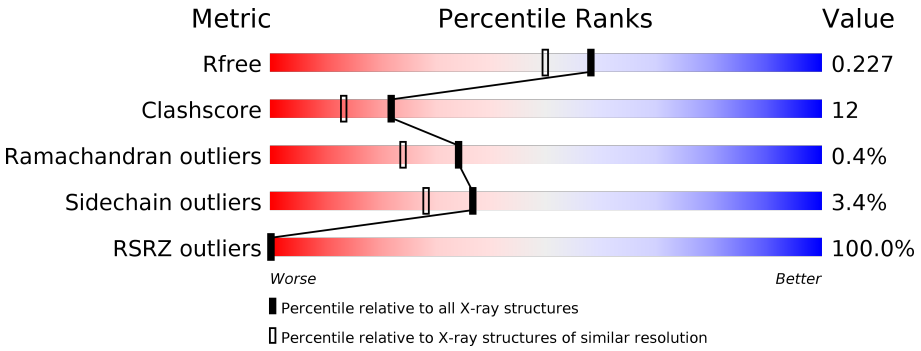
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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))
R_{free}	130704	6207 (1.90-1.90)
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 on 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 <=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	266	100% 86% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2338 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 ZYG-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2109	1338	364	396	11	0	1	0

- Molecule 2 is water.

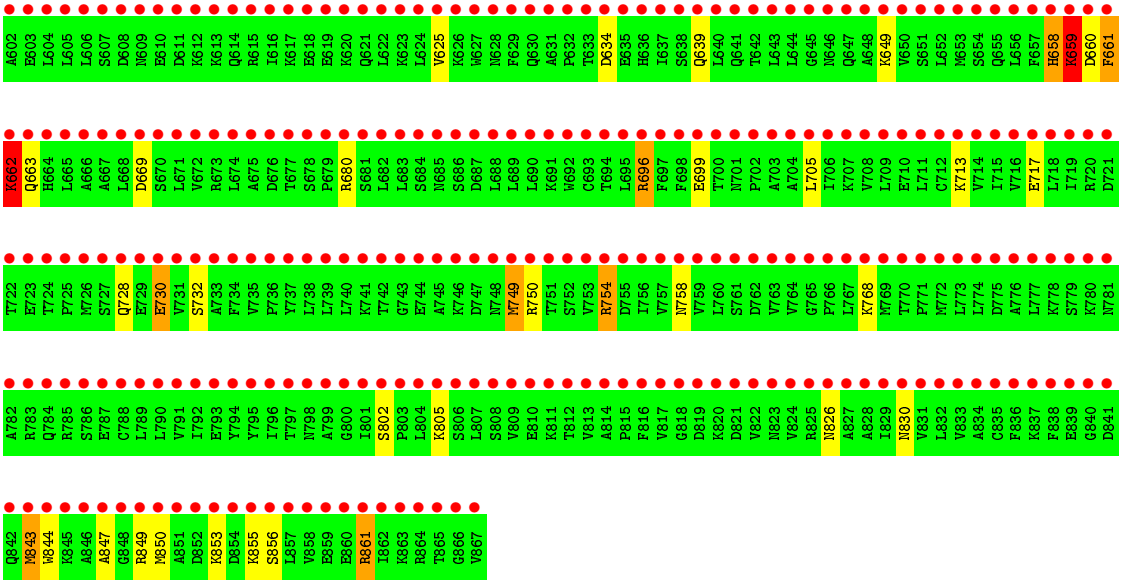
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	229	229	229	0	0

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: ZYG-9

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	54.13Å 54.13Å 116.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 1.90 19.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.83-1.90) 99.9 (19.83-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	0.03 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.224 0.174 , 0.227	Depositor DCC
R_{free} test set	1335 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	-6.8	Xtriage
Anisotropy	-0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2338	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% 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, 0.333 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	0.97	1/2138 (0.0%)	0.96	8/2885 (0.3%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	730	GLU	CD-OE1	5.08	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	754	ARG	NE-CZ-NH1	14.63	127.61	120.30
1	A	754	ARG	NE-CZ-NH2	-14.63	112.99	120.30
1	A	663	GLN	N-CA-C	-8.09	89.15	111.00
1	A	634	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	749	MET	CG-SD-CE	-5.55	91.33	100.20
1	A	750	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	750	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	861	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	659	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	662	LYS	Peptide

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	2109	0	2195	51	0
2	A	229	0	0	12	0
All	All	2338	0	2195	51	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 12.

All (51) 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:705:LEU:HD23	1:A:749:MET:CE	1.55	1.36
1:A:730:GLU:HB3	2:A:227:HOH:O	1.40	1.16
1:A:659:LYS:CD	1:A:659:LYS:H	1.53	1.10
1:A:659:LYS:H	1:A:659:LYS:HD2	1.11	1.08
1:A:705:LEU:HD23	1:A:749:MET:HE3	1.30	1.06
1:A:705:LEU:CD2	1:A:749:MET:HE3	1.89	1.02
1:A:659:LYS:HD2	1:A:659:LYS:N	1.71	1.02
1:A:705:LEU:CD2	1:A:749:MET:CE	2.43	0.96
1:A:705:LEU:HD23	1:A:749:MET:HE1	1.43	0.95
1:A:659:LYS:H	1:A:659:LYS:CE	1.80	0.94
1:A:660:ASP:HB2	2:A:131:HOH:O	1.71	0.90
1:A:625:VAL:H	1:A:639:GLN:HE22	1.19	0.90
1:A:659:LYS:CD	1:A:659:LYS:N	2.30	0.90
1:A:660:ASP:O	1:A:662:LYS:N	2.13	0.81
1:A:843:MET:CE	1:A:847:ALA:HB2	2.10	0.80
1:A:660:ASP:CB	2:A:131:HOH:O	2.32	0.76
1:A:730:GLU:OE2	2:A:150:HOH:O	2.04	0.74
1:A:768:LYS:HE3	2:A:176:HOH:O	1.86	0.72
1:A:669:ASP:HB2	2:A:38:HOH:O	1.91	0.71
1:A:658:HIS:ND1	1:A:659:LYS:CD	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:ARG:NH2	2:A:199:HOH:O	2.25	0.70
1:A:830:ASN:HD21	1:A:861:ARG:HH11	1.39	0.70
1:A:658:HIS:CE1	2:A:131:HOH:O	2.45	0.68
1:A:658:HIS:ND1	1:A:659:LYS:HD3	2.09	0.68
1:A:713:LYS:HE2	1:A:717:GLU:OE2	1.96	0.66
1:A:659:LYS:HE2	1:A:659:LYS:H	1.60	0.66
1:A:843:MET:HE2	1:A:847:ALA:HB2	1.80	0.63
1:A:660:ASP:O	1:A:661:PHE:C	2.38	0.61
1:A:659:LYS:N	1:A:659:LYS:CE	2.61	0.60
1:A:658:HIS:ND1	1:A:659:LYS:HD2	2.16	0.59
1:A:696:ARG:NH1	1:A:699:GLU:OE2	2.36	0.59
1:A:830:ASN:ND2	1:A:861:ARG:HH11	2.01	0.59
1:A:660:ASP:C	1:A:662:LYS:N	2.54	0.57
1:A:826:ASN:ND2	1:A:861:ARG:HH22	2.02	0.57
1:A:660:ASP:C	1:A:662:LYS:H	2.07	0.57
1:A:843:MET:HE1	1:A:847:ALA:CB	2.35	0.57
1:A:659:LYS:HE2	1:A:659:LYS:N	2.18	0.57
1:A:680:ARG:HD3	2:A:198:HOH:O	2.05	0.56
1:A:802:SER:HA	1:A:805:LYS:HG2	1.87	0.56
1:A:728:GLN:HG2	2:A:154:HOH:O	2.05	0.55
1:A:705:LEU:CD2	1:A:749:MET:HE1	2.27	0.53
1:A:843:MET:CE	1:A:847:ALA:CB	2.83	0.53
1:A:826:ASN:HD21	1:A:861:ARG:HH22	1.57	0.52
1:A:754:ARG:HD2	1:A:758:ASN:OD1	2.09	0.51
1:A:849:ARG:CZ	1:A:849:ARG:HB2	2.47	0.44
1:A:847:ALA:CB	1:A:850:MET:HE2	2.49	0.43
1:A:658:HIS:ND1	2:A:131:HOH:O	2.37	0.42
1:A:696:ARG:HH11	1:A:699:GLU:CD	2.23	0.42
1:A:649:LYS:HG2	1:A:649:LYS:HZ2	1.70	0.41
1:A:659:LYS:HE3	2:A:171:HOH:O	2.20	0.41
1:A:844:TRP:CZ3	1:A:855:LYS:HG3	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	265/266 (100%)	262 (99%)	2 (1%)	1 (0%)	34 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	661	PHE

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	239/238 (100%)	231 (97%)	8 (3%)	38 29

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

Mol	Chain	Res	Type
1	A	658	HIS
1	A	659	LYS
1	A	662	LYS
1	A	696	ARG
1	A	732	SER
1	A	843	MET
1	A	853	LYS
1	A	856	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	GLN
1	A	826	ASN
1	A	830	ASN

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	266/266 (100%)	84.27	266 (100%)	0	0	17, 27, 46, 69	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	788	CYS	152.6
1	A	627	TRP	149.5
1	A	835	CYS	144.4
1	A	622	LEU	136.4
1	A	637	ILE	135.1
1	A	719	ILE	133.4
1	A	693	CYS	132.8
1	A	763	VAL	132.2
1	A	718	LEU	130.4
1	A	605	LEU	128.5
1	A	726	MET	126.2
1	A	836	PHE	124.4
1	A	801	ILE	124.2
1	A	697	PHE	123.5
1	A	737	TYR	120.6
1	A	749	MET	120.5
1	A	712	CYS	120.4
1	A	640	LEU	119.8
1	A	795	TYR	117.8
1	A	631	ALA	116.8
1	A	698	PHE	115.9
1	A	629	PHE	115.9
1	A	657	PHE	115.7
1	A	643	LEU	115.4
1	A	653	MET	115.4
1	A	684	SER	115.4
1	A	814	ALA	114.8

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Mol	Chain	Res	Type	RSRZ
1	A	609	ASN	114.7
1	A	817	VAL	114.4
1	A	716	VAL	112.6
1	A	764	VAL	112.2
1	A	738	LEU	111.7
1	A	794	TYR	111.1
1	A	690	LEU	111.1
1	A	692	TRP	110.8
1	A	803	PRO	110.3
1	A	683	LEU	109.6
1	A	727	SER	109.5
1	A	734	PHE	108.9
1	A	822	VAL	108.6
1	A	767	LEU	107.5
1	A	743	GLY	107.2
1	A	695	LEU	107.0
1	A	772	MET	106.7
1	A	725	PRO	106.5
1	A	645	GLY	106.5
1	A	818	GLY	106.0
1	A	752	SER	105.9
1	A	828	ALA	105.8
1	A	761	SER	105.6
1	A	644	LEU	105.4
1	A	800	GLY	105.2
1	A	852	ASP	105.0
1	A	722	THR	104.8
1	A	608	ASP	104.8
1	A	709	LEU	104.6
1	A	833	VAL	104.4
1	A	681	SER	104.2
1	A	667	ALA	103.9
1	A	773	LEU	103.9
1	A	861	ARG	103.8
1	A	769	MET	103.5
1	A	677	THR	103.2
1	A	759	VAL	103.1
1	A	715	ILE	103.0
1	A	829	ILE	101.6
1	A	675	ALA	101.0
1	A	688	LEU	100.9
1	A	774	LEU	100.8

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Mol	Chain	Res	Type	RSRZ
1	A	624	LEU	100.3
1	A	625	VAL	100.3
1	A	606	LEU	100.3
1	A	703	ALA	99.8
1	A	694	THR	99.7
1	A	739	LEU	99.5
1	A	733	ALA	99.2
1	A	682	LEU	98.7
1	A	807	LEU	98.5
1	A	731	VAL	98.5
1	A	824	VAL	97.7
1	A	634	ASP	97.1
1	A	642	THR	97.1
1	A	648	ALA	96.7
1	A	711	LEU	96.6
1	A	646	ASN	96.5
1	A	771	PRO	95.6
1	A	791	VAL	95.4
1	A	760	LEU	95.3
1	A	706	ILE	95.0
1	A	826	ASN	95.0
1	A	811	LYS	94.8
1	A	632	PRO	94.5
1	A	602	ALA	94.3
1	A	757	VAL	94.0
1	A	844	TRP	93.8
1	A	843	MET	93.7
1	A	823	ASN	93.5
1	A	816	PHE	93.2
1	A	636	HIS	92.3
1	A	827	ALA	92.2
1	A	638	SER	91.9
1	A	720	ARG	91.7
1	A	756	ILE	91.2
1	A	633	THR	90.7
1	A	747	ASP	90.4
1	A	724	THR	90.1
1	A	668	LEU	89.9
1	A	689	LEU	89.9
1	A	710	GLU	89.1
1	A	790	LEU	89.1
1	A	686	SER	88.7

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Mol	Chain	Res	Type	RSRZ
1	A	700	THR	88.3
1	A	765	GLY	88.2
1	A	781	ASN	87.8
1	A	611	ASP	87.7
1	A	607	SER	87.2
1	A	655	GLN	87.1
1	A	618	GLU	86.7
1	A	672	VAL	86.5
1	A	735	VAL	86.3
1	A	650	VAL	86.2
1	A	705	LEU	86.1
1	A	714	VAL	85.8
1	A	652	LEU	85.8
1	A	656	LEU	85.4
1	A	702	PRO	85.3
1	A	777	LEU	85.3
1	A	728	GLN	85.1
1	A	647	GLN	84.4
1	A	865	THR	84.4
1	A	754	ARG	84.1
1	A	830	ASN	83.9
1	A	616	ILE	83.9
1	A	639	GLN	83.7
1	A	628	ASN	83.6
1	A	729	GLU	83.5
1	A	670	SER	82.8
1	A	732	SER	82.5
1	A	740	LEU	82.0
1	A	664	HIS	81.7
1	A	745	ALA	81.6
1	A	812	THR	80.9
1	A	770	THR	80.9
1	A	859	GLU	80.8
1	A	785	ARG	80.8
1	A	758	ASN	80.3
1	A	857	LEU	80.2
1	A	834	ALA	80.1
1	A	847	ALA	80.1
1	A	615	ARG	79.4
1	A	802	SER	79.3
1	A	809	VAL	79.2
1	A	621	GLN	79.2

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Mol	Chain	Res	Type	RSRZ
1	A	736	PRO	79.1
1	A	797	THR	78.6
1	A	766	PRO	78.2
1	A	798	ASN	78.0
1	A	674	LEU	77.7
1	A	784	GLN	77.6
1	A	746	LYS	77.3
1	A	685	ASN	77.1
1	A	841	ASP	76.6
1	A	782	ALA	75.9
1	A	614	GLN	75.9
1	A	641	GLN	75.7
1	A	619	GLU	75.7
1	A	806	SER	75.6
1	A	708	VAL	75.4
1	A	679	PRO	75.0
1	A	792	ILE	74.7
1	A	783	ARG	74.7
1	A	730	GLU	74.1
1	A	635	GLU	74.0
1	A	832	LEU	73.8
1	A	623	LYS	73.7
1	A	666	ALA	73.3
1	A	661	PHE	73.1
1	A	742	THR	72.7
1	A	819	ASP	72.4
1	A	680	ARG	72.0
1	A	846	ALA	71.8
1	A	626	LYS	71.7
1	A	691	LYS	71.4
1	A	687	ASP	71.1
1	A	856	SER	70.7
1	A	821	ASP	70.4
1	A	665	LEU	70.3
1	A	704	ALA	70.0
1	A	776	ALA	69.9
1	A	860	GLU	69.5
1	A	786	SER	69.4
1	A	678	SER	69.1
1	A	604	LEU	69.1
1	A	713	LYS	69.0
1	A	804	LEU	68.9

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Mol	Chain	Res	Type	RSRZ
1	A	787	GLU	68.6
1	A	799	ALA	68.5
1	A	789	LEU	67.9
1	A	721	ASP	67.5
1	A	707	LYS	67.2
1	A	815	PRO	67.1
1	A	813	VAL	66.4
1	A	744	GLU	65.7
1	A	838	PHE	65.2
1	A	696	ARG	64.6
1	A	768	LYS	64.4
1	A	810	GLU	64.4
1	A	864	ARG	64.1
1	A	620	LYS	63.8
1	A	862	ILE	63.7
1	A	751	THR	63.6
1	A	658	HIS	63.5
1	A	753	VAL	63.4
1	A	723	GLU	63.3
1	A	654	SER	63.2
1	A	717	GLU	62.9
1	A	671	LEU	62.8
1	A	796	ILE	62.6
1	A	850	MET	62.1
1	A	762	ASP	61.9
1	A	741	LYS	61.8
1	A	750	ARG	61.6
1	A	610	GLU	61.5
1	A	858	VAL	61.4
1	A	617	LYS	61.0
1	A	825	ARG	60.4
1	A	837	LYS	60.1
1	A	851	ALA	59.5
1	A	676	ASP	58.9
1	A	612	LYS	58.8
1	A	673	ARG	58.8
1	A	613	LYS	58.3
1	A	831	VAL	58.2
1	A	808	SER	57.5
1	A	755	ASP	57.5
1	A	701	ASN	54.8
1	A	651	SER	53.9

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Mol	Chain	Res	Type	RSRZ
1	A	778	LYS	53.0
1	A	793	GLU	52.9
1	A	820	LYS	52.7
1	A	660	ASP	52.3
1	A	669	ASP	52.0
1	A	603	GLU	51.5
1	A	842	GLN	51.0
1	A	867	VAL	50.7
1	A	748[A]	ASN	50.6
1	A	630	GLN	50.5
1	A	663	GLN	50.4
1	A	848	GLY	50.2
1	A	840	GLY	48.8
1	A	854	ASP	48.2
1	A	775	ASP	47.5
1	A	855	LYS	47.3
1	A	780	LYS	47.2
1	A	805	LYS	46.8
1	A	839	GLU	46.6
1	A	779	SER	46.4
1	A	659	LYS	46.3
1	A	853	LYS	45.4
1	A	649	LYS	45.1
1	A	863	LYS	38.7
1	A	699	GLU	37.5
1	A	849	ARG	36.6
1	A	845	LYS	33.6
1	A	866	GLY	31.0
1	A	662	LYS	22.5

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.