



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:50 AM GMT

PDB ID : 2OF3  
Title : TOG domain structure from C.elegans Zyg9  
Authors : Al-Bassam, J.; Larsen, N.A.; Hyman, A.A.; Harrison, S.C.  
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](mailto: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.

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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

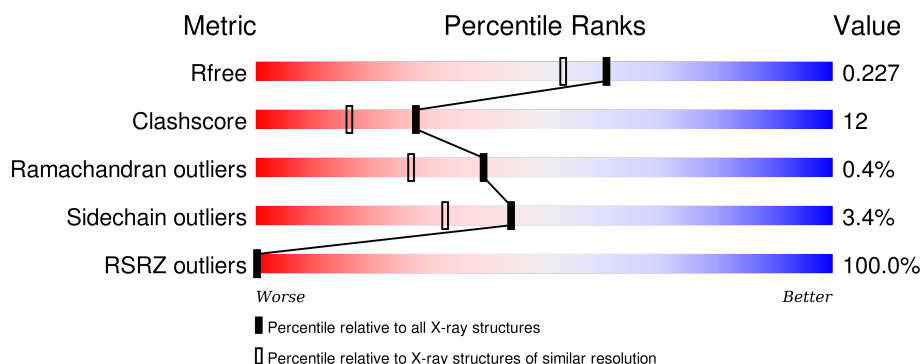
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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  $\geq 3$ , 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	266	<div> <div>100%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>••</div> </div> </div>

## 2 Entry composition

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
1	A	266	Total	C	N	O	S	0	1	0
			2109	1338	364	396	11			

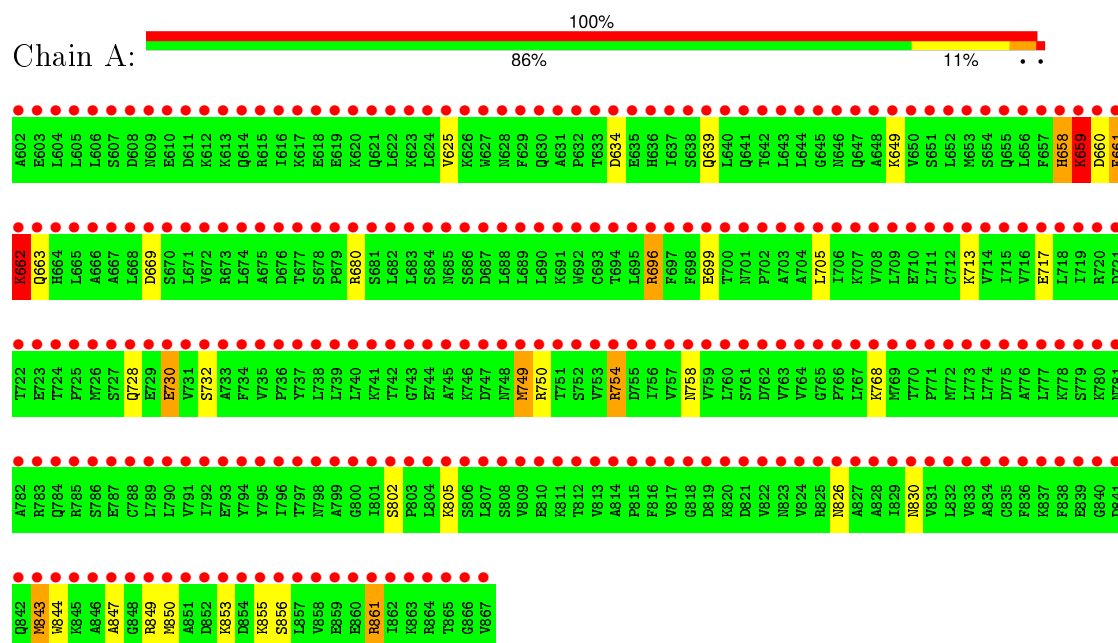
- Molecule 2 is water.

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

### 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: ZYG-9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	-6.8	Xtriage
Anisotropy	-0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.5	EDS
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26372 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2338	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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(°)	Ideal(°)
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 ⓘ

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:830:ASN:HD21	1:A:861:ARG:HH11	1.39	0.70
1:A:696:ARG:NH2	2:A:199:HOH:O	2.25	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:HB2	1:A:849:ARG:CZ	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%)	39	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	661	PHE

### 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	239/238 (100%)	231 (97%)	8 (3%)	45	34

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	266/266 (100%)	85.28	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	154.1
1	A	627	TRP	151.1
1	A	835	CYS	145.8
1	A	622	LEU	138.6
1	A	637	ILE	137.3
1	A	719	ILE	135.6
1	A	763	VAL	134.7
1	A	693	CYS	134.2
1	A	718	LEU	132.4
1	A	605	LEU	130.7
1	A	836	PHE	126.6
1	A	801	ILE	126.3
1	A	726	MET	126.2
1	A	697	PHE	125.6
1	A	640	LEU	121.7
1	A	712	CYS	121.7
1	A	737	TYR	121.1
1	A	749	MET	120.5
1	A	631	ALA	118.6
1	A	795	TYR	118.3
1	A	698	PHE	117.8
1	A	629	PHE	117.8
1	A	657	PHE	117.7
1	A	643	LEU	117.3
1	A	684	SER	116.9
1	A	814	ALA	116.8
1	A	817	VAL	116.5

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Mol	Chain	Res	Type	RSRZ
1	A	609	ASN	115.6
1	A	653	MET	115.5
1	A	716	VAL	114.7
1	A	764	VAL	114.2
1	A	738	LEU	113.6
1	A	690	LEU	113.0
1	A	692	TRP	112.0
1	A	803	PRO	111.6
1	A	794	TYR	111.6
1	A	683	LEU	111.4
1	A	727	SER	110.8
1	A	734	PHE	110.8
1	A	822	VAL	110.6
1	A	767	LEU	109.3
1	A	743	GLY	108.5
1	A	695	LEU	108.5
1	A	645	GLY	107.9
1	A	725	PRO	107.8
1	A	828	ALA	107.5
1	A	818	GLY	107.4
1	A	752	SER	107.1
1	A	644	LEU	107.1
1	A	761	SER	106.9
1	A	772	MET	106.7
1	A	800	GLY	106.6
1	A	852	ASP	106.4
1	A	709	LEU	106.4
1	A	833	VAL	106.2
1	A	608	ASP	106.1
1	A	722	THR	105.6
1	A	667	ALA	105.6
1	A	681	SER	105.6
1	A	773	LEU	105.5
1	A	759	VAL	105.0
1	A	715	ILE	104.7
1	A	677	THR	104.0
1	A	861	ARG	104.0
1	A	769	MET	103.5
1	A	829	ILE	103.3
1	A	675	ALA	102.7
1	A	688	LEU	102.6
1	A	774	LEU	102.4

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Mol	Chain	Res	Type	RSRZ
1	A	625	VAL	102.2
1	A	606	LEU	102.0
1	A	624	LEU	101.9
1	A	703	ALA	101.5
1	A	739	LEU	101.2
1	A	733	ALA	100.9
1	A	694	THR	100.4
1	A	731	VAL	100.4
1	A	682	LEU	100.3
1	A	807	LEU	100.1
1	A	824	VAL	99.4
1	A	634	ASP	98.3
1	A	648	ALA	98.3
1	A	711	LEU	98.2
1	A	642	THR	97.8
1	A	646	ASN	97.2
1	A	791	VAL	97.1
1	A	760	LEU	96.9
1	A	771	PRO	96.8
1	A	706	ILE	96.5
1	A	602	ALA	95.8
1	A	826	ASN	95.8
1	A	757	VAL	95.7
1	A	632	PRO	95.4
1	A	811	LYS	95.2
1	A	844	TRP	94.8
1	A	816	PHE	94.8
1	A	823	ASN	94.2
1	A	827	ALA	93.8
1	A	843	MET	93.8
1	A	636	HIS	93.3
1	A	638	SER	93.1
1	A	756	ILE	92.7
1	A	720	ARG	91.8
1	A	747	ASP	91.5
1	A	633	THR	91.4
1	A	689	LEU	91.4
1	A	668	LEU	91.4
1	A	724	THR	90.8
1	A	790	LEU	90.5
1	A	686	SER	89.8
1	A	710	GLU	89.6

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Mol	Chain	Res	Type	RSRZ
1	A	765	GLY	89.3
1	A	700	THR	89.0
1	A	611	ASP	88.9
1	A	781	ASN	88.5
1	A	607	SER	88.4
1	A	672	VAL	88.2
1	A	650	VAL	87.9
1	A	735	VAL	87.9
1	A	655	GLN	87.7
1	A	705	LEU	87.4
1	A	714	VAL	87.4
1	A	652	LEU	87.2
1	A	618	GLU	87.1
1	A	656	LEU	86.8
1	A	777	LEU	86.7
1	A	702	PRO	86.2
1	A	728	GLN	85.8
1	A	616	ILE	85.3
1	A	647	GLN	85.1
1	A	865	THR	85.0
1	A	830	ASN	84.7
1	A	639	GLN	84.4
1	A	628	ASN	84.3
1	A	754	ARG	84.2
1	A	729	GLU	84.0
1	A	670	SER	83.7
1	A	732	SER	83.5
1	A	740	LEU	83.3
1	A	745	ALA	82.9
1	A	664	HIS	82.6
1	A	812	THR	81.6
1	A	857	LEU	81.6
1	A	770	THR	81.5
1	A	834	ALA	81.5
1	A	847	ALA	81.4
1	A	859	GLU	81.4
1	A	758	ASN	81.0
1	A	785	ARG	80.9
1	A	809	VAL	80.7
1	A	802	SER	80.4
1	A	736	PRO	80.0
1	A	621	GLN	79.8

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Mol	Chain	Res	Type	RSRZ
1	A	615	ARG	79.6
1	A	797	THR	79.4
1	A	766	PRO	79.2
1	A	674	LEU	79.0
1	A	798	ASN	78.7
1	A	784	GLN	78.2
1	A	685	ASN	77.7
1	A	746	LYS	77.7
1	A	841	ASP	77.5
1	A	782	ALA	77.1
1	A	708	VAL	76.9
1	A	806	SER	76.7
1	A	614	GLN	76.4
1	A	641	GLN	76.4
1	A	619	GLU	76.2
1	A	792	ILE	75.9
1	A	679	PRO	75.9
1	A	832	LEU	75.1
1	A	783	ARG	74.8
1	A	730	GLU	74.6
1	A	666	ALA	74.5
1	A	635	GLU	74.4
1	A	661	PHE	74.4
1	A	623	LYS	74.0
1	A	819	ASP	73.4
1	A	742	THR	73.3
1	A	846	ALA	73.0
1	A	687	ASP	72.1
1	A	680	ARG	72.0
1	A	626	LYS	72.0
1	A	691	LYS	71.8
1	A	856	SER	71.6
1	A	665	LEU	71.4
1	A	821	ASP	71.3
1	A	704	ALA	71.2
1	A	776	ALA	71.0
1	A	786	SER	70.2
1	A	604	LEU	70.1
1	A	804	LEU	70.0
1	A	678	SER	70.0
1	A	860	GLU	69.9
1	A	799	ALA	69.6

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Mol	Chain	Res	Type	RSRZ
1	A	713	LYS	69.3
1	A	787	GLU	69.0
1	A	789	LEU	69.0
1	A	721	ASP	68.4
1	A	815	PRO	67.8
1	A	813	VAL	67.6
1	A	707	LYS	67.5
1	A	838	PHE	66.4
1	A	744	GLU	66.1
1	A	862	ILE	64.8
1	A	810	GLU	64.7
1	A	696	ARG	64.7
1	A	753	VAL	64.7
1	A	768	LYS	64.7
1	A	864	ARG	64.2
1	A	658	HIS	64.2
1	A	751	THR	64.2
1	A	620	LYS	64.1
1	A	654	SER	64.1
1	A	671	LEU	63.8
1	A	796	ILE	63.7
1	A	723	GLU	63.7
1	A	717	GLU	63.2
1	A	762	ASP	62.7
1	A	858	VAL	62.6
1	A	850	MET	62.2
1	A	741	LYS	62.1
1	A	610	GLU	61.9
1	A	750	ARG	61.7
1	A	617	LYS	61.3
1	A	825	ARG	60.5
1	A	851	ALA	60.5
1	A	837	LYS	60.3
1	A	676	ASP	59.6
1	A	831	VAL	59.3
1	A	612	LYS	59.1
1	A	673	ARG	58.9
1	A	613	LYS	58.6
1	A	808	SER	58.3
1	A	755	ASP	58.2
1	A	701	ASN	55.2
1	A	651	SER	54.7

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Mol	Chain	Res	Type	RSRZ
1	A	778	LYS	53.2
1	A	793	GLU	53.2
1	A	660	ASP	53.0
1	A	820	LYS	53.0
1	A	669	ASP	52.7
1	A	603	GLU	51.8
1	A	867	VAL	51.7
1	A	842	GLN	51.3
1	A	748[A]	ASN	51.0
1	A	848	GLY	50.9
1	A	630	GLN	50.9
1	A	663	GLN	50.8
1	A	840	GLY	49.4
1	A	854	ASP	48.8
1	A	775	ASP	48.1
1	A	855	LYS	47.5
1	A	780	LYS	47.4
1	A	779	SER	47.1
1	A	805	LYS	47.0
1	A	839	GLU	46.9
1	A	659	LYS	46.5
1	A	853	LYS	45.6
1	A	649	LYS	45.3
1	A	863	LYS	38.9
1	A	699	GLU	37.8
1	A	849	ARG	36.7
1	A	845	LYS	33.8
1	A	866	GLY	31.5
1	A	662	LYS	22.6

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.