



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:39 AM UTC

PDB ID : 9NU9 / pdb\_00009nu9  
Title : X-ray Crystal Structure of Fission Yeast Fsc1 protein in C2 Symmetry  
Authors : Azuka, C.D.; Jin, X.  
Deposited on : 2025-03-19  
Resolution : 2.45 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

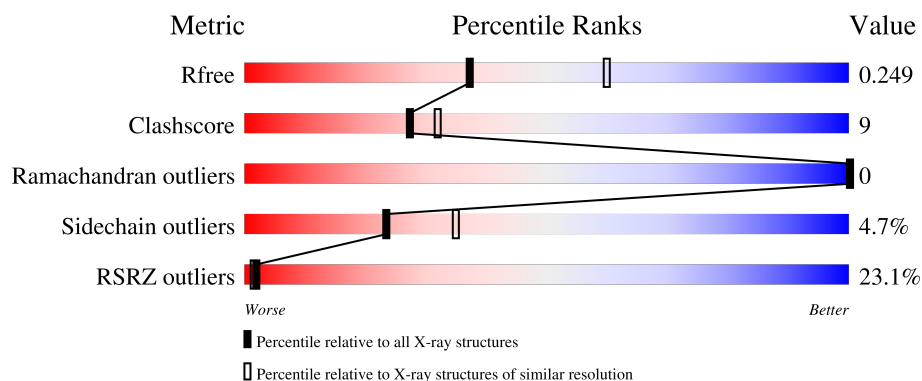
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	649	<div> <div>18%</div> <div>62%</div> <div>14%</div> <div>•</div> <div>22%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4252 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 FAS1 domain-containing protein fsc1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4018	2581	648	781	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	ALA	GLU	conflict	UNP O94439

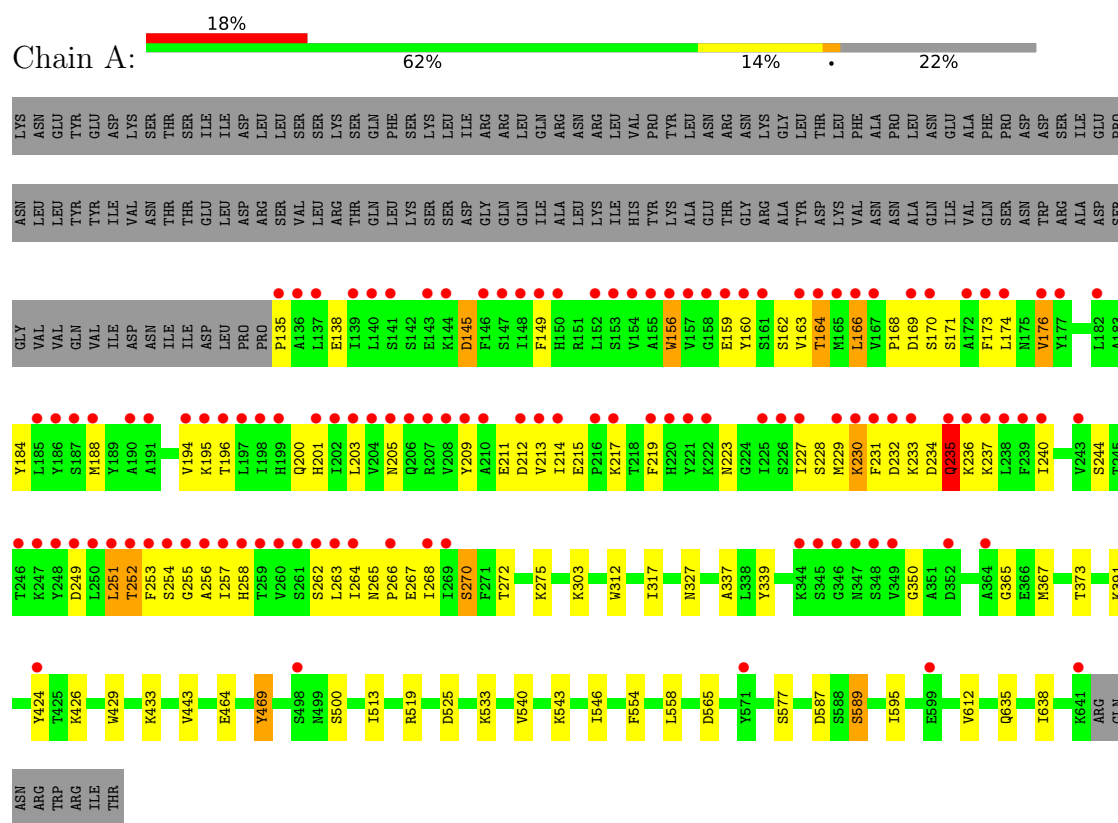
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	234	Total	O	0	0
			234	234		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: FAS1 domain-containing protein fsc1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	347.82Å 40.91Å 59.09Å 90.00° 92.57° 90.00°	Depositor
Resolution (Å)	47.84 – 2.45 47.84 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.84-2.45) 88.5 (47.84-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.204 , 0.250 0.205 , 0.249	Depositor DCC
$R_{free}$ test set	1462 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	1.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.48	0/4104	0.70	4/5578 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	TYR	N-CA-C	-5.70	103.83	112.04
1	A	235	GLN	N-CA-C	-5.52	106.62	113.19
1	A	188	MET	N-CA-C	-5.23	106.74	113.02
1	A	365	GLY	N-CA-C	5.08	121.61	115.31

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	4018	0	3976	73	0
2	A	234	0	0	8	0
All	All	4252	0	3976	73	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 (73) 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:200:GLN:HE21	1:A:265:ASN:HB2	1.34	0.91
1:A:214:ILE:HG23	1:A:231:PHE:HB3	1.69	0.75
1:A:237:LYS:HB3	1:A:244:SER:HB2	1.68	0.75
1:A:215:GLU:N	1:A:215:GLU:OE1	2.22	0.73
1:A:267:GLU:OE1	1:A:267:GLU:N	2.27	0.66
1:A:546:ILE:HD12	2:A:773:HOH:O	1.94	0.66
1:A:211:GLU:HA	1:A:214:ILE:HG13	1.78	0.65
1:A:443:VAL:HG13	1:A:540:VAL:HG21	1.82	0.62
1:A:215:GLU:OE2	1:A:217:LYS:HB2	2.01	0.61
1:A:543:LYS:HA	2:A:773:HOH:O	2.01	0.60
1:A:171:SER:HA	1:A:174:LEU:HD12	1.82	0.60
1:A:464:GLU:HG2	2:A:702:HOH:O	2.00	0.60
1:A:135:PRO:HA	1:A:253:PHE:HD2	1.67	0.59
1:A:350:GLY:HA2	1:A:525:ASP:OD1	2.02	0.59
1:A:270:SER:O	1:A:275:LYS:NZ	2.35	0.59
1:A:211:GLU:HA	1:A:214:ILE:CG1	2.33	0.58
1:A:426:LYS:NZ	2:A:706:HOH:O	2.35	0.58
1:A:229:MET:HG2	1:A:240:ILE:HD12	1.85	0.58
1:A:184:TYR:CE2	1:A:275:LYS:HD3	2.39	0.56
1:A:162:SER:O	1:A:205:ASN:HA	2.05	0.56
1:A:217:LYS:HD3	1:A:219:PHE:HE1	1.70	0.56
1:A:201:HIS:HA	1:A:264:ILE:HD12	1.88	0.56
1:A:166:LEU:HD22	1:A:258:HIS:HD2	1.71	0.55
1:A:252:THR:HG21	1:A:257:ILE:HD12	1.88	0.55
1:A:612:VAL:HG11	1:A:638:ILE:HD13	1.88	0.55
1:A:254:SER:OG	1:A:255:GLY:N	2.37	0.54
1:A:265:ASN:HB3	1:A:268:ILE:HB	1.90	0.54
1:A:262:SER:OG	1:A:263:LEU:N	2.41	0.54
1:A:337:ALA:HB3	1:A:339:TYR:CE1	2.44	0.53
1:A:173:PHE:CD1	1:A:263:LEU:HD21	2.45	0.52
1:A:145:ASP:HB3	1:A:169:ASP:HB2	1.91	0.51
1:A:176:VAL:HG21	1:A:266:PRO:HB2	1.90	0.51
1:A:200:GLN:HG3	1:A:264:ILE:HB	1.93	0.50
1:A:219:PHE:HB2	1:A:227:ILE:HB	1.93	0.50
1:A:433:LYS:NZ	2:A:713:HOH:O	2.45	0.50
1:A:587:ASP:HB3	1:A:589:SER:H	1.78	0.49
1:A:233:LYS:O	1:A:236:LYS:HG3	2.13	0.49
1:A:138:GLU:HA	1:A:138:GLU:OE2	2.13	0.48
1:A:235:GLN:HB3	1:A:237:LYS:HE3	1.95	0.47
1:A:235:GLN:HB3	1:A:237:LYS:CE	2.44	0.47
1:A:196:THR:HG22	1:A:268:ILE:HD11	1.97	0.47
1:A:303:LYS:HD3	1:A:327:ASN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:HB2	1:A:212:ASP:HB2	1.97	0.46
1:A:554:PHE:CE2	1:A:558:LEU:HD11	2.50	0.46
1:A:214:ILE:O	1:A:230:LYS:HD2	2.15	0.46
1:A:424:TYR:HD1	1:A:424:TYR:HA	1.61	0.46
1:A:231:PHE:CG	1:A:232:ASP:N	2.84	0.46
1:A:312:TRP:NE1	2:A:717:HOH:O	2.48	0.45
1:A:159:GLU:HG3	1:A:160:TYR:N	2.32	0.45
1:A:156:TRP:CH2	1:A:195:LYS:HB2	2.51	0.45
1:A:272:THR:OG1	1:A:275:LYS:HG3	2.16	0.45
1:A:233:LYS:O	1:A:236:LYS:CG	2.64	0.45
1:A:577:SER:HB2	2:A:701:HOH:O	2.16	0.45
1:A:251:LEU:HD22	1:A:251:LEU:HA	1.82	0.45
1:A:164:THR:HG23	1:A:203:LEU:HB2	1.99	0.45
1:A:135:PRO:HA	1:A:253:PHE:CD2	2.49	0.45
1:A:145:ASP:O	1:A:170:SER:N	2.48	0.45
1:A:249:ASP:HA	1:A:256:ALA:HB1	2.00	0.44
1:A:373:THR:HG23	1:A:391:LYS:HB3	1.99	0.44
1:A:513:ILE:O	1:A:533:LYS:NZ	2.46	0.43
1:A:145:ASP:OD1	1:A:145:ASP:N	2.51	0.43
1:A:219:PHE:O	1:A:227:ILE:N	2.40	0.43
1:A:565:ASP:OD1	1:A:565:ASP:C	2.62	0.43
1:A:429:TRP:HE3	2:A:845:HOH:O	2.01	0.43
1:A:469:TYR:CD1	1:A:519:ARG:HG2	2.54	0.43
1:A:233:LYS:HA	1:A:236:LYS:HA	2.01	0.42
1:A:230:LYS:HB3	1:A:230:LYS:HE2	1.72	0.42
1:A:211:GLU:OE2	1:A:231:PHE:HE2	2.03	0.42
1:A:184:TYR:CZ	1:A:275:LYS:HD3	2.56	0.41
1:A:237:LYS:HD2	1:A:244:SER:OG	2.19	0.41
1:A:176:VAL:HG21	1:A:266:PRO:CB	2.50	0.41
1:A:156:TRP:HZ2	1:A:194:VAL:HG12	1.85	0.41
1:A:149:PHE:CD2	1:A:168:PRO:HD2	2.57	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	505/649 (78%)	467 (92%)	38 (8%)	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	450/584 (77%)	429 (95%)	21 (5%)	23	35

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	ASP
1	A	156	TRP
1	A	163	VAL
1	A	164	THR
1	A	166	LEU
1	A	176	VAL
1	A	213	VAL
1	A	223	ASN
1	A	228	SER
1	A	230	LYS
1	A	234	ASP
1	A	235	GLN
1	A	251	LEU
1	A	252	THR
1	A	270	SER
1	A	317	ILE
1	A	367	MET
1	A	500	SER
1	A	589	SER
1	A	595	ILE
1	A	635	GLN

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

Mol	Chain	Res	Type
1	A	377	GLN
1	A	439	GLN
1	A	450	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 oligosaccharides 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	507/649 (78%)	0.86	117 (23%) 2 1	20, 41, 138, 148	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	ILE	7.1
1	A	135	PRO	6.7
1	A	137	LEU	6.6
1	A	208	VAL	6.5
1	A	140	LEU	6.2
1	A	238	LEU	6.1
1	A	227	ILE	5.8
1	A	166	LEU	5.8
1	A	225	ILE	5.6
1	A	203	LEU	5.6
1	A	251	LEU	5.6
1	A	349	VAL	5.5
1	A	204	VAL	5.5
1	A	156	TRP	5.1
1	A	239	PHE	5.0
1	A	165	MET	4.9
1	A	216	PRO	4.6
1	A	153	SER	4.6
1	A	157	VAL	4.5
1	A	348	SER	4.5
1	A	136	ALA	4.4
1	A	243	VAL	4.4
1	A	146	PHE	4.4
1	A	345	SER	4.4
1	A	201	HIS	4.2
1	A	149	PHE	4.1
1	A	347	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	247	LYS	4.0
1	A	209	TYR	4.0
1	A	167	VAL	4.0
1	A	240	ILE	3.9
1	A	257	ILE	3.9
1	A	173	PHE	3.9
1	A	174	LEU	3.9
1	A	164	THR	3.9
1	A	352	ASP	3.9
1	A	250	LEU	3.8
1	A	219	PHE	3.8
1	A	258	HIS	3.8
1	A	152	LEU	3.7
1	A	424	TYR	3.7
1	A	148	ILE	3.7
1	A	253	PHE	3.7
1	A	160	TYR	3.7
1	A	155	ALA	3.6
1	A	176	VAL	3.6
1	A	217	LYS	3.6
1	A	229	MET	3.6
1	A	139	ILE	3.5
1	A	254	SER	3.5
1	A	266	PRO	3.4
1	A	197	LEU	3.4
1	A	226	SER	3.4
1	A	191	ALA	3.4
1	A	220	HIS	3.3
1	A	213	VAL	3.3
1	A	269	ILE	3.3
1	A	255	GLY	3.2
1	A	214	ILE	3.2
1	A	177	TYR	3.2
1	A	263	LEU	3.2
1	A	196	THR	3.2
1	A	231	PHE	3.2
1	A	264	ILE	3.2
1	A	206	GLN	3.1
1	A	161	SER	3.1
1	A	261	SER	3.1
1	A	147	SER	3.0
1	A	194	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	246	THR	3.0
1	A	262	SER	2.9
1	A	259	THR	2.9
1	A	221	TYR	2.9
1	A	158	GLY	2.9
1	A	212	ASP	2.9
1	A	249	ASP	2.9
1	A	237	LYS	2.8
1	A	163	VAL	2.8
1	A	190	ALA	2.8
1	A	256	ALA	2.8
1	A	346	GLY	2.8
1	A	199	HIS	2.8
1	A	205	ASN	2.8
1	A	641	LYS	2.8
1	A	260	VAL	2.7
1	A	233	LYS	2.7
1	A	248	TYR	2.7
1	A	207	ARG	2.6
1	A	195	LYS	2.6
1	A	222	LYS	2.6
1	A	198	ILE	2.6
1	A	232	ASP	2.6
1	A	150	HIS	2.6
1	A	252	THR	2.6
1	A	185	LEU	2.5
1	A	230	LYS	2.5
1	A	236	LYS	2.5
1	A	154	VAL	2.5
1	A	188	MET	2.4
1	A	169	ASP	2.4
1	A	143	GLU	2.4
1	A	599	GLU	2.4
1	A	571	TYR	2.3
1	A	182	LEU	2.3
1	A	268	ILE	2.2
1	A	187	SER	2.2
1	A	159	GLU	2.2
1	A	210	ALA	2.2
1	A	172	ALA	2.2
1	A	141	SER	2.1
1	A	170	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	144	LYS	2.1
1	A	344	LYS	2.1
1	A	235	GLN	2.0
1	A	364	ALA	2.0
1	A	186	TYR	2.0
1	A	498	SER	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 oligosaccharides 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.