

wwPDB X-ray Structure Validation Summary Report (i)

Jan 24, 2023 – 06:51 AM EST

PDB ID : 3GZS

Title : Crystal structure of a susd superfamily protein (bf3413) from bacteroides frag-

ilis netc 9343 at 2.10 A resolution

Authors : Joint Center for Structural Genomics (JCSG)

Deposited on : 2009-04-07

Resolution : 2.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.31.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

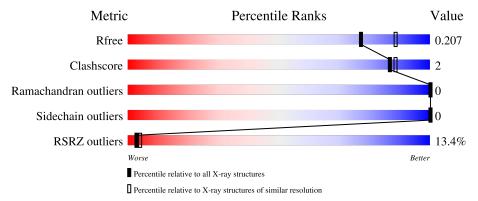
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.09 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 >=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	515	92%	•	-	
1	В	515	90%	6%	•	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	В	9	_	_	X	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8328 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.

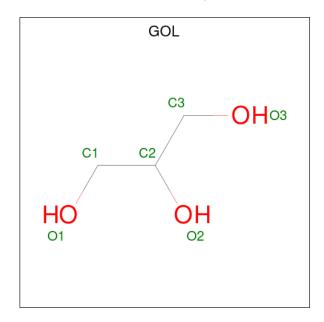
• Molecule 1 is a protein called Uncharacterized SusD superfamily protein.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
1	А	495	Total	С	N	_	S	Se	0	2	0
1	11	450	3879	2457	659	748	2	13	U	2	
1	D	495	Total	С	N	О	S	Se	0	2	0
1	Б	490	3881	2457	660	749	2	13	0	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Α	0	GLY	-	expression tag	UNP Q5L9X2
В	0	GLY	-	expression tag	UNP Q5L9X2

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 3 4	0	1

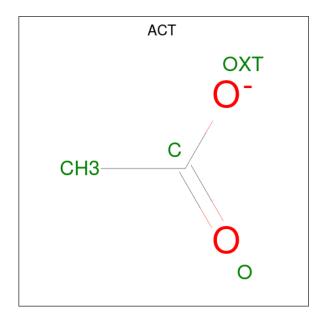
Continued on next page...



 $Continued\ from\ previous\ page...$

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	В	1	Total C O 6 3 3	0	0
2	В	1	Total C O 6 3 3	0	0

 \bullet Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	В	1	Total C O 4 2 2	0	0
3	В	1	Total C O 4 2 2	0	0
3	В	1	Total C O 4 2 2	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	В	1	Total C 4 2	O 2	0	0

• Molecule 4 is water.

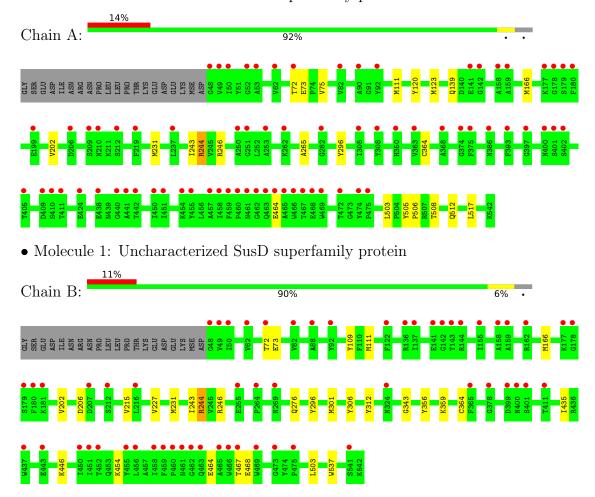
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	243	Total O 243 243	0	0
4	В	260	Total O 260 260	0	0



3 Residue-property plots (i)

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: Uncharacterized SusD superfamily protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	88.92Å 50.38Å 117.95Å	Donositor
a, b, c, α , β , γ	90.00° 108.05° 90.00°	Depositor
Resolution (Å)	29.63 - 2.09	Depositor
Resolution (A)	29.63 - 2.09	EDS
% Data completeness	97.3 (29.63-2.09)	Depositor
(in resolution range)	97.3 (29.63-2.09)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.16 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
D D.	0.156 , 0.198	Depositor
R, R_{free}	0.166 , 0.207	DCC
R_{free} test set	2934 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 58.9	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8328	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 41.67 % 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 2.2811e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, OCS, ACT

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		nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.62	$2/3953 \ (0.1\%)$	0.58	2/5337~(0.0%)	
1	В	0.65	1/3958 (0.0%)	0.58	2/5345~(0.0%)	
All	All	0.64	3/7911 (0.0%)	0.58	$4/10682 \ (0.0\%)$	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\text{\AA})$
1	В	73	GLU	CB-CG	5.92	1.63	1.52
1	A	73	GLU	CB-CG	5.35	1.62	1.52
1	A	111	MSE	SE-CE	-5.15	1.65	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	244	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	244	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	В	244	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	244	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	3879	0	3681	13	0
1	В	3881	0	3681	20	0
2	A	25	0	30	0	0
2	В	12	0	16	0	0
3	A	12	0	9	0	0
3	В	16	0	12	2	0
4	A	243	0	0	0	0
4	В	260	0	0	1	0
All	All	8328	0	7429	32	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 2.

The worst 5 of 32 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	overlap (Å)
1:B:72:THR:HG23	1:B:296:TYR:OH	1.81	0.80
1:A:72:THR:HG23	1:A:296:TYR:OH	1.97	0.65
1:B:202:VAL:HG13	1:B:231:MSE:HE3	1.82	0.62
1:A:166:MSE:SE	1:A:503:LEU:HD13	2.54	0.57
1:B:215[A]:VAL:HG23	1:B:227:VAL:HG22	1.88	0.55

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	494/515~(96%)	478 (97%)	16 (3%)	0	100	100	
1	В	495/515~(96%)	477 (96%)	18 (4%)	0	100	100	
All	All	989/1030~(96%)	955 (97%)	34 (3%)	0	100	100	

There are no Ramachandran outliers to report.



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	Percer	ntiles
1	A	389/409 (95%)	389 (100%)	0	100	100
1	В	390/409 (95%)	390 (100%)	0	100	100
All	All	779/818 (95%)	779 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	428	ASN
1	В	210	ASN
1	В	428	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trme	Chain	Dog	Link	Bond lengths			Bond angles		
Mol Type Chain	rtes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
1	OCS	A	364	1	7,8,9	0.97	0	6,11,13	1.67	1 (16%)
1	OCS	В	364	1	7,8,9	0.99	0	6,11,13	1.56	2 (33%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	A	364	1	-	0/4/7/9	-
1	OCS	В	364	1	-	0/4/7/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathrm{Ideal}(^{o})$
1	В	364	OCS	OD2-SG-CB	2.77	110.16	105.74
1	A	364	OCS	OD2-SG-CB	2.76	110.14	105.74
1	В	364	OCS	OD1-SG-CB	2.07	109.40	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Dag	es Link	В	Bond lengths			Bond angles		
MIOI	туре	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	GOL	В	3	-	5,5,5	0.28	0	5,5,5	0.36	0	
3	ACT	В	9	-	3,3,3	0.87	0	3,3,3	1.38	0	



N / - 1	Т	Clasica	Das	Link	В	ond leng	$_{ m gths}$	В	ond ang	gles
Mol	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1[A]	-	5,5,5	0.69	0	5,5,5	1.61	1 (20%)
3	ACT	A	11	-	3,3,3	0.74	0	3,3,3	1.39	0
2	GOL	В	2	-	5,5,5	0.38	0	5,5,5	0.23	0
3	ACT	A	13	-	3,3,3	0.75	0	3,3,3	1.23	0
2	GOL	A	5	-	5,5,5	0.46	0	5,5,5	0.27	0
3	ACT	A	8	-	3,3,3	0.77	0	3,3,3	1.29	0
3	ACT	В	10	-	3,3,3	0.67	0	3,3,3	1.33	0
2	GOL	A	1[B]	-	5,5,5	0.69	0	5,5,5	1.49	1 (20%)
2	GOL	A	4	-	5,5,5	0.50	0	5,5,5	0.32	0
3	ACT	В	7	-	3,3,3	0.79	0	3,3,3	1.45	0
3	ACT	В	12	-	3,3,3	0.73	0	3,3,3	1.43	0
2	GOL	A	6	-	5,5,5	0.33	0	5,5,5	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	В	3	-	-	1/4/4/4	-
2	GOL	A	1[A]	-	-	4/4/4/4	-
2	GOL	В	2	-	-	4/4/4/4	-
2	GOL	A	5	-	-	2/4/4/4	-
2	GOL	A	1[B]	-	-	3/4/4/4	-
2	GOL	A	4	-	-	2/4/4/4	-
2	GOL	A	6	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	A	1[A]	GOL	O1-C1-C2	-3.52	93.33	110.20
2	A	1[B]	GOL	O1-C1-C2	-3.24	94.68	110.20

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1[A]	GOL	O1-C1-C2-C3

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1[A]	GOL	C1-C2-C3-O3
2	A	1[A]	GOL	O2-C2-C3-O3
2	A	1[B]	GOL	C1-C2-C3-O3
2	A	1[B]	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	9	ACT	2	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q<0.9	
1	A	481/515~(93%)	0.84	72 (14%)	2	3	43, 50, 61, 86	0
1	В	$481/515 \ (93\%)$	0.74	57 (11%)	4	5	43, 50, 62, 88	0
All	All	962/1030 (93%)	0.79	129 (13%)	3	4	43, 50, 62, 88	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	VAL	10.1
1	В	178	GLY	10.1
1	A	48	GLY	9.2
1	В	179	SER	7.2
1	В	142	GLY	5.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	OCS	A	364	9/10	0.94	0.12	51,52,60,61	0
1	OCS	В	364	9/10	0.95	0.11	50,51,60,64	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GOL	A	1[A]	6/6	0.61	0.34	53,71,77,79	1
2	GOL	A	1[B]	6/6	0.61	0.34	59,71,77,79	1
3	ACT	A	11	4/4	0.62	0.24	82,83,84,84	0
2	GOL	A	5	6/6	0.74	0.37	73,76,79,81	0
2	GOL	A	6	6/6	0.84	0.30	57,70,72,73	0
3	ACT	В	9	4/4	0.84	0.20	66,66,67,68	0
3	ACT	В	12	4/4	0.86	0.15	68,73,74,75	0
2	GOL	В	2	6/6	0.90	0.33	45,55,64,68	0
2	GOL	В	3	6/6	0.91	0.25	46,61,70,70	0
3	ACT	В	10	4/4	0.94	0.15	44,52,52,52	0
2	GOL	A	4	6/6	0.94	0.15	49,55,68,74	0
3	ACT	A	8	4/4	0.95	0.23	49,51,54,56	0
3	ACT	В	7	4/4	0.98	0.10	36,36,38,40	0
3	ACT	A	13	4/4	0.98	0.10	43,43,45,46	0

6.5 Other polymers (i)

There are no such residues in this entry.

