

Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2024 – 09:19 pm GMT

PDB ID : 5JT1

Title: The 3D structure of Ni-reconstituted U489C variant of [NiFeSe] hydroge-

nase from Desulfovibrio vulgaris Hildenborough in the oxidized state at 1.35

Angstrom resolution

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Deposited on : 2016-05-09

Resolution : 1.35 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 (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 : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

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)

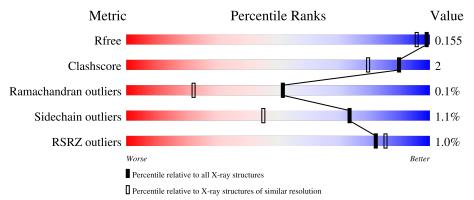
Validation Pipeline (wwPDB-VP) : 2.36

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 1.35 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ range(\AA)}) \end{array}$
R_{free}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	317	86%	11'	%	
2	В	509	91%	•	5%	



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13001 atoms, of which 6094 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 Periplasmic [NiFeSe] hydrogenase, small subunit.

Mol	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace
1	A	283	Total 4394	C 1419	H 2179	N 366	O 409	S 21	0	20	0

• Molecule 2 is a protein called Periplasmic [NiFeSe] hydrogenase, large subunit, selenocystei ne-containing.

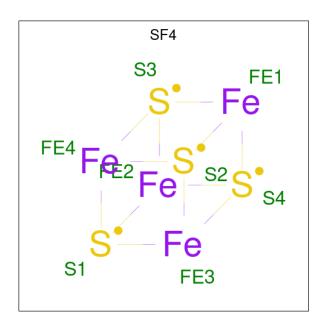
N	/Iol	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace
	2	В	483	Total 7792	C 2481	H 3913	N 671	O 701	S 26	0	23	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	4	TRP	-	expression tag	UNP Q72AS3
В	5	SER	-	expression tag	UNP Q72AS3
В	6	HIS	-	expression tag	UNP Q72AS3
В	7	PRO	-	expression tag	UNP Q72AS3
В	8	GLN	-	expression tag	UNP Q72AS3
В	9	PHE	-	expression tag	UNP Q72AS3
В	10	GLU	-	expression tag	UNP Q72AS3
В	11	LYS	-	expression tag	UNP Q72AS3
В	489	CYS	SEC	engineered mutation	UNP Q72AS3

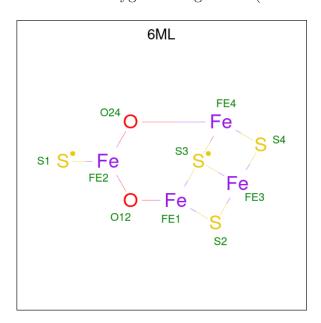
• Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	1

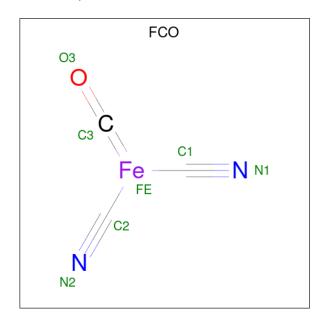
 \bullet Molecule 4 is oxygen-damaged SF4 (three-letter code: 6ML) (formula: Fe $_4{\rm O}_2{\rm S}_4).$



Mol	Chain	Residues	A	tom	ıs		ZeroOcc	AltConf
4	A	1	Total	Fe	0	S	0	1



 \bullet Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: $C_3FeN_2O).$



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
5	В	1	Total 7	C 3	Fe 1	N 2	O 1	0	0

• Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

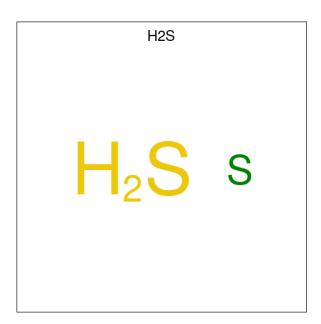
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Ni 1 1	0	1

• Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

I	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	7	В	1	Total Fe 1 1	0	0

• Molecule 8 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S).





Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
8	В	1	Total 3	H 2	S 1	0	0

• Molecule 9 is water.

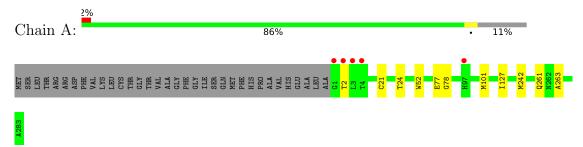
\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	286	Total O 290 290	0	4
9	В	472	Total O 479 479	0	8



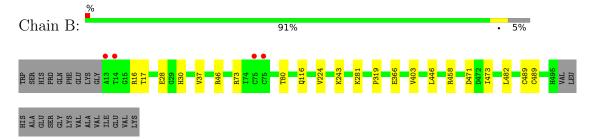
3 Residue-property plots (i)

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: Periplasmic [NiFeSe] hydrogenase, small subunit



• Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	106.78Å 63.18Å 110.66Å	Donositon
a, b, c, α , β , γ	90.00° 105.27° 90.00°	Depositor
Resolution (Å)	45.63 - 1.35	Depositor
Resolution (A)	45.63 - 1.35	EDS
% Data completeness	97.5 (45.63-1.35)	Depositor
(in resolution range)	97.5 (45.63-1.35)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.52 (at 1.35Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
D D.	0.116 , 0.145	Depositor
R, R_{free}	0.129 , 0.155	DCC
R_{free} test set	7575 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41, 50.8	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13001	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.

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: CSX, SF4, 6ML, FE2, NI, CSD, FCO, H2S

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).

ſ	Mol	Chain	Bond lengths		Bond angles	
	IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
	1	A	0.45	0/2329	0.63	0/3167
	2	В	0.46	0/4007	0.67	$2/5412 \ (0.0\%)$
	All	All	0.46	0/6336	0.65	2/8579 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	458	ARG	NE-CZ-NH1	6.23	123.41	120.30
2	В	458	ARG	NE-CZ-NH2	-5.17	117.72	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	2215	2179	2160	5	0
2	В	3879	3913	3913	16	0
3	A	24	0	0	0	0
4	A	10	0	0	0	0
5	В	7	0	0	0	0
6	В	1	0	0	0	0
7	В	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	В	1	2	0	0	0
9	A	290	0	0	4	2
9	В	479	0	0	7	1
All	All	6907	6094	6073	20	2

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.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:A:2:THR:OG1	9:A:401:HOH:O	2.10	0.69
2:B:281:LYS:NZ	9:B:703:HOH:O	2.29	0.63
9:A:639[A]:HOH:O	2:B:30[A]:HIS:HD2	1.92	0.52
2:B:46[A]:ARG:NH2	9:B:707:HOH:O	2.43	0.50
2:B:243:LYS:HE3	9:B:1005:HOH:O	2.13	0.49
2:B:30[B]:HIS:CE1	9:B:1052:HOH:O	2.68	0.47
1:A:21[B]:CYS:O	1:A:24:THR:HG22	2.15	0.47
2:B:471:ASP:OD1	9:B:701:HOH:O	2.21	0.44
1:A:77[B]:GLU:HG2	1:A:78[B]:GLY:N	2.32	0.44
9:A:639[A]:HOH:O	2:B:30[A]:HIS:CD2	2.70	0.44
1:A:127:ILE:HD12	2:B:73:ARG:HG2	2.00	0.43
2:B:28:GLU:OE1	2:B:489[A]:CYS:SG	2.77	0.43
2:B:489[A]:CYS:CB	9:B:1056[A]:HOH:O	2.66	0.43
1:A:242:MET:HG2	9:A:628:HOH:O	2.19	0.42
2:B:17:THR:HG21	2:B:473[B]:ILE:HG21	2.01	0.42
2:B:319:PRO:HG3	2:B:446:LEU:HG	2.02	0.41
2:B:366:GLU:HG2	9:B:1063:HOH:O	2.21	0.40
2:B:482:LEU:HD13	2:B:482:LEU:C	2.41	0.40
2:B:16:ARG:HA	2:B:37:VAL:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:605:HOH:O	9:A:605:HOH:O[2_658]	1.50	0.70
9:A:401:HOH:O	9:B:1053:HOH:O[3_545]	2.08	0.12



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	Perce	ntiles
1	A	301/317~(95%)	293 (97%)	7 (2%)	1 (0%)	41	18
2	В	500/509~(98%)	492 (98%)	8 (2%)	0	100	100
All	All	801/826 (97%)	785 (98%)	15 (2%)	1 (0%)	51	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ALA

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	Percen	tiles
1	A	244/253 (96%)	240 (98%)	4 (2%)	62	30
2	В	414/413 (100%)	410 (99%)	4 (1%)	76	49
All	All	658/666 (99%)	650 (99%)	8 (1%)	73	42

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

Mol	Chain	Res	Type
1	A	52	TRP
1	A	101[A]	MET
1	A	101[B]	MET
1	A	261	GLN
2	В	80	THR

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Mol	Chain	Res	Type
2	В	116	GLN
2	В	224	VAL
2	В	403	VAL

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	Type	Chain	Res	Dag	Dec	Dec	Dag	Das	Dag	Dec	Pos	Dec	Dag	Dag Link		ond leng	$_{ m gths}$	Bond angles		
				Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2										
2	CSD	В	489[B]	2	3,7,8	1.02	0	1,8,10	0.91	0										
2	CSX	В	75[A]	2,6	3,6,7	0.98	0	1,6,8	0.26	0										
2	CSX	В	75[B]	2	3,6,7	1.06	0	1,6,8	0.42	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	В	489[B]	2	-	0/2/6/8	-
2	CSX	В	75[A]	2,6	-	0/1/5/7	-
2	CSX	В	75[B]	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.



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)

Of 8 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 5 for Mogul analysis.

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	Res	Dag	Das	Dag	Link	В	ond leng	gths	Bond angles		
MIOI				LIIIK	Counts	RMSZ	# Z > 2	Counts	$\mid \text{RMSZ} \mid \# Z > 2$				
4	6ML	A	304[B]	1	0,12,12	-	-	-					
3	SF4	A	303[A]	1	0,12,12	-	-	-					
3	SF4	A	302	1	0,12,12	-	-	-					
5	FCO	В	601	2,9	0,6,6	-	-	-					
3	SF4	A	301	1	0,12,12	-	-	-					

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
4	6ML	A	304[B]	1	=	-	0/2/3/3
3	SF4	A	303[A]	1	=	-	0/6/5/5
3	SF4	A	302	1	-	-	0/6/5/5
3	SF4	A	301	1	=	-	0/6/5/5

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	<RSRZ $>$	# RSRZ > 2		$OWAB(A^2)$	Q<0.9
1	A	283/317 (89%)	-0.32	5 (1%) 68	73	9, 14, 27, 69	1 (0%)
2	В	481/509 (94%)	-0.40	2 (0%) 92	93	9, 14, 24, 47	3 (0%)
All	All	764/826 (92%)	-0.37	7 (0%) 82	87	9, 14, 25, 69	4 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	13	ALA	6.8
1	A	3	LEU	6.1
1	A	2	THR	3.9
1	A	1	GLY	3.8
1	A	4	THR	3.1
1	A	97	HIS	2.2
2	В	14	THR	2.1

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
2	CSX	В	75[A]	7/8	0.97	0.15	11,13,17,17	11
2	CSX	В	75[B]	7/8	0.97	0.15	11,13,17,17	11
2	CSD	В	489[B]	8/9	0.98	0.10	10,13,18,19	11

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
6	NI	В	602[A]	1/1	0.99	0.14	16,16,16,16	1
3	SF4	A	302	8/8	1.00	0.07	9,10,10,10	0
3	SF4	A	303[A]	8/8	1.00	0.07	9,9,11,11	8
4	6ML	A	304[B]	10/10	1.00	0.08	9,11,12,12	10
5	FCO	В	601	7/7	1.00	0.08	11,12,14,16	0
3	SF4	A	301	8/8	1.00	0.06	11,11,12,12	0
7	FE2	В	603	1/1	1.00	0.05	11,11,11,11	0
8	H2S	В	604	1/1	1.00	0.07	11,11,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.

