wwPDB X-ray Structure Validation Summary Report (i)

Dec 20, 2023 – 01:21 pm GMT

PDB ID	:	8PP5
Title	:	Unitary crystal structure of positively supercharged ferritin variant Ftn(pos)-m1 (Mg Formate condition)
Authors	:	Lang, L.; Beck, T.
Deposited on	:	2023-07-06
Resolution	:	2.00 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:

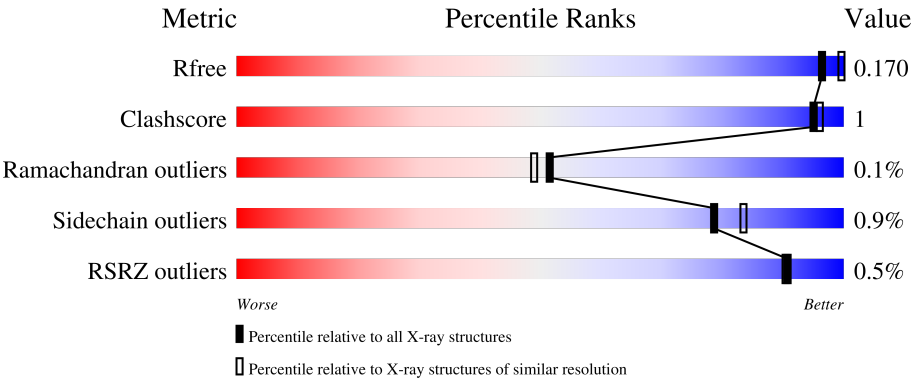
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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.



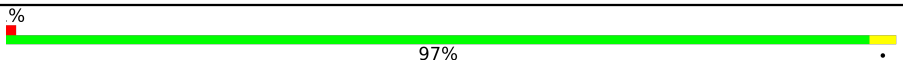
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	172	97%
1	B	172	98%
1	C	172	96%
1	D	172	95% 5%
1	E	172	95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	172	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18041 atoms, of which 8538 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 Ferritin heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	172	Total	C	H	N	O	S	42	1	0
			2865	905	1428	258	269	5			
1	B	172	Total	C	H	N	O	S	42	0	0
			2850	900	1422	257	266	5			
1	C	172	Total	C	H	N	O	S	42	0	0
			2850	900	1422	257	266	5			
1	D	172	Total	C	H	N	O	S	42	0	0
			2850	900	1422	257	266	5			
1	E	172	Total	C	H	N	O	S	42	0	0
			2850	900	1422	257	266	5			
1	F	172	Total	C	H	N	O	S	42	0	0
			2850	900	1422	257	266	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	ASN	engineered mutation	UNP P02794
A	86	GLN	LYS	engineered mutation	UNP P02794
A	90	LYS	CYS	engineered mutation	UNP P02794
A	98	ARG	ASN	engineered mutation	UNP P02794
A	102	LYS	CYS	engineered mutation	UNP P02794
A	105	LYS	HIS	engineered mutation	UNP P02794
A	109	LYS	ASN	engineered mutation	UNP P02794
A	123	LYS	ASP	engineered mutation	UNP P02794
A	162	ARG	GLU	engineered mutation	UNP P02794
B	25	ARG	ASN	engineered mutation	UNP P02794
B	86	GLN	LYS	engineered mutation	UNP P02794
B	90	LYS	CYS	engineered mutation	UNP P02794
B	98	ARG	ASN	engineered mutation	UNP P02794
B	102	LYS	CYS	engineered mutation	UNP P02794
B	105	LYS	HIS	engineered mutation	UNP P02794
B	109	LYS	ASN	engineered mutation	UNP P02794
B	123	LYS	ASP	engineered mutation	UNP P02794

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	162	ARG	GLU	engineered mutation	UNP P02794
C	25	ARG	ASN	engineered mutation	UNP P02794
C	86	GLN	LYS	engineered mutation	UNP P02794
C	90	LYS	CYS	engineered mutation	UNP P02794
C	98	ARG	ASN	engineered mutation	UNP P02794
C	102	LYS	CYS	engineered mutation	UNP P02794
C	105	LYS	HIS	engineered mutation	UNP P02794
C	109	LYS	ASN	engineered mutation	UNP P02794
C	123	LYS	ASP	engineered mutation	UNP P02794
C	162	ARG	GLU	engineered mutation	UNP P02794
D	25	ARG	ASN	engineered mutation	UNP P02794
D	86	GLN	LYS	engineered mutation	UNP P02794
D	90	LYS	CYS	engineered mutation	UNP P02794
D	98	ARG	ASN	engineered mutation	UNP P02794
D	102	LYS	CYS	engineered mutation	UNP P02794
D	105	LYS	HIS	engineered mutation	UNP P02794
D	109	LYS	ASN	engineered mutation	UNP P02794
D	123	LYS	ASP	engineered mutation	UNP P02794
D	162	ARG	GLU	engineered mutation	UNP P02794
E	25	ARG	ASN	engineered mutation	UNP P02794
E	86	GLN	LYS	engineered mutation	UNP P02794
E	90	LYS	CYS	engineered mutation	UNP P02794
E	98	ARG	ASN	engineered mutation	UNP P02794
E	102	LYS	CYS	engineered mutation	UNP P02794
E	105	LYS	HIS	engineered mutation	UNP P02794
E	109	LYS	ASN	engineered mutation	UNP P02794
E	123	LYS	ASP	engineered mutation	UNP P02794
E	162	ARG	GLU	engineered mutation	UNP P02794
F	25	ARG	ASN	engineered mutation	UNP P02794
F	86	GLN	LYS	engineered mutation	UNP P02794
F	90	LYS	CYS	engineered mutation	UNP P02794
F	98	ARG	ASN	engineered mutation	UNP P02794
F	102	LYS	CYS	engineered mutation	UNP P02794
F	105	LYS	HIS	engineered mutation	UNP P02794
F	109	LYS	ASN	engineered mutation	UNP P02794
F	123	LYS	ASP	engineered mutation	UNP P02794
F	162	ARG	GLU	engineered mutation	UNP P02794

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is water.

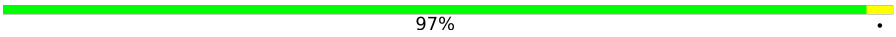
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	151	Total O 151 151	0	0
4	B	154	Total O 154 154	0	0
4	C	154	Total O 154 154	0	0
4	D	154	Total O 154 154	0	0
4	E	156	Total O 156 156	0	0
4	F	147	Total O 147 147	0	0

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.

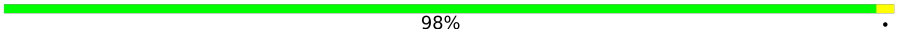
• Molecule 1: Ferritin heavy chain, N-terminally processed

Chain A:



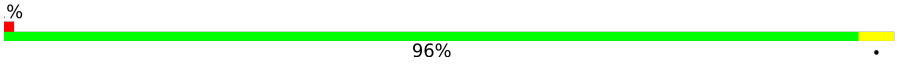
• Molecule 1: Ferritin heavy chain, N-terminally processed

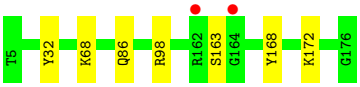
Chain B:



• Molecule 1: Ferritin heavy chain, N-terminally processed

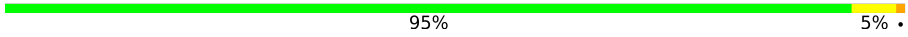
Chain C:





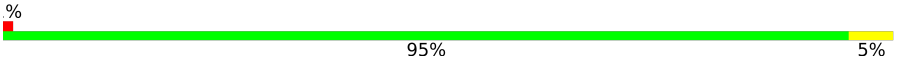
• Molecule 1: Ferritin heavy chain, N-terminally processed

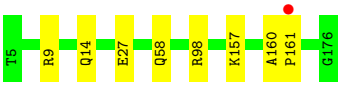
Chain D:



• Molecule 1: Ferritin heavy chain, N-terminally processed

Chain E:





• Molecule 1: Ferritin heavy chain, N-terminally processed

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	126.90Å 126.90Å 187.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.09 – 2.00 105.09 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (105.09-2.00) 98.7 (105.09-1.75)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.160 , 0.193 0.171 , 0.170	Depositor DCC
R_{free} test set	6971 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.000 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.000 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.000 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.008 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18041	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

Bond lengths and bond angles in the following residue types are not validated in this section: FE, MG

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	0.46	0/1465	0.77	2/1965 (0.1%)
1	B	0.51	0/1456	0.73	0/1953
1	C	0.47	0/1456	0.76	0/1953
1	D	0.49	0/1456	0.77	0/1953
1	E	0.48	1/1456 (0.1%)	0.72	0/1953
1	F	0.48	0/1456	0.71	0/1953
All	All	0.48	1/8745 (0.0%)	0.74	2/11730 (0.0%)

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	27	GLU	CD-OE1	-5.60	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	ARG	NE-CZ-NH2	-5.34	117.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	98	ARG	Sidechain
1	C	98	ARG	Sidechain
1	D	162	ARG	Sidechain
1	E	98	ARG	Sidechain
1	F	98	ARG	Sidechain

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	1437	1428	1416	4	0
1	B	1428	1422	1411	2	0
1	C	1428	1422	1411	2	0
1	D	1428	1422	1411	7	0
1	E	1428	1422	1411	6	0
1	F	1428	1422	1411	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
4	A	151	0	0	2	0
4	B	154	0	0	0	0
4	C	154	0	0	1	0
4	D	154	0	0	4	0
4	E	156	0	0	3	0
4	F	147	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9503	8538	8471	21	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 1.

The worst 5 of 21 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:D:162:ARG:HG3	1:D:162:ARG:HH11	1.50	0.76
1:E:58:GLN:NE2	4:E:301:HOH:O	2.22	0.72
1:A:164:GLY:N	4:A:301:HOH:O	2.29	0.65
4:D:323:HOH:O	1:E:157:LYS:HE3	1.95	0.65
1:D:63:ARG:HG2	1:F:63:ARG:NH1	2.18	0.58

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	171/172 (99%)	168 (98%)	2 (1%)	1 (1%)	25 19
1	B	170/172 (99%)	168 (99%)	2 (1%)	0	100 100
1	C	170/172 (99%)	168 (99%)	2 (1%)	0	100 100
1	D	170/172 (99%)	168 (99%)	2 (1%)	0	100 100
1	E	170/172 (99%)	168 (99%)	2 (1%)	0	100 100
1	F	170/172 (99%)	167 (98%)	3 (2%)	0	100 100
All	All	1021/1032 (99%)	1007 (99%)	13 (1%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU

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	154/153 (101%)	154 (100%)	0	100 100
1	B	153/153 (100%)	152 (99%)	1 (1%)	84 88
1	C	153/153 (100%)	150 (98%)	3 (2%)	55 58
1	D	153/153 (100%)	150 (98%)	3 (2%)	55 58
1	E	153/153 (100%)	153 (100%)	0	100 100
1	F	153/153 (100%)	152 (99%)	1 (1%)	84 88
All	All	919/918 (100%)	911 (99%)	8 (1%)	78 83

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	32	TYR
1	D	119	LYS
1	D	32	TYR
1	C	163	SER
1	D	49	LYS

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

Mol	Chain	Res	Type
1	C	86	GLN
1	E	60	HIS
1	F	14	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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

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	172/172 (100%)	-0.62	0 100 100	21, 25, 42, 91	0
1	B	172/172 (100%)	-0.64	0 100 100	20, 25, 42, 88	0
1	C	172/172 (100%)	-0.60	2 (1%) 79 78	21, 26, 44, 97	0
1	D	172/172 (100%)	-0.63	0 100 100	20, 25, 43, 75	0
1	E	172/172 (100%)	-0.62	1 (0%) 89 88	21, 26, 44, 89	0
1	F	172/172 (100%)	-0.60	2 (1%) 79 78	21, 26, 44, 89	0
All	All	1032/1032 (100%)	-0.62	5 (0%) 91 90	20, 25, 44, 97	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	GLY	3.2
1	C	162	ARG	2.8
1	F	161	PRO	2.8
1	F	164	GLY	2.1
1	E	161	PRO	2.0

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 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	B-factors(Å^2)	Q<0.9
3	MG	B	202	1/1	0.89	0.38	63,63,63,63	0
3	MG	A	202	1/1	0.97	0.08	32,32,32,32	0
3	MG	C	202	1/1	0.98	0.04	52,52,52,52	0
3	MG	C	203	1/1	0.98	0.08	28,28,28,28	0
2	FE	F	201	1/1	0.99	0.05	47,47,47,47	0
2	FE	A	201	1/1	0.99	0.05	41,41,41,41	0
2	FE	C	201	1/1	0.99	0.06	43,43,43,43	0
2	FE	D	201	1/1	0.99	0.07	47,47,47,47	0
2	FE	E	201	1/1	0.99	0.04	44,44,44,44	0
2	FE	B	201	1/1	1.00	0.05	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.