

wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 07:25 PM EDT

PDB ID : 3H02

Title: 2.15 Angstrom Resolution Crystal Structure of Naphthoate Synthase from

Salmonella typhimurium.

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GID)

Deposited on : 2009-04-08

Resolution : 2.15 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 2022.3.0, CSD as543be (2022)

Xtriage (Phenix) : 1.20.1

EDS : 2.37.1

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

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

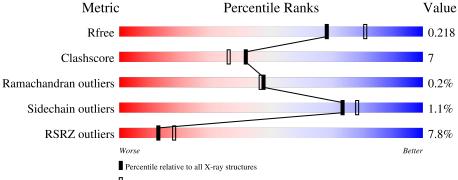
Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

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 2.15 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.



Percentile relative to X-ray structures of similar resolution

Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	288	80%	12%	8%
1	В	288	79%	12%	9%
1	С	288	12% 78%	12%	9%
1	D	288	7% 79%	12%	8%



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Mol	Chain	Length	Quality of chain		
1	Е	288	7%		10% • 8%
1	F	288	70%	12%	17%

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
2	SO4	A	286	-	-	X	-
2	SO4	F	286	-	-	X	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13009 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 Naphthoate synthase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	A	266	Total	С	Ν	О	S	Se	0	5	0
1	Λ	200	2111	1318	378	396	8	11		9	
1	В	262	Total	С	N	О	S	Se	0	4	0
1	Ъ	202	2071	1294	372	386	8	11	0	4	U
1	C	262	Total	С	N	Ο	S	Se	0	5	0
1		202	2075	1297	369	390	8	11	0		
1	D	264	Total	С	N	O	S	Se	0	4	0
1	D	204	2081	1302	367	393	8	11	0	4	
1	Е	264	Total	С	N	Ο	S	Se	0	4	0
1	ш	204	2088	1306	368	395	8	11	0	4	
1	F	239	Total	С	N	О	S	Se	0	6	0
1	I.	239	1893	1186	332	356	8	11		6	U

There are 18 discrepancies between the modelled and reference sequences:

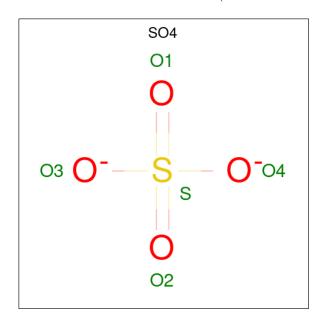
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
A	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
A	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
В	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
В	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
В	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
С	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
С	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
С	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
D	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
D	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
D	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
Е	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
Е	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
Е	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
F	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
F	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56



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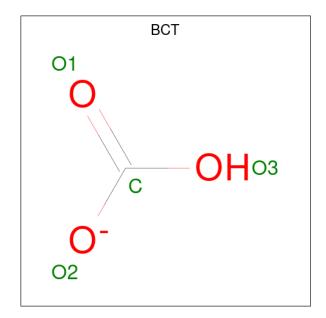
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56

 \bullet Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

 \bullet Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 1 3	0	0
3	В	1	Total C O 4 1 3	0	0
3	С	1	Total C O 4 1 3	0	0
3	D	1	Total C O 4 1 3	0	0
3	Е	1	Total C O 4 1 3	0	0
3	F	1	Total C O 4 1 3	0	0
3	F	1	Total C O 4 1 3	0	0

• Molecule 4 is water.

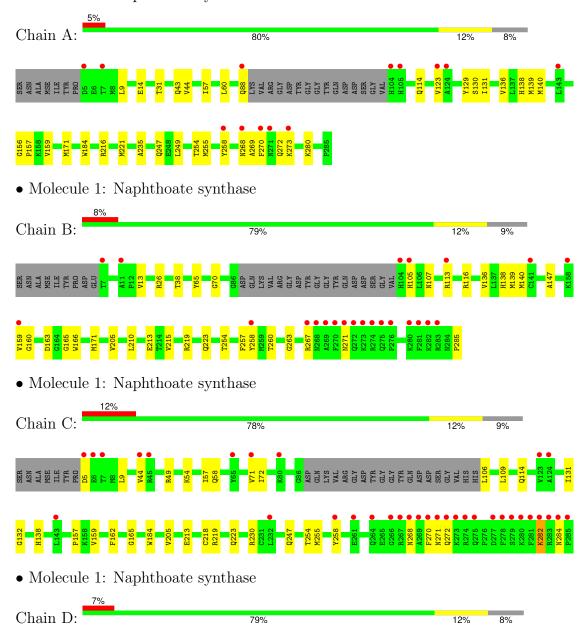
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 117 117	0	2
4	В	109	Total O 115 115	0	9
4	С	93	Total O 97 97	0	5
4	D	94	Total O 97 97	0	4
4	E	101	Total O 108 108	0	9
4	F	114	Total O 118 118	0	9



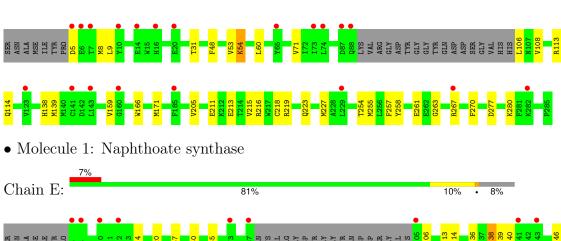
3 Residue-property plots (i)

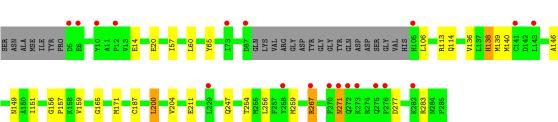
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Naphthoate synthase

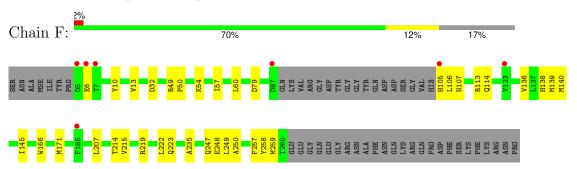








• Molecule 1: Naphthoate synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	75.90Å 132.82Å 151.79Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 - 2.15	Depositor
Resolution (A)	29.60 - 2.15	EDS
% Data completeness	98.6 (29.83-2.15)	Depositor
(in resolution range)	98.6 (29.60-2.15)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	6.61 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0051	Depositor
D D.	0.169 , 0.215	Depositor
R, R_{free}	0.176 , 0.218	DCC
R_{free} test set	4153 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 58.4	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	0.95	EDS
Total number of atoms	13009	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.29% 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: BCT, SO4

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.51	0/2139	0.66	0/2867	
1	В	0.54	0/2099	0.70	0/2812	
1	С	0.48	0/2101	0.65	0/2815	
1	D	0.49	0/2107	0.67	0/2825	
1	Е	0.51	0/2115	0.66	0/2833	
1	F	0.54	0/1915	0.68	0/2569	
All	All	0.51	0/12476	0.67	0/16721	

There are no bond length outliers.

There are no bond angle outliers.

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	2111	0	2062	26	0
1	В	2071	0	2027	35	0
1	С	2075	0	2034	30	0
1	D	2081	0	2038	30	0
1	Е	2088	0	2032	35	0
1	F	1893	0	1858	30	0
2	A	5	0	0	2	0



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	5	0	0	2	0
3	A	4	0	0	0	0
3	В	4	0	0	0	0
3	С	4	0	0	0	0
3	D	4	0	0	0	0
3	Ε	4	0	0	0	0
3	F	8	0	0	1	0
4	A	117	0	0	4	0
4	В	115	0	0	4	0
4	С	97	0	0	2	0
4	D	97	0	0	2	0
4	Ε	108	0	0	1	0
4	F	118	0	0	5	0
All	All	13009	0	12051	172	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 7.

The worst 5 of 172 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:C:44:VAL:HG12	1:C:44:VAL:O	1.65	0.96
1:C:268:ASN:O	1:C:272:GLN:HG3	1.69	0.92
1:C:5:ASP:O	1:C:9:LEU:HD13	1.71	0.89
1:F:13:VAL:HG23	4:F:407:HOH:O	1.72	0.89
1:D:205:VAL:HG11	1:D:213:GLU:HG2	1.55	0.88

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	Perce	ntiles
1	A	$267/288 \; (93\%)$	258 (97%)	8 (3%)	1 (0%)	34	29
1	В	262/288 (91%)	255 (97%)	7 (3%)	0	100	100
1	С	263/288 (91%)	254 (97%)	9 (3%)	0	100	100
1	D	264/288 (92%)	258 (98%)	6 (2%)	0	100	100
1	E	264/288 (92%)	252 (96%)	11 (4%)	1 (0%)	34	29
1	F	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	34	29
All	All	1561/1728 (90%)	1509 (97%)	49 (3%)	3 (0%)	47	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	GLY
1	F	258	TYR
1	Е	156	GLY

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	$220/220\ (100\%)$	218 (99%)	2 (1%)	78 83
1	В	$215/220\ (98\%)$	214 (100%)	1 (0%)	88 92
1	С	216/220 (98%)	213 (99%)	3 (1%)	67 72
1	D	217/220 (99%)	215 (99%)	2 (1%)	78 83
1	E	217/220 (99%)	213 (98%)	4 (2%)	59 63
1	F	197/220 (90%)	194 (98%)	3 (2%)	65 69
All	All	$1282/1320\ (97\%)$	1267 (99%)	15 (1%)	73 76

5 of 15 residues with a non-rotameric sidechain are listed below:

\mathbf{Mol}	Chain	Res	Type
1	D	138	HIS
1	F	54[B]	LYS



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Mol	Chain	Res	Type
1	Е	138	HIS
1	F	138	HIS
1	Е	271	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	С	284	ASN
1	Ε	271	ASN
1	F	193	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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 R		Dag	Link	В	Bond lengths			Bond angles		
MIOI	туре	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	286	-	4,4,4	0.32	0	6,6,6	0.08	0
3	BCT	F	287	-	3,3,3	0.73	0	2,3,3	0.29	0



Mol Type		Chain	Dog	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	BCT	D	286	-	3,3,3	0.70	0	2,3,3	0.22	0
3	BCT	F	288	-	3,3,3	0.52	0	2,3,3	0.25	0
3	BCT	Е	286	-	3,3,3	0.56	0	2,3,3	0.89	0
3	BCT	A	287	-	3,3,3	0.67	0	2,3,3	0.42	0
3	BCT	С	286	-	3,3,3	0.81	0	2,3,3	0.94	0
3	BCT	В	286	-	3,3,3	0.48	0	2,3,3	0.16	0
2	SO4	F	286	-	4,4,4	0.30	0	6,6,6	0.19	0

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	286	SO4	2	0
3	F	287	BCT	1	0
2	F	286	SO4	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	<rsrz></rsrz>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	255/288~(88%)	0.15	13 (5%) 28 36	15, 22, 36, 65	0
1	В	251/288 (87%)	0.31	23 (9%) 9 13	12, 20, 33, 53	0
1	С	251/288 (87%)	0.53	34 (13%) 3 3	15, 21, 41, 65	0
1	D	253/288 (87%)	0.35	20 (7%) 12 17	14, 22, 32, 51	0
1	E	253/288 (87%)	0.22	19 (7%) 14 19	10, 21, 34, 59	0
1	F	228/288 (79%)	0.01	7 (3%) 49 58	6, 17, 29, 44	0
All	All	1491/1728 (86%)	0.27	116 (7%) 13 18	6, 21, 35, 65	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	271	ASN	11.9
1	В	104	HIS	9.1
1	С	270	PHE	8.2
1	A	104	HIS	7.2
1	С	269	ALA	6.8

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 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
2	SO4	A	286	5/5	0.90	0.20	37,39,45,53	5
3	BCT	F	288	4/4	0.90	0.22	54,54,55,58	0
3	BCT	A	287	4/4	0.91	0.16	27,30,33,37	0
2	SO4	F	286	5/5	0.91	0.23	42,42,44,54	5
3	BCT	С	286	4/4	0.94	0.15	28,33,36,38	0
3	BCT	В	286	4/4	0.94	0.13	26,35,38,40	0
3	BCT	D	286	4/4	0.95	0.14	23,29,33,35	0
3	BCT	F	287	4/4	0.96	0.12	18,27,32,36	0
3	BCT	Ε	286	4/4	0.97	0.10	22,30,34,36	0

6.5 Other polymers (i)

There are no such residues in this entry.

