



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:37 PM EDT

PDB ID : 3RQN
Title : Structure of the neuronal nitric oxide synthase heme domain in complex with 6-((((3*R*,4*R*)-4-(2-(((S*)-1-(3-fluorophenyl)propan-2-yl)amino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : unknown
Resolution : 1.95 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

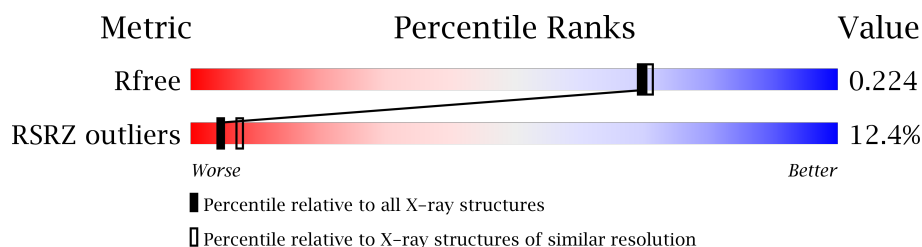
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	100719	2004 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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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
5	ACT	A	860	-	-	-	X
5	ACT	B	860	-	-	-	X

2 Entry composition [i](#)

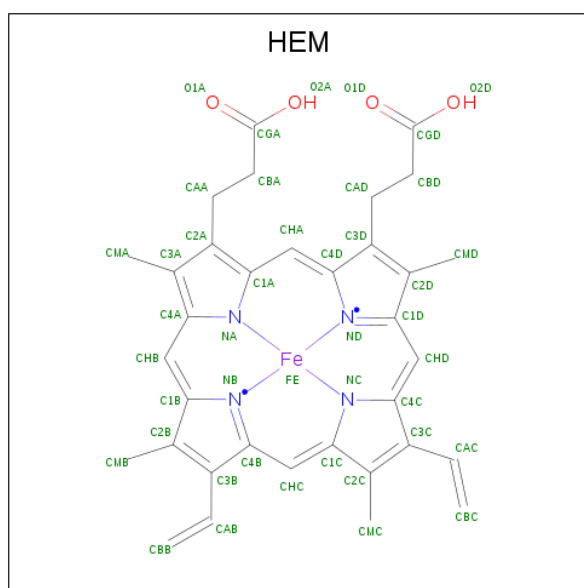
There are 7 unique types of molecules in this entry. The entry contains 7277 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	3	0
			3343	2140	571	610	22			
1	B	411	Total	C	N	O	S	0	2	0
			3354	2146	574	612	22			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



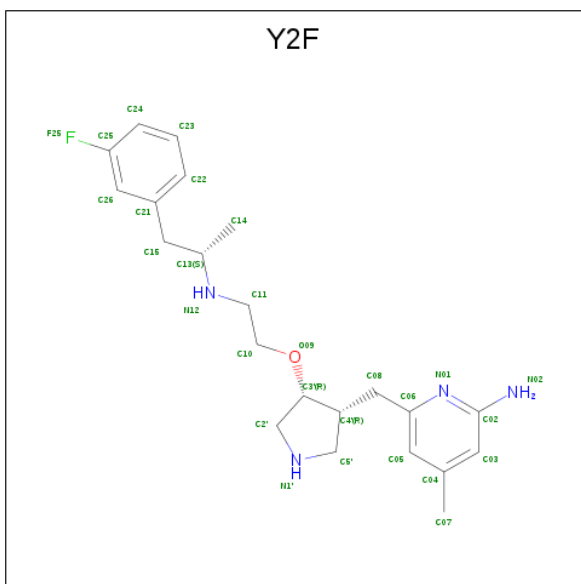
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-{{[(3R,4R)-4-(2-{{[(2S)-1-(3-fluorophenyl)propan-2-yl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: Y2F) (formula: C₂₂H₃₁FN₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			28	22	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			28	22	1	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	169	Total	O	0	0
			169	169		
7	B	226	Total	O	0	0
			226	226		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.94Å 110.63Å 164.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 1.95 38.49 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.26-1.95) 99.9 (38.49-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.209 0.193 , 0.224	Depositor DCC
R_{free} test set	3465 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7277	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	750	1	28,50,50	2.20	8 (28%)	17,82,82	2.19	4 (23%)
3	H4B	A	760	-	14,18,18	1.01	2 (14%)	12,26,26	2.46	5 (41%)
4	Y2F	A	800	-	27,30,30	0.89	1 (3%)	34,40,40	1.97	7 (20%)
5	ACT	A	860	-	1,3,3	1.62	0	0,3,3	0.00	-
2	HEM	B	750	1	28,50,50	2.23	10 (35%)	17,82,82	2.11	4 (23%)
3	H4B	B	760	-	14,18,18	1.09	1 (7%)	12,26,26	2.37	5 (41%)
4	Y2F	B	800	-	27,30,30	0.66	0	34,40,40	1.96	7 (20%)
5	ACT	B	860	-	1,3,3	1.55	0	0,3,3	0.00	-

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	HEM	A	750	1	-	0/6/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	Y2F	A	800	-	-	0/15/25/25	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/6/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	Y2F	B	800	-	-	0/15/25/25	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-4.86	1.33	1.40
2	A	750	HEM	C3B-C2B	-4.71	1.34	1.40
2	B	750	HEM	C3C-C2C	-4.41	1.34	1.40
2	A	750	HEM	C3C-C2C	-3.98	1.35	1.40
4	A	800	Y2F	C13-N12	-2.69	1.44	1.48
2	A	750	HEM	C4D-ND	2.08	1.39	1.36
2	B	750	HEM	CAA-C2A	2.12	1.55	1.52
2	B	750	HEM	C4A-NA	2.12	1.40	1.36
2	B	750	HEM	C4D-ND	2.22	1.39	1.36
3	A	760	H4B	C2-N2	2.22	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	760	H4B	C4-N3	2.24	1.37	1.33
2	B	750	HEM	CAD-C3D	2.30	1.56	1.52
3	A	760	H4B	C4-N3	2.31	1.37	1.33
2	A	750	HEM	CMA-C3A	2.32	1.56	1.51
2	A	750	HEM	C1C-NC	2.50	1.39	1.36
2	B	750	HEM	C1C-NC	2.86	1.40	1.36
2	A	750	HEM	C3B-CAB	3.07	1.54	1.47
2	B	750	HEM	C3B-CAB	3.08	1.54	1.47
2	B	750	HEM	C3C-CAC	3.58	1.54	1.47
2	A	750	HEM	C3C-CAC	3.70	1.55	1.47
2	B	750	HEM	C3D-C2D	4.38	1.50	1.37
2	A	750	HEM	C3D-C2D	5.05	1.52	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CBA-CAA-C2A	-5.74	101.51	112.48
2	A	750	HEM	CBD-CAD-C3D	-5.67	101.65	112.47
2	A	750	HEM	CBA-CAA-C2A	-4.71	103.49	112.48
2	B	750	HEM	CBD-CAD-C3D	-4.21	104.44	112.47
3	A	760	H4B	N3-C2-N1	-3.77	119.33	125.45
4	B	800	Y2F	C05-C06-N01	-3.00	119.65	122.91
3	B	760	H4B	N3-C2-N1	-2.82	120.88	125.45
4	A	800	Y2F	C05-C06-N01	-2.74	119.94	122.91
2	A	750	HEM	C1D-C2D-C3D	-2.60	105.19	107.00
2	B	750	HEM	C1D-C2D-C3D	-2.39	105.34	107.00
3	B	760	H4B	C6-C7-N8	-2.29	107.38	111.01
4	A	800	Y2F	C15-C21-C26	-2.08	116.64	120.43
4	A	800	Y2F	C04-C05-C06	-2.03	118.98	120.26
3	A	760	H4B	C4A-N5-C6	-2.00	115.71	121.16
3	B	760	H4B	C2-N1-C8A	2.19	119.43	114.51
2	B	750	HEM	C4C-C3C-C2C	2.20	108.44	106.90
2	A	750	HEM	C4C-C3C-C2C	2.31	108.51	106.90
4	B	800	Y2F	F25-C25-C24	2.33	122.61	118.53
4	B	800	Y2F	C21-C26-C25	2.50	120.89	118.84
4	A	800	Y2F	N02-C02-N01	2.68	121.16	116.64
4	B	800	Y2F	N02-C02-N01	2.78	121.32	116.64
4	B	800	Y2F	C2'-N1'-C5'	2.78	111.86	105.40
4	A	800	Y2F	C2'-N1'-C5'	3.12	112.66	105.40
3	A	760	H4B	C2-N1-C8A	3.25	121.84	114.51
3	B	760	H4B	C4-N3-C2	3.81	121.53	116.06
3	A	760	H4B	C4-N3-C2	3.92	121.70	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C4-C4A-C8A	3.97	118.15	114.56
4	B	800	Y2F	C11-N12-C13	4.86	121.40	114.08
3	B	760	H4B	C4-C4A-C8A	4.87	118.97	114.56
4	A	800	Y2F	C11-N12-C13	5.46	122.31	114.08
4	A	800	Y2F	C02-N01-C06	6.05	122.45	118.17
4	B	800	Y2F	C02-N01-C06	6.59	122.83	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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, 95th 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	409/422 (96%)	0.93	70 (17%) 2 2	22, 42, 75, 96	0
1	B	411/422 (97%)	0.45	32 (7%) 14 22	21, 34, 57, 69	0
All	All	820/844 (97%)	0.69	102 (12%) 4 7	21, 38, 68, 96	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.4
1	A	488	PRO	7.5
1	A	348	VAL	7.1
1	A	713	THR	5.8
1	B	348	VAL	5.6
1	A	355	PHE	5.4
1	A	715	VAL	5.2
1	A	716	TRP	5.0
1	A	300	PHE	4.8
1	A	352	ASP	4.6
1	A	507	GLN	4.5
1	A	350	THR	4.5
1	A	321	THR	4.5
1	A	351	LYS	4.4
1	A	486	LYS	4.2
1	B	619	ARG	4.2
1	B	350	THR	4.1
1	A	680	VAL	4.0
1	B	299	ARG	4.0
1	A	619	ARG	3.9
1	A	391	THR	3.8
1	A	506	ILE	3.8
1	A	678	TRP	3.7
1	A	567	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	469	LYS	3.6
1	B	620	LYS	3.6
1	A	299	ARG	3.5
1	A	491	SER	3.4
1	A	392	SER	3.4
1	A	386	LYS	3.4
1	A	390	SER	3.4
1	B	321	THR	3.4
1	A	677	VAL	3.4
1	A	389	GLU	3.3
1	A	388	ILE	3.3
1	A	593	ILE	3.2
1	B	389	GLU	3.2
1	A	490	GLY	3.2
1	B	691	PHE	3.2
1	A	514	ARG	3.1
1	B	667	ARG	3.0
1	A	714	HIS	3.0
1	A	592[A]	GLU	2.9
1	A	487	GLN	2.9
1	B	680	VAL	2.9
1	A	489	ASP	2.9
1	A	385	ASN	2.9
1	B	718	GLY	2.8
1	A	679	ILE	2.8
1	A	353	GLN	2.8
1	A	588	TYR	2.8
1	B	567	VAL	2.8
1	A	415	CYS	2.8
1	A	551	PHE	2.7
1	A	595	VAL	2.7
1	B	616	LEU	2.7
1	A	511	LYS	2.7
1	B	352	ASP	2.7
1	A	371	ARG	2.7
1	A	492	THR	2.6
1	B	677	VAL	2.6
1	A	503	GLU	2.6
1	A	480	ILE	2.5
1	A	309	ASP	2.5
1	B	615	ASP	2.5
1	A	584	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	2.5
1	B	591	THR	2.5
1	A	676	TRP	2.5
1	B	679	ILE	2.5
1	A	667	ARG	2.5
1	A	505	CYS	2.5
1	A	682	PRO	2.4
1	B	310	VAL	2.4
1	B	676	TRP	2.4
1	A	591	THR	2.4
1	A	479	LEU	2.4
1	A	512	ALA	2.3
1	B	678	TRP	2.3
1	B	593	ILE	2.3
1	A	356	PRO	2.3
1	B	309	ASP	2.3
1	A	712	ASN	2.3
1	A	681	PRO	2.2
1	B	715	VAL	2.2
1	A	686	SER	2.2
1	A	416	VAL	2.2
1	A	561	TRP	2.2
1	B	592[A]	GLU	2.2
1	B	416	VAL	2.2
1	B	322	LEU	2.2
1	A	349	ARG	2.2
1	A	645	LYS	2.1
1	B	682	PRO	2.1
1	B	355	PHE	2.1
1	A	594	GLY	2.1
1	B	617	ASP	2.1
1	A	467	ASP	2.1
1	A	508	GLN	2.1
1	B	550	LYS	2.0
1	A	685	GLY	2.0
1	A	330	ILE	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
5	ACT	A	860	4/4	0.96	0.26	7.65	51,52,53,54	0
5	ACT	B	860	4/4	0.94	0.15	2.80	40,43,43,43	0
3	H4B	B	760	17/17	0.97	0.18	0.58	22,24,29,29	0
4	Y2F	A	800	28/28	0.88	0.24	0.57	33,37,40,42	0
2	HEM	B	750	43/43	0.98	0.18	0.46	21,24,31,35	0
4	Y2F	B	800	28/28	0.92	0.20	0.44	29,35,38,40	0
3	H4B	A	760	17/17	0.97	0.18	0.34	23,27,30,31	0
2	HEM	A	750	43/43	0.97	0.21	0.34	22,26,33,34	0
6	ZN	A	900	1/1	0.99	0.08	-1.01	30,30,30,30	0

5.5 Other polymers [i](#)

There are no such residues in this entry.