WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 06:46 PM EDT

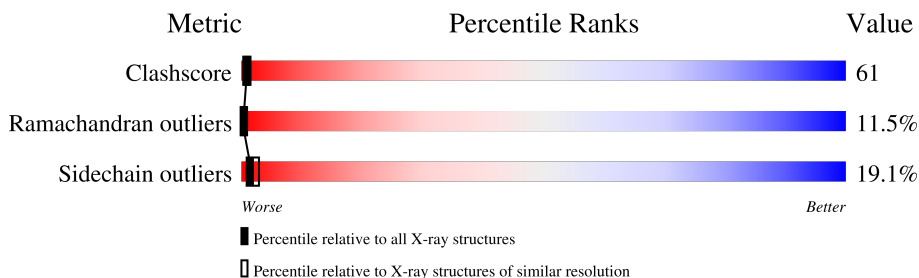|		
PDB ID	:	1MDA
Title	:	CRYSTAL STRUCTURE OF AN ELECTRON-TRANSFER COMPLEX BE-TWEEN METHYLAMINE DEHYDROGENASE AND AMICYANIN
Authors	:	Chen, L.; Durley, R.; Mathews, F.S.
Deposited on	:	1992-03-02
Resolution	:	2.50 Å(reported)

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 2.50 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	Percentile Ranks	Value
Clashscore		61
Ramachandran outliers		11.5%
Sidechain outliers		19.1%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	368	39% 42% 15% ·
1	J	368	41% 40% 15% ·
2	L	121	40% 43% 14% ·
2	M	121	31% 50% 14% 5%
3	A	103	9% 36% 38% 17%
3	B	103	16% 38% 33% 14%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRQ	M	57	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8567 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 METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	368	Total 2582	C 1585	N 451	O 532	S 14	0	0	0
1	J	368	Total 2583	C 1585	N 451	O 533	S 14	0	0	0

- Molecule 2 is a protein called METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	121	Total 910	C 558	N 155	O 184	S 13	0	0	0
2	M	121	Total 910	C 558	N 155	O 184	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	TRQ	TRP	conflict	UNP A44544
M	57	TRQ	TRP	conflict	UNP A44544

- Molecule 3 is a protein called AMICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	103	Total 790	C 506	N 130	O 148	S 6	0	0	0
3	B	103	Total 790	C 506	N 130	O 148	S 6	0	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cu 1	0	0

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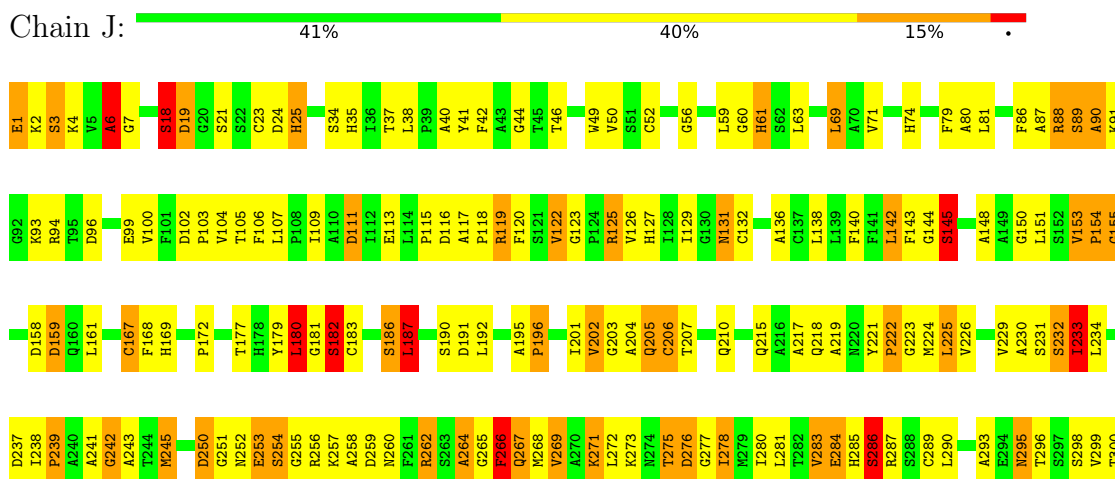| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cu	0	0
			1	1		

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS was not executed.

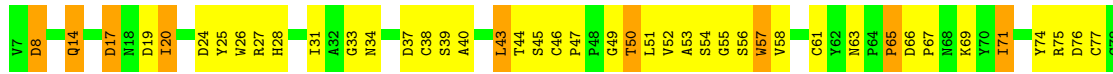• Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

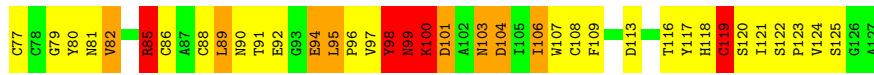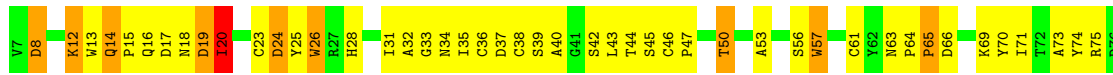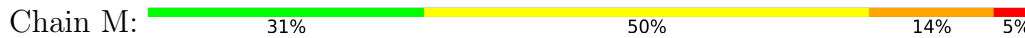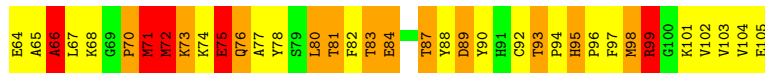• Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

A301 S302 V303 G304 Q305 T306 S307 G308 P309 I310 D315 S316 D317 A318 I319 I320 A321 A322 Q323 D324 D328 N329 Y330 A331 T336 E337 V338 L339 D340 I341 Y342 D343 A344 A345 S346 D347 Q348 D349 Q350 S351 S352 V353 E354 L355 D356 K357 G358 P359 E360 S361 L362 Q365 N366 E367 A368

• Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain L:

40% 43% 14% ·

V7 D8 Q14 D17 N18 D19 I20 D24 Y25 W26 R27 H28 I31 A32 G33 N34 D37 C38 S39 A40 L43 T44 S45 C46 P47 P48 G49 T50 L51 V52 A53 S54 G55 S56 W57 V58 C61 Y62 N63 P64 P65 D66 P67 N68 K69 Y70 I71 Y74 R75 D76 C77 C78

G79 Y80 N81 V82 R85 C88 L89 E94 L95 P96 V97 Y98 N99 K100 D101 A102 N103 D104 I105 I106 W107 C108 F109 E112 D113 G114 M115 T116 Y117 H118 C119 S120 I121 S122 P123 V124 A127
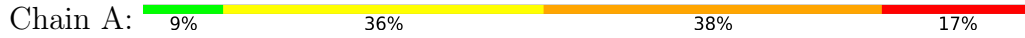
• Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain M:

31% 50% 14% 5%

V7 D8 K12 W13 Q14 P15 Q16 D17 N18 D19 I20 C23 D24 Y25 W26 R27 H28 I31 A32 G33 N34 I35 C36 D37 C38 S39 A40 G41 S42 L43 T44 S45 C46 P47 T50 A53 S56 W57 C61 Y62 N63 P64 P65 D66 K69 Y70 I71 T72 A73 Y74 R75 D76

C77 C78 G79 Y80 N81 V82 R85 C86 A87 C88 L89 N90 T91 E92 G93 E94 L95 P96 V97 Y98 N99 K100 D101 A102 N103 D104 I105 I106 W107 C108 F109 D113 T116 Y117 H118 C119 S120 I121 S122 P123 V124 S125 G126 A127

• Molecule 3: AMICYANIN

Chain A:

9% 36% 38% 17%

A3 T4 I5 P6 S7 E8 S9 P10 F11 A12 A13 A14 E15 V16 A17 D18 G19 A20 I21 V22 V23 D24 I25 A26 K27 M28 K29 Y30 E31 E34 L35 H36 V37 K38 V39 G40 D41 T42 V43 T44 W45 I46 N47 R48 E49 A50 M51 P52 H53 N54 V55 H56 F57 V58 A59 G60 V61 L62 G63

E64 A65 A66 L67 K68 G69 P70 M71 M72 K73 K74 E75 Q76 A77 Y78 S79 L80 T81 F82 T83 E84 T87 Y88 D89 Y90 H91 C92 T93 P94 H95 P96 F97 M98 R99 G100 K101 V102 V103 V104 E105

• Molecule 3: AMICYANIN

Chain B:

16% 38% 33% 14%

A3 T4 I5 P6 S7 E8 S9 P10 F11 A12 A13 A14 E15 V16 A17 D18 G19 A20 I21 V22 V23 D24 I25 A26 K27 M28 K29 Y30 E31 T32 P33 E34 L35 H36 V37 K38 V39 G40 D41 T42 V43 T44 W45 I46 N47 R48 E49 A50 M51 P52 H53 N54 V55 H56 F57 V58 A59 G60 V61 L62

G63 E64 A65 A66 L67 K68 G69 P70 M71 M72 K73 K74 E75 Q76 A77 Y78 S79 L80 T81 F82 T83 T87 Y88 D89 Y90 H91 C92 T93 P94 H95 P96 F97 M98 R99 G100 K101 V102 V103 V104 E105

4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.70Å 124.70Å 247.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, TNT	Depositor
R, R_{free}	0.285 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8567	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	H	0.87	9/2629 (0.3%)	1.76	77/3577 (2.2%)
1	J	0.84	7/2630 (0.3%)	1.65	69/3577 (1.9%)
2	L	0.86	2/917 (0.2%)	1.59	21/1250 (1.7%)
2	M	0.84	2/917 (0.2%)	1.59	25/1250 (2.0%)
3	A	1.09	7/811 (0.9%)	1.99	32/1102 (2.9%)
3	B	1.08	4/811 (0.5%)	2.06	29/1102 (2.6%)
All	All	0.90	31/8715 (0.4%)	1.74	253/11858 (2.1%)

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	H	3	0
1	J	1	1
2	M	1	1
3	B	0	1
All	All	5	3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	253	GLU	CD-OE1	6.93	1.33	1.25
2	L	94	GLU	CD-OE1	6.83	1.33	1.25
1	J	113	GLU	CD-OE1	6.74	1.33	1.25
1	H	284	GLU	CD-OE2	6.46	1.32	1.25
1	H	47	GLU	CD-OE1	6.40	1.32	1.25

The worst 5 of 253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5	ILE	C-N-CD	-19.12	78.54	120.60
3	B	5	ILE	C-N-CD	-18.21	80.53	120.60
1	H	240	ALA	N-CA-CB	-14.04	90.45	110.10
3	B	9	SER	C-N-CD	-11.45	95.41	120.60
1	J	182	SER	N-CA-CB	10.74	126.61	110.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	232	SER	CA
1	H	310	ILE	CA
1	H	320	ILE	CA
1	J	232	SER	CA
2	M	94	GLU	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	11	PHE	Mainchain
1	J	180	LEU	Mainchain
2	M	98	TYR	Mainchain

5.2 Too-close contacts ⓘ

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	H	2582	0	2472	219	0
1	J	2583	0	2472	237	0
2	L	910	0	808	85	0
2	M	910	0	809	108	0
3	A	790	0	774	226	0
3	B	790	0	774	206	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8567	0	8109	1009	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 61.

The worst 5 of 1009 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)
3:B:6:PRO:HB3	3:B:83:THR:HG23	1.22	1.19
1:H:222:PRO:HG3	1:H:273:LYS:HD2	1.21	1.15
2:M:121:ILE:HG23	2:M:123:PRO:HD3	1.22	1.15
2:L:121:ILE:HG23	2:L:123:PRO:HD3	1.27	1.12
2:L:81:ASN:H	1:J:63:LEU:HD11	1.16	1.10

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	H	366/368 (100%)	290 (79%)	45 (12%)	31 (8%)	1	1
1	J	366/368 (100%)	291 (80%)	42 (12%)	33 (9%)	1	0
2	L	118/121 (98%)	98 (83%)	12 (10%)	8 (7%)	1	1
2	M	118/121 (98%)	94 (80%)	14 (12%)	10 (8%)	1	1
3	A	101/103 (98%)	49 (48%)	23 (23%)	29 (29%)	0	0
3	B	101/103 (98%)	60 (59%)	18 (18%)	23 (23%)	0	0
All	All	1170/1184 (99%)	882 (75%)	154 (13%)	134 (12%)	0	0

5 of 134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	182	SER
1	H	186	SER
1	H	206	CYS
1	H	222	PRO
1	H	223	GLY

5.3.2 Protein sidechains ⓘ

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	H	264/264 (100%)	219 (83%)	45 (17%)	2	3
1	J	264/264 (100%)	225 (85%)	39 (15%)	3	5
2	L	99/99 (100%)	83 (84%)	16 (16%)	2	4
2	M	99/99 (100%)	85 (86%)	14 (14%)	3	6
3	A	83/83 (100%)	54 (65%)	29 (35%)	0	0
3	B	83/83 (100%)	56 (68%)	27 (32%)	0	0
All	All	892/892 (100%)	722 (81%)	170 (19%)	1	2

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	5	ILE
3	B	4	THR
3	A	16	VAL
3	A	46	ILE
3	B	24	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	48	ASN
2	M	81	ASN
1	J	205	GLN
3	A	95	HIS
1	J	323	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	TRQ	M	57	2	13,17,18	4.85	5 (38%)	14,24,26	2.66	7 (50%)
2	TRQ	L	57	2	13,17,18	4.48	4 (30%)	14,24,26	2.79	5 (35%)

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	TRQ	M	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	L	57	2	-	1/4/19/21	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	57	TRQ	CH2-CZ2	-14.82	1.37	1.54
2	L	57	TRQ	CH2-CZ2	-12.70	1.39	1.54
2	L	57	TRQ	CE2-CZ2	-8.99	1.38	1.50
2	M	57	TRQ	CE2-CZ2	-7.92	1.39	1.50
2	M	57	TRQ	CZ3-CH2	-3.42	1.36	1.45

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	57	TRQ	CZ2-CE2-NE1	6.87	130.92	119.94
2	M	57	TRQ	CZ2-CE2-NE1	6.30	129.99	119.94
2	M	57	TRQ	O6-CH2-CZ2	4.43	121.52	118.51
2	L	57	TRQ	O6-CH2-CZ2	4.24	121.39	118.51
2	L	57	TRQ	O7-CZ2-CE2	-3.92	117.69	121.84

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	57	TRQ	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	57	TRQ	7	0
2	L	57	TRQ	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.