Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 05:37 PM EST

PDB ID	:	1MXA
Title	:	S-ADENOSYLMETHIONINE SYNTHETASE WITH PPI
Authors	:	Takusagawa, F.; Kamitori, S.; Markham, G.D.
Deposited on	:	1996-01-10
Resolution	:	2.80 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 (i)) were used in the production of this report:

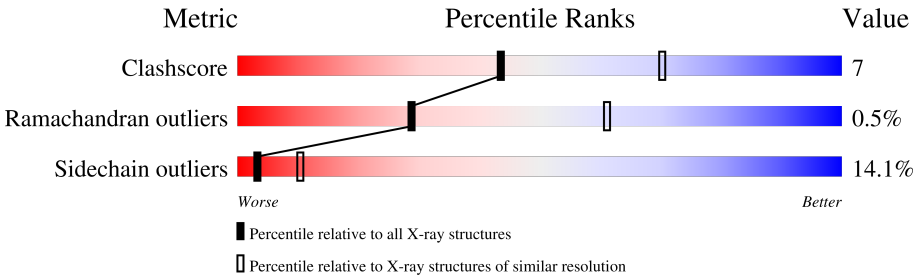
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	A	383	69% 22% 7% ••

2 Entry composition (i)

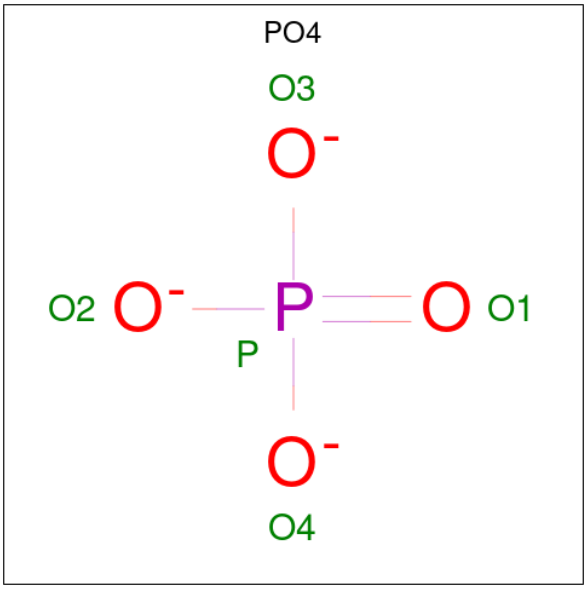
There are 5 unique types of molecules in this entry. The entry contains 3517 atoms, of which 600 are hydrogens and 0 are deuteriums.

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 S-ADENOSYLMETHIONINE SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	378	3499	1830	600	496	560	13	600	0	1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

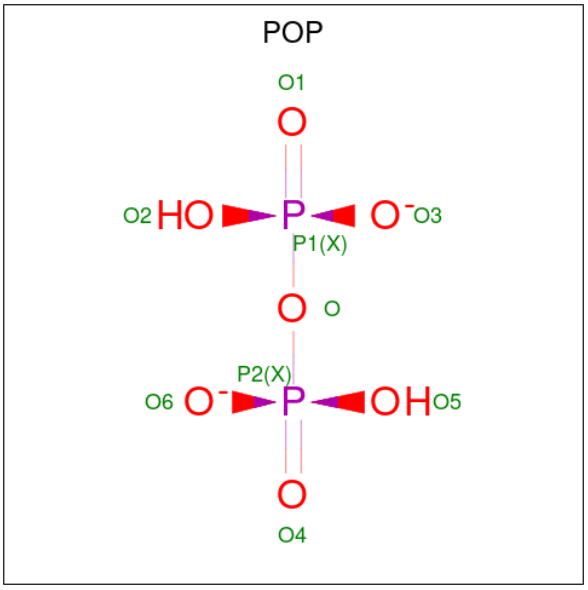
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	2	2	2	0	0

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
5	A	1	9	7	2	0	0

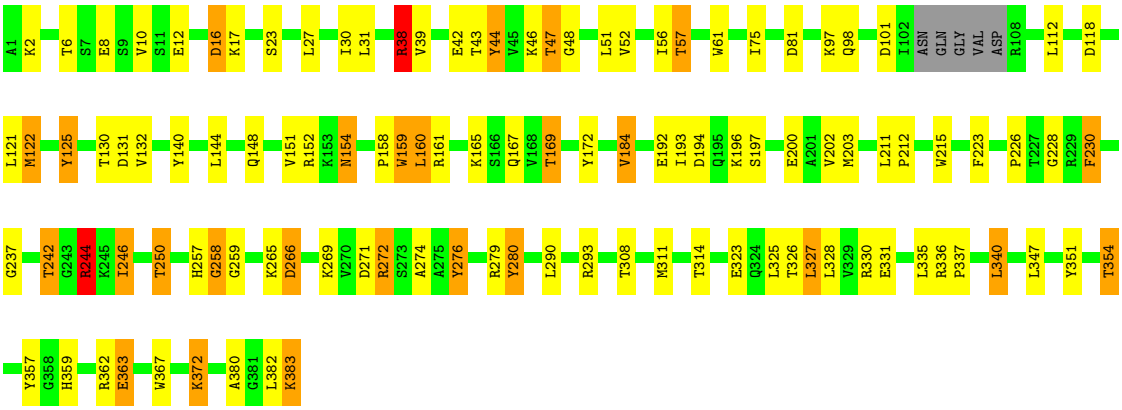
3 Residue-property plots (i)

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. 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: S-ADENOSYLMETHIONINE SYNTHETASE

Chain A: 69% 22% 7% ••



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	128.90Å 128.90Å 139.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3517	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

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: POP, PO4, K, 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	0.76	0/2957	1.49	40/4007 (1.0%)

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	A	0	10

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	A	61	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	A	271	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	244	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	159	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	A	336	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	250	THR	N-CA-CB	-7.68	95.72	110.30
1	A	38	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	367	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	A	159	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	A	16	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	61	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	250	THR	CA-CB-CG2	7.35	122.69	112.40
1	A	215	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	A	367	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	160	LEU	CA-CB-CG	6.88	131.12	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	GLU	CA-CB-CG	6.72	128.19	113.40
1	A	161	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	279	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	159	TRP	CB-CG-CD1	-6.19	118.95	127.00
1	A	159	TRP	CG-CD2-CE3	6.17	139.46	133.90
1	A	293	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	258	GLY	CA-C-N	5.98	128.15	116.20
1	A	118	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	382	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	215	TRP	CG-CD1-NE1	-5.75	104.34	110.10
1	A	161	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	61	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	44	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	A	230	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	A	46	LYS	CA-CB-CG	5.56	125.63	113.40
1	A	42	GLU	OE1-CD-OE2	-5.49	116.72	123.30
1	A	362	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	327	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	125	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	276	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	362	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	314	THR	N-CA-C	-5.16	97.06	111.00
1	A	363	GLU	N-CA-C	5.11	124.78	111.00
1	A	271	ASP	OD1-CG-OD2	-5.01	113.78	123.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	TYR	Sidechain
1	A	140	TYR	Sidechain
1	A	194	ASP	Peptide
1	A	228	GLY	Peptide
1	A	244	ARG	Sidechain
1	A	259	GLY	Peptide
1	A	272	ARG	Sidechain
1	A	280	TYR	Sidechain
1	A	44	TYR	Sidechain
1	A	48	GLY	Peptide

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	2899	600	2866	39	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	9	0	0	0	0
All	All	2917	600	2866	39	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.

All (39) 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:A:57:THR:HB	1:A:98:GLN:HB3	1.62	0.81
1:A:265:LYS:HB3	1:A:269:LYS:HG3	1.62	0.80
1:A:257:HIS:HD2	1:A:258:GLY:O	1.74	0.71
1:A:151:VAL:HA	1:A:154:ASN:ND2	2.11	0.65
1:A:167:GLN:HB3	1:A:184:VAL:HG13	1.80	0.64
1:A:43:THR:H	1:A:242:THR:HG23	1.62	0.63
1:A:56:ILE:HG22	1:A:97:LYS:HA	1.80	0.63
1:A:272:ARG:HH12	1:A:354:THR:HG21	1.63	0.62
1:A:10:VAL:HG12	1:A:165:LYS:HG2	1.82	0.61
1:A:23:SER:OG	1:A:242:THR:HG21	2.00	0.61
1:A:223:PHE:HB3	1:A:226:PRO:HG3	1.85	0.57
1:A:290:LEU:HD23	1:A:325:LEU:HD21	1.86	0.57
1:A:151:VAL:HA	1:A:154:ASN:HD21	1.68	0.56
1:A:244:ARG:O	1:A:246:ILE:HG22	2.05	0.56
1:A:354:THR:HG23	1:A:359:HIS:NE2	2.21	0.55
1:A:12:GLU:HG2	1:A:357:TYR:OH	2.08	0.54
1:A:47:THR:HG22	1:A:237:GLY:H	1.77	0.50
1:A:337:PRO:HA	1:A:340:LEU:HD22	1.93	0.50
1:A:159:TRP:CE3	1:A:193:ILE:HG21	2.46	0.49
1:A:75:ILE:O	1:A:152:ARG:NH2	2.46	0.48
1:A:351:TYR:O	1:A:354:THR:HG22	2.14	0.48
1:A:276:TYR:OH	1:A:359:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:MET:HG3	1:A:274:ALA:HB3	1.98	0.46
1:A:27:LEU:HD13	1:A:39:VAL:HG22	1.98	0.45
1:A:266:ASP:OD1	1:A:269:LYS:NZ	2.49	0.45
1:A:57:THR:HA	1:A:98:GLN:O	2.17	0.45
1:A:122:MET:N	1:A:122:MET:SD	2.89	0.45
1:A:17:LYS:HA	1:A:17:LYS:HD3	1.81	0.44
1:A:56:ILE:HD13	1:A:56:ILE:HG21	1.71	0.44
1:A:38:ARG:HA	1:A:38:ARG:HE	1.83	0.43
1:A:211:LEU:HA	1:A:212:PRO:HD3	1.89	0.42
1:A:2:LYS:HA	1:A:172:TYR:O	2.19	0.42
1:A:30:ILE:CD1	1:A:56:ILE:HD11	2.49	0.42
1:A:6:THR:OG1	1:A:169:THR:HB	2.20	0.42
1:A:380:ALA:O	1:A:383:LYS:HG2	2.21	0.41
1:A:280:TYR:OH	1:A:372:LYS:NZ	2.51	0.41
1:A:130:THR:HG22	1:A:132:VAL:H	1.85	0.41
1:A:335:LEU:HA	1:A:340:LEU:CD1	2.51	0.41
1:A:30:ILE:HD11	1:A:56:ILE:HD11	2.03	0.40

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	374/383 (98%)	346 (92%)	26 (7%)	2 (0%)	29 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	GLU
1	A	250	THR

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	306/311 (98%)	263 (86%)	43 (14%)	3 10

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	31	LEU
1	A	38	ARG
1	A	47	THR
1	A	51	LEU
1	A	52	VAL
1	A	57	THR
1	A	81	ASP
1	A	101	ASP
1	A	112	LEU
1	A	121	LEU
1	A	122	MET
1	A	131	ASP
1	A	144	LEU
1	A	148	GLN
1	A	154	ASN
1	A	158	PRO
1	A	160	LEU
1	A	169	THR
1	A	184	VAL
1	A	192	GLU
1	A	196	LYS
1	A	197	SER
1	A	200	GLU
1	A	202	VAL
1	A	203	MET
1	A	230	PHE
1	A	242	THR
1	A	246	ILE
1	A	266	ASP

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Mol	Chain	Res	Type
1	A	308	THR
1	A	311	MET
1	A	323	GLU
1	A	326	THR
1	A	327	LEU
1	A	328	LEU
1	A	330	ARG
1	A	331	GLU
1	A	340	LEU
1	A	347	LEU
1	A	354	THR
1	A	372	LYS
1	A	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	A	148	GLN
1	A	154	ASN
1	A	189	HIS
1	A	195	GLN
1	A	257	HIS
1	A	297	GLN
1	A	342	GLN
1	A	359	HIS
1	A	374	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)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	POP	A	385	3	6,8,8	1.50	1 (16%)	13,13,13	1.73	1 (7%)
2	PO4	A	384	3	4,4,4	2.02	2 (50%)	6,6,6	0.69	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POP	A	385	3	-	0/6/6/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	384	PO4	P-O3	-2.35	1.47	1.54
5	A	385	POP	P2-O5	-2.22	1.46	1.54
2	A	384	PO4	P-O1	-2.13	1.45	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	385	POP	P2-O-P1	-5.31	114.61	132.83

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.