



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:32 am BST

PDB ID : 1MDL  
Title : MANDELATE RACEMASE MUTANT K166R CO-CRYSTALLIZED WITH (R)-MANDELATE  
Authors : Clifton, J.G.; Petsko, G.A.  
Deposited on : 1996-03-29  
Resolution : 1.85 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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)	:	2.11

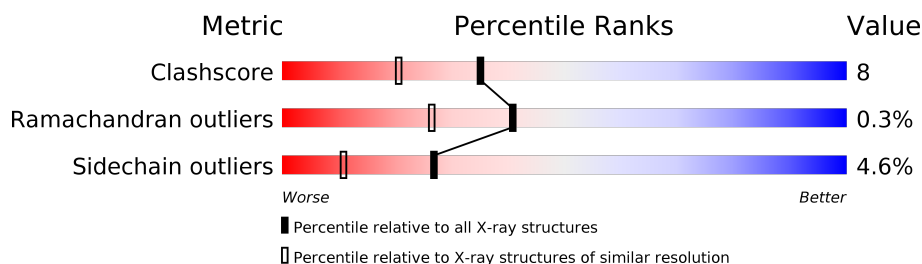
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	359	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2895 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 MANDELATE RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2700	1727	464	496	13			

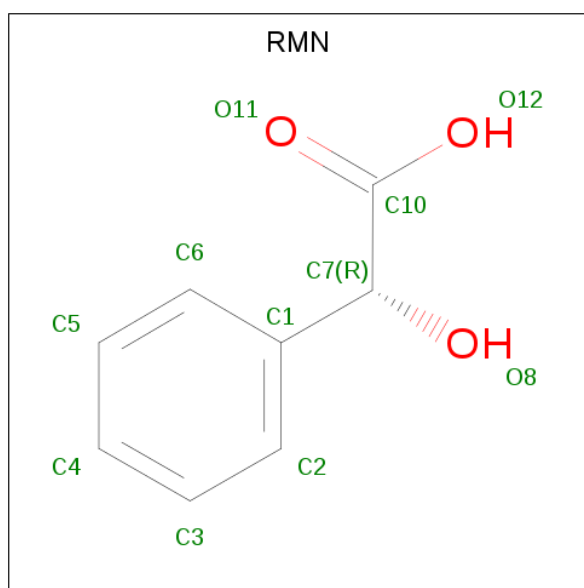
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ARG	LYS	ENGINEERED MUTATION	UNP P11444

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

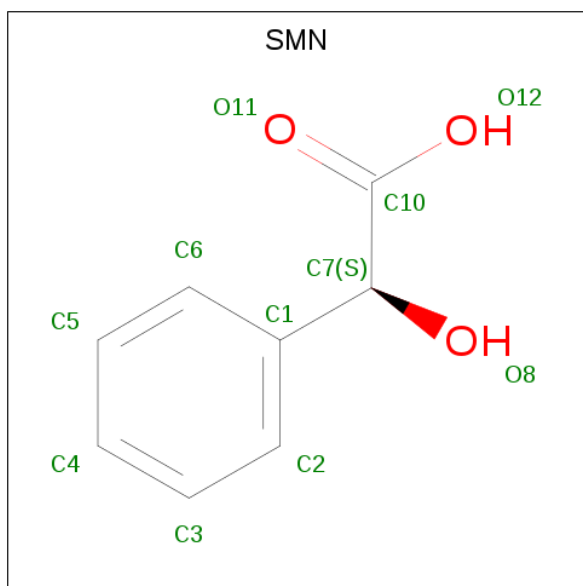
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (R)-MANDELIC ACID (three-letter code: RMN) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	8	3		

- Molecule 4 is (S)-MANDELIC ACID (three-letter code: SMN) (formula:  $C_8H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	8	3		

- Molecule 5 is water.

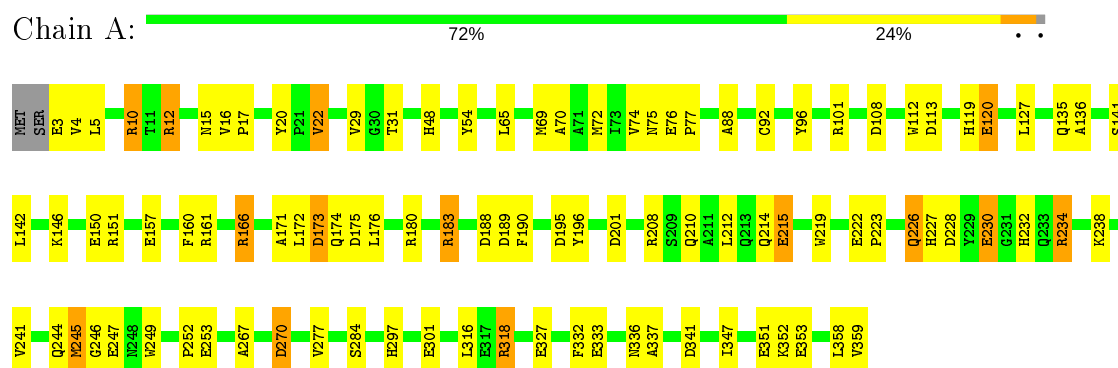
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: MANDELATE RACEMASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.32Å 125.32Å 106.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.85)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	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: SMN, MG, RMN

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	1.02	14/2756 (0.5%)	1.63	38/3753 (1.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLU	CD-OE2	8.80	1.35	1.25
1	A	333	GLU	CD-OE2	7.38	1.33	1.25
1	A	301	GLU	CD-OE1	6.67	1.32	1.25
1	A	157	GLU	CD-OE1	6.63	1.32	1.25
1	A	253	GLU	CD-OE1	6.54	1.32	1.25
1	A	120	GLU	CD-OE1	6.34	1.32	1.25
1	A	230	GLU	CD-OE2	6.29	1.32	1.25
1	A	150	GLU	CD-OE2	5.97	1.32	1.25
1	A	3	GLU	CD-OE2	5.84	1.32	1.25
1	A	353	GLU	CD-OE1	5.80	1.32	1.25
1	A	222	GLU	CD-OE1	5.62	1.31	1.25
1	A	327	GLU	CD-OE1	5.51	1.31	1.25
1	A	351	GLU	CD-OE1	5.36	1.31	1.25
1	A	76	GLU	CD-OE1	5.03	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ARG	NE-CZ-NH1	15.87	128.23	120.30
1	A	183	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	A	166	ARG	NE-CZ-NH2	-13.03	113.78	120.30
1	A	101	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	A	341	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	175	ASP	CB-CG-OD1	-8.32	110.81	118.30
1	A	108	ASP	CB-CG-OD1	-7.86	111.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	CB-CG-OD1	7.78	125.30	118.30
1	A	188	ASP	CB-CG-OD1	7.16	124.75	118.30
1	A	151	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	101	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	A	318	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	A	188	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	A	201	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	241	VAL	CG1-CB-CG2	-6.81	100.01	110.90
1	A	10	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	A	270	ASP	CB-CG-OD1	-6.58	112.37	118.30
1	A	234	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	189	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	284	SER	N-CA-CB	-6.25	101.12	110.50
1	A	166	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	10	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	A	337	ALA	CB-CA-C	-6.03	101.06	110.10
1	A	54	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	A	173	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	245	MET	CG-SD-CE	5.96	109.74	100.20
1	A	12	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	A	196	TYR	CB-CG-CD2	5.79	124.48	121.00
1	A	92	CYS	CA-CB-SG	-5.75	103.65	114.00
1	A	195	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	A	4	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	A	270	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	238	LYS	CB-CA-C	-5.36	99.67	110.40
1	A	201	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	20	TYR	CA-CB-CG	5.26	123.39	113.40
1	A	113	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	A	166	ARG	CB-CA-C	-5.03	100.34	110.40
1	A	113	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	A	2700	0	2748	43	0
2	A	1	0	0	0	0
3	A	11	0	7	2	0
4	A	11	0	6	1	0
5	A	172	0	0	1	0
All	All	2895	0	2761	45	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 8.

All (45) 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:171:ALA:HB3	1:A:174:GLN:HE21	1.31	0.93
1:A:171:ALA:HB3	1:A:174:GLN:NE2	1.93	0.83
1:A:223:PRO:HD2	1:A:232:HIS:CE1	2.15	0.82
1:A:135:GLN:HA	1:A:336:ASN:HD22	1.47	0.80
1:A:141:SER:HA	1:A:166:ARG:HG3	1.78	0.65
1:A:166:ARG:NH2	3:A:398:RMN:O11	2.23	0.62
1:A:10:ARG:HH21	1:A:12:ARG:NH1	1.97	0.62
1:A:65:LEU:O	1:A:69:MET:HG3	2.01	0.61
4:A:399:SMN:H7	5:A:480:HOH:O	2.04	0.57
1:A:112:TRP:CD1	1:A:277:VAL:HB	2.41	0.55
1:A:10:ARG:HH21	1:A:12:ARG:CZ	2.19	0.54
1:A:70:ALA:O	1:A:74:VAL:HG23	2.07	0.54
1:A:88:ALA:HB2	1:A:96:TYR:CE2	2.42	0.54
1:A:212:LEU:O	1:A:215:GLU:HB2	2.08	0.54
1:A:22:VAL:HG22	1:A:22:VAL:O	2.07	0.53
1:A:176:LEU:O	1:A:180:ARG:HG3	2.09	0.53
3:A:398:RMN:H6	3:A:398:RMN:O11	2.08	0.52
1:A:172:LEU:HD13	1:A:208:ARG:HG2	1.92	0.52
1:A:223:PRO:HD2	1:A:232:HIS:HE1	1.70	0.52
1:A:16:VAL:O	1:A:31:THR:HA	2.10	0.51
1:A:74:VAL:O	1:A:75:ASN:HB2	2.12	0.50
1:A:171:ALA:CB	1:A:174:GLN:NE2	2.71	0.50
1:A:160:PHE:HZ	1:A:318:ARG:HD2	1.76	0.50
1:A:160:PHE:CZ	1:A:318:ARG:HD2	2.48	0.49
1:A:135:GLN:HA	1:A:336:ASN:ND2	2.24	0.47
1:A:244:GLN:HE21	1:A:245:MET:H	1.61	0.47
1:A:142:LEU:HD12	1:A:166:ARG:O	2.16	0.46
1:A:226:GLN:HG3	1:A:227:HIS:N	2.31	0.45
1:A:270:ASP:OD2	1:A:297:HIS:ND1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:VAL:O	1:A:359:VAL:HG12	2.16	0.44
1:A:119:HIS:O	1:A:120:GLU:C	2.57	0.43
1:A:210:GLN:O	1:A:214:GLN:NE2	2.52	0.43
1:A:246:GLY:HA2	1:A:249:TRP:CD2	2.53	0.43
1:A:230:GLU:O	1:A:234:ARG:HG3	2.20	0.42
1:A:358:LEU:HA	1:A:358:LEU:HD12	1.67	0.42
1:A:244:GLN:HE22	1:A:267:ALA:N	2.18	0.42
1:A:48:HIS:HD2	1:A:347:ILE:O	2.02	0.42
1:A:5:LEU:HD23	1:A:77:PRO:HA	2.02	0.42
1:A:5:LEU:HA	1:A:5:LEU:HD23	1.73	0.42
1:A:16:VAL:HA	1:A:17:PRO:HD3	1.83	0.42
1:A:228:ASP:O	1:A:232:HIS:HD2	2.03	0.41
1:A:318:ARG:HG3	1:A:332:PHE:CZ	2.56	0.41
1:A:161:ARG:HD2	1:A:161:ARG:HH11	1.70	0.41
1:A:136:ALA:HA	1:A:316:LEU:O	2.22	0.40
1:A:223:PRO:HD2	1:A:232:HIS:ND1	2.33	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	355/359 (99%)	340 (96%)	14 (4%)	1 (0%)	41	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	PHE

### 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	A	280/282 (99%)	267 (95%)	13 (5%)	27	11

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	22	VAL
1	A	29	VAL
1	A	72	MET
1	A	127	LEU
1	A	146	LYS
1	A	173	ASP
1	A	183	ARG
1	A	215	GLU
1	A	219	TRP
1	A	226	GLN
1	A	252	PRO
1	A	352	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	48	HIS
1	A	135	GLN
1	A	174	GLN
1	A	197	ASN
1	A	227	HIS
1	A	232	HIS
1	A	244	GLN
1	A	336	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
4	SMN	A	399	2	8,11,11	1.01	1 (12%)	9,14,14	0.82	0
3	RMN	A	398	-	8,11,11	0.96	1 (12%)	9,14,14	0.73	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
4	SMN	A	399	2	-	0/4/8/8	0/1/1/1
3	RMN	A	398	-	-	0/4/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	398	RMN	C1-C7	2.16	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	399	SMN	C1-C7	2.15	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	399	SMN	1	0
3	A	398	RMN	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

### 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.