



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 07:46 AM EDT

PDB ID : 1KH7  
Title : E. COLI ALKALINE PHOSPHATASE MUTANT (D153GD330N)  
Authors : Le Du, M.H.; Lamoure, C.; Muller, B.H.; Bulgakov, O.V.; Lajeunesse, E.  
Deposited on : 2001-11-29  
Resolution : 2.40 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) : 2.23.2

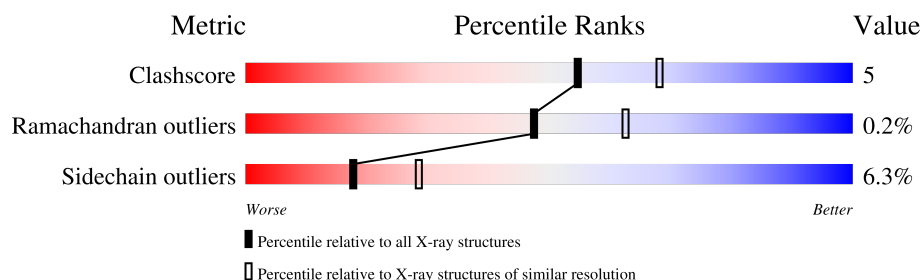
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\geq 3$ , 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	449	 86% 12% ..
1	B	449	 80% 17% ..

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6887 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 alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3256	2012	578	655	11			
1	B	444	Total	C	N	O	S	0	0	0
			3256	2012	578	655	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASN	ASP	conflict	UNP P00634
A	35	ASN	ASP	conflict	UNP P00634
A	153	GLY	ASP	engineered mutation	UNP P00634
A	173	LYS	ALA	conflict	UNP P00634
A	176	GLN	GLU	conflict	UNP P00634
A	228	GLU	GLN	conflict	UNP P00634
A	230	GLU	GLN	conflict	UNP P00634
A	330	ASN	ASP	engineered mutation	UNP P00634
B	15	ASN	ASP	conflict	UNP P00634
B	35	ASN	ASP	conflict	UNP P00634
B	153	GLY	ASP	engineered mutation	UNP P00634
B	173	LYS	ALA	conflict	UNP P00634
B	176	GLN	GLU	conflict	UNP P00634
B	228	GLU	GLN	conflict	UNP P00634
B	230	GLU	GLN	conflict	UNP P00634
B	330	ASN	ASP	engineered mutation	UNP P00634

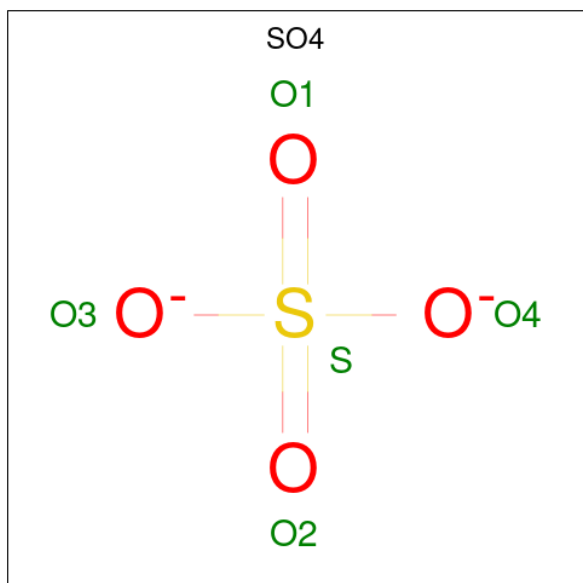
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total	O	0	0
			187	187		
5	B	172	Total	O	0	0
			172	172		

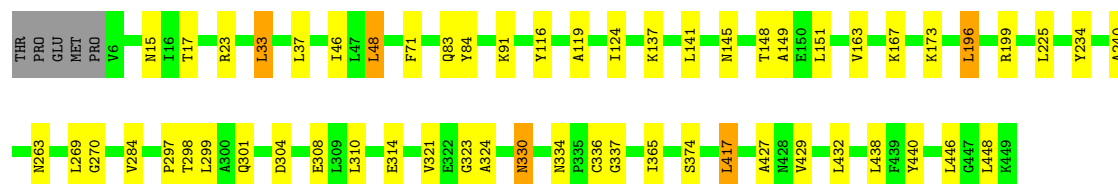
### 3 Residue-property plots [i](#)

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.

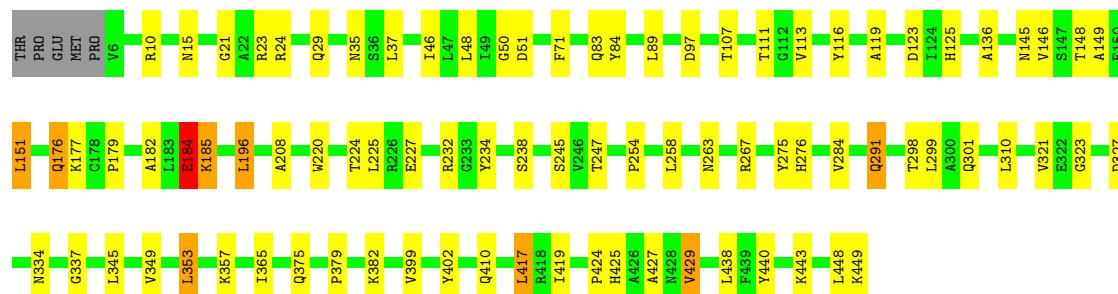
#### • Molecule 1: alkaline phosphatase

Chain A: 



#### • Molecule 1: alkaline phosphatase

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.51Å 163.51Å 138.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (10.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.178 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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: MG, ZN, 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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	0/3309	0.73	2/4490 (0.0%)
1	B	0.46	0/3309	0.74	4/4490 (0.1%)
All	All	0.46	0/6618	0.73	6/8980 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	LEU	CA-CB-CG	6.92	131.21	115.30
1	A	323	GLY	N-CA-C	-6.28	97.41	113.10
1	B	417	LEU	CA-CB-CG	5.94	128.96	115.30
1	B	323	GLY	N-CA-C	-5.57	99.19	113.10
1	B	97	ASP	N-CA-C	-5.29	96.72	111.00
1	B	50	GLY	N-CA-C	-5.00	100.60	113.10

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	3256	0	3198	26	2
1	B	3256	0	3198	45	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	187	0	0	1	0
5	B	172	0	0	3	2
All	All	6887	0	6396	67	2

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 5.

All (67) 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:91:LYS:HA	1:A:124:ILE:HD11	1.61	0.83
1:B:182:ALA:HB1	1:B:184:GLU:OE1	1.88	0.72
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.71	0.72
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.72	0.71
1:A:334:ASN:HD22	1:A:337:GLY:H	1.36	0.70
1:B:111:THR:HG22	1:B:113:VAL:HG12	1.73	0.70
1:B:334:ASN:HD22	1:B:337:GLY:H	1.39	0.70
1:B:111:THR:CG2	1:B:113:VAL:HG12	2.22	0.69
1:A:334:ASN:ND2	1:A:337:GLY:H	1.95	0.63
1:A:298:THR:OG1	1:A:301:GLN:HG3	1.99	0.62
1:B:15:ASN:O	1:B:21:GLY:HA3	2.00	0.62
1:B:179:PRO:O	1:B:185:LYS:HD3	2.01	0.60
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.84	0.59
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.39	0.57
1:A:149:ALA:HA	1:A:263:ASN:HD22	1.70	0.57
1:A:141:LEU:HD21	1:A:446:LEU:HD22	1.89	0.55
1:B:443:LYS:HE2	1:B:449:LYS:HA	1.88	0.54
1:B:176:GLN:HG2	1:B:177:LYS:HG3	1.88	0.54
1:B:107:THR:O	1:B:111:THR:HB	2.07	0.54
1:A:37:LEU:HD22	1:A:427:ALA:HB2	1.91	0.52
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.45	0.52
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.40	0.51
1:B:224:THR:OG1	1:B:227:GLU:HG3	2.11	0.50
1:B:148:THR:HG23	1:B:299:LEU:HD13	1.94	0.50
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.95	0.49
1:A:330:ASN:HD21	1:A:374:SER:H	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:HD13	1:B:438:LEU:HD11	1.95	0.49
1:B:10:ARG:NH2	1:B:29:GLN:OE1	2.45	0.49
1:B:234:TYR:CD2	1:B:254:PRO:HB2	2.49	0.48
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.13	0.48
1:B:424:PRO:O	1:B:425:HIS:HB2	2.14	0.48
1:B:37:LEU:HD22	1:B:427:ALA:HB2	1.95	0.47
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.96	0.47
1:B:125:HIS:NE2	5:B:1139:HOH:O	2.30	0.47
1:A:91:LYS:HA	1:A:124:ILE:CD1	2.39	0.47
1:B:111:THR:HG21	1:B:113:VAL:HG12	1.95	0.47
1:B:275:TYR:O	1:B:276:HIS:HB2	2.16	0.46
1:A:167:LYS:O	1:A:173:LYS:HD2	2.16	0.46
1:B:136:ALA:HA	1:B:448:LEU:HD11	1.98	0.46
1:A:17:THR:HG22	1:B:89:LEU:HD13	1.98	0.45
1:A:33:LEU:HD22	1:A:33:LEU:HA	1.81	0.45
1:B:291:GLN:HG3	5:B:1320:HOH:O	2.17	0.45
1:A:240:ALA:HA	1:A:297:PRO:HG3	1.99	0.44
1:B:10:ARG:O	1:B:24:ARG:HD3	2.17	0.44
1:A:46:ILE:HG22	1:A:48:LEU:HD22	1.99	0.44
1:B:345:LEU:O	1:B:349:VAL:HG23	2.17	0.44
1:A:440:TYR:CD2	1:B:23:ARG:HD3	2.52	0.44
1:B:196:LEU:HD12	1:B:196:LEU:HA	1.83	0.44
1:A:199:ARG:HA	1:A:234:TYR:OH	2.18	0.43
1:B:149:ALA:HA	1:B:263:ASN:HD22	1.82	0.43
1:B:379:PRO:HA	1:B:399:VAL:CG2	2.48	0.43
1:A:148:THR:HG23	1:A:299:LEU:HD13	2.01	0.43
1:B:220:TRP:CZ2	1:B:232:ARG:HD3	2.53	0.43
1:A:23:ARG:HD2	1:B:440:TYR:CE2	2.53	0.43
1:A:270:GLY:HA3	1:A:336:CYS:HB2	2.00	0.43
1:A:432:LEU:O	1:B:10:ARG:HD2	2.19	0.43
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.93	0.42
1:B:419:ILE:CD1	1:B:429:VAL:HG22	2.50	0.42
1:B:51:ASP:O	1:B:327:ASP:HB2	2.20	0.41
1:B:185:LYS:HE3	1:B:185:LYS:HB3	1.72	0.41
1:B:353:LEU:O	1:B:357:LYS:HG3	2.20	0.41
1:B:46:ILE:HG22	1:B:48:LEU:HD22	2.02	0.41
1:B:208:ALA:HB2	1:B:258:LEU:HB3	2.03	0.41
5:A:1008:HOH:O	1:B:123:ASP:HB2	2.21	0.41
1:A:149:ALA:HB2	1:A:324:ALA:HB1	2.03	0.40
1:B:375:GLN:NE2	5:B:1048:HOH:O	2.49	0.40
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.93	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASP:OD2	5:B:1139:HOH:O[9_766]	1.87	0.33
1:A:308:GLU:OE2	5:B:1139:HOH:O[9_766]	2.12	0.08

## 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	442/449 (98%)	433 (98%)	9 (2%)	0	100	100
1	B	442/449 (98%)	429 (97%)	11 (2%)	2 (0%)	29	41
All	All	884/898 (98%)	862 (98%)	20 (2%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	LYS
1	B	184	GLU

### 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	332/340 (98%)	312 (94%)	20 (6%)	19	31
1	B	332/340 (98%)	310 (93%)	22 (7%)	16	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	664/680 (98%)	622 (94%)	42 (6%)	18	28

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	33	LEU
1	A	48	LEU
1	A	71	PHE
1	A	83	GLN
1	A	84	TYR
1	A	137	LYS
1	A	145	ASN
1	A	151	LEU
1	A	163	VAL
1	A	196	LEU
1	A	225	LEU
1	A	269	LEU
1	A	284	VAL
1	A	310	LEU
1	A	314	GLU
1	A	330	ASN
1	A	417	LEU
1	A	429	VAL
1	A	448	LEU
1	B	35	ASN
1	B	71	PHE
1	B	83	GLN
1	B	84	TYR
1	B	145	ASN
1	B	146	VAL
1	B	151	LEU
1	B	176	GLN
1	B	184	GLU
1	B	196	LEU
1	B	225	LEU
1	B	238	SER
1	B	245	SER
1	B	247	THR
1	B	267	ARG
1	B	284	VAL
1	B	291	GLN

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Mol	Chain	Res	Type
1	B	310	LEU
1	B	353	LEU
1	B	382	LYS
1	B	417	LEU
1	B	429	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	35	ASN
1	A	83	GLN
1	A	145	ASN
1	A	235	GLN
1	A	251	GLN
1	A	263	ASN
1	A	330	ASN
1	A	334	ASN
1	B	15	ASN
1	B	35	ASN
1	B	83	GLN
1	B	145	ASN
1	B	244	ASN
1	B	263	ASN
1	B	301	GLN
1	B	334	ASN
1	B	375	GLN
1	B	410	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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	$\# Z  > 2$
4	SO4	B	2453	-	4,4,4	0.74	0	6,6,6	0.55	0
4	SO4	A	1453	-	4,4,4	0.68	0	6,6,6	1.15	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.

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

### 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.