



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 08:01 AM EST

PDB ID : 1FBH  
Title : CRYSTALLOGRAPHIC STUDIES OF THE CATALYTIC MECHANISM OF  
THE NEUTRAL FORM OF FRUCTOSE-1,6-BISPHOSPHATASE  
Authors : Zhang, Y.; Liang, J.-Y.; Huang, S.; Ke, H.; Lipscomb, W.N.  
Deposited on : unknown  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

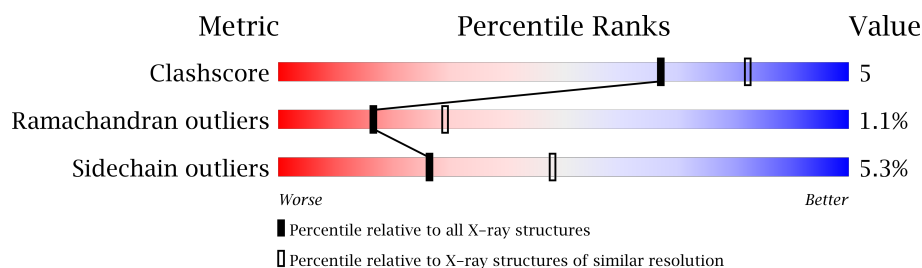
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	 79% 14% • 5%
1	B	335	 79% 14% •• 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6366 atoms, of which 1317 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.

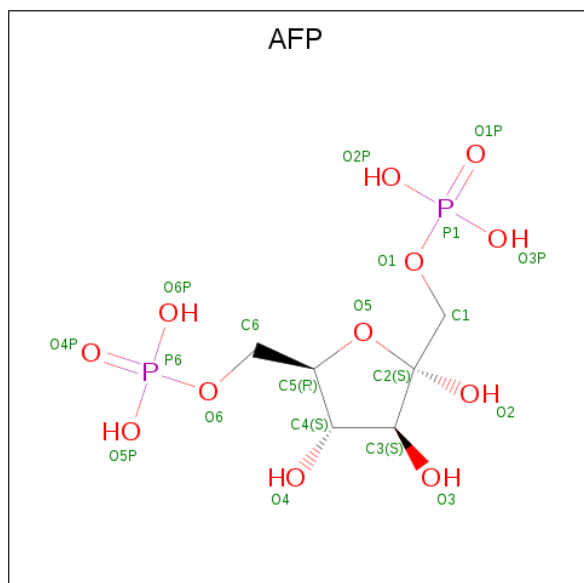
- Molecule 1 is a protein called FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	317	Total	C	H	N	O	S	0	0	1
			2962	1540	538	409	460	15			
1	B	318	Total	C	H	N	O	S	0	0	1
			2974	1549	539	410	461	15			

There are 6 discrepancies between the modelled and reference sequences:

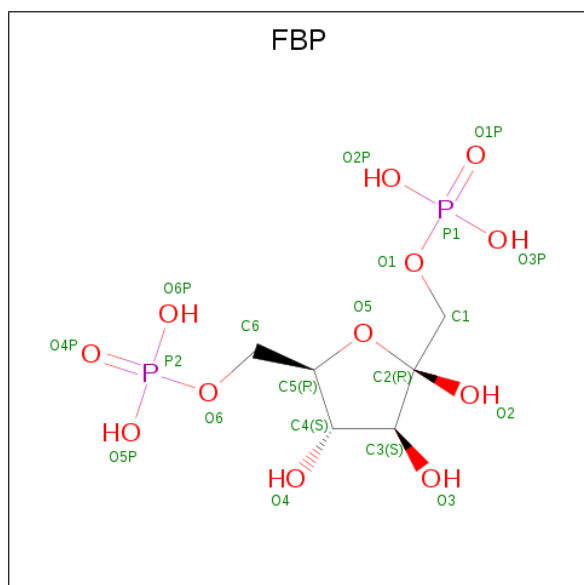
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	CONFLICT	UNP P00636
A	96	THR	SER	CONFLICT	UNP P00636
A	199	ASN	ASP	CONFLICT	UNP P00636
B	20	GLN	GLU	CONFLICT	UNP P00636
B	96	THR	SER	CONFLICT	UNP P00636
B	199	ASN	ASP	CONFLICT	UNP P00636

- Molecule 2 is ALPHA FRUCTOSE 1,6-DIPHOSPHATE (three-letter code: AFP) (formula:  $C_6H_{14}O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			25	6	5	12	2		
2	B	1	Total	C	H	O	P	0	0
			25	6	5	12	2		

- Molecule 3 is BETA-FRUCTOSE-1,6-DIPHOSPHATE (three-letter code: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			25	6	5	12	2		
3	B	1	Total	C	H	O	P	0	0
			25	6	5	12	2		

- Molecule 4 is water.

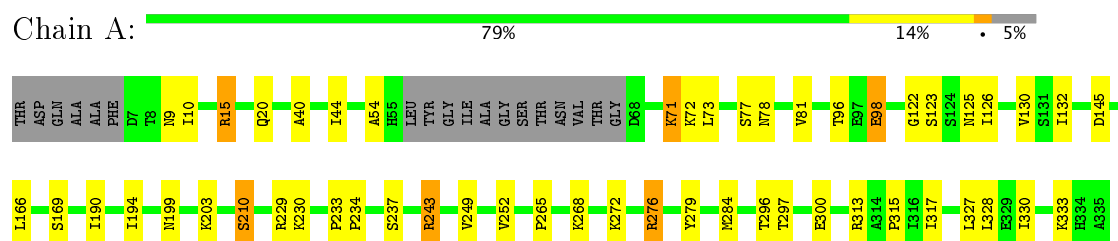
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	56	Total	H	O	0	0
			168	112	56		
4	B	54	Total	H	O	0	0
			162	108	54		

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

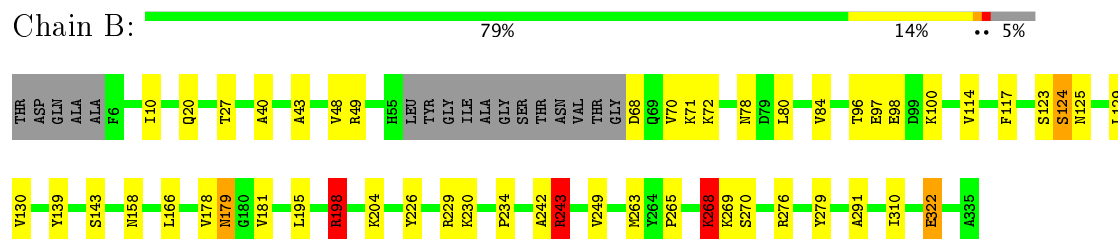
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: FRUCTOSE 1,6-BISPHOSPHATASE



#### • Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.20 Å 131.20 Å 69.30 Å 90.00° 90.00° 120.00°	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	X-PLOR	Depositor
R, $R_{free}$	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: FBP, AFP

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	0.64	0/2463	1.24	7/3330 (0.2%)
1	B	0.62	0/2475	1.24	6/3346 (0.2%)
All	All	0.63	0/4938	1.24	13/6676 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	243	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	203	LYS	CA-CB-CG	6.26	127.17	113.40
1	B	243	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	15	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	243	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	279	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	313	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	268	LYS	CA-CB-CG	5.49	125.47	113.40
1	A	279	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	B	49	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	198	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	179	ASN	CB-CG-ND2	5.06	128.85	116.70

There are no chirality outliers.

There are no planarity outliers.

### 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	2424	538	2482	21	0
1	B	2435	539	2491	25	0
2	A	20	5	5	1	0
2	B	20	5	5	1	0
3	A	20	5	4	1	0
3	B	20	5	7	1	0
4	A	56	112	0	0	0
4	B	54	108	0	0	0
All	All	5049	1317	4994	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 5.

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)
2:B:336:AFP:O3P	3:B:337:FBP:C1	2.14	0.83
1:B:78:ASN:OD1	1:B:96:THR:HG21	1.86	0.76
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.69	0.74
1:B:70:VAL:HG22	1:B:124:SER:HA	1.76	0.68
1:B:125:ASN:HB3	1:B:130:VAL:HB	1.75	0.67
1:A:78:ASN:OD1	1:A:96:THR:HG21	1.96	0.66
1:A:96:THR:HG22	1:A:98:GLU:H	1.61	0.64
1:A:210:SER:HB3	1:A:243:ARG:O	1.97	0.63
1:B:195:LEU:HD21	1:B:198:ARG:HG3	1.82	0.61
1:A:122:GLY:HA2	2:A:336:AFP:O1P	2.00	0.61
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.83	0.59
3:A:337:FBP:O4P	1:B:243:ARG:NH2	2.41	0.54
1:B:226:TYR:CZ	1:B:230:LYS:HE2	2.44	0.52
1:A:317:ILE:HG21	1:A:327:LEU:HD23	1.92	0.52
1:A:126:ILE:HG12	1:A:132:ILE:HD13	1.92	0.51
1:A:166:LEU:HD23	1:B:129:LEU:HD12	1.93	0.50
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.95	0.49
1:B:96:THR:HG23	1:B:117:PHE:CE1	2.47	0.49
1:B:181:VAL:HG21	1:B:291:ALA:HB2	1.94	0.48
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.95	0.48
1:A:9:ASN:HD21	1:A:15:ARG:NH2	2.12	0.48
1:B:43:ALA:HB3	1:B:80:LEU:HD21	1.96	0.48
1:A:229:ARG:HH11	1:A:330:ILE:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:HG21	1:A:328:LEU:HD21	1.97	0.46
1:A:233:PRO:HA	1:A:234:PRO:HD2	1.93	0.44
1:B:242:ALA:O	1:B:243:ARG:HD3	2.17	0.44
1:A:252:VAL:HG11	1:A:284:MET:SD	2.58	0.44
1:A:40:ALA:O	1:A:44:ILE:HG13	2.18	0.44
1:A:297:THR:HB	1:A:315:PRO:HG2	1.99	0.43
1:B:100:LYS:O	1:B:310:ILE:HD11	2.18	0.43
1:B:268:LYS:HZ2	1:B:269:LYS:H	1.66	0.43
1:A:73:LEU:HD23	1:A:126:ILE:HD13	2.01	0.43
1:B:166:LEU:HD13	1:B:249:VAL:HG12	2.00	0.42
1:B:226:TYR:CE1	1:B:230:LYS:HE2	2.54	0.42
1:B:263:MET:HB3	1:B:265:PRO:HD3	2.02	0.42
1:A:71:LYS:HB2	1:A:71:LYS:NZ	2.34	0.42
1:A:169:SER:HB2	1:B:48:VAL:HG12	2.02	0.42
1:B:229:ARG:CG	1:B:234:PRO:HD3	2.50	0.41
1:B:68:ASP:N	1:B:71:LYS:O	2.54	0.41
1:B:96:THR:HG22	1:B:98:GLU:H	1.85	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.87	0.41
1:A:190:ILE:HD11	1:A:194:ILE:HD11	2.02	0.41
1:A:77:SER:O	1:A:81:VAL:HG23	2.20	0.41
1:B:229:ARG:HG3	1:B:234:PRO:HD3	2.02	0.41
1:B:204:LYS:O	1:B:322:GLU:HB2	2.22	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	313/335 (93%)	294 (94%)	15 (5%)	4 (1%)	14	25
1	B	314/335 (94%)	293 (93%)	18 (6%)	3 (1%)	18	32
All	All	627/670 (94%)	587 (94%)	33 (5%)	7 (1%)	17	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	268	LYS
1	B	27	THR
1	B	72	LYS
1	A	54	ALA
1	A	333	LYS
1	B	178	VAL

### 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	265/278 (95%)	251 (95%)	14 (5%)	26	48
1	B	266/278 (96%)	252 (95%)	14 (5%)	26	48
All	All	531/556 (96%)	503 (95%)	28 (5%)	26	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	20	GLN
1	A	71	LYS
1	A	98	GLU
1	A	123	SER
1	A	145	ASP
1	A	199	ASN
1	A	210	SER
1	A	230	LYS
1	A	237	SER
1	A	265	PRO
1	A	272	LYS
1	A	276	ARG
1	A	300	GLU
1	B	10	ILE
1	B	20	GLN

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Mol	Chain	Res	Type
1	B	97	GLU
1	B	123	SER
1	B	124	SER
1	B	143	SER
1	B	158	ASN
1	B	179	ASN
1	B	198	ARG
1	B	243	ARG
1	B	268	LYS
1	B	270	SER
1	B	276	ARG
1	B	322	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	154	GLN
1	A	158	ASN
1	A	182	ASN
1	A	199	ASN
1	A	282	ASN
1	B	142	ASN
1	B	154	GLN
1	B	158	ASN
1	B	179	ASN
1	B	182	ASN
1	B	282	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands 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	AFP	A	336	3	18,20,20	0.71	0	23,32,32	1.00	1 (4%)
3	FBP	A	337	2	18,20,20	0.63	0	23,32,32	0.96	1 (4%)
2	AFP	B	336	3	18,20,20	0.75	0	23,32,32	0.97	1 (4%)
3	FBP	B	337	2	18,20,20	0.62	0	23,32,32	0.96	1 (4%)

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	AFP	A	336	3	-	0/13/32/32	0/1/1/1
3	FBP	A	337	2	-	0/13/32/32	0/1/1/1
2	AFP	B	336	3	-	0/13/32/32	0/1/1/1
3	FBP	B	337	2	-	0/13/32/32	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	336	AFP	O2P-P1-O1P	2.18	119.02	110.50
3	B	337	FBP	O2P-P1-O1P	2.18	119.03	110.50
3	A	337	FBP	O2P-P1-O1P	2.20	119.11	110.50
2	A	336	AFP	O2P-P1-O1P	2.24	119.25	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	336	AFP	1	0
3	A	337	FBP	1	0
2	B	336	AFP	1	0
3	B	337	FBP	1	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.