



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:39 PM GMT

PDB ID : 1UMI  
Title : Structural basis of sugar-recognizing ubiquitin ligase  
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Deposited on : 2003-10-01  
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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

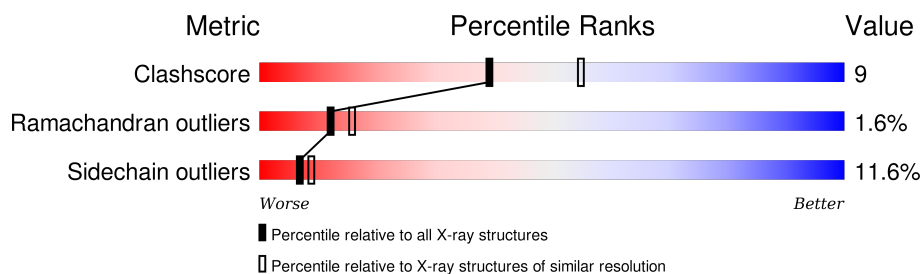
# 1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 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	184	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1562 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 F-box only protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1488	946	249	291	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	GLY	-	CLONING ARTIFACT	GB 28436805
A	115	SER	-	CLONING ARTIFACT	GB 28436805
A	116	HIS	-	CLONING ARTIFACT	GB 28436805
A	132	ALA	CYS	ENGINEERED	GB 28436805
A	151	LYS	ARG	SEE REMARK 999	GB 28436805

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			29	16	2	11		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		

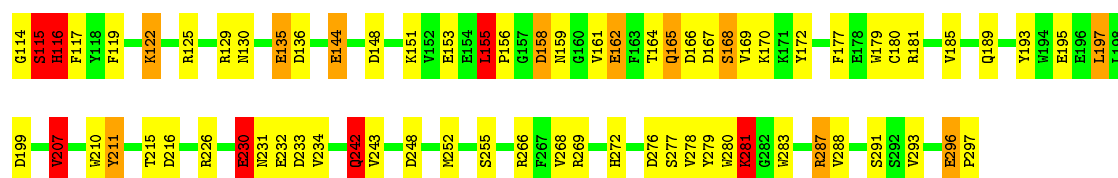
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: F-box only protein 2

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.81Å 63.81Å 147.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.72 – 2.40	Depositor
% Data completeness (in resolution range)	99.7 (58.72-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.197 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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: NAG, NDG

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	2.17	50/1532 (3.3%)	1.70	38/2080 (1.8%)

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	3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	GLU	CG-CD	13.94	1.72	1.51
1	A	135	GLU	CD-OE2	13.79	1.40	1.25
1	A	281	LYS	CE-NZ	13.40	1.82	1.49
1	A	230	GLU	CG-CD	12.87	1.71	1.51
1	A	281	LYS	CB-CG	11.62	1.83	1.52
1	A	207	VAL	CB-CG1	-10.35	1.31	1.52
1	A	279	TYR	CD2-CE2	10.27	1.54	1.39
1	A	242	GLN	CG-CD	9.86	1.73	1.51
1	A	296	GLU	CD-OE1	8.86	1.35	1.25
1	A	281	LYS	CD-CE	8.52	1.72	1.51
1	A	242	GLN	CB-CG	8.38	1.75	1.52
1	A	162	GLU	CG-CD	7.85	1.63	1.51
1	A	114	GLY	N-CA	7.76	1.57	1.46
1	A	211	TYR	CD2-CE2	7.51	1.50	1.39
1	A	189	GLN	CG-CD	7.33	1.68	1.51
1	A	193	TYR	CD2-CE2	7.29	1.50	1.39
1	A	277	SER	CB-OG	-7.26	1.32	1.42
1	A	125	ARG	NE-CZ	7.24	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	GLU	CB-CG	7.21	1.65	1.52
1	A	181	ARG	CZ-NH1	7.18	1.42	1.33
1	A	162	GLU	CD-OE1	7.14	1.33	1.25
1	A	114	GLY	C-O	-7.12	1.12	1.23
1	A	122	LYS	CE-NZ	7.04	1.66	1.49
1	A	122	LYS	CG-CD	7.01	1.76	1.52
1	A	210	TRP	CE3-CZ3	6.90	1.50	1.38
1	A	122	LYS	CD-CE	6.89	1.68	1.51
1	A	230	GLU	CD-OE2	6.87	1.33	1.25
1	A	119	PHE	CG-CD1	6.62	1.48	1.38
1	A	195	GLU	CD-OE2	6.21	1.32	1.25
1	A	280	TRP	CE3-CZ3	6.17	1.49	1.38
1	A	119	PHE	CE1-CZ	6.09	1.49	1.37
1	A	168	SER	CB-OG	-6.09	1.34	1.42
1	A	180	CYS	CB-SG	-6.06	1.72	1.82
1	A	116	HIS	N-CA	6.04	1.58	1.46
1	A	169	VAL	CB-CG2	6.04	1.65	1.52
1	A	135	GLU	CD-OE1	6.02	1.32	1.25
1	A	162	GLU	CB-CG	5.92	1.63	1.52
1	A	268	VAL	CB-CG1	-5.83	1.40	1.52
1	A	177	PHE	CD2-CE2	5.79	1.50	1.39
1	A	156	PRO	CG-CD	5.62	1.69	1.50
1	A	185	VAL	CB-CG1	5.55	1.64	1.52
1	A	125	ARG	CZ-NH1	5.33	1.40	1.33
1	A	283	TRP	CE2-CZ2	5.29	1.48	1.39
1	A	234	VAL	CB-CG2	5.27	1.64	1.52
1	A	162	GLU	CD-OE2	5.26	1.31	1.25
1	A	170	LYS	CD-CE	5.17	1.64	1.51
1	A	288	VAL	C-O	5.15	1.33	1.23
1	A	291	SER	N-CA	-5.13	1.36	1.46
1	A	266	ARG	CG-CD	5.03	1.64	1.51
1	A	230	GLU	CD-OE1	5.00	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH1	15.50	128.05	120.30
1	A	155	LEU	CA-C-N	10.90	147.63	117.10
1	A	155	LEU	C-N-CD	10.77	151.03	128.40
1	A	181	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	A	155	LEU	N-CA-C	8.12	132.93	111.00
1	A	166	ASP	CB-CG-OD2	8.12	125.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASP	CB-CG-OD2	7.83	125.35	118.30
1	A	248	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	233	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	155	LEU	CA-C-O	-7.71	103.90	120.10
1	A	216	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	122	LYS	CA-CB-CG	7.34	129.56	113.40
1	A	116	HIS	N-CA-C	7.32	130.76	111.00
1	A	252	MET	CG-SD-CE	7.30	111.87	100.20
1	A	155	LEU	C-N-CA	-7.10	92.18	122.00
1	A	158	ASP	CB-CG-OD1	-7.08	111.93	118.30
1	A	135	GLU	OE1-CD-OE2	-7.03	114.86	123.30
1	A	233	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	A	155	LEU	O-C-N	-6.80	108.19	121.10
1	A	181	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	195	GLU	CA-CB-CG	6.68	128.09	113.40
1	A	269	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	125	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	281	LYS	CD-CE-NZ	6.48	126.60	111.70
1	A	199	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	122	LYS	CD-CE-NZ	6.07	125.65	111.70
1	A	276	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	230	GLU	OE1-CD-OE2	-5.88	116.25	123.30
1	A	166	ASP	CB-CA-C	5.78	121.95	110.40
1	A	148	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	144	GLU	CA-CB-CG	5.72	125.99	113.40
1	A	207	VAL	N-CA-CB	-5.67	99.02	111.50
1	A	115	SER	N-CA-C	5.50	125.85	111.00
1	A	136	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	279	TYR	CD1-CE1-CZ	5.33	124.59	119.80
1	A	287	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	287	ARG	CG-CD-NE	-5.04	101.21	111.80
1	A	226	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	SER	Peptide
1	A	116	HIS	Peptide
1	A	155	LEU	Peptide



## 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	1488	0	1368	26	0
2	A	29	0	25	0	0
3	A	45	0	0	2	0
All	All	1562	0	1393	26	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 9.

All (26) 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:242:GLN:CG	1:A:242:GLN:CB	1.75	1.65
1:A:122:LYS:CG	1:A:122:LYS:CD	1.76	1.62
1:A:281:LYS:CG	1:A:281:LYS:CB	1.83	1.53
1:A:281:LYS:NZ	1:A:281:LYS:CE	1.82	1.42
1:A:115:SER:HB3	3:A:43:HOH:O	1.37	1.24
1:A:197:LEU:HD12	1:A:197:LEU:C	2.00	0.81
1:A:155:LEU:HD13	1:A:172:TYR:HD2	1.45	0.80
1:A:122:LYS:CD	1:A:122:LYS:CB	2.60	0.79
1:A:230:GLU:HB3	3:A:10:HOH:O	1.84	0.77
1:A:115:SER:HA	1:A:116:HIS:CB	2.14	0.76
1:A:155:LEU:HD13	1:A:172:TYR:CD2	2.29	0.66
1:A:197:LEU:HD12	1:A:197:LEU:O	1.95	0.65
1:A:231:ASN:O	1:A:232:GLU:HB2	2.05	0.57
1:A:115:SER:HA	1:A:116:HIS:HB2	1.88	0.54
1:A:197:LEU:CD1	1:A:197:LEU:C	2.79	0.49
1:A:117:PHE:CD1	1:A:297:PRO:HB2	2.51	0.46
1:A:117:PHE:CE1	1:A:297:PRO:HB2	2.51	0.45
1:A:159:ASN:HB3	1:A:215:THR:OG1	2.17	0.45
1:A:122:LYS:CD	1:A:122:LYS:HB2	2.48	0.44
1:A:207:VAL:HG22	1:A:293:VAL:HG22	1.99	0.44
1:A:281:LYS:CG	1:A:281:LYS:CA	2.86	0.43
1:A:179:TRP:HZ2	1:A:242:GLN:HG3	1.84	0.43
1:A:151:LYS:HE3	1:A:153:GLU:OE2	2.19	0.42
1:A:164:THR:O	1:A:165:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:ND2	1:A:135:GLU:H	2.19	0.41
1:A:211:TYR:HA	1:A:287:ARG:O	2.21	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	182/184 (99%)	169 (93%)	10 (6%)	3 (2%)	12 16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	165	GLN
1	A	167	ASP

### 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	155/155 (100%)	137 (88%)	18 (12%)	7 9

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	129	ARG
1	A	144	GLU
1	A	155	LEU
1	A	158	ASP
1	A	161	VAL
1	A	162	GLU
1	A	168	SER
1	A	197	LEU
1	A	207	VAL
1	A	230	GLU
1	A	242	GLN
1	A	243	VAL
1	A	255	SER
1	A	272	HIS
1	A	278	VAL
1	A	281	LYS
1	A	296	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	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](#)

2 carbohydrates 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	NDG	A	298	2	15,15,15	2.04	5 (33%)	17,21,21	2.98	9 (52%)
2	NAG	A	299	2	14,14,15	1.49	2 (14%)	15,19,21	3.03	7 (46%)

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	NDG	A	298	2	-	0/6/26/26	0/1/1/1
2	NAG	A	299	2	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	299	NAG	O7-C7	-3.41	1.15	1.23
2	A	298	NDG	O6-C6	-3.32	1.28	1.42
2	A	298	NDG	O-C1	-2.92	1.37	1.43
2	A	299	NAG	O5-C1	-2.82	1.39	1.43
2	A	298	NDG	O-C5	-2.13	1.39	1.44
2	A	298	NDG	C8-C7	2.12	1.54	1.50
2	A	298	NDG	O1L-C1	4.27	1.54	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	NAG	O7-C7-C8	-6.66	109.84	122.06
2	A	298	NDG	O1L-C1-O	-3.53	100.58	110.25
2	A	298	NDG	C8-C7-N2	-3.15	110.07	116.11
2	A	298	NDG	O3-C3-C4	2.00	114.84	110.34
2	A	299	NAG	O3-C3-C2	2.48	114.02	109.11
2	A	298	NDG	O4-C4-C5	2.61	116.16	109.24
2	A	298	NDG	C4-C3-C2	2.79	114.30	110.43
2	A	299	NAG	C4-C3-C2	2.79	115.57	111.23
2	A	298	NDG	O6-C6-C5	3.01	121.28	111.33
2	A	299	NAG	O4-C4-C3	3.54	118.30	110.34
2	A	298	NDG	O-C5-C6	3.65	115.58	106.36
2	A	298	NDG	O7-C7-N2	3.68	129.37	121.86
2	A	299	NAG	C2-N2-C7	4.13	128.35	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	NAG	O7-C7-N2	4.29	130.60	121.86
2	A	299	NAG	C1-O5-C5	4.41	117.84	112.25
2	A	298	NDG	O-C5-C4	8.12	124.91	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.