



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:31 PM GMT

PDB ID : 1B52
Title : OLIGO-PEPTIDE BINDING PROTEIN (OPPA) COMPLEXED WITH KTK
Authors : Tame, J.R.H.; Wilkinson, A.J.
Deposited on : 1999-01-11
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

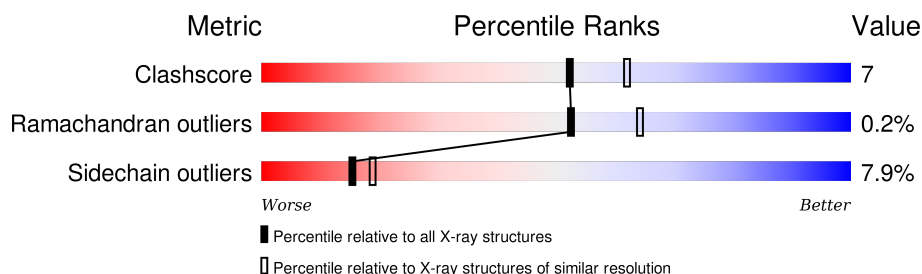
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 ≥ 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	517	 73% 22% •
2	B	3	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4301 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.

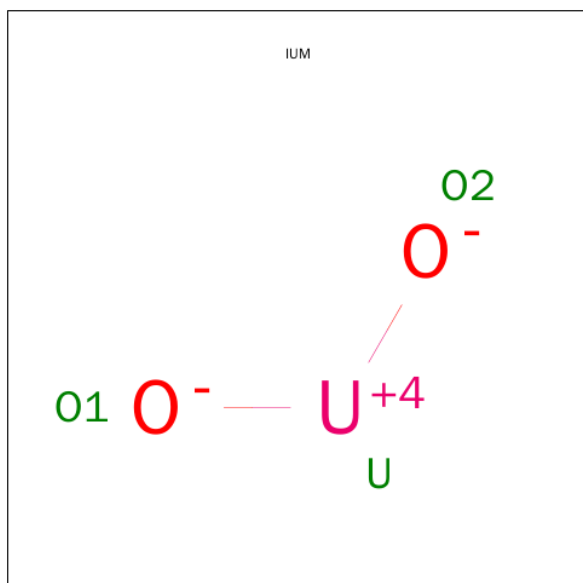
- Molecule 1 is a protein called PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	1	0	0
			4148	2656	697	790	5			

- Molecule 2 is a protein called PROTEIN (LYS-THR-LYS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			26	16	5	5			

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		

- Molecule 4 is water.

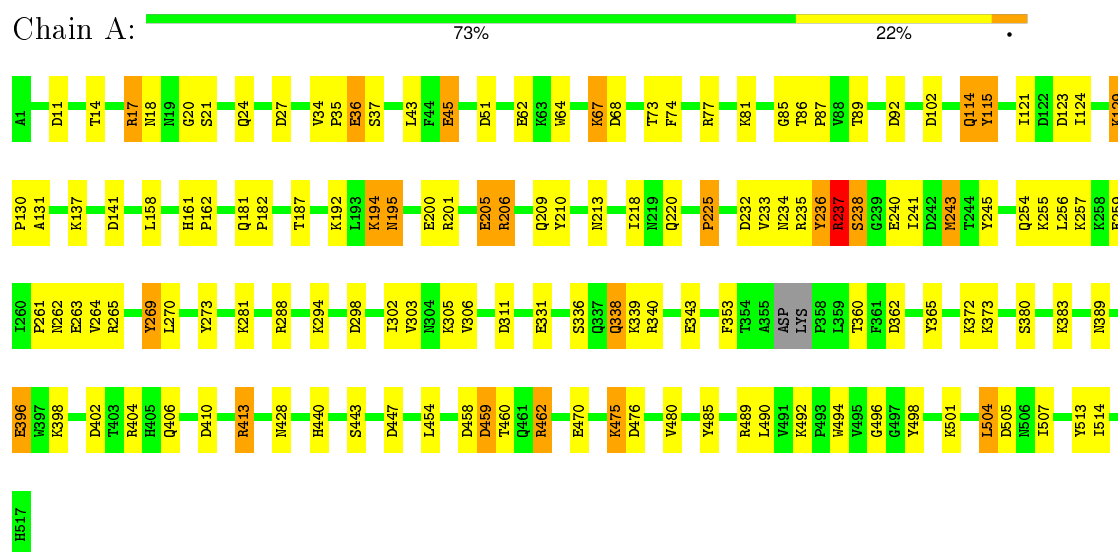
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total 122	O 122	0	0
4	B	3	Total 3	O 3	0	0

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 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 ($RSRZ > 2$). 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: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



• Molecule 2: PROTEIN (LYS-THR-LYS)



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2 A	Depositor
Cell constants a, b, c, α , β , γ	106.35Å 76.80Å 69.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	98.5 (15.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4301	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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: IUM

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	1/4258 (0.0%)	1.65	57/5804 (1.0%)
2	B	0.93	0/25	1.33	0/29
All	All	0.76	1/4283 (0.0%)	1.65	57/5833 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	PHE	C-O	-14.54	0.95	1.23

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ARG	NE-CZ-NH2	-15.65	112.47	120.30
1	A	362	ASP	CB-CG-OD2	15.11	131.90	118.30
1	A	362	ASP	CB-CG-OD1	-14.75	105.03	118.30
1	A	265	ARG	CD-NE-CZ	14.64	144.10	123.60
1	A	340	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	298	ASP	CB-CG-OD2	-11.57	107.89	118.30
1	A	447	ASP	CB-CG-OD1	10.57	127.81	118.30
1	A	17	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	353	PHE	O-C-N	-10.41	106.04	122.70
1	A	265	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	A	353	PHE	CA-C-O	10.33	141.80	120.10
1	A	288	ARG	NE-CZ-NH2	9.59	125.10	120.30
1	A	237	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	77	ARG	CD-NE-CZ	8.99	136.19	123.60
1	A	102	ASP	CB-CG-OD1	8.66	126.09	118.30
1	A	17	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	288	ARG	CD-NE-CZ	8.05	134.87	123.60
1	A	102	ASP	CB-CG-OD2	-7.82	111.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	413	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	459	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	413	ARG	CD-NE-CZ	7.40	133.96	123.60
1	A	27	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	343	GLU	CG-CD-OE1	7.03	132.36	118.30
1	A	476	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	462	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	A	158	LEU	CB-CA-C	-6.98	96.93	110.20
1	A	245	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	A	206	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	236	TYR	CB-CG-CD1	6.77	125.06	121.00
1	A	114	GLN	CB-CG-CD	6.58	128.71	111.60
1	A	288	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	A	237	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	195	ASN	N-CA-CB	6.39	122.10	110.60
1	A	36	GLU	OE1-CD-OE2	-6.33	115.70	123.30
1	A	51	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	413	ARG	CG-CD-NE	-6.24	98.70	111.80
1	A	458	ASP	N-CA-CB	-6.20	99.44	110.60
1	A	489	ARG	NH1-CZ-NH2	6.17	126.19	119.40
1	A	485	TYR	CA-CB-CG	6.07	124.93	113.40
1	A	498	TYR	CB-CG-CD1	5.96	124.58	121.00
1	A	273	TYR	CB-CG-CD1	5.92	124.56	121.00
1	A	45	GLU	OE1-CD-OE2	-5.91	116.20	123.30
1	A	410	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	302	ILE	CB-CG1-CD1	-5.57	98.30	113.90
1	A	115	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	A	470	GLU	CG-CD-OE1	5.46	129.23	118.30
1	A	137	LYS	CA-CB-CG	5.45	125.38	113.40
1	A	331	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	A	210	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	27	ASP	OD1-CG-OD2	-5.37	113.09	123.30
1	A	269	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	447	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	A	269	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	475	LYS	N-CA-CB	5.31	120.16	110.60
1	A	413	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	505	ASP	CB-CG-OD2	5.11	122.90	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	4148	0	4059	55	0
2	B	26	0	35	0	0
3	A	2	0	0	0	0
4	A	122	0	0	4	0
4	B	3	0	0	0	0
All	All	4301	0	4094	55	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 (55) 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:37:SER:HB2	4:A:578:HOH:O	1.70	0.90
1:A:17:ARG:HG2	1:A:243:MET:HG3	1.68	0.75
1:A:402:ASP:HB2	4:A:641:HOH:O	1.91	0.69
1:A:129:LYS:HB3	1:A:130:PRO:HD2	1.76	0.67
1:A:236:TYR:CZ	1:A:492:LYS:HD3	2.31	0.66
1:A:206:ARG:HD3	1:A:213:ASN:OD1	1.94	0.66
1:A:194:LYS:HG3	1:A:205:GLU:HG2	1.79	0.65
1:A:365:TYR:OH	1:A:372:LYS:HG3	2.01	0.60
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.37	0.58
1:A:234:ASN:ND2	4:A:615:HOH:O	2.08	0.57
1:A:200:GLU:O	1:A:201:ARG:HB3	2.05	0.56
1:A:238:SER:OG	1:A:240:GLU:HG3	2.06	0.56
1:A:236:TYR:CE2	1:A:492:LYS:HD3	2.40	0.55
1:A:263:GLU:O	1:A:490:LEU:HA	2.05	0.55
1:A:67:LYS:O	1:A:68:ASP:HB2	2.09	0.53
1:A:85:GLY:HA2	1:A:209:GLN:NE2	2.25	0.51
1:A:235:ARG:HB2	1:A:241:ILE:HD12	1.93	0.50
1:A:270:LEU:HD12	1:A:504:LEU:CD2	2.42	0.49
1:A:396:GLU:HB2	4:A:634:HOH:O	2.12	0.49
1:A:192:LYS:HG2	1:A:205:GLU:O	2.12	0.49
1:A:194:LYS:HG3	1:A:205:GLU:CG	2.42	0.48
1:A:459:ASP:OD1	1:A:462:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:NE2	1:A:182:PRO:HD2	2.30	0.47
1:A:89:THR:O	1:A:92:ASP:HB2	2.14	0.47
1:A:114:GLN:HA	1:A:121:ILE:HG21	1.95	0.47
1:A:129:LYS:HB3	1:A:130:PRO:CD	2.44	0.47
1:A:43:LEU:O	1:A:187:THR:HB	2.15	0.47
1:A:338:GLN:HG3	1:A:339:LYS:N	2.30	0.46
1:A:89:THR:HB	1:A:141:ASP:O	2.16	0.46
1:A:20:GLY:O	1:A:21:SER:HB3	2.16	0.45
1:A:86:THR:HB	1:A:87:PRO:CD	2.46	0.45
1:A:360:THR:HA	1:A:389:ASN:O	2.17	0.44
1:A:492:LYS:HG3	1:A:494:TRP:CZ2	2.53	0.44
1:A:218:ILE:HD11	1:A:514:ILE:HG12	2.00	0.44
1:A:124:ILE:HD13	1:A:131:ALA:HA	2.00	0.44
1:A:123:ASP:HB3	1:A:129:LYS:HG3	2.00	0.44
1:A:64:TRP:HA	1:A:73:THR:O	2.18	0.44
1:A:218:ILE:HD11	1:A:514:ILE:CD1	2.48	0.44
1:A:257:LYS:HZ2	1:A:264:VAL:HG11	1.83	0.43
1:A:257:LYS:O	1:A:261:PRO:HD3	2.17	0.43
1:A:129:LYS:CB	1:A:130:PRO:HD2	2.45	0.43
1:A:129:LYS:CB	1:A:130:PRO:CD	2.97	0.43
1:A:24:GLN:HG3	1:A:36:GLU:OE2	2.19	0.43
1:A:237:ARG:NH1	1:A:259:GLU:OE1	2.51	0.43
1:A:294:LYS:HA	1:A:480:VAL:HG13	2.00	0.43
1:A:64:TRP:HB3	1:A:74:PHE:CD2	2.55	0.42
1:A:496:GLY:HA3	1:A:513:TYR:CE1	2.54	0.42
1:A:303:VAL:HG13	1:A:311:ASP:HB2	2.02	0.41
1:A:233:VAL:HG11	1:A:256:LEU:HD11	2.02	0.41
1:A:404:ARG:O	1:A:440:HIS:HE1	2.03	0.41
1:A:161:HIS:CD2	1:A:162:PRO:HD2	2.56	0.41
1:A:34:VAL:N	1:A:35:PRO:CD	2.84	0.41
1:A:14:THR:HG22	1:A:220:GLN:HB3	2.04	0.40
1:A:18:ASN:HD22	1:A:232:ASP:CG	2.24	0.40
1:A:233:VAL:HG22	1:A:490:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	511/517 (99%)	480 (94%)	30 (6%)	1 (0%)	52	64
2	B	1/3 (33%)	1 (100%)	0	0	100	100
All	All	512/520 (98%)	481 (94%)	30 (6%)	1 (0%)	52	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO

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	453/455 (100%)	417 (92%)	36 (8%)	15	19
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	456/458 (100%)	420 (92%)	36 (8%)	15	19

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	45	GLU
1	A	62	GLU
1	A	67	LYS
1	A	81	LYS

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Mol	Chain	Res	Type
1	A	129	LYS
1	A	194	LYS
1	A	195	ASN
1	A	205	GLU
1	A	225	PRO
1	A	237	ARG
1	A	238	SER
1	A	243	MET
1	A	254	GLN
1	A	255	LYS
1	A	262	ASN
1	A	269	TYR
1	A	281	LYS
1	A	305	LYS
1	A	306	VAL
1	A	336	SER
1	A	338	GLN
1	A	373	LYS
1	A	380	SER
1	A	383	LYS
1	A	396	GLU
1	A	398	LYS
1	A	406	GLN
1	A	413	ARG
1	A	443	SER
1	A	454	LEU
1	A	460	THR
1	A	475	LYS
1	A	501	LYS
1	A	504	LEU
1	A	507	ILE

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

Mol	Chain	Res	Type
1	A	161	HIS
1	A	181	GLN
1	A	199	ASN
1	A	209	GLN
1	A	262	ASN
1	A	279	ASN
1	A	308	ASN

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Mol	Chain	Res	Type
1	A	338	GLN
1	A	395	GLN
1	A	440	HIS

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 ⓘ

Of 2 ligands modelled in this entry, 2 are modelled with single atom - leaving 0 for Mogul analysis.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.