wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 03:19 PM EDT

PDB ID	:	1KX5
Title	:	X-Ray Structure of the Nucleosome Core Particle, NCP147, at 1.9 A Resolution
Authors	:	Davey, C.A.; Sargent, D.F.; Luger, K.; Maeder, A.W.; Richmond, T.J.
Deposited on	:	2002-01-31
Resolution	:	1.94 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

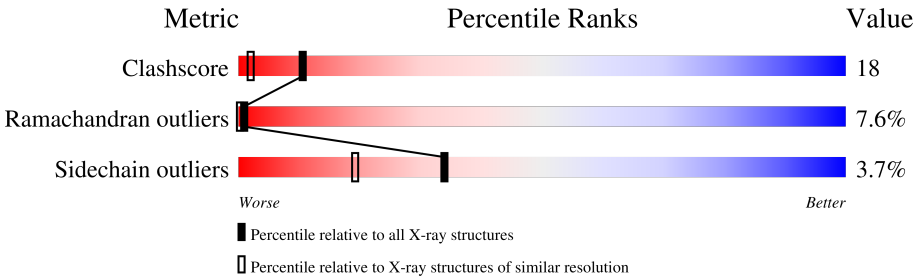
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	147	54% 46%
2	J	147	55% 42% .
3	A	135	69% 26% . .
3	E	135	77% 15% 7% .
4	B	102	75% 20% . .
4	F	102	78% 19% . .
5	C	128	84% 12% . .
5	G	128	74% 23% .

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Mol	Chain	Length	Quality of chain
6	D	125	
6	H	125	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16755 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 DNA chain called DNA (5'(ATCAATATCCACCTGCAGATACTACCAA AAGTGTATTTGGAAACTGCTCCATCAAAAGGCATGTTCAGCTGGAATCCAGCT GAACATGCCTTTTGATGGAGCAGTTTCCAAATACACTTTTGGTAGTATCTGCA GGTGGATATTGAT)3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	147	Total	C	N	O	P	0	0	0
			3011	1440	546	879	146			

- Molecule 2 is a DNA chain called DNA (5'(ATCAATATCCACCTGCAGATACTACCAA AAGTGTATTTGGAAACTGCTCCATCAAAAGGCATGTTCAGCTGGATTCCAGCT GAACATGCCTTTTGATGGAGCAGTTTCCAAATACACTTTTGGTAGTATCTGCA GGTGGATATTGAT)3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	147	Total	C	N	O	P	0	0	0
			3010	1440	543	881	146			

- Molecule 3 is a protein called histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	135	Total	C	N	O	S	134	0	0
			1074	670	215	186	3			
3	E	135	Total	C	N	O	S	94	0	0
			1074	670	215	186	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P16105
E	102	ALA	GLY	conflict	UNP P16105

- Molecule 4 is a protein called histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	102	Total	C	N	O	S	74	0	0
			792	494	163	134	1			
4	F	102	Total	C	N	O	S	42	0	0
			792	494	163	134	1			

- Molecule 5 is a protein called histone H2A.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	128	Total	C	N	O	98	0	0
			978	608	195	175			
5	G	128	Total	C	N	O	105	0	0
			978	608	195	175			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	variant	UNP P06897
C	123	SER	ALA	conflict	UNP P06897
C	?	-	ALA	deletion	UNP P06897
G	99	ARG	GLY	variant	UNP P06897
G	123	SER	ALA	conflict	UNP P06897
G	?	-	ALA	deletion	UNP P06897

- Molecule 6 is a protein called histone H2B.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	122	Total	C	N	O	S	106	0	0
			949	595	178	174	2			
6	H	122	Total	C	N	O	S	139	0	0
			949	595	178	174	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	variant	UNP P02281
H	29	THR	SER	variant	UNP P02281

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	7	Total	Mn	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	6	Total Mn 6 6	0	0
7	E	1	Total Mn 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0
8	E	1	Total Cl 1 1	0	0
8	H	1	Total Cl 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	780	Total O 780 780	0	0
9	J	802	Total O 802 802	0	0
9	A	219	Total O 219 219	0	0
9	B	129	Total O 129 129	0	0
9	C	214	Total O 214 214	0	0
9	D	196	Total O 196 196	0	0
9	E	221	Total O 221 221	0	0
9	F	202	Total O 202 202	0	0
9	G	188	Total O 188 188	0	0
9	H	179	Total O 179 179	0	0

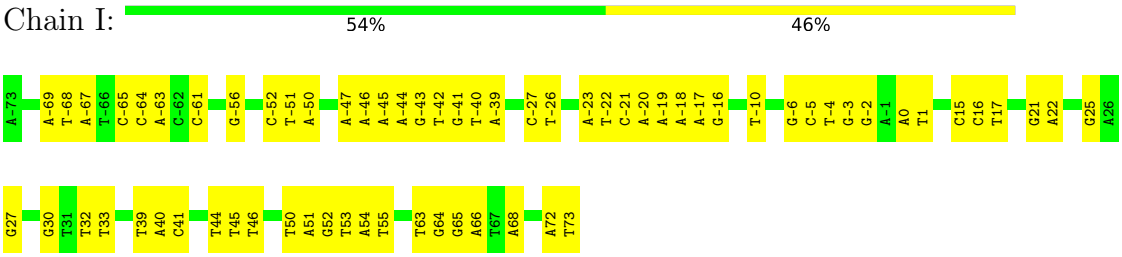
3 Residue-property plots (i)

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.

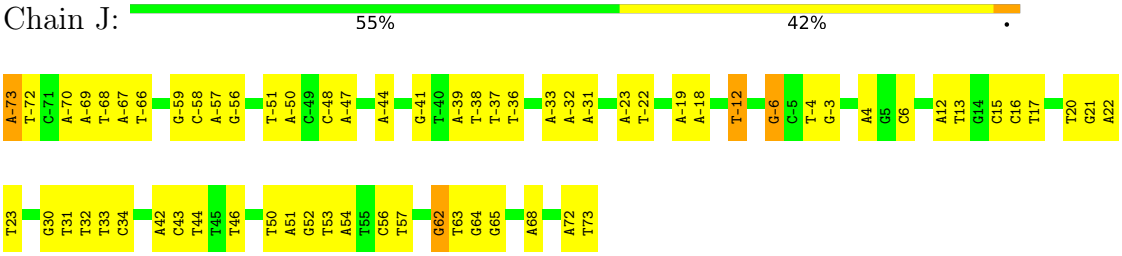
• Molecule 1: DNA (5'(ATCAATATCCACCTGCAGATACTACCAAAAGTGTATTTGGAAA CTGCTCCATCAAAAGGCATGTTCAGCTGGAATCCAGCTGAACATGCCTTTTGATGGA GCAGTTTCCAAATACACTTTTGGTAGTATCTGCAGGTGGATATTGAT)3')

Chain I:



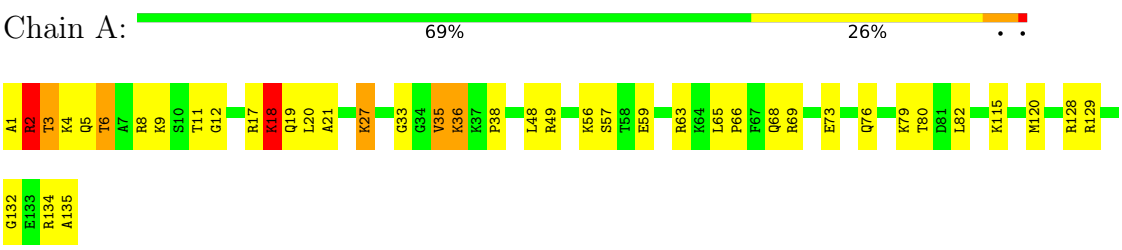
• Molecule 2: DNA (5'(ATCAATATCCACCTGCAGATACTACCAAAAGTGTATTTGGAAA CTGCTCCATCAAAAGGCATGTTCAGCTGGATTCCAGCTGAACATGCCTTTTGATGGA GCAGTTTCCAAATACACTTTTGGTAGTATCTGCAGGTGGATATTGAT)3')

Chain J:



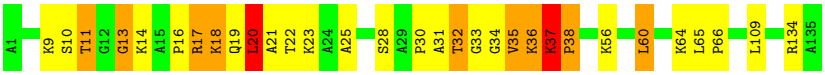
• Molecule 3: histone H3

Chain A:



• Molecule 3: histone H3

Chain E:

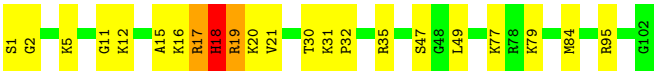


• Molecule 4: histone H4

Chain B:

• Molecule 4: histone H4

Chain F:

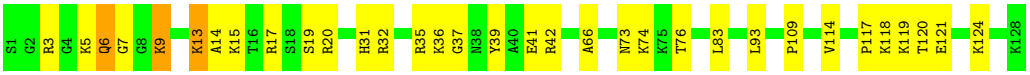


• Molecule 5: histone H2A.1

Chain C:

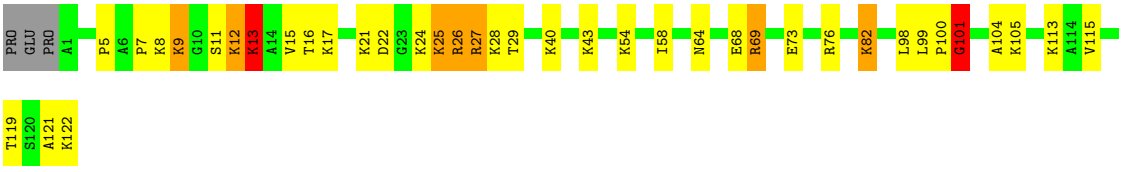
• Molecule 5: histone H2A.1

Chain G:



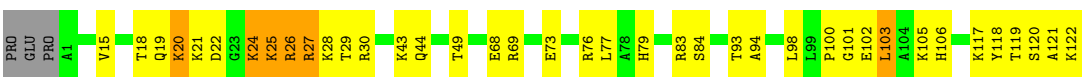
• Molecule 6: histone H2B.2

Chain D:



• Molecule 6: histone H2B.2

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.95Å 181.17Å 109.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.94	Depositor
% Data completeness (in resolution range)	95.6 (6.00-1.94)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16755	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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: CL, MN

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	I	0.41	0/3378	0.76	0/5212
2	J	0.42	0/3376	0.76	1/5209 (0.0%)
3	A	0.52	0/1088	0.68	0/1455
3	E	0.59	0/1088	0.79	2/1455 (0.1%)
4	B	0.53	0/800	0.75	0/1061
4	F	0.63	0/800	0.78	0/1061
5	C	0.57	0/988	0.68	0/1322
5	G	0.44	0/988	0.63	0/1322
6	D	0.56	0/962	0.71	3/1284 (0.2%)
6	H	0.44	0/962	0.62	0/1284
All	All	0.48	0/14430	0.73	6/20665 (0.0%)

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	I	0	1
2	J	0	7
All	All	0	8

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	37	LYS	N-CA-C	5.62	126.16	111.00
3	E	20	LEU	N-CA-C	5.39	125.55	111.00
6	D	69	ARG	NE-CZ-NH2	-5.36	117.62	120.30
6	D	101	GLY	N-CA-C	5.13	125.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	76	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	-6	DG	Sidechain
2	J	-12	DT	Sidechain
2	J	-3	DG	Sidechain
2	J	-6	DG	Sidechain
2	J	-73	DA	Sidechain

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	I	3011	0	1662	84	0
2	J	3010	0	1663	81	0
3	A	1074	0	1151	55	0
3	E	1074	0	1151	34	0
4	B	792	0	855	38	0
4	F	792	0	855	30	0
5	C	978	0	1054	33	0
5	G	978	0	1054	28	0
6	D	949	0	1017	49	0
6	H	949	0	1017	52	0
7	E	1	0	0	0	0
7	I	7	0	0	0	0
7	J	6	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	H	1	0	0	0	0
9	A	219	0	0	8	0
9	B	129	0	0	6	0
9	C	214	0	0	4	0
9	D	196	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	221	0	0	11	0
9	F	202	0	0	8	0
9	G	188	0	0	7	0
9	H	179	0	0	8	0
9	I	780	0	0	15	0
9	J	802	0	0	23	0
All	All	16755	0	11479	431	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 18.

The worst 5 of 431 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:I:72:DA:H2"	1:I:73:DT:H5"	1.25	1.14
6:D:13:LYS:HG3	6:D:25:LYS:HA	1.25	1.12
5:C:12:ALA:HB1	5:C:15:LYS:HB3	1.29	1.07
1:I:-42:DT:OP1	5:C:12:ALA:HB3	1.60	1.00
5:C:12:ALA:CB	5:C:15:LYS:HB3	1.92	0.99

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	
3	A	133/135 (98%)	106 (80%)	14 (10%)	13 (10%)	0	0
3	E	133/135 (98%)	105 (79%)	12 (9%)	16 (12%)	0	0
4	B	100/102 (98%)	83 (83%)	8 (8%)	9 (9%)	1	0
4	F	100/102 (98%)	88 (88%)	8 (8%)	4 (4%)	3	0
5	C	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	G	126/128 (98%)	106 (84%)	15 (12%)	5 (4%)	3 0
6	D	120/125 (96%)	101 (84%)	7 (6%)	12 (10%)	0 0
6	H	120/125 (96%)	104 (87%)	6 (5%)	10 (8%)	1 0
All	All	958/980 (98%)	806 (84%)	79 (8%)	73 (8%)	1 0

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	2	ARG
3	A	3	THR
3	A	4	LYS
4	B	24	ASP
6	D	5	PRO

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
3	A	110/110 (100%)	105 (96%)	5 (4%)	27 12
3	E	110/110 (100%)	106 (96%)	4 (4%)	35 20
4	B	78/78 (100%)	76 (97%)	2 (3%)	46 32
4	F	78/78 (100%)	75 (96%)	3 (4%)	33 18
5	C	101/101 (100%)	96 (95%)	5 (5%)	24 9
5	G	101/101 (100%)	96 (95%)	5 (5%)	24 9
6	D	102/105 (97%)	99 (97%)	3 (3%)	42 28
6	H	102/105 (97%)	100 (98%)	2 (2%)	55 42
All	All	782/788 (99%)	753 (96%)	29 (4%)	34 19

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	82	LYS

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Mol	Chain	Res	Type
6	H	25	LYS
3	E	60	LEU
5	G	9	LYS
3	E	36	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	110	ASN
6	H	92	GLN
6	D	92	GLN
3	E	125	GLN
5	G	6	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 18 are monoatomic - 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 (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.