



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 12:08 am GMT

PDB ID : 1A12
Title : REGULATOR OF CHROMOSOME CONDENSATION (RCC1) OF HUMAN
Authors : Renault, L.; Nassar, N.; Vetter, I.; Becker, J.; Roth, M.; Wittinghofer, A.
Deposited on : 1997-12-19
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

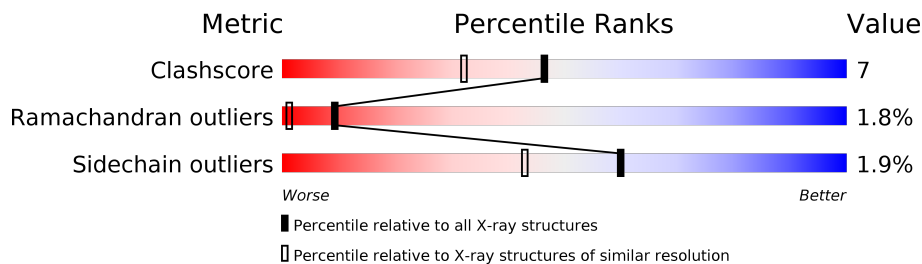
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	122078	4165 (1.70-1.70)
Ramachandran outliers	120005	4098 (1.70-1.70)
Sidechain outliers	119972	4098 (1.70-1.70)

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	413	
1	B	413	
1	C	413	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9884 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 REGULATOR OF CHROMOSOME CONDENSATION 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3000	1867	532	582	19			
1	B	401	Total	C	N	O	S	0	0	0
			3000	1867	532	582	19			
1	C	401	Total	C	N	O	S	0	0	0
			3000	1867	532	582	19			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	296	Total	O	0	0
			296	296		
2	B	309	Total	O	0	0
			309	309		
2	C	279	Total	O	0	0
			279	279		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.96Å 82.90Å 83.11Å 112.88° 104.09° 103.42°	Depositor
Resolution (Å)	41.00 – 1.70	Depositor
% Data completeness (in resolution range)	92.0 (41.00-1.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.189 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9884	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.53	0/3055	0.70	3/4121 (0.1%)
1	B	0.60	4/3055 (0.1%)	0.80	7/4121 (0.2%)
1	C	0.94	3/3055 (0.1%)	1.21	7/4121 (0.2%)
All	All	0.71	7/9165 (0.1%)	0.93	17/12363 (0.1%)

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	1
1	B	0	2
1	C	0	4
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	209	GLU	C-N	-36.07	0.51	1.34
1	C	210	LEU	C-N	-19.57	0.89	1.34
1	C	209	GLU	C-O	8.14	1.38	1.23
1	B	420	GLN	N-CA	-7.82	1.30	1.46
1	B	216	GLY	N-CA	5.81	1.54	1.46
1	B	219	GLY	N-CA	5.51	1.54	1.46
1	B	215	GLY	CA-C	5.40	1.60	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	GLU	O-C-N	-52.78	38.25	122.70
1	C	210	LEU	O-C-N	-32.34	70.95	122.70
1	C	210	LEU	CA-C-N	9.96	139.11	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	GLU	O-C-N	9.26	137.51	122.70
1	B	419	GLU	CA-C-N	-7.72	100.22	117.20
1	C	210	LEU	C-N-CA	7.25	139.82	121.70
1	A	235	GLY	O-C-N	6.97	133.85	122.70
1	B	57	ARG	C-N-CA	6.71	138.48	121.70
1	B	234	ARG	O-C-N	6.46	134.19	123.20
1	C	209	GLU	C-N-CA	-6.43	105.62	121.70
1	A	235	GLY	N-CA-C	-5.65	98.97	113.10
1	C	149	ASN	C-N-CA	5.51	135.46	121.70
1	B	232	LYS	O-C-N	5.41	131.35	122.70
1	A	235	GLY	CA-C-N	-5.36	105.41	117.20
1	B	148	ASP	N-CA-C	-5.29	96.70	111.00
1	B	218	GLN	O-C-N	5.28	132.17	123.20
1	C	209	GLU	CA-C-O	-5.16	109.26	120.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	VAL	Mainchain
1	B	231	LEU	Mainchain
1	B	291	ASN	Mainchain
1	C	209	GLU	Mainchain
1	C	210	LEU	Mainchain
1	C	228	CYS	Mainchain
1	C	43	GLY	Mainchain

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	3000	0	2952	29	0
1	B	3000	0	2952	53	0
1	C	3000	0	2950	42	0
2	A	296	0	0	9	0
2	B	309	0	0	10	0
2	C	279	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9884	0	8854	122	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 (122) 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:B:233:SER:O	1:B:235:GLY:N	2.12	0.83
1:A:200:GLU:HG3	2:A:611:HOH:O	1.83	0.77
1:C:295:SER:HA	2:C:635:HOH:O	1.88	0.72
1:B:400:VAL:HG13	1:B:418:LYS:HG3	1.73	0.71
1:B:221:GLU:OE2	2:B:675:HOH:O	2.08	0.71
1:C:57:ARG:NE	1:C:57:ARG:HA	2.06	0.70
1:C:166:VAL:HG13	2:C:598:HOH:O	1.91	0.69
1:B:362:LYS:NZ	2:B:653:HOH:O	2.11	0.69
1:C:84:LYS:HD2	2:C:699:HOH:O	1.93	0.67
1:C:218:GLN:HG3	2:C:666:HOH:O	1.95	0.67
1:A:231:LEU:HD11	1:A:283:PRO:HB2	1.75	0.67
1:C:218:GLN:HB2	2:C:616:HOH:O	1.94	0.66
1:A:120:LYS:HE3	2:A:702:HOH:O	1.96	0.66
1:B:392:MET:O	2:B:477:HOH:O	2.12	0.66
1:A:291:ASN:O	2:A:666:HOH:O	2.13	0.66
1:B:208:PRO:HD2	1:B:211:PHE:HD2	1.61	0.65
1:C:234:ARG:O	1:C:235:GLY:C	2.35	0.64
1:A:258:GLU:O	1:B:292:SER:HB3	1.98	0.64
1:B:236:SER:O	1:B:237:ARG:HB2	2.00	0.61
1:B:207:VAL:HG13	1:B:211:PHE:HB2	1.82	0.60
1:A:208:PRO:HG2	1:A:209:GLU:H	1.67	0.58
1:B:399:ARG:HG2	1:B:417:ASP:HA	1.85	0.58
1:B:292:SER:OG	2:B:718:HOH:O	2.17	0.58
1:C:215:GLY:O	2:C:616:HOH:O	2.17	0.57
1:C:21:LYS:HG2	1:C:22:LYS:H	1.68	0.57
1:B:119:GLU:HG3	1:B:139:ARG:HH12	1.68	0.56
1:C:213:ASN:HB3	2:C:613:HOH:O	2.06	0.56
1:B:210:LEU:H	1:B:210:LEU:HD12	1.69	0.56
1:C:196:LEU:HD23	1:C:226:PRO:HG3	1.88	0.55
1:B:236:SER:O	1:B:237:ARG:CB	2.55	0.55
1:B:196:LEU:HD23	1:B:226:PRO:HG3	1.88	0.55
1:C:237:ARG:NH1	1:C:237:ARG:HB2	2.22	0.55
1:A:366:VAL:HG13	1:A:391:MET:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:HD2	2:A:618:HOH:O	2.08	0.54
1:B:231:LEU:HD11	1:B:283:PRO:HB2	1.90	0.54
1:C:148:ASP:OD2	2:C:655:HOH:O	2.18	0.54
1:B:139:ARG:HG2	2:B:640:HOH:O	2.08	0.53
1:A:234:ARG:HH12	1:A:285:ASN:HD22	1.57	0.53
1:A:266:LEU:HD12	2:A:577:HOH:O	2.09	0.53
1:B:116:GLU:HG3	2:B:657:HOH:O	2.08	0.53
1:B:291:ASN:HD22	1:C:292:SER:HB3	1.74	0.52
1:B:420:GLN:O	1:B:421:SER:C	2.47	0.52
1:C:227:LYS:HD2	2:C:596:HOH:O	2.08	0.52
1:B:180:GLY:HA3	1:B:183:HIS:CE1	2.45	0.52
1:C:142:LEU:HG	1:C:155:LEU:HD11	1.91	0.52
1:A:196:LEU:CD2	1:A:226:PRO:HG3	2.40	0.52
1:A:234:ARG:O	1:A:235:GLY:C	2.47	0.52
1:B:287:THR:HA	1:B:290:LYS:HG3	1.92	0.52
1:C:196:LEU:CD2	1:C:226:PRO:HG3	2.42	0.50
1:C:180:GLY:HA3	1:C:183:HIS:CE1	2.46	0.50
1:C:211:PHE:O	1:C:215:GLY:HA2	2.13	0.49
1:C:366:VAL:HG13	1:C:391:MET:HB2	1.94	0.49
1:B:232:LYS:O	1:B:238:GLY:O	2.30	0.49
1:B:232:LYS:O	1:B:239:HIS:HA	2.13	0.49
1:B:207:VAL:HG21	1:B:223:LEU:CD2	2.42	0.49
1:B:231:LEU:HB3	1:B:232:LYS:HD2	1.95	0.49
1:A:147:ARG:HD2	2:A:466:HOH:O	2.14	0.48
1:A:25:VAL:HG23	2:A:580:HOH:O	2.14	0.48
1:C:87:GLN:HG2	1:C:114:LYS:HD2	1.94	0.48
1:B:399:ARG:CA	1:B:418:LYS:HB2	2.44	0.48
1:C:374:ASN:O	1:C:375:TYR:HB2	2.14	0.48
1:C:21:LYS:HG2	1:C:22:LYS:N	2.30	0.47
1:C:87:GLN:HE21	1:C:88:VAL:H	1.63	0.47
1:A:234:ARG:NH1	1:A:285:ASN:HD22	2.13	0.47
1:B:142:LEU:HG	1:B:155:LEU:HD11	1.97	0.47
1:A:395:GLN:O	1:A:399:ARG:HD2	2.16	0.46
1:C:217:ARG:HG2	1:C:218:GLN:N	2.30	0.46
1:B:120:LYS:NZ	2:B:527:HOH:O	2.48	0.46
1:B:196:LEU:CD2	1:B:226:PRO:HG3	2.45	0.46
1:B:290:LYS:O	1:B:292:SER:N	2.48	0.46
1:C:269:TYR:O	1:C:319:GLY:HA2	2.15	0.46
1:C:395:GLN:O	1:C:399:ARG:HD2	2.15	0.46
1:B:213:ASN:O	1:B:214:ARG:HB2	2.15	0.46
1:C:237:ARG:HH11	1:C:237:ARG:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:MET:HG3	2:A:645:HOH:O	2.15	0.46
1:A:233:SER:O	1:A:234:ARG:O	2.34	0.45
1:C:24:LYS:NZ	2:C:560:HOH:O	2.45	0.45
1:C:149:ASN:OD1	1:C:150:ASN:N	2.49	0.45
1:B:221:GLU:O	1:B:225:VAL:HG23	2.17	0.45
1:B:366:VAL:HG13	1:B:391:MET:HB2	1.99	0.45
1:B:185:VAL:HG12	1:B:195:THR:HG22	1.99	0.44
1:B:60:PRO:O	1:B:395:GLN:HG3	2.17	0.44
1:C:185:VAL:HG12	1:C:195:THR:HG22	1.98	0.44
1:C:207:VAL:HG22	1:C:222:ARG:NH1	2.32	0.44
1:A:209:GLU:HG2	1:A:210:LEU:N	2.33	0.44
1:A:212:ALA:O	1:A:213:ASN:HB3	2.17	0.44
1:B:234:ARG:CG	1:B:234:ARG:O	2.66	0.43
1:B:362:LYS:NZ	2:B:654:HOH:O	2.50	0.43
1:B:86:GLY:HA3	1:B:120:LYS:HG3	2.01	0.43
1:B:80:VAL:HG21	1:B:131:THR:HG23	2.01	0.43
1:C:275:PRO:HD2	2:C:619:HOH:O	2.17	0.43
1:C:79:THR:HB	1:C:91:PHE:CE2	2.54	0.43
1:A:225:VAL:HA	1:A:226:PRO:HD3	1.91	0.43
1:C:207:VAL:HG22	1:C:222:ARG:HH12	1.84	0.43
1:A:185:VAL:HG12	1:A:195:THR:HG22	1.99	0.43
1:A:213:ASN:O	1:A:214:ARG:O	2.37	0.42
1:B:234:ARG:C	1:B:234:ARG:HD2	2.39	0.42
1:B:167:GLN:CD	2:B:640:HOH:O	2.58	0.42
1:C:303:GLN:HG3	2:C:532:HOH:O	2.19	0.42
1:C:166:VAL:CG1	2:C:598:HOH:O	2.58	0.42
1:B:147:ARG:HG2	2:B:470:HOH:O	2.19	0.42
1:C:217:ARG:HG2	2:C:666:HOH:O	2.19	0.42
1:B:211:PHE:HB3	1:B:222:ARG:HH22	1.84	0.41
1:C:200:GLU:HA	1:C:212:ALA:HB1	2.03	0.41
1:A:208:PRO:HG3	1:A:282:ILE:HD11	2.02	0.41
1:B:233:SER:HB3	1:B:238:GLY:O	2.21	0.41
1:C:150:ASN:ND2	2:C:664:HOH:O	2.52	0.41
1:C:87:GLN:NE2	1:C:88:VAL:H	2.19	0.41
1:A:210:LEU:HD23	1:A:223:LEU:HD21	2.03	0.41
1:B:207:VAL:HG22	1:B:222:ARG:HH21	1.84	0.41
1:C:149:ASN:OD1	2:C:609:HOH:O	2.20	0.41
1:A:201:GLN:OE1	1:A:201:GLN:HA	2.21	0.41
1:B:79:THR:HB	1:B:91:PHE:CE2	2.55	0.41
1:A:241:ARG:HD3	2:A:713:HOH:O	2.21	0.40
1:B:232:LYS:HB3	1:B:233:SER:H	1.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLN:O	1:B:399:ARG:HD2	2.21	0.40
1:B:79:THR:HG23	1:B:412:VAL:HG21	2.03	0.40
1:A:374:ASN:O	1:A:375:TYR:HB2	2.22	0.40
1:A:79:THR:HB	1:A:91:PHE:CE2	2.56	0.40
1:B:208:PRO:HD2	1:B:211:PHE:CD2	2.48	0.40
1:B:233:SER:C	1:B:235:GLY:N	2.69	0.40
1:B:418:LYS:O	1:B:418:LYS:HG2	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	399/413 (97%)	380 (95%)	13 (3%)	6 (2%)	11	2
1	B	399/413 (97%)	376 (94%)	14 (4%)	9 (2%)	7	1
1	C	399/413 (97%)	380 (95%)	12 (3%)	7 (2%)	9	1
All	All	1197/1239 (97%)	1136 (95%)	39 (3%)	22 (2%)	9	1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ARG
1	A	234	ARG
1	B	232	LYS
1	B	233	SER
1	B	234	ARG
1	B	237	ARG
1	B	291	ASN
1	B	419	GLU
1	C	211	PHE
1	C	236	SER

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Mol	Chain	Res	Type
1	B	22	LYS
1	B	293	THR
1	C	234	ARG
1	C	418	LYS
1	C	419	GLU
1	A	213	ASN
1	A	22	LYS
1	B	214	ARG
1	C	209	GLU
1	C	235	GLY
1	A	209	GLU
1	A	238	GLY

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	324/334 (97%)	316 (98%)	8 (2%)	50	31
1	B	324/334 (97%)	320 (99%)	4 (1%)	74	62
1	C	324/334 (97%)	318 (98%)	6 (2%)	60	43
All	All	972/1002 (97%)	954 (98%)	18 (2%)	60	43

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

Mol	Chain	Res	Type
1	A	21	LYS
1	A	22	LYS
1	A	33	GLU
1	A	128	ASP
1	A	207	VAL
1	A	209	GLU
1	A	232	LYS
1	A	318	LEU
1	B	33	GLU
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	293	THR
1	B	318	LEU
1	C	57	ARG
1	C	217	ARG
1	C	220	LEU
1	C	237	ARG
1	C	322	GLU
1	C	418	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	B	201	GLN
1	B	291	ASN
1	C	87	GLN
1	C	150	ASN
1	C	169	GLN
1	C	218	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 carbohydrates in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	210:LEU	C	211:PHE	N	0.89
1	C	209:GLU	C	210:LEU	N	0.51

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.