



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2018 – 12:27 AM EDT

PDB ID : 1JSV
Title : The structure of cyclin-dependent kinase 2 (CDK2) in complex with 4-[(6-amino-4-pyrimidinyl)amino]benzenesulfonamide
Authors : Watenpaugh, K.D.; Kelley, L.C.
Deposited on : 2001-08-19
Resolution : 1.96 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
Mogul : 1.7.3 (157068), CSD as539be (2018)
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) : rb-20031021

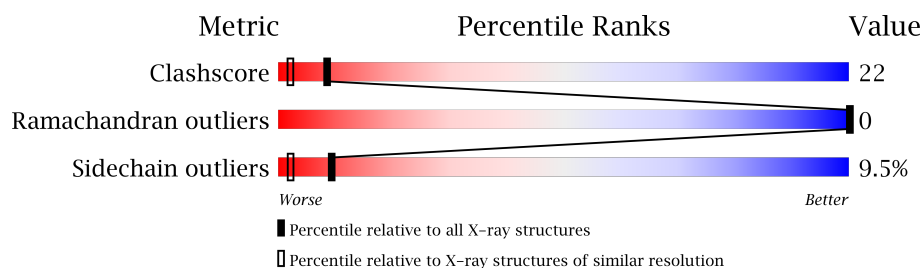
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	U55	A	400	-	-	X	-

2 Entry composition [i](#)

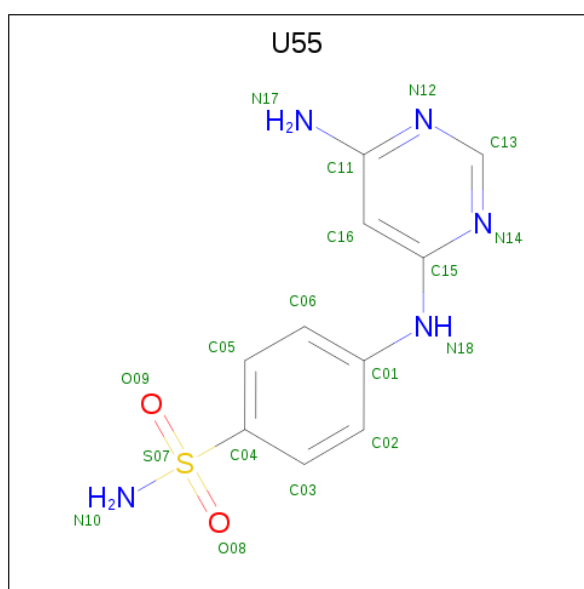
There are 3 unique types of molecules in this entry. The entry contains 2702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	1
			2316	1510	395	403	8			

- Molecule 2 is 4-[(6-AMINO-4-PYRIMIDINYL)AMINO]BENZENESULFONAMIDE (three-letter code: U55) (formula: C₁₀H₁₁N₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	10	5	2	1		

- Molecule 3 is water.

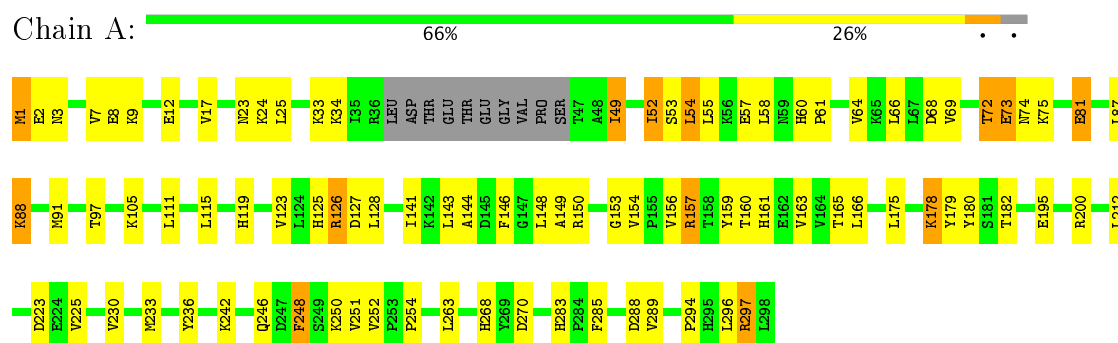
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	368	Total	O	0	0
			368	368		

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 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: CELL DIVISION PROTEIN KINASE 2



4 Data and refinement statistics

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	54.03 Å 72.06 Å 72.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.96	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.96)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2702	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: U55

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	0.66	0/2376	1.00	2/3222 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	254	PRO	CA-C-O	-5.68	106.57	120.20
1	A	254	PRO	O-C-N	5.53	131.54	122.70

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	2316	0	2371	100	1
2	A	18	0	11	7	0
3	A	368	0	0	1	0
All	All	2702	0	2382	104	1

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 22.

All (104) 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:17:VAL:CG1	1:A:34:LYS:HE3	1.27	1.58
1:A:17:VAL:HG12	1:A:34:LYS:CE	1.44	1.43
1:A:17:VAL:CG1	1:A:34:LYS:CE	2.05	1.17
1:A:54:LEU:CD2	1:A:55:LEU:HD23	1.76	1.15
1:A:33:LYS:NZ	2:A:400:U55:H171	1.49	1.10
1:A:73:GLU:O	1:A:73:GLU:HG3	1.36	1.06
1:A:54:LEU:HD22	1:A:55:LEU:HD23	1.42	0.98
1:A:283:HIS:HD2	1:A:285:PHE:H	1.01	0.97
1:A:33:LYS:HZ1	2:A:400:U55:H171	0.95	0.93
1:A:54:LEU:HD23	1:A:55:LEU:HD23	1.55	0.87
1:A:17:VAL:HG11	1:A:34:LYS:CE	2.05	0.87
1:A:88:LYS:HD2	1:A:88:LYS:O	1.75	0.86
1:A:33:LYS:NZ	2:A:400:U55:N17	2.25	0.84
1:A:157:ARG:HH11	1:A:157:ARG:HG2	1.43	0.83
1:A:125:HIS:HD2	1:A:127:ASP:H	1.27	0.83
1:A:91:MET:HE3	1:A:195:GLU:HG2	1.62	0.81
1:A:283:HIS:CD2	1:A:285:PHE:H	1.93	0.81
1:A:297:ARG:CG	1:A:297:ARG:O	2.29	0.80
1:A:17:VAL:CG1	1:A:34:LYS:HE2	2.11	0.80
1:A:73:GLU:O	1:A:73:GLU:CG	2.21	0.80
1:A:52:ILE:CG2	1:A:69:VAL:HG21	2.13	0.78
1:A:297:ARG:O	1:A:297:ARG:HG2	1.82	0.77
1:A:251:VAL:HG12	1:A:252:VAL:HG13	1.70	0.74
1:A:149:ALA:O	1:A:153:GLY:N	2.20	0.73
1:A:12:GLU:HG2	1:A:159:TYR:OH	1.90	0.72
1:A:17:VAL:HG11	1:A:34:LYS:HE2	1.69	0.71
1:A:230:VAL:O	1:A:233:MET:HG3	1.90	0.71
1:A:54:LEU:HD22	1:A:55:LEU:CD2	2.18	0.70
1:A:1:MET:HG2	1:A:3:ASN:HD22	1.56	0.70
1:A:54:LEU:C	1:A:54:LEU:HD23	2.12	0.69
1:A:157:ARG:HH11	1:A:157:ARG:CG	2.06	0.68
1:A:125:HIS:CG	1:A:128:LEU:HD12	2.30	0.66
1:A:54:LEU:HD23	1:A:55:LEU:N	2.10	0.66
1:A:156:VAL:HG12	1:A:157:ARG:HD3	1.76	0.66
1:A:175:LEU:HD21	1:A:212:LEU:HD21	1.78	0.65
1:A:1:MET:HG3	1:A:2:GLU:H	1.62	0.63
1:A:1:MET:HG3	1:A:2:GLU:N	2.14	0.63
1:A:157:ARG:NH1	1:A:157:ARG:HG2	2.06	0.63
1:A:54:LEU:CD2	1:A:55:LEU:CD2	2.67	0.63
1:A:88:LYS:O	1:A:88:LYS:CD	2.47	0.62
1:A:111:LEU:HD21	1:A:141:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:O	1:A:24:LYS:HG3	2.01	0.61
1:A:9:LYS:HE2	1:A:17:VAL:HG21	1.82	0.61
1:A:125:HIS:HE1	1:A:144:ALA:O	1.84	0.61
1:A:88:LYS:C	1:A:88:LYS:CD	2.70	0.59
1:A:88:LYS:HD2	1:A:88:LYS:C	2.23	0.59
1:A:72:THR:O	1:A:75:LYS:HB2	2.03	0.58
1:A:165:THR:O	1:A:165:THR:HG23	2.01	0.58
1:A:54:LEU:HD21	1:A:58:LEU:HD11	1.85	0.57
1:A:149:ALA:O	1:A:153:GLY:CA	2.52	0.57
1:A:248:PHE:O	1:A:251:VAL:HB	2.05	0.56
1:A:268:HIS:CD2	1:A:270:ASP:H	2.23	0.56
1:A:72:THR:O	1:A:72:THR:CG2	2.52	0.56
1:A:159:TYR:CE1	1:A:160:THR:HG23	2.41	0.56
1:A:52:ILE:HG21	1:A:69:VAL:HG21	1.87	0.56
1:A:23:ASN:OD1	1:A:25:LEU:N	2.40	0.55
1:A:268:HIS:HD2	1:A:270:ASP:N	2.04	0.55
1:A:160:THR:O	1:A:161:HIS:HB2	2.07	0.55
1:A:91:MET:CE	1:A:195:GLU:HG2	2.36	0.55
1:A:125:HIS:O	1:A:126:ARG:HB3	2.07	0.54
1:A:72:THR:HG22	1:A:72:THR:O	2.06	0.54
1:A:7:VAL:O	1:A:8:GLU:HB3	2.07	0.54
1:A:149:ALA:O	1:A:153:GLY:HA2	2.07	0.54
2:A:400:U55:H021	2:A:400:U55:H161	1.90	0.54
1:A:126:ARG:HD2	1:A:149:ALA:HB1	1.90	0.53
1:A:125:HIS:O	1:A:126:ARG:CB	2.58	0.52
1:A:119:HIS:CE1	1:A:182:THR:HB	2.45	0.51
1:A:165:THR:O	1:A:165:THR:CG2	2.57	0.51
1:A:1:MET:CG	1:A:3:ASN:HD22	2.23	0.49
1:A:268:HIS:CD2	1:A:270:ASP:N	2.79	0.49
1:A:2:GLU:CD	1:A:2:GLU:N	2.66	0.49
1:A:58:LEU:CD1	1:A:123:VAL:HG21	2.42	0.49
1:A:73:GLU:O	1:A:74:ASN:HB2	2.13	0.49
2:A:400:U55:H021	2:A:400:U55:C16	2.44	0.48
1:A:2:GLU:H	1:A:2:GLU:CD	2.17	0.47
2:A:400:U55:C02	2:A:400:U55:H161	2.45	0.47
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.48	0.47
1:A:52:ILE:HG21	1:A:69:VAL:HG11	1.97	0.47
1:A:157:ARG:HG3	1:A:161:HIS:O	2.16	0.46
1:A:288:ASP:OD1	1:A:288:ASP:C	2.54	0.46
1:A:49:ILE:HD12	1:A:49:ILE:HA	1.78	0.46
1:A:126:ARG:HD3	1:A:154:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:HD2	1:A:285:PHE:N	1.86	0.45
1:A:175:LEU:CD2	1:A:212:LEU:HD21	2.45	0.44
1:A:64:VAL:HG13	1:A:81:GLU:HG2	1.99	0.44
1:A:223:ASP:OD1	1:A:225:VAL:HB	2.17	0.44
1:A:54:LEU:C	1:A:54:LEU:CD2	2.82	0.44
1:A:178:LYS:HB3	1:A:179:TYR:CE2	2.54	0.43
1:A:17:VAL:HG12	1:A:34:LYS:HE3	0.47	0.43
1:A:157:ARG:HD2	1:A:163:VAL:HA	2.00	0.43
1:A:246:GLN:NE2	1:A:250:LYS:NZ	2.67	0.43
1:A:248:PHE:CE2	1:A:263:LEU:HD23	2.53	0.42
1:A:248:PHE:HE2	1:A:263:LEU:HD23	1.85	0.42
1:A:178:LYS:HB3	1:A:179:TYR:CD2	2.55	0.42
1:A:242:LYS:HE2	3:A:600:HOH:O	2.20	0.42
1:A:125:HIS:HB3	1:A:128:LEU:CD1	2.49	0.42
1:A:52:ILE:HG22	1:A:53:SER:N	2.34	0.42
1:A:105:LYS:HG2	1:A:289:VAL:HG23	2.01	0.41
1:A:125:HIS:CD2	1:A:127:ASP:H	2.19	0.41
2:A:400:U55:C16	2:A:400:U55:C02	2.99	0.41
1:A:58:LEU:N	1:A:58:LEU:HD23	2.36	0.41
1:A:87:LEU:O	1:A:91:MET:HG3	2.21	0.40
1:A:88:LYS:HA	1:A:88:LYS:HD3	1.64	0.40
1:A:294:PRO:HG2	1:A:296:LEU:HG	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:NH2	1:A:236:TYR:O[4_446]	1.86	0.34

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	284/298 (95%)	278 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	253/263 (96%)	229 (90%)	24 (10%)	9	2

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	49	ILE
1	A	52	ILE
1	A	54	LEU
1	A	57	GLU
1	A	66	LEU
1	A	68	ASP
1	A	72	THR
1	A	73	GLU
1	A	81	GLU
1	A	88	LYS
1	A	97	THR
1	A	115	LEU
1	A	126	ARG
1	A	143	LEU
1	A	146	PHE
1	A	148	LEU
1	A	150	ARG
1	A	157	ARG
1	A	166	LEU
1	A	178	LYS
1	A	180	TYR
1	A	248	PHE

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Mol	Chain	Res	Type
1	A	297	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	5	GLN
1	A	125	HIS
1	A	246	GLN
1	A	268	HIS
1	A	283	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 ⓘ

1 ligand is 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	U55	A	400	-	19,19,19	1.93	7 (36%)	25,27,27	1.86	5 (20%)

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	U55	A	400	-	-	0/10/10/10	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	U55	C15-N18	-3.24	1.33	1.38
2	A	400	U55	C01-N18	-3.11	1.34	1.40
2	A	400	U55	C04-S07	-2.47	1.73	1.77
2	A	400	U55	C05-C04	2.22	1.42	1.38
2	A	400	U55	C15-N14	2.60	1.39	1.34
2	A	400	U55	C13-N12	3.02	1.39	1.33
2	A	400	U55	O09-S07	3.23	1.50	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	U55	O09-S07-O08	-5.93	108.41	118.71
2	A	400	U55	C16-C15-N14	-2.78	118.87	122.77
2	A	400	U55	N14-C13-N12	-2.60	124.42	128.63
2	A	400	U55	O08-S07-N10	2.37	110.99	107.36
2	A	400	U55	C04-S07-N10	4.37	114.63	108.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	U55	7	0

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 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.