



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 11:31 am BST

PDB ID : 1EK1
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE
COMPLEXED WITH CIU INHIBITOR
Authors : Argiriadi, M.A.; Morisseau, C.; Goodrow, M.H.; Dowdy, D.L.; Hammock,
B.D.; Christianson, D.W.
Deposited on : 2000-03-06
Resolution : 3.10 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
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) : 2.11

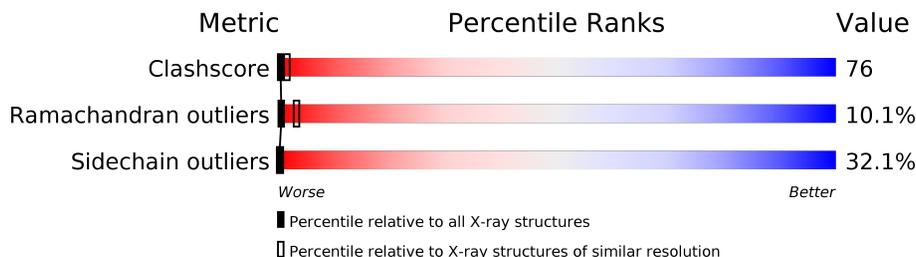
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	
1	B	554	

2 Entry composition [i](#)

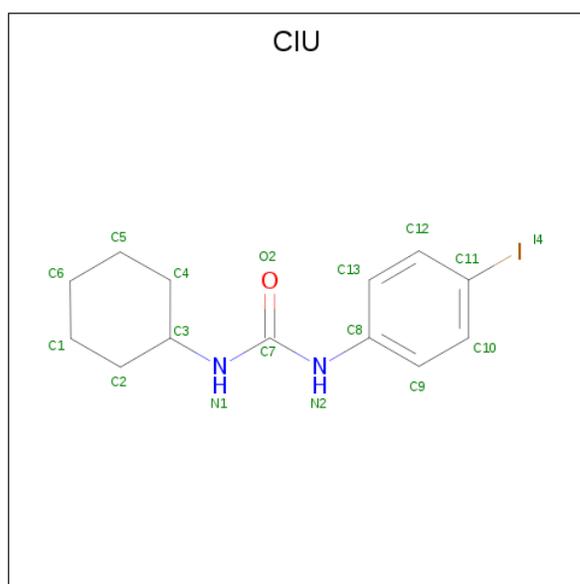
There are 3 unique types of molecules in this entry. The entry contains 8255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	Total 3901	C 2517	N 651	O 704	S 29	61	0	0
1	B	541	Total 4299	C 2766	N 719	O 783	S 31	71	0	0

- Molecule 2 is N-CYCLOHEXYL-N'-(4-IODOPHENYL)UREA (three-letter code: CIU) (formula: C₁₃H₁₇IN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	I	N	O		
2	A	1	Total 17	C 13	I 1	N 2	O 1	0	0
2	B	1	Total 17	C 13	I 1	N 2	O 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	17	Total O 17 17	0	0

P495	P496	I496	Y497	I498	I499	R499	P500	P500	E501	M502	S503	K504	K505	M505	M506	E507	K508	M509	I510	F511	F512	F512	L513	K514	M515	G516	G521	G522	H523	M524	T525	Q526	I527	E528	K529	P530	T531	E532	V533	M534	Q535	I536	L537	F538	K539	M540	S541	L541	Q542	E543	VAL	GLN	ASN	PRO	SER	SER	THR	SER	LYS	ILE				
E432	E433	D434	I435	M436	I437	S438	K439	K440	T441	T442	E445	I446	F447	F448	Y449	I450	Q451	Q452	F453	K454	K455	T456	G457	F458	R459	G460	P461	L462	M463	W464	R465	R466	T468	E469	R470	N471	W472	K473	W474	S475	C476	K477	G478	L479	G480	R481	K482	I483	L484	L488	M489	W490	T491	A492	E493	K494								
F369	M370	K371	V372	I373	I374	S375	I376	F377	V378	F379	N380	Y381	Q382	L383	Y384	F385	Q386	E387	F388	G389	V390	L395	E396	K397	N398	M399	S400	R401	L402	F403	K404	S405	F406	M342	F407	R408	A409	S410	D411	E412	T413	G414	F415	I416	A417	Y418	H419	K420	A421	T422	E423	I424	G425	G426	I427	L428	V429	H430	T431					
A307	M308	E309	L310	L311	C312	K313	E314	M315	V316	T317	F318	L319	D320	K321	L322	G323	I324	P325	Q326	V328	F329	I330	G331	H332	D333	W334	Q335	G336	V337	M338	V339	M340	M341	M342	A343	L344	P347	E348	R349	V350	R351	A352	F353	A354	S355	L356	M357	T358	P359	F360	M361	P362	P363	D364	V367	S368								
P244	G245	I246	R247	L248	H249	F250	V251	E252	M253	G254	S255	G256	L259	H263	G264	F265	P266	E267	S268	W269	F270	S271	W272	R273	Y274	Q275	I276	L277	E278	L279	A280	Q281	A282	G283	F284	R285	V286	L287	A288	L289	D290	M291	K292	G293	Y294	G295	G296	D297	M298	C299	N230	N231	N232	N233	D234	V235	S236	H237	G238	Y239	L303	E304	E305	V306
D184	D185	F186	G187	M188	N189	L190	K191	P192	A193	R194	D195	M196	G197	M198	V199	T200	I201	L202	V203	H204	N205	T206	A207	S208	A209	L210	R211	E212	L213	E214	K215	V216	T217	G218	G219	M220	Q221	F222	E223	P225	A224	P226	L227	V228	P229	C230	N231	P232	N233	D234	V235	S236	H237	G238	Y239	V240	T241	V242	K243					
T123	M124	M125	W126	L127	D128	D129	G130	P131	K132	R133	D134	S135	L136	A137	Q138	M139	M140	C141	E142	L143	S144	Q145	H146	F147	D148	F149	L150	I151	E152	F153	C154	Q155	G156	G157	M158	I159	K160	P161	E162	P163	Q164	I165	Y166	M167	F168	L169	L170	L171	L172	K173	A174	A175	K176	P177	M178	E179	V180	V181	F182	I183				
Q62	M63	V64	P65	M66	M67	D68	E69	S70	Y71	R72	K73	S74	S75	K76	A77	C78	G79	A80	M81	L82	P83	E84	M85	F86	S87	I88	S89	I90	I91	F92	S93	Q94	A95	M96	R99	S100	I101	M102	R103	P104	M105	L106	Q107	A108	A109	I110	A111	L112	K113	K114	K115	G116	F117	M118	T119	C120	I121	V122						

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.90Å 143.00Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8255	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: CIU

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	0.77	1/4004 (0.0%)	0.95	11/5430 (0.2%)
1	B	0.77	0/4413	0.96	11/5984 (0.2%)
All	All	0.77	1/8417 (0.0%)	0.96	22/11414 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	CYS	CB-SG	5.35	1.91	1.82

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ASN	C-N-CD	-12.52	93.07	120.60
1	B	231	ASN	C-N-CA	7.61	153.97	122.00
1	A	218	GLY	N-CA-C	-6.85	95.98	113.10
1	B	66	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	231	ASN	N-CA-C	5.82	126.72	111.00

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	3901	0	3890	581	0
1	B	4299	0	4270	676	0
2	A	17	0	17	2	0
2	B	17	0	17	5	0
3	A	4	0	0	0	0
3	B	17	0	0	5	0
All	All	8255	0	8194	1220	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 76.

The worst 5 of 1220 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:293:GLY:HA2	1:A:299:SER:HB2	1.33	1.10
1:B:141:CYS:O	1:B:144:SER:HB3	1.52	1.10
1:B:61:SER:O	1:B:64:VAL:HG23	1.51	1.09
1:B:223:GLU:H	1:B:223:GLU:CD	1.53	1.08
1:B:183:LEU:HD23	1:B:201:ILE:HD12	1.31	1.08

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	484/554 (87%)	345 (71%)	90 (19%)	49 (10%)	0 3
1	B	539/554 (97%)	384 (71%)	101 (19%)	54 (10%)	0 3
All	All	1023/1108 (92%)	729 (71%)	191 (19%)	103 (10%)	0 3

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	18	SER
1	A	63	TRP
1	A	65	PRO
1	A	91	ILE

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	427/480 (89%)	291 (68%)	136 (32%)	0	0
1	B	468/480 (98%)	317 (68%)	151 (32%)	0	0
All	All	895/960 (93%)	608 (68%)	287 (32%)	0	0

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	ARG
1	B	73	LYS
1	B	459	ARG
1	A	531	THR
1	B	43	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	B	146	HIS
1	B	463	ASN
1	A	526	GLN
1	B	94	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](#)

2 ligands 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	CIU	A	1100	-	18,18,18	2.82	11 (61%)	23,23,23	2.03	4 (17%)
2	CIU	B	1200	-	18,18,18	2.83	11 (61%)	23,23,23	2.03	4 (17%)

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	CIU	A	1100	-	-	0/8/16/16	0/2/2/2
2	CIU	B	1200	-	-	0/8/16/16	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CIU	C11-I4	6.73	2.27	2.10
2	A	1100	CIU	C11-I4	6.71	2.27	2.10
2	B	1200	CIU	C4-C3	3.96	1.61	1.52
2	A	1100	CIU	C4-C3	3.94	1.61	1.52
2	B	1200	CIU	C12-C11	3.86	1.47	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1200	CIU	N2-C7-N1	5.36	121.25	113.76
2	A	1100	CIU	N2-C7-N1	5.36	121.24	113.76
2	B	1200	CIU	C8-N2-C7	4.55	135.92	126.61
2	A	1100	CIU	O2-C7-N1	-4.55	114.34	122.62
2	A	1100	CIU	C8-N2-C7	4.53	135.89	126.61

There are no chirality outliers.

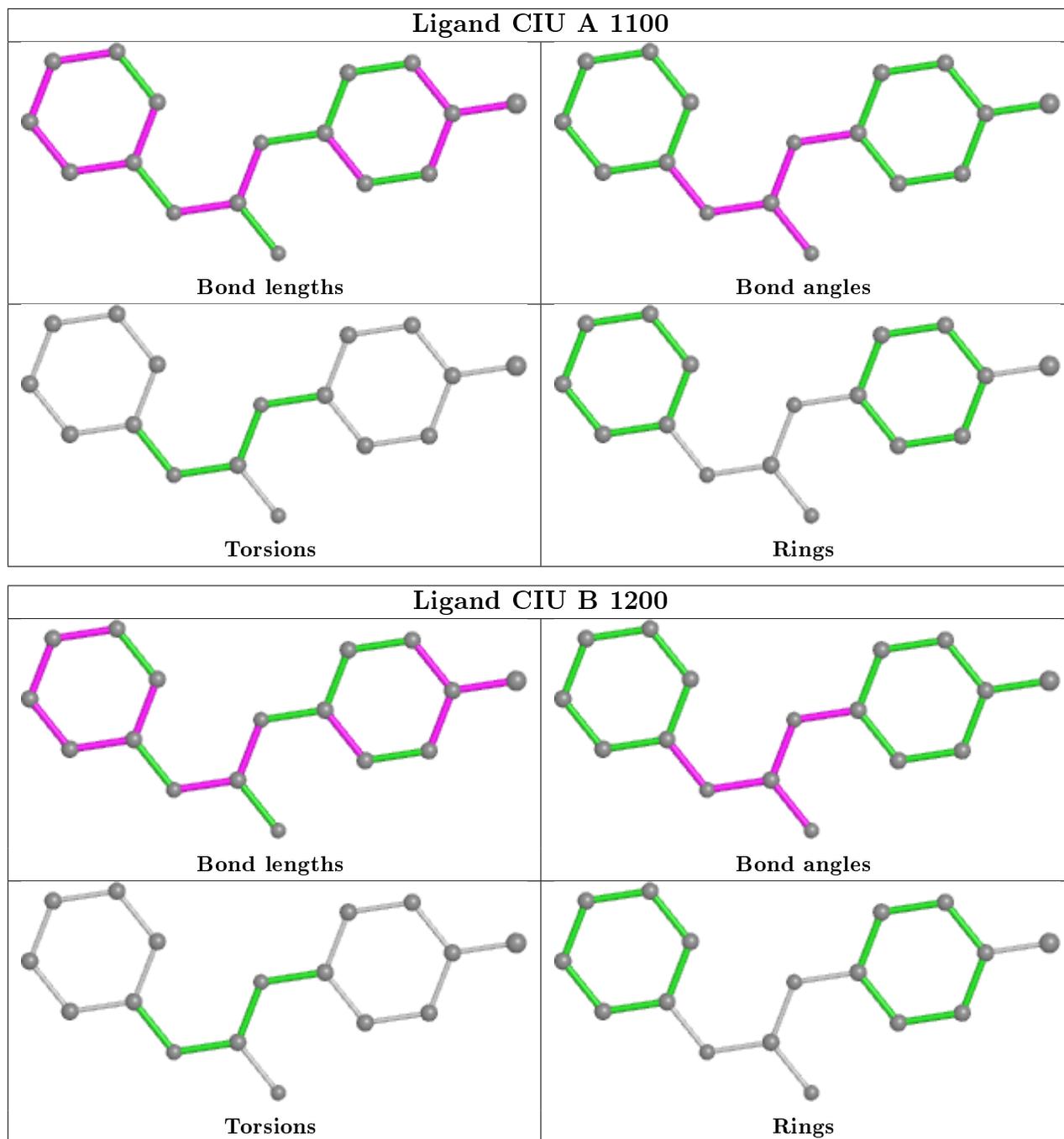
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CIU	2	0
2	B	1200	CIU	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.