



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2019 – 03:37 AM EDT

PDB ID : 1DS1  
Title : CRYSTAL STRUCTURE OF CLAVAMINATE SYNTHASE IN COMPLEX WITH FE(II) AND 2-OXOGLUTARATE  
Authors : Zhang, Z.H.; Ren, J.; Stammers, D.K.; Baldwin, J.E.; Harlos, K.; Schofield, C.J.  
Deposited on : 2000-01-06  
Resolution : 1.08 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](mailto: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	:	1.8.0 (224370), CSD as540be (2019)
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)	:	2.3.2

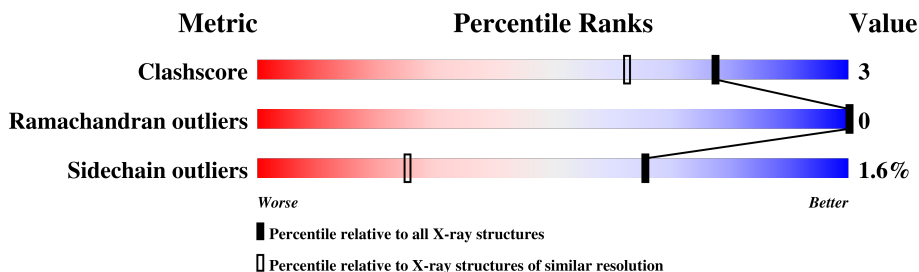
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.08 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	1154 (1.12-1.04)
Ramachandran outliers	120053	1107 (1.12-1.04)
Sidechain outliers	120020	1105 (1.12-1.04)

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  $\geq 3$ , 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	324	

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
5	PGO	A	331	-	X	-	-

## 2 Entry composition [i](#)

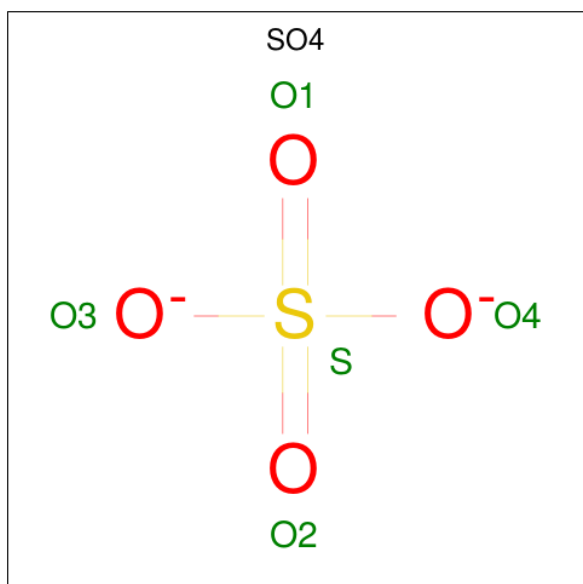
There are 6 unique types of molecules in this entry. The entry contains 2927 atoms, of which 2 are hydrogens and 0 are deuteriums.

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 CLAVAMINATE SYNTHASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2481	1545	449	478	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

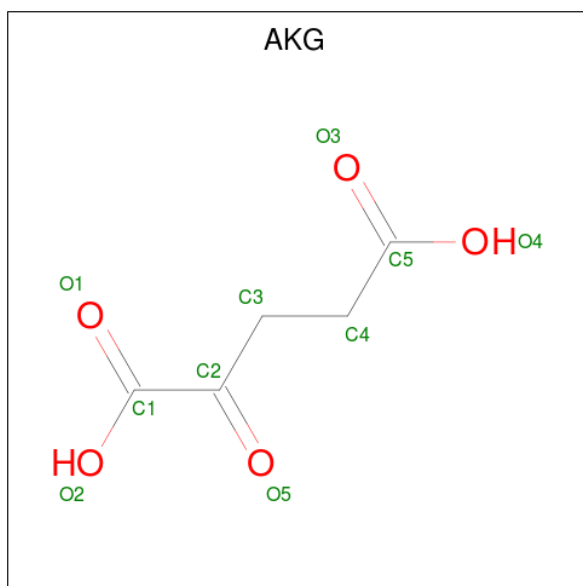


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

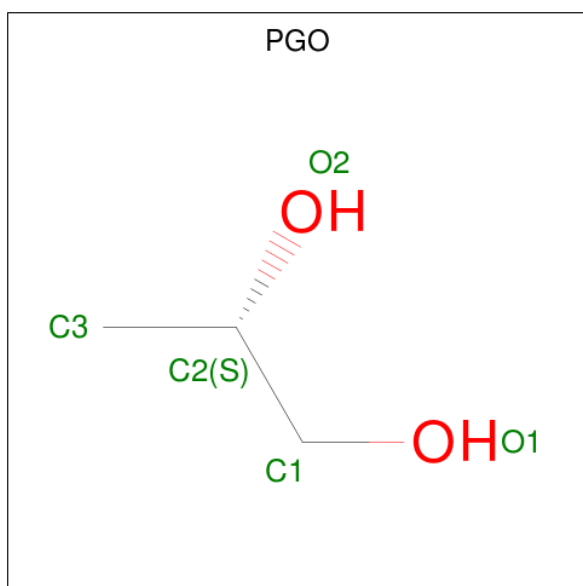
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula:  $C_3H_8O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			6	3	1	2		
5	A	1	Total	C	H	O	0	0
			6	3	1	2		

- Molecule 6 is water.

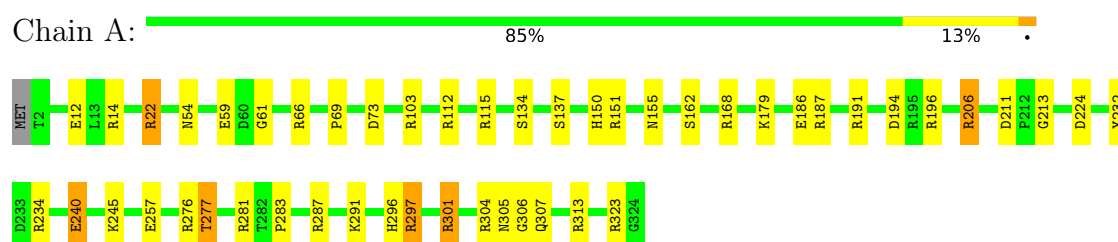
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	403	Total	O	0	0
			403	403		

### 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 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: CLAVAMINATE SYNTHASE 1



## 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, $\alpha$ , $\beta$ , $\gamma$	67.08Å 67.94Å 68.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.08	Depositor
% Data completeness (in resolution range)	88.6 (8.00-1.08)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	SHELXL-97, CNS	Depositor
R, $R_{free}$	0.135 , 0.166	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGO, AKG, SO4, FE2

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	0.82	1/2537 (0.0%)	1.79	60/3457 (1.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	PRO	C-N	-5.51	1.21	1.34

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	28.07	134.33	120.30
1	A	234	ARG	CD-NE-CZ	26.63	160.89	123.60
1	A	234	ARG	NE-CZ-NH1	-25.94	107.33	120.30
1	A	297	ARG	NE-CZ-NH2	21.90	131.25	120.30
1	A	112	ARG	NE-CZ-NH2	-15.76	112.42	120.30
1	A	115	ARG	NE-CZ-NH1	14.39	127.50	120.30
1	A	168	ARG	NE-CZ-NH2	-13.53	113.54	120.30
1	A	115	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	A	206	ARG	NE-CZ-NH2	13.11	126.86	120.30
1	A	168	ARG	NE-CZ-NH1	12.43	126.52	120.30
1	A	179	LYS	CD-CE-NZ	11.18	137.42	111.70
1	A	281	ARG	NE-CZ-NH1	-11.16	114.72	120.30
1	A	191	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	305	ASN	CA-C-N	10.15	136.50	116.20
1	A	103	ARG	CD-NE-CZ	9.97	137.56	123.60
1	A	103	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	A	287	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	305	ASN	O-C-N	-9.29	107.40	123.20
1	A	66	ARG	CD-NE-CZ	9.02	136.22	123.60
1	A	187	ARG	NE-CZ-NH2	8.88	124.74	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH1	-8.75	115.93	120.30
1	A	22	ARG	NE-CZ-NH1	-8.55	116.03	120.30
1	A	134	SER	C-N-CA	8.46	142.86	121.70
1	A	304	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	206	ARG	CD-NE-CZ	8.18	135.05	123.60
1	A	297	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	134	SER	O-C-N	-7.33	110.97	122.70
1	A	12	GLU	OE1-CD-OE2	7.08	131.80	123.30
1	A	313	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	22	ARG	NH1-CZ-NH2	6.78	126.85	119.40
1	A	150	HIS	CG-ND1-CE1	6.73	117.62	108.20
1	A	277	THR	CA-CB-OG1	-6.69	94.96	109.00
1	A	306	GLY	N-CA-C	6.53	129.42	113.10
1	A	297	ARG	NH1-CZ-NH2	-6.45	112.30	119.40
1	A	179	LYS	CG-CD-CE	6.42	131.15	111.90
1	A	276	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	73	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	277	THR	OG1-CB-CG2	6.38	124.67	110.00
1	A	22	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	257	GLU	OE1-CD-OE2	-6.35	115.68	123.30
1	A	232	TYR	CZ-CE2-CD2	-6.34	114.09	119.80
1	A	301	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	A	206	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	A	115	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	22	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	306	GLY	O-C-N	-5.98	113.14	122.70
1	A	168	ARG	CD-NE-CZ	-5.84	115.42	123.60
1	A	196	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	224	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	69	PRO	O-C-N	-5.48	113.93	122.70
1	A	281	ARG	NH1-CZ-NH2	5.46	125.40	119.40
1	A	194	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	A	232	TYR	CG-CD2-CE2	5.35	125.58	121.30
1	A	323	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	A	313	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	112	ARG	NH1-CZ-NH2	5.27	125.19	119.40
1	A	306	GLY	CA-C-O	5.25	130.04	120.60
1	A	234	ARG	CG-CD-NE	5.13	122.57	111.80
1	A	151	ARG	O-C-N	-5.12	114.51	122.70
1	A	194	ASP	CB-CG-OD2	5.08	122.87	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	2481	0	2419	16	0
2	A	20	0	0	2	0
3	A	1	0	0	0	0
4	A	10	0	4	0	0
5	A	10	2	16	2	0
6	A	403	0	0	4	0
All	All	2925	2	2439	16	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 3.

All (16) 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:22:ARG:HG2	2:A:335:SO4:O1	1.91	0.70
1:A:291:LYS:HD3	6:A:681:HOH:O	1.98	0.63
1:A:297:ARG:HG2	6:A:788:HOH:O	1.99	0.62
1:A:22:ARG:HH12	5:A:331:PGO:H12	1.67	0.59
1:A:22:ARG:HH12	5:A:331:PGO:C1	2.15	0.59
1:A:162:SER:OG	1:A:296:HIS:HE1	1.87	0.58
1:A:277:THR:O	1:A:277:THR:OG1	2.29	0.49
1:A:206:ARG:NE	6:A:617:HOH:O	2.47	0.46
1:A:61:GLY:O	1:A:277:THR:HG21	2.15	0.46
1:A:240:GLU:O	1:A:245:LYS:NZ	2.48	0.46
1:A:14:ARG:NH1	6:A:702:HOH:O	2.49	0.46
1:A:211:ASP:OD2	1:A:213:GLY:N	2.49	0.45
1:A:61:GLY:HA3	1:A:277:THR:CG2	2.47	0.44
1:A:59:GLU:N	2:A:336:SO4:O3	2.48	0.43
1:A:301:ARG:HA	1:A:307:GLN:NE2	2.36	0.41
1:A:137:SER:O	1:A:283:PRO:HA	2.20	0.41

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	321/324 (99%)	318 (99%)	3 (1%)	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	258/259 (100%)	254 (98%)	4 (2%)	65	25

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	155	ASN
1	A	186	GLU
1	A	240	GLU

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	54	ASN
1	A	108	HIS
1	A	131	HIS
1	A	217	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	296	HIS
1	A	307	GLN

### 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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	$\# Z  > 2$
4	AKG	A	330	3	3,9,9	1.64	1 (33%)	4,11,11	1.00	0
5	PGO	A	331	-	4,4,4	1.28	1 (25%)	4,4,4	1.86	2 (50%)
5	PGO	A	332	-	4,4,4	1.46	1 (25%)	4,4,4	1.31	1 (25%)
2	SO4	A	335	-	4,4,4	0.56	0	6,6,6	0.76	0
2	SO4	A	336	-	4,4,4	0.54	0	6,6,6	0.47	0
2	SO4	A	339	-	4,4,4	0.67	0	6,6,6	0.83	0
2	SO4	A	340	-	4,4,4	0.64	0	6,6,6	0.71	0

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
4	AKG	A	330	3	-	2/3/9/9	-
5	PGO	A	331	-	-	2/2/2/2	-
5	PGO	A	332	-	-	0/2/2/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	330	AKG	O5-C2	2.67	1.26	1.22
5	A	331	PGO	C1-C2	2.31	1.58	1.50
5	A	332	PGO	C1-C2	2.22	1.58	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	331	PGO	O1-C1-C2	-2.69	104.68	111.31
5	A	332	PGO	O1-C1-C2	-2.41	105.38	111.31
5	A	331	PGO	O2-C2-C3	2.05	118.12	109.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	331	PGO	O1-C1-C2-O2
4	A	330	AKG	C1-C2-C3-C4
4	A	330	AKG	O5-C2-C3-C4
5	A	331	PGO	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	331	PGO	2	0

## 5.7 Other polymers [i](#)

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.