Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 05:59 am GMT

PDB ID	:	8BII
Title	:	O-Methyltransferase Plu4895 (mutant H229N) in complex with SAH
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2022-11-02
Resolution	:	2.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (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)	:	2.36

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 2.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20635 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 methyltransferase Plu4895 H229N mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2554	1642	413	488	11			
1	B	318	Total	C	N	O	S	0	1	0
			2562	1646	415	490	11			
1	C	318	Total	C	N	O	S	0	0	0
			2554	1642	413	488	11			
1	D	318	Total	C	N	O	S	0	0	0
			2554	1642	413	488	11			
1	E	318	Total	C	N	O	S	0	0	0
			2554	1642	413	488	11			
1	F	318	Total	C	N	O	S	0	0	0
			2554	1642	413	488	11			
1	G	316	Total	C	N	O	S	0	0	0
			2537	1633	410	483	11			
1	H	312	Total	C	N	O	S	0	0	0
			2505	1611	405	478	11			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
A	-16	ARG	-	expression tag	UNP A0A6L9JQS9
A	-15	GLY	-	expression tag	UNP A0A6L9JQS9
A	-14	SER	-	expression tag	UNP A0A6L9JQS9
A	-13	HIS	-	expression tag	UNP A0A6L9JQS9
A	-12	HIS	-	expression tag	UNP A0A6L9JQS9
A	-11	HIS	-	expression tag	UNP A0A6L9JQS9
A	-10	HIS	-	expression tag	UNP A0A6L9JQS9
A	-9	HIS	-	expression tag	UNP A0A6L9JQS9
A	-8	HIS	-	expression tag	UNP A0A6L9JQS9
A	-7	GLU	-	expression tag	UNP A0A6L9JQS9
A	-6	ASN	-	expression tag	UNP A0A6L9JQS9
A	-5	LEU	-	expression tag	UNP A0A6L9JQS9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	expression tag	UNP A0A6L9JQS9
A	-3	PHE	-	expression tag	UNP A0A6L9JQS9
A	-2	GLN	-	expression tag	UNP A0A6L9JQS9
A	-1	GLY	-	expression tag	UNP A0A6L9JQS9
A	0	SER	-	expression tag	UNP A0A6L9JQS9
A	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9
B	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
B	-16	ARG	-	expression tag	UNP A0A6L9JQS9
B	-15	GLY	-	expression tag	UNP A0A6L9JQS9
B	-14	SER	-	expression tag	UNP A0A6L9JQS9
B	-13	HIS	-	expression tag	UNP A0A6L9JQS9
B	-12	HIS	-	expression tag	UNP A0A6L9JQS9
B	-11	HIS	-	expression tag	UNP A0A6L9JQS9
B	-10	HIS	-	expression tag	UNP A0A6L9JQS9
B	-9	HIS	-	expression tag	UNP A0A6L9JQS9
B	-8	HIS	-	expression tag	UNP A0A6L9JQS9
B	-7	GLU	-	expression tag	UNP A0A6L9JQS9
B	-6	ASN	-	expression tag	UNP A0A6L9JQS9
B	-5	LEU	-	expression tag	UNP A0A6L9JQS9
B	-4	TYR	-	expression tag	UNP A0A6L9JQS9
B	-3	PHE	-	expression tag	UNP A0A6L9JQS9
B	-2	GLN	-	expression tag	UNP A0A6L9JQS9
B	-1	GLY	-	expression tag	UNP A0A6L9JQS9
B	0	SER	-	expression tag	UNP A0A6L9JQS9
B	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9
C	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
C	-16	ARG	-	expression tag	UNP A0A6L9JQS9
C	-15	GLY	-	expression tag	UNP A0A6L9JQS9
C	-14	SER	-	expression tag	UNP A0A6L9JQS9
C	-13	HIS	-	expression tag	UNP A0A6L9JQS9
C	-12	HIS	-	expression tag	UNP A0A6L9JQS9
C	-11	HIS	-	expression tag	UNP A0A6L9JQS9
C	-10	HIS	-	expression tag	UNP A0A6L9JQS9
C	-9	HIS	-	expression tag	UNP A0A6L9JQS9
C	-8	HIS	-	expression tag	UNP A0A6L9JQS9
C	-7	GLU	-	expression tag	UNP A0A6L9JQS9
C	-6	ASN	-	expression tag	UNP A0A6L9JQS9
C	-5	LEU	-	expression tag	UNP A0A6L9JQS9
C	-4	TYR	-	expression tag	UNP A0A6L9JQS9
C	-3	PHE	-	expression tag	UNP A0A6L9JQS9
C	-2	GLN	-	expression tag	UNP A0A6L9JQS9
C	-1	GLY	-	expression tag	UNP A0A6L9JQS9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP A0A6L9JQS9
C	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9
D	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
D	-16	ARG	-	expression tag	UNP A0A6L9JQS9
D	-15	GLY	-	expression tag	UNP A0A6L9JQS9
D	-14	SER	-	expression tag	UNP A0A6L9JQS9
D	-13	HIS	-	expression tag	UNP A0A6L9JQS9
D	-12	HIS	-	expression tag	UNP A0A6L9JQS9
D	-11	HIS	-	expression tag	UNP A0A6L9JQS9
D	-10	HIS	-	expression tag	UNP A0A6L9JQS9
D	-9	HIS	-	expression tag	UNP A0A6L9JQS9
D	-8	HIS	-	expression tag	UNP A0A6L9JQS9
D	-7	GLU	-	expression tag	UNP A0A6L9JQS9
D	-6	ASN	-	expression tag	UNP A0A6L9JQS9
D	-5	LEU	-	expression tag	UNP A0A6L9JQS9
D	-4	TYR	-	expression tag	UNP A0A6L9JQS9
D	-3	PHE	-	expression tag	UNP A0A6L9JQS9
D	-2	GLN	-	expression tag	UNP A0A6L9JQS9
D	-1	GLY	-	expression tag	UNP A0A6L9JQS9
D	0	SER	-	expression tag	UNP A0A6L9JQS9
D	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9
E	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
E	-16	ARG	-	expression tag	UNP A0A6L9JQS9
E	-15	GLY	-	expression tag	UNP A0A6L9JQS9
E	-14	SER	-	expression tag	UNP A0A6L9JQS9
E	-13	HIS	-	expression tag	UNP A0A6L9JQS9
E	-12	HIS	-	expression tag	UNP A0A6L9JQS9
E	-11	HIS	-	expression tag	UNP A0A6L9JQS9
E	-10	HIS	-	expression tag	UNP A0A6L9JQS9
E	-9	HIS	-	expression tag	UNP A0A6L9JQS9
E	-8	HIS	-	expression tag	UNP A0A6L9JQS9
E	-7	GLU	-	expression tag	UNP A0A6L9JQS9
E	-6	ASN	-	expression tag	UNP A0A6L9JQS9
E	-5	LEU	-	expression tag	UNP A0A6L9JQS9
E	-4	TYR	-	expression tag	UNP A0A6L9JQS9
E	-3	PHE	-	expression tag	UNP A0A6L9JQS9
E	-2	GLN	-	expression tag	UNP A0A6L9JQS9
E	-1	GLY	-	expression tag	UNP A0A6L9JQS9
E	0	SER	-	expression tag	UNP A0A6L9JQS9
E	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9
F	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
F	-16	ARG	-	expression tag	UNP A0A6L9JQS9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	GLY	-	expression tag	UNP A0A6L9JQS9
F	-14	SER	-	expression tag	UNP A0A6L9JQS9
F	-13	HIS	-	expression tag	UNP A0A6L9JQS9
F	-12	HIS	-	expression tag	UNP A0A6L9JQS9
F	-11	HIS	-	expression tag	UNP A0A6L9JQS9
F	-10	HIS	-	expression tag	UNP A0A6L9JQS9
F	-9	HIS	-	expression tag	UNP A0A6L9JQS9
F	-8	HIS	-	expression tag	UNP A0A6L9JQS9
F	-7	GLU	-	expression tag	UNP A0A6L9JQS9
F	-6	ASN	-	expression tag	UNP A0A6L9JQS9
F	-5	LEU	-	expression tag	UNP A0A6L9JQS9
F	-4	TYR	-	expression tag	UNP A0A6L9JQS9
F	-3	PHE	-	expression tag	UNP A0A6L9JQS9
F	-2	GLN	-	expression tag	UNP A0A6L9JQS9
F	-1	GLY	-	expression tag	UNP A0A6L9JQS9
F	0	SER	-	expression tag	UNP A0A6L9JQS9
F	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9
G	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
G	-16	ARG	-	expression tag	UNP A0A6L9JQS9
G	-15	GLY	-	expression tag	UNP A0A6L9JQS9
G	-14	SER	-	expression tag	UNP A0A6L9JQS9
G	-13	HIS	-	expression tag	UNP A0A6L9JQS9
G	-12	HIS	-	expression tag	UNP A0A6L9JQS9
G	-11	HIS	-	expression tag	UNP A0A6L9JQS9
G	-10	HIS	-	expression tag	UNP A0A6L9JQS9
G	-9	HIS	-	expression tag	UNP A0A6L9JQS9
G	-8	HIS	-	expression tag	UNP A0A6L9JQS9
G	-7	GLU	-	expression tag	UNP A0A6L9JQS9
G	-6	ASN	-	expression tag	UNP A0A6L9JQS9
G	-5	LEU	-	expression tag	UNP A0A6L9JQS9
G	-4	TYR	-	expression tag	UNP A0A6L9JQS9
G	-3	PHE	-	expression tag	UNP A0A6L9JQS9
G	-2	GLN	-	expression tag	UNP A0A6L9JQS9
G	-1	GLY	-	expression tag	UNP A0A6L9JQS9
G	0	SER	-	expression tag	UNP A0A6L9JQS9
G	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9
H	-17	MET	-	initiating methionine	UNP A0A6L9JQS9
H	-16	ARG	-	expression tag	UNP A0A6L9JQS9
H	-15	GLY	-	expression tag	UNP A0A6L9JQS9
H	-14	SER	-	expression tag	UNP A0A6L9JQS9
H	-13	HIS	-	expression tag	UNP A0A6L9JQS9
H	-12	HIS	-	expression tag	UNP A0A6L9JQS9

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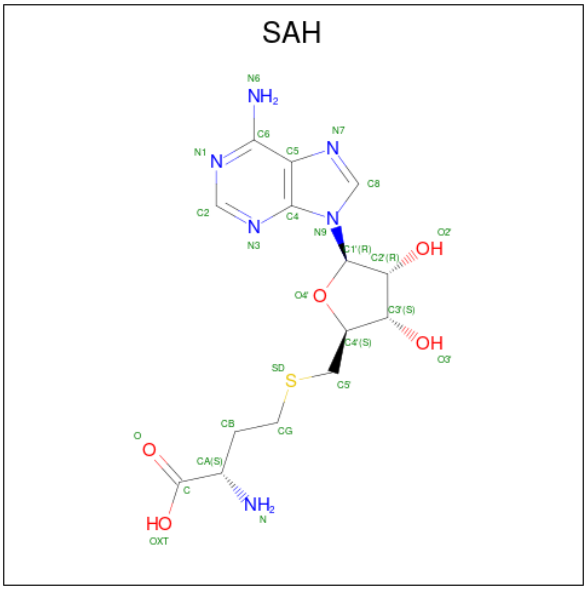
Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	HIS	-	expression tag	UNP A0A6L9JQS9
H	-10	HIS	-	expression tag	UNP A0A6L9JQS9
H	-9	HIS	-	expression tag	UNP A0A6L9JQS9
H	-8	HIS	-	expression tag	UNP A0A6L9JQS9
H	-7	GLU	-	expression tag	UNP A0A6L9JQS9
H	-6	ASN	-	expression tag	UNP A0A6L9JQS9
H	-5	LEU	-	expression tag	UNP A0A6L9JQS9
H	-4	TYR	-	expression tag	UNP A0A6L9JQS9
H	-3	PHE	-	expression tag	UNP A0A6L9JQS9
H	-2	GLN	-	expression tag	UNP A0A6L9JQS9
H	-1	GLY	-	expression tag	UNP A0A6L9JQS9
H	0	SER	-	expression tag	UNP A0A6L9JQS9
H	229	ASN	HIS	engineered mutation	UNP A0A6L9JQS9

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	10	Total	O	0	0
			10	10		
4	C	9	Total	O	0	0
			9	9		
4	D	7	Total	O	0	0
			7	7		
4	E	4	Total	O	0	0
			4	4		
4	F	5	Total	O	0	0
			5	5		
4	G	6	Total	O	0	0
			6	6		
4	H	7	Total	O	0	0
			7	7		

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 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	58.92Å 98.30Å 531.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.9 (30.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20635	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	SAH	H	900	-	24,28,28	0.69	1 (4%)	25,40,40	0.90	3 (12%)
2	SAH	E	401	-	24,28,28	0.70	1 (4%)	25,40,40	0.94	3 (12%)
2	SAH	A	900	-	24,28,28	0.70	1 (4%)	25,40,40	0.96	3 (12%)
2	SAH	C	900	-	24,28,28	0.71	1 (4%)	25,40,40	0.93	3 (12%)
2	SAH	F	900	-	24,28,28	0.71	1 (4%)	25,40,40	0.96	3 (12%)
2	SAH	G	900	-	24,28,28	0.71	1 (4%)	25,40,40	0.97	3 (12%)
2	SAH	B	900	-	24,28,28	0.70	1 (4%)	25,40,40	0.97	3 (12%)
2	SAH	D	900	-	24,28,28	0.70	1 (4%)	25,40,40	0.98	3 (12%)

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	SAH	H	900	-	-	3/11/31/31	0/3/3/3
2	SAH	E	401	-	-	1/11/31/31	0/3/3/3
2	SAH	A	900	-	-	1/11/31/31	0/3/3/3
2	SAH	C	900	-	-	2/11/31/31	0/3/3/3
2	SAH	F	900	-	-	3/11/31/31	0/3/3/3
2	SAH	G	900	-	-	4/11/31/31	0/3/3/3
2	SAH	B	900	-	-	1/11/31/31	0/3/3/3
2	SAH	D	900	-	-	0/11/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	SAH	OXT-C	-2.18	1.23	1.30
2	C	900	SAH	OXT-C	-2.12	1.23	1.30
2	F	900	SAH	OXT-C	-2.10	1.23	1.30
2	H	900	SAH	OXT-C	-2.10	1.23	1.30
2	A	900	SAH	OXT-C	-2.09	1.23	1.30
2	D	900	SAH	OXT-C	-2.07	1.23	1.30
2	B	900	SAH	OXT-C	-2.04	1.23	1.30
2	E	401	SAH	OXT-C	-2.02	1.23	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	900	SAH	OXT-C-O	-2.65	118.07	124.09
2	B	900	SAH	OXT-C-O	-2.57	118.26	124.09
2	G	900	SAH	OXT-C-O	-2.56	118.28	124.09
2	F	900	SAH	OXT-C-O	-2.50	118.42	124.09
2	A	900	SAH	OXT-C-O	-2.46	118.51	124.09
2	C	900	SAH	OXT-C-O	-2.42	118.58	124.09
2	H	900	SAH	OXT-C-O	-2.38	118.69	124.09
2	G	900	SAH	OXT-C-CA	2.37	121.47	113.38
2	B	900	SAH	OXT-C-CA	2.36	121.44	113.38
2	E	401	SAH	OXT-C-O	-2.32	118.81	124.09
2	A	900	SAH	C5-C6-N6	2.29	123.84	120.35
2	D	900	SAH	OXT-C-CA	2.27	121.13	113.38
2	F	900	SAH	C5-C6-N6	2.23	123.75	120.35
2	C	900	SAH	OXT-C-CA	2.21	120.91	113.38
2	D	900	SAH	C5-C6-N6	2.20	123.70	120.35
2	F	900	SAH	OXT-C-CA	2.20	120.86	113.38
2	E	401	SAH	C5-C6-N6	2.18	123.66	120.35
2	C	900	SAH	C5-C6-N6	2.17	123.65	120.35
2	A	900	SAH	OXT-C-CA	2.15	120.72	113.38
2	H	900	SAH	C5-C6-N6	2.13	123.59	120.35
2	G	900	SAH	C5-C6-N6	2.11	123.56	120.35
2	E	401	SAH	OXT-C-CA	2.08	120.45	113.38
2	B	900	SAH	C5-C6-N6	2.07	123.50	120.35
2	H	900	SAH	OXT-C-CA	2.03	120.31	113.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	900	SAH	O-C-CA-N
2	H	900	SAH	OXT-C-CA-N
2	C	900	SAH	C-CA-CB-CG
2	F	900	SAH	C-CA-CB-CG
2	G	900	SAH	C-CA-CB-CG
2	H	900	SAH	C4'-C5'-SD-CG
2	E	401	SAH	OXT-C-CA-N
2	C	900	SAH	N-CA-CB-CG
2	F	900	SAH	N-CA-CB-CG
2	G	900	SAH	N-CA-CB-CG
2	A	900	SAH	CB-CG-SD-C5'
2	G	900	SAH	CB-CG-SD-C5'

Continued on next page...

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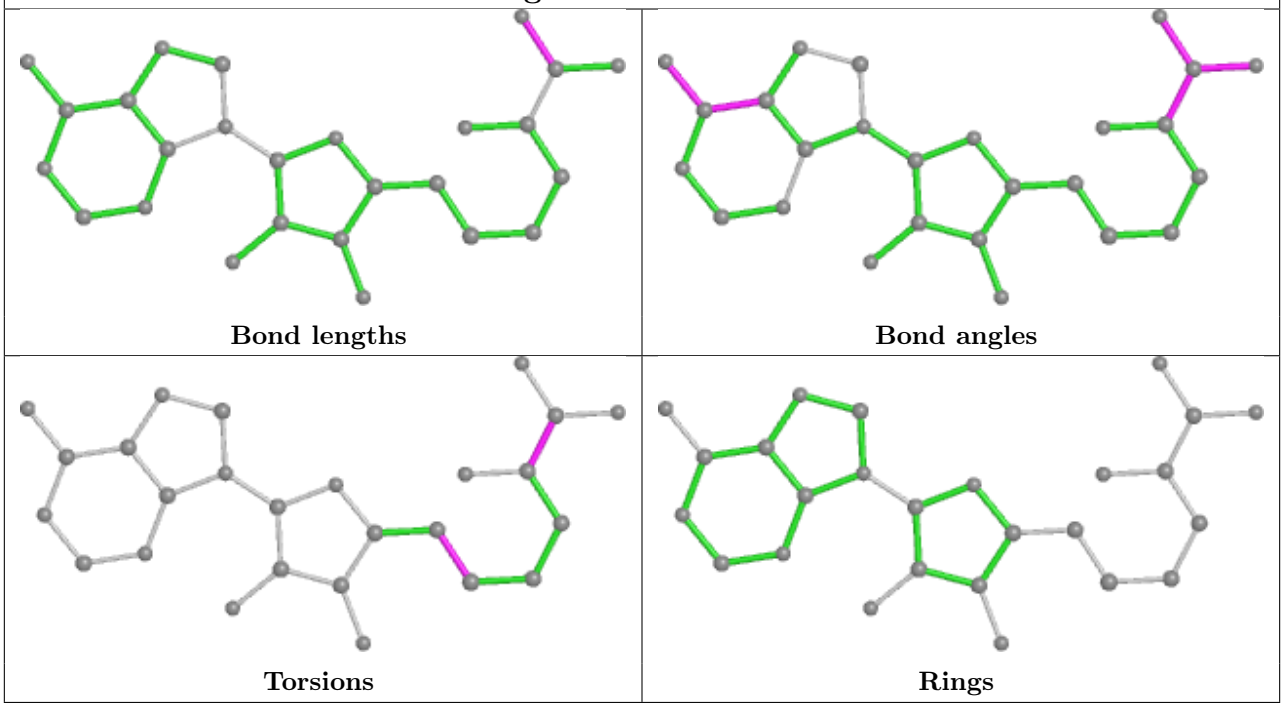
Mol	Chain	Res	Type	Atoms
2	B	900	SAH	C-CA-CB-CG
2	F	900	SAH	OXT-C-CA-N
2	G	900	SAH	OXT-C-CA-N

There are no ring outliers.

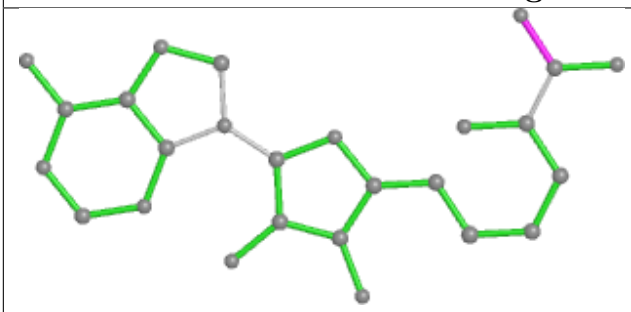
No monomer is involved in short contacts.

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 then 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.

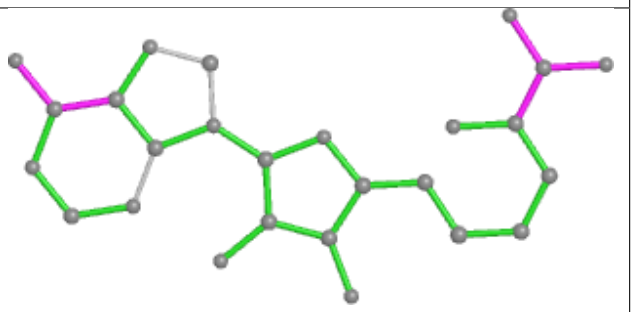
Ligand SAH H 900



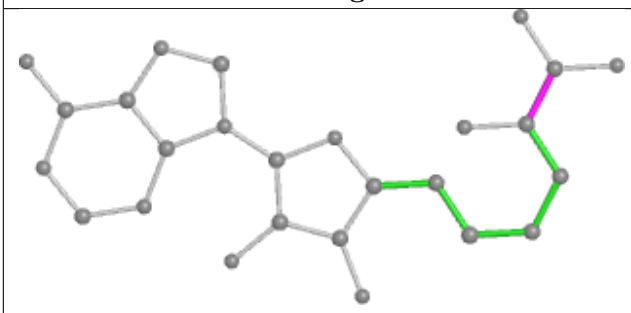
Ligand SAH E 401



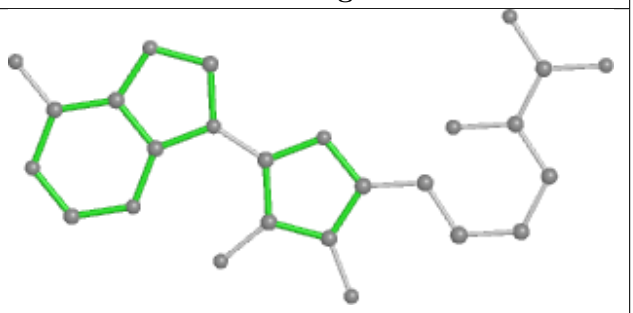
Bond lengths



Bond angles

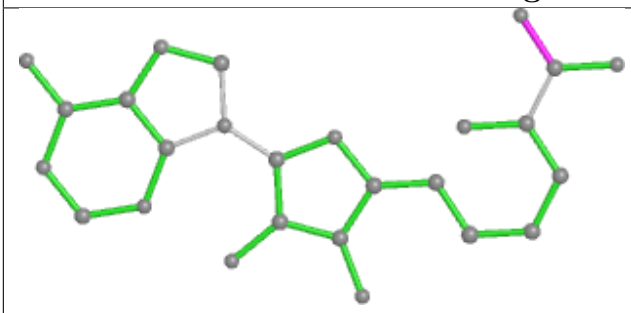


Torsions

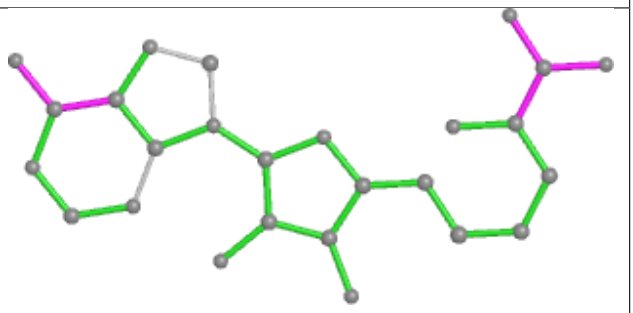


Rings

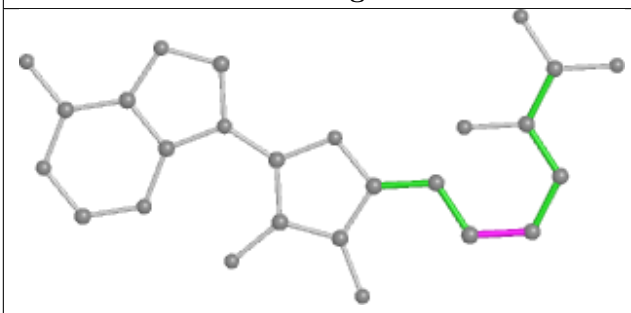
Ligand SAH A 900



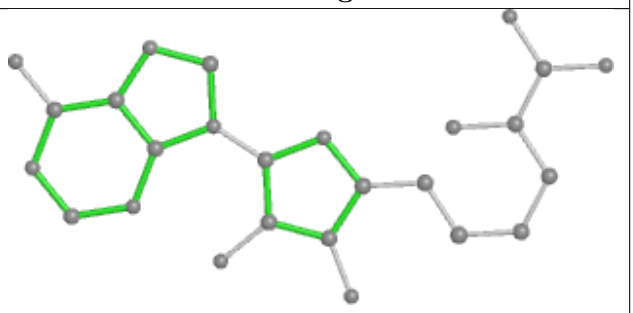
Bond lengths



Bond angles

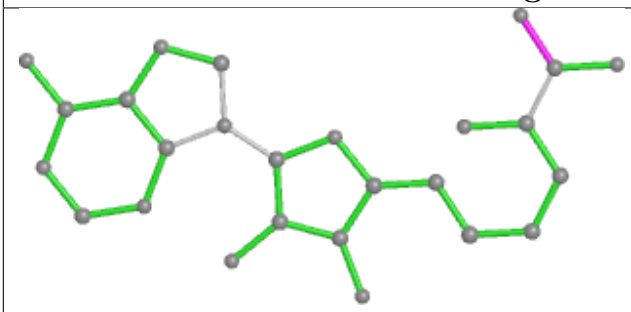


Torsions

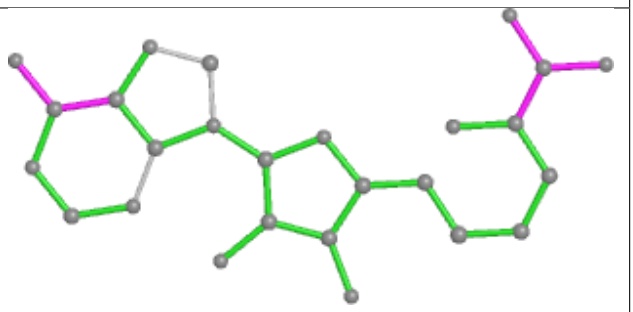


Rings

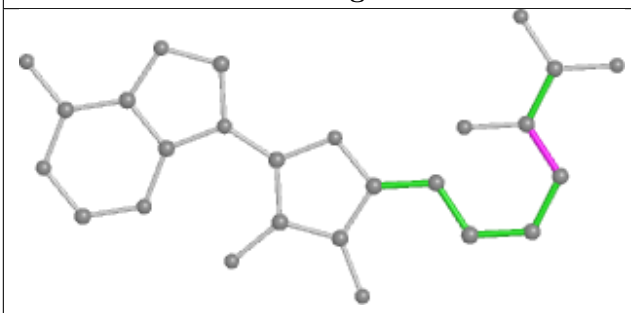
Ligand SAH C 900



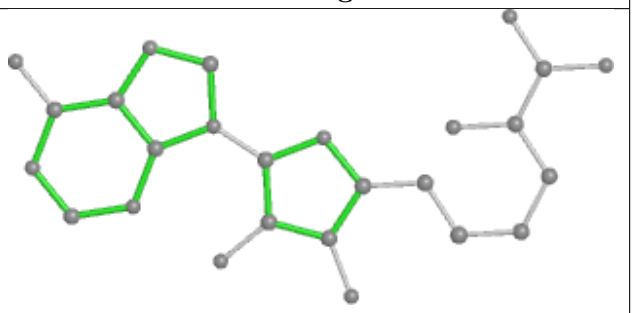
Bond lengths



Bond angles

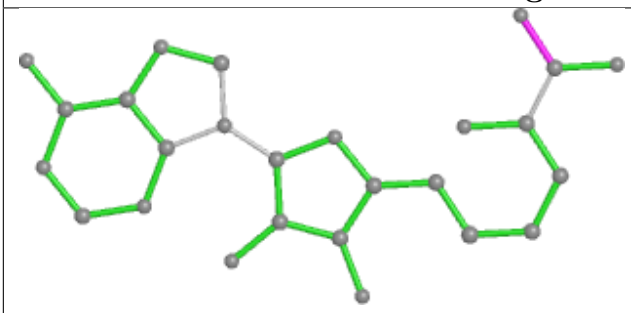


Torsions

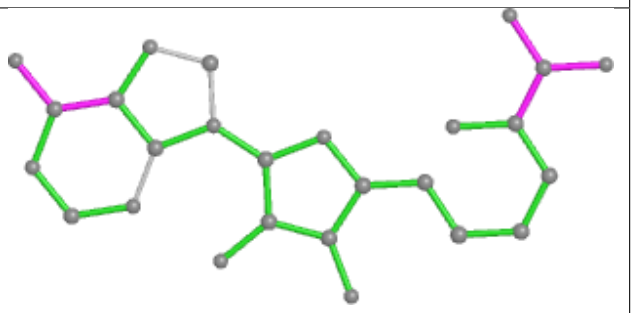


Rings

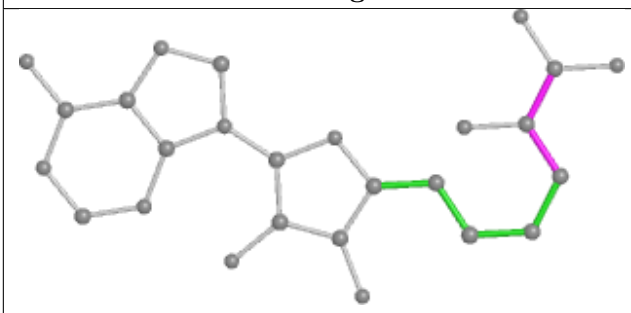
Ligand SAH F 900



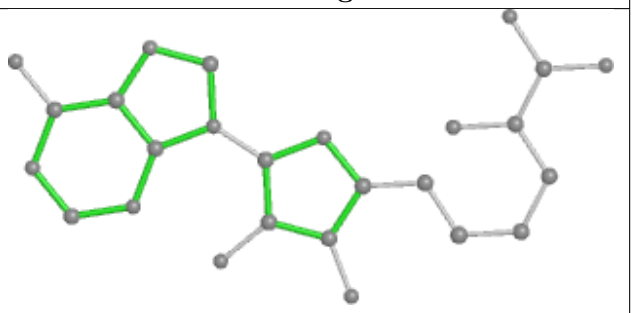
Bond lengths



Bond angles

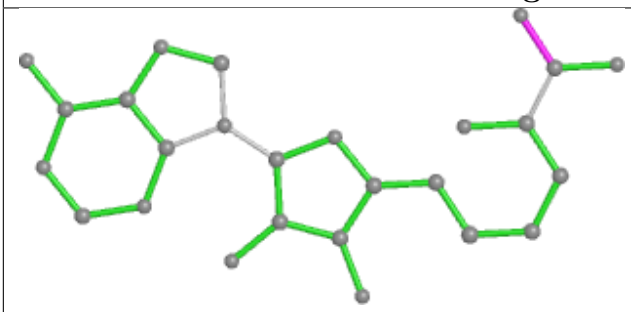


Torsions

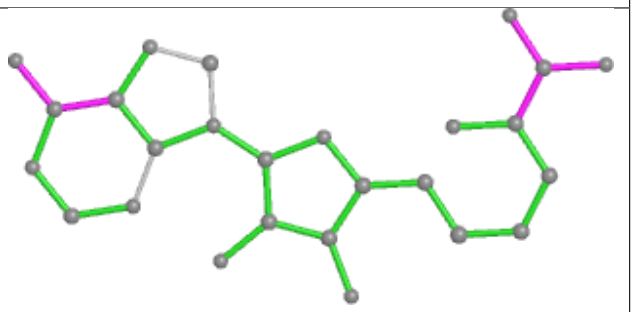


Rings

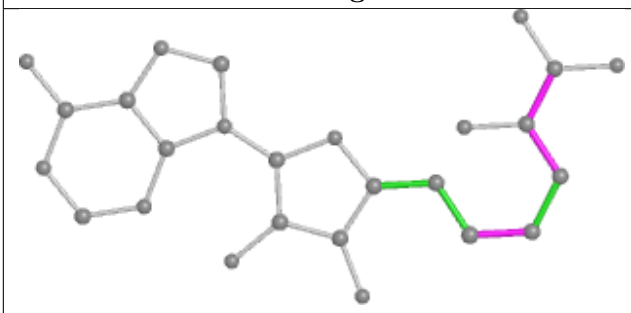
Ligand SAH G 900



Bond lengths



Bond angles



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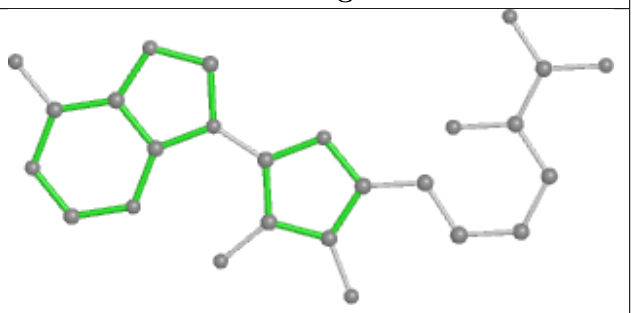
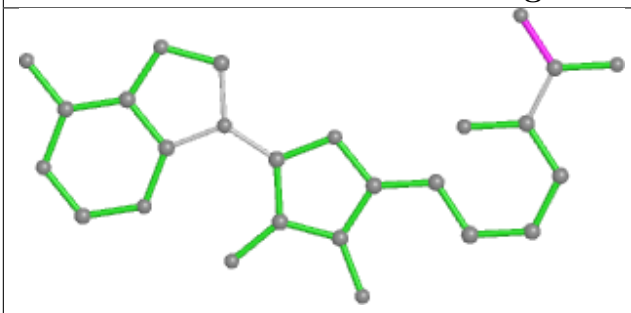


Rings

Ligand SAH B 900



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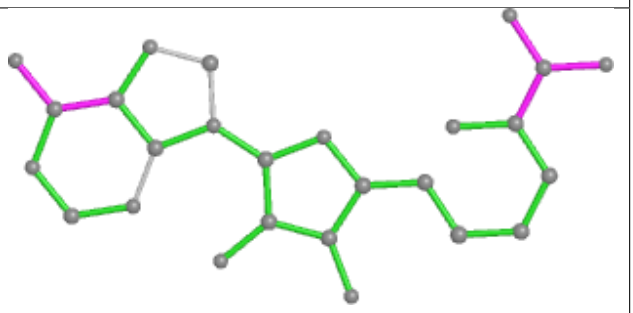
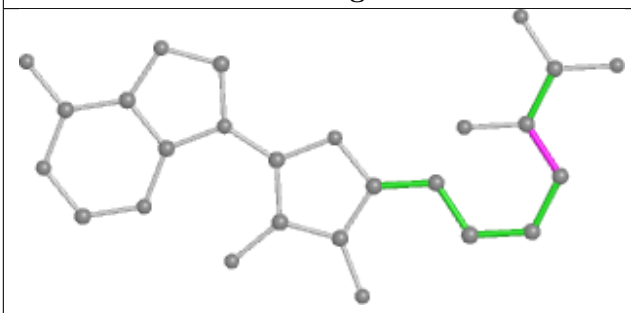


Bond angles



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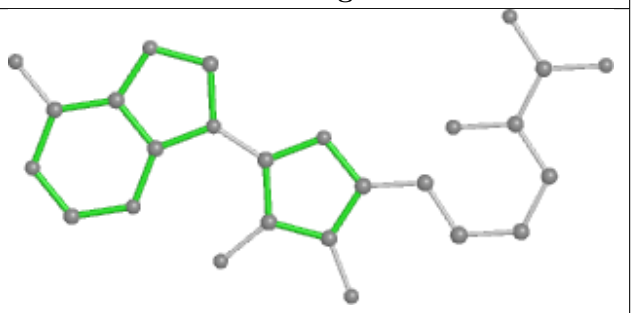
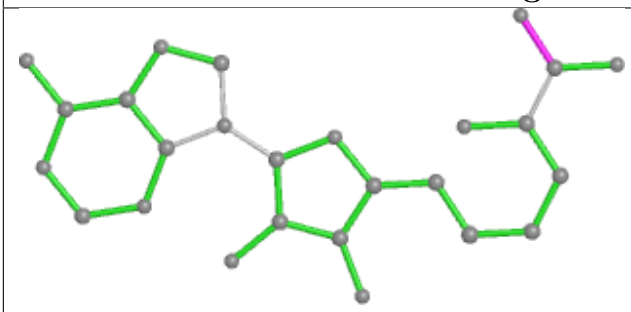


Rings

Ligand SAH D 900



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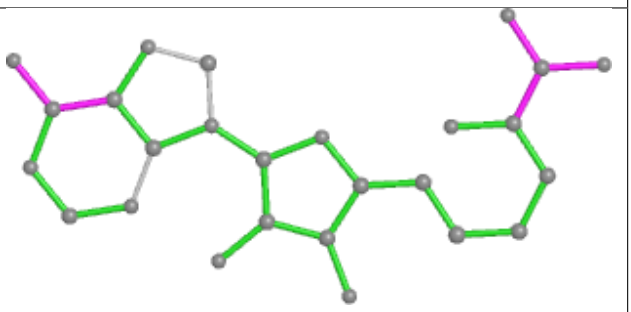
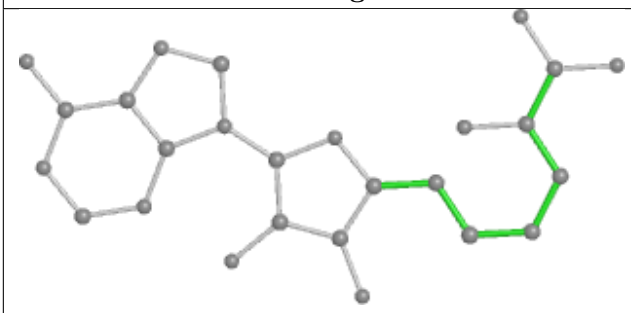


Bond angles



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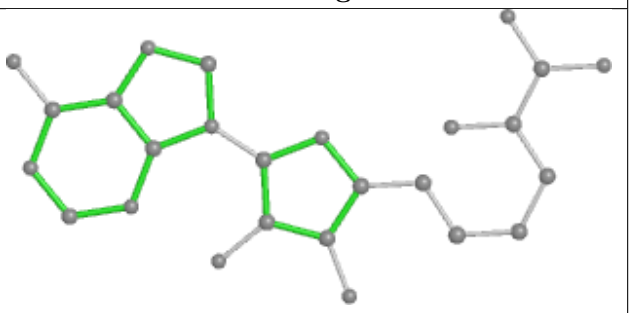

Rings

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.