wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 05:24 pm BST

PDB ID	:	5O4H
Title	:	HcgC from Methanococcus maripaludis cocrystallized with SAM and pyridinol
Authors	:	Wagner, T.; Bai, L.; Xu, T.; Hu, X.; Ermler, U.; Shima, S.
Deposited on	:	2017-05-29
Resolution	:	1.75 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 (i) symbol.

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

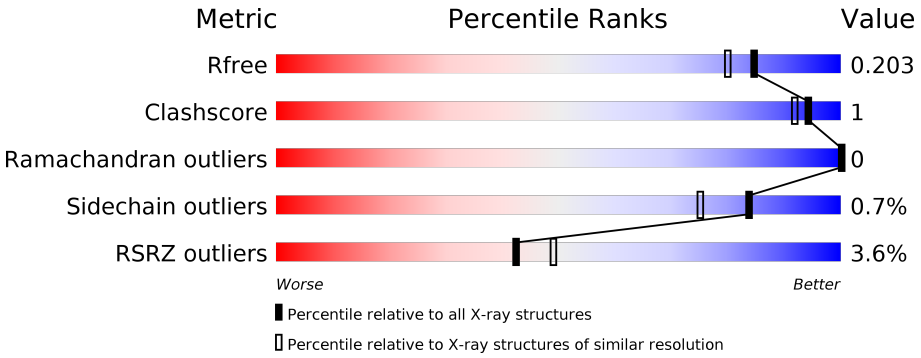
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	274	4% 93% • 5%
1	B	274	4% 90% • 5%
1	C	274	3% 91% • •
1	D	274	3% 91% • 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9179 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 HcgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			2056	1318	332	399	7			
1	B	259	Total	C	N	O	S	0	0	0
			2040	1308	331	394	7			
1	C	262	Total	C	N	O	S	0	8	0
			2110	1359	336	407	8			
1	D	258	Total	C	N	O	S	0	6	0
			2074	1332	336	399	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ASP	-	expression tag	UNP Q6LX54
A	262	LYS	-	expression tag	UNP Q6LX54
A	263	LEU	-	expression tag	UNP Q6LX54
A	264	ALA	-	expression tag	UNP Q6LX54
A	265	ALA	-	expression tag	UNP Q6LX54
A	266	ALA	-	expression tag	UNP Q6LX54
A	267	LEU	-	expression tag	UNP Q6LX54
A	268	GLU	-	expression tag	UNP Q6LX54
A	269	HIS	-	expression tag	UNP Q6LX54
A	270	HIS	-	expression tag	UNP Q6LX54
A	271	HIS	-	expression tag	UNP Q6LX54
A	272	HIS	-	expression tag	UNP Q6LX54
A	273	HIS	-	expression tag	UNP Q6LX54
A	274	HIS	-	expression tag	UNP Q6LX54
B	261	ASP	-	expression tag	UNP Q6LX54
B	262	LYS	-	expression tag	UNP Q6LX54
B	263	LEU	-	expression tag	UNP Q6LX54
B	264	ALA	-	expression tag	UNP Q6LX54
B	265	ALA	-	expression tag	UNP Q6LX54
B	266	ALA	-	expression tag	UNP Q6LX54
B	267	LEU	-	expression tag	UNP Q6LX54

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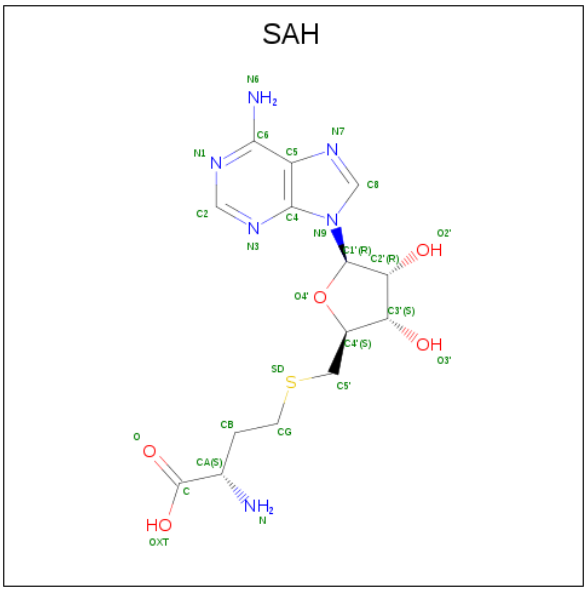
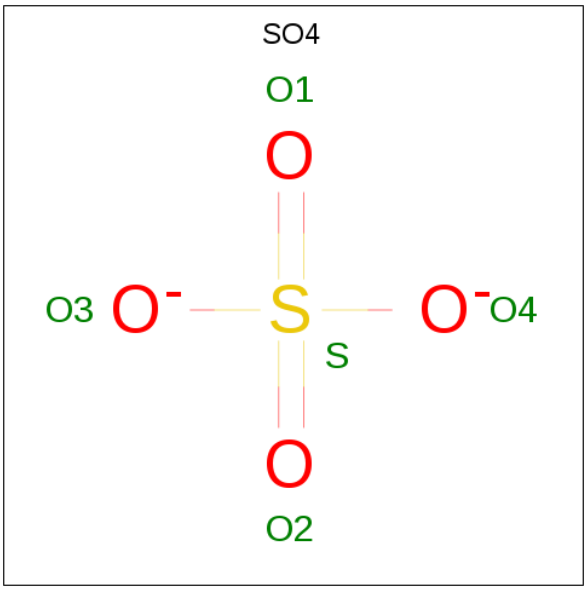
Chain	Residue	Modelled	Actual	Comment	Reference
B	268	GLU	-	expression tag	UNP Q6LX54
B	269	HIS	-	expression tag	UNP Q6LX54
B	270	HIS	-	expression tag	UNP Q6LX54
B	271	HIS	-	expression tag	UNP Q6LX54
B	272	HIS	-	expression tag	UNP Q6LX54
B	273	HIS	-	expression tag	UNP Q6LX54
B	274	HIS	-	expression tag	UNP Q6LX54
C	261	ASP	-	expression tag	UNP Q6LX54
C	262	LYS	-	expression tag	UNP Q6LX54
C	263	LEU	-	expression tag	UNP Q6LX54
C	264	ALA	-	expression tag	UNP Q6LX54
C	265	ALA	-	expression tag	UNP Q6LX54
C	266	ALA	-	expression tag	UNP Q6LX54
C	267	LEU	-	expression tag	UNP Q6LX54
C	268	GLU	-	expression tag	UNP Q6LX54
C	269	HIS	-	expression tag	UNP Q6LX54
C	270	HIS	-	expression tag	UNP Q6LX54
C	271	HIS	-	expression tag	UNP Q6LX54
C	272	HIS	-	expression tag	UNP Q6LX54
C	273	HIS	-	expression tag	UNP Q6LX54
C	274	HIS	-	expression tag	UNP Q6LX54
D	261	ASP	-	expression tag	UNP Q6LX54
D	262	LYS	-	expression tag	UNP Q6LX54
D	263	LEU	-	expression tag	UNP Q6LX54
D	264	ALA	-	expression tag	UNP Q6LX54
D	265	ALA	-	expression tag	UNP Q6LX54
D	266	ALA	-	expression tag	UNP Q6LX54
D	267	LEU	-	expression tag	UNP Q6LX54
D	268	GLU	-	expression tag	UNP Q6LX54
D	269	HIS	-	expression tag	UNP Q6LX54
D	270	HIS	-	expression tag	UNP Q6LX54
D	271	HIS	-	expression tag	UNP Q6LX54
D	272	HIS	-	expression tag	UNP Q6LX54
D	273	HIS	-	expression tag	UNP Q6LX54
D	274	HIS	-	expression tag	UNP Q6LX54

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



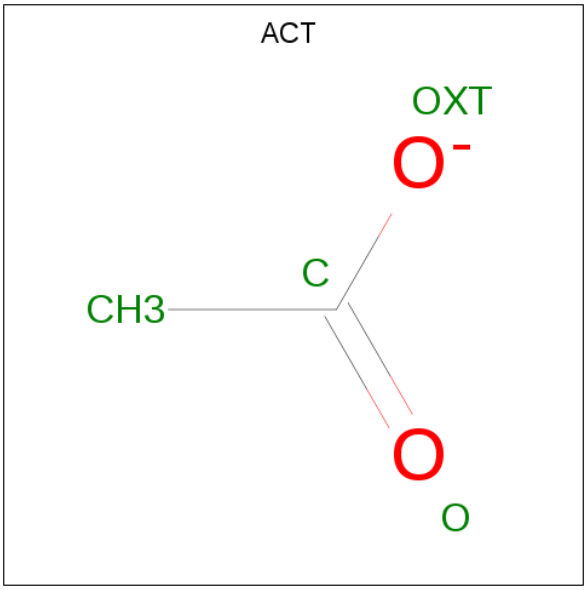
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



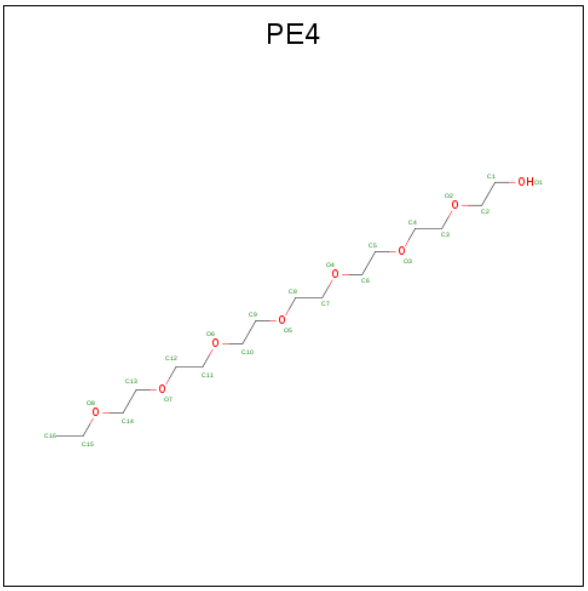
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 15 10 5	0	0
5	B	1	Total C O 11 7 4	0	0
5	B	1	Total C O 14 9 5	0	0
5	C	1	Total C O 10 7 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Na 1 1	0	0

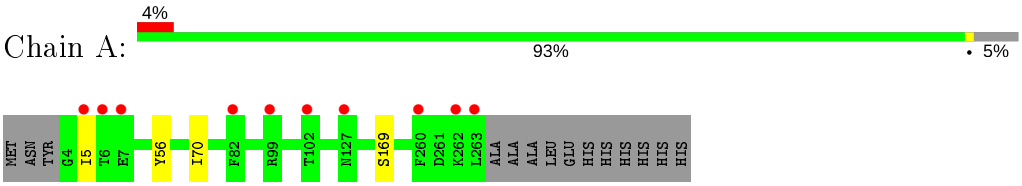
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	157	Total O 157 157	0	0
7	B	182	Total O 182 182	0	0
7	C	184	Total O 184 184	0	0
7	D	176	Total O 176 176	0	0

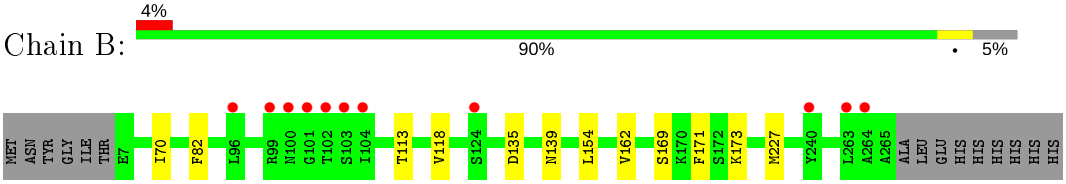
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

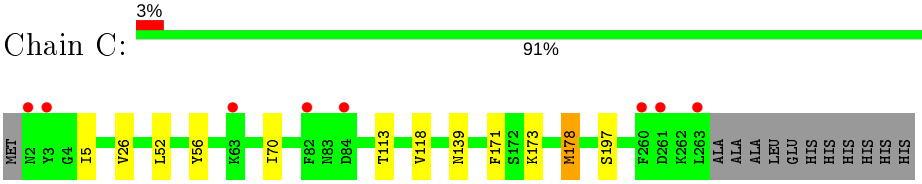
- Molecule 1: HcgC



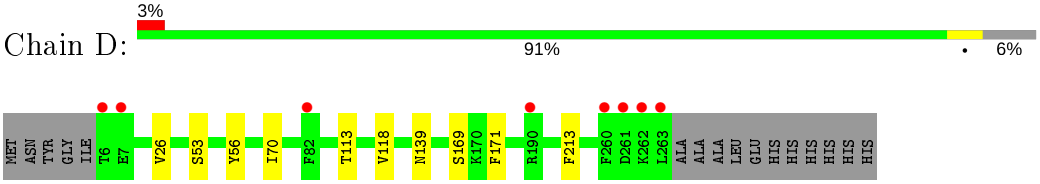
- Molecule 1: HcgC



- Molecule 1: HcgC



- Molecule 1: HcgC



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.17Å 77.74Å 100.99Å 90.00° 110.87° 90.00°	Depositor
Resolution (Å)	47.85 – 1.75 47.85 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.85-1.75) 99.6 (47.85-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.168 , 0.193 0.180 , 0.203	Depositor DCC
R_{free} test set	5307 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9179	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PE4, NA, SAH, SO4, ACT

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	0.49	0/2088	0.68	0/2810
1	B	0.47	0/2069	0.68	0/2785
1	C	0.48	0/2165	0.70	2/2915 (0.1%)
1	D	0.46	0/2121	0.68	0/2854
All	All	0.47	0/8443	0.69	2/11364 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178[A]	MET	CB-CG-SD	5.10	127.69	112.40
1	C	178[B]	MET	CB-CG-SD	5.10	127.69	112.40

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	2056	0	2127	3	0
1	B	2040	0	2107	9	0
1	C	2110	0	2193	8	0
1	D	2074	0	2163	6	0
2	A	26	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	19	1	0
2	C	26	0	19	0	0
2	D	26	0	19	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	D	5	0	0	0	0
4	A	8	0	6	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	A	15	0	18	1	0
5	B	25	0	28	1	0
5	C	10	0	13	0	0
6	D	1	0	0	0	0
7	A	157	0	0	0	0
7	B	182	0	0	1	0
7	C	184	0	0	0	0
7	D	176	0	0	1	0
All	All	9179	0	8740	22	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 1.

The worst 5 of 22 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:169:SER:OG	7:B:401:HOH:O	2.18	0.53
1:B:171:PHE:CZ	1:D:169:SER:HA	2.47	0.50
1:D:26[B]:VAL:CG1	1:D:56:TYR:HB3	2.42	0.48
1:C:139[A]:ASN:HB2	1:C:171[A]:PHE:CE2	2.48	0.48
1:C:5:ILE:HG12	1:D:213:PHE:CE2	2.48	0.48

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	259/274 (94%)	258 (100%)	1 (0%)	0	100	100
1	B	257/274 (94%)	255 (99%)	2 (1%)	0	100	100
1	C	268/274 (98%)	267 (100%)	1 (0%)	0	100	100
1	D	262/274 (96%)	260 (99%)	2 (1%)	0	100	100
All	All	1046/1096 (95%)	1040 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	239/249 (96%)	238 (100%)	1 (0%)	91	87
1	B	235/249 (94%)	233 (99%)	2 (1%)	78	67
1	C	248/249 (100%)	246 (99%)	2 (1%)	81	72
1	D	243/249 (98%)	241 (99%)	2 (1%)	81	72
All	All	965/996 (97%)	958 (99%)	7 (1%)	84	75

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	70	ILE
1	D	70	ILE
1	C	197	SER
1	B	70	ILE
1	D	53	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	A	301	-	21,28,28	1.17	2 (9%)	20,40,40	1.45	3 (15%)
5	PE4	B	306	-	13,13,23	0.54	0	12,12,22	0.45	0
2	SAH	D	301	-	21,28,28	1.17	3 (14%)	20,40,40	1.59	5 (25%)
2	SAH	B	301	-	21,28,28	1.17	1 (4%)	20,40,40	1.58	5 (25%)
4	ACT	B	304	-	1,3,3	7.55	1 (100%)	0,3,3	0.00	-
4	ACT	A	304	-	1,3,3	7.10	1 (100%)	0,3,3	0.00	-
3	SO4	B	302	-	4,4,4	0.37	0	6,6,6	0.17	0
4	ACT	C	302	-	1,3,3	6.13	1 (100%)	0,3,3	0.00	-
4	ACT	D	304	-	1,3,3	5.34	1 (100%)	0,3,3	0.00	-
5	PE4	C	303	-	9,9,23	0.53	0	8,8,22	0.52	0
4	ACT	A	305	-	1,3,3	4.44	1 (100%)	0,3,3	0.00	-
3	SO4	A	303	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	B	303	-	4,4,4	0.34	0	6,6,6	0.04	0
5	PE4	B	305	-	10,10,23	0.58	0	9,9,22	0.28	0
3	SO4	A	302	-	4,4,4	0.32	0	6,6,6	0.11	0
3	SO4	D	303	-	4,4,4	0.32	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SAH	C	301	-	21,28,28	1.15	2 (9%)	20,40,40	1.57	3 (15%)
5	PE4	A	306	-	14,14,23	0.51	0	13,13,22	0.45	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
2	SAH	A	301	-	-	0/7/31/31	0/3/3/3
2	SAH	D	301	-	-	1/7/31/31	0/3/3/3
2	SAH	B	301	-	-	1/7/31/31	0/3/3/3
5	PE4	C	303	-	-	3/7/7/21	-
5	PE4	A	306	-	-	6/12/12/21	-
5	PE4	B	305	-	-	5/8/8/21	-
5	PE4	B	306	-	-	9/11/11/21	-
2	SAH	C	301	-	-	1/7/31/31	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	ACT	CH3-C	7.55	1.58	1.48
4	A	304	ACT	CH3-C	7.10	1.57	1.48
4	C	302	ACT	CH3-C	6.13	1.56	1.48
4	D	304	ACT	CH3-C	5.34	1.55	1.48
4	A	305	ACT	CH3-C	4.44	1.54	1.48

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	SAH	N3-C2-N1	-4.25	122.03	128.68
2	D	301	SAH	N3-C2-N1	-4.22	122.09	128.68
2	B	301	SAH	N3-C2-N1	-4.12	122.23	128.68
2	A	301	SAH	N3-C2-N1	-3.85	122.66	128.68
2	A	301	SAH	C1'-N9-C4	-2.98	121.41	126.64

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	305	PE4	O6-C10-C9-O5
5	B	306	PE4	O6-C11-C12-O7
5	B	305	PE4	O6-C11-C12-O7
5	B	305	PE4	O7-C13-C14-O8
5	A	306	PE4	O3-C5-C6-O4

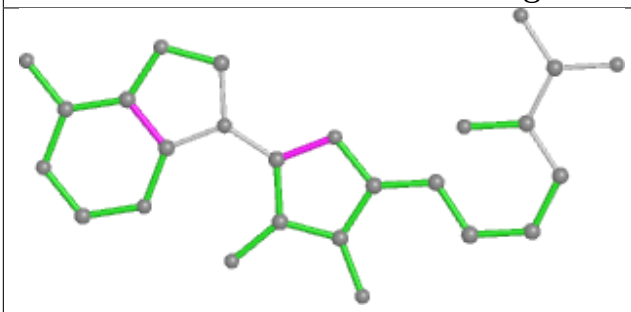
There are no ring outliers.

4 monomers are involved in 4 short contacts:

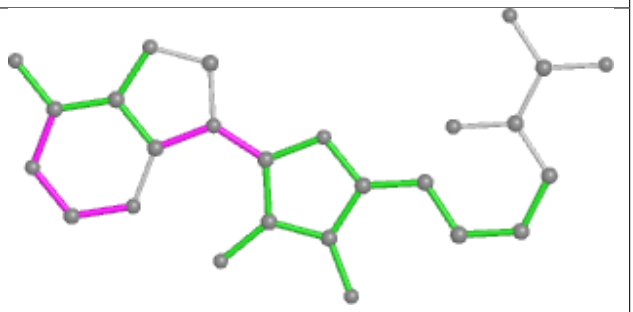
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	306	PE4	1	0
2	D	301	SAH	1	0
2	B	301	SAH	1	0
5	A	306	PE4	1	0

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 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.

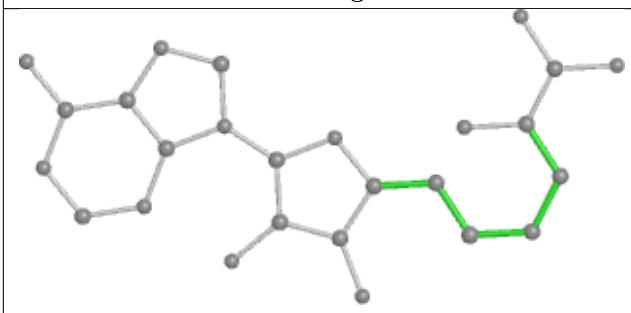
Ligand SAH A 301



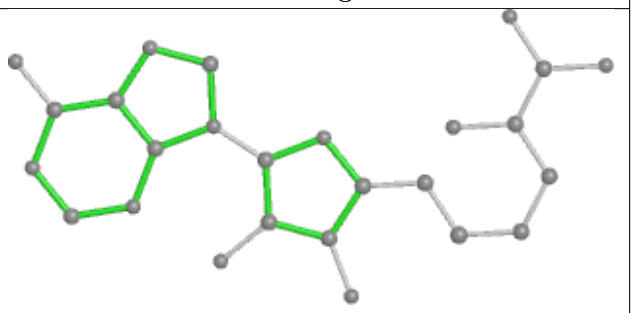
Bond lengths



Bond angles



Torsions



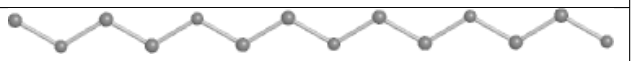
Rings

Ligand PE4 B 306

Bond lengths

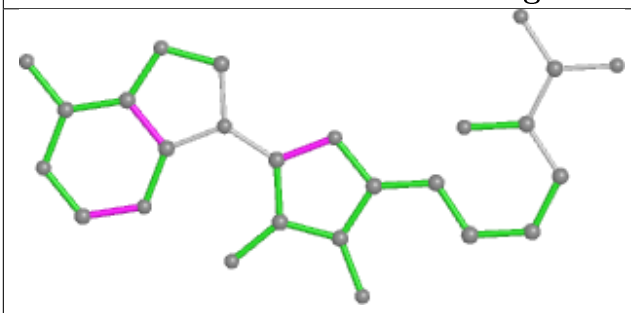
Bond angles

Torsions

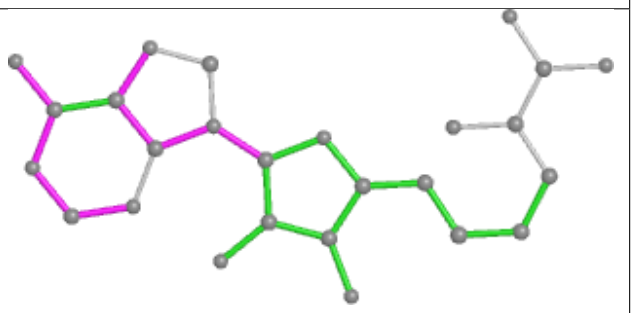


Rings

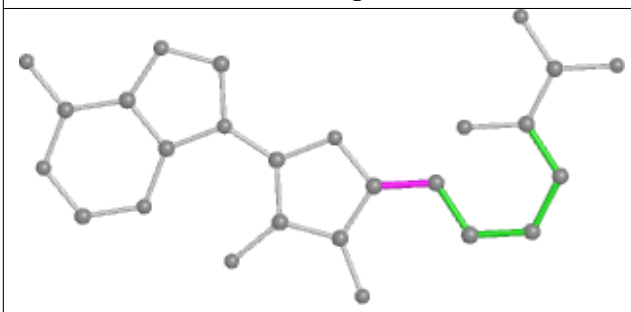
Ligand SAH D 301



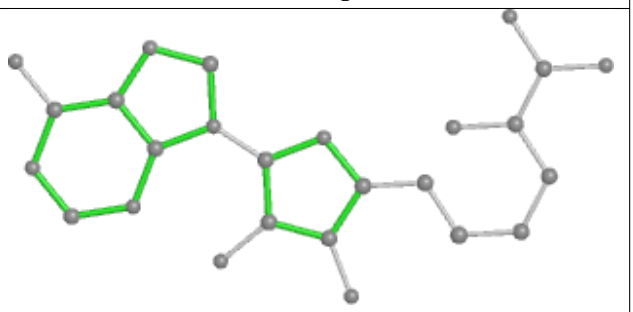
Bond lengths



Bond angles

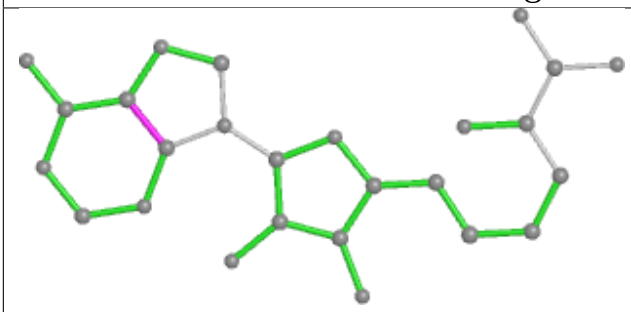


Torsions

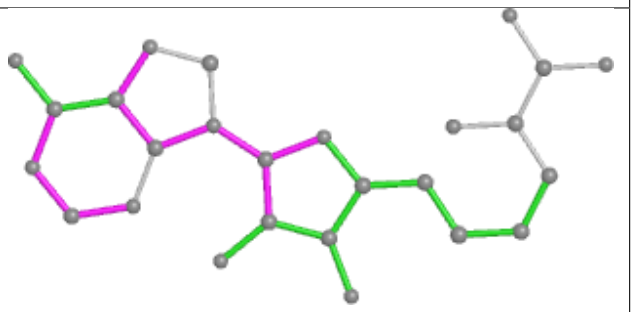


Rings

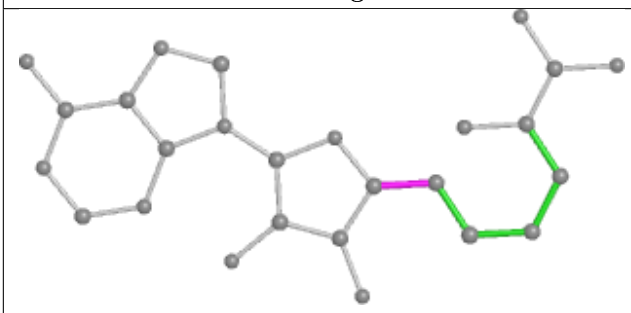
Ligand SAH B 301



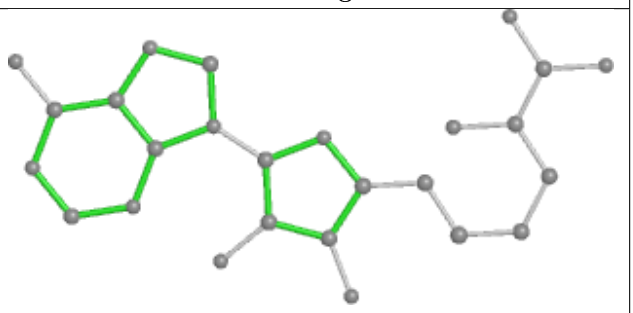
Bond lengths



Bond angles

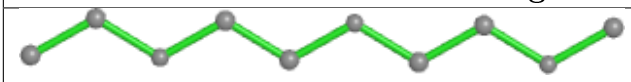


Torsions

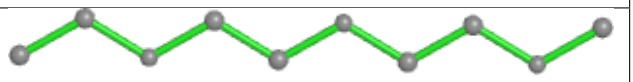


Rings

Ligand PE4 C 303

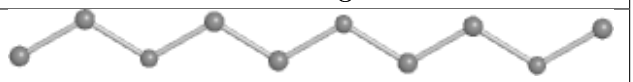


Bond lengths



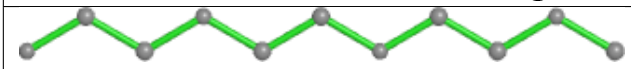
Bond angles

Torsions

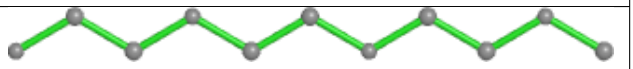


Rings

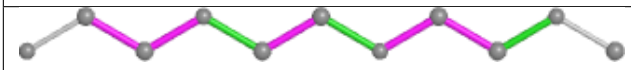
Ligand PE4 B 305



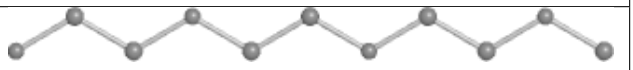
Bond lengths



Bond angles

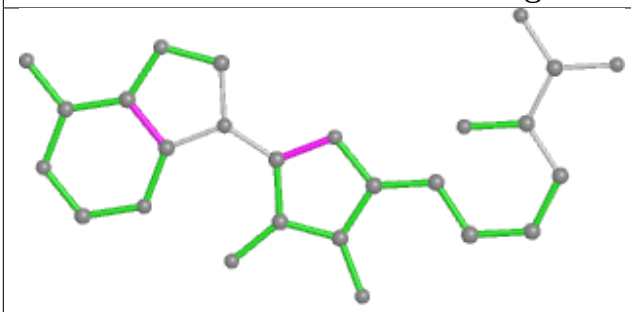


Torsions

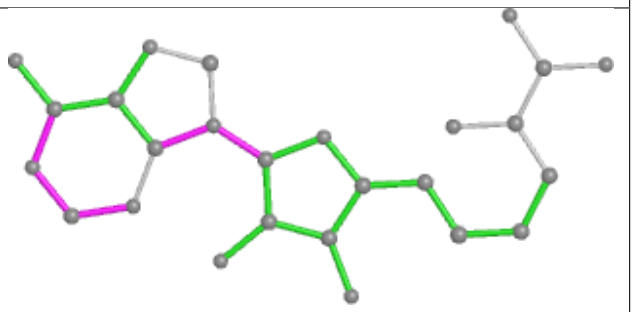


Rings

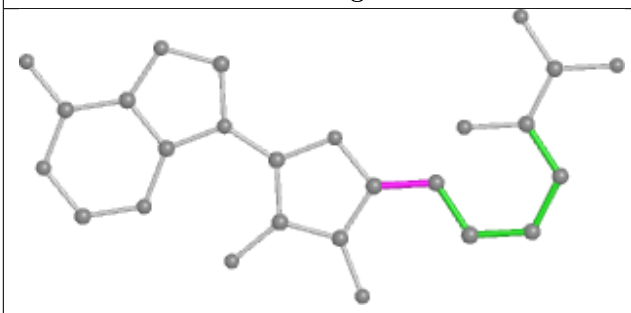
Ligand SAH C 301



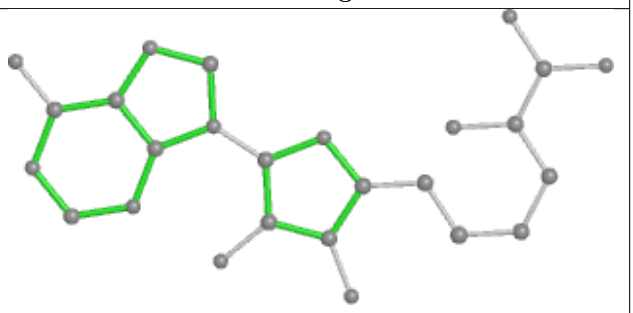
Bond lengths



Bond angles



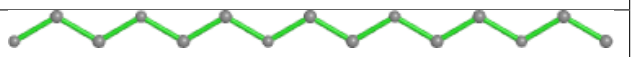
Torsions



Rings

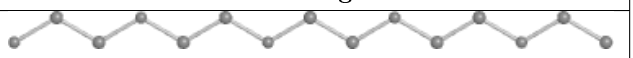
Ligand PE4 A 306

Bond lengths



Bond angles

Torsions



Rings

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	260/274 (94%)	-0.03	10 (3%) 40 47	19, 31, 59, 123	0
1	B	259/274 (94%)	0.08	11 (4%) 36 42	22, 34, 68, 113	0
1	C	262/274 (95%)	-0.05	8 (3%) 49 55	20, 34, 61, 97	0
1	D	258/274 (94%)	-0.09	8 (3%) 49 55	20, 33, 60, 97	0
All	All	1039/1096 (94%)	-0.02	37 (3%) 42 49	19, 33, 61, 123	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	THR	8.2
1	C	82	PHE	5.9
1	B	264	ALA	5.3
1	A	262	LYS	5.1
1	C	3	TYR	5.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

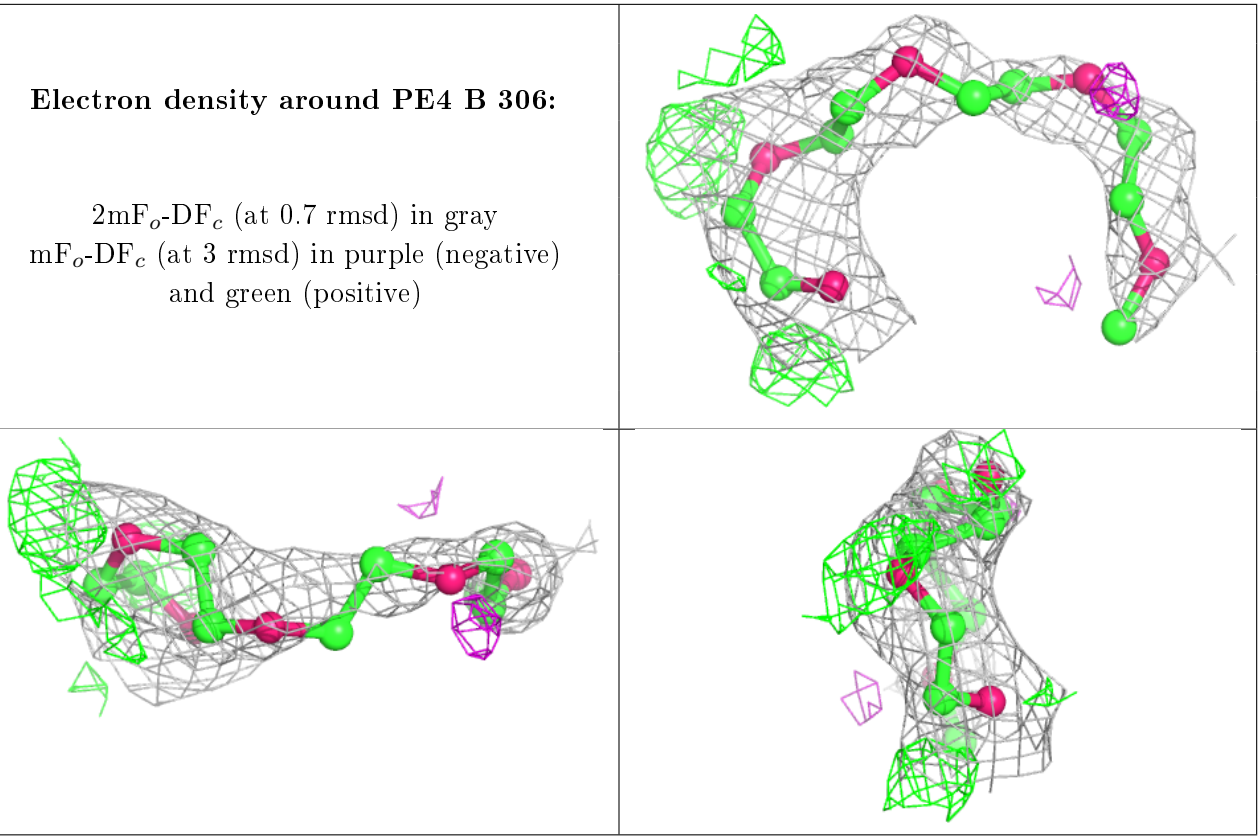
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PE4	B	306	14/24	0.64	0.23	78,80,82,82	0
5	PE4	B	305	11/24	0.69	0.14	62,67,68,69	0
4	ACT	D	304	4/4	0.70	0.22	63,64,66,69	0
5	PE4	C	303	10/24	0.76	0.14	75,77,78,78	0
5	PE4	A	306	15/24	0.78	0.15	56,60,68,70	0
3	SO4	A	303	5/5	0.82	0.21	81,82,86,86	0
4	ACT	A	305	4/4	0.84	0.22	62,62,62,63	0
3	SO4	B	303	5/5	0.88	0.23	75,75,76,76	5
4	ACT	C	302	4/4	0.88	0.20	33,48,53,56	0
3	SO4	B	302	5/5	0.91	0.10	78,79,80,81	0
3	SO4	D	303	5/5	0.91	0.24	52,58,63,65	0
3	SO4	A	302	5/5	0.93	0.11	119,120,120,120	0
4	ACT	B	304	4/4	0.94	0.14	28,38,45,47	0
6	NA	D	302	1/1	0.95	0.14	32,32,32,32	0
4	ACT	A	304	4/4	0.95	0.12	35,38,38,45	0
2	SAH	A	301	26/26	0.96	0.07	24,27,30,34	0
2	SAH	B	301	26/26	0.97	0.06	27,30,34,36	0
2	SAH	D	301	26/26	0.98	0.05	25,29,31,33	0
2	SAH	C	301	26/26	0.98	0.06	23,27,29,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

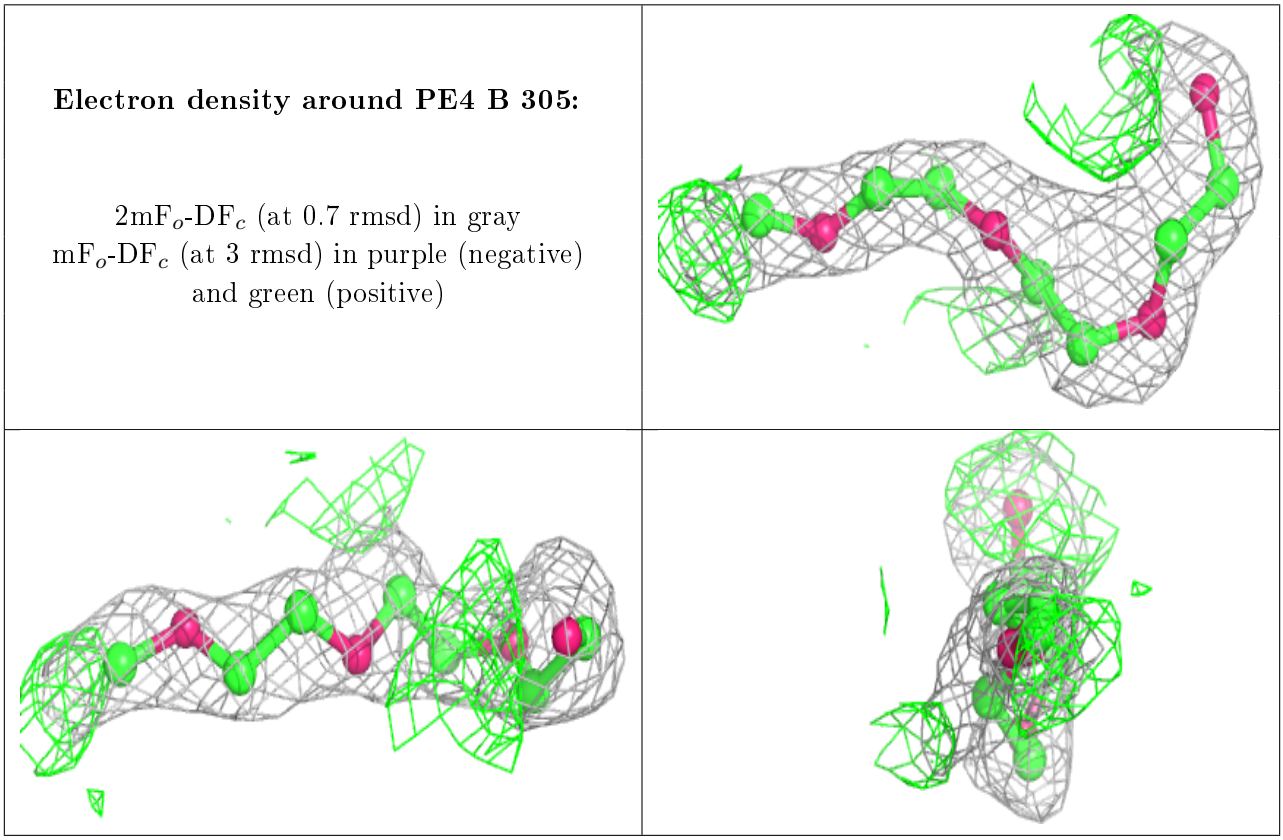
Electron density around PE4 B 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



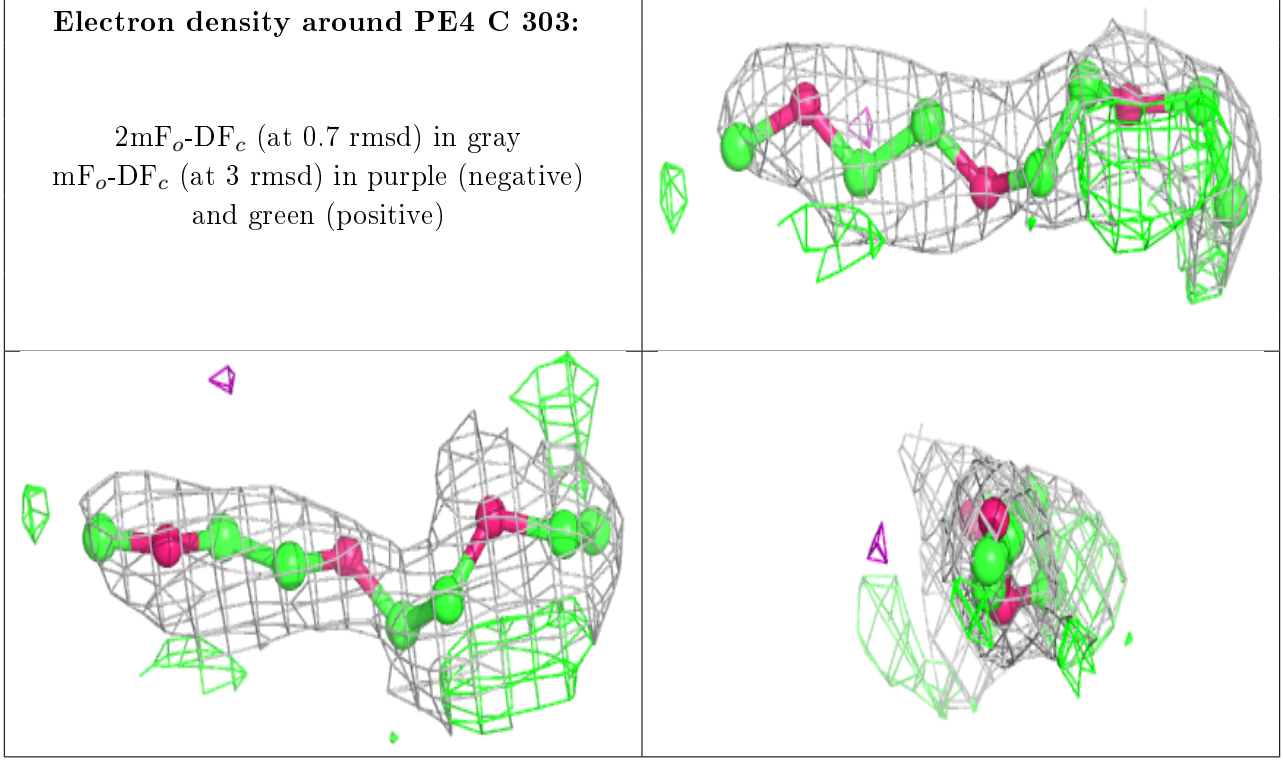
Electron density around PE4 B 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



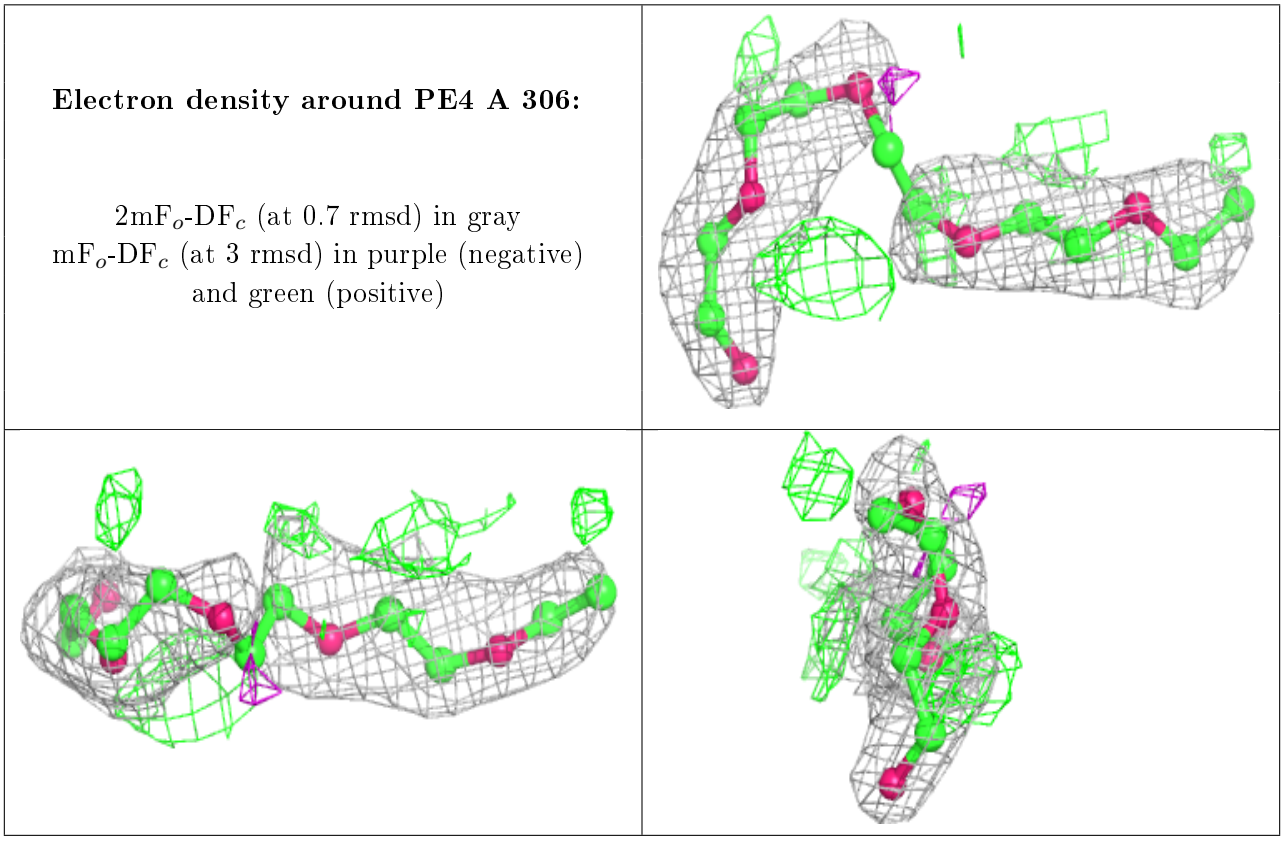
Electron density around PE4 C 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



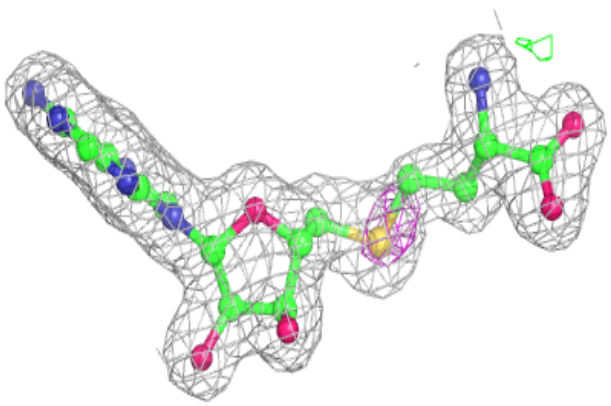
Electron density around PE4 A 306:

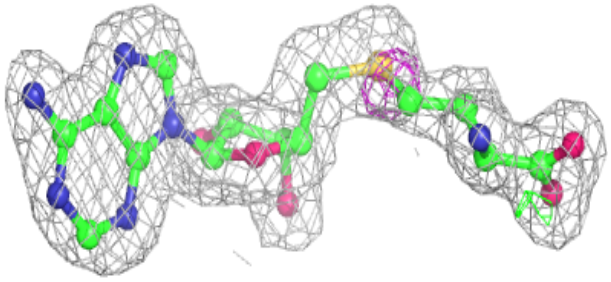
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

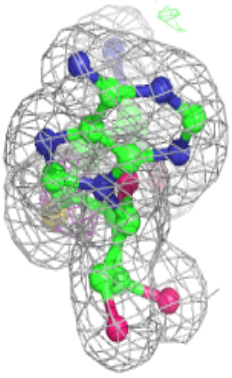


Electron density around SAH A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

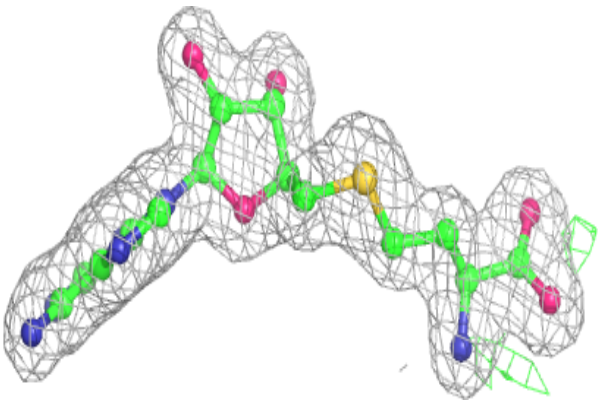


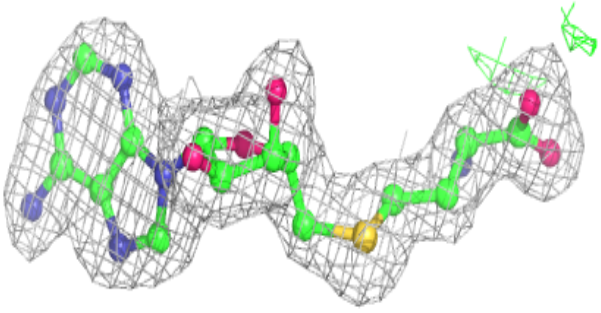


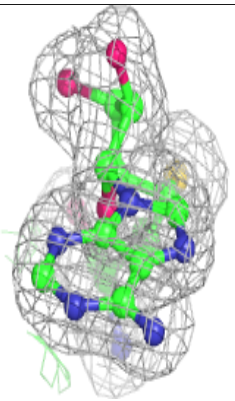


Electron density around SAH B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

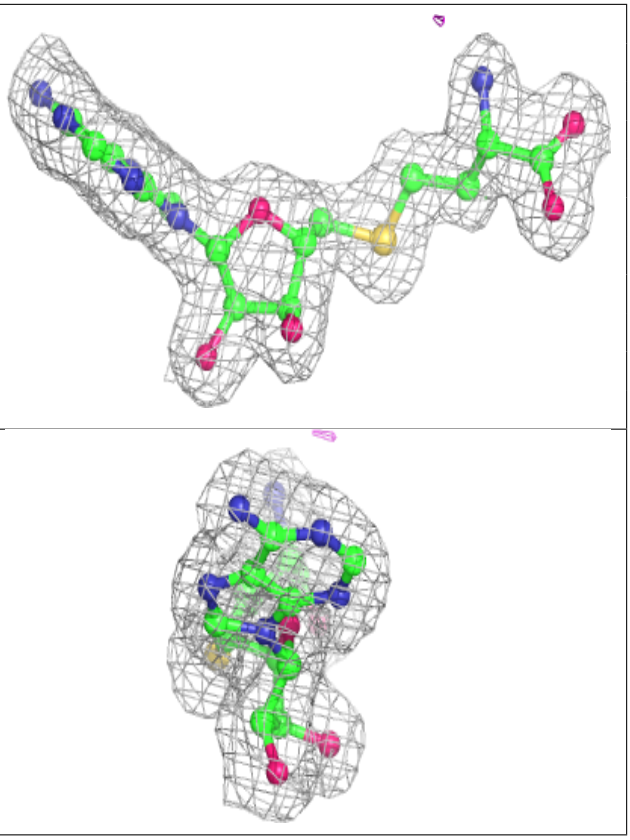






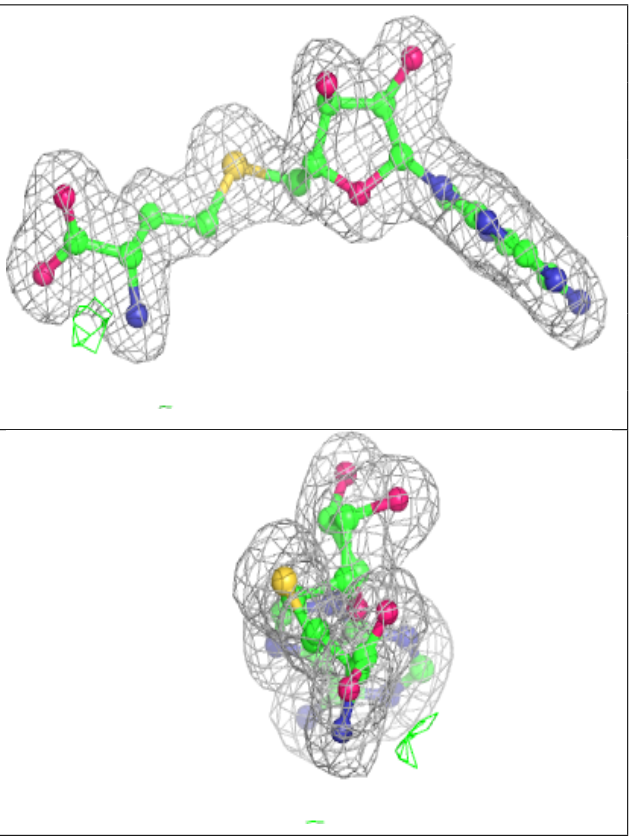
Electron density around SAH D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SAH C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.