



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 06:43 PM EDT

PDB ID : 5O4J  
Title : HcgC from Methanococcus maripaludis cocrystallized with SAH and pyridinol  
Authors : Wagner, T.; Bai, L.; Xu, T.; Hu, X.; Ermler, U.; Shima, S.  
Deposited on : 2017-05-29  
Resolution : 1.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

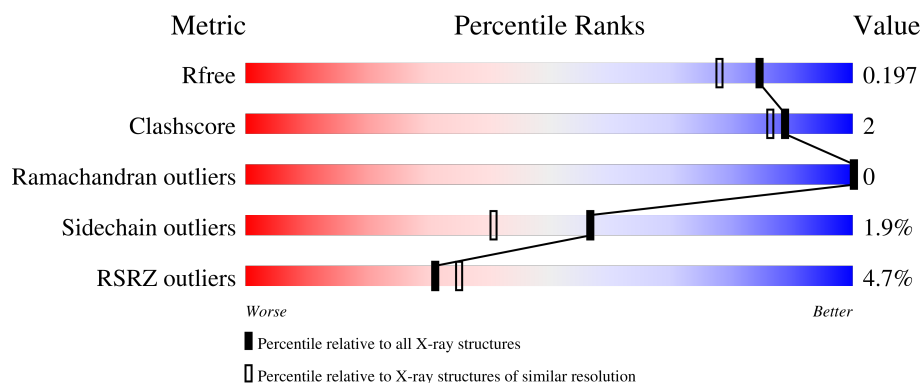
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	274	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	C	274	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>.</div> </div> </div>
1	D	274	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9403 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	264	Total	C	N	O	S	0	6	0
			2113	1354	338	413	8			
1	B	261	Total	C	N	O	S	0	3	0
			2078	1330	335	404	9			
1	C	262	Total	C	N	O	S	0	5	0
			2094	1344	336	407	7			
1	D	261	Total	C	N	O	S	0	3	0
			2074	1329	334	403	8			

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<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



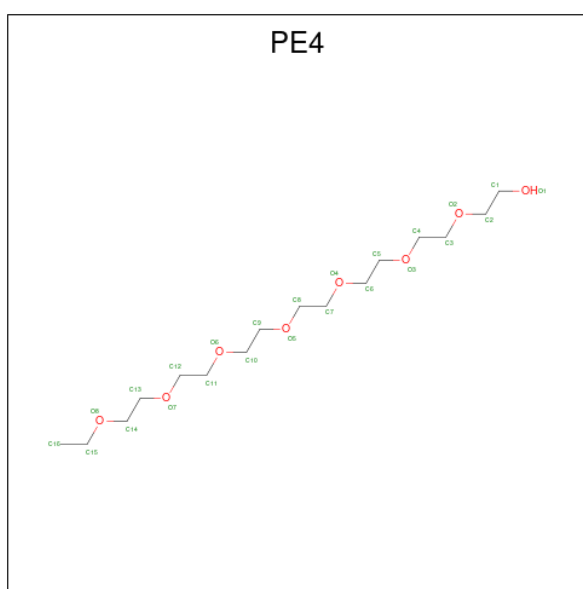
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



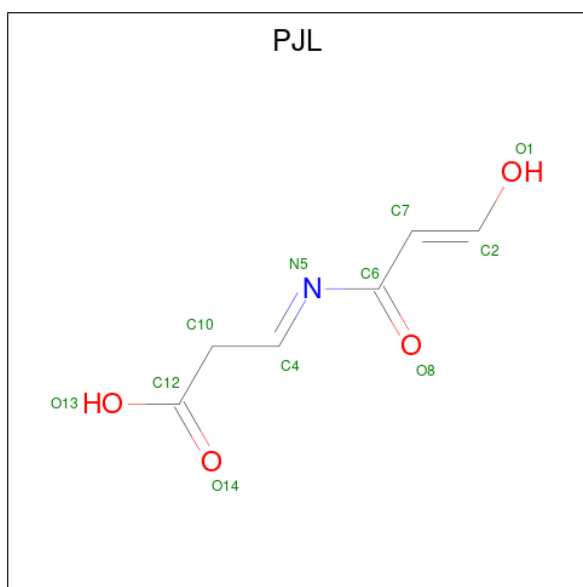
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 15 10 5	0	0
4	B	1	Total C O 14 9 5	0	0
4	C	1	Total C O 13 9 4	0	0

- Molecule 5 is (3 {E})-3-[( {E})-3-oxidanylprop-2-enoyl]iminopropanoic acid (three-letter code: PJJ) (formula: C<sub>6</sub>H<sub>7</sub>NO<sub>4</sub>).

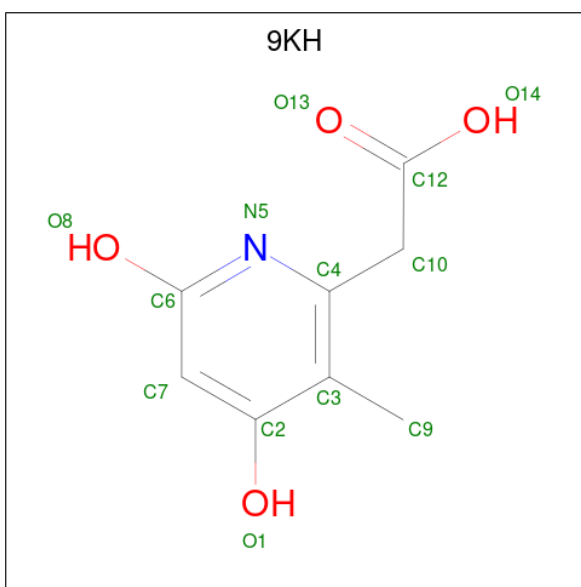


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Li	0	0
			1	1		
6	D	1	Total	Li	0	0
			1	1		

- Molecule 7 is 6-carboxy methyl-4-hydroxy-2-pyridinol (three-letter code: 9KH) (formula: C<sub>8</sub>H<sub>9</sub>NO<sub>4</sub>).

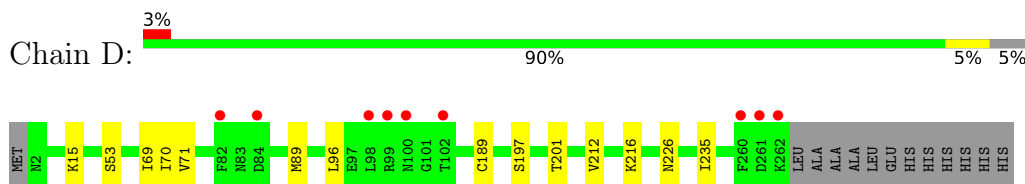


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			13	8	1	4		
7	C	1	Total	C	N	O	0	0
			13	8	1	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	241	Total	O	0	0
			241	241		
8	B	226	Total	O	0	0
			226	226		
8	C	173	Total	O	0	0
			173	173		
8	D	199	Total	O	0	0
			199	199		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.74Å 83.00Å 96.12Å 90.00° 108.03° 90.00°	Depositor
Resolution (Å)	45.70 – 1.70 45.70 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.70-1.70) 99.6 (45.70-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.159 , 0.192 0.169 , 0.197	Depositor DCC
$R_{free}$ test set	6067 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: LI, SAH, SO4, PJJ, PE4, 9KH

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	0.32	0/2158	0.52	0/2905
1	B	0.31	0/2114	0.50	0/2846
1	C	0.30	0/2139	0.49	0/2879
1	D	0.31	0/2113	0.50	0/2844
All	All	0.31	0/8524	0.50	0/11474

There are no bond length outliers.

There are no bond angle outliers.

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	2113	0	2186	11	0
1	B	2078	0	2140	9	0
1	C	2094	0	2171	4	0
1	D	2074	0	2141	6	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	15	0	18	5	0
4	B	14	0	16	0	0
4	C	13	0	17	0	0
5	A	11	0	0	1	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	13	0	0	0	0
7	C	13	0	0	0	0
8	A	241	0	0	1	1
8	B	226	0	0	2	0
8	C	173	0	0	0	0
8	D	199	0	0	1	1
All	All	9403	0	8765	32	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (32) 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)
5:A:304:PJL:C2	5:A:304:PJL:C4	2.73	0.66
1:B:2:ASN:ND2	8:B:401:HOH:O	2.30	0.64
1:A:23[A]:SER:OG	4:A:303:PE4:H52	2.04	0.57
1:A:23[B]:SER:HA	4:A:303:PE4:H41	1.88	0.56
1:A:23[A]:SER:HA	4:A:303:PE4:H41	1.89	0.55
1:D:15:LYS:NZ	8:D:402:HOH:O	2.32	0.53
1:A:187:ASP:OD1	1:A:190:ARG:NH1	2.44	0.46
1:B:69:ILE:HG21	1:B:89:MET:HE3	1.98	0.46
1:A:26:VAL:HG21	4:A:303:PE4:H42	1.98	0.46
1:C:160:LYS:HE3	1:C:262:LYS:HD3	1.98	0.45
1:B:1:MET:HE1	1:B:10:LYS:HD3	1.99	0.45
1:B:197:SER:HB2	1:B:235:ILE:HB	1.99	0.45
1:A:69:ILE:HG21	1:A:89:MET:HE3	1.99	0.45
1:D:212:VAL:O	1:D:216:LYS:HA	2.17	0.44
1:A:23[A]:SER:OG	4:A:303:PE4:H41	2.17	0.44
1:B:170:LYS:NZ	8:B:408:HOH:O	2.49	0.44
1:C:212:VAL:O	1:C:216:LYS:HA	2.17	0.43
1:D:197:SER:HB2	1:D:235:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189[B]:CYS:SG	1:D:201:THR:HG22	2.59	0.43
1:A:69:ILE:HG21	1:A:89:MET:CE	2.48	0.43
1:A:197:SER:HB2	1:A:235:ILE:HB	2.00	0.43
2:A:301:SAH:N	8:A:401:HOH:O	2.24	0.43
1:C:113:THR:HG21	1:C:118:VAL:HG13	1.98	0.43
1:D:71:VAL:HA	1:D:89:MET:O	2.19	0.42
1:B:113:THR:HG21	1:B:118:VAL:HG13	2.02	0.42
1:B:212:VAL:O	1:B:216:LYS:HA	2.19	0.42
1:A:113:THR:HG21	1:A:118:VAL:HG13	2.02	0.42
1:B:189[B]:CYS:SG	1:B:201:THR:HG22	2.61	0.41
1:D:69:ILE:HG21	1:D:89:MET:HE3	2.03	0.41
1:C:197:SER:HB2	1:C:235:ILE:HB	2.02	0.41
1:B:69:ILE:HG21	1:B:89:MET:CE	2.50	0.41
1:A:135:ASP:HB2	1:A:162:VAL:CG1	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:430:HOH:O	8:D:438:HOH:O[2_559]	2.08	0.12

## 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	268/274 (98%)	266 (99%)	2 (1%)	0	100	100
1	B	262/274 (96%)	260 (99%)	2 (1%)	0	100	100
1	C	265/274 (97%)	262 (99%)	3 (1%)	0	100	100
1	D	262/274 (96%)	259 (99%)	3 (1%)	0	100	100
All	All	1057/1096 (96%)	1047 (99%)	10 (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	247/249 (99%)	242 (98%)	5 (2%)	55	38
1	B	242/249 (97%)	240 (99%)	2 (1%)	81	74
1	C	245/249 (98%)	238 (97%)	7 (3%)	42	23
1	D	242/249 (97%)	238 (98%)	4 (2%)	60	46
All	All	976/996 (98%)	958 (98%)	18 (2%)	57	43

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	70	ILE
1	A	92	ASN
1	A	97	GLU
1	A	261	ASP
1	B	53	SER
1	B	70	ILE
1	C	2	ASN
1	C	53	SER
1	C	70	ILE
1	C	93	LYS
1	C	97	GLU
1	C	100	ASN
1	C	226	ASN
1	D	53	SER
1	D	70	ILE
1	D	96	LEU
1	D	226	ASN

Sometimes 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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$
5	PJL	A	304	-	8,10,10	0.99	0	7,11,11	1.06	1 (14%)
2	SAH	C	301	-	24,28,28	1.02	1 (4%)	25,40,40	1.25	2 (8%)
3	SO4	C	303	-	4,4,4	0.28	0	6,6,6	0.11	0
4	PE4	B	304	-	13,13,23	0.49	0	12,12,22	0.29	0
7	9KH	B	302	-	12,13,13	0.73	0	16,18,18	1.97	6 (37%)
3	SO4	B	303	-	4,4,4	0.33	0	6,6,6	0.04	0
2	SAH	A	301	-	24,28,28	1.03	1 (4%)	25,40,40	1.26	3 (12%)
2	SAH	B	301	-	24,28,28	0.99	0	25,40,40	1.24	3 (12%)
3	SO4	D	302	-	4,4,4	0.34	0	6,6,6	0.13	0
4	PE4	C	304	-	12,12,23	0.49	0	11,11,22	0.23	0
7	9KH	C	302	-	12,13,13	0.85	0	16,18,18	2.02	5 (31%)
4	PE4	A	303	-	14,14,23	0.49	0	13,13,22	0.34	0
3	SO4	A	302	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SAH	D	301	-	24,28,28	1.08	2 (8%)	25,40,40	1.31	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
5	PJL	A	304	-	-	1/3/9/9	-
2	SAH	C	301	-	-	2/11/31/31	0/3/3/3
4	PE4	B	304	-	-	6/11/11/21	-
7	9KH	B	302	-	-	2/4/4/4	0/1/1/1
2	SAH	A	301	-	-	2/11/31/31	0/3/3/3
2	SAH	B	301	-	-	3/11/31/31	0/3/3/3
4	PE4	C	304	-	-	4/10/10/21	-
7	9KH	C	302	-	-	0/4/4/4	0/1/1/1
4	PE4	A	303	-	-	5/12/12/21	-
2	SAH	D	301	-	-	2/11/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	SAH	O4'-C1'	2.54	1.44	1.41
2	C	301	SAH	C5-C4	2.33	1.47	1.40
2	D	301	SAH	C5-C4	2.28	1.47	1.40
2	A	301	SAH	C5-C4	2.05	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	302	9KH	C2-C3-C4	4.62	119.92	116.51
7	B	302	9KH	C2-C3-C4	4.23	119.63	116.51
2	A	301	SAH	N3-C2-N1	-3.59	123.06	128.68
2	B	301	SAH	N3-C2-N1	-3.54	123.14	128.68
7	C	302	9KH	C3-C4-N5	-3.41	120.27	123.87
2	D	301	SAH	N3-C2-N1	-3.34	123.46	128.68
7	C	302	9KH	C9-C3-C4	-3.33	119.78	122.69
2	C	301	SAH	N3-C2-N1	-3.29	123.54	128.68
7	B	302	9KH	C3-C4-N5	-3.10	120.59	123.87
7	B	302	9KH	C9-C3-C4	-2.78	120.26	122.69
2	D	301	SAH	C4-C5-N7	-2.72	106.57	109.40
7	B	302	9KH	C7-C2-C3	-2.65	119.35	121.98
7	C	302	9KH	C7-C2-C3	-2.60	119.39	121.98
7	B	302	9KH	O13-C12-C10	-2.40	116.20	123.04
7	B	302	9KH	C6-N5-C4	2.31	120.94	117.64
2	C	301	SAH	C4-C5-N7	-2.29	107.02	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	SAH	C2-N1-C6	2.28	122.66	118.75
7	C	302	9KH	C6-N5-C4	2.27	120.88	117.64
2	B	301	SAH	C1'-N9-C4	-2.26	122.68	126.64
5	A	304	PJL	O8-C6-C7	-2.21	117.43	122.08
2	A	301	SAH	C1'-N9-C4	-2.20	122.78	126.64
2	B	301	SAH	C4-C5-N7	-2.10	107.21	109.40
2	D	301	SAH	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (27) torsion outliers are listed below:

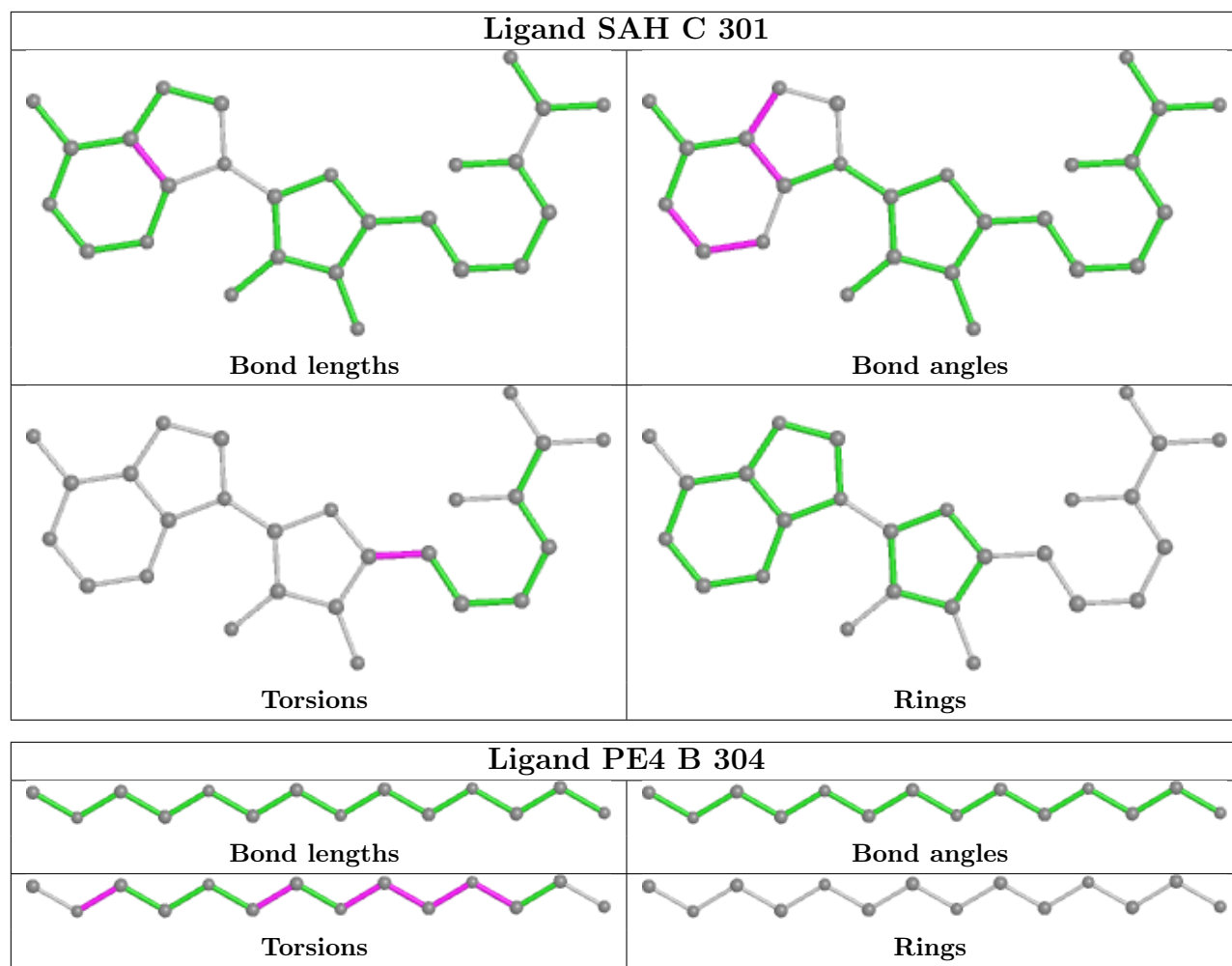
Mol	Chain	Res	Type	Atoms
2	C	301	SAH	C3'-C4'-C5'-SD
4	B	304	PE4	O6-C10-C9-O5
4	A	303	PE4	O4-C7-C8-O5
4	A	303	PE4	O2-C3-C4-O3
4	C	304	PE4	O7-C13-C14-O8
4	A	303	PE4	C7-C8-O5-C9
5	A	304	PJL	O8-C6-C7-C2
4	A	303	PE4	O3-C5-C6-O4
4	C	304	PE4	C10-C9-O5-C8
4	A	303	PE4	C6-C5-O3-C4
2	C	301	SAH	O4'-C4'-C5'-SD
2	D	301	SAH	O4'-C4'-C5'-SD
4	B	304	PE4	C13-C14-O8-C15
4	B	304	PE4	C7-C8-O5-C9
4	C	304	PE4	O6-C11-C12-O7
4	B	304	PE4	C10-C9-O5-C8
4	B	304	PE4	O6-C11-C12-O7
2	B	301	SAH	OXT-C-CA-CB
2	A	301	SAH	O-C-CA-N
4	C	304	PE4	C9-C10-O6-C11
2	B	301	SAH	O-C-CA-CB
7	B	302	9KH	C4-C10-C12-O13
7	B	302	9KH	C4-C10-C12-O14
2	A	301	SAH	C3'-C4'-C5'-SD
2	B	301	SAH	C3'-C4'-C5'-SD
2	D	301	SAH	C3'-C4'-C5'-SD
4	B	304	PE4	C9-C10-O6-C11

There are no ring outliers.

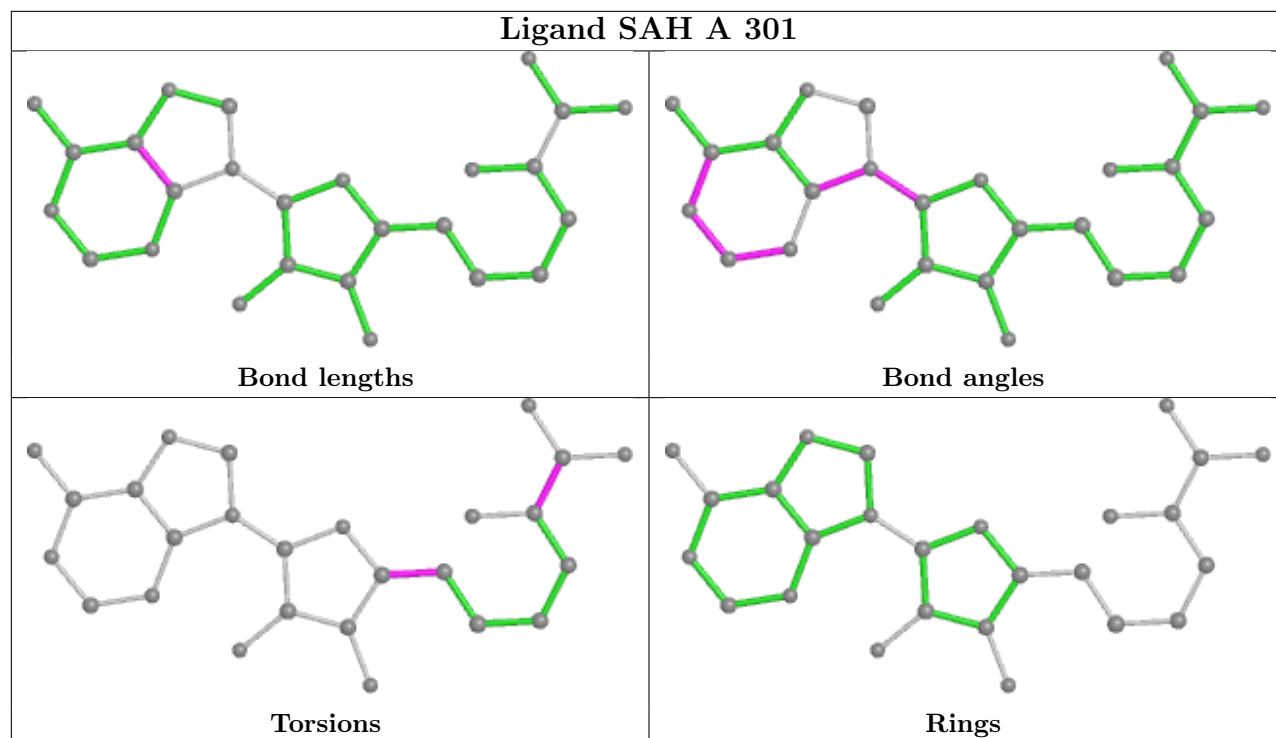
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	PJL	1	0
2	A	301	SAH	1	0
4	A	303	PE4	5	0

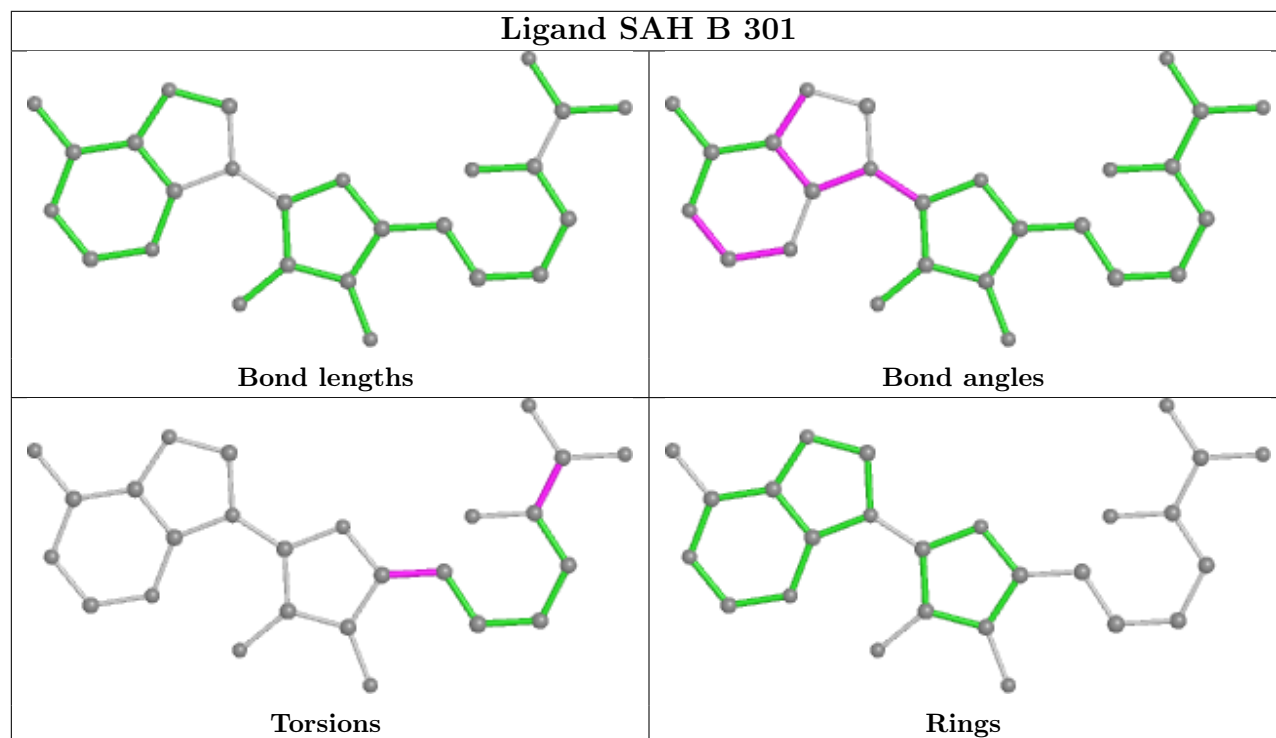
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



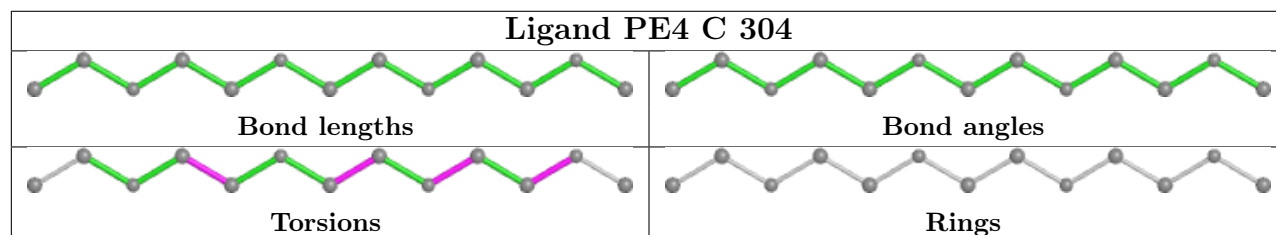
## Ligand SAH A 301

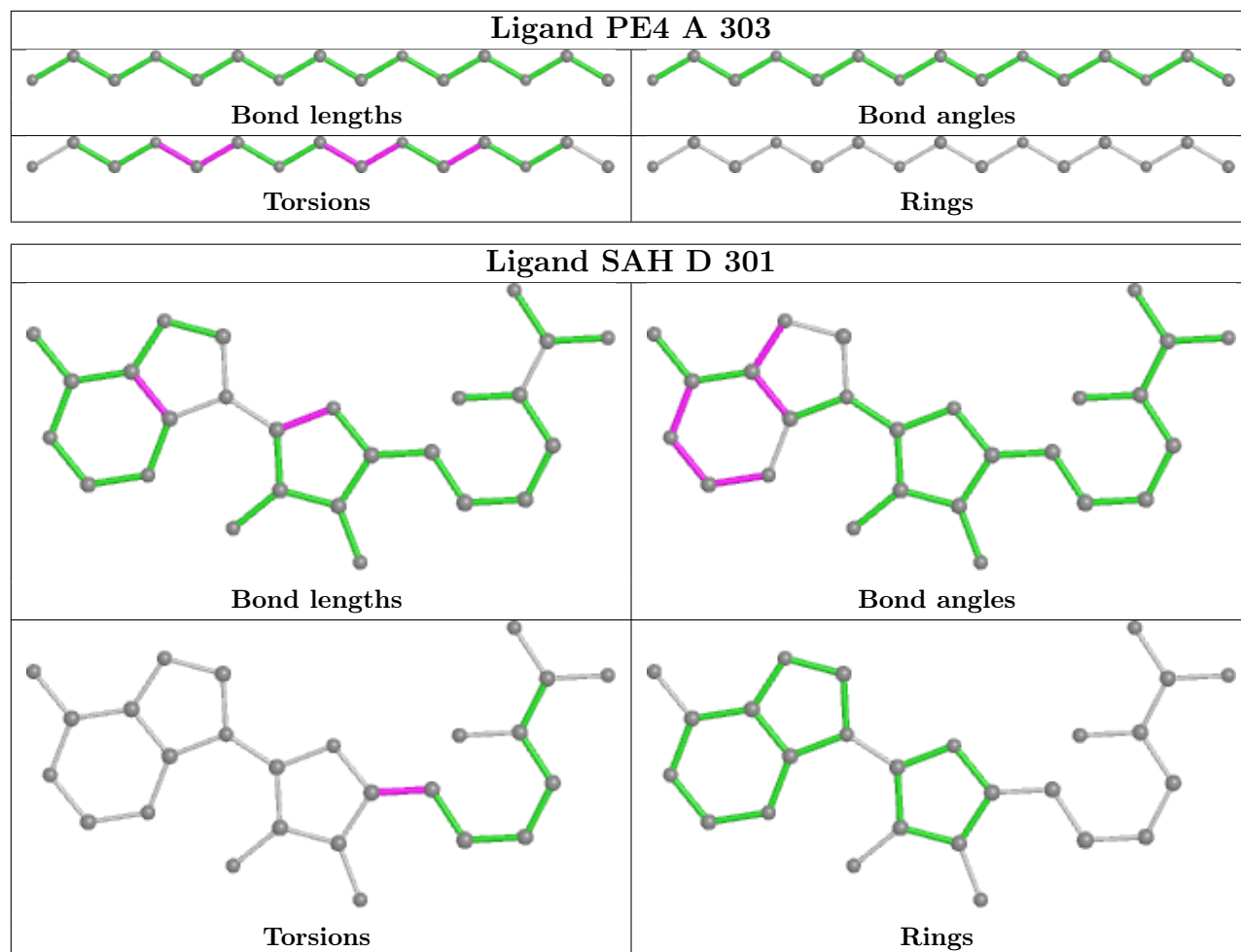


## Ligand SAH B 301



## Ligand PE4 C 304





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/274 (96%)	-0.12	11 (4%) 36 40	16, 26, 63, 123	0
1	B	261/274 (95%)	-0.08	12 (4%) 32 36	18, 29, 58, 104	0
1	C	262/274 (95%)	0.11	17 (6%) 18 21	18, 37, 70, 118	0
1	D	261/274 (95%)	-0.10	9 (3%) 45 50	19, 34, 69, 110	0
All	All	1048/1096 (95%)	-0.05	49 (4%) 31 35	16, 31, 66, 123	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	7.7
1	C	263	LEU	7.2
1	A	102	THR	6.7
1	C	82	PHE	5.6
1	B	102	THR	5.4
1	C	99	ARG	5.3
1	A	82	PHE	5.0
1	C	96	LEU	4.7
1	C	260	PHE	4.7
1	A	1	MET	4.7
1	B	98	LEU	4.6
1	C	262	LYS	4.4
1	B	96	LEU	4.3
1	B	99	ARG	4.2
1	B	101	GLY	4.0
1	A	263	LEU	4.0
1	B	261	ASP	4.0
1	D	102	THR	3.7
1	C	240	TYR	3.5
1	A	100	ASN	3.3
1	C	3	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	82	PHE	3.3
1	D	100	ASN	3.3
1	D	84	ASP	3.2
1	D	262	LYS	3.1
1	A	99	ARG	3.0
1	B	103	SER	2.8
1	D	261	ASP	2.7
1	C	125	LYS	2.6
1	B	82	PHE	2.6
1	A	84	ASP	2.6
1	C	83	ASN	2.4
1	D	98	LEU	2.4
1	C	126	PHE	2.4
1	B	100	ASN	2.4
1	C	77	LEU	2.4
1	B	43	LYS	2.3
1	B	260	PHE	2.3
1	C	158	ALA	2.3
1	A	101	GLY	2.3
1	D	99	ARG	2.3
1	A	260	PHE	2.2
1	C	100	ASN	2.2
1	C	156	VAL	2.2
1	C	98	LEU	2.2
1	B	126	PHE	2.1
1	C	2	ASN	2.1
1	D	260	PHE	2.0
1	A	83	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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,

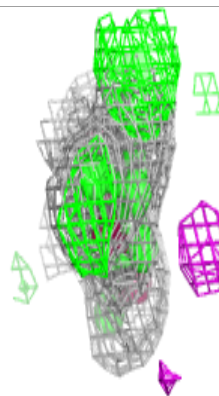
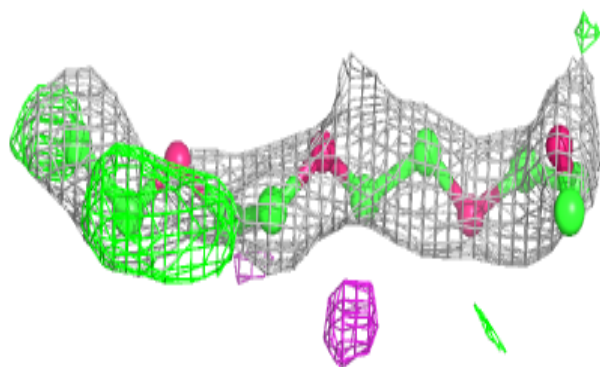
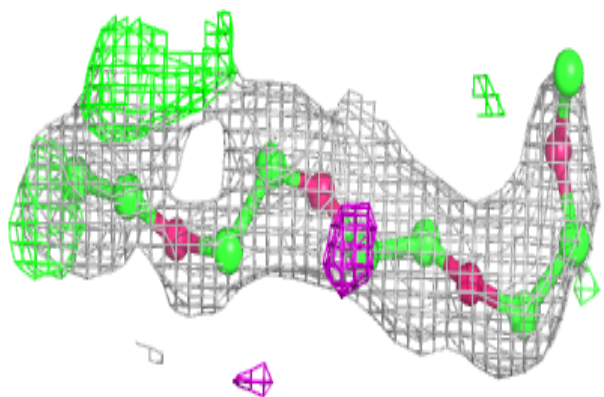
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PE4	C	304	13/24	0.61	0.17	69,75,80,81	0
4	PE4	B	304	14/24	0.68	0.21	61,76,84,85	0
4	PE4	A	303	15/24	0.75	0.16	48,54,68,68	0
7	9KH	C	302	13/13	0.85	0.12	29,37,44,45	0
2	SAH	C	301	26/26	0.88	0.09	26,31,47,77	0
5	PJL	A	304	11/11	0.90	0.11	20,38,44,44	0
2	SAH	D	301	26/26	0.91	0.10	27,32,62,79	0
2	SAH	B	301	26/26	0.91	0.09	21,26,46,83	0
6	LI	D	303	1/1	0.91	0.31	20,20,20,20	0
7	9KH	B	302	13/13	0.91	0.13	22,42,50,51	0
2	SAH	A	301	26/26	0.91	0.09	16,21,40,71	0
3	SO4	D	302	5/5	0.92	0.17	53,59,70,77	0
3	SO4	C	303	5/5	0.94	0.11	55,56,57,59	0
6	LI	A	305	1/1	0.96	0.57	9,9,9,9	0
3	SO4	A	302	5/5	0.96	0.14	44,48,60,78	0
3	SO4	B	303	5/5	0.98	0.06	59,60,61,67	0

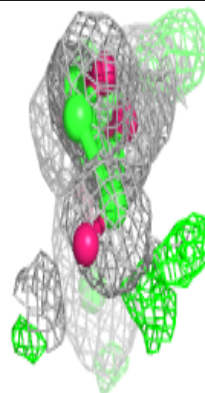
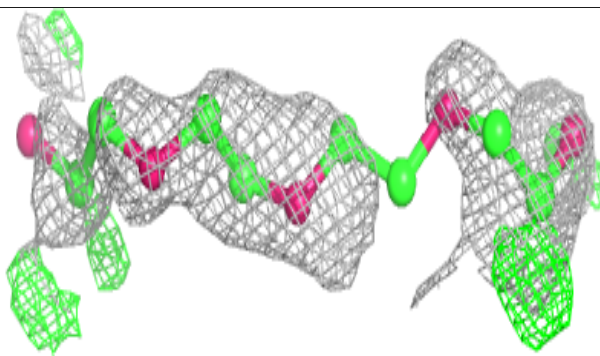
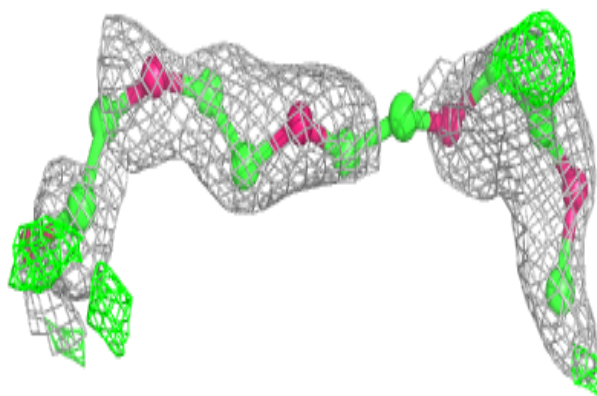
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PE4 C 304:**

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

**Electron density around PE4 B 304:**

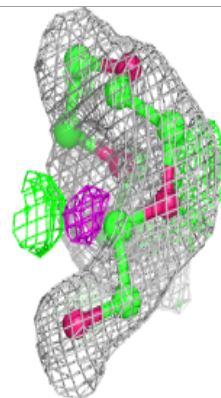
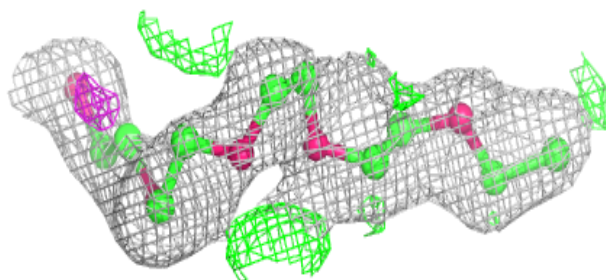
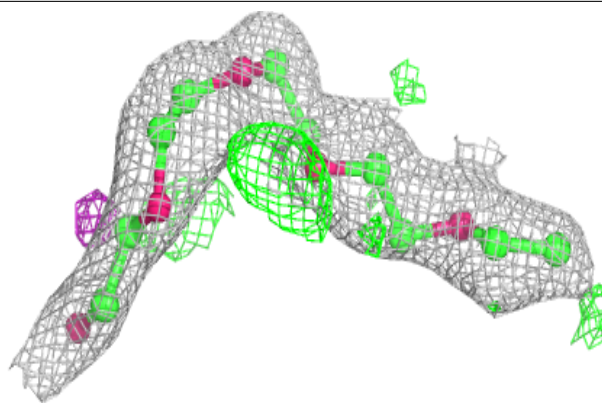
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



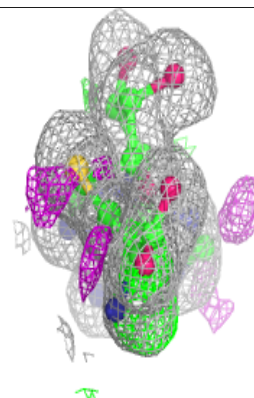
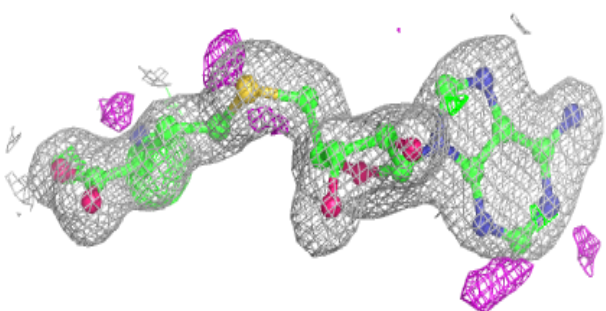
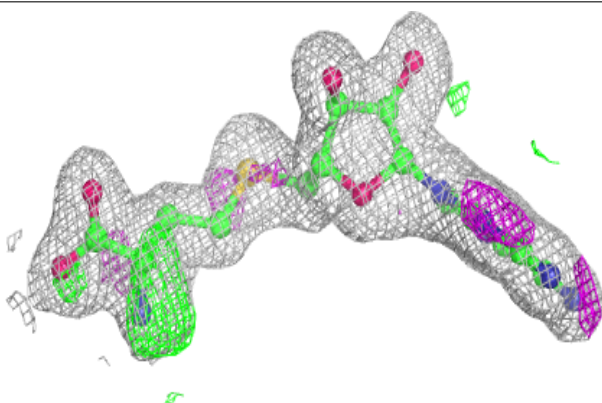


**Electron density around PE4 A 303:**

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

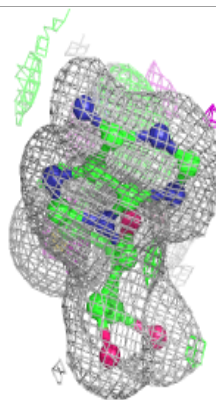
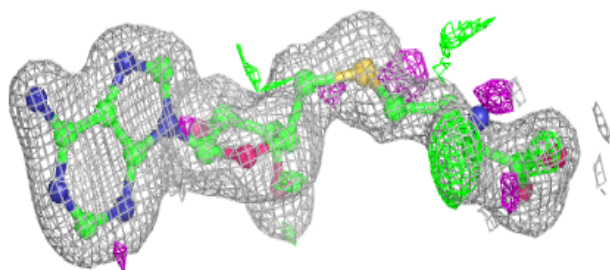
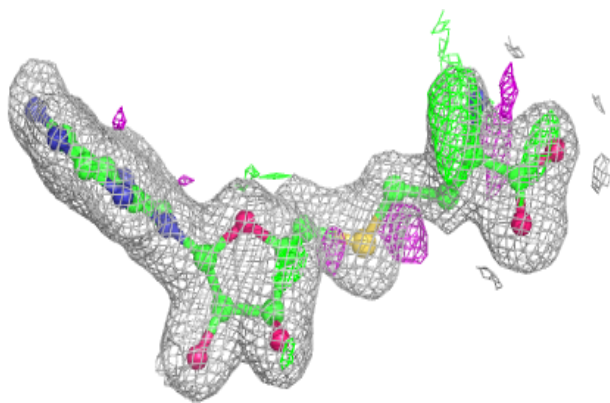
**Electron density around SAH C 301:**

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

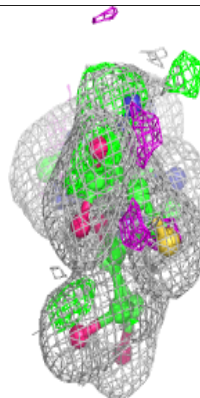
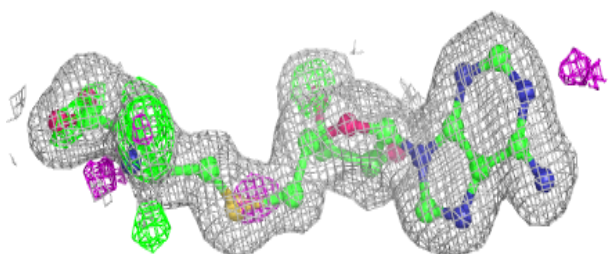
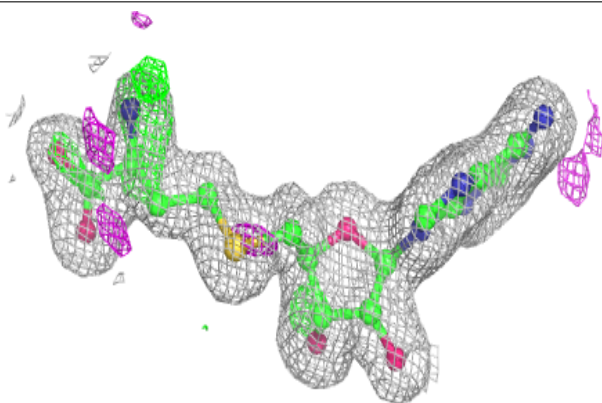


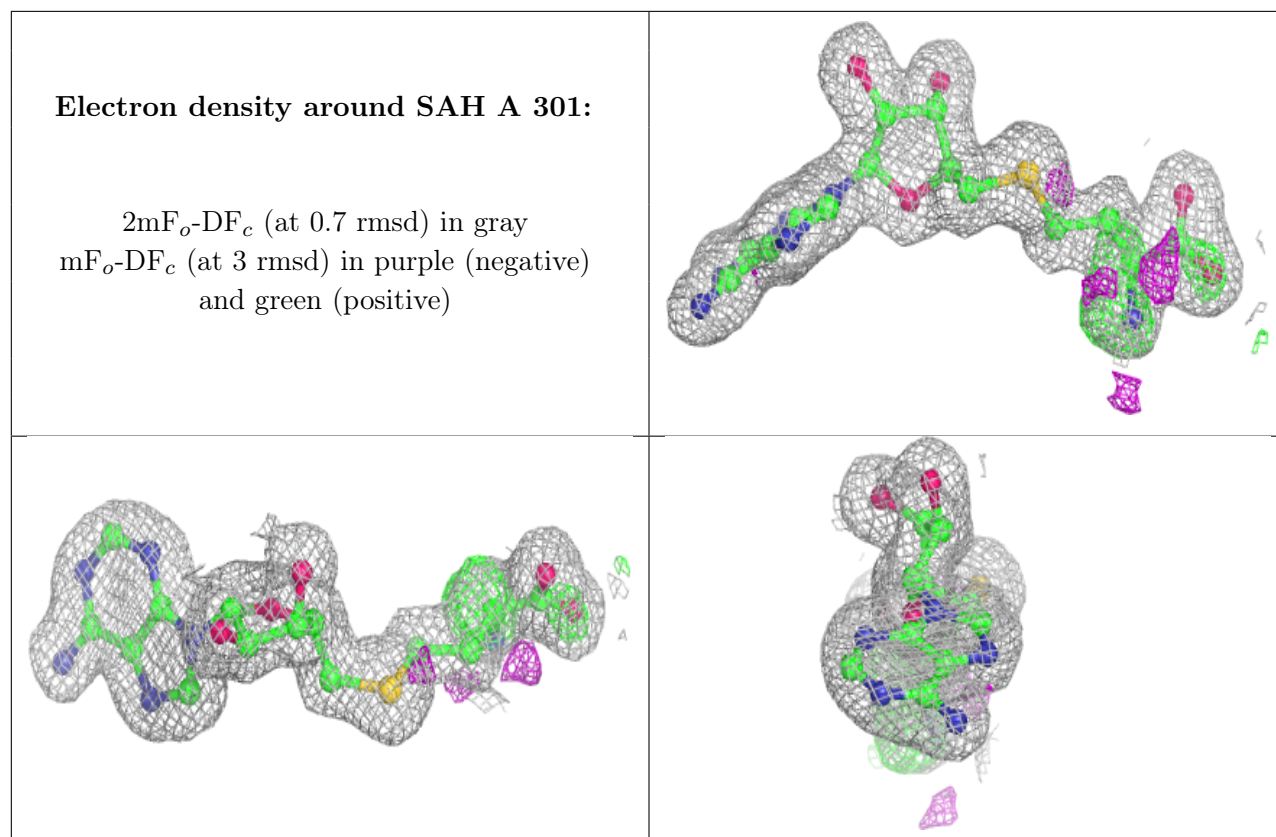
**Electron density around SAH D 301:**

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

**Electron density around SAH 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.