



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2022 – 08:15 PM EDT

PDB ID : 5CCV  
Title : Crystal structure of full-length NS5 from dengue virus type 3  
Authors : Klema, V.J.; Choi, K.H.  
Deposited on : 2015-07-02  
Resolution : 3.60 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](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.

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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 : 2.27  
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) : 2.27

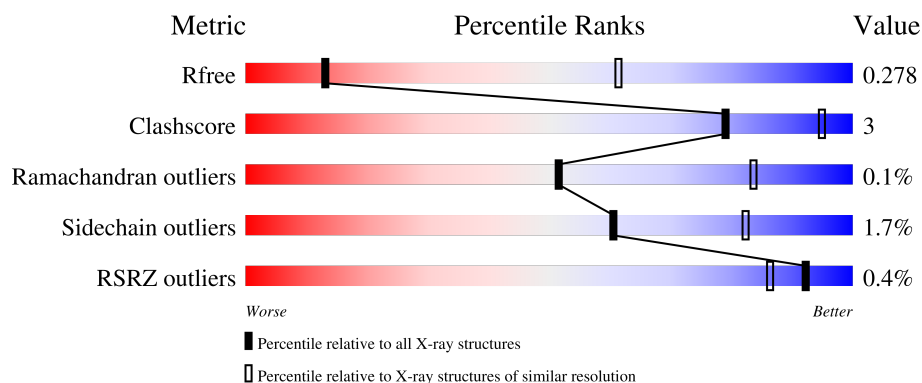
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	905	
1	B	905	
1	C	905	
1	D	905	
1	E	905	

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Mol	Chain	Length	Quality of chain
1	F	905	<div><div></div><div>86%</div><div>7% • 6%</div></div>
1	G	905	<div><div></div><div>86%</div><div>8% 6%</div></div>
1	H	905	<div><div>%</div><div></div><div>80%</div><div>• 15%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 52681 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 RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6831	4301	1229	1255	46			
1	B	851	Total	C	N	O	S	0	0	0
			6892	4346	1236	1263	47			
1	C	852	Total	C	N	O	S	0	0	0
			6879	4339	1229	1263	48			
1	D	848	Total	C	N	O	S	0	0	0
			6827	4302	1226	1252	47			
1	E	852	Total	C	N	O	S	0	0	0
			6885	4341	1231	1266	47			
1	F	850	Total	C	N	O	S	0	0	0
			6846	4311	1231	1257	47			
1	G	847	Total	C	N	O	S	0	0	0
			6813	4292	1222	1252	47			
1	H	767	Total	C	N	O	S	0	0	0
			4484	2739	870	866	9			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	763	ALA	THR	conflict	UNP P27915
A	?	-	TRP	deletion	UNP P27915
A	?	-	SER	deletion	UNP P27915
A	?	-	ILE	deletion	UNP P27915
A	?	-	HIS	deletion	UNP P27915
A	?	-	ALA	deletion	UNP P27915
A	?	-	HIS	deletion	UNP P27915
A	901	ALA	-	expression tag	UNP P27915
A	902	ALA	-	expression tag	UNP P27915
A	903	ALA	-	expression tag	UNP P27915
A	904	LEU	-	expression tag	UNP P27915
A	905	GLU	-	expression tag	UNP P27915
A	906	HIS	-	expression tag	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
A	907	HIS	-	expression tag	UNP P27915
A	908	HIS	-	expression tag	UNP P27915
A	909	HIS	-	expression tag	UNP P27915
A	910	HIS	-	expression tag	UNP P27915
A	911	HIS	-	expression tag	UNP P27915
B	763	ALA	THR	conflict	UNP P27915
B	?	-	TRP	deletion	UNP P27915
B	?	-	SER	deletion	UNP P27915
B	?	-	ILE	deletion	UNP P27915
B	?	-	HIS	deletion	UNP P27915
B	?	-	ALA	deletion	UNP P27915
B	?	-	HIS	deletion	UNP P27915
B	901	ALA	-	expression tag	UNP P27915
B	902	ALA	-	expression tag	UNP P27915
B	903	ALA	-	expression tag	UNP P27915
B	904	LEU	-	expression tag	UNP P27915
B	905	GLU	-	expression tag	UNP P27915
B	906	HIS	-	expression tag	UNP P27915
B	907	HIS	-	expression tag	UNP P27915
B	908	HIS	-	expression tag	UNP P27915
B	909	HIS	-	expression tag	UNP P27915
B	910	HIS	-	expression tag	UNP P27915
B	911	HIS	-	expression tag	UNP P27915
C	763	ALA	THR	conflict	UNP P27915
C	?	-	TRP	deletion	UNP P27915
C	?	-	SER	deletion	UNP P27915
C	?	-	ILE	deletion	UNP P27915
C	?	-	HIS	deletion	UNP P27915
C	?	-	ALA	deletion	UNP P27915
C	?	-	HIS	deletion	UNP P27915
C	901	ALA	-	expression tag	UNP P27915
C	902	ALA	-	expression tag	UNP P27915
C	903	ALA	-	expression tag	UNP P27915
C	904	LEU	-	expression tag	UNP P27915
C	905	GLU	-	expression tag	UNP P27915
C	906	HIS	-	expression tag	UNP P27915
C	907	HIS	-	expression tag	UNP P27915
C	908	HIS	-	expression tag	UNP P27915
C	909	HIS	-	expression tag	UNP P27915
C	910	HIS	-	expression tag	UNP P27915
C	911	HIS	-	expression tag	UNP P27915
D	763	ALA	THR	conflict	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	TRP	deletion	UNP P27915
D	?	-	SER	deletion	UNP P27915
D	?	-	ILE	deletion	UNP P27915
D	?	-	HIS	deletion	UNP P27915
D	?	-	ALA	deletion	UNP P27915
D	?	-	HIS	deletion	UNP P27915
D	901	ALA	-	expression tag	UNP P27915
D	902	ALA	-	expression tag	UNP P27915
D	903	ALA	-	expression tag	UNP P27915
D	904	LEU	-	expression tag	UNP P27915
D	905	GLU	-	expression tag	UNP P27915
D	906	HIS	-	expression tag	UNP P27915
D	907	HIS	-	expression tag	UNP P27915
D	908	HIS	-	expression tag	UNP P27915
D	909	HIS	-	expression tag	UNP P27915
D	910	HIS	-	expression tag	UNP P27915
D	911	HIS	-	expression tag	UNP P27915
E	763	ALA	THR	conflict	UNP P27915
E	?	-	TRP	deletion	UNP P27915
E	?	-	SER	deletion	UNP P27915
E	?	-	ILE	deletion	UNP P27915
E	?	-	HIS	deletion	UNP P27915
E	?	-	ALA	deletion	UNP P27915
E	?	-	HIS	deletion	UNP P27915
E	901	ALA	-	expression tag	UNP P27915
E	902	ALA	-	expression tag	UNP P27915
E	903	ALA	-	expression tag	UNP P27915
E	904	LEU	-	expression tag	UNP P27915
E	905	GLU	-	expression tag	UNP P27915
E	906	HIS	-	expression tag	UNP P27915
E	907	HIS	-	expression tag	UNP P27915
E	908	HIS	-	expression tag	UNP P27915
E	909	HIS	-	expression tag	UNP P27915
E	910	HIS	-	expression tag	UNP P27915
E	911	HIS	-	expression tag	UNP P27915
F	763	ALA	THR	conflict	UNP P27915
F	?	-	TRP	deletion	UNP P27915
F	?	-	SER	deletion	UNP P27915
F	?	-	ILE	deletion	UNP P27915
F	?	-	HIS	deletion	UNP P27915
F	?	-	ALA	deletion	UNP P27915
F	?	-	HIS	deletion	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
F	901	ALA	-	expression tag	UNP P27915
F	902	ALA	-	expression tag	UNP P27915
F	903	ALA	-	expression tag	UNP P27915
F	904	LEU	-	expression tag	UNP P27915
F	905	GLU	-	expression tag	UNP P27915
F	906	HIS	-	expression tag	UNP P27915
F	907	HIS	-	expression tag	UNP P27915
F	908	HIS	-	expression tag	UNP P27915
F	909	HIS	-	expression tag	UNP P27915
F	910	HIS	-	expression tag	UNP P27915
F	911	HIS	-	expression tag	UNP P27915
G	763	ALA	THR	conflict	UNP P27915
G	?	-	TRP	deletion	UNP P27915
G	?	-	SER	deletion	UNP P27915
G	?	-	ILE	deletion	UNP P27915
G	?	-	HIS	deletion	UNP P27915
G	?	-	ALA	deletion	UNP P27915
G	?	-	HIS	deletion	UNP P27915
G	901	ALA	-	expression tag	UNP P27915
G	902	ALA	-	expression tag	UNP P27915
G	903	ALA	-	expression tag	UNP P27915
G	904	LEU	-	expression tag	UNP P27915
G	905	GLU	-	expression tag	UNP P27915
G	906	HIS	-	expression tag	UNP P27915
G	907	HIS	-	expression tag	UNP P27915
G	908	HIS	-	expression tag	UNP P27915
G	909	HIS	-	expression tag	UNP P27915
G	910	HIS	-	expression tag	UNP P27915
G	911	HIS	-	expression tag	UNP P27915
H	763	ALA	THR	conflict	UNP P27915
H	?	-	TRP	deletion	UNP P27915
H	?	-	SER	deletion	UNP P27915
H	?	-	ILE	deletion	UNP P27915
H	?	-	HIS	deletion	UNP P27915
H	?	-	ALA	deletion	UNP P27915
H	?	-	HIS	deletion	UNP P27915
H	901	ALA	-	expression tag	UNP P27915
H	902	ALA	-	expression tag	UNP P27915
H	903	ALA	-	expression tag	UNP P27915
H	904	LEU	-	expression tag	UNP P27915
H	905	GLU	-	expression tag	UNP P27915
H	906	HIS	-	expression tag	UNP P27915

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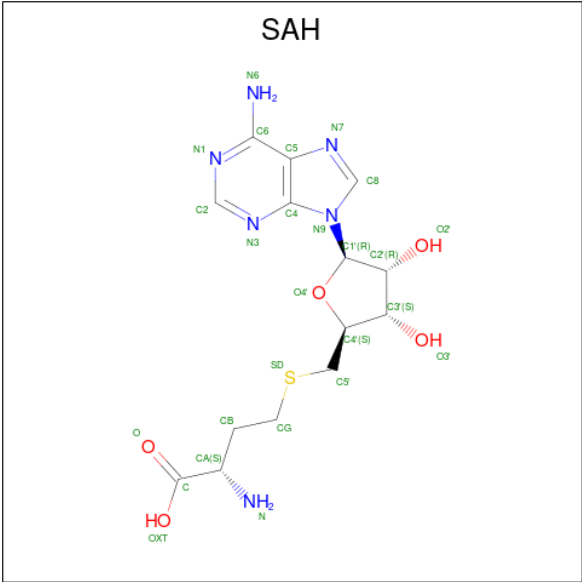
Chain	Residue	Modelled	Actual	Comment	Reference
H	907	HIS	-	expression tag	UNP P27915
H	908	HIS	-	expression tag	UNP P27915
H	909	HIS	-	expression tag	UNP P27915
H	910	HIS	-	expression tag	UNP P27915
H	911	HIS	-	expression tag	UNP P27915

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0

- Molecule 3 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).



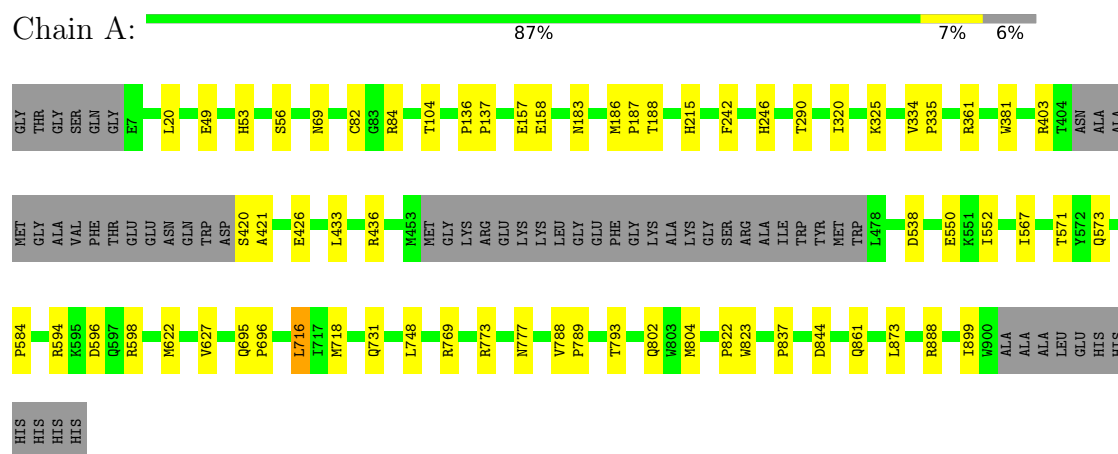


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	G	1	Total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

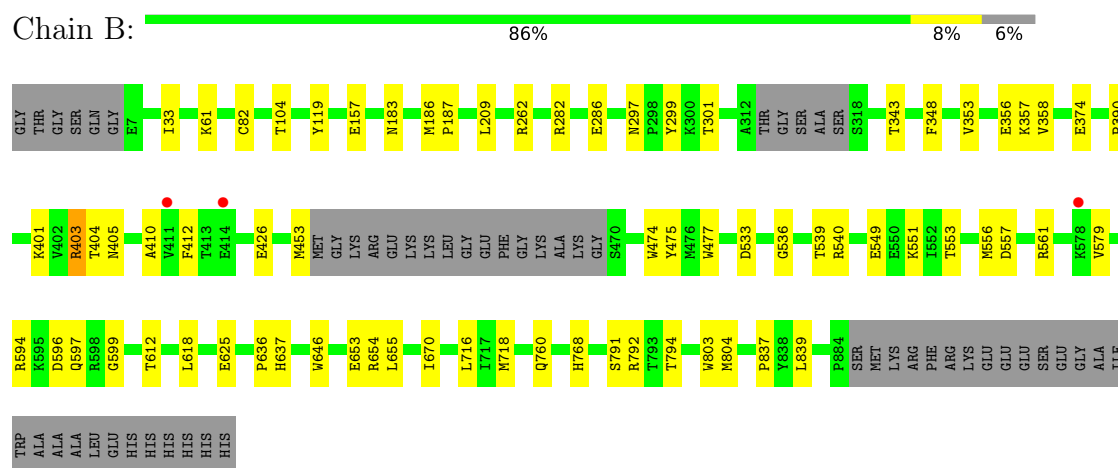
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

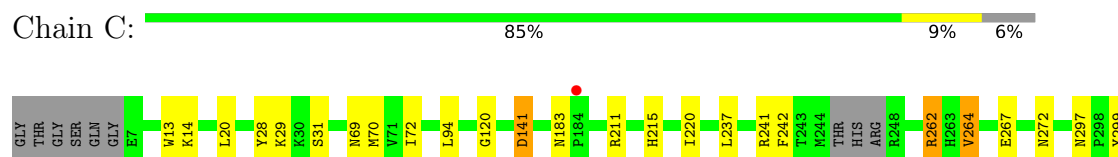
#### • Molecule 1: RNA-directed RNA polymerase NS5

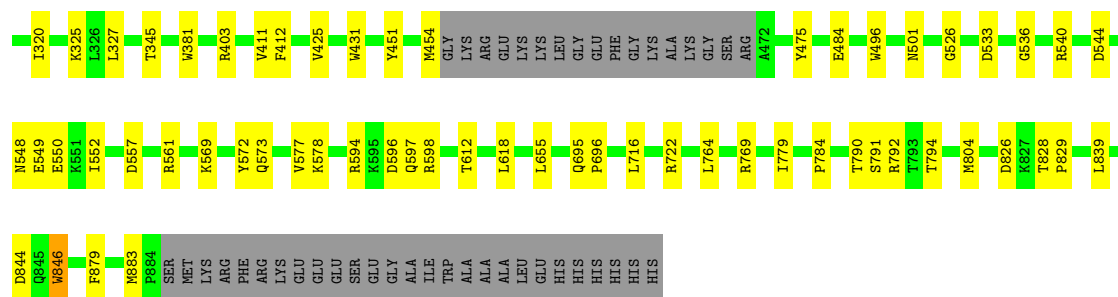


#### • Molecule 1: RNA-directed RNA polymerase NS5



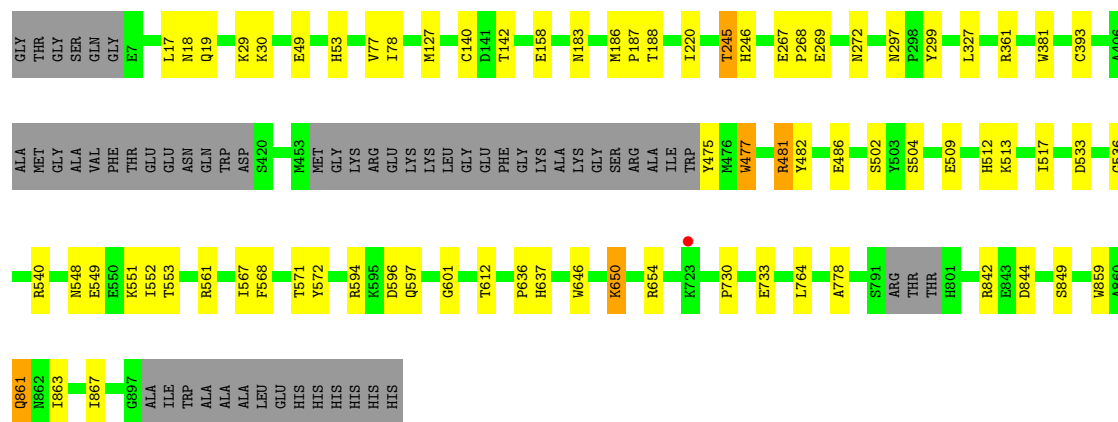
#### • Molecule 1: RNA-directed RNA polymerase NS5





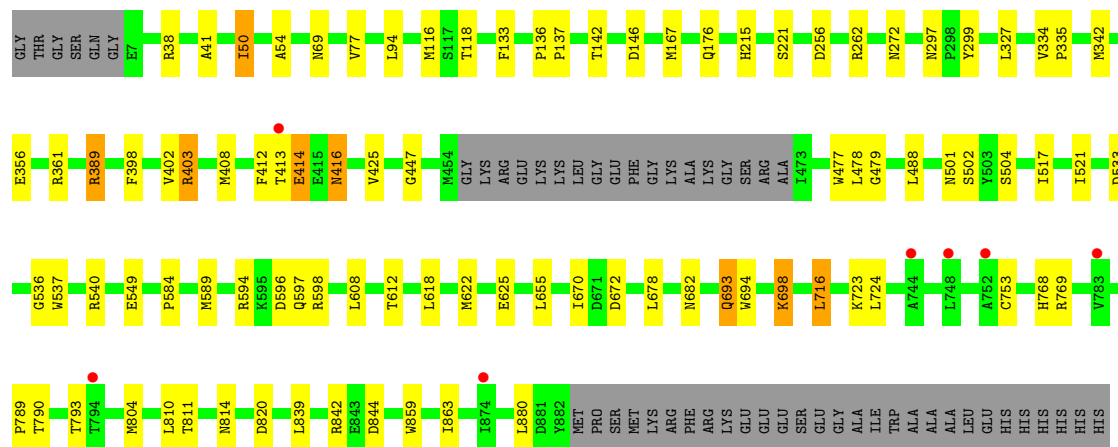
• Molecule 1: RNA-directed RNA polymerase NS5

Chain D: 85% 8% 6%



• Molecule 1: RNA-directed RNA polymerase NS5

Chain E: 84% 9% 6%



• Molecule 1: RNA-directed RNA polymerase NS5

Chain F: 86% 7% 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.31Å 215.31Å 480.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.22 – 3.60 49.22 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-3.60) 94.3 (49.22-3.60)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.94 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.238 , 0.274 0.247 , 0.278	Depositor DCC
$R_{free}$ test set	2004 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	52681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: SAH, ZN

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	0.20	0/6992	0.36	1/9454 (0.0%)
1	B	0.21	0/7060	0.36	0/9551
1	C	0.21	0/7046	0.36	0/9533
1	D	0.21	0/6990	0.36	0/9452
1	E	0.21	0/7053	0.36	0/9544
1	F	0.21	0/7009	0.36	0/9477
1	G	0.21	0/6976	0.36	0/9434
1	H	0.19	0/4563	0.35	0/6318
All	All	0.21	0/53689	0.36	1/72763 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	LEU	CA-CB-CG	5.38	127.68	115.30

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	6831	0	6746	35	0
1	B	6892	0	6803	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6879	0	6788	43	0
1	D	6827	0	6724	48	0
1	E	6885	0	6788	51	0
1	F	6846	0	6757	36	0
1	G	6813	0	6712	40	0
1	H	4484	0	2810	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
3	E	26	0	19	1	0
3	F	26	0	19	0	0
3	G	26	0	19	0	0
3	H	26	0	19	0	0
All	All	52681	0	50280	290	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 290 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:G:420:SER:O	1:G:422:ARG:N	1.97	0.97
1:A:82:CYS:HG	1:A:104:THR:HG1	1.35	0.72
1:D:361:ARG:HA	1:D:594:ARG:HH22	1.58	0.68
1:D:245:THR:O	1:G:861:GLN:NE2	2.27	0.68
1:G:13:TRP:HZ2	1:G:215:HIS:HB2	1.58	0.67

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	843/905 (93%)	811 (96%)	32 (4%)	0	100	100
1	B	845/905 (93%)	806 (95%)	38 (4%)	1 (0%)	51	83
1	C	846/905 (94%)	808 (96%)	37 (4%)	1 (0%)	51	83
1	D	840/905 (93%)	808 (96%)	32 (4%)	0	100	100
1	E	848/905 (94%)	812 (96%)	34 (4%)	2 (0%)	47	79
1	F	844/905 (93%)	804 (95%)	38 (4%)	2 (0%)	47	79
1	G	841/905 (93%)	796 (95%)	42 (5%)	3 (0%)	34	71
1	H	747/905 (82%)	706 (94%)	41 (6%)	0	100	100
All	All	6654/7240 (92%)	6351 (95%)	294 (4%)	9 (0%)	51	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	VAL
1	F	264	VAL
1	G	421	ALA
1	G	11	GLU
1	E	413	THR

### 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	739/786 (94%)	733 (99%)	6 (1%)	81	91

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	747/786 (95%)	737 (99%)	10 (1%)	69	86
1	C	745/786 (95%)	728 (98%)	17 (2%)	50	76
1	D	737/786 (94%)	729 (99%)	8 (1%)	73	88
1	E	746/786 (95%)	725 (97%)	21 (3%)	43	72
1	F	741/786 (94%)	730 (98%)	11 (2%)	65	84
1	G	736/786 (94%)	728 (99%)	8 (1%)	73	88
1	H	193/786 (25%)	182 (94%)	11 (6%)	20	55
All	All	5384/6288 (86%)	5292 (98%)	92 (2%)	60	82

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	723	LYS
1	F	742	GLN
1	E	804	MET
1	F	264	VAL
1	G	333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	742	GLN
1	G	554	GLN
1	G	861	GLN
1	G	613	ASN
1	B	597	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are 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
3	SAH	H	1003	-	21,28,28	1.16	2 (9%)	20,40,40	1.13	2 (10%)
3	SAH	C	1003	-	21,28,28	1.24	2 (9%)	20,40,40	1.14	1 (5%)
3	SAH	E	1003	-	21,28,28	1.13	2 (9%)	20,40,40	1.14	1 (5%)
3	SAH	D	1003	-	21,28,28	1.10	1 (4%)	20,40,40	1.13	2 (10%)
3	SAH	F	1003	-	21,28,28	1.13	2 (9%)	20,40,40	1.13	1 (5%)
3	SAH	G	1003	-	21,28,28	1.15	2 (9%)	20,40,40	1.14	2 (10%)
3	SAH	B	1003	-	21,28,28	1.16	2 (9%)	20,40,40	1.16	2 (10%)
3	SAH	A	1003	-	21,28,28	1.17	2 (9%)	20,40,40	1.14	2 (10%)

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
3	SAH	H	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	C	1003	-	-	1/7/31/31	0/3/3/3
3	SAH	E	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	D	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	F	1003	-	-	1/7/31/31	0/3/3/3
3	SAH	G	1003	-	-	0/7/31/31	0/3/3/3
3	SAH	B	1003	-	-	1/7/31/31	0/3/3/3
3	SAH	A	1003	-	-	1/7/31/31	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	SAH	C2'-C1'	2.87	1.58	1.53
3	C	1003	SAH	C2-N3	2.44	1.36	1.32
3	F	1003	SAH	C2-N3	2.39	1.35	1.32
3	H	1003	SAH	C2-N3	2.36	1.35	1.32
3	B	1003	SAH	C2-N3	2.35	1.35	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1003	SAH	C5'-C4'-C3'	-2.24	109.46	115.06
3	B	1003	SAH	O4'-C1'-C2'	-2.16	103.77	106.93
3	D	1003	SAH	O4'-C1'-C2'	-2.13	103.82	106.93
3	A	1003	SAH	O4'-C1'-C2'	-2.12	103.82	106.93
3	H	1003	SAH	O4'-C1'-C2'	-2.12	103.83	106.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

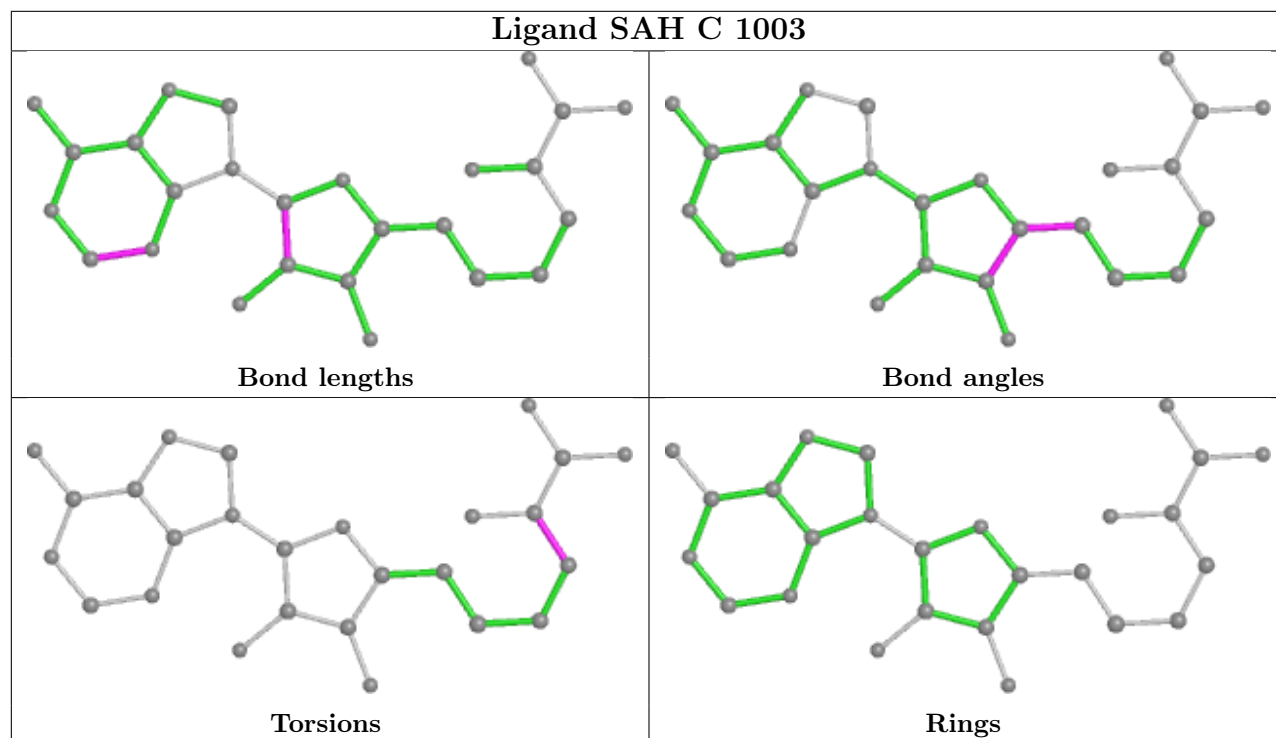
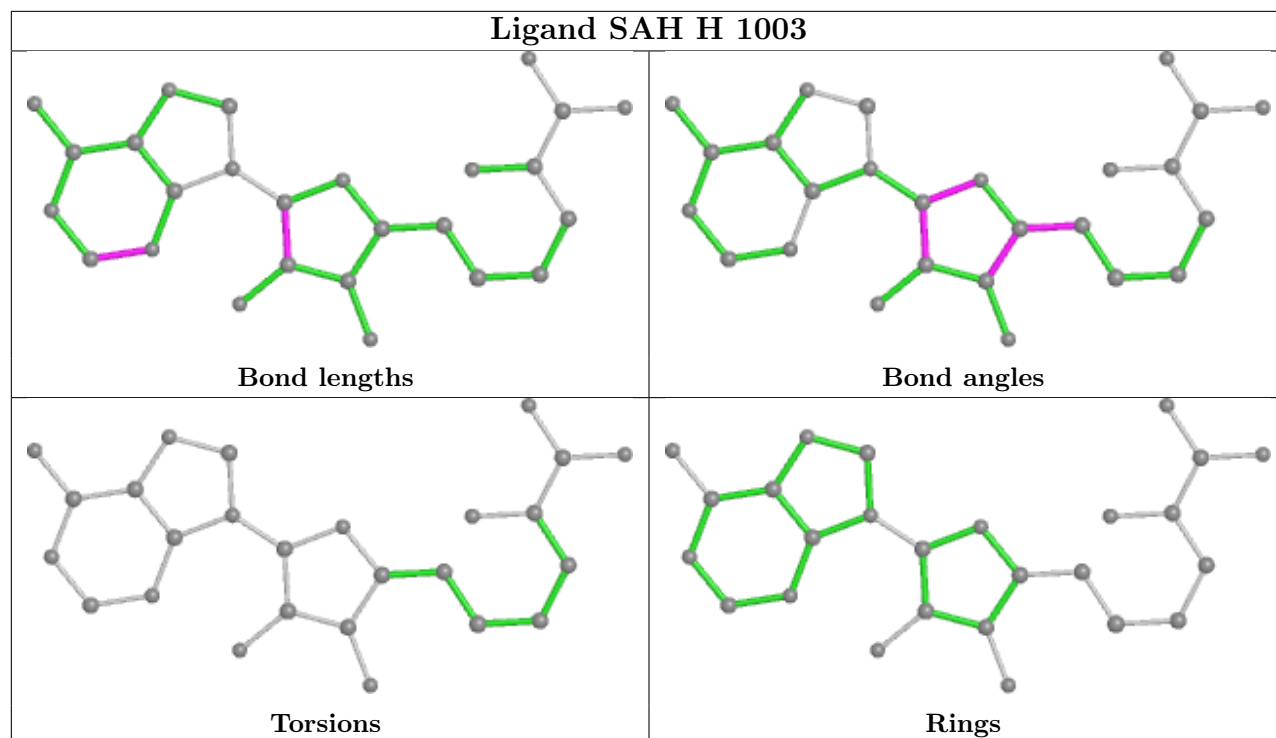
Mol	Chain	Res	Type	Atoms
3	A	1003	SAH	C-CA-CB-CG
3	B	1003	SAH	C-CA-CB-CG
3	C	1003	SAH	C-CA-CB-CG
3	F	1003	SAH	C-CA-CB-CG

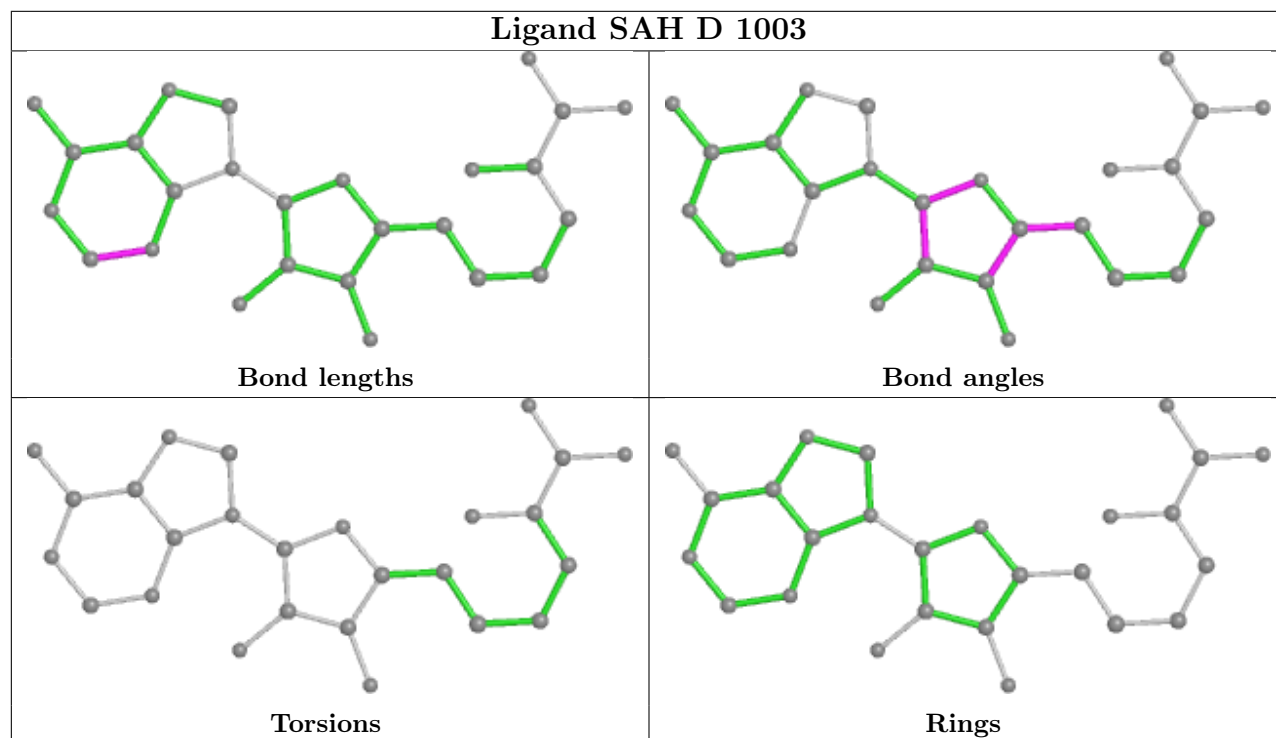
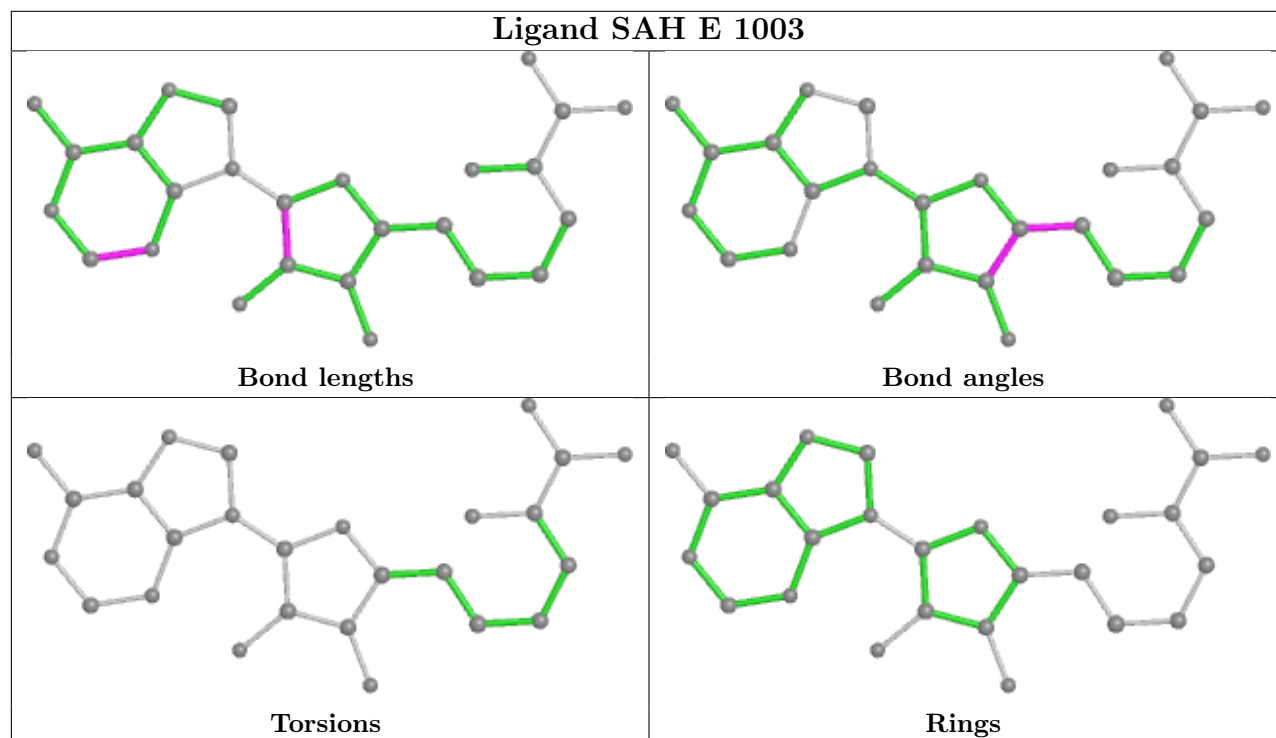
There are no ring outliers.

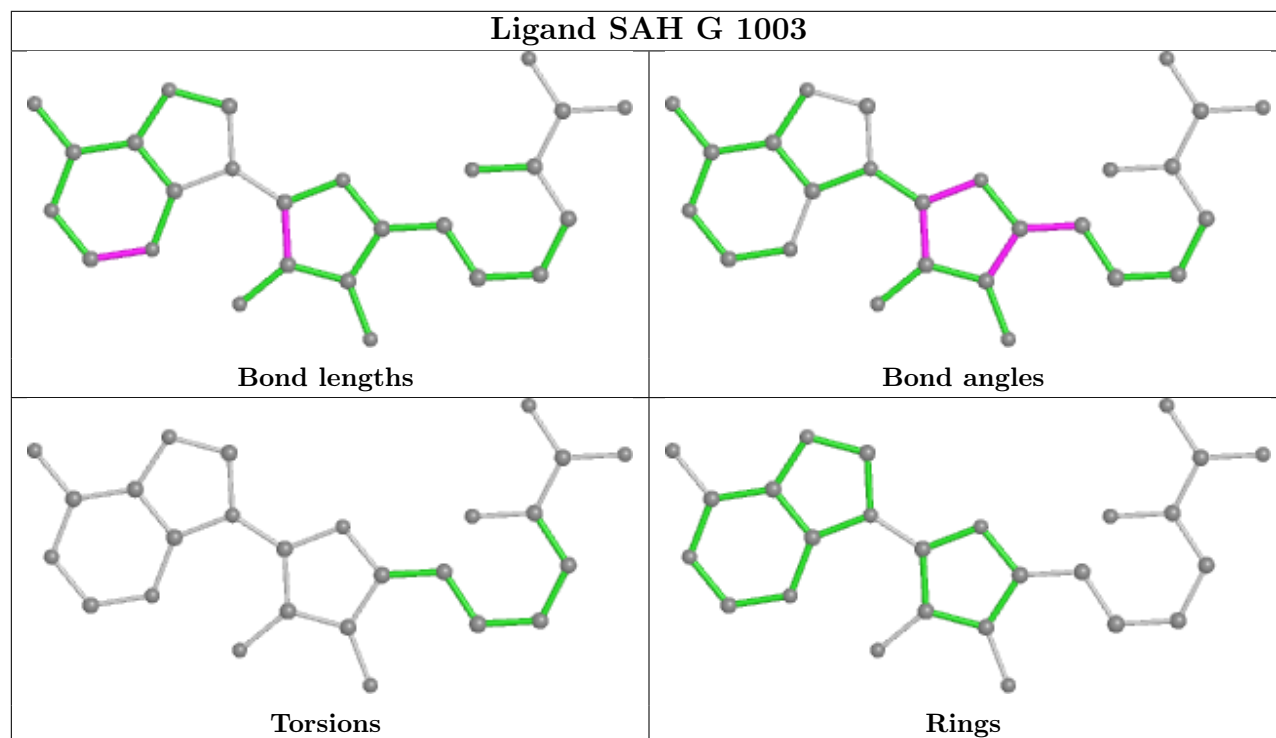
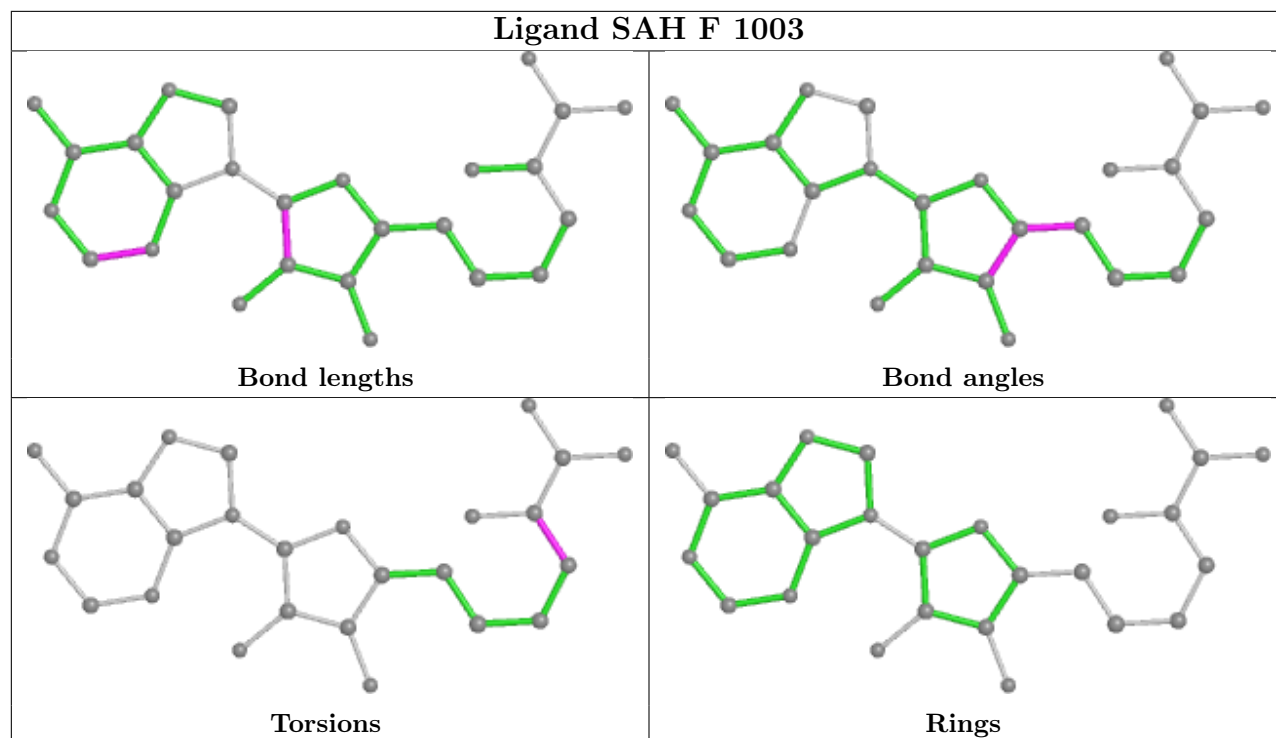
1 monomer is involved in 1 short contact:

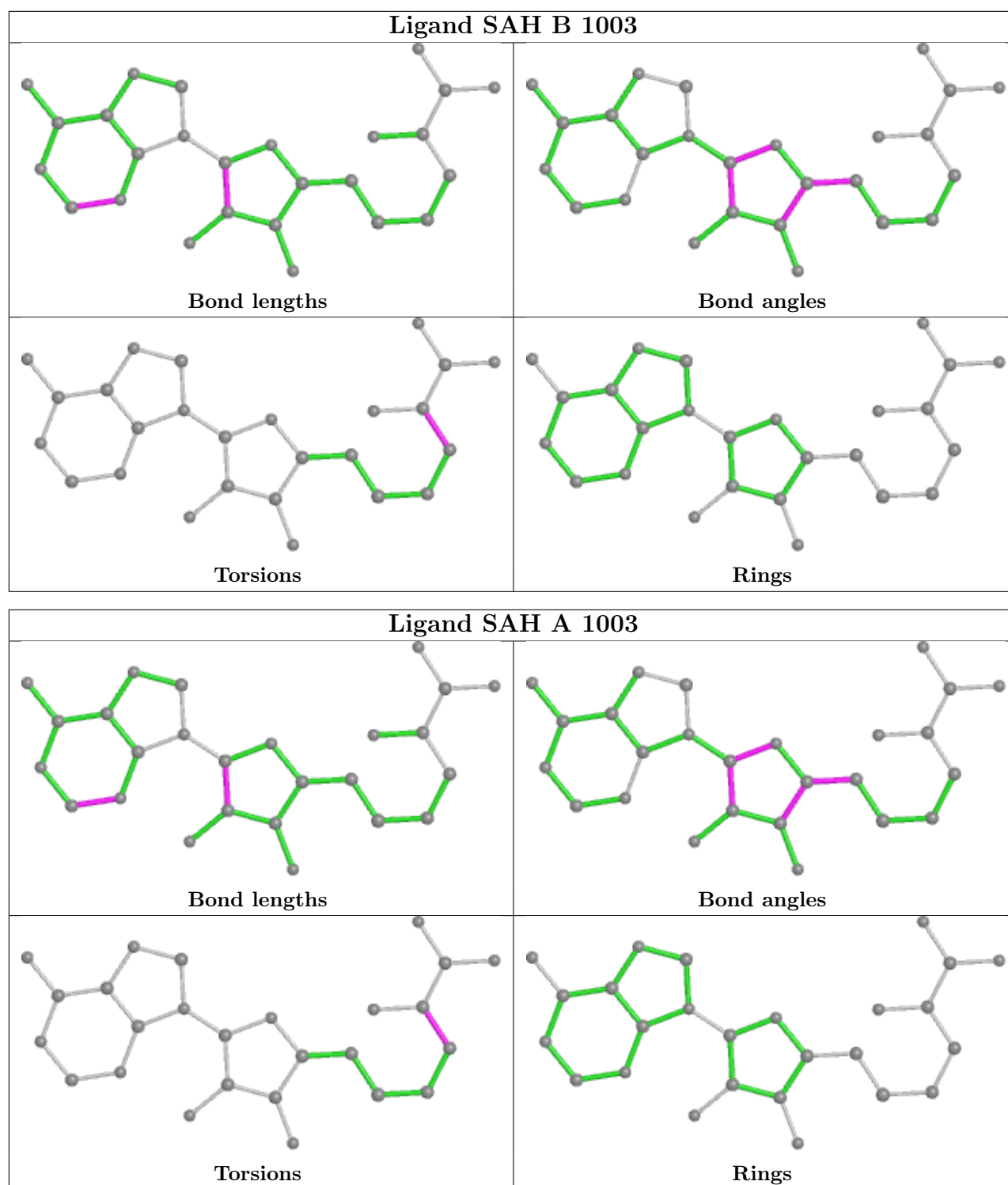
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1003	SAH	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	849/905 (93%)	-0.26	0 100 100	72, 85, 130, 207	0
1	B	851/905 (94%)	-0.18	3 (0%) 92 86	75, 86, 123, 201	0
1	C	852/905 (94%)	-0.19	1 (0%) 95 93	72, 87, 142, 187	0
1	D	848/905 (93%)	-0.24	1 (0%) 95 93	72, 83, 114, 232	0
1	E	852/905 (94%)	-0.13	7 (0%) 86 75	78, 101, 142, 188	0
1	F	850/905 (93%)	-0.23	0 100 100	74, 93, 116, 173	0
1	G	847/905 (93%)	-0.22	2 (0%) 95 91	77, 97, 116, 189	0
1	H	767/905 (84%)	-0.05	12 (1%) 72 57	93, 122, 171, 211	0
All	All	6716/7240 (92%)	-0.19	26 (0%) 92 86	72, 93, 140, 232	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	783	VAL	3.6
1	E	748	LEU	3.1
1	E	744	ALA	3.0
1	H	751	THR	2.9
1	B	578	LYS	2.8

### 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 ⓘ

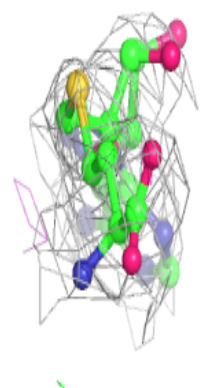
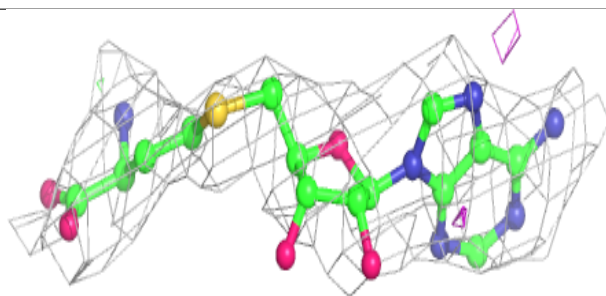
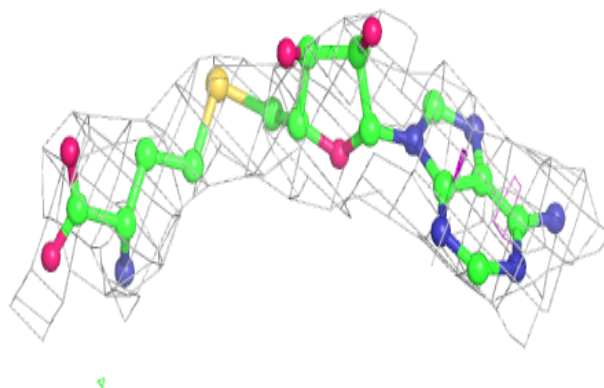
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	SAH	H	1003	26/26	0.88	0.40	96,106,159,164	0
2	ZN	H	1002	1/1	0.91	0.17	146,146,146,146	0
3	SAH	C	1003	26/26	0.92	0.21	88,110,137,210	0
3	SAH	F	1003	26/26	0.92	0.19	76,83,114,118	0
3	SAH	G	1003	26/26	0.92	0.35	94,98,143,184	0
3	SAH	B	1003	26/26	0.92	0.23	77,79,94,100	0
3	SAH	E	1003	26/26	0.93	0.24	93,96,103,171	0
2	ZN	A	1002	1/1	0.93	0.06	101,101,101,101	0
3	SAH	D	1003	26/26	0.94	0.27	71,72,124,177	0
3	SAH	A	1003	26/26	0.95	0.18	78,79,92,153	0
2	ZN	H	1001	1/1	0.96	0.07	99,99,99,99	0
2	ZN	E	1001	1/1	0.97	0.13	100,100,100,100	0
2	ZN	F	1002	1/1	0.98	0.16	99,99,99,99	0
2	ZN	G	1001	1/1	0.98	0.23	98,98,98,98	0
2	ZN	D	1001	1/1	0.98	0.12	83,83,83,83	0
2	ZN	C	1001	1/1	0.98	0.18	82,82,82,82	0
2	ZN	B	1002	1/1	0.99	0.12	77,77,77,77	0
2	ZN	E	1002	1/1	0.99	0.08	79,79,79,79	0
2	ZN	F	1001	1/1	0.99	0.18	84,84,84,84	0
2	ZN	A	1001	1/1	0.99	0.06	75,75,75,75	0
2	ZN	C	1002	1/1	0.99	0.10	76,76,76,76	0
2	ZN	G	1002	1/1	0.99	0.10	84,84,84,84	0
2	ZN	B	1001	1/1	0.99	0.15	90,90,90,90	0
2	ZN	D	1002	1/1	0.99	0.14	82,82,82,82	0

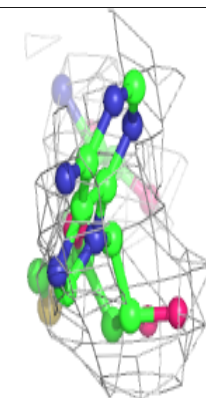
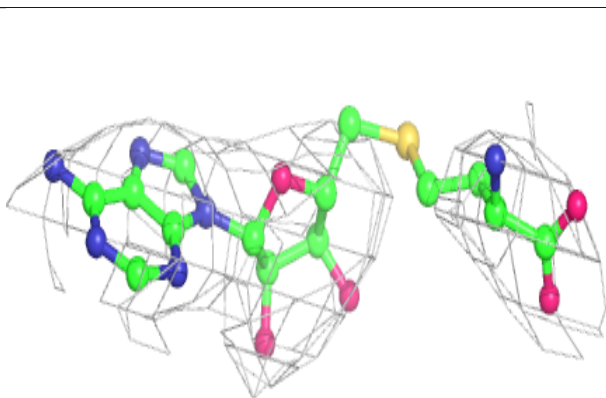
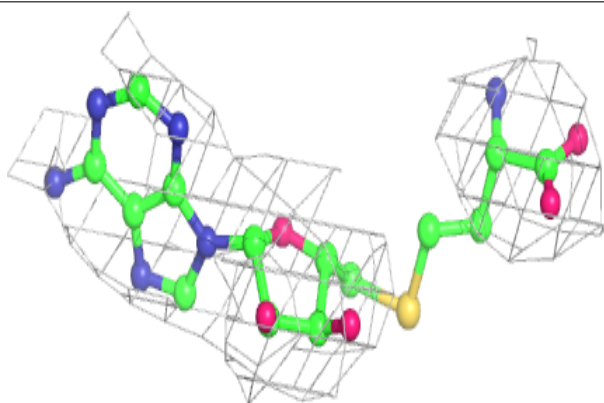
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAH H 1003:**

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

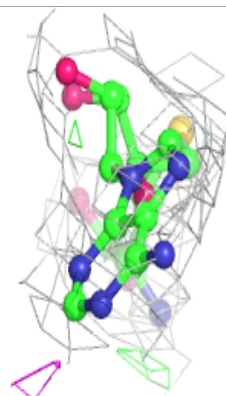
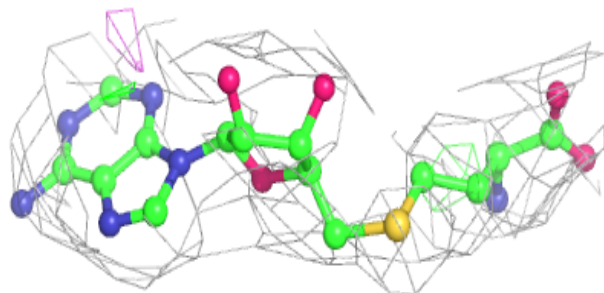
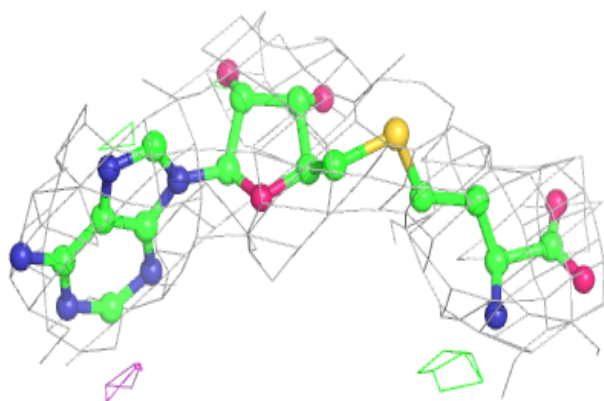
**Electron density around SAH C 1003:**

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

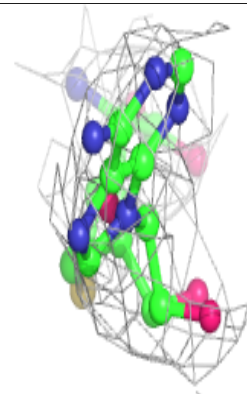
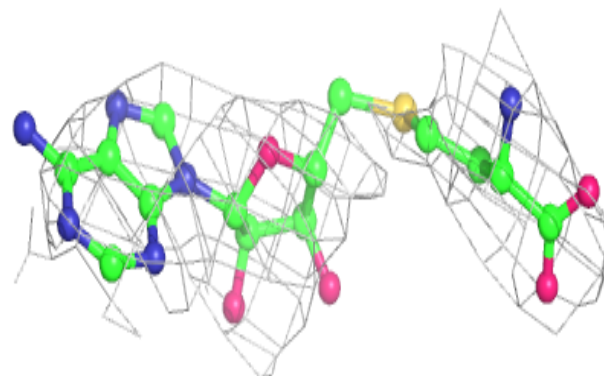
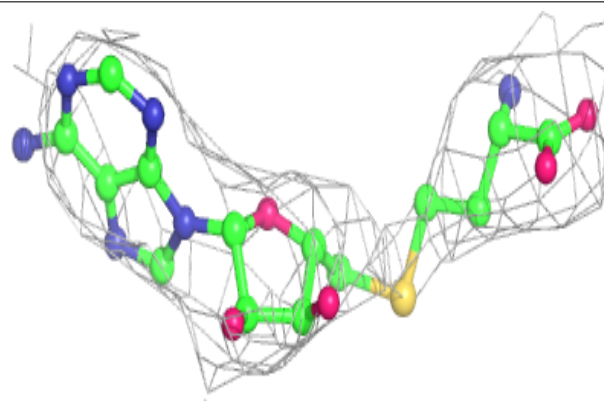


**Electron density around SAH F 1003:**

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and green (positive)

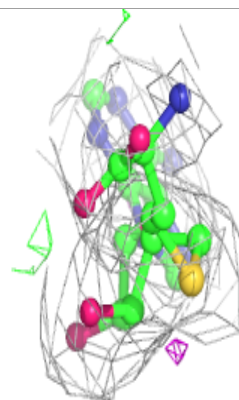
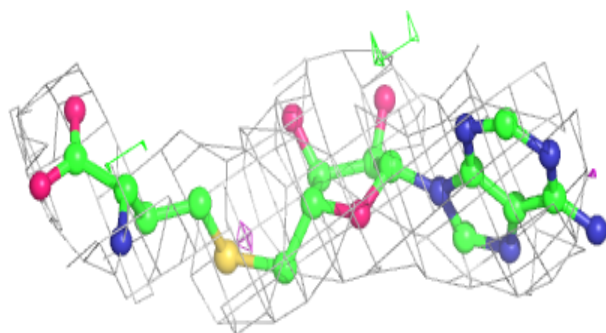
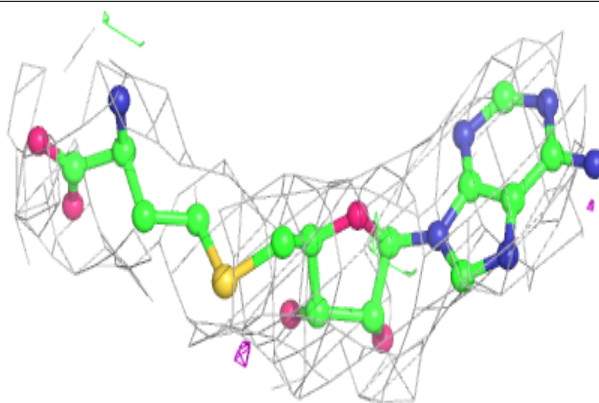
**Electron density around SAH G 1003:**

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and green (positive)

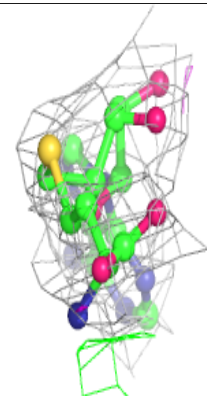
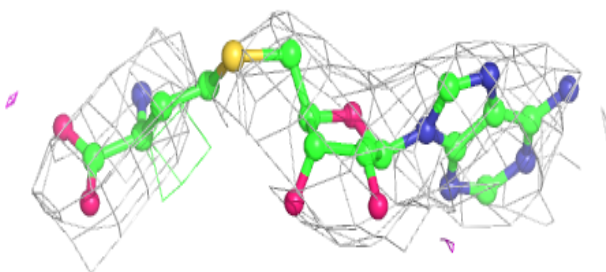
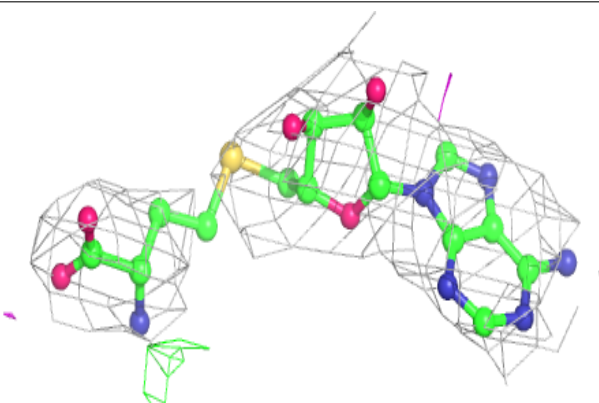


**Electron density around SAH B 1003:**

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

**Electron density around SAH E 1003:**

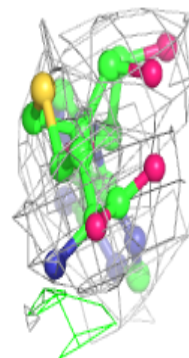
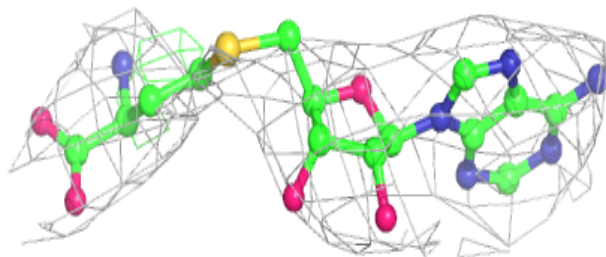
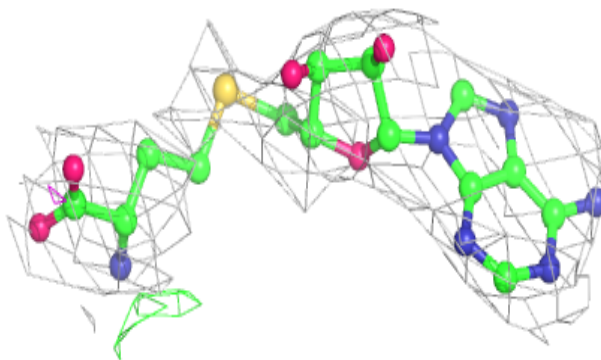
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



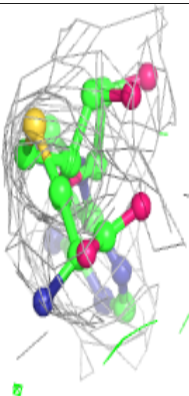
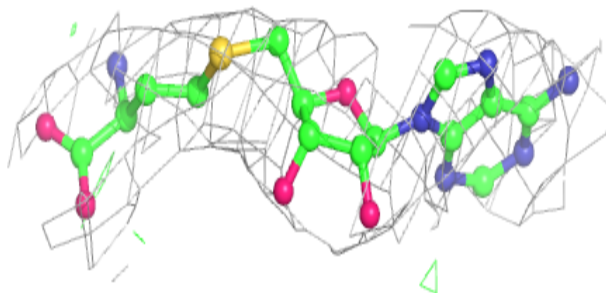
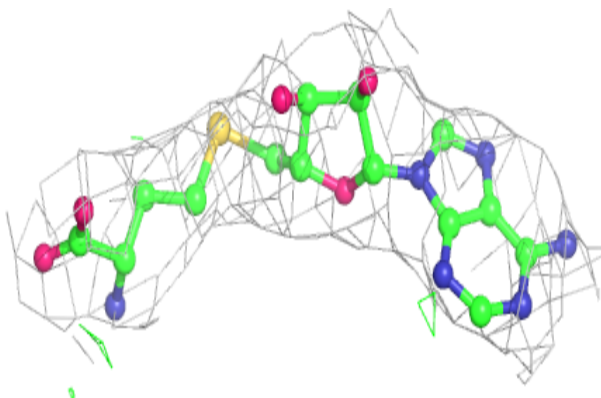


**Electron density around SAH D 1003:**

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

**Electron density around SAH A 1003:**

$2mF_o-DF_c$  (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.