



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2025 – 12:07 PM EST

PDB ID : 9DFW  
Title : X-ray crystal structure of an engineered Viperin-like enzyme from *T. virens* with bound CTP and SAM  
Authors : Lachowicz, J.C.; Bonanno, J.B.; Grove, T.L.  
Deposited on : 2024-08-30  
Resolution : 1.68 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.

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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

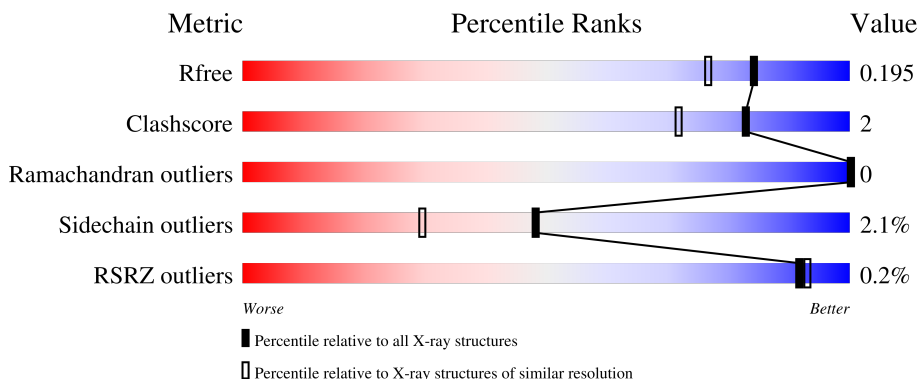
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




The reported resolution of this entry is 1.68 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))
$R_{free}$	164625	8422 (1.70-1.66)
Clashscore	180529	1005 (1.68-1.68)
Ramachandran outliers	177936	9065 (1.70-1.66)
Sidechain outliers	177891	9064 (1.70-1.66)
RSRZ outliers	164620	8421 (1.70-1.66)

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	317	
1	B	317	
1	C	317	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7953 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 Radical SAM core domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	2	0
			2299	1455	398	431	15			
1	B	294	Total	C	N	O	S	0	4	0
			2393	1508	416	453	16			
1	C	283	Total	C	N	O	S	0	6	0
			2320	1466	403	436	15			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP G9MQB8
A	-4	HIS	-	expression tag	UNP G9MQB8
A	-3	HIS	-	expression tag	UNP G9MQB8
A	-2	HIS	-	expression tag	UNP G9MQB8
A	-1	HIS	-	expression tag	UNP G9MQB8
A	0	HIS	-	expression tag	UNP G9MQB8
A	1	HIS	-	expression tag	UNP G9MQB8
A	2	SER	-	expression tag	UNP G9MQB8
A	3	SER	-	expression tag	UNP G9MQB8
A	4	GLY	-	expression tag	UNP G9MQB8
A	5	VAL	-	expression tag	UNP G9MQB8
A	6	ASP	-	expression tag	UNP G9MQB8
A	7	LEU	-	expression tag	UNP G9MQB8
A	8	GLY	-	expression tag	UNP G9MQB8
A	9	THR	-	expression tag	UNP G9MQB8
A	10	GLU	-	expression tag	UNP G9MQB8
A	11	ASN	-	expression tag	UNP G9MQB8
A	12	LEU	-	expression tag	UNP G9MQB8
A	13	TYR	-	expression tag	UNP G9MQB8
A	14	PHE	-	expression tag	UNP G9MQB8
A	15	GLN	-	expression tag	UNP G9MQB8
A	16	SER	-	expression tag	UNP G9MQB8
A	17	MET	-	expression tag	UNP G9MQB8

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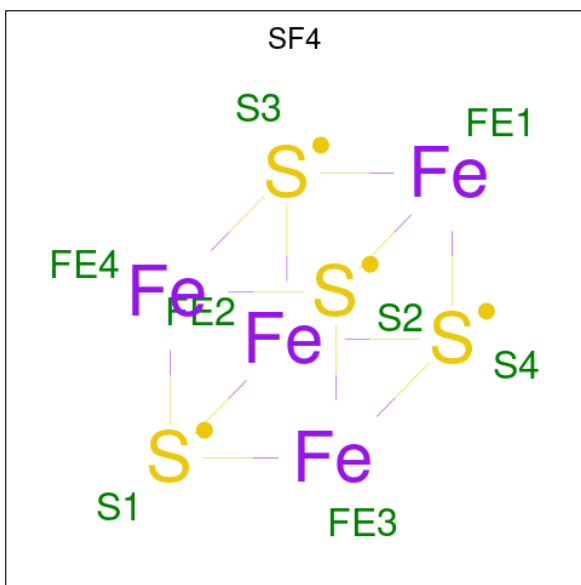
Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ILE	VAL	engineered mutation	UNP G9MQB8
A	199	GLU	THR	engineered mutation	UNP G9MQB8
A	257	ASN	ASP	engineered mutation	UNP G9MQB8
A	258	CYS	ARG	engineered mutation	UNP G9MQB8
A	259	THR	ASN	engineered mutation	UNP G9MQB8
A	261	GLY	-	insertion	UNP G9MQB8
A	262	ARG	-	insertion	UNP G9MQB8
A	263	LYS	GLN	engineered mutation	UNP G9MQB8
A	264	ASP	GLN	engineered mutation	UNP G9MQB8
B	-5	MET	-	initiating methionine	UNP G9MQB8
B	-4	HIS	-	expression tag	UNP G9MQB8
B	-3	HIS	-	expression tag	UNP G9MQB8
B	-2	HIS	-	expression tag	UNP G9MQB8
B	-1	HIS	-	expression tag	UNP G9MQB8
B	0	HIS	-	expression tag	UNP G9MQB8
B	1	HIS	-	expression tag	UNP G9MQB8
B	2	SER	-	expression tag	UNP G9MQB8
B	3	SER	-	expression tag	UNP G9MQB8
B	4	GLY	-	expression tag	UNP G9MQB8
B	5	VAL	-	expression tag	UNP G9MQB8
B	6	ASP	-	expression tag	UNP G9MQB8
B	7	LEU	-	expression tag	UNP G9MQB8
B	8	GLY	-	expression tag	UNP G9MQB8
B	9	THR	-	expression tag	UNP G9MQB8
B	10	GLU	-	expression tag	UNP G9MQB8
B	11	ASN	-	expression tag	UNP G9MQB8
B	12	LEU	-	expression tag	UNP G9MQB8
B	13	TYR	-	expression tag	UNP G9MQB8
B	14	PHE	-	expression tag	UNP G9MQB8
B	15	GLN	-	expression tag	UNP G9MQB8
B	16	SER	-	expression tag	UNP G9MQB8
B	17	MET	-	expression tag	UNP G9MQB8
B	198	ILE	VAL	engineered mutation	UNP G9MQB8
B	199	GLU	THR	engineered mutation	UNP G9MQB8
B	257	ASN	ASP	engineered mutation	UNP G9MQB8
B	258	CYS	ARG	engineered mutation	UNP G9MQB8
B	259	THR	ASN	engineered mutation	UNP G9MQB8
B	261	GLY	-	insertion	UNP G9MQB8
B	262	ARG	-	insertion	UNP G9MQB8
B	263	LYS	GLN	engineered mutation	UNP G9MQB8
B	264	ASP	GLN	engineered mutation	UNP G9MQB8
C	-5	MET	-	initiating methionine	UNP G9MQB8

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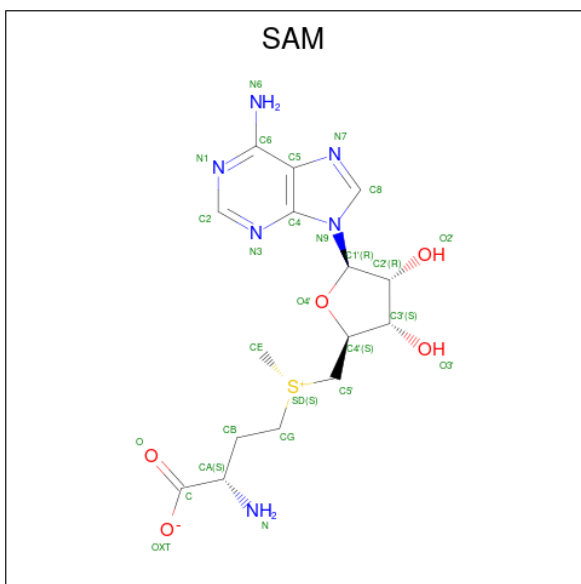
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP G9MQB8
C	-3	HIS	-	expression tag	UNP G9MQB8
C	-2	HIS	-	expression tag	UNP G9MQB8
C	-1	HIS	-	expression tag	UNP G9MQB8
C	0	HIS	-	expression tag	UNP G9MQB8
C	1	HIS	-	expression tag	UNP G9MQB8
C	2	SER	-	expression tag	UNP G9MQB8
C	3	SER	-	expression tag	UNP G9MQB8
C	4	GLY	-	expression tag	UNP G9MQB8
C	5	VAL	-	expression tag	UNP G9MQB8
C	6	ASP	-	expression tag	UNP G9MQB8
C	7	LEU	-	expression tag	UNP G9MQB8
C	8	GLY	-	expression tag	UNP G9MQB8
C	9	THR	-	expression tag	UNP G9MQB8
C	10	GLU	-	expression tag	UNP G9MQB8
C	11	ASN	-	expression tag	UNP G9MQB8
C	12	LEU	-	expression tag	UNP G9MQB8
C	13	TYR	-	expression tag	UNP G9MQB8
C	14	PHE	-	expression tag	UNP G9MQB8
C	15	GLN	-	expression tag	UNP G9MQB8
C	16	SER	-	expression tag	UNP G9MQB8
C	17	MET	-	expression tag	UNP G9MQB8
C	198	ILE	VAL	engineered mutation	UNP G9MQB8
C	199	GLU	THR	engineered mutation	UNP G9MQB8
C	257	ASN	ASP	engineered mutation	UNP G9MQB8
C	258	CYS	ARG	engineered mutation	UNP G9MQB8
C	259	THR	ASN	engineered mutation	UNP G9MQB8
C	261	GLY	-	insertion	UNP G9MQB8
C	262	ARG	-	insertion	UNP G9MQB8
C	263	LYS	GLN	engineered mutation	UNP G9MQB8
C	264	ASP	GLN	engineered mutation	UNP G9MQB8

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



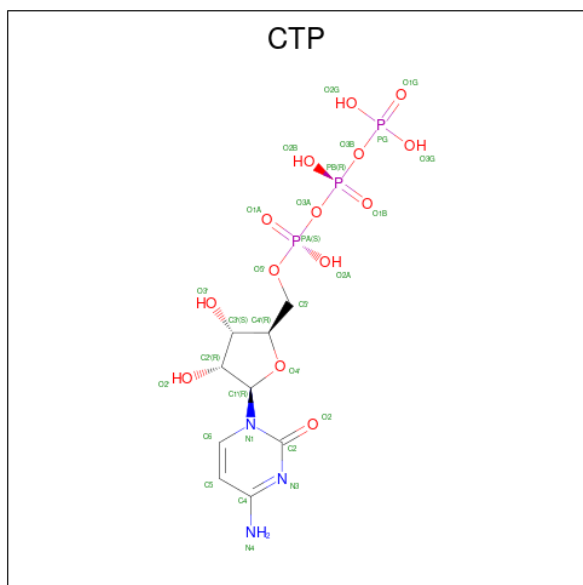
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ) (labeled as "Ligand of Interest" by depositor).



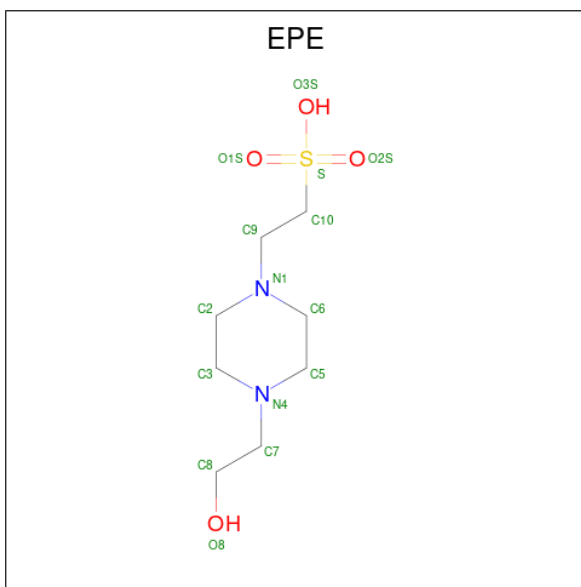
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula:  $C_9H_{16}N_3O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		


- Molecule 8 is water.

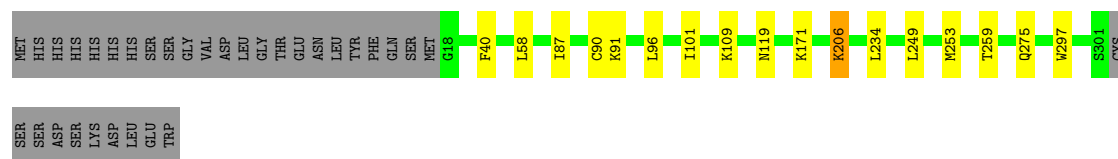
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	241	Total	O	0	0
			241	241		
8	B	252	Total	O	0	0
			252	252		
8	C	217	Total	O	0	0
			217	217		

### 3 Residue-property plots


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.

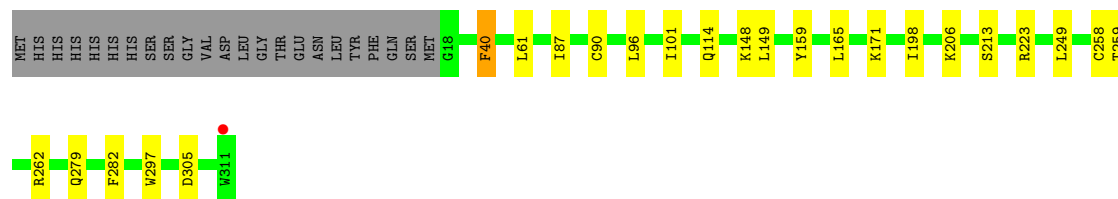
- Molecule 1: Radical SAM core domain-containing protein

Chain A: 




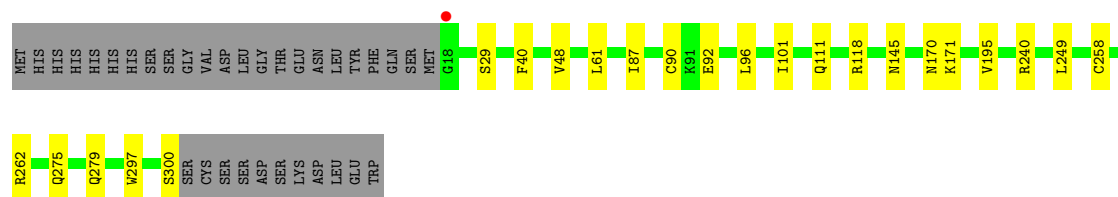
- Molecule 1: Radical SAM core domain-containing protein

Chain B: 



- Molecule 1: Radical SAM core domain-containing protein

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.13Å 85.13Å 110.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.86 – 1.68 19.86 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.86-1.68) 99.9 (19.86-1.68)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.155 , 0.188 0.165 , 0.195	Depositor DCC
$R_{free}$ test set	4941 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l 0.033 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: GOL, MG, EPE, SF4, CTP, SAM

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	0.72	0/2347	0.81	0/3160
1	B	0.73	0/2446	0.82	1/3293 (0.0%)
1	C	0.73	0/2371	0.80	0/3192
All	All	0.72	0/7164	0.81	1/9645 (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	B	223	ARG	NE-CZ-NH1	-5.05	117.77	120.30

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	2299	0	2255	9	0
1	B	2393	0	2334	12	0
1	C	2320	0	2272	13	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
3	A	27	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	21	0	0
3	C	27	0	22	0	0
4	A	29	0	12	0	0
4	B	29	0	12	0	0
4	C	29	0	12	0	0
5	A	30	0	36	0	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
7	C	6	0	8	0	0
8	A	241	0	0	2	0
8	B	252	0	0	1	0
8	C	217	0	0	4	0
All	All	7953	0	7006	33	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 2.

The worst 5 of 33 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:C:87:ILE:HD11	1:C:101:ILE:HD11	1.75	0.68
1:C:29[A]:SER:OG	8:C:501:HOH:O	2.07	0.67
1:A:87:ILE:HD11	1:A:101:ILE:HD11	1.76	0.66
1:A:249:LEU:HG	1:A:253:MET:HA	1.82	0.61
1:B:149:LEU:HD11	1:B:165:LEU:HD21	1.84	0.60

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	284/317 (90%)	277 (98%)	7 (2%)	0	100	100
1	B	296/317 (93%)	291 (98%)	5 (2%)	0	100	100
1	C	287/317 (90%)	277 (96%)	10 (4%)	0	100	100
All	All	867/951 (91%)	845 (98%)	22 (2%)	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	256/285 (90%)	250 (98%)	6 (2%)	45	26
1	B	268/285 (94%)	263 (98%)	5 (2%)	52	34
1	C	259/285 (91%)	254 (98%)	5 (2%)	52	34
All	All	783/855 (92%)	767 (98%)	16 (2%)	48	32

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	297	TRP
1	C	275	GLN
1	B	279	GLN
1	C	171	LYS
1	B	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	B	114	GLN
1	B	239	ASN
1	C	157	GLN
1	C	279	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	EPE	A	404	-	15,15,15	0.68	1 (6%)	19,20,20	0.84	1 (5%)
2	SF4	B	401	3,1	0,12,12	-	-	-		
2	SF4	C	401	3,1	0,12,12	-	-	-		
3	SAM	C	402	2	23,29,29	0.96	2 (8%)	20,42,42	0.98	2 (10%)
3	SAM	B	402	2	23,29,29	0.62	0	20,42,42	1.19	2 (10%)
4	CTP	C	403	-	29,30,30	0.90	1 (3%)	43,47,47	0.80	0
7	GOL	C	404	-	5,5,5	0.12	0	5,5,5	0.26	0
4	CTP	B	403	-	29,30,30	0.88	0	43,47,47	0.79	0
2	SF4	A	401	3,1	0,12,12	-	-	-		
4	CTP	A	403	-	29,30,30	1.00	2 (6%)	43,47,47	0.89	2 (4%)
5	EPE	A	405	-	15,15,15	0.70	1 (6%)	19,20,20	0.88	0
3	SAM	A	402	2	23,29,29	0.74	0	20,42,42	1.08	1 (5%)

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	SAM	C	402	2	-	1/13/33/33	0/3/3/3
2	SF4	B	401	3,1	-	-	0/6/5/5
2	SF4	C	401	3,1	-	-	0/6/5/5
3	SAM	B	402	2	-	4/13/33/33	0/3/3/3
4	CTP	C	403	-	-	4/22/38/38	0/2/2/2
7	GOL	C	404	-	-	0/4/4/4	-
4	CTP	B	403	-	-	2/22/38/38	0/2/2/2
2	SF4	A	401	3,1	-	-	0/6/5/5
4	CTP	A	403	-	-	2/22/38/38	0/2/2/2
5	EPE	A	404	-	-	4/9/19/19	0/1/1/1
5	EPE	A	405	-	-	1/9/19/19	0/1/1/1
3	SAM	A	402	2	-	1/13/33/33	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	CTP	PA-O3A	3.08	1.62	1.59
4	A	403	CTP	PA-O3A	2.88	1.62	1.59
3	C	402	SAM	OXT-C	-2.46	1.22	1.30
5	A	404	EPE	O3S-S	2.39	1.56	1.47
5	A	405	EPE	O3S-S	2.36	1.56	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	SAM	C5-C6-N6	2.80	124.57	120.31
3	B	402	SAM	C5-C6-N6	2.78	124.55	120.31
3	B	402	SAM	CG-SD-C5'	-2.57	97.15	103.43
3	C	402	SAM	CG-SD-C5'	-2.54	97.21	103.43
5	A	404	EPE	O1S-S-C10	-2.30	103.25	106.73

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

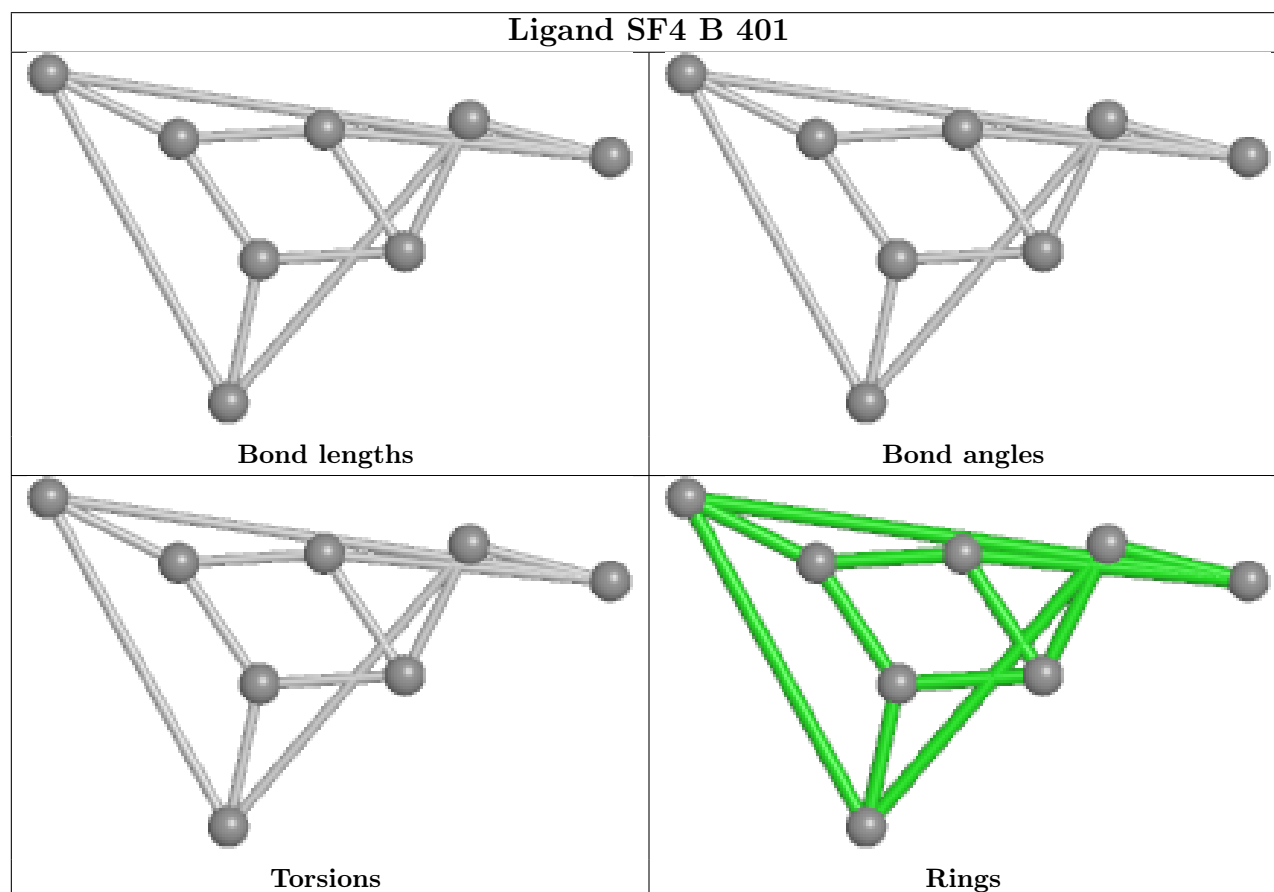
Mol	Chain	Res	Type	Atoms
4	B	403	CTP	C5'-O5'-PA-O1A
4	C	403	CTP	C5'-O5'-PA-O1A
5	A	404	EPE	N4-C7-C8-O8
5	A	405	EPE	S-C10-C9-N1
5	A	404	EPE	C8-C7-N4-C5

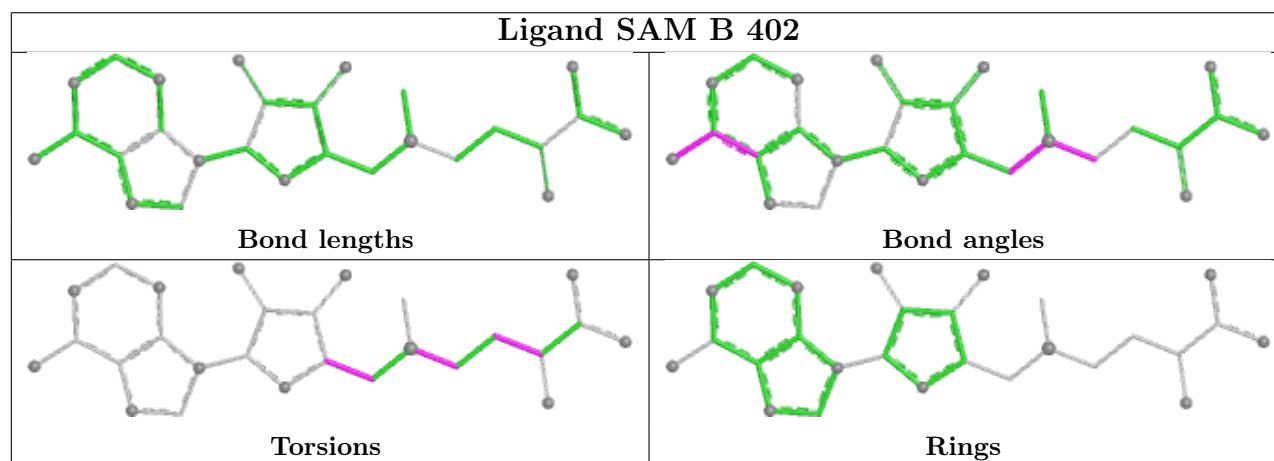
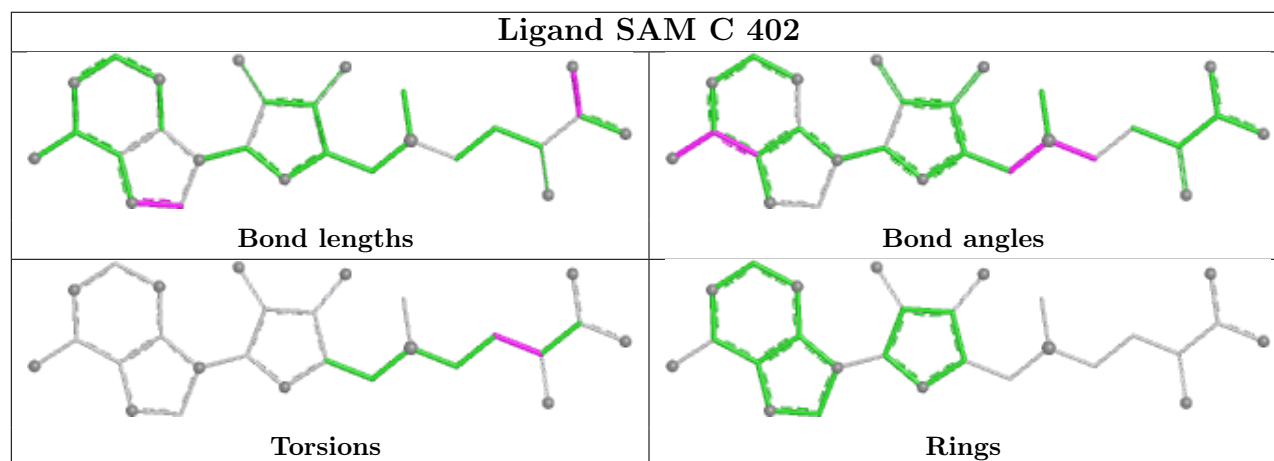
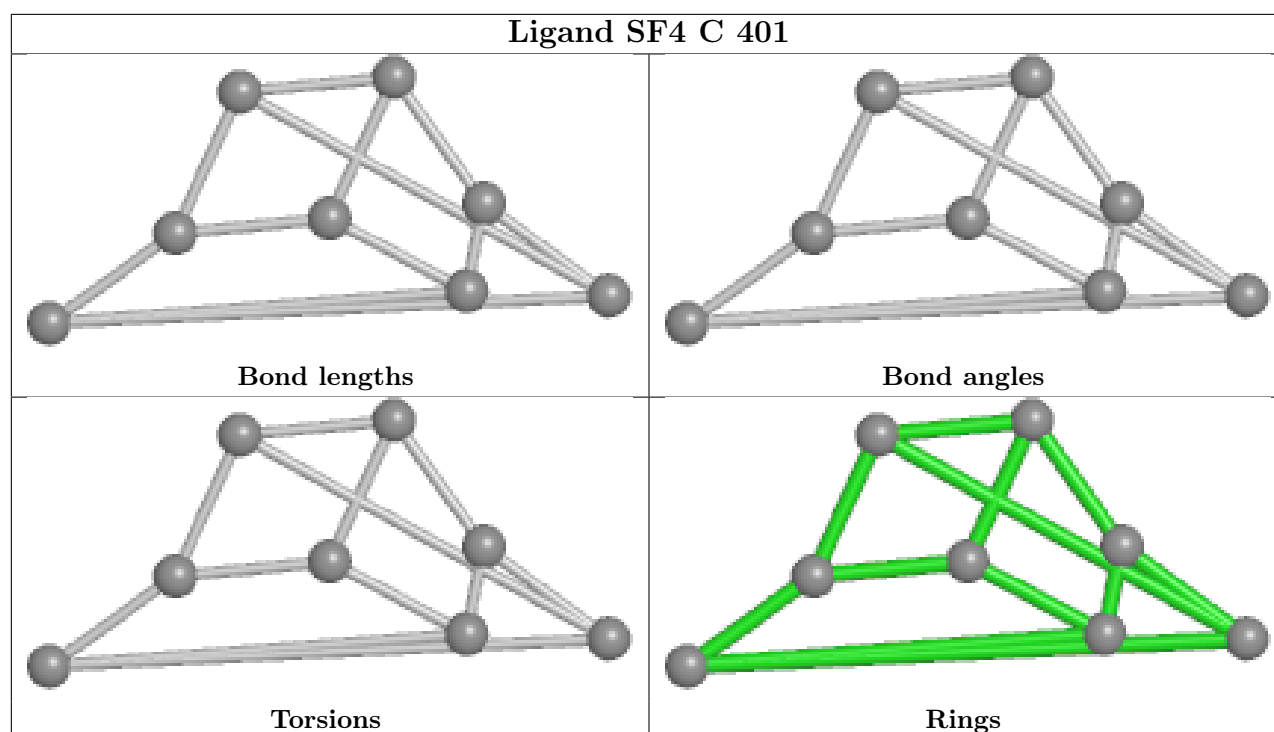


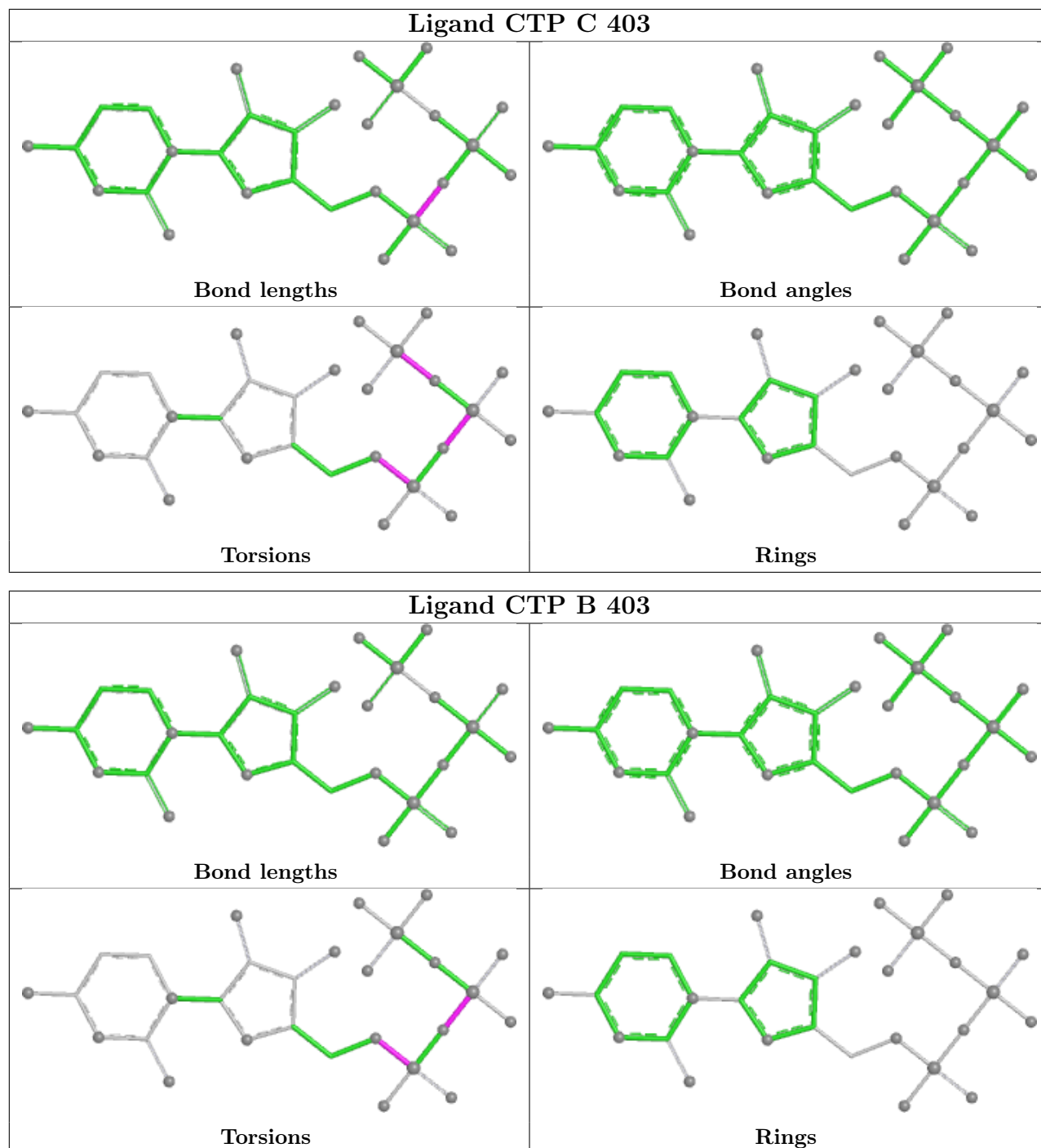
There are no ring outliers.

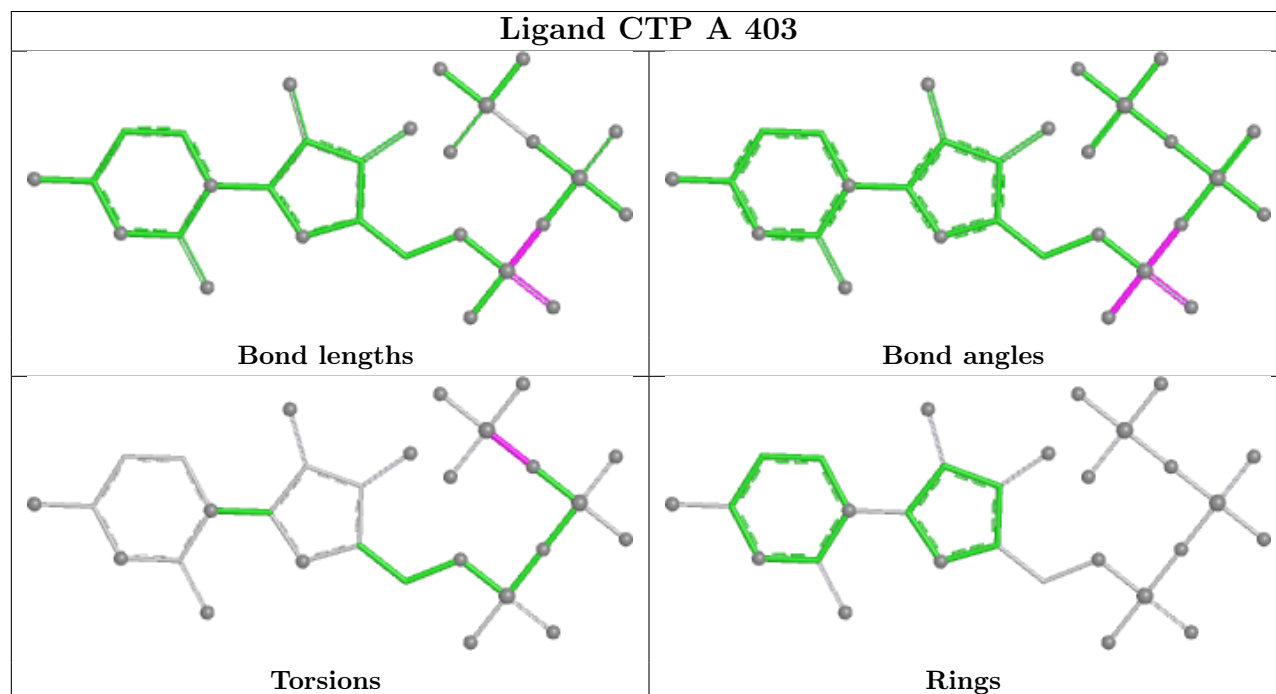
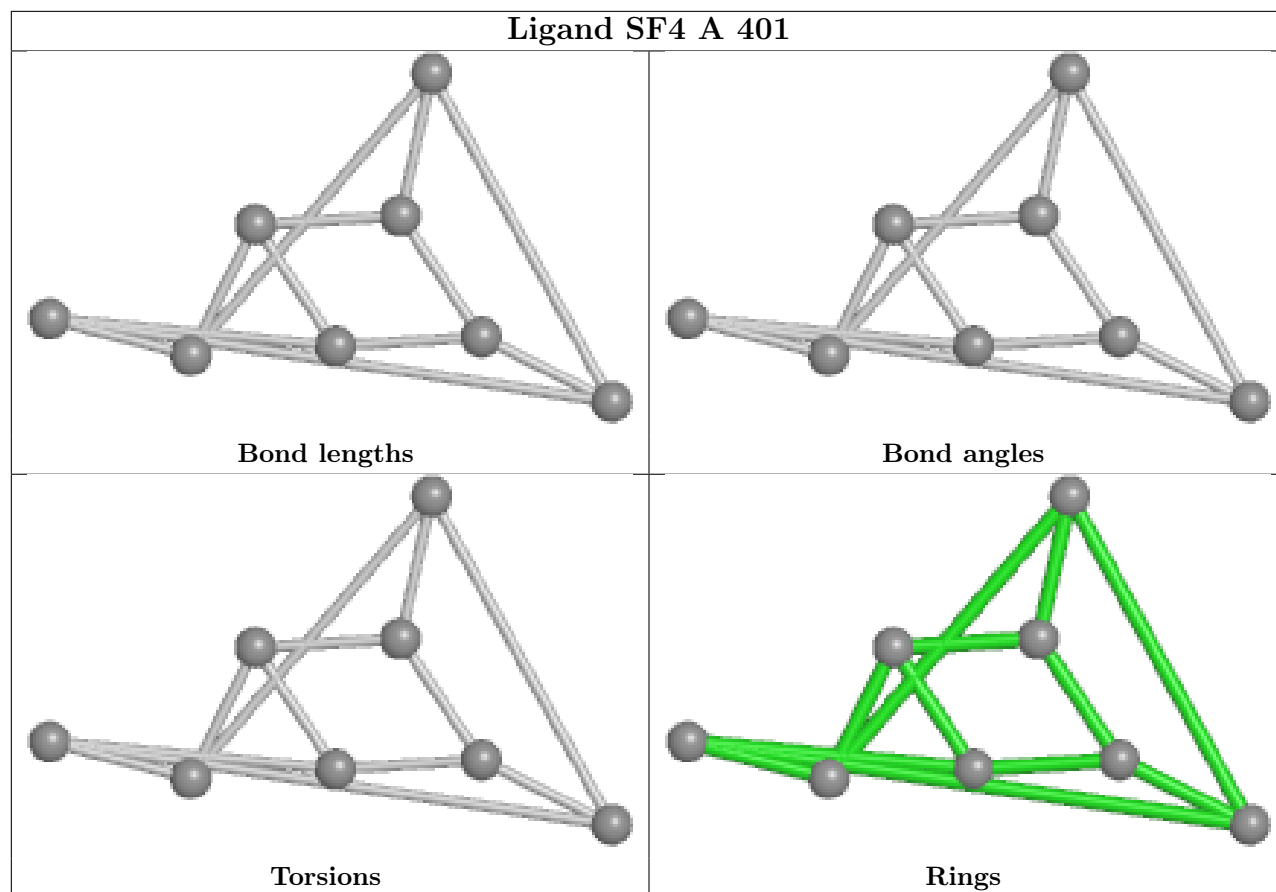
No monomer is involved in short contacts.

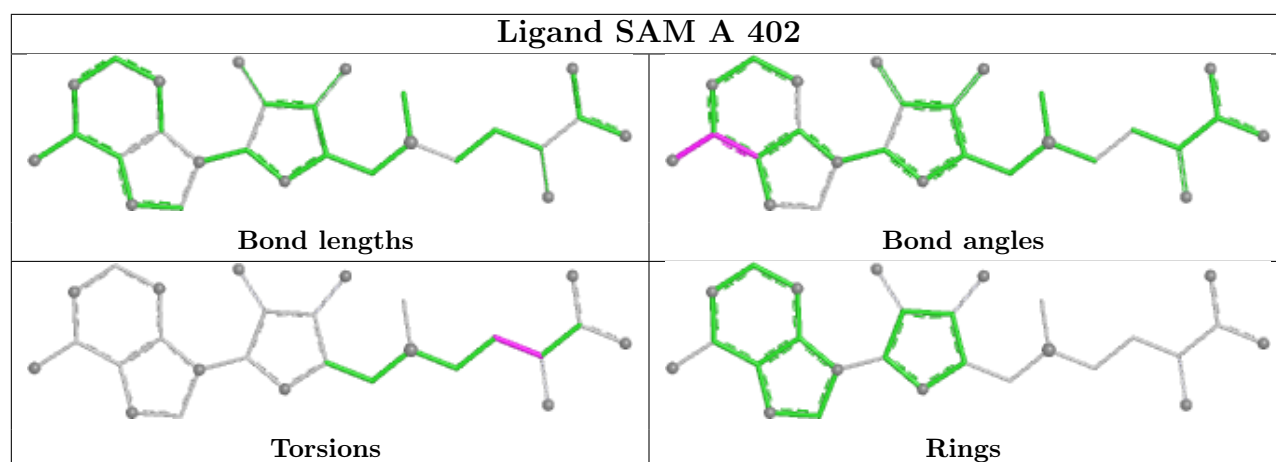
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	284/317 (89%)	-0.41	0	100   100	11, 26, 44, 85	2 (0%)
1	B	294/317 (92%)	-0.35	1 (0%)	90   92	11, 26, 43, 62	4 (1%)
1	C	283/317 (89%)	-0.31	1 (0%)	89   91	10, 26, 47, 81	6 (2%)
All	All	861/951 (90%)	-0.36	2 (0%)	92   93	10, 26, 45, 85	12 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	GLY	2.8
1	B	311	TRP	2.2

### 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.

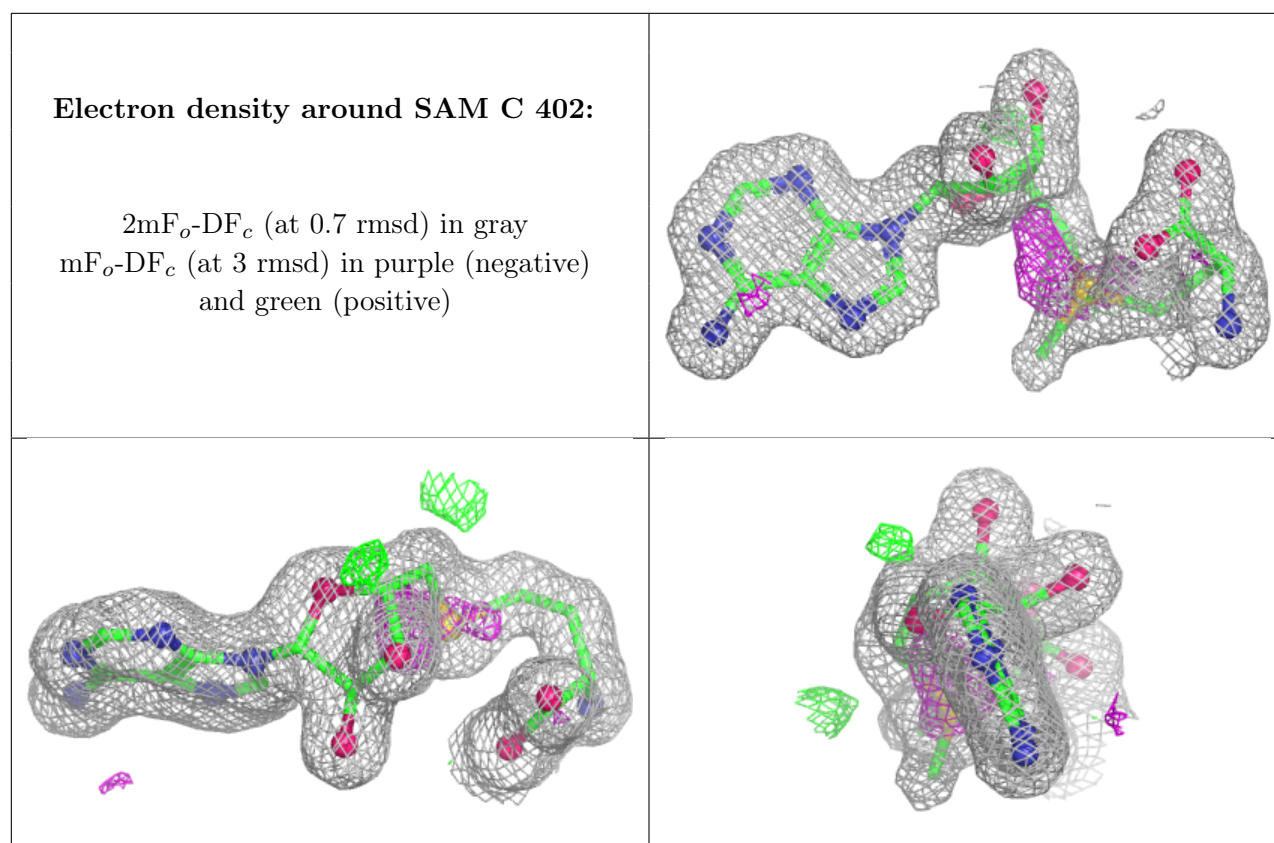
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
5	EPE	A	404	15/15	0.82	0.15	36,66,80,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	C	404	6/6	0.90	0.09	29,32,33,36	0
5	EPE	A	405	15/15	0.91	0.09	39,42,57,66	0
3	SAM	C	402	27/27	0.96	0.05	16,22,31,33	0
6	MG	A	407	1/1	0.96	0.09	43,43,43,43	0
3	SAM	A	402	27/27	0.96	0.06	14,20,27,30	0
3	SAM	B	402	27/27	0.97	0.05	17,22,30,40	0
6	MG	C	405	1/1	0.97	0.05	26,26,26,26	0
6	MG	A	406	1/1	0.97	0.09	30,30,30,30	0
4	CTP	B	403	29/29	0.99	0.03	18,20,25,28	0
4	CTP	C	403	29/29	0.99	0.03	18,20,24,26	0
2	SF4	C	401	8/8	0.99	0.02	20,21,22,22	0
4	CTP	A	403	29/29	0.99	0.04	17,20,24,27	0
2	SF4	B	401	8/8	1.00	0.02	19,20,21,22	0
2	SF4	A	401	8/8	1.00	0.02	18,19,20,20	0

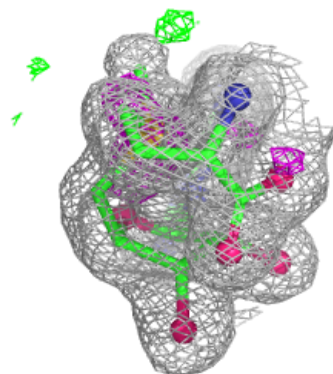
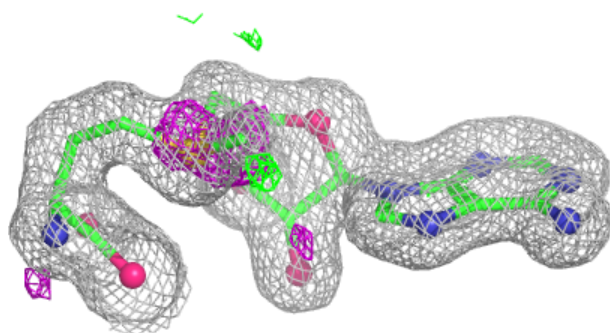
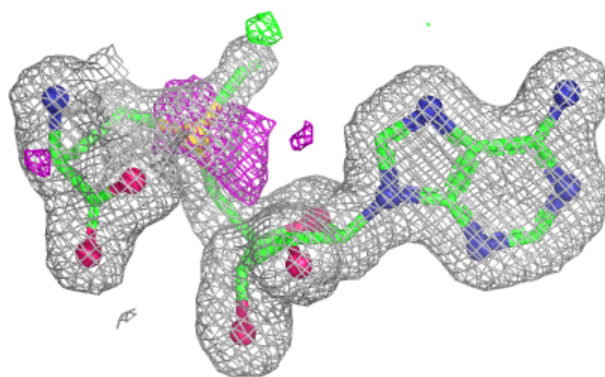
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



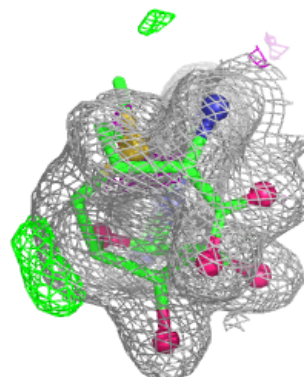
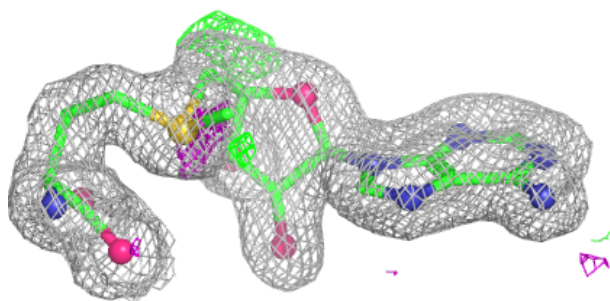
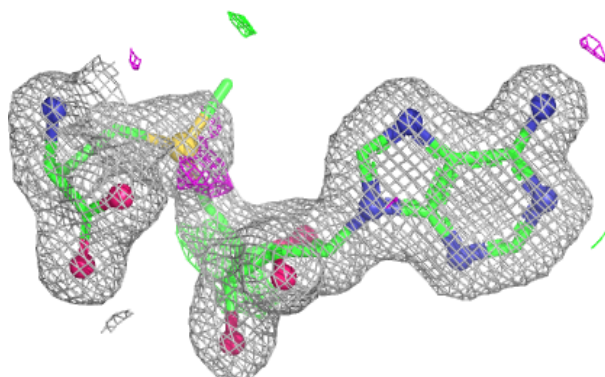


**Electron density around SAM A 402:**

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

**Electron density around SAM B 402:**

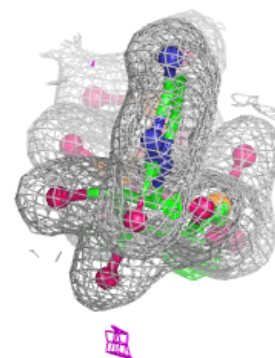
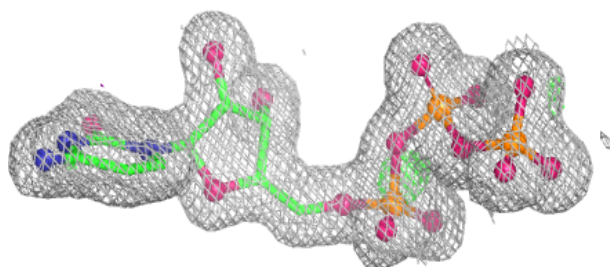
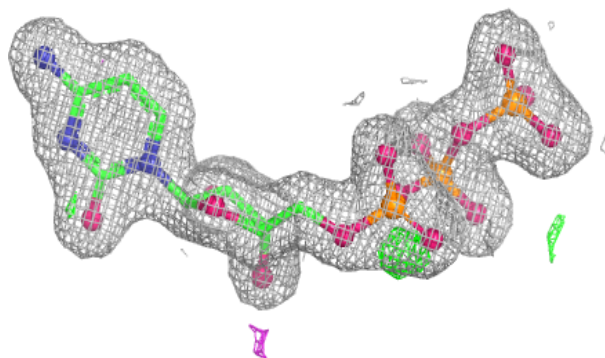
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



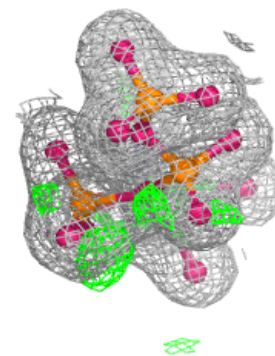
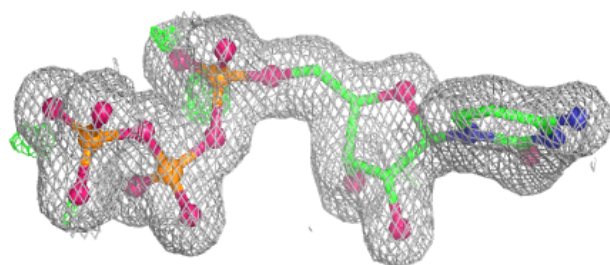
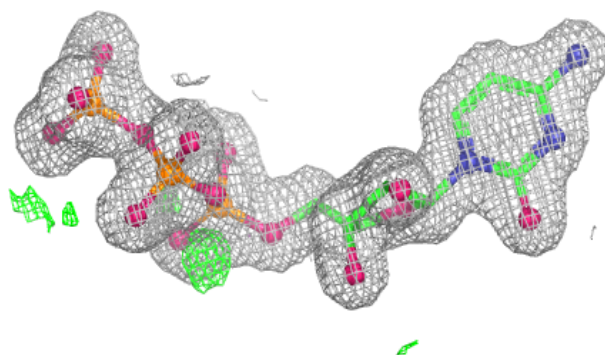


**Electron density around CTP B 403:**

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

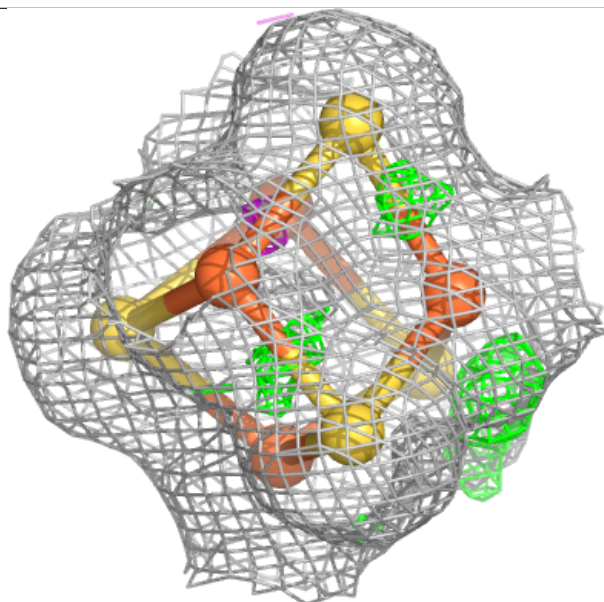
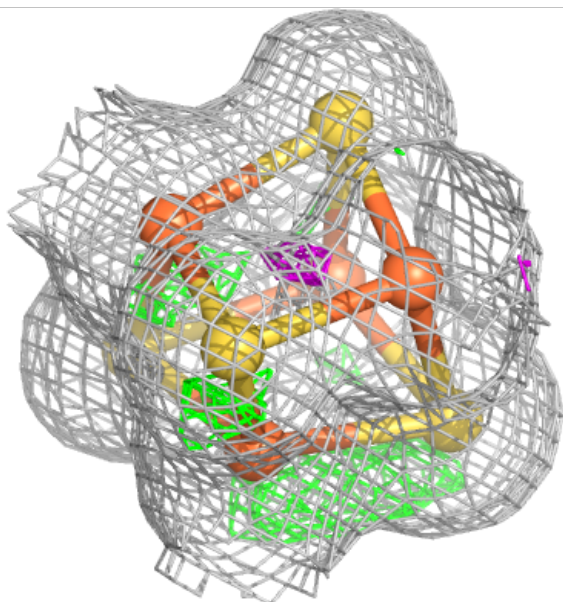
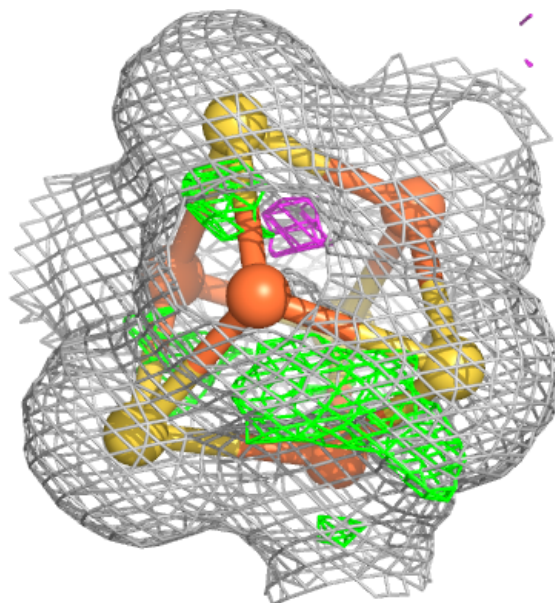
**Electron density around CTP C 403:**

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



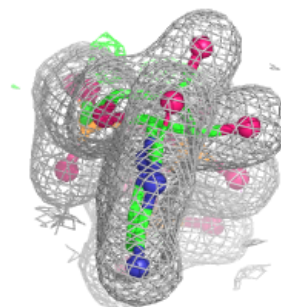
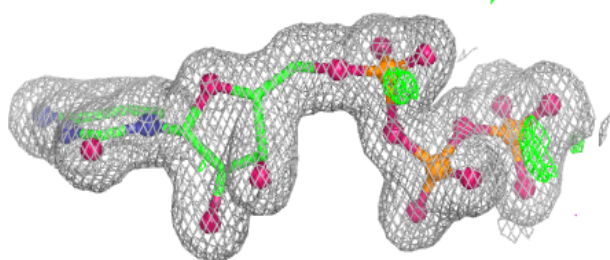
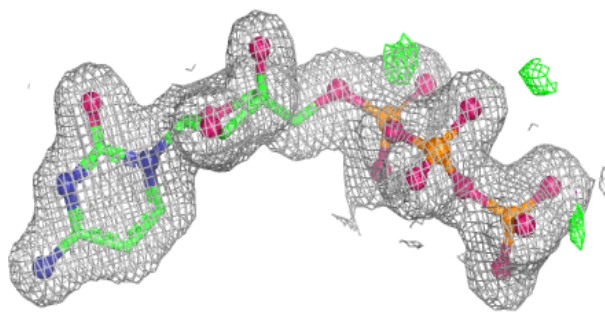
**Electron density around SF4 C 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CTP A 403:**

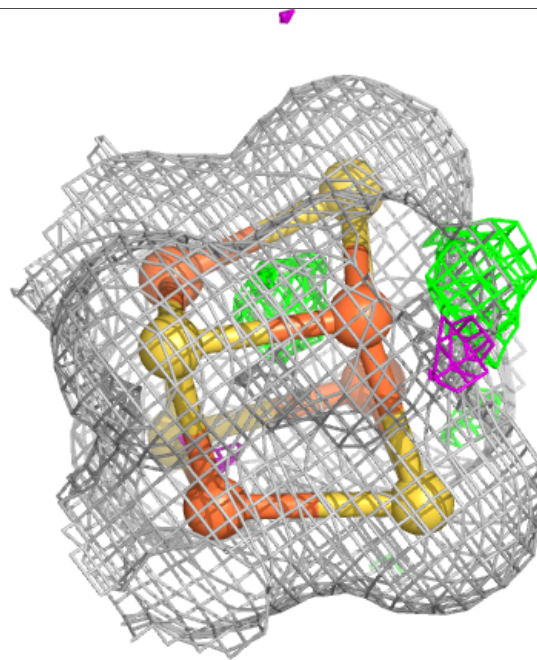
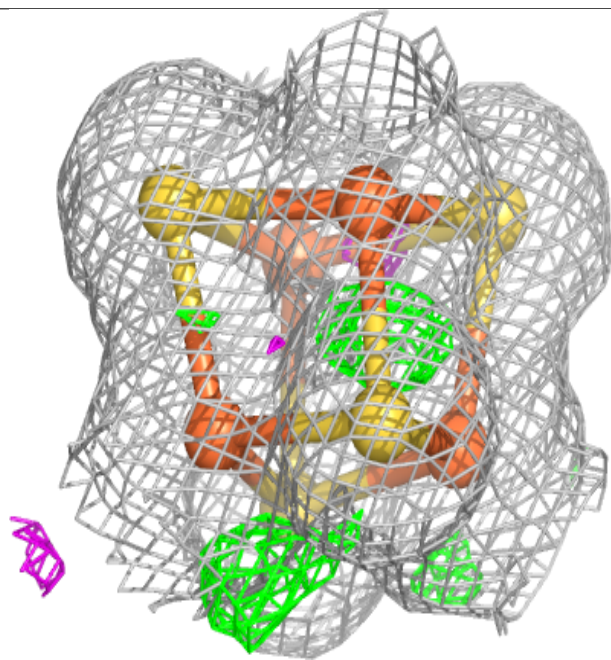
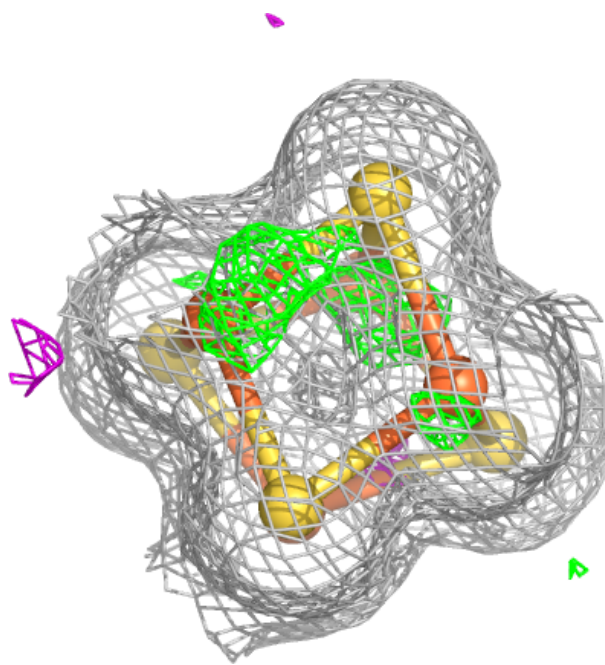
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





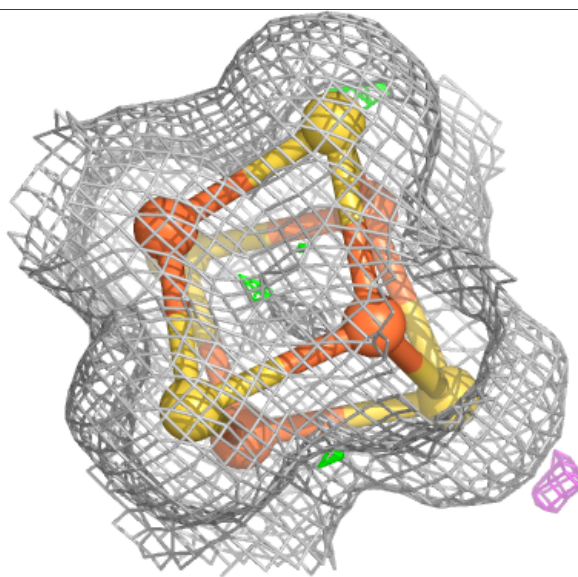
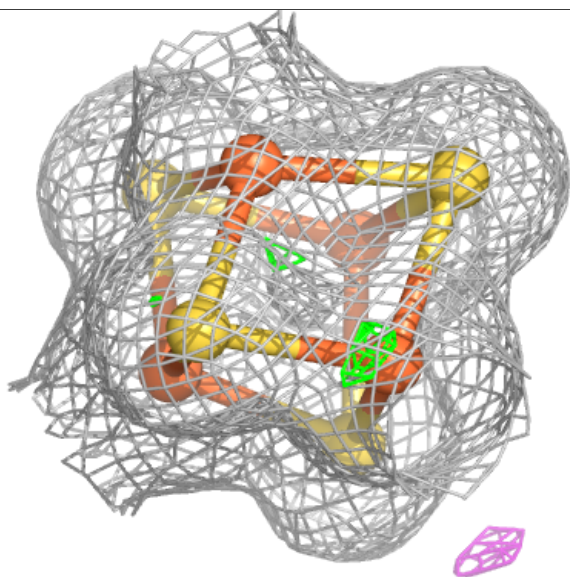
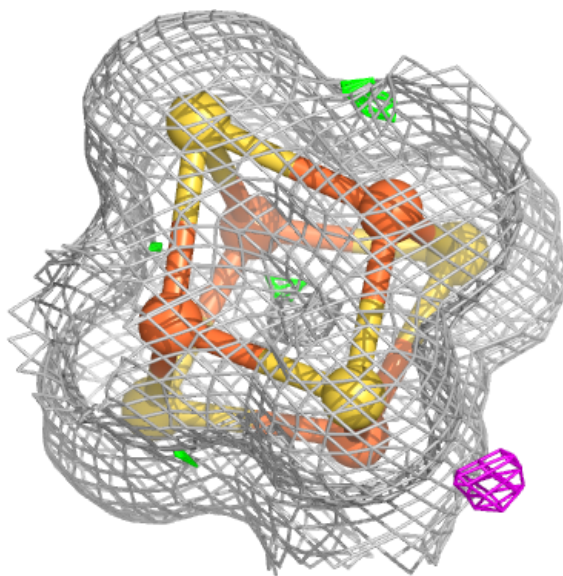
**Electron density around SF4 B 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SF4 A 401:**

$2mF_o-DF_c$  (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.