



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 12:34 PM UTC

PDB ID : 9DGW / pdb_00009dgw
Title : X-ray crystal structure of the Viperin-like enzyme from T. virens with bound CTP and SAM
Authors : Lachowicz, J.C.; Bonanno, J.B.; Grove, T.L.
Deposited on : 2024-09-03
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

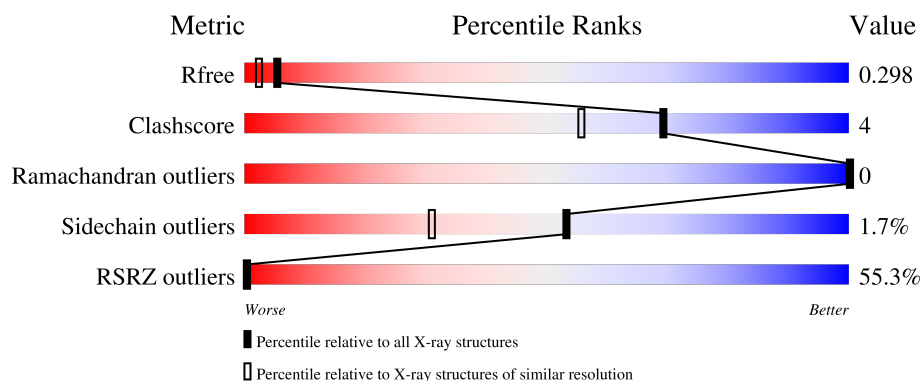
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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 ≥ 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	315	<div> <div>34%</div> <div>80% 8% 11%</div> </div>
1	B	315	<div> <div>35%</div> <div>83% 7% 10%</div> </div>
1	C	315	<div> <div>78%</div> <div>78% 10% 12%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	C	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7261 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	279	Total	C	N	O	S	0	0	0
			2250	1424	390	422	14			
1	B	282	Total	C	N	O	S	0	1	0
			2277	1439	395	429	14			
1	C	276	Total	C	N	O	S	0	3	0
			2243	1425	387	417	14			

There are 69 discrepancies between the modelled and reference sequences:

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

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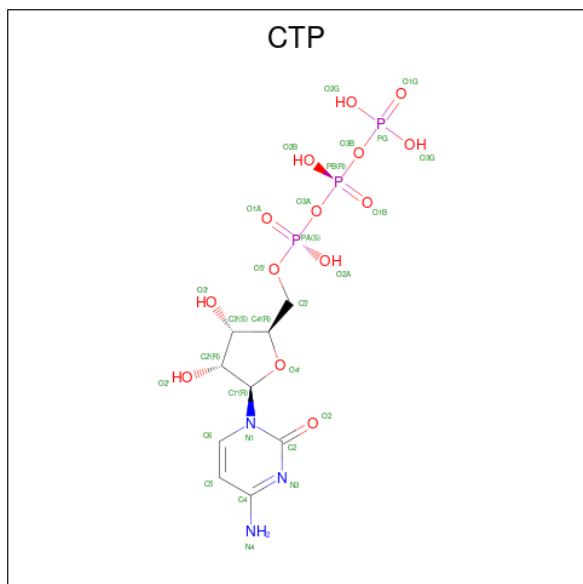
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	initiating methionine	UNP G9MQB8
B	-5	HIS	-	expression tag	UNP G9MQB8
B	-4	HIS	-	expression tag	UNP G9MQB8
B	-3	HIS	-	expression tag	UNP G9MQB8
B	-2	HIS	-	expression tag	UNP G9MQB8
B	-1	HIS	-	expression tag	UNP G9MQB8
B	0	HIS	-	expression tag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

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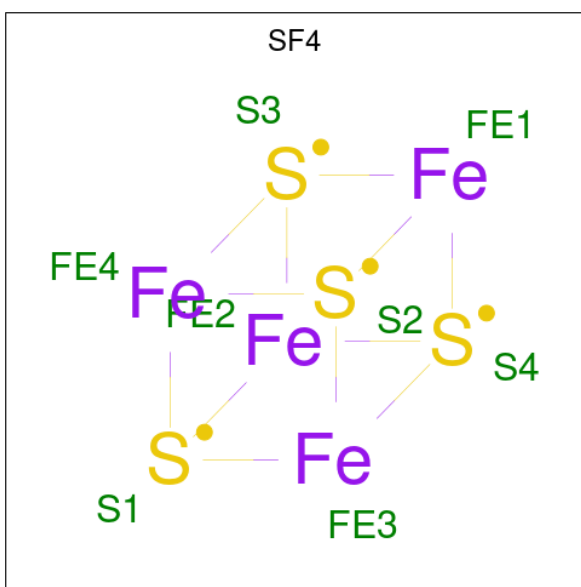
Chain	Residue	Modelled	Actual	Comment	Reference
C	13	PHE	-	expression tag	UNP G9MQB8
C	14	GLN	-	expression tag	UNP G9MQB8
C	15	SER	-	expression tag	UNP G9MQB8
C	16	MET	-	expression tag	UNP G9MQB8

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



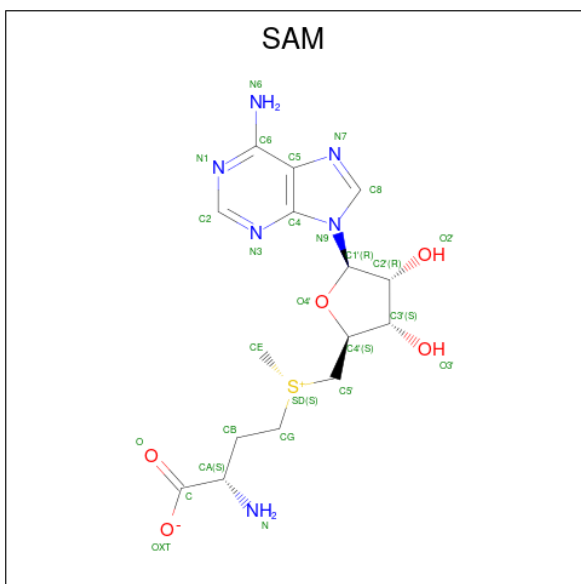
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



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

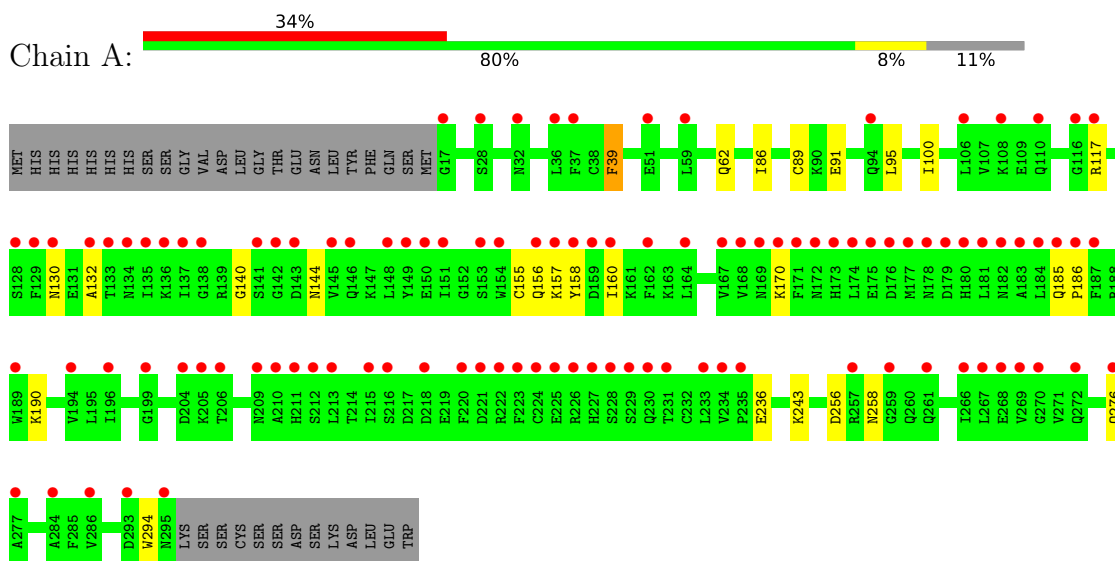
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	134	Total	O	0	0
			134	134		
5	C	44	Total	O	0	0
			44	44		

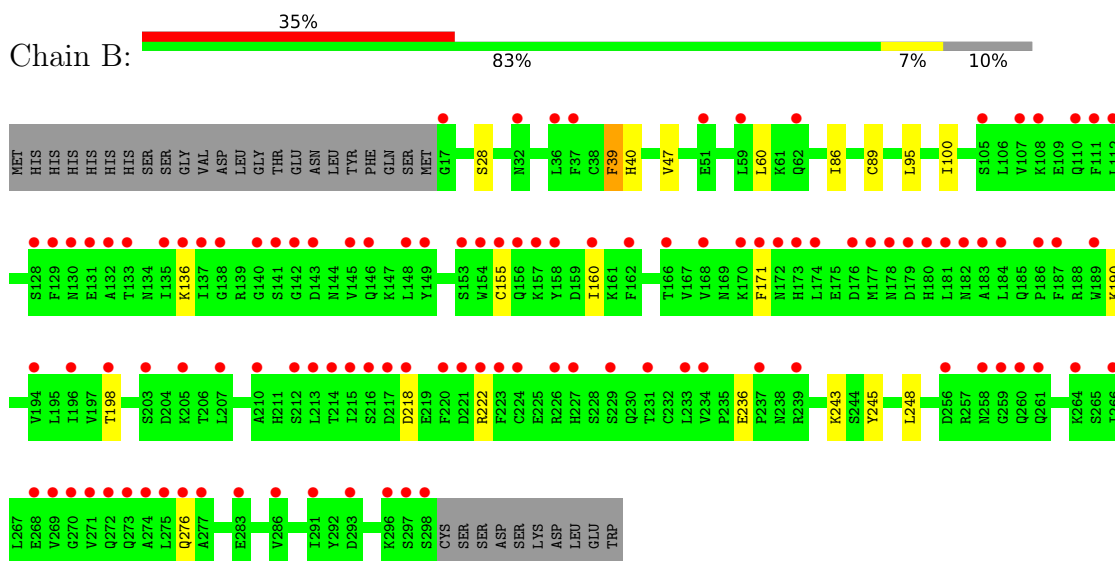
3 Residue-property plots [i](#)

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.

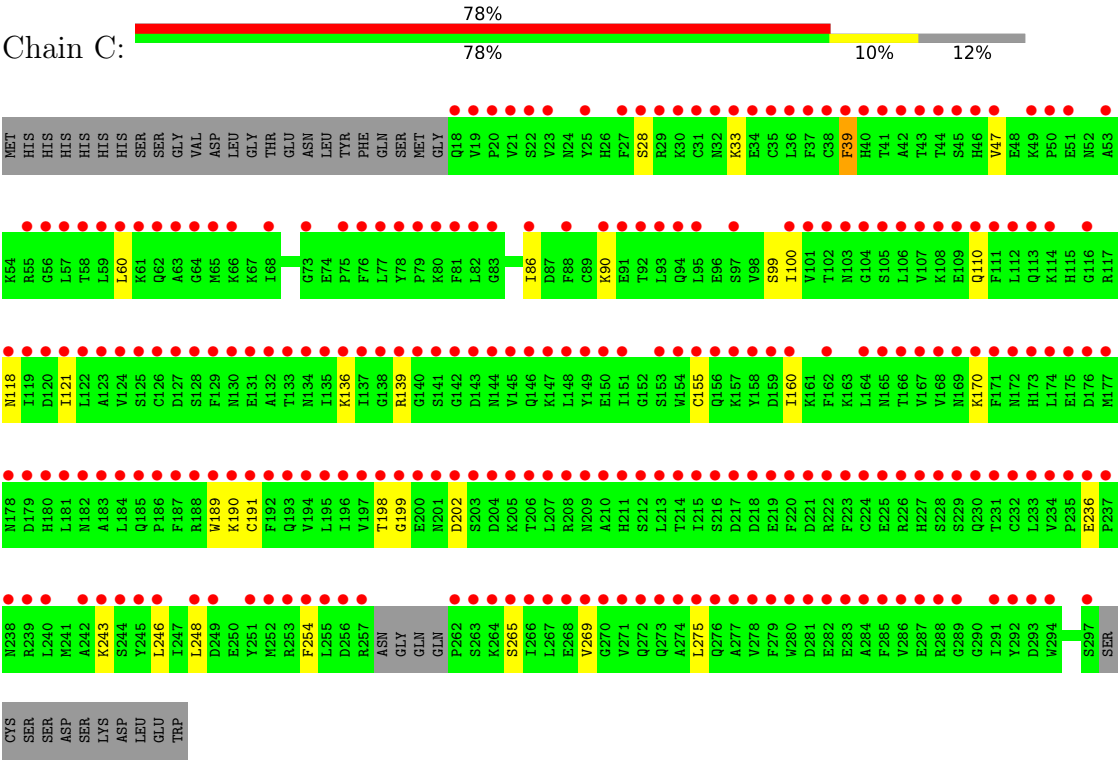
- Molecule 1: Radical SAM core domain-containing protein



- Molecule 1: Radical SAM core domain-containing protein



- Molecule 1: Radical SAM core domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.57Å 80.31Å 105.61Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	28.59 – 1.72 28.59 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.59-1.72) 99.1 (28.59-1.72)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.261 , 0.292 0.269 , 0.298	Depositor DCC
R_{free} test set	4454 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7261	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CTP, SF4, 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	0.58	0/2298	0.97	1/3098 (0.0%)
1	B	0.58	0/2325	0.95	2/3133 (0.1%)
1	C	0.54	0/2290	0.94	0/3086
All	All	0.57	0/6913	0.95	3/9317 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	HIS	CB-CA-C	5.32	119.67	111.95
1	B	39	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	39	PHE	CA-CB-CG	5.05	118.85	113.80

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	2250	0	2197	14	0
1	B	2277	0	2224	13	0
1	C	2243	0	2196	19	0
2	A	29	0	12	0	0
2	B	29	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	29	0	12	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	C	8	0	0	2	0
4	A	27	0	21	0	0
4	B	27	0	22	0	0
4	C	27	0	22	1	0
5	A	121	0	0	1	0
5	B	134	0	0	0	0
5	C	44	0	0	1	0
All	All	7261	0	6718	48	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 4.

All (48) 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)
3:C:403:SF4:FE1	3:C:403:SF4:S2	1.88	0.65
4:C:401:SAM:N	3:C:403:SF4:S2	2.71	0.63
1:C:86[B]:ILE:HD11	1:C:100:ILE:HD11	1.82	0.60
1:B:218:ASP:HB3	1:B:222:ARG:HH12	1.72	0.54
1:B:190:LYS:HE2	1:B:236:GLU:OE2	2.08	0.54
1:B:28[B]:SER:HB2	1:B:47:VAL:HG22	1.92	0.52
1:B:89:CYS:HB3	1:B:95:LEU:HD12	1.92	0.51
1:B:60:LEU:HD11	1:B:248:LEU:HD11	1.92	0.50
1:B:86:ILE:HD11	1:B:100:ILE:HD11	1.94	0.50
1:B:190:LYS:CE	1:B:236:GLU:OE2	2.59	0.50
1:C:199:GLY:N	1:C:202:ASP:OD1	2.42	0.50
1:C:170:LYS:HE2	1:C:170:LYS:HA	1.94	0.49
1:C:90:LYS:HG2	1:C:118:ASN:HA	1.95	0.48
1:C:33:LYS:NZ	1:C:139:ARG:O	2.38	0.46
1:A:190:LYS:HE2	1:A:236:GLU:OE2	2.16	0.46
1:A:86:ILE:CD1	1:A:100:ILE:HD11	2.47	0.45
1:C:190:LYS:CE	1:C:236:GLU:OE1	2.64	0.45
1:A:243:LYS:NZ	1:A:258:ASN:HB3	2.32	0.45
1:B:136:LYS:HE3	1:B:171:PHE:CZ	2.52	0.45
1:C:28[A]:SER:HB3	1:C:47:VAL:HG22	1.99	0.45
1:C:190:LYS:HE2	1:C:236:GLU:OE1	2.16	0.45
1:C:110:GLN:NE2	5:C:502:HOH:O	2.50	0.44
1:A:140:GLY:HA3	1:A:144:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:CYS:HB3	1:A:160:ILE:O	2.18	0.44
1:B:245:TYR:CD2	2:B:403:CTP:H2'	2.52	0.44
1:C:86[B]:ILE:CD1	1:C:100:ILE:HD11	2.47	0.44
1:A:130:ASN:OD1	1:A:132:ALA:HB3	2.18	0.44
1:C:60:LEU:HD11	1:C:248:LEU:HD11	2.01	0.43
1:A:86:ILE:HD11	1:A:100:ILE:HD11	2.01	0.43
1:A:91:GLU:OE1	1:A:117:ARG:NH2	2.50	0.43
1:A:157:LYS:HE3	1:A:158:TYR:OH	2.19	0.42
1:C:28[B]:SER:HB2	1:C:47:VAL:HG22	2.01	0.42
1:A:190:LYS:CE	1:A:236:GLU:OE2	2.67	0.42
1:C:246:LEU:HD22	1:C:275:LEU:HD11	2.01	0.42
1:B:155:CYS:HB3	1:B:160:ILE:O	2.20	0.42
1:C:155:CYS:HB3	1:C:160:ILE:O	2.20	0.42
1:B:190:LYS:NZ	2:B:403:CTP:O1A	2.52	0.41
1:C:39:PHE:C	1:C:39:PHE:CD1	2.98	0.41
1:C:189:TRP:CE2	1:C:191:CYS:SG	3.14	0.41
1:A:185:GLN:N	1:A:186:PRO:CD	2.83	0.41
1:C:254:PHE:CZ	1:C:275:LEU:HD13	2.56	0.41
1:B:136:LYS:HE3	1:B:171:PHE:CE2	2.55	0.41
1:C:99:SER:HA	1:C:121:ILE:O	2.20	0.41
1:C:265:SER:O	1:C:269:VAL:HG22	2.21	0.40
1:A:62:GLN:NE2	5:A:510:HOH:O	2.52	0.40
1:A:243:LYS:NZ	1:A:256:ASP:O	2.45	0.40
1:A:89:CYS:HB3	1:A:95:LEU:HD12	2.03	0.40
1:B:218:ASP:HB3	1:B:222:ARG:NH1	2.37	0.40

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	277/315 (88%)	270 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	281/315 (89%)	275 (98%)	6 (2%)	0	100	100
1	C	275/315 (87%)	268 (98%)	7 (2%)	0	100	100
All	All	833/945 (88%)	813 (98%)	20 (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	250/284 (88%)	245 (98%)	5 (2%)	48	26
1	B	254/284 (89%)	250 (98%)	4 (2%)	55	34
1	C	249/284 (88%)	245 (98%)	4 (2%)	55	34
All	All	753/852 (88%)	740 (98%)	13 (2%)	53	31

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PHE
1	A	156	GLN
1	A	170	LYS
1	A	276	GLN
1	A	294	TRP
1	B	39	PHE
1	B	198	THR
1	B	243	LYS
1	B	276	GLN
1	C	39	PHE
1	C	136	LYS
1	C	198	THR
1	C	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	62	GLN
1	A	238	ASN
1	B	173	HIS
1	B	273	GLN
1	C	40	HIS
1	C	110	GLN
1	C	273	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 ⓘ

9 ligands are modelled in this entry.

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	$\# Z > 2$
4	SAM	C	401	3	27,29,29	0.59	1 (3%)	34,42,42	0.83	3 (8%)
3	SF4	A	402	4,1	0,12,12	-	-	-		
4	SAM	B	402	3	27,29,29	0.63	1 (3%)	34,42,42	0.54	0
2	CTP	C	402	-	29,30,30	1.02	2 (6%)	43,47,47	0.99	3 (6%)
3	SF4	C	403	4,1	0,12,12	-	-	-		
2	CTP	B	403	-	29,30,30	1.04	3 (10%)	43,47,47	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	B	401	4,1	0,12,12	-	-	-		
2	CTP	A	401	-	29,30,30	0.80	0	43,47,47	0.96	2 (4%)
4	SAM	A	403	3	27,29,29	0.44	0	34,42,42	0.76	1 (2%)

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
4	SAM	C	401	3	-	3/17/33/33	0/3/3/3
3	SF4	A	402	4,1	-	-	0/6/5/5
4	SAM	B	402	3	-	1/17/33/33	0/3/3/3
2	CTP	C	402	-	-	1/22/38/38	0/2/2/2
3	SF4	C	403	4,1	-	-	0/6/5/5
2	CTP	B	403	-	-	1/22/38/38	0/2/2/2
3	SF4	B	401	4,1	-	-	0/6/5/5
2	CTP	A	401	-	-	1/22/38/38	0/2/2/2
4	SAM	A	403	3	-	3/17/33/33	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	CTP	PA-O3A	3.60	1.63	1.59
2	B	403	CTP	PA-O3A	3.05	1.62	1.59
2	B	403	CTP	PG-O1G	-2.82	1.41	1.50
4	C	401	SAM	OXT-C	-2.68	1.22	1.30
2	B	403	CTP	PB-O2B	-2.28	1.44	1.55
4	B	402	SAM	O-C	2.23	1.28	1.22
2	C	402	CTP	PG-O2G	-2.07	1.47	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	CTP	O2A-PA-O1A	3.23	127.47	112.44
2	A	401	CTP	O2A-PA-O1A	3.03	126.55	112.44
4	A	403	SAM	CG-SD-C5'	-2.84	96.49	103.43
2	C	402	CTP	O2A-PA-O1A	2.79	125.40	112.44
4	C	401	SAM	O3'-C3'-C2'	-2.75	103.01	111.82
2	C	402	CTP	O3A-PB-O1B	-2.66	102.72	110.70
4	C	401	SAM	O3'-C3'-C4'	2.19	117.38	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	CTP	O3A-PA-O1A	-2.09	104.42	110.70
2	A	401	CTP	O2A-PA-O3A	-2.06	101.70	107.27
2	C	402	CTP	O2B-PB-O3A	2.02	112.73	107.27
4	C	401	SAM	O2'-C2'-C1'	2.00	117.00	110.10

There are no chirality outliers.

All (10) torsion outliers are listed below:

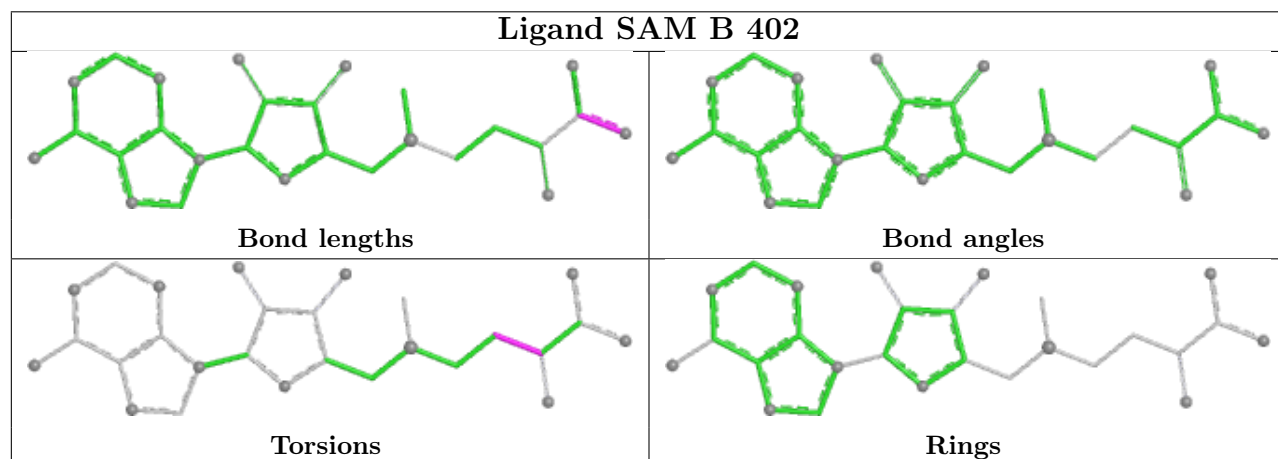
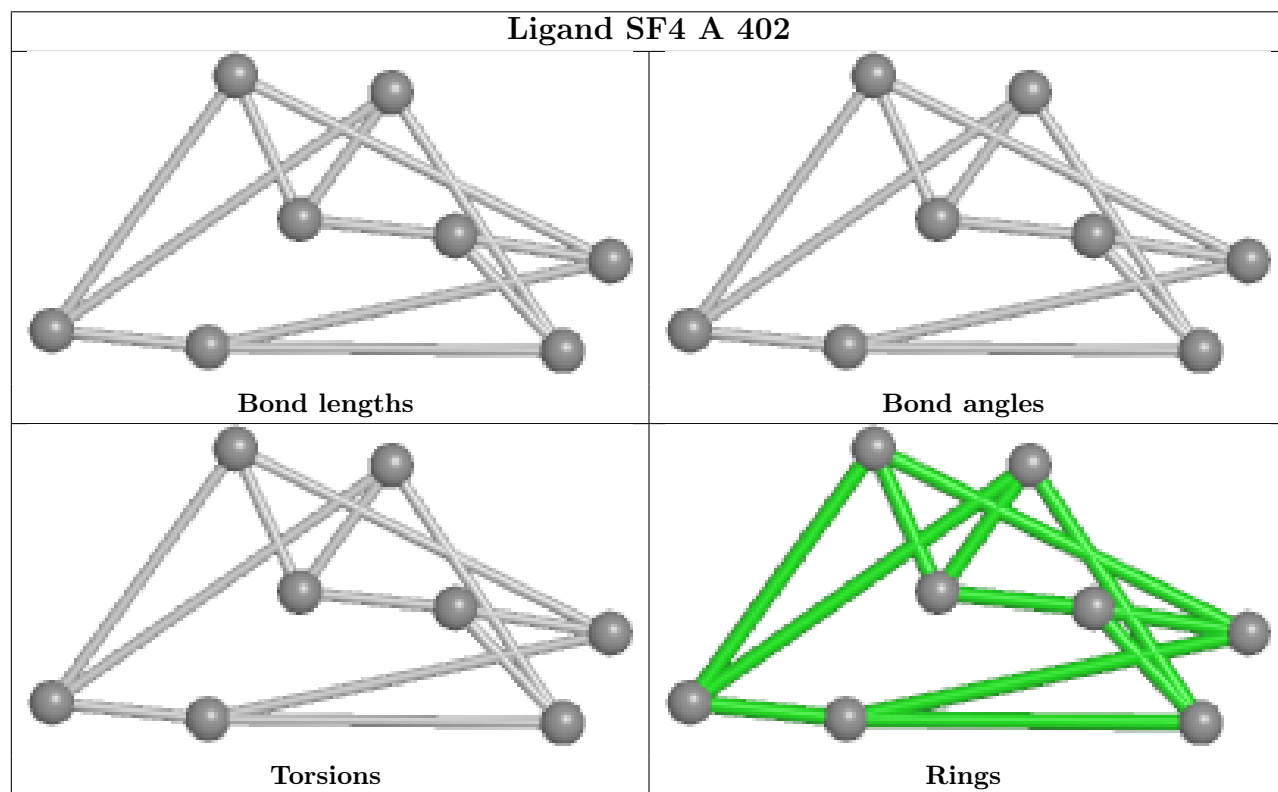
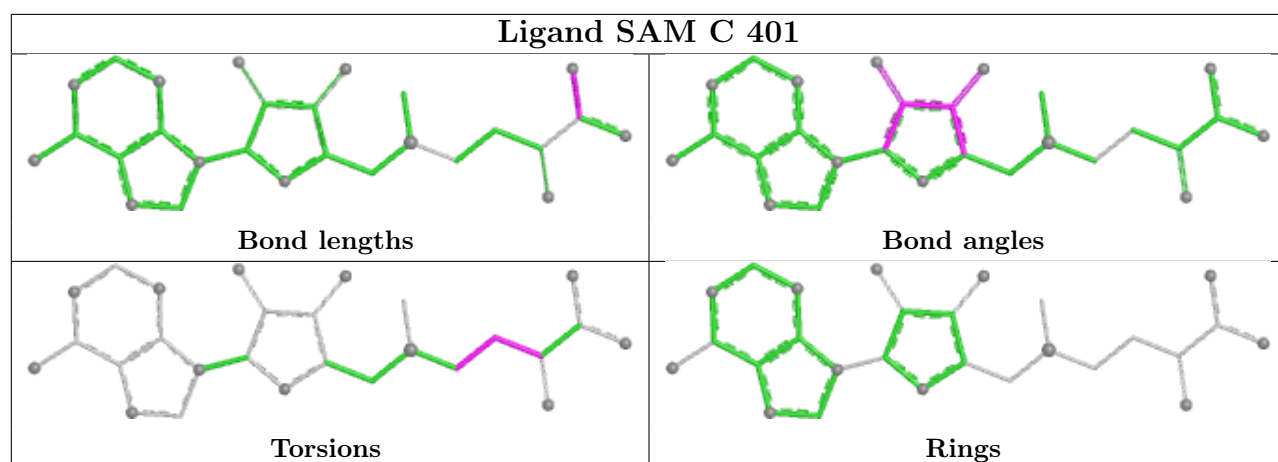
Mol	Chain	Res	Type	Atoms
4	C	401	SAM	N-CA-CB-CG
4	C	401	SAM	C-CA-CB-CG
2	B	403	CTP	PB-O3B-PG-O2G
4	B	402	SAM	C-CA-CB-CG
2	A	401	CTP	PB-O3B-PG-O1G
4	A	403	SAM	C-CA-CB-CG
2	C	402	CTP	PB-O3B-PG-O3G
4	C	401	SAM	CA-CB-CG-SD
4	A	403	SAM	C2'-C1'-N9-C8
4	A	403	SAM	CB-CG-SD-C5'

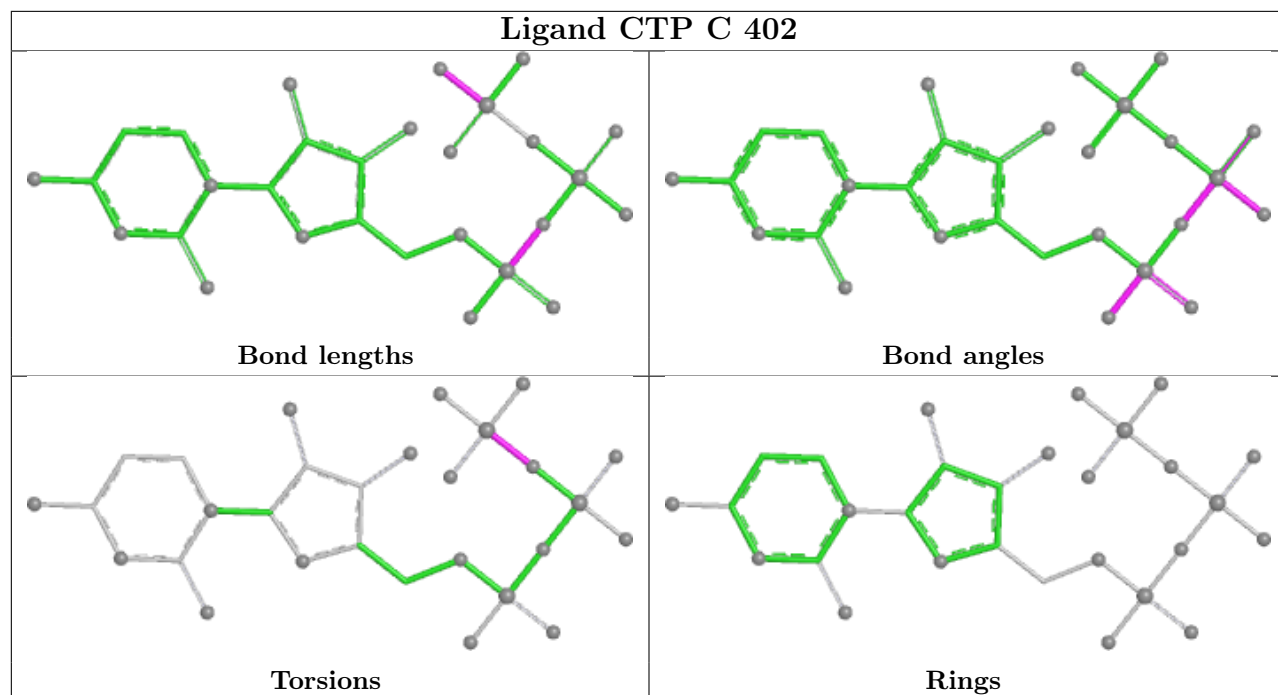
There are no ring outliers.

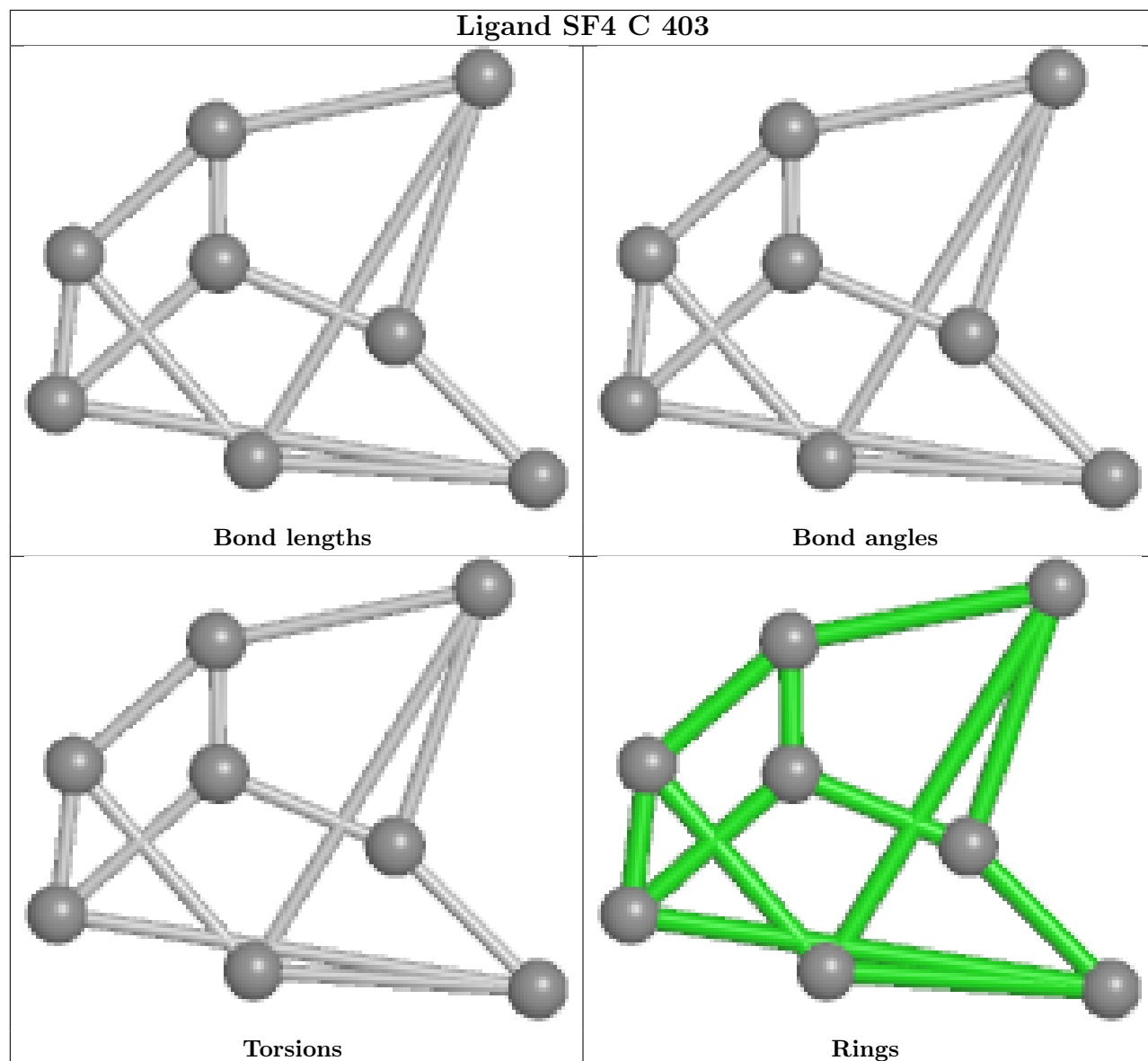
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	SAM	1	0
3	C	403	SF4	2	0
2	B	403	CTP	2	0

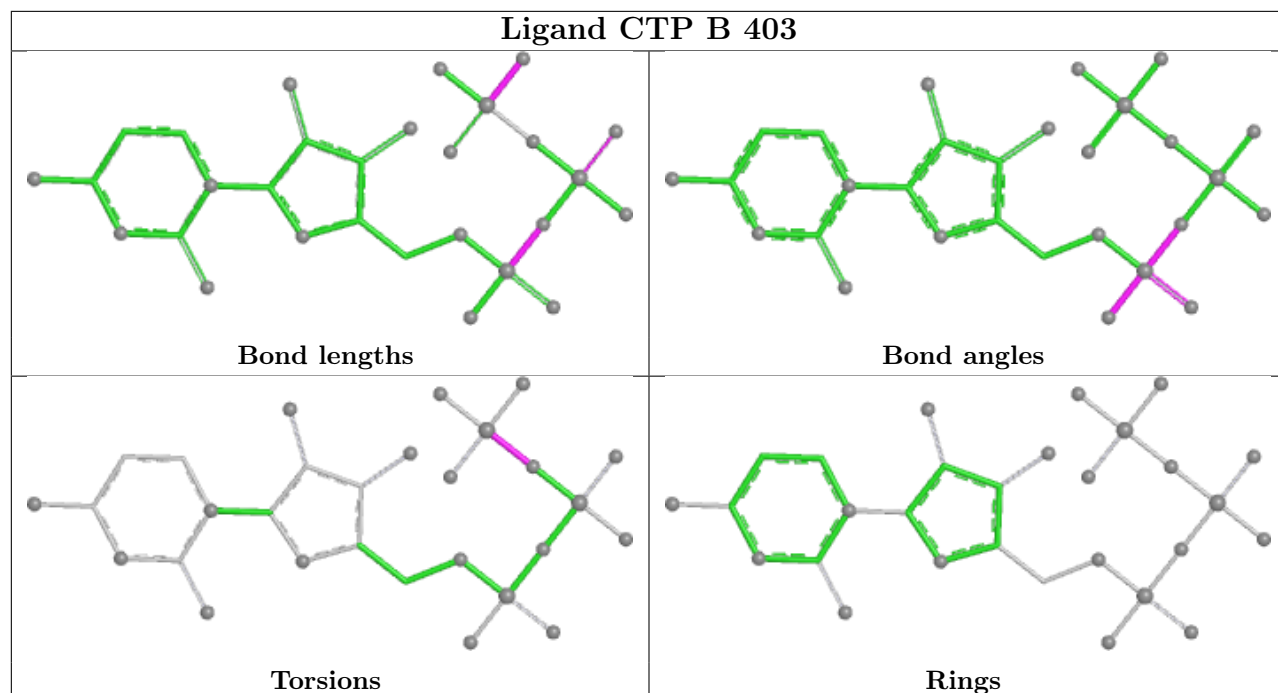
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



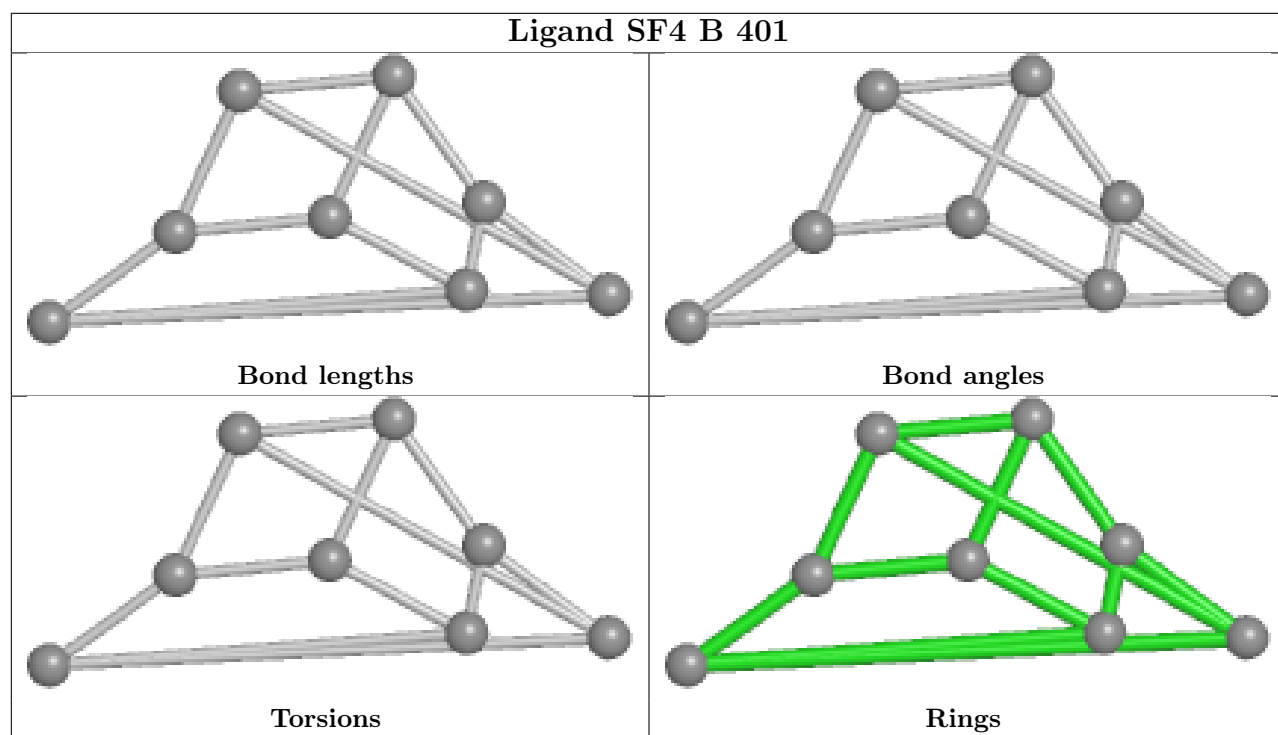


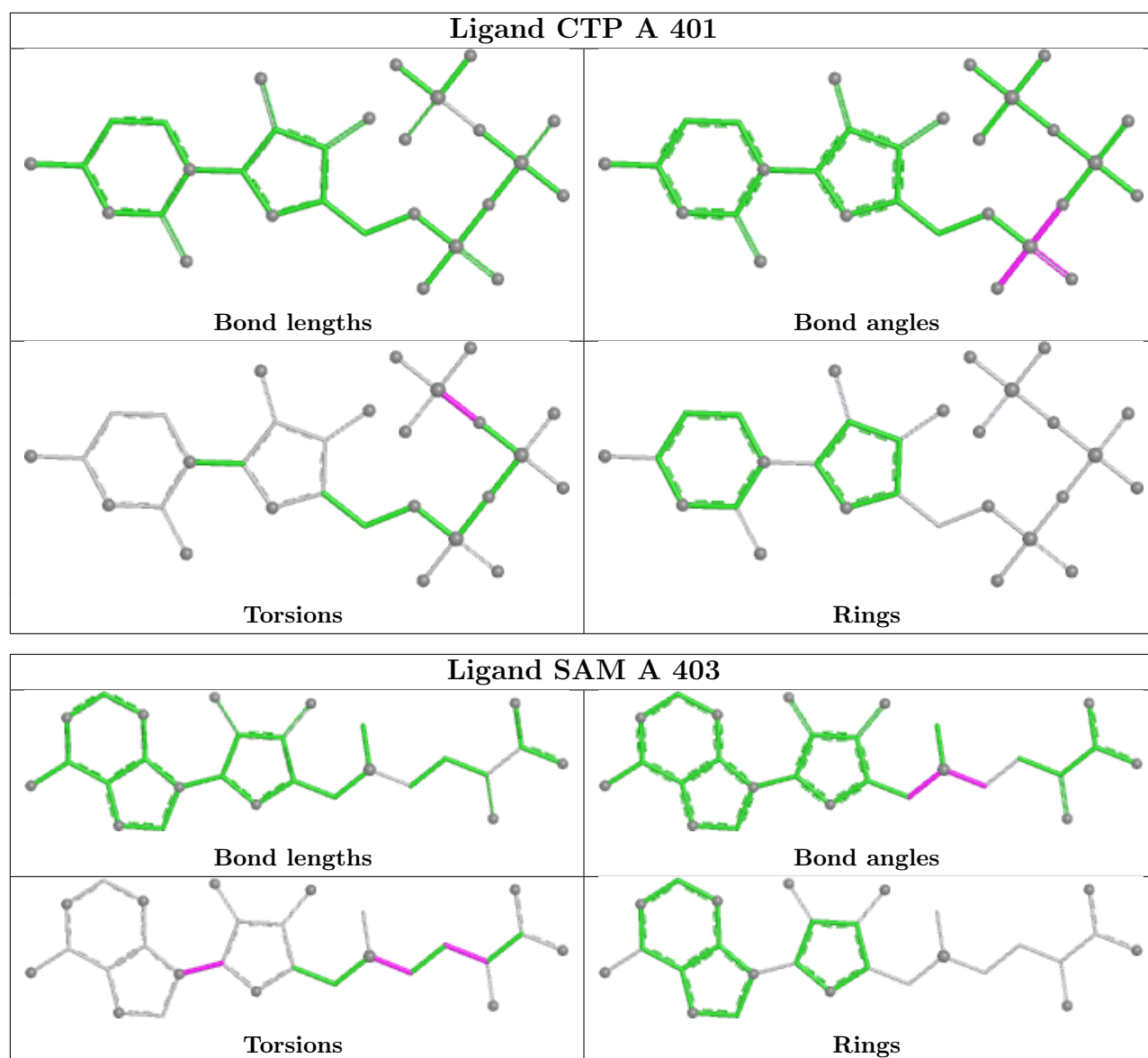


Ligand CTP B 403



Ligand SF4 B 401





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/315 (88%)	1.72	107 (38%) 1 1	25, 44, 77, 92	0
1	B	282/315 (89%)	1.70	109 (38%) 1 1	14, 45, 73, 81	1 (0%)
1	C	276/315 (87%)	3.95	247 (89%) 0 0	24, 69, 118, 134	3 (1%)
All	All	837/945 (88%)	2.45	463 (55%) 0 0	14, 52, 99, 134	4 (0%)

All (463) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	174	LEU	9.5
1	C	129	PHE	9.5
1	C	36	LEU	9.1
1	C	223	PHE	8.8
1	C	137	ILE	8.8
1	C	135	ILE	8.5
1	C	168	VAL	8.4
1	C	233	LEU	8.2
1	C	184	LEU	8.0
1	C	189	TRP	7.9
1	C	148	LEU	7.9
1	C	171	PHE	7.8
1	C	269	VAL	7.5
1	C	167	VAL	7.1
1	C	128	SER	7.1
1	C	37	PHE	7.1
1	C	38	CYS	7.1
1	C	130	ASN	7.0
1	C	132	ALA	7.0
1	C	145	VAL	6.9
1	C	214	THR	6.9
1	C	140	GLY	6.8
1	C	181	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	126	CYS	6.8
1	C	224	CYS	6.8
1	C	149	TYR	6.7
1	C	191	CYS	6.5
1	C	220	PHE	6.5
1	C	175	GLU	6.5
1	C	213	LEU	6.4
1	C	154	TRP	6.3
1	C	31	CYS	6.1
1	C	43	THR	6.1
1	C	215	ILE	6.0
1	C	286	VAL	5.9
1	C	166	THR	5.8
1	C	178	ASN	5.8
1	C	35	CYS	5.7
1	C	136	LYS	5.6
1	C	197	VAL	5.6
1	C	227	HIS	5.6
1	C	133	THR	5.5
1	C	180	HIS	5.5
1	C	266	ILE	5.5
1	C	107[A]	VAL	5.5
1	C	231	THR	5.4
1	C	144	ASN	5.4
1	C	146	GLN	5.4
1	C	210	ALA	5.3
1	C	207	LEU	5.3
1	C	232	CYS	5.2
1	C	271	VAL	5.2
1	C	267	LEU	5.2
1	C	42	ALA	5.2
1	C	186	PRO	5.2
1	A	174	LEU	5.2
1	C	173	HIS	5.1
1	B	174	LEU	5.1
1	C	194	VAL	5.1
1	C	275	LEU	5.1
1	C	127	ASP	5.0
1	C	172	ASN	5.0
1	C	59	LEU	5.0
1	C	151	ILE	5.0
1	B	171	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	177	MET	5.0
1	C	63	ALA	5.0
1	C	39	PHE	5.0
1	C	187	PHE	5.0
1	C	183	ALA	4.9
1	C	164	LEU	4.9
1	C	77	LEU	4.9
1	C	196	ILE	4.9
1	C	234	VAL	4.9
1	C	195	LEU	4.8
1	C	240	LEU	4.8
1	C	226	ARG	4.8
1	C	134	ASN	4.8
1	A	145	VAL	4.8
1	C	294	TRP	4.7
1	C	169	ASN	4.7
1	A	149	TYR	4.6
1	C	278	VAL	4.6
1	C	206	THR	4.6
1	C	19	VAL	4.5
1	C	124	VAL	4.5
1	C	60	LEU	4.5
1	C	139	ARG	4.5
1	C	229	SER	4.4
1	C	208	ARG	4.4
1	C	142	GLY	4.4
1	C	41	THR	4.4
1	B	135	ILE	4.4
1	C	201	ASN	4.4
1	C	176	ASP	4.4
1	C	280	TRP	4.3
1	C	251	TYR	4.3
1	A	132	ALA	4.3
1	C	243	LYS	4.3
1	C	235	PRO	4.3
1	C	147	LYS	4.3
1	C	162	PHE	4.3
1	C	284	ALA	4.3
1	C	212	SER	4.3
1	C	199	GLY	4.3
1	A	171	PHE	4.3
1	C	32	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	160	ILE	4.3
1	B	259	GLY	4.2
1	C	53	ALA	4.2
1	C	40	HIS	4.2
1	C	216	SER	4.2
1	A	135	ILE	4.2
1	C	222	ARG	4.2
1	C	56	GLY	4.2
1	A	269	VAL	4.2
1	C	209	ASN	4.2
1	C	198	THR	4.2
1	C	274	ALA	4.1
1	B	36	LEU	4.1
1	C	270	GLY	4.1
1	A	222	ARG	4.1
1	C	179	ASP	4.1
1	C	93	LEU	4.1
1	A	129	PHE	4.1
1	B	145	VAL	4.1
1	A	154	TRP	4.0
1	C	28[A]	SER	4.0
1	C	170	LYS	4.0
1	C	225	GLU	4.0
1	A	183	ALA	4.0
1	C	125	SER	4.0
1	C	158	TYR	4.0
1	B	17	GLY	4.0
1	A	173	HIS	3.9
1	C	153	SER	3.9
1	C	156	GLN	3.9
1	C	192	PHE	3.9
1	C	58	THR	3.9
1	C	228	SER	3.9
1	A	182	ASN	3.9
1	B	129	PHE	3.9
1	C	205	LYS	3.9
1	C	44	THR	3.8
1	A	181	LEU	3.8
1	C	78	TYR	3.8
1	C	202	ASP	3.8
1	C	218	ASP	3.8
1	C	254	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	297	SER	3.8
1	A	168	VAL	3.8
1	A	36	LEU	3.8
1	C	106	LEU	3.8
1	C	292	TYR	3.8
1	C	103	ASN	3.8
1	C	204	ASP	3.8
1	B	183	ALA	3.8
1	C	262	PRO	3.8
1	A	223	PHE	3.7
1	C	64	GLY	3.7
1	C	211	HIS	3.7
1	C	221	ASP	3.7
1	C	122	LEU	3.7
1	C	138	GLY	3.7
1	C	131	GLU	3.7
1	B	269	VAL	3.7
1	C	47	VAL	3.7
1	C	272	GLN	3.7
1	C	277	ALA	3.7
1	C	289	GLY	3.7
1	C	155	CYS	3.7
1	A	128	SER	3.7
1	C	203	SER	3.7
1	C	86[A]	ILE	3.6
1	C	88	PHE	3.6
1	B	132	ALA	3.6
1	C	104	GLY	3.6
1	A	231	THR	3.6
1	C	182	ASN	3.6
1	C	33	LYS	3.6
1	B	173	HIS	3.6
1	A	133	THR	3.5
1	C	92	THR	3.5
1	C	105	SER	3.5
1	B	215	ILE	3.5
1	C	21	VAL	3.5
1	C	219	GLU	3.5
1	C	217	ASP	3.5
1	C	255	LEU	3.5
1	C	265	SER	3.5
1	C	159	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	141	SER	3.5
1	A	153	SER	3.4
1	C	264	LYS	3.4
1	B	223	PHE	3.4
1	B	213	LEU	3.4
1	B	179	ASP	3.4
1	B	189	TRP	3.4
1	C	283	GLU	3.4
1	C	238	ASN	3.4
1	C	68	ILE	3.4
1	B	273	GLN	3.4
1	C	34	GLU	3.4
1	C	287	GLU	3.4
1	C	50	PRO	3.4
1	C	45	SER	3.4
1	B	216	SER	3.3
1	A	213	LEU	3.3
1	A	233	LEU	3.3
1	B	181	LEU	3.3
1	C	20	PRO	3.3
1	B	178	ASN	3.3
1	B	298	SER	3.3
1	B	220	PHE	3.3
1	C	279	PHE	3.3
1	C	30	LYS	3.2
1	C	61	LYS	3.2
1	A	176	ASP	3.2
1	A	220	PHE	3.2
1	C	285	PHE	3.2
1	A	142	GLY	3.2
1	B	229	SER	3.2
1	C	29	ARG	3.2
1	B	196	ILE	3.2
1	C	121	ILE	3.2
1	C	23	VAL	3.2
1	C	101	VAL	3.2
1	C	143	ASP	3.2
1	A	130	ASN	3.2
1	B	110	GLN	3.2
1	A	229	SER	3.2
1	A	179	ASP	3.2
1	B	143	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	295	ASN	3.1
1	B	222	ARG	3.1
1	A	184	LEU	3.1
1	B	293	ASP	3.1
1	B	168	VAL	3.1
1	B	170	LYS	3.1
1	A	148	LEU	3.1
1	C	242	ALA	3.1
1	A	110	GLN	3.1
1	A	32	ASN	3.1
1	B	182	ASN	3.1
1	C	253	ARG	3.1
1	B	286	VAL	3.1
1	B	142	GLY	3.1
1	A	215	ILE	3.1
1	B	231	THR	3.1
1	C	76	PHE	3.1
1	B	154	TRP	3.0
1	B	156	GLN	3.0
1	C	62	GLN	3.0
1	C	95	LEU	3.0
1	C	268	GLU	3.0
1	A	216	SER	3.0
1	C	111	PHE	3.0
1	A	225	GLU	3.0
1	C	248	LEU	3.0
1	C	165	ASN	3.0
1	B	234	VAL	3.0
1	A	117	ARG	3.0
1	C	119	ILE	3.0
1	C	81	PHE	3.0
1	B	297	SER	2.9
1	C	27	PHE	2.9
1	C	230	GLN	2.9
1	B	214	THR	2.9
1	C	123	ALA	2.9
1	B	140	GLY	2.9
1	B	224	CYS	2.9
1	C	97	SER	2.9
1	C	157	LYS	2.9
1	C	244	SER	2.9
1	B	187	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	158	TYR	2.9
1	A	138	GLY	2.9
1	C	193	GLN	2.9
1	A	143	ASP	2.9
1	C	79	PRO	2.9
1	A	180	HIS	2.9
1	C	46	HIS	2.9
1	A	178	ASN	2.9
1	B	198	THR	2.8
1	A	234	VAL	2.8
1	B	210	ALA	2.8
1	B	136	LYS	2.8
1	C	237	PRO	2.8
1	A	196	ILE	2.8
1	C	55	ARG	2.8
1	A	205	LYS	2.8
1	B	218	ASP	2.8
1	C	80	LYS	2.8
1	A	277	ALA	2.8
1	A	167	VAL	2.8
1	A	59	LEU	2.8
1	B	184	LEU	2.8
1	A	151	ILE	2.8
1	B	137	ILE	2.8
1	A	170	LYS	2.8
1	B	296	LYS	2.8
1	A	189	TRP	2.8
1	A	162	PHE	2.8
1	B	158	TYR	2.8
1	C	51	GLU	2.8
1	C	273	GLN	2.8
1	C	112	LEU	2.8
1	A	227	HIS	2.8
1	A	228	SER	2.8
1	C	83	GLY	2.8
1	A	284	ALA	2.7
1	A	261	GLN	2.7
1	C	110	GLN	2.7
1	C	108	LYS	2.7
1	B	275	LEU	2.7
1	C	293	ASP	2.7
1	B	270	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	239	ARG	2.7
1	B	133	THR	2.7
1	C	22	SER	2.7
1	C	263	SER	2.7
1	C	150	GLU	2.7
1	B	260	GLN	2.7
1	C	120	ASP	2.7
1	B	37	PHE	2.7
1	C	257	ARG	2.7
1	C	246	LEU	2.7
1	C	245	TYR	2.7
1	B	258	ASN	2.7
1	A	226	ARG	2.6
1	B	105	SER	2.6
1	B	130	ASN	2.6
1	C	82	LEU	2.6
1	A	293	ASP	2.6
1	B	153	SER	2.6
1	A	218	ASP	2.6
1	B	233	LEU	2.6
1	B	256	ASP	2.6
1	C	190	LYS	2.6
1	B	226	ARG	2.6
1	C	236	GLU	2.6
1	C	185	GLN	2.6
1	A	212	SER	2.6
1	B	160	ILE	2.6
1	B	172	ASN	2.6
1	A	221	ASP	2.5
1	C	102	THR	2.5
1	C	57	LEU	2.5
1	A	209	ASN	2.5
1	C	25	TYR	2.5
1	A	194	VAL	2.5
1	C	188	ARG	2.5
1	A	160	ILE	2.5
1	A	185	GLN	2.5
1	C	116	GLY	2.5
1	B	227	HIS	2.5
1	B	141	SER	2.5
1	A	286	VAL	2.5
1	B	176	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	32	ASN	2.5
1	C	113	GLN	2.5
1	A	187	PHE	2.5
1	A	235	PRO	2.5
1	B	186	PRO	2.5
1	C	90	LYS	2.4
1	A	204	ASP	2.4
1	A	177	MET	2.4
1	B	155	CYS	2.4
1	B	112	LEU	2.4
1	B	237	PRO	2.4
1	A	94	GLN	2.4
1	C	94	GLN	2.4
1	C	282	GLU	2.4
1	A	146	GLN	2.4
1	B	276	GLN	2.4
1	C	75	PRO	2.4
1	A	164	LEU	2.4
1	B	149	TYR	2.4
1	C	288	ARG	2.4
1	B	212	SER	2.3
1	A	210	ALA	2.3
1	C	249	ASP	2.3
1	B	205	LYS	2.3
1	C	291	ILE	2.3
1	A	172	ASN	2.3
1	A	116	GLY	2.3
1	A	175	GLU	2.3
1	A	257	ARG	2.3
1	A	159	ASP	2.3
1	B	274	ALA	2.3
1	A	106	LEU	2.3
1	A	156	GLN	2.3
1	A	230	GLN	2.3
1	A	276	GLN	2.3
1	B	261	GLN	2.3
1	B	283	GLU	2.3
1	C	109	GLU	2.3
1	B	148	LEU	2.3
1	B	107	VAL	2.3
1	B	62	GLN	2.2
1	C	91	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	224	CYS	2.2
1	B	239	ARG	2.2
1	B	59	LEU	2.2
1	B	203	SER	2.2
1	C	49	LYS	2.2
1	C	114	LYS	2.2
1	B	162	PHE	2.2
1	C	252	MET	2.2
1	B	266	ILE	2.2
1	C	18	GLN	2.2
1	C	100	ILE	2.2
1	C	276	GLN	2.2
1	A	211	HIS	2.2
1	B	271	VAL	2.2
1	A	169	ASN	2.2
1	B	128	SER	2.2
1	B	264	LYS	2.2
1	A	259	GLY	2.2
1	A	150	GLU	2.2
1	B	194	VAL	2.2
1	A	141	SER	2.2
1	C	65	MET	2.2
1	B	138	GLY	2.2
1	B	166	THR	2.2
1	B	131	GLU	2.1
1	A	199	GLY	2.1
1	A	28	SER	2.1
1	B	221	ASP	2.1
1	C	281	ASP	2.1
1	A	268	GLU	2.1
1	B	291	ILE	2.1
1	B	108	LYS	2.1
1	B	157	LYS	2.1
1	B	146	GLN	2.1
1	A	37	PHE	2.1
1	A	17	GLY	2.1
1	A	136	LYS	2.1
1	B	277	ALA	2.1
1	A	134	ASN	2.1
1	C	118	ASN	2.1
1	A	272	GLN	2.1
1	A	267	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	137	ILE	2.1
1	B	268	GLU	2.0
1	C	200	GLU	2.0
1	B	272	GLN	2.0
1	C	256	ASP	2.0
1	B	207	LEU	2.0
1	A	206	THR	2.0
1	A	108	LYS	2.0
1	A	186	PRO	2.0
1	C	66	LYS	2.0
1	A	51	GLU	2.0
1	B	51	GLU	2.0
1	A	270	GLY	2.0
1	B	177	MET	2.0
1	C	73	GLY	2.0
1	A	266	ILE	2.0
1	B	111	PHE	2.0
1	B	217	ASP	2.0
1	A	157	LYS	2.0
1	B	180	HIS	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

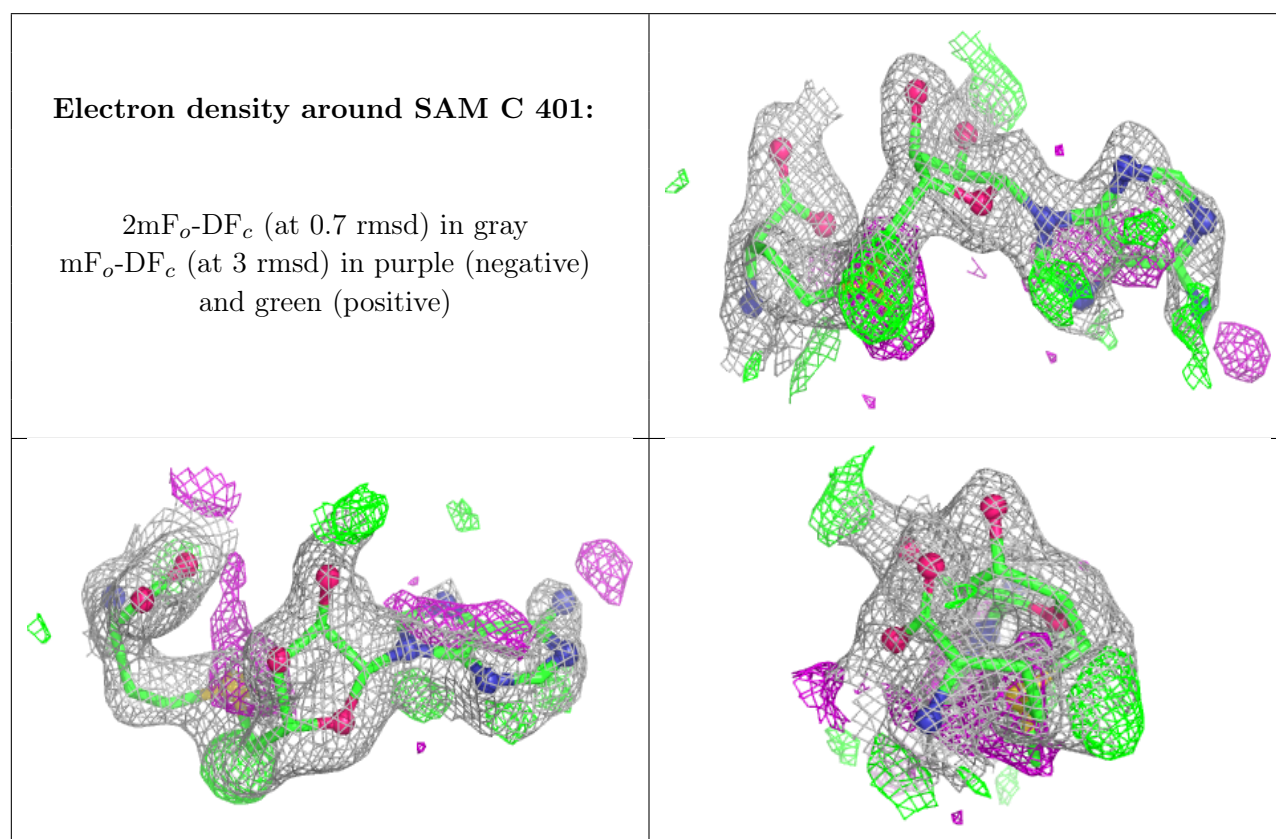
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SAM	C	401	27/27	0.73	0.22	46,51,60,64	0
3	SF4	C	403	8/8	0.87	0.16	56,61,65,67	0
4	SAM	B	402	27/27	0.89	0.12	27,31,38,40	0

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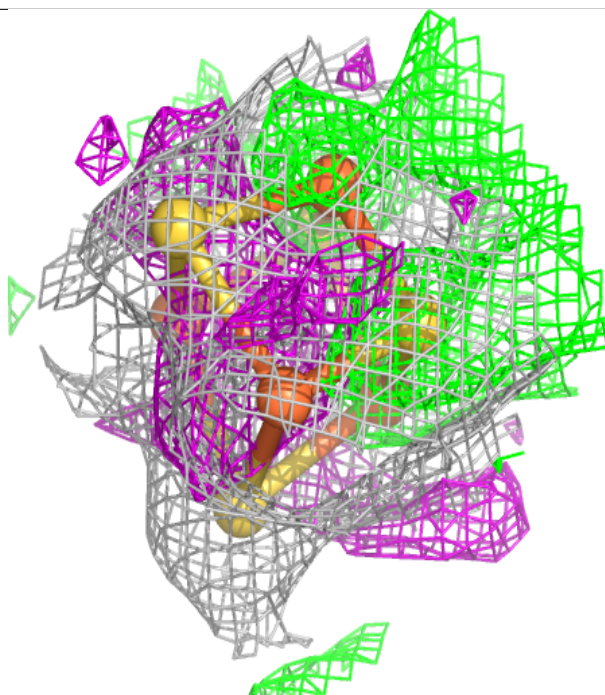
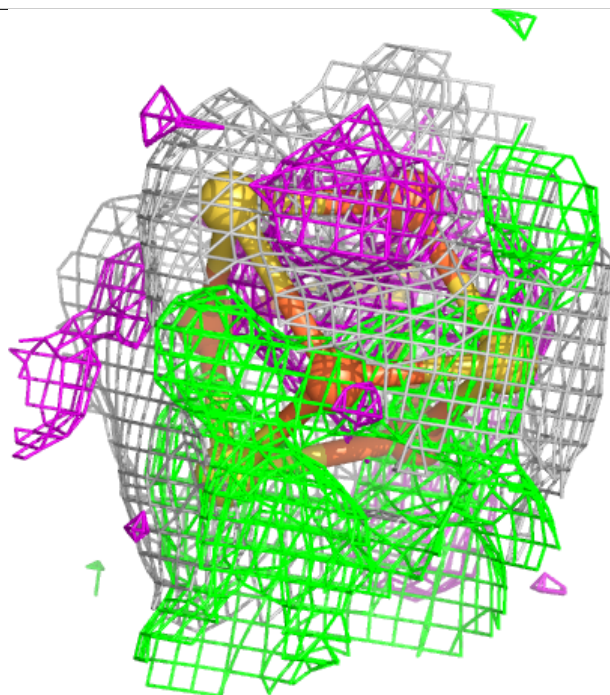
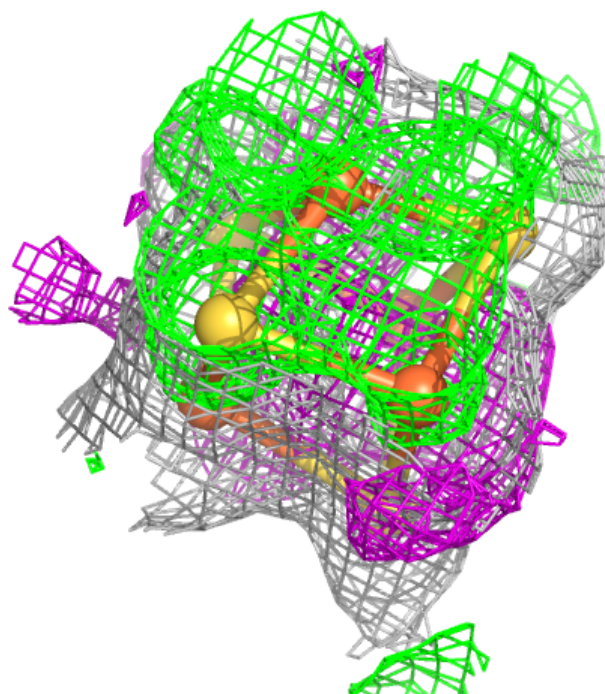
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SAM	A	403	27/27	0.92	0.10	27,31,35,37	0
2	CTP	C	402	29/29	0.95	0.11	40,43,49,51	0
2	CTP	B	403	29/29	0.96	0.08	26,29,33,36	0
2	CTP	A	401	29/29	0.96	0.08	25,27,30,32	0
3	SF4	A	402	8/8	0.99	0.04	30,33,36,36	0
3	SF4	B	401	8/8	0.99	0.04	31,34,36,37	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.



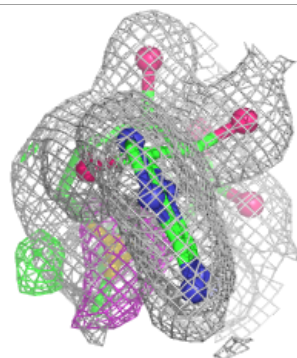
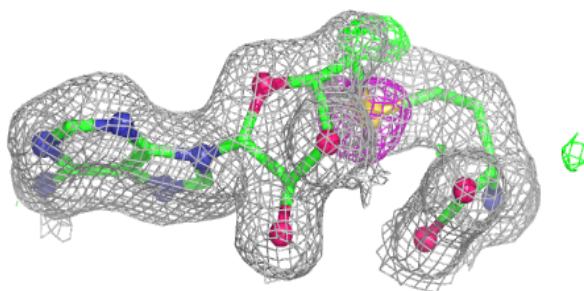
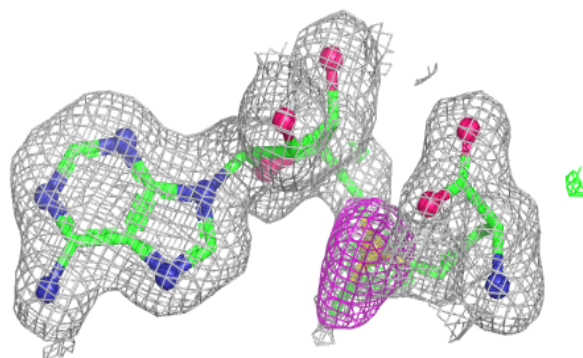
Electron density around SF4 C 403:

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

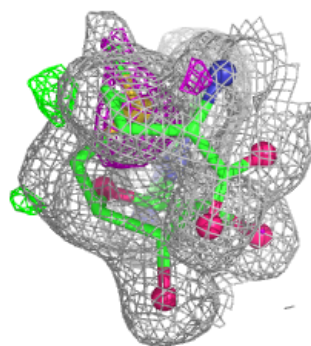
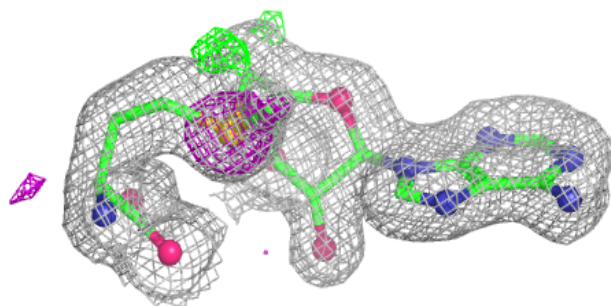
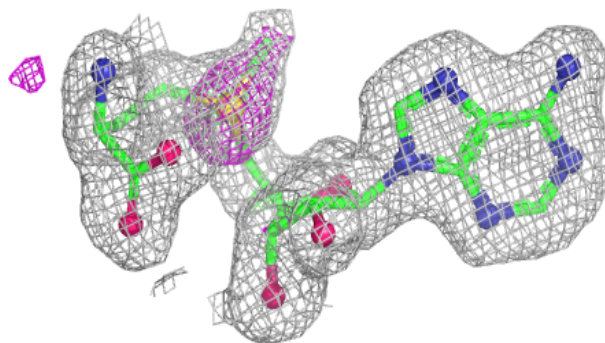


Electron density around SAM B 402:

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

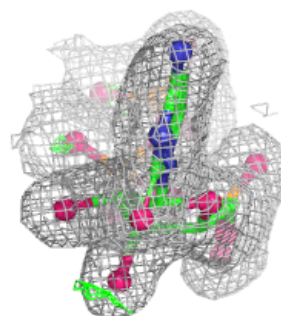
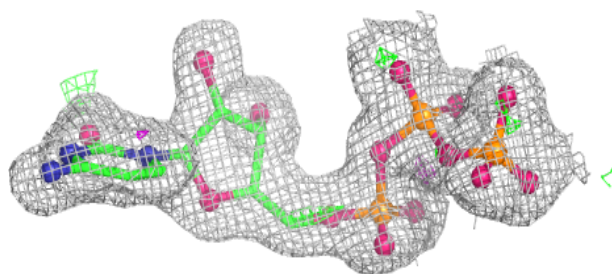
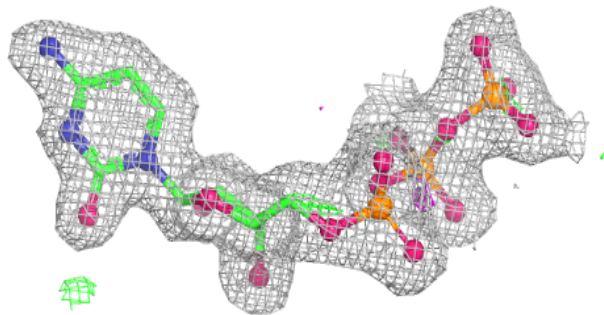
**Electron density around SAM A 403:**

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

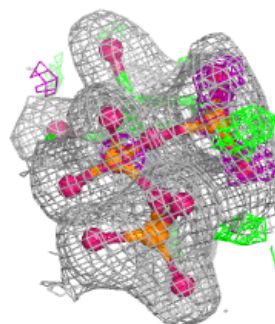
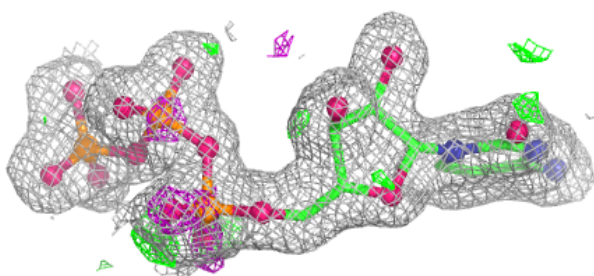
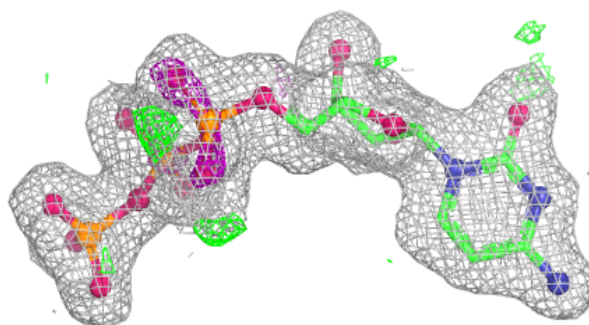


Electron density around CTP C 402:

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

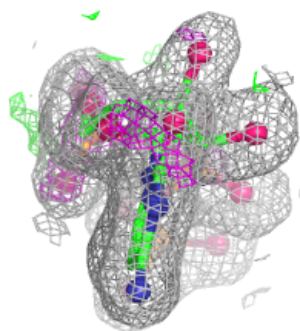
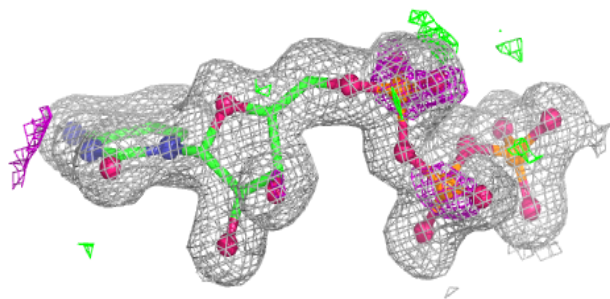
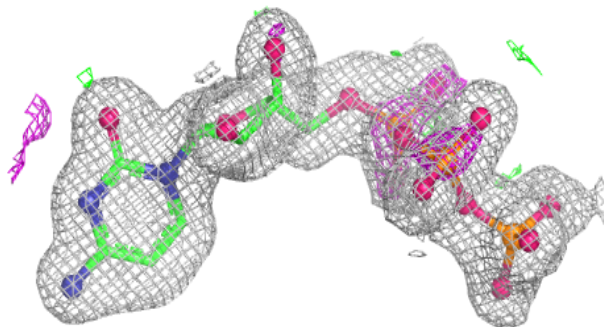
**Electron density around CTP B 403:**

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



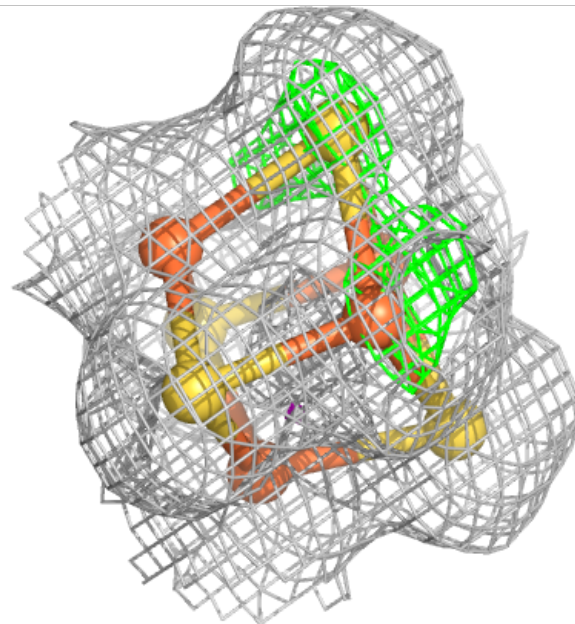
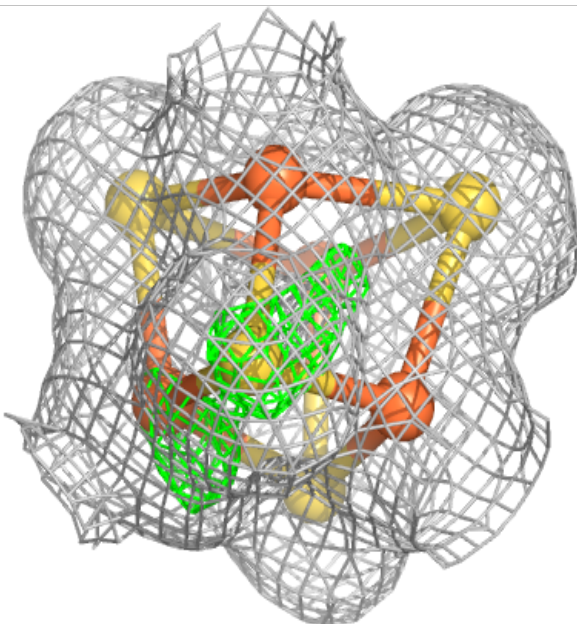
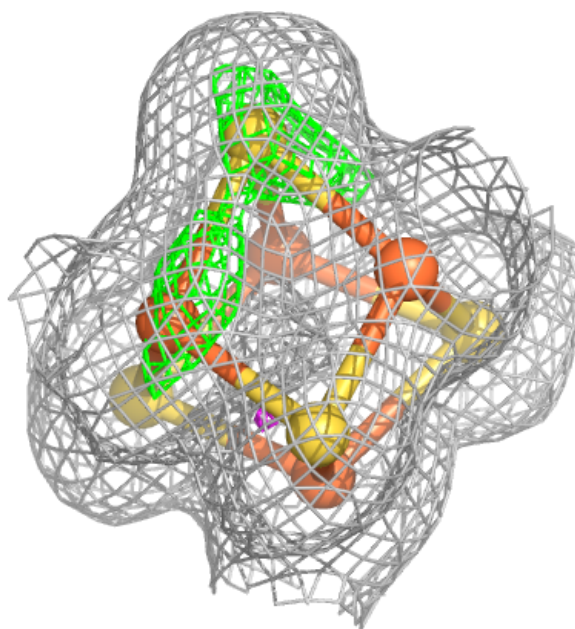
Electron density around CTP A 401:

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



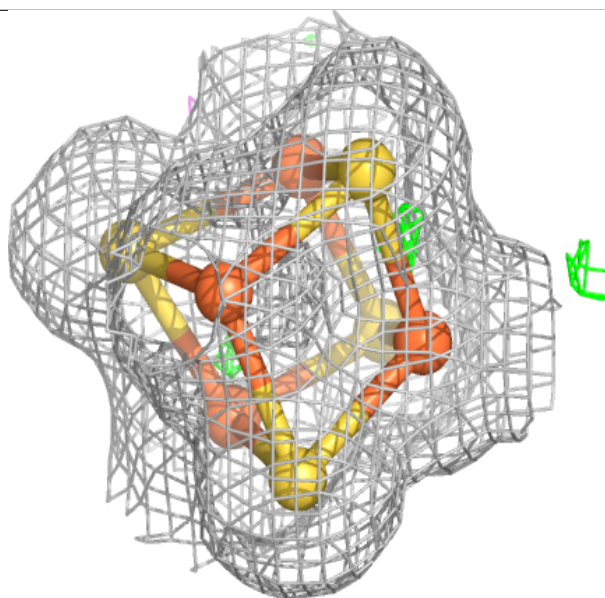
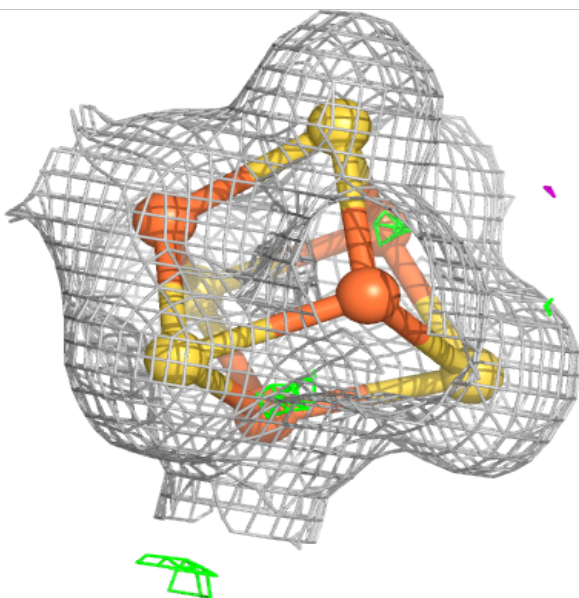
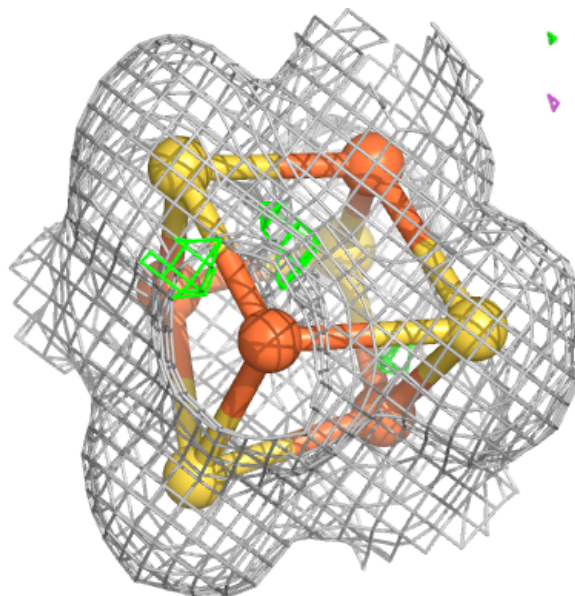
Electron density around SF4 A 402:

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 SF4 B 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.