



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2025 – 12:06 PM EST

PDB ID : 9DGW
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 4.02b-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

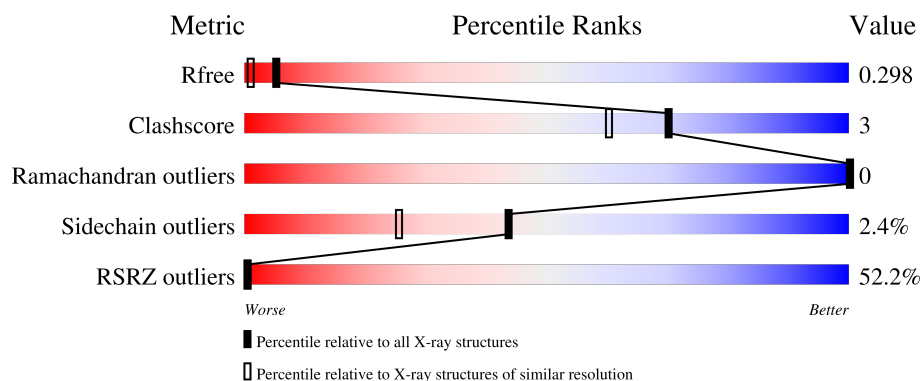
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	164625	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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>30%</div> <div>80%</div> <div>8%</div> <div>11%</div> </div>
1	B	315	<div> <div>32%</div> <div>82%</div> <div>7%</div> <div>10%</div> </div>
1	C	315	<div> <div>77%</div> <div>77%</div> <div>11%</div> <div>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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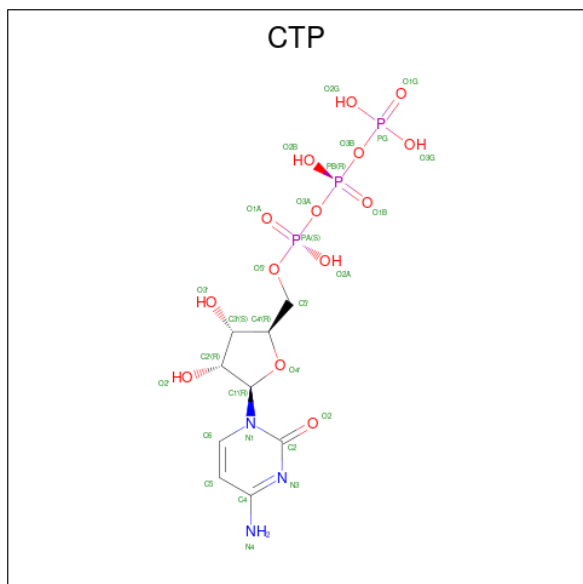
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	initiating methionine	UNP G9MQB8
B	-5	HIS	-	expression tag	UNP G9MQB8
B	-4	HIS	-	expression tag	UNP G9MQB8
B	-3	HIS	-	expression tag	UNP G9MQB8
B	-2	HIS	-	expression tag	UNP G9MQB8
B	-1	HIS	-	expression tag	UNP G9MQB8
B	0	HIS	-	expression tag	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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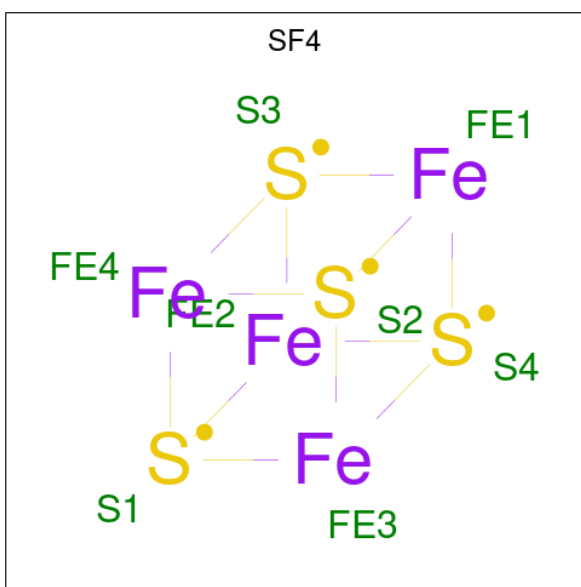
Chain	Residue	Modelled	Actual	Comment	Reference
C	13	PHE	-	expression tag	UNP G9MQB8
C	14	GLN	-	expression tag	UNP G9MQB8
C	15	SER	-	expression tag	UNP G9MQB8
C	16	MET	-	expression tag	UNP G9MQB8

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



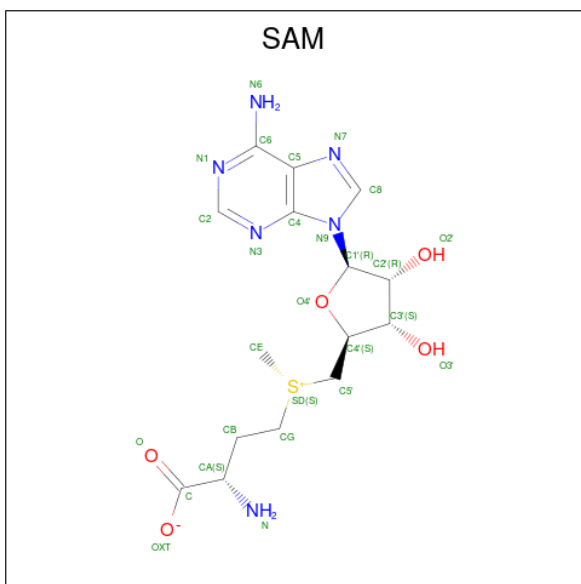
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

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



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

- Molecule 4 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
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		

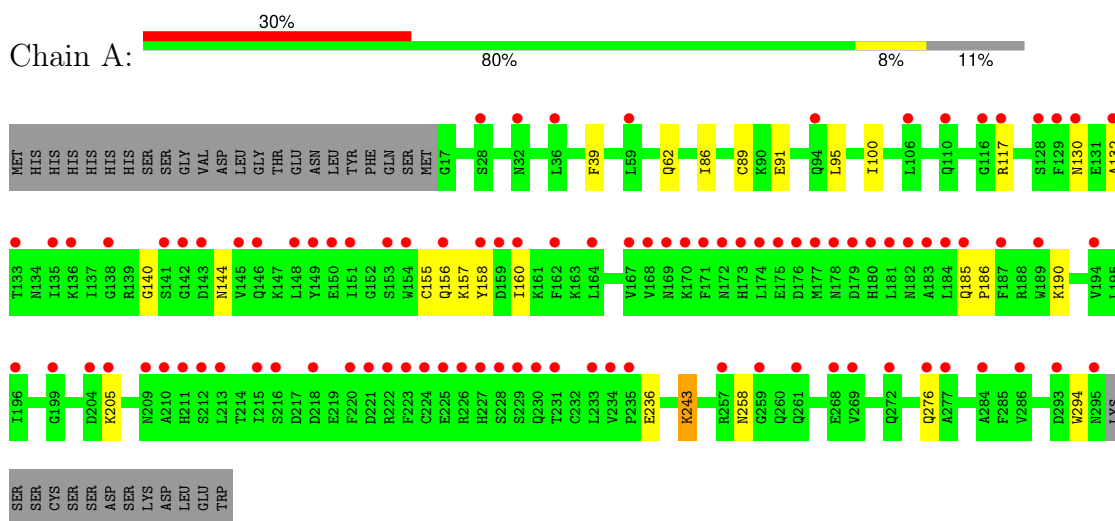
- Molecule 5 is water.

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		

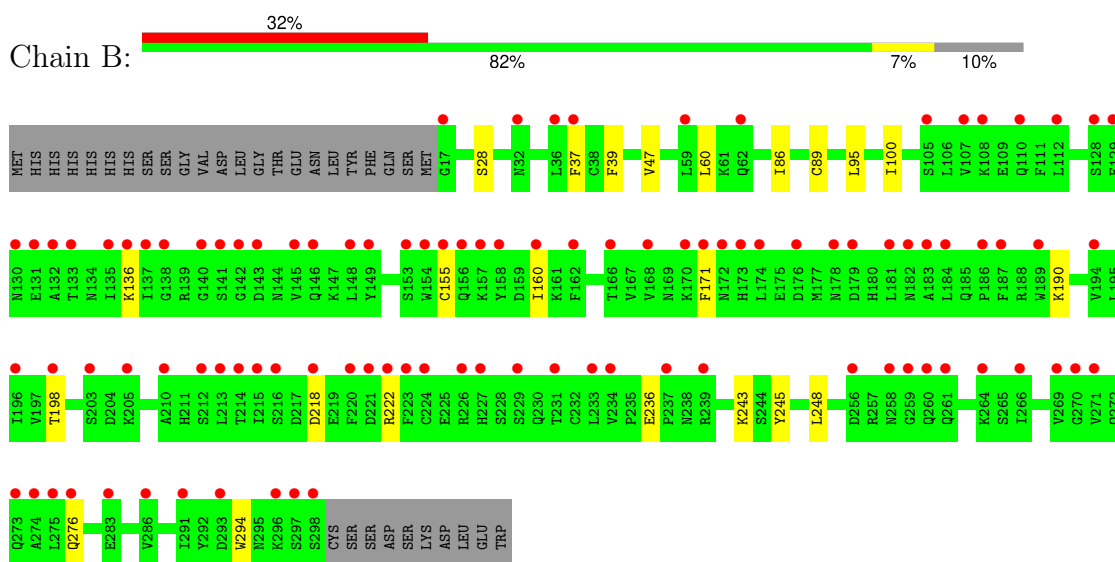
3 Residue-property plots

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.

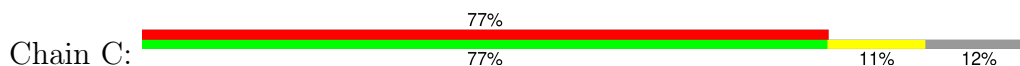
- Molecule 1: Radical SAM core domain-containing protein



- Molecule 1: Radical SAM core domain-containing protein



- Molecule 1: Radical SAM core domain-containing protein



ASP	ASP	W241	L181	I121	K64	MET
SER	N182	A242	N183	L122	R55	HIS
LYS	A183	K243	A184	A123	G56	HIS
ASP	L184	S244	Q185	V124	L57	HIS
LEU	Q186	Y245	P186	S125	T58	HIS
GLU	L246	L247	F187	C126	L59	HIS
TRP	L248	L249	R188	D127	L60	HIS
	D249	E250	W189	S128	K61	SER
	E250	K190	K190	F129	Q62	SER
	Y251	C191	C191	N130	A63	SER
	M252	F192	F192	A132	G64	GLY
	R253	Q193	Q193	T133	M65	ASP
	F254	V194	V194	N134	LEU	ASP
	L255	L195	L195	I135	GLY	LEU
	D256	I196	I196	K136	THR	GLY
	R257	T198	V197	I137	P75	THR
	ASN	G199	T198	G138	F76	GLU
	GLY	E200	G199	R139	L77	ASN
	GLN	H201	E200	G140	Y78	LEU
	GLN	D202	D202	S141	P79	TYR
	P262	S203	S203	G142	K90	PHE
	S263	D204	D204	D143	F81	GLN
	K264	K205	K205	N144	L82	SER
	S265	T206	T206	V145	G83	MET
	L266	L207	L207	Q146		GLY
	L267	R208	R208	K147	I86	Q18
	E268	V269	V269	L148	D87	V19
	V270	Q270	Q270	Y149	F88	P20
	Q271	H211	H211	E150	C89	V21
	Q272	S212	S212	I151	K90	S22
	Q273	L213	L213	G152	E91	V23
	A274	T214	T214	S153	T92	N24
	L275	L215	L215	W154	L93	Y25
	Q276	S216	S216	C155	Q94	H26
	A277	D217	D217	Q156	L95	F27
	A278	D218	D218	E96	S28	S28
	V279	E219	E219	K157	R29	K29
	W280	F220	F220	Y158	K30	K30
	D281	D221	D221	D159	C31	C31
	E282	R222	R222	I160	N32	N32
	E283	F223	F223	K161	K33	K33
	A284	C224	C224	F162	E34	E34
	F285	E225	E225	K163	C35	C35
	V286	R226	R226	L164	L36	L36
	E287	H227	H227	N165	F37	F37
	R288	S228	S228	T166	S105	C38
	Q289	Q229	Q229	V167	F39	F39
	Q290	Q230	Q230	V168	H40	H40
	T291	T231	T231	M169	T41	T41
	Y292	C232	C232	K170	A42	A42
	D293	L233	L233	F171	T43	T43
	Y294	V234	V234	M172	T44	T44
	S297	P235	P235	H173	S45	S45
	SER	E236	E236	H174	H46	H46
	SER	F237	F237	L174	V47	V47
	CYS	R238	R238	E175	E48	E48
	SER	R239	R239	D176	G116	G116
	SER	L240	L240	M177	R117	K49
				M178	N118	P50
				D179	I119	E51
				H180	D120	N52
						A53

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	4492 reflections (4.95%)	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 , 30.9	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, SAM, SF4

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	0.42	0/2298	0.71	0/3098
1	B	0.42	0/2325	0.70	0/3133
1	C	0.38	0/2290	0.68	1/3086 (0.0%)
All	All	0.41	0/6913	0.69	1/9317 (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	C	288	ARG	NE-CZ-NH2	-5.09	117.76	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	2250	0	2197	13	0
1	B	2277	0	2224	12	0
1	C	2243	0	2196	18	0
2	A	29	0	12	0	0
2	B	29	0	12	1	0
2	C	29	0	12	0	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	45	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 45 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

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	277/315 (88%)	270 (98%)	7 (2%)	0	100	100
1	B	281/315 (89%)	275 (98%)	6 (2%)	0	100	100
1	C	275/315 (87%)	268 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	244 (98%)	6 (2%)	44	25
1	B	254/284 (89%)	248 (98%)	6 (2%)	44	25
1	C	249/284 (88%)	243 (98%)	6 (2%)	44	25
All	All	753/852 (88%)	735 (98%)	18 (2%)	44	25

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	198	THR
1	C	294	TRP
1	C	243	LYS
1	B	198	THR
1	C	136	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	276	GLN
1	C	110	GLN
1	C	273	GLN
1	A	238	ASN
1	A	62	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
2	CTP	A	401	-	29,30,30	0.80	0	43,47,47	0.96	2 (4%)
4	SAM	C	401	3	23,29,29	0.89	1 (4%)	20,42,42	1.11	2 (10%)
3	SF4	A	402	4,1	0,12,12	-	-	-		
3	SF4	C	403	4,1	0,12,12	-	-	-		
3	SF4	B	401	4,1	0,12,12	-	-	-		
4	SAM	B	402	3	23,29,29	0.86	1 (4%)	20,42,42	0.77	0
4	SAM	A	403	3	23,29,29	0.78	1 (4%)	20,42,42	1.00	1 (5%)
2	CTP	B	403	-	29,30,30	1.04	3 (10%)	43,47,47	1.08	2 (4%)
2	CTP	C	402	-	29,30,30	1.02	2 (6%)	43,47,47	0.99	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTP	A	401	-	-	1/22/38/38	0/2/2/2
4	SAM	C	401	3	-	3/13/33/33	0/3/3/3
3	SF4	A	402	4,1	-	-	0/6/5/5
3	SF4	C	403	4,1	-	-	0/6/5/5
3	SF4	B	401	4,1	-	-	0/6/5/5
4	SAM	B	402	3	-	1/13/33/33	0/3/3/3
4	SAM	A	403	3	-	2/13/33/33	0/3/3/3
2	CTP	B	403	-	-	1/22/38/38	0/2/2/2
2	CTP	C	402	-	-	1/22/38/38	0/2/2/2

The worst 5 of 8 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
4	A	403	SAM	C8-N7	-2.29	1.30	1.34

The worst 5 of 10 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

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

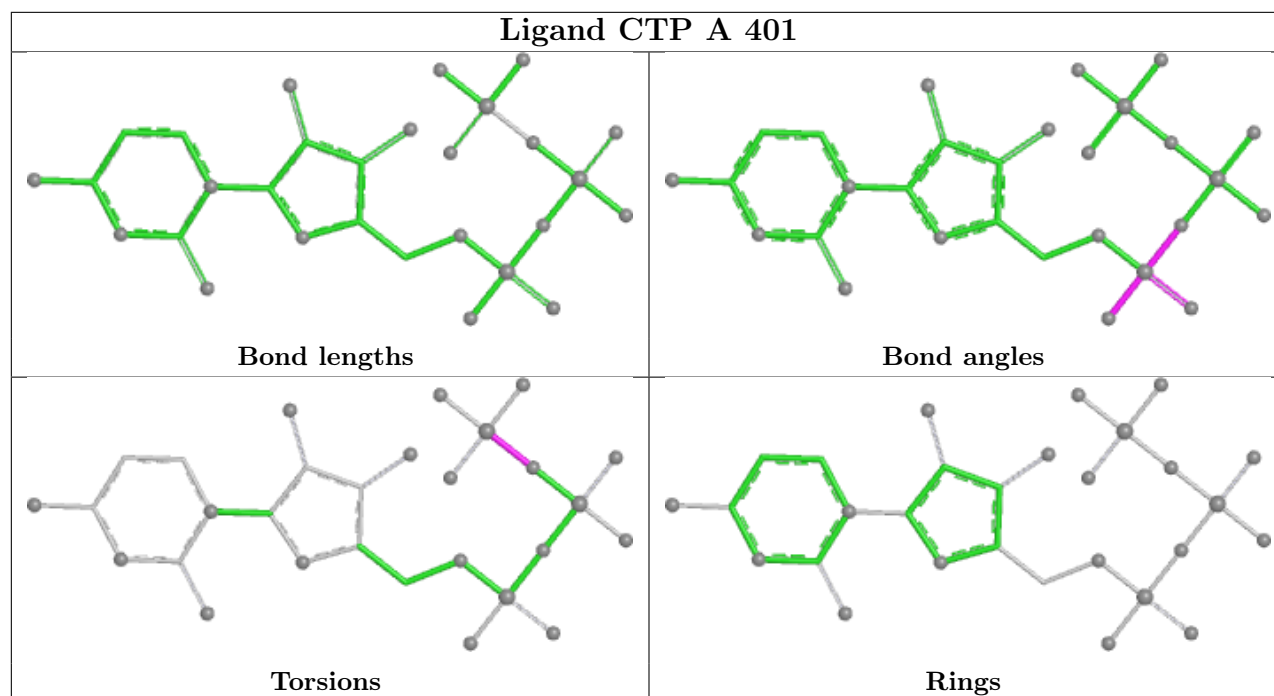
Mol	Chain	Res	Type	Atoms
4	C	401	SAM	N-CA-CB-CG
4	C	401	SAM	C-CA-CB-CG
2	B	403	CTP	PB-O3B-PG-O2G
4	B	402	SAM	C-CA-CB-CG
2	A	401	CTP	PB-O3B-PG-O1G

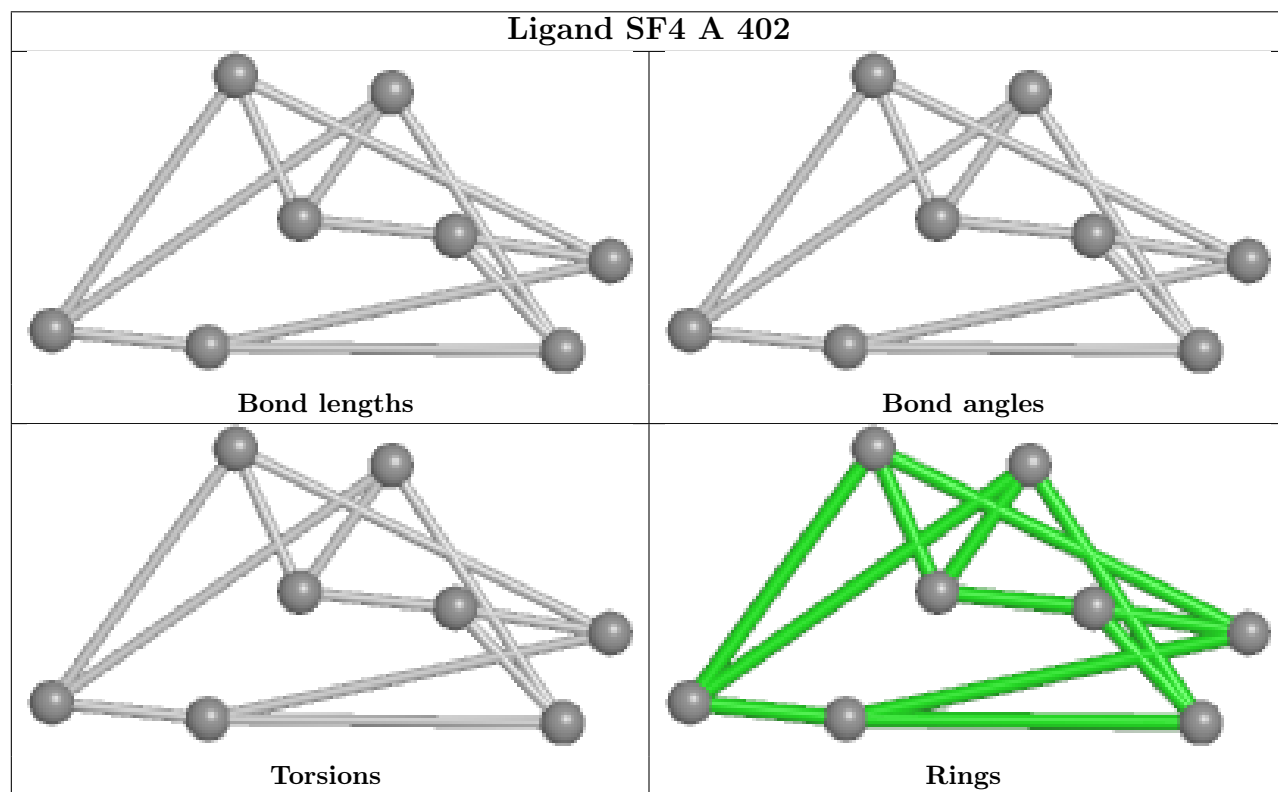
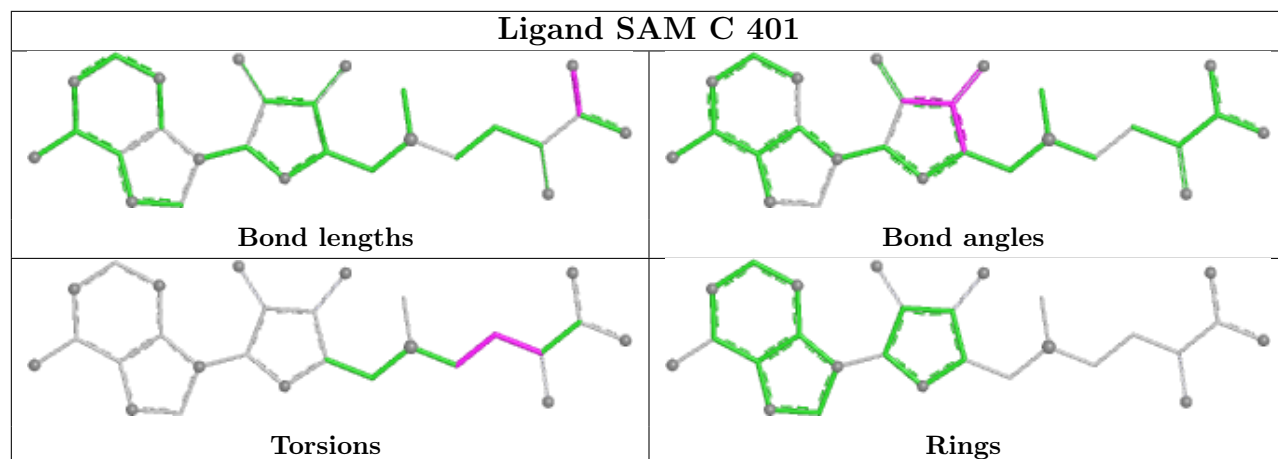
There are no ring outliers.

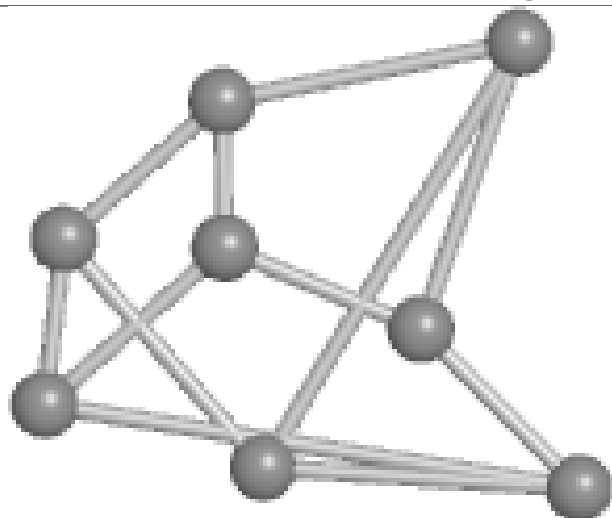
3 monomers are involved in 3 short contacts:

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

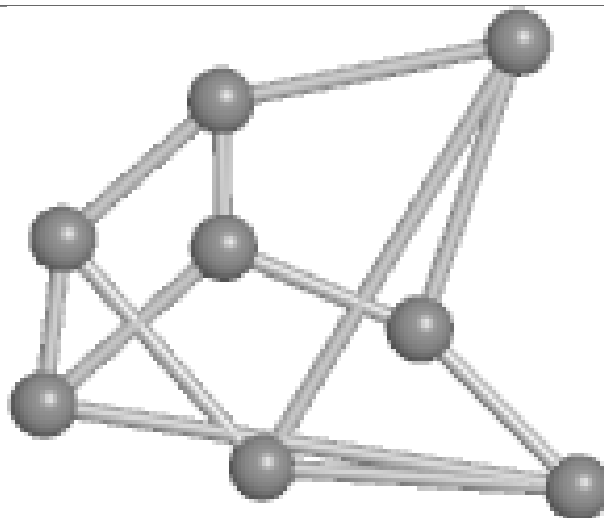
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



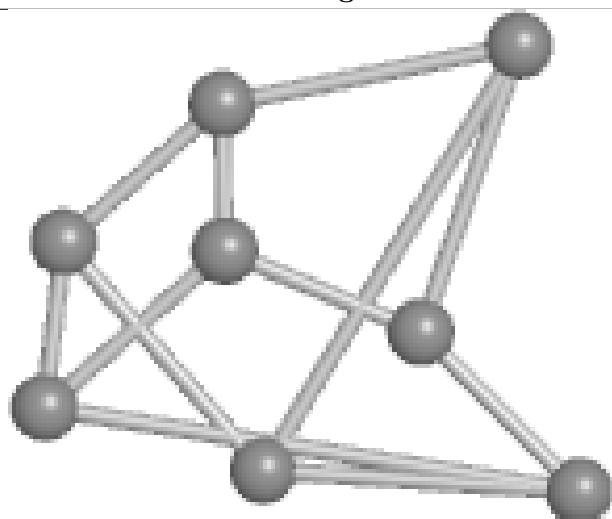


Ligand SF4 C 403

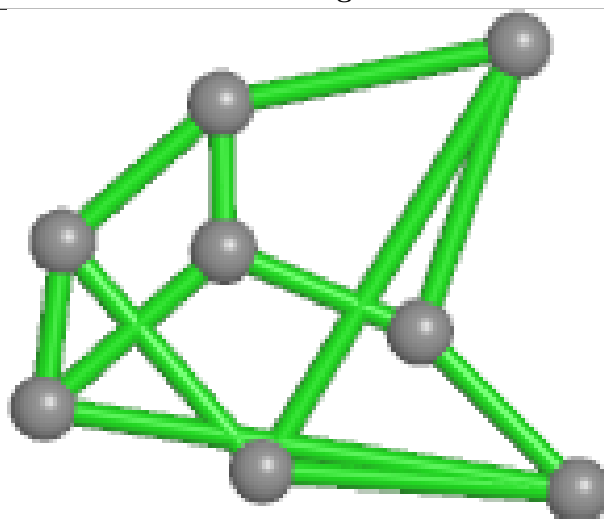
Bond lengths



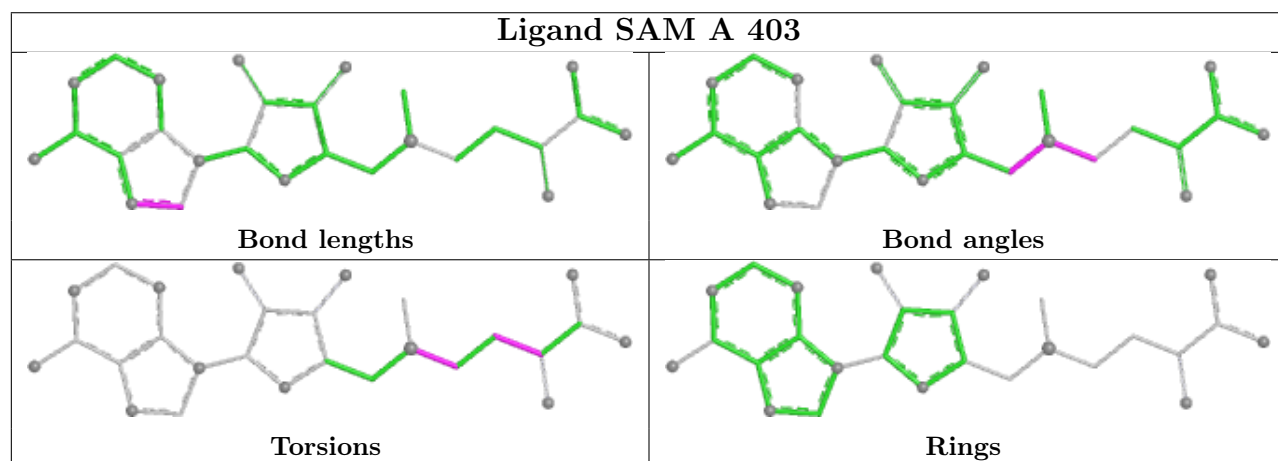
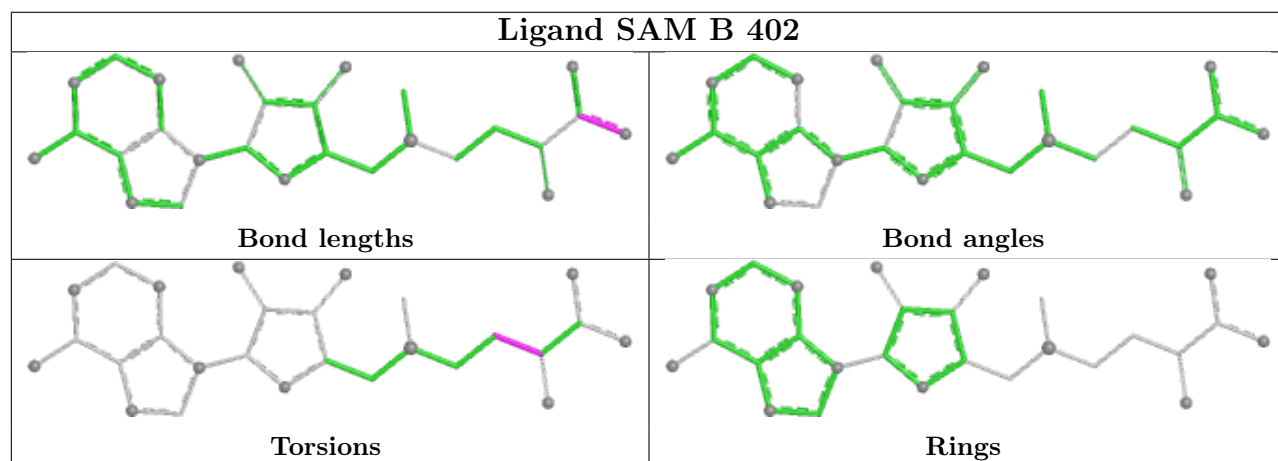
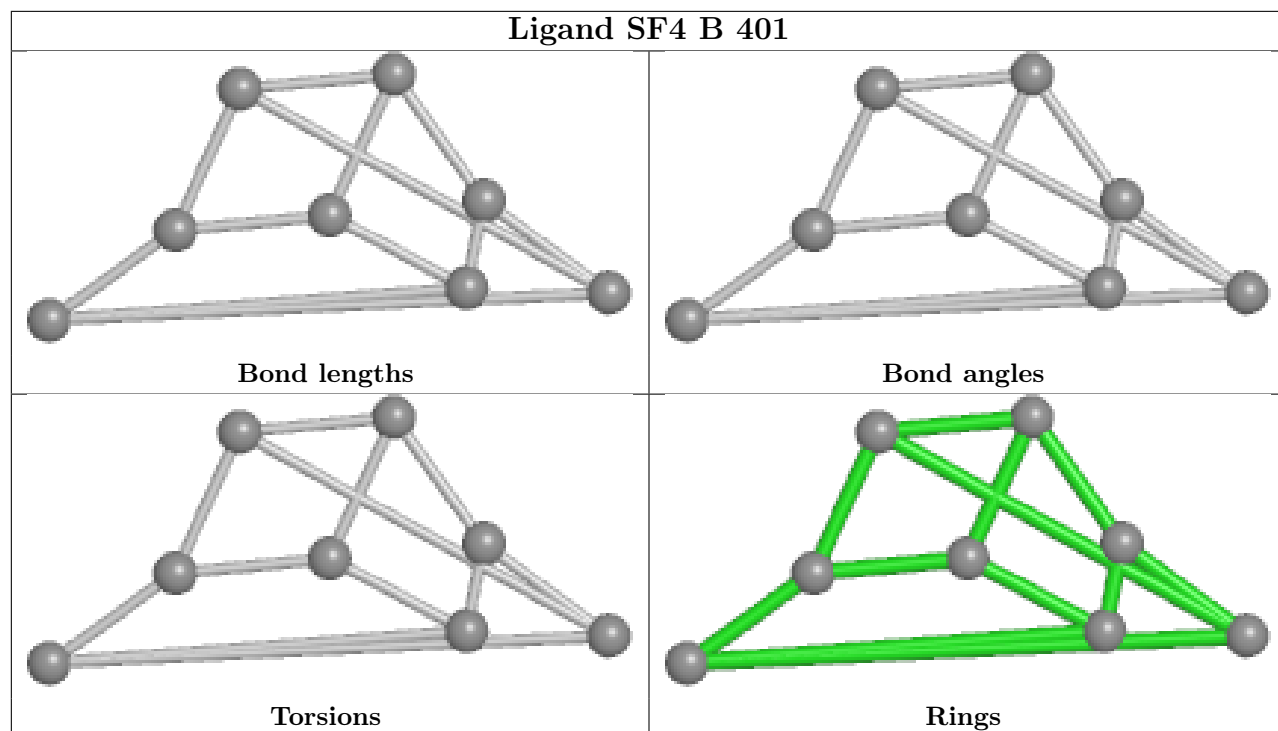
Bond angles

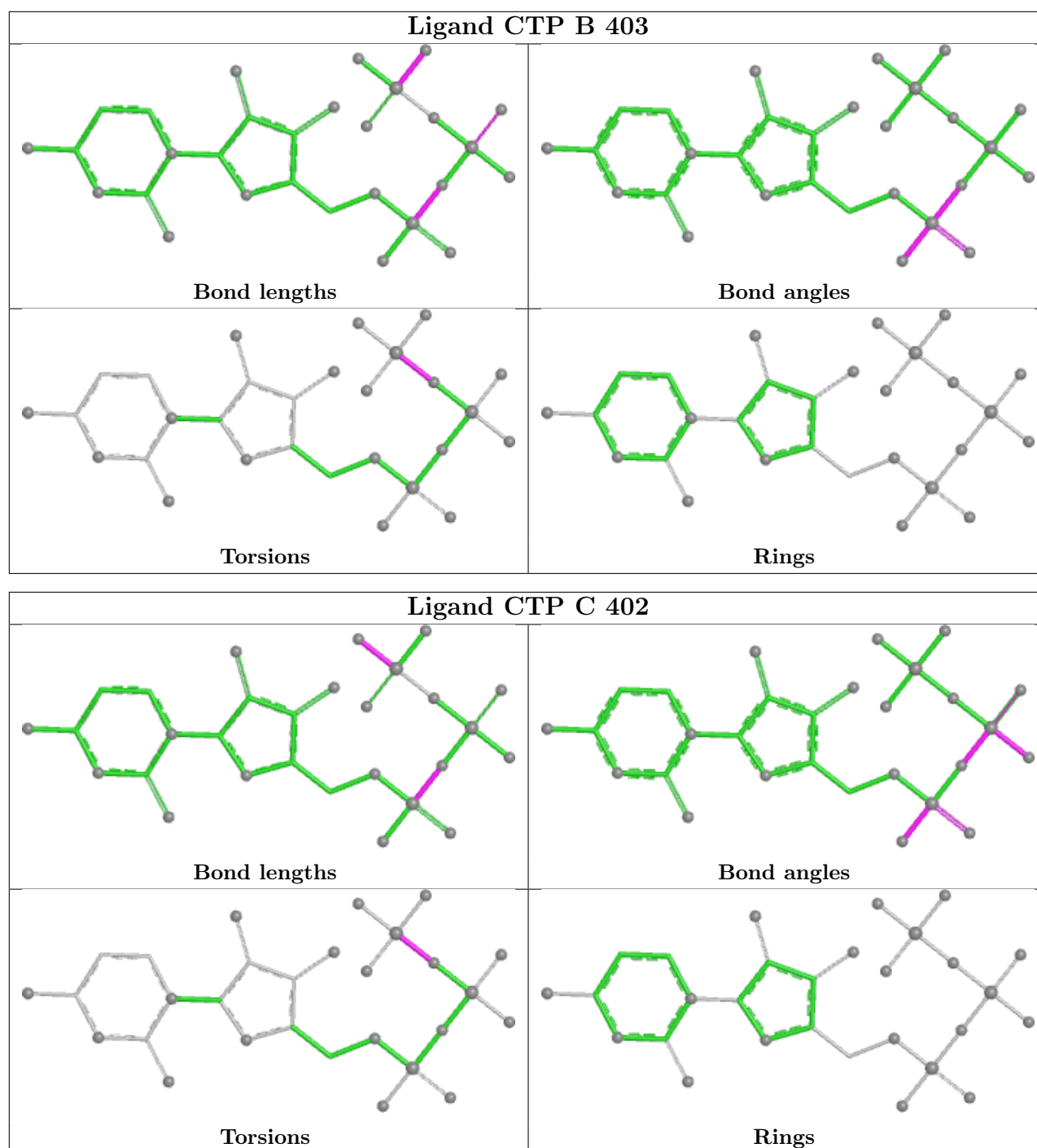


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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%)	1.63	95 (34%) 1 1	25, 44, 77, 92	0
1	B	282/315 (89%)	1.61	100 (35%) 1 1	14, 45, 73, 81	1 (0%)
1	C	276/315 (87%)	3.83	242 (87%) 0 0	24, 69, 118, 134	3 (1%)
All	All	837/945 (88%)	2.35	437 (52%) 0 0	14, 52, 99, 134	4 (0%)

The worst 5 of 437 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	PHE	9.3
1	C	174	LEU	9.2
1	C	36	LEU	8.8
1	C	223	PHE	8.7
1	C	137	ILE	8.5

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](#)

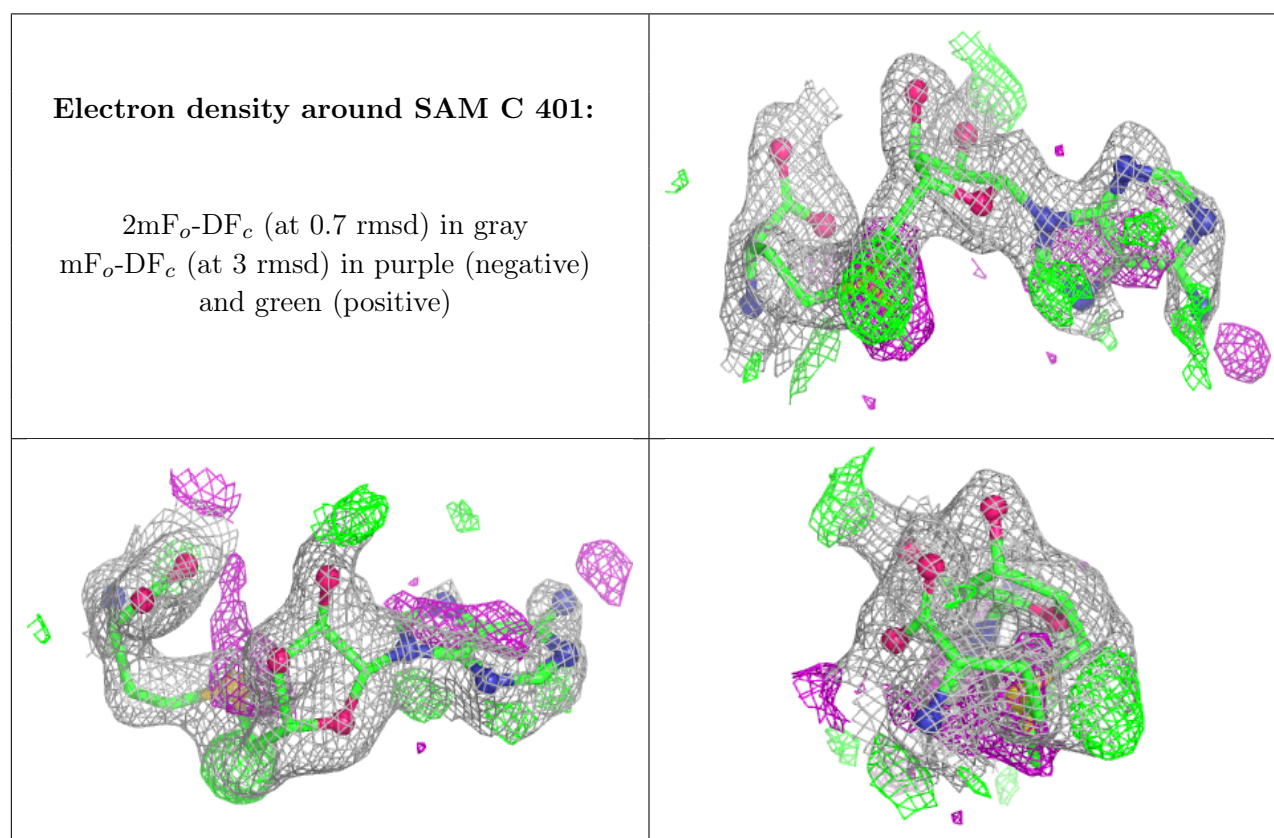
There are no monosaccharides in this entry.

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, 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.

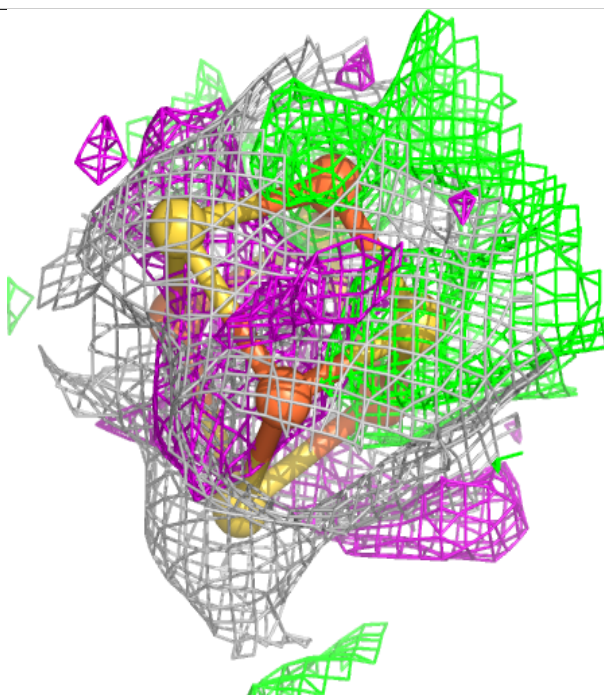
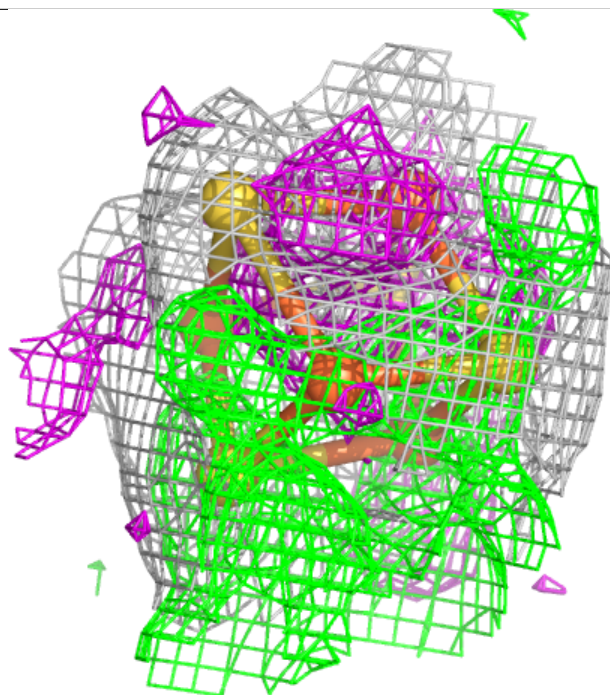
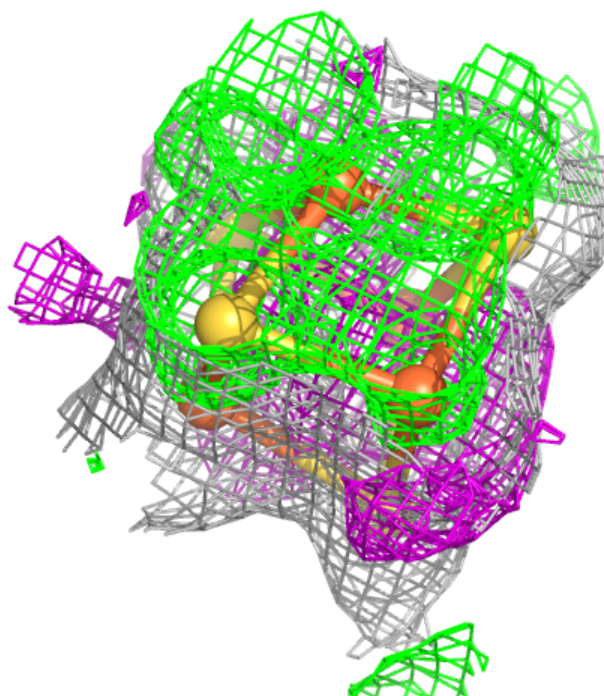
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SAM	C	401	27/27	0.73	0.22	46,51,60,64	0
3	SF4	C	403	8/8	0.87	0.16	56,61,65,67	0
4	SAM	B	402	27/27	0.89	0.12	27,31,38,40	0
4	SAM	A	403	27/27	0.92	0.10	27,31,35,37	0
2	CTP	C	402	29/29	0.95	0.11	40,43,49,51	0
2	CTP	B	403	29/29	0.96	0.08	26,29,33,36	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.



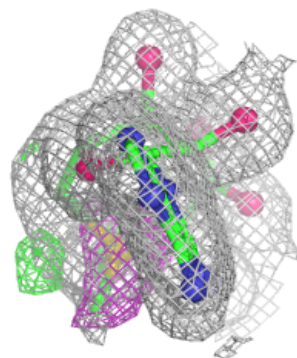
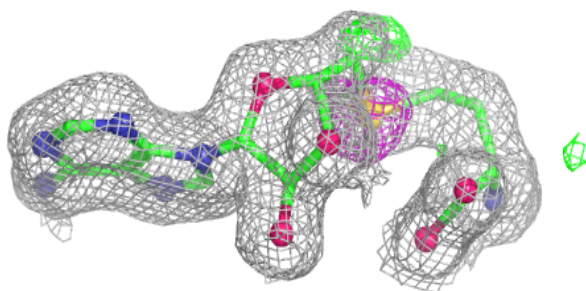
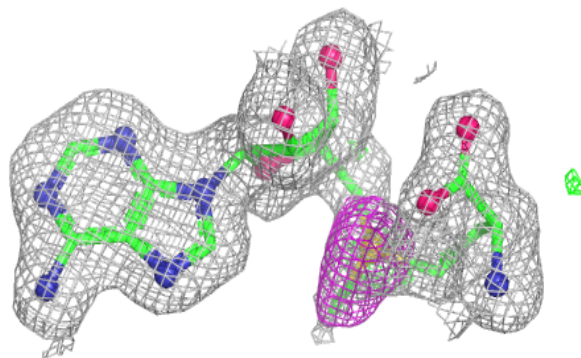
Electron density around SF4 C 403:

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

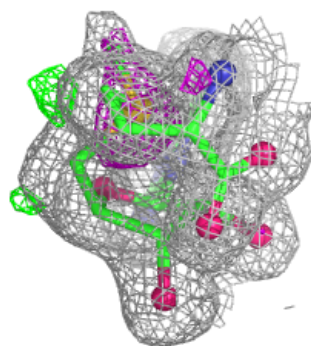
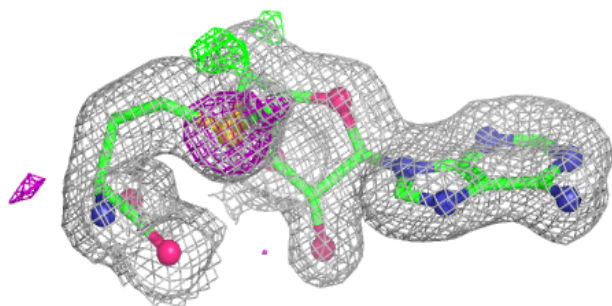
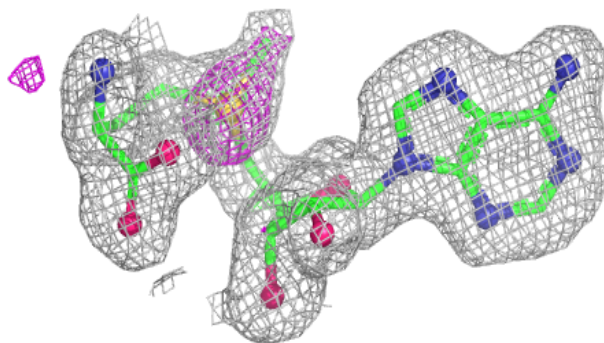


Electron density around SAM B 402:

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

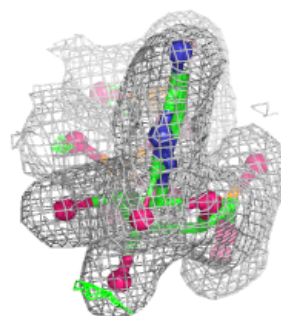
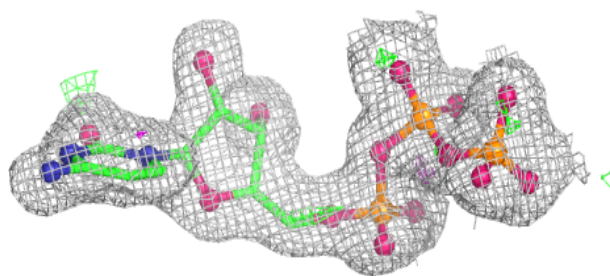
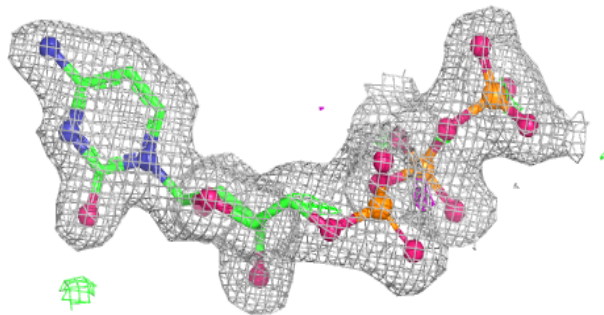
**Electron density around SAM A 403:**

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

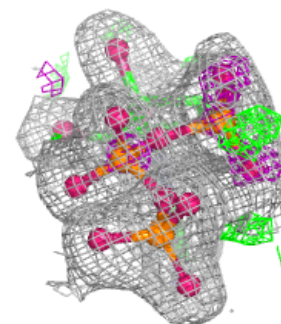
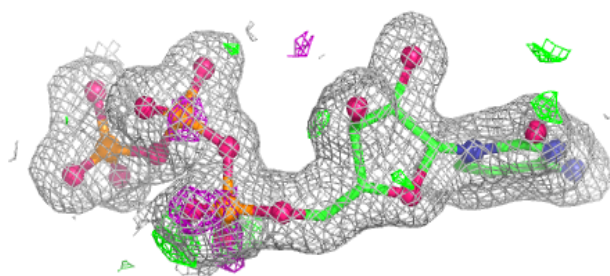
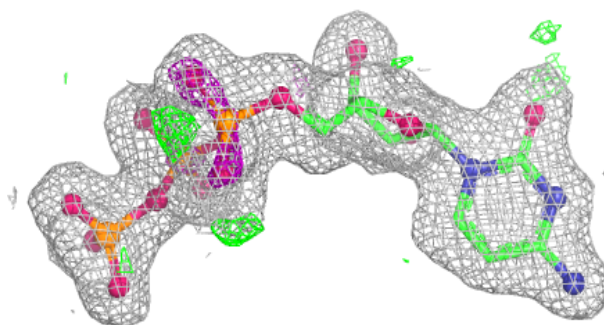


Electron density around CTP C 402:

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

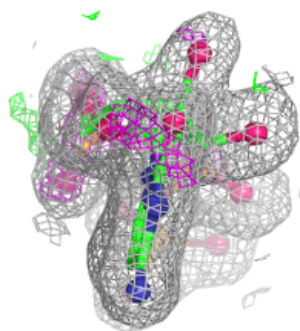
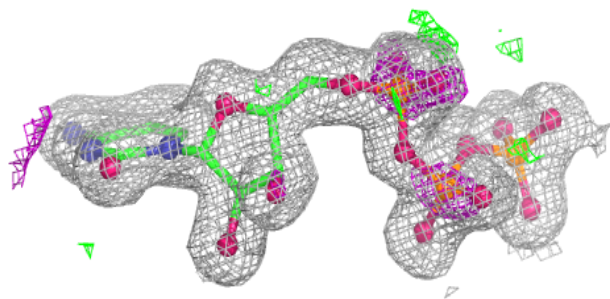
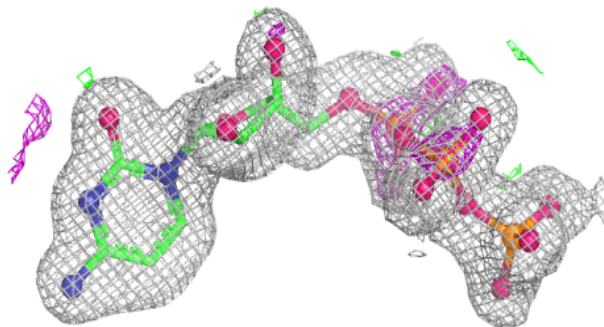
**Electron density around CTP B 403:**

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



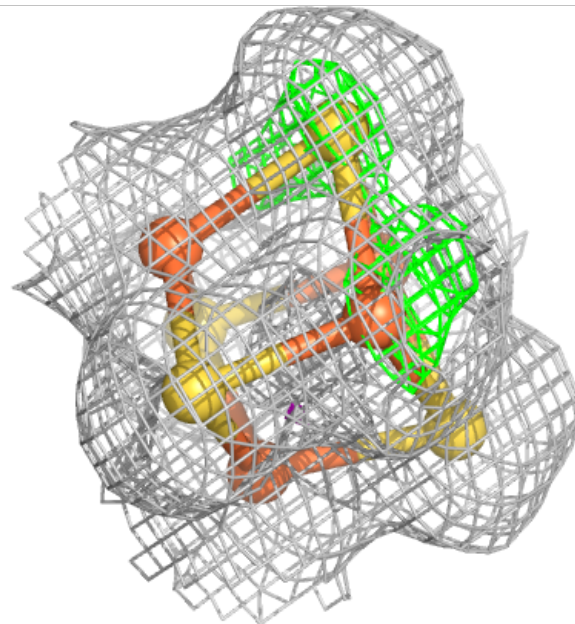
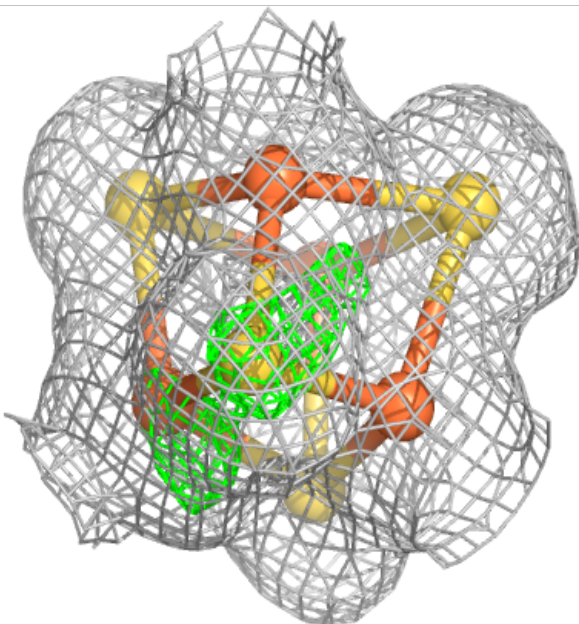
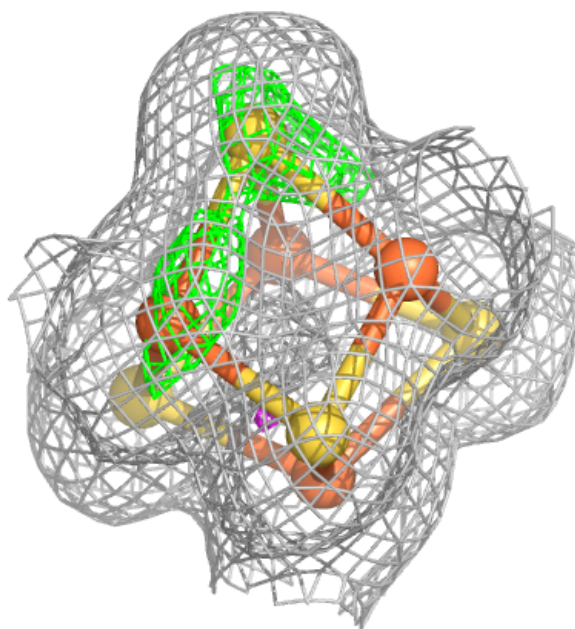
Electron density around CTP A 401:

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



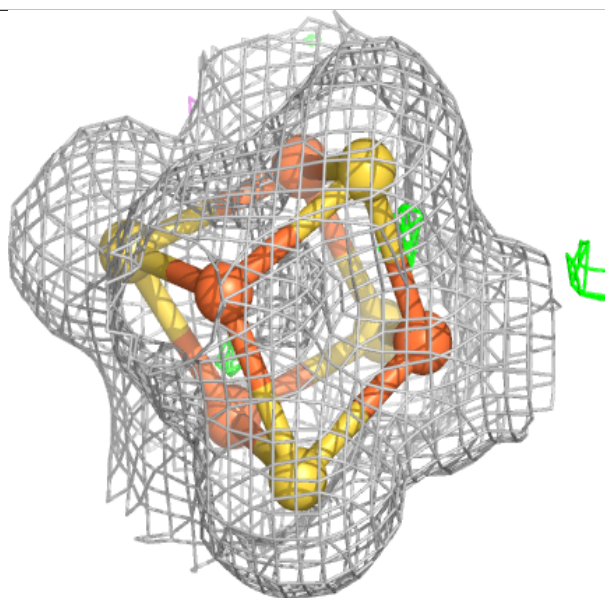
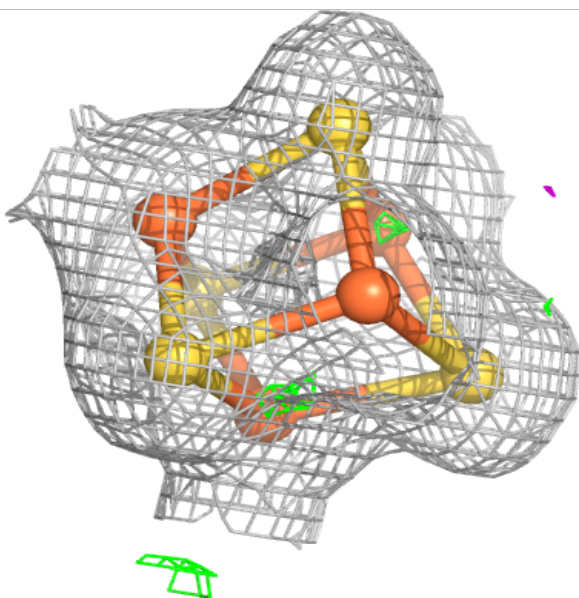
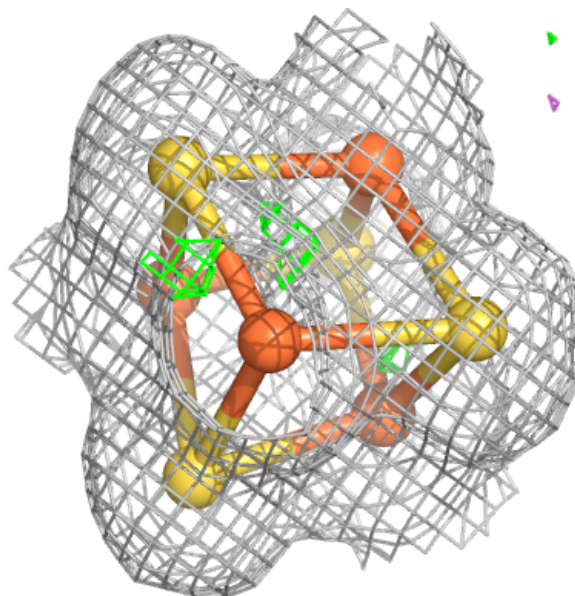
Electron density around SF4 A 402:

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 ⓘ

There are no such residues in this entry.