



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:42 AM UTC

PDB ID : 4NEC / pdb_00004nec
Title : Conversion of a Disulfide Bond into a Thioacetal Group during Echinomycin Biosynthesis
Authors : Hotta, K.; Keegan, R.M.; Ranganathan, S.; Fang, M.; Bibby, J.; Winn, M.D.; Sato, M.; Lian, M.; Watanabe, K.; Rigden, D.J.; Kim, C.-Y.
Deposited on : 2013-10-29
Resolution : 1.50 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	:	4-5-2 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

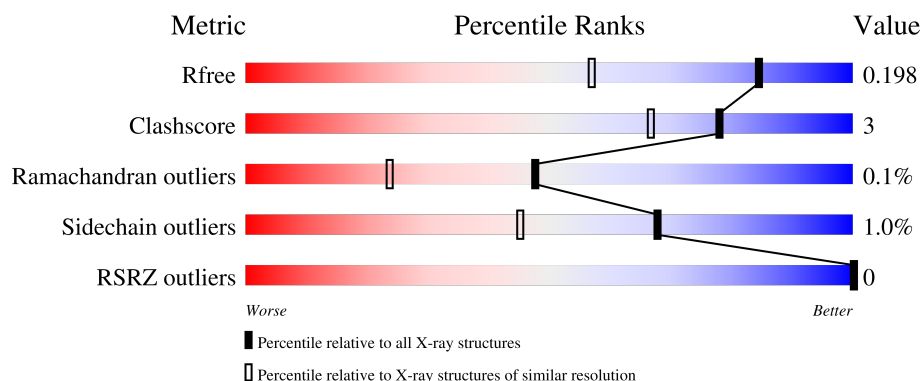
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	264	84% 6% 10%
1	B	264	86% 6% 8%
1	C	264	85% 12%
1	D	264	85% 6% 9%

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Mol	Chain	Length	Quality of chain
2	E	8	 50%50%
2	F	8	 75%25%
2	G	8	 50%50%
2	H	8	 50%25%25%

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
7	ACT	B	402	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8028 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 Putative SAM-dependent methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	2	0
			1801	1129	318	349	5			
1	B	244	Total	C	N	O	S	0	1	0
			1858	1160	334	359	5			
1	C	233	Total	C	N	O	S	0	4	0
			1793	1122	320	346	5			
1	D	239	Total	C	N	O	S	0	1	0
			1799	1128	318	348	5			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q0X0A7
A	-18	GLY	-	expression tag	UNP Q0X0A7
A	-17	SER	-	expression tag	UNP Q0X0A7
A	-16	SER	-	expression tag	UNP Q0X0A7
A	-15	HIS	-	expression tag	UNP Q0X0A7
A	-14	HIS	-	expression tag	UNP Q0X0A7
A	-13	HIS	-	expression tag	UNP Q0X0A7
A	-12	HIS	-	expression tag	UNP Q0X0A7
A	-11	HIS	-	expression tag	UNP Q0X0A7
A	-10	HIS	-	expression tag	UNP Q0X0A7
A	-9	SER	-	expression tag	UNP Q0X0A7
A	-8	SER	-	expression tag	UNP Q0X0A7
A	-7	GLY	-	expression tag	UNP Q0X0A7
A	-6	LEU	-	expression tag	UNP Q0X0A7
A	-5	VAL	-	expression tag	UNP Q0X0A7
A	-4	PRO	-	expression tag	UNP Q0X0A7
A	-3	ARG	-	expression tag	UNP Q0X0A7
A	-2	GLY	-	expression tag	UNP Q0X0A7
A	-1	SER	-	expression tag	UNP Q0X0A7
A	0	HIS	-	expression tag	UNP Q0X0A7
A	225	TRP	-	expression tag	UNP Q0X0A7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	226	ASN	-	expression tag	UNP Q0X0A7
A	227	SER	-	expression tag	UNP Q0X0A7
A	228	SER	-	expression tag	UNP Q0X0A7
A	229	SER	-	expression tag	UNP Q0X0A7
A	230	VAL	-	expression tag	UNP Q0X0A7
A	231	ASP	-	expression tag	UNP Q0X0A7
A	232	LYS	-	expression tag	UNP Q0X0A7
A	233	LEU	-	expression tag	UNP Q0X0A7
A	234	ALA	-	expression tag	UNP Q0X0A7
A	235	ALA	-	expression tag	UNP Q0X0A7
A	236	ALA	-	expression tag	UNP Q0X0A7
A	237	LEU	-	expression tag	UNP Q0X0A7
A	238	GLU	-	expression tag	UNP Q0X0A7
A	239	HIS	-	expression tag	UNP Q0X0A7
A	240	HIS	-	expression tag	UNP Q0X0A7
A	241	HIS	-	expression tag	UNP Q0X0A7
A	242	HIS	-	expression tag	UNP Q0X0A7
A	243	HIS	-	expression tag	UNP Q0X0A7
A	244	HIS	-	expression tag	UNP Q0X0A7
B	-19	MET	-	expression tag	UNP Q0X0A7
B	-18	GLY	-	expression tag	UNP Q0X0A7
B	-17	SER	-	expression tag	UNP Q0X0A7
B	-16	SER	-	expression tag	UNP Q0X0A7
B	-15	HIS	-	expression tag	UNP Q0X0A7
B	-14	HIS	-	expression tag	UNP Q0X0A7
B	-13	HIS	-	expression tag	UNP Q0X0A7
B	-12	HIS	-	expression tag	UNP Q0X0A7
B	-11	HIS	-	expression tag	UNP Q0X0A7
B	-10	HIS	-	expression tag	UNP Q0X0A7
B	-9	SER	-	expression tag	UNP Q0X0A7
B	-8	SER	-	expression tag	UNP Q0X0A7
B	-7	GLY	-	expression tag	UNP Q0X0A7
B	-6	LEU	-	expression tag	UNP Q0X0A7
B	-5	VAL	-	expression tag	UNP Q0X0A7
B	-4	PRO	-	expression tag	UNP Q0X0A7
B	-3	ARG	-	expression tag	UNP Q0X0A7
B	-2	GLY	-	expression tag	UNP Q0X0A7
B	-1	SER	-	expression tag	UNP Q0X0A7
B	0	HIS	-	expression tag	UNP Q0X0A7
B	225	TRP	-	expression tag	UNP Q0X0A7
B	226	ASN	-	expression tag	UNP Q0X0A7
B	227	SER	-	expression tag	UNP Q0X0A7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	228	SER	-	expression tag	UNP Q0X0A7
B	229	SER	-	expression tag	UNP Q0X0A7
B	230	VAL	-	expression tag	UNP Q0X0A7
B	231	ASP	-	expression tag	UNP Q0X0A7
B	232	LYS	-	expression tag	UNP Q0X0A7
B	233	LEU	-	expression tag	UNP Q0X0A7
B	234	ALA	-	expression tag	UNP Q0X0A7
B	235	ALA	-	expression tag	UNP Q0X0A7
B	236	ALA	-	expression tag	UNP Q0X0A7
B	237	LEU	-	expression tag	UNP Q0X0A7
B	238	GLU	-	expression tag	UNP Q0X0A7
B	239	HIS	-	expression tag	UNP Q0X0A7
B	240	HIS	-	expression tag	UNP Q0X0A7
B	241	HIS	-	expression tag	UNP Q0X0A7
B	242	HIS	-	expression tag	UNP Q0X0A7
B	243	HIS	-	expression tag	UNP Q0X0A7
B	244	HIS	-	expression tag	UNP Q0X0A7
C	-19	MET	-	expression tag	UNP Q0X0A7
C	-18	GLY	-	expression tag	UNP Q0X0A7
C	-17	SER	-	expression tag	UNP Q0X0A7
C	-16	SER	-	expression tag	UNP Q0X0A7
C	-15	HIS	-	expression tag	UNP Q0X0A7
C	-14	HIS	-	expression tag	UNP Q0X0A7
C	-13	HIS	-	expression tag	UNP Q0X0A7
C	-12	HIS	-	expression tag	UNP Q0X0A7
C	-11	HIS	-	expression tag	UNP Q0X0A7
C	-10	HIS	-	expression tag	UNP Q0X0A7
C	-9	SER	-	expression tag	UNP Q0X0A7
C	-8	SER	-	expression tag	UNP Q0X0A7
C	-7	GLY	-	expression tag	UNP Q0X0A7
C	-6	LEU	-	expression tag	UNP Q0X0A7
C	-5	VAL	-	expression tag	UNP Q0X0A7
C	-4	PRO	-	expression tag	UNP Q0X0A7
C	-3	ARG	-	expression tag	UNP Q0X0A7
C	-2	GLY	-	expression tag	UNP Q0X0A7
C	-1	SER	-	expression tag	UNP Q0X0A7
C	0	HIS	-	expression tag	UNP Q0X0A7
C	225	TRP	-	expression tag	UNP Q0X0A7
C	226	ASN	-	expression tag	UNP Q0X0A7
C	227	SER	-	expression tag	UNP Q0X0A7
C	228	SER	-	expression tag	UNP Q0X0A7
C	229	SER	-	expression tag	UNP Q0X0A7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	230	VAL	-	expression tag	UNP Q0X0A7
C	231	ASP	-	expression tag	UNP Q0X0A7
C	232	LYS	-	expression tag	UNP Q0X0A7
C	233	LEU	-	expression tag	UNP Q0X0A7
C	234	ALA	-	expression tag	UNP Q0X0A7
C	235	ALA	-	expression tag	UNP Q0X0A7
C	236	ALA	-	expression tag	UNP Q0X0A7
C	237	LEU	-	expression tag	UNP Q0X0A7
C	238	GLU	-	expression tag	UNP Q0X0A7
C	239	HIS	-	expression tag	UNP Q0X0A7
C	240	HIS	-	expression tag	UNP Q0X0A7
C	241	HIS	-	expression tag	UNP Q0X0A7
C	242	HIS	-	expression tag	UNP Q0X0A7
C	243	HIS	-	expression tag	UNP Q0X0A7
C	244	HIS	-	expression tag	UNP Q0X0A7
D	-19	MET	-	expression tag	UNP Q0X0A7
D	-18	GLY	-	expression tag	UNP Q0X0A7
D	-17	SER	-	expression tag	UNP Q0X0A7
D	-16	SER	-	expression tag	UNP Q0X0A7
D	-15	HIS	-	expression tag	UNP Q0X0A7
D	-14	HIS	-	expression tag	UNP Q0X0A7
D	-13	HIS	-	expression tag	UNP Q0X0A7
D	-12	HIS	-	expression tag	UNP Q0X0A7
D	-11	HIS	-	expression tag	UNP Q0X0A7
D	-10	HIS	-	expression tag	UNP Q0X0A7
D	-9	SER	-	expression tag	UNP Q0X0A7
D	-8	SER	-	expression tag	UNP Q0X0A7
D	-7	GLY	-	expression tag	UNP Q0X0A7
D	-6	LEU	-	expression tag	UNP Q0X0A7
D	-5	VAL	-	expression tag	UNP Q0X0A7
D	-4	PRO	-	expression tag	UNP Q0X0A7
D	-3	ARG	-	expression tag	UNP Q0X0A7
D	-2	GLY	-	expression tag	UNP Q0X0A7
D	-1	SER	-	expression tag	UNP Q0X0A7
D	0	HIS	-	expression tag	UNP Q0X0A7
D	225	TRP	-	expression tag	UNP Q0X0A7
D	226	ASN	-	expression tag	UNP Q0X0A7
D	227	SER	-	expression tag	UNP Q0X0A7
D	228	SER	-	expression tag	UNP Q0X0A7
D	229	SER	-	expression tag	UNP Q0X0A7
D	230	VAL	-	expression tag	UNP Q0X0A7
D	231	ASP	-	expression tag	UNP Q0X0A7

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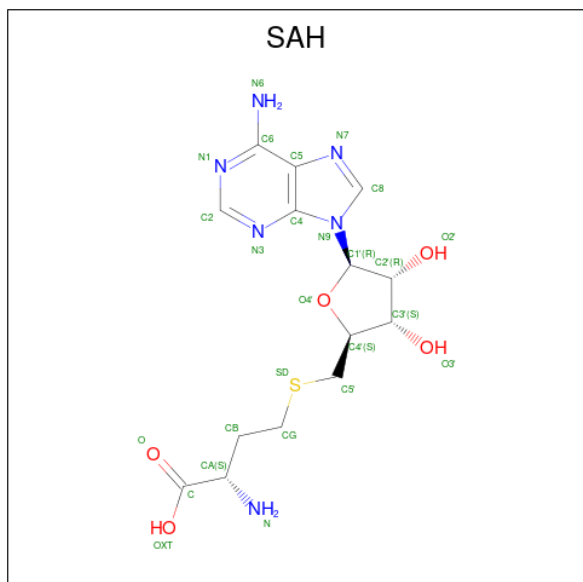
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Chain	Residue	Modelled	Actual	Comment	Reference
D	232	LYS	-	expression tag	UNP Q0X0A7
D	233	LEU	-	expression tag	UNP Q0X0A7
D	234	ALA	-	expression tag	UNP Q0X0A7
D	235	ALA	-	expression tag	UNP Q0X0A7
D	236	ALA	-	expression tag	UNP Q0X0A7
D	237	LEU	-	expression tag	UNP Q0X0A7
D	238	GLU	-	expression tag	UNP Q0X0A7
D	239	HIS	-	expression tag	UNP Q0X0A7
D	240	HIS	-	expression tag	UNP Q0X0A7
D	241	HIS	-	expression tag	UNP Q0X0A7
D	242	HIS	-	expression tag	UNP Q0X0A7
D	243	HIS	-	expression tag	UNP Q0X0A7
D	244	HIS	-	expression tag	UNP Q0X0A7

- Molecule 2 is a protein called Echinomycin.

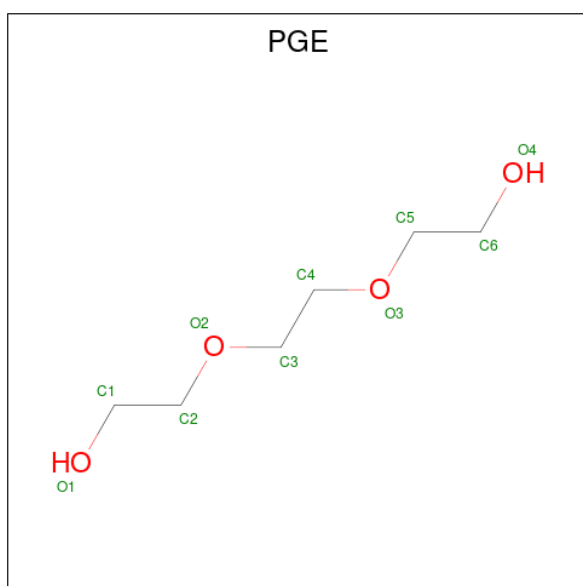
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	S	0	0	0
			53	33	8	10	2			
2	F	8	Total	C	N	O	S	0	0	0
			53	33	8	10	2			
2	G	8	Total	C	N	O	S	0	0	0
			53	33	8	10	2			
2	H	8	Total	C	N	O	S	0	0	0
			53	33	8	10	2			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

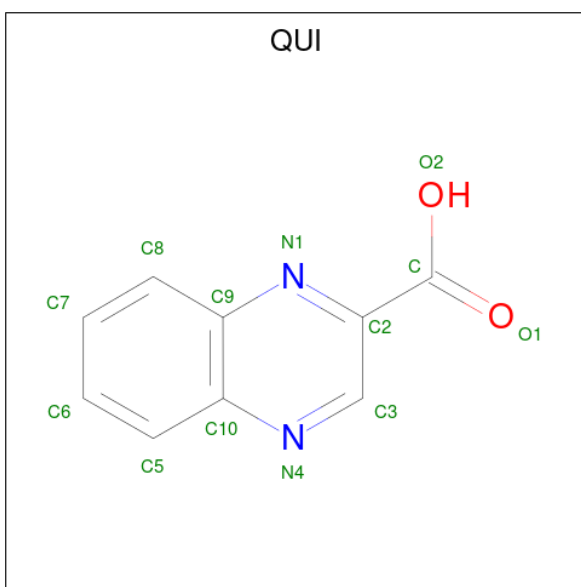


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

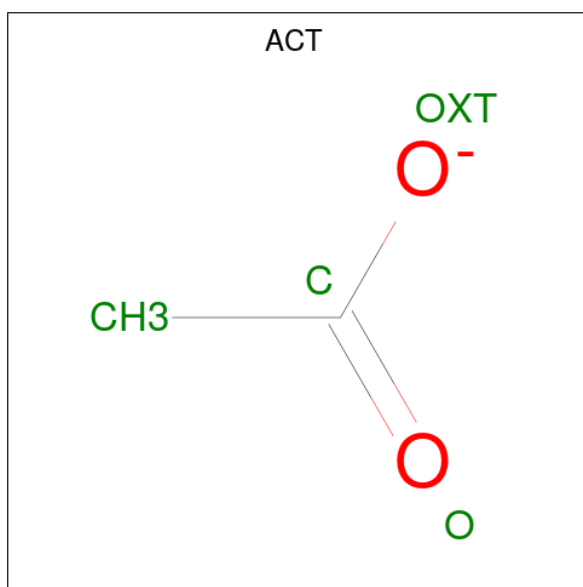
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is 2-CARBOXYQUINOXALINE (CCD ID: QUI) (formula: $C_9H_6N_2O_2$).



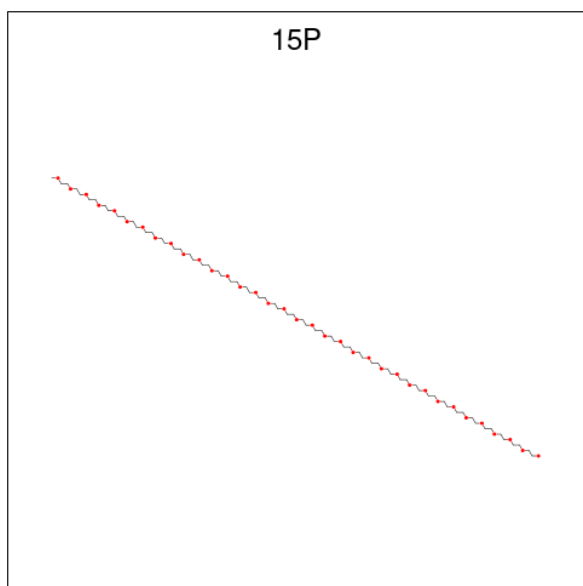
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			12	9	2	1		
6	E	1	Total	C	N	O	0	0
			12	9	2	1		
6	F	1	Total	C	N	O	0	0
			12	9	2	1		
6	F	1	Total	C	N	O	0	0
			12	9	2	1		
6	G	1	Total	C	N	O	0	0
			12	9	2	1		
6	G	1	Total	C	N	O	0	0
			12	9	2	1		
6	H	1	Total	C	N	O	0	0
			12	9	2	1		
6	H	1	Total	C	N	O	0	0
			12	9	2	1		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is POLYETHYLENE GLYCOL (N=34) (CCD ID: 15P) (formula: $C_{69}H_{140}O_{35}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			9	6	3		
8	D	1	Total	C	O	0	0
			18	13	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	54	Total 54	O 54	0	0
9	B	86	Total 86	O 86	0	0
9	F	2	Total 2	O 2	0	0
9	C	78	Total 78	O 78	0	0
9	G	2	Total 2	O 2	0	0
9	D	97	Total 97	O 97	0	0
9	H	1	Total 1	O 1	0	0

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: Putative SAM-dependent methyltransferase

Chain A: 



- Molecule 1: Putative SAM-dependent methyltransferase

Chain B: 



- Molecule 1: Putative SAM-dependent methyltransferase

Chain C: 



- Molecule 1: Putative SAM-dependent methyltransferase

Chain D: 



- Molecule 2: Echinomycin

Chain E: 



- Molecule 2: Echinomycin

Chain F:  75% 25%



● Molecule 2: Echinomycin

Chain G:  50% 50%



● Molecule 2: Echinomycin

Chain H:  50% 25% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.19Å 146.88Å 58.19Å 90.00° 102.63° 90.00°	Depositor
Resolution (Å)	45.42 – 1.50 45.42 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.42-1.50) 99.7 (45.42-1.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.150 , 0.190 (Not available) , 0.198	Depositor DCC
R_{free} test set	7597 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 16.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.447 for l,-k,h	Xtriage
Reported twinning fraction	0.530 for H, K, L 0.470 for L, -K, H	Depositor
Outliers	0 of 151251 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8028	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 15P, PGE, NCY, NA, ACT, QUI, N2C, MVA, DSN, SAH

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	0.41	0/1842	0.67	0/2505
1	B	0.41	0/1904	0.66	0/2591
1	C	0.43	0/1836	0.66	0/2498
1	D	0.44	0/1841	0.68	0/2505
2	E	0.45	0/8	1.22	0/8
2	F	0.54	0/8	1.54	0/8
2	G	0.42	0/8	1.09	0/8
2	H	0.49	0/8	1.69	0/8
All	All	0.42	0/7455	0.67	0/10131

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	G	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	6	ALA	Peptide
2	G	6	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	H	6	ALA	Peptide

5.2 Too-close contacts ⓘ

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	1801	0	1740	9	0
1	B	1858	0	1787	13	0
1	C	1793	0	1714	6	0
1	D	1799	0	1737	9	0
2	E	53	0	54	1	0
2	F	53	0	54	0	0
2	G	53	0	54	2	0
2	H	53	0	54	2	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
3	D	26	0	19	1	0
4	A	7	0	9	0	0
4	D	4	0	4	5	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
6	E	24	0	10	0	0
6	F	24	0	10	0	0
6	G	24	0	10	0	0
6	H	24	0	10	0	0
7	B	4	0	3	2	0
8	D	27	0	26	1	0
9	A	54	0	0	0	0
9	B	86	0	0	1	0
9	C	78	0	0	0	0
9	D	97	0	0	1	0
9	F	2	0	0	0	0
9	G	2	0	0	0	0
9	H	1	0	0	0	0
All	All	8028	0	7352	42	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 42 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:106[A]:ASP:OD1	1:C:134[A]:ARG:HD3	1.47	1.13
1:B:33:LEU:HD23	1:B:39:ILE:HD11	1.65	0.79
1:D:155:ARG:NH1	9:D:596:HOH:O	2.22	0.73
1:A:212:LEU:HD13	1:A:214:VAL:HG13	1.74	0.69
1:B:18[B]:ARG:NH2	1:B:22:ASP:O	2.26	0.68

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	236/264 (89%)	230 (98%)	6 (2%)	0	100	100
1	B	243/264 (92%)	236 (97%)	6 (2%)	1 (0%)	30	12
1	C	233/264 (88%)	227 (97%)	6 (3%)	0	100	100
1	D	236/264 (89%)	232 (98%)	4 (2%)	0	100	100
2	E	2/8 (25%)	2 (100%)	0	0	100	100
2	F	2/8 (25%)	2 (100%)	0	0	100	100
2	G	2/8 (25%)	2 (100%)	0	0	100	100
2	H	2/8 (25%)	2 (100%)	0	0	100	100
All	All	956/1088 (88%)	933 (98%)	22 (2%)	1 (0%)	48	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	GLY

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	179/204 (88%)	177 (99%)	2 (1%)	65	41
1	B	187/204 (92%)	187 (100%)	0	100	100
1	C	177/204 (87%)	176 (99%)	1 (1%)	78	62
1	D	179/204 (88%)	175 (98%)	4 (2%)	45	17
All	All	722/816 (88%)	715 (99%)	7 (1%)	68	45

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	GLU
1	D	40	GLN
1	D	183	LEU
1	D	118	GLU
1	C	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	B	226	ASN
1	C	182	HIS
1	D	241	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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	NCY	H	7	2	5,6,7	1.29	1 (20%)	5,6,8	1.50	1 (20%)
2	MVA	H	4	2	6,7,8	0.28	0	6,8,10	0.80	0
2	NCY	E	7	2	5,6,7	1.27	1 (20%)	5,6,8	1.58	1 (20%)
2	NCY	G	7	2	5,6,7	1.26	1 (20%)	5,6,8	1.43	1 (20%)
2	MVA	G	8	2	6,7,8	0.35	0	6,8,10	0.56	0
2	N2C	G	3	2	6,7,8	0.78	0	6,7,9	1.40	1 (16%)
2	NCY	F	7	2	5,6,7	1.21	1 (20%)	5,6,8	1.04	0
2	MVA	F	4	2	6,7,8	0.40	0	6,8,10	1.04	0
2	MVA	E	4	2	6,7,8	0.37	0	6,8,10	1.04	0
2	MVA	H	8	2	6,7,8	0.40	0	6,8,10	0.31	0
2	N2C	H	3	2	6,7,8	0.77	0	6,7,9	1.24	1 (16%)
2	MVA	F	8	2	6,7,8	0.31	0	6,8,10	0.63	0
2	MVA	E	8	2	6,7,8	0.33	0	6,8,10	0.52	0
2	N2C	E	3	2	6,7,8	0.71	0	6,7,9	1.25	1 (16%)
2	N2C	F	3	2	6,7,8	0.60	0	6,7,9	1.05	1 (16%)
2	MVA	G	4	2	6,7,8	0.26	0	6,8,10	0.97	0

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	NCY	H	7	2	-	0/3/6/8	-
2	MVA	H	4	2	-	1/6/8/10	-
2	NCY	E	7	2	-	0/3/6/8	-
2	NCY	G	7	2	-	0/3/6/8	-
2	MVA	G	8	2	-	1/6/8/10	-
2	N2C	G	3	2	-	1/4/7/9	-
2	NCY	F	7	2	-	0/3/6/8	-
2	MVA	F	4	2	-	1/6/8/10	-
2	MVA	E	4	2	-	1/6/8/10	-
2	MVA	H	8	2	-	0/6/8/10	-
2	N2C	H	3	2	-	1/4/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MVA	F	8	2	-	0/6/8/10	-
2	MVA	E	8	2	-	2/6/8/10	-
2	N2C	E	3	2	-	1/4/7/9	-
2	N2C	F	3	2	-	1/4/7/9	-
2	MVA	G	4	2	-	1/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	7	NCY	CB-SG	-2.28	1.76	1.81
2	G	7	NCY	CB-SG	-2.16	1.77	1.81
2	F	7	NCY	CB-SG	-2.13	1.77	1.81
2	E	7	NCY	CB-SG	-2.07	1.77	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	NCY	O-C-CA	-2.89	117.34	124.77
2	E	7	NCY	O-C-CA	-2.71	117.81	124.77
2	G	3	N2C	O-C-CA	-2.58	118.14	124.77
2	G	7	NCY	O-C-CA	-2.43	118.51	124.77
2	E	3	N2C	O-C-CA	-2.34	118.76	124.77

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	MVA	CB-CA-N-CN
2	F	4	MVA	CB-CA-N-CN
2	G	4	MVA	CB-CA-N-CN
2	H	4	MVA	CB-CA-N-CN
2	E	3	N2C	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	7	NCY	1	0
2	E	4	MVA	1	0
2	H	8	MVA	2	0
2	G	4	MVA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SAH	C	401	-	27,28,28	1.47	6 (22%)	36,40,40	1.95	11 (30%)
6	QUI	F	101	2	13,13,14	1.61	2 (15%)	17,17,19	1.99	8 (47%)
8	15P	D	403	-	16,16,103	0.55	0	14,14,102	0.12	0
8	15P	D	402	-	8,8,103	0.49	0	7,7,102	0.14	0
3	SAH	D	401	-	27,28,28	1.47	6 (22%)	36,40,40	1.92	9 (25%)
4	PGE	A	402	-	6,6,9	0.40	0	5,5,8	0.34	0
7	ACT	B	402	-	3,3,3	0.88	0	3,3,3	0.76	0
6	QUI	G	101	2	13,13,14	1.71	2 (15%)	17,17,19	2.21	8 (47%)
6	QUI	G	102	2	13,13,14	1.73	2 (15%)	17,17,19	2.30	8 (47%)
3	SAH	A	401	-	27,28,28	1.44	5 (18%)	36,40,40	1.91	10 (27%)
6	QUI	F	102	2	13,13,14	1.72	2 (15%)	17,17,19	2.25	7 (41%)
3	SAH	B	401	-	27,28,28	1.45	5 (18%)	36,40,40	1.92	10 (27%)
4	PGE	D	404	-	3,3,9	0.36	0	2,2,8	0.29	0
6	QUI	E	102	2	13,13,14	1.80	2 (15%)	17,17,19	1.97	7 (41%)
6	QUI	H	101	2	13,13,14	1.75	2 (15%)	17,17,19	2.38	8 (47%)
6	QUI	H	102	2	13,13,14	1.71	2 (15%)	17,17,19	2.06	7 (41%)
6	QUI	E	101	2	13,13,14	1.75	2 (15%)	17,17,19	2.21	9 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	C	401	-	-	0/15/31/31	0/3/3/3
6	QUI	F	101	2	-	0/2/2/4	0/2/2/2
8	15P	D	403	-	-	8/12/12/101	-
8	15P	D	402	-	-	4/6/6/101	-
3	SAH	D	401	-	-	0/15/31/31	0/3/3/3
4	PGE	A	402	-	-	2/4/4/7	-
6	QUI	G	101	2	-	0/2/2/4	0/2/2/2
6	QUI	G	102	2	-	2/2/2/4	0/2/2/2
3	SAH	A	401	-	-	0/15/31/31	0/3/3/3
6	QUI	F	102	2	-	0/2/2/4	0/2/2/2
3	SAH	B	401	-	-	0/15/31/31	0/3/3/3
4	PGE	D	404	-	-	0/1/1/7	-
6	QUI	E	102	2	-	1/2/2/4	0/2/2/2
6	QUI	H	101	2	-	0/2/2/4	0/2/2/2
6	QUI	H	102	2	-	2/2/2/4	0/2/2/2
6	QUI	E	101	2	-	0/2/2/4	0/2/2/2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	SAH	C5-C4	4.63	1.47	1.39
3	D	401	SAH	C5-C4	4.61	1.47	1.39
3	C	401	SAH	C5-C4	4.60	1.47	1.39
3	A	401	SAH	C5-C4	4.49	1.47	1.39
6	E	102	QUI	C10-C9	3.55	1.49	1.42

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	101	QUI	O1-C-C2	-5.35	119.28	124.22
3	B	401	SAH	C5-C4-N3	-5.15	119.62	126.72
3	C	401	SAH	C5-C4-N3	-5.14	119.64	126.72
3	D	401	SAH	C5-C4-N3	-5.07	119.73	126.72
3	A	401	SAH	C5-C4-N3	-4.98	119.86	126.72

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	102	QUI	O1-C-C2-N1
6	G	102	QUI	O1-C-C2-C3

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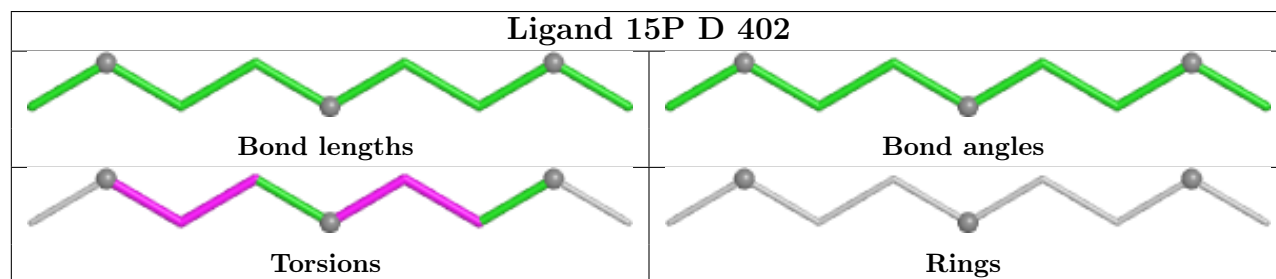
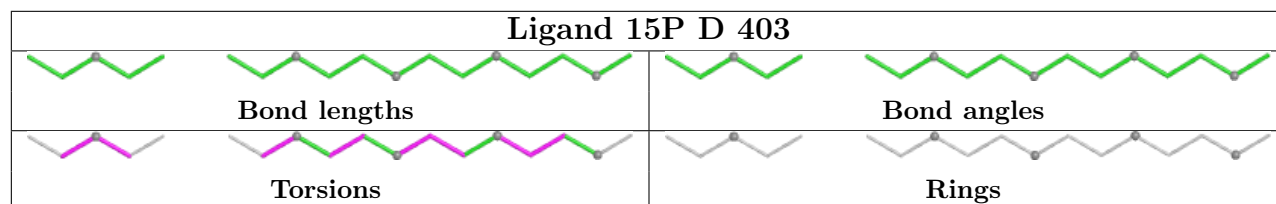
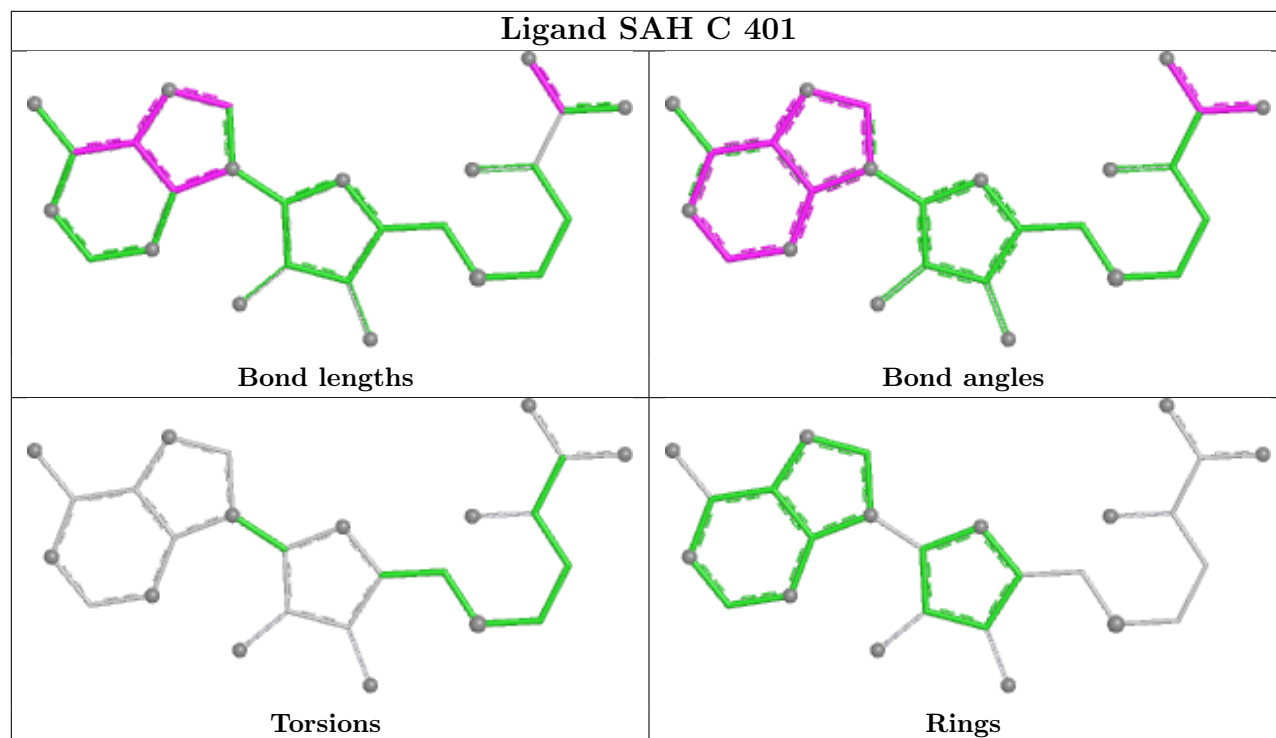
Mol	Chain	Res	Type	Atoms
6	H	102	QUI	O1-C-C2-N1
6	H	102	QUI	O1-C-C2-C3
8	D	402	15P	O5-C10-C9-O4

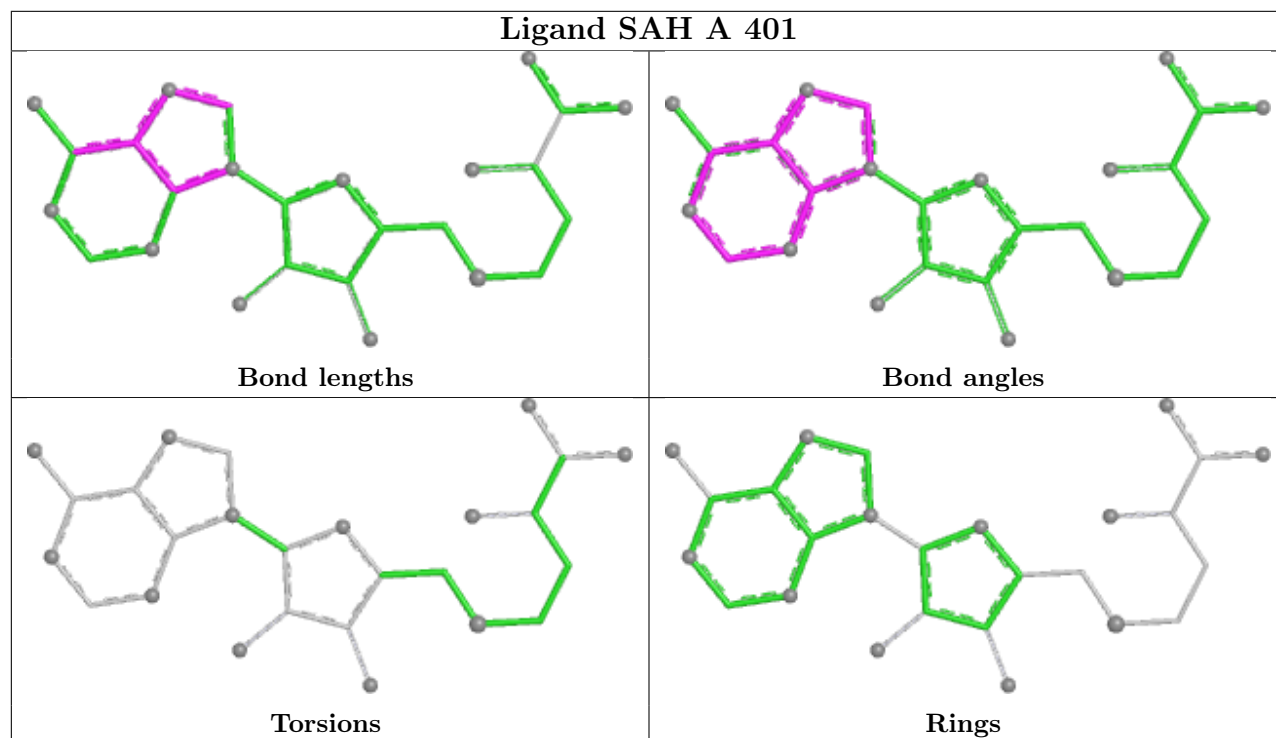
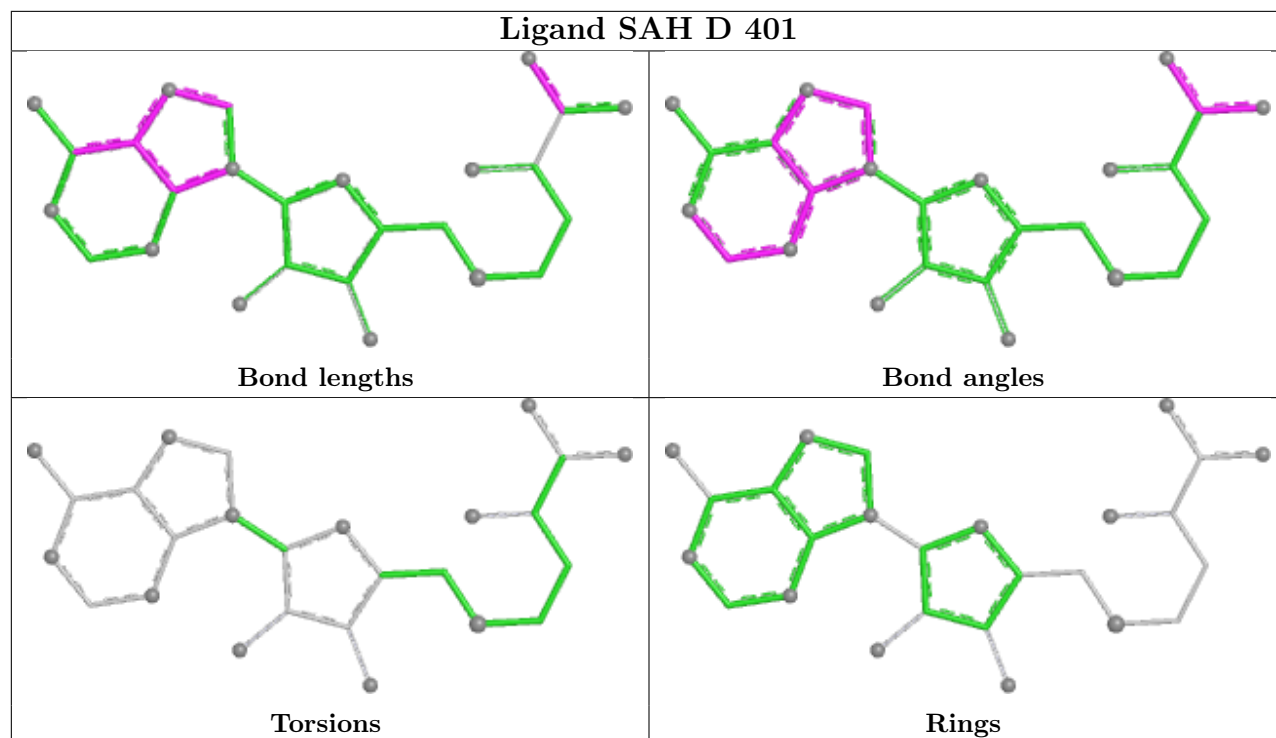
There are no ring outliers.

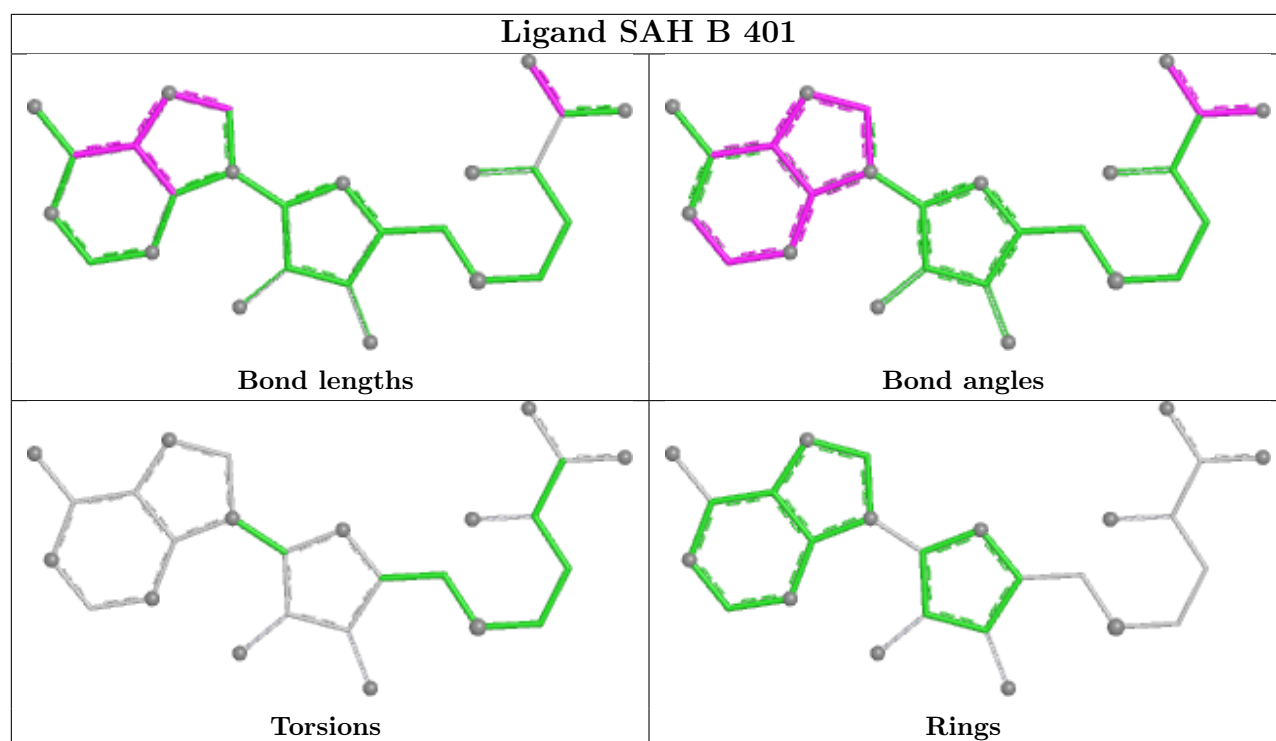
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	402	15P	1	0
3	D	401	SAH	1	0
7	B	402	ACT	2	0
4	D	404	PGE	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	238/264 (90%)	-1.18	0 100 100	5, 18, 35, 58	2 (0%)
1	B	244/264 (92%)	-1.21	0 100 100	7, 17, 30, 61	2 (0%)
1	C	233/264 (88%)	-1.20	0 100 100	4, 19, 31, 45	5 (2%)
1	D	239/264 (90%)	-1.29	0 100 100	8, 15, 27, 44	2 (0%)
2	E	2/8 (25%)	-1.03	0 100 100	21, 21, 21, 22	0
2	F	2/8 (25%)	-1.25	0 100 100	16, 16, 16, 17	0
2	G	2/8 (25%)	-0.96	0 100 100	21, 21, 21, 23	0
2	H	2/8 (25%)	-1.36	0 100 100	12, 12, 12, 17	0
All	All	962/1088 (88%)	-1.22	0 100 100	4, 17, 31, 61	11 (1%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	MVA	E	4	8/9	0.98	0.05	21,25,27,28	0
2	MVA	E	8	8/9	0.99	0.03	16,18,20,22	0
2	MVA	F	4	8/9	0.99	0.03	15,16,18,20	0
2	MVA	F	8	8/9	0.99	0.03	13,16,17,17	0
2	MVA	G	4	8/9	0.99	0.04	24,26,29,30	0
2	MVA	G	8	8/9	0.99	0.03	20,22,24,24	0
2	MVA	H	4	8/9	0.99	0.03	13,14,15,15	0
2	MVA	H	8	8/9	0.99	0.03	13,14,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DSN	G	1	6/7	0.99	0.02	18,19,20,22	0
2	DSN	E	5	6/7	0.99	0.03	21,22,25,26	0
2	DSN	H	5	6/7	0.99	0.02	16,16,17,18	0
2	DSN	H	1	6/7	1.00	0.02	13,13,14,15	0
2	N2C	E	3	8/9	1.00	0.03	20,21,22,22	0
2	N2C	F	3	8/9	1.00	0.02	13,15,16,16	0
2	N2C	G	3	8/9	1.00	0.03	16,22,23,24	0
2	N2C	H	3	8/9	1.00	0.02	12,13,14,15	0
2	DSN	F	1	6/7	1.00	0.02	15,16,16,18	0
2	DSN	F	5	6/7	1.00	0.02	16,17,18,18	0
2	DSN	G	5	6/7	1.00	0.03	22,24,25,26	0
2	DSN	E	1	6/7	1.00	0.02	17,19,19,20	0
2	NCY	E	7	7/8	1.00	0.02	17,18,19,19	0
2	NCY	F	7	7/8	1.00	0.01	13,14,15,16	0
2	NCY	G	7	7/8	1.00	0.02	18,20,21,22	0
2	NCY	H	7	7/8	1.00	0.02	14,15,15,16	0

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($\text{\AA}^2$)	Q<0.9
4	PGE	D	404	4/10	0.97	0.07	12,14,16,16	4
8	15P	D	403	18/104	0.97	0.06	20,28,34,35	0
8	15P	D	402	9/104	0.98	0.06	16,28,33,36	0
4	PGE	A	402	7/10	0.98	0.05	29,31,33,34	0
6	QUI	F	101	12/13	0.99	0.02	16,18,20,21	0
6	QUI	F	102	12/13	0.99	0.03	21,23,25,25	0
6	QUI	G	101	12/13	0.99	0.03	21,25,28,29	0
6	QUI	G	102	12/13	0.99	0.04	26,32,39,39	0
6	QUI	H	101	12/13	0.99	0.02	13,16,18,19	0
6	QUI	H	102	12/13	0.99	0.02	19,20,22,22	0
7	ACT	B	402	4/4	0.99	0.05	16,16,21,24	0
6	QUI	E	101	12/13	0.99	0.03	19,21,22,23	0

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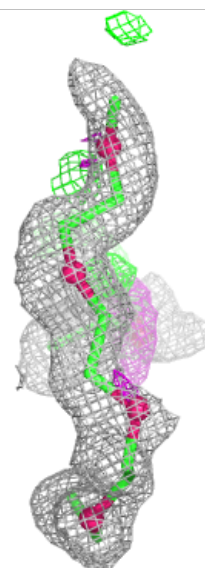
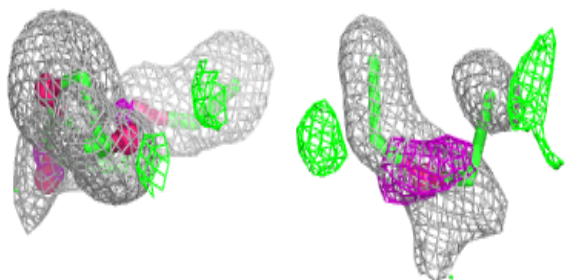
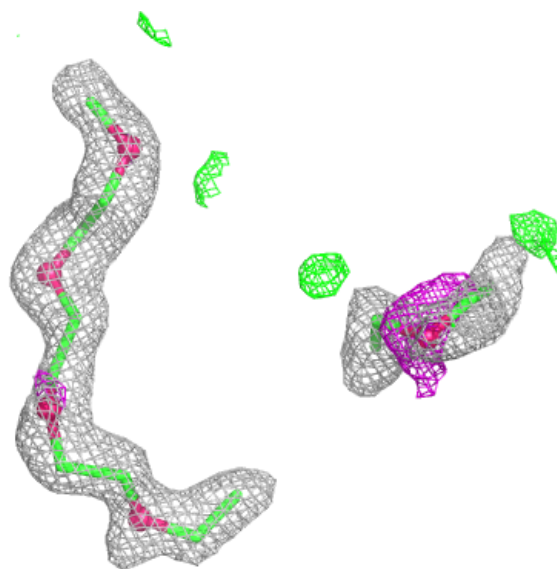
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	QUI	E	102	12/13	0.99	0.04	21,23,24,24	0
5	NA	A	403	1/1	1.00	0.02	26,26,26,26	0
5	NA	A	404	1/1	1.00	0.03	29,29,29,29	0
5	NA	C	402	1/1	1.00	0.06	45,45,45,45	0
3	SAH	C	401	26/26	1.00	0.02	15,16,18,19	0
3	SAH	D	401	26/26	1.00	0.02	9,11,14,15	0
3	SAH	A	401	26/26	1.00	0.02	12,14,16,17	0
3	SAH	B	401	26/26	1.00	0.02	10,12,13,15	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.

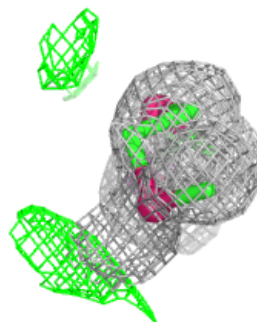
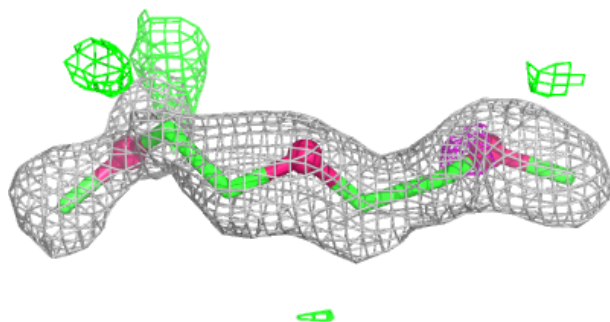
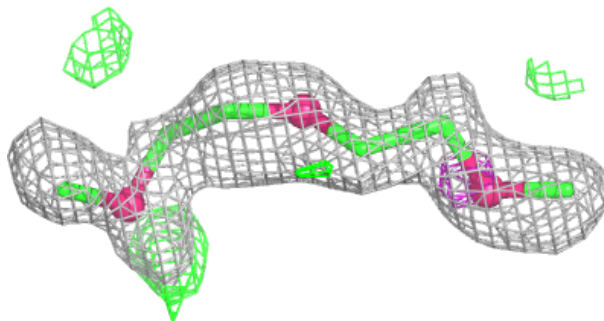
Electron density around 15P D 403:

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

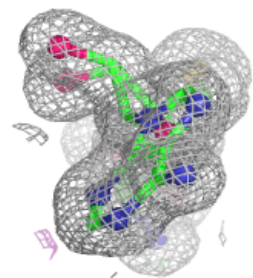
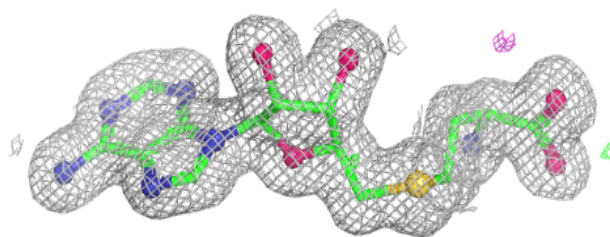
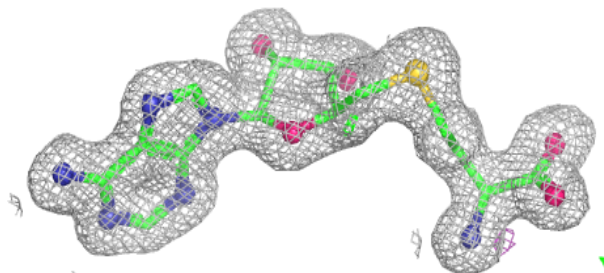


Electron density around 15P D 402:

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

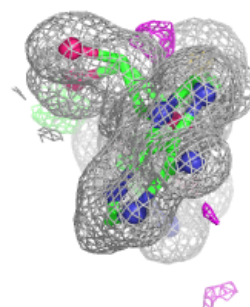
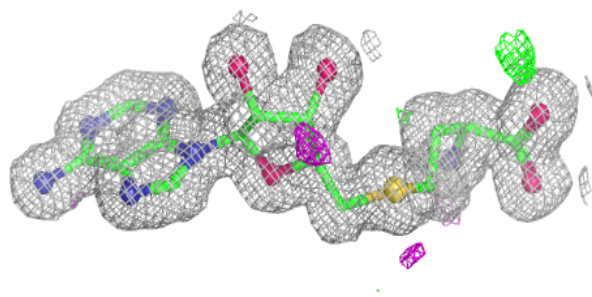
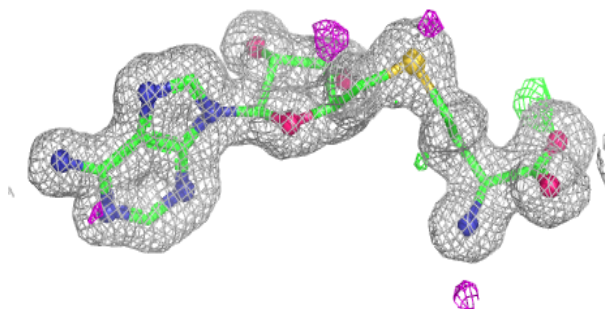
**Electron density around SAH C 401:**

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

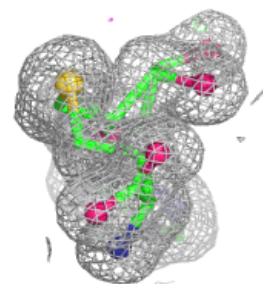
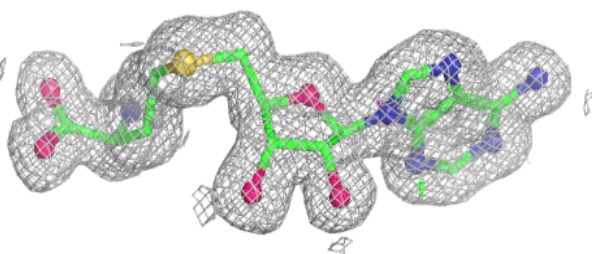
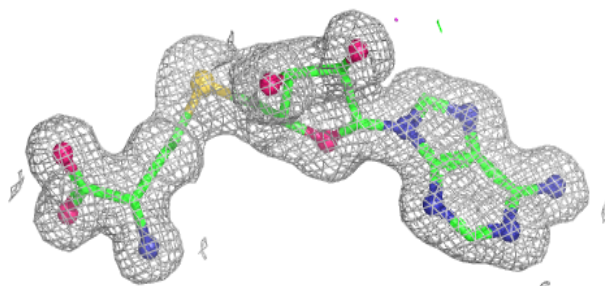


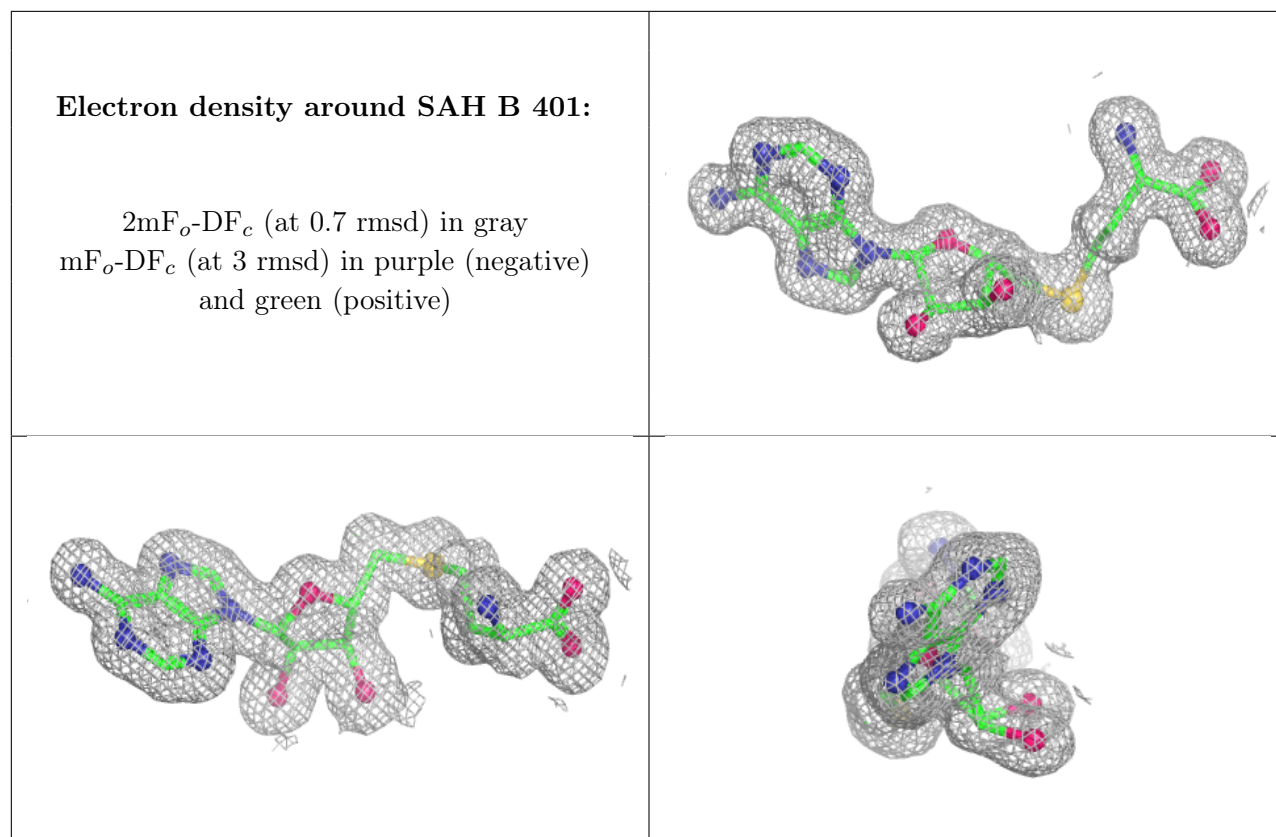
Electron density around SAH D 401:

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

**Electron density around SAH 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.