



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:01 PM UTC

PDB ID : 5EEH / pdb_00005eeh
Title : Crystal structure of carminomycin-4-O-methyltransferase DnrK in complex with SAH and 2-chloro-4-nitrophenol
Authors : Wang, F.; Singh, S.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2015-10-22
Resolution : 1.82 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

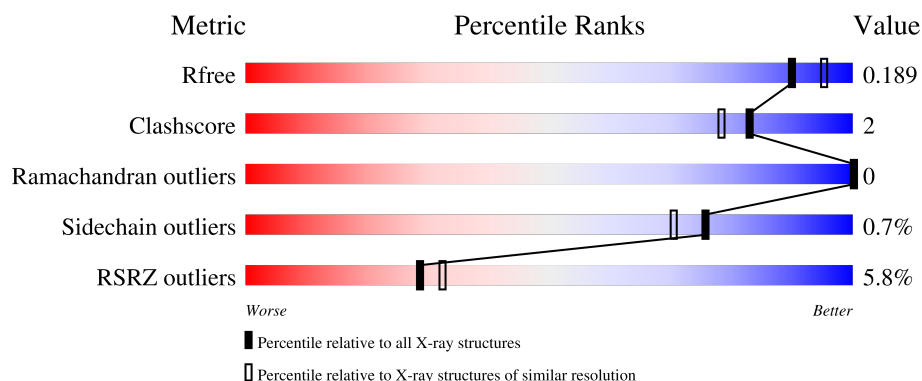
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	376	 3% 85% 6% 9%
1	B	376	 2% 87% 10% 3%
1	C	376	 11% 85% 6% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9261 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 Carminomycin 4-O-methyltransferase DnrK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	10	0
			2734	1723	496	510	5			
1	B	340	Total	C	N	O	S	0	4	0
			2664	1681	480	498	5			
1	C	343	Total	C	N	O	S	0	2	0
			2662	1683	476	498	5			

There are 60 discrepancies between the modelled and reference sequences:

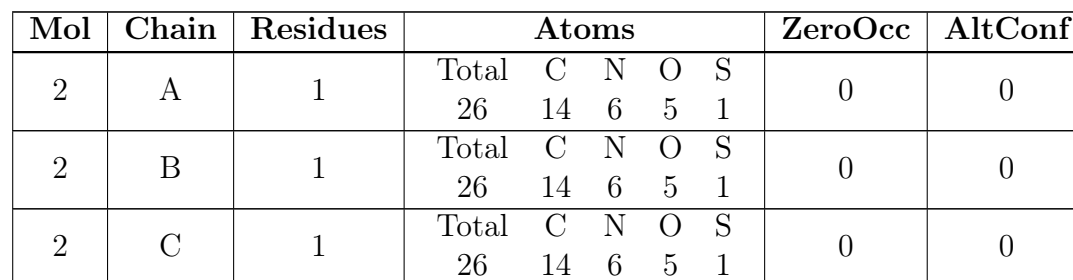
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q06528
A	-18	GLY	-	expression tag	UNP Q06528
A	-17	SER	-	expression tag	UNP Q06528
A	-16	SER	-	expression tag	UNP Q06528
A	-15	HIS	-	expression tag	UNP Q06528
A	-14	HIS	-	expression tag	UNP Q06528
A	-13	HIS	-	expression tag	UNP Q06528
A	-12	HIS	-	expression tag	UNP Q06528
A	-11	HIS	-	expression tag	UNP Q06528
A	-10	HIS	-	expression tag	UNP Q06528
A	-9	SER	-	expression tag	UNP Q06528
A	-8	SER	-	expression tag	UNP Q06528
A	-7	GLY	-	expression tag	UNP Q06528
A	-6	LEU	-	expression tag	UNP Q06528
A	-5	VAL	-	expression tag	UNP Q06528
A	-4	PRO	-	expression tag	UNP Q06528
A	-3	ARG	-	expression tag	UNP Q06528
A	-2	GLY	-	expression tag	UNP Q06528
A	-1	SER	-	expression tag	UNP Q06528
A	0	HIS	-	expression tag	UNP Q06528
B	-19	MET	-	initiating methionine	UNP Q06528
B	-18	GLY	-	expression tag	UNP Q06528
B	-17	SER	-	expression tag	UNP Q06528

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q06528
B	-15	HIS	-	expression tag	UNP Q06528
B	-14	HIS	-	expression tag	UNP Q06528
B	-13	HIS	-	expression tag	UNP Q06528
B	-12	HIS	-	expression tag	UNP Q06528
B	-11	HIS	-	expression tag	UNP Q06528
B	-10	HIS	-	expression tag	UNP Q06528
B	-9	SER	-	expression tag	UNP Q06528
B	-8	SER	-	expression tag	UNP Q06528
B	-7	GLY	-	expression tag	UNP Q06528
B	-6	LEU	-	expression tag	UNP Q06528
B	-5	VAL	-	expression tag	UNP Q06528
B	-4	PRO	-	expression tag	UNP Q06528
B	-3	ARG	-	expression tag	UNP Q06528
B	-2	GLY	-	expression tag	UNP Q06528
B	-1	SER	-	expression tag	UNP Q06528
B	0	HIS	-	expression tag	UNP Q06528
C	-19	MET	-	initiating methionine	UNP Q06528
C	-18	GLY	-	expression tag	UNP Q06528
C	-17	SER	-	expression tag	UNP Q06528
C	-16	SER	-	expression tag	UNP Q06528
C	-15	HIS	-	expression tag	UNP Q06528
C	-14	HIS	-	expression tag	UNP Q06528
C	-13	HIS	-	expression tag	UNP Q06528
C	-12	HIS	-	expression tag	UNP Q06528
C	-11	HIS	-	expression tag	UNP Q06528
C	-10	HIS	-	expression tag	UNP Q06528
C	-9	SER	-	expression tag	UNP Q06528
C	-8	SER	-	expression tag	UNP Q06528
C	-7	GLY	-	expression tag	UNP Q06528
C	-6	LEU	-	expression tag	UNP Q06528
C	-5	VAL	-	expression tag	UNP Q06528
C	-4	PRO	-	expression tag	UNP Q06528
C	-3	ARG	-	expression tag	UNP Q06528
C	-2	GLY	-	expression tag	UNP Q06528
C	-1	SER	-	expression tag	UNP Q06528
C	0	HIS	-	expression tag	UNP Q06528

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



- P9P
-
- Chemical structure of P9P (2-chloro-4-nitrophenol). The structure shows a benzene ring with a nitro group (NO₂) at position 4, a chlorine atom (Cl) at position 2, and a hydroxyl group (OH) at position 1. Atoms are labeled with IDs: O06, O07, N05, C03, C02, C04, C08, C09, C10, CL1, O11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	A	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	A	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	A	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	A	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	B	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	B	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	B	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	B	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	B	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	B	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	C	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	C	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		
3	C	1	Total	C	Cl	N	O	0	0
			11	6	1	1	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

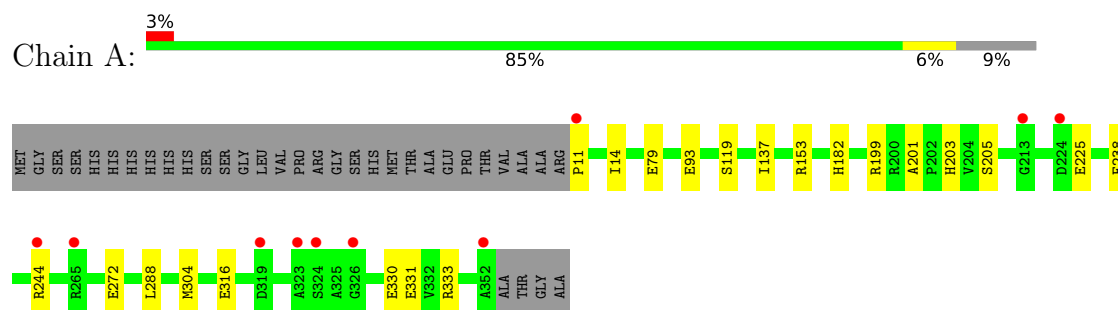
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	372	Total	O	0	0
			372	372		
5	B	321	Total	O	0	0
			321	321		
5	C	220	Total	O	0	0
			220	220		

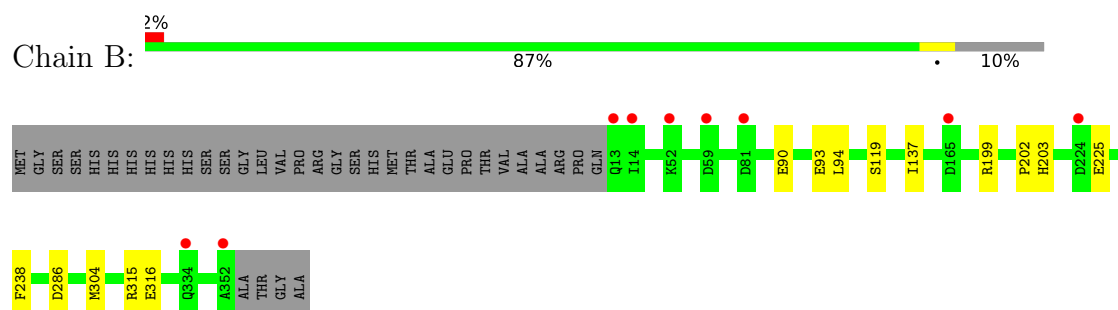
3 Residue-property plots [i](#)

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.

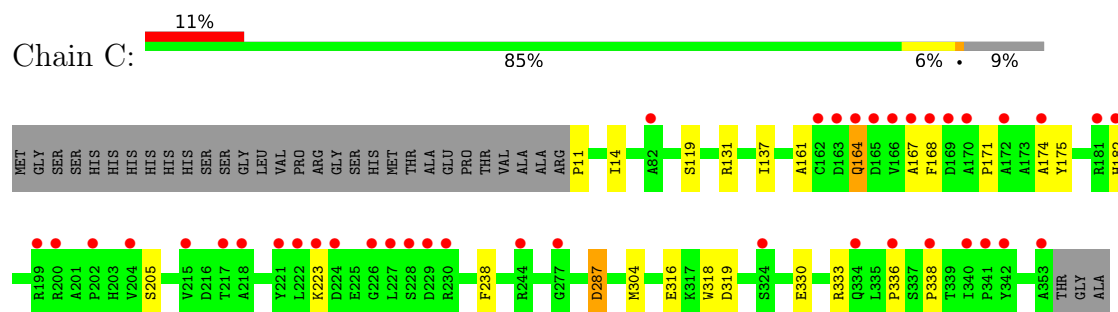
• Molecule 1: Carminomycin 4-O-methyltransferase DnrK



• Molecule 1: Carminomycin 4-O-methyltransferase DnrK



• Molecule 1: Carminomycin 4-O-methyltransferase DnrK



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.35Å 110.68Å 116.87Å 90.00° 120.24° 90.00°	Depositor
Resolution (Å)	48.50 – 1.82 48.50 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.50-1.82) 98.3 (48.50-1.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.154 , 0.185 0.159 , 0.189	Depositor DCC
R_{free} test set	2000 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9261	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: SO4, SAH, P9P

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	0.51	0/2791	0.75	2/3800 (0.1%)
1	B	0.47	0/2718	0.73	0/3702
1	C	0.43	0/2717	0.76	2/3703 (0.1%)
All	All	0.47	0/8226	0.75	4/11205 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	GLN	N-CA-C	8.58	121.77	111.82
1	C	318	TRP	N-CA-C	5.31	117.15	111.36
1	A	201	ALA	CA-C-N	5.28	124.94	119.56
1	A	201	ALA	C-N-CA	5.28	124.94	119.56

There are no chirality outliers.

There are no planarity outliers.

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	2734	0	2716	15	0
1	B	2664	0	2657	11	0
1	C	2662	0	2659	16	0
2	A	26	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	19	0	0
2	C	26	0	19	0	0
3	A	66	0	24	1	0
3	B	66	0	24	1	0
3	C	33	0	12	2	0
4	A	20	0	0	2	0
4	B	20	0	0	0	0
4	C	5	0	0	0	0
5	A	372	0	0	5	7
5	B	321	0	0	2	1
5	C	220	0	0	5	6
All	All	9261	0	8149	40	8

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (40) 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:B:316:GLU:OE1	5:B:501:HOH:O	1.98	0.82
1:C:161:ALA:O	1:C:164:GLN:HG3	1.88	0.74
1:C:319:ASP:OD1	5:C:501:HOH:O	2.12	0.67
3:C:402:P9P:O11	5:C:502:HOH:O	2.14	0.64
4:A:410:SO4:O3	5:A:502:HOH:O	2.12	0.64
1:C:131:ARG:NH1	5:C:503:HOH:O	2.22	0.64
1:C:223:LYS:NZ	5:C:504:HOH:O	2.31	0.64
1:A:288:LEU:HD11	1:C:330:GLU:HB2	1.80	0.62
4:A:411:SO4:O2	5:A:501:HOH:O	2.09	0.61
1:C:167:ALA:N	5:C:508:HOH:O	2.35	0.58
1:A:203:HIS:ND1	1:B:93:GLU:OE1	2.36	0.58
1:A:79:GLU:OE2	5:A:503:HOH:O	2.17	0.56
1:A:93:GLU:OE1	1:B:203:HIS:ND1	2.38	0.55
1:C:11:PRO:HB2	1:C:14[A]:ILE:HG23	1.92	0.52
1:A:199[A]:ARG:NH2	1:A:225:GLU:O	2.42	0.52
1:C:182:HIS:ND1	1:C:205:SER:OG	2.39	0.51
1:A:330:GLU:HA	1:C:316:GLU:HB2	1.91	0.51
1:C:174:ALA:O	1:C:333:ARG:NH1	2.43	0.50
1:C:119:SER:HA	1:C:137:ILE:HD12	1.93	0.50
1:A:153:ARG:HD3	5:A:509:HOH:O	2.13	0.48
1:A:182[A]:HIS:NE2	1:A:244:ARG:HD2	2.29	0.48
1:B:119:SER:HA	1:B:137:ILE:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:HA	1:A:137:ILE:HD12	1.96	0.47
1:C:304:MET:HE1	3:C:402:P9P:C02	2.45	0.47
1:B:202:PRO:HG3	5:B:534:HOH:O	2.14	0.47
1:B:304:MET:HE1	3:B:403:P9P:C02	2.45	0.46
1:A:304:MET:HE1	3:A:402:P9P:C02	2.45	0.46
1:A:203:HIS:HD1	1:B:93:GLU:CD	2.25	0.45
1:B:286:ASP:OD1	1:B:315[B]:ARG:HA	2.16	0.45
1:C:168:PHE:C	1:C:171:PRO:HD2	2.42	0.44
1:A:182[A]:HIS:ND1	1:A:205:SER:OG	2.42	0.44
1:A:11:PRO:O	1:A:14:ILE:HG22	2.19	0.43
1:B:286:ASP:OD1	1:B:315[A]:ARG:HA	2.18	0.43
1:C:336:PRO:O	1:C:338:PRO:HD3	2.18	0.43
1:A:331:GLU:CD	1:A:333:ARG:HE	2.27	0.42
1:C:175:TYR:HA	1:C:333:ARG:NH1	2.34	0.41
1:B:90[B]:GLU:H	1:B:90[B]:GLU:CD	2.27	0.41
1:C:287:ASP:OD2	1:C:287:ASP:N	2.53	0.41
1:B:199:ARG:NH2	1:B:225:GLU:O	2.50	0.41
1:A:272:GLU:OE1	5:A:505:HOH:O	2.22	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:767:HOH:O	5:C:593:HOH:O[3_444]	1.98	0.22
5:A:522:HOH:O	5:A:527:HOH:O[2_757]	2.00	0.20
5:A:542:HOH:O	5:C:533:HOH:O[3_444]	2.02	0.18
5:B:761:HOH:O	5:C:603:HOH:O[2_858]	2.04	0.16
5:A:628:HOH:O	5:C:507:HOH:O[4_748]	2.05	0.15
5:A:661:HOH:O	5:C:708:HOH:O[3_444]	2.17	0.03
5:A:684:HOH:O	5:C:703:HOH:O[3_444]	2.18	0.02
5:A:838:HOH:O	5:A:838:HOH:O[2_757]	2.19	0.01

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	350/376 (93%)	345 (99%)	5 (1%)	0	100	100
1	B	342/376 (91%)	336 (98%)	6 (2%)	0	100	100
1	C	343/376 (91%)	335 (98%)	8 (2%)	0	100	100
All	All	1035/1128 (92%)	1016 (98%)	19 (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	284/299 (95%)	282 (99%)	2 (1%)	76	70
1	B	276/299 (92%)	274 (99%)	2 (1%)	76	70
1	C	276/299 (92%)	274 (99%)	2 (1%)	76	70
All	All	836/897 (93%)	830 (99%)	6 (1%)	76	70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	PHE
1	A	316	GLU
1	B	94	LEU
1	B	238	PHE
1	C	238	PHE
1	C	287	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	C	179	ASN

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 ⓘ

27 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	SO4	C	405	-	4,4,4	0.22	0	6,6,6	0.14	0
4	SO4	A	409	-	4,4,4	0.17	0	6,6,6	0.36	0
4	SO4	A	408	-	4,4,4	0.22	0	6,6,6	0.21	0
4	SO4	A	410	-	4,4,4	0.21	0	6,6,6	0.23	0
4	SO4	B	408	-	4,4,4	0.27	0	6,6,6	0.25	0
3	P9P	B	407	-	11,11,11	2.68	2 (18%)	13,15,15	0.92	1 (7%)
4	SO4	B	410	-	4,4,4	0.24	0	6,6,6	0.09	0
3	P9P	C	402	-	11,11,11	2.68	2 (18%)	13,15,15	1.21	2 (15%)
3	P9P	B	403	-	11,11,11	2.68	2 (18%)	13,15,15	0.99	1 (7%)
3	P9P	A	407	-	11,11,11	2.62	2 (18%)	13,15,15	0.95	1 (7%)
3	P9P	B	404	-	11,11,11	2.59	2 (18%)	13,15,15	0.88	1 (7%)
2	SAH	A	401	-	27,28,28	1.04	4 (14%)	36,40,40	1.95	9 (25%)
3	P9P	A	403	-	11,11,11	2.49	2 (18%)	13,15,15	0.85	0
3	P9P	B	405	-	11,11,11	2.49	2 (18%)	13,15,15	0.91	0
2	SAH	B	402	-	27,28,28	1.01	3 (11%)	36,40,40	1.94	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	C	401	-	27,28,28	1.06	4 (14%)	36,40,40	1.94	9 (25%)
4	SO4	B	411	-	4,4,4	0.23	0	6,6,6	0.11	0
3	P9P	C	403	-	11,11,11	2.66	2 (18%)	13,15,15	0.81	0
3	P9P	A	405	-	11,11,11	2.73	2 (18%)	13,15,15	1.22	2 (15%)
3	P9P	A	406	-	11,11,11	2.69	2 (18%)	13,15,15	1.00	1 (7%)
4	SO4	B	409	-	4,4,4	0.25	0	6,6,6	0.24	0
3	P9P	B	406	-	11,11,11	2.72	2 (18%)	13,15,15	1.41	4 (30%)
3	P9P	C	404	-	11,11,11	2.67	2 (18%)	13,15,15	0.78	0
4	SO4	A	411	-	4,4,4	0.21	0	6,6,6	0.17	0
3	P9P	A	404	-	11,11,11	2.59	2 (18%)	13,15,15	1.12	1 (7%)
3	P9P	B	401	-	11,11,11	2.61	2 (18%)	13,15,15	1.04	2 (15%)
3	P9P	A	402	-	11,11,11	2.50	2 (18%)	13,15,15	1.16	1 (7%)

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	SAH	C	401	-	-	1/15/31/31	0/3/3/3
3	P9P	A	406	-	-	0/2/4/4	0/1/1/1
3	P9P	C	403	-	-	0/2/4/4	0/1/1/1
3	P9P	B	406	-	-	0/2/4/4	0/1/1/1
3	P9P	B	407	-	-	0/2/4/4	0/1/1/1
3	P9P	A	405	-	-	0/2/4/4	0/1/1/1
3	P9P	C	404	-	-	0/2/4/4	0/1/1/1
3	P9P	C	402	-	-	0/2/4/4	0/1/1/1
3	P9P	B	403	-	-	0/2/4/4	0/1/1/1
3	P9P	A	407	-	-	0/2/4/4	0/1/1/1
3	P9P	B	404	-	-	0/2/4/4	0/1/1/1
3	P9P	A	404	-	-	0/2/4/4	0/1/1/1
3	P9P	B	401	-	-	0/2/4/4	0/1/1/1
2	SAH	A	401	-	-	2/15/31/31	0/3/3/3
3	P9P	A	403	-	-	0/2/4/4	0/1/1/1
3	P9P	A	402	-	-	0/2/4/4	0/1/1/1
3	P9P	B	405	-	-	0/2/4/4	0/1/1/1
2	SAH	B	402	-	-	2/15/31/31	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	406	P9P	O06-N05	8.38	1.37	1.22
3	A	405	P9P	O06-N05	8.35	1.37	1.22
3	A	406	P9P	O06-N05	8.29	1.37	1.22
3	B	407	P9P	O06-N05	8.26	1.37	1.22
3	C	404	P9P	O06-N05	8.21	1.36	1.22
3	C	403	P9P	O06-N05	8.16	1.36	1.22
3	B	403	P9P	O06-N05	8.14	1.36	1.22
3	C	402	P9P	O06-N05	8.14	1.36	1.22
3	A	407	P9P	O06-N05	8.03	1.36	1.22
3	B	401	P9P	O06-N05	7.88	1.36	1.22
3	A	404	P9P	O06-N05	7.88	1.36	1.22
3	B	404	P9P	O06-N05	7.86	1.36	1.22
3	B	405	P9P	O06-N05	7.61	1.35	1.22
3	A	403	P9P	O06-N05	7.42	1.35	1.22
3	A	402	P9P	O06-N05	7.37	1.35	1.22
2	A	401	SAH	C8-N7	2.66	1.36	1.31
2	C	401	SAH	C2-N1	2.55	1.38	1.33
3	A	405	P9P	O11-C10	2.53	1.41	1.36
3	B	401	P9P	O11-C10	2.53	1.41	1.36
3	A	403	P9P	O11-C10	2.47	1.41	1.36
2	A	401	SAH	C2-N1	2.47	1.38	1.33
2	B	402	SAH	C2-N3	2.42	1.38	1.33
2	B	402	SAH	C8-N7	2.38	1.36	1.31
3	A	404	P9P	O11-C10	2.38	1.41	1.36
2	C	401	SAH	OXT-C	-2.35	1.23	1.30
3	C	404	P9P	O11-C10	2.34	1.41	1.36
3	C	403	P9P	O11-C10	2.33	1.41	1.36
3	B	407	P9P	O11-C10	2.28	1.40	1.36
3	A	407	P9P	O11-C10	2.27	1.40	1.36
2	C	401	SAH	C2-N3	2.26	1.37	1.33
2	B	402	SAH	C2-N1	2.25	1.37	1.33
3	B	404	P9P	O11-C10	2.22	1.40	1.36
3	A	406	P9P	O11-C10	2.20	1.40	1.36
3	A	402	P9P	O11-C10	2.19	1.40	1.36
3	C	402	P9P	O11-C10	2.15	1.40	1.36
2	A	401	SAH	OXT-C	-2.13	1.23	1.30
3	B	405	P9P	O11-C10	2.13	1.40	1.36
3	B	406	P9P	O11-C10	2.12	1.40	1.36
3	B	403	P9P	O11-C10	2.09	1.40	1.36
2	A	401	SAH	C2-N3	2.08	1.37	1.33
2	C	401	SAH	C8-N7	2.06	1.35	1.31

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	N3-C2-N1	-6.16	119.26	128.58
2	C	401	SAH	N3-C2-N1	-5.74	119.89	128.58
2	B	402	SAH	N3-C2-N1	-5.67	120.00	128.58
2	B	402	SAH	N9-C8-N7	-4.24	107.92	113.94
2	A	401	SAH	N9-C8-N7	-4.22	107.94	113.94
2	C	401	SAH	C5-C4-N3	-4.18	120.95	126.72
2	B	402	SAH	C5-C4-N3	-3.81	121.47	126.72
2	A	401	SAH	C5-C4-N3	-3.68	121.65	126.72
2	C	401	SAH	N9-C8-N7	-3.56	108.89	113.94
2	B	402	SAH	C5-N7-C8	3.39	108.78	103.45
2	C	401	SAH	C2-N3-C4	3.39	120.11	111.83
2	C	401	SAH	C5'-SD-CG	-3.32	92.41	102.26
2	A	401	SAH	C2-N3-C4	3.29	119.88	111.83
2	B	402	SAH	C2-N3-C4	3.24	119.73	111.83
2	C	401	SAH	C5-N7-C8	3.09	108.31	103.45
2	A	401	SAH	C5-N7-C8	3.00	108.17	103.45
2	B	402	SAH	OXT-C-O	-3.00	117.28	124.08
2	A	401	SAH	OXT-C-O	-2.88	117.55	124.08
2	C	401	SAH	OXT-C-O	-2.85	117.61	124.08
3	A	402	P9P	C09-C10-C02	2.77	121.09	118.49
2	B	402	SAH	C4-C5-N7	-2.67	107.52	110.58
2	C	401	SAH	N3-C4-N9	2.66	131.69	127.17
2	A	401	SAH	C4-N9-C8	2.56	108.43	105.74
2	B	402	SAH	C4-N9-C8	2.49	108.36	105.74
3	A	405	P9P	C09-C10-C02	2.40	120.74	118.49
2	A	401	SAH	N3-C4-N9	2.39	131.24	127.17
2	A	401	SAH	C5'-SD-CG	-2.39	95.17	102.26
2	C	401	SAH	C4-C5-N7	-2.39	107.85	110.58
3	B	406	P9P	C03-C02-CL1	2.38	122.34	118.45
3	B	403	P9P	C09-C10-C02	2.37	120.72	118.49
2	B	402	SAH	N3-C4-N9	2.32	131.11	127.17
2	B	402	SAH	C5'-SD-CG	-2.30	95.43	102.26
3	B	406	P9P	C09-C10-C02	2.27	120.62	118.49
3	A	407	P9P	C09-C10-C02	2.26	120.61	118.49
3	B	401	P9P	C09-C10-C02	2.25	120.61	118.49
3	A	405	P9P	C03-C02-CL1	2.23	122.10	118.45
3	A	406	P9P	C09-C10-C02	2.22	120.58	118.49
3	B	401	P9P	C03-C02-C10	-2.18	119.65	120.92
3	C	402	P9P	C09-C10-C02	2.16	120.52	118.49
3	B	406	P9P	O06-N05-C04	2.12	121.74	118.82
3	B	407	P9P	C09-C10-C02	2.11	120.48	118.49
3	B	404	P9P	C09-C10-C02	2.10	120.46	118.49
3	B	406	P9P	C08-C04-N05	2.07	121.15	119.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	P9P	C08-C04-N05	2.05	121.13	119.34
3	A	404	P9P	C09-C10-C02	2.00	120.37	118.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SAH	C-CA-CB-CG
2	B	402	SAH	C-CA-CB-CG
2	C	401	SAH	CB-CG-SD-C5'
2	A	401	SAH	CB-CG-SD-C5'
2	B	402	SAH	CB-CG-SD-C5'

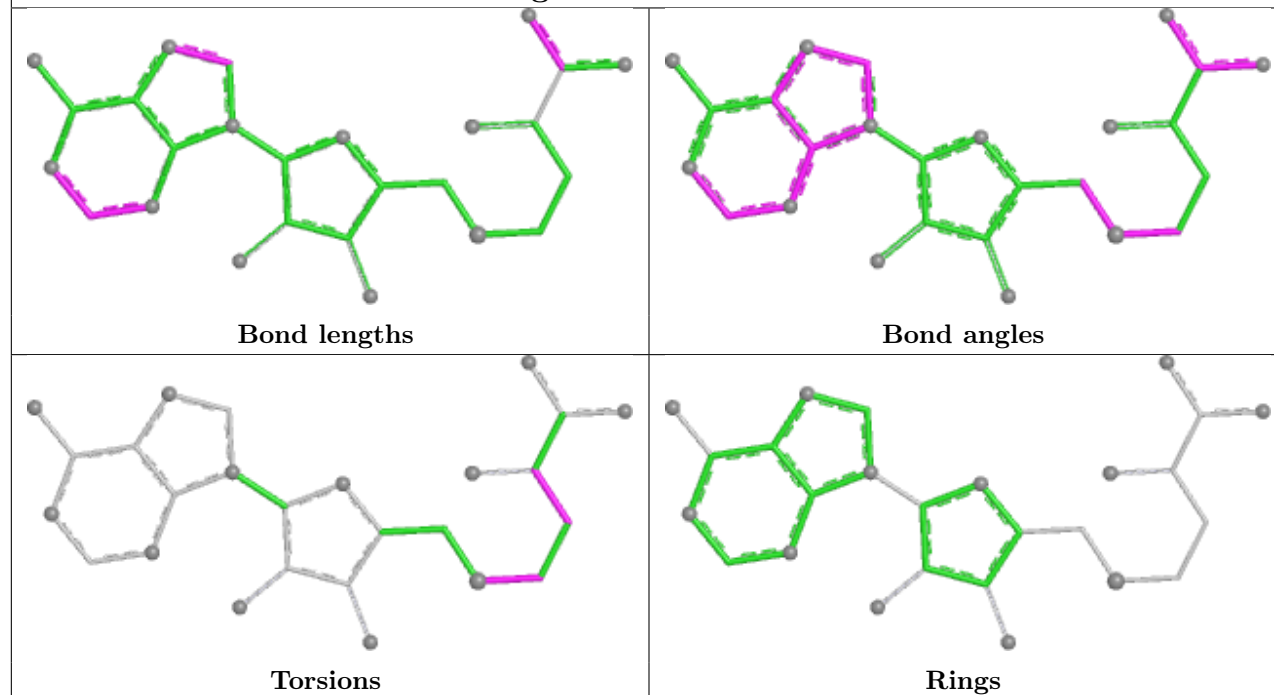
There are no ring outliers.

5 monomers are involved in 6 short contacts:

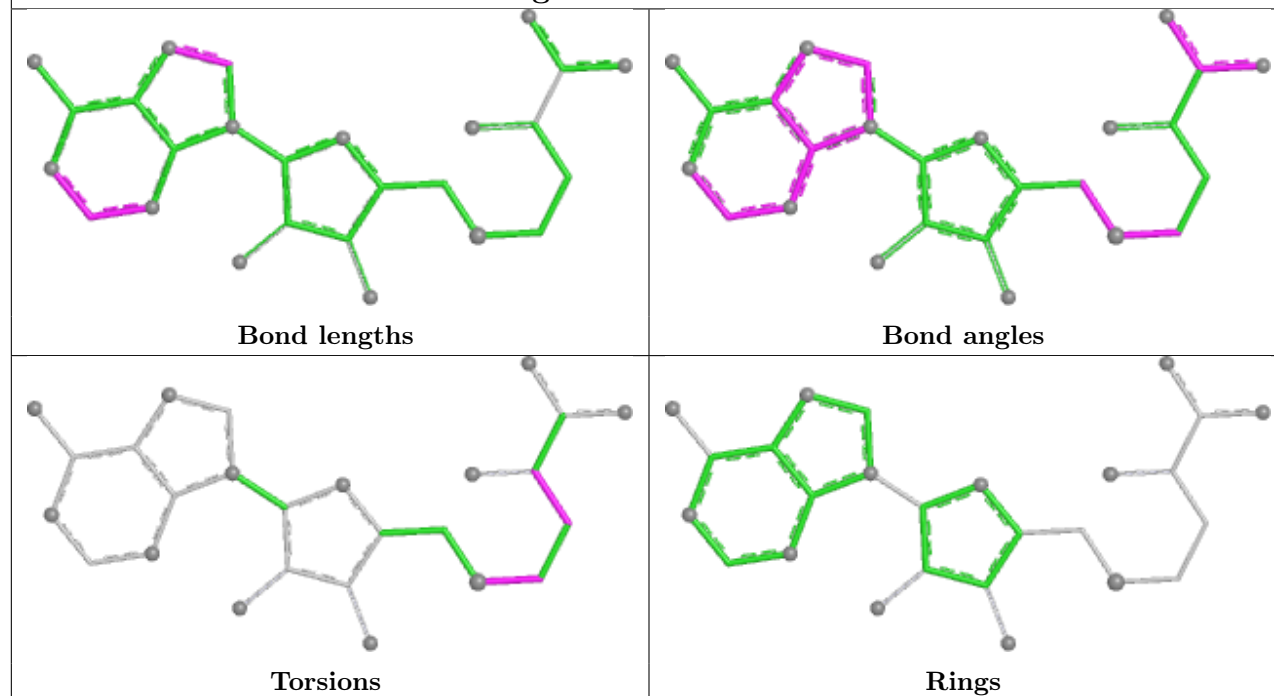
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	410	SO4	1	0
3	C	402	P9P	2	0
3	B	403	P9P	1	0
4	A	411	SO4	1	0
3	A	402	P9P	1	0

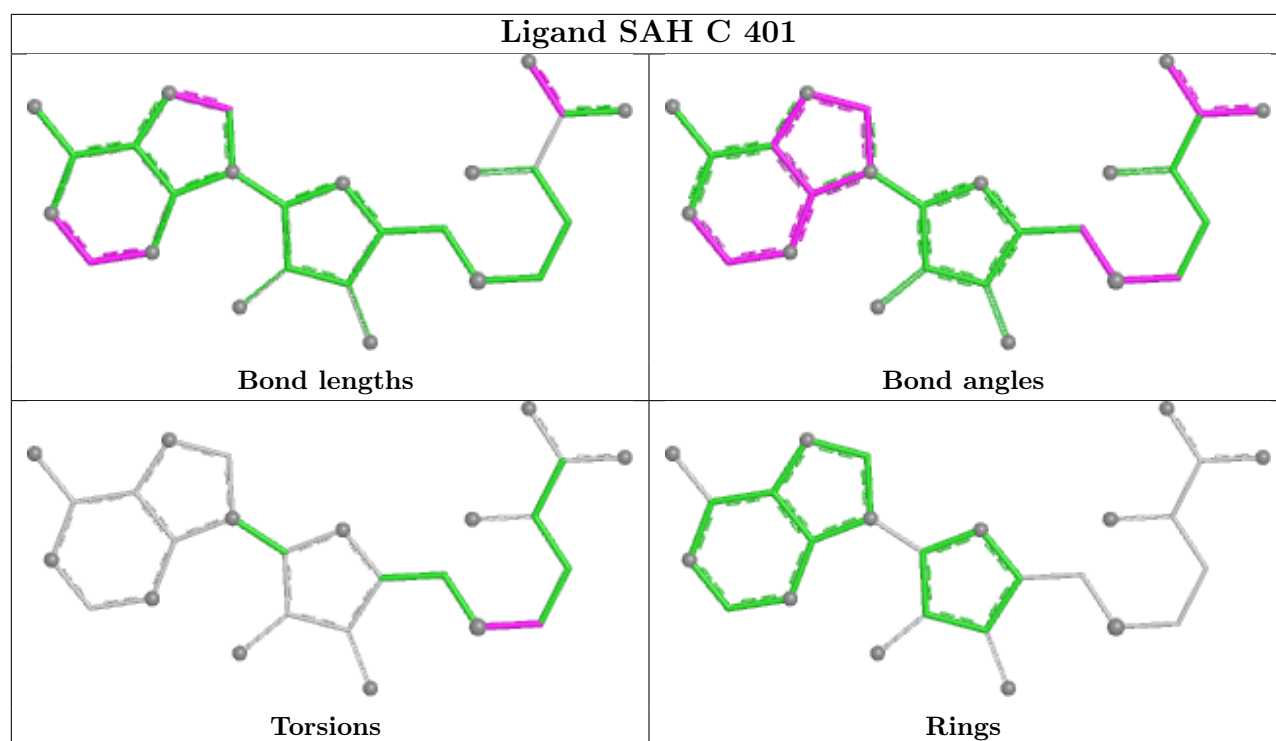
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 SAH A 401



Ligand SAH B 402





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	342/376 (90%)	-0.19	10 (2%) 53 60	7, 21, 44, 56	10 (2%)
1	B	340/376 (90%)	-0.20	9 (2%) 57 62	11, 24, 46, 73	4 (1%)
1	C	343/376 (91%)	0.55	40 (11%) 9 10	10, 39, 79, 111	2 (0%)
All	All	1025/1128 (90%)	0.06	59 (5%) 29 32	7, 26, 63, 111	16 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	VAL	6.4
1	C	167	ALA	5.5
1	C	168	PHE	5.5
1	C	163	ASP	5.2
1	C	223	LYS	4.5
1	C	353	ALA	4.3
1	C	165	ASP	4.2
1	C	170	ALA	3.5
1	C	200	ARG	3.4
1	B	52	LYS	3.2
1	C	218	ALA	3.2
1	C	164	GLN	3.2
1	C	82	ALA	3.1
1	C	244	ARG	3.0
1	C	199	ARG	2.9
1	C	222	LEU	2.8
1	C	341	PRO	2.8
1	B	13	GLN	2.7
1	B	14	ILE	2.7
1	A	213	GLY	2.6
1	B	81	ASP	2.6
1	C	342	TYR	2.5
1	A	324	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	352	ALA	2.5
1	C	169	ASP	2.5
1	C	215	VAL	2.5
1	C	338	PRO	2.5
1	C	230	ARG	2.4
1	C	224	ASP	2.4
1	A	224	ASP	2.4
1	B	165	ASP	2.4
1	B	224	ASP	2.4
1	C	217	THR	2.4
1	B	334	GLN	2.4
1	C	277	GLY	2.4
1	A	265[A]	ARG	2.3
1	C	229	ASP	2.3
1	C	227	LEU	2.3
1	A	326	GLY	2.3
1	B	59	ASP	2.3
1	C	182	HIS	2.3
1	C	202	PRO	2.2
1	C	221	TYR	2.2
1	A	244	ARG	2.2
1	C	340	ILE	2.2
1	C	204	VAL	2.2
1	A	319	ASP	2.2
1	C	162	CYS	2.1
1	C	181	ARG	2.1
1	C	336	PRO	2.1
1	C	172	ALA	2.1
1	C	334	GLN	2.1
1	C	228	SER	2.1
1	C	226	GLY	2.1
1	A	323	ALA	2.1
1	C	174	ALA	2.1
1	A	11	PRO	2.0
1	B	352	ALA	2.0
1	C	324	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

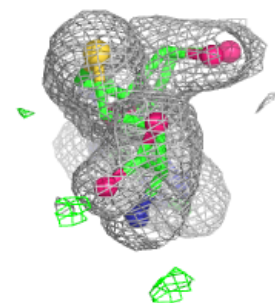
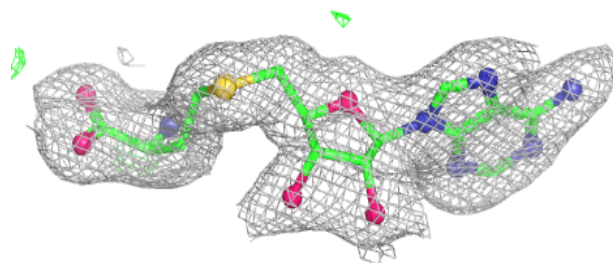
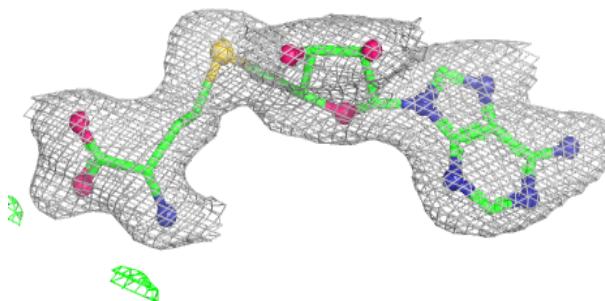
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	P9P	C	404	11/11	0.79	0.16	47,51,55,62	11
4	SO4	A	411	5/5	0.79	0.17	56,59,62,63	5
3	P9P	C	402	11/11	0.84	0.18	33,37,42,50	11
3	P9P	C	403	11/11	0.85	0.14	38,49,59,59	11
4	SO4	B	411	5/5	0.85	0.12	72,74,76,76	0
3	P9P	B	401	11/11	0.88	0.13	25,30,37,38	11
4	SO4	B	410	5/5	0.89	0.11	69,70,72,79	0
3	P9P	B	407	11/11	0.89	0.14	33,36,59,60	11
3	P9P	A	407	11/11	0.91	0.11	27,32,37,37	11
4	SO4	B	408	5/5	0.92	0.11	39,41,44,51	0
4	SO4	A	410	5/5	0.92	0.11	44,47,57,60	0
3	P9P	A	406	11/11	0.92	0.12	23,33,60,63	11
4	SO4	A	408	5/5	0.93	0.11	36,41,46,50	0
4	SO4	B	409	5/5	0.94	0.15	19,20,32,46	5
4	SO4	A	409	5/5	0.94	0.14	15,19,32,36	5
3	P9P	A	402	11/11	0.94	0.09	13,18,22,23	11
4	SO4	C	405	5/5	0.94	0.09	49,56,60,67	0
3	P9P	B	405	11/11	0.96	0.08	20,22,27,27	11
3	P9P	B	406	11/11	0.96	0.09	18,21,35,37	11
3	P9P	B	403	11/11	0.96	0.09	17,21,25,29	11
2	SAH	C	401	26/26	0.97	0.07	34,38,45,46	0
3	P9P	A	403	11/11	0.97	0.07	21,23,26,29	11
3	P9P	A	404	11/11	0.97	0.07	13,20,25,27	11
3	P9P	A	405	11/11	0.97	0.07	19,22,33,35	11
3	P9P	B	404	11/11	0.97	0.06	20,23,30,31	11
2	SAH	B	402	26/26	0.98	0.05	15,18,27,32	0
2	SAH	A	401	26/26	0.98	0.05	14,18,26,28	0

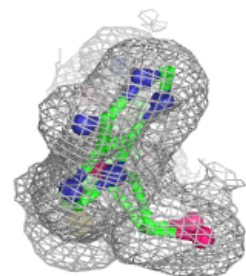
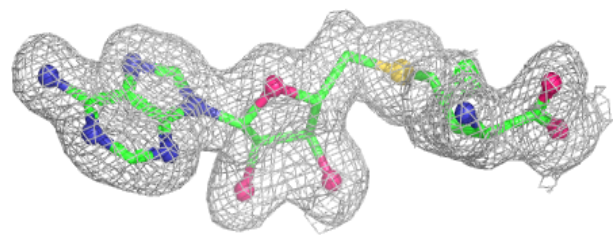
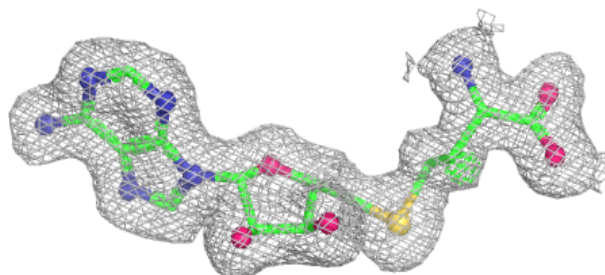
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

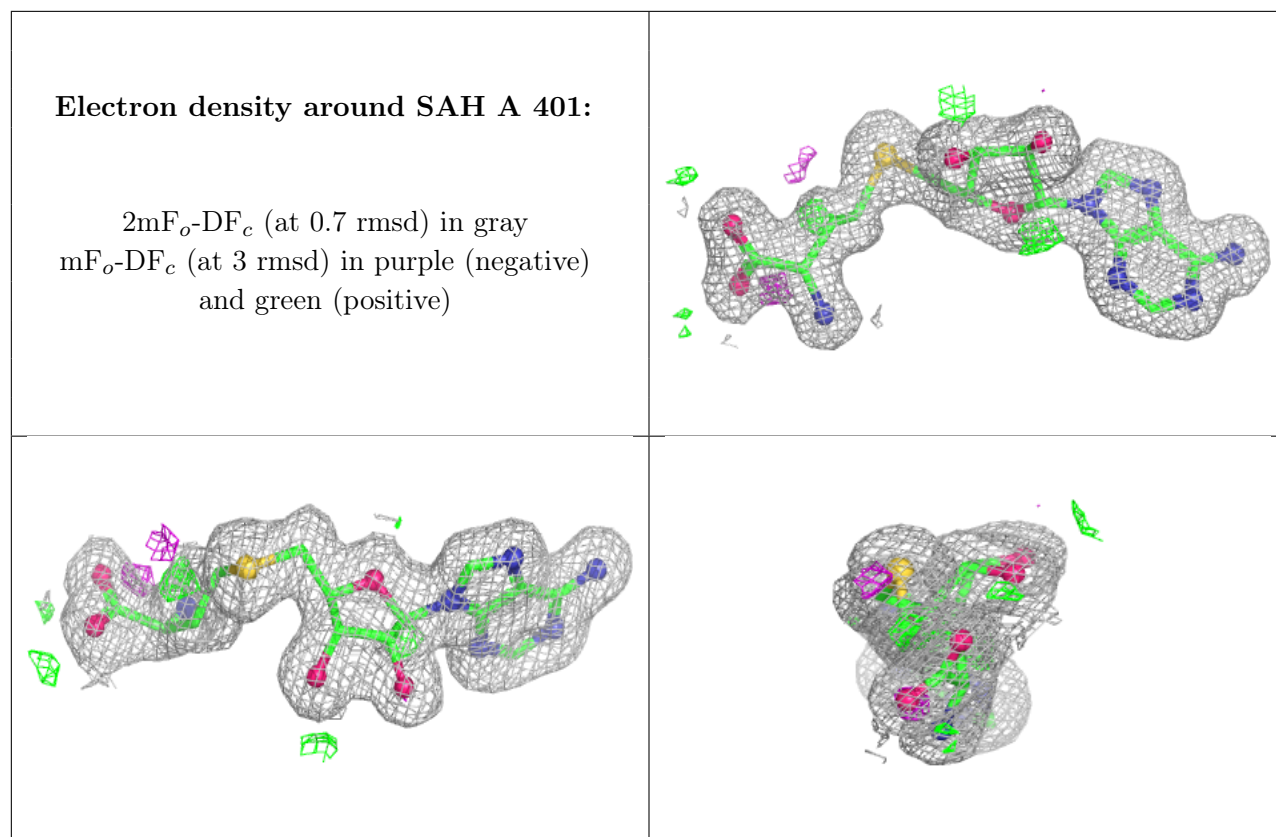
Electron density around SAH C 401:

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

**Electron density around SAH 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.