



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2026 – 02:20 AM JST

PDB ID : 9WBM / pdb_00009wbm
Title : O-methyltransferase CcOMT8
Authors : Wei, H.
Deposited on : 2025-08-14
Resolution : 2.58 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

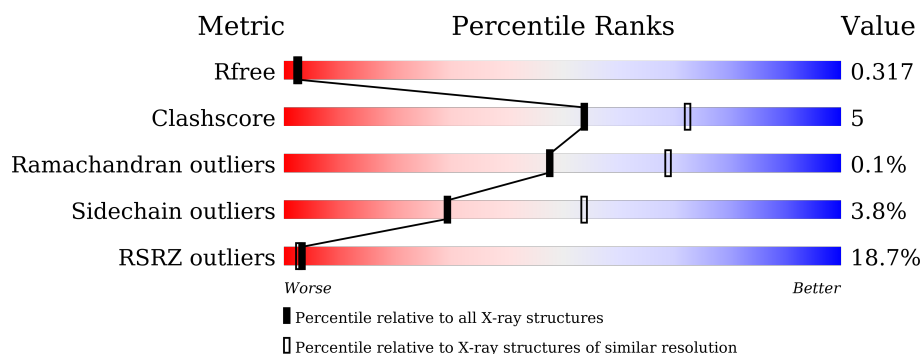
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	347	18% 87% 10% ..
1	B	347	18% 83% 15% ..
1	C	347	17% 84% 14% ..
1	D	347	21% 86% 12% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10935 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.

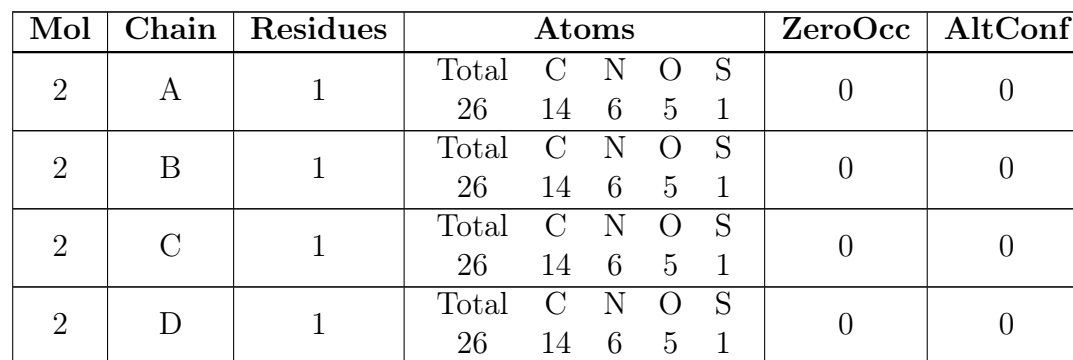
- Molecule 1 is a protein called 6-O-methyltransferase 2 (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2671	1706	446	496	23			
1	B	342	Total	C	N	O	S	0	0	0
			2671	1706	446	496	23			
1	C	342	Total	C	N	O	S	0	0	0
			2671	1706	446	496	23			
1	D	342	Total	C	N	O	S	0	0	0
			2671	1706	446	496	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A2Z5FRS5
A	2	GLU	-	expression tag	UNP A0A2Z5FRS5
B	1	MET	-	initiating methionine	UNP A0A2Z5FRS5
B	2	GLU	-	expression tag	UNP A0A2Z5FRS5
C	1	MET	-	initiating methionine	UNP A0A2Z5FRS5
C	2	GLU	-	expression tag	UNP A0A2Z5FRS5
D	1	MET	-	initiating methionine	UNP A0A2Z5FRS5
D	2	GLU	-	expression tag	UNP A0A2Z5FRS5

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

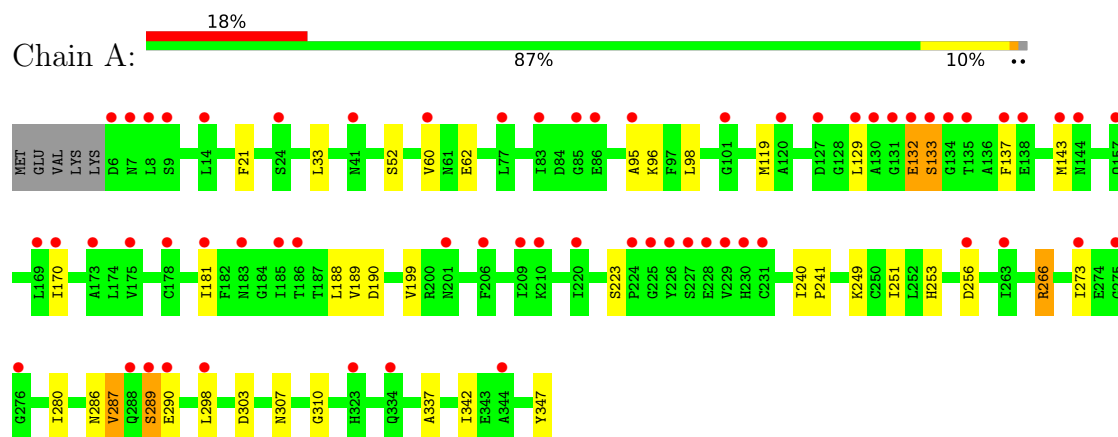


- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3 | A | 32 | Total O
32 32 | 0 | 0 |
| 3 | B | 34 | Total O
34 34 | 0 | 0 |
| 3 | C | 45 | Total O
45 45 | 0 | 0 |
| 3 | D | 36 | Total O
36 36 | 0 | 0 |

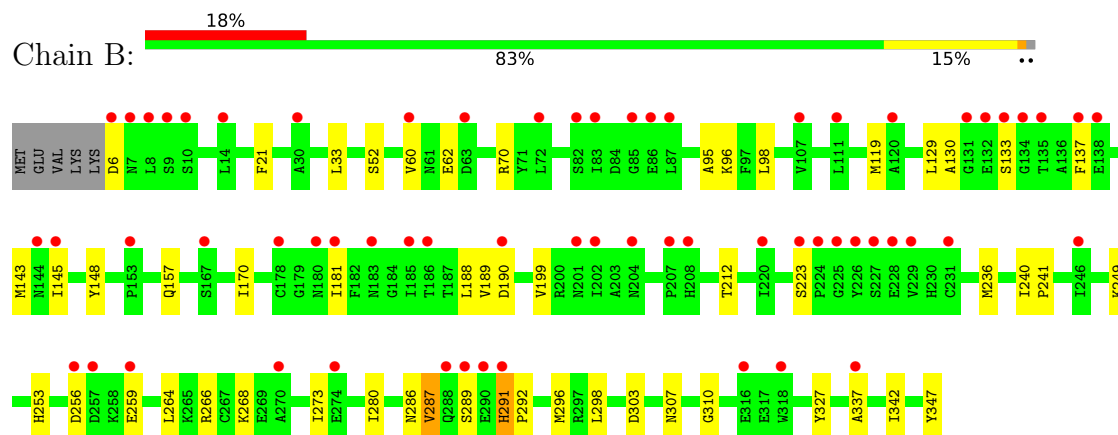
3 Residue-property plots [i](#)

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.

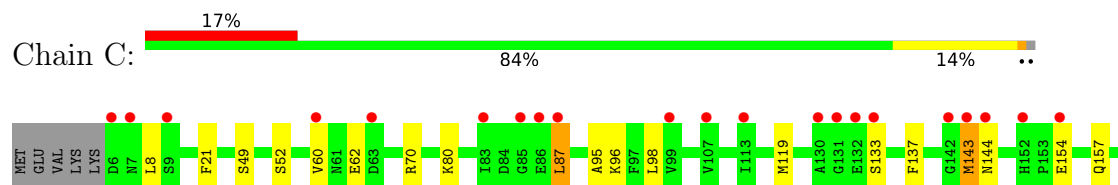
• Molecule 1: 6-O-methyltransferase 2 (Fragment)

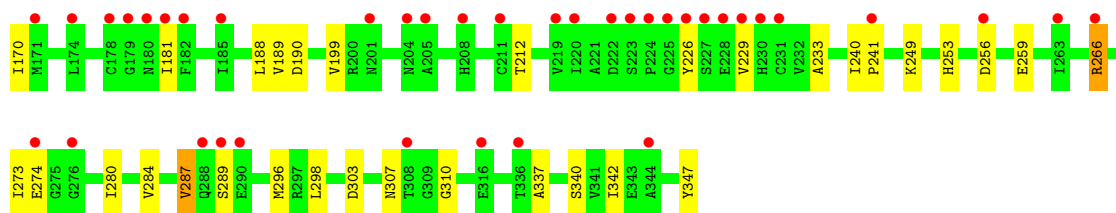


• Molecule 1: 6-O-methyltransferase 2 (Fragment)

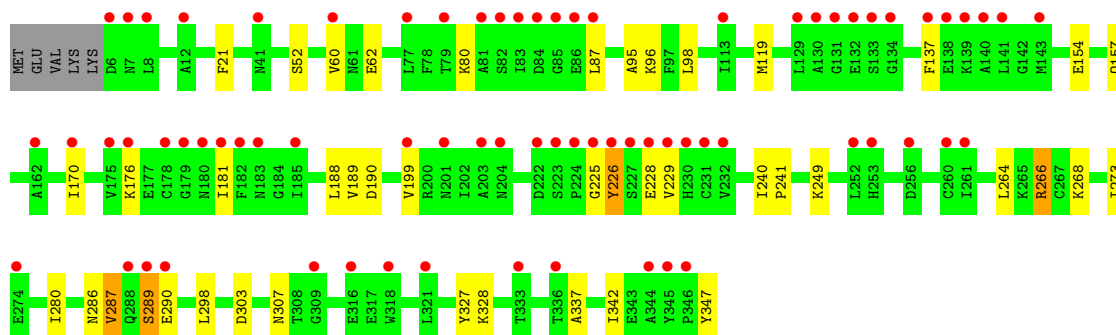
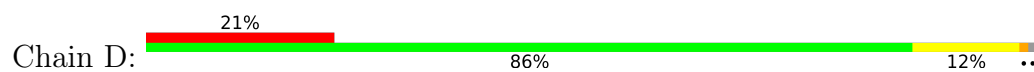


• Molecule 1: 6-O-methyltransferase 2 (Fragment)





● Molecule 1: 6-O-methyltransferase 2 (Fragment)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.99Å 78.04Å 90.62Å 86.22° 89.57° 84.28°	Depositor
Resolution (Å)	49.21 – 2.58 49.21 – 2.58	Depositor EDS
% Data completeness (in resolution range)	94.3 (49.21-2.58) 94.3 (49.21-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.269 , 0.310 0.275 , 0.317	Depositor DCC
R_{free} test set	2385 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10935	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.42% 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: 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	0.72	0/2729	0.88	1/3692 (0.0%)
1	B	0.72	0/2729	0.88	2/3692 (0.1%)
1	C	0.72	0/2729	0.88	1/3692 (0.0%)
1	D	0.71	0/2729	0.88	0/3692
All	All	0.72	0/10916	0.88	4/14768 (0.0%)

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
1	A	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ALA	N-CA-C	5.97	118.13	108.41
1	C	289	SER	N-CA-C	5.51	117.81	110.53
1	A	251	ILE	CB-CA-C	-5.24	106.46	111.44
1	B	145	ILE	N-CA-C	5.15	115.77	110.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLU	Peptide
1	A	290	GLU	Peptide
1	D	290	GLU	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	2671	0	2667	23	0
1	B	2671	0	2667	33	0
1	C	2671	0	2667	29	0
1	D	2671	0	2667	29	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
2	C	26	0	19	1	0
2	D	26	0	19	1	0
3	A	32	0	0	1	0
3	B	34	0	0	2	0
3	C	45	0	0	2	0
3	D	36	0	0	4	0
All	All	10935	0	10744	106	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 5.

All (106) 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:A:52:SER:HB3	1:A:60:VAL:HG11	1.46	0.95
1:D:52:SER:HB3	1:D:60:VAL:HG11	1.48	0.95
1:B:52:SER:HB3	1:B:60:VAL:HG11	1.46	0.94
1:C:52:SER:HB3	1:C:60:VAL:HG11	1.48	0.93
1:C:143:MET:HE3	1:C:144:ASN:HD22	1.32	0.93
1:B:291:HIS:HB2	1:B:292:PRO:CD	2.20	0.71
1:C:154:GLU:HB2	3:C:738:HOH:O	1.94	0.66
1:D:225:GLY:O	1:D:226:TYR:C	2.39	0.66
1:D:154:GLU:HB2	3:D:731:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:N	1:D:87:LEU:HD12	2.15	0.61
1:A:190:ASP:HB2	1:A:199:VAL:CG1	2.30	0.61
1:D:328:LYS:HD2	3:D:703:HOH:O	2.01	0.60
1:B:190:ASP:HB2	1:B:199:VAL:CG1	2.32	0.59
1:C:190:ASP:HB2	1:C:199:VAL:CG1	2.33	0.59
1:B:253:HIS:HA	3:B:716:HOH:O	2.02	0.58
1:D:190:ASP:HB2	1:D:199:VAL:CG1	2.33	0.58
1:B:291:HIS:HB2	1:B:292:PRO:HD3	1.87	0.57
1:C:143:MET:HE3	1:C:144:ASN:ND2	2.12	0.57
1:D:137:PHE:HB2	1:D:307:ASN:HA	1.87	0.57
1:A:137:PHE:HB2	1:A:307:ASN:HA	1.87	0.56
1:A:249:LYS:O	2:A:601:SAH:N	2.39	0.56
1:D:286:ASN:ND2	1:D:289:SER:OG	2.38	0.56
1:B:236:MET:O	1:B:266:ARG:NH1	2.39	0.55
1:A:286:ASN:ND2	1:A:289:SER:OG	2.39	0.55
1:C:95:ALA:HA	1:C:98:LEU:HG	1.89	0.55
1:B:95:ALA:HA	1:B:98:LEU:HG	1.89	0.54
1:D:170:ILE:HD11	1:D:249:LYS:CE	2.37	0.54
1:C:137:PHE:HB2	1:C:307:ASN:HA	1.87	0.54
1:B:137:PHE:HB2	1:B:307:ASN:HA	1.88	0.54
1:A:95:ALA:HA	1:A:98:LEU:HG	1.90	0.53
1:D:273:ILE:HA	1:D:347:TYR:CD2	2.44	0.53
1:C:170:ILE:HD11	1:C:249:LYS:CE	2.39	0.53
1:C:256:ASP:OD1	1:C:256:ASP:C	2.52	0.53
1:D:95:ALA:HA	1:D:98:LEU:HG	1.90	0.53
1:C:273:ILE:HA	1:C:347:TYR:CD2	2.43	0.53
1:A:273:ILE:HA	1:A:347:TYR:CD2	2.44	0.52
1:B:256:ASP:OD1	1:B:256:ASP:C	2.52	0.52
1:A:170:ILE:HD11	1:A:249:LYS:CE	2.39	0.52
1:A:303:ASP:OD1	1:A:307:ASN:ND2	2.43	0.52
1:A:256:ASP:OD1	1:A:256:ASP:C	2.52	0.52
1:B:170:ILE:HD11	1:B:249:LYS:CE	2.40	0.52
1:D:303:ASP:OD1	1:D:307:ASN:ND2	2.43	0.52
1:B:273:ILE:HA	1:B:347:TYR:CD2	2.44	0.52
1:D:80:LYS:HE3	1:D:87:LEU:HD23	1.91	0.52
1:B:291:HIS:CB	1:B:292:PRO:CD	2.87	0.51
1:B:303:ASP:OD1	1:B:307:ASN:ND2	2.43	0.51
1:C:303:ASP:OD1	1:C:307:ASN:ND2	2.43	0.51
1:C:280:ILE:HB	1:C:342:ILE:HB	1.93	0.51
1:B:286:ASN:ND2	1:B:289:SER:OG	2.42	0.50
1:C:274:GLU:O	1:C:274:GLU:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:CG	1:B:119:MET:HE3	2.48	0.49
1:C:21:PHE:CG	1:D:119:MET:HE3	2.47	0.49
1:C:119:MET:HE3	1:D:21:PHE:CG	2.48	0.48
1:D:240:ILE:HD12	1:D:266:ARG:HB3	1.94	0.48
1:A:240:ILE:HD12	1:A:266:ARG:HB3	1.95	0.48
1:B:280:ILE:HB	1:B:342:ILE:HB	1.96	0.48
1:D:280:ILE:HB	1:D:342:ILE:HB	1.94	0.48
1:D:189:VAL:HG21	1:D:241:PRO:HB2	1.96	0.48
1:B:189:VAL:HG21	1:B:241:PRO:HB2	1.95	0.48
1:D:170:ILE:CG2	3:D:727:HOH:O	2.61	0.48
1:D:287:VAL:HG22	1:D:298:LEU:HD22	1.95	0.48
1:B:240:ILE:HD12	1:B:266:ARG:HB3	1.96	0.47
1:A:129:LEU:HD12	1:B:33:LEU:HD11	1.95	0.47
1:A:287:VAL:HG22	1:A:298:LEU:HD22	1.96	0.47
1:C:240:ILE:HD12	1:C:266:ARG:HB3	1.96	0.47
1:C:287:VAL:HG22	1:C:298:LEU:HD22	1.97	0.47
1:A:280:ILE:HB	1:A:342:ILE:HB	1.96	0.47
1:C:189:VAL:HG21	1:C:241:PRO:HB2	1.97	0.46
1:D:170:ILE:HG23	3:D:727:HOH:O	2.16	0.46
1:A:119:MET:HE3	1:B:21:PHE:CG	2.50	0.46
1:B:199:VAL:HG22	3:B:721:HOH:O	2.15	0.46
1:A:199:VAL:HG22	3:A:710:HOH:O	2.16	0.45
1:D:249:LYS:O	2:D:601:SAH:N	2.49	0.45
1:B:287:VAL:HG22	1:B:298:LEU:HD22	1.99	0.45
1:C:233:ALA:N	3:C:704:HOH:O	2.37	0.45
1:C:170:ILE:HG22	1:C:337:ALA:HB1	1.99	0.44
1:D:87:LEU:HD12	1:D:87:LEU:H	1.82	0.44
1:A:189:VAL:HG21	1:A:241:PRO:HB2	1.99	0.44
1:A:132:GLU:O	1:A:133:SER:HB2	2.18	0.44
1:D:170:ILE:HD11	1:D:249:LYS:HE2	1.99	0.44
1:C:80:LYS:HD2	1:C:87:LEU:HD21	2.00	0.43
1:C:226:TYR:HB2	1:C:229:VAL:O	2.18	0.43
1:C:249:LYS:O	2:C:601:SAH:N	2.52	0.43
1:C:70:ARG:HD2	1:D:287:VAL:HG21	2.00	0.42
1:B:291:HIS:HB2	1:B:292:PRO:HD2	1.96	0.42
1:B:264:LEU:O	1:B:327:TYR:OH	2.36	0.42
1:D:80:LYS:CE	1:D:87:LEU:HD23	2.49	0.42
1:A:170:ILE:HG22	1:A:337:ALA:HB1	2.02	0.42
1:B:170:ILE:HD11	1:B:249:LYS:HE2	2.01	0.42
1:B:143:MET:HG3	1:B:148:TYR:HB2	2.01	0.42
1:A:287:VAL:HG21	1:B:70:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ILE:HD11	1:C:249:LYS:HE2	2.02	0.41
1:C:296:MET:HE2	1:C:296:MET:HB2	1.99	0.41
1:B:253:HIS:O	1:B:310:GLY:HA3	2.20	0.41
1:A:253:HIS:O	1:A:310:GLY:HA3	2.21	0.41
1:D:264:LEU:O	1:D:327:TYR:OH	2.36	0.41
1:B:189:VAL:HG22	1:B:212:THR:HB	2.03	0.41
1:B:296:MET:HE2	1:B:296:MET:HB2	2.00	0.41
1:C:253:HIS:O	1:C:310:GLY:HA3	2.21	0.41
1:B:170:ILE:HG22	1:B:337:ALA:HB1	2.03	0.41
1:C:284:VAL:HG23	1:C:340:SER:HB2	2.03	0.41
1:A:33:LEU:HD11	1:B:129:LEU:HD12	2.02	0.40
1:D:268:LYS:HE2	1:D:347:TYR:CE1	2.56	0.40
1:D:170:ILE:HG22	1:D:337:ALA:HB1	2.02	0.40
1:B:268:LYS:HE2	1:B:347:TYR:CE1	2.57	0.40
1:C:189:VAL:HG22	1:C:212:THR:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/347 (98%)	335 (98%)	5 (2%)	0	100	100
1	B	340/347 (98%)	334 (98%)	5 (2%)	1 (0%)	36	56
1	C	340/347 (98%)	335 (98%)	5 (2%)	0	100	100
1	D	340/347 (98%)	337 (99%)	2 (1%)	1 (0%)	36	56
All	All	1360/1388 (98%)	1341 (99%)	17 (1%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	226	TYR
1	B	291	HIS

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	289/294 (98%)	279 (96%)	10 (4%)	32	57
1	B	289/294 (98%)	279 (96%)	10 (4%)	32	57
1	C	289/294 (98%)	276 (96%)	13 (4%)	24	47
1	D	289/294 (98%)	278 (96%)	11 (4%)	29	54
All	All	1156/1176 (98%)	1112 (96%)	44 (4%)	29	54

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	96	LYS
1	A	133	SER
1	A	143	MET
1	A	181	ILE
1	A	188	LEU
1	A	223	SER
1	A	266	ARG
1	A	287	VAL
1	A	289	SER
1	B	6	ASP
1	B	62	GLU
1	B	96	LYS
1	B	133	SER
1	B	157	GLN
1	B	181	ILE
1	B	188	LEU
1	B	223	SER
1	B	259	GLU
1	B	287	VAL

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Mol	Chain	Res	Type
1	C	8	LEU
1	C	49	SER
1	C	62	GLU
1	C	87	LEU
1	C	96	LYS
1	C	133	SER
1	C	143	MET
1	C	157	GLN
1	C	181	ILE
1	C	188	LEU
1	C	259	GLU
1	C	266	ARG
1	C	287	VAL
1	D	62	GLU
1	D	96	LYS
1	D	157	GLN
1	D	176	LYS
1	D	181	ILE
1	D	188	LEU
1	D	228	GLU
1	D	229	VAL
1	D	266	ARG
1	D	287	VAL
1	D	289	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	40	HIS
1	A	61	ASN
1	A	144	ASN
1	A	286	ASN
1	B	11	GLN
1	B	40	HIS
1	B	144	ASN
1	C	11	GLN
1	C	40	HIS
1	C	61	ASN
1	C	144	ASN
1	C	288	GLN
1	D	11	GLN

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Mol	Chain	Res	Type
1	D	40	HIS
1	D	144	ASN
1	D	286	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	SAH	D	601	-	27,28,28	1.32	5 (18%)	38,40,40	2.00	9 (23%)
2	SAH	B	601	-	27,28,28	1.26	4 (14%)	38,40,40	2.25	12 (31%)
2	SAH	A	601	-	27,28,28	1.38	5 (18%)	38,40,40	2.25	13 (34%)
2	SAH	C	601	-	27,28,28	1.36	4 (14%)	38,40,40	2.31	14 (36%)

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	D	601	-	-	0/15/31/31	0/3/3/3
2	SAH	B	601	-	-	0/15/31/31	0/3/3/3
2	SAH	A	601	-	-	0/15/31/31	0/3/3/3
2	SAH	C	601	-	-	4/15/31/31	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	SAH	C5-C4	3.70	1.45	1.39
2	A	601	SAH	C5-C4	3.17	1.44	1.39
2	D	601	SAH	C5-C4	3.14	1.44	1.39
2	B	601	SAH	C4-N9	-2.88	1.31	1.37
2	B	601	SAH	C5-C4	2.61	1.43	1.39
2	A	601	SAH	C5-C6	2.58	1.48	1.41
2	A	601	SAH	C4-N9	-2.55	1.32	1.37
2	C	601	SAH	C5-C6	2.54	1.48	1.41
2	D	601	SAH	C4-N9	-2.48	1.32	1.37
2	A	601	SAH	C5-N7	-2.44	1.34	1.39
2	C	601	SAH	C4-N9	-2.37	1.32	1.37
2	D	601	SAH	OXT-C	-2.33	1.22	1.30
2	B	601	SAH	OXT-C	-2.31	1.23	1.30
2	D	601	SAH	CG-SD	-2.21	1.73	1.81
2	B	601	SAH	C5-N7	-2.17	1.34	1.39
2	D	601	SAH	C5-N7	-2.08	1.35	1.39
2	C	601	SAH	OXT-C	-2.05	1.23	1.30
2	A	601	SAH	OXT-C	-2.01	1.24	1.30

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SAH	C5-C4-N3	-5.37	119.74	126.75
2	C	601	SAH	N3-C2-N1	-5.35	120.23	128.60
2	D	601	SAH	N3-C2-N1	-5.04	120.72	128.60
2	B	601	SAH	N3-C2-N1	-4.84	121.03	128.60
2	C	601	SAH	C5-C4-N3	-4.83	120.44	126.75
2	C	601	SAH	N3-C4-N9	4.64	134.73	127.08
2	A	601	SAH	O4'-C1'-N9	4.61	117.15	108.06
2	B	601	SAH	C4-N9-C8	4.61	110.72	105.73
2	C	601	SAH	C2-N3-C4	4.55	122.49	111.75
2	D	601	SAH	C5-C4-N3	-4.42	120.98	126.75
2	C	601	SAH	C4-N9-C8	4.38	110.47	105.73
2	A	601	SAH	C2-N3-C4	4.33	121.99	111.75
2	B	601	SAH	C5-C4-N3	-4.29	121.16	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SAH	N3-C2-N1	-4.28	121.91	128.60
2	B	601	SAH	C2-N3-C4	4.10	121.43	111.75
2	B	601	SAH	N3-C4-N9	4.08	133.81	127.08
2	D	601	SAH	N3-C4-N9	4.05	133.75	127.08
2	D	601	SAH	C2-N3-C4	4.01	121.22	111.75
2	B	601	SAH	O4'-C1'-N9	3.93	115.80	108.06
2	A	601	SAH	N3-C4-N9	3.73	133.23	127.08
2	D	601	SAH	C4-N9-C8	3.62	109.65	105.73
2	A	601	SAH	C4-C5-N7	-3.52	106.33	110.62
2	B	601	SAH	N9-C8-N7	-3.25	109.47	113.91
2	A	601	SAH	C6-C5-N7	3.23	138.04	132.02
2	C	601	SAH	N9-C8-N7	-3.00	109.81	113.91
2	C	601	SAH	C6-C5-N7	2.94	137.49	132.02
2	A	601	SAH	C5-N7-C8	2.90	107.63	103.51
2	B	601	SAH	C4-N9-C1'	-2.88	119.72	126.59
2	B	601	SAH	C6-C5-N7	2.78	137.19	132.02
2	D	601	SAH	C2-N1-C6	2.59	123.21	118.77
2	C	601	SAH	C2-N1-C6	2.56	123.17	118.77
2	A	601	SAH	OXT-C-O	-2.55	118.29	124.09
2	A	601	SAH	C4-N9-C8	2.54	108.48	105.73
2	C	601	SAH	OXT-C-CA	2.53	122.00	113.38
2	C	601	SAH	C5-N7-C8	2.52	107.08	103.51
2	D	601	SAH	OXT-C-O	-2.51	118.39	124.09
2	B	601	SAH	C5-N7-C8	2.50	107.06	103.51
2	A	601	SAH	N9-C8-N7	-2.47	110.53	113.91
2	B	601	SAH	C4-C5-N7	-2.39	107.71	110.62
2	D	601	SAH	N9-C8-N7	-2.35	110.70	113.91
2	C	601	SAH	C4-C5-N7	-2.30	107.82	110.62
2	C	601	SAH	OXT-C-O	-2.29	118.89	124.09
2	D	601	SAH	C6-C5-N7	2.28	136.27	132.02
2	B	601	SAH	OXT-C-O	-2.20	119.09	124.09
2	C	601	SAH	O2'-C2'-C1'	2.12	117.10	110.02
2	A	601	SAH	OXT-C-CA	2.10	120.55	113.38
2	C	601	SAH	C4-N9-C1'	-2.10	121.59	126.59
2	A	601	SAH	C4-N9-C1'	-2.06	121.70	126.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	SAH	C-CA-CB-CG
2	C	601	SAH	CB-CG-SD-C5'

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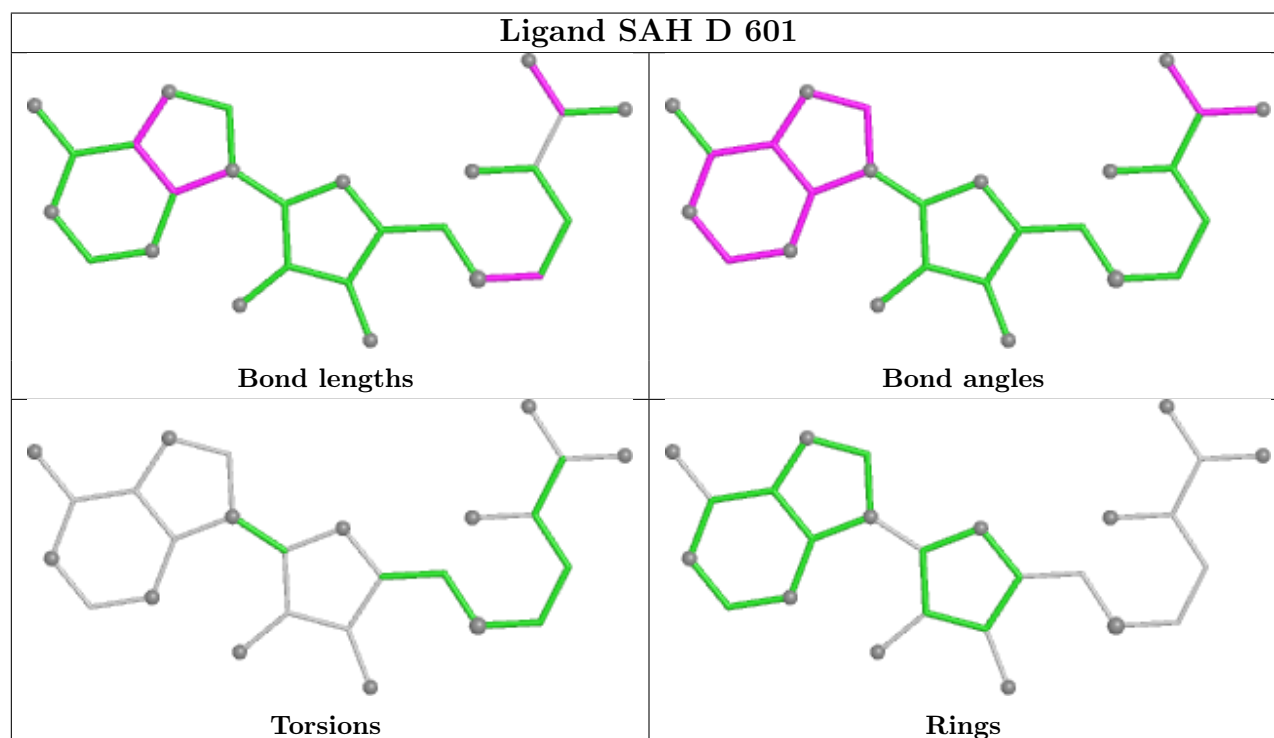
Mol	Chain	Res	Type	Atoms
2	C	601	SAH	N-CA-CB-CG
2	C	601	SAH	OXT-C-CA-N

There are no ring outliers.

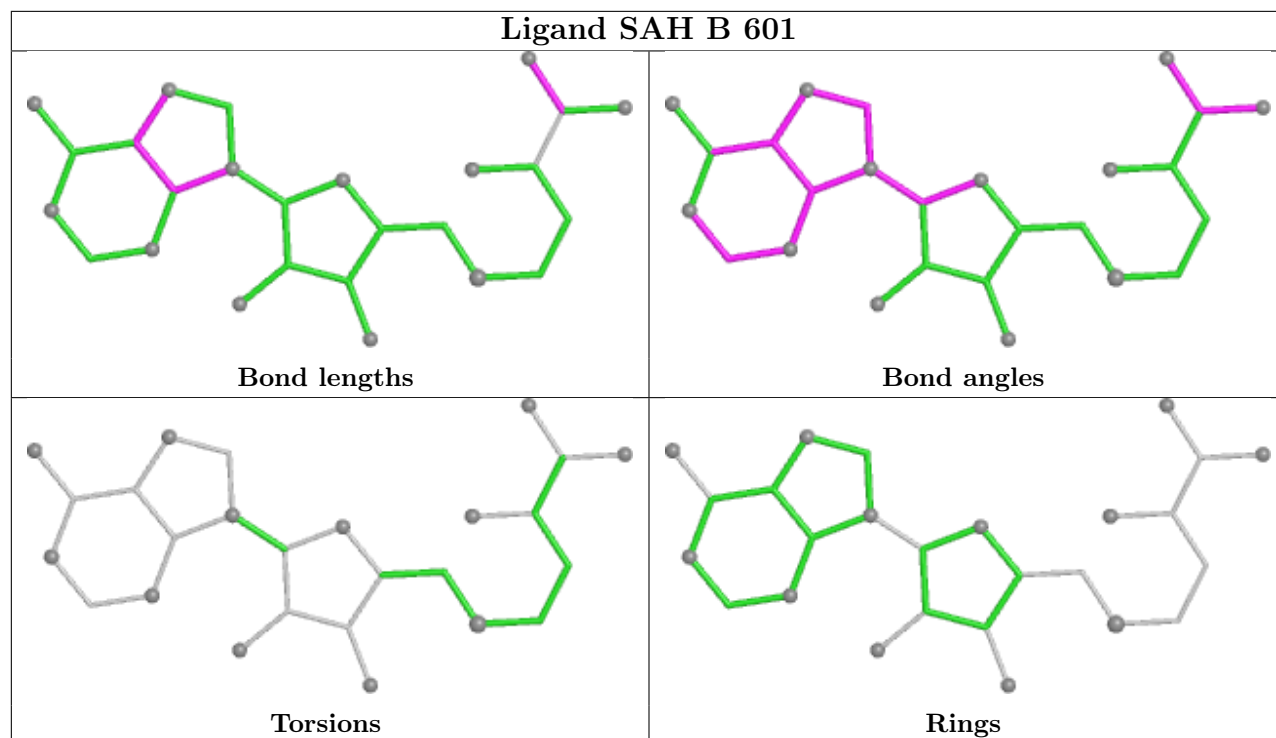
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	SAH	1	0
2	A	601	SAH	1	0
2	C	601	SAH	1	0

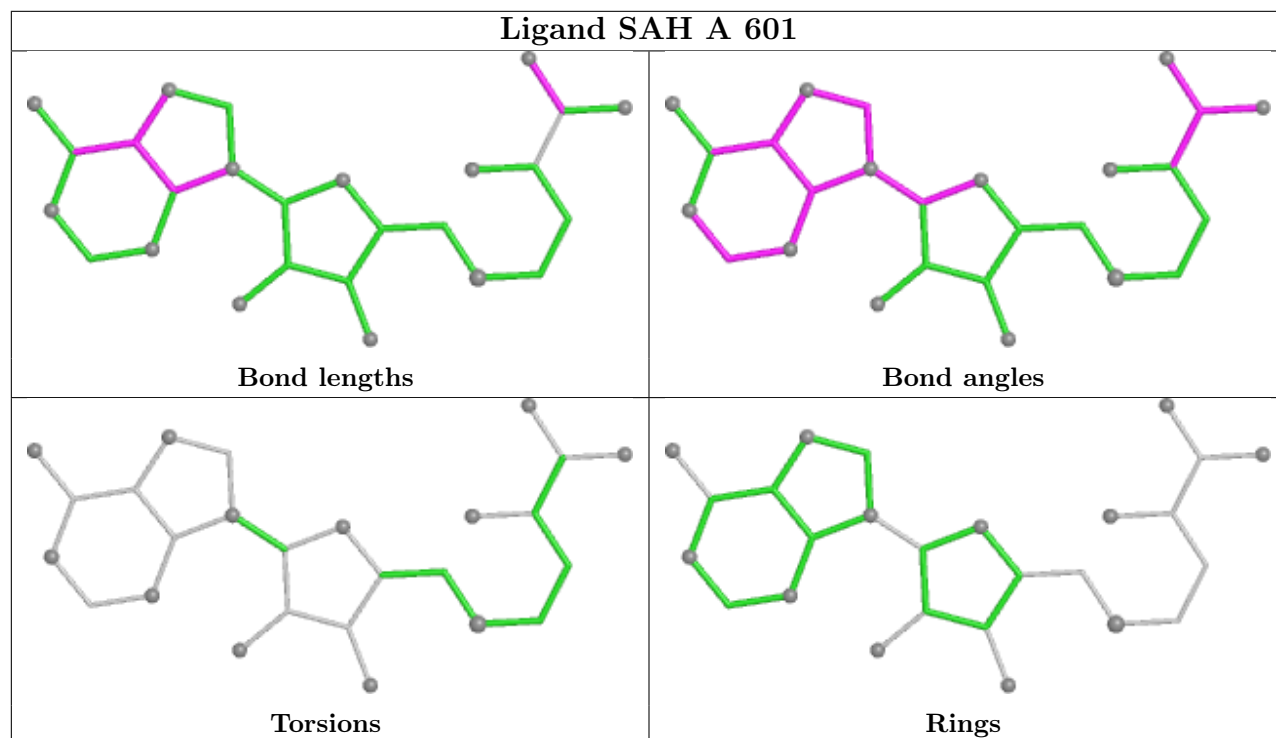
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

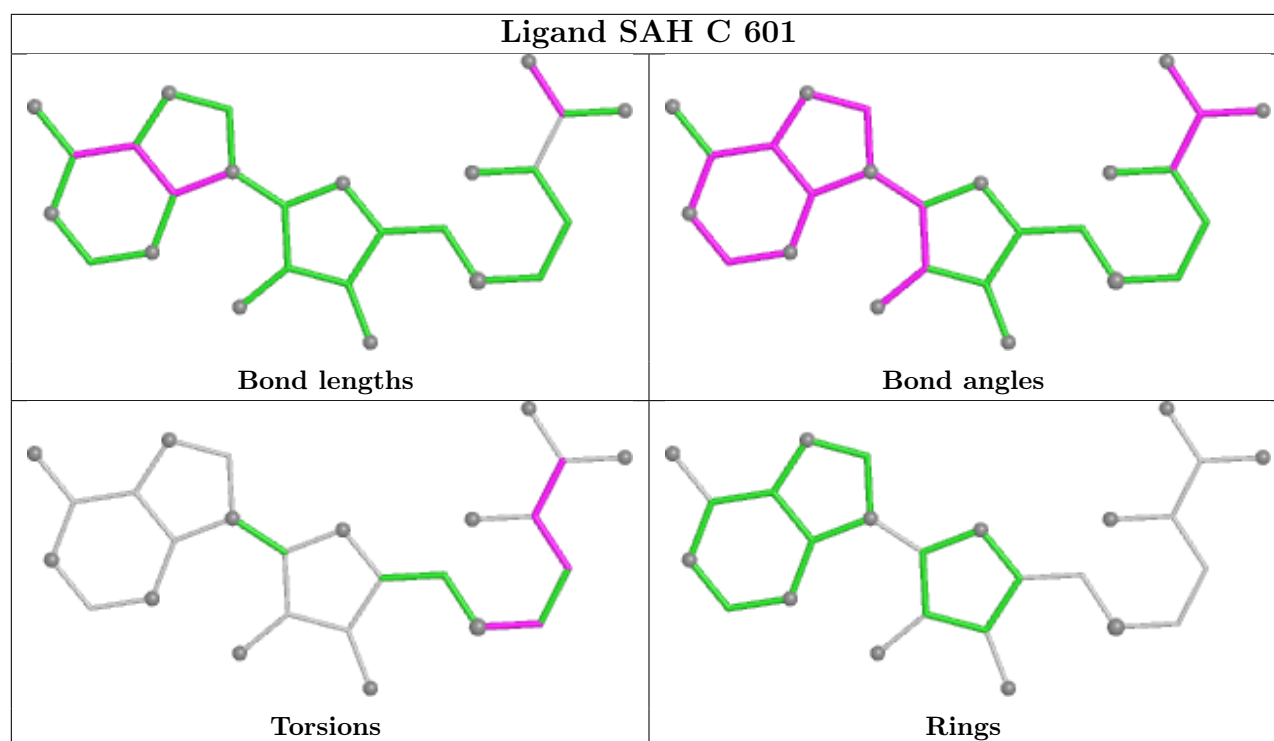


Ligand SAH B 601



Ligand SAH A 601





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	342/347 (98%)	1.31	62 (18%) 3 3	11, 21, 45, 80	0
1	B	342/347 (98%)	1.32	63 (18%) 3 3	13, 22, 48, 89	0
1	C	342/347 (98%)	1.28	59 (17%) 4 3	13, 23, 46, 73	0
1	D	342/347 (98%)	1.33	72 (21%) 2 2	11, 22, 49, 83	0
All	All	1368/1388 (98%)	1.31	256 (18%) 3 3	11, 22, 49, 89	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	ASN	8.4
1	C	226	TYR	7.6
1	D	226	TYR	7.6
1	D	130	ALA	7.3
1	D	131	GLY	7.3
1	A	131	GLY	7.2
1	B	229	VAL	6.7
1	C	201	ASN	6.6
1	A	6	ASP	6.6
1	C	131	GLY	6.5
1	B	6	ASP	6.5
1	B	225	GLY	6.5
1	A	226	TYR	6.4
1	B	226	TYR	6.3
1	A	227	SER	5.8
1	C	6	ASP	5.6
1	A	290	GLU	5.5
1	A	132	GLU	5.4
1	B	132	GLU	5.4
1	B	227	SER	5.2
1	A	225	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	344	ALA	5.1
1	B	131	GLY	5.1
1	D	224	PRO	5.1
1	C	228	GLU	5.0
1	D	133	SER	5.0
1	A	229	VAL	5.0
1	A	201	ASN	4.8
1	C	227	SER	4.7
1	A	101	GLY	4.7
1	D	289	SER	4.6
1	B	290	GLU	4.6
1	C	133	SER	4.6
1	D	7	ASN	4.6
1	A	224	PRO	4.5
1	B	228	GLU	4.5
1	B	7	ASN	4.4
1	D	290	GLU	4.4
1	A	181	ILE	4.4
1	D	182	PHE	4.4
1	A	289	SER	4.3
1	B	134	GLY	4.3
1	B	144	ASN	4.3
1	A	133	SER	4.3
1	D	227	SER	4.3
1	D	228	GLU	4.2
1	B	224	PRO	4.2
1	A	228	GLU	4.2
1	D	179	GLY	4.1
1	D	181	ILE	4.1
1	A	143	MET	4.1
1	C	229	VAL	4.0
1	A	288	GLN	4.0
1	B	289	SER	3.9
1	B	83	ILE	3.8
1	C	130	ALA	3.8
1	C	256	ASP	3.8
1	A	7	ASN	3.7
1	B	256	ASP	3.7
1	A	231	CYS	3.7
1	A	8	LEU	3.7
1	A	129	LEU	3.7
1	C	224	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	288	GLN	3.6
1	B	60	VAL	3.6
1	D	178	CYS	3.6
1	D	85	GLY	3.5
1	B	231	CYS	3.5
1	D	336	THR	3.5
1	D	316	GLU	3.5
1	C	7	ASN	3.4
1	A	186	THR	3.4
1	D	288	GLN	3.4
1	C	276	GLY	3.4
1	C	225	GLY	3.4
1	D	225	GLY	3.4
1	C	132	GLU	3.4
1	C	204	ASN	3.4
1	C	143	MET	3.3
1	C	231	CYS	3.3
1	A	334	GLN	3.3
1	B	82	SER	3.3
1	D	222	ASP	3.3
1	D	132	GLU	3.3
1	D	12	ALA	3.3
1	B	181	ILE	3.3
1	D	180	ASN	3.2
1	B	138	GLU	3.2
1	B	133	SER	3.2
1	D	6	ASP	3.2
1	B	201	ASN	3.2
1	C	179	GLY	3.2
1	C	220	ILE	3.1
1	D	8	LEU	3.1
1	A	185	ILE	3.1
1	D	143	MET	3.1
1	D	253	HIS	3.1
1	B	63	ASP	3.1
1	B	291	HIS	3.1
1	D	229	VAL	3.1
1	A	24	SER	3.0
1	C	185	ILE	3.0
1	D	87	LEU	3.0
1	B	178	CYS	3.0
1	C	87	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	230	HIS	3.0
1	A	134	GLY	3.0
1	D	86	GLU	2.9
1	B	186	THR	2.9
1	B	316	GLU	2.9
1	C	180	ASN	2.9
1	B	220	ILE	2.9
1	D	140	ALA	2.8
1	C	222	ASP	2.8
1	C	171	MET	2.8
1	C	83	ILE	2.8
1	C	344	ALA	2.8
1	D	321	LEU	2.8
1	D	113	ILE	2.7
1	A	77	LEU	2.7
1	D	333	THR	2.7
1	A	138	GLU	2.7
1	C	274	GLU	2.7
1	A	170	ILE	2.7
1	C	181	ILE	2.7
1	D	83	ILE	2.7
1	A	130	ALA	2.7
1	B	86	GLU	2.7
1	D	185	ILE	2.7
1	D	318	TRP	2.7
1	A	135	THR	2.7
1	A	157	GLN	2.7
1	B	85	GLY	2.7
1	C	60	VAL	2.7
1	B	30	ALA	2.7
1	D	223	SER	2.6
1	A	120	ALA	2.6
1	C	182	PHE	2.6
1	B	8	LEU	2.6
1	D	199	VAL	2.6
1	D	79	THR	2.6
1	A	276	GLY	2.6
1	D	346	PRO	2.6
1	B	9	SER	2.6
1	A	95	ALA	2.6
1	D	203	ALA	2.6
1	D	176	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	113	ILE	2.6
1	D	141	LEU	2.6
1	A	173	ALA	2.6
1	B	223	SER	2.6
1	D	134	GLY	2.5
1	A	83	ILE	2.5
1	A	137	PHE	2.5
1	B	107	VAL	2.5
1	D	41	ASN	2.5
1	C	223	SER	2.5
1	A	127	ASP	2.5
1	B	135	THR	2.5
1	C	154	GLU	2.5
1	D	309	GLY	2.5
1	D	261	ILE	2.5
1	B	87	LEU	2.5
1	C	174	LEU	2.5
1	D	175	VAL	2.5
1	B	337	ALA	2.5
1	A	275	GLY	2.4
1	B	10	SER	2.4
1	C	290	GLU	2.4
1	A	178	CYS	2.4
1	C	263	ILE	2.4
1	D	230	HIS	2.4
1	A	41	ASN	2.4
1	D	139	LYS	2.4
1	B	185	ILE	2.4
1	C	211	CYS	2.4
1	D	260	CYS	2.4
1	C	99	VAL	2.4
1	B	270	ALA	2.4
1	A	273	ILE	2.4
1	A	85	GLY	2.3
1	D	252	LEU	2.3
1	D	77	LEU	2.3
1	B	257	ASP	2.3
1	C	219	VAL	2.3
1	D	274	GLU	2.3
1	A	183	ASN	2.3
1	D	81	ALA	2.3
1	C	142	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	82	SER	2.3
1	B	208	HIS	2.3
1	A	256	ASP	2.3
1	D	138	GLU	2.3
1	D	232	VAL	2.3
1	B	204	ASN	2.3
1	C	241	PRO	2.3
1	B	137	PHE	2.3
1	D	204	ASN	2.2
1	A	14	LEU	2.2
1	C	9	SER	2.2
1	B	190	ASP	2.2
1	C	86	GLU	2.2
1	B	180	ASN	2.2
1	A	323	HIS	2.2
1	B	72	LEU	2.2
1	A	209	ILE	2.2
1	D	60	VAL	2.2
1	C	152	HIS	2.2
1	D	129	LEU	2.2
1	C	316	GLU	2.2
1	A	144	ASN	2.2
1	A	230	HIS	2.2
1	A	344	ALA	2.2
1	C	85	GLY	2.2
1	A	220	ILE	2.2
1	C	63	ASP	2.2
1	D	84	ASP	2.2
1	B	153	PRO	2.2
1	B	207	PRO	2.2
1	C	288	GLN	2.1
1	D	162	ALA	2.1
1	C	308	THR	2.1
1	B	145	ILE	2.1
1	D	231	CYS	2.1
1	A	9	SER	2.1
1	C	107	VAL	2.1
1	B	14	LEU	2.1
1	C	266	ARG	2.1
1	B	167	SER	2.1
1	A	210	LYS	2.1
1	C	205	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	183	ASN	2.1
1	A	169	LEU	2.1
1	C	336	THR	2.1
1	A	60	VAL	2.1
1	A	206	PHE	2.1
1	C	144	ASN	2.1
1	B	202	ILE	2.1
1	B	246	ILE	2.1
1	D	256	ASP	2.1
1	D	345	TYR	2.1
1	C	178	CYS	2.1
1	D	137	PHE	2.0
1	B	120	ALA	2.0
1	D	183	ASN	2.0
1	B	259	GLU	2.0
1	B	274	GLU	2.0
1	B	318	TRP	2.0
1	C	289	SER	2.0
1	C	208	HIS	2.0
1	A	175	VAL	2.0
1	A	86	GLU	2.0
1	A	298	LEU	2.0
1	B	111	LEU	2.0
1	A	263	ILE	2.0
1	D	170	ILE	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 ⓘ

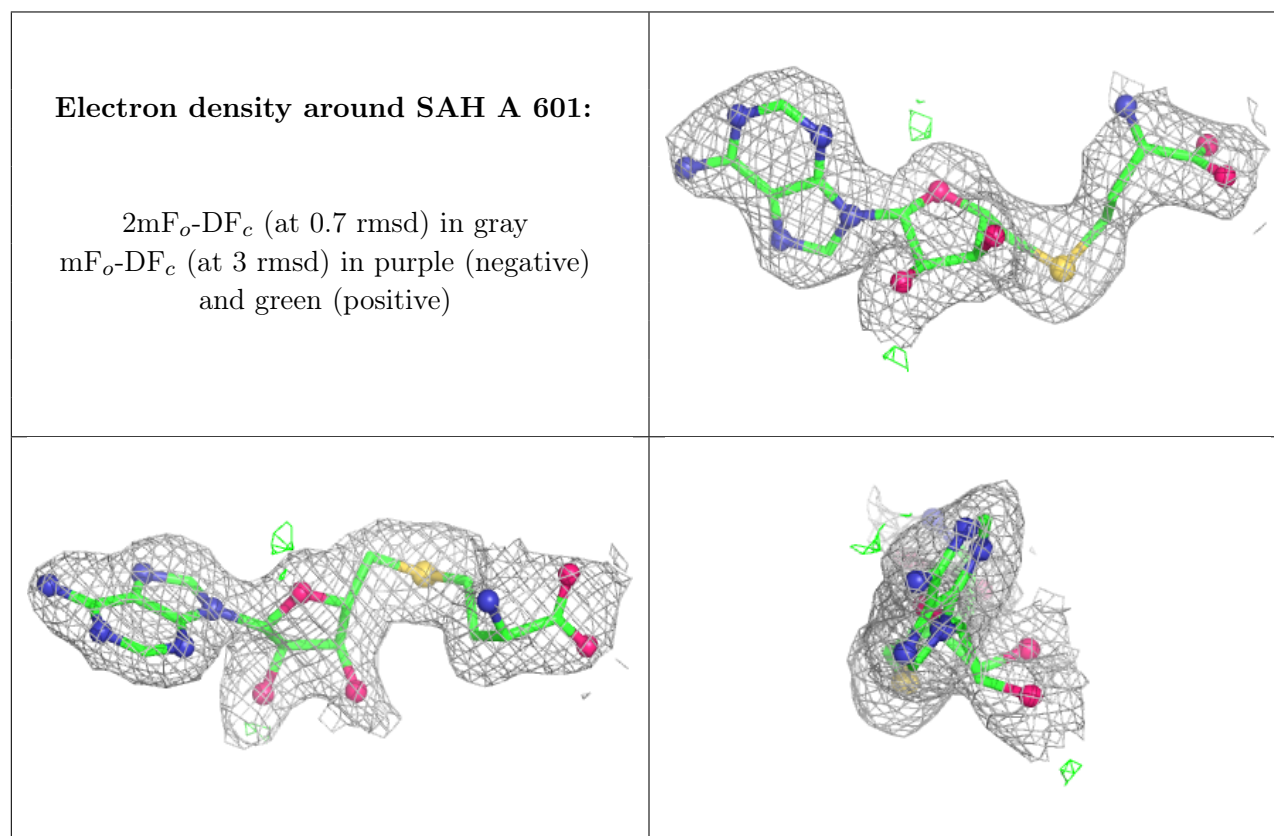
There are no oligosaccharides in this entry.

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.

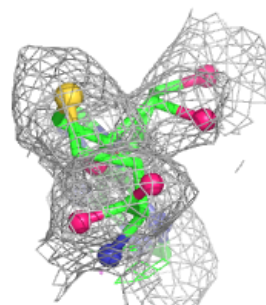
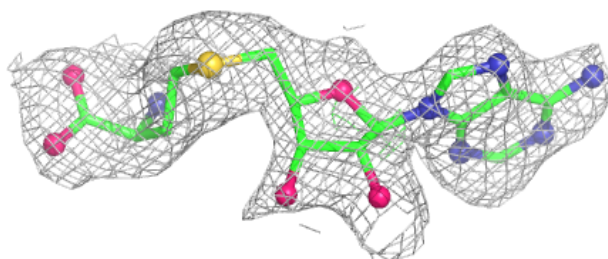
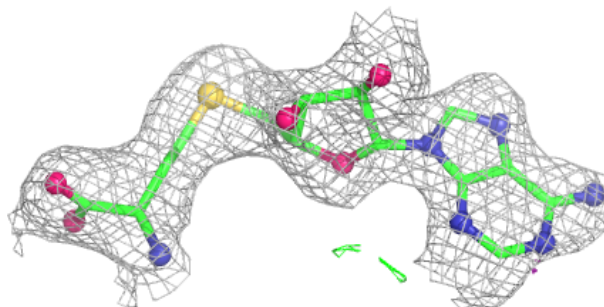
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	A	601	26/26	0.90	0.12	13,14,18,18	0
2	SAH	D	601	26/26	0.91	0.11	13,14,15,16	0
2	SAH	C	601	26/26	0.93	0.10	12,13,15,16	0
2	SAH	B	601	26/26	0.94	0.10	10,11,13,13	0

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.

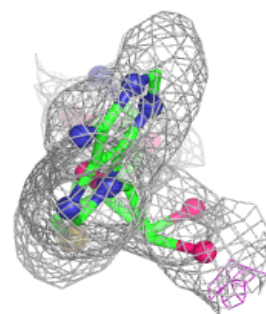
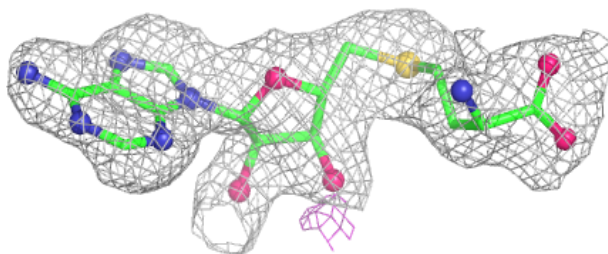
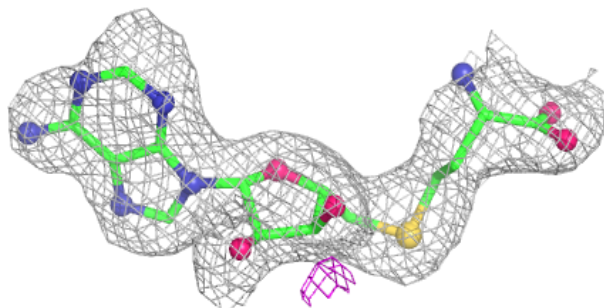


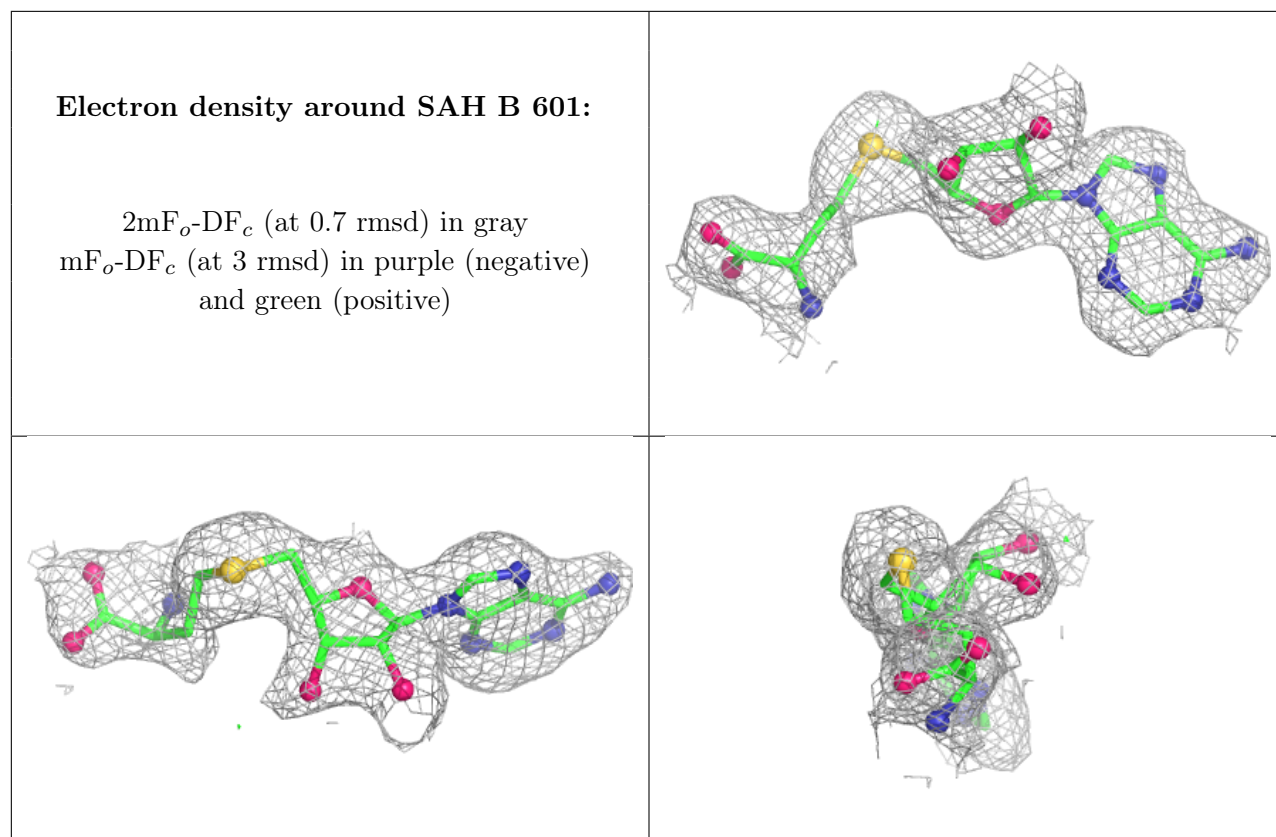
Electron density around SAH D 601:

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

**Electron density around SAH C 601:**

$2mF_o-DF_c$ (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.