



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 AM UTC

PDB ID : 5WT1 / pdb_00005wt1
Title : Pyrococcus abyssi methyltransferase PaTrm5a bound by SAH and cognate tRNA
Authors : Xie, W.; Wang, C.; Jia, Q.
Deposited on : 2016-12-09
Resolution : 2.60 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

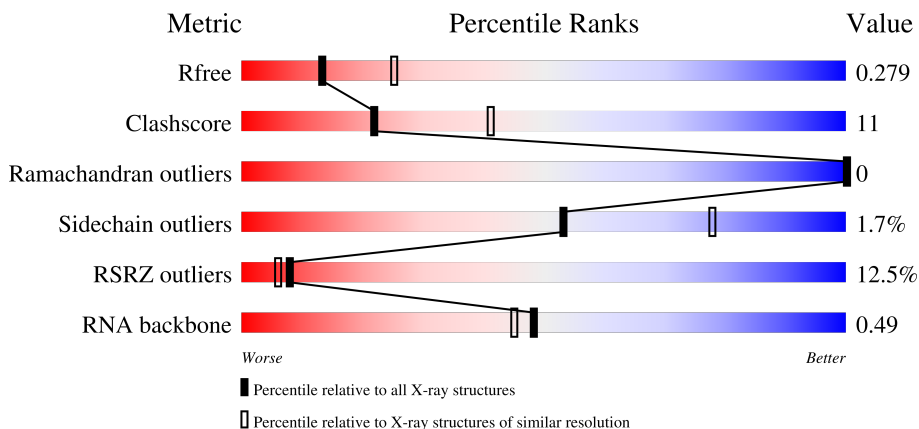
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	333	9% 74% 25% .
1	B	333	19% 73% 25% ..
2	C	76	3% 51% 33% . 12%
2	F	76	5% 54% 32% . 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7973 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 tRNA (guanine(37)-N1)-methyltransferase Trm5a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2558	1642	453	459	4			
1	B	330	Total	C	N	O	S	0	0	0
			2408	1533	430	441	4			

- Molecule 2 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	P	0	0	0
			1436	639	263	467	67			
2	F	68	Total	C	N	O	P	0	0	0
			1459	649	268	474	68			

- 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		

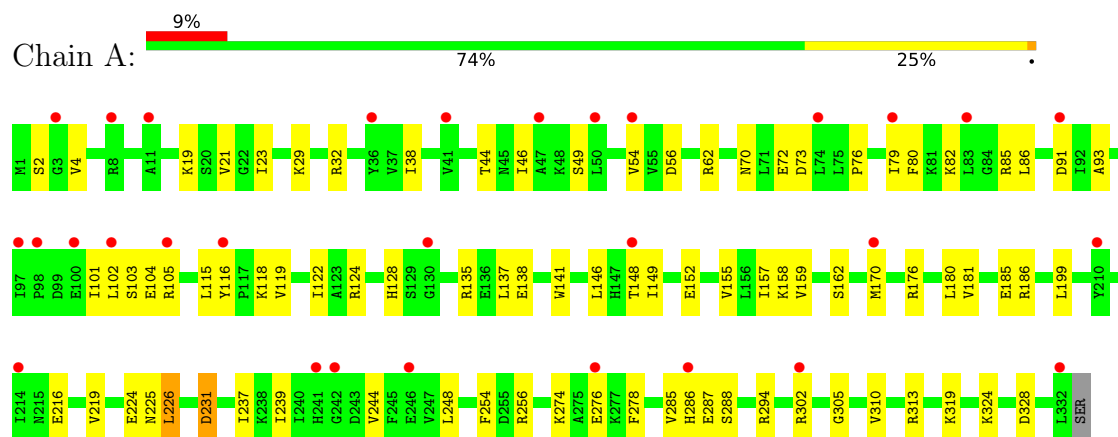
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	C	17	Total	O	0	0
			17	17		
4	B	11	Total	O	0	0
			11	11		
4	F	10	Total	O	0	0
			10	10		

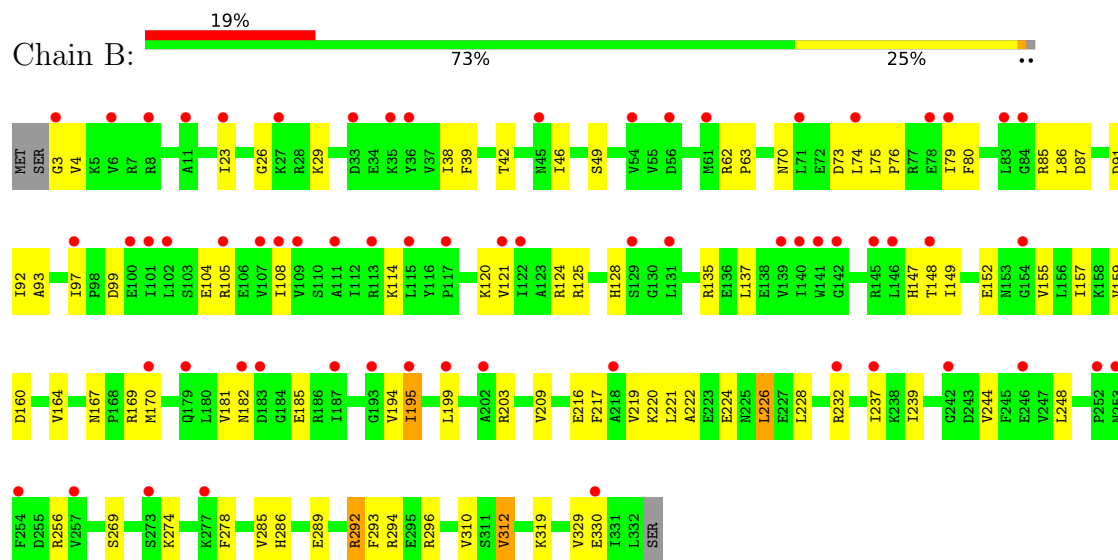
3 Residue-property plots [i](#)

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: tRNA (guanine(37)-N1)-methyltransferase Trm5a

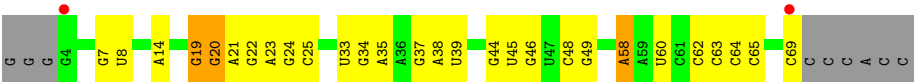


- Molecule 1: tRNA (guanine(37)-N1)-methyltransferase Trm5a

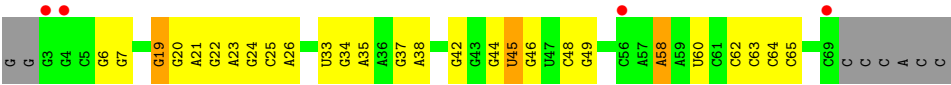


- Molecule 2: RNA (76-MER)





● Molecule 2: RNA (76-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.10Å 57.02Å 115.81Å 90.00° 101.53° 90.00°	Depositor
Resolution (Å)	40.22 – 2.60 40.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.22-2.60) 98.7 (40.22-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.247 , 0.274 0.251 , 0.279	Depositor DCC
R_{free} test set	2024 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7973	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2655e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.26	0/2603	0.56	0/3532
1	B	0.41	2/2453 (0.1%)	0.73	7/3345 (0.2%)
2	C	0.15	0/1605	0.40	0/2502
2	F	0.18	0/1631	0.45	1/2543 (0.0%)
All	All	0.29	2/8292 (0.0%)	0.56	8/11922 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	ARG	NE-CZ	-7.90	1.24	1.33
1	B	232	ARG	CZ-NH1	-6.21	1.24	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ARG	NE-CZ-NH1	-10.42	111.08	121.50
1	B	232	ARG	NE-CZ-NH2	10.41	128.57	119.20
1	B	232	ARG	CG-CD-NE	9.77	133.49	112.00
1	B	195	ILE	CA-CB-CG1	5.47	119.70	110.40
1	B	195	ILE	N-CA-CB	-5.30	103.79	111.21
2	F	45	U	P-O3'-C3'	5.26	128.10	120.20
1	B	232	ARG	CD-NE-CZ	-5.22	117.08	124.40
1	B	195	ILE	CB-CA-C	5.14	120.71	111.36

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	2558	0	2533	67	0
1	B	2408	0	2196	67	0
2	C	1436	0	728	17	0
2	F	1459	0	739	11	0
3	A	26	0	19	2	0
3	B	26	0	19	1	0
4	A	22	0	0	0	0
4	B	11	0	0	1	0
4	C	17	0	0	1	0
4	F	10	0	0	0	0
All	All	7973	0	6234	152	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 11.

All (152) 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:91:ASP:H	1:A:148:THR:HG21	1.31	0.92
1:B:292:ARG:HG2	1:B:292:ARG:HH11	1.36	0.90
1:A:23:ILE:HG21	1:A:46:ILE:HD11	1.55	0.89
1:B:29:LYS:NZ	2:F:19:G:OP2	2.08	0.86
1:B:91:ASP:H	1:B:148:THR:HG21	1.41	0.85
1:A:4:VAL:O	1:A:38:ILE:HA	1.78	0.84
1:B:99:ASP:OD2	1:B:124:ARG:NH2	2.13	0.81
1:B:164:VAL:HG21	1:B:194:VAL:HG13	1.63	0.79
1:A:286:HIS:HD2	1:A:288:SER:H	1.32	0.77
2:F:58:A:O2'	2:F:60:U:OP2	2.05	0.74
1:B:79:ILE:HD11	1:B:104:GLU:HG2	1.70	0.73
1:A:248:LEU:O	1:A:274:LYS:NZ	2.21	0.73
1:B:76:PRO:HG2	1:B:79:ILE:HD12	1.74	0.70
1:B:248:LEU:O	1:B:274:LYS:NZ	2.23	0.70
1:A:23:ILE:HG21	1:A:46:ILE:CD1	2.22	0.68
2:C:58:A:O2'	2:C:60:U:OP2	2.11	0.68
1:B:4:VAL:O	1:B:38:ILE:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PRO:HD2	1:A:79:ILE:HD11	1.77	0.66
1:A:286:HIS:CD2	1:A:288:SER:H	2.13	0.66
1:A:91:ASP:N	1:A:148:THR:HG21	2.10	0.64
1:A:23:ILE:CG2	1:A:46:ILE:HD11	2.25	0.63
1:B:125:ARG:HD3	1:B:135:ARG:CZ	2.28	0.63
1:A:294:ARG:NH1	1:A:310:VAL:O	2.32	0.63
1:B:296:ARG:NH1	4:B:501:HOH:O	2.32	0.62
1:B:195:ILE:O	1:B:199:LEU:HD13	2.00	0.62
1:B:182:ASN:O	1:B:185:GLU:HG3	1.99	0.62
2:C:23:A:H2'	2:C:24:G:C8	2.35	0.61
2:F:23:A:H2'	2:F:24:G:C8	2.36	0.61
1:B:62:ARG:HG3	1:B:63:PRO:HD2	1.82	0.61
1:A:231:ASP:OD1	1:A:231:ASP:N	2.29	0.59
1:B:26:GLY:O	1:B:62:ARG:NH2	2.36	0.59
1:B:220:LYS:HE3	1:B:221:LEU:HG	1.85	0.58
1:A:148:THR:HG22	1:A:149:ILE:N	2.19	0.58
1:A:286:HIS:HD2	1:A:288:SER:N	2.02	0.58
1:A:44:THR:HB	1:A:54:VAL:HG21	1.87	0.57
1:B:289:GLU:OE1	1:B:292:ARG:NH1	2.38	0.56
2:F:7:G:O2'	2:F:49:G:OP2	2.22	0.56
1:A:158:LYS:NZ	1:A:224:GLU:OE1	2.28	0.56
1:A:70:ASN:OD1	1:A:73:ASP:N	2.36	0.56
1:A:219:VAL:HG23	1:A:239:ILE:HG21	1.88	0.56
1:B:148:THR:HG22	1:B:149:ILE:N	2.21	0.56
1:B:219:VAL:HG23	1:B:239:ILE:HD11	1.87	0.55
1:A:199:LEU:HD11	1:A:225:ASN:HB3	1.89	0.55
1:B:292:ARG:HG2	1:B:292:ARG:NH1	2.13	0.55
1:B:70:ASN:OD1	1:B:73:ASP:N	2.34	0.55
1:B:97:ILE:O	1:B:124:ARG:NH2	2.40	0.55
1:A:32:ARG:NH2	2:C:19:G:N7	2.54	0.55
1:A:102:LEU:O	1:A:105:ARG:CB	2.54	0.55
1:A:313:ARG:NH2	1:A:328:ASP:OD2	2.40	0.54
1:B:167:ASN:HB3	1:B:170:MET:HE2	1.88	0.54
2:C:63:C:H2'	2:C:64:C:C6	2.44	0.53
1:A:23:ILE:HD13	1:A:46:ILE:HD11	1.91	0.52
2:C:63:C:H2'	2:C:64:C:H6	1.74	0.52
1:A:146:LEU:HD23	1:A:162:SER:HB3	1.91	0.52
1:A:244:VAL:HG23	3:A:401:SAH:C2	2.40	0.52
1:A:104:GLU:N	1:A:104:GLU:OE1	2.43	0.51
1:B:46:ILE:HA	1:B:49:SER:HB3	1.93	0.51
1:A:216:GLU:HA	1:A:219:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:HG13	1:B:248:LEU:HD13	1.92	0.51
1:B:3:GLY:HA2	1:B:39:PHE:O	2.11	0.50
1:A:158:LYS:N	1:A:225:ASN:OD1	2.22	0.50
1:B:209:VAL:CG1	1:B:237:ILE:HG12	2.41	0.50
1:A:219:VAL:HG23	1:A:239:ILE:CG2	2.42	0.50
1:A:2:SER:OG	1:A:56:ASP:OD1	2.28	0.50
1:B:105:ARG:O	1:B:108:ILE:HB	2.12	0.49
1:A:85:ARG:N	4:C:101:HOH:O	2.43	0.49
1:A:128:HIS:CD2	2:C:37:G:H2'	2.47	0.49
2:C:62:C:H2'	2:C:63:C:H6	1.77	0.49
1:B:256:ARG:HG3	1:B:278:PHE:HB2	1.94	0.49
1:B:293:PHE:O	1:B:296:ARG:HB3	2.13	0.49
1:A:19:LYS:HE3	2:C:20:G:H4'	1.95	0.49
1:A:148:THR:HG22	1:A:149:ILE:H	1.78	0.49
1:A:226:LEU:CD2	1:A:237:ILE:HB	2.43	0.49
1:B:216:GLU:HA	1:B:219:VAL:HG12	1.95	0.49
1:A:93:ALA:HB2	1:A:119:VAL:HG21	1.93	0.48
1:A:276:GLU:N	1:A:276:GLU:OE1	2.46	0.48
1:B:92:ILE:HG23	1:B:121:VAL:HG13	1.94	0.48
1:A:29:LYS:HB2	1:A:62:ARG:HG2	1.95	0.48
1:A:152:GLU:O	1:A:155:VAL:HG22	2.14	0.48
1:A:186:ARG:HG2	1:A:254:PHE:CD2	2.48	0.48
1:A:256:ARG:HG3	1:A:278:PHE:HB2	1.96	0.48
1:B:199:LEU:O	1:B:203:ARG:CB	2.62	0.47
2:C:7:G:O2'	2:C:49:G:OP2	2.29	0.47
1:A:137:LEU:HB2	1:A:146:LEU:HD21	1.95	0.47
1:B:87:ASP:CG	1:B:169:ARG:HH21	2.23	0.47
1:B:195:ILE:HG12	1:B:222:ALA:HB1	1.97	0.47
1:B:86:LEU:HD11	1:B:93:ALA:HB1	1.96	0.47
1:B:148:THR:HG22	1:B:149:ILE:H	1.81	0.46
1:B:310:VAL:HG12	1:B:329:VAL:HG13	1.95	0.46
1:B:160:ASP:O	1:B:164:VAL:HG12	2.15	0.46
1:B:294:ARG:HB2	1:B:312:VAL:HG11	1.98	0.46
1:B:319:LYS:NZ	2:F:35:A:OP2	2.49	0.46
1:A:128:HIS:CE1	1:A:135:ARG:HB2	2.51	0.46
1:B:147:HIS:HA	1:B:160:ASP:HA	1.98	0.46
1:B:125:ARG:HA	1:B:137:LEU:HD23	1.97	0.45
1:B:128:HIS:CE1	1:B:135:ARG:HB2	2.50	0.45
1:A:302:ARG:HH12	1:A:305:GLY:C	2.25	0.45
1:A:319:LYS:NZ	2:C:35:A:OP2	2.49	0.45
1:B:226:LEU:CD2	1:B:237:ILE:HB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:HG23	3:B:401:SAH:C2	2.47	0.45
1:B:62:ARG:HG3	1:B:63:PRO:CD	2.45	0.45
1:A:85:ARG:HB2	2:C:39:U:OP1	2.17	0.45
1:B:226:LEU:HD21	1:B:237:ILE:HB	1.98	0.44
2:F:62:C:H2'	2:F:63:C:H6	1.81	0.44
1:A:23:ILE:HG21	1:A:46:ILE:CG1	2.47	0.44
1:A:85:ARG:HH21	2:C:25:C:P	2.41	0.44
1:A:116:TYR:O	1:A:119:VAL:HG12	2.18	0.44
1:B:219:VAL:HG23	1:B:239:ILE:CD1	2.48	0.44
1:A:79:ILE:HD12	1:A:80:PHE:N	2.33	0.43
1:A:124:ARG:N	1:A:138:GLU:O	2.46	0.43
1:A:176:ARG:O	1:A:180:LEU:HD22	2.17	0.43
1:B:91:ASP:N	1:B:148:THR:HG21	2.21	0.43
2:C:62:C:H2'	2:C:63:C:C6	2.53	0.43
1:B:220:LYS:HE3	1:B:221:LEU:CG	2.46	0.43
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.86	0.43
1:B:157:ILE:HG22	1:B:159:VAL:HG13	2.01	0.43
1:A:157:ILE:HG22	1:A:159:VAL:HG13	2.01	0.43
1:B:85:ARG:NH2	2:F:26:A:OP2	2.44	0.43
1:B:285:VAL:HG12	1:B:286:HIS:O	2.18	0.43
1:A:122:ILE:HB	1:A:141:TRP:HB3	2.01	0.42
1:B:181:VAL:HG13	1:B:185:GLU:OE1	2.19	0.42
2:F:6:G:O2'	2:F:7:G:H5'	2.19	0.42
1:A:286:HIS:CD2	1:A:287:GLU:N	2.87	0.42
1:B:278:PHE:CE2	1:B:330:GLU:HB2	2.54	0.42
1:B:91:ASP:OD1	1:B:120:LYS:N	2.53	0.42
1:B:224:GLU:O	1:B:228:LEU:HD13	2.19	0.42
1:A:19:LYS:HZ1	2:C:20:G:P	2.43	0.41
3:A:401:SAH:HG1	3:A:401:SAH:H4'	1.51	0.41
1:B:217:PHE:HA	1:B:220:LYS:HE2	2.02	0.41
2:F:63:C:H2'	2:F:64:C:C6	2.55	0.41
1:A:46:ILE:HA	1:A:49:SER:OG	2.20	0.41
2:F:64:C:H2'	2:F:65:C:H6	1.86	0.41
1:A:170:MET:HE3	1:A:324:LYS:NZ	2.36	0.41
1:B:23:ILE:O	1:B:42:THR:N	2.47	0.41
1:B:209:VAL:HG13	1:B:237:ILE:HG23	2.02	0.41
1:B:220:LYS:HE2	1:B:220:LYS:HB3	1.85	0.41
1:A:21:VAL:HG11	1:A:46:ILE:HD13	2.03	0.41
1:A:72:GLU:HB2	1:A:80:PHE:CZ	2.55	0.41
1:A:118:LYS:HZ2	2:C:14:A:P	2.43	0.41
1:A:181:VAL:HG13	1:A:185:GLU:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG13	1:A:248:LEU:HD13	2.03	0.40
1:B:195:ILE:HG12	1:B:222:ALA:CB	2.50	0.40
2:F:24:G:H2'	2:F:25:C:O4'	2.21	0.40
1:A:285:VAL:HG12	1:A:286:HIS:O	2.21	0.40
2:C:64:C:H2'	2:C:65:C:H6	1.86	0.40
1:B:75:LEU:HD23	1:B:80:PHE:HB2	2.03	0.40
1:B:148:THR:CG2	1:B:149:ILE:N	2.83	0.40
1:A:82:LYS:CB	1:A:101:ILE:HD13	2.52	0.40
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.91	0.40
1:B:152:GLU:O	1:B:155:VAL:HG22	2.20	0.40
2:C:14:A:C5	2:C:22:G:C2	3.09	0.40
1:B:74:LEU:HD21	1:B:114:LYS:CB	2.52	0.40

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	330/333 (99%)	327 (99%)	3 (1%)	0	100	100
1	B	328/333 (98%)	322 (98%)	6 (2%)	0	100	100
All	All	658/666 (99%)	649 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	262/301 (87%)	258 (98%)	4 (2%)	57 80
1	B	220/301 (73%)	216 (98%)	4 (2%)	51 76
All	All	482/602 (80%)	474 (98%)	8 (2%)	53 78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	103	SER
1	A	226	LEU
1	A	231	ASP
1	B	226	LEU
1	B	269	SER
1	B	292	ARG
1	B	312	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	286	HIS
1	B	153	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	66/76 (86%)	12 (18%)	2 (3%)
2	F	67/76 (88%)	14 (20%)	1 (1%)
All	All	133/152 (87%)	26 (19%)	3 (2%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	8	U
2	C	19	G
2	C	20	G
2	C	21	A
2	C	33	U

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Mol	Chain	Res	Type
2	C	34	G
2	C	38	A
2	C	44	G
2	C	45	U
2	C	48	C
2	C	58	A
2	C	69	C
2	F	19	G
2	F	20	G
2	F	21	A
2	F	22	G
2	F	33	U
2	F	34	G
2	F	37	G
2	F	38	A
2	F	42	G
2	F	44	G
2	F	45	U
2	F	46	G
2	F	48	C
2	F	58	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	20	G
2	C	46	G
2	F	45	U

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](#)

2 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$
3	SAH	A	401	-	27,28,28	1.44	5 (18%)	36,40,40	1.91	9 (25%)
3	SAH	B	401	-	27,28,28	1.44	5 (18%)	36,40,40	1.97	10 (27%)

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	A	401	-	-	5/15/31/31	0/3/3/3
3	SAH	B	401	-	-	2/15/31/31	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	SAH	C5-C4	4.64	1.47	1.39
3	B	401	SAH	C5-C4	4.44	1.47	1.39
3	A	401	SAH	C5-C6	2.72	1.48	1.41
3	B	401	SAH	C5-C6	2.61	1.48	1.41
3	A	401	SAH	C8-N7	2.40	1.36	1.31
3	B	401	SAH	C8-N7	2.35	1.36	1.31
3	B	401	SAH	C4-N9	-2.22	1.33	1.37
3	B	401	SAH	C5-N7	-2.15	1.35	1.39
3	A	401	SAH	C5-N7	-2.12	1.35	1.39
3	A	401	SAH	C4-N9	-2.04	1.33	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SAH	C5-C4-N3	-5.35	119.35	126.72
3	B	401	SAH	C5-C4-N3	-5.11	119.69	126.72
3	B	401	SAH	N3-C4-N9	4.27	134.43	127.17
3	A	401	SAH	N3-C4-N9	4.19	134.30	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	SAH	C4-N9-C8	3.67	109.59	105.74
3	A	401	SAH	C4-C5-N7	-3.59	106.48	110.58
3	A	401	SAH	C2-N3-C4	3.56	120.52	111.83
3	B	401	SAH	C2-N3-C4	3.51	120.40	111.83
3	B	401	SAH	N3-C2-N1	-3.38	123.46	128.58
3	B	401	SAH	C4-C5-N7	-3.38	106.72	110.58
3	A	401	SAH	N3-C2-N1	-3.25	123.66	128.58
3	A	401	SAH	C4-N9-C8	2.98	108.87	105.74
3	B	401	SAH	C5-N7-C8	2.64	107.60	103.45
3	B	401	SAH	N9-C8-N7	-2.62	110.22	113.94
3	A	401	SAH	C5-N7-C8	2.62	107.57	103.45
3	B	401	SAH	C4'-C5'-SD	-2.36	105.35	113.78
3	B	401	SAH	C6-C5-N7	2.36	136.65	132.09
3	A	401	SAH	C6-C5-N7	2.36	136.63	132.09
3	A	401	SAH	N9-C8-N7	-2.26	110.73	113.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	SAH	N-CA-CB-CG
3	A	401	SAH	C-CA-CB-CG
3	A	401	SAH	C2'-C1'-N9-C8
3	A	401	SAH	C4'-C5'-SD-CG
3	A	401	SAH	O4'-C1'-N9-C8
3	B	401	SAH	C2'-C1'-N9-C8
3	B	401	SAH	C-CA-CB-CG

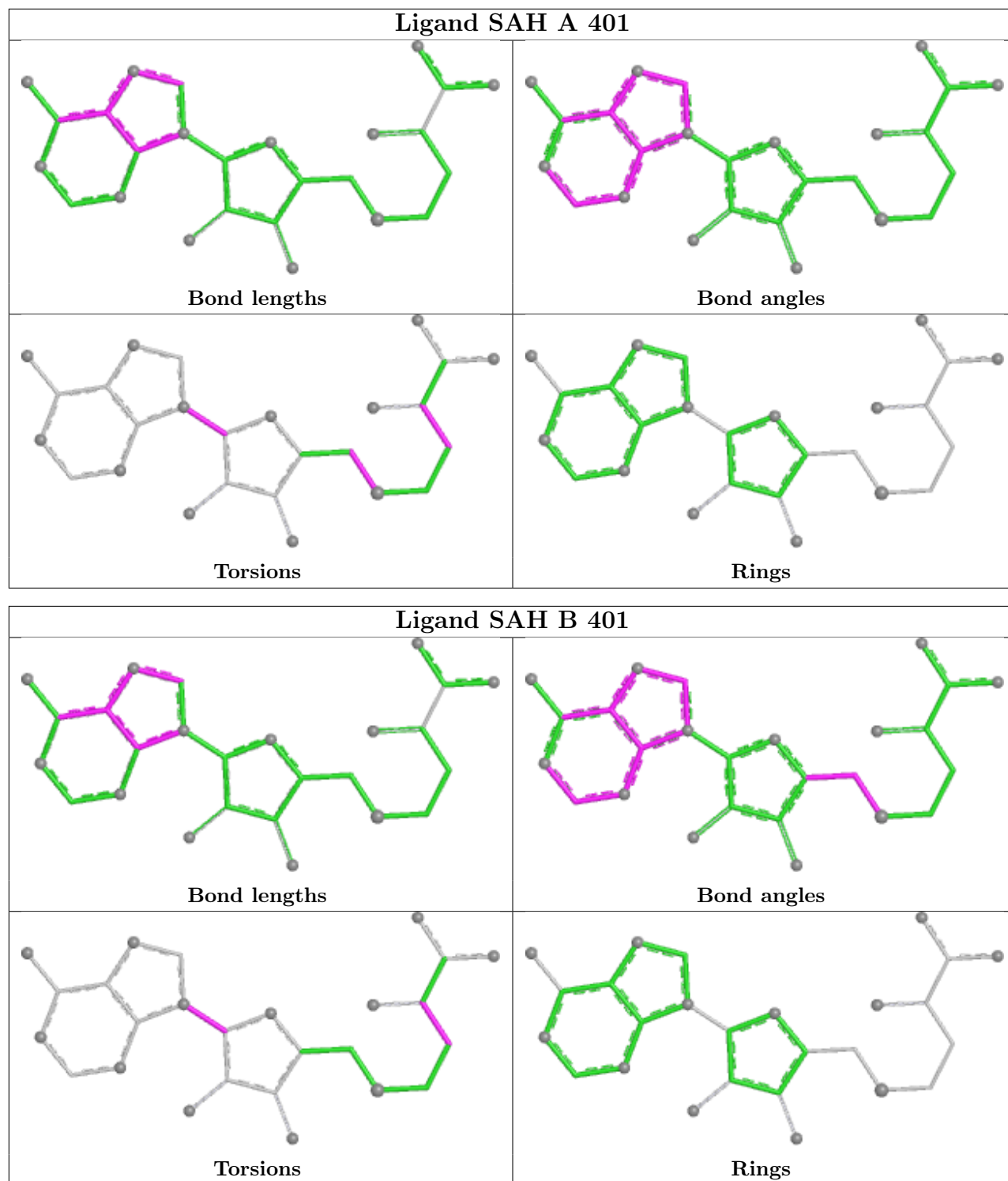
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SAH	2	0
3	B	401	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.



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	332/333 (99%)	0.84	30 (9%) 15 11	36, 64, 97, 126	0
1	B	330/333 (99%)	1.34	64 (19%) 3 2	37, 76, 117, 130	0
2	C	67/76 (88%)	0.36	2 (2%) 52 47	41, 57, 104, 157	0
2	F	68/76 (89%)	0.58	4 (5%) 28 23	48, 64, 99, 158	0
All	All	797/818 (97%)	0.98	100 (12%) 8 6	36, 69, 112, 158	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	THR	4.9
1	B	79	ILE	4.6
1	B	74	LEU	4.3
1	A	105	ARG	4.0
1	A	79	ILE	3.9
1	B	154	GLY	3.8
1	A	50	LEU	3.6
1	B	242	GLY	3.6
1	B	6	VAL	3.5
1	B	36	TYR	3.5
1	A	3	GLY	3.3
1	B	139	VAL	3.3
1	B	142	GLY	3.3
1	B	71	LEU	3.2
1	B	56	ASP	3.2
2	C	69	C	3.1
1	B	45	ASN	3.1
1	B	101	ILE	3.1
1	B	195	ILE	3.1
1	B	122	ILE	3.1
1	B	202	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLY	3.0
1	B	141	TRP	2.9
1	B	97	ILE	2.9
1	A	8	ARG	2.9
1	B	237	ILE	2.9
1	B	115	LEU	2.9
1	B	199	LEU	2.9
1	B	218	ALA	2.9
1	B	83	LEU	2.8
1	B	102	LEU	2.8
1	A	54	VAL	2.7
1	B	170	MET	2.7
1	A	302	ARG	2.7
1	B	61	MET	2.7
1	A	276	GLU	2.7
1	B	330	GLU	2.7
1	B	140	ILE	2.7
1	B	8	ARG	2.7
1	B	113	ARG	2.7
1	A	170	MET	2.6
1	A	214	ILE	2.6
1	B	27	LYS	2.6
1	B	145	ARG	2.6
1	A	83	LEU	2.6
2	F	56	C	2.6
1	B	257	VAL	2.6
1	B	117	PRO	2.5
1	B	254	PHE	2.5
1	B	54	VAL	2.5
1	B	11	ALA	2.5
1	A	102	LEU	2.5
1	A	148	THR	2.5
1	B	129	SER	2.5
1	B	35	LYS	2.5
1	B	121	VAL	2.5
2	C	4	G	2.5
1	B	100	GLU	2.4
1	A	246	GLU	2.4
1	A	74	LEU	2.4
1	B	23	ILE	2.4
1	B	105	ARG	2.4
2	F	69	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	2.4
1	A	332	LEU	2.3
1	B	109	VAL	2.3
1	B	78	GLU	2.3
1	B	252	PRO	2.3
1	A	91	ASP	2.3
1	B	253	ASN	2.3
1	B	146	LEU	2.3
1	A	210	TYR	2.3
1	A	98	PRO	2.3
1	A	241	HIS	2.2
1	A	242	GLY	2.2
1	B	131	LEU	2.2
1	B	183	ASP	2.2
1	A	11	ALA	2.2
1	B	277	LYS	2.2
1	A	97	ILE	2.2
1	B	187	ILE	2.2
1	B	273	SER	2.2
1	A	41	VAL	2.2
1	B	111	ALA	2.2
2	F	4	G	2.2
1	A	100	GLU	2.2
1	B	3	GLY	2.1
2	F	3	G	2.1
1	B	84	GLY	2.1
1	B	232	ARG	2.1
1	B	182	ASN	2.1
1	A	36	TYR	2.1
1	B	33	ASP	2.1
1	B	179	GLN	2.1
1	B	108	ILE	2.1
1	A	286	HIS	2.1
1	B	107	VAL	2.0
1	A	47	ALA	2.0
1	A	116	TYR	2.0
1	B	246	GLU	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 [i](#)

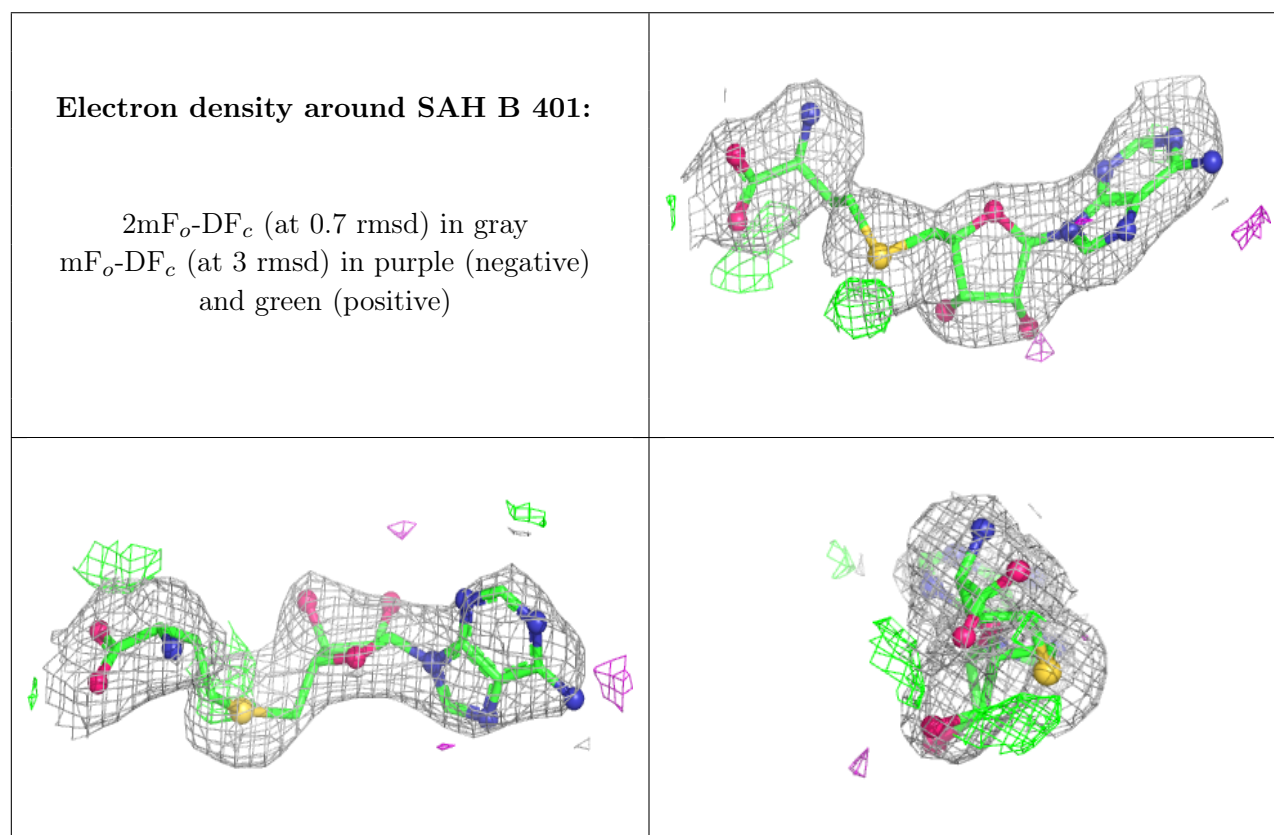
There are no oligosaccharides in this entry.

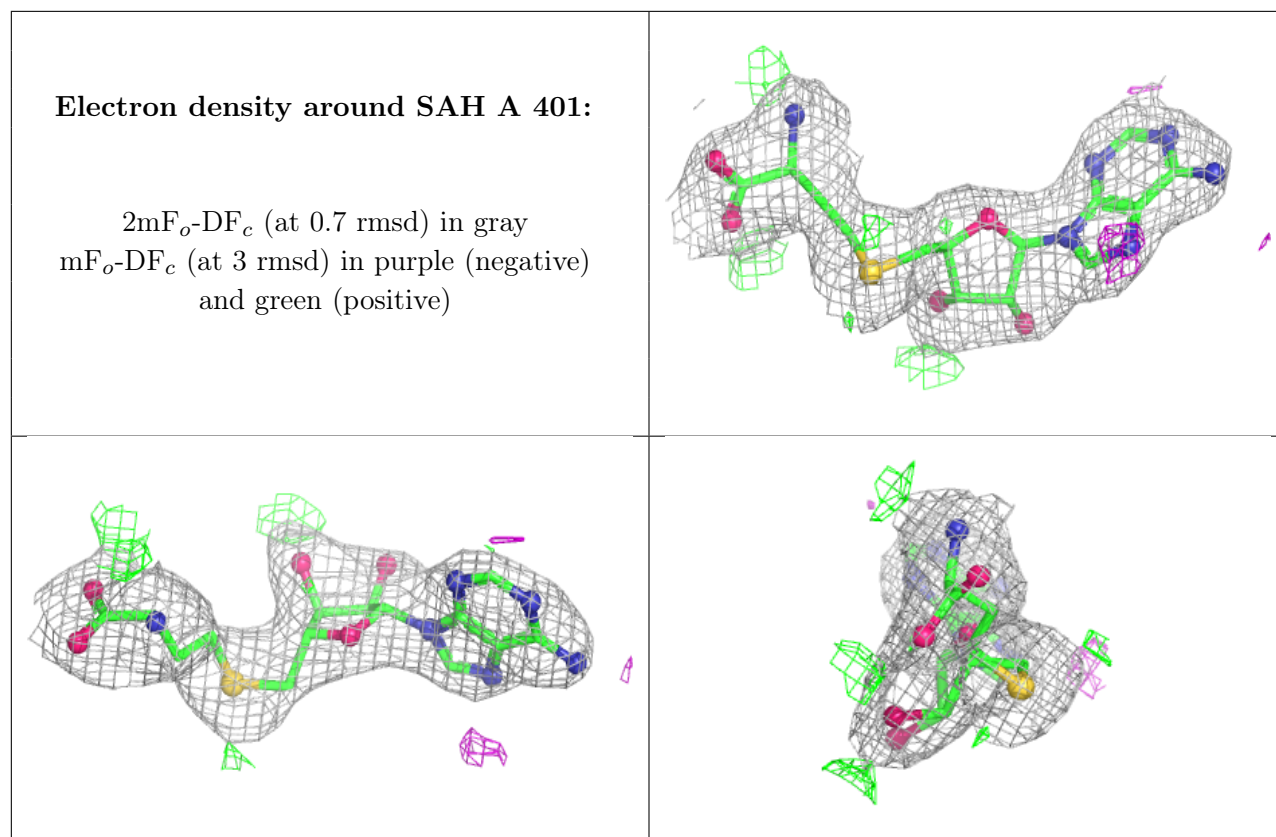
6.4 Ligands [i](#)

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
3	SAH	B	401	26/26	0.90	0.12	52,61,70,71	0
3	SAH	A	401	26/26	0.91	0.12	33,47,55,57	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.