



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:08 am BST

PDB ID : 1MT6  
Title : Structure of histone H3 K4-specific methyltransferase SET7/9 with AdoHcy  
Authors : Jacobs, S.A.; Harp, J.M.; Devarakonda, S.; Kim, Y.; Rastinejad, F.; Khorasanizadeh, S.  
Deposited on : 2002-09-20  
Resolution : 2.20 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

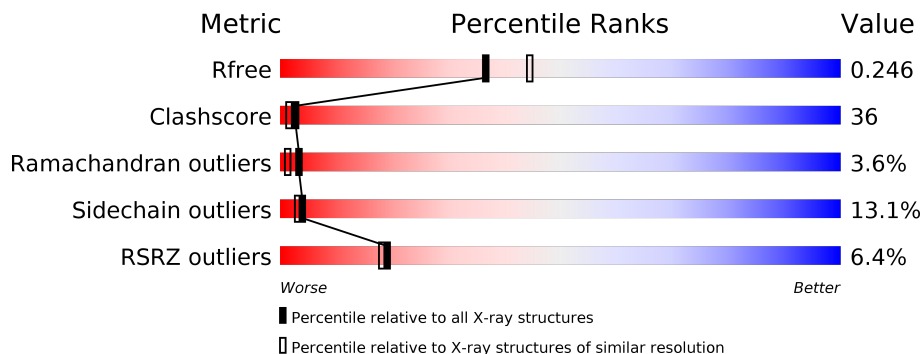
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	280	

## 2 Entry composition [i](#)

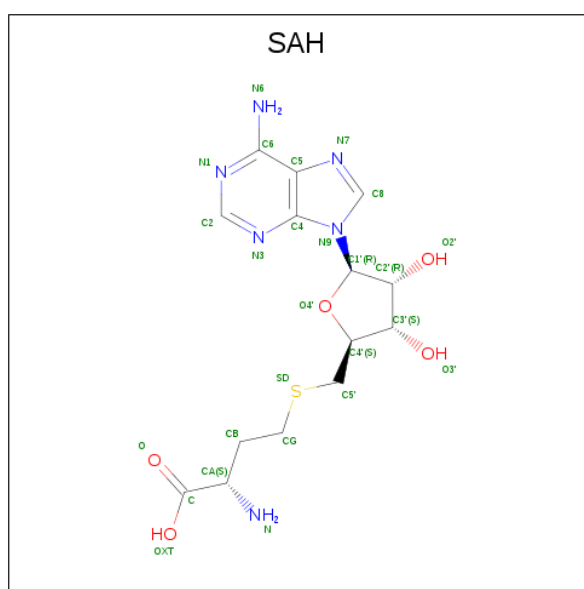
There are 3 unique types of molecules in this entry. The entry contains 2389 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SET9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2192	1382	356	443	11	0	0	0

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



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

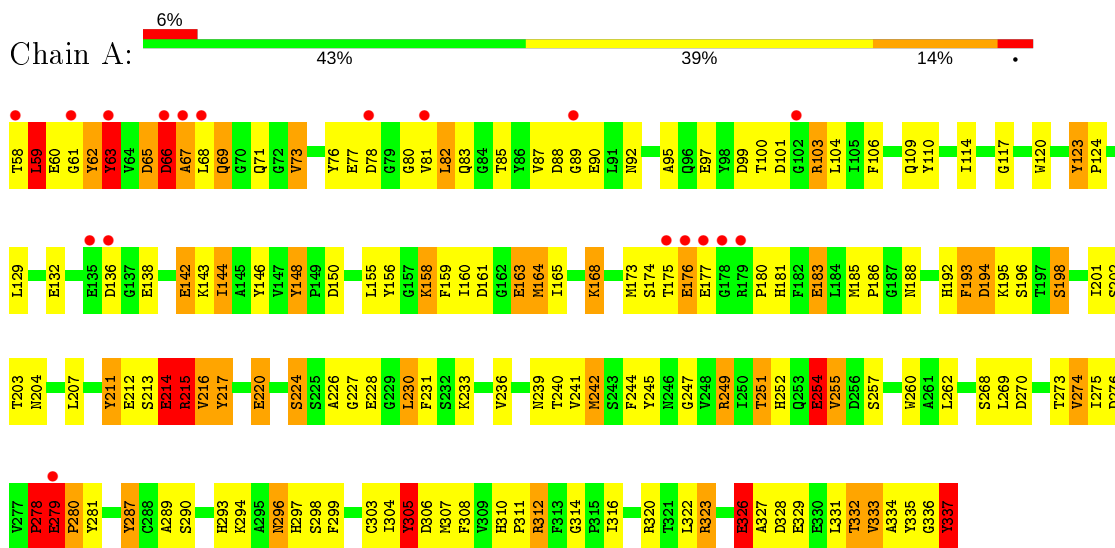
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: SET9



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.35Å 76.04Å 166.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.64 – 2.20 28.64 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (28.64-2.20) 93.0 (28.64-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.20Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.226 , 0.263 0.204 , 0.246	Depositor DCC
$R_{free}$ test set	2132 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtrriage
Anisotropy	0.914	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2389	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.00	60/2246 (2.7%)	1.57	24/3051 (0.8%)

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	6

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	GLU	C-O	13.29	1.48	1.23
1	A	220	GLU	CG-CD	10.87	1.68	1.51
1	A	193	PHE	CE1-CZ	9.91	1.56	1.37
1	A	337	TYR	CD2-CE2	9.35	1.53	1.39
1	A	215	ARG	CZ-NH1	9.34	1.45	1.33
1	A	156	TYR	CD2-CE2	9.28	1.53	1.39
1	A	216	VAL	CA-CB	8.59	1.72	1.54
1	A	305	TYR	CD1-CE1	8.17	1.51	1.39
1	A	148	TYR	CE2-CZ	-8.14	1.27	1.38
1	A	215	ARG	CZ-NH2	8.07	1.43	1.33
1	A	215	ARG	CB-CG	-8.07	1.30	1.52
1	A	120	TRP	CB-CG	-7.77	1.36	1.50
1	A	296	ASN	C-O	7.67	1.38	1.23
1	A	332	THR	C-O	7.58	1.37	1.23
1	A	298	SER	CB-OG	7.37	1.51	1.42
1	A	305	TYR	CD2-CE2	7.14	1.50	1.39
1	A	144	ILE	CA-CB	7.01	1.71	1.54
1	A	228	GLU	CG-CD	6.98	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	VAL	CA-CB	-6.97	1.40	1.54
1	A	214	GLU	CG-CD	6.87	1.62	1.51
1	A	287	TYR	CD1-CE1	6.85	1.49	1.39
1	A	326	GLU	CD-OE1	6.76	1.33	1.25
1	A	148	TYR	CD2-CE2	6.75	1.49	1.39
1	A	163	GLU	CD-OE1	6.75	1.33	1.25
1	A	254	GLU	CG-CD	6.72	1.62	1.51
1	A	333	VAL	CB-CG1	6.68	1.66	1.52
1	A	244	PHE	CD1-CE1	6.68	1.52	1.39
1	A	77	GLU	CG-CD	6.62	1.61	1.51
1	A	333	VAL	C-O	6.55	1.35	1.23
1	A	214	GLU	CD-OE2	6.50	1.32	1.25
1	A	123	TYR	CE2-CZ	6.35	1.46	1.38
1	A	312	ARG	CB-CG	6.30	1.69	1.52
1	A	308	PHE	CE1-CZ	6.25	1.49	1.37
1	A	230	LEU	CG-CD1	6.19	1.74	1.51
1	A	215	ARG	NE-CZ	6.07	1.41	1.33
1	A	164	MET	CG-SD	6.04	1.96	1.81
1	A	183	GLU	CG-CD	5.92	1.60	1.51
1	A	312	ARG	CZ-NH2	5.78	1.40	1.33
1	A	138	GLU	CG-CD	5.76	1.60	1.51
1	A	337	TYR	CA-C	5.57	1.67	1.52
1	A	194	ASP	CB-CG	5.51	1.63	1.51
1	A	211	TYR	CD2-CE2	-5.51	1.31	1.39
1	A	245	TYR	CD2-CE2	5.46	1.47	1.39
1	A	241	VAL	CA-CB	5.43	1.66	1.54
1	A	334	ALA	C-O	-5.36	1.13	1.23
1	A	287	TYR	CD2-CE2	5.34	1.47	1.39
1	A	148	TYR	CD1-CE1	5.30	1.47	1.39
1	A	196	SER	CB-OG	5.30	1.49	1.42
1	A	337	TYR	CD1-CE1	5.26	1.47	1.39
1	A	281	TYR	CE1-CZ	5.25	1.45	1.38
1	A	279	GLU	C-N	-5.24	1.24	1.34
1	A	164	MET	CB-CG	5.20	1.68	1.51
1	A	217	TYR	CD1-CE1	-5.20	1.31	1.39
1	A	281	TYR	CG-CD1	5.17	1.45	1.39
1	A	97	GLU	CB-CG	-5.16	1.42	1.52
1	A	168	LYS	CD-CE	5.13	1.64	1.51
1	A	337	TYR	CB-CG	5.10	1.59	1.51
1	A	110	TYR	CB-CG	-5.04	1.44	1.51
1	A	142	GLU	CD-OE2	-5.02	1.20	1.25
1	A	220	GLU	CD-OE1	5.01	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ARG	NE-CZ-NH1	-11.11	114.74	120.30
1	A	279	GLU	CA-C-O	-8.81	101.61	120.10
1	A	194	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	323	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	A	59	LEU	CA-CB-CG	8.32	134.44	115.30
1	A	306	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	185	MET	CG-SD-CE	-7.68	87.92	100.20
1	A	242	MET	CG-SD-CE	-7.41	88.34	100.20
1	A	224	SER	C-N-CA	-6.70	104.95	121.70
1	A	312	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	164	MET	CG-SD-CE	-6.52	89.77	100.20
1	A	224	SER	CA-C-N	6.17	130.78	117.20
1	A	136	ASP	CB-CA-C	-5.93	98.54	110.40
1	A	202	SER	CB-CA-C	-5.82	99.05	110.10
1	A	323	ARG	CB-CG-CD	-5.74	96.69	111.60
1	A	66	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	278	PRO	CA-C-N	-5.63	104.81	117.20
1	A	194	ASP	OD1-CG-OD2	-5.54	112.78	123.30
1	A	144	ILE	CB-CA-C	-5.43	100.75	111.60
1	A	65	ASP	N-CA-C	5.38	125.54	111.00
1	A	279	GLU	CB-CA-C	5.31	121.02	110.40
1	A	242	MET	CB-CA-C	-5.24	99.91	110.40
1	A	323	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	A	337	TYR	CB-CG-CD2	5.13	124.08	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	TYR	Sidechain
1	A	215	ARG	Mainchain
1	A	278	PRO	Mainchain
1	A	279	GLU	Mainchain
1	A	305	TYR	Sidechain
1	A	337	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2192	0	2053	153	0
2	A	26	0	18	3	0
3	A	171	0	0	24	0
All	All	2389	0	2071	153	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 36.

All (153) 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:230:LEU:CG	1:A:230:LEU:CD1	1.74	1.60
1:A:326:GLU:HG3	3:A:477:HOH:O	1.54	1.03
1:A:188:ASN:HA	3:A:501:HOH:O	1.63	0.98
1:A:62:TYR:O	1:A:63:TYR:HB3	1.64	0.95
1:A:297:HIS:HD2	1:A:335:TYR:H	1.01	0.94
1:A:239:ASN:ND2	1:A:320:ARG:HD3	1.83	0.93
1:A:310:HIS:HD2	1:A:312:ARG:H	1.08	0.93
1:A:335:TYR:OH	2:A:1:SAH:H5'2	1.69	0.93
1:A:216:VAL:HB	3:A:505:HOH:O	1.70	0.89
1:A:297:HIS:CD2	1:A:335:TYR:H	1.91	0.89
1:A:251:THR:HG23	1:A:254:GLU:HB2	1.54	0.88
1:A:326:GLU:HA	1:A:326:GLU:OE2	1.72	0.88
1:A:307:MET:CE	3:A:440:HOH:O	2.21	0.87
1:A:336:GLY:C	1:A:337:TYR:CD1	2.47	0.87
1:A:251:THR:CG2	1:A:254:GLU:HB2	2.05	0.87
1:A:61:GLY:C	1:A:62:TYR:HD1	1.79	0.86
1:A:337:TYR:HB3	3:A:465:HOH:O	1.74	0.85
1:A:155:LEU:CB	1:A:164:MET:HE1	2.07	0.85
1:A:279:GLU:HB3	1:A:280:PRO:HD3	1.60	0.83
1:A:242:MET:HB3	3:A:505:HOH:O	1.79	0.82
1:A:310:HIS:CD2	1:A:311:PRO:HD2	2.14	0.82
1:A:269:LEU:HD22	1:A:275:ILE:HD11	1.63	0.81
1:A:239:ASN:HB2	3:A:428:HOH:O	1.81	0.80
1:A:279:GLU:CB	1:A:280:PRO:HD3	2.12	0.79
1:A:61:GLY:C	1:A:62:TYR:CD1	2.54	0.79
1:A:155:LEU:HB2	1:A:164:MET:CE	2.12	0.79
1:A:230:LEU:CB	1:A:230:LEU:CD1	2.59	0.79
1:A:239:ASN:HD22	1:A:320:ARG:HD3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HG21	1:A:242:MET:HE3	1.63	0.78
1:A:155:LEU:HB3	1:A:164:MET:HE1	1.67	0.76
1:A:252:HIS:HE1	1:A:270:ASP:O	1.68	0.76
1:A:155:LEU:HB2	1:A:164:MET:HE1	1.69	0.75
1:A:326:GLU:OE2	1:A:326:GLU:CA	2.36	0.74
1:A:142:GLU:OE1	1:A:158:LYS:NZ	2.21	0.74
1:A:310:HIS:CD2	1:A:312:ARG:H	1.99	0.73
1:A:296:ASN:HD21	2:A:1:SAH:HN1	1.33	0.73
1:A:63:TYR:C	1:A:63:TYR:CD2	2.62	0.73
1:A:216:VAL:CB	3:A:505:HOH:O	2.34	0.73
1:A:69:GLN:HG2	1:A:88:ASP:H	1.54	0.72
1:A:58:THR:O	1:A:59:LEU:HD22	1.89	0.71
1:A:279:GLU:CB	1:A:280:PRO:CD	2.69	0.71
1:A:62:TYR:O	1:A:63:TYR:CB	2.39	0.71
1:A:216:VAL:CG2	3:A:505:HOH:O	2.37	0.70
1:A:62:TYR:N	1:A:62:TYR:CD1	2.55	0.70
1:A:69:GLN:CG	1:A:88:ASP:H	2.04	0.70
1:A:159:PHE:CE1	1:A:164:MET:HB2	2.26	0.69
1:A:63:TYR:C	1:A:63:TYR:HD2	1.96	0.69
1:A:251:THR:HG23	1:A:254:GLU:H	1.57	0.69
1:A:230:LEU:CD2	1:A:230:LEU:CD1	2.69	0.68
1:A:236:VAL:HG11	1:A:242:MET:HE1	1.75	0.68
1:A:297:HIS:HD2	1:A:335:TYR:N	1.83	0.68
1:A:251:THR:HG23	1:A:254:GLU:CB	2.24	0.67
1:A:336:GLY:C	1:A:337:TYR:HD1	1.95	0.66
1:A:336:GLY:O	1:A:337:TYR:HD1	1.80	0.65
1:A:165:ILE:HD13	1:A:165:ILE:N	2.10	0.65
1:A:175:THR:O	1:A:176:GLU:C	2.36	0.64
1:A:58:THR:HG22	1:A:59:LEU:N	2.13	0.63
1:A:249:ARG:HH21	1:A:249:ARG:HG2	1.62	0.63
1:A:198:SER:HA	1:A:249:ARG:O	1.99	0.62
1:A:144:ILE:HB	1:A:159:PHE:CD2	2.34	0.62
1:A:81:VAL:HG12	1:A:82:LEU:H	1.65	0.61
1:A:155:LEU:HB2	1:A:164:MET:HE3	1.82	0.61
1:A:236:VAL:HG21	1:A:242:MET:CE	2.31	0.61
1:A:337:TYR:CD2	3:A:503:HOH:O	2.51	0.60
1:A:143:LYS:HE3	3:A:474:HOH:O	2.01	0.60
1:A:71:GLN:OE1	1:A:85:THR:HG22	2.02	0.59
1:A:61:GLY:O	1:A:62:TYR:HD1	1.84	0.59
1:A:159:PHE:CZ	1:A:164:MET:HE2	2.37	0.59
1:A:87:VAL:O	1:A:88:ASP:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLY:O	1:A:132:GLU:HA	2.03	0.58
1:A:287:TYR:CE1	1:A:289:ALA:HB3	2.39	0.58
1:A:123:TYR:OH	1:A:129:LEU:HD22	2.03	0.57
1:A:327:ALA:O	1:A:328:ASP:HB2	2.04	0.57
1:A:305:TYR:CZ	1:A:333:VAL:HG21	2.39	0.57
1:A:146:TYR:CD2	1:A:311:PRO:HG3	2.40	0.57
1:A:310:HIS:CG	1:A:311:PRO:HD2	2.39	0.57
1:A:304:ILE:HB	1:A:322:LEU:HD21	1.85	0.56
1:A:337:TYR:N	1:A:337:TYR:CD1	2.72	0.56
1:A:63:TYR:HD2	1:A:63:TYR:O	1.88	0.56
1:A:217:TYR:HD2	1:A:233:LYS:HG3	1.71	0.56
1:A:255:VAL:HG11	1:A:274:VAL:HG11	1.88	0.56
1:A:226:ALA:O	1:A:227:GLY:C	2.39	0.56
1:A:99:ASP:C	1:A:101:ASP:N	2.59	0.56
1:A:99:ASP:C	1:A:101:ASP:H	2.10	0.55
1:A:213:SER:HB2	3:A:364:HOH:O	2.07	0.55
1:A:254:GLU:OE2	1:A:254:GLU:O	2.25	0.54
1:A:251:THR:HG23	1:A:254:GLU:N	2.23	0.54
1:A:160:ILE:HD12	1:A:165:ILE:HG13	1.90	0.54
1:A:99:ASP:N	1:A:103:ARG:O	2.40	0.54
1:A:106:PHE:C	1:A:106:PHE:CD1	2.82	0.53
1:A:168:LYS:HG2	3:A:421:HOH:O	2.09	0.53
1:A:69:GLN:HB3	1:A:89:GLY:H	1.75	0.52
1:A:99:ASP:O	1:A:101:ASP:N	2.43	0.52
1:A:279:GLU:HB2	1:A:280:PRO:CD	2.40	0.51
1:A:278:PRO:C	1:A:279:GLU:O	2.49	0.51
1:A:303:CYS:N	1:A:332:THR:O	2.42	0.51
1:A:68:LEU:HB2	1:A:69:GLN:NE2	2.25	0.51
1:A:81:VAL:HG12	1:A:82:LEU:N	2.25	0.51
1:A:150:ASP:OD1	1:A:150:ASP:C	2.47	0.50
1:A:201:ILE:HD11	1:A:247:GLY:HA2	1.93	0.50
1:A:76:TYR:HD1	1:A:80:GLY:O	1.95	0.49
1:A:66:ASP:OD2	1:A:67:ALA:N	2.46	0.49
1:A:173:MET:HE2	1:A:183:GLU:OE2	2.13	0.49
1:A:158:LYS:HB3	1:A:165:ILE:HB	1.94	0.48
1:A:337:TYR:CE2	3:A:503:HOH:O	2.65	0.48
1:A:307:MET:HE2	3:A:440:HOH:O	1.98	0.48
1:A:212:GLU:OE1	1:A:290:SER:HA	2.14	0.48
1:A:249:ARG:HG2	1:A:249:ARG:NH2	2.28	0.48
1:A:323:ARG:NH1	1:A:329:GLU:OE2	2.37	0.47
1:A:336:GLY:O	1:A:337:TYR:CD1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TYR:HB3	1:A:124:PRO:HD2	1.97	0.46
1:A:231:PHE:CD2	1:A:231:PHE:N	2.82	0.46
1:A:87:VAL:HB	1:A:92:ASN:HD22	1.79	0.46
1:A:297:HIS:HA	1:A:333:VAL:O	2.15	0.46
1:A:217:TYR:CD2	1:A:233:LYS:HG3	2.49	0.46
1:A:103:ARG:HD2	3:A:487:HOH:O	2.16	0.45
1:A:204:ASN:O	1:A:312:ARG:NH2	2.48	0.45
1:A:165:ILE:O	1:A:192:HIS:HD2	1.99	0.45
1:A:254:GLU:OE2	1:A:254:GLU:HA	2.16	0.45
1:A:260:TRP:C	1:A:262:LEU:H	2.19	0.45
1:A:76:TYR:C	1:A:78:ASP:N	2.70	0.45
1:A:194:ASP:OD1	1:A:203:THR:HB	2.16	0.45
1:A:68:LEU:HA	3:A:360:HOH:O	2.16	0.44
1:A:240:THR:HB	1:A:242:MET:CE	2.48	0.44
1:A:294:LYS:HD3	1:A:294:LYS:HA	1.80	0.44
1:A:230:LEU:HD12	1:A:230:LEU:HA	2.00	0.43
1:A:337:TYR:CB	3:A:465:HOH:O	2.50	0.43
1:A:173:MET:O	1:A:174:SER:HB3	2.18	0.43
1:A:181:HIS:CD2	3:A:436:HOH:O	2.71	0.43
1:A:254:GLU:OE2	1:A:254:GLU:CA	2.66	0.43
1:A:61:GLY:HA3	3:A:453:HOH:O	2.18	0.43
1:A:76:TYR:C	1:A:78:ASP:H	2.21	0.43
1:A:90:GLU:HG2	3:A:424:HOH:O	2.20	0.42
1:A:173:MET:O	1:A:174:SER:CB	2.66	0.42
1:A:83:GLN:O	1:A:95:ALA:HA	2.19	0.42
1:A:297:HIS:HE1	1:A:299:PHE:CE2	2.37	0.42
1:A:290:SER:O	1:A:293:HIS:HE1	2.03	0.42
1:A:310:HIS:HD2	1:A:312:ARG:N	1.92	0.42
1:A:73:VAL:CG2	1:A:73:VAL:O	2.66	0.42
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.69	0.42
1:A:192:HIS:O	1:A:193:PHE:C	2.56	0.42
1:A:304:ILE:HG12	3:A:356:HOH:O	2.19	0.42
1:A:68:LEU:CA	3:A:360:HOH:O	2.67	0.41
1:A:214:GLU:HB2	3:A:444:HOH:O	2.20	0.41
1:A:307:MET:HE2	1:A:307:MET:HB3	1.77	0.41
1:A:314:GLY:O	1:A:316:ILE:HG12	2.20	0.41
1:A:66:ASP:CG	1:A:67:ALA:H	2.24	0.41
1:A:247:GLY:HA3	1:A:276:ASP:O	2.20	0.41
1:A:58:THR:CG2	1:A:59:LEU:N	2.83	0.41
1:A:220:GLU:CD	1:A:220:GLU:H	2.24	0.40
1:A:260:TRP:C	1:A:262:LEU:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:TYR:CE2	1:A:215:ARG:HD3	2.57	0.40
1:A:296:ASN:ND2	2:A:1:SAH:HG2	2.37	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	278/280 (99%)	240 (86%)	28 (10%)	10 (4%)	<b>3</b> <b>1</b>

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	66	ASP
1	A	67	ALA
1	A	224	SER
1	A	279	GLU
1	A	176	GLU
1	A	177	GLU
1	A	180	PRO
1	A	278	PRO
1	A	100	THR

### 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	236/236 (100%)	205 (87%)	31 (13%)	<b>4</b> <b>3</b>

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	60	GLU
1	A	62	TYR
1	A	63	TYR
1	A	65	ASP
1	A	69	GLN
1	A	73	VAL
1	A	82	LEU
1	A	103	ARG
1	A	104	LEU
1	A	109	GLN
1	A	114	ILE
1	A	158	LYS
1	A	161	ASP
1	A	163	GLU
1	A	186	PRO
1	A	195	LYS
1	A	198	SER
1	A	207	LEU
1	A	214	GLU
1	A	249	ARG
1	A	251	THR
1	A	254	GLU
1	A	255	VAL
1	A	257	SER
1	A	268	SER
1	A	273	THR
1	A	278	PRO
1	A	280	PRO
1	A	326	GLU
1	A	337	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	109	GLN

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Mol	Chain	Res	Type
1	A	192	HIS
1	A	239	ASN
1	A	252	HIS
1	A	296	ASN
1	A	297	HIS
1	A	310	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is 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	A	1	-	21,28,28	2.68	8 (38%)	20,40,40	2.99	11 (55%)

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	A	1	-	-	2/7/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SAH	CA-N	5.99	1.60	1.47
2	A	1	SAH	O4'-C1'	4.84	1.47	1.41
2	A	1	SAH	C2-N1	4.30	1.41	1.33
2	A	1	SAH	C8-N7	-3.61	1.28	1.34
2	A	1	SAH	C6-N6	3.57	1.47	1.34
2	A	1	SAH	CG-SD	3.45	1.94	1.81
2	A	1	SAH	C2'-C3'	2.92	1.61	1.53
2	A	1	SAH	C2'-C1'	-2.76	1.49	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	SAH	C5'-C4'-C3'	5.53	128.87	115.06
2	A	1	SAH	CB-CG-SD	-4.72	102.72	113.31
2	A	1	SAH	O2'-C2'-C1'	-4.08	95.77	110.85
2	A	1	SAH	C2-N1-C6	3.97	125.55	118.75
2	A	1	SAH	O4'-C4'-C3'	3.96	112.96	105.11
2	A	1	SAH	C5-C6-N6	3.94	126.34	120.35
2	A	1	SAH	N3-C2-N1	-3.65	122.98	128.68
2	A	1	SAH	C5-C6-N1	-3.64	112.10	120.35
2	A	1	SAH	C4-C5-N7	3.51	113.06	109.40
2	A	1	SAH	O2'-C2'-C3'	-2.83	102.67	111.82
2	A	1	SAH	O4'-C1'-C2'	2.66	110.81	106.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	SAH	C3'-C4'-C5'-SD
2	A	1	SAH	CB-CG-SD-C5'

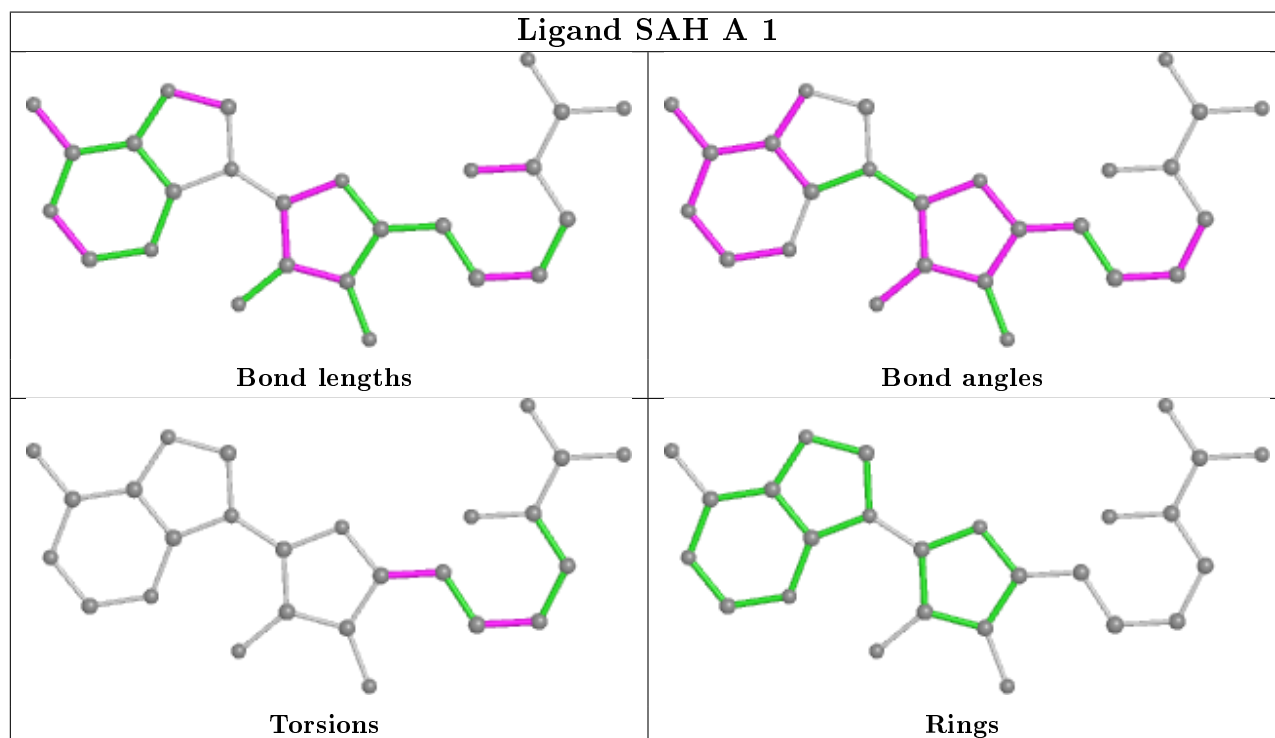
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SAH	3	0



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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	280/280 (100%)	0.07	18 (6%) <b>19</b> <b>18</b>	23, 45, 93, 102	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	LEU	5.4
1	A	61	GLY	5.0
1	A	178	GLY	4.8
1	A	177	GLU	4.2
1	A	102	GLY	4.1
1	A	66	ASP	4.0
1	A	175	THR	4.0
1	A	63	TYR	3.8
1	A	89	GLY	3.2
1	A	176	GLU	3.1
1	A	67	ALA	3.1
1	A	135	GLU	2.9
1	A	179	ARG	2.8
1	A	279	GLU	2.8
1	A	81	VAL	2.6
1	A	58	THR	2.5
1	A	136	ASP	2.4
1	A	78	ASP	2.2

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

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

### 6.3 Carbohydrates [i](#)

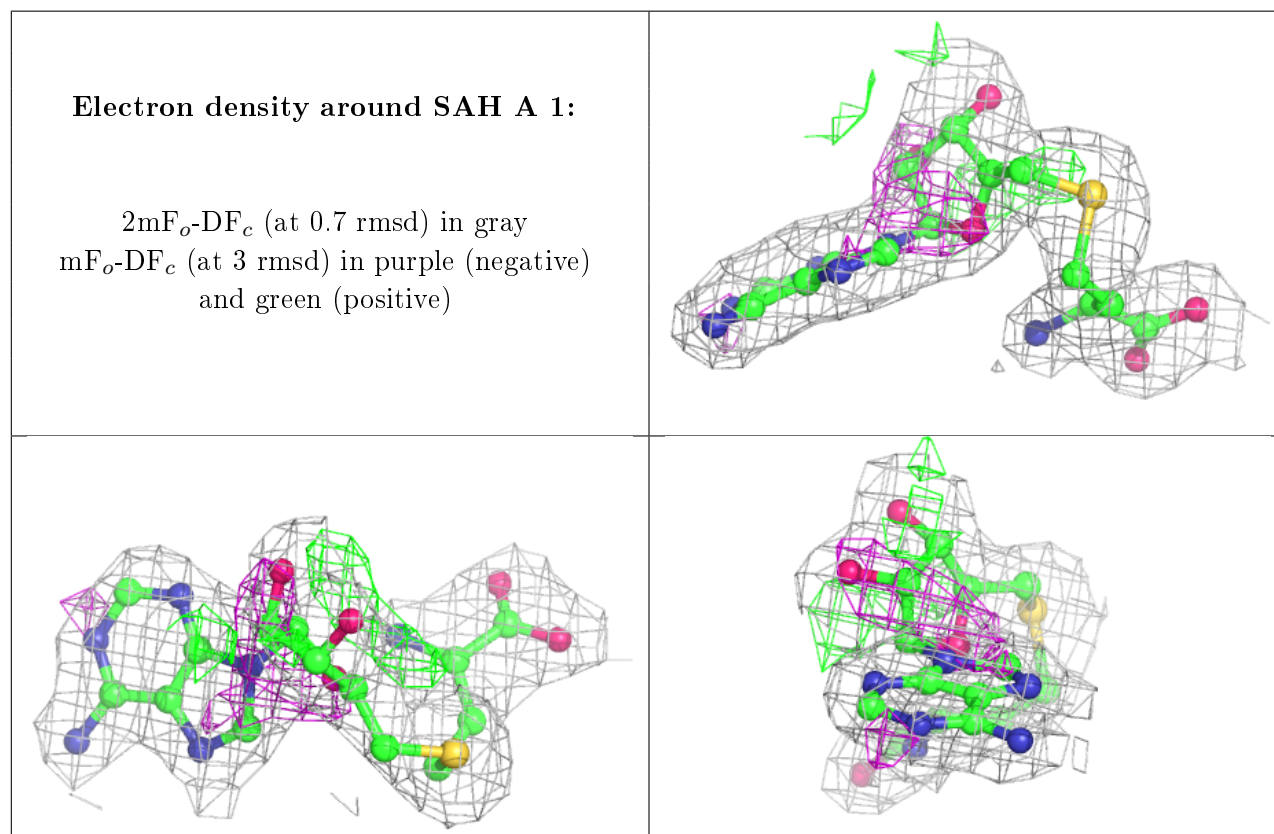
There are no carbohydrates in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SAH	A	1	26/26	0.92	0.13	26,42,49,51	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.