



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:00 am BST

PDB ID : 4H0N  
Title : Crystal structure of Spodoptera frugiperda DNMT2 E260A/E261A/K263A mutant  
Authors : Li, S.; Du, J.; Yang, H.; Yin, J.; Zhong, J.; Ding, J.  
Deposited on : 2012-09-09  
Resolution : 2.71 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

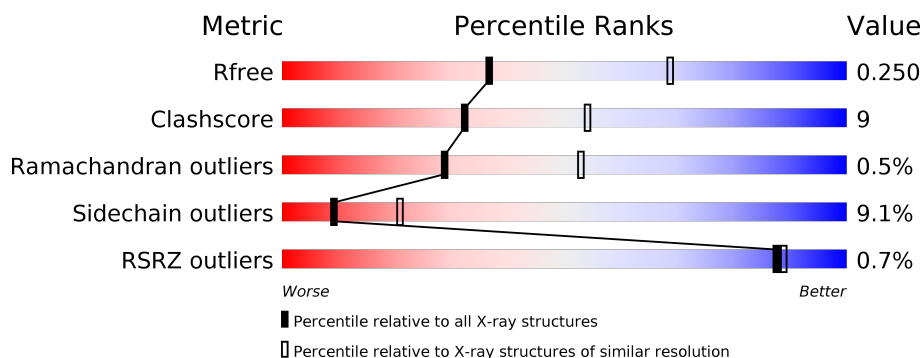
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	333	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>••</div> </div> </div>
1	B	333	<div> <div></div> <div>72%</div> <div>24%</div> <div>••</div> </div>
1	C	333	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>••</div> </div> </div>
1	D	333	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11038 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 DNMT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2684	1722	451	492	19			
1	B	331	Total	C	N	O	S	0	0	0
			2684	1722	451	492	19			
1	C	331	Total	C	N	O	S	0	0	0
			2684	1722	451	492	19			
1	D	331	Total	C	N	O	S	0	0	0
			2684	1722	451	492	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
A	261	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
A	263	ALA	LYS	ENGINEERED MUTATION	PDB 4H0N
B	260	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
B	261	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
B	263	ALA	LYS	ENGINEERED MUTATION	PDB 4H0N
C	260	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
C	261	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
C	263	ALA	LYS	ENGINEERED MUTATION	PDB 4H0N
D	260	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
D	261	ALA	GLU	ENGINEERED MUTATION	PDB 4H0N
D	263	ALA	LYS	ENGINEERED MUTATION	PDB 4H0N

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	55	Total 55	O 55	0	0
4	C	34	Total 34	O 34	0	0
4	D	53	Total 53	O 53	0	0

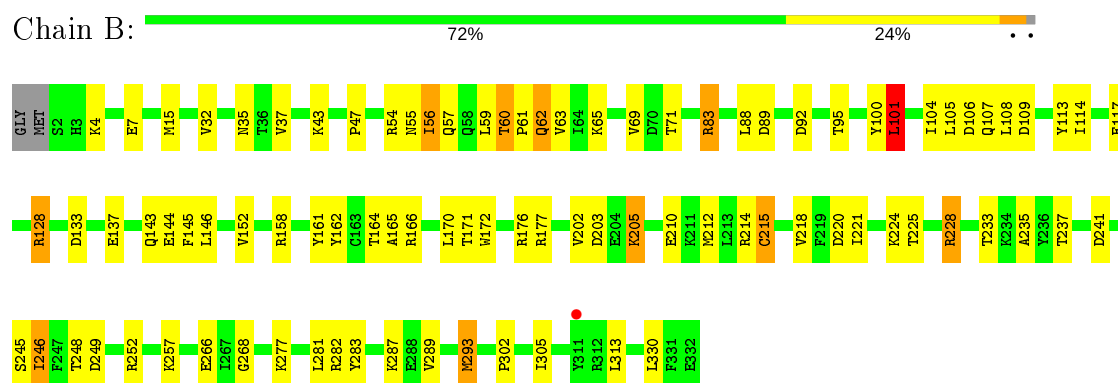
### 3 Residue-property plots [i](#)

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.

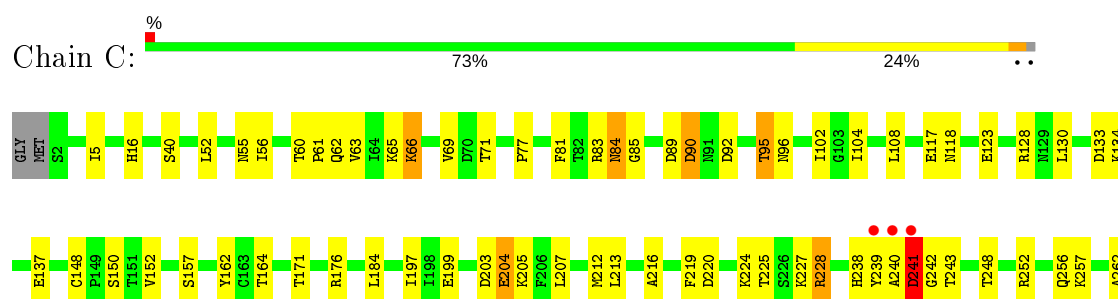
#### • Molecule 1: DNMT2

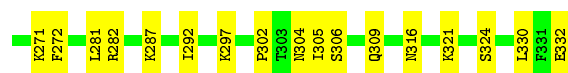


#### • Molecule 1: DNMT2

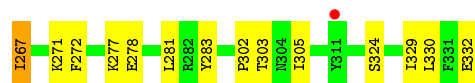
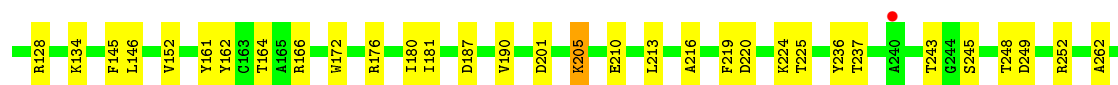
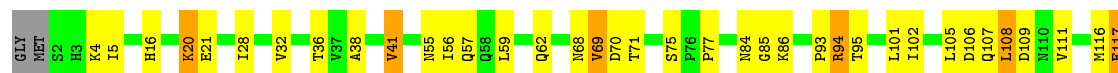
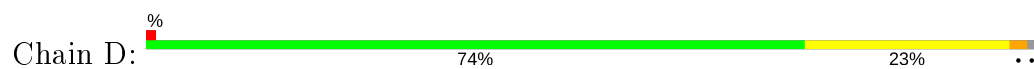


#### • Molecule 1: DNMT2





• Molecule 1: DNMT2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.39Å 106.15Å 151.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.71 48.70 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.70-2.71) 99.0 (48.70-2.71)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.202 , 0.256 0.200 , 0.250	Depositor DCC
$R_{free}$ test set	2148 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	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 69.74 % 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 3.5163e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CA, 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	0.32	0/2743	0.48	0/3709
1	B	0.29	0/2743	0.49	1/3709 (0.0%)
1	C	0.33	0/2743	0.48	0/3709
1	D	0.32	0/2743	0.51	0/3709
All	All	0.32	0/10972	0.49	1/14836 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2684	0	2700	48	0
1	B	2684	0	2700	44	0
1	C	2684	0	2700	53	0
1	D	2684	0	2700	44	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	26	0	19	3	0
2	D	26	0	19	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	52	0	0	4	0
4	B	55	0	0	4	0
4	C	34	0	0	2	0
4	D	53	0	0	1	0
All	All	11038	0	10876	190	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 9.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:TYR:HE1	1:C:241:ASP:CG	1.57	1.07
1:C:239:TYR:CE1	1:C:241:ASP:CG	2.30	1.04
1:B:15:MET:HG3	4:B:554:HOH:O	1.61	1.00
1:D:108:LEU:H	1:D:108:LEU:HD23	1.24	0.99
1:C:241:ASP:CG	1:C:242:GLY:H	1.55	0.98
1:D:108:LEU:N	1:D:108:LEU:CD2	2.36	0.89
1:D:108:LEU:H	1:D:108:LEU:CD2	1.88	0.86
1:C:241:ASP:CG	1:C:242:GLY:N	2.30	0.84
1:C:302:PRO:HG2	1:C:305:ILE:HD13	1.59	0.84
1:C:239:TYR:CE1	1:C:241:ASP:OD1	2.30	0.82
1:C:77:PRO:HG3	2:C:401:SAH:H5'1	1.63	0.81
1:C:239:TYR:HE1	1:C:241:ASP:CB	1.95	0.79
1:A:83:ARG:HB2	1:A:83:ARG:CZ	2.12	0.79
1:D:16:HIS:CD2	1:D:28:ILE:HG13	2.19	0.77
1:B:224:LYS:NZ	1:B:249:ASP:OD1	2.20	0.74
1:A:55:ASN:OD1	1:A:57:GLN:NE2	2.20	0.74
1:D:32:VAL:HG21	1:D:59:LEU:HD11	1.71	0.73
1:B:15:MET:CG	4:B:554:HOH:O	2.23	0.73
1:C:241:ASP:OD1	1:C:243:THR:HG23	1.89	0.72
1:C:134:LYS:HA	1:C:137:GLU:OE1	1.90	0.72
1:D:224:LYS:NZ	1:D:249:ASP:OD1	2.23	0.70
1:B:145:PHE:HB2	1:B:162:TYR:HB2	1.76	0.67
1:A:306:SER:OG	1:A:309:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASN:OD1	1:D:57:GLN:NE2	2.26	0.66
1:D:4:LYS:HB2	1:D:69:VAL:HA	1.76	0.66
1:B:43:LYS:NZ	1:B:47:PRO:O	2.28	0.65
1:D:16:HIS:O	1:D:20:LYS:NZ	2.30	0.65
1:C:241:ASP:OD1	1:C:242:GLY:N	2.30	0.65
1:C:227:LYS:NZ	4:C:534:HOH:O	2.30	0.65
1:C:164:THR:HB	1:C:330:LEU:HD13	1.77	0.65
1:A:195:GLU:HG2	1:A:224:LYS:HB2	1.80	0.63
1:B:55:ASN:ND2	1:B:57:GLN:OE1	2.31	0.63
1:D:164:THR:HB	1:D:330:LEU:HD13	1.81	0.62
1:D:145:PHE:HB2	1:D:162:TYR:HB2	1.81	0.62
1:C:55:ASN:ND2	4:C:515:HOH:O	2.29	0.61
1:A:83:ARG:CB	1:A:83:ARG:CZ	2.78	0.61
1:A:81:PHE:CE1	1:A:96:ASN:HB3	2.35	0.61
1:C:239:TYR:HE1	1:C:241:ASP:HB3	1.65	0.61
1:A:158:ARG:NH2	1:A:317:SER:O	2.33	0.60
1:B:133:ASP:O	1:B:137:GLU:HG3	2.01	0.60
1:A:164:THR:HB	1:A:330:LEU:HD13	1.83	0.60
1:A:4:LYS:HB2	1:A:69:VAL:HA	1.83	0.59
1:A:248:THR:HB	1:A:281:LEU:HD23	1.85	0.58
1:D:108:LEU:N	1:D:108:LEU:HD22	2.17	0.58
1:C:90:ASP:OD1	1:C:90:ASP:N	2.32	0.58
1:C:89:ASP:O	1:C:95:THR:HG21	2.04	0.58
1:D:324:SER:HB3	4:D:549:HOH:O	2.04	0.57
1:C:60:THR:HG23	1:C:63:VAL:H	1.70	0.56
1:C:248:THR:HB	1:C:281:LEU:HD23	1.87	0.56
1:A:79:GLN:NE2	4:A:534:HOH:O	2.33	0.56
1:D:220:ASP:OD2	1:D:245:SER:OG	2.23	0.56
1:D:267:ILE:HD12	1:D:267:ILE:H	1.70	0.56
1:C:212:MET:HE1	1:C:238:HIS:O	2.07	0.55
1:C:239:TYR:CE1	1:C:241:ASP:CB	2.82	0.55
1:D:146:LEU:HD23	1:D:161:TYR:HA	1.89	0.55
1:B:164:THR:HB	1:B:330:LEU:HD13	1.87	0.55
1:B:83:ARG:HB2	1:B:88:LEU:HD21	1.88	0.55
1:B:220:ASP:OD2	1:B:228:ARG:NH2	2.39	0.55
1:B:233:THR:HG22	1:B:235:ALA:H	1.71	0.54
1:A:83:ARG:NH2	1:A:83:ARG:CB	2.71	0.54
1:B:246:ILE:HD11	1:B:283:TYR:CD1	2.43	0.54
1:A:141:ILE:HG23	1:A:168:ASN:HB3	1.88	0.53
1:A:183:ARG:NH1	4:A:543:HOH:O	2.41	0.53
1:C:239:TYR:CE1	1:C:241:ASP:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASP:OD2	1:B:245:SER:OG	2.24	0.53
1:D:248:THR:HB	1:D:281:LEU:HD23	1.91	0.52
1:B:248:THR:HB	1:B:281:LEU:HD23	1.91	0.52
1:C:62:GLN:N	1:C:62:GLN:OE1	2.41	0.52
1:B:166:ARG:HD3	1:B:172:TRP:CG	2.45	0.52
1:D:77:PRO:HG3	2:D:401:SAH:H8	1.90	0.52
1:D:70:ASP:HA	1:D:111:VAL:HA	1.93	0.51
1:D:93:PRO:O	1:D:94:ARG:HB2	2.09	0.51
1:B:32:VAL:HG11	1:B:59:LEU:HD11	1.93	0.51
1:D:210:GLU:HA	1:D:213:LEU:HD12	1.91	0.51
1:D:302:PRO:HG2	1:D:305:ILE:HG12	1.93	0.51
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.46	0.51
1:D:107:GLN:OE1	1:D:109:ASP:OD2	2.30	0.50
1:D:102:ILE:O	1:D:134:LYS:HE2	2.10	0.50
1:D:329:ILE:O	1:D:332:GLU:HB2	2.12	0.50
1:B:60:THR:HB	1:B:62:GLN:HG2	1.93	0.50
1:B:4:LYS:HB2	1:B:69:VAL:HA	1.94	0.50
1:C:102:ILE:HD13	1:C:130:LEU:HD23	1.94	0.50
1:C:92:ASP:HB3	1:C:95:THR:HG22	1.93	0.49
1:B:106:ASP:OD1	1:B:107:GLN:NE2	2.45	0.49
1:D:107:GLN:OE1	1:D:109:ASP:OD1	2.30	0.49
1:B:101:LEU:HA	1:B:104:ILE:HG12	1.95	0.49
1:C:81:PHE:CE1	1:C:96:ASN:HB3	2.47	0.49
1:A:211:LYS:HE3	1:A:212:MET:HG2	1.94	0.48
1:A:37:VAL:HG12	1:A:313:LEU:HD11	1.96	0.48
1:C:207:LEU:HD23	1:C:282:ARG:HB3	1.96	0.48
1:C:148:CYS:SG	1:C:157:SER:HA	2.53	0.48
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.48	0.48
1:B:237:THR:HG22	1:B:283:TYR:CD1	2.48	0.48
1:B:92:ASP:O	1:B:95:THR:HG22	2.13	0.48
1:C:133:ASP:O	1:C:137:GLU:HG3	2.13	0.48
1:C:63:VAL:HA	1:C:66:LYS:HE3	1.95	0.48
1:C:61:PRO:O	1:C:65:LYS:HG2	2.14	0.48
1:A:37:VAL:HG11	1:A:309:GLN:HG2	1.95	0.48
1:B:146:LEU:HD23	1:B:161:TYR:HA	1.95	0.48
1:B:62:GLN:OE1	1:B:62:GLN:N	2.46	0.47
1:C:316:ASN:O	2:C:401:SAH:HG1	2.14	0.47
1:B:71:THR:HG23	1:B:113:TYR:HB2	1.95	0.47
1:A:63:VAL:HG23	1:A:66:LYS:HD3	1.95	0.47
1:C:212:MET:CE	1:C:239:TYR:HA	2.44	0.47
1:A:277:LYS:HB3	1:A:277:LYS:HE3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HG3	1:A:84:ASN:OD1	2.15	0.47
1:A:5:ILE:HG13	1:A:71:THR:HB	1.96	0.47
1:B:114:ILE:HB	1:B:165:ALA:HB3	1.96	0.47
1:B:37:VAL:HG12	1:B:313:LEU:HD11	1.97	0.47
1:C:252:ARG:O	1:C:256:GLN:HG2	2.13	0.47
1:A:203:ASP:HB3	1:A:205:LYS:HD3	1.97	0.47
1:C:240:ALA:O	1:C:241:ASP:O	2.32	0.47
1:B:214:ARG:NH1	1:B:268:GLY:O	2.49	0.46
1:B:166:ARG:HD2	1:B:330:LEU:O	2.15	0.46
1:A:120:LYS:HD3	1:A:121:GLY:N	2.31	0.46
1:A:104:ILE:O	1:A:108:LEU:HG	2.16	0.46
1:A:152:VAL:HG12	1:A:321:LYS:HE3	1.98	0.46
1:C:83:ARG:O	1:C:85:GLY:N	2.49	0.46
1:B:61:PRO:O	1:B:65:LYS:HG3	2.15	0.46
1:A:237:THR:HG22	1:A:283:TYR:CD1	2.51	0.45
1:A:14:GLY:HA3	1:A:318:VAL:HG22	1.97	0.45
1:C:84:ASN:OD1	1:C:85:GLY:N	2.47	0.45
1:C:197:ILE:HD13	1:C:292:ILE:HG13	1.99	0.45
1:D:237:THR:HG22	1:D:283:TYR:CD1	2.51	0.45
1:A:208:VAL:HA	1:A:209:PRO:HD3	1.80	0.45
1:C:117:GLU:HG3	1:C:162:TYR:CE1	2.52	0.45
1:A:83:ARG:HB3	1:A:88:LEU:HD21	1.99	0.44
1:B:203:ASP:HB3	1:B:205:LYS:HB2	1.99	0.44
1:A:177:ARG:NH1	1:A:179:GLU:HB3	2.32	0.44
1:B:56:ILE:HD11	1:B:100:TYR:HB3	1.98	0.44
1:D:225:THR:OG1	1:D:252:ARG:NH1	2.50	0.44
1:D:262:ALA:HB1	1:D:272:PHE:CD1	2.53	0.44
1:D:38:ALA:O	1:D:41:VAL:HG13	2.18	0.44
1:B:225:THR:OG1	1:B:252:ARG:NH1	2.51	0.44
1:A:24:LEU:O	4:A:506:HOH:O	2.21	0.44
1:A:59:LEU:O	1:A:100:TYR:OH	2.25	0.44
1:A:92:ASP:O	1:A:95:THR:HG23	2.17	0.44
1:D:101:LEU:HD22	1:D:101:LEU:HA	1.76	0.44
1:D:146:LEU:HG	1:D:180:ILE:HG21	2.00	0.44
1:D:166:ARG:HD3	1:D:172:TRP:CG	2.53	0.44
1:B:143:GLN:HA	4:B:501:HOH:O	2.18	0.43
1:C:271:LYS:HA	1:C:271:LYS:HD2	1.83	0.43
1:B:7:GLU:OE1	4:B:553:HOH:O	2.21	0.43
1:A:191:PRO:O	1:A:227:LYS:HG2	2.19	0.43
1:C:306:SER:OG	1:C:309:GLN:HG3	2.18	0.43
2:C:401:SAH:HB1	2:C:401:SAH:H5'2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLN:HE21	1:A:309:GLN:HB2	1.45	0.43
1:D:75:SER:OG	2:D:401:SAH:N	2.52	0.43
1:A:297:LYS:HD2	1:A:297:LYS:H	1.82	0.43
1:A:197:ILE:HG21	1:A:291:MET:HB3	2.00	0.42
1:B:215:CYS:O	1:B:218:VAL:HG22	2.19	0.42
1:B:221:ILE:HG12	1:B:246:ILE:HG22	2.02	0.42
1:C:203:ASP:OD1	1:C:204:GLU:N	2.52	0.42
1:D:216:ALA:HA	1:D:219:PHE:CD2	2.54	0.42
1:C:220:ASP:OD2	1:C:228:ARG:NH2	2.52	0.42
1:D:145:PHE:CE2	1:D:181:ILE:HD12	2.53	0.42
1:B:166:ARG:NH2	1:B:171:THR:OG1	2.52	0.42
1:B:289:VAL:O	1:B:293:MET:HB2	2.20	0.42
1:C:305:ILE:HG23	1:C:309:GLN:HB2	2.02	0.42
1:D:205:LYS:HE2	1:D:205:LYS:HB2	1.93	0.42
1:A:153:GLY:N	4:A:527:HOH:O	2.52	0.42
1:B:202:VAL:HG11	1:B:282:ARG:CD	2.50	0.42
1:D:16:HIS:CD2	1:D:20:LYS:NZ	2.87	0.42
1:A:219:PHE:CE1	1:A:240:ALA:HB1	2.55	0.42
1:A:110:ASN:C	1:A:110:ASN:HD22	2.22	0.41
1:A:148:CYS:SG	1:A:157:SER:HA	2.59	0.41
1:D:84:ASN:HB3	1:D:85:GLY:H	1.63	0.41
1:A:274:GLU:HG3	1:A:275:LEU:N	2.35	0.41
1:B:302:PRO:HG2	1:B:305:ILE:HD12	2.01	0.41
1:D:106:ASP:C	1:D:107:GLN:HG2	2.40	0.41
1:D:5:ILE:HG13	1:D:71:THR:HB	2.02	0.41
1:A:246:ILE:HD13	1:A:246:ILE:HA	1.88	0.41
1:C:262:ALA:HB1	1:C:272:PHE:CD1	2.55	0.41
1:A:92:ASP:HB3	1:A:95:THR:CG2	2.50	0.41
1:A:57:GLN:HA	1:A:100:TYR:CD1	2.55	0.41
1:C:241:ASP:OD1	1:C:243:THR:CG2	2.62	0.41
1:D:237:THR:HG22	1:D:283:TYR:CG	2.56	0.41
1:B:54:ARG:HH11	1:B:54:ARG:CG	2.34	0.41
1:C:224:LYS:HE2	1:C:224:LYS:HB3	1.89	0.41
1:A:134:LYS:HA	1:A:134:LYS:HD2	1.84	0.41
1:B:237:THR:HG22	1:B:283:TYR:CG	2.56	0.41
1:A:214:ARG:NE	1:A:268:GLY:O	2.53	0.40
1:C:65:LYS:HD3	1:C:65:LYS:HA	1.83	0.40
1:C:5:ILE:HG13	1:C:71:THR:HB	2.02	0.40
1:B:128:ARG:NE	1:B:144:GLU:OE2	2.45	0.40
1:C:104:ILE:O	1:C:108:LEU:HG	2.22	0.40
1:C:152:VAL:O	1:C:321:LYS:HE3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLU:HG3	1:D:162:TYR:CE1	2.56	0.40
1:D:236:TYR:HA	1:D:243:THR:HB	2.03	0.40
1:C:239:TYR:CZ	1:C:241:ASP:CG	2.92	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	329/333 (99%)	319 (97%)	10 (3%)	0	100	100
1	B	329/333 (99%)	318 (97%)	9 (3%)	2 (1%)	25	48
1	C	329/333 (99%)	318 (97%)	8 (2%)	3 (1%)	17	38
1	D	329/333 (99%)	315 (96%)	13 (4%)	1 (0%)	41	65
All	All	1316/1332 (99%)	1270 (96%)	40 (3%)	6 (0%)	29	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	84	ASN
1	C	241	ASP
1	B	158	ARG
1	C	171	THR
1	B	266	GLU
1	D	267	ILE

### 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	304/305 (100%)	274 (90%)	30 (10%)	8	17
1	B	304/305 (100%)	276 (91%)	28 (9%)	9	20
1	C	304/305 (100%)	277 (91%)	27 (9%)	9	22
1	D	304/305 (100%)	278 (91%)	26 (9%)	10	23
All	All	1216/1220 (100%)	1105 (91%)	111 (9%)	9	21

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	36	THR
1	A	43	LYS
1	A	66	LYS
1	A	69	VAL
1	A	83	ARG
1	A	84	ASN
1	A	90	ASP
1	A	95	THR
1	A	97	SER
1	A	110	ASN
1	A	118	ASN
1	A	125	SER
1	A	128	ARG
1	A	176	ARG
1	A	180	ILE
1	A	184	LEU
1	A	196	SER
1	A	198	ILE
1	A	199	GLU
1	A	201	ASP
1	A	205	LYS
1	A	211	LYS
1	A	221	ILE
1	A	234	LYS
1	A	277	LYS
1	A	297	LYS
1	A	304	ASN
1	A	305	ILE
1	A	309	GLN

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Mol	Chain	Res	Type
1	B	35	ASN
1	B	56	ILE
1	B	60	THR
1	B	62	GLN
1	B	63	VAL
1	B	83	ARG
1	B	89	ASP
1	B	101	LEU
1	B	105	LEU
1	B	108	LEU
1	B	109	ASP
1	B	117	GLU
1	B	128	ARG
1	B	152	VAL
1	B	170	LEU
1	B	176	ARG
1	B	177	ARG
1	B	205	LYS
1	B	210	GLU
1	B	212	MET
1	B	215	CYS
1	B	228	ARG
1	B	241	ASP
1	B	246	ILE
1	B	257	LYS
1	B	277	LYS
1	B	287	LYS
1	B	293	MET
1	C	16	HIS
1	C	40	SER
1	C	52	LEU
1	C	56	ILE
1	C	66	LYS
1	C	69	VAL
1	C	90	ASP
1	C	95	THR
1	C	118	ASN
1	C	123	GLU
1	C	128	ARG
1	C	150	SER
1	C	176	ARG
1	C	184	LEU

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Mol	Chain	Res	Type
1	C	199	GLU
1	C	204	GLU
1	C	205	LYS
1	C	213	LEU
1	C	225	THR
1	C	228	ARG
1	C	241	ASP
1	C	257	LYS
1	C	287	LYS
1	C	297	LYS
1	C	304	ASN
1	C	324	SER
1	C	332	GLU
1	D	20	LYS
1	D	21	GLU
1	D	36	THR
1	D	41	VAL
1	D	56	ILE
1	D	62	GLN
1	D	68	ASN
1	D	69	VAL
1	D	86	LYS
1	D	94	ARG
1	D	95	THR
1	D	105	LEU
1	D	108	LEU
1	D	116	MET
1	D	117	GLU
1	D	128	ARG
1	D	152	VAL
1	D	176	ARG
1	D	187	ASP
1	D	190	VAL
1	D	201	ASP
1	D	205	LYS
1	D	271	LYS
1	D	277	LYS
1	D	278	GLU
1	D	303	THR

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

Mol	Chain	Res	Type
1	A	309	GLN
1	B	55	ASN
1	B	84	ASN
1	D	16	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SAH	D	401	-	21,28,28	1.20	2 (9%)	20,40,40	1.68	2 (10%)
2	SAH	C	401	-	21,28,28	1.20	2 (9%)	20,40,40	1.67	3 (15%)
2	SAH	B	401	-	21,28,28	1.22	2 (9%)	20,40,40	1.73	3 (15%)
2	SAH	A	401	-	21,28,28	1.19	2 (9%)	20,40,40	1.66	3 (15%)

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	401	-	-	2/7/31/31	0/3/3/3
2	SAH	C	401	-	-	3/7/31/31	0/3/3/3
2	SAH	B	401	-	-	2/7/31/31	0/3/3/3
2	SAH	A	401	-	-	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	B	401	SAH	C2-N3	4.07	1.38	1.32
2	C	401	SAH	C2-N3	4.02	1.38	1.32
2	D	401	SAH	C2-N3	3.99	1.38	1.32
2	A	401	SAH	C2-N3	3.96	1.38	1.32
2	D	401	SAH	C2-N1	2.55	1.38	1.33
2	C	401	SAH	C2-N1	2.53	1.38	1.33
2	A	401	SAH	C2-N1	2.50	1.38	1.33
2	B	401	SAH	C2-N1	2.49	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	N3-C2-N1	-5.45	120.16	128.68
2	D	401	SAH	N3-C2-N1	-5.44	120.18	128.68
2	B	401	SAH	N3-C2-N1	-5.42	120.21	128.68
2	C	401	SAH	N3-C2-N1	-5.33	120.35	128.68
2	B	401	SAH	C5'-SD-CG	-3.80	90.86	102.27
2	D	401	SAH	C5'-SD-CG	-3.41	92.03	102.27
2	C	401	SAH	C5'-SD-CG	-3.38	92.12	102.27
2	A	401	SAH	C5'-SD-CG	-3.06	93.07	102.27
2	C	401	SAH	C3'-C2'-C1'	3.06	105.58	100.98
2	A	401	SAH	C3'-C2'-C1'	2.69	105.03	100.98
2	B	401	SAH	C3'-C2'-C1'	2.47	104.70	100.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	SAH	N-CA-CB-CG
2	D	401	SAH	C-CA-CB-CG
2	C	401	SAH	N-CA-CB-CG
2	C	401	SAH	C-CA-CB-CG
2	B	401	SAH	N-CA-CB-CG

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

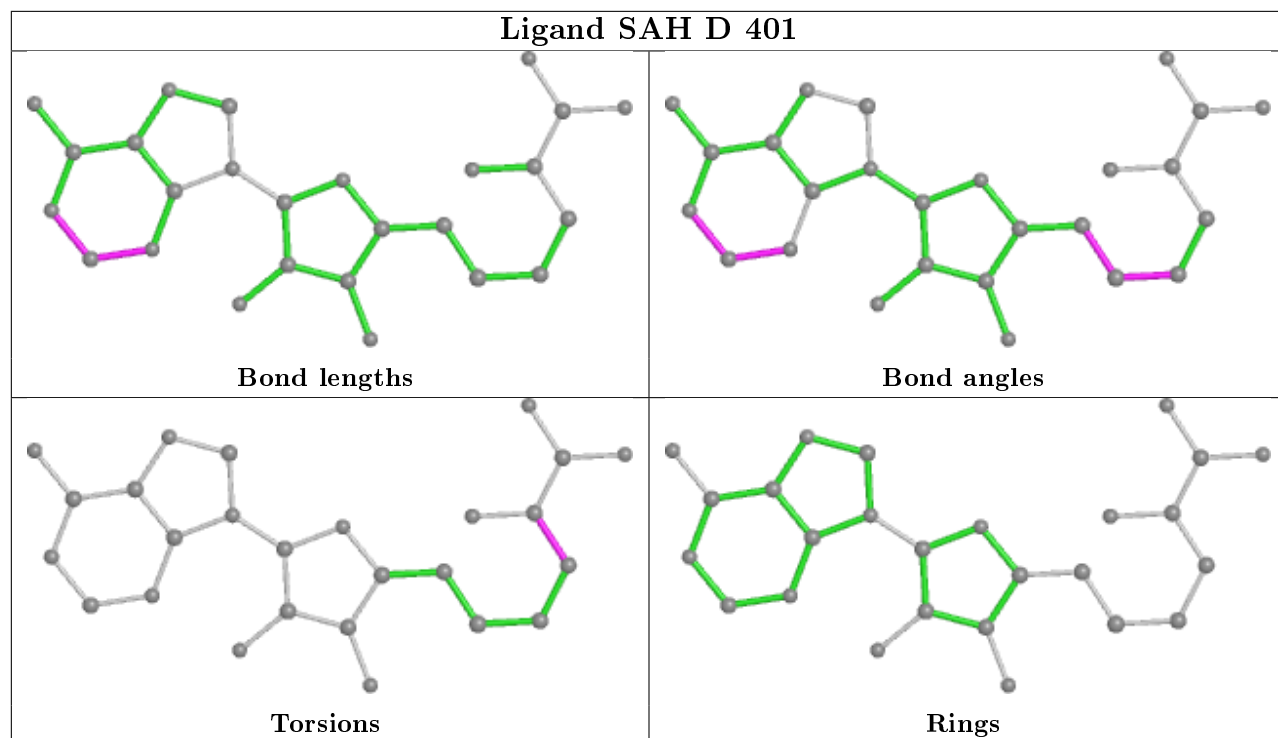
There are no ring outliers.

2 monomers are involved in 5 short contacts:

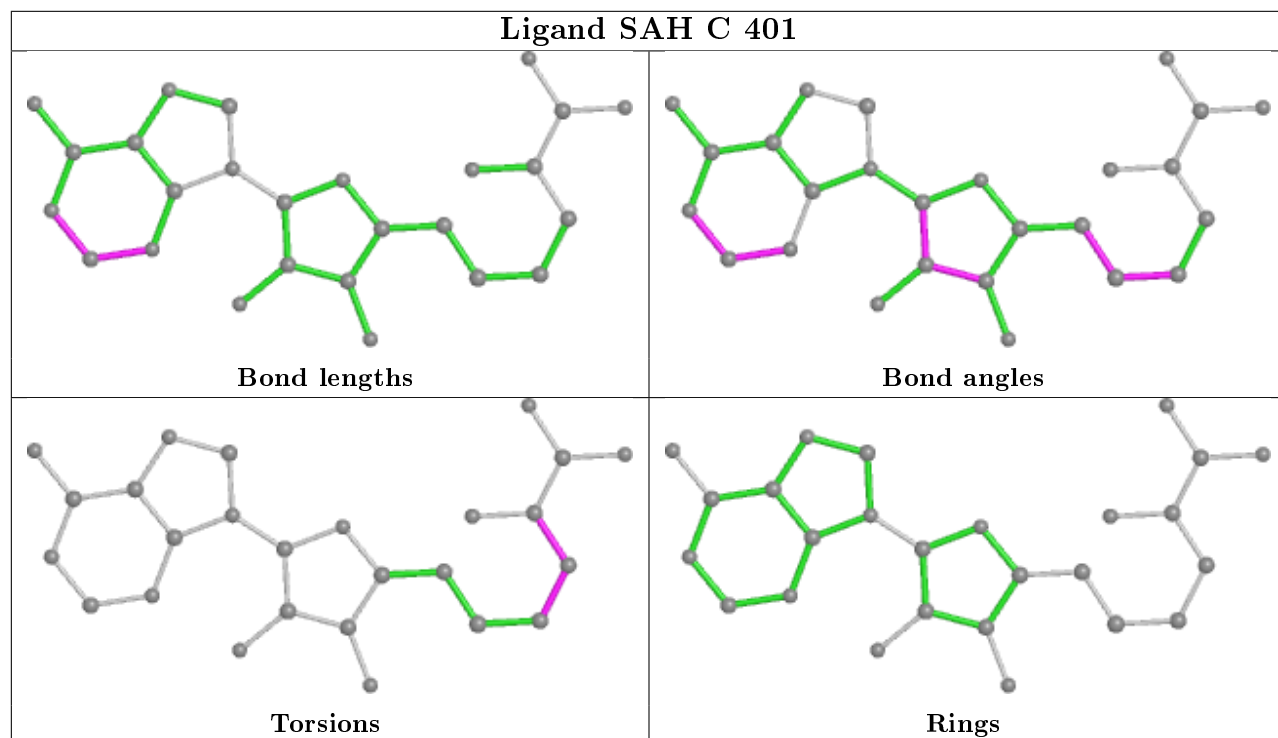
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	SAH	2	0
2	C	401	SAH	3	0

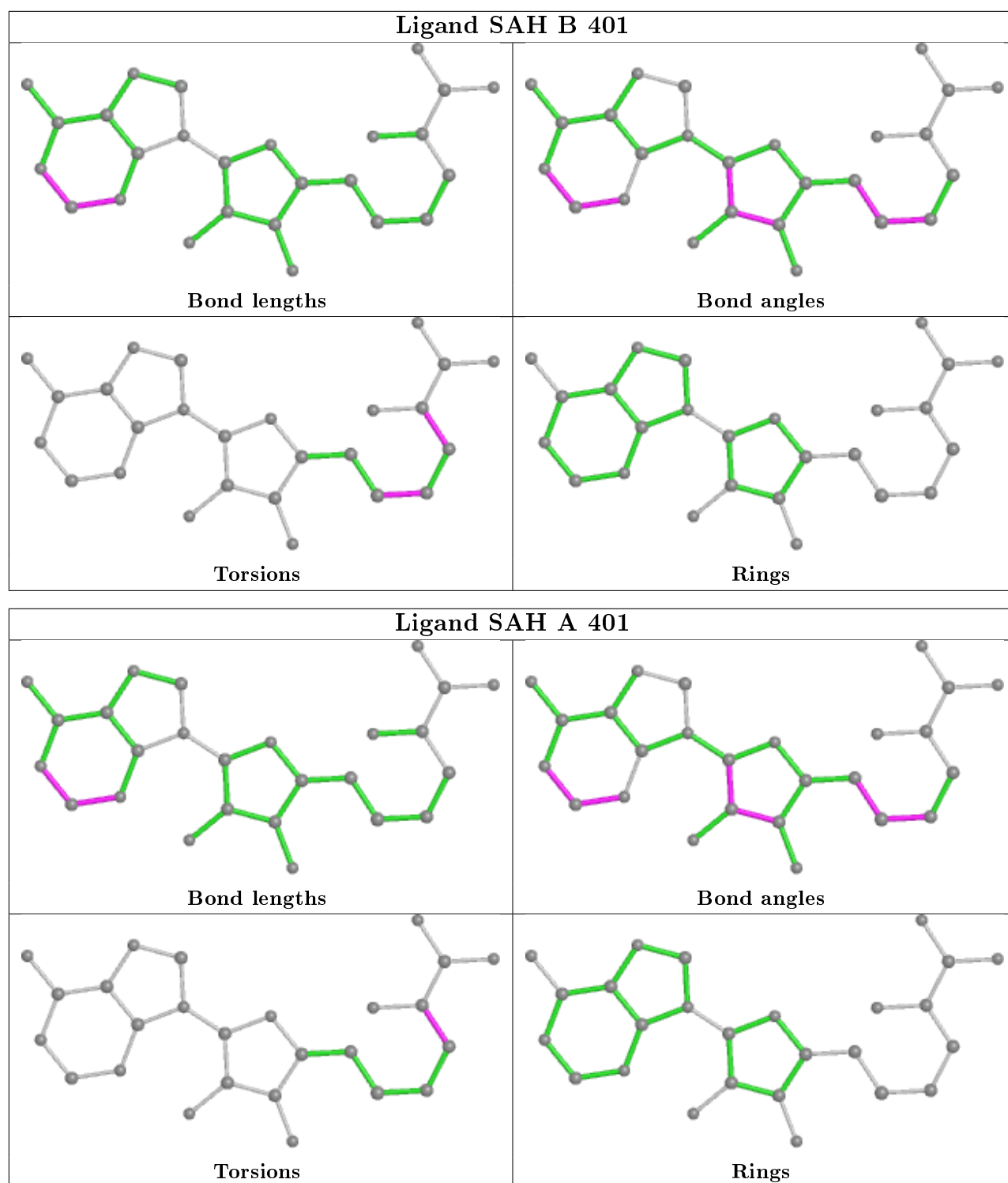
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand SAH D 401



## Ligand SAH C 401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	331/333 (99%)	-0.21	3 (0%) 84 85	17, 36, 73, 110	0
1	B	331/333 (99%)	-0.18	1 (0%) 94 95	20, 36, 70, 90	0
1	C	331/333 (99%)	-0.14	3 (0%) 84 85	21, 40, 73, 139	0
1	D	331/333 (99%)	-0.15	2 (0%) 89 90	21, 38, 77, 96	0
All	All	1324/1332 (99%)	-0.17	9 (0%) 87 89	17, 38, 73, 139	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	TYR	3.4
1	C	240	ALA	3.4
1	C	241	ASP	3.1
1	B	311	TYR	3.0
1	A	239	TYR	2.7
1	D	240	ALA	2.6
1	A	240	ALA	2.6
1	A	241	ASP	2.3
1	D	311	TYR	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](#)

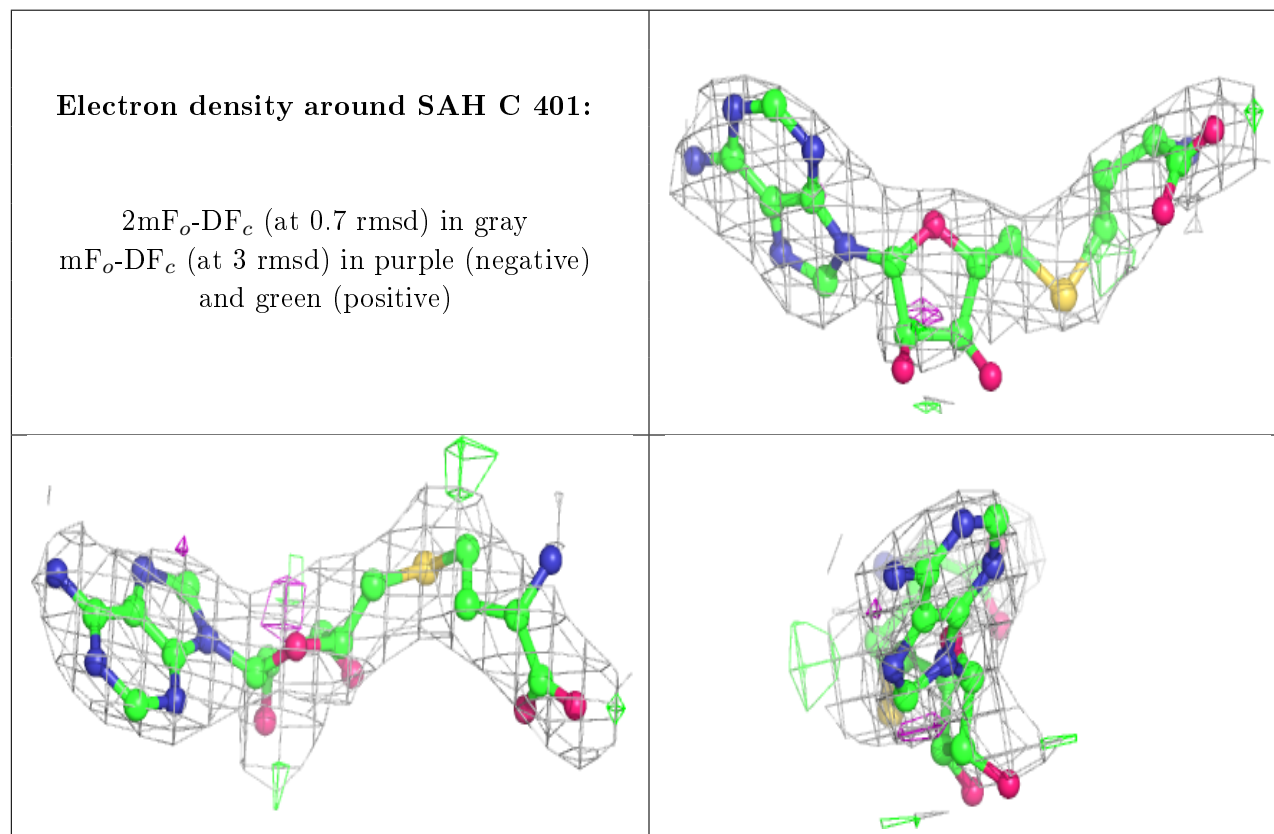
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

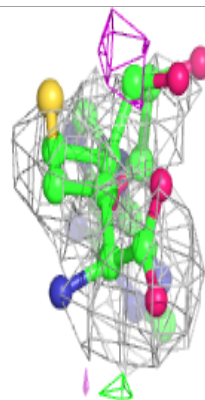
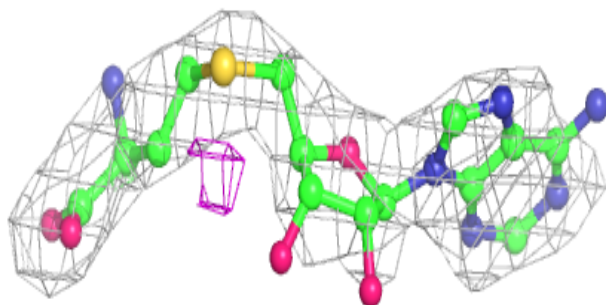
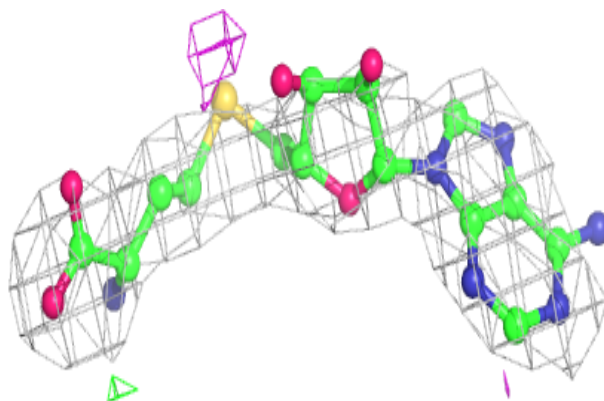
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	A	402	1/1	0.43	0.15	47,47,47,47	0
3	CA	D	402	1/1	0.72	0.14	62,62,62,62	0
3	CA	B	402	1/1	0.81	0.14	64,64,64,64	0
2	SAH	C	401	26/26	0.86	0.27	48,73,104,109	0
3	CA	C	402	1/1	0.87	0.17	62,62,62,62	0
2	SAH	B	401	26/26	0.87	0.31	43,88,97,142	0
2	SAH	D	401	26/26	0.94	0.24	14,56,68,70	0
2	SAH	A	401	26/26	0.94	0.17	28,57,78,87	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.

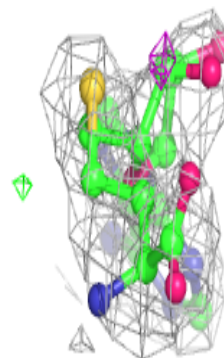
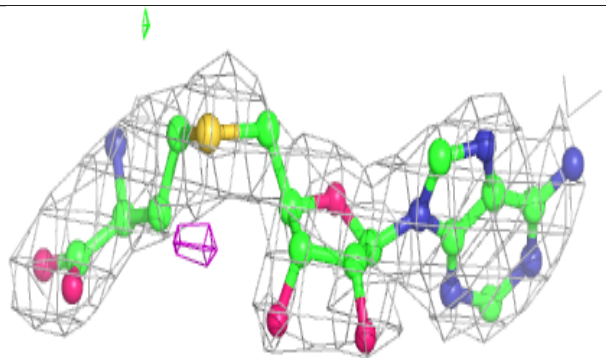
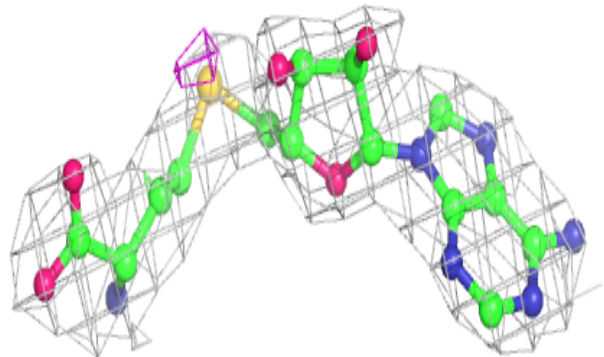


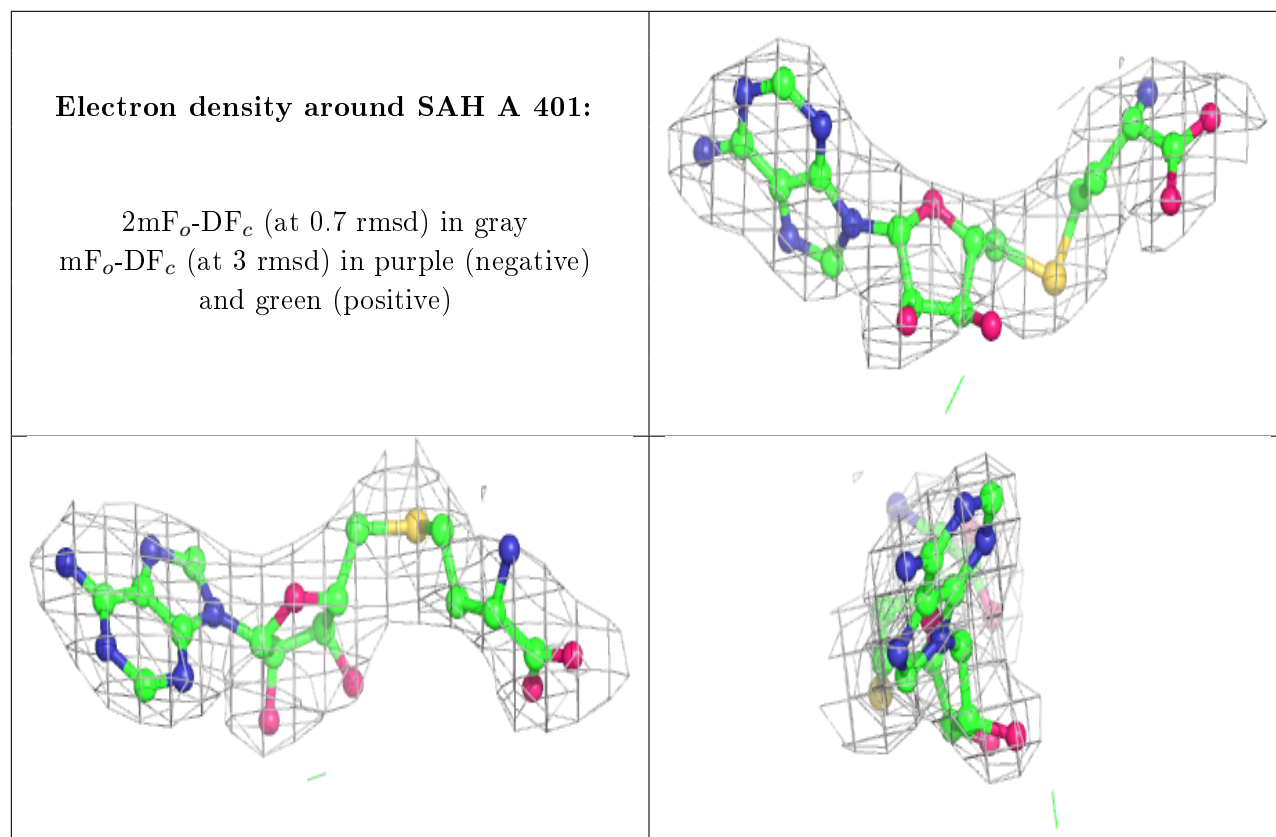
**Electron density around SAH B 401:**

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

**Electron density around SAH D 401:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.