



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 10:23 AM BST

PDB ID : 5EGS  
Title : Human PRMT6 with bound fragment-type inhibitor  
Authors : Steuber, H.; Egner, U.; Kania, J.; Wu, H.; Brown, P.J.  
Deposited on : 2015-10-27  
Resolution : 2.15 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 : 2.13  
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) : 2.13

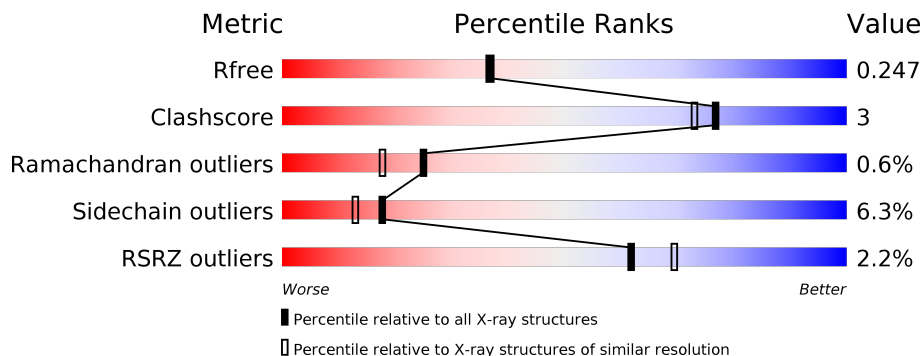
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	376	 2% 76% 11% • 11%
1	B	376	 % 79% 10% • 10%
1	C	376	 2% 78% 9% •• 10%
1	D	376	 2% 77% 10% • 11%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11269 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 Protein arginine N-methyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2645	1677	467	487	14	0	0	0
1	B	338	2687	1700	476	497	14	0	1	0
1	C	337	2681	1701	470	496	14	0	2	0
1	D	334	2651	1680	468	489	14	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

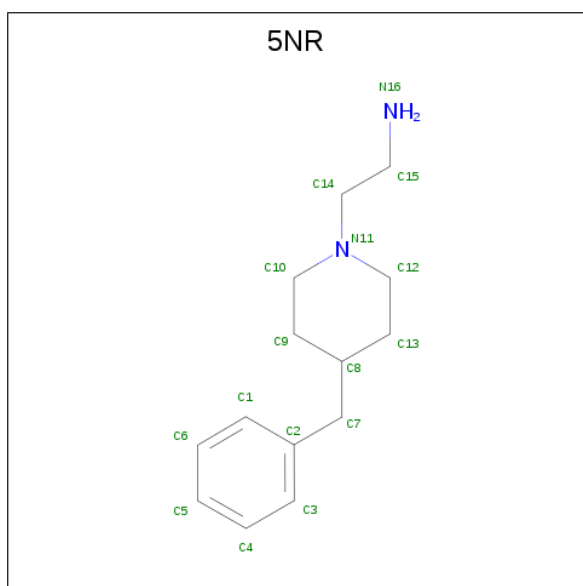
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q96LA8
A	194	VAL	ALA	conflict	UNP Q96LA8
B	0	GLY	-	expression tag	UNP Q96LA8
B	194	VAL	ALA	conflict	UNP Q96LA8
C	0	GLY	-	expression tag	UNP Q96LA8
C	194	VAL	ALA	conflict	UNP Q96LA8
D	0	GLY	-	expression tag	UNP Q96LA8
D	194	VAL	ALA	conflict	UNP Q96LA8

- 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
			Total	C	N	O	S		
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 2-[4-(phenylmethyl)piperidin-1-yl]ethanamine (three-letter code: 5NR) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			16	14	2		
3	A	1	Total	C	N	0	0
			16	14	2		
3	B	1	Total	C	N	0	0
			16	14	2		
3	C	1	Total	C	N	0	0
			16	14	2		
3	C	1	Total	C	N	0	0
			16	14	2		
3	D	1	Total	C	N	0	0
			16	14	2		

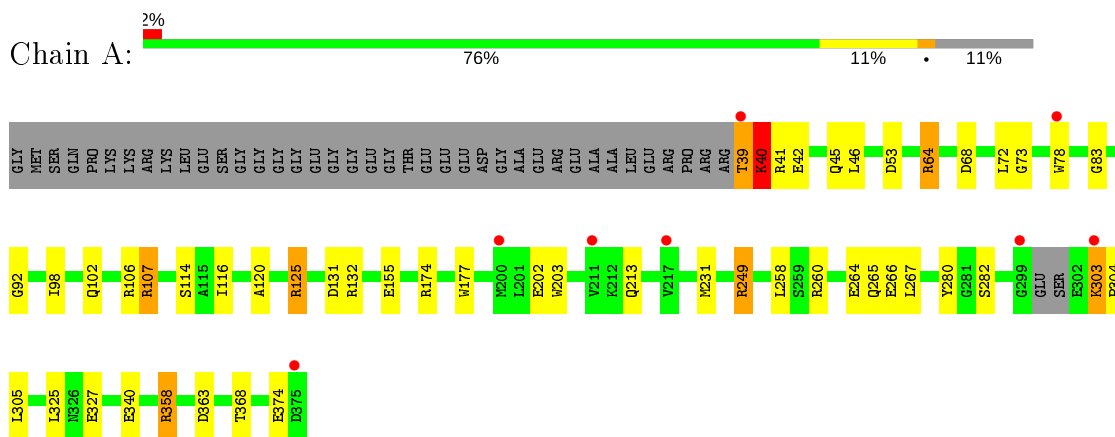
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	119	Total	O	0	0
			119	119		
4	C	85	Total	O	0	0
			85	85		
4	D	91	Total	O	0	0
			91	91		

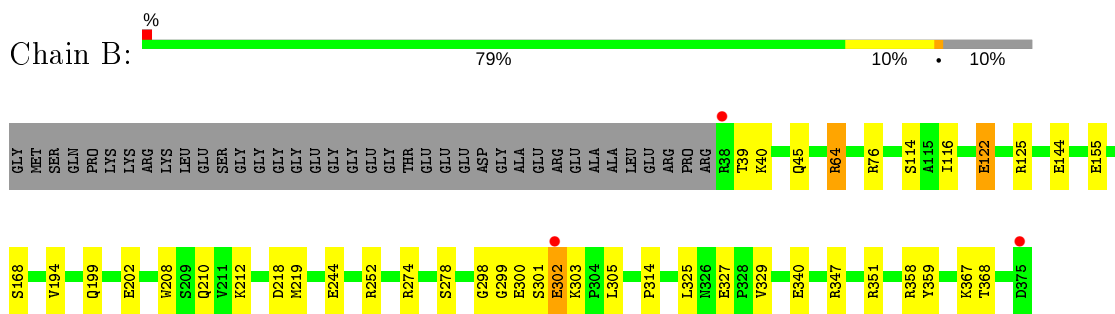
### 3 Residue-property plots [i](#)

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.

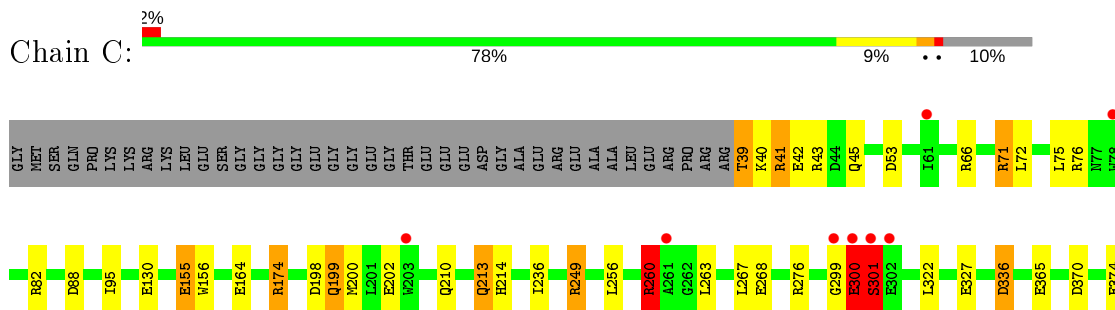
- Molecule 1: Protein arginine N-methyltransferase 6



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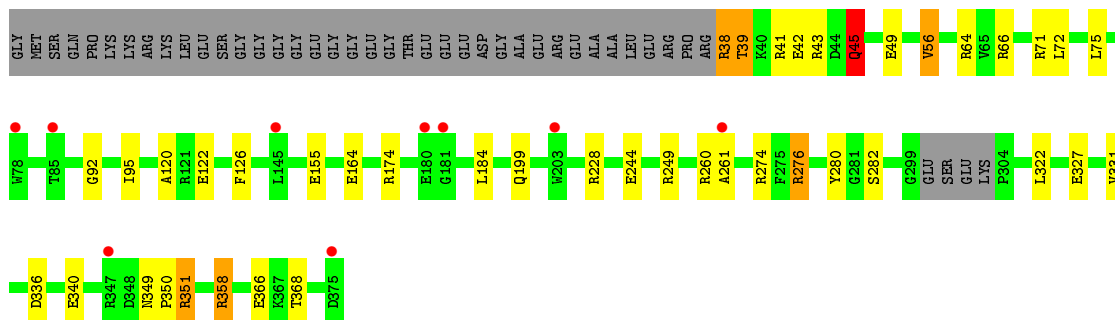
- Molecule 1: Protein arginine N-methyltransferase 6



E375

• Molecule 1: Protein arginine N-methyltransferase 6

Chain D: 2% 77% 10% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.16Å 135.62Å 83.09Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	41.26 – 2.15 41.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.26-2.15) 99.3 (41.26-2.15)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.201 , 0.246 0.207 , 0.247	Depositor DCC
$R_{free}$ test set	2101 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11269	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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: 5NR, 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	1.11	6/2704 (0.2%)	1.14	15/3662 (0.4%)
1	B	1.15	3/2750 (0.1%)	1.12	10/3723 (0.3%)
1	C	1.07	2/2749 (0.1%)	1.14	20/3725 (0.5%)
1	D	1.07	3/2713 (0.1%)	1.11	14/3674 (0.4%)
All	All	1.10	14/10916 (0.1%)	1.13	59/14784 (0.4%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	GLU	CD-OE2	7.22	1.33	1.25
1	D	280	TYR	CG-CD2	-7.18	1.29	1.39
1	B	368	THR	CB-CG2	-6.63	1.30	1.52
1	B	340	GLU	CD-OE1	-6.61	1.18	1.25
1	D	340	GLU	CD-OE1	-5.77	1.19	1.25
1	A	202	GLU	CD-OE1	5.72	1.31	1.25
1	C	156	TRP	CB-CG	5.52	1.60	1.50
1	A	177	TRP	CB-CG	5.46	1.60	1.50
1	A	282	SER	CB-OG	-5.46	1.35	1.42
1	D	244	GLU	CD-OE2	5.43	1.31	1.25
1	A	78	TRP	CB-CG	5.35	1.59	1.50
1	A	73	GLY	N-CA	5.04	1.53	1.46
1	A	280	TYR	CG-CD1	5.04	1.45	1.39
1	C	155	GLU	CD-OE2	5.01	1.31	1.25

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	D	260	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	B	64	ARG	NE-CZ-NH1	9.10	124.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	A	107	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	C	41	ARG	NE-CZ-NH2	8.97	124.79	120.30
1	C	88	ASP	CB-CG-OD1	8.61	126.05	118.30
1	D	351	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	C	198	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	64	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	252	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	174	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	64	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	B	351	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	C	370	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	C	370	ASP	CB-CG-OD2	7.31	124.88	118.30
1	D	228	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	64	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	125	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	131	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	274	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	64	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	C	174	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	C	249	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	C	301	SER	N-CA-C	-6.15	94.40	111.00
1	D	56	VAL	CB-CA-C	-6.06	99.89	111.40
1	D	351	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	C	88	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	249	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	C	41	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	B	202	GLU	CG-CD-OE1	-5.67	106.96	118.30
1	C	276	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	132	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	174	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	66	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	340	GLU	OE1-CD-OE2	-5.46	116.74	123.30
1	C	41	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	322	LEU	CB-CG-CD1	5.39	120.17	111.00
1	D	274	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	D	71	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	125	ARG	CD-NE-CZ	5.30	131.02	123.60
1	B	218	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	53	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	C	76	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	41	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	64	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	66	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	329	VAL	CB-CA-C	-5.15	101.61	111.40
1	B	274	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	D	276	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	363	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	45	GLN	CB-CA-C	5.06	120.52	110.40
1	A	358	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	D	56	VAL	CG1-CB-CG2	5.03	118.94	110.90
1	A	53	ASP	CB-CG-OD2	5.02	122.81	118.30
1	B	252	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	C	336	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	71	ARG	NE-CZ-NH2	5.00	122.80	120.30

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	2645	0	2603	19	0
1	B	2687	0	2649	13	0
1	C	2681	0	2635	19	0
1	D	2651	0	2612	15	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	32	0	44	4	0
3	B	16	0	22	0	0
3	C	32	0	44	1	0
3	D	16	0	22	0	0
4	A	110	0	0	0	0
4	B	119	0	0	1	0
4	C	85	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	91	0	0	1	0
All	All	11269	0	10707	64	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 3.

All (64) 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:40:LYS:NZ	4:C:501:HOH:O	1.99	0.93
1:B:122:GLU:OE1	1:B:125:ARG:NH1	2.08	0.86
1:A:39:THR:O	1:A:40:LYS:HB2	1.78	0.82
1:C:260:ARG:HH21	1:C:260:ARG:HG3	1.45	0.82
1:D:39:THR:HG23	1:D:42:GLU:H	1.49	0.78
1:D:351:ARG:NH1	4:D:501:HOH:O	2.08	0.77
1:A:39:THR:HG21	1:A:42:GLU:OE1	1.88	0.73
1:A:114:SER:HB3	1:A:116:ILE:HG22	1.71	0.71
1:D:39:THR:HG22	1:D:42:GLU:CD	2.12	0.70
1:D:39:THR:HG22	1:D:42:GLU:OE1	1.91	0.70
1:A:40:LYS:C	1:A:40:LYS:HD3	2.12	0.69
1:A:83:GLY:O	1:A:106:ARG:NH1	2.28	0.66
1:B:114:SER:HB3	1:B:116:ILE:HG22	1.77	0.66
1:B:219:MET:HE3	1:C:95:ILE:HD12	1.77	0.65
1:C:299:GLY:O	1:C:300:GLU:HB2	1.97	0.64
1:C:213:GLN:HG2	1:D:72:LEU:HD11	1.78	0.64
1:A:267:LEU:HD23	3:A:403:5NR:H9	1.80	0.63
1:B:298:GLY:O	4:B:501:HOH:O	2.15	0.63
1:B:219:MET:CE	1:C:95:ILE:HD12	2.30	0.62
1:A:267:LEU:HB3	3:A:403:5NR:H8	1.80	0.61
1:B:76:ARG:O	1:B:299:GLY:HA3	2.00	0.61
1:C:39:THR:HG23	1:C:42:GLU:OE2	2.01	0.60
1:A:340:GLU:OE2	1:A:358:ARG:NH2	2.35	0.59
1:D:39:THR:CG2	1:D:42:GLU:CG	2.83	0.57
1:A:40:LYS:HD3	1:A:40:LYS:O	2.05	0.57
1:C:260:ARG:NH2	1:C:260:ARG:HG3	2.16	0.57
1:A:98:ILE:O	1:A:102:GLN:HG3	2.05	0.56
1:D:174:ARG:HD2	1:D:184:LEU:HD11	1.88	0.55
1:C:71:ARG:O	1:C:75:LEU:HG	2.09	0.53
1:A:265:GLN:O	1:A:266:GLU:C	2.46	0.53
1:C:260:ARG:HH21	1:C:260:ARG:CG	2.15	0.52
1:B:199:GLN:HG3	1:B:244:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:NH2	1:C:214:HIS:CD2	2.79	0.50
1:D:39:THR:CG2	1:D:42:GLU:HG3	2.43	0.49
1:C:200:MET:HA	1:C:200:MET:CE	2.43	0.49
1:B:302:GLU:OE2	1:B:303:LYS:N	2.47	0.48
1:D:39:THR:HG22	1:D:42:GLU:CG	2.44	0.47
1:C:199:GLN:HG3	4:C:504:HOH:O	2.14	0.47
1:A:203:TRP:CZ2	1:B:314:PRO:HD3	2.51	0.46
1:C:263:LEU:HG	1:C:267:LEU:HD22	1.97	0.46
1:B:39:THR:CG2	1:B:40:LYS:N	2.78	0.45
1:B:208:TRP:HB3	1:B:219:MET:O	2.16	0.45
1:D:45:GLN:NE2	1:D:49[A]:GLU:OE2	2.50	0.44
1:A:231:MET:HB3	1:A:325:LEU:O	2.17	0.44
1:D:38:ARG:N	1:D:38:ARG:HH11	2.15	0.44
1:C:236:ILE:O	1:C:374:GLU:HB2	2.19	0.43
1:A:40:LYS:CD	1:A:40:LYS:C	2.86	0.43
1:D:349:ASN:HA	1:D:350:PRO:HD2	1.91	0.43
1:C:260:ARG:NH2	1:C:260:ARG:CG	2.73	0.43
1:D:92:GLY:O	1:D:120:ALA:HB2	2.19	0.43
1:A:303:LYS:CB	1:A:304:PRO:CD	2.97	0.42
1:A:305:LEU:C	1:A:305:LEU:HD23	2.40	0.42
1:D:358:ARG:NH2	1:D:366:GLU:OE2	2.48	0.42
3:C:403:5NR:H22	3:C:403:5NR:H13	1.84	0.42
1:C:43:ARG:NE	4:C:503:HOH:O	2.38	0.42
1:C:256:LEU:N	1:C:256:LEU:HD12	2.35	0.41
3:A:403:5NR:H22	3:A:403:5NR:H13	1.85	0.41
1:A:64:ARG:O	1:A:68:ASP:HB2	2.21	0.41
1:B:325:LEU:HD22	1:B:359:TYR:CZ	2.55	0.41
1:C:39:THR:N	1:C:42:GLU:OE2	2.54	0.41
1:A:92:GLY:O	1:A:120:ALA:HB2	2.21	0.41
3:A:402:5NR:C3	3:A:402:5NR:H10	2.48	0.40
1:A:303:LYS:HB3	1:A:304:PRO:HD3	2.03	0.40
1:D:282:SER:HA	1:D:331:VAL:O	2.20	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	331/376 (88%)	320 (97%)	9 (3%)	2 (1%)	25	18
1	B	337/376 (90%)	329 (98%)	8 (2%)	0	100	100
1	C	337/376 (90%)	321 (95%)	12 (4%)	4 (1%)	13	7
1	D	331/376 (88%)	319 (96%)	10 (3%)	2 (1%)	25	18
All	All	1336/1504 (89%)	1289 (96%)	39 (3%)	8 (1%)	25	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	C	260	ARG
1	C	300	GLU
1	C	301	SER
1	D	261	ALA
1	C	164	GLU
1	D	164	GLU
1	A	374	GLU

### 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	279/310 (90%)	264 (95%)	15 (5%)	22	18
1	B	285/310 (92%)	268 (94%)	17 (6%)	19	14
1	C	284/310 (92%)	264 (93%)	20 (7%)	15	10
1	D	281/310 (91%)	262 (93%)	19 (7%)	16	10
All	All	1129/1240 (91%)	1058 (94%)	71 (6%)	18	13

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	40	LYS
1	A	45	GLN
1	A	46	LEU
1	A	72	LEU
1	A	107	ARG
1	A	125	ARG
1	A	155	GLU
1	A	213	GLN
1	A	249	ARG
1	A	258	LEU
1	A	264	GLU
1	A	303	LYS
1	A	327	GLU
1	A	368	THR
1	B	45	GLN
1	B	122	GLU
1	B	144	GLU
1	B	155	GLU
1	B	168	SER
1	B	194	VAL
1	B	210	GLN
1	B	212	LYS
1	B	278	SER
1	B	300	GLU
1	B	301	SER
1	B	302	GLU
1	B	305	LEU
1	B	327	GLU
1	B	347	ARG
1	B	358	ARG
1	B	367	LYS
1	C	39	THR
1	C	41	ARG
1	C	45	GLN
1	C	72	LEU
1	C	82	ARG
1	C	130	GLU
1	C	155	GLU
1	C	174	ARG
1	C	199	GLN
1	C	202	GLU
1	C	210	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	213	GLN
1	C	249	ARG
1	C	260	ARG
1	C	268	GLU
1	C	300	GLU
1	C	301	SER
1	C	327	GLU
1	C	336	ASP
1	C	365	GLU
1	D	38	ARG
1	D	39	THR
1	D	41	ARG
1	D	43	ARG
1	D	45	GLN
1	D	56	VAL
1	D	75	LEU
1	D	95	ILE
1	D	122	GLU
1	D	126	PHE
1	D	155	GLU
1	D	199	GLN
1	D	249	ARG
1	D	276	ARG
1	D	322	LEU
1	D	327	GLU
1	D	336	ASP
1	D	358	ARG
1	D	368	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	210	GLN
1	B	45	GLN
1	B	210	GLN
1	C	214	HIS
1	C	364	GLN
1	D	45	GLN



### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	5NR	C	403	-	17,17,17	0.75	0	21,21,21	1.12	1 (4%)
3	5NR	C	402	-	17,17,17	0.75	0	21,21,21	1.08	2 (9%)
3	5NR	A	402	-	17,17,17	0.62	0	21,21,21	1.33	3 (14%)
3	5NR	D	402	-	17,17,17	0.88	0	21,21,21	0.59	0
3	5NR	B	402	-	17,17,17	0.72	0	21,21,21	1.17	1 (4%)
2	SAH	C	401	-	21,28,28	1.12	4 (19%)	20,40,40	1.67	3 (15%)
2	SAH	B	401	-	21,28,28	1.04	0	20,40,40	1.61	4 (20%)
2	SAH	D	401	-	21,28,28	1.32	2 (9%)	20,40,40	1.76	4 (20%)
2	SAH	A	401	-	21,28,28	1.07	1 (4%)	20,40,40	1.46	3 (15%)
3	5NR	A	403	-	17,17,17	0.93	0	21,21,21	1.20	3 (14%)

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	5NR	C	403	-	-	0/7/17/17	0/2/2/2
3	5NR	C	402	-	-	0/7/17/17	0/2/2/2
3	5NR	A	402	-	-	0/7/17/17	0/2/2/2
3	5NR	D	402	-	-	0/7/17/17	0/2/2/2
3	5NR	B	402	-	-	0/7/17/17	0/2/2/2
2	SAH	C	401	-	-	0/7/31/31	0/3/3/3
2	SAH	B	401	-	-	0/7/31/31	0/3/3/3
2	SAH	D	401	-	-	0/7/31/31	0/3/3/3
2	SAH	A	401	-	-	0/7/31/31	0/3/3/3
3	5NR	A	403	-	-	2/7/17/17	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	SAH	C2-N3	3.13	1.37	1.32
2	C	401	SAH	C2-N3	3.03	1.37	1.32
2	D	401	SAH	C2'-C1'	-2.59	1.49	1.53
2	A	401	SAH	C5-C4	2.34	1.47	1.40
2	C	401	SAH	C5-C4	2.04	1.46	1.40
2	C	401	SAH	CA-N	2.03	1.51	1.47
2	C	401	SAH	C5-N7	-2.01	1.32	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	SAH	N3-C2-N1	-4.96	120.93	128.68
2	D	401	SAH	N3-C2-N1	-4.73	121.28	128.68
2	B	401	SAH	N3-C2-N1	-4.24	122.06	128.68
2	C	401	SAH	O4'-C1'-C2'	-3.51	101.79	106.93
2	A	401	SAH	N3-C2-N1	-3.48	123.24	128.68
3	B	402	5NR	C14-C15-N16	-3.21	102.16	112.69
3	A	402	5NR	C2-C7-C8	-2.83	109.20	114.50
2	D	401	SAH	C1'-N9-C4	-2.59	122.09	126.64
3	A	403	5NR	C5-C6-C1	-2.55	116.30	120.19
3	A	402	5NR	C10-C9-C8	2.53	118.40	111.99
2	A	401	SAH	C4-C5-N7	-2.52	106.77	109.40
3	A	403	5NR	C14-N11-C10	-2.48	104.90	111.23
2	B	401	SAH	C5-C6-N6	-2.41	116.69	120.35
3	A	402	5NR	C9-C8-C7	-2.39	106.30	111.88
2	B	401	SAH	C2'-C3'-C4'	2.37	107.24	102.64
3	C	403	5NR	C5-C6-C1	-2.30	116.69	120.19
2	B	401	SAH	N6-C6-N1	2.29	123.33	118.57
2	D	401	SAH	C2-N1-C6	2.21	122.54	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	O4'-C1'-C2'	-2.19	103.73	106.93
3	A	403	5NR	C9-C10-N11	2.07	114.33	111.11
2	C	401	SAH	N6-C6-N1	2.05	122.83	118.57
2	D	401	SAH	N6-C6-N1	2.03	122.80	118.57
3	C	402	5NR	C13-C8-C7	-2.02	107.14	111.88
3	C	402	5NR	C1-C2-C3	2.02	121.34	118.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

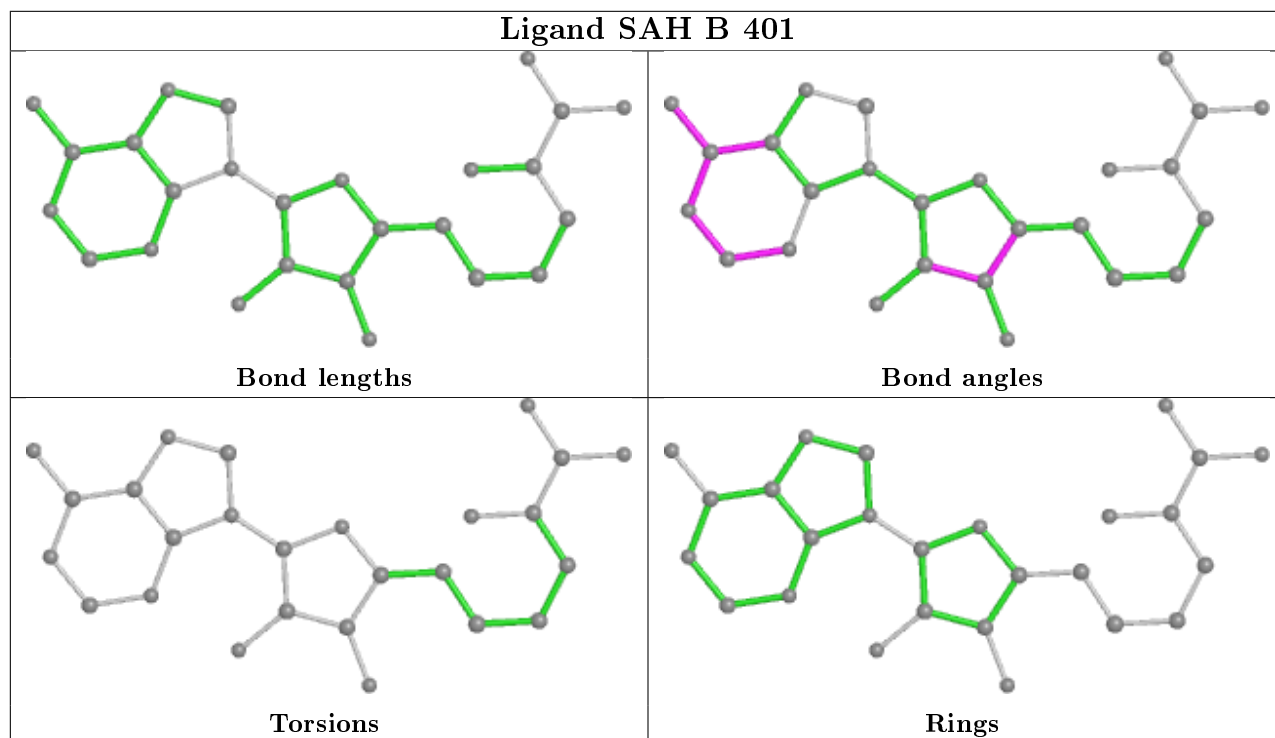
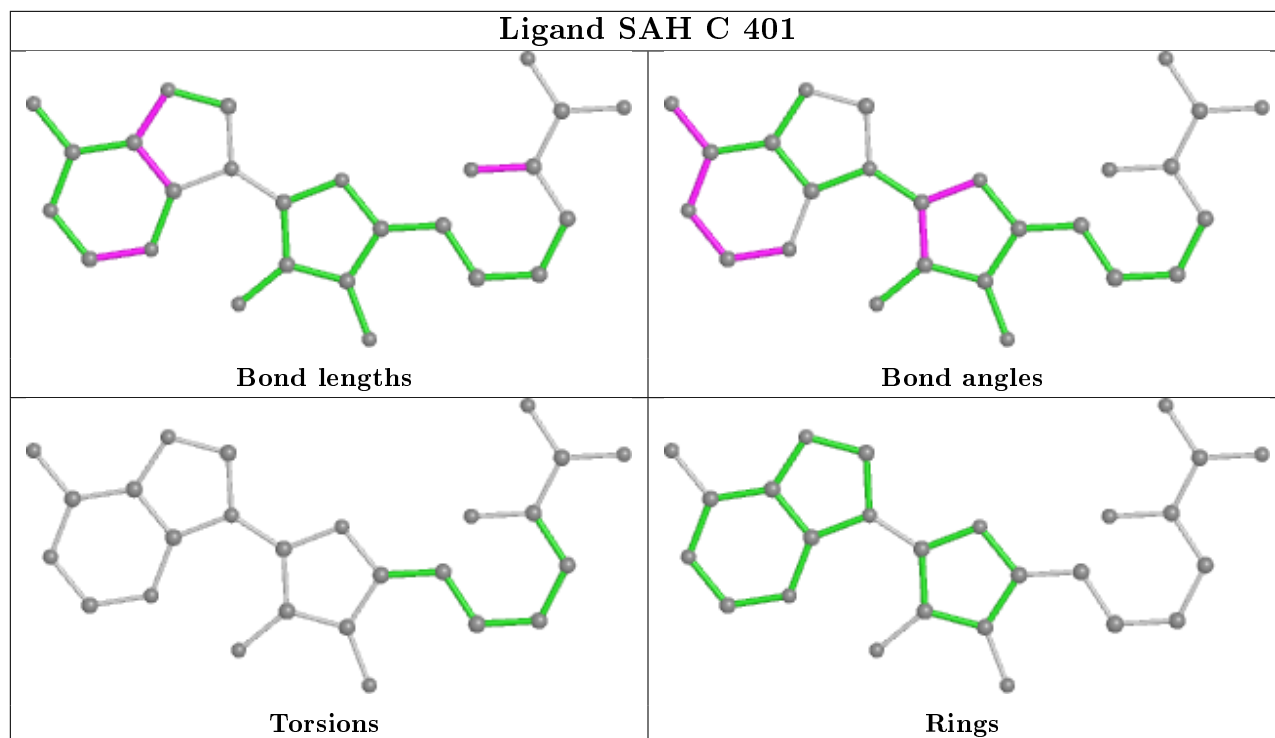
Mol	Chain	Res	Type	Atoms
3	A	403	5NR	C15-C14-N11-C12
3	A	403	5NR	C15-C14-N11-C10

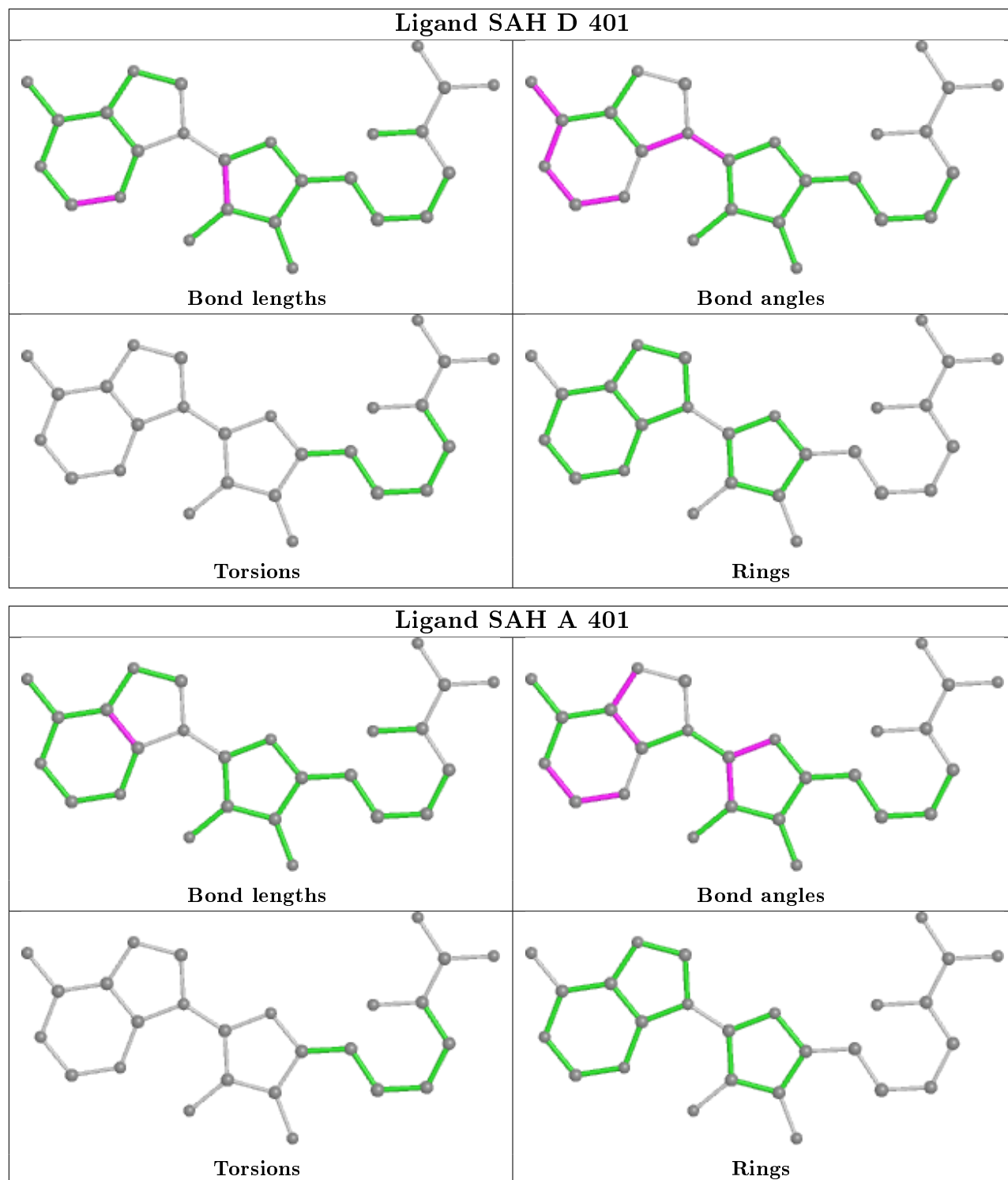
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	5NR	1	0
3	A	402	5NR	1	0
3	A	403	5NR	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

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	335/376 (89%)	0.11	8 (2%) 59 67	16, 31, 50, 68	5 (1%)
1	B	338/376 (89%)	0.00	3 (0%) 84 88	14, 26, 46, 72	1 (0%)
1	C	337/376 (89%)	0.17	9 (2%) 54 63	18, 29, 54, 87	6 (1%)
1	D	334/376 (88%)	0.14	9 (2%) 54 63	19, 32, 53, 67	5 (1%)
All	All	1344/1504 (89%)	0.10	29 (2%) 62 69	14, 29, 52, 87	17 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	SER	4.8
1	C	300	GLU	4.4
1	A	303	LYS	4.3
1	C	61	ILE	3.5
1	A	78	TRP	3.5
1	A	375	ASP	3.1
1	D	375	ASP	3.0
1	C	261	ALA	3.0
1	D	145	LEU	2.9
1	C	299	GLY	2.9
1	D	180	GLU	2.9
1	B	375	ASP	2.9
1	D	85	THR	2.7
1	C	375	ASP	2.7
1	A	299	GLY	2.7
1	A	39	THR	2.5
1	D	347	ARG	2.5
1	A	200	MET	2.5
1	D	203	TRP	2.4
1	D	181	GLY	2.4
1	C	203[A]	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	217	VAL	2.2
1	D	261	ALA	2.2
1	C	302	GLU	2.2
1	D	78	TRP	2.1
1	A	211	VAL	2.1
1	B	38	ARG	2.1
1	C	78	TRP	2.1
1	B	302	GLU	2.0

## 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 monosaccharides 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.

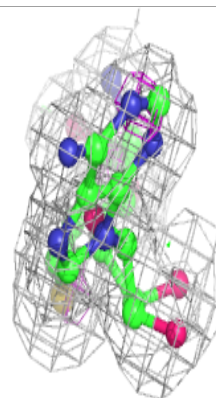
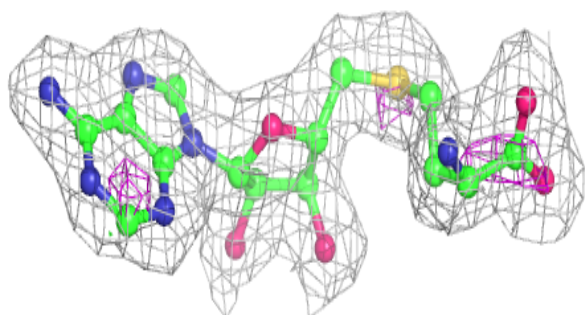
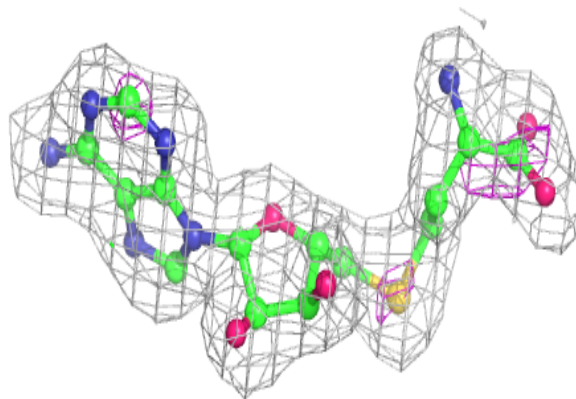
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	5NR	C	403	16/16	0.85	0.21	32,41,51,51	0
3	5NR	B	402	16/16	0.86	0.17	16,19,25,26	0
3	5NR	C	402	16/16	0.91	0.17	19,22,34,35	0
3	5NR	D	402	16/16	0.92	0.13	16,18,24,24	0
3	5NR	A	403	16/16	0.92	0.17	25,33,37,37	0
3	5NR	A	402	16/16	0.94	0.15	15,20,27,28	0
2	SAH	D	401	26/26	0.95	0.10	21,25,27,29	0
2	SAH	A	401	26/26	0.96	0.10	18,22,23,24	0
2	SAH	C	401	26/26	0.96	0.11	18,20,23,24	0
2	SAH	B	401	26/26	0.97	0.11	15,19,21,23	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.

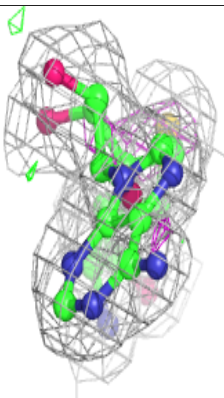
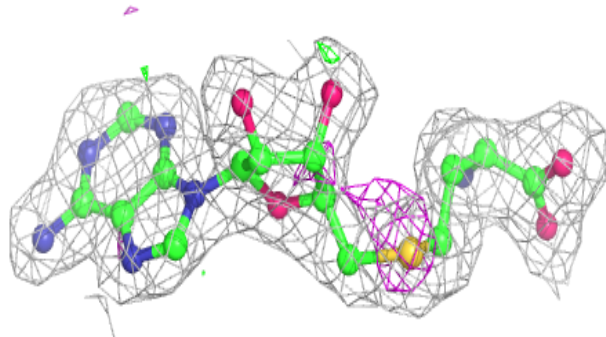
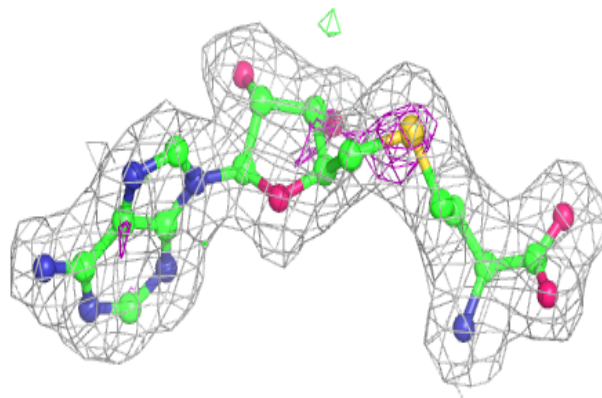


**Electron density around SAH D 401:**

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

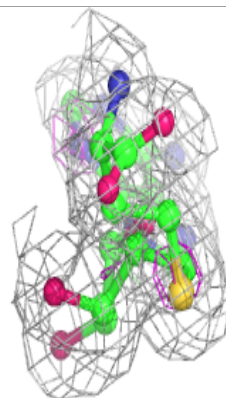
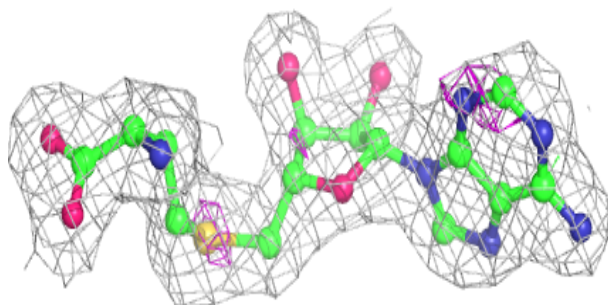
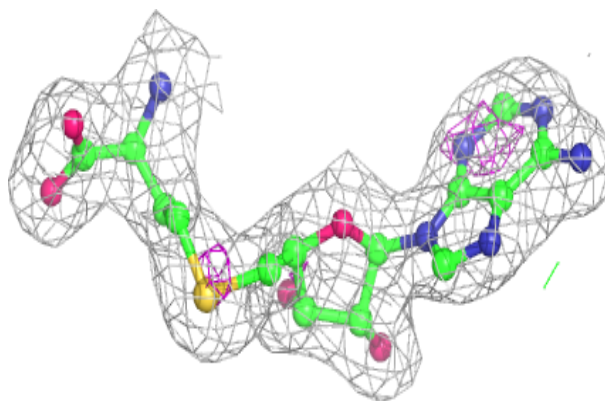
**Electron density around SAH A 401:**

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

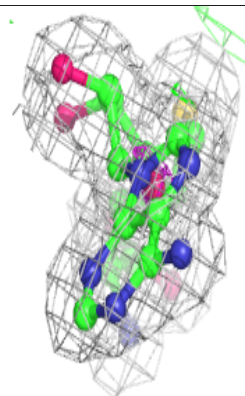
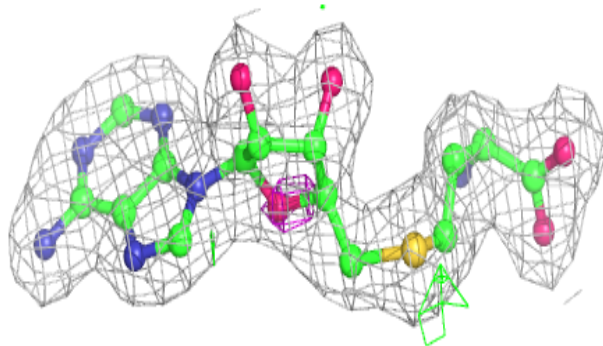
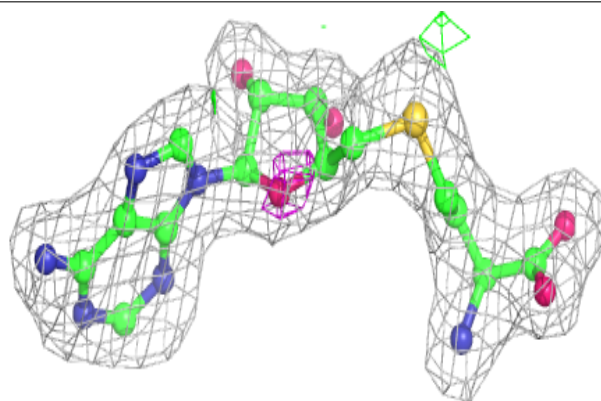


**Electron density around SAH C 401:**

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

**Electron density around SAH B 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

There are no such residues in this entry.