



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 11:09 AM EDT

PDB ID : 5VSD  
Title : Structure of human GLP SET-domain (EHMT1) in complex with inhibitor 13  
Authors : Babault, N.; Xiong, Y.; Liu, J.; Jin, J.  
Deposited on : 2017-05-11  
Resolution : 1.85 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

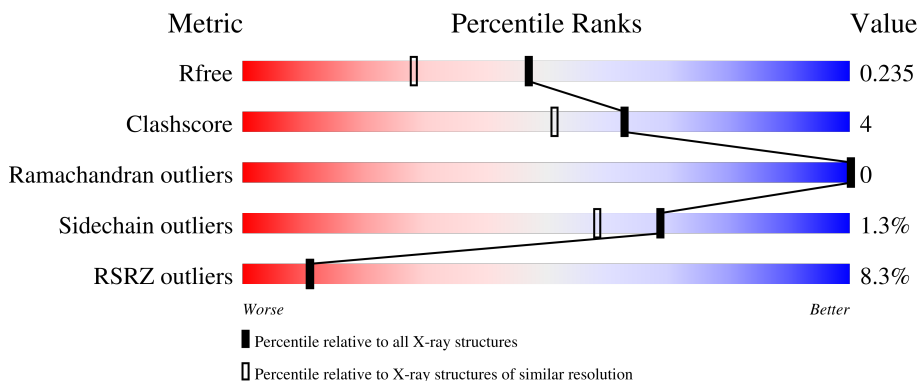
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

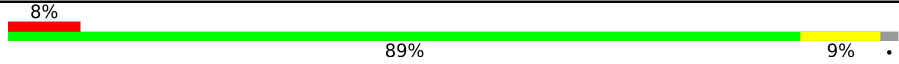
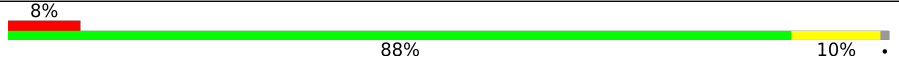
The reported resolution of this entry is 1.85 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	261	
1	B	261	

## 2 Entry composition [i](#)

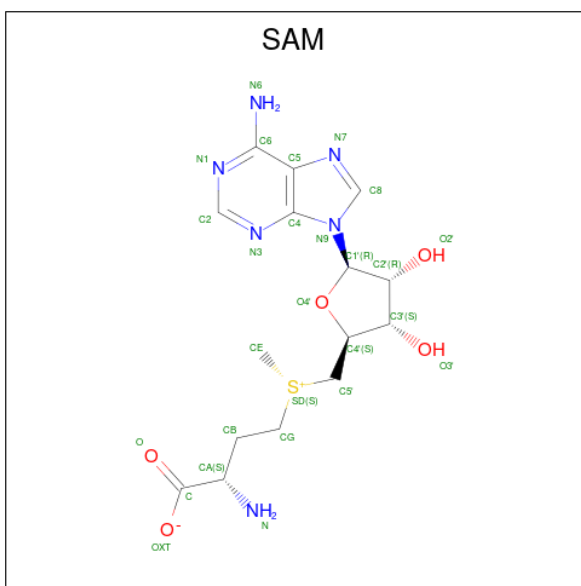
There are 7 unique types of molecules in this entry. The entry contains 4829 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histone-lysine N-methyltransferase EHMT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	Total 2081	C 1298	N 375	O 383	S 25	0	0	0
1	B	258	Total 2085	C 1300	N 376	O 384	S 25	1	0	0

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S).

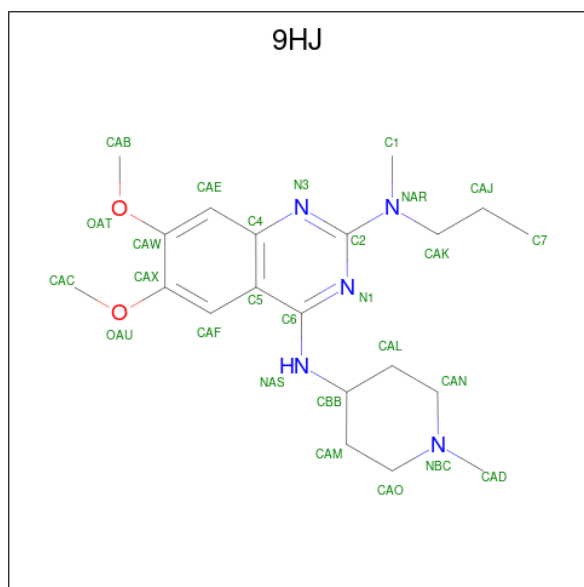


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	B	1	Total 27	C 15	N 6	O 5	S 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

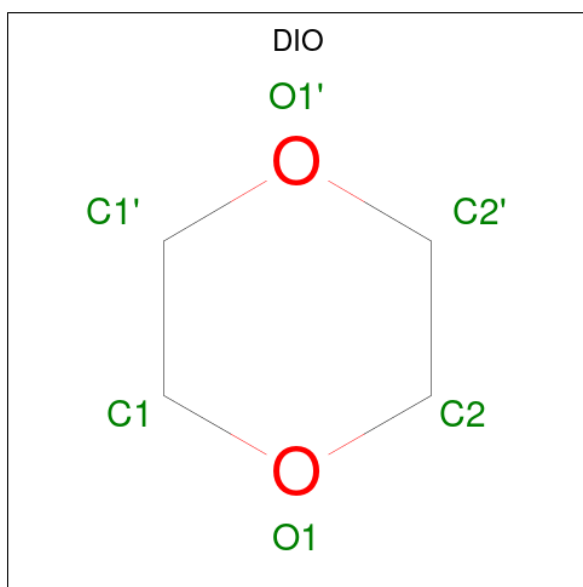
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Zn 4 4	0	0
3	B	4	Total Zn 4 4	0	0

- Molecule 4 is 6,7-dimethoxy-N 2 -methyl-N 4 -(1-methylpiperidin-4-yl)-N 2 -propylquinazoli ne-2,4-diamine (three-letter code: 9HJ) (formula: C<sub>20</sub>H<sub>31</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 27 20 5 2	0	0
4	B	1	Total C N O 27 20 5 2	0	0

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

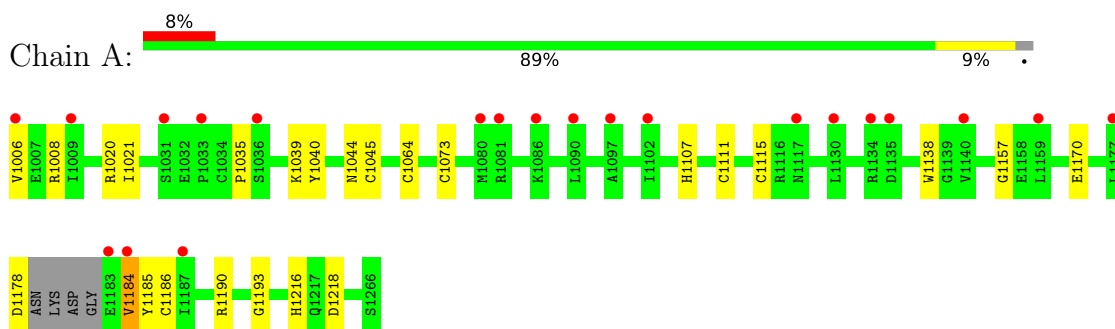
- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	273	Total 273	O 273	0	0
7	B	256	Total 256	O 256	0	0

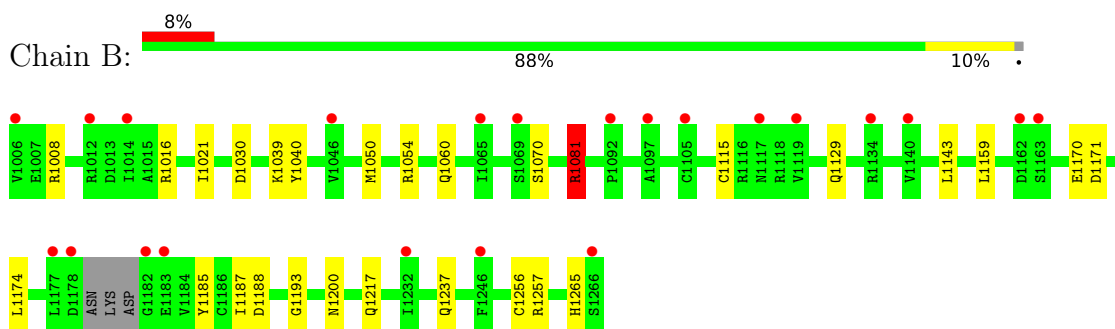
### 3 Residue-property plots

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: Histone-lysine N-methyltransferase EHMT1



- Molecule 1: Histone-lysine N-methyltransferase EHMT1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.86Å 96.59Å 102.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.85 19.91 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.91-1.85) 98.2 (19.91-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 1.85Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.192 , 0.235 0.192 , 0.235	Depositor DCC
$R_{free}$ test set	3239 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtrriage
Anisotropy	0.952	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4829	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 4.49% 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: GOL, 9HJ, DIO, SAM, ZN

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	0.42	1/2131 (0.0%)	0.63	2/2881 (0.1%)
1	B	0.40	0/2135	0.64	2/2886 (0.1%)
All	All	0.41	1/4266 (0.0%)	0.64	4/5767 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1186	CYS	CB-SG	-5.76	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1081	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	1184	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	B	1170	GLU	CA-CB-CG	-5.36	101.61	113.40
1	A	1006	VAL	N-CA-C	-5.19	96.98	111.00

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	2081	0	1972	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2085	0	1975	21	0
2	A	27	0	22	0	0
2	B	27	0	22	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	27	0	0	0	0
4	B	27	0	0	1	0
5	A	6	0	8	0	0
6	B	12	0	16	2	0
7	A	273	0	0	4	0
7	B	256	0	0	1	0
All	All	4829	0	4015	36	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 4.

All (36) 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:B:1060:GLN:H	1:B:1217:GLN:HE22	1.29	0.78
1:A:1216:HIS:HD2	1:A:1218:ASP:H	1.34	0.76
1:A:1178:ASP:HB3	1:A:1184:VAL:HG13	1.68	0.75
1:A:1008:ARG:NH2	7:A:3102:HOH:O	2.22	0.72
1:A:1020:ARG:NH2	7:A:3103:HOH:O	2.23	0.71
1:B:1200:ASN:HD22	1:B:1237:GLN:HE22	1.43	0.67
1:B:1060:GLN:H	1:B:1217:GLN:NE2	1.93	0.66
1:B:1257:ARG:NH2	7:B:3102:HOH:O	2.30	0.65
1:A:1044:ASN:HD22	1:A:1157:GLY:H	1.44	0.63
1:B:1081:ARG:HH21	1:B:1081:ARG:HG3	1.64	0.62
1:A:1107:HIS:O	1:B:1039:LYS:HE2	2.02	0.59
1:A:1044:ASN:ND2	1:A:1157:GLY:H	2.01	0.56
1:B:1021:ILE:HD12	1:B:1021:ILE:O	2.10	0.52
1:B:1159:LEU:HD23	1:B:1187:ILE:HG12	1.92	0.51
1:B:1081:ARG:HH21	1:B:1081:ARG:CG	2.23	0.51
1:B:1129:GLN:HB2	1:B:1143:LEU:HD11	1.95	0.49
1:A:1111:CYS:O	1:B:1016:ARG:NH1	2.45	0.48
1:B:1081:ARG:HG3	1:B:1081:ARG:NH2	2.30	0.47
1:B:1050:MET:HE1	1:B:1185:TYR:CD1	2.50	0.46
1:A:1035:PRO:HG3	1:A:1138:TRP:NE1	2.32	0.45
1:A:1184:VAL:HG12	1:A:1185:TYR:N	2.32	0.45
1:B:1054:ARG:NH2	6:B:3007:GOL:H31	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:HIS:CD2	1:A:1218:ASP:H	2.25	0.44
1:A:1040:TYR:HA	1:A:1193:GLY:O	2.17	0.44
1:A:1184:VAL:HG12	1:A:1185:TYR:H	1.82	0.44
1:B:1200:ASN:HD22	1:B:1237:GLN:NE2	2.11	0.44
1:A:1008:ARG:HD3	7:A:3153:HOH:O	2.17	0.43
1:A:1064:CYS:SG	1:A:1073:CYS:HA	2.59	0.43
1:B:1040:TYR:HA	1:B:1193:GLY:O	2.19	0.43
1:B:1256:CYS:HB2	1:B:1265:HIS:HB2	2.01	0.43
1:A:1045:CYS:HB3	7:A:3205:HOH:O	2.18	0.43
1:A:1170:GLU:HG2	1:A:1190:ARG:HD3	2.02	0.41
1:B:1171:ASP:HB2	4:B:3006:9HJ:CAF	2.50	0.41
1:B:1159:LEU:HD21	6:B:3008:GOL:H32	2.03	0.40
1:B:1008:ARG:NH2	1:B:1030:ASP:O	2.52	0.40
1:B:1174:LEU:HD23	1:B:1188:ASP:HA	2.04	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	253/261 (97%)	244 (96%)	9 (4%)	0	100	100
1	B	254/261 (97%)	245 (96%)	9 (4%)	0	100	100
All	All	507/522 (97%)	489 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/236 (99%)	230 (99%)	3 (1%)	69	58
1	B	233/236 (99%)	230 (99%)	3 (1%)	69	58
All	All	466/472 (99%)	460 (99%)	6 (1%)	69	58

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1021	ILE
1	A	1039	LYS
1	A	1115	CYS
1	B	1070	SER
1	B	1081	ARG
1	B	1115	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1044	ASN
1	A	1216	HIS
1	B	1077	GLN
1	B	1217	GLN
1	B	1237	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

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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
4	9HJ	B	3006	-	28,29,29	1.22	2 (7%)	35,40,40	3.33	17 (48%)
4	9HJ	A	3006	-	28,29,29	1.31	3 (10%)	35,40,40	3.16	18 (51%)
6	GOL	B	3008	-	5,5,5	0.54	0	5,5,5	0.46	0
2	SAM	A	3001	-	24,29,29	0.98	2 (8%)	23,42,42	1.33	2 (8%)
2	SAM	B	3001	-	24,29,29	0.92	1 (4%)	23,42,42	1.40	3 (13%)
6	GOL	B	3007	-	5,5,5	0.29	0	5,5,5	0.43	0
5	DIO	A	3007	-	6,6,6	0.48	0	6,6,6	0.79	0

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
4	9HJ	B	3006	-	-	1/15/37/37	0/3/3/3
4	9HJ	A	3006	-	-	3/15/37/37	0/3/3/3
6	GOL	B	3008	-	-	2/4/4/4	-
2	SAM	A	3001	-	-	2/12/33/33	0/3/3/3
2	SAM	B	3001	-	-	2/12/33/33	0/3/3/3
6	GOL	B	3007	-	-	2/4/4/4	-
5	DIO	A	3007	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3006	9HJ	C6-C5	-4.37	1.39	1.44
4	B	3006	9HJ	C6-C5	-3.99	1.39	1.44
4	A	3006	9HJ	C6-N1	2.32	1.36	1.32
2	A	3001	SAM	O4'-C1'	2.08	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	SAM	O4'-C1'	2.07	1.44	1.41
4	B	3006	9HJ	CAE-CAW	2.04	1.40	1.36
4	A	3006	9HJ	CAE-CAW	2.03	1.40	1.36
2	A	3001	SAM	CE-SD	-2.02	1.66	1.78

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3006	9HJ	CAJ-CAK-NAR	-11.00	102.32	113.58
4	A	3006	9HJ	CAJ-CAK-NAR	-8.07	105.32	113.58
4	A	3006	9HJ	C5-C6-NAS	-6.51	114.49	120.63
4	A	3006	9HJ	C6-C5-C4	6.13	119.74	115.88
4	A	3006	9HJ	CAF-C5-C6	-5.92	119.54	124.88
4	B	3006	9HJ	C6-C5-C4	5.91	119.60	115.88
4	B	3006	9HJ	CAF-C5-C6	-5.48	119.94	124.88
4	B	3006	9HJ	CAO-CAM-CBB	-4.93	101.86	110.50
4	B	3006	9HJ	C6-NAS-CBB	4.86	133.40	124.16
4	B	3006	9HJ	CAM-CBB-NAS	4.69	117.91	110.60
4	A	3006	9HJ	C6-NAS-CBB	4.64	132.99	124.16
2	A	3001	SAM	N3-C2-N1	-4.55	121.56	128.68
2	B	3001	SAM	N3-C2-N1	-4.55	121.56	128.68
4	B	3006	9HJ	C5-C6-NAS	-4.42	116.46	120.63
4	B	3006	9HJ	CAO-NBC-CAN	4.36	115.62	109.52
4	A	3006	9HJ	CAO-CAM-CBB	-4.29	102.97	110.50
4	A	3006	9HJ	CAO-NBC-CAN	4.13	115.30	109.52
4	A	3006	9HJ	C5-C4-N3	-3.75	118.83	122.81
4	B	3006	9HJ	CAC-OAU-CAX	3.75	123.18	117.53
4	A	3006	9HJ	CAN-CAL-CBB	-3.42	104.49	110.50
4	B	3006	9HJ	C5-C4-N3	-3.41	119.19	122.81
4	A	3006	9HJ	OAT-CAW-CAE	-3.27	121.00	125.24
4	A	3006	9HJ	OAU-CAX-CAF	-3.07	121.27	125.24
4	A	3006	9HJ	NAS-C6-N1	3.07	125.41	118.90
4	B	3006	9HJ	OAT-CAW-CAE	-3.06	121.28	125.24
4	A	3006	9HJ	CAC-OAU-CAX	2.91	121.92	117.53
4	B	3006	9HJ	CAD-NBC-CAN	-2.76	106.53	110.66
4	A	3006	9HJ	CAD-NBC-CAN	-2.63	106.73	110.66
4	B	3006	9HJ	CAN-CAL-CBB	-2.62	105.90	110.50
4	B	3006	9HJ	OAU-CAX-CAF	-2.53	121.96	125.24
4	B	3006	9HJ	NAS-C6-N1	2.47	124.13	118.90
2	B	3001	SAM	CG-SD-C5'	2.40	109.53	103.40
4	A	3006	9HJ	OAT-CAW-CAX	2.39	118.74	115.41
4	A	3006	9HJ	C1-NAR-CAK	2.26	121.58	115.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3001	SAM	C4-C5-N7	-2.14	107.17	109.40
4	B	3006	9HJ	OAT-CAW-CAX	2.13	118.38	115.41
4	B	3006	9HJ	OAU-CAX-CAW	2.08	118.31	115.41
2	A	3001	SAM	O4'-C4'-C5'	2.06	114.08	108.88
4	A	3006	9HJ	OAU-CAX-CAW	2.03	118.23	115.41
4	A	3006	9HJ	CAM-CBB-NAS	2.01	113.73	110.60

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	SAM	CB-CG-SD-CE
2	A	3001	SAM	CB-CG-SD-C5'
2	B	3001	SAM	CB-CG-SD-CE
2	B	3001	SAM	CB-CG-SD-C5'
4	A	3006	9HJ	CAJ-CAK-NAR-C2
4	A	3006	9HJ	CAL-CBB-NAS-C6
4	B	3006	9HJ	CAL-CBB-NAS-C6
6	B	3007	GOL	O1-C1-C2-O2
6	B	3007	GOL	O1-C1-C2-C3
6	B	3008	GOL	O1-C1-C2-C3
4	A	3006	9HJ	CAJ-CAK-NAR-C1
6	B	3008	GOL	O1-C1-C2-O2

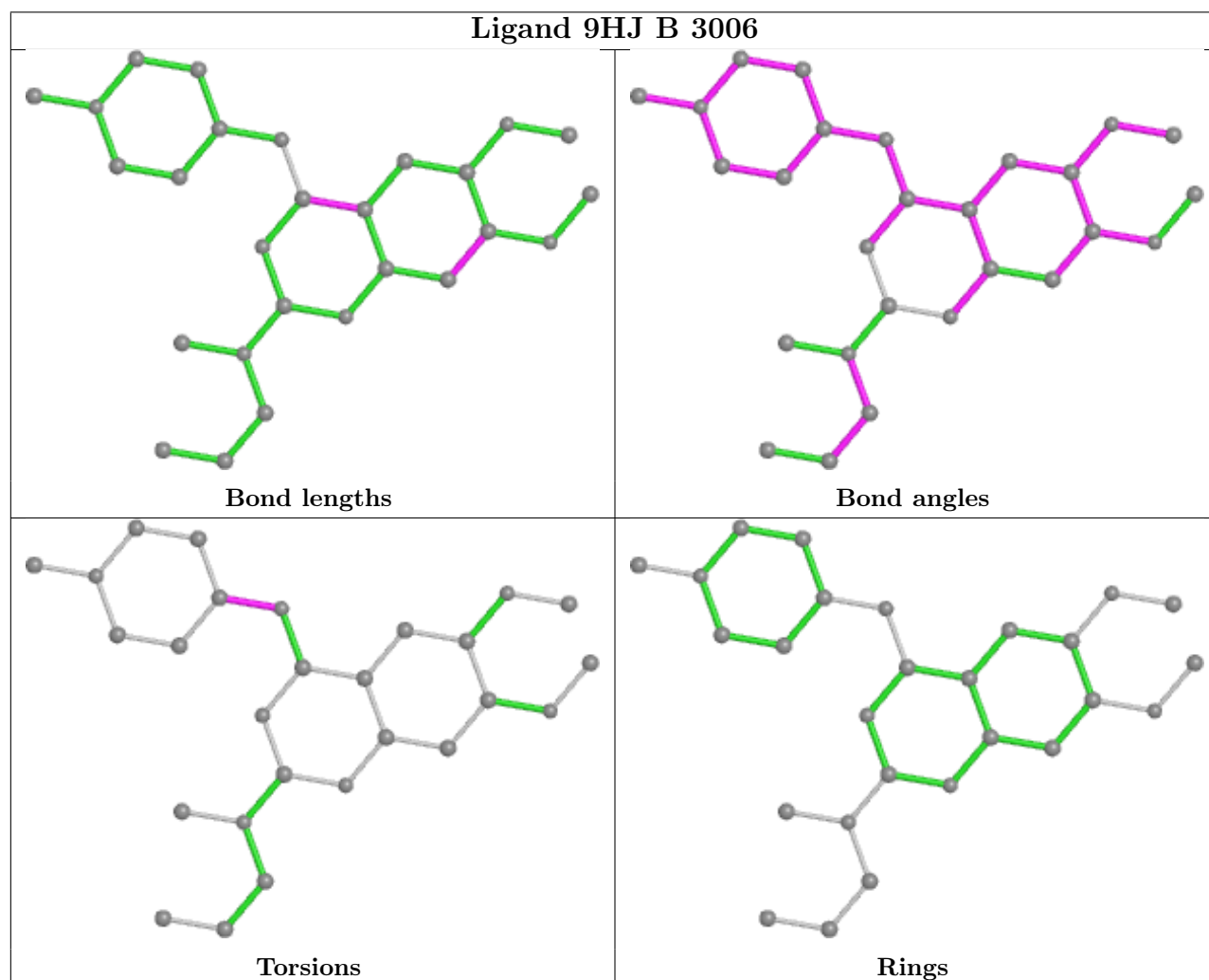
There are no ring outliers.

3 monomers are involved in 3 short contacts:

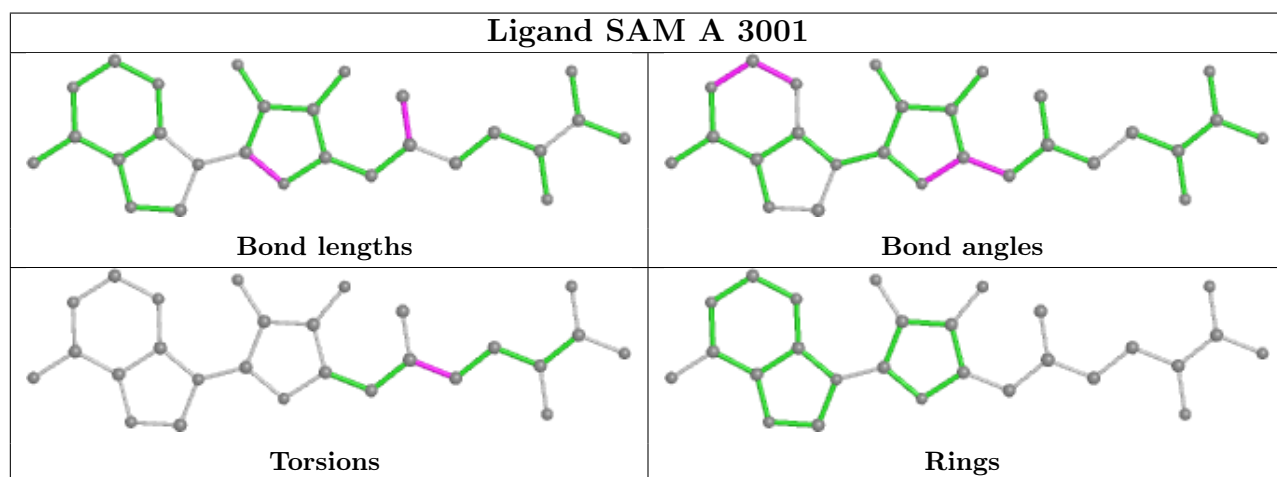
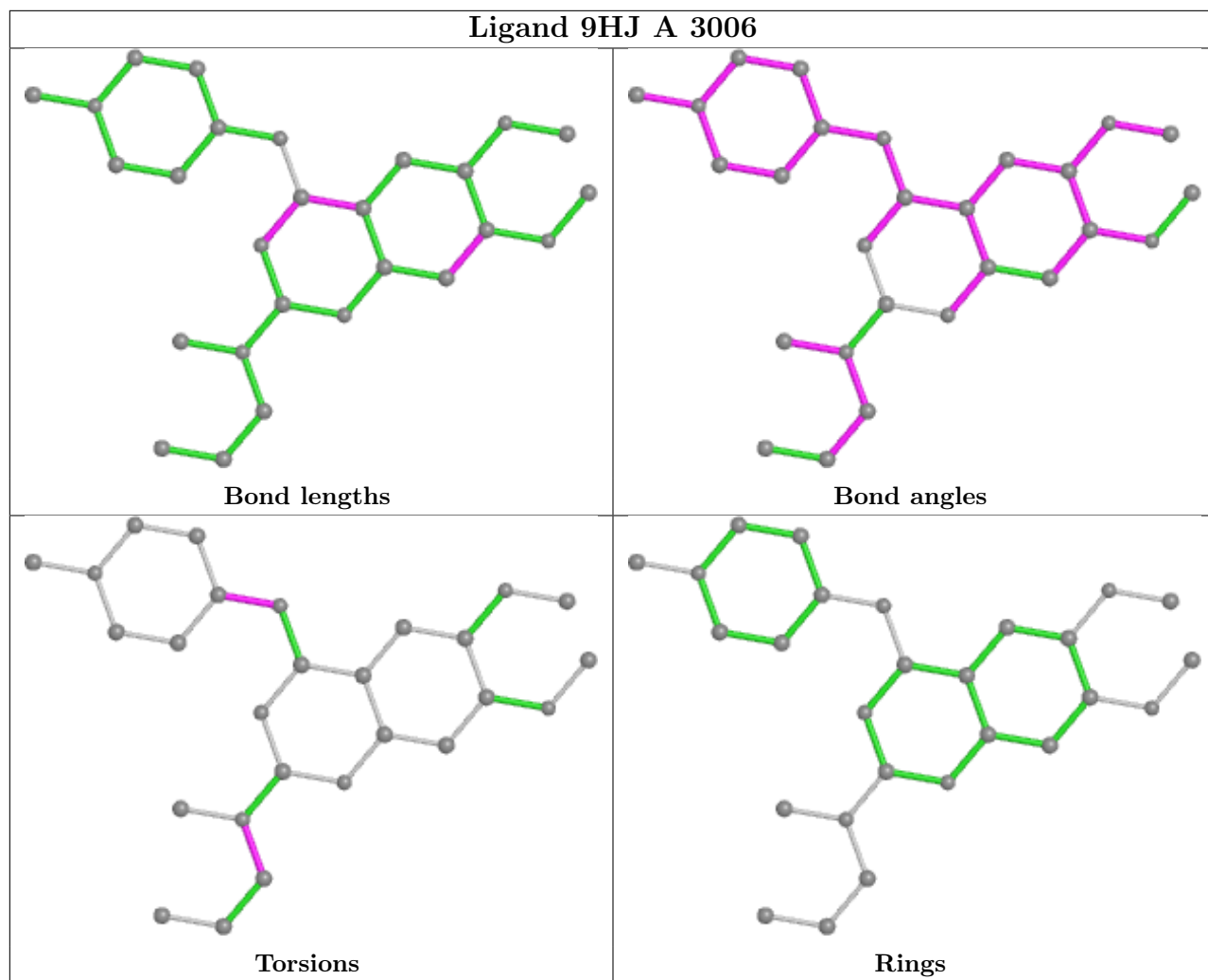
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3006	9HJ	1	0
6	B	3008	GOL	1	0
6	B	3007	GOL	1	0

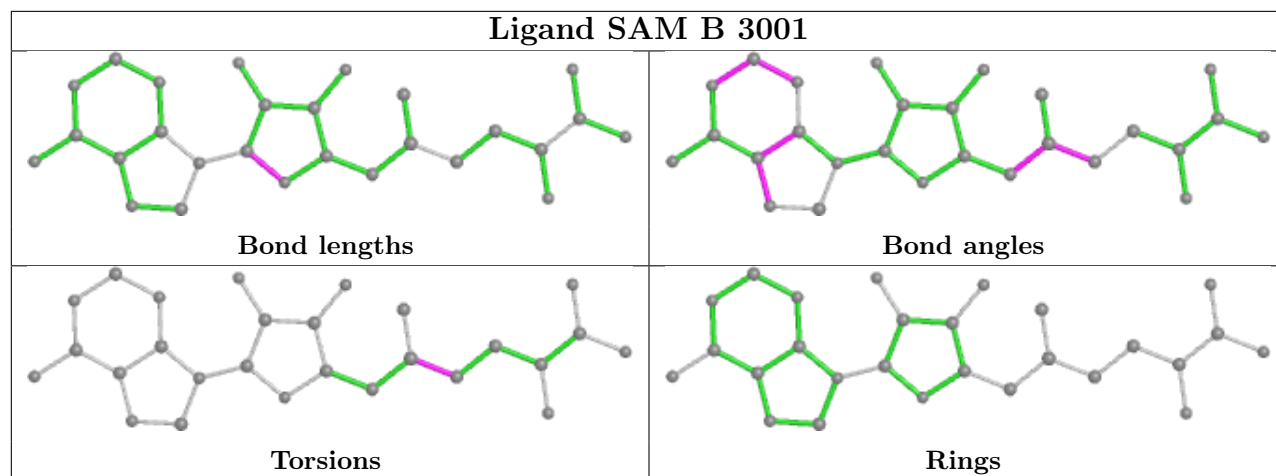
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	257/261 (98%)	0.81	21 (8%) <b>11</b> <b>11</b>	16, 27, 51, 100	1 (0%)
1	B	258/261 (98%)	0.80	22 (8%) <b>10</b> <b>10</b>	17, 27, 50, 82	1 (0%)
All	All	515/522 (98%)	0.81	43 (8%) <b>11</b> <b>11</b>	16, 27, 51, 100	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1006	VAL	7.2
1	A	1183	GLU	6.6
1	A	1006	VAL	6.0
1	B	1065	ILE	5.8
1	A	1184	VAL	5.7
1	A	1031	SER	5.1
1	B	1163	SER	4.8
1	A	1080	MET	4.4
1	A	1009	ILE	4.1
1	B	1134	ARG	3.9
1	B	1178	ASP	3.9
1	B	1097	ALA	3.7
1	B	1182	GLY	3.5
1	A	1134	ARG	3.4
1	B	1183	GLU	3.3
1	A	1187	ILE	3.3
1	A	1081	ARG	3.0
1	A	1097	ALA	3.0
1	B	1117	ASN	3.0
1	A	1033	PRO	2.9
1	B	1140	VAL	2.7
1	B	1105	CYS	2.6
1	B	1092	PRO	2.5
1	A	1102	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1266	SER	2.5
1	A	1159	LEU	2.5
1	A	1090	LEU	2.5
1	A	1086	LYS	2.4
1	A	1130	LEU	2.4
1	B	1046	VAL	2.4
1	A	1177	LEU	2.3
1	B	1119	VAL	2.3
1	B	1069	SER	2.2
1	B	1246	PHE	2.2
1	B	1014	ILE	2.2
1	B	1162	ASP	2.2
1	A	1140	VAL	2.2
1	A	1135	ASP	2.1
1	B	1232	ILE	2.1
1	A	1117	ASN	2.1
1	A	1036	SER	2.1
1	B	1177	LEU	2.0
1	B	1012	ARG	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
6	GOL	B	3007	6/6	0.64	0.27	41,54,59,59	0
4	9HJ	B	3006	27/27	0.82	0.17	26,32,48,60	0
4	9HJ	A	3006	27/27	0.83	0.18	20,31,53,55	0
2	SAM	B	3001	27/27	0.89	0.14	22,29,35,38	0

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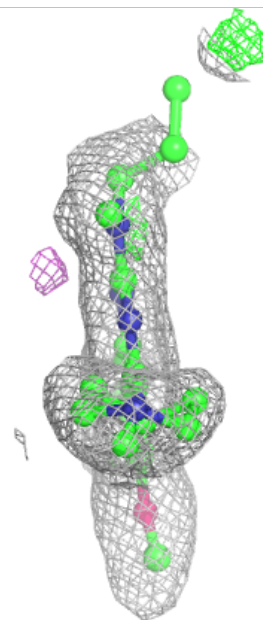
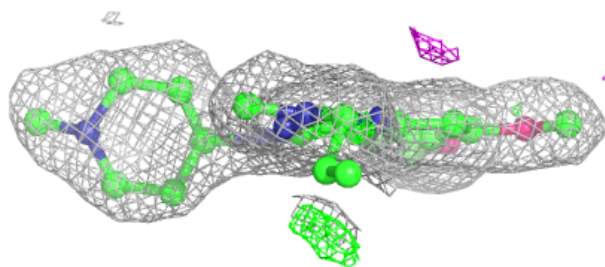
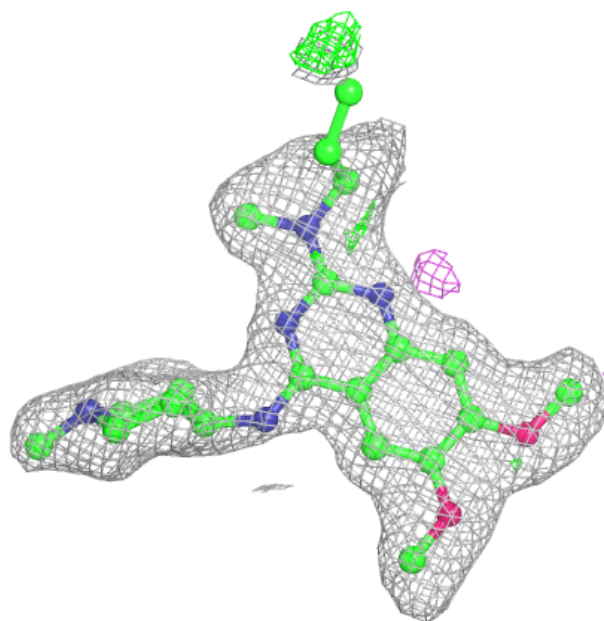
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SAM	A	3001	27/27	0.90	0.14	18,27,32,33	0
6	GOL	B	3008	6/6	0.92	0.17	26,31,38,43	0
5	DIO	A	3007	6/6	0.95	0.12	25,32,33,35	0
3	ZN	B	3005	1/1	0.97	0.04	30,30,30,30	0
3	ZN	A	3004	1/1	0.98	0.05	21,21,21,21	0
3	ZN	A	3003	1/1	0.99	0.06	22,22,22,22	0
3	ZN	A	3002	1/1	0.99	0.07	22,22,22,22	0
3	ZN	A	3005	1/1	0.99	0.06	22,22,22,22	0
3	ZN	B	3002	1/1	0.99	0.04	23,23,23,23	0
3	ZN	B	3003	1/1	0.99	0.06	21,21,21,21	0
3	ZN	B	3004	1/1	0.99	0.04	23,23,23,23	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.

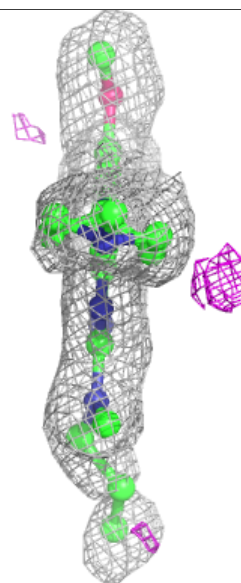
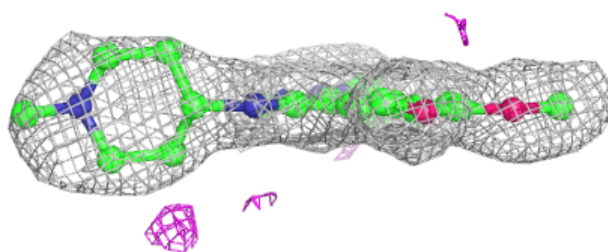
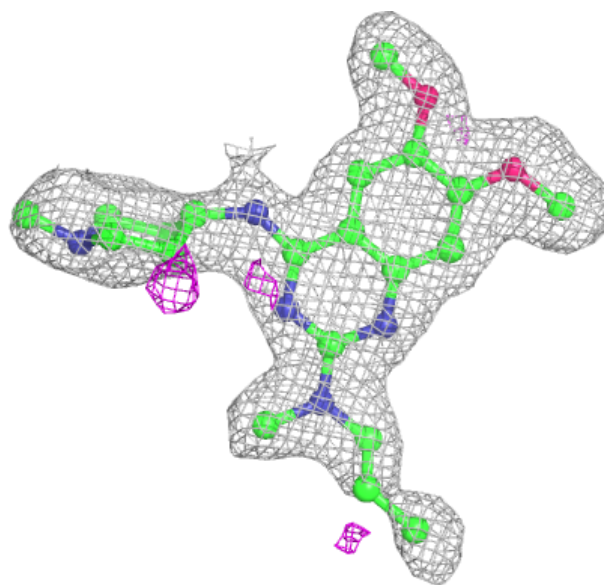
**Electron density around 9HJ B 3006:**

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



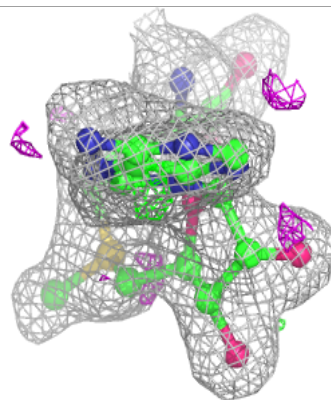
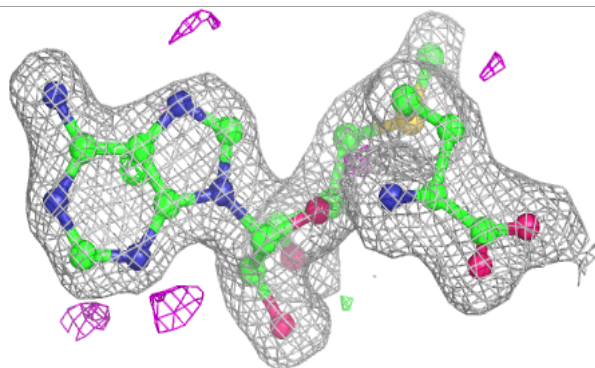
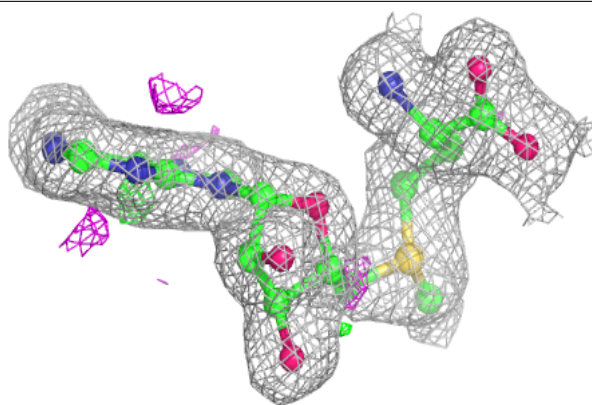
**Electron density around 9HJ A 3006:**

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

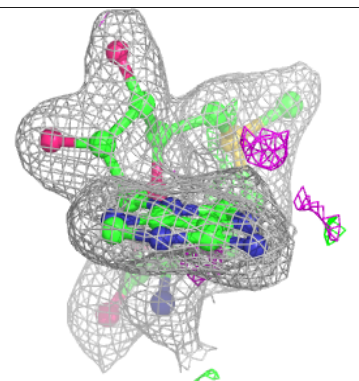
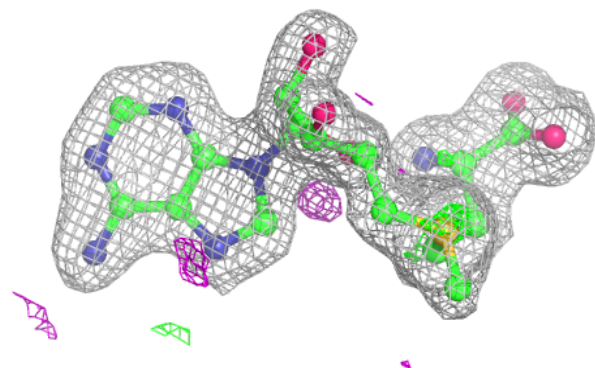
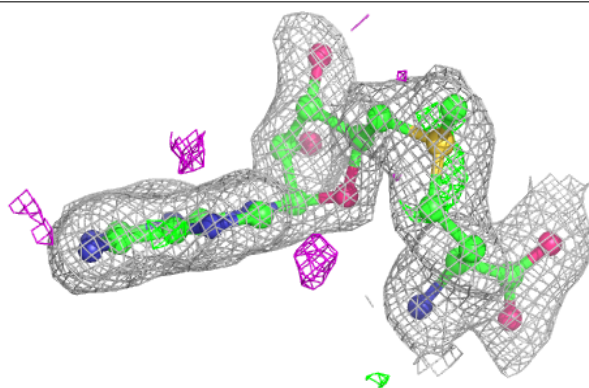


**Electron density around SAM B 3001:**

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

**Electron density around SAM A 3001:**

$2mF_o-DF_c$  (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.