



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 04:16 PM EDT

PDB ID : 9YKS / pdb\_00009yks  
Title : Crystal structure of the G9a (EHMT2) SET domain in complex with SAM and TNG917  
Authors : Whittington, D.A.  
Deposited on : 2025-10-07  
Resolution : 1.79 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

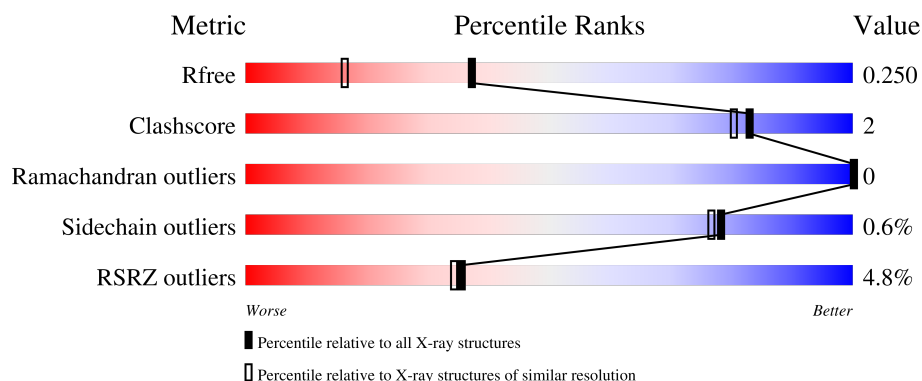
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	282	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	B	282	<div> <div>4%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	C	282	<div> <div>8%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	282	<div> <div>3%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10403 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.

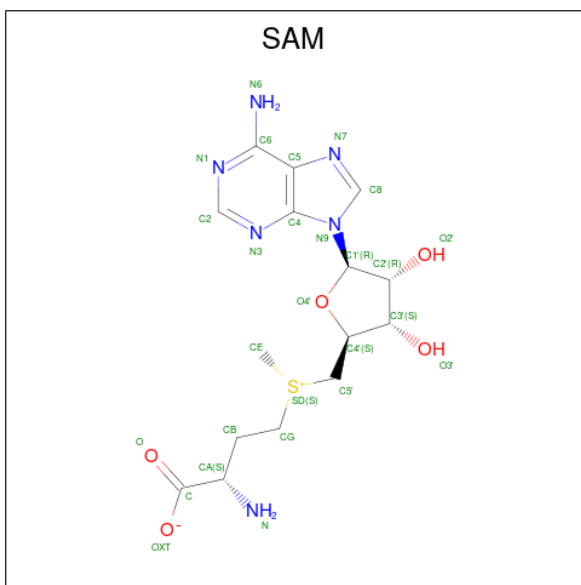
- Molecule 1 is a protein called Histone-lysine N-methyltransferase EHMT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	11	0
			2282	1419	406	433	24			
1	B	274	Total	C	N	O	S	0	7	0
			2254	1405	395	428	26			
1	C	272	Total	C	N	O	S	0	9	0
			2247	1401	393	428	25			
1	D	276	Total	C	N	O	S	0	10	0
			2291	1430	404	433	24			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

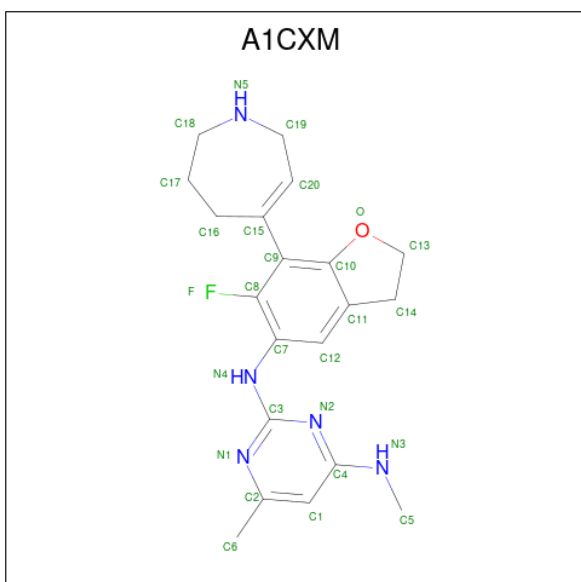
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	B	4	Total	Zn	0	0
			4	4		
2	C	4	Total	Zn	0	0
			4	4		
2	D	4	Total	Zn	0	0
			4	4		

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: 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
3	A	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	B	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	C	1	Total 27	C 15	N 6	O 5	S 1	0	0
3	D	1	Total 27	C 15	N 6	O 5	S 1	0	0

- Molecule 4 is N 2 -[(7M)-6-fluoro-7-(2,5,6,7-tetrahydro-1H-azepin-4-yl)-2,3-dihydro-1-benzofuran-5-yl]-N 4 ,6-dimethylpyrimidine-2,4-diamine (CCD ID: A1CXM) (formula: C<sub>20</sub>H<sub>24</sub>FN<sub>5</sub>O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



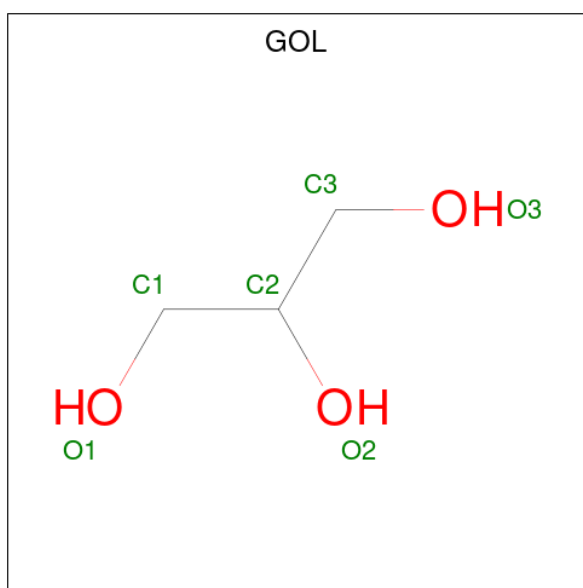
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	282	Total O 283 283	0	4
7	B	301	Total O 302 302	0	1

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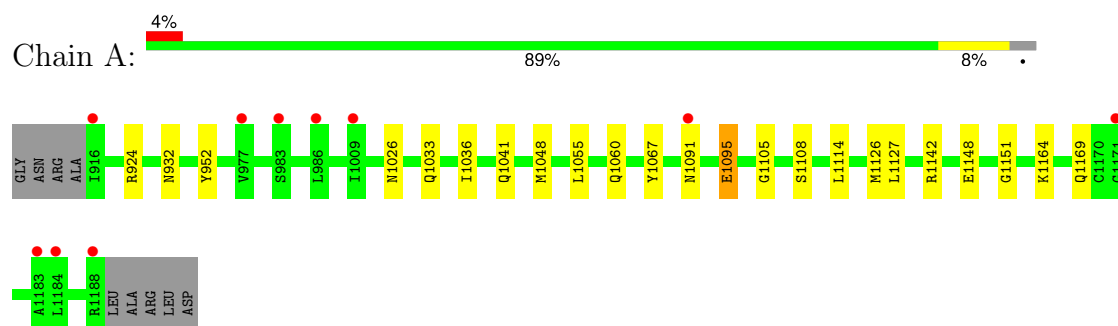
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	199	Total 199	O 199	0	1
7	D	247	Total 249	O 249	0	2

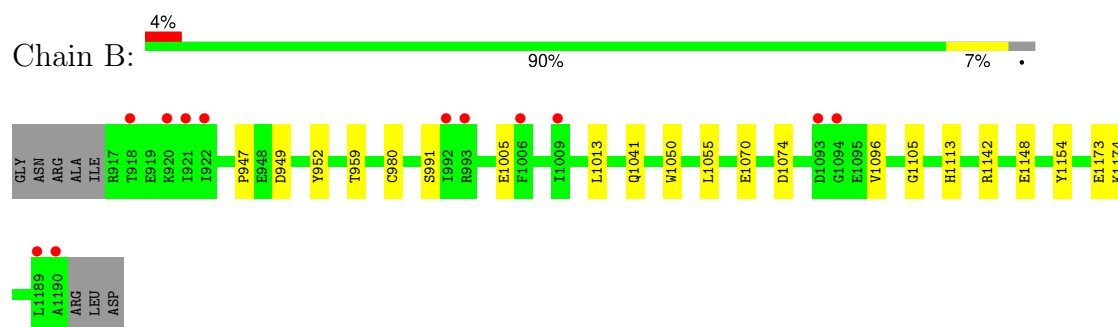
### 3 Residue-property plots [i](#)

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.

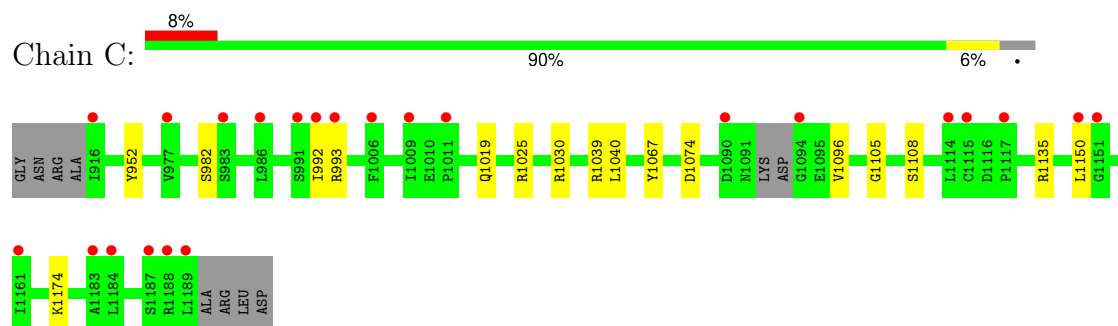
- Molecule 1: Histone-lysine N-methyltransferase EHMT2



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- Molecule 1: Histone-lysine N-methyltransferase EHMT2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.60Å 76.98Å 134.14Å 90.00° 89.80° 90.00°	Depositor
Resolution (Å)	45.60 – 1.79 45.60 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.60-1.79) 99.9 (45.60-1.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.192 , 0.252 0.199 , 0.250	Depositor DCC
$R_{free}$ test set	5358 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	1.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 42.09 % 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 2.1448e-04. 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: SAM, EDO, A1CXM, GOL, 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	0.26	0/2343	0.45	0/3161
1	B	0.26	0/2309	0.42	0/3116
1	C	0.21	0/2304	0.39	0/3109
1	D	0.24	0/2352	0.44	0/3175
All	All	0.24	0/9308	0.42	0/12561

There are no bond length outliers.

There are no bond angle outliers.

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	2282	0	2188	14	0
1	B	2254	0	2158	13	0
1	C	2247	0	2151	10	0
1	D	2291	0	2210	8	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	27	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	22	0	0
3	C	27	0	22	0	0
3	D	27	0	22	0	0
4	A	27	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	0	0
5	A	16	0	24	0	0
5	B	12	0	18	1	0
5	C	12	0	18	1	0
5	D	12	0	18	0	0
6	B	12	0	16	0	0
7	A	283	0	0	2	0
7	B	302	0	0	2	0
7	C	199	0	0	0	0
7	D	249	0	0	1	0
All	All	10403	0	8889	44	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 2.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:GLN:HB3	1:A:1126[B]:MET:HG2	1.70	0.74
1:C:992:ILE:HG22	1:C:993:ARG:HG3	1.69	0.73
1:A:1142[A]:ARG:NH2	1:A:1148:GLU:OE2	2.27	0.64
1:C:1074:ASP:HB2	1:C:1096:VAL:HG23	1.79	0.63
1:D:959:THR:OG1	1:D:1070:GLU:OE2	2.15	0.60
1:B:1142:ARG:NH2	1:B:1148:GLU:OE2	2.31	0.58
1:A:1127:LEU:HD13	5:B:1210:EDO:H12	1.86	0.56
1:B:1173:GLU:OE2	1:B:1174:LYS:NZ	2.39	0.56
1:B:1074:ASP:HB3	1:B:1096:VAL:HG23	1.88	0.54
1:A:1091[B]:ASN:ND2	1:A:1095:GLU:O	2.32	0.52
1:D:1033:GLN:HB3	1:D:1126[B]:MET:HG2	1.92	0.51
1:D:1145:ARG:NH2	1:D:1148[B]:GLU:OE2	2.46	0.48
1:C:1135:ARG:HD2	5:C:1207:EDO:H12	1.94	0.48
1:A:1048:MET:HE2	1:A:1169:GLN:O	2.13	0.48
1:B:1041:GLN:NE2	7:B:1315:HOH:O	2.39	0.48
1:C:952:TYR:HA	1:C:1105:GLY:O	2.14	0.48
1:A:1095:GLU:H	1:A:1095:GLU:HG3	1.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:LEU:HG	1:A:1151:GLY:HA3	1.97	0.47
1:D:956:ASN:HB3	1:D:1071[B]:LEU:CD2	2.45	0.47
1:D:1067:TYR:HA	1:D:1108[A]:SER:OG	2.16	0.46
1:B:991:SER:HB3	1:B:1013:LEU:O	2.16	0.46
1:B:1005:GLU:CD	1:C:1174:LYS:HE3	2.41	0.45
1:C:1019:GLN:H	1:C:1019:GLN:CD	2.24	0.45
1:B:1041:GLN:HB2	1:B:1055:LEU:HD11	1.99	0.45
1:A:1041:GLN:HB2	1:A:1055:LEU:HD21	1.99	0.44
1:A:924[B]:ARG:CZ	1:A:924[B]:ARG:H	2.30	0.44
1:C:1067:TYR:HA	1:C:1108[B]:SER:OG	2.17	0.44
1:A:1060:GLN:HG2	7:A:1475:HOH:O	2.18	0.43
1:A:952:TYR:HA	1:A:1105:GLY:O	2.18	0.43
1:D:956:ASN:HB3	1:D:1071[B]:LEU:HD21	2.01	0.43
1:C:1040:LEU:HD22	1:C:1150:LEU:HD11	2.00	0.43
1:A:1067:TYR:HA	1:A:1108[B]:SER:OG	2.19	0.43
1:B:949:ASP:OD1	1:B:949:ASP:N	2.46	0.42
1:D:1123[B]:ARG:NH2	7:D:1324:HOH:O	2.53	0.42
1:B:1113:HIS:HB2	1:B:1154:TYR:CG	2.56	0.41
1:B:947:PRO:HD3	1:B:1050:TRP:CZ2	2.55	0.41
1:B:952:TYR:HA	1:B:1105:GLY:O	2.20	0.41
1:C:1025:ARG:O	1:C:1030:ARG:HD2	2.21	0.41
1:D:952:TYR:HA	1:D:1105:GLY:O	2.21	0.41
1:A:1026:ASN:ND2	7:A:1302:HOH:O	2.34	0.41
1:B:980:CYS:HA	7:B:1323:HOH:O	2.22	0.40
1:C:1039[B]:ARG:HA	1:C:1039[B]:ARG:HD2	1.81	0.40
1:A:932:ASN:HB2	1:A:1036:ILE:O	2.21	0.40
1:B:959:THR:OG1	1:B:1070:GLU:OE2	2.34	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	282/282 (100%)	269 (95%)	13 (5%)	0	100	100
1	B	279/282 (99%)	263 (94%)	16 (6%)	0	100	100
1	C	277/282 (98%)	264 (95%)	13 (5%)	0	100	100
1	D	284/282 (101%)	272 (96%)	12 (4%)	0	100	100
All	All	1122/1128 (100%)	1068 (95%)	54 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	257/252 (102%)	255 (99%)	2 (1%)	73	70
1	B	253/252 (100%)	253 (100%)	0	100	100
1	C	254/252 (101%)	253 (100%)	1 (0%)	84	83
1	D	258/252 (102%)	254 (98%)	4 (2%)	55	47
All	All	1022/1008 (101%)	1015 (99%)	7 (1%)	78	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1095	GLU
1	A	1164	LYS
1	C	982	SER
1	D	920	LYS
1	D	1096	VAL
1	D	1142[A]	ARG
1	D	1142[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1186	GLN

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Mol	Chain	Res	Type
1	C	973	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 16 are monoatomic - leaving 23 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	$\# Z  > 2$
3	SAM	D	1205	-	27,29,29	1.17	5 (18%)	34,42,42	1.93	9 (26%)
5	EDO	B	1209	-	3,3,3	0.45	0	2,2,2	0.39	0
4	A1CXM	B	1206	-	28,30,30	0.81	0	31,42,42	2.13	8 (25%)
5	EDO	A	1209	-	3,3,3	0.44	0	2,2,2	0.33	0
5	EDO	C	1209	-	3,3,3	0.46	0	2,2,2	0.26	0
5	EDO	A	1210	-	3,3,3	0.46	0	2,2,2	0.37	0
4	A1CXM	C	1206	-	28,30,30	0.74	0	31,42,42	2.18	7 (22%)
5	EDO	D	1207	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	D	1208	-	3,3,3	0.47	0	2,2,2	0.44	0
6	GOL	B	1207	-	5,5,5	0.83	0	5,5,5	1.10	0
5	EDO	D	1209	-	3,3,3	0.36	0	2,2,2	0.48	0
5	EDO	A	1208	-	3,3,3	0.44	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	B	1208	-	5,5,5	1.03	0	5,5,5	1.10	0
4	A1CXM	A	1206	-	28,30,30	0.80	0	31,42,42	2.09	10 (32%)
3	SAM	A	1205	-	27,29,29	1.15	5 (18%)	34,42,42	1.91	8 (23%)
5	EDO	B	1211	-	3,3,3	0.37	0	2,2,2	0.55	0
5	EDO	B	1210	-	3,3,3	0.43	0	2,2,2	0.43	0
5	EDO	C	1207	-	3,3,3	0.42	0	2,2,2	0.42	0
4	A1CXM	D	1206	-	28,30,30	0.77	0	31,42,42	2.05	8 (25%)
5	EDO	C	1208	-	3,3,3	0.44	0	2,2,2	0.40	0
3	SAM	B	1205	-	27,29,29	1.07	4 (14%)	34,42,42	1.77	7 (20%)
3	SAM	C	1205	-	27,29,29	1.14	4 (14%)	34,42,42	1.92	10 (29%)
5	EDO	A	1207	-	3,3,3	0.48	0	2,2,2	0.45	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
3	SAM	D	1205	-	-	2/17/33/33	0/3/3/3
5	EDO	B	1209	-	-	0/1/1/1	-
4	A1CXM	B	1206	-	-	0/8/25/25	0/3/4/4
5	EDO	A	1209	-	-	0/1/1/1	-
5	EDO	C	1209	-	-	0/1/1/1	-
5	EDO	A	1210	-	-	1/1/1/1	-
4	A1CXM	C	1206	-	-	0/8/25/25	0/3/4/4
5	EDO	D	1207	-	-	0/1/1/1	-
5	EDO	D	1208	-	-	1/1/1/1	-
6	GOL	B	1207	-	-	2/4/4/4	-
5	EDO	D	1209	-	-	0/1/1/1	-
5	EDO	A	1208	-	-	0/1/1/1	-
6	GOL	B	1208	-	-	3/4/4/4	-
4	A1CXM	A	1206	-	-	0/8/25/25	0/3/4/4
3	SAM	A	1205	-	-	2/17/33/33	0/3/3/3
5	EDO	B	1211	-	-	0/1/1/1	-
5	EDO	B	1210	-	-	0/1/1/1	-
5	EDO	C	1207	-	-	0/1/1/1	-
4	A1CXM	D	1206	-	-	0/8/25/25	0/3/4/4
5	EDO	C	1208	-	-	0/1/1/1	-
3	SAM	B	1205	-	-	2/17/33/33	0/3/3/3
3	SAM	C	1205	-	-	2/17/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1207	-	-	0/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1205	SAM	C2-N3	2.93	1.39	1.33
3	D	1205	SAM	C5-N7	-2.90	1.33	1.39
3	D	1205	SAM	C2-N3	2.84	1.39	1.33
3	C	1205	SAM	C2-N3	2.81	1.38	1.33
3	C	1205	SAM	C2-N1	2.56	1.38	1.33
3	A	1205	SAM	C8-N7	2.53	1.36	1.31
3	B	1205	SAM	C2-N1	2.46	1.38	1.33
3	C	1205	SAM	C8-N7	2.31	1.36	1.31
3	A	1205	SAM	C2-N1	2.30	1.38	1.33
3	B	1205	SAM	C8-N7	2.30	1.36	1.31
3	B	1205	SAM	C2-N3	2.25	1.37	1.33
3	A	1205	SAM	C5-N7	-2.25	1.35	1.39
3	D	1205	SAM	C8-N7	2.20	1.35	1.31
3	D	1205	SAM	C2-N1	2.16	1.37	1.33
3	D	1205	SAM	OXT-C	-2.15	1.23	1.30
3	C	1205	SAM	OXT-C	-2.05	1.24	1.30
3	B	1205	SAM	C5-N7	-2.02	1.35	1.39
3	A	1205	SAM	OXT-C	-2.01	1.24	1.30

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1206	A1CXM	O-C13-C14	-6.27	101.40	107.86
3	A	1205	SAM	N3-C2-N1	-6.22	119.17	128.58
4	D	1206	A1CXM	O-C13-C14	-5.98	101.70	107.86
3	D	1205	SAM	N3-C2-N1	-5.84	119.74	128.58
3	C	1205	SAM	N3-C2-N1	-5.68	119.99	128.58
3	B	1205	SAM	N3-C2-N1	-5.46	120.32	128.58
4	A	1206	A1CXM	O-C13-C14	-5.43	102.26	107.86
4	B	1206	A1CXM	O-C13-C14	-5.30	102.40	107.86
4	C	1206	A1CXM	C5-N3-C4	-4.94	118.39	122.96
3	C	1205	SAM	C5-C4-N3	-4.51	120.51	126.72
3	D	1205	SAM	C5-C4-N3	-4.44	120.60	126.72
4	B	1206	A1CXM	O-C10-C11	-4.44	110.69	113.59
4	C	1206	A1CXM	O-C10-C11	-4.13	110.89	113.59
3	B	1205	SAM	C5-C4-N3	-3.96	121.26	126.72
4	A	1206	A1CXM	N2-C3-N1	-3.90	119.86	126.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1206	A1CXM	N2-C3-N1	-3.90	119.86	126.26
3	A	1205	SAM	C5-C4-N3	-3.84	121.42	126.72
4	B	1206	A1CXM	C5-N3-C4	-3.82	119.43	122.96
3	A	1205	SAM	N9-C8-N7	-3.65	108.75	113.94
4	A	1206	A1CXM	O-C10-C11	-3.49	111.31	113.59
4	D	1206	A1CXM	O-C10-C11	-3.47	111.32	113.59
4	A	1206	A1CXM	C5-N3-C4	-3.47	119.75	122.96
3	C	1205	SAM	N9-C8-N7	-3.46	109.02	113.94
4	D	1206	A1CXM	N2-C3-N1	-3.42	120.66	126.26
4	C	1206	A1CXM	N2-C3-N1	-3.40	120.69	126.26
3	C	1205	SAM	C2-N3-C4	3.37	120.07	111.83
4	A	1206	A1CXM	C3-N1-C2	3.33	122.45	115.98
4	B	1206	A1CXM	C3-N1-C2	3.33	122.45	115.98
3	A	1205	SAM	C5-N7-C8	3.28	108.61	103.45
3	A	1205	SAM	C2-N3-C4	3.23	119.72	111.83
3	D	1205	SAM	N9-C8-N7	-3.22	109.37	113.94
3	D	1205	SAM	C2-N3-C4	3.17	119.56	111.83
3	C	1205	SAM	C5-N7-C8	3.13	108.37	103.45
4	D	1206	A1CXM	C3-N1-C2	3.13	122.05	115.98
4	B	1206	A1CXM	C8-C9-C15	-3.10	120.99	122.95
4	B	1206	A1CXM	C13-O-C10	3.08	109.30	107.07
4	D	1206	A1CXM	C5-N3-C4	-3.07	120.12	122.96
4	C	1206	A1CXM	C3-N1-C2	3.01	121.82	115.98
3	B	1205	SAM	C2-N3-C4	3.01	119.17	111.83
3	D	1205	SAM	N3-C4-N9	2.94	132.16	127.17
3	B	1205	SAM	N9-C8-N7	-2.92	109.79	113.94
3	A	1205	SAM	OXT-C-O	-2.82	117.68	124.08
3	C	1205	SAM	N3-C4-N9	2.79	131.91	127.17
3	D	1205	SAM	C5-N7-C8	2.76	107.79	103.45
3	B	1205	SAM	C5-N7-C8	2.72	107.72	103.45
4	D	1206	A1CXM	C8-C9-C15	-2.71	121.23	122.95
3	D	1205	SAM	C2'-C1'-N9	-2.69	106.62	113.30
4	D	1206	A1CXM	C14-C11-C10	-2.59	106.22	107.98
4	C	1206	A1CXM	C14-C11-C10	-2.58	106.23	107.98
4	A	1206	A1CXM	C8-C9-C15	-2.54	121.34	122.95
3	C	1205	SAM	C2'-C1'-N9	-2.46	107.18	113.30
4	A	1206	A1CXM	C13-O-C10	2.46	108.85	107.07
3	D	1205	SAM	OXT-C-O	-2.46	118.50	124.08
3	B	1205	SAM	C2'-C1'-N9	-2.46	107.20	113.30
3	B	1205	SAM	N3-C4-N9	2.43	131.31	127.17
4	C	1206	A1CXM	C6-C2-N1	2.40	120.19	116.56
4	A	1206	A1CXM	C6-C2-N1	2.38	120.15	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1205	SAM	C6-C5-C4	2.26	120.27	117.18
4	A	1206	A1CXM	C14-C11-C10	-2.26	106.44	107.98
3	C	1205	SAM	OXT-C-O	-2.21	119.07	124.08
3	A	1205	SAM	N3-C4-N9	2.18	130.88	127.17
4	D	1206	A1CXM	C6-C2-N1	2.18	119.85	116.56
3	C	1205	SAM	C4-C5-N7	-2.17	108.10	110.58
4	B	1206	A1CXM	C6-C2-N1	2.10	119.74	116.56
3	A	1205	SAM	C2'-C1'-N9	-2.06	108.19	113.30
3	C	1205	SAM	C6-C5-C4	2.03	119.94	117.18
4	A	1206	A1CXM	N3-C4-N2	2.01	121.24	116.36

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1205	SAM	CB-CG-SD-CE
3	A	1205	SAM	CB-CG-SD-C5'
3	B	1205	SAM	CB-CG-SD-CE
3	B	1205	SAM	CB-CG-SD-C5'
3	C	1205	SAM	CB-CG-SD-CE
3	C	1205	SAM	CB-CG-SD-C5'
3	D	1205	SAM	CB-CG-SD-CE
3	D	1205	SAM	CB-CG-SD-C5'
6	B	1207	GOL	O1-C1-C2-C3
6	B	1208	GOL	O1-C1-C2-C3
6	B	1207	GOL	O1-C1-C2-O2
6	B	1208	GOL	O1-C1-C2-O2
6	B	1208	GOL	O2-C2-C3-O3
5	A	1210	EDO	O1-C1-C2-O2
5	D	1208	EDO	O1-C1-C2-O2

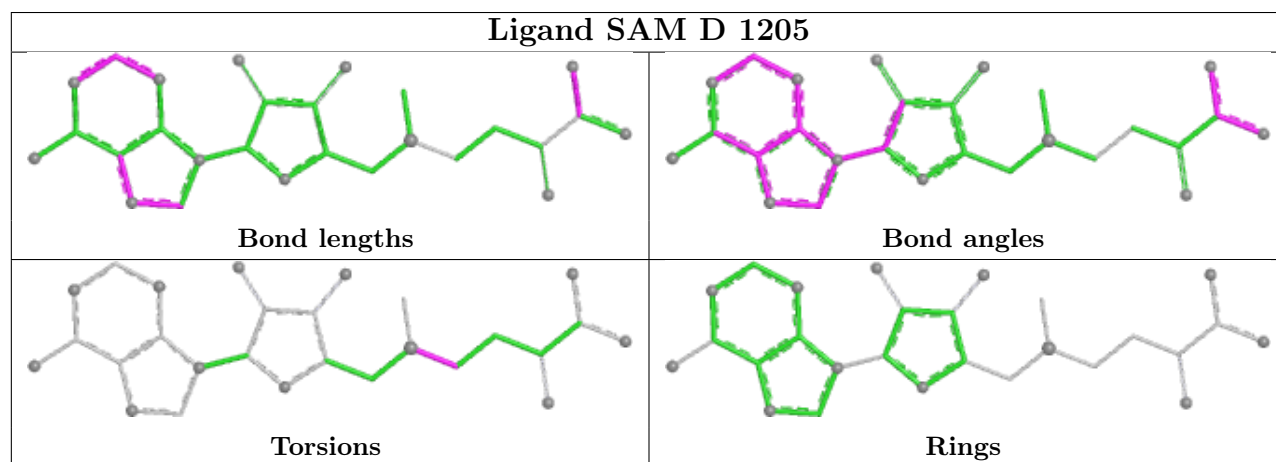
There are no ring outliers.

2 monomers are involved in 2 short contacts:

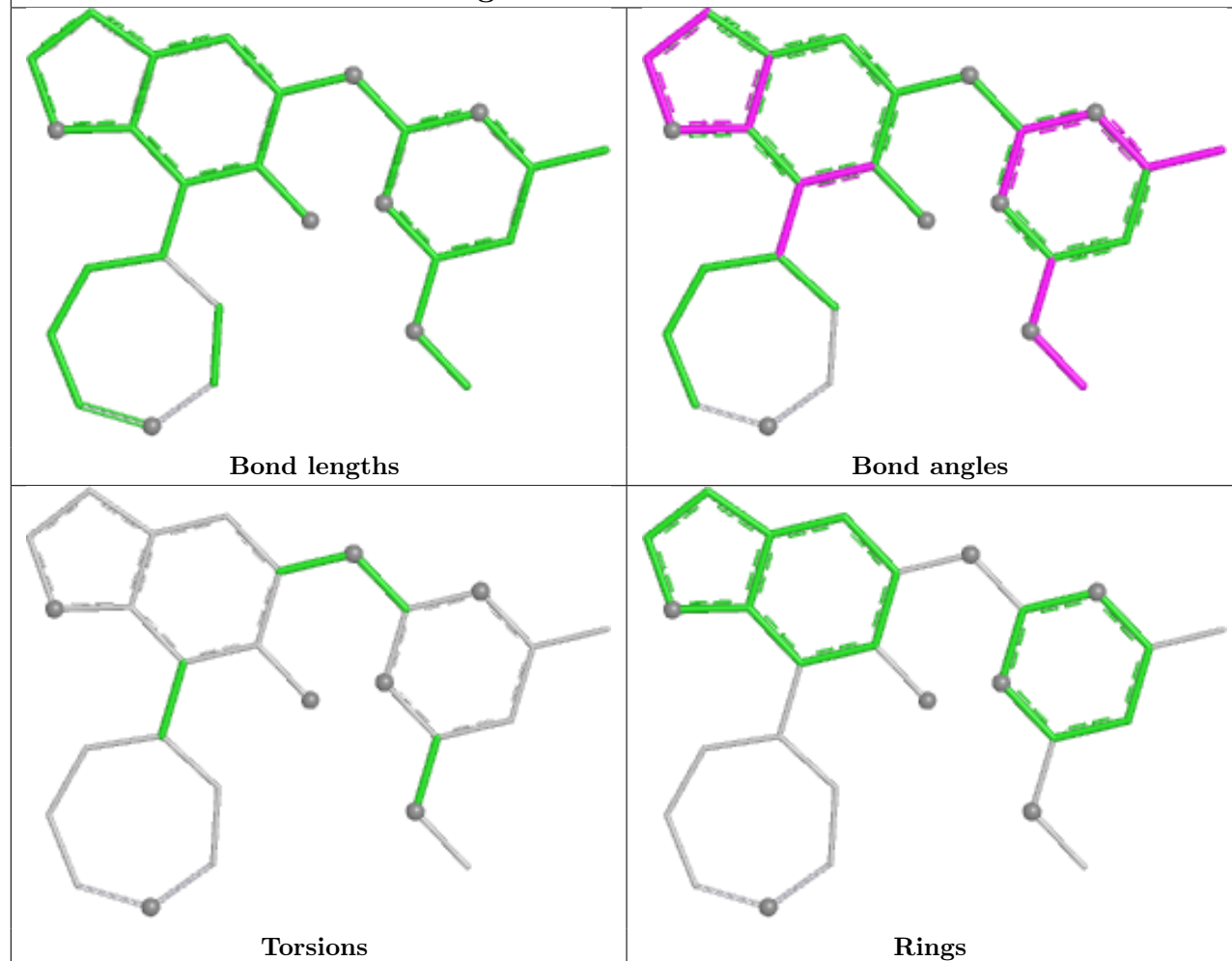
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1210	EDO	1	0
5	C	1207	EDO	1	0

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

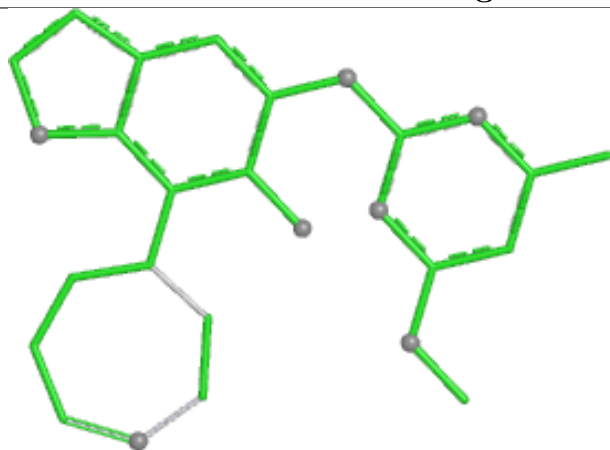
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



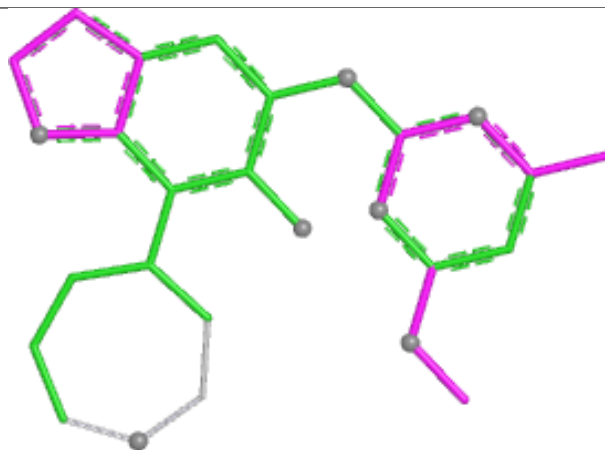
## Ligand A1CXM B 1206



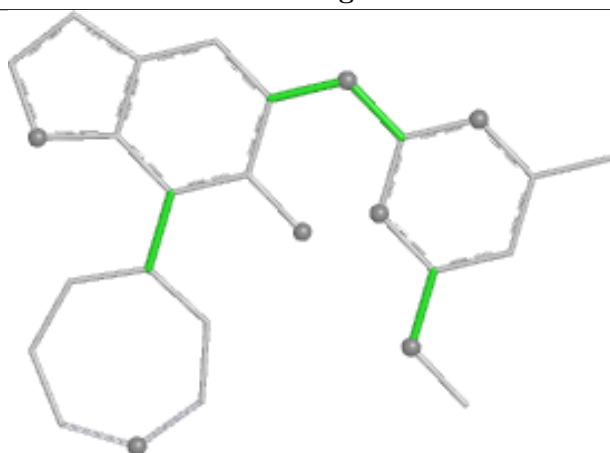
## Ligand A1CXM C 1206



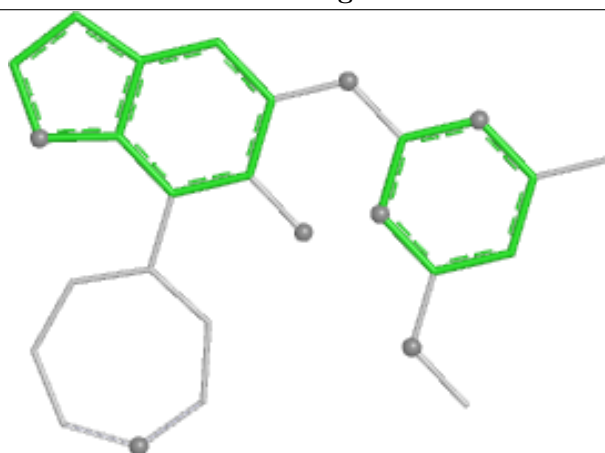
Bond lengths



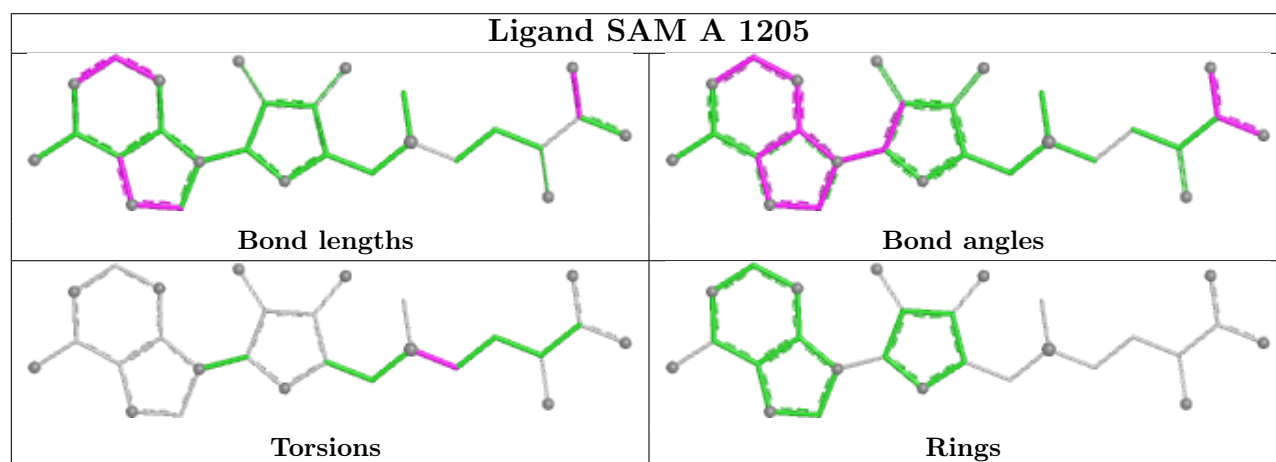
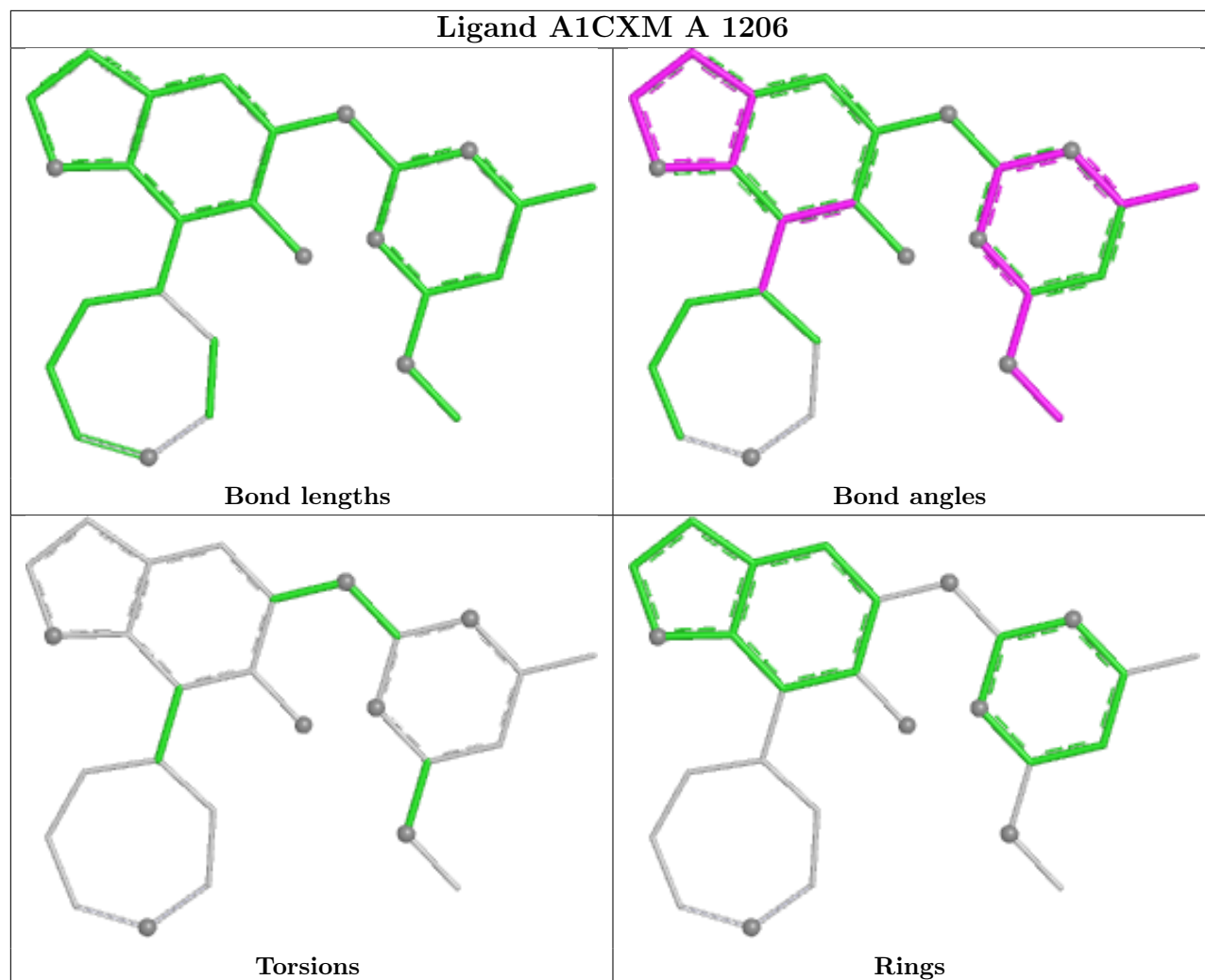
Bond angles

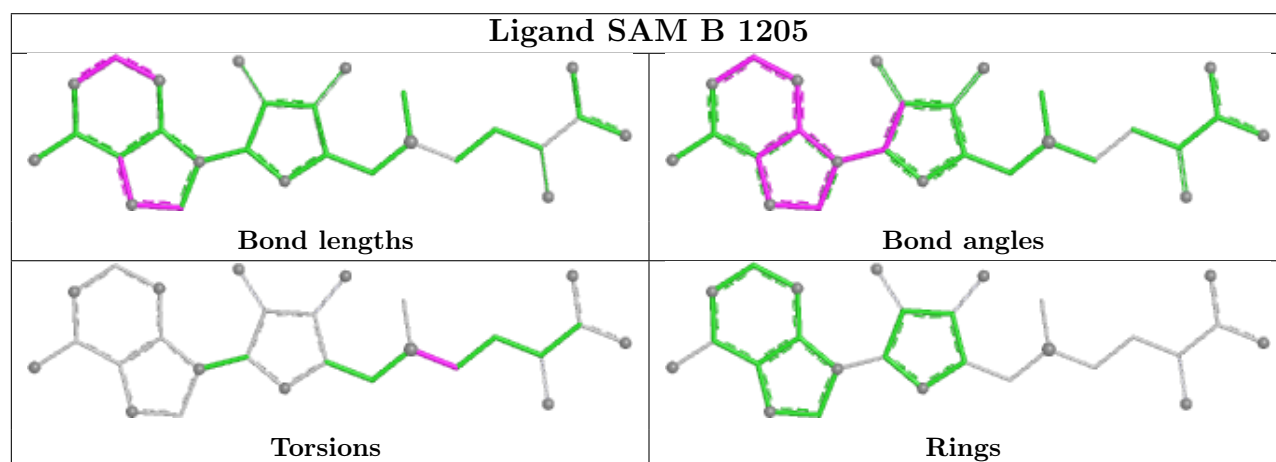
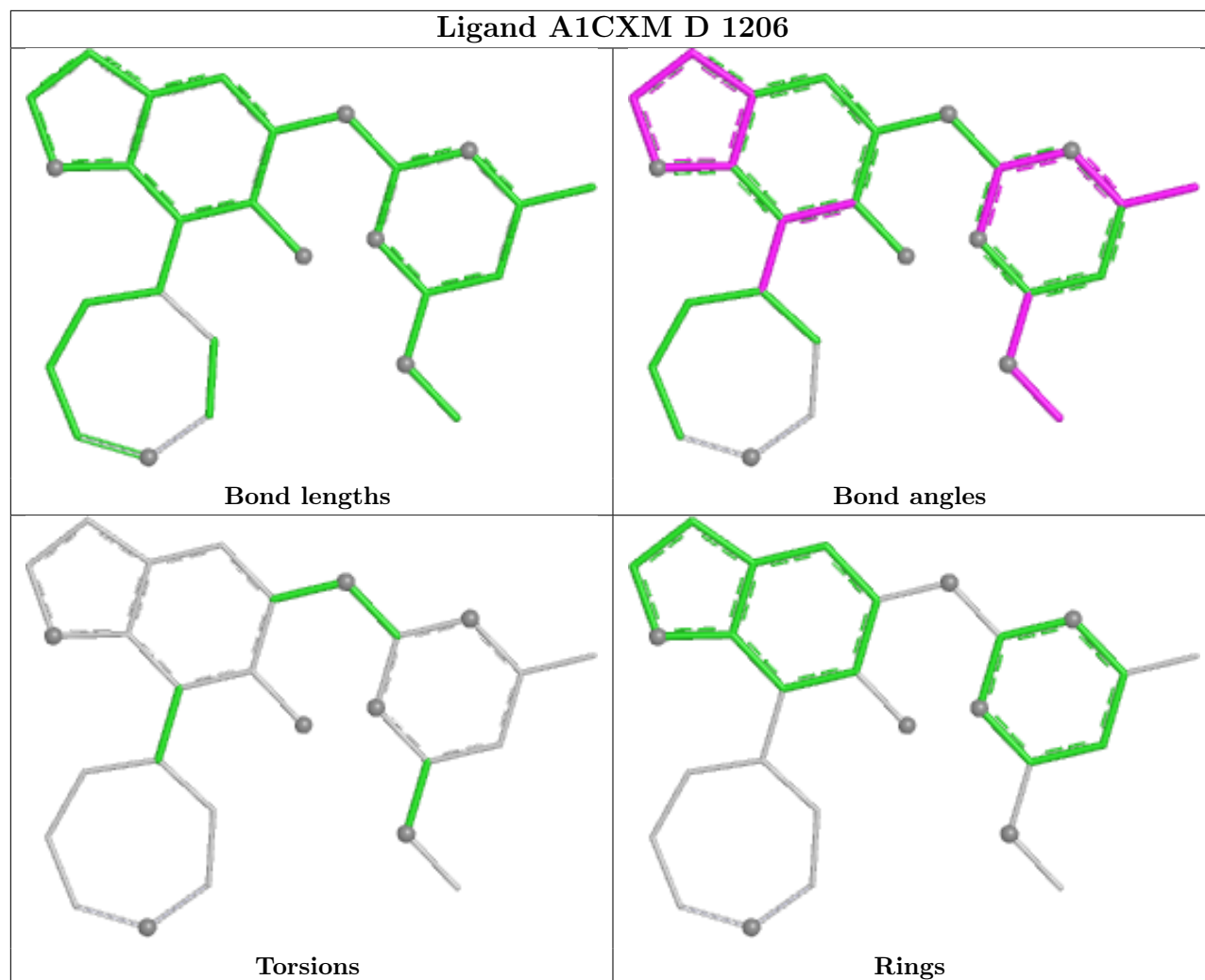


Torsions

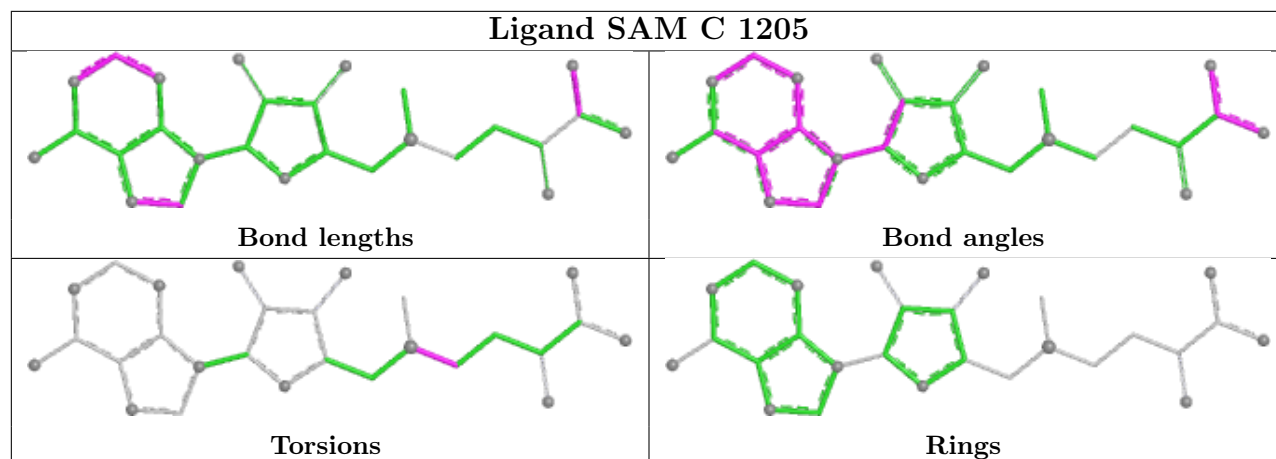


Rings









## 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	273/282 (96%)	0.41	10 (3%) 45 45	10, 26, 48, 75	11 (4%)
1	B	274/282 (97%)	0.40	12 (4%) 39 38	9, 27, 55, 69	7 (2%)
1	C	272/282 (96%)	0.90	23 (8%) 16 14	14, 32, 59, 72	9 (3%)
1	D	276/282 (97%)	0.41	8 (2%) 53 53	11, 27, 52, 89	10 (3%)
All	All	1095/1128 (97%)	0.53	53 (4%) 35 34	9, 28, 54, 89	37 (3%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1192	LEU	5.9
1	B	992	ILE	4.5
1	C	992	ILE	4.1
1	D	1189	LEU	3.6
1	C	1188	ARG	3.6
1	B	1190	ALA	3.6
1	B	1189	LEU	3.6
1	D	992	ILE	3.4
1	C	1009	ILE	3.4
1	C	1151	GLY	3.4
1	A	916	ILE	3.3
1	C	1189	LEU	3.1
1	C	1006	PHE	3.1
1	C	986	LEU	2.9
1	A	977	VAL	2.8
1	C	1184	LEU	2.8
1	B	920	LYS	2.8
1	C	1161	ILE	2.8
1	C	1114	LEU	2.7
1	A	1188	ARG	2.7
1	D	1190	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1093	ASP	2.7
1	C	1094	GLY	2.6
1	D	918	THR	2.6
1	C	1090	ASP	2.5
1	B	918	THR	2.5
1	C	916	ILE	2.4
1	C	993	ARG	2.4
1	B	1006	PHE	2.4
1	C	1150	LEU	2.4
1	A	1009	ILE	2.3
1	D	1191	ARG	2.3
1	B	1094	GLY	2.3
1	A	1184	LEU	2.3
1	A	986	LEU	2.2
1	A	983	SER	2.2
1	A	1091[A]	ASN	2.2
1	C	1115	CYS	2.2
1	B	1009	ILE	2.2
1	C	1011	PRO	2.2
1	C	983	SER	2.2
1	C	991[A]	SER	2.2
1	C	977	VAL	2.1
1	C	1187	SER	2.1
1	A	1171	GLY	2.1
1	D	963	ASN	2.1
1	B	922	ILE	2.1
1	D	921	ILE	2.1
1	C	1183	ALA	2.0
1	C	1117	PRO	2.0
1	B	921	ILE	2.0
1	B	993[A]	ARG	2.0
1	A	1183	ALA	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 oligosaccharides 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
5	EDO	D	1208	4/4	0.69	0.19	46,50,51,54	0
5	EDO	C	1208	4/4	0.72	0.15	35,37,44,52	0
5	EDO	B	1209	4/4	0.73	0.17	45,50,50,54	0
6	GOL	B	1207	6/6	0.77	0.15	32,35,43,46	0
5	EDO	D	1209	4/4	0.79	0.22	27,31,34,41	0
5	EDO	B	1210	4/4	0.80	0.17	40,40,44,52	0
5	EDO	A	1207	4/4	0.81	0.15	33,35,45,54	0
5	EDO	A	1210	4/4	0.82	0.14	30,32,34,40	0
5	EDO	B	1211	4/4	0.83	0.16	28,32,33,37	0
5	EDO	C	1209	4/4	0.84	0.13	32,38,39,40	0
5	EDO	C	1207	4/4	0.84	0.14	33,35,36,43	0
5	EDO	A	1209	4/4	0.86	0.14	31,35,37,39	0
5	EDO	A	1208	4/4	0.87	0.11	45,46,47,57	0
6	GOL	B	1208	6/6	0.87	0.12	30,36,37,43	0
5	EDO	D	1207	4/4	0.90	0.09	22,28,29,31	0
4	A1CXM	C	1206	27/27	0.92	0.09	23,32,36,41	0
3	SAM	C	1205	27/27	0.92	0.09	26,30,35,36	0
4	A1CXM	D	1206	27/27	0.93	0.08	19,27,35,42	0
4	A1CXM	A	1206	27/27	0.93	0.08	17,27,30,33	0
4	A1CXM	B	1206	27/27	0.94	0.08	16,27,34,40	0
3	SAM	D	1205	27/27	0.95	0.07	17,21,25,26	0
3	SAM	A	1205	27/27	0.95	0.07	14,21,24,27	0
3	SAM	B	1205	27/27	0.96	0.06	16,21,26,27	0
2	ZN	C	1203	1/1	0.97	0.05	34,34,34,34	0
2	ZN	D	1203	1/1	0.98	0.06	24,24,24,24	0
2	ZN	C	1201	1/1	0.98	0.04	32,32,32,32	0
2	ZN	C	1202	1/1	0.98	0.04	33,33,33,33	0
2	ZN	A	1203	1/1	0.98	0.04	32,32,32,32	0
2	ZN	C	1204	1/1	0.98	0.04	40,40,40,40	0
2	ZN	D	1202	1/1	0.98	0.05	24,24,24,24	0
2	ZN	B	1201	1/1	0.99	0.05	22,22,22,22	0
2	ZN	B	1202	1/1	0.99	0.05	23,23,23,23	0
2	ZN	D	1201	1/1	0.99	0.05	22,22,22,22	0
2	ZN	B	1203	1/1	0.99	0.05	23,23,23,23	0
2	ZN	B	1204	1/1	0.99	0.04	29,29,29,29	0
2	ZN	A	1202	1/1	0.99	0.03	29,29,29,29	0
2	ZN	A	1201	1/1	0.99	0.05	29,29,29,29	0

*Continued on next page...*

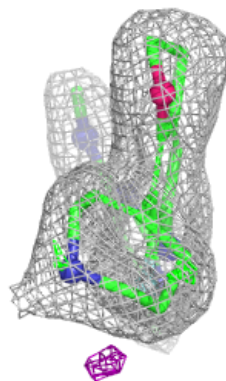
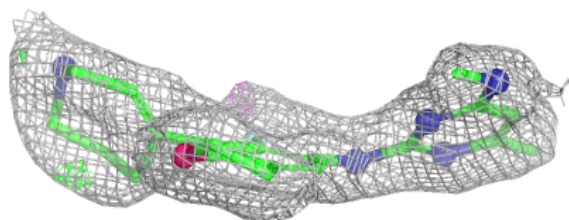
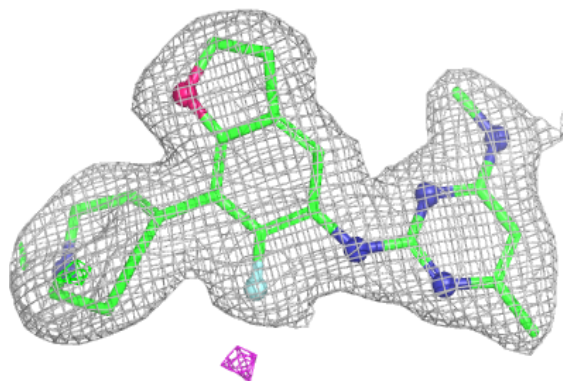
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	D	1204	1/1	1.00	0.03	27,27,27,27	0
2	ZN	A	1204	1/1	1.00	0.02	30,30,30,30	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.

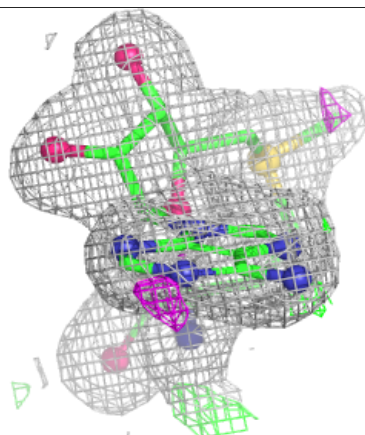
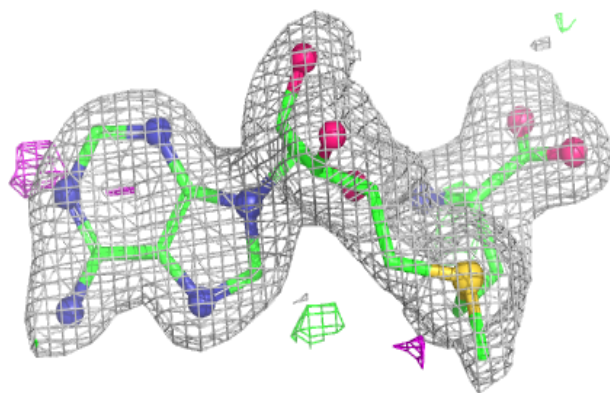
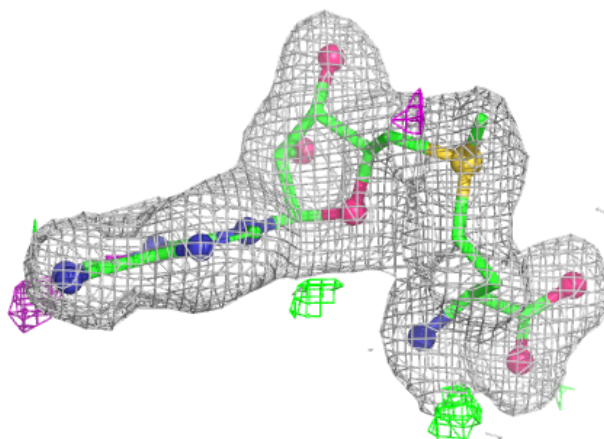
**Electron density around A1CXM C 1206:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



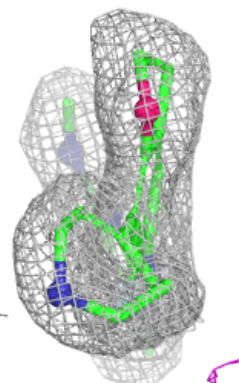
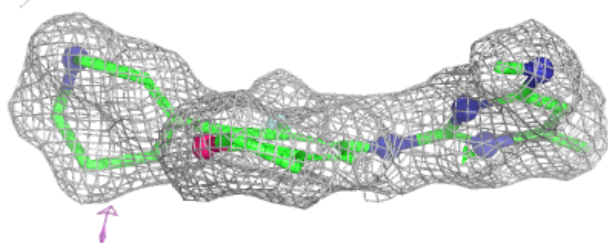
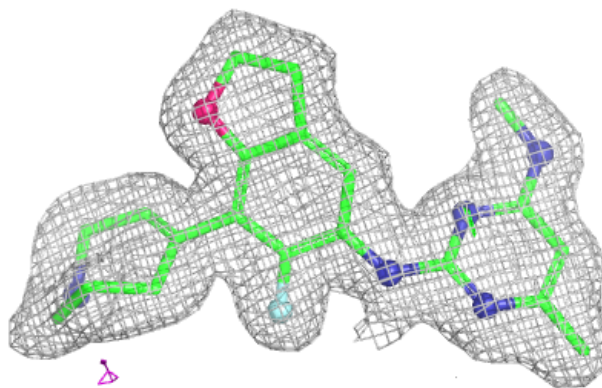
**Electron density around SAM C 1205:**

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

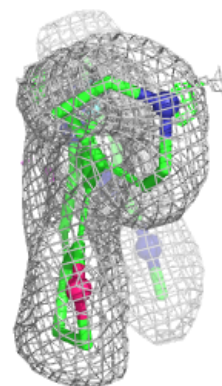
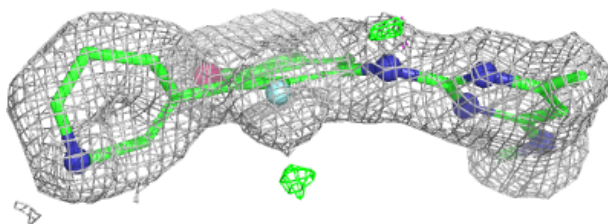
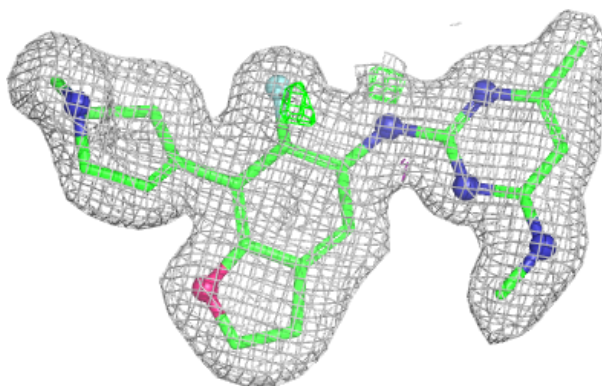


**Electron density around A1CXM D 1206:**

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

**Electron density around A1CXM A 1206:**

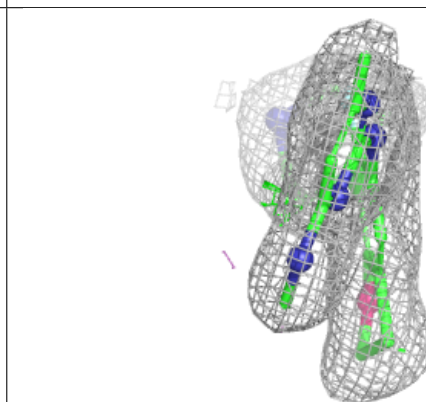
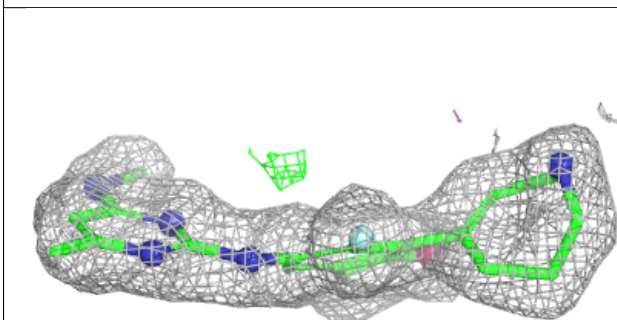
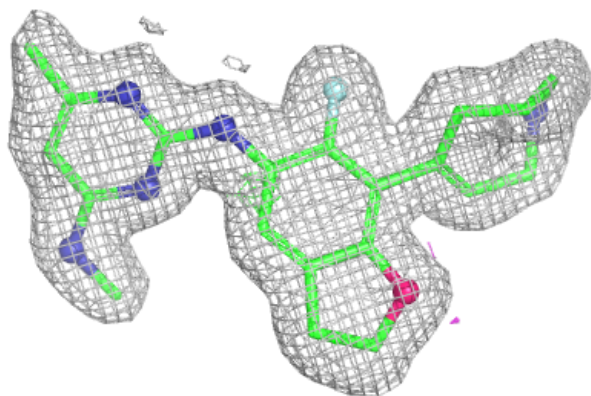
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



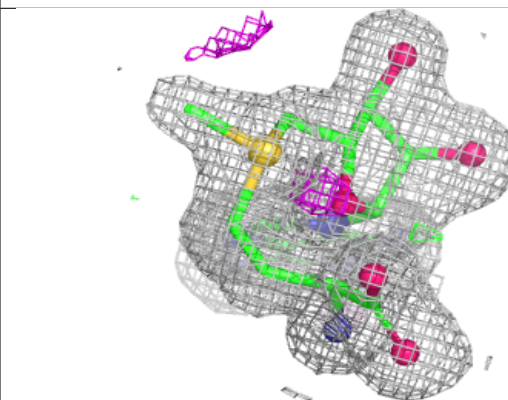
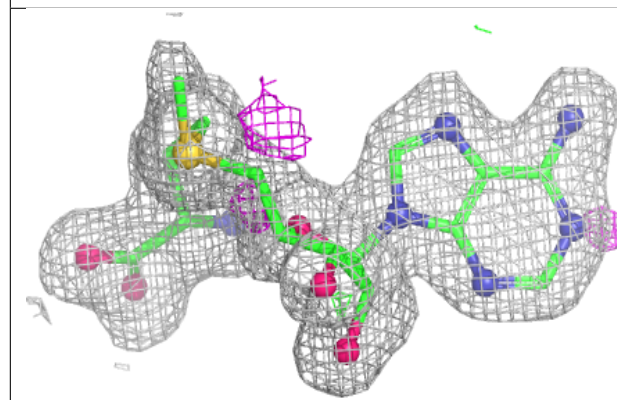
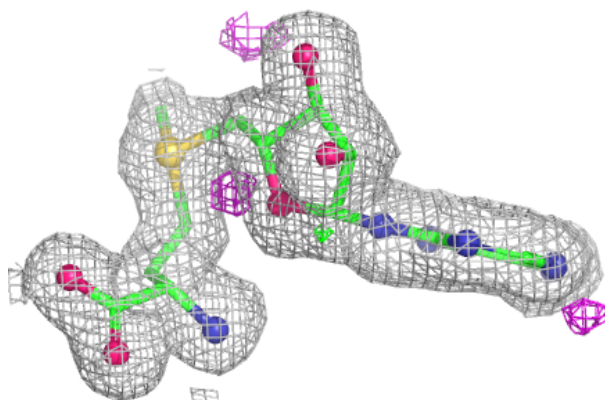


**Electron density around A1CXM B 1206:**

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

**Electron density around SAM D 1205:**

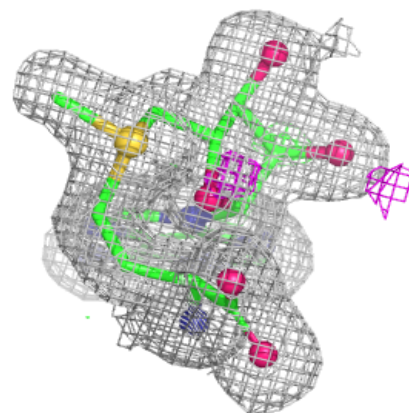
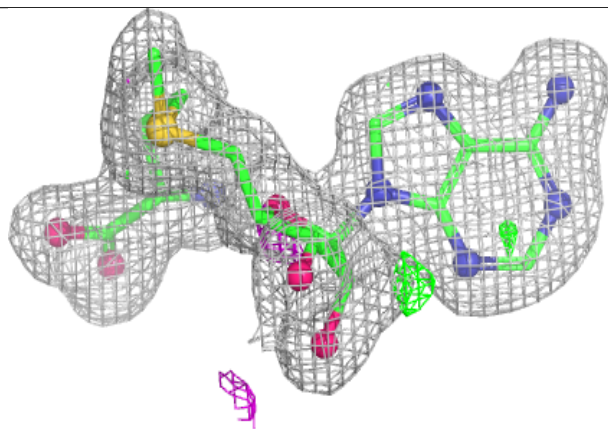
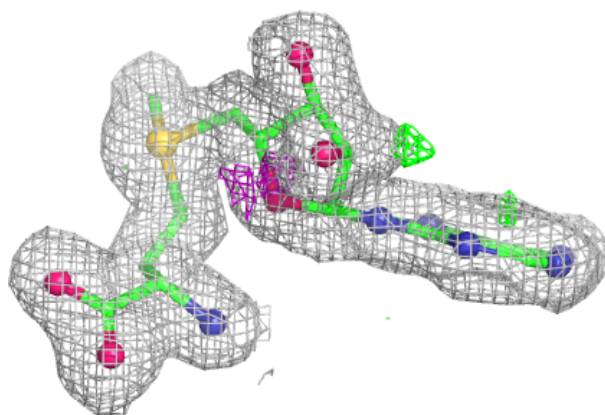
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





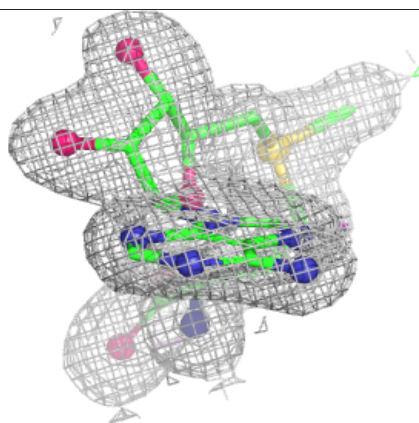
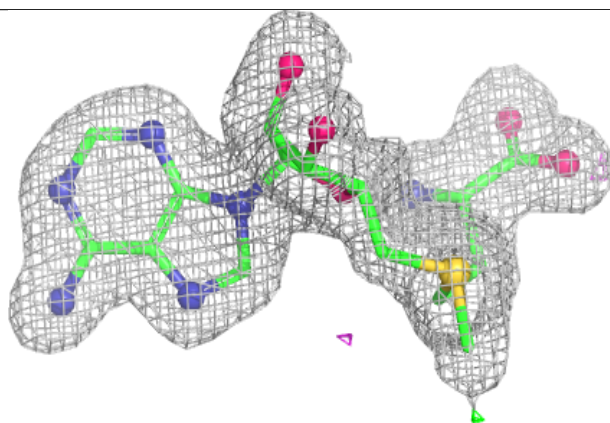
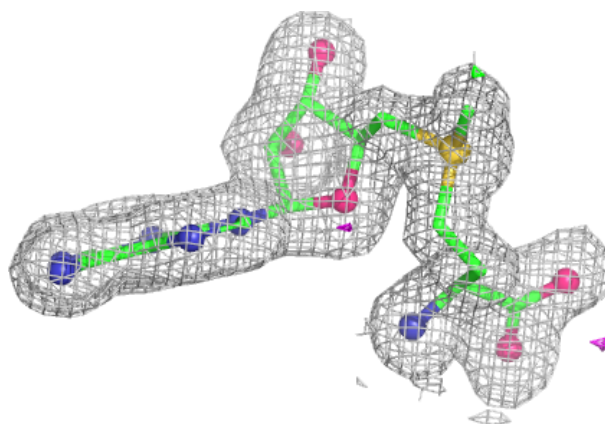
**Electron density around SAM A 1205:**

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



**Electron density around SAM B 1205:**

$2mF_o-DF_c$  (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.