Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 06:12 PM EDT

PDB ID	:	5V9I
Title	:	Crystal structure of catalytic domain of G9a with MS0105
Authors	:	Dong, A.; Zeng, H.; Liu, J.; Xiong, Y.; Babault, N.; Jin, J.; Walker, J.R.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Wu, H.; Brown, P.J.; Structural Genomics Consortium (SGC)
Deposited on	:	2017-03-23
Resolution	:	1.74 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

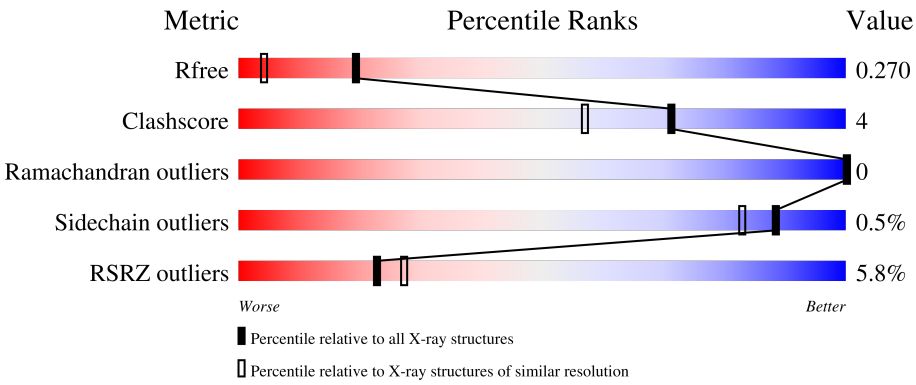
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 >=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 <=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	283	7% 87% 7% 6%
1	B	283	5% 90% 5% 5%
1	C	283	5% 89% 5% 6%
1	D	283	5% 92% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1507	-	-	X	-
5	GOL	A	1509	-	-	X	-
5	GOL	B	1507	-	-	X	-
5	GOL	B	1509	-	-	X	-
5	GOL	C	1507	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9547 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
			Total	C	N	O	S			
1	A	266	2128	1345	362	397	24	0	11	0
1	B	268	2164	1362	376	403	23	0	9	0
1	C	265	2125	1339	364	397	25	0	11	1
1	D	265	2126	1330	373	400	23	0	6	0

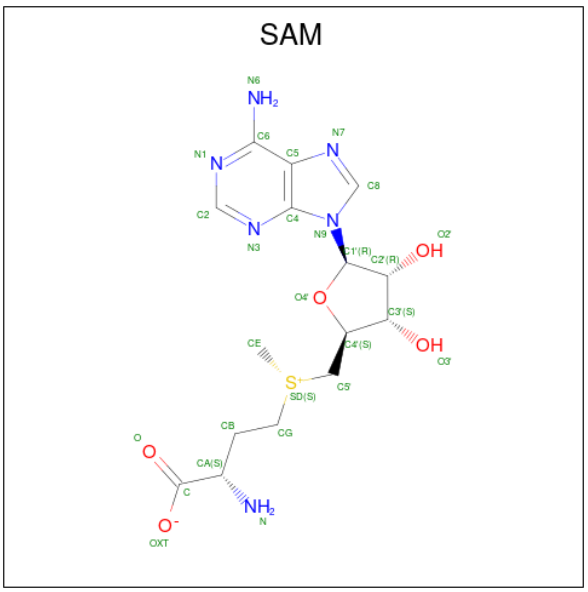
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	911	GLY	-	expression tag	UNP Q96KQ7
A	912	SER	-	expression tag	UNP Q96KQ7
B	911	GLY	-	expression tag	UNP Q96KQ7
B	912	SER	-	expression tag	UNP Q96KQ7
C	911	GLY	-	expression tag	UNP Q96KQ7
C	912	SER	-	expression tag	UNP Q96KQ7
D	911	GLY	-	expression tag	UNP Q96KQ7
D	912	SER	-	expression tag	UNP Q96KQ7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

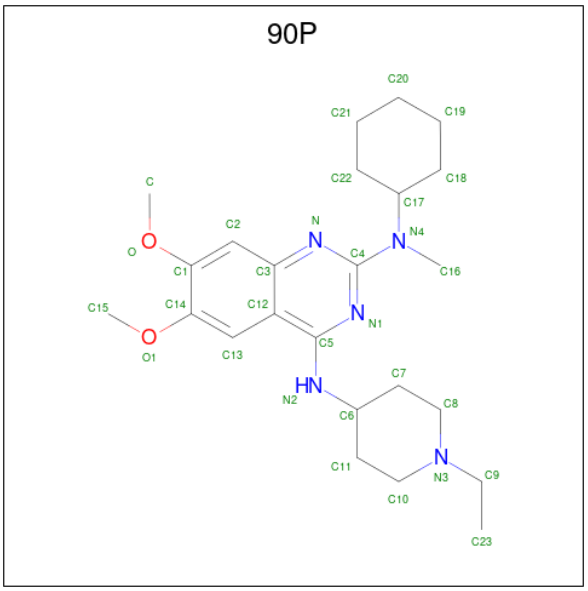
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	4	4	4	0	0
2	B	4	4	4	0	0
2	C	4	4	4	0	0
2	D	4	4	4	0	0

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



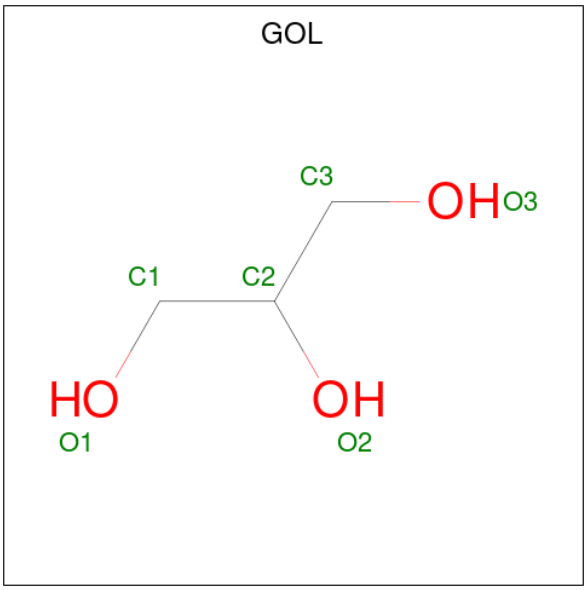
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	27	15	6	5	1	0	0
			Total	C	N	O	S		
3	B	1	27	15	6	5	1	0	0
			Total	C	N	O	S		
3	C	1	27	15	6	5	1	0	0
			Total	C	N	O	S		
3	D	1	27	15	6	5	1	0	0

- Molecule 4 is N 2 -cyclohexyl-N 4 -(1-ethylpiperidin-4-yl)-6,7-dimethoxy-N 2 -methylquinazoline-2,4-diamine (three-letter code: 90P) (formula: $C_{24}H_{37}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	27	20	5	2	0	0
			Total	C	N	O		
4	B	1	27	20	5	2	0	0
			Total	C	N	O		
4	C	1	32	24	6	2	0	1
			Total	C	N	O		
4	D	1	32	24	6	2	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	X			
6	A	1	1	1		0	0
			Total	X			
6	B	2	2	2		0	0
			Total	X			
6	C	1	1	1		0	0

- Molecule 7 is water.

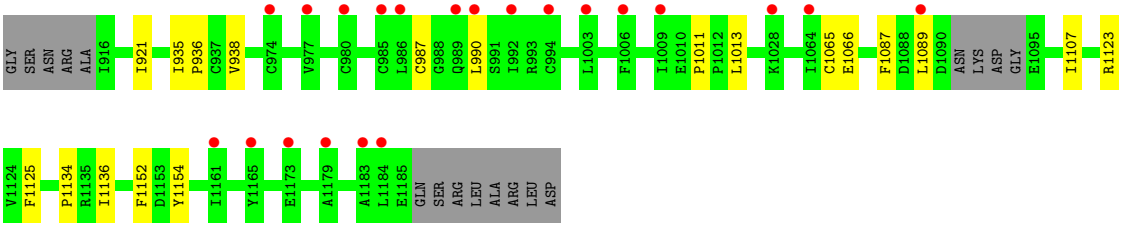
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
7	A	143	143	143		0	0
			Total	O			
7	B	187	188	188		0	1
			Total	O			
7	C	186	189	189		0	3
			Total	O			
7	D	184	184	184		0	0

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.

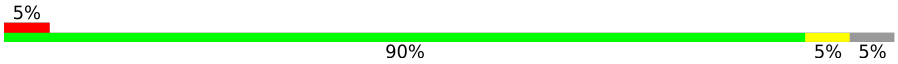
• Molecule 1: Histone-lysine N-methyltransferase EHMT2

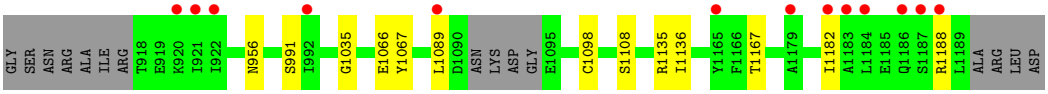
Chain A:



• Molecule 1: Histone-lysine N-methyltransferase EHMT2

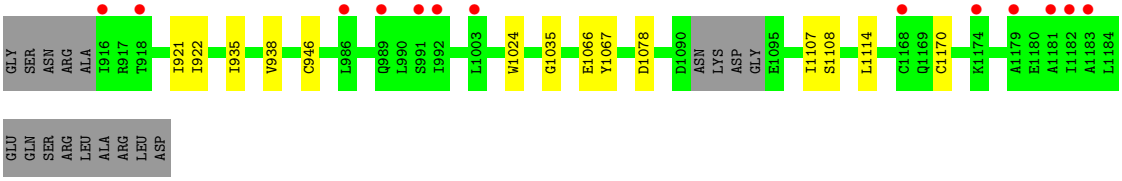
Chain B:





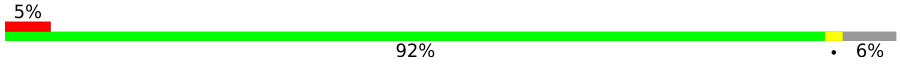
• Molecule 1: Histone-lysine N-methyltransferase EHMT2

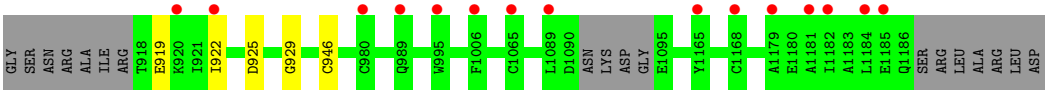
Chain C:



• Molecule 1: Histone-lysine N-methyltransferase EHMT2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.61Å 77.51Å 134.79Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	25.48 – 1.74 43.02 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.48-1.74) 99.3 (43.02-1.74)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 1.74Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.234 , 0.275 0.228 , 0.270	Depositor DCC
R_{free} test set	1191 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9547	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 51.53 % 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 5.5352e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: UNX, ZN, 90P, GOL, SAM

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	0.49	0/2203	0.60	0/2987
1	B	0.52	0/2230	0.62	0/3018
1	C	0.52	0/2198	0.61	0/2977
1	D	0.55	0/2177	0.62	0/2948
All	All	0.52	0/8808	0.61	0/11930

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	2128	0	1987	21	0
1	B	2164	0	2055	20	0
1	C	2125	0	1986	13	0
1	D	2126	0	1973	4	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

Continued on next page...

Continued from previous page...

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	1	0
4	B	27	0	0	1	0
4	C	32	0	0	0	0
4	D	32	0	0	0	0
5	A	18	0	24	12	0
5	B	18	0	24	15	0
5	C	6	0	8	5	0
5	D	12	0	16	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	A	143	0	0	0	0
7	B	188	0	0	2	0
7	C	189	0	0	0	0
7	D	184	0	0	0	0
All	All	9547	0	8161	60	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 (60) 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:935:ILE:HG21	1:C:1107[B]:ILE:HD12	1.38	1.02
1:B:956:ASN:HD22	5:B:1509:GOL:H11	1.23	0.99
1:B:956:ASN:ND2	5:B:1509:GOL:H11	1.80	0.95
1:B:1089:LEU:HD22	1:B:1136[B]:ILE:HD11	1.55	0.86
1:A:1087:PHE:HA	5:A:1509:GOL:H31	1.59	0.84
5:B:1507:GOL:H2	7:B:1638:HOH:O	1.80	0.81
1:B:956:ASN:HD22	5:B:1509:GOL:C1	1.93	0.81
1:B:1098:CYS:SG	4:B:1506:90P:C22	2.71	0.79
1:C:1066:GLU:N	5:C:1507:GOL:H31	1.96	0.79
1:A:1152:PHE:HE2	5:A:1509:GOL:H11	1.47	0.79
1:C:921:ILE:HD13	1:C:938:VAL:HG12	1.63	0.78
1:B:1135:ARG:HD2	5:B:1509:GOL:H31	1.71	0.72
1:C:1066:GLU:H	5:C:1507:GOL:H31	1.56	0.67
1:A:1089[B]:LEU:HD22	1:A:1136[B]:ILE:HD11	1.76	0.66
1:B:1135:ARG:CG	5:B:1509:GOL:H12	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1135:ARG:HG2	5:B:1509:GOL:H12	1.79	0.65
1:A:935:ILE:HG21	1:A:1107[B]:ILE:HD12	1.79	0.64
1:A:1011:PRO:HB2	1:A:1123[B]:ARG:HH22	1.63	0.63
1:A:1152:PHE:HE2	5:A:1509:GOL:C1	2.11	0.63
1:C:1066:GLU:H	5:C:1507:GOL:C3	2.11	0.62
5:B:1507:GOL:H31	7:B:1648:HOH:O	1.99	0.62
1:A:1123[B]:ARG:CZ	1:A:1123[B]:ARG:H	2.13	0.61
1:C:922[B]:ILE:HG23	1:C:946:CYS:HB2	1.84	0.60
1:B:1089:LEU:CD2	1:B:1136[B]:ILE:HD11	2.32	0.59
1:C:1066:GLU:HB2	5:C:1507:GOL:H11	1.85	0.58
1:A:1066:GLU:N	5:A:1507:GOL:H31	2.18	0.58
1:D:929:GLY:HA2	5:D:1507:GOL:H32	1.85	0.57
1:B:1067:TYR:HA	1:B:1108[B]:SER:OG	2.05	0.57
1:B:956:ASN:ND2	5:B:1509:GOL:C1	2.57	0.55
1:C:935:ILE:CG2	1:C:1107[B]:ILE:HD12	2.26	0.55
1:A:1066:GLU:H	5:A:1507:GOL:C3	2.20	0.54
1:B:1066:GLU:HB3	5:B:1507:GOL:H12	1.90	0.54
1:A:1065:CYS:HA	5:A:1507:GOL:H32	1.89	0.54
1:A:921:ILE:HD12	1:A:938:VAL:HG12	1.89	0.54
1:A:1152:PHE:CE2	5:A:1509:GOL:H11	2.37	0.53
1:C:1035:GLY:HA2	5:C:1507:GOL:O2	2.10	0.52
1:B:1066:GLU:HB2	5:B:1507:GOL:H11	1.91	0.50
1:A:1123[B]:ARG:HB3	1:A:1134:PRO:HB2	1.94	0.50
1:B:1135:ARG:HG3	5:B:1509:GOL:H12	1.93	0.50
1:B:1035:GLY:HA2	5:B:1507:GOL:O2	2.12	0.49
1:A:1089[B]:LEU:CD2	1:A:1136[B]:ILE:HD11	2.40	0.48
1:C:1067:TYR:HA	1:C:1108[B]:SER:OG	2.13	0.48
1:A:936:PRO:HB2	5:A:1508:GOL:H32	1.95	0.48
1:A:1013:LEU:HD22	1:A:1125:PHE:HE2	1.80	0.46
1:C:921:ILE:HD13	1:C:938:VAL:CG1	2.39	0.46
1:A:1066:GLU:H	5:A:1507:GOL:H31	1.77	0.45
1:D:922[A]:ILE:HG22	1:D:946:CYS:HB2	1.97	0.45
1:A:1154:TYR:HA	5:A:1509:GOL:H12	2.00	0.44
1:B:1066:GLU:CB	5:B:1507:GOL:C1	2.96	0.44
1:A:921:ILE:HD12	5:A:1508:GOL:H31	1.99	0.43
4:A:1506:90P:C	5:A:1509:GOL:H2	2.48	0.43
1:C:1024:TRP:CH2	1:D:925:ASP:HB3	2.54	0.42
1:B:1089:LEU:HD22	1:B:1136[B]:ILE:CD1	2.39	0.42
1:A:987:CYS:HA	1:A:990:LEU:HD12	2.02	0.42
1:D:922[A]:ILE:CG2	1:D:946:CYS:HB2	2.50	0.41
1:C:1114:LEU:HD23	1:C:1170:CYS:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1066:GLU:CB	5:B:1507:GOL:H11	2.50	0.41
1:B:1167:THR:HG22	1:B:1182:ILE:CD1	2.50	0.41

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	273/283 (96%)	264 (97%)	9 (3%)	0	100	100
1	B	273/283 (96%)	263 (96%)	10 (4%)	0	100	100
1	C	272/283 (96%)	262 (96%)	10 (4%)	0	100	100
1	D	267/283 (94%)	258 (97%)	9 (3%)	0	100	100
All	All	1085/1132 (96%)	1047 (96%)	38 (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	226/253 (89%)	226 (100%)	0	100	100
1	B	236/253 (93%)	233 (99%)	3 (1%)	69	52
1	C	228/253 (90%)	227 (100%)	1 (0%)	91	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	228/253 (90%)	227 (100%)	1 (0%)	91 86
All	All	918/1012 (91%)	913 (100%)	5 (0%)	88 83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	991[A]	SER
1	B	991[B]	SER
1	B	1188	ARG
1	C	1078	ASP
1	D	919	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 39 ligands modelled in this entry, 16 are monoatomic and 4 are unknown - leaving 19 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	$\#\|Z\| > 2$
5	GOL	A	1508	-	5,5,5	0.11	0	5,5,5	0.32	0
5	GOL	B	1507	-	5,5,5	0.36	0	5,5,5	0.62	0
5	GOL	B	1509	-	5,5,5	0.38	0	5,5,5	0.55	0
5	GOL	C	1507	-	5,5,5	0.42	0	5,5,5	0.57	0
4	90P	C	1506[B]	-	27,29,34	0.45	0	37,41,47	1.17	2 (5%)
5	GOL	A	1507	-	5,5,5	0.12	0	5,5,5	0.59	0
5	GOL	D	1508	-	5,5,5	0.04	0	5,5,5	0.11	0
4	90P	B	1506	-	27,29,34	0.44	0	37,41,47	0.74	1 (2%)
4	90P	D	1506[A]	-	27,29,34	0.44	0	37,41,47	0.79	1 (2%)
5	GOL	D	1507	-	5,5,5	0.13	0	5,5,5	0.29	0
5	GOL	B	1508	-	5,5,5	0.09	0	5,5,5	0.29	0
4	90P	D	1506[B]	-	27,29,34	0.43	0	37,41,47	1.23	2 (5%)
3	SAM	A	1505	-	24,29,29	0.76	0	23,42,42	0.94	1 (4%)
3	SAM	B	1505	-	24,29,29	0.87	1 (4%)	23,42,42	0.90	1 (4%)
4	90P	C	1506[A]	-	27,29,34	0.45	0	37,41,47	0.90	2 (5%)
5	GOL	A	1509	-	5,5,5	0.24	0	5,5,5	0.60	0
4	90P	A	1506	-	27,29,34	0.39	0	37,41,47	1.43	3 (8%)
3	SAM	C	1505	-	24,29,29	0.85	0	23,42,42	0.86	1 (4%)
3	SAM	D	1505	-	24,29,29	0.86	0	23,42,42	0.92	1 (4%)

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
5	GOL	A	1508	-	-	0/4/4/4	-
5	GOL	B	1507	-	-	0/4/4/4	-
5	GOL	B	1509	-	-	0/4/4/4	-
5	GOL	C	1507	-	-	2/4/4/4	-
4	90P	C	1506[B]	-	-	3/16/26/36	0/3/3/4
5	GOL	A	1507	-	-	2/4/4/4	-
5	GOL	D	1508	-	-	0/4/4/4	-
4	90P	B	1506	-	-	0/16/26/36	0/3/3/4
4	90P	D	1506[A]	-	-	3/16/26/36	0/3/3/4
5	GOL	D	1507	-	-	2/4/4/4	-
5	GOL	B	1508	-	-	4/4/4/4	-
4	90P	D	1506[B]	-	-	5/16/26/36	0/3/3/4
3	SAM	A	1505	-	-	2/12/33/33	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	B	1505	-	-	2/12/33/33	0/3/3/3
4	90P	C	1506[A]	-	-	2/16/26/36	0/3/3/4
5	GOL	A	1509	-	-	0/4/4/4	-
4	90P	A	1506	-	-	2/16/26/36	0/3/3/4
3	SAM	C	1505	-	-	3/12/33/33	0/3/3/3
3	SAM	D	1505	-	-	2/12/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1505	SAM	CG-CB	2.14	1.58	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1506	90P	C22-C17-N4	6.59	121.04	111.45
4	D	1506[B]	90P	C22-C17-N4	5.58	119.57	111.45
4	C	1506[B]	90P	C22-C17-N4	4.76	118.38	111.45
4	C	1506[B]	90P	C18-C17-N4	4.67	118.25	111.45
4	D	1506[B]	90P	C18-C17-N4	4.52	118.02	111.45
4	A	1506	90P	C18-C17-N4	4.25	117.64	111.45
4	D	1506[A]	90P	C22-C17-N4	4.03	117.31	111.45
4	C	1506[A]	90P	C22-C17-N4	3.94	117.18	111.45
4	B	1506	90P	C18-C17-N4	3.70	116.83	111.45
4	A	1506	90P	C4-N4-C17	-3.35	113.12	120.34
4	C	1506[A]	90P	C18-C17-N4	2.75	115.45	111.45
3	D	1505	SAM	C5-C6-N6	2.70	124.45	120.35
3	A	1505	SAM	C5-C6-N6	2.44	124.07	120.35
3	B	1505	SAM	C5-C6-N6	2.43	124.05	120.35
3	C	1505	SAM	C5-C6-N6	2.26	123.79	120.35

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1505	SAM	CB-CG-SD-CE
3	A	1505	SAM	CB-CG-SD-C5'
3	B	1505	SAM	CB-CG-SD-CE
3	B	1505	SAM	CB-CG-SD-C5'
3	C	1505	SAM	CB-CG-SD-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1505	SAM	CB-CG-SD-C5'
3	D	1505	SAM	CB-CG-SD-CE
3	D	1505	SAM	CB-CG-SD-C5'
4	A	1506	90P	N1-C4-N4-C17
4	A	1506	90P	N-C4-N4-C17
4	C	1506[A]	90P	N1-C4-N4-C17
4	C	1506[A]	90P	N-C4-N4-C17
4	C	1506[B]	90P	N1-C4-N4-C17
4	C	1506[B]	90P	N-C4-N4-C17
4	D	1506[A]	90P	C18-C17-N4-C4
4	D	1506[A]	90P	C22-C17-N4-C16
4	D	1506[A]	90P	C18-C17-N4-C16
4	D	1506[B]	90P	N1-C4-N4-C17
4	D	1506[B]	90P	N-C4-N4-C16
4	D	1506[B]	90P	N-C4-N4-C17
5	C	1507	GOL	C1-C2-C3-O3
4	D	1506[B]	90P	N1-C4-N4-C16
5	A	1507	GOL	O1-C1-C2-C3
5	B	1508	GOL	O1-C1-C2-C3
5	B	1508	GOL	C1-C2-C3-O3
5	D	1507	GOL	O1-C1-C2-C3
5	A	1507	GOL	O1-C1-C2-O2
5	C	1507	GOL	O2-C2-C3-O3
4	C	1506[B]	90P	N-C4-N4-C16
4	D	1506[B]	90P	C22-C17-N4-C16
5	B	1508	GOL	O1-C1-C2-O2
5	D	1507	GOL	O1-C1-C2-O2
5	B	1508	GOL	O2-C2-C3-O3
3	C	1505	SAM	O4'-C4'-C5'-SD

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1508	GOL	2	0
5	B	1507	GOL	7	0
5	B	1509	GOL	8	0
5	C	1507	GOL	5	0
5	A	1507	GOL	4	0
4	B	1506	90P	1	0
5	D	1507	GOL	1	0
5	A	1509	GOL	6	0

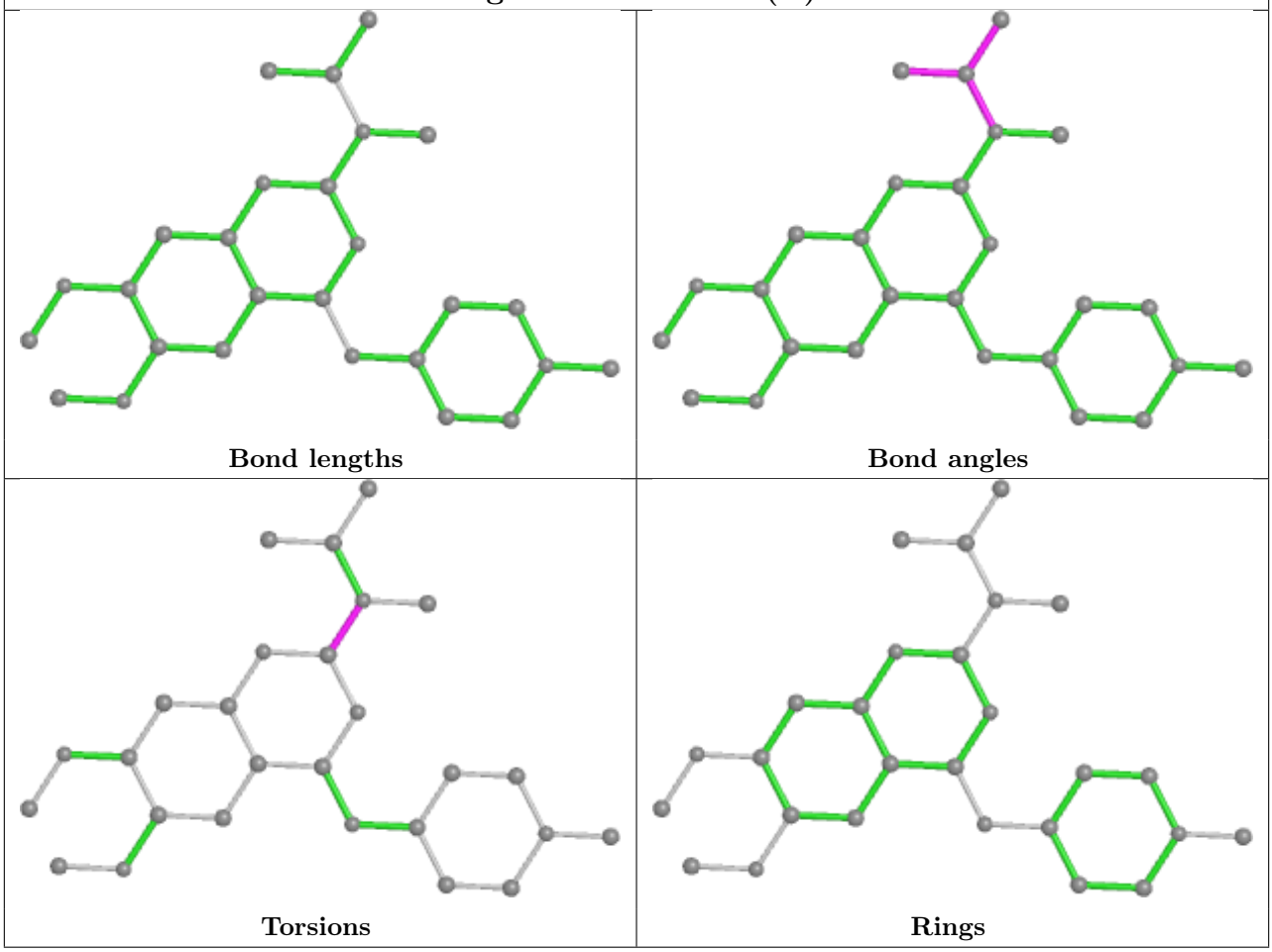
Continued on next page...

Continued from previous page...

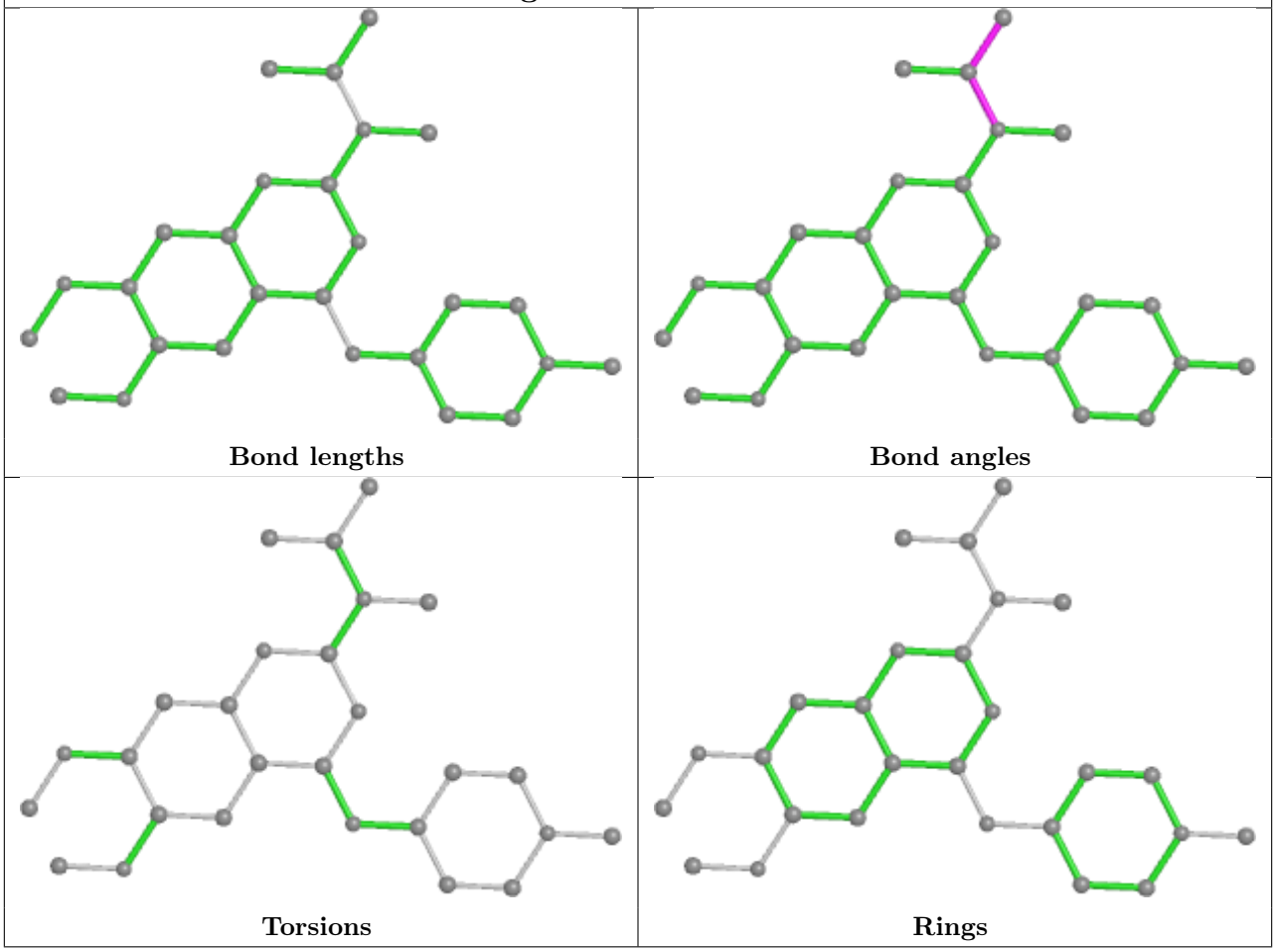
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1506	90P	1	0

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 then 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.

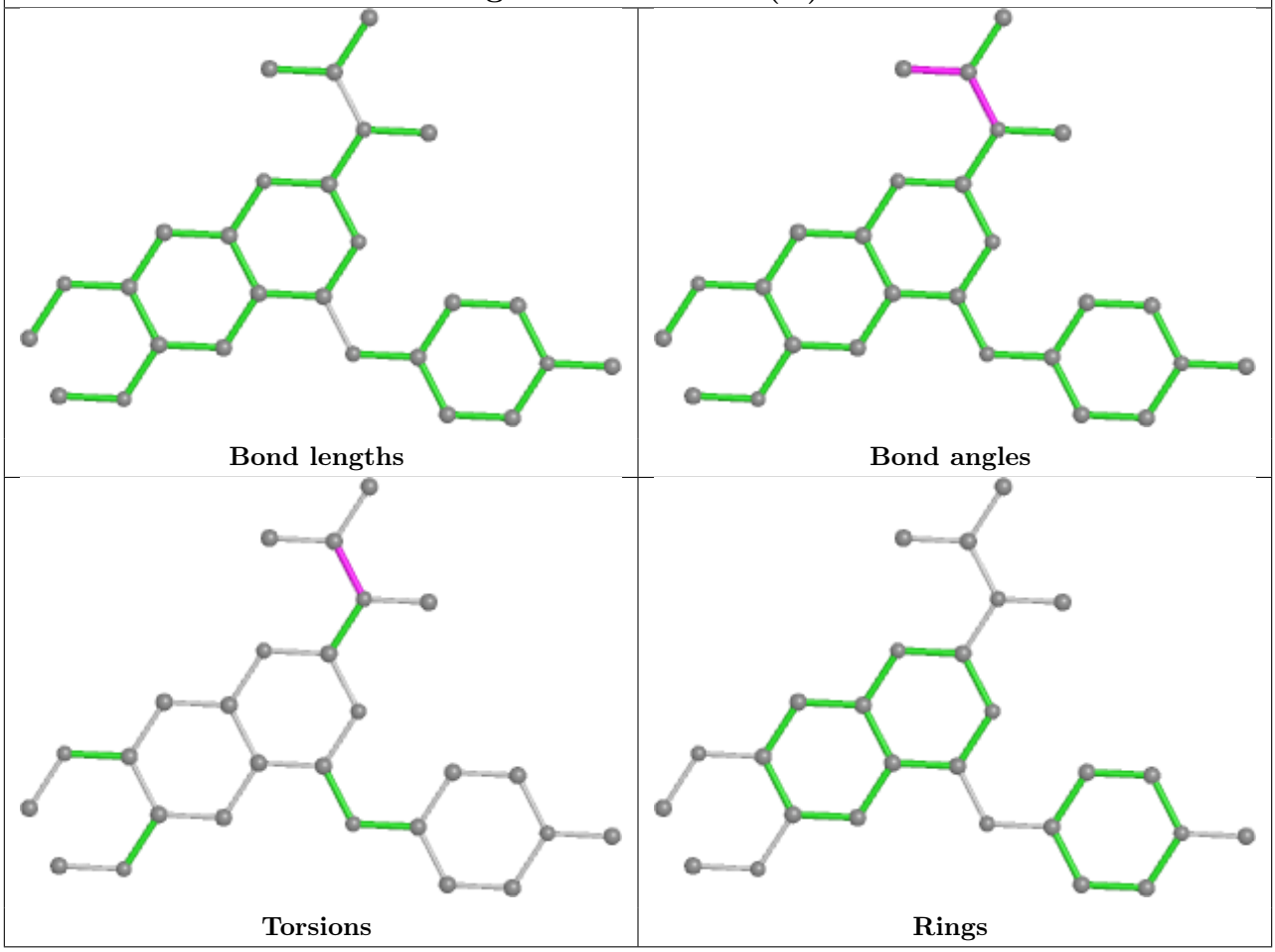
Ligand 90P C 1506 (B)



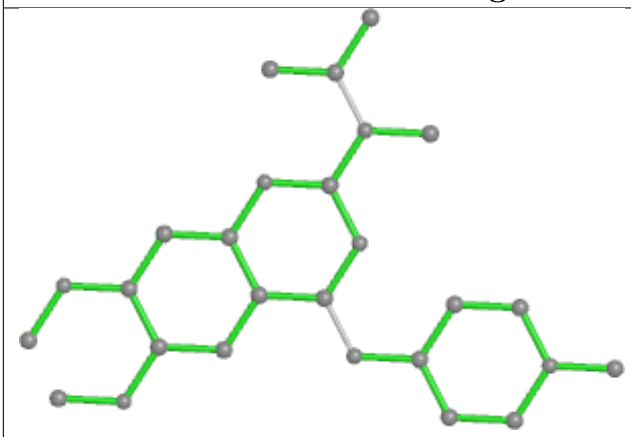
Ligand 90P B 1506



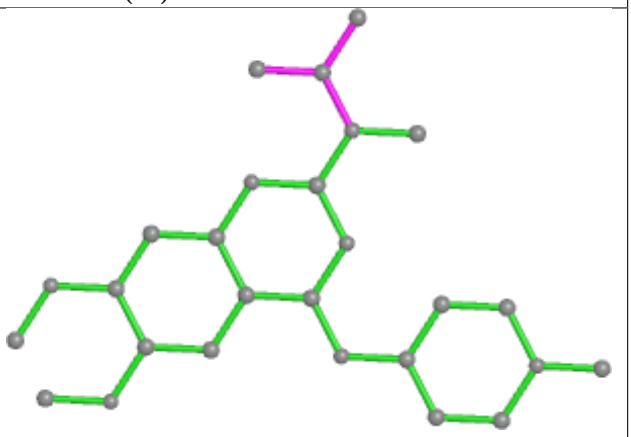
Ligand 90P D 1506 (A)



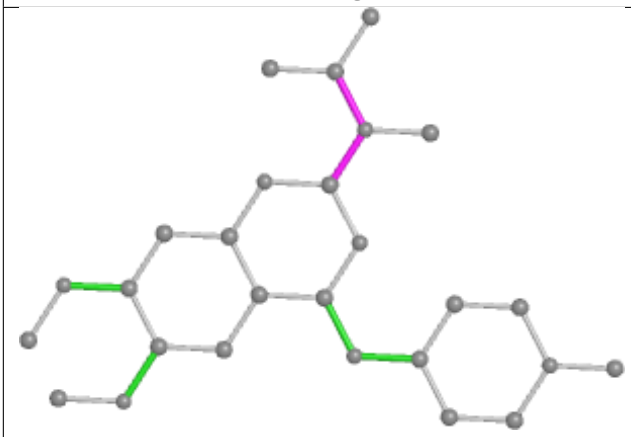
Ligand 90P D 1506 (B)



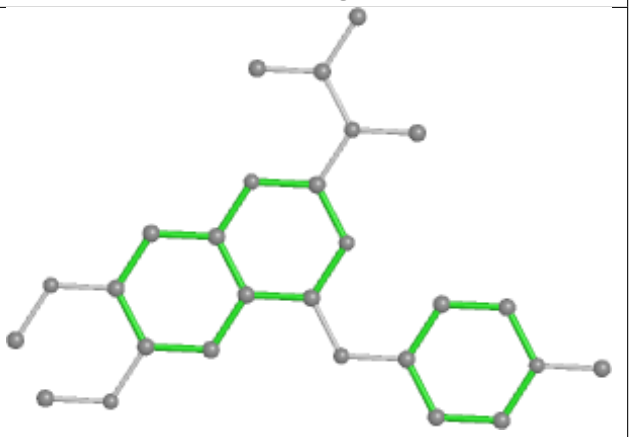
Bond lengths



Bond angles

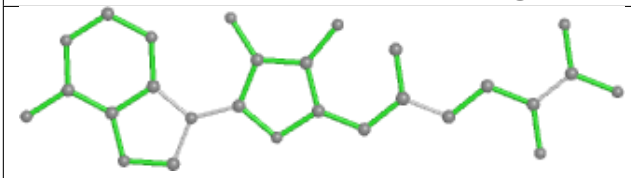


Torsions

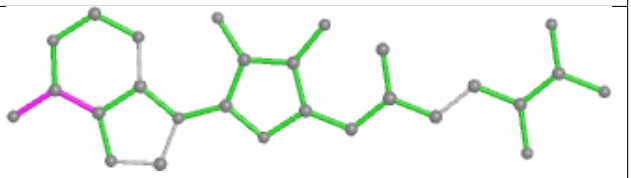


Rings

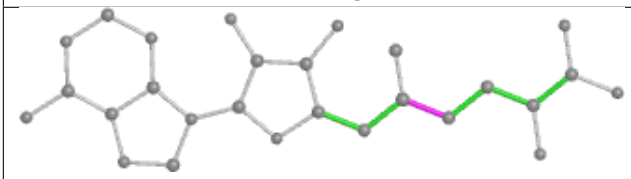
Ligand SAM A 1505



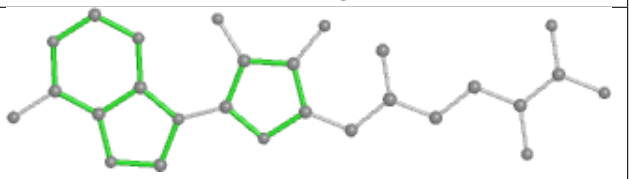
Bond lengths



Bond angles

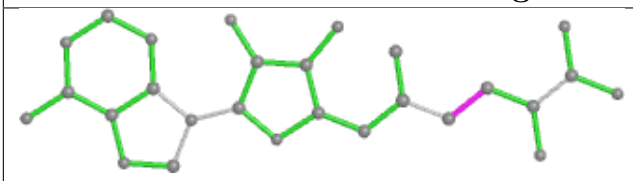


Torsions

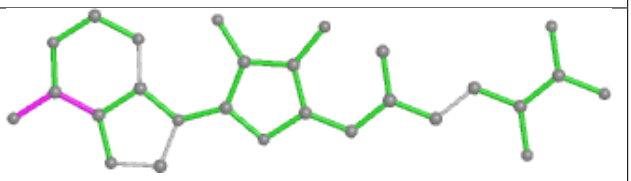


Rings

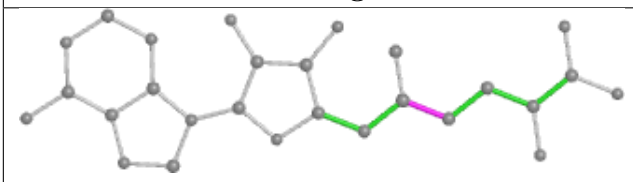
Ligand SAM B 1505



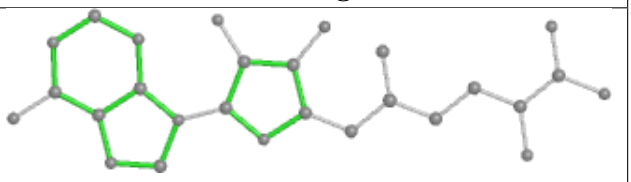
Bond lengths



Bond angles

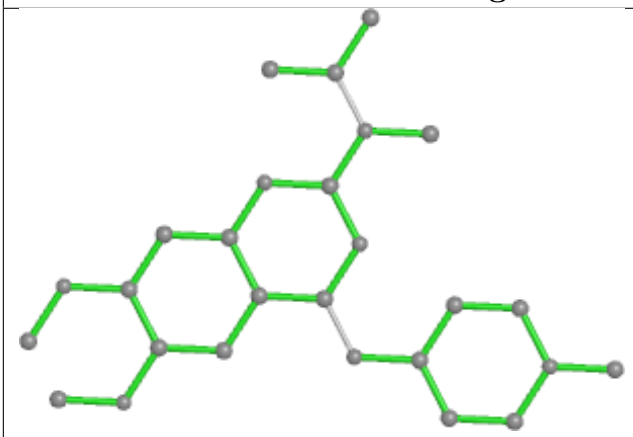


Torsions

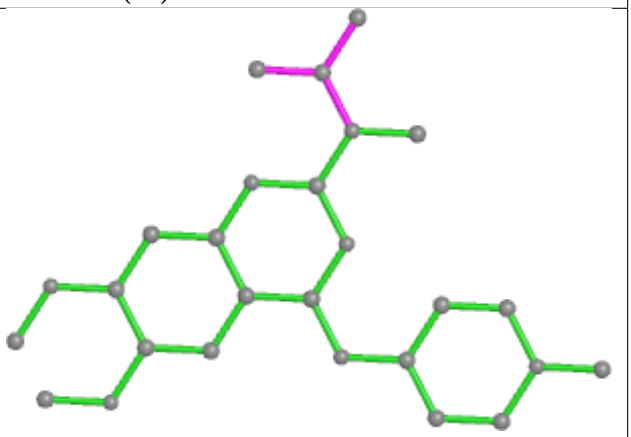


Rings

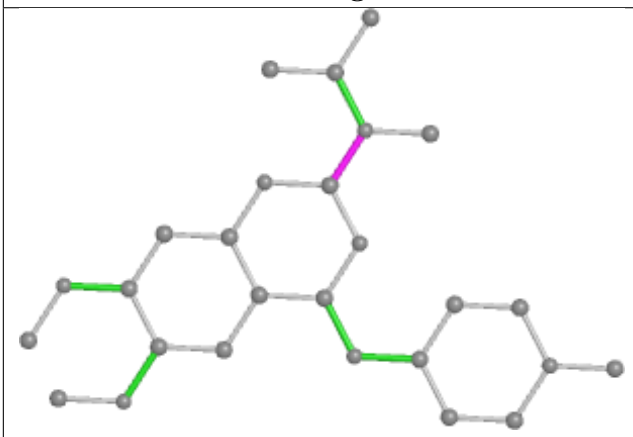
Ligand 90P C 1506 (A)



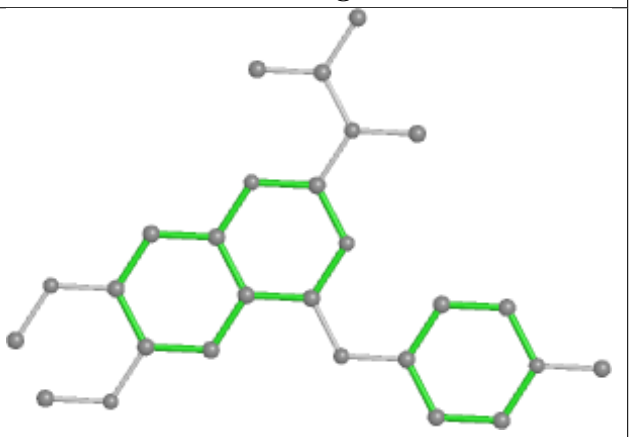
Bond lengths



Bond angles

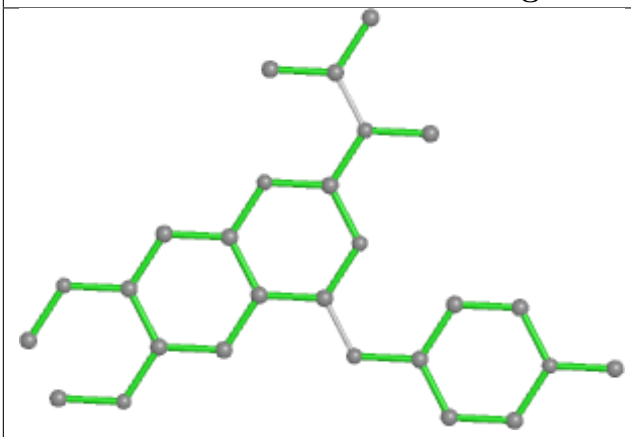


Torsions

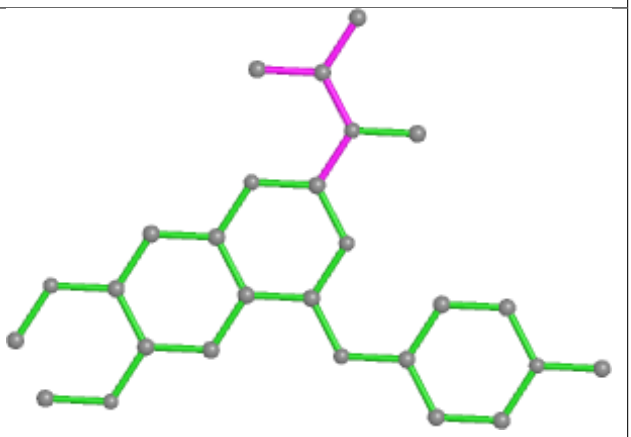


Rings

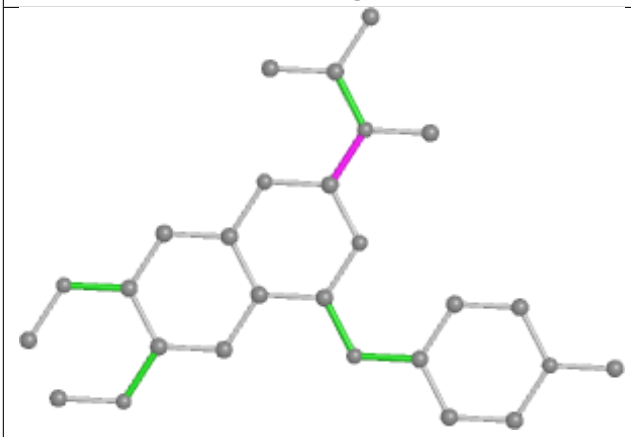
Ligand 90P A 1506



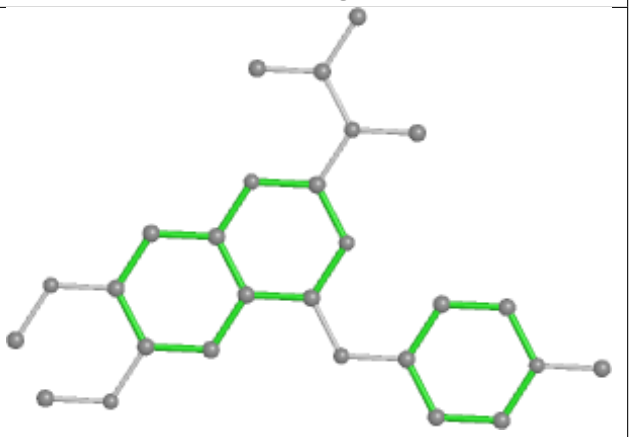
Bond lengths



Bond angles

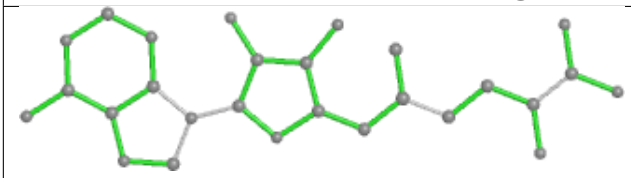


Torsions

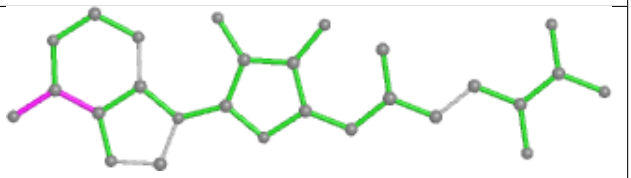


Rings

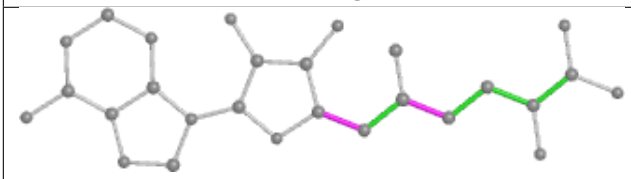
Ligand SAM C 1505



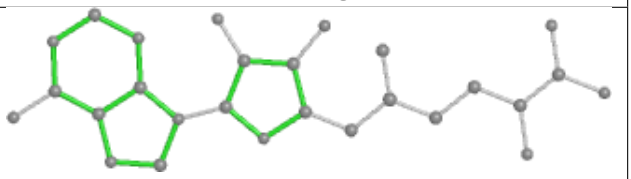
Bond lengths



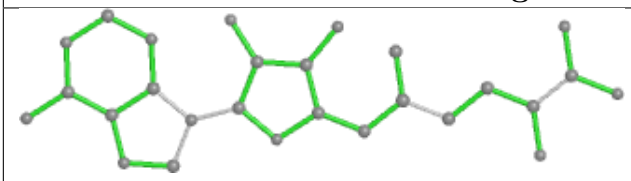
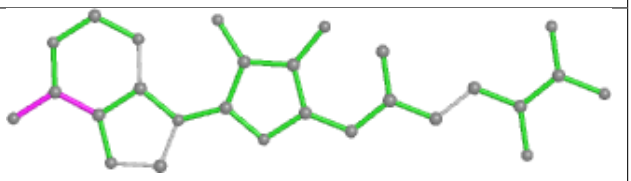
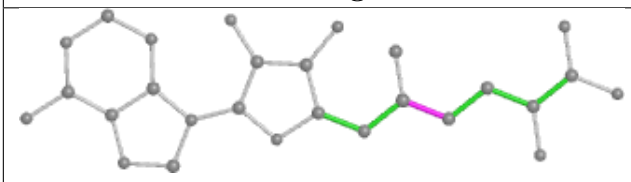
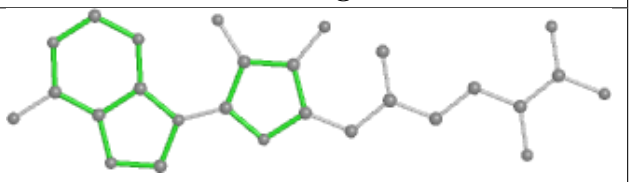
Bond angles



Torsions



Rings

Ligand SAM D 1505	
 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 (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, 95th 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^2)	Q<0.9
1	A	266/283 (93%)	0.72	21 (7%)	12	16	19, 33, 55, 83	0
1	B	268/283 (94%)	0.38	13 (4%)	29	34	15, 25, 45, 76	0
1	C	265/283 (93%)	0.43	13 (4%)	29	34	15, 24, 43, 80	0
1	D	265/283 (93%)	0.44	15 (5%)	23	28	14, 24, 44, 83	0
All	All	1064/1132 (93%)	0.49	62 (5%)	23	27	14, 27, 50, 83	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1184	LEU	6.1
1	C	1182	ILE	5.7
1	A	986	LEU	5.1
1	B	1184	LEU	4.9
1	D	922[A]	ILE	4.8
1	A	1183	ALA	4.5
1	D	920	LYS	4.4
1	A	1003	LEU	4.4
1	D	1181	ALA	4.3
1	A	1009	ILE	4.1
1	D	1184	LEU	4.0
1	C	986	LEU	4.0
1	A	992	ILE	4.0
1	D	995	TRP	3.9
1	A	989	GLN	3.9
1	C	916	ILE	3.9
1	A	977	VAL	3.9
1	C	1003	LEU	3.6
1	A	1006	PHE	3.3
1	D	1006	PHE	3.3
1	B	1089	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1181	ALA	3.2
1	D	1185	GLU	3.2
1	A	1089[A]	LEU	3.0
1	B	1183	ALA	3.0
1	B	992	ILE	2.9
1	B	920	LYS	2.9
1	B	1179	ALA	2.9
1	A	974	CYS	2.8
1	C	1168	CYS	2.8
1	A	985	CYS	2.7
1	B	922	ILE	2.7
1	B	1165	TYR	2.7
1	A	1179	ALA	2.6
1	D	980	CYS	2.6
1	A	1165	TYR	2.6
1	C	1179	ALA	2.6
1	C	992	ILE	2.5
1	C	989	GLN	2.4
1	B	1187	SER	2.4
1	A	1064[A]	ILE	2.3
1	D	1182	ILE	2.3
1	C	1174	LYS	2.3
1	B	921	ILE	2.3
1	D	1165	TYR	2.3
1	D	1179	ALA	2.2
1	C	918	THR	2.2
1	B	1182	ILE	2.2
1	C	1183	ALA	2.2
1	D	1065	CYS	2.2
1	D	989	GLN	2.2
1	A	980	CYS	2.1
1	A	990	LEU	2.1
1	C	991	SER	2.1
1	A	1028	LYS	2.1
1	A	1173	GLU	2.1
1	A	994	CYS	2.1
1	D	1168	CYS	2.1
1	B	1186	GLN	2.0
1	A	1161	ILE	2.0
1	B	1188	ARG	2.0
1	D	1089	LEU	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, 95th 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^2)	Q<0.9
5	GOL	D	1508	6/6	0.65	0.29	47,50,52,55	0
5	GOL	B	1508	6/6	0.73	0.26	43,47,50,53	0
5	GOL	D	1507	6/6	0.77	0.17	36,40,43,44	0
5	GOL	B	1509	6/6	0.80	0.25	28,34,38,40	0
5	GOL	A	1509	6/6	0.81	0.22	29,33,34,39	0
5	GOL	A	1507	6/6	0.82	0.23	29,35,37,39	0
4	90P	B	1506	27/31	0.84	0.13	22,25,33,38	0
4	90P	A	1506	27/31	0.85	0.16	29,34,45,49	0
5	GOL	C	1507	6/6	0.87	0.19	22,29,30,34	0
4	90P	C	1506[A]	27/31	0.87	0.14	22,26,35,36	5
4	90P	C	1506[B]	27/31	0.87	0.14	21,26,34,36	5
6	UNX	A	1510	1/1	0.87	0.32	30,30,30,30	0
5	GOL	A	1508	6/6	0.88	0.23	36,39,40,41	0
5	GOL	B	1507	6/6	0.88	0.30	19,28,31,31	0
6	UNX	C	1508	1/1	0.88	0.60	30,30,30,30	0
4	90P	D	1506[B]	27/31	0.90	0.14	20,25,31,33	5
3	SAM	A	1505	27/27	0.90	0.11	24,31,33,34	0
4	90P	D	1506[A]	27/31	0.90	0.14	20,25,32,36	5
6	UNX	B	1511	1/1	0.92	0.33	30,30,30,30	0
6	UNX	B	1510	1/1	0.94	0.28	30,30,30,30	0
3	SAM	C	1505	27/27	0.94	0.10	19,23,25,27	0
3	SAM	D	1505	27/27	0.94	0.10	18,21,24,24	0
3	SAM	B	1505	27/27	0.95	0.09	16,19,24,26	0
2	ZN	A	1501	1/1	0.98	0.09	30,30,30,30	0
2	ZN	A	1503	1/1	0.99	0.05	36,36,36,36	0
2	ZN	A	1504	1/1	0.99	0.03	40,40,40,40	0
2	ZN	B	1501	1/1	0.99	0.10	18,18,18,18	0

Continued on next page...

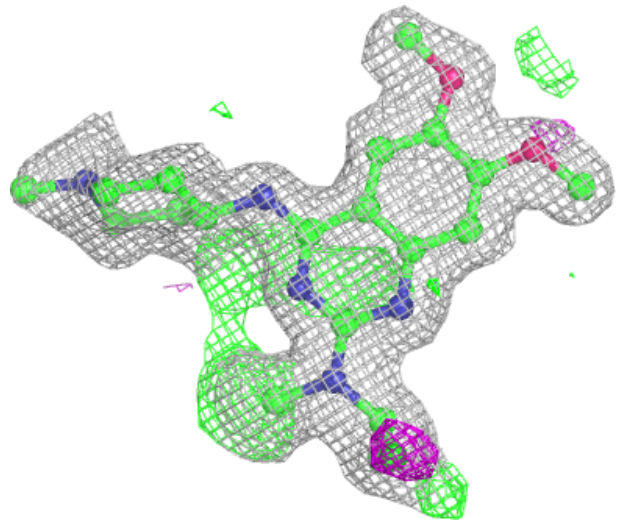
Continued from previous page...

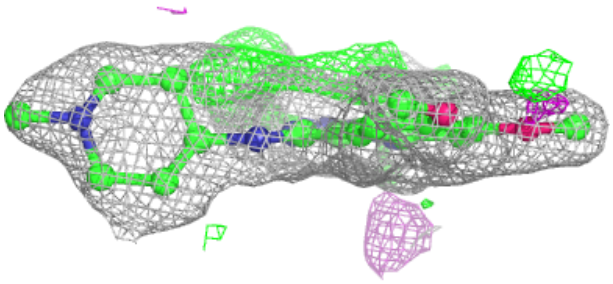
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	1504	1/1	0.99	0.07	24,24,24,24	0
2	ZN	C	1501	1/1	0.99	0.06	22,22,22,22	0
2	ZN	C	1502	1/1	0.99	0.08	22,22,22,22	0
2	ZN	C	1504	1/1	0.99	0.07	28,28,28,28	0
2	ZN	D	1501	1/1	0.99	0.09	19,19,19,19	0
2	ZN	D	1502	1/1	0.99	0.07	19,19,19,19	0
2	ZN	D	1504	1/1	0.99	0.06	27,27,27,27	0
2	ZN	A	1502	1/1	0.99	0.06	32,32,32,32	0
2	ZN	B	1503	1/1	1.00	0.08	19,19,19,19	0
2	ZN	B	1502	1/1	1.00	0.06	19,19,19,19	0
2	ZN	C	1503	1/1	1.00	0.04	24,24,24,24	0
2	ZN	D	1503	1/1	1.00	0.05	19,19,19,19	0

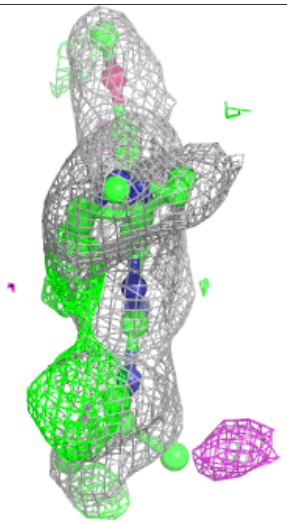
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 90P B 1506:

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

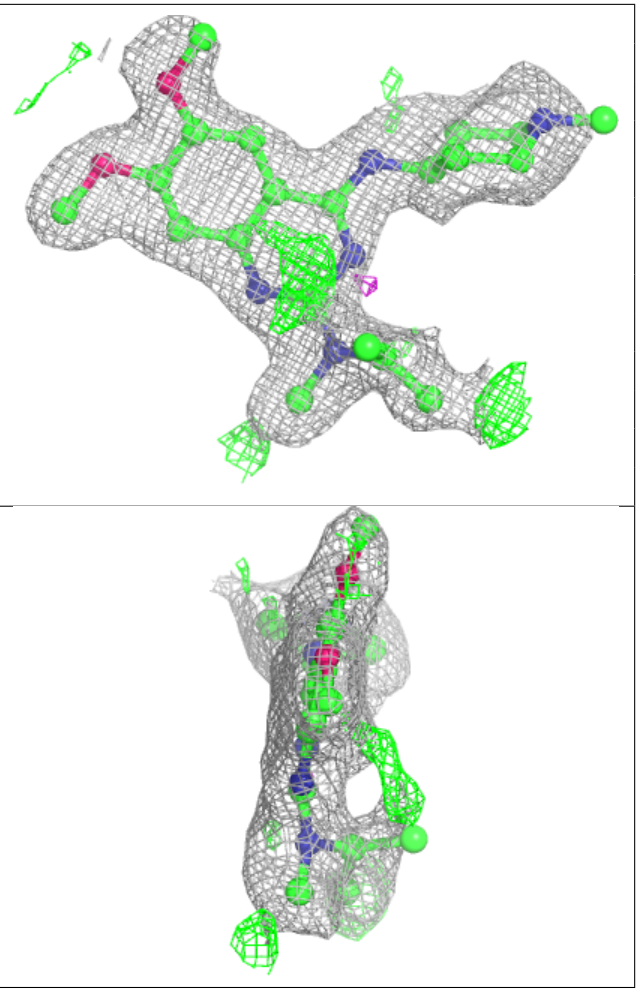


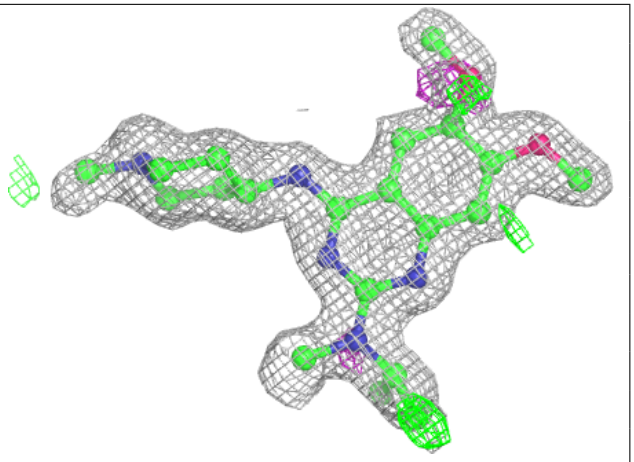
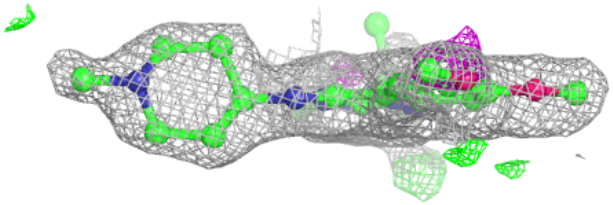
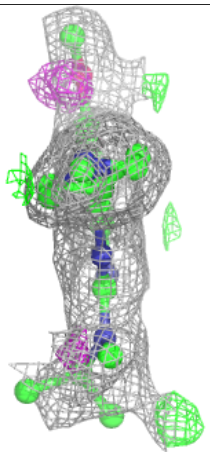


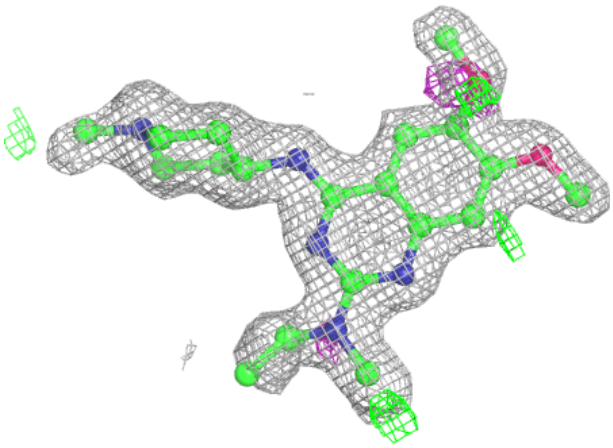
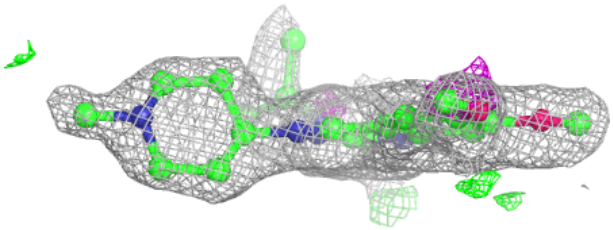
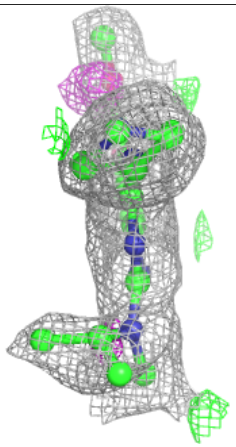


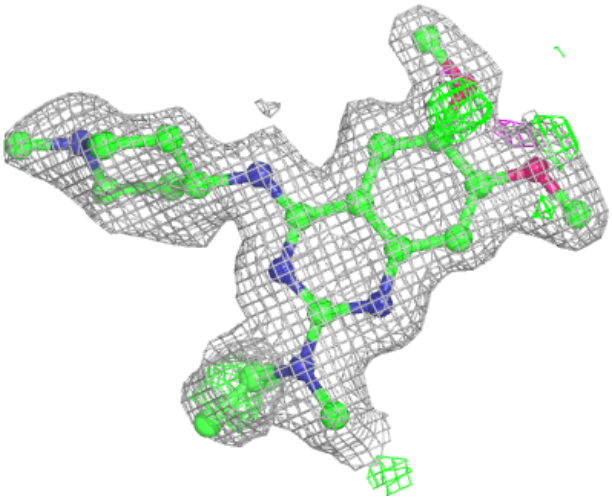
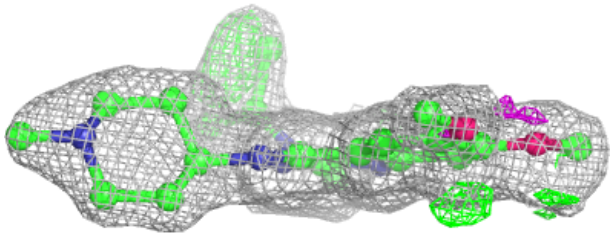
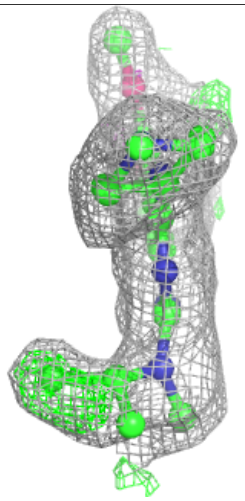
Electron density around 90P A 1506:

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



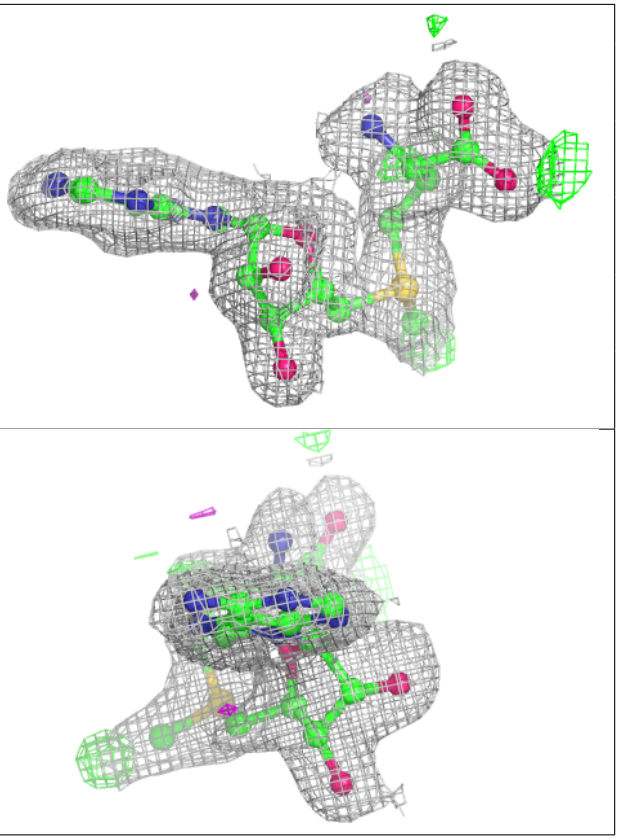
Electron density around 90P C 1506 (A): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

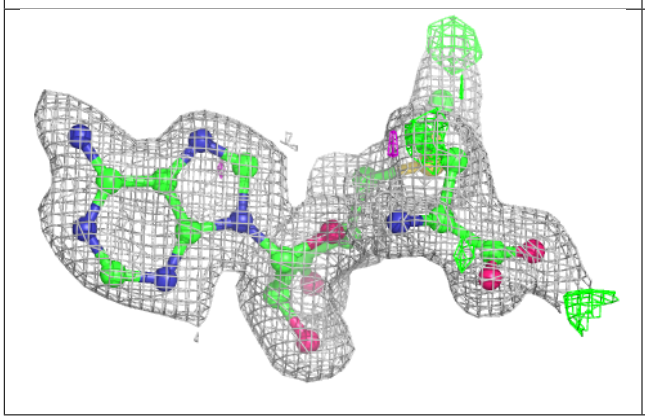
Electron density around 90P C 1506 (B): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

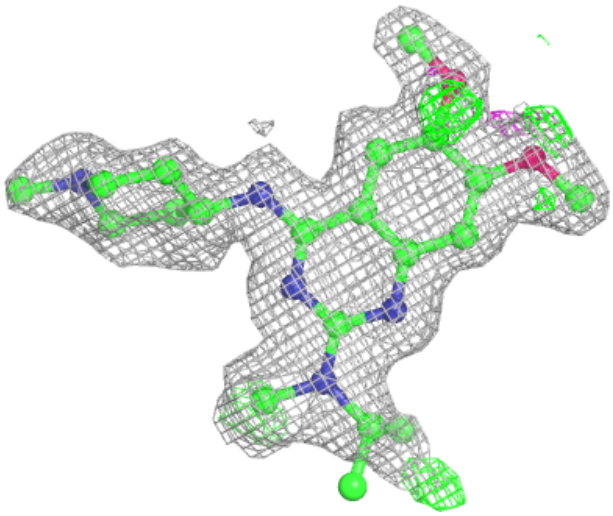
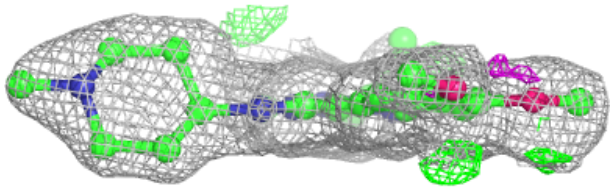
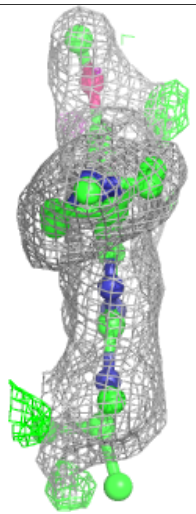
Electron density around 90P D 1506 (B): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around SAM A 1505:

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

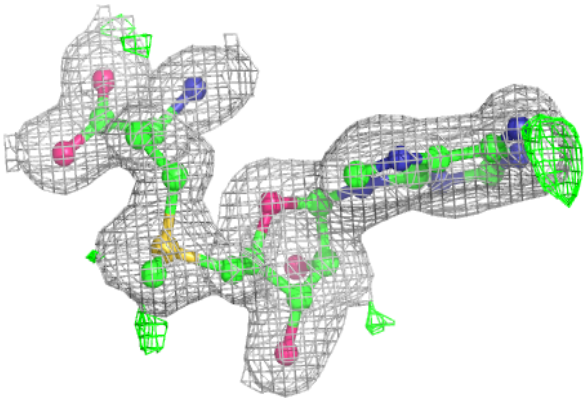


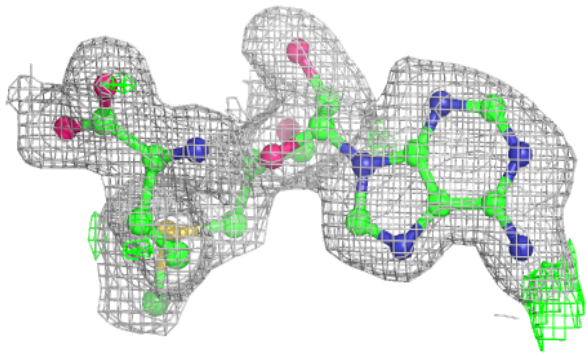


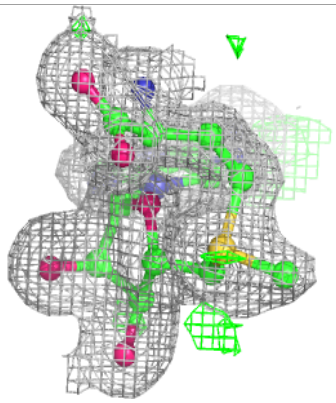
Electron density around 90P D 1506 (A): 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around SAM C 1505:

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

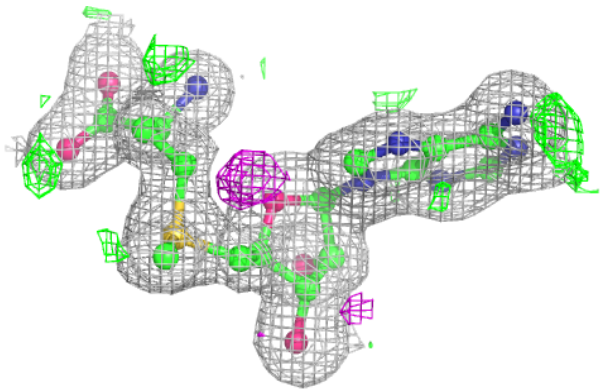


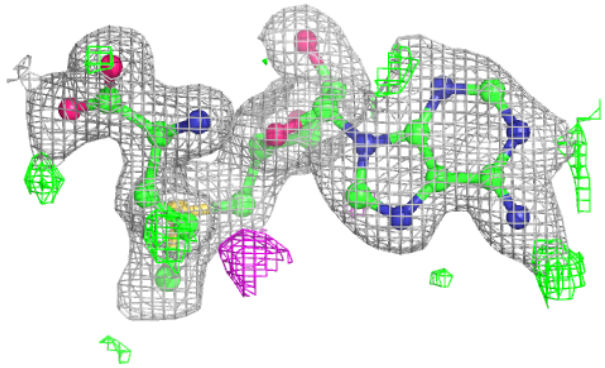


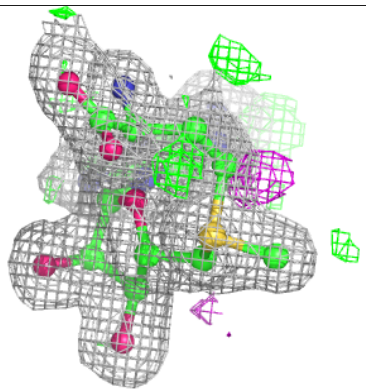


Electron density around SAM D 1505:

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

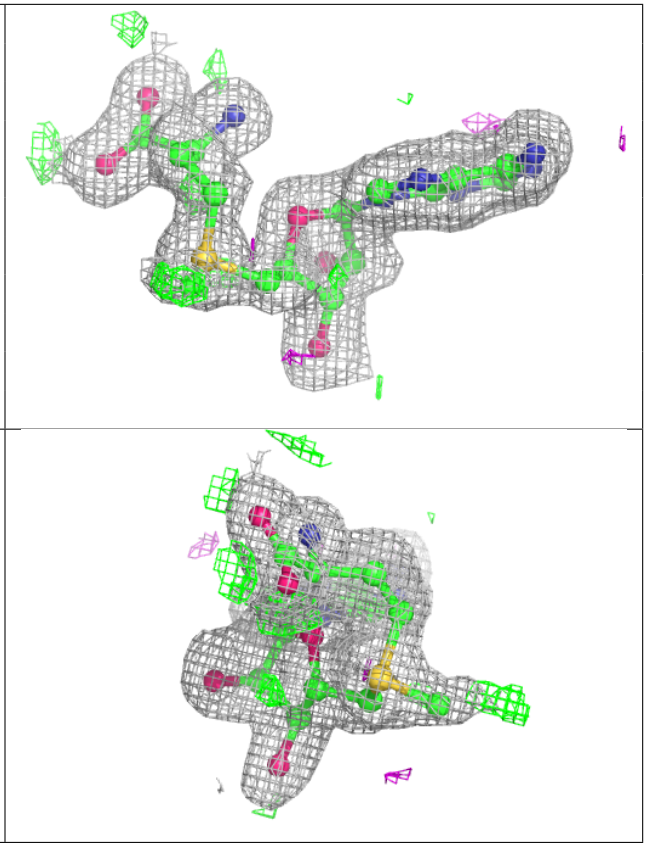






Electron density around SAM B 1505:

$2mF_o$-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.