



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 03:56 AM EDT

PDB ID : 7T7L
Title : Structure of human G9a SET-domain (EHMT2) in complex with covalent inhibitor (Compound 1)
Authors : Park, K.-S.; Kumar, P.
Deposited on : 2021-12-15
Resolution : 2.20 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 ⓘ 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 ⓘ](#)) 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

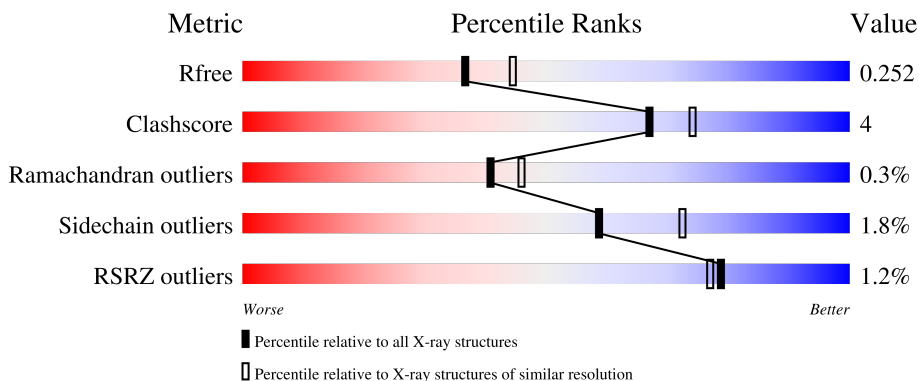
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	283	
1	B	283	
1	C	283	
1	D	283	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9210 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.

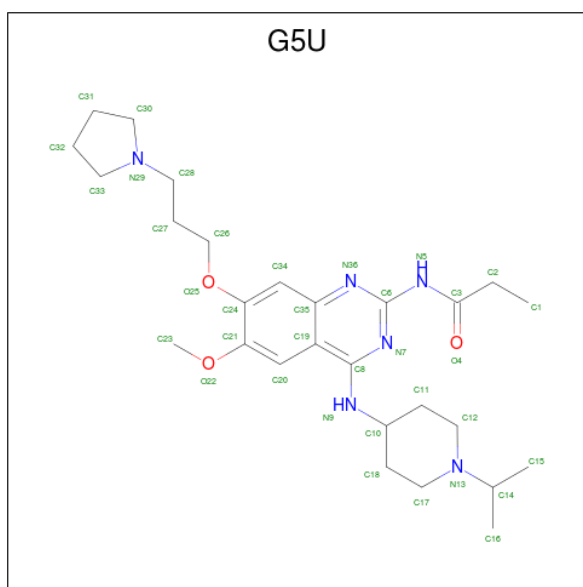
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2161	1350	379	409	23	0	4	0
1	B	264	2125	1327	369	405	24	0	2	0
1	C	266	2139	1336	371	409	23	0	1	0
1	D	269	2172	1354	381	414	23	0	1	0

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

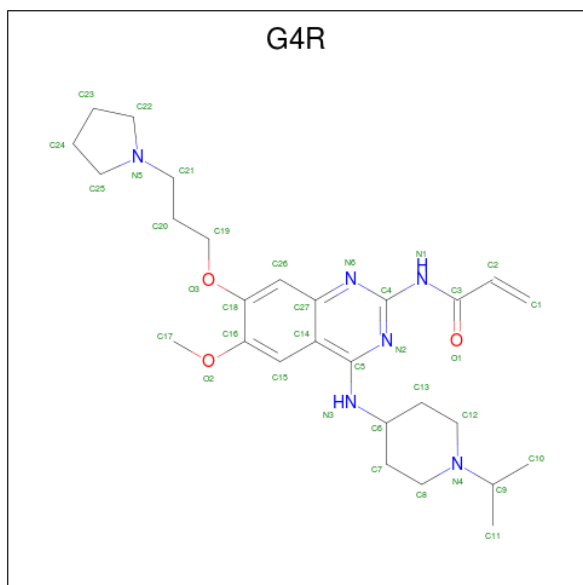
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	36	27	6	3	0	0
4	B	1	36	27	6	3	1	0
4	D	1	36	27	6	3	0	0

- Molecule 5 is N-(6-methoxy-4-{[1-(propan-2-yl)piperidin-4-yl]amino}-7-[3-(pyrrolidin-1-yl)propoxy]quinazolin-2-yl)prop-2-enamide (three-letter code: G4R) (formula: C₂₇H₄₀N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			36	27	6	3		

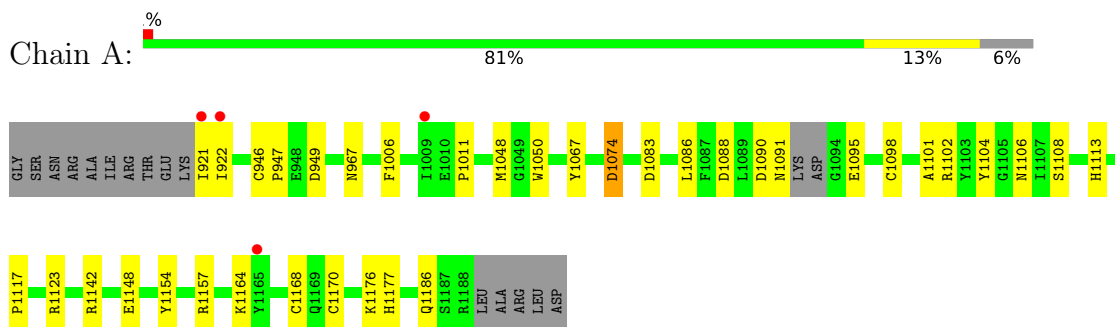
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	B	81	Total	O	0	0
			81	81		
6	C	77	Total	O	0	0
			77	77		
6	D	111	Total	O	0	0
			111	111		

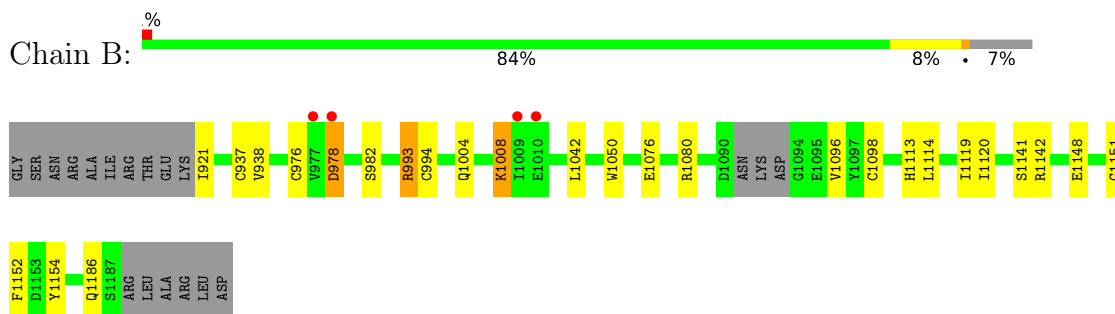
3 Residue-property plots [i](#)

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.

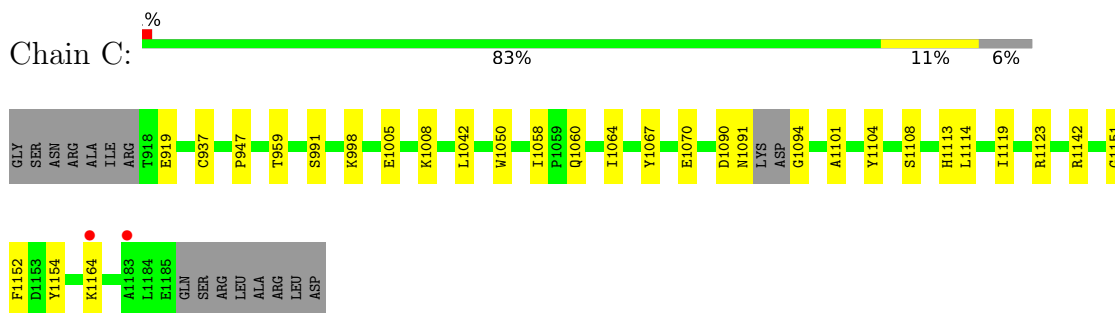
- Molecule 1: Histone-lysine N-methyltransferase EHMT2



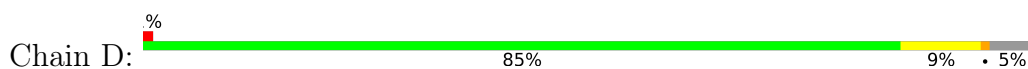
- Molecule 1: Histone-lysine N-methyltransferase EHMT2

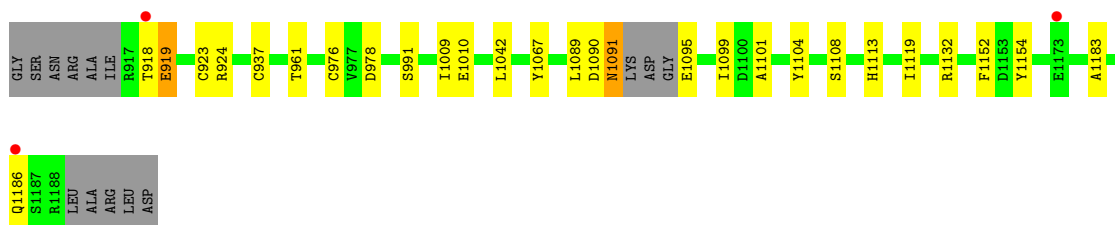


- Molecule 1: Histone-lysine N-methyltransferase EHMT2



- Molecule 1: Histone-lysine N-methyltransferase EHMT2





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.82Å 72.30Å 85.03Å 71.15° 86.17° 89.10°	Depositor
Resolution (Å)	68.42 – 2.20 68.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (68.42-2.20) 98.2 (68.42-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.204 , 0.251 0.206 , 0.252	Depositor DCC
R_{free} test set	3099 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtrriage
Anisotropy	0.863	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9210	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.23 % 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 4.8573e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: G4R, ZN, SAM, G5U

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	0.25	0/2218	0.44	0/2995
1	B	0.28	0/2176	0.44	0/2941
1	C	0.28	0/2187	0.43	0/2957
1	D	0.25	0/2220	0.44	0/3000
All	All	0.26	0/8801	0.44	0/11893

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	2161	0	2066	22	0
1	B	2125	0	2012	14	0
1	C	2139	0	2027	16	0
1	D	2172	0	2059	17	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	36	0	0	2	0
4	B	36	0	0	0	0
4	D	36	0	0	0	0
5	C	36	0	0	0	0
6	A	76	0	0	1	0
6	B	81	0	0	0	0
6	C	77	0	0	0	0
6	D	111	0	0	1	0
All	All	9210	0	8252	67	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 (67) 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:D:1091:ASN:O	1:D:1091:ASN:ND2	2.16	0.78
1:A:1090:ASP:O	1:A:1123:ARG:NH2	2.18	0.71
1:B:978:ASP:OD1	1:B:978:ASP:N	2.25	0.70
1:B:921:ILE:HA	1:B:938:VAL:HG12	1.76	0.67
1:D:1095:GLU:N	1:D:1095:GLU:OE2	2.30	0.65
1:D:1009:ILE:HG13	1:D:1010:GLU:HG2	1.77	0.65
1:A:1106:ASN:OD1	1:A:1108[B]:SER:OG	2.18	0.61
1:D:924:ARG:NH1	6:D:1602:HOH:O	2.33	0.61
1:A:1074:ASP:HB2	4:A:1506:G5U:C2	2.31	0.60
1:B:1142:ARG:NH2	1:B:1148:GLU:OE2	2.34	0.60
1:A:921:ILE:N	6:A:1603:HOH:O	2.34	0.59
1:A:1048:MET:HE3	1:A:1170:CYS:HA	1.87	0.57
1:B:1004:GLN:O	1:B:1008:LYS:NZ	2.38	0.57
1:A:1088:ASP:HA	1:A:1098:CYS:HB3	1.88	0.56
1:A:1176:LYS:O	1:A:1176:LYS:HD2	2.08	0.53
1:B:1113:HIS:HB2	1:B:1154:TYR:CG	2.44	0.53
1:B:976:CYS:HB3	1:B:978:ASP:OD1	2.10	0.52
1:D:1183:ALA:HA	1:D:1186:GLN:HG2	1.92	0.51
1:B:1008:LYS:H	1:B:1008:LYS:HD2	1.75	0.51
1:D:918:THR:O	1:D:919:GLU:HG2	2.10	0.51
1:A:1157:ARG:NH1	4:A:1506:G5U:O4	2.46	0.49
1:C:1114:LEU:HG	1:C:1151:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:THR:OG1	1:C:1070:GLU:OE2	2.20	0.48
1:C:1008:LYS:NZ	1:C:1060:GLN:OE1	2.47	0.48
1:A:949:ASP:OD2	1:A:1102:ARG:NH2	2.47	0.47
1:A:1142[A]:ARG:NH2	1:A:1148:GLU:OE2	2.33	0.47
1:A:1083:ASP:HA	1:A:1086:LEU:HD13	1.96	0.47
1:B:1076:GLU:O	1:B:1080:ARG:HG3	2.14	0.47
1:C:1067:TYR:HA	1:C:1108[B]:SER:OG	2.14	0.47
1:D:1113:HIS:HB2	1:D:1154:TYR:CG	2.49	0.47
1:C:919:GLU:OE2	1:D:961:THR:OG1	2.30	0.46
1:D:937:CYS:HA	1:D:1042:LEU:O	2.15	0.46
1:A:967:ASN:ND2	1:C:959:THR:O	2.47	0.46
1:A:1117:PRO:O	1:A:1142[B]:ARG:NH1	2.48	0.46
1:D:1119:ILE:HG13	1:D:1152:PHE:HB3	1.97	0.46
1:D:1089:LEU:HD11	1:D:1099:ILE:HG13	1.97	0.46
1:B:1119:ILE:HG13	1:B:1152:PHE:HB3	1.98	0.46
1:C:1113:HIS:HB2	1:C:1154:TYR:CG	2.51	0.46
1:A:1006:PHE:CE2	1:A:1011:PRO:HB3	2.51	0.45
1:B:1114:LEU:HG	1:B:1151:GLY:HA3	1.98	0.45
1:A:1095:GLU:H	1:A:1095:GLU:HG2	1.55	0.45
1:A:1176:LYS:HG3	1:A:1177:HIS:CE1	2.52	0.45
1:B:1120:ILE:HG23	1:B:1141:SER:HB3	1.99	0.44
1:D:1067:TYR:HA	1:D:1108[B]:SER:OG	2.17	0.44
1:C:1101:ALA:HA	1:C:1104:TYR:O	2.17	0.44
1:C:1060:GLN:HB2	1:C:1142:ARG:HA	1.99	0.44
1:A:1067:TYR:HA	1:A:1108[B]:SER:OG	2.17	0.44
1:C:1005:GLU:OE1	1:C:1005:GLU:N	2.47	0.44
1:B:937:CYS:HA	1:B:1042:LEU:O	2.18	0.43
1:A:1113:HIS:HB2	1:A:1154:TYR:CG	2.53	0.43
1:B:1042:LEU:HD11	1:B:1050:TRP:HB3	1.99	0.43
1:A:1101:ALA:HA	1:A:1104:TYR:O	2.18	0.43
1:C:998:LYS:HE2	1:C:998:LYS:HB3	1.82	0.42
1:B:993:ARG:HD3	1:B:994:CYS:O	2.20	0.42
1:C:947:PRO:HG3	1:C:1050:TRP:NE1	2.33	0.42
1:D:976:CYS:HB3	1:D:978:ASP:OD1	2.18	0.42
1:A:1168:CYS:HB2	1:A:1177:HIS:HB2	2.02	0.42
1:C:937:CYS:HA	1:C:1042:LEU:O	2.20	0.42
1:D:1091:ASN:ND2	1:D:1091:ASN:C	2.72	0.41
1:A:922:ILE:HB	1:A:946:CYS:SG	2.61	0.41
1:D:923:CYS:HB3	1:D:937:CYS:HB3	2.02	0.41
1:D:1183:ALA:O	1:D:1186:GLN:HG3	2.20	0.41
1:A:947:PRO:HD3	1:A:1050:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1058:ILE:HG21	1:C:1064:ILE:HD11	2.04	0.40
1:C:1091:ASN:O	1:C:1094:GLY:N	2.54	0.40
1:D:1101:ALA:HA	1:D:1104:TYR:O	2.21	0.40
1:C:1119:ILE:HG13	1:C:1152:PHE:HB3	2.03	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	266/283 (94%)	254 (96%)	12 (4%)	0	100	100
1	B	262/283 (93%)	244 (93%)	17 (6%)	1 (0%)	34	37
1	C	263/283 (93%)	251 (95%)	12 (5%)	0	100	100
1	D	266/283 (94%)	246 (92%)	18 (7%)	2 (1%)	19	19
All	All	1057/1132 (93%)	995 (94%)	59 (6%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1090	ASP
1	B	978	ASP
1	D	919	GLU

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/253 (96%)	239 (98%)	4 (2%)	62	76
1	B	238/253 (94%)	232 (98%)	6 (2%)	47	60
1	C	239/253 (94%)	235 (98%)	4 (2%)	60	74
1	D	243/253 (96%)	240 (99%)	3 (1%)	71	83
All	All	963/1012 (95%)	946 (98%)	17 (2%)	59	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1074	ASP
1	A	1091	ASN
1	A	1164	LYS
1	A	1186	GLN
1	B	982	SER
1	B	993	ARG
1	B	1008	LYS
1	B	1096	VAL
1	B	1098	CYS
1	B	1186	GLN
1	C	991	SER
1	C	1090	ASP
1	C	1123	ARG
1	C	1164	LYS
1	D	991	SER
1	D	1091	ASN
1	D	1132	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	1177	HIS
1	D	1091	ASN

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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	C	1505	-	24,29,29	1.22	3 (12%)	23,42,42	1.49	3 (13%)
4	G5U	A	1506	1	38,39,39	4.40	14 (36%)	53,53,53	1.86	12 (22%)
3	SAM	B	1505	-	24,29,29	1.21	3 (12%)	23,42,42	1.46	3 (13%)
4	G5U	D	1506	1	38,39,39	4.43	14 (36%)	53,53,53	2.19	21 (39%)
3	SAM	A	1505	-	24,29,29	1.22	3 (12%)	23,42,42	1.50	4 (17%)
5	G4R	C	1506	-	38,39,39	4.02	15 (39%)	52,53,53	2.39	19 (36%)
4	G5U	B	1506	1	38,39,39	4.46	16 (42%)	53,53,53	2.17	15 (28%)
3	SAM	D	1505	-	24,29,29	1.22	3 (12%)	23,42,42	1.49	3 (13%)

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	C	1505	-	-	2/12/33/33	0/3/3/3
4	G5U	A	1506	1	-	15/23/40/40	0/4/4/4
3	SAM	B	1505	-	-	2/12/33/33	0/3/3/3
4	G5U	D	1506	1	-	12/23/40/40	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	A	1505	-	-	2/12/33/33	0/3/3/3
5	G4R	C	1506	-	-	8/23/40/40	0/4/4/4
4	G5U	B	1506	1	-	4/23/40/40	0/4/4/4
3	SAM	D	1505	-	-	2/12/33/33	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1506	G4R	C9-N4	-14.04	1.20	1.48
4	B	1506	G5U	C14-N13	-13.88	1.20	1.48
4	A	1506	G5U	C14-N13	-13.52	1.21	1.48
4	D	1506	G5U	C14-N13	-13.36	1.21	1.48
4	B	1506	G5U	C28-N29	-13.12	1.17	1.47
4	D	1506	G5U	C28-N29	-13.05	1.17	1.47
4	A	1506	G5U	C28-N29	-12.78	1.18	1.47
5	C	1506	G4R	C21-N5	-11.70	1.20	1.47
4	A	1506	G5U	C33-N29	-11.47	1.26	1.47
4	D	1506	G5U	C33-N29	-11.45	1.26	1.47
4	B	1506	G5U	C33-N29	-11.43	1.26	1.47
5	C	1506	G4R	C22-N5	-10.48	1.27	1.47
4	D	1506	G5U	C6-N5	8.21	1.49	1.38
4	B	1506	G5U	C6-N5	8.10	1.49	1.38
4	A	1506	G5U	C6-N5	7.86	1.49	1.38
4	D	1506	G5U	C30-N29	6.21	1.59	1.47
4	A	1506	G5U	C30-N29	6.19	1.59	1.47
4	B	1506	G5U	C30-N29	6.18	1.59	1.47
4	D	1506	G5U	C3-N5	5.94	1.48	1.35
5	C	1506	G4R	C3-N1	5.91	1.45	1.35
5	C	1506	G4R	C4-N1	5.85	1.46	1.38
4	B	1506	G5U	C3-N5	5.77	1.48	1.35
4	A	1506	G5U	C3-N5	5.62	1.48	1.35
4	B	1506	G5U	C31-C30	-5.60	1.32	1.51
4	D	1506	G5U	C31-C30	-5.54	1.32	1.51
4	A	1506	G5U	C31-C30	-5.48	1.32	1.51
4	A	1506	G5U	C10-N9	4.38	1.56	1.46
4	D	1506	G5U	C10-N9	4.27	1.56	1.46
4	B	1506	G5U	C10-N9	4.05	1.56	1.46
3	A	1505	SAM	C2-N3	3.96	1.38	1.32
3	C	1505	SAM	C2-N3	3.95	1.38	1.32
3	D	1505	SAM	C2-N3	3.95	1.38	1.32
3	B	1505	SAM	C2-N3	3.92	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1506	G4R	C6-N3	3.63	1.55	1.46
4	B	1506	G5U	C11-C10	-3.33	1.44	1.52
4	A	1506	G5U	C20-C21	3.22	1.42	1.36
5	C	1506	G4R	C14-C27	-3.20	1.37	1.42
5	C	1506	G4R	C7-C6	-3.18	1.44	1.52
4	D	1506	G5U	C11-C10	-3.18	1.44	1.52
5	C	1506	G4R	C24-C23	-3.17	1.26	1.48
4	A	1506	G5U	C11-C10	-3.15	1.44	1.52
4	D	1506	G5U	C8-N7	3.11	1.37	1.32
4	A	1506	G5U	C8-N7	3.08	1.37	1.32
4	B	1506	G5U	O25-C24	3.08	1.43	1.37
4	A	1506	G5U	O25-C24	3.08	1.43	1.37
4	D	1506	G5U	O25-C24	3.07	1.43	1.37
4	D	1506	G5U	C20-C21	3.05	1.42	1.36
5	C	1506	G4R	C23-C22	3.02	1.62	1.51
5	C	1506	G4R	O1-C3	-2.92	1.18	1.24
5	C	1506	G4R	C2-C3	2.90	1.53	1.48
4	B	1506	G5U	C20-C21	2.78	1.41	1.36
4	D	1506	G5U	C19-C35	-2.67	1.38	1.42
4	A	1506	G5U	C19-C35	-2.55	1.38	1.42
4	B	1506	G5U	C19-C35	-2.55	1.38	1.42
3	D	1505	SAM	C2-N1	2.47	1.38	1.33
3	C	1505	SAM	C2-N1	2.47	1.38	1.33
3	A	1505	SAM	C2-N1	2.44	1.38	1.33
4	A	1506	G5U	O4-C3	-2.42	1.18	1.23
3	B	1505	SAM	C2-N1	2.42	1.38	1.33
4	B	1506	G5U	O4-C3	-2.36	1.18	1.23
4	B	1506	G5U	C34-C24	2.33	1.40	1.36
4	B	1506	G5U	C8-N7	2.32	1.36	1.32
5	C	1506	G4R	O3-C18	2.24	1.42	1.37
4	D	1506	G5U	O4-C3	-2.21	1.18	1.23
4	B	1506	G5U	C34-C35	2.18	1.45	1.41
3	A	1505	SAM	OXT-C	-2.14	1.23	1.30
3	B	1505	SAM	OXT-C	-2.13	1.23	1.30
3	C	1505	SAM	OXT-C	-2.13	1.23	1.30
3	D	1505	SAM	OXT-C	-2.12	1.23	1.30
5	C	1506	G4R	O2-C16	2.06	1.40	1.37
5	C	1506	G4R	C13-C6	-2.05	1.47	1.52

All (80) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1506	G4R	C2-C3-N1	8.75	119.61	113.84
4	B	1506	G5U	C6-N5-C3	-8.35	117.63	130.28
4	D	1506	G5U	C6-N5-C3	-7.27	119.27	130.28
4	A	1506	G5U	C6-N5-C3	-5.74	121.59	130.28
3	D	1505	SAM	N3-C2-N1	-5.56	119.98	128.68
3	C	1505	SAM	N3-C2-N1	-5.44	120.17	128.68
3	B	1505	SAM	N3-C2-N1	-5.44	120.18	128.68
3	A	1505	SAM	N3-C2-N1	-5.41	120.23	128.68
4	A	1506	G5U	O22-C21-C20	-4.79	119.05	125.24
4	B	1506	G5U	O22-C21-C20	-4.75	119.10	125.24
4	D	1506	G5U	O22-C21-C20	-4.58	119.32	125.24
5	C	1506	G4R	C1-C2-C3	-4.48	117.15	122.27
5	C	1506	G4R	O2-C16-C15	-4.46	119.47	125.24
5	C	1506	G4R	C5-C14-C27	4.42	118.66	115.88
4	B	1506	G5U	C8-C19-C35	4.10	118.46	115.88
5	C	1506	G4R	C8-N4-C12	4.00	116.39	109.08
4	B	1506	G5U	C19-C8-N9	-3.97	116.89	120.63
4	D	1506	G5U	C18-C10-C11	3.95	117.67	110.82
4	B	1506	G5U	C18-C10-C11	3.84	117.48	110.82
4	D	1506	G5U	C8-C19-C35	3.80	118.27	115.88
5	C	1506	G4R	N6-C4-N2	-3.80	120.22	126.23
5	C	1506	G4R	C4-N6-C27	3.72	121.67	115.60
4	A	1506	G5U	O25-C24-C34	-3.63	119.05	125.19
5	C	1506	G4R	C15-C14-C5	-3.61	121.63	124.88
5	C	1506	G4R	C14-C27-N6	-3.59	119.01	122.81
4	B	1506	G5U	O22-C21-C24	3.51	120.29	115.41
4	B	1506	G5U	C20-C19-C8	-3.44	121.78	124.88
4	D	1506	G5U	C19-C8-N9	-3.44	117.38	120.63
5	C	1506	G4R	O2-C16-C18	3.37	120.10	115.41
5	C	1506	G4R	C13-C12-N4	3.31	116.50	111.43
4	A	1506	G5U	C11-C10-N9	3.30	115.74	110.60
4	D	1506	G5U	O25-C24-C34	-3.19	119.79	125.19
4	A	1506	G5U	N5-C6-N7	3.18	125.78	116.46
4	A	1506	G5U	O25-C24-C21	3.13	122.19	115.73
4	A	1506	G5U	O22-C21-C24	2.94	119.51	115.41
4	D	1506	G5U	O22-C21-C24	2.93	119.49	115.41
4	D	1506	G5U	C8-N9-C10	2.92	129.71	124.16
4	A	1506	G5U	C8-C19-C35	2.90	117.70	115.88
4	D	1506	G5U	N5-C6-N7	2.89	124.91	116.46
5	C	1506	G4R	O3-C18-C26	-2.83	120.40	125.19
4	A	1506	G5U	C18-C10-C11	2.73	115.55	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1505	SAM	OXT-C-O	-2.68	118.01	124.09
4	D	1506	G5U	C18-C10-N9	2.66	114.75	110.60
5	C	1506	G4R	C4-N2-C5	2.65	122.45	116.39
3	B	1505	SAM	OXT-C-O	-2.63	118.12	124.09
5	C	1506	G4R	O1-C3-C2	-2.63	118.52	122.72
3	D	1505	SAM	OXT-C-O	-2.62	118.14	124.09
4	D	1506	G5U	O25-C24-C21	2.61	121.13	115.73
3	A	1505	SAM	OXT-C-O	-2.60	118.18	124.09
4	A	1506	G5U	C23-O22-C21	-2.59	113.62	117.53
4	D	1506	G5U	C23-O22-C21	-2.56	113.66	117.53
4	D	1506	G5U	C6-N36-C35	2.56	119.78	115.60
5	C	1506	G4R	C17-O2-C16	-2.54	113.69	117.53
4	B	1506	G5U	O25-C24-C34	-2.49	120.98	125.19
4	A	1506	G5U	C6-N36-C35	2.47	119.63	115.60
4	B	1506	G5U	C19-C35-N36	-2.44	120.22	122.81
5	C	1506	G4R	C14-C5-N2	-2.43	117.99	121.98
4	B	1506	G5U	C23-O22-C21	-2.42	113.87	117.53
4	B	1506	G5U	N9-C8-N7	2.36	123.90	118.90
4	B	1506	G5U	O4-C3-N5	-2.29	119.45	123.63
4	D	1506	G5U	N9-C8-N7	2.28	123.75	118.90
4	D	1506	G5U	C33-N29-C30	2.28	106.26	104.04
5	C	1506	G4R	C11-C9-N4	-2.27	107.27	112.20
4	D	1506	G5U	C19-C35-N36	-2.23	120.45	122.81
4	D	1506	G5U	C31-C30-N29	2.23	106.52	103.92
4	A	1506	G5U	C34-C35-C19	2.22	122.21	119.65
3	C	1505	SAM	OXT-C-CA	2.18	120.81	113.38
3	B	1505	SAM	OXT-C-CA	2.17	120.76	113.38
3	A	1505	SAM	OXT-C-CA	2.16	120.74	113.38
4	B	1506	G5U	C8-N9-C10	2.16	128.27	124.16
3	D	1505	SAM	OXT-C-CA	2.15	120.72	113.38
4	B	1506	G5U	C2-C3-N5	2.15	120.51	114.75
5	C	1506	G4R	C13-C6-N3	-2.15	107.25	110.60
4	D	1506	G5U	C17-C18-C10	2.10	114.18	110.50
3	A	1505	SAM	C3'-C2'-C1'	2.08	104.11	100.98
4	D	1506	G5U	C28-N29-C33	-2.08	107.53	113.29
5	C	1506	G4R	C12-C13-C6	2.04	114.08	110.50
4	D	1506	G5U	C32-C33-N29	2.02	106.28	103.92
4	D	1506	G5U	C34-C35-C19	2.01	121.97	119.65
4	B	1506	G5U	C6-N36-C35	2.01	118.88	115.60

There are no chirality outliers.

All (47) 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
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	G5U	C11-C10-N9-C8
4	A	1506	G5U	C27-C28-N29-C30
4	A	1506	G5U	C27-C28-N29-C33
4	A	1506	G5U	N36-C6-N5-C3
4	A	1506	G5U	N7-C6-N5-C3
4	A	1506	G5U	C19-C8-N9-C10
4	A	1506	G5U	N7-C8-N9-C10
4	B	1506	G5U	C27-C28-N29-C30
4	B	1506	G5U	N36-C6-N5-C3
4	B	1506	G5U	N7-C6-N5-C3
4	D	1506	G5U	C18-C10-N9-C8
4	D	1506	G5U	C15-C14-N13-C12
4	D	1506	G5U	C15-C14-N13-C17
4	D	1506	G5U	C16-C14-N13-C12
4	D	1506	G5U	C27-C28-N29-C30
4	D	1506	G5U	N36-C6-N5-C3
4	D	1506	G5U	N7-C6-N5-C3
4	D	1506	G5U	C19-C8-N9-C10
4	D	1506	G5U	N7-C8-N9-C10
5	C	1506	G4R	C1-C2-C3-N1
5	C	1506	G4R	C1-C2-C3-O1
5	C	1506	G4R	C20-C21-N5-C22
5	C	1506	G4R	C20-C21-N5-C25
5	C	1506	G4R	C10-C9-N4-C12
5	C	1506	G4R	C11-C9-N4-C12
4	A	1506	G5U	O25-C26-C27-C28
4	A	1506	G5U	C24-C21-O22-C23
5	C	1506	G4R	C19-C20-C21-N5
4	A	1506	G5U	C1-C2-C3-O4
4	A	1506	G5U	C1-C2-C3-N5
4	A	1506	G5U	C20-C21-O22-C23
4	B	1506	G5U	C26-C27-C28-N29
4	A	1506	G5U	C15-C14-N13-C17
4	A	1506	G5U	C16-C14-N13-C12
5	C	1506	G4R	C10-C9-N4-C8

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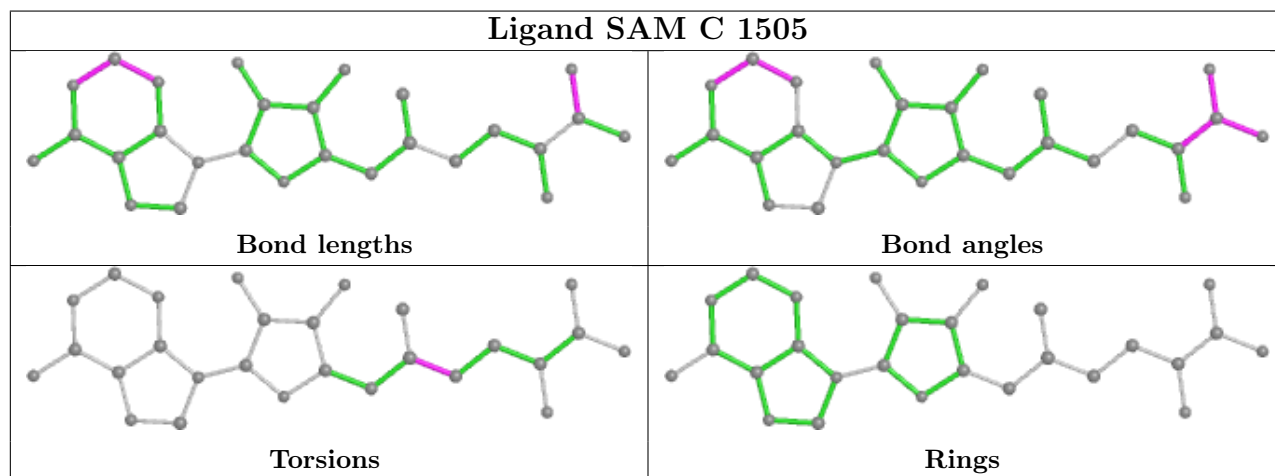
Mol	Chain	Res	Type	Atoms
4	D	1506	G5U	C26-C27-C28-N29
4	D	1506	G5U	C1-C2-C3-N5
4	A	1506	G5U	C21-C24-O25-C26
4	D	1506	G5U	C1-C2-C3-O4

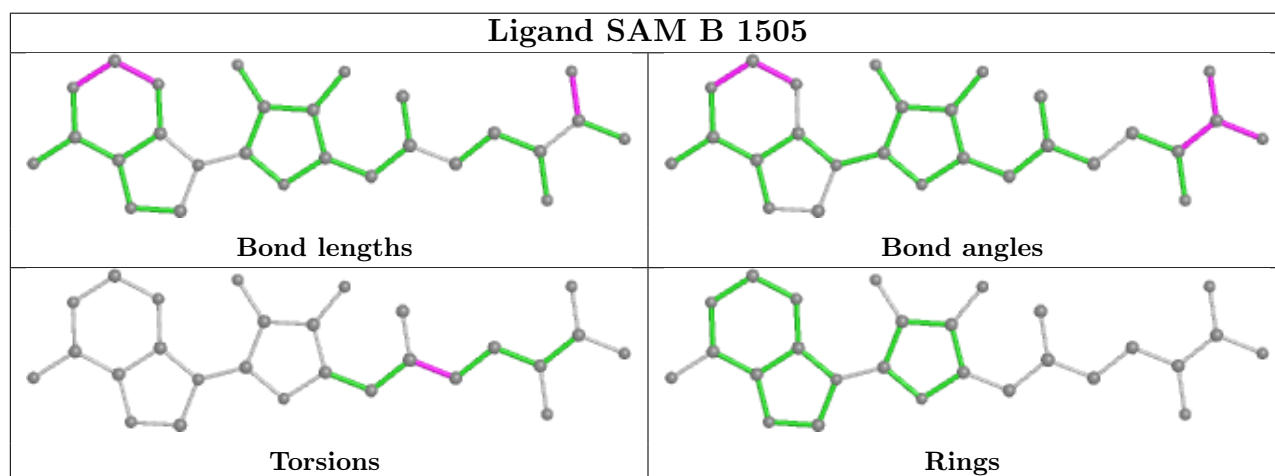
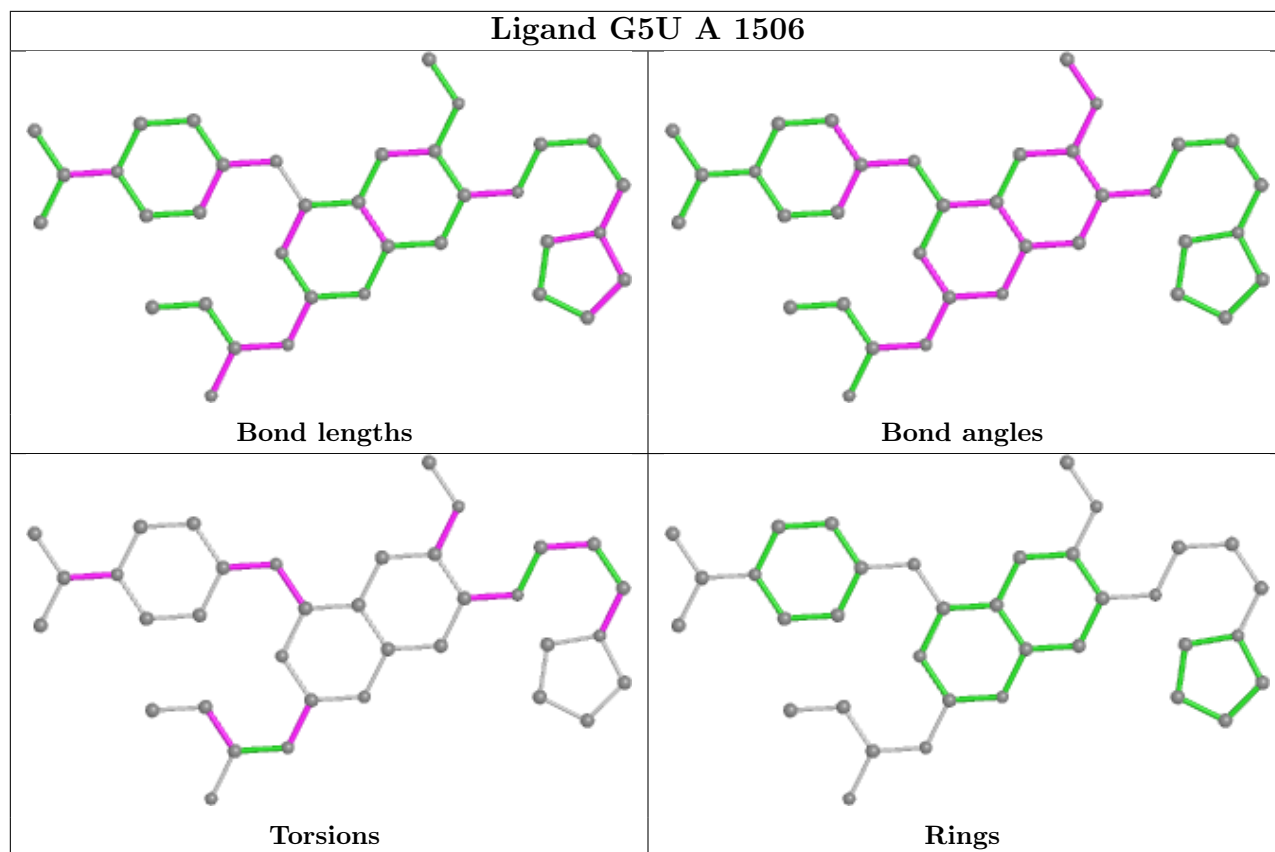
There are no ring outliers.

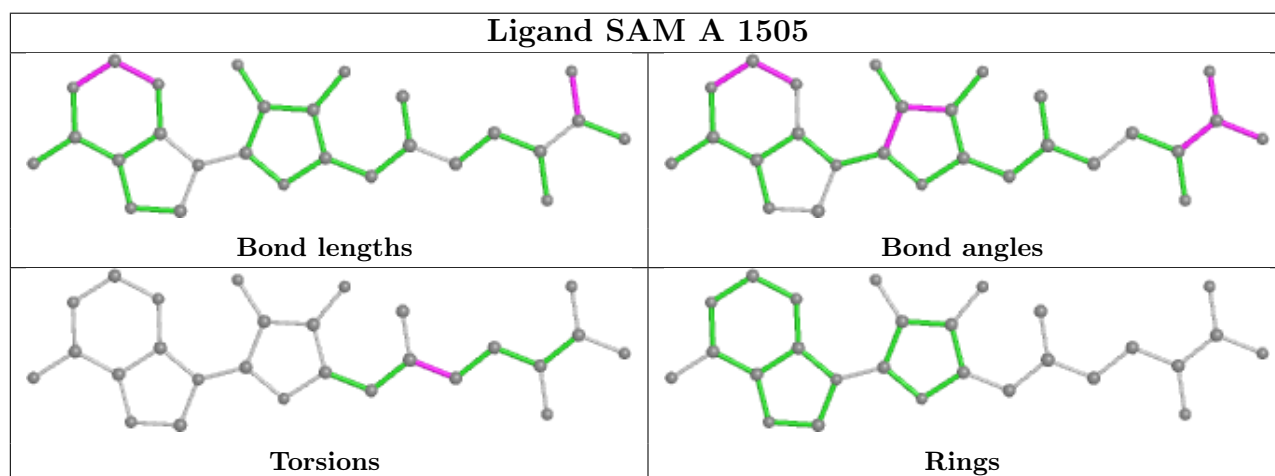
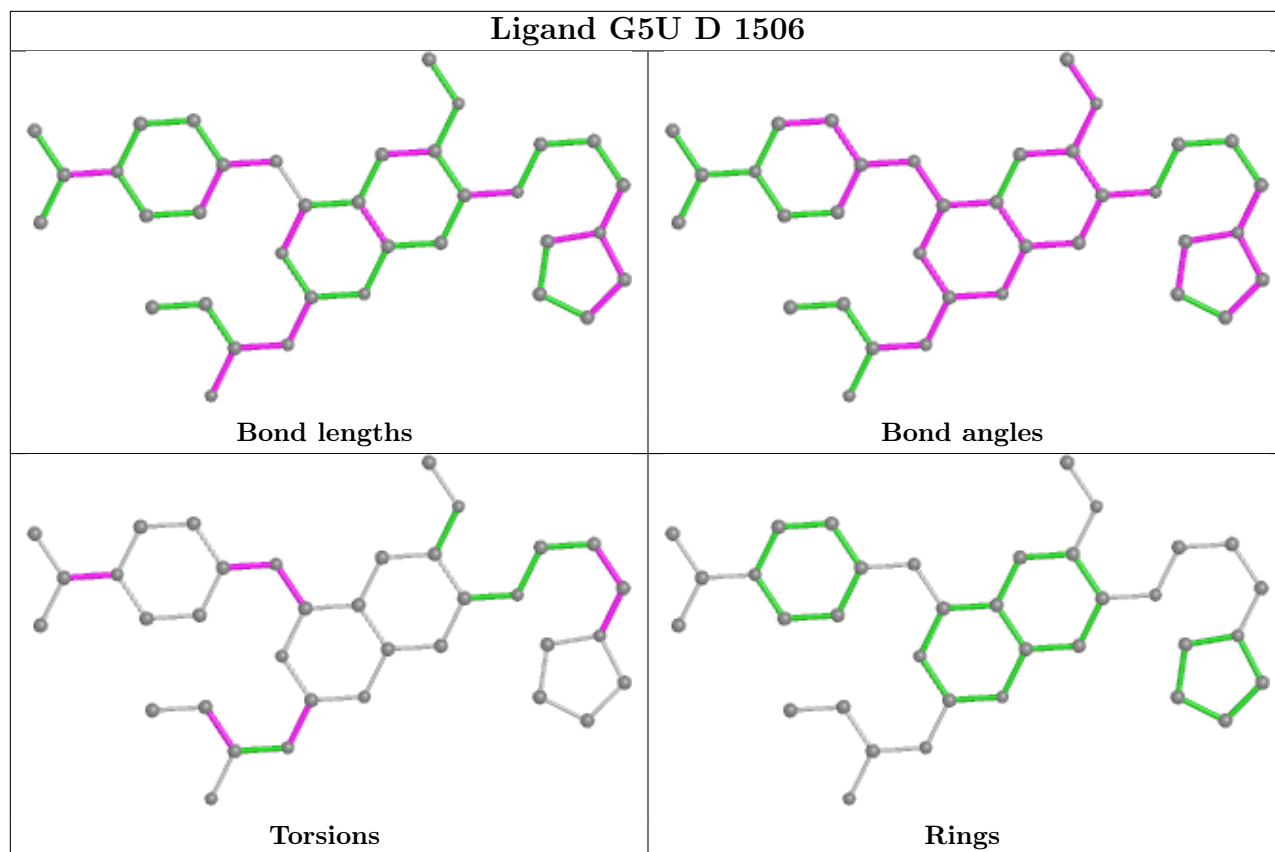
1 monomer is involved in 2 short contacts:

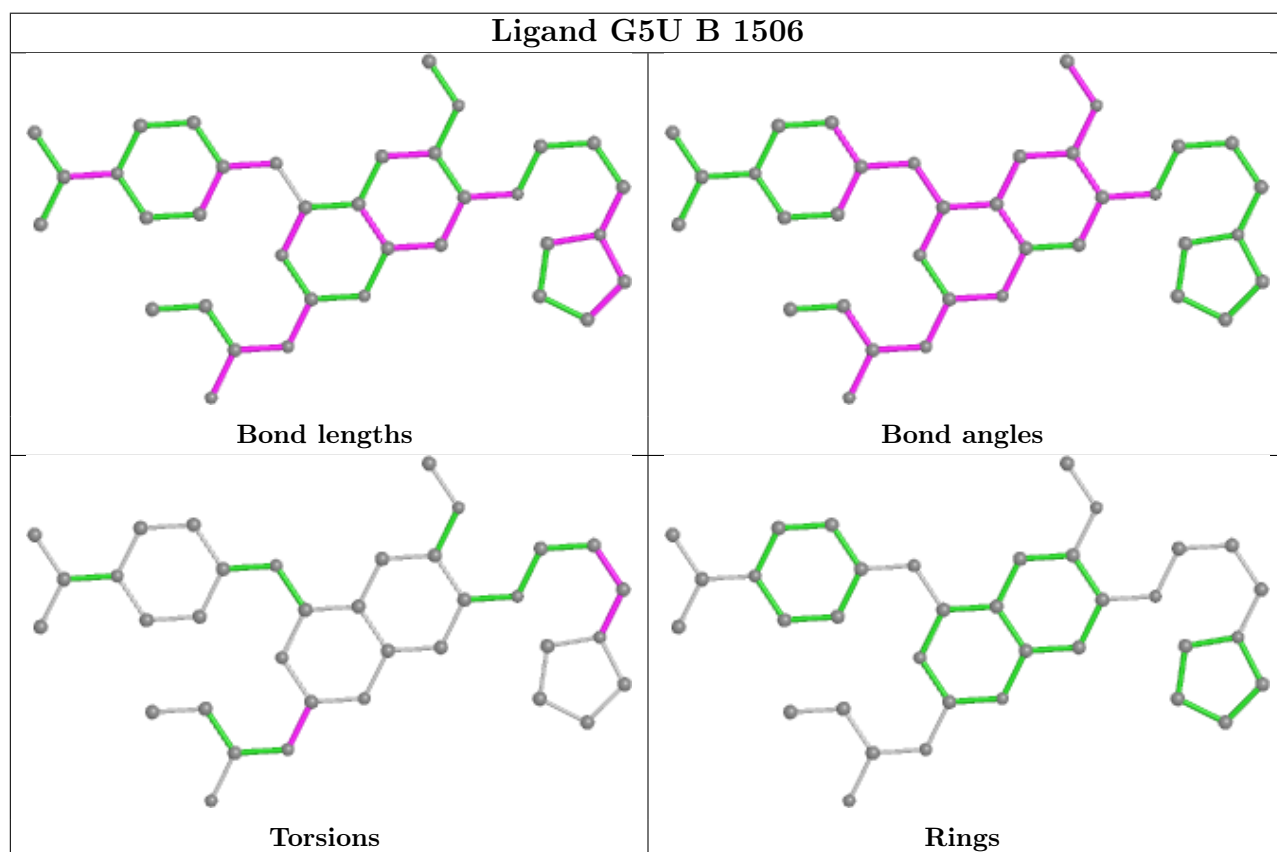
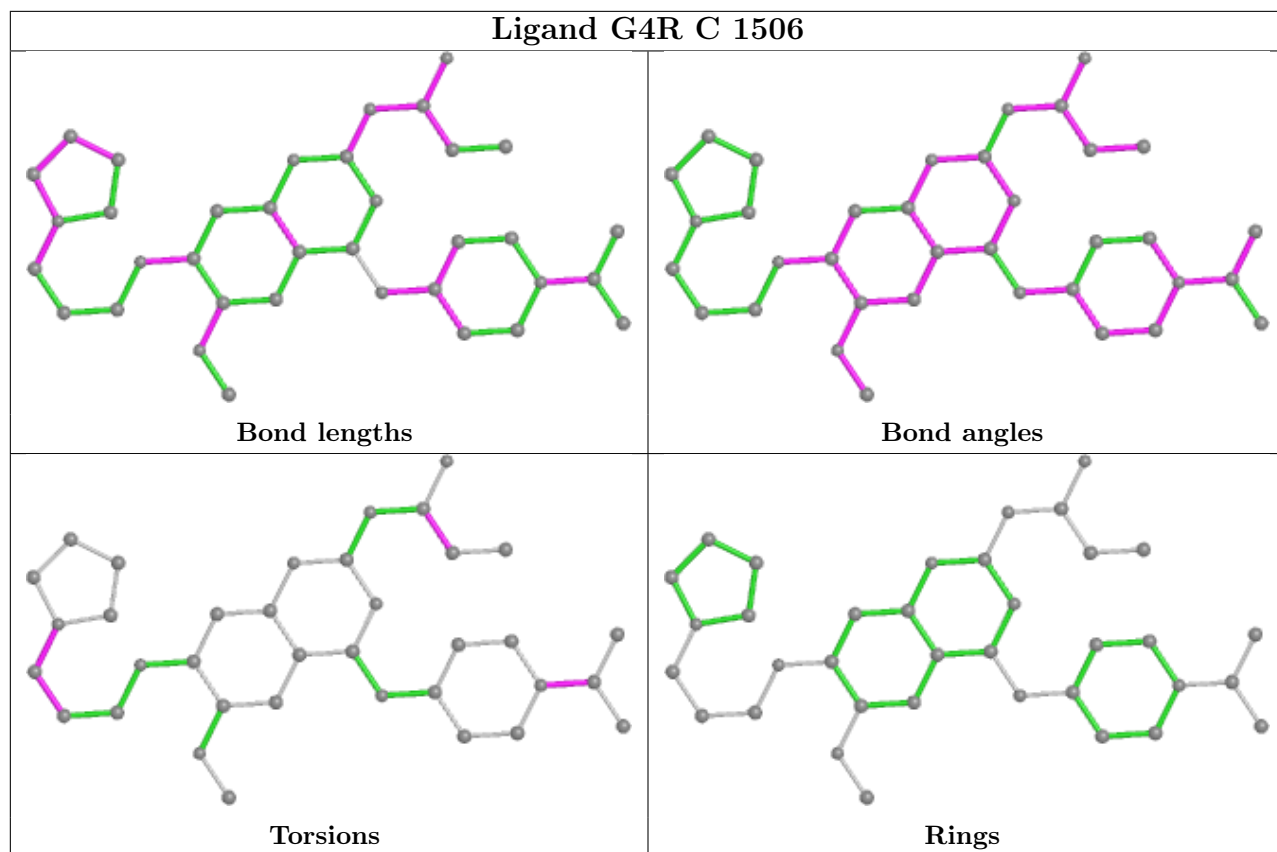
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1506	G5U	2	0

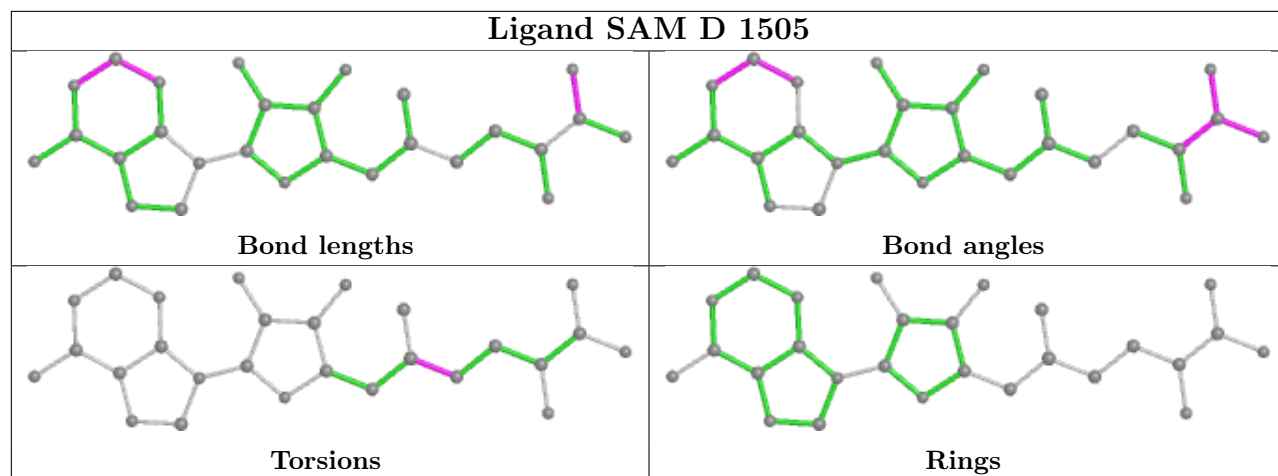
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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%)	-0.07	4 (1%) 73 72	28, 39, 66, 80	0
1	B	264/283 (93%)	0.01	4 (1%) 73 72	29, 44, 66, 85	0
1	C	266/283 (93%)	0.06	2 (0%) 86 85	30, 46, 66, 84	0
1	D	269/283 (95%)	-0.04	3 (1%) 80 79	28, 40, 63, 77	0
All	All	1065/1132 (94%)	-0.01	13 (1%) 79 77	28, 42, 66, 85	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	921	ILE	3.9
1	D	918	THR	3.6
1	B	1009	ILE	3.4
1	A	1009	ILE	2.7
1	D	1186	GLN	2.7
1	A	922	ILE	2.6
1	D	1173	GLU	2.5
1	B	978	ASP	2.5
1	A	1165	TYR	2.3
1	B	1010	GLU	2.2
1	C	1164	LYS	2.1
1	C	1183	ALA	2.1
1	B	977	VAL	2.1

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](#)

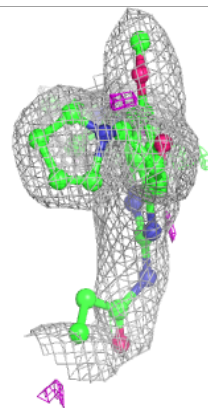
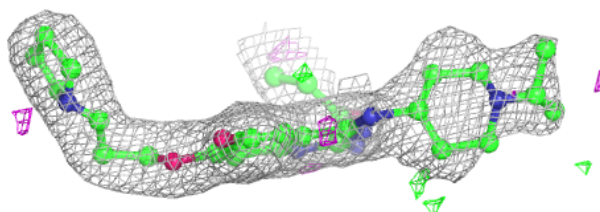
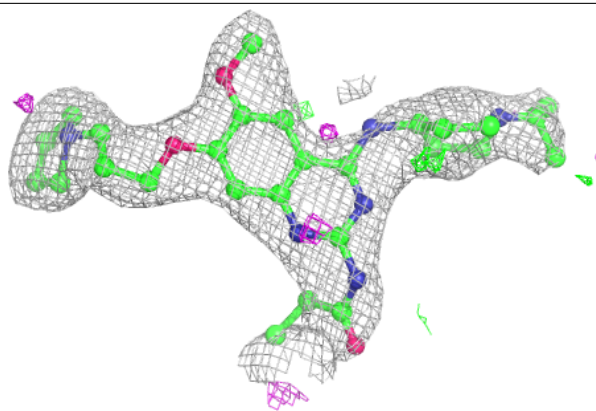
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	G5U	B	1506	36/36	0.88	0.19	34,49,63,66	1
4	G5U	D	1506	36/36	0.88	0.21	38,54,75,76	3
4	G5U	A	1506	36/36	0.91	0.20	33,54,66,68	3
5	G4R	C	1506	36/36	0.91	0.19	35,45,61,63	3
3	SAM	C	1505	27/27	0.93	0.11	34,41,47,53	0
3	SAM	D	1505	27/27	0.94	0.12	29,38,41,46	0
2	ZN	C	1504	1/1	0.95	0.12	52,52,52,52	0
3	SAM	A	1505	27/27	0.95	0.12	29,40,45,51	0
3	SAM	B	1505	27/27	0.95	0.12	27,36,43,44	0
2	ZN	A	1504	1/1	0.96	0.16	51,51,51,51	0
2	ZN	B	1501	1/1	0.97	0.17	43,43,43,43	0
2	ZN	B	1503	1/1	0.97	0.15	47,47,47,47	0
2	ZN	C	1501	1/1	0.97	0.19	45,45,45,45	0
2	ZN	C	1502	1/1	0.98	0.14	39,39,39,39	0
2	ZN	C	1503	1/1	0.98	0.12	45,45,45,45	0
2	ZN	B	1504	1/1	0.98	0.14	50,50,50,50	0
2	ZN	D	1503	1/1	0.98	0.15	33,33,33,33	0
2	ZN	A	1502	1/1	0.99	0.14	29,29,29,29	0
2	ZN	D	1504	1/1	0.99	0.14	45,45,45,45	0
2	ZN	B	1502	1/1	0.99	0.14	44,44,44,44	0
2	ZN	D	1501	1/1	0.99	0.15	32,32,32,32	0
2	ZN	D	1502	1/1	0.99	0.16	31,31,31,31	0
2	ZN	A	1503	1/1	1.00	0.17	30,30,30,30	0
2	ZN	A	1501	1/1	1.00	0.13	28,28,28,28	0

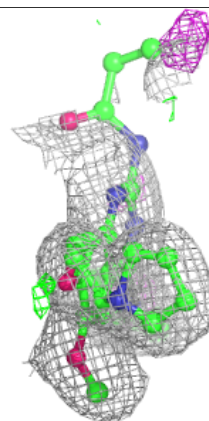
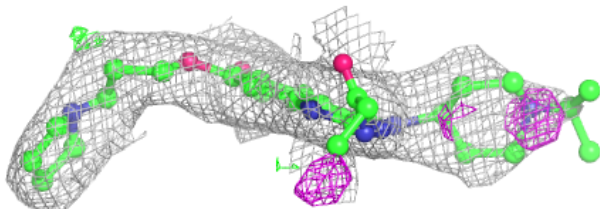
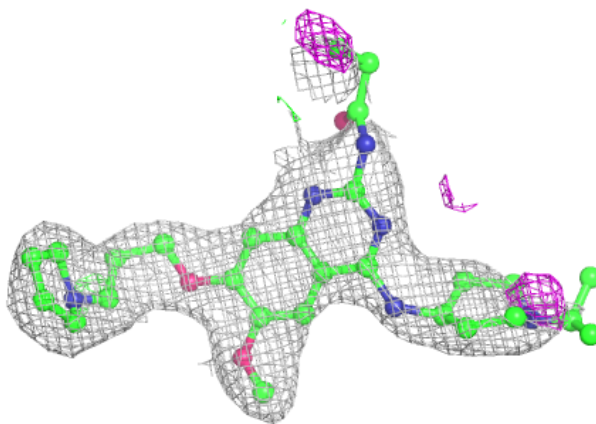
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G5U 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)

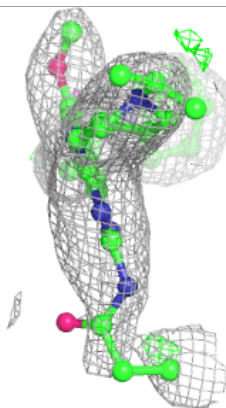
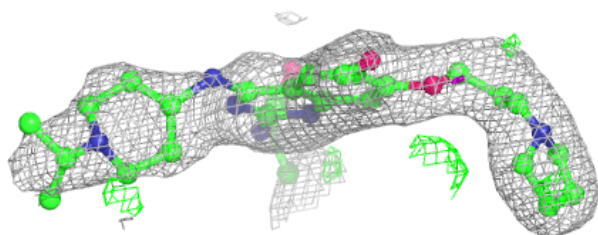
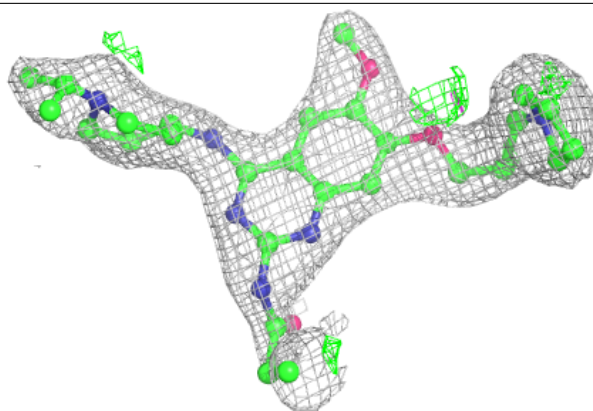
**Electron density around G5U D 1506:**

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

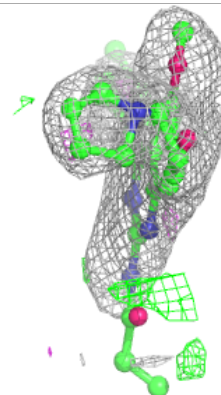
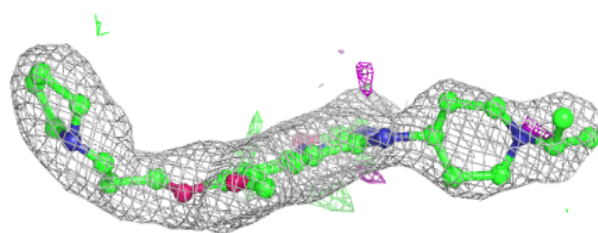
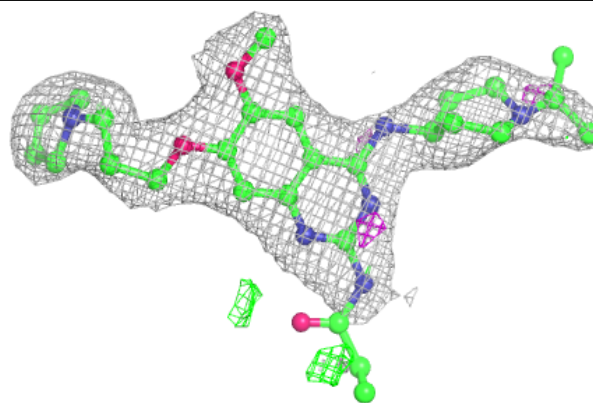


Electron density around G5U A 1506:

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

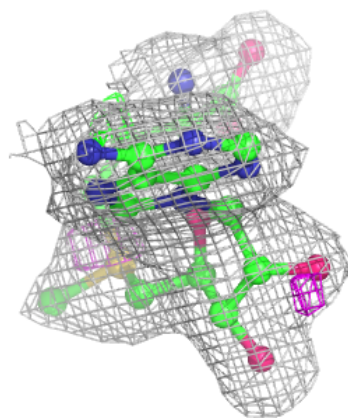
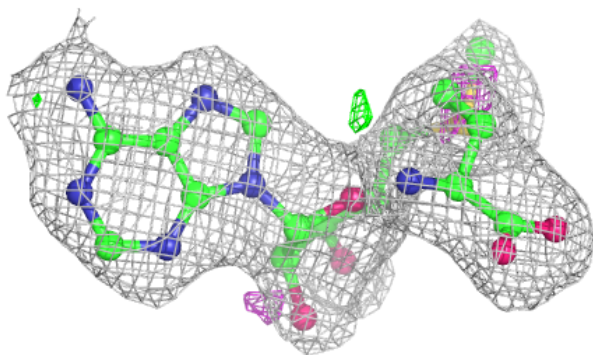
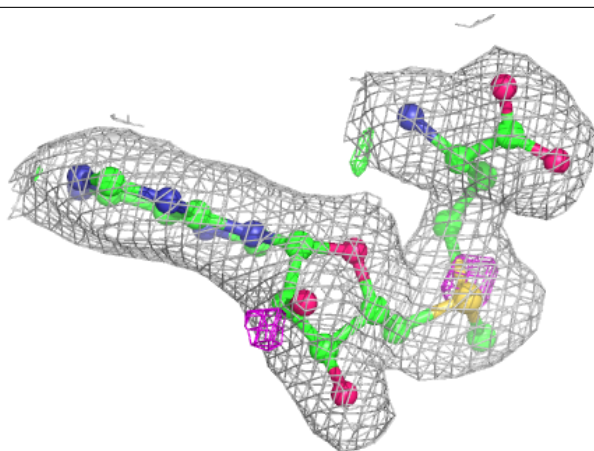
**Electron density around G4R C 1506:**

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

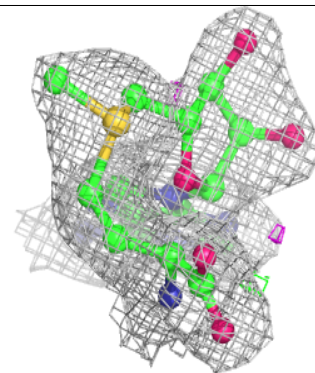
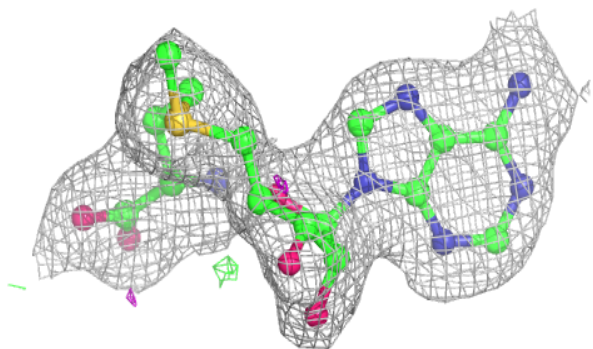
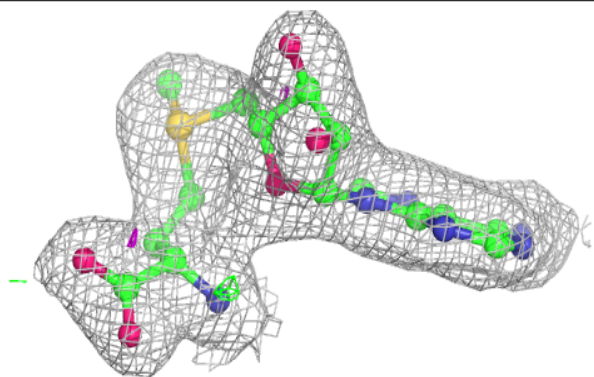


Electron density around SAM C 1505:

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

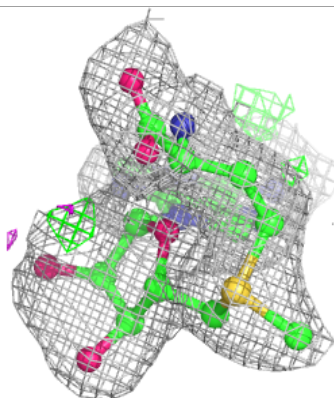
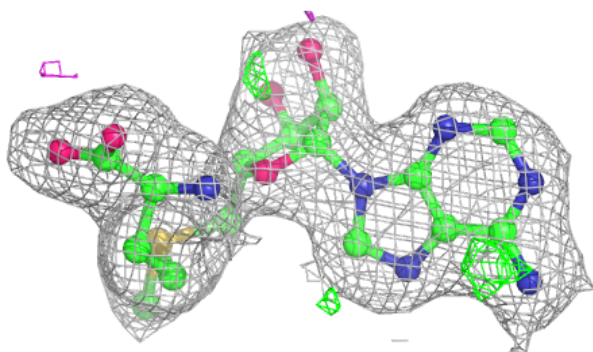
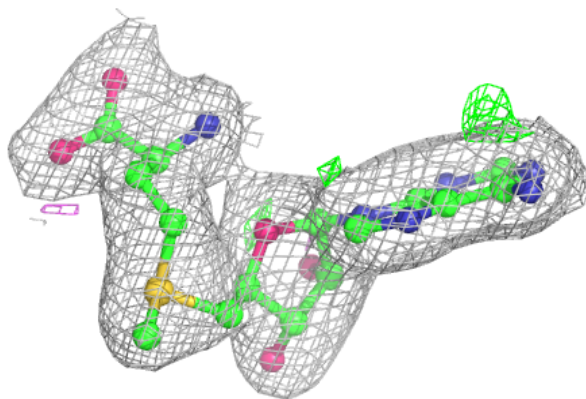
**Electron density around SAM D 1505:**

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

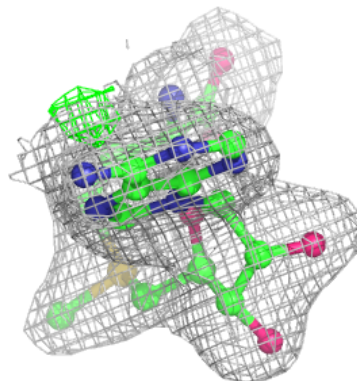
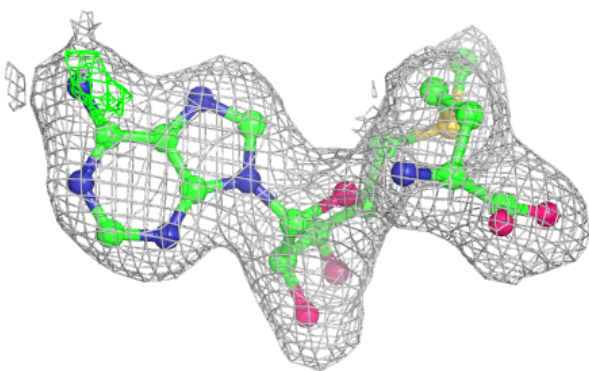
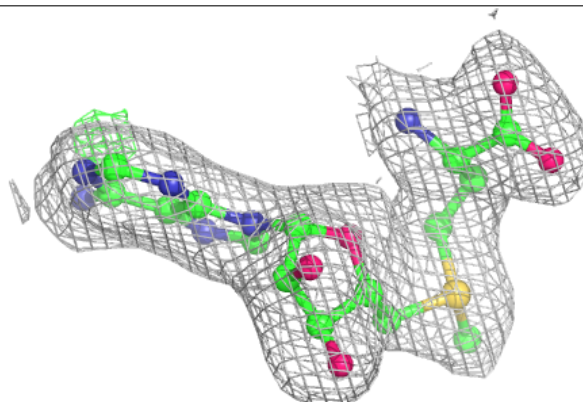


Electron density around SAM A 1505:

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

**Electron density around 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.