



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:27 AM UTC

PDB ID : 6X0P / pdb_00006x0p
Title : Ash1L SET domain Q2265A mutant in complex with AS-5
Authors : Rogawski, D.S.; Li, H.; Borkin, D.; Cierpicki, T.; Grembecka, J.
Deposited on : 2020-05-17
Resolution : 1.69 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 : 4-5-2 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

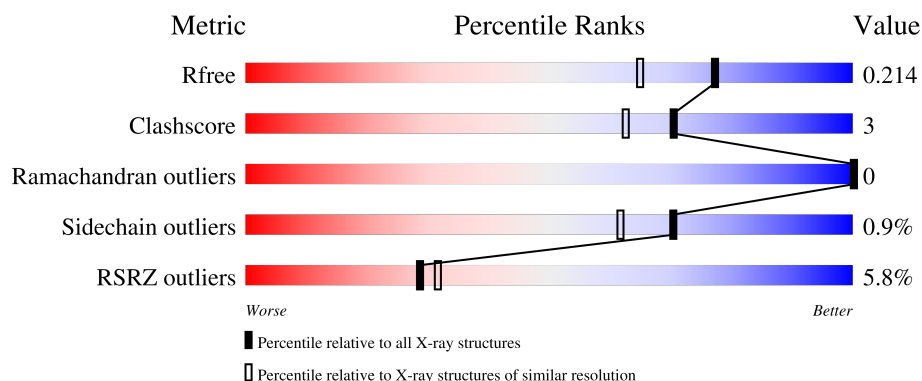
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	226	3% 90% 7% .
1	B	226	12% 87% 10% .
1	C	226	4% 93% . .
1	D	226	4% 88% 9% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8288 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 ASH1L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1739	1078	309	329	23			
1	B	220	Total	C	N	O	S	0	2	0
			1751	1089	312	326	24			
1	C	220	Total	C	N	O	S	0	1	0
			1750	1087	312	328	23			
1	D	220	Total	C	N	O	S	0	2	0
			1765	1097	314	330	24			

There are 28 discrepancies between the modelled and reference sequences:

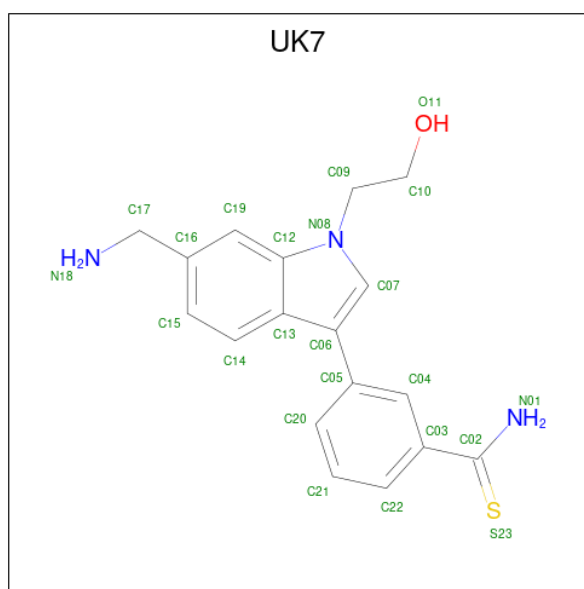
Chain	Residue	Modelled	Actual	Comment	Reference
A	2063	GLY	-	expression tag	UNP Q9NR48
A	2064	ALA	-	expression tag	UNP Q9NR48
A	2065	MET	-	expression tag	UNP Q9NR48
A	2066	ALA	-	expression tag	UNP Q9NR48
A	2067	GLY	-	expression tag	UNP Q9NR48
A	2068	SER	-	expression tag	UNP Q9NR48
A	2265	ALA	GLN	engineered mutation	UNP Q9NR48
B	2063	GLY	-	expression tag	UNP Q9NR48
B	2064	ALA	-	expression tag	UNP Q9NR48
B	2065	MET	-	expression tag	UNP Q9NR48
B	2066	ALA	-	expression tag	UNP Q9NR48
B	2067	GLY	-	expression tag	UNP Q9NR48
B	2068	SER	-	expression tag	UNP Q9NR48
B	2265	ALA	GLN	engineered mutation	UNP Q9NR48
C	2063	GLY	-	expression tag	UNP Q9NR48
C	2064	ALA	-	expression tag	UNP Q9NR48
C	2065	MET	-	expression tag	UNP Q9NR48
C	2066	ALA	-	expression tag	UNP Q9NR48
C	2067	GLY	-	expression tag	UNP Q9NR48
C	2068	SER	-	expression tag	UNP Q9NR48
C	2265	ALA	GLN	engineered mutation	UNP Q9NR48

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2063	GLY	-	expression tag	UNP Q9NR48
D	2064	ALA	-	expression tag	UNP Q9NR48
D	2065	MET	-	expression tag	UNP Q9NR48
D	2066	ALA	-	expression tag	UNP Q9NR48
D	2067	GLY	-	expression tag	UNP Q9NR48
D	2068	SER	-	expression tag	UNP Q9NR48
D	2265	ALA	GLN	engineered mutation	UNP Q9NR48

- Molecule 2 is 3-[6-(aminomethyl)-1-(2-hydroxyethyl)-1H-indol-3-yl]benzene-1-carbothioamide (CCD ID: UK7) (formula: C₁₈H₁₉N₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	18	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			23	18	3	1	1		
2	C	1	Total	C	N	O	S	0	0
			23	18	3	1	1		
2	D	1	Total	C	N	O	S	0	0
			23	18	3	1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

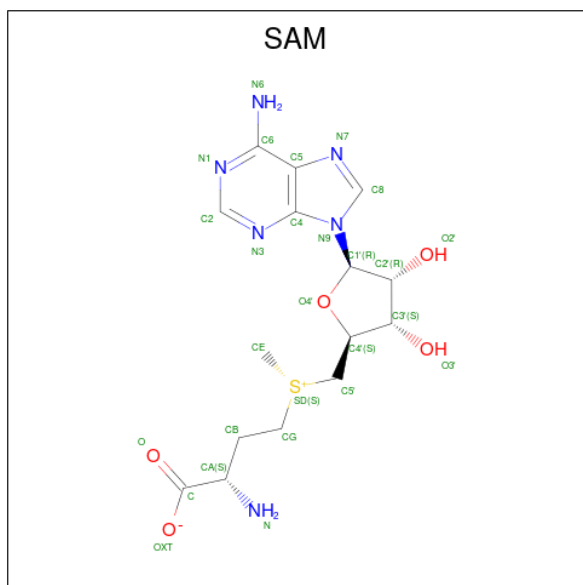
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0
3	C	3	Total 3	Zn 3	0	0
3	D	3	Total 3	Zn 3	0	0

- Molecule 4 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	276	Total 276	O 276	0	0
5	B	237	Total 237	O 237	0	0

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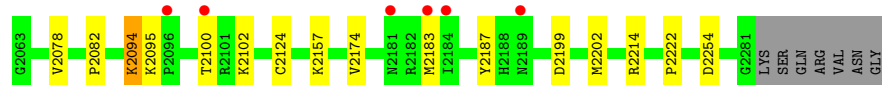
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	272	Total 272	O 272	0	0
5	D	286	Total 286	O 286	0	0

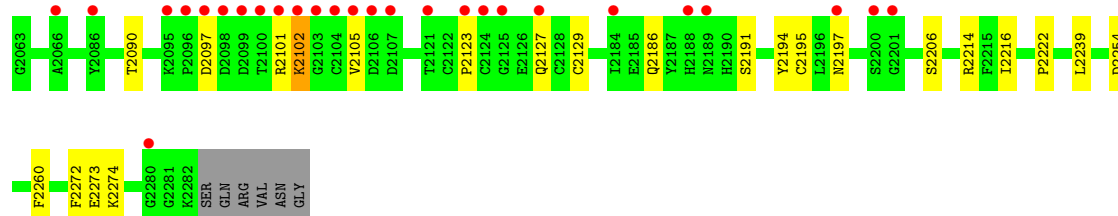
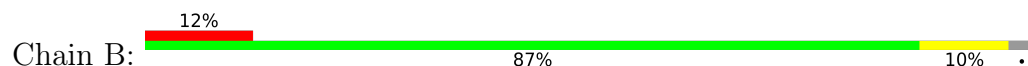
3 Residue-property plots [i](#)

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.

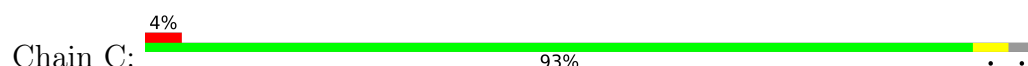
- Molecule 1: Histone-lysine N-methyltransferase ASH1L



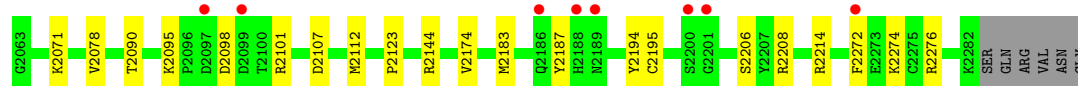
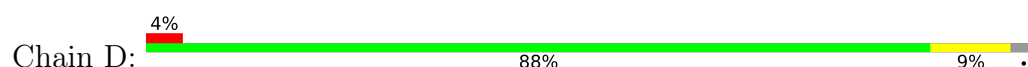
- Molecule 1: Histone-lysine N-methyltransferase ASH1L



- Molecule 1: Histone-lysine N-methyltransferase ASH1L



- Molecule 1: Histone-lysine N-methyltransferase ASH1L



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.13Å 62.31Å 72.97Å 87.76° 85.55° 90.04°	Depositor
Resolution (Å)	40.86 – 1.69 40.86 – 1.69	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.86-1.69) 95.8 (40.86-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.177 , 0.213 0.178 , 0.214	Depositor DCC
R_{free} test set	5052 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.103 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8288	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SAM, UK7, 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	0/1776	0.53	0/2390
1	B	0.25	0/1795	0.50	0/2416
1	C	0.28	0/1790	0.50	0/2407
1	D	0.27	0/1809	0.56	0/2432
All	All	0.26	0/7170	0.52	0/9645

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	1739	0	1635	12	0
1	B	1751	0	1647	13	0
1	C	1750	0	1657	7	0
1	D	1765	0	1673	15	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	1	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	27	0	22	1	0
4	B	27	0	22	1	0
4	C	27	0	22	1	0
4	D	27	0	22	1	0
5	A	276	0	0	1	0
5	B	237	0	0	1	0
5	C	272	0	0	3	0
5	D	286	0	0	4	0
All	All	8288	0	6700	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (47) 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:2208:ARG:NH1	5:D:2401:HOH:O	2.26	0.68
1:A:2082:PRO:HB3	1:A:2202:MET:HE1	1.76	0.68
1:B:2097:ASP:H	1:B:2101:ARG:HH21	1.46	0.62
1:D:2144:ARG:NH1	5:D:2403:HOH:O	2.29	0.62
1:D:2095:LYS:NZ	5:D:2407:HOH:O	2.33	0.61
1:B:2097:ASP:N	1:B:2101:ARG:HH21	2.04	0.55
1:C:2102:LYS:HG3	1:C:2129:CYS:HB3	1.88	0.55
1:C:2070:LYS:NZ	5:C:2403:HOH:O	2.34	0.54
1:A:2214:ARG:O	4:A:2305:SAM:HE2	2.09	0.52
1:B:2272[B]:PHE:CE2	1:B:2274:LYS:HB2	2.47	0.50
1:C:2214:ARG:O	4:C:2305:SAM:HE2	2.12	0.49
1:D:2078:VAL:HB	1:D:2174:VAL:HG12	1.95	0.48
1:D:2183:MET:HA	1:D:2187:TYR:HB2	1.96	0.48
1:C:2077:TYR:OH	5:C:2401:HOH:O	2.16	0.48
1:B:2214:ARG:O	4:B:2305:SAM:HE2	2.13	0.48
1:D:2195[B]:CYS:SG	2:D:2301:UK7:N01	2.86	0.48
1:D:2090:THR:HG23	1:D:2123:PRO:HD3	1.96	0.47
1:B:2273:GLU:HG3	1:B:2274:LYS:HG3	1.97	0.47
1:B:2090:THR:HG23	1:B:2123:PRO:HD3	1.97	0.47
1:D:2098:ASP:HB3	1:D:2101:ARG:HG3	1.97	0.46
5:C:2413:HOH:O	1:D:2071:LYS:HE3	2.15	0.46
1:A:2199:ASP:HB3	1:A:2202:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2193:HIS:CE1	1:C:2264:LYS:HE2	2.51	0.46
1:B:2197:ASN:ND2	5:B:2412:HOH:O	2.49	0.46
1:B:2101:ARG:O	1:B:2127:GLN:HB3	2.16	0.45
1:A:2202:MET:HE3	1:A:2202:MET:HB2	1.70	0.45
1:D:2214:ARG:O	4:D:2305:SAM:HE2	2.16	0.45
1:D:2098:ASP:HB3	1:D:2101:ARG:CG	2.47	0.44
1:B:2194:TYR:HB3	1:B:2206:SER:OG	2.16	0.44
1:A:2094:LYS:HD2	1:A:2095:LYS:H	1.83	0.43
1:A:2078:VAL:HB	1:A:2174:VAL:HG12	1.99	0.43
1:A:2095:LYS:NZ	5:A:2401:HOH:O	2.24	0.42
1:A:2183:MET:HA	1:A:2187:TYR:HB2	2.01	0.42
1:A:2222:PRO:HG3	1:A:2254:ASP:HB2	2.01	0.42
1:B:2102:LYS:HB3	1:B:2129:CYS:SG	2.59	0.42
1:D:2112:MET:HA	1:D:2112:MET:HE2	2.00	0.42
1:C:2080:VAL:HB	1:C:2202:MET:HE3	2.02	0.42
1:A:2157:LYS:HA	1:A:2157:LYS:HD2	1.90	0.42
1:D:2276:ARG:NH1	5:D:2419:HOH:O	2.53	0.41
1:A:2095:LYS:HB2	1:A:2124:CYS:HA	2.02	0.41
1:C:2102:LYS:HD2	1:C:2102:LYS:HA	1.76	0.41
1:D:2272[B]:PHE:CE2	1:D:2274:LYS:HB2	2.55	0.41
1:B:2195[A]:CYS:SG	1:B:2260:PHE:HB3	2.61	0.41
1:B:2216:ILE:HD13	1:B:2239:LEU:HD22	2.02	0.41
1:A:2102:LYS:HD3	1:A:2102:LYS:HA	1.79	0.41
1:B:2222:PRO:HG3	1:B:2254:ASP:HB2	2.02	0.40
1:D:2194:TYR:HB3	1:D:2206:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	217/226 (96%)	208 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	220/226 (97%)	212 (96%)	8 (4%)	0	100	100
1	C	219/226 (97%)	211 (96%)	8 (4%)	0	100	100
1	D	220/226 (97%)	209 (95%)	11 (5%)	0	100	100
All	All	876/904 (97%)	840 (96%)	36 (4%)	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	188/197 (95%)	186 (99%)	2 (1%)	65	54
1	B	188/197 (95%)	184 (98%)	4 (2%)	47	30
1	C	189/197 (96%)	189 (100%)	0	100	100
1	D	192/197 (98%)	191 (100%)	1 (0%)	81	76
All	All	757/788 (96%)	750 (99%)	7 (1%)	70	62

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

Mol	Chain	Res	Type
1	A	2094	LYS
1	A	2100	THR
1	B	2102	LYS
1	B	2105	VAL
1	B	2186	GLN
1	B	2191	SER
1	D	2107	ASP

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

Mol	Chain	Res	Type
1	A	2266	GLN

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Mol	Chain	Res	Type
1	B	2266	GLN
1	D	2120	ASN
1	D	2177	GLN
1	D	2266	GLN

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 20 ligands modelled in this entry, 12 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
2	UK7	A	2301	-	25,25,25	2.63	6 (24%)	34,35,35	1.28	3 (8%)
2	UK7	C	2301	-	25,25,25	2.71	6 (24%)	34,35,35	1.28	3 (8%)
4	SAM	D	2305	-	27,29,29	1.09	4 (14%)	34,42,42	1.71	9 (26%)
2	UK7	B	2301	-	25,25,25	2.83	6 (24%)	34,35,35	1.03	2 (5%)
2	UK7	D	2301	-	25,25,25	2.76	6 (24%)	34,35,35	1.09	3 (8%)
4	SAM	B	2305	-	27,29,29	1.03	3 (11%)	34,42,42	1.65	7 (20%)
4	SAM	C	2305	-	27,29,29	1.08	4 (14%)	34,42,42	1.80	8 (23%)
4	SAM	A	2305	-	27,29,29	1.12	4 (14%)	34,42,42	1.79	8 (23%)

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
2	UK7	A	2301	-	-	1/13/13/13	0/3/3/3
2	UK7	C	2301	-	-	1/13/13/13	0/3/3/3
4	SAM	D	2305	-	-	4/17/33/33	0/3/3/3
2	UK7	B	2301	-	-	1/13/13/13	0/3/3/3
2	UK7	D	2301	-	-	1/13/13/13	0/3/3/3
4	SAM	B	2305	-	-	2/17/33/33	0/3/3/3
4	SAM	C	2305	-	-	4/17/33/33	0/3/3/3
4	SAM	A	2305	-	-	4/17/33/33	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2301	UK7	C02-N01	11.99	1.45	1.32
2	D	2301	UK7	C02-N01	11.87	1.45	1.32
2	C	2301	UK7	C02-N01	11.38	1.44	1.32
2	A	2301	UK7	C02-N01	11.19	1.44	1.32
2	B	2301	UK7	C02-S23	-4.25	1.60	1.66
2	D	2301	UK7	C02-S23	-3.95	1.60	1.66
2	C	2301	UK7	C02-S23	-3.91	1.60	1.66
2	A	2301	UK7	C02-S23	-3.30	1.61	1.66
2	B	2301	UK7	C05-C06	2.82	1.53	1.49
2	C	2301	UK7	C05-C06	2.74	1.53	1.49
4	D	2305	SAM	C2-N3	2.73	1.38	1.33
2	D	2301	UK7	C05-C06	2.69	1.53	1.49
4	A	2305	SAM	C8-N7	2.67	1.36	1.31
2	C	2301	UK7	C07-N08	-2.60	1.32	1.36
2	A	2301	UK7	C07-N08	-2.59	1.33	1.36
2	C	2301	UK7	C13-C06	-2.58	1.41	1.47
4	A	2305	SAM	C2-N3	2.57	1.38	1.33
2	A	2301	UK7	C13-C06	-2.57	1.41	1.47
4	B	2305	SAM	C2-N3	2.56	1.38	1.33
2	A	2301	UK7	C05-C06	2.50	1.52	1.49
4	C	2305	SAM	C2-N1	2.49	1.38	1.33
2	B	2301	UK7	C13-C12	-2.47	1.37	1.41
2	A	2301	UK7	C13-C12	-2.46	1.37	1.41
4	D	2305	SAM	C2-N1	2.38	1.38	1.33
4	C	2305	SAM	OXT-C	-2.32	1.23	1.30
2	D	2301	UK7	C13-C06	-2.27	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2305	SAM	OXT-C	-2.24	1.23	1.30
4	C	2305	SAM	C8-N7	2.23	1.36	1.31
2	B	2301	UK7	C13-C06	-2.22	1.42	1.47
4	C	2305	SAM	C2-N3	2.21	1.37	1.33
4	A	2305	SAM	C2-N1	2.21	1.37	1.33
4	B	2305	SAM	C2-N1	2.21	1.37	1.33
4	D	2305	SAM	C8-N7	2.20	1.35	1.31
2	D	2301	UK7	C13-C12	-2.15	1.38	1.41
2	D	2301	UK7	C07-N08	-2.14	1.33	1.36
4	B	2305	SAM	OXT-C	-2.10	1.23	1.30
2	C	2301	UK7	C13-C12	-2.06	1.38	1.41
2	B	2301	UK7	C19-C12	2.06	1.43	1.39
4	A	2305	SAM	OXT-C	-2.02	1.24	1.30

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2305	SAM	N3-C2-N1	-5.52	120.22	128.58
4	A	2305	SAM	N3-C2-N1	-5.25	120.63	128.58
4	B	2305	SAM	N3-C2-N1	-5.11	120.85	128.58
4	D	2305	SAM	N3-C2-N1	-4.99	121.03	128.58
4	A	2305	SAM	C5-C4-N3	-4.00	121.21	126.72
4	D	2305	SAM	C5-C4-N3	-3.93	121.31	126.72
4	C	2305	SAM	N9-C8-N7	-3.91	108.38	113.94
4	A	2305	SAM	N9-C8-N7	-3.84	108.48	113.94
2	A	2301	UK7	C13-C06-C07	3.74	107.96	106.02
2	C	2301	UK7	C13-C06-C07	3.66	107.92	106.02
4	C	2305	SAM	C5-C4-N3	-3.50	121.89	126.72
4	B	2305	SAM	C5-C4-N3	-3.45	121.97	126.72
4	A	2305	SAM	C5-N7-C8	3.09	108.31	103.45
4	B	2305	SAM	N9-C8-N7	-3.06	109.60	113.94
4	A	2305	SAM	C2-N3-C4	3.03	119.22	111.83
4	C	2305	SAM	C5-N7-C8	3.01	108.18	103.45
4	D	2305	SAM	N9-C8-N7	-3.01	109.67	113.94
2	D	2301	UK7	C13-C06-C07	2.94	107.55	106.02
4	C	2305	SAM	C2-N3-C4	2.92	118.97	111.83
4	D	2305	SAM	C2-N3-C4	2.90	118.92	111.83
2	B	2301	UK7	C12-N08-C07	2.87	110.20	108.49
4	D	2305	SAM	C5-N7-C8	2.78	107.82	103.45
2	C	2301	UK7	C12-N08-C07	2.71	110.11	108.49
4	B	2305	SAM	C5-N7-C8	2.71	107.71	103.45
4	B	2305	SAM	C2-N3-C4	2.52	117.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2301	UK7	C12-C13-C06	-2.51	105.40	106.83
2	D	2301	UK7	C12-N08-C07	2.49	109.98	108.49
4	D	2305	SAM	OXT-C-O	-2.45	118.52	124.08
4	A	2305	SAM	C4-C5-N7	-2.40	107.83	110.58
4	B	2305	SAM	OXT-C-O	-2.40	118.64	124.08
4	C	2305	SAM	C4-N9-C8	2.32	108.17	105.74
2	B	2301	UK7	C13-C06-C07	2.30	107.22	106.02
4	D	2305	SAM	C4-C5-N7	-2.28	107.98	110.58
4	B	2305	SAM	N3-C4-N9	2.27	131.02	127.17
4	D	2305	SAM	O4'-C1'-N9	-2.24	103.79	108.09
4	C	2305	SAM	C4-C5-N7	-2.23	108.03	110.58
4	C	2305	SAM	N3-C4-N9	2.18	130.88	127.17
4	D	2305	SAM	N3-C4-N9	2.18	130.88	127.17
4	A	2305	SAM	N3-C4-N9	2.12	130.78	127.17
2	A	2301	UK7	C12-N08-C07	2.10	109.74	108.49
2	C	2301	UK7	C03-C02-N01	2.10	119.26	116.25
2	D	2301	UK7	C03-C02-N01	2.07	119.22	116.25
4	A	2305	SAM	C5-C4-N9	2.01	108.01	105.81

There are no chirality outliers.

All (18) torsion outliers are listed below:

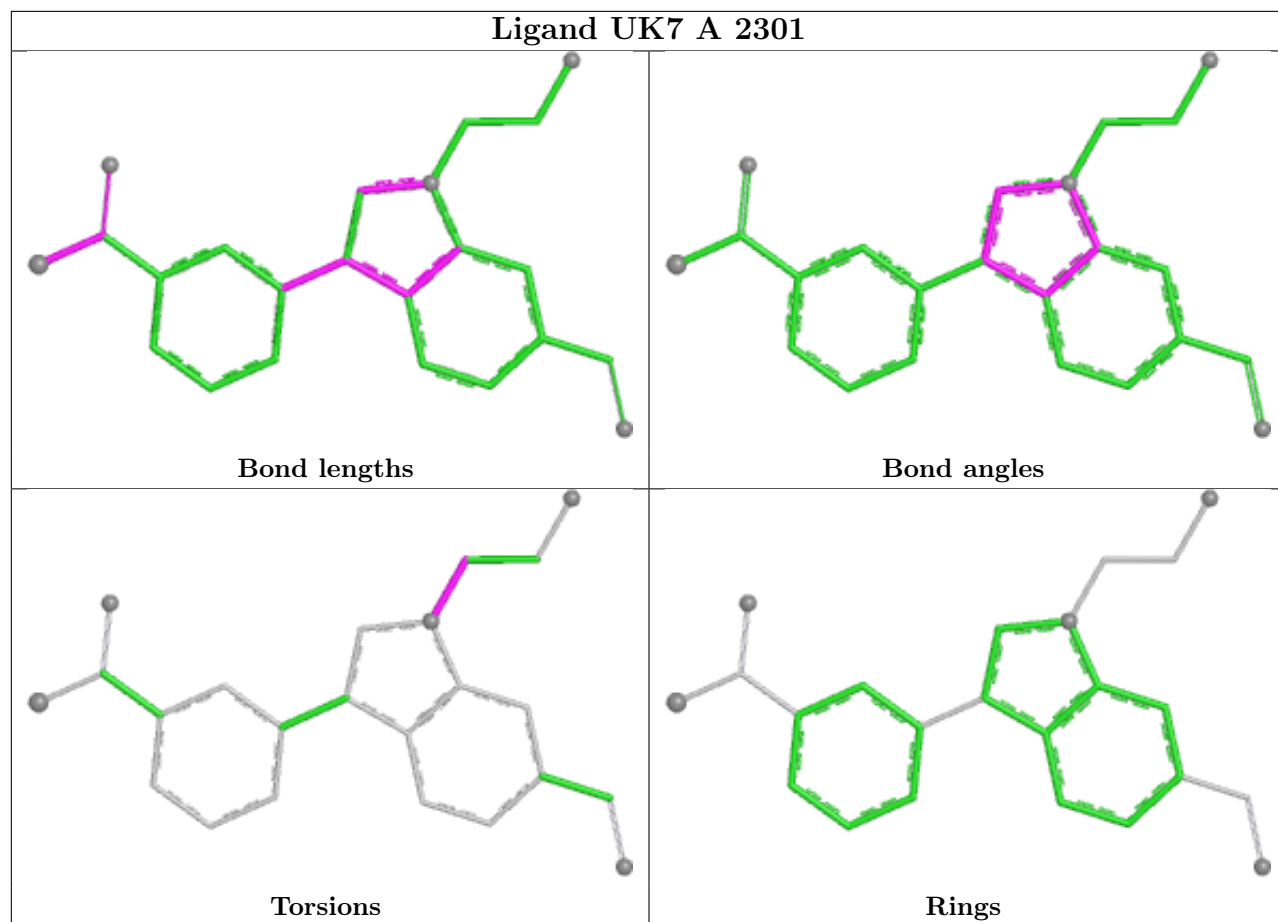
Mol	Chain	Res	Type	Atoms
2	B	2301	UK7	C10-C09-N08-C07
2	C	2301	UK7	C10-C09-N08-C07
4	A	2305	SAM	CB-CG-SD-CE
4	A	2305	SAM	CB-CG-SD-C5'
4	B	2305	SAM	CB-CG-SD-CE
4	B	2305	SAM	CB-CG-SD-C5'
4	C	2305	SAM	CB-CG-SD-CE
4	C	2305	SAM	CB-CG-SD-C5'
4	D	2305	SAM	CB-CG-SD-CE
4	D	2305	SAM	CB-CG-SD-C5'
2	A	2301	UK7	C10-C09-N08-C12
2	D	2301	UK7	C10-C09-N08-C12
4	C	2305	SAM	O-C-CA-CB
4	D	2305	SAM	O-C-CA-CB
4	C	2305	SAM	OXT-C-CA-CB
4	D	2305	SAM	OXT-C-CA-CB
4	A	2305	SAM	OXT-C-CA-CB
4	A	2305	SAM	O-C-CA-CB

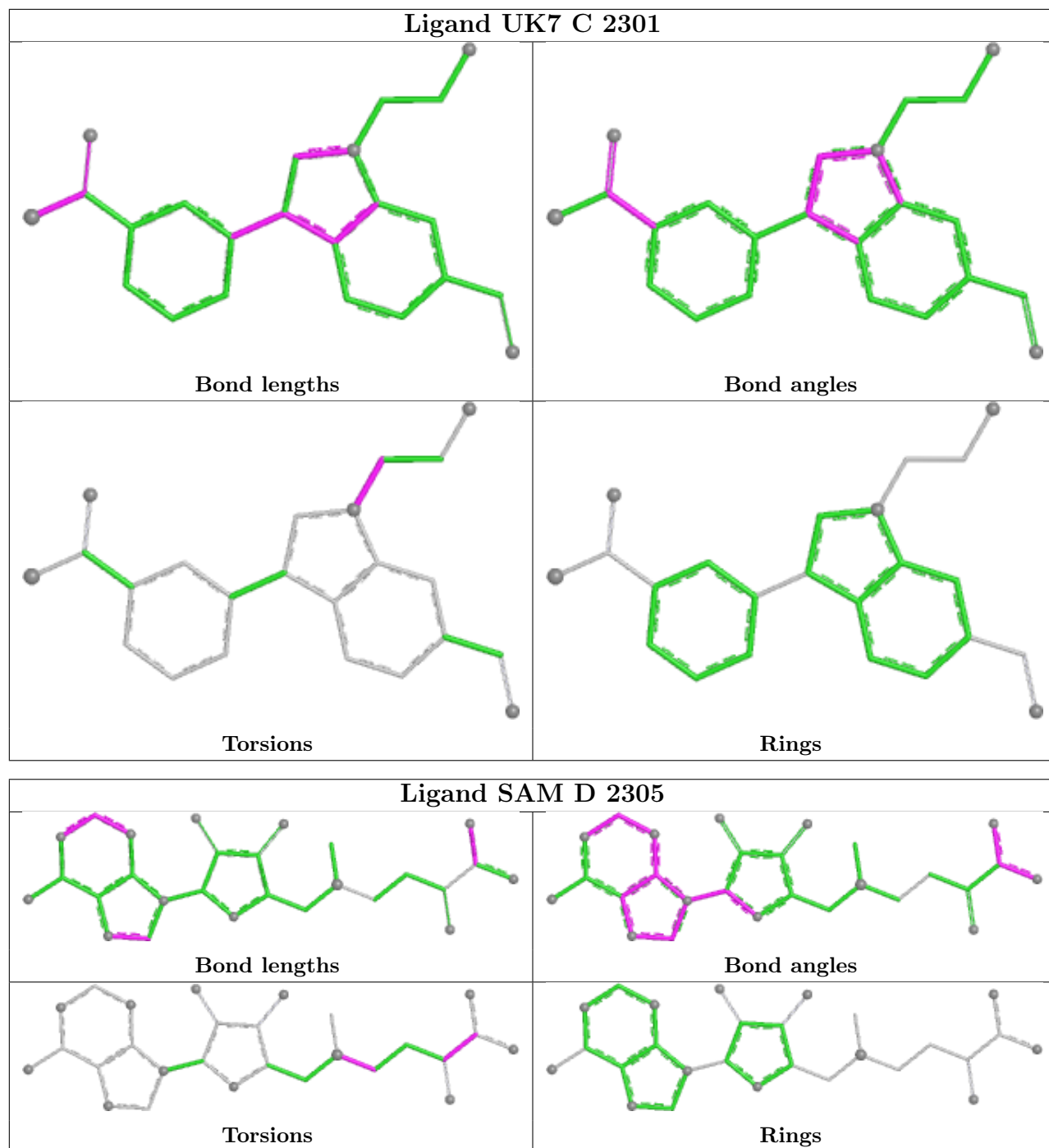
There are no ring outliers.

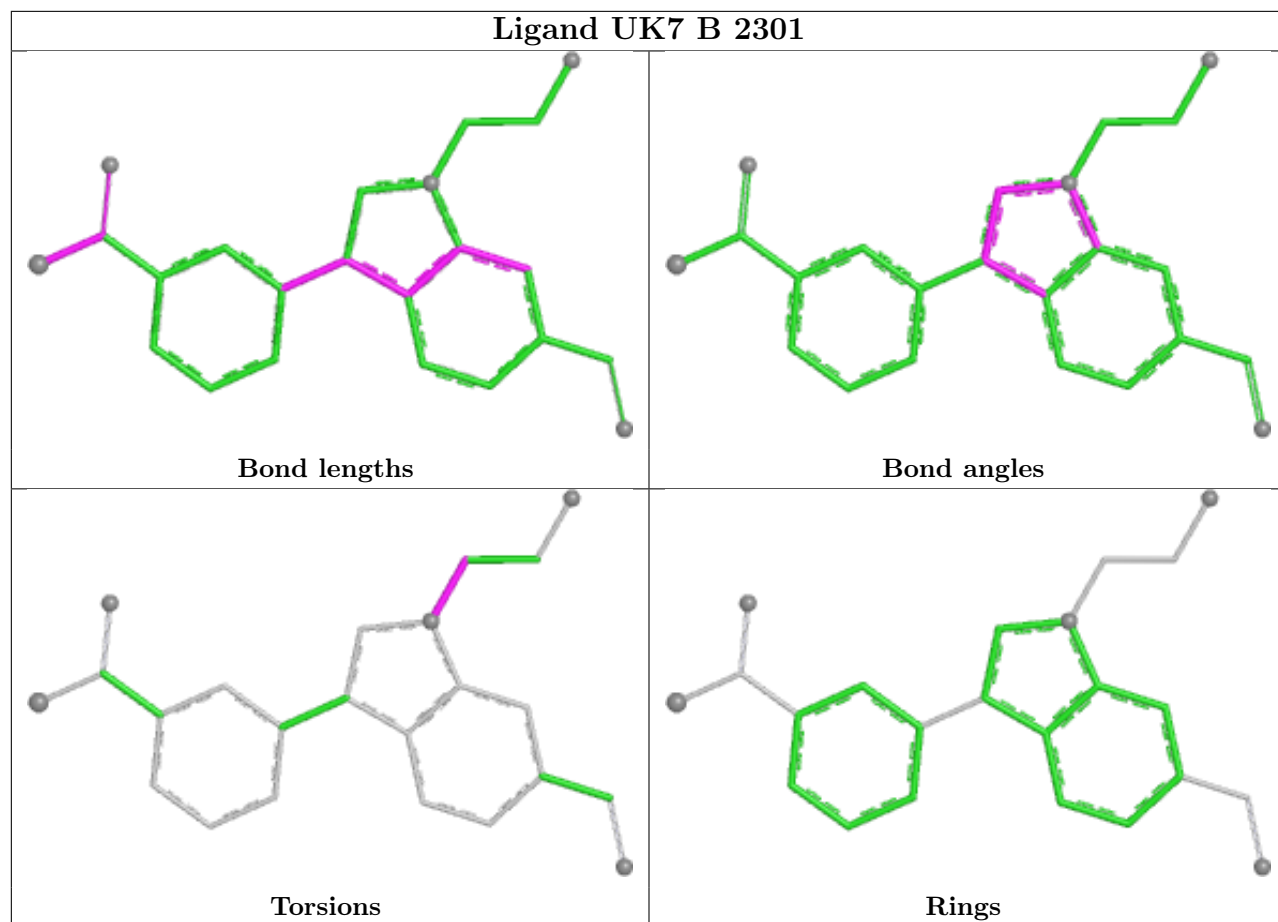
5 monomers are involved in 5 short contacts:

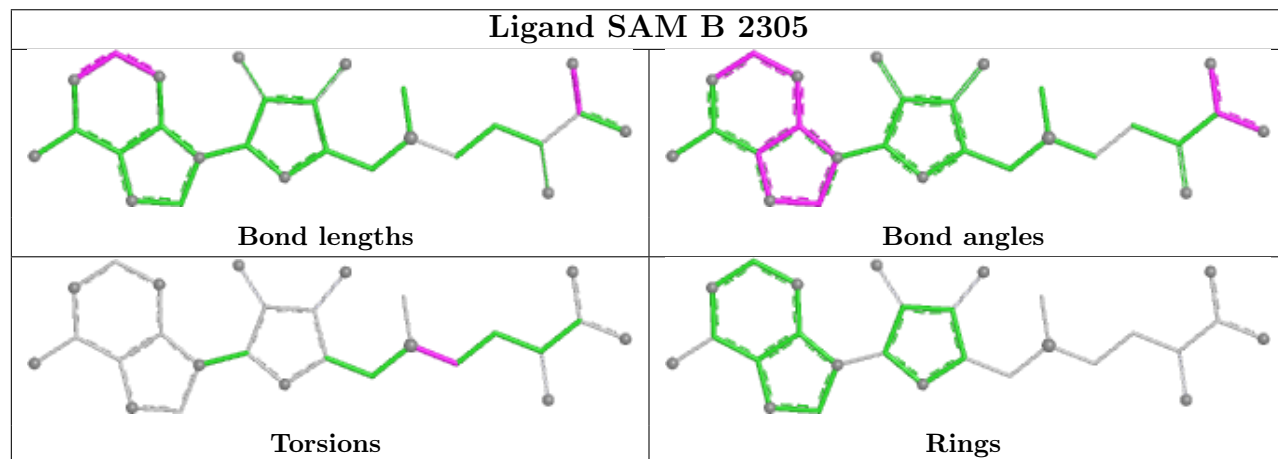
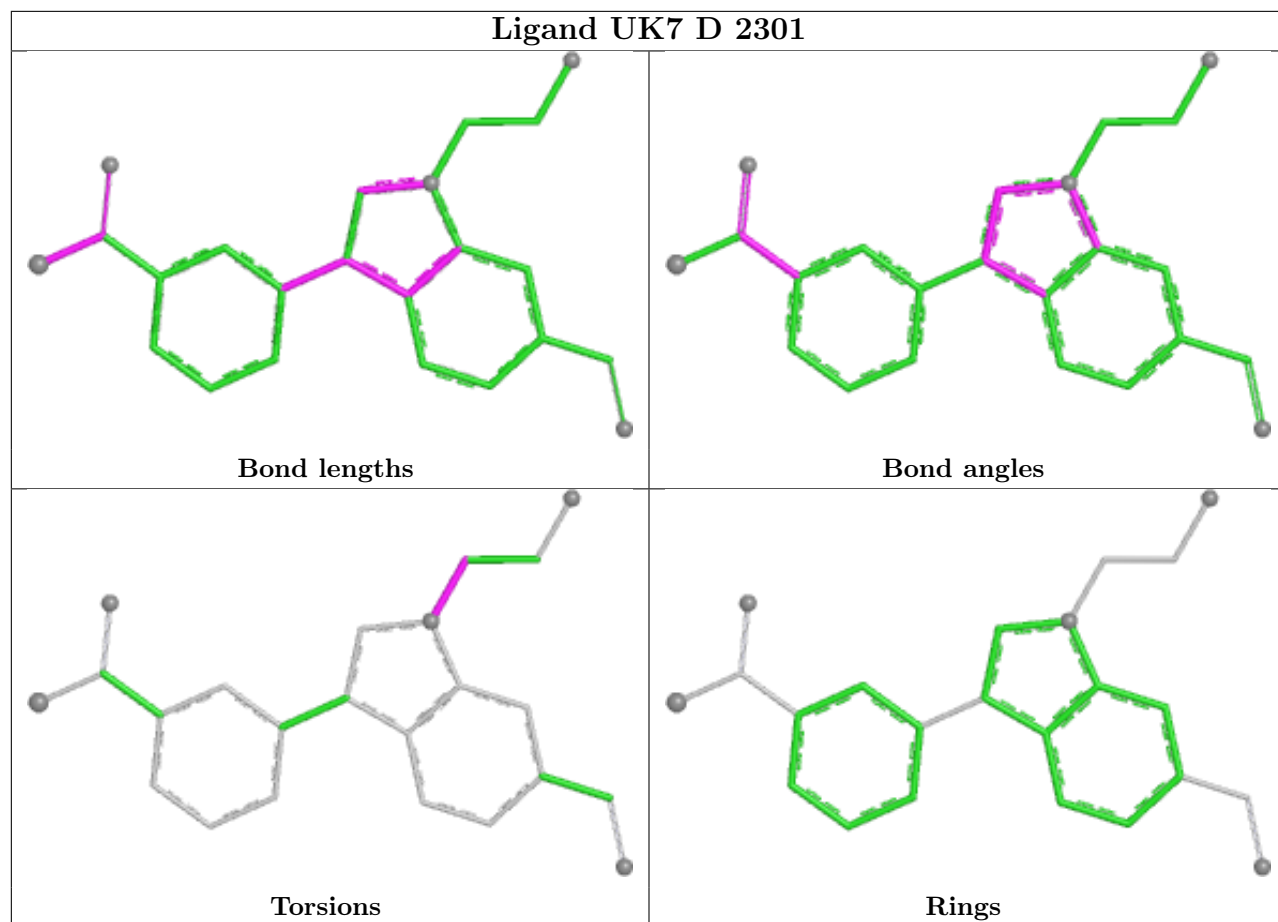
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2305	SAM	1	0
2	D	2301	UK7	1	0
4	B	2305	SAM	1	0
4	C	2305	SAM	1	0
4	A	2305	SAM	1	0

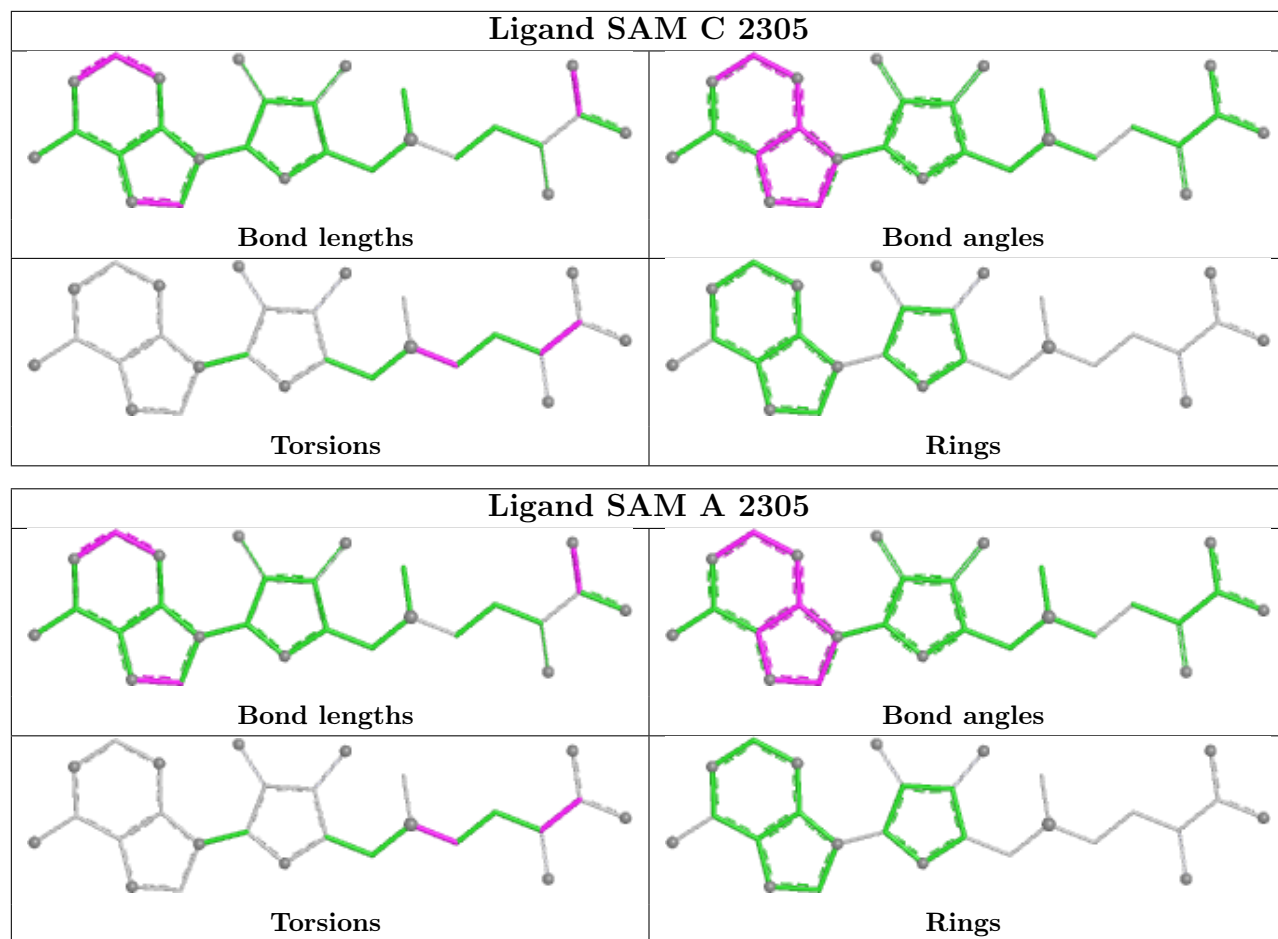
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	219/226 (96%)	0.04	6 (2%) 56 60	7, 15, 33, 49	0
1	B	220/226 (97%)	0.43	27 (12%) 8 8	8, 17, 40, 55	2 (0%)
1	C	220/226 (97%)	0.06	10 (4%) 38 42	7, 15, 32, 48	1 (0%)
1	D	220/226 (97%)	0.09	8 (3%) 46 50	7, 15, 32, 41	2 (0%)
All	All	879/904 (97%)	0.15	51 (5%) 29 32	7, 15, 35, 55	5 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2088	ALA	4.8
1	C	2087	GLU	4.3
1	B	2096	PRO	4.0
1	C	2086	TYR	3.6
1	B	2099	ASP	3.3
1	C	2085	GLY	3.2
1	B	2184	ILE	3.2
1	B	2105	VAL	3.1
1	B	2123	PRO	3.1
1	B	2098	ASP	3.1
1	B	2100	THR	3.0
1	B	2103	GLY	2.9
1	B	2095	LYS	2.9
1	B	2197	ASN	2.9
1	C	2105	VAL	2.8
1	B	2106	ASP	2.8
1	D	2201	GLY	2.7
1	A	2189	ASN	2.7
1	D	2186	GLN	2.7
1	A	2184	ILE	2.7
1	B	2200	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2125	GLY	2.6
1	B	2124	CYS	2.6
1	D	2189	ASN	2.5
1	B	2097	ASP	2.5
1	C	2097	ASP	2.5
1	B	2121	THR	2.5
1	B	2104	CYS	2.5
1	A	2100	THR	2.5
1	D	2200	SER	2.5
1	C	2181	ASN	2.4
1	B	2101	ARG	2.4
1	D	2099	ASP	2.4
1	D	2188	HIS	2.4
1	A	2181	ASN	2.4
1	D	2272[A]	PHE	2.4
1	B	2107	ASP	2.3
1	B	2189	ASN	2.3
1	A	2183	MET	2.2
1	B	2127	GLN	2.2
1	B	2086	TYR	2.2
1	A	2096	PRO	2.2
1	C	2100	THR	2.2
1	B	2201	GLY	2.1
1	D	2097	ASP	2.1
1	C	2101	ARG	2.1
1	B	2188	HIS	2.1
1	B	2280	GLY	2.1
1	B	2102	LYS	2.1
1	B	2066	ALA	2.0
1	C	2098	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

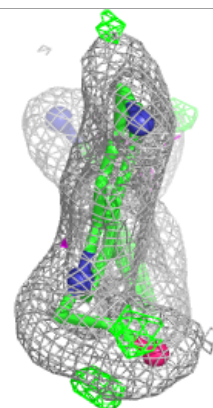
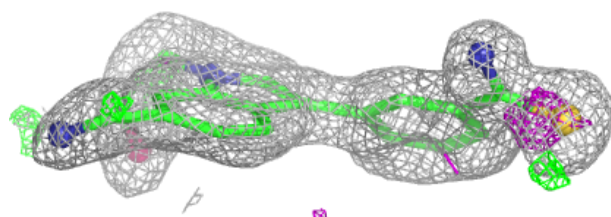
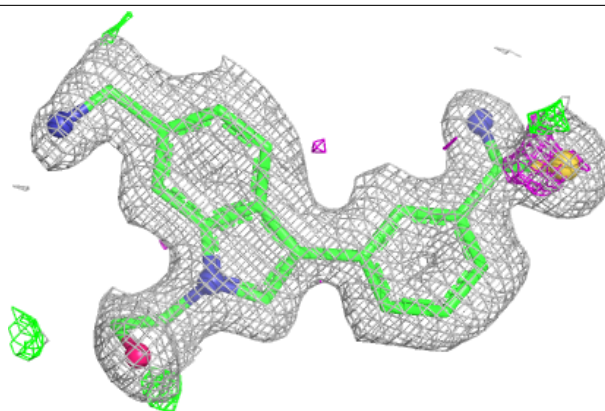
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UK7	C	2301	23/23	0.94	0.08	10,14,20,24	0
2	UK7	D	2301	23/23	0.94	0.07	13,16,18,24	0
2	UK7	A	2301	23/23	0.95	0.07	9,13,20,21	0
2	UK7	B	2301	23/23	0.95	0.08	13,17,23,27	0
3	ZN	B	2303	1/1	0.96	0.04	19,19,19,19	0
3	ZN	B	2302	1/1	0.98	0.04	18,18,18,18	0
4	SAM	A	2305	27/27	0.98	0.05	6,9,11,16	0
4	SAM	B	2305	27/27	0.98	0.05	8,11,15,16	0
4	SAM	C	2305	27/27	0.98	0.05	7,10,11,13	0
4	SAM	D	2305	27/27	0.98	0.05	7,10,13,15	0
3	ZN	A	2303	1/1	0.99	0.02	13,13,13,13	0
3	ZN	B	2304	1/1	0.99	0.02	11,11,11,11	0
3	ZN	C	2303	1/1	0.99	0.01	12,12,12,12	0
3	ZN	C	2304	1/1	0.99	0.02	11,11,11,11	0
3	ZN	D	2303	1/1	1.00	0.02	13,13,13,13	0
3	ZN	D	2304	1/1	1.00	0.01	10,10,10,10	0
3	ZN	C	2302	1/1	1.00	0.01	14,14,14,14	0
3	ZN	A	2304	1/1	1.00	0.02	11,11,11,11	0
3	ZN	A	2302	1/1	1.00	0.02	15,15,15,15	0
3	ZN	D	2302	1/1	1.00	0.01	13,13,13,13	0

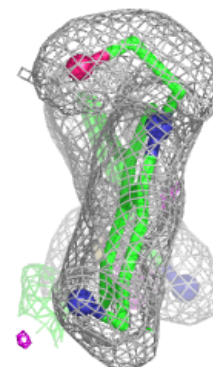
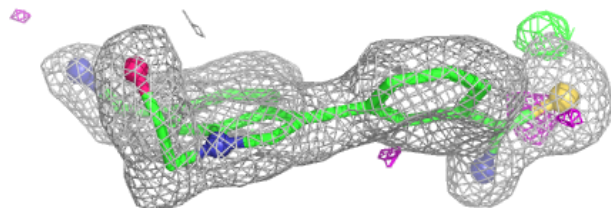
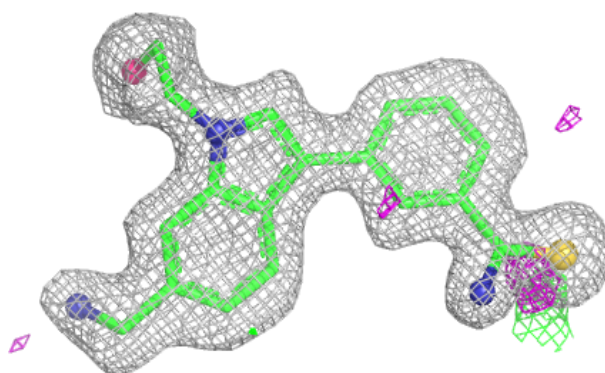
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UK7 C 2301:

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

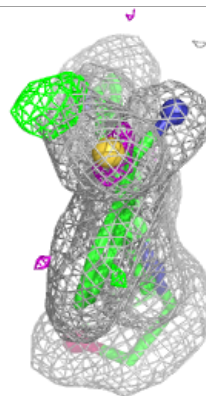
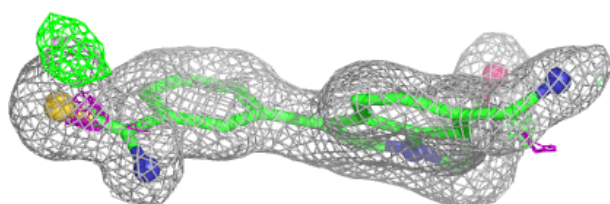
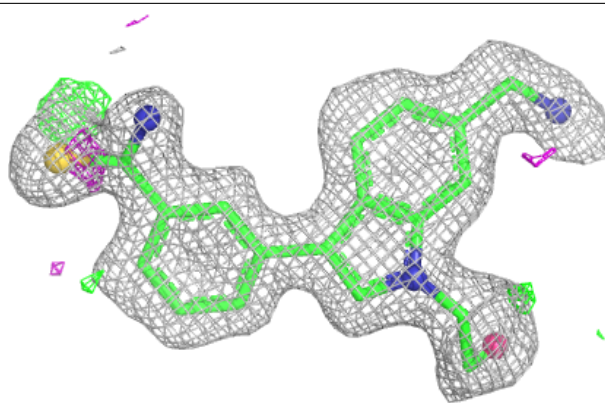
**Electron density around UK7 D 2301:**

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

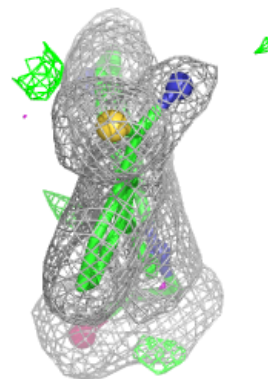
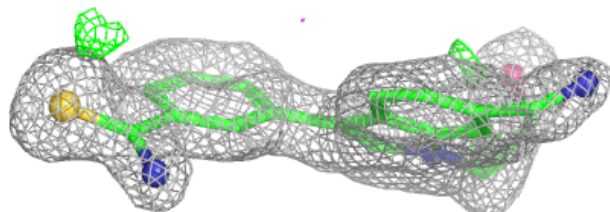
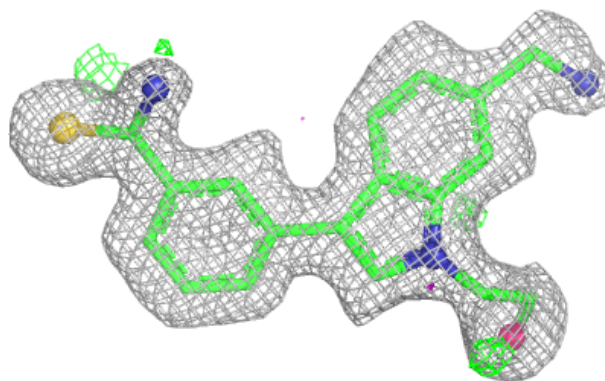


Electron density around UK7 A 2301:

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

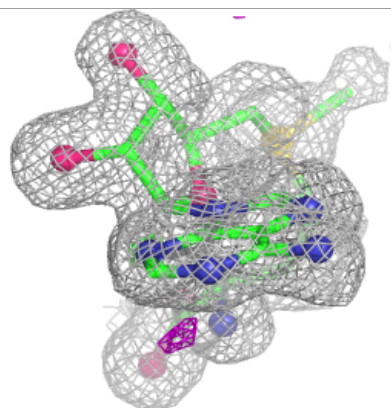
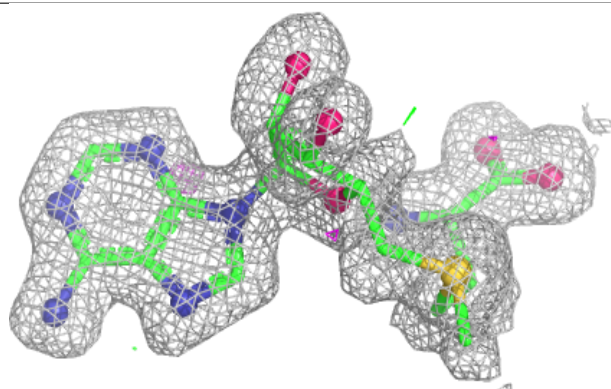
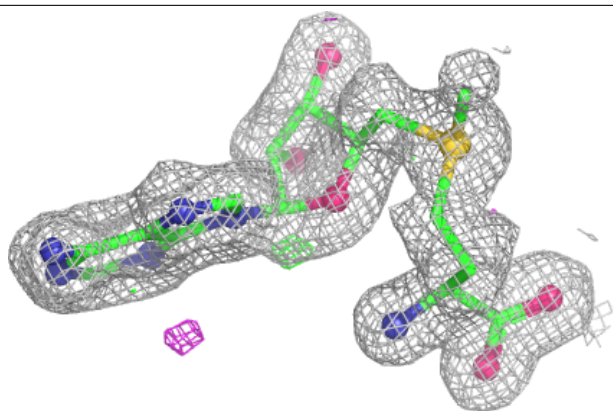
**Electron density around UK7 B 2301:**

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

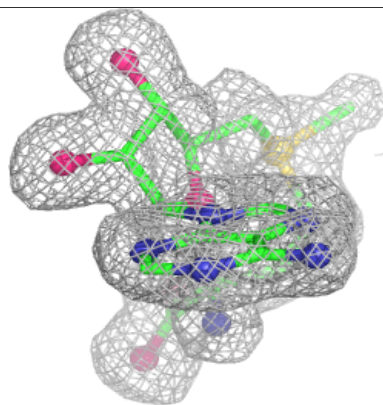
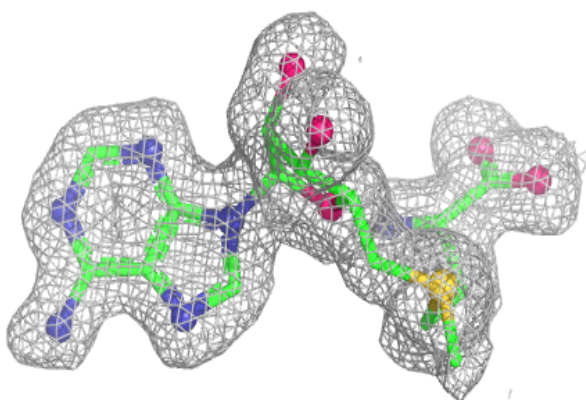
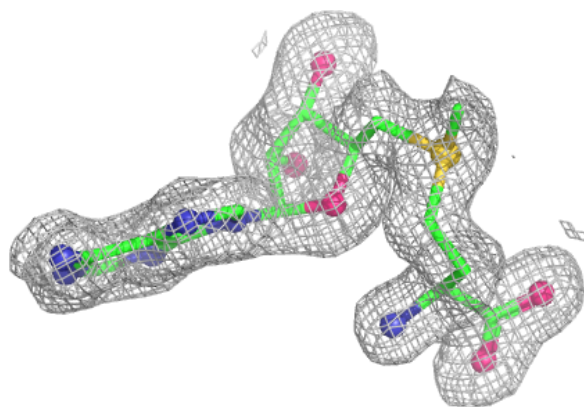


Electron density around SAM A 2305:

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

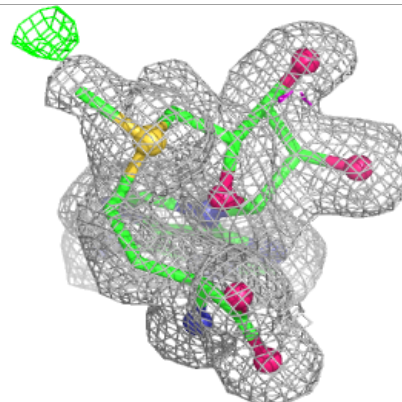
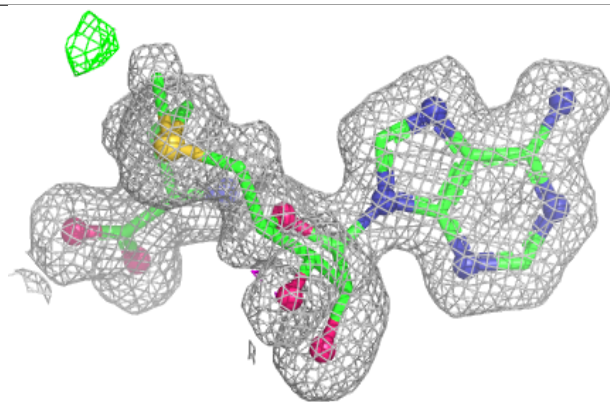
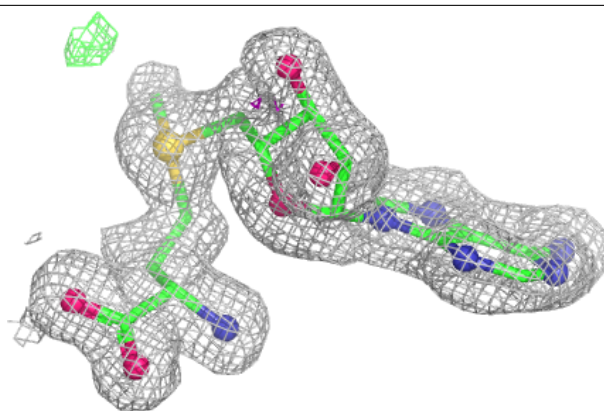
**Electron density around SAM B 2305:**

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

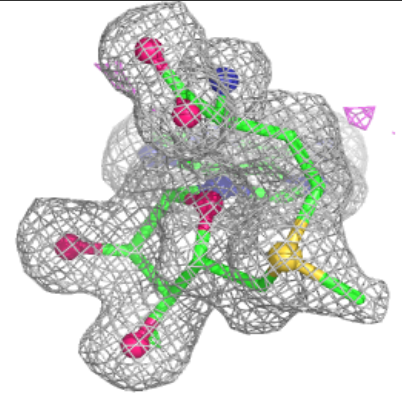
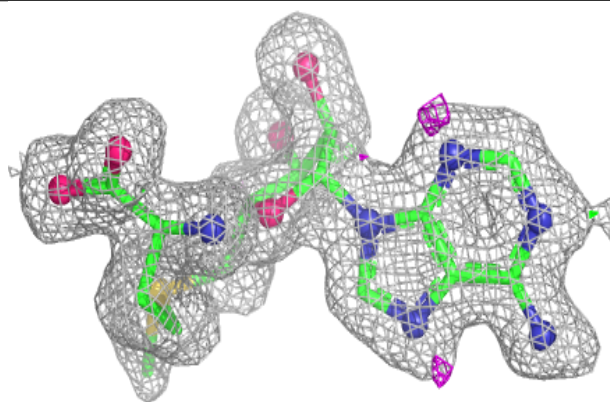
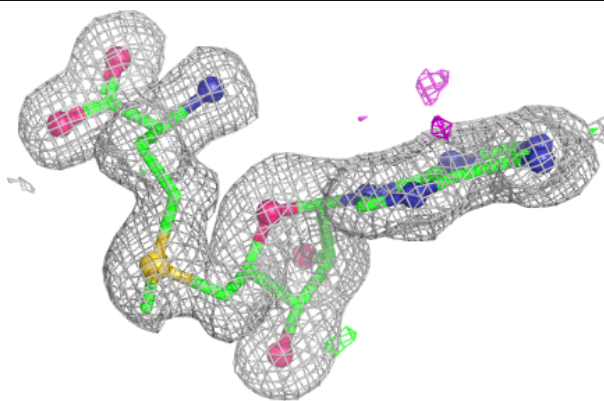


Electron density around SAM C 2305:

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

**Electron density around SAM D 2305:**

$2mF_o-DF_c$ (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.