



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 07:10 am BST

PDB ID : 6B1U
Title : Structure of full-length human AMPK (a2b1g1) in complex with a small molecule activator SC4
Authors : Ngoei, K.R.W.; Langendorf, C.G.; Ling, N.X.Y.; Hoque, A.; Johnson, S.; Camerino, M.C.; Walker, S.R.; Bozikis, Y.E.; Dite, T.A.; Ovens, A.J.; Smiles, W.J.; Jacobs, R.; Huang, H.; Parker, M.W.; Scott, J.W.; Rider, M.H.; Kemp, B.E.; Foitzik, R.C.; Baell, J.B.; Oakhill, J.S.
Deposited on : 2017-09-19
Resolution : 2.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.11
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) : 2.11

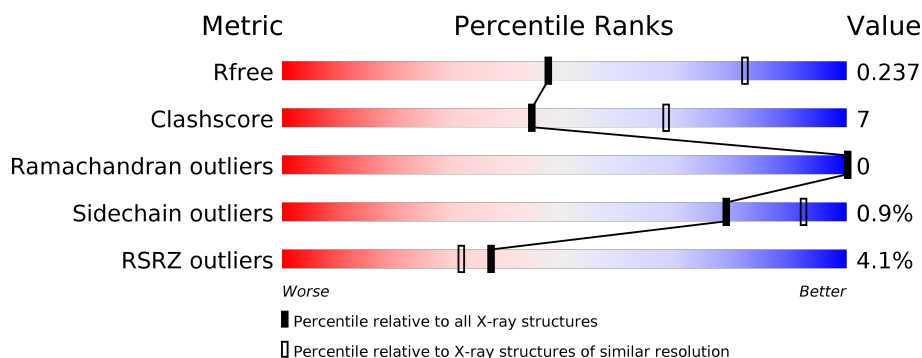
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on 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	565	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>22%</div> </div> </div>
1	C	565	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>8%</div> <div>19%</div> </div> </div>
2	B	270	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>8%</div> <div>32%</div> </div> </div>
2	D	270	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>9%</div> <div>33%</div> </div> </div>
3	E	336	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>11%</div> </div> </div>
3	F	336	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14977 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 5'-AMP-activated protein kinase catalytic subunit alpha-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	P	S	0	0	0
			3456	2221	588	622	1	24			
1	C	460	Total	C	N	O	P	S	0	0	0
			3585	2295	610	654	1	25			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP P54646
A	-11	GLY	-	expression tag	UNP P54646
A	-10	SER	-	expression tag	UNP P54646
A	-9	SER	-	expression tag	UNP P54646
A	-8	HIS	-	expression tag	UNP P54646
A	-7	HIS	-	expression tag	UNP P54646
A	-6	HIS	-	expression tag	UNP P54646
A	-5	HIS	-	expression tag	UNP P54646
A	-4	HIS	-	expression tag	UNP P54646
A	-3	HIS	-	expression tag	UNP P54646
A	-2	SER	-	expression tag	UNP P54646
A	-1	GLN	-	expression tag	UNP P54646
A	0	ASP	-	expression tag	UNP P54646
A	1	PRO	-	expression tag	UNP P54646
A	271	GLY	ASP	conflict	UNP P54646
C	-12	MET	-	initiating methionine	UNP P54646
C	-11	GLY	-	expression tag	UNP P54646
C	-10	SER	-	expression tag	UNP P54646
C	-9	SER	-	expression tag	UNP P54646
C	-8	HIS	-	expression tag	UNP P54646
C	-7	HIS	-	expression tag	UNP P54646
C	-6	HIS	-	expression tag	UNP P54646
C	-5	HIS	-	expression tag	UNP P54646
C	-4	HIS	-	expression tag	UNP P54646
C	-3	HIS	-	expression tag	UNP P54646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP P54646
C	-1	GLN	-	expression tag	UNP P54646
C	0	ASP	-	expression tag	UNP P54646
C	1	PRO	-	expression tag	UNP P54646
C	271	GLY	ASP	conflict	UNP P54646

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	P	S	0	0	0
			1401	904	232	259	1	5			
2	D	182	Total	C	N	O	P	S	0	0	0
			1423	916	235	265	1	6			

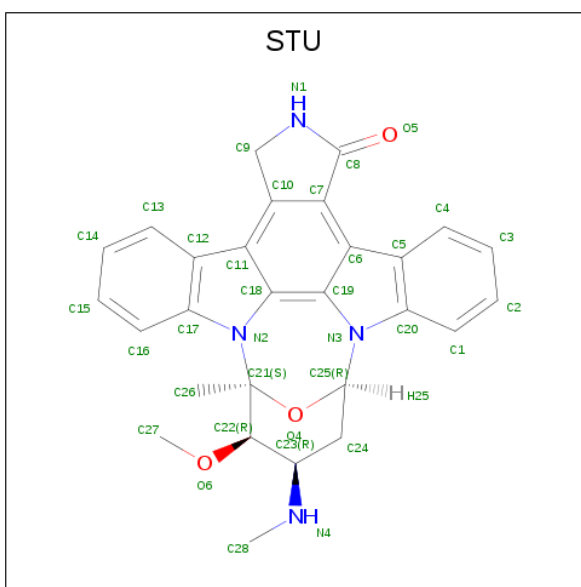
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	299	Total	C	N	O	S	0	0	0
			2332	1522	383	420	7			
3	F	299	Total	C	N	O	S	0	0	0
			2340	1525	389	419	7			

There are 12 discrepancies between the modelled and reference sequences:

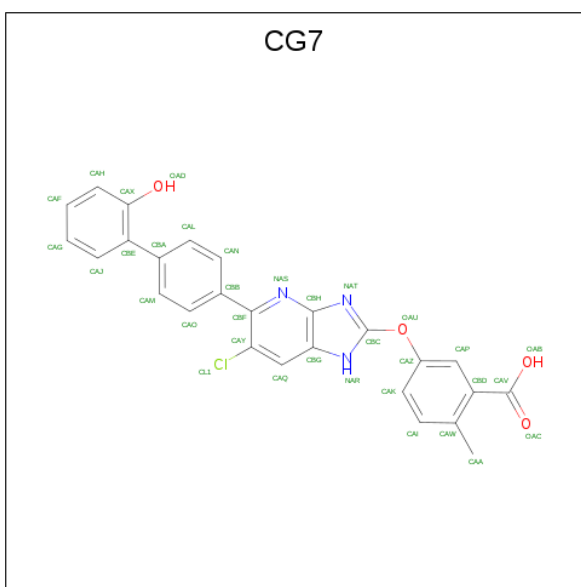
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine	UNP P54619
F	-3	ALA	-	expression tag	UNP P54619
F	-2	ASP	-	expression tag	UNP P54619
F	-1	LEU	-	expression tag	UNP P54619
F	0	ASN	-	expression tag	UNP P54619
F	1	TRP	-	expression tag	UNP P54619

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: C₂₈H₂₆N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	C	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 5 is 5-{[6-chloro-5-(2'-hydroxy[1,1'-biphenyl]-4-yl)-1H-imidazo[4,5-b]pyridin-2-yl]oxy}-2-methylbenzoic acid (three-letter code: CG7) (formula: C₂₆H₁₈ClN₃O₄) (labeled as "Ligand of Interest" by author).



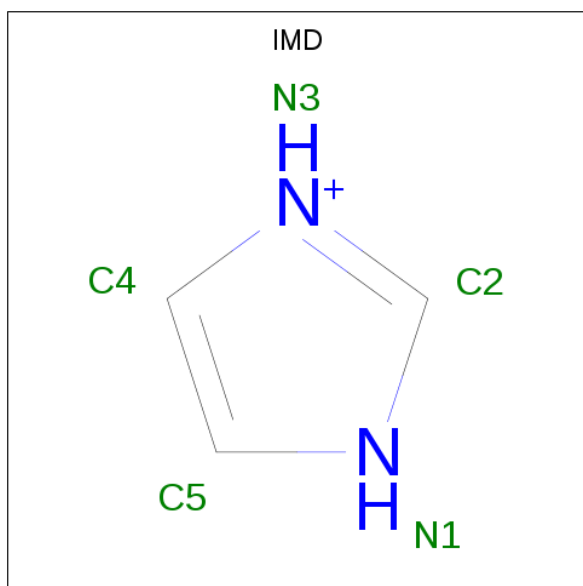
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0
			68	52	2	6	8	

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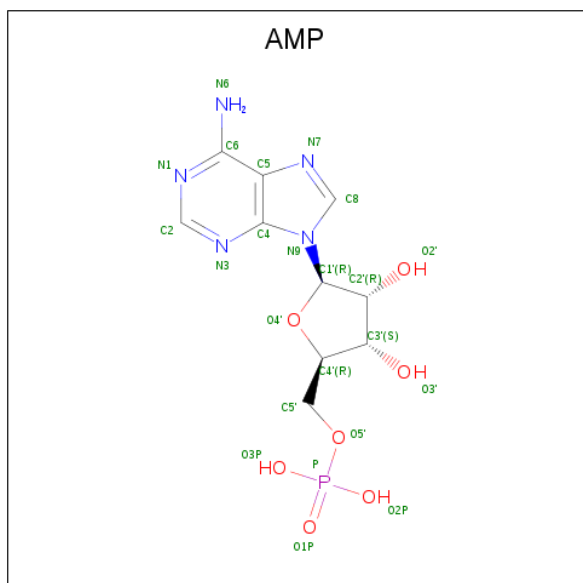
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Cl	N	O	0	0
			34	26	1	3	4		

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			5	3	2		

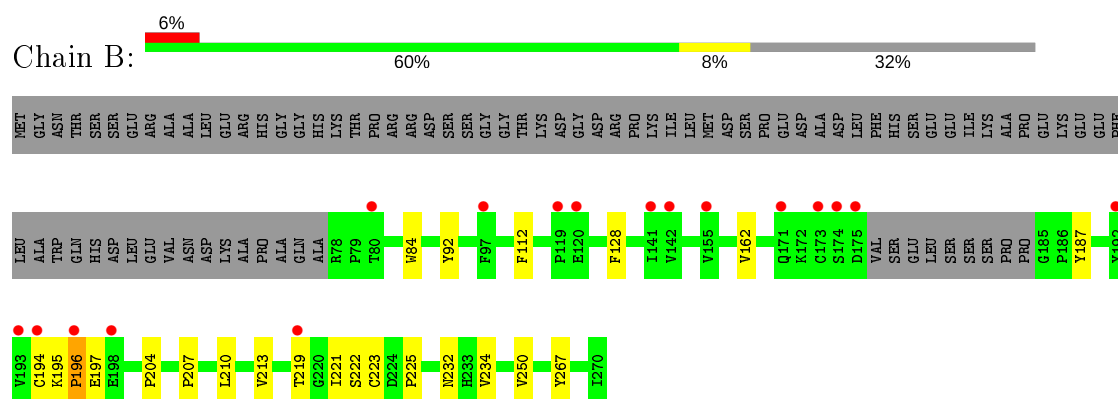
- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



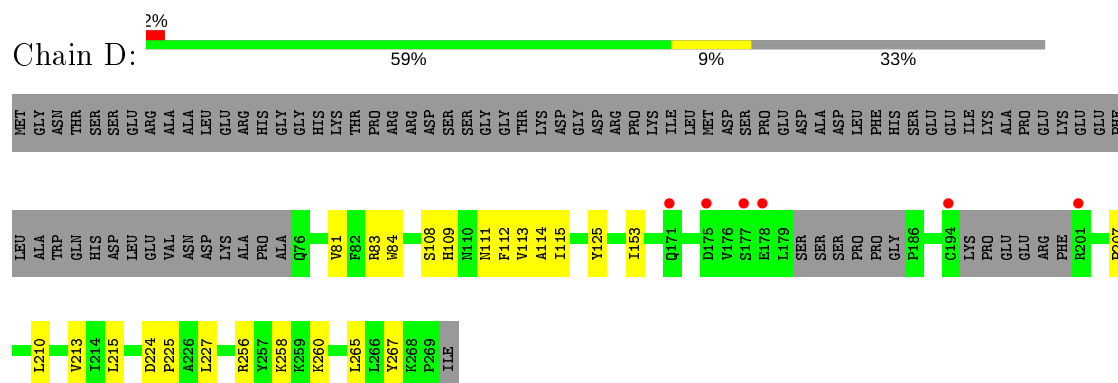
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 8 is water.

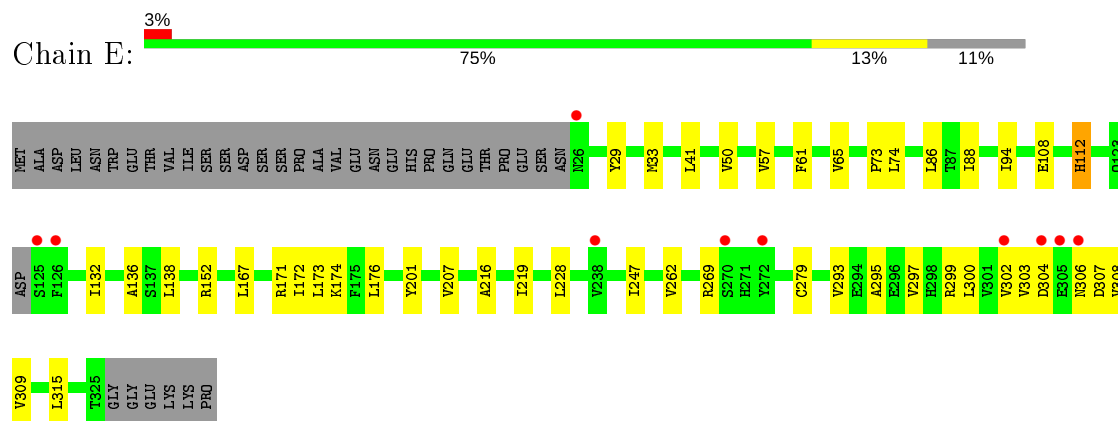
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	48	Total	O	0	0
			48	48		
8	B	5	Total	O	0	0
			5	5		
8	C	37	Total	O	0	0
			37	37		
8	D	22	Total	O	0	0
			22	22		
8	E	35	Total	O	0	0
			35	35		
8	F	24	Total	O	0	0
			24	24		



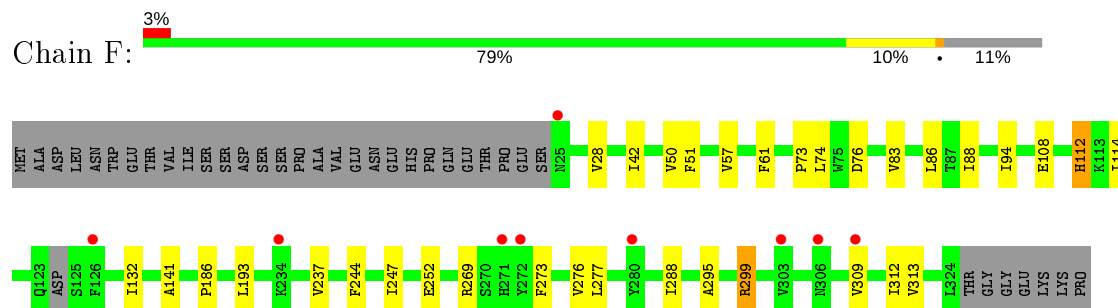
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.83Å 133.90Å 141.72Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	48.64 – 2.77 48.64 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.64-2.77) 99.8 (48.64-2.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.194 , 0.226 0.211 , 0.237	Depositor DCC
R_{free} test set	3627 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, SEP, TPO, STU, AMP, CG7

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	0.38	0/3523	0.57	0/4771
1	C	0.39	0/3659	0.58	0/4963
2	B	0.41	1/1432 (0.1%)	0.61	1/1965 (0.1%)
2	D	0.38	0/1453	0.58	0/1987
3	E	0.39	0/2381	0.57	0/3244
3	F	0.39	0/2388	0.57	0/3250
All	All	0.39	1/14836 (0.0%)	0.58	1/20180 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	196	PRO	N-CD	5.12	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	LYS	C-N-CD	5.64	140.25	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3456	0	3339	48	0
1	C	3585	0	3440	38	1
2	B	1401	0	1310	30	0
2	D	1423	0	1351	16	0
3	E	2332	0	2339	41	1
3	F	2340	0	2358	30	0
4	A	35	0	26	12	0
4	C	35	0	26	5	0
5	A	68	0	0	4	0
5	C	34	0	0	2	0
6	C	5	0	5	0	0
7	E	46	0	24	4	0
7	F	46	0	24	1	0
8	A	48	0	0	0	0
8	B	5	0	0	0	0
8	C	37	0	0	0	0
8	D	22	0	0	0	0
8	E	35	0	0	0	0
8	F	24	0	0	0	0
All	All	14977	0	14242	192	1

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 7.

The worst 5 of 192 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:185:ILE:CD1	1:C:226:ILE:HD12	1.66	1.24
1:C:185:ILE:HD13	1:C:226:ILE:CD1	1.76	1.15
3:E:303:VAL:HG11	3:E:307:ASP:HA	1.44	0.98
1:A:365:PRO:HB3	2:B:221:ILE:CG2	1.93	0.97
1:A:370:MET:HE2	3:E:65:VAL:HA	1.46	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:HIS:O	3:E:309:VAL:N[1_445]	2.01	0.19

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	429/565 (76%)	420 (98%)	9 (2%)	0	100	100
1	C	451/565 (80%)	442 (98%)	9 (2%)	0	100	100
2	B	179/270 (66%)	175 (98%)	4 (2%)	0	100	100
2	D	175/270 (65%)	171 (98%)	4 (2%)	0	100	100
3	E	295/336 (88%)	289 (98%)	6 (2%)	0	100	100
3	F	295/336 (88%)	290 (98%)	5 (2%)	0	100	100
All	All	1824/2342 (78%)	1787 (98%)	37 (2%)	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	358/497 (72%)	357 (100%)	1 (0%)	92	97
1	C	373/497 (75%)	368 (99%)	5 (1%)	69	89
2	B	146/239 (61%)	144 (99%)	2 (1%)	67	87
2	D	154/239 (64%)	154 (100%)	0	100	100
3	E	254/308 (82%)	250 (98%)	4 (2%)	62	86
3	F	255/308 (83%)	253 (99%)	2 (1%)	81	93
All	All	1540/2088 (74%)	1526 (99%)	14 (1%)	78	92

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	453	LEU
1	C	455	ASP
3	E	299	ARG
1	C	345	SER
3	E	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	HIS
1	A	450	GLN
1	C	335	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SEP	D	108	2	8,9,10	1.01	0	8,12,14	1.60	1 (12%)
2	SEP	B	108	2	8,9,10	0.86	0	8,12,14	1.51	1 (12%)
1	TPO	C	172	1	8,10,11	0.85	0	10,14,16	1.02	1 (10%)
1	TPO	A	172	1	8,10,11	1.09	0	10,14,16	1.41	1 (10%)

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	SEP	D	108	2	-	1/5/8/10	-
2	SEP	B	108	2	-	0/5/8/10	-
1	TPO	C	172	1	-	2/9/11/13	-
1	TPO	A	172	1	-	0/9/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	108	SEP	OG-CB-CA	3.49	111.55	108.14
2	B	108	SEP	O3P-P-OG	2.75	114.04	106.73
1	A	172	TPO	O2P-P-O1P	-2.10	102.45	110.68
1	C	172	TPO	O-C-CA	-2.04	119.42	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	108	SEP	N-CA-CB-OG
1	C	172	TPO	C-CA-CB-CG2
1	C	172	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	108	SEP	2	0
1	A	172	TPO	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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
7	AMP	E	401	-	22,25,25	1.09	2 (9%)	25,38,38	1.40	5 (20%)
6	IMD	C	603	-	3,5,5	0.39	0	4,5,5	0.72	0
5	CG7	A	602[B]	-	35,38,38	2.65	6 (17%)	39,55,55	1.33	5 (12%)
5	CG7	A	602[A]	-	35,38,38	2.64	6 (17%)	39,55,55	1.32	5 (12%)
7	AMP	F	402	-	22,25,25	1.06	1 (4%)	25,38,38	1.56	6 (24%)
7	AMP	F	401	-	22,25,25	1.09	2 (9%)	25,38,38	1.45	5 (20%)
7	AMP	E	402	-	22,25,25	1.05	1 (4%)	25,38,38	1.43	3 (12%)
4	STU	A	601	-	30,42,42	2.52	10 (33%)	31,68,68	2.45	13 (41%)
4	STU	C	601	-	30,42,42	2.53	10 (33%)	31,68,68	2.44	12 (38%)
5	CG7	C	602	-	35,38,38	2.66	6 (17%)	39,55,55	1.33	5 (12%)

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
7	AMP	E	401	-	-	1/6/26/26	0/3/3/3
6	IMD	C	603	-	-	-	0/1/1/1
5	CG7	A	602[B]	-	-	1/10/16/16	0/5/5/5
5	CG7	A	602[A]	-	-	0/10/16/16	0/5/5/5
7	AMP	F	402	-	-	1/6/26/26	0/3/3/3
7	AMP	F	401	-	-	3/6/26/26	0/3/3/3
7	AMP	E	402	-	-	3/6/26/26	0/3/3/3
4	STU	A	601	-	-	4/4/42/42	-
4	STU	C	601	-	-	2/4/42/42	-
5	CG7	C	602	-	-	0/10/16/16	0/5/5/5

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602[B]	CG7	CBB-CBF	-8.50	1.39	1.49
5	C	602	CG7	CBB-CBF	-8.44	1.39	1.49
5	A	602[A]	CG7	CBB-CBF	-8.42	1.39	1.49
5	C	602	CG7	CBD-CAV	-8.05	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602[A]	CG7	CBD-CAV	-7.92	1.39	1.47

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C7-C8-N1	5.51	111.95	106.37
4	C	601	STU	C7-C8-N1	5.45	111.89	106.37
4	A	601	STU	C9-N1-C8	-5.09	108.95	113.85
4	C	601	STU	C9-N1-C8	-5.06	108.98	113.85
4	A	601	STU	O5-C8-C7	-4.46	124.02	129.32

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	401	AMP	C5'-O5'-P-O1P
7	F	401	AMP	C5'-O5'-P-O2P
7	E	402	AMP	C5'-O5'-P-O1P
7	E	402	AMP	C5'-O5'-P-O2P
4	A	601	STU	C23-C22-O6-C27

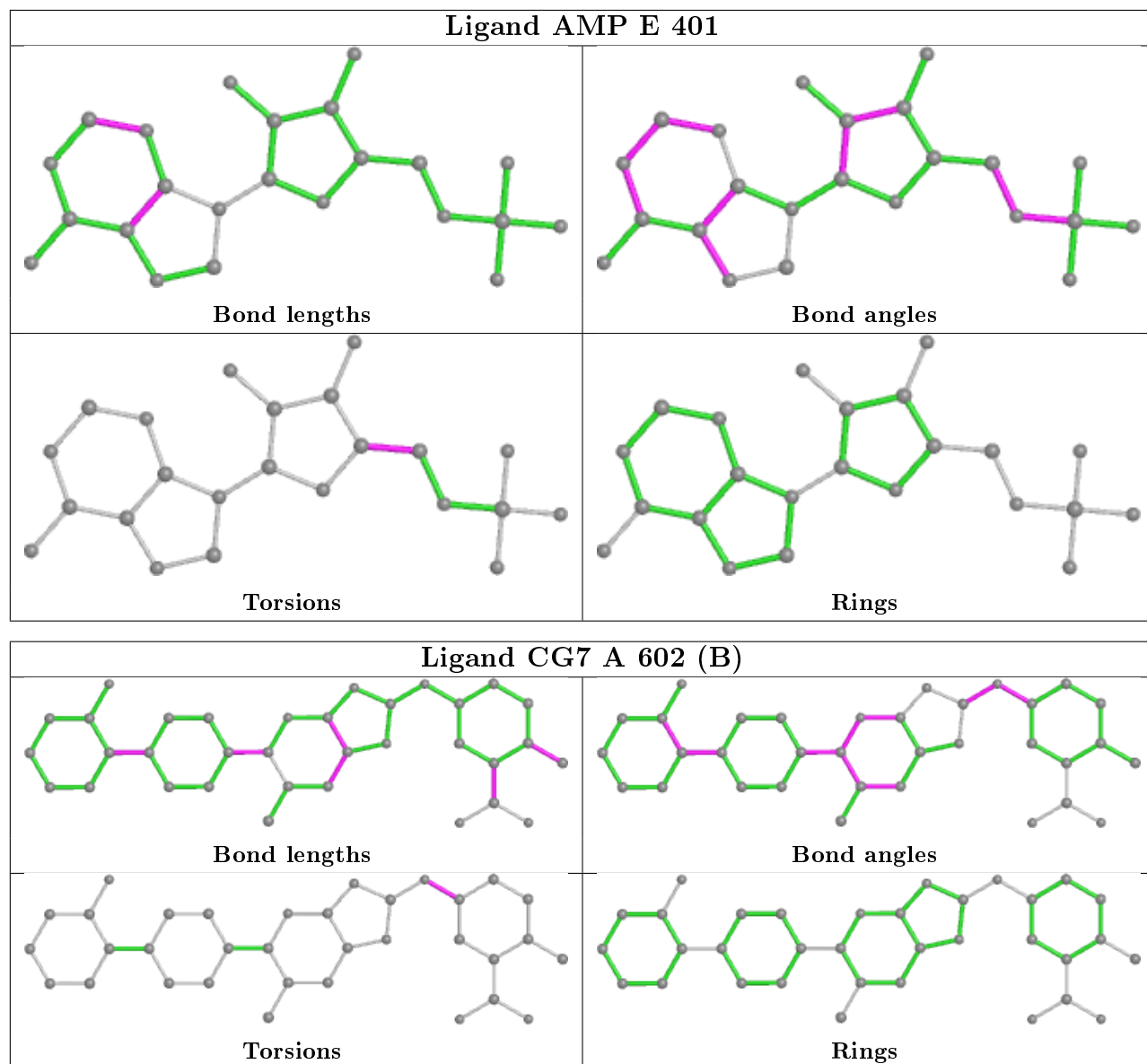
There are no ring outliers.

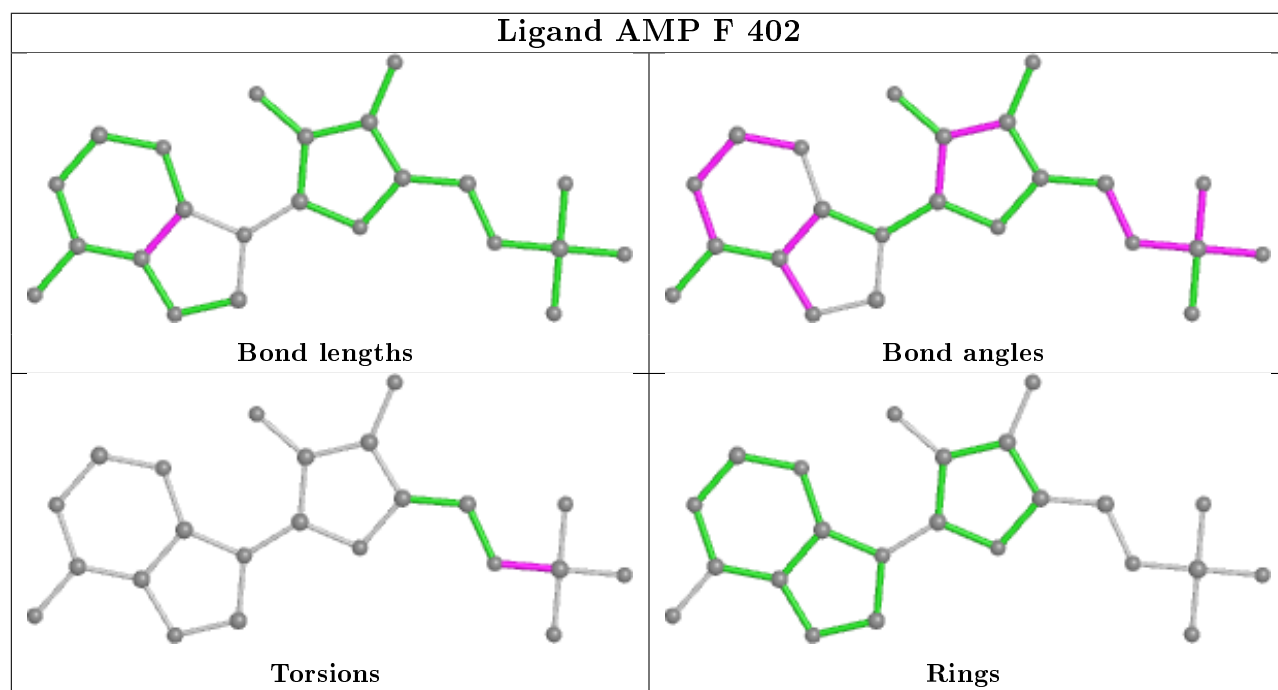
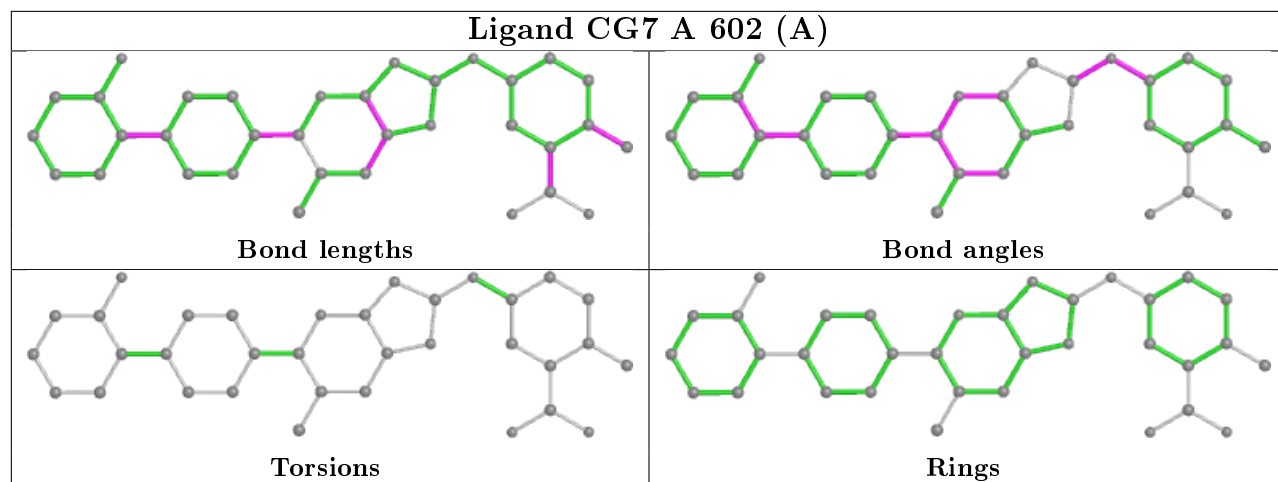
7 monomers are involved in 28 short contacts:

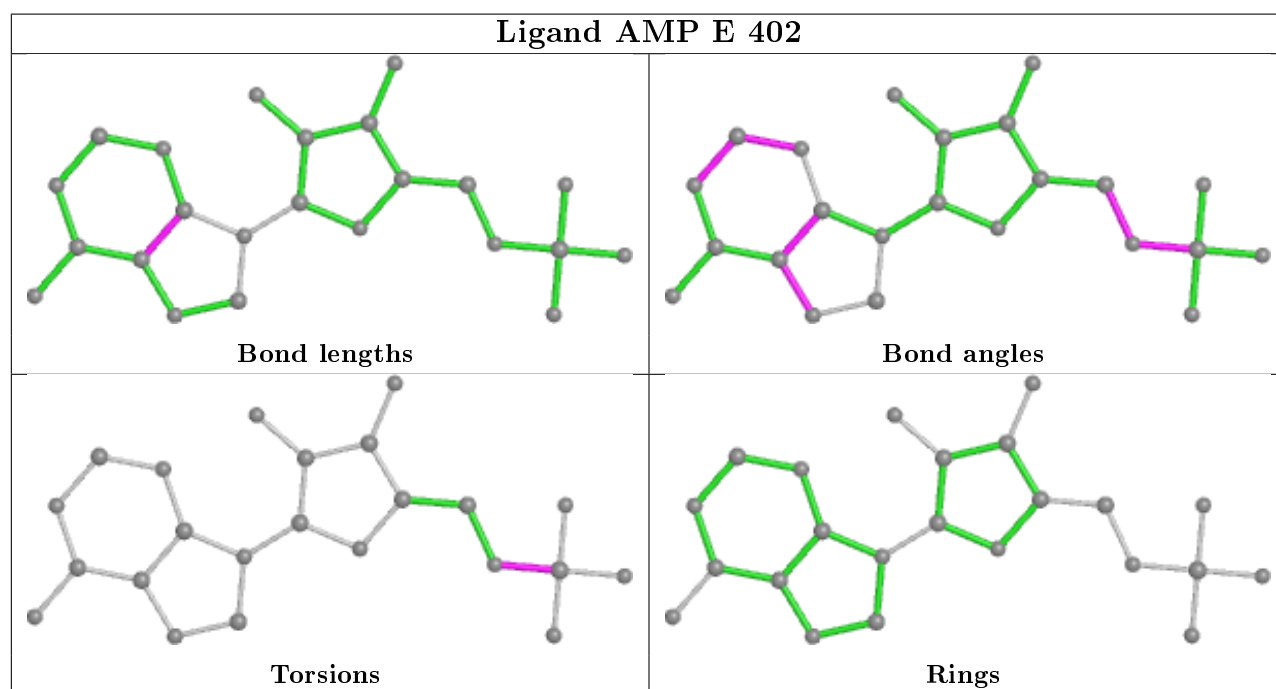
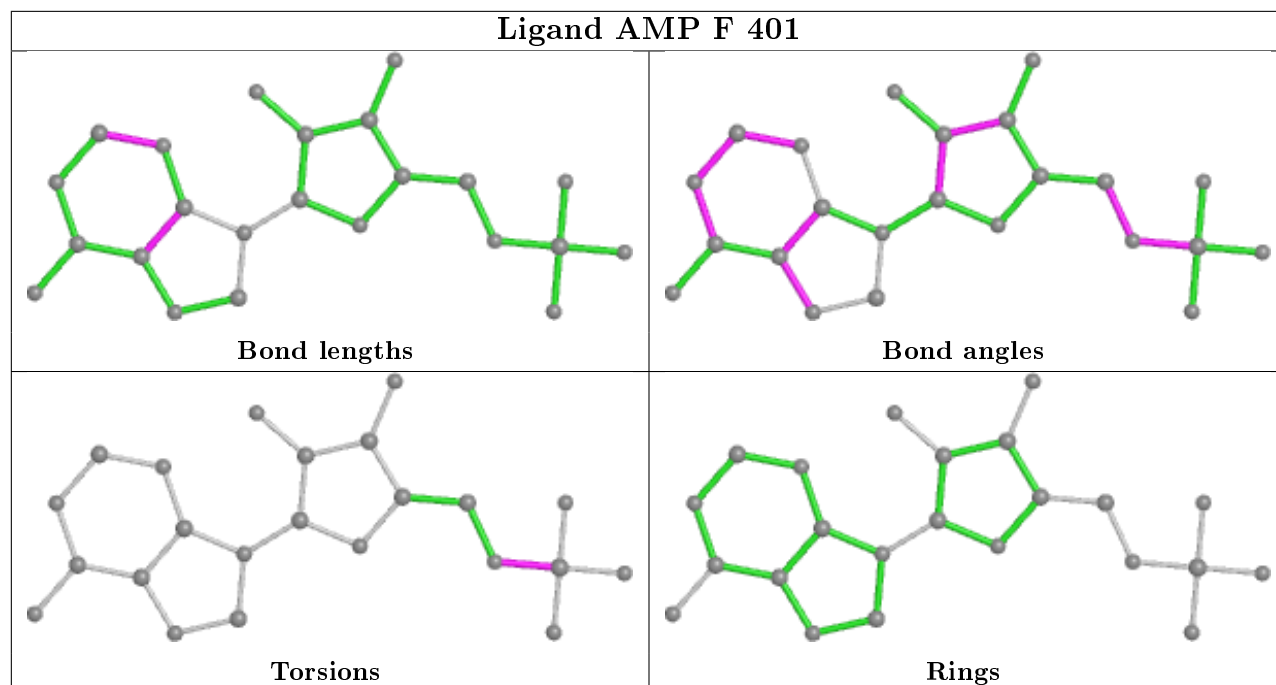
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	401	AMP	4	0
5	A	602[B]	CG7	3	0
5	A	602[A]	CG7	1	0
7	F	402	AMP	1	0
4	A	601	STU	12	0
4	C	601	STU	5	0
5	C	602	CG7	2	0

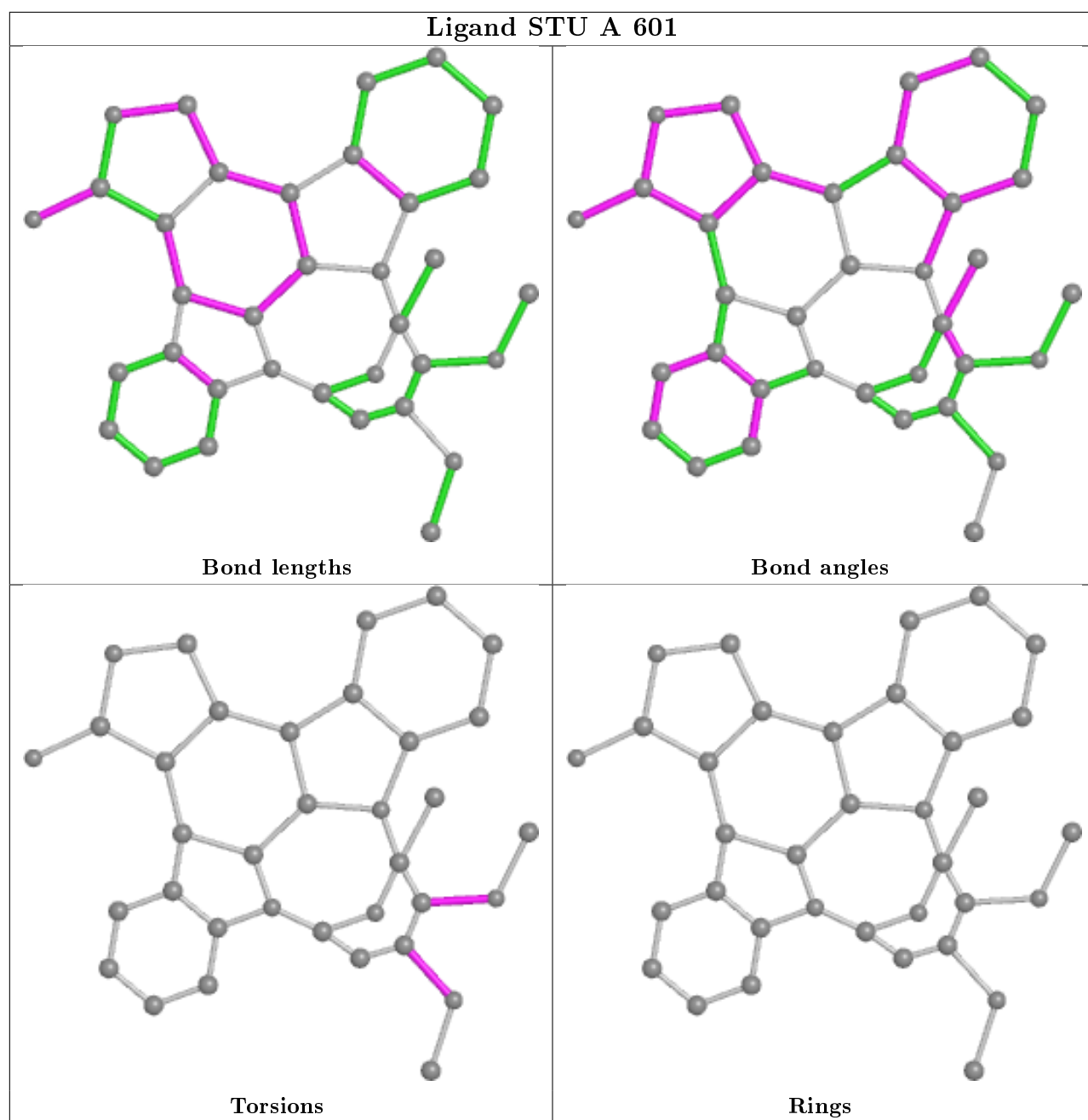
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

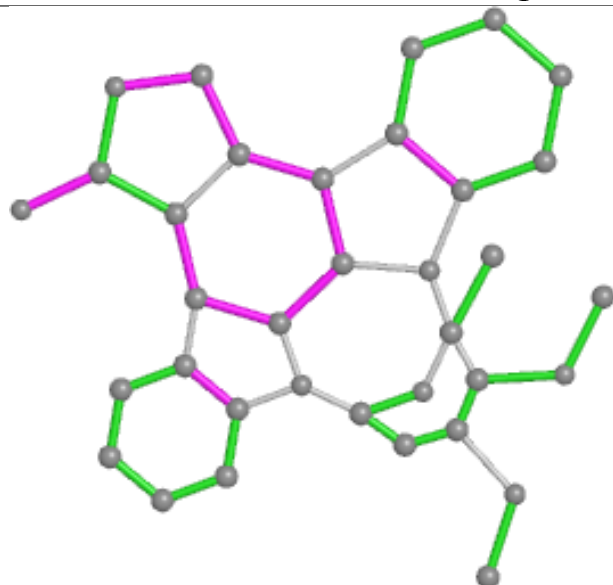




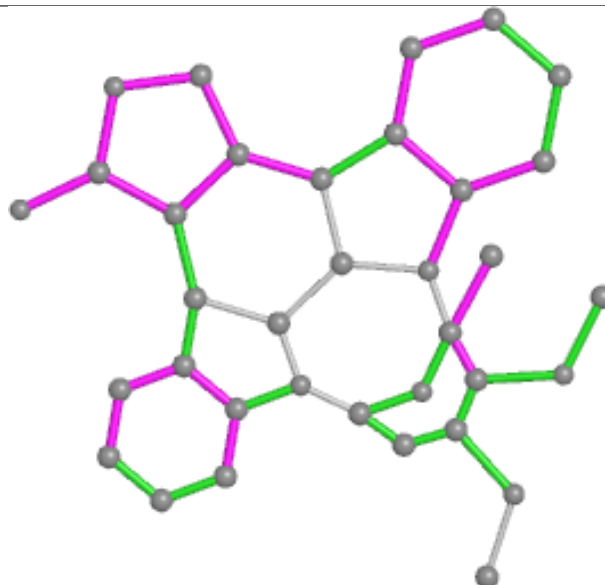




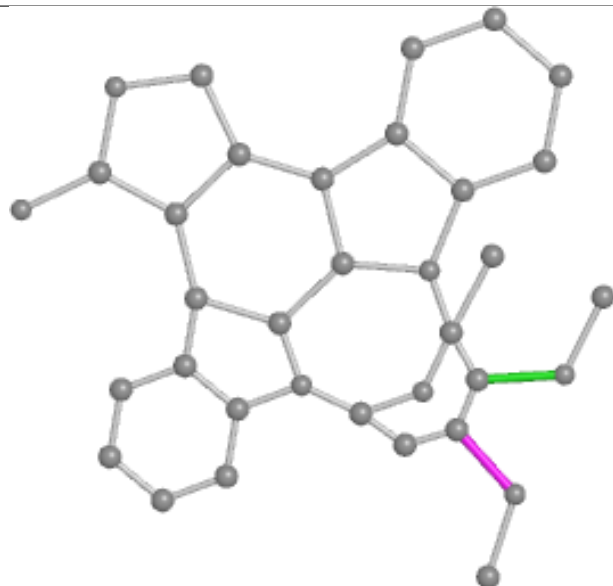
Ligand STU C 601



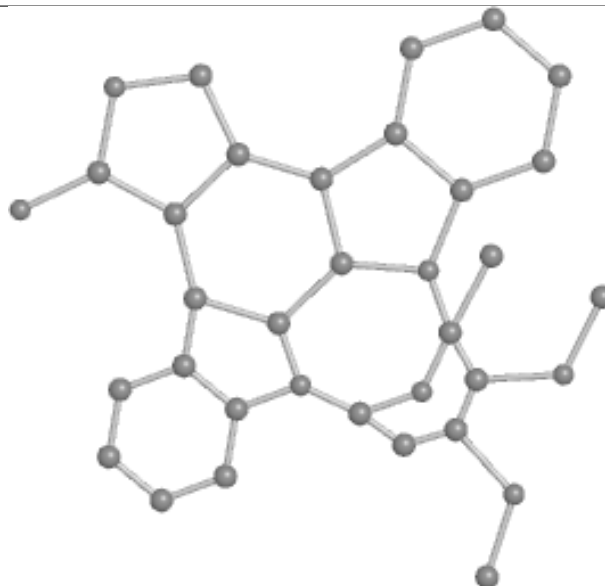
Bond lengths



Bond angles

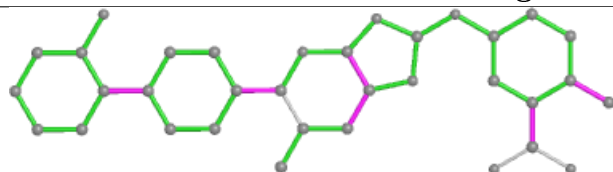


Torsions

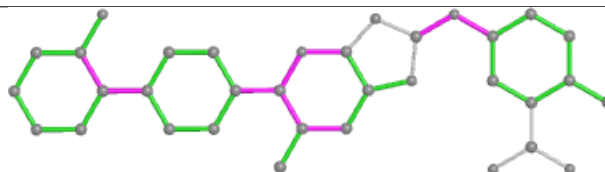


Rings

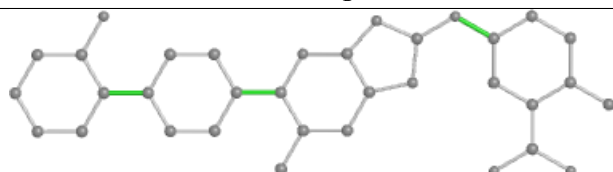
Ligand CG7 C 602



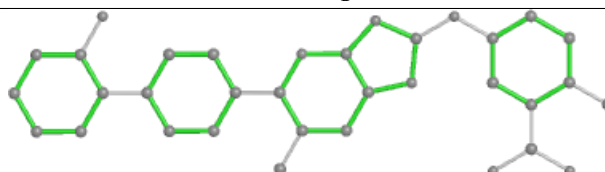
Bond lengths



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	441/565 (78%)	0.16	13 (2%) 51 46	39, 66, 111, 144	0
1	C	459/565 (81%)	0.17	22 (4%) 30 24	35, 63, 105, 128	0
2	B	183/270 (67%)	0.56	17 (9%) 8 6	38, 76, 121, 149	0
2	D	181/270 (67%)	0.19	6 (3%) 46 41	41, 60, 106, 151	0
3	E	299/336 (88%)	0.12	10 (3%) 46 41	37, 56, 94, 129	0
3	F	299/336 (88%)	0.06	9 (3%) 50 45	37, 59, 89, 134	0
All	All	1862/2342 (79%)	0.18	77 (4%) 37 32	35, 63, 106, 151	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	407	TYR	5.7
1	A	524	PRO	5.1
3	E	304	ASP	5.0
2	B	175	ASP	4.7
2	B	196	PRO	4.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	C	172	11/12	0.85	0.22	76,79,85,86	4
1	TPO	A	172	11/12	0.87	0.22	67,69,75,76	4
2	SEP	B	108	10/11	0.95	0.14	63,64,71,71	0
2	SEP	D	108	10/11	0.97	0.12	57,59,66,66	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

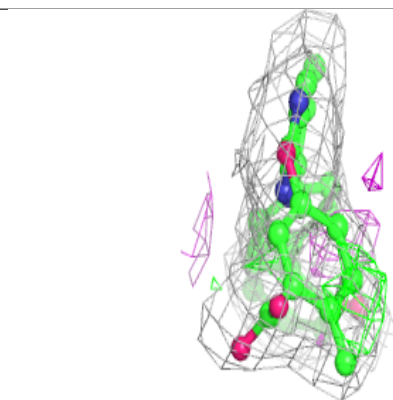
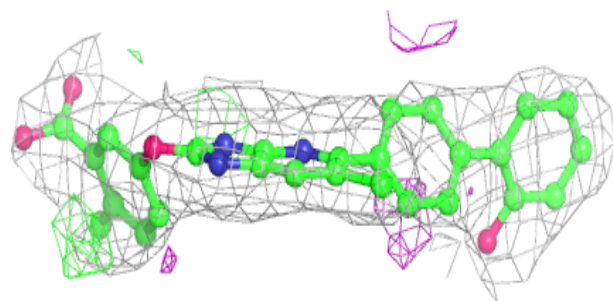
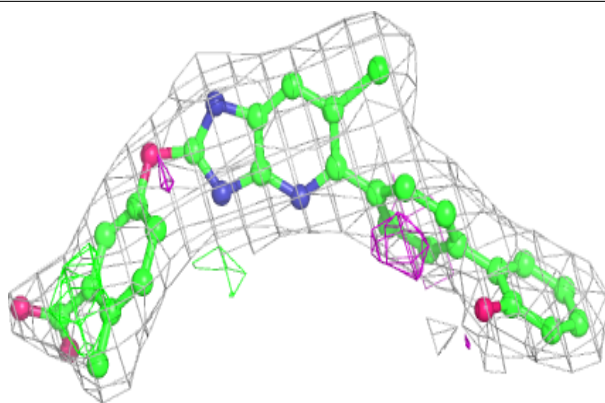
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	IMD	C	603	5/5	0.89	0.33	86,87,87,87	0
5	CG7	A	602[B]	34/34	0.89	0.22	49,56,58,58	34
5	CG7	A	602[A]	34/34	0.89	0.22	54,62,66,66	34
5	CG7	C	602	34/34	0.94	0.21	41,45,67,69	0
4	STU	C	601	35/35	0.96	0.18	36,38,43,43	0
4	STU	A	601	35/35	0.96	0.18	40,41,43,44	0
7	AMP	F	402	23/23	0.97	0.16	47,52,56,57	0
7	AMP	E	401	23/23	0.97	0.16	49,52,57,58	0
7	AMP	E	402	23/23	0.98	0.14	48,51,54,55	0
7	AMP	F	401	23/23	0.98	0.17	46,48,50,51	0

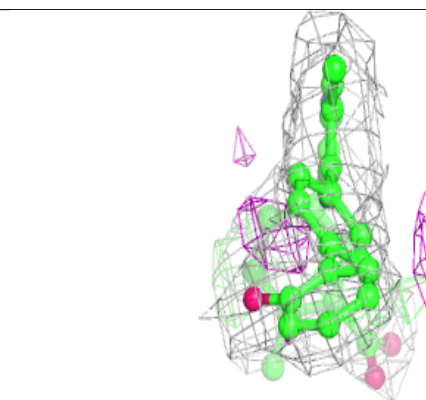
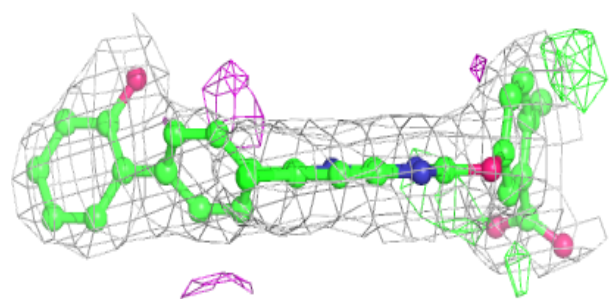
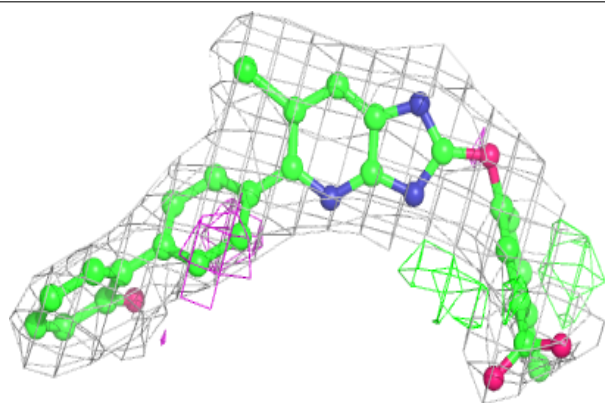
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CG7 A 602 (B):

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

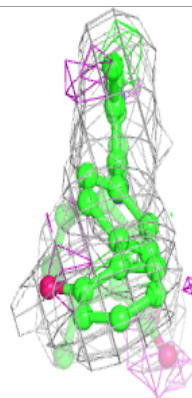
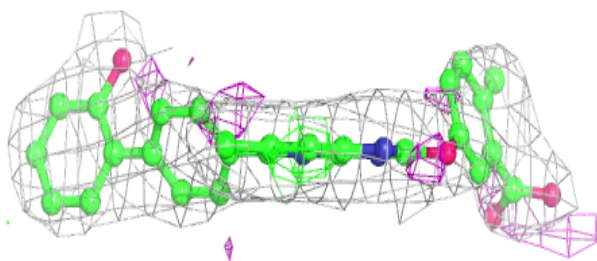
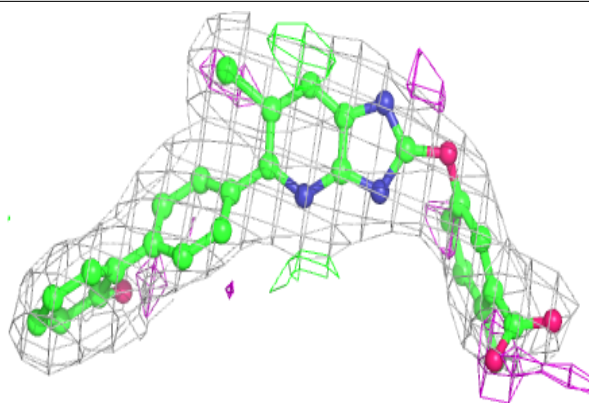
**Electron density around CG7 A 602 (A):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



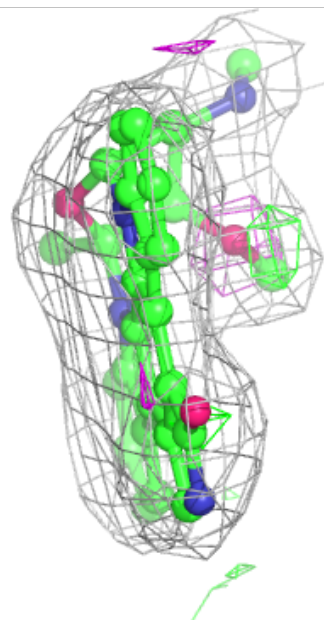
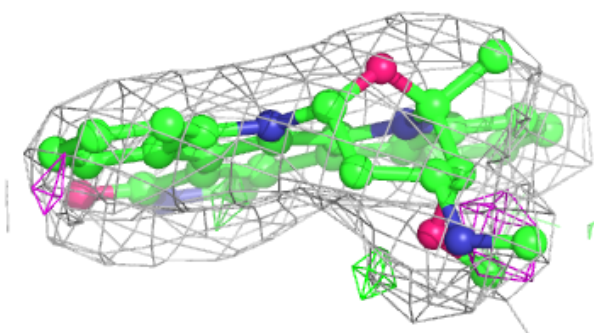
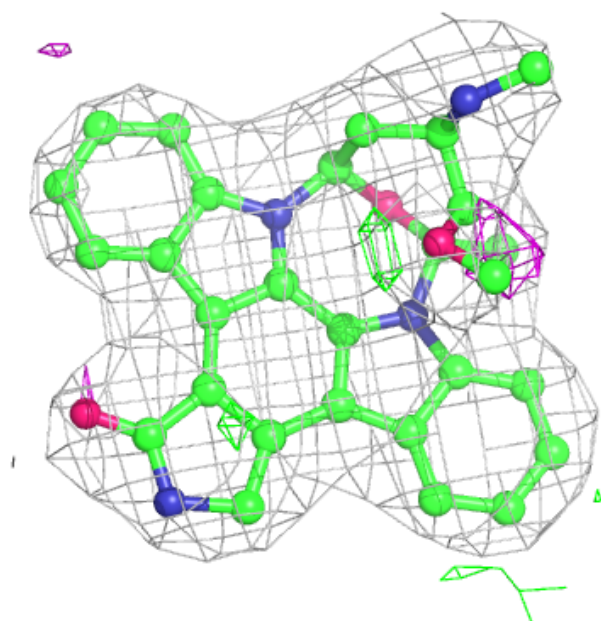
Electron density around CG7 C 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



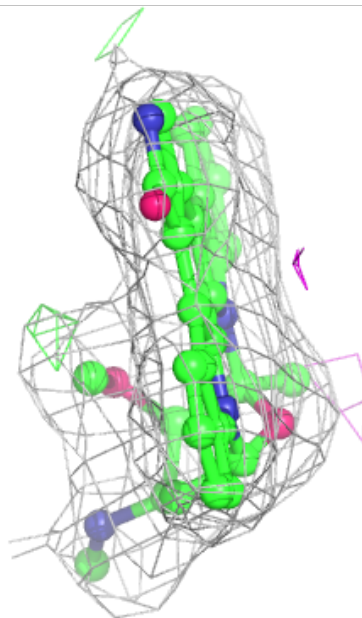
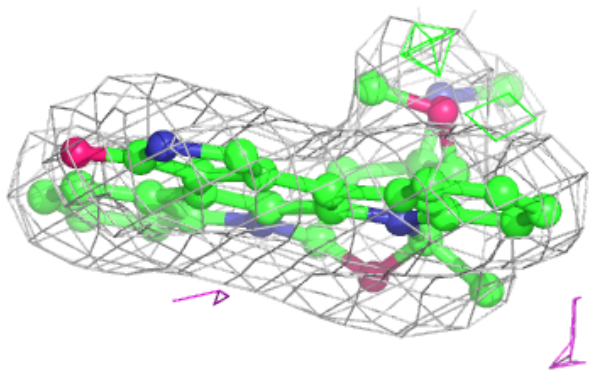
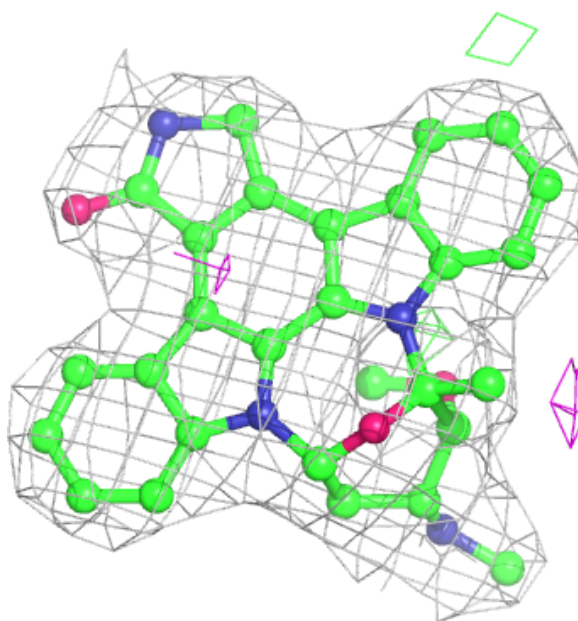
Electron density around STU C 601:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



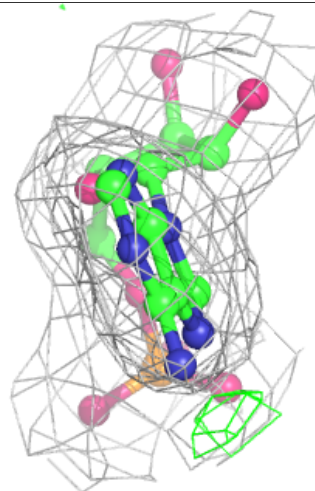
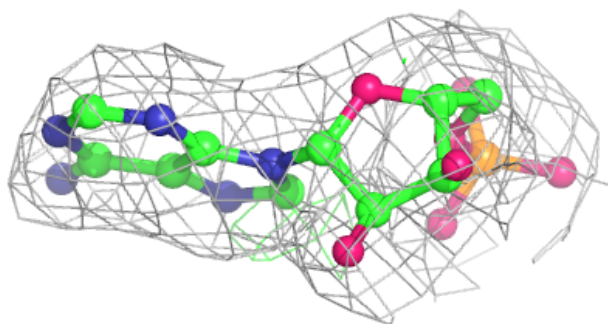
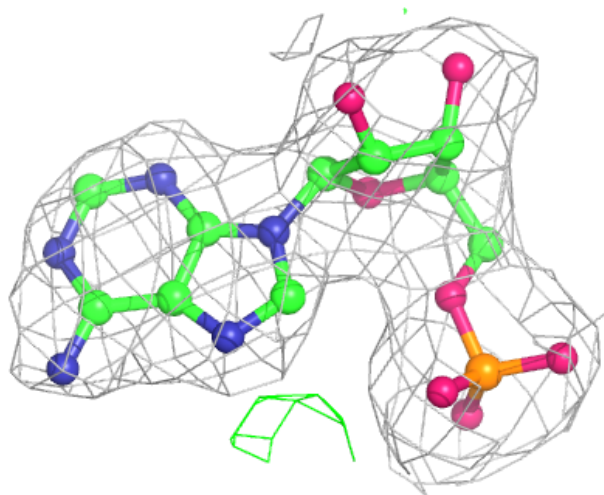
Electron density around STU A 601:

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and green (positive)



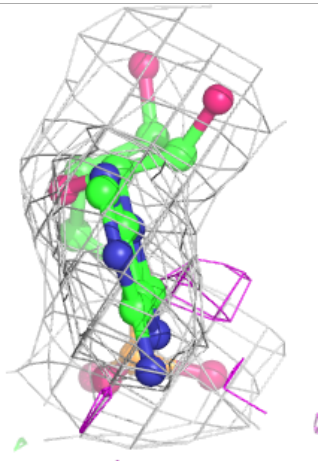
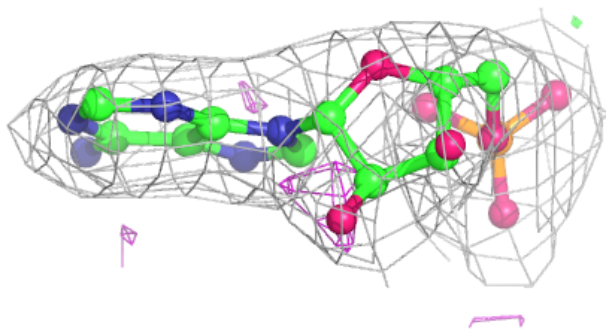
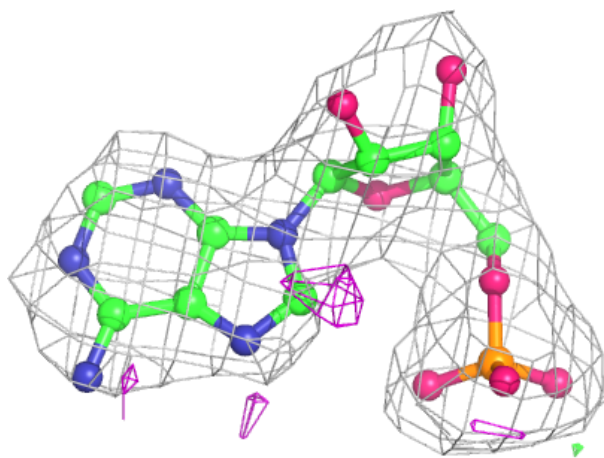
Electron density around AMP F 402:

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and green (positive)



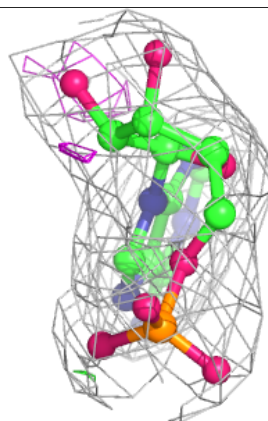
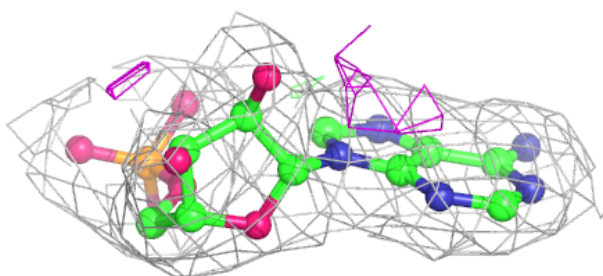
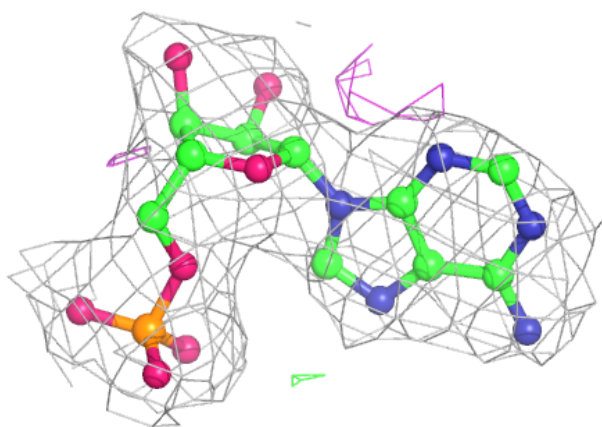
Electron density around AMP E 401:

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and green (positive)



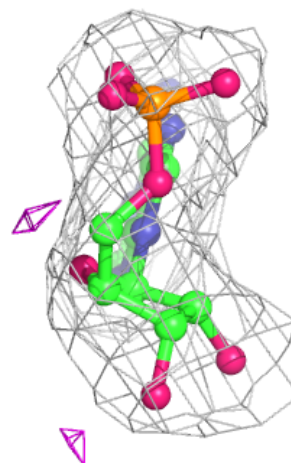
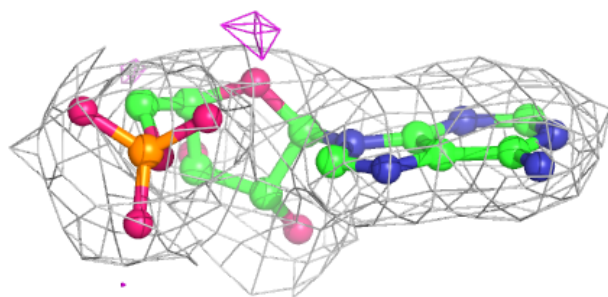
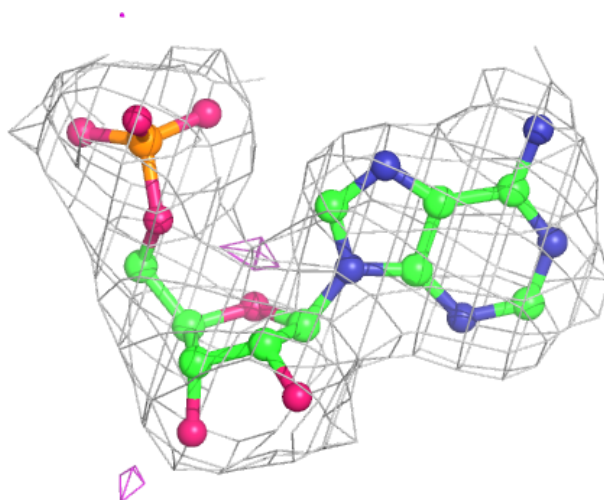
Electron density around AMP E 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP F 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.