



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 02:15 AM EDT

PDB ID : 7MYJ  
Title : Structure of full length human AMPK (a2b1g1) in complex with a small molecule activator MSG011  
Authors : Ovens, A.J.; Gee, Y.S.; Ling, N.X.Y.; Waters, N.J.; Yu, D.; Scott, J.W.; Parker, M.W.; Hoffman, N.J.; Kemp, B.E.; Baell, J.B.; Oakhill, J.S.; Langendorf, C.G.  
Deposited on : 2021-05-21  
Resolution : 2.95 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

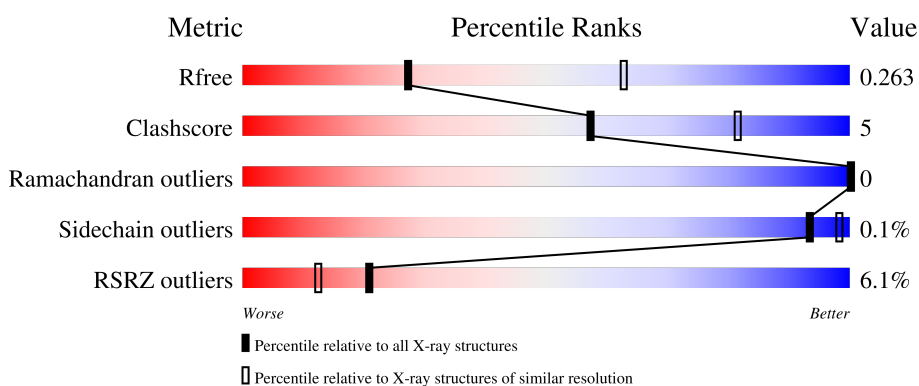
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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.



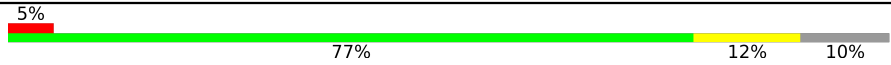
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	565	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: grey;"></div> </div>
1	C	565	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey;"></div> </div>
2	B	270	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 58%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: grey;"></div> </div>
2	D	270	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: grey;"></div> </div>
3	E	336	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	F	336	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	C	172	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14740 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
			Total	C	N	O	P	S			
1	A	435	3379	2172	571	612	1	23	0	0	0
1	C	465	3601	2308	610	658	1	24	1	0	0

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
			Total	C	N	O	P	S			
2	B	184	1397	906	229	257	1	4	0	0	0
2	D	187	1446	936	238	265	1	6	0	0	0

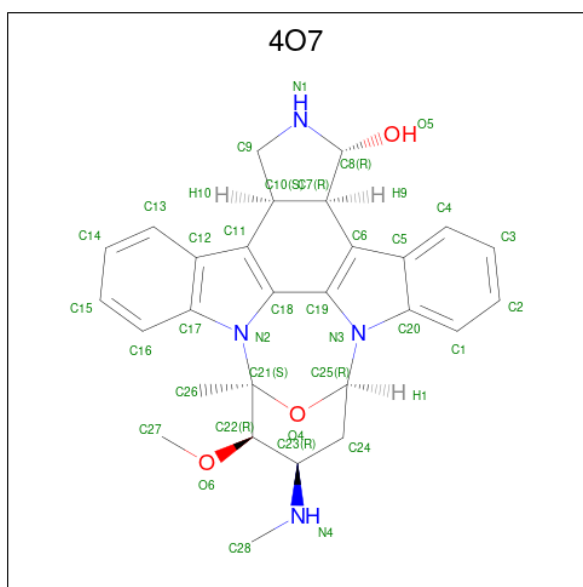
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	303	2342	1527	385	423	7	0	0	0
3	F	303	2339	1524	386	422	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

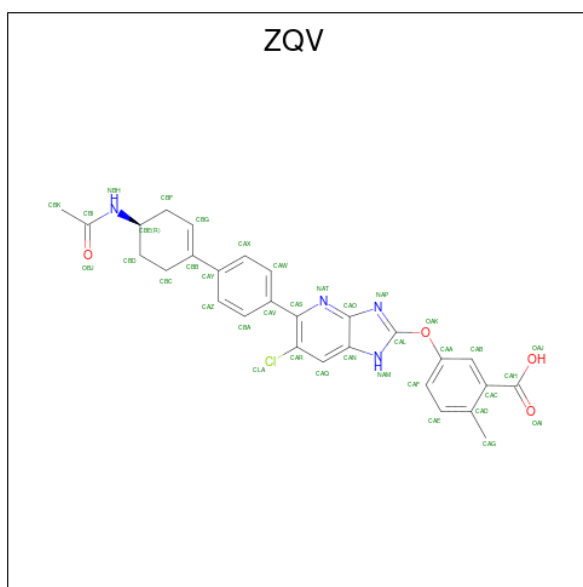
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine	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 (5S,6R,7R,9R,13cR,14R,16aS)-6-methoxy-5-methyl-7-(methylamino)-6,7,8,9,14,15,16,16a-octahydro-5H,13cH-5,9-epoxy-4b,9a,1 5-triazadibenzo[b,h]cyclohepta[1,2,3,4-jkl]cyclopenta[e]-as-indacen-14-ol (three-letter code: 4O7) (formula: C<sub>28</sub>H<sub>30</sub>N<sub>4</sub>O<sub>3</sub>).



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

- Molecule 5 is 5-({5-[(4'R)-4'-acetamido-2',3',4',5'-tetrahydro[1,1'-biphenyl]-4-yl]-6-chloro-1H-imidazo[4,5-b]pyridin-2-yl}oxy)-2-methylbenzoic acid (three-letter code: ZQV) (formula: C<sub>28</sub>H<sub>25</sub>ClN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



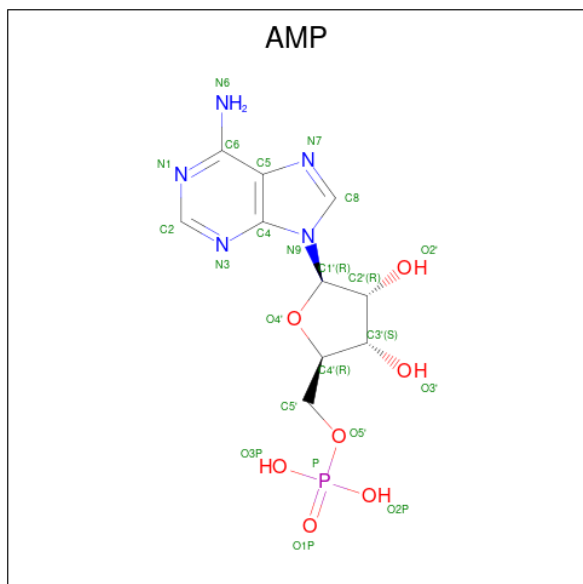
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
5	A	1	37	28	1	4	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
5	D	1	37	28	1	4	4	0	0

- Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).

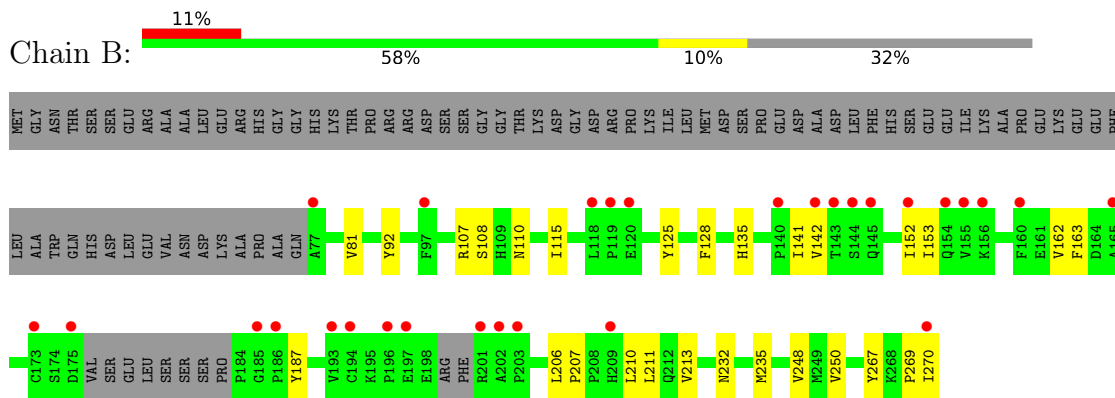


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	E	1	23	10	5	7	1	0	0
6	E	1	23	10	5	7	1	0	0
6	F	1	23	10	5	7	1	0	0
6	F	1	23	10	5	7	1	0	0

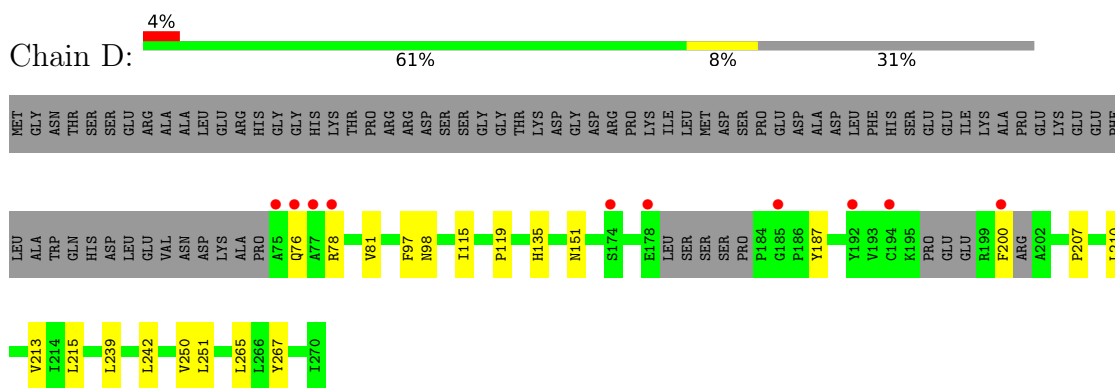




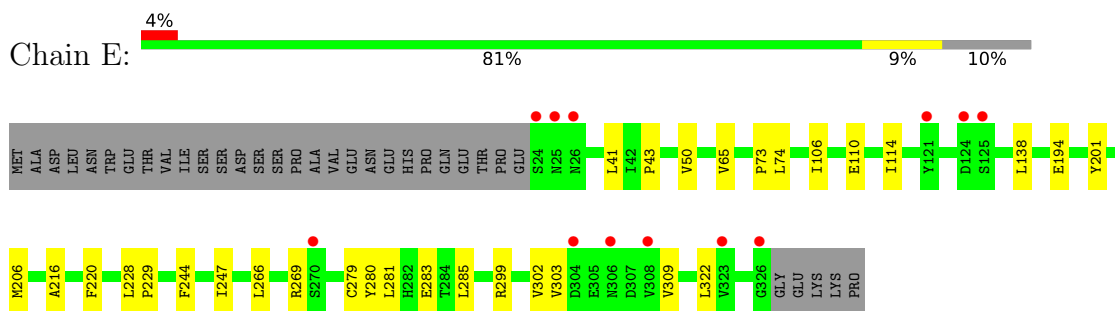
• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



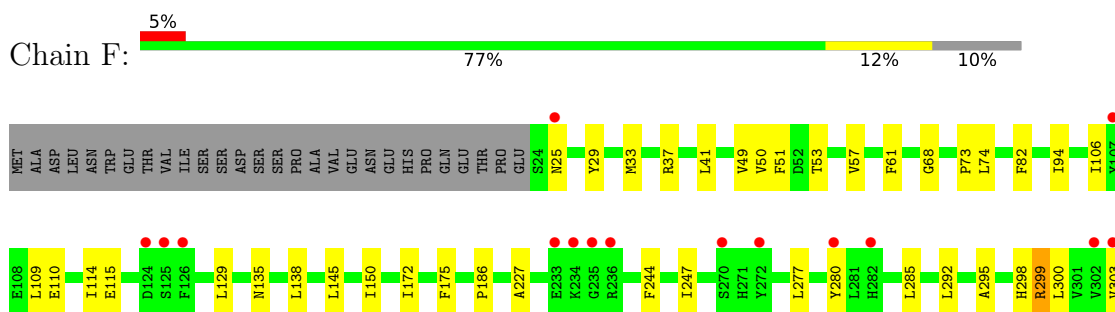
• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

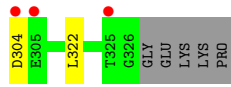


• Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1



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





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.84Å 134.20Å 141.82Å 90.00° 92.55° 90.00°	Depositor
Resolution (Å)	48.72 – 2.95 48.72 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.72-2.95) 99.0 (48.72-2.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.96Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.213 , 0.243 0.234 , 0.263	Depositor DCC
$R_{free}$ test set	2991 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.8	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, ZQV, TPO, AMP, 4O7

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	0.44	0/3448	0.60	0/4678
1	C	0.43	0/3674	0.58	0/4982
2	B	0.44	0/1428	0.58	0/1959
2	D	0.45	0/1477	0.61	0/2018
3	E	0.43	0/2391	0.59	0/3260
3	F	0.47	0/2388	0.59	0/3258
All	All	0.44	0/14806	0.59	0/20155

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	3379	0	3216	41	0
1	C	3601	0	3435	22	0
2	B	1397	0	1305	23	0
2	D	1446	0	1359	17	0
3	E	2342	0	2341	27	0
3	F	2339	0	2316	27	0
4	A	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	0	0	0
5	A	37	0	0	0	0
5	D	37	0	0	0	0
6	E	46	0	24	0	0
6	F	46	0	24	0	0
All	All	14740	0	14020	141	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 5.

The worst 5 of 141 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)
3:F:292:LEU:HD21	3:F:300:LEU:HG	1.18	1.16
3:E:41:LEU:HD13	3:E:138:LEU:HD21	1.26	1.09
2:B:125:TYR:HE1	2:B:153:ILE:HG12	1.15	1.06
3:E:41:LEU:CD1	3:E:138:LEU:HD21	1.86	1.06
3:F:292:LEU:CD2	3:F:300:LEU:HG	1.93	0.99

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	422/565 (75%)	418 (99%)	4 (1%)	0	100	100
1	C	452/565 (80%)	447 (99%)	5 (1%)	0	100	100
2	B	177/270 (66%)	176 (99%)	1 (1%)	0	100	100
2	D	178/270 (66%)	175 (98%)	3 (2%)	0	100	100
3	E	301/336 (90%)	299 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	301/336 (90%)	295 (98%)	6 (2%)	0	100	100
All	All	1831/2342 (78%)	1810 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/497 (69%)	345 (100%)	0	100	100
1	C	370/497 (74%)	370 (100%)	0	100	100
2	B	143/239 (60%)	143 (100%)	0	100	100
2	D	150/239 (63%)	150 (100%)	0	100	100
3	E	253/308 (82%)	252 (100%)	1 (0%)	91	96
3	F	248/308 (80%)	247 (100%)	1 (0%)	91	96
All	All	1509/2088 (72%)	1507 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	299	ARG
3	F	299	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	248	ASN
3	E	290	ASN
3	F	320	GLN
3	F	80	GLN
1	C	444	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](#)

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
1	TPO	A	172	1	8,10,11	0.73	0	10,14,16	0.98	1 (10%)
2	SEP	B	108	2	8,9,10	0.85	0	8,12,14	1.90	2 (25%)
2	SEP	D	108	2	8,9,10	0.64	0	8,12,14	0.64	0
1	TPO	C	172	1	8,10,11	0.78	0	10,14,16	1.04	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	172	1	-	0/9/11/13	-
2	SEP	B	108	2	-	4/5/8/10	-
2	SEP	D	108	2	-	3/5/8/10	-
1	TPO	C	172	1	-	4/9/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	SEP	OG-CB-CA	3.77	111.81	108.14
2	B	108	SEP	OG-P-O1P	3.46	116.17	106.47
1	C	172	TPO	O-C-CA	-2.72	117.64	124.78
1	A	172	TPO	O-C-CA	-2.42	118.43	124.78



There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	108	SEP	CB-OG-P-O1P
2	B	108	SEP	CB-OG-P-O2P
2	B	108	SEP	CB-OG-P-O3P
1	C	172	TPO	N-CA-CB-CG2
1	C	172	TPO	N-CA-CB-OG1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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
5	ZQV	D	701	-	40,41,41	2.29	10 (25%)	46,59,59	1.18	3 (6%)
4	4O7	A	601	-	30,42,42	2.49	8 (26%)	21,68,68	1.96	7 (33%)
4	4O7	C	601	-	30,42,42	2.50	8 (26%)	21,68,68	1.98	8 (38%)
6	AMP	F	401	-	22,25,25	0.60	0	25,38,38	0.73	1 (4%)
6	AMP	E	402	-	22,25,25	0.62	0	25,38,38	0.75	1 (4%)
6	AMP	F	402	-	22,25,25	0.62	0	25,38,38	0.70	1 (4%)
6	AMP	E	401	-	22,25,25	0.61	0	25,38,38	0.72	1 (4%)
5	ZQV	A	602	-	40,41,41	2.33	9 (22%)	46,59,59	1.38	5 (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
5	ZQV	D	701	-	-	8/18/30/30	0/5/5/5
4	4O7	A	601	-	-	2/4/58/58	-
4	4O7	C	601	-	-	2/4/58/58	-
6	AMP	F	401	-	-	1/6/26/26	0/3/3/3
6	AMP	E	402	-	-	1/6/26/26	0/3/3/3
6	AMP	F	402	-	-	4/6/26/26	0/3/3/3
6	AMP	E	401	-	-	4/6/26/26	0/3/3/3
5	ZQV	A	602	-	-	8/18/30/30	0/5/5/5

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	ZQV	CAV-CAS	-7.25	1.40	1.49
5	D	701	ZQV	CAV-CAS	-7.23	1.40	1.49
4	C	601	4O7	C8-N1	-6.77	1.35	1.45
4	A	601	4O7	C8-N1	-6.70	1.35	1.45
5	D	701	ZQV	CAG-CAD	-5.42	1.40	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	4O7	C16-C17-N2	4.79	138.09	132.29
4	C	601	4O7	C16-C17-N2	4.68	137.96	132.29
5	A	602	ZQV	CAS-NAT-CAO	4.01	121.76	117.99
5	D	701	ZQV	CAS-NAT-CAO	3.84	121.60	117.99
4	A	601	4O7	C9-C10-C7	3.53	110.59	101.92

There are no chirality outliers.

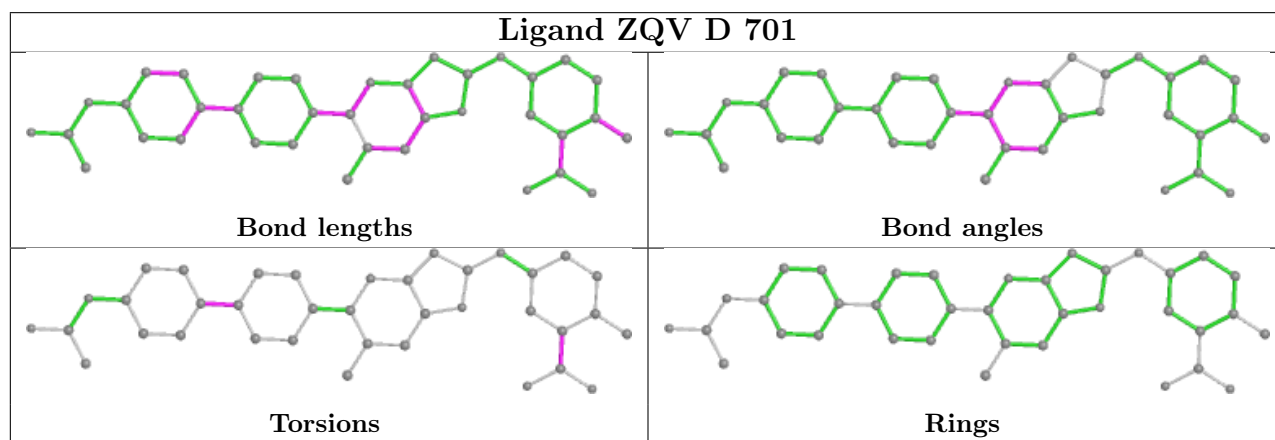
5 of 30 torsion outliers are listed below:

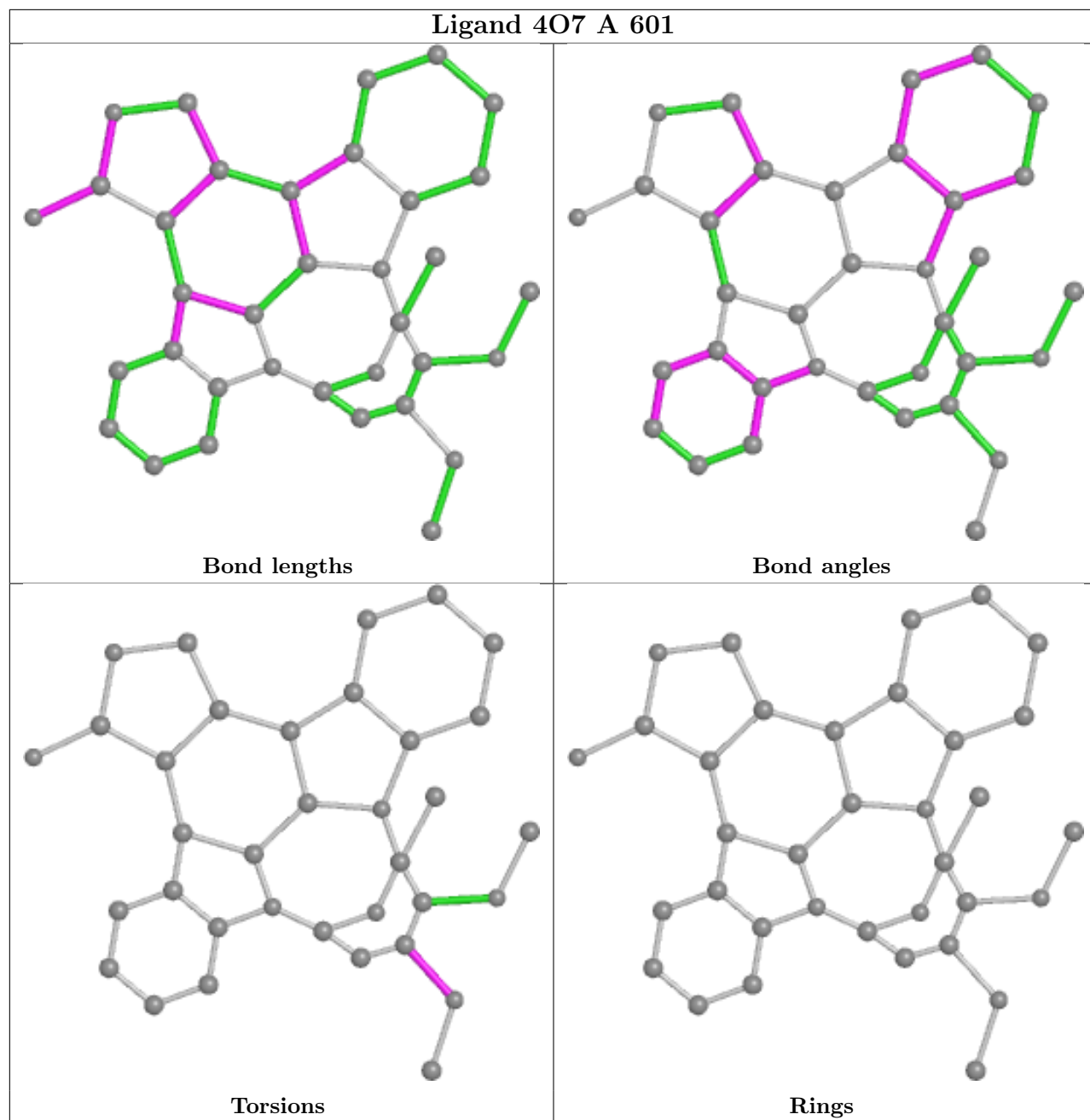
Mol	Chain	Res	Type	Atoms
6	E	401	AMP	C5'-O5'-P-O2P
6	E	401	AMP	C5'-O5'-P-O3P
6	F	402	AMP	C5'-O5'-P-O2P
6	F	402	AMP	C5'-O5'-P-O3P
6	F	402	AMP	O4'-C4'-C5'-O5'

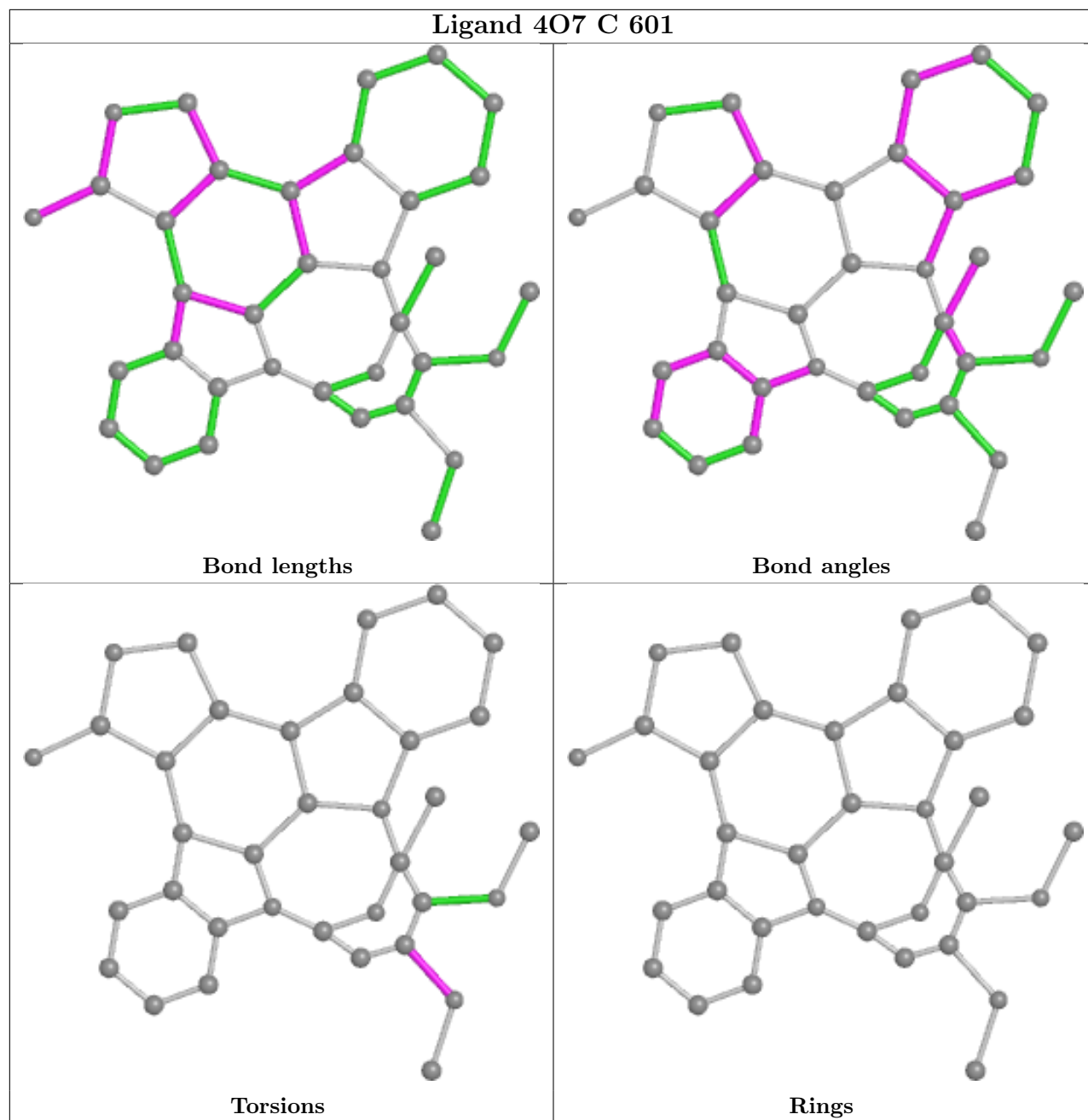
There are no ring outliers.

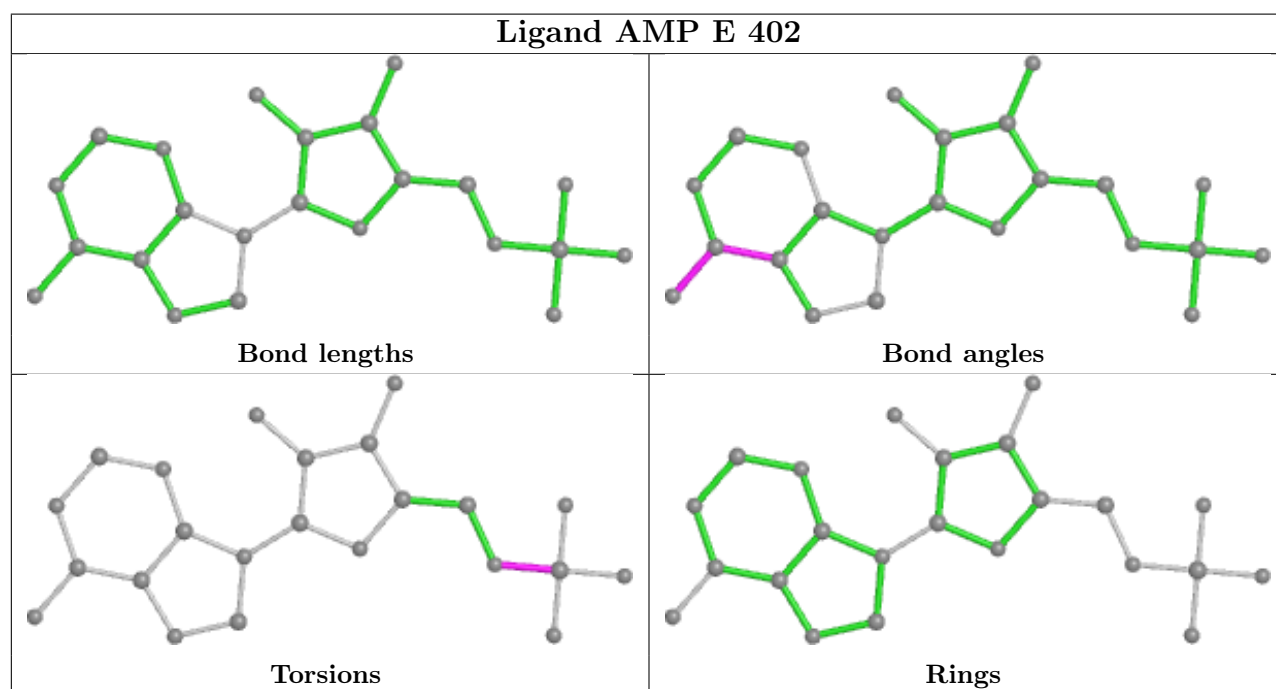
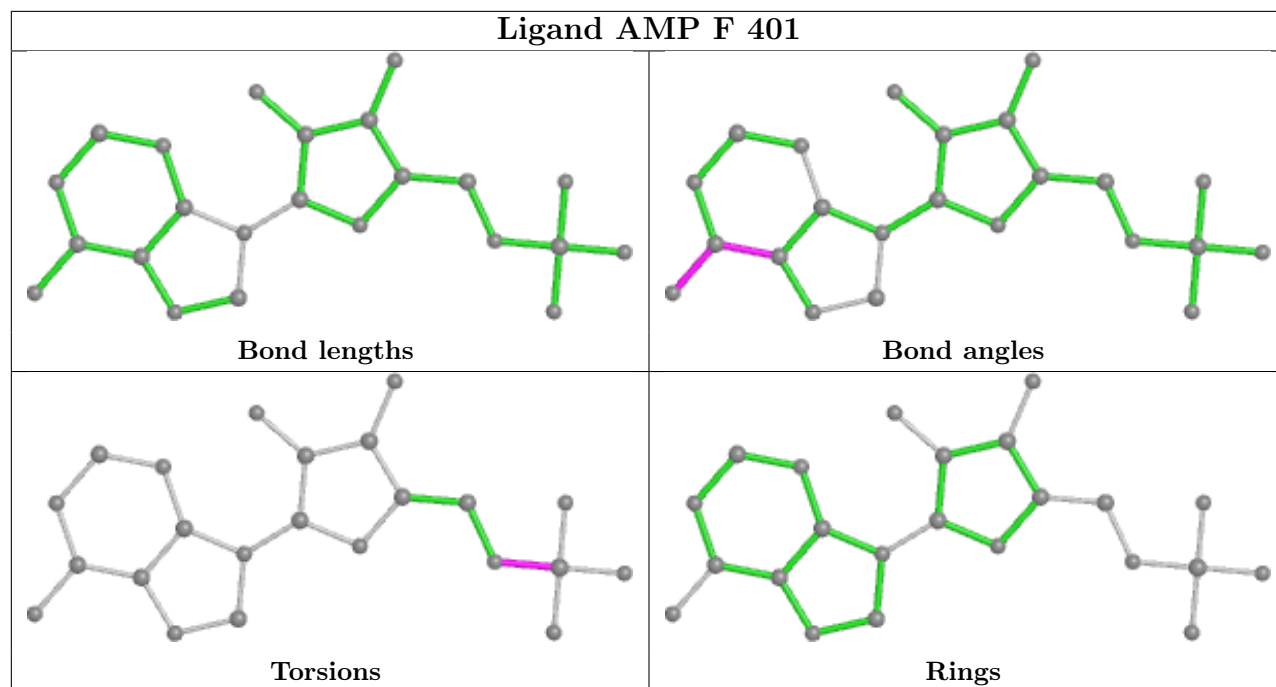
No monomer is involved in short contacts.

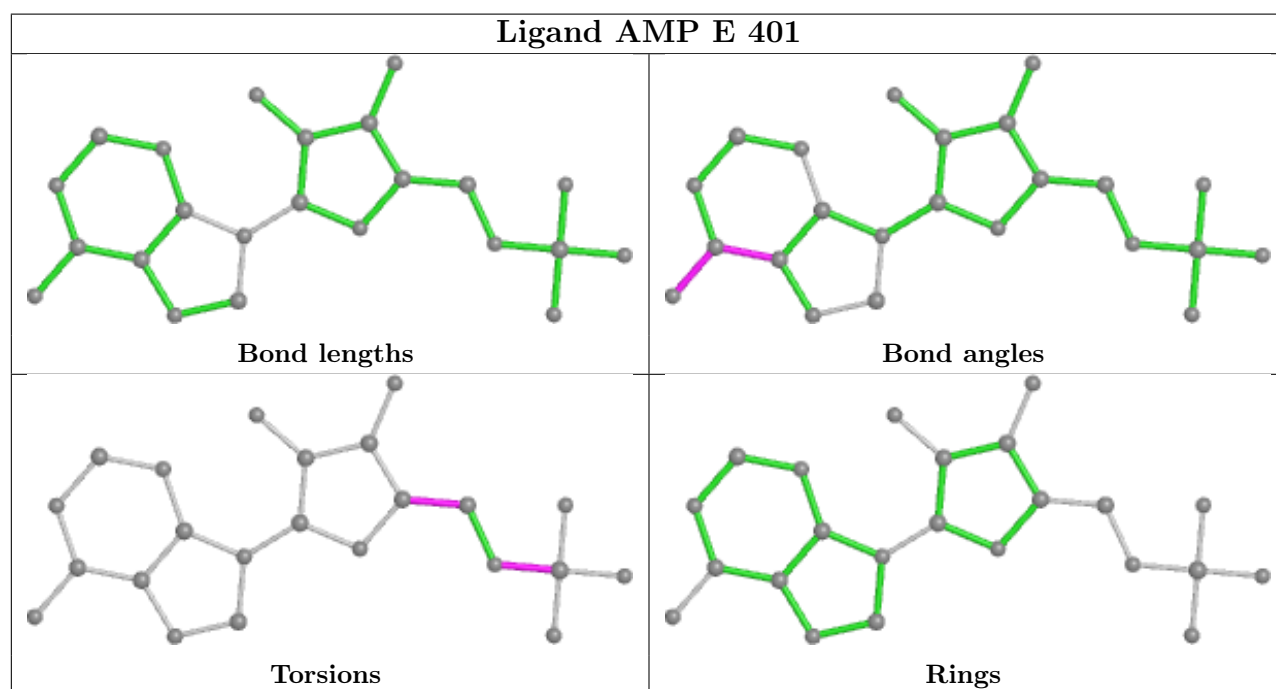
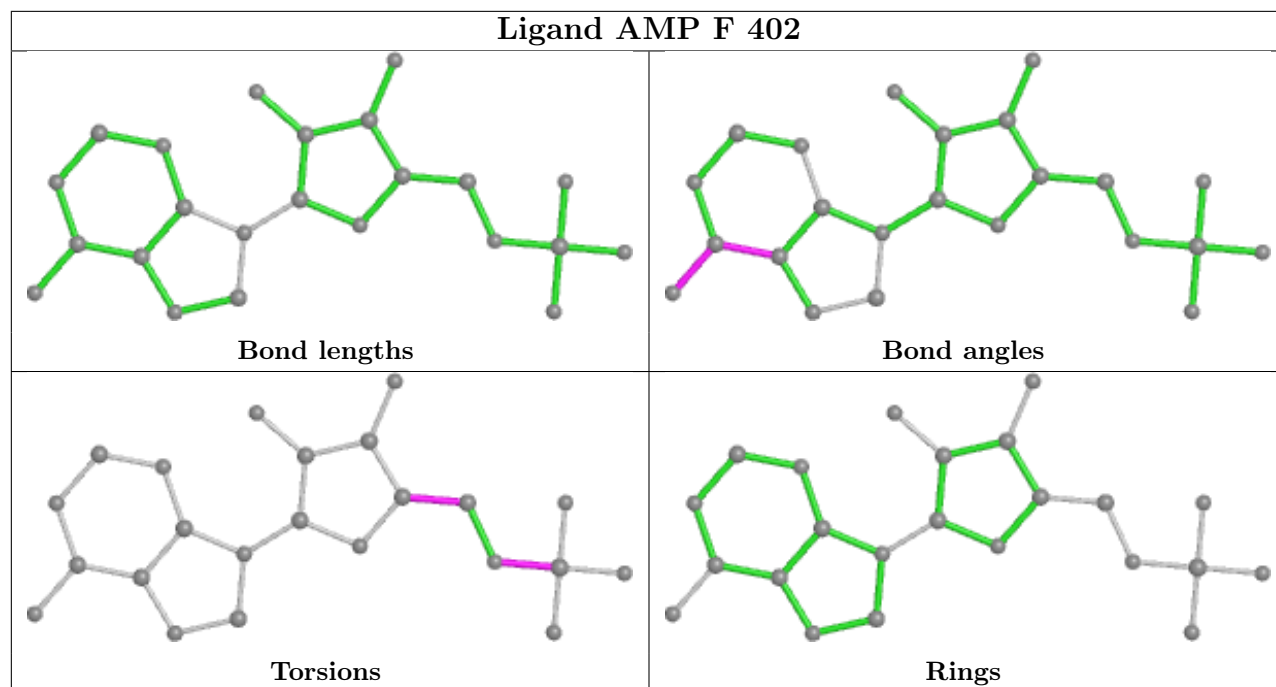
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

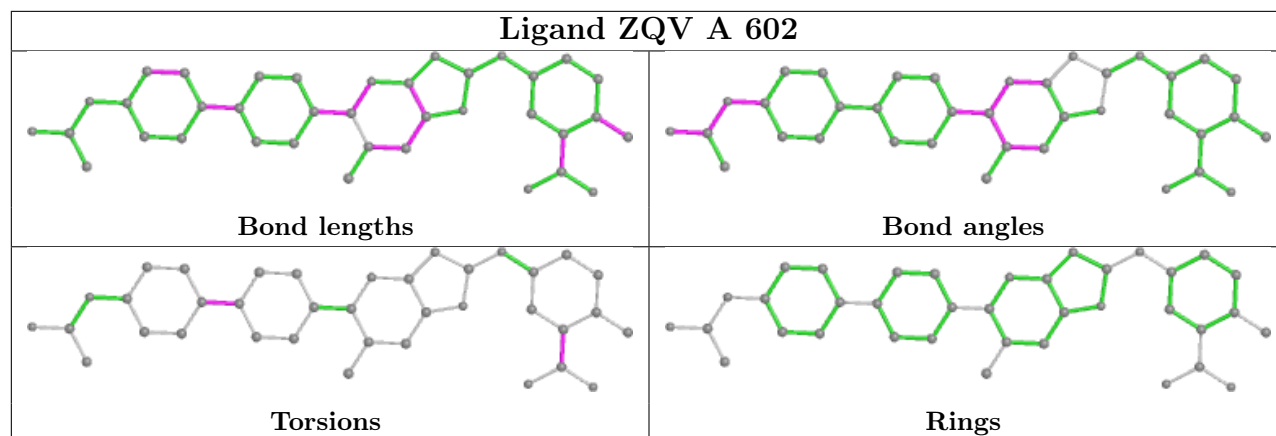












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	434/565 (76%)	0.35	22 (5%) 28 17	52, 78, 115, 159	0
1	C	464/565 (82%)	0.27	23 (4%) 28 18	43, 69, 112, 139	0
2	B	183/270 (67%)	0.78	29 (15%) 2 1	52, 88, 162, 207	0
2	D	186/270 (68%)	0.47	10 (5%) 25 16	41, 66, 138, 173	0
3	E	303/336 (90%)	0.29	12 (3%) 38 25	44, 68, 103, 134	0
3	F	303/336 (90%)	0.32	18 (5%) 22 13	41, 66, 96, 116	0
All	All	1873/2342 (79%)	0.37	114 (6%) 21 12	41, 72, 116, 207	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	304	ASP	6.4
3	E	304	ASP	6.1
2	D	194	CYS	5.0
2	D	76	GLN	4.9
2	D	178	GLU	4.7

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	C	172	11/12	0.67	0.42	92,95,96,97	1
1	TPO	A	172	11/12	0.76	0.23	90,92,94,94	0
2	SEP	D	108	10/11	0.89	0.17	69,73,77,78	0
2	SEP	B	108	10/11	0.92	0.14	80,81,86,86	0

### 6.3 Carbohydrates [i](#)

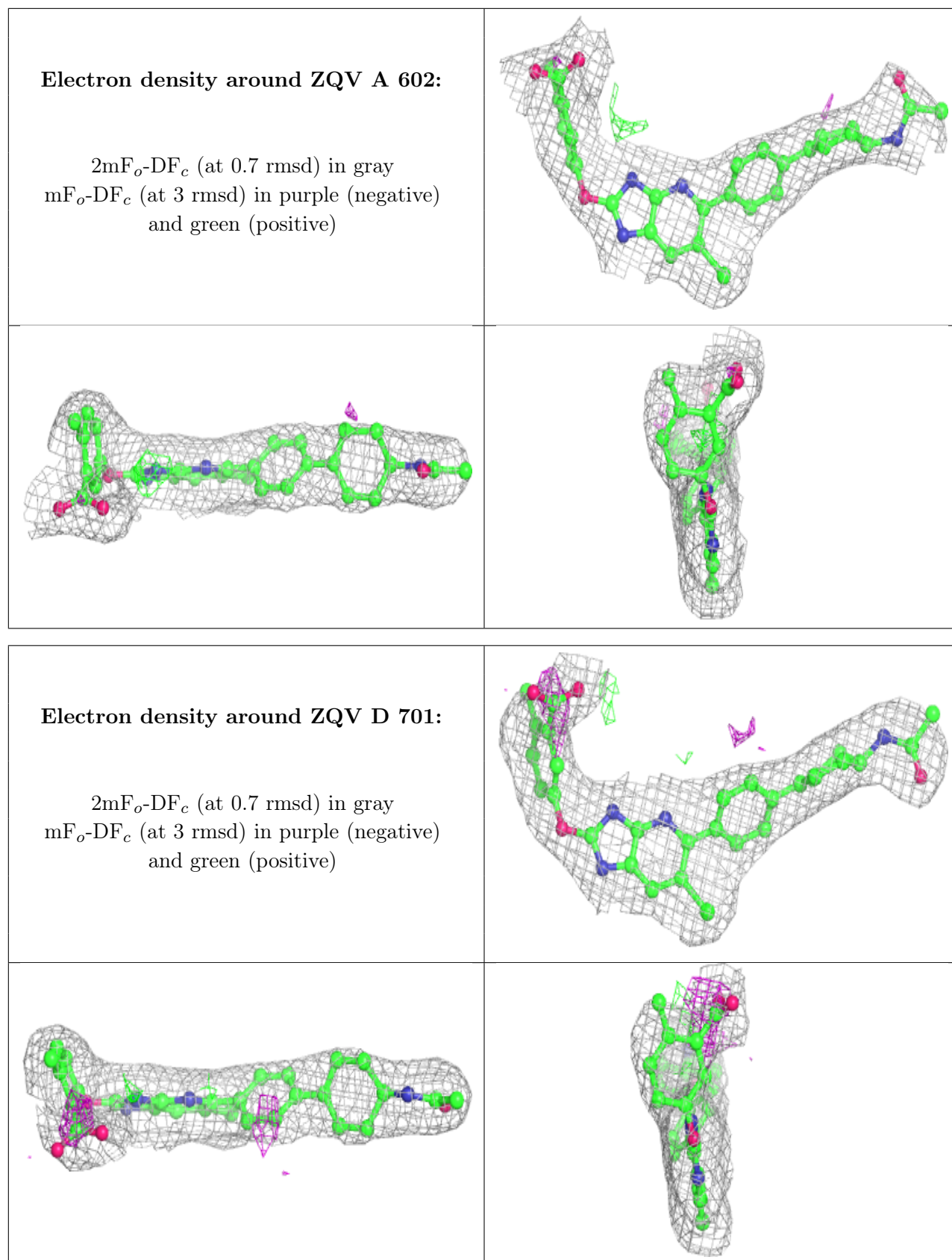
There are no monosaccharides in this entry.

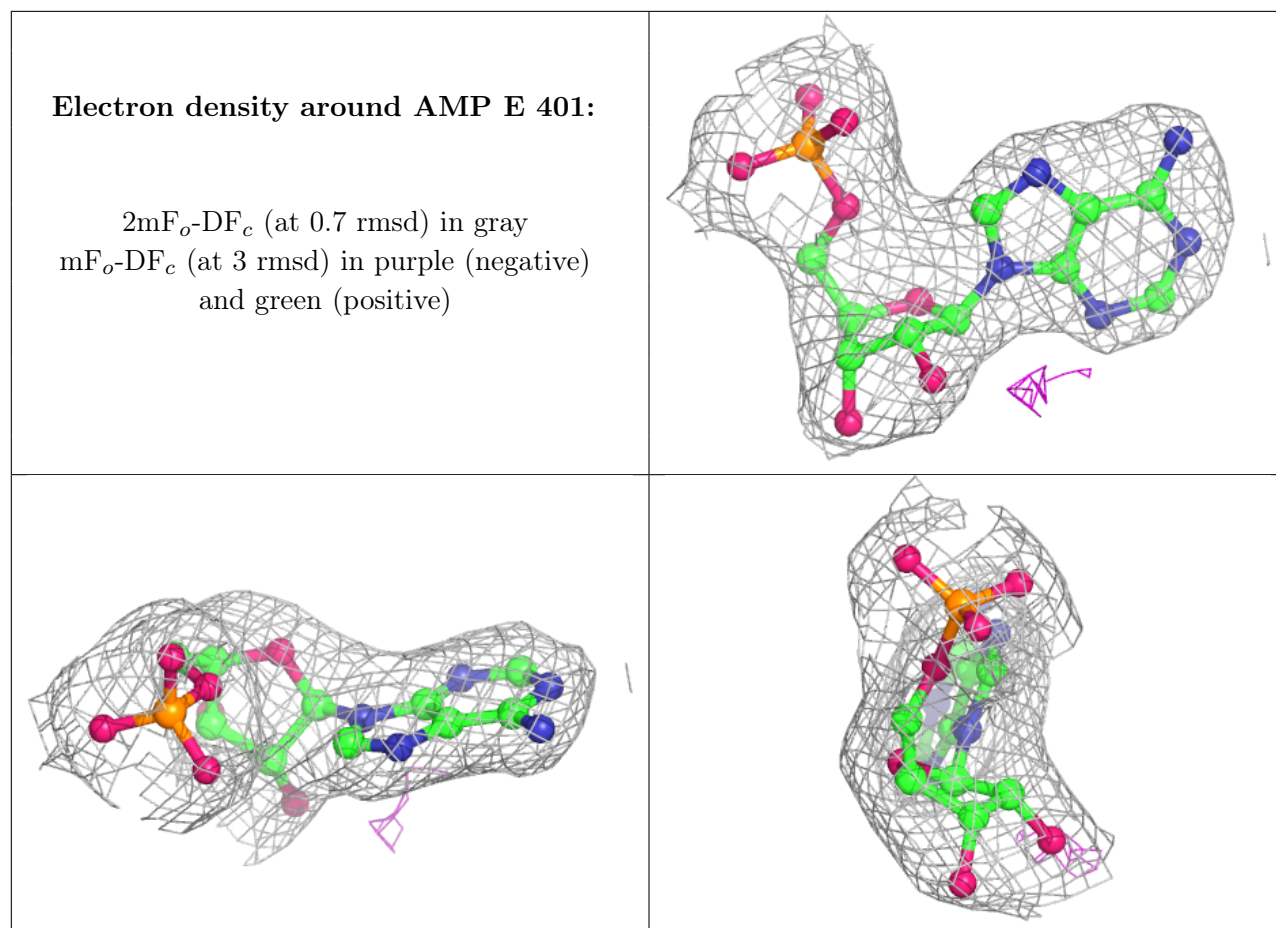
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ZQV	A	602	37/37	0.88	0.21	70,72,78,78	0
5	ZQV	D	701	37/37	0.93	0.21	54,60,76,78	0
6	AMP	E	401	23/23	0.95	0.19	59,62,64,65	0
6	AMP	F	402	23/23	0.95	0.18	53,57,60,61	0
6	AMP	F	401	23/23	0.96	0.18	55,57,61,62	0
6	AMP	E	402	23/23	0.96	0.17	61,63,70,70	0
4	4O7	A	601	35/35	0.97	0.20	45,46,48,49	0
4	4O7	C	601	35/35	0.97	0.20	44,46,48,50	0

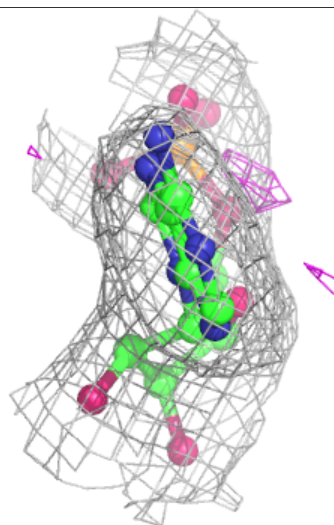
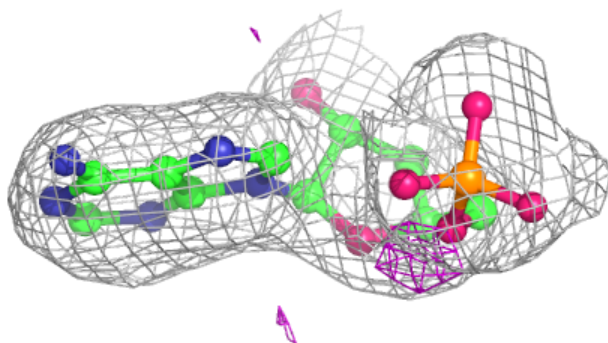
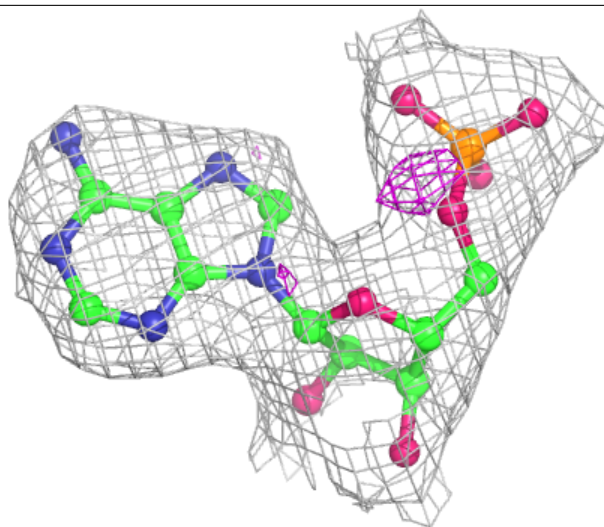
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





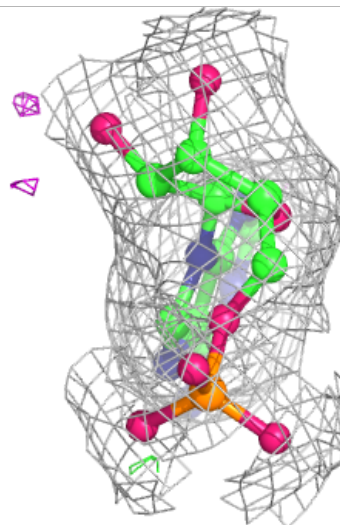
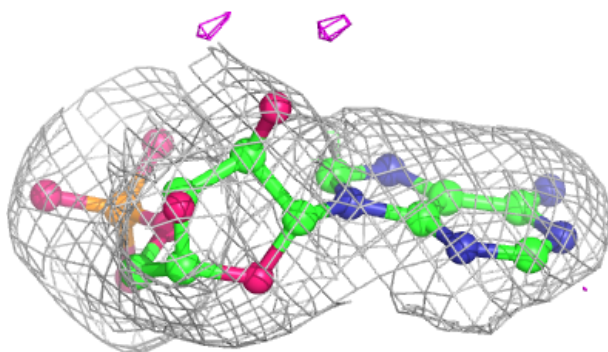
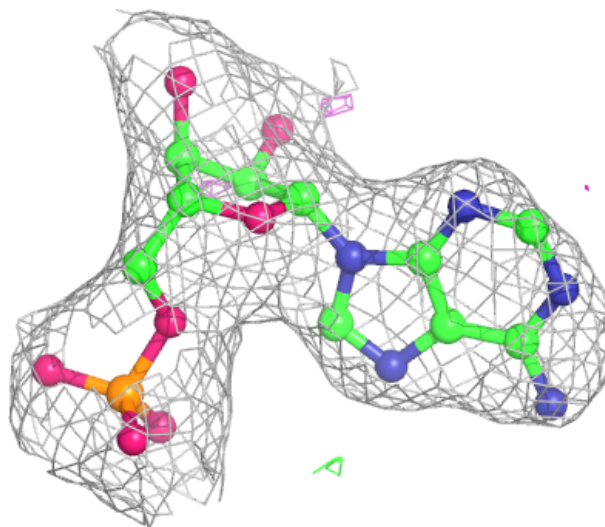
**Electron density around AMP F 402:**

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



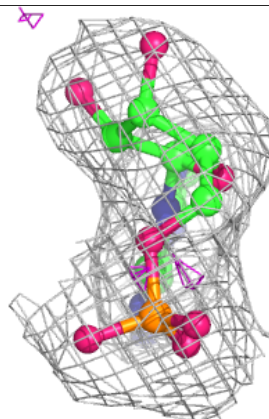
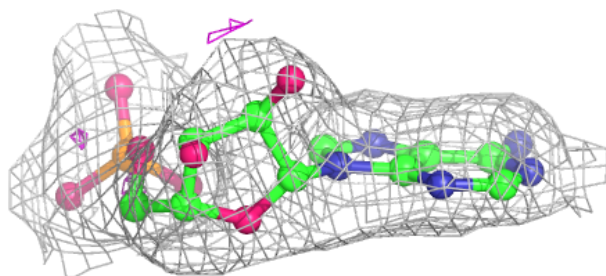
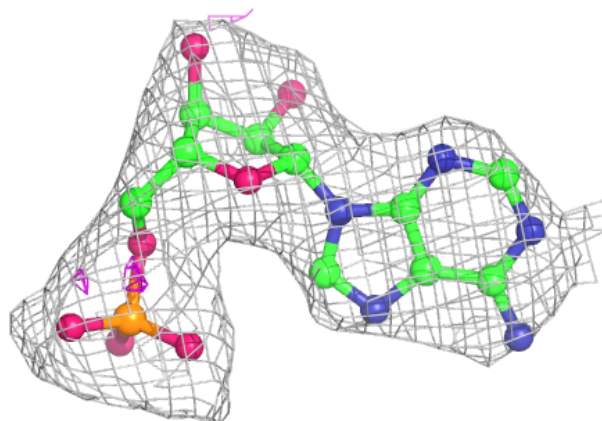
**Electron density around AMP F 401:**

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



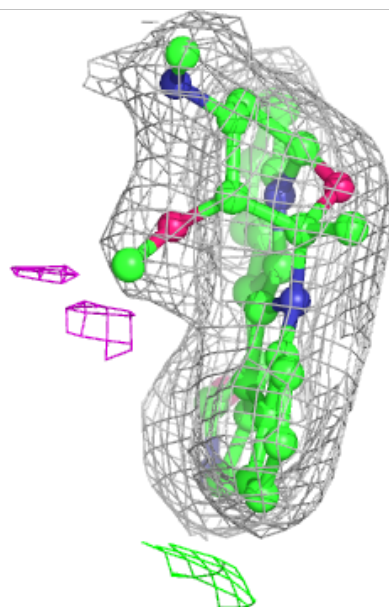
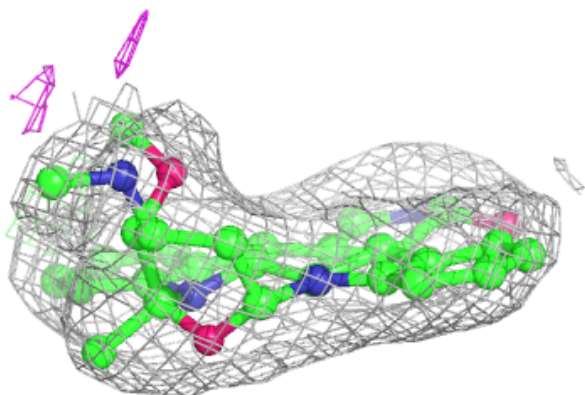
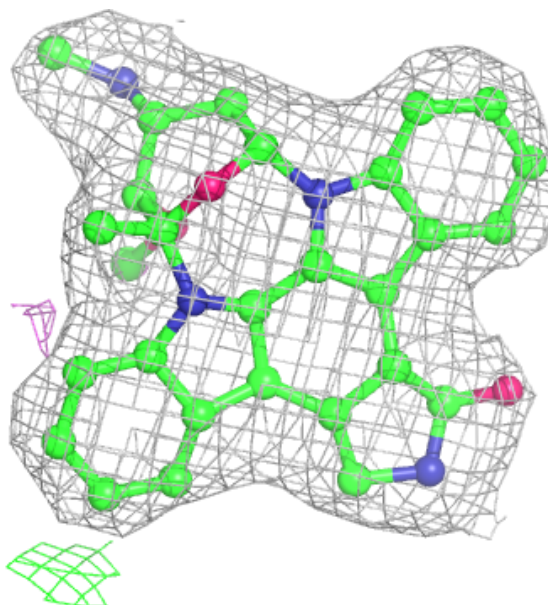
**Electron density around AMP E 402:**

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

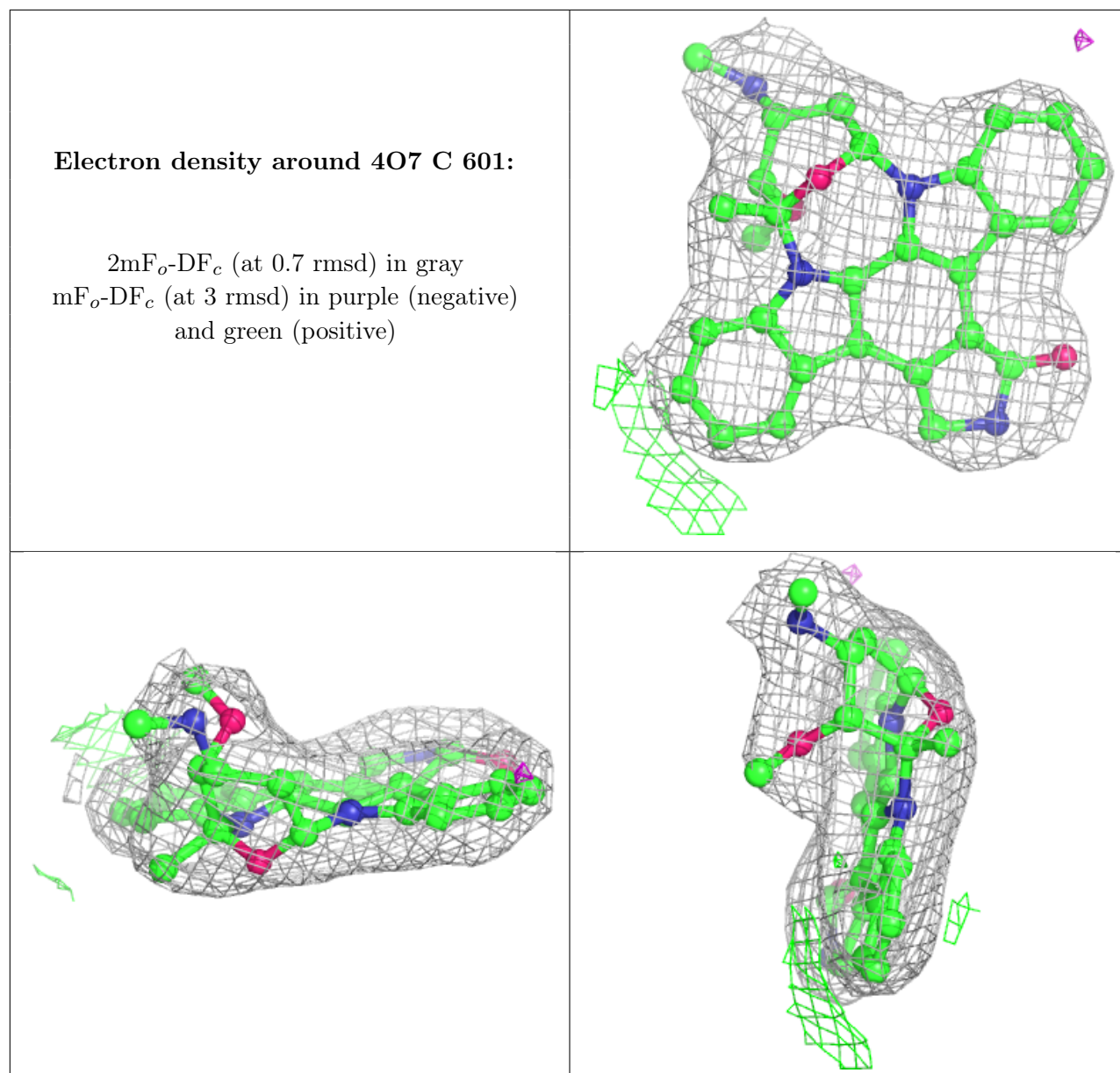


**Electron density around 4O7 A 601:**

$2mF_o-DF_c$  (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.