



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 13, 2023 – 11:10 am GMT

PDB ID : 4CFE  
Title : Structure of full length human AMPK in complex with a small molecule activator, a benzimidazole derivative (991)  
Authors : Xiao, B.; Sanders, M.J.; Carmena, D.; Bright, N.J.; Haire, L.F.; Underwood, E.; Patel, B.R.; Heath, R.B.; Walker, P.A.; Hallen, S.; Giordanetto, F.; Martin, S.R.; Carling, D.; Gamblin, S.J.  
Deposited on : 2013-11-14  
Resolution : 3.02 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

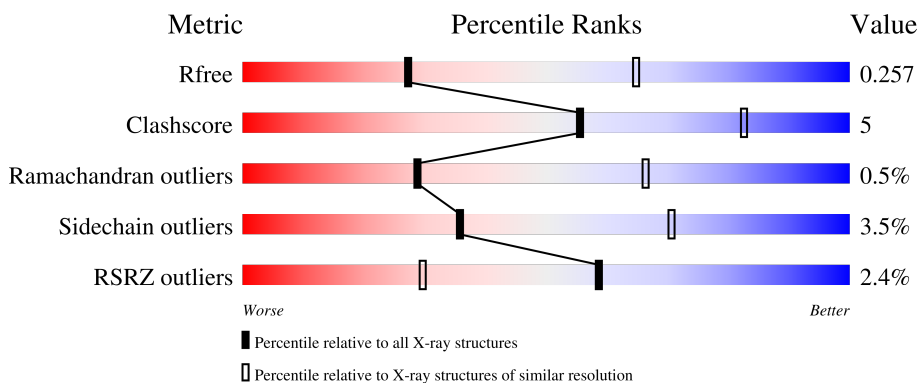
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	571	
1	C	571	
2	B	286	
2	D	286	
3	E	331	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	331	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '74%', a yellow segment labeled '13%', and a small grey segment at the end labeled '13%'.</p>

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 14322 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 SUB-UNIT ALPHA-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	426	3411	2191	593	604	1	22	3	0	0
1	C	404	3268	2101	568	576	1	22	7	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P54646
A	-17	SER	-	expression tag	UNP P54646
A	-16	HIS	-	expression tag	UNP P54646
A	-15	HIS	-	expression tag	UNP P54646
A	-14	HIS	-	expression tag	UNP P54646
A	-13	HIS	-	expression tag	UNP P54646
A	-12	HIS	-	expression tag	UNP P54646
A	-11	HIS	-	expression tag	UNP P54646
A	-10	SER	-	expression tag	UNP P54646
A	-9	SER	-	expression tag	UNP P54646
A	-8	GLY	-	expression tag	UNP P54646
A	-7	LEU	-	expression tag	UNP P54646
A	-6	GLU	-	expression tag	UNP P54646
A	-5	VAL	-	expression tag	UNP P54646
A	-4	LEU	-	expression tag	UNP P54646
A	-3	PHE	-	expression tag	UNP P54646
A	-2	GLN	-	expression tag	UNP P54646
A	-1	GLY	-	expression tag	UNP P54646
A	0	PRO	-	expression tag	UNP P54646
C	-18	MET	-	expression tag	UNP P54646
C	-17	SER	-	expression tag	UNP P54646
C	-16	HIS	-	expression tag	UNP P54646
C	-15	HIS	-	expression tag	UNP P54646
C	-14	HIS	-	expression tag	UNP P54646

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP P54646
C	-12	HIS	-	expression tag	UNP P54646
C	-11	HIS	-	expression tag	UNP P54646
C	-10	SER	-	expression tag	UNP P54646
C	-9	SER	-	expression tag	UNP P54646
C	-8	GLY	-	expression tag	UNP P54646
C	-7	LEU	-	expression tag	UNP P54646
C	-6	GLU	-	expression tag	UNP P54646
C	-5	VAL	-	expression tag	UNP P54646
C	-4	LEU	-	expression tag	UNP P54646
C	-3	PHE	-	expression tag	UNP P54646
C	-2	GLN	-	expression tag	UNP P54646
C	-1	GLY	-	expression tag	UNP P54646
C	0	PRO	-	expression tag	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	168	1336	863	224	243	1	5	0	0	0
2	D	167	1322	855	221	241	1	4	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP Q9Y478
B	-14	GLY	-	expression tag	UNP Q9Y478
B	-13	LEU	-	expression tag	UNP Q9Y478
B	-12	ASN	-	expression tag	UNP Q9Y478
B	-11	ASP	-	expression tag	UNP Q9Y478
B	-10	ILE	-	expression tag	UNP Q9Y478
B	-9	PHE	-	expression tag	UNP Q9Y478
B	-8	GLU	-	expression tag	UNP Q9Y478
B	-7	ALA	-	expression tag	UNP Q9Y478
B	-6	GLN	-	expression tag	UNP Q9Y478
B	-5	LYS	-	expression tag	UNP Q9Y478
B	-4	ILE	-	expression tag	UNP Q9Y478
B	-3	GLU	-	expression tag	UNP Q9Y478
B	-2	TRP	-	expression tag	UNP Q9Y478
B	-1	HIS	-	expression tag	UNP Q9Y478

*Continued on next page...*

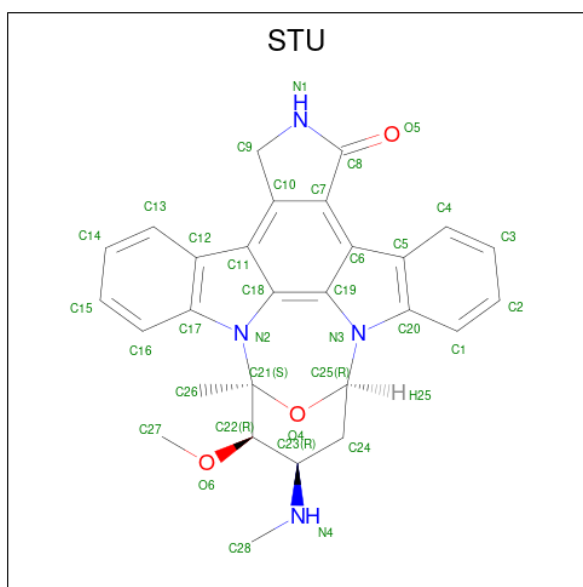
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLU	-	expression tag	UNP Q9Y478
D	-15	MET	-	expression tag	UNP Q9Y478
D	-14	GLY	-	expression tag	UNP Q9Y478
D	-13	LEU	-	expression tag	UNP Q9Y478
D	-12	ASN	-	expression tag	UNP Q9Y478
D	-11	ASP	-	expression tag	UNP Q9Y478
D	-10	ILE	-	expression tag	UNP Q9Y478
D	-9	PHE	-	expression tag	UNP Q9Y478
D	-8	GLU	-	expression tag	UNP Q9Y478
D	-7	ALA	-	expression tag	UNP Q9Y478
D	-6	GLN	-	expression tag	UNP Q9Y478
D	-5	LYS	-	expression tag	UNP Q9Y478
D	-4	ILE	-	expression tag	UNP Q9Y478
D	-3	GLU	-	expression tag	UNP Q9Y478
D	-2	TRP	-	expression tag	UNP Q9Y478
D	-1	HIS	-	expression tag	UNP Q9Y478
D	0	GLU	-	expression tag	UNP Q9Y478

- Molecule 3 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1.

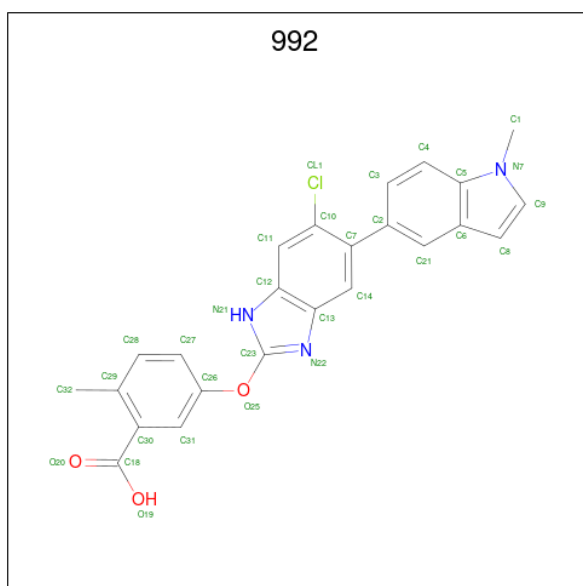
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	294	2369	1541	393	428	7	8	0	0
3	F	288	2315	1504	385	419	7	15	0	0

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: C<sub>28</sub>H<sub>26</sub>N<sub>4</sub>O<sub>3</sub>).



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-chloranyl-5-(1-methylindol-5-yl)-1H-benzimidazol-2-yl]oxy]-2-methylbenzoic acid (three-letter code: 992) (formula: C<sub>24</sub>H<sub>18</sub>ClN<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			31	24	1	3	3		

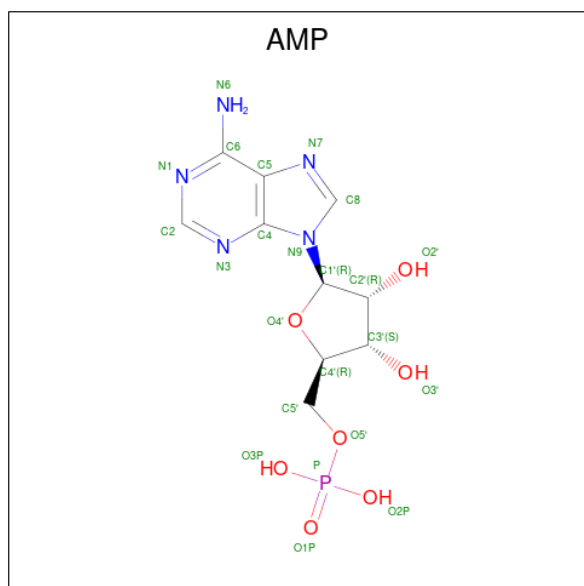
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
5	C	1	31	24	1	3	3	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	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
6	F	1	23	10	5	7	1	0	0

- Molecule 7 is water.

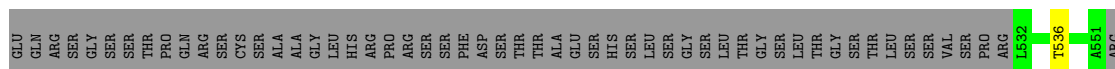
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	13	13	13	0	0
7	B	6	6	6	0	0

Continued on next page...

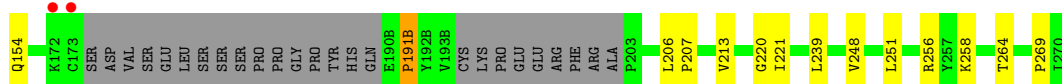
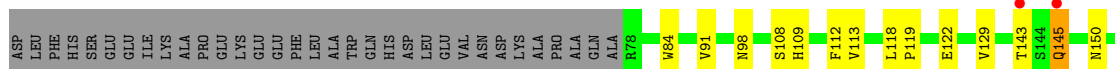
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
7	C	6	Total O 6 6	0	0
7	D	1	Total O 1 1	0	0
7	E	2	Total O 2 2	0	0
7	F	3	Total O 3 3	0	0

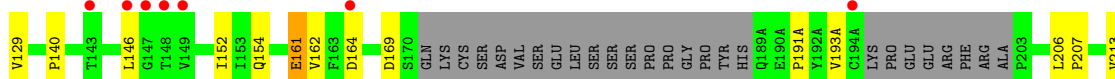
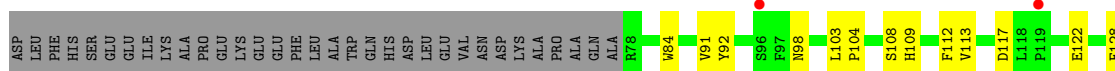




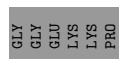
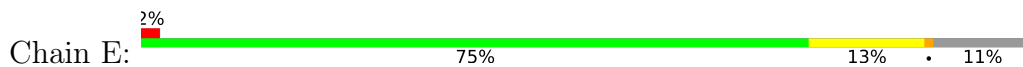
● Molecule 2: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-1



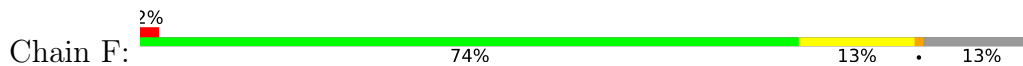
● Molecule 2: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-1

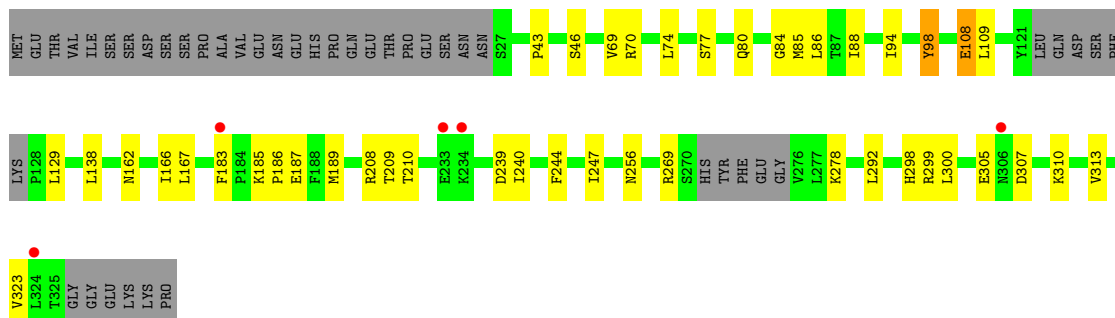


● Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1



● Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.03Å 134.14Å 140.56Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.91 – 3.02 19.91 – 3.02	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.91-3.02) 92.0 (19.91-3.02)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.04Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.218 , 0.253 0.224 , 0.257	Depositor DCC
$R_{free}$ test set	2550 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.0	Xtrriage
Anisotropy	0.303	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 67.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: STU, SEP, TPO, AMP, 992

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	0.21	0/3478	0.36	0/4698
1	C	0.22	0/3333	0.37	0/4497
2	B	0.22	0/1361	0.43	1/1851 (0.1%)
2	D	0.23	0/1347	0.45	1/1834 (0.1%)
3	E	0.21	0/2418	0.40	0/3282
3	F	0.22	0/2360	0.39	0/3202
All	All	0.22	0/14297	0.39	2/19364 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	191(A)	PRO	N-CA-CB	6.22	110.77	103.30
2	B	191(B)	PRO	N-CA-CB	5.89	110.37	103.30

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	3411	0	3398	43	0
1	C	3268	0	3277	35	0
2	B	1336	0	1322	15	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1322	0	1300	17	0
3	E	2369	0	2444	25	0
3	F	2315	0	2398	19	0
4	A	35	0	26	2	0
4	C	35	0	26	1	0
5	A	31	0	17	2	0
5	C	31	0	17	2	0
6	E	69	0	36	2	0
6	F	69	0	36	0	0
7	A	13	0	0	0	0
7	B	6	0	0	0	0
7	C	6	0	0	1	0
7	D	1	0	0	0	0
7	E	2	0	0	0	0
7	F	3	0	0	0	0
All	All	14322	0	14297	146	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 146 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:430:TRP:HB3	1:C:440:VAL:HA	1.71	0.72
1:C:179:TYR:HA	1:C:202:VAL:HG11	1.77	0.67
1:C:158:PHE:O	1:C:160:LEU:N	2.28	0.66
1:C:423:MET:HB3	1:C:428:PHE:HB2	1.78	0.65
2:D:122:GLU:HG2	2:D:154:GLN:HG2	1.79	0.65

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	415/571 (73%)	394 (95%)	21 (5%)	0	100	100
1	C	393/571 (69%)	369 (94%)	23 (6%)	1 (0%)	41	75
2	B	161/286 (56%)	155 (96%)	5 (3%)	1 (1%)	25	62
2	D	160/286 (56%)	150 (94%)	8 (5%)	2 (1%)	12	43
3	E	290/331 (88%)	279 (96%)	7 (2%)	4 (1%)	11	41
3	F	282/331 (85%)	271 (96%)	10 (4%)	1 (0%)	34	71
All	All	1701/2376 (72%)	1618 (95%)	74 (4%)	9 (0%)	29	66

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	159	GLY
2	D	193(A)	VAL
2	B	191(B)	PRO
3	E	185	LYS
2	D	221	ILE

### 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	365/503 (73%)	356 (98%)	9 (2%)	47	78
1	C	355/503 (71%)	345 (97%)	10 (3%)	43	76
2	B	149/253 (59%)	144 (97%)	5 (3%)	37	72
2	D	146/253 (58%)	139 (95%)	7 (5%)	25	60
3	E	270/304 (89%)	260 (96%)	10 (4%)	34	69
3	F	265/304 (87%)	252 (95%)	13 (5%)	25	60
All	All	1550/2120 (73%)	1496 (96%)	54 (4%)	36	70

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	161	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	E	208	ARG
3	F	269	ARG
2	D	221	ILE
3	E	98	TYR

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

Mol	Chain	Res	Type
1	A	48	ASN
2	B	145	GLN
3	F	162	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
2	SEP	B	108	2	8,9,10	0.91	0	8,12,14	0.98	0
2	SEP	D	108	2	8,9,10	0.90	0	8,12,14	0.84	0
1	TPO	C	172	1	8,10,11	0.79	0	10,14,16	1.02	0
1	TPO	A	172	1	8,10,11	0.76	0	10,14,16	0.95	0

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	TPO	CB-OG1-P-O2P
2	B	108	SEP	N-CA-CB-OG
2	D	108	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	108	SEP	2	0
2	D	108	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
6	AMP	F	1327	-	22,25,25	0.89	1 (4%)	25,38,38	1.21	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	AMP	E	1326	-	22,25,25	0.90	1 (4%)	25,38,38	1.20	2 (8%)
6	AMP	E	1328	-	22,25,25	0.90	1 (4%)	25,38,38	1.22	2 (8%)
6	AMP	F	1328	-	22,25,25	0.89	1 (4%)	25,38,38	1.24	2 (8%)
6	AMP	E	1327	-	22,25,25	0.90	1 (4%)	25,38,38	1.16	2 (8%)
5	992	C	1553	-	34,35,35	1.22	3 (8%)	39,52,52	1.30	3 (7%)
4	STU	C	1552	-	30,42,42	1.01	2 (6%)	31,68,68	2.14	9 (29%)
5	992	A	1553	-	34,35,35	1.23	4 (11%)	39,52,52	1.32	3 (7%)
4	STU	A	1552	-	30,42,42	1.00	2 (6%)	31,68,68	2.11	8 (25%)
6	AMP	F	1326	-	22,25,25	0.88	1 (4%)	25,38,38	1.20	2 (8%)

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
6	AMP	F	1327	-	-	1/6/26/26	0/3/3/3
6	AMP	E	1326	-	-	2/6/26/26	0/3/3/3
6	AMP	E	1328	-	-	4/6/26/26	0/3/3/3
6	AMP	F	1328	-	-	0/6/26/26	0/3/3/3
6	AMP	E	1327	-	-	3/6/26/26	0/3/3/3
5	992	C	1553	-	-	4/10/12/12	0/5/5/5
4	STU	C	1552	-	-	1/4/42/42	-
5	992	A	1553	-	-	4/10/12/12	0/5/5/5
4	STU	A	1552	-	-	1/4/42/42	-
6	AMP	F	1326	-	-	0/6/26/26	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1553	992	C9-N7	-2.91	1.32	1.37
5	C	1553	992	C9-N7	-2.88	1.32	1.37
5	C	1553	992	C11-C10	2.87	1.41	1.36
5	A	1553	992	C11-C10	2.80	1.41	1.36
5	A	1553	992	O25-C23	2.67	1.41	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1552	STU	C9-N1-C8	-5.37	108.69	113.85
4	A	1552	STU	C9-N1-C8	-5.35	108.71	113.85
4	A	1552	STU	C10-C9-N1	4.12	105.95	101.76
4	C	1552	STU	C10-C9-N1	4.07	105.90	101.76
4	C	1552	STU	C7-C8-N1	4.01	110.43	106.37

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

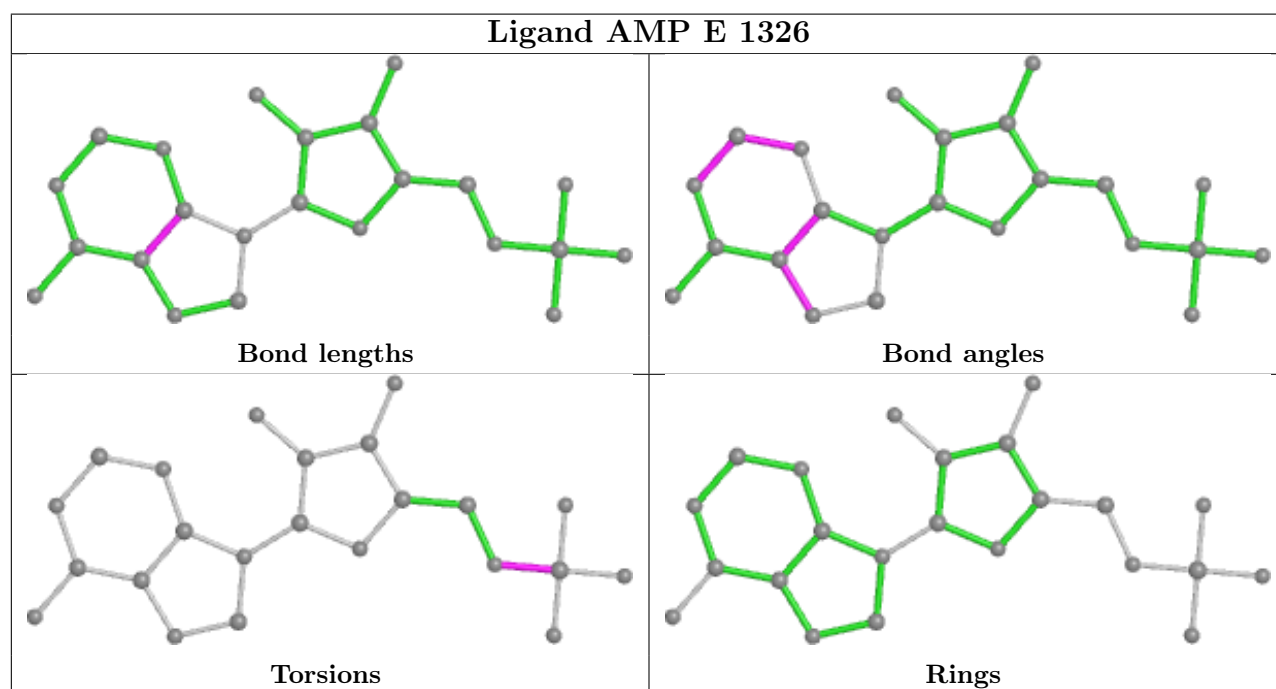
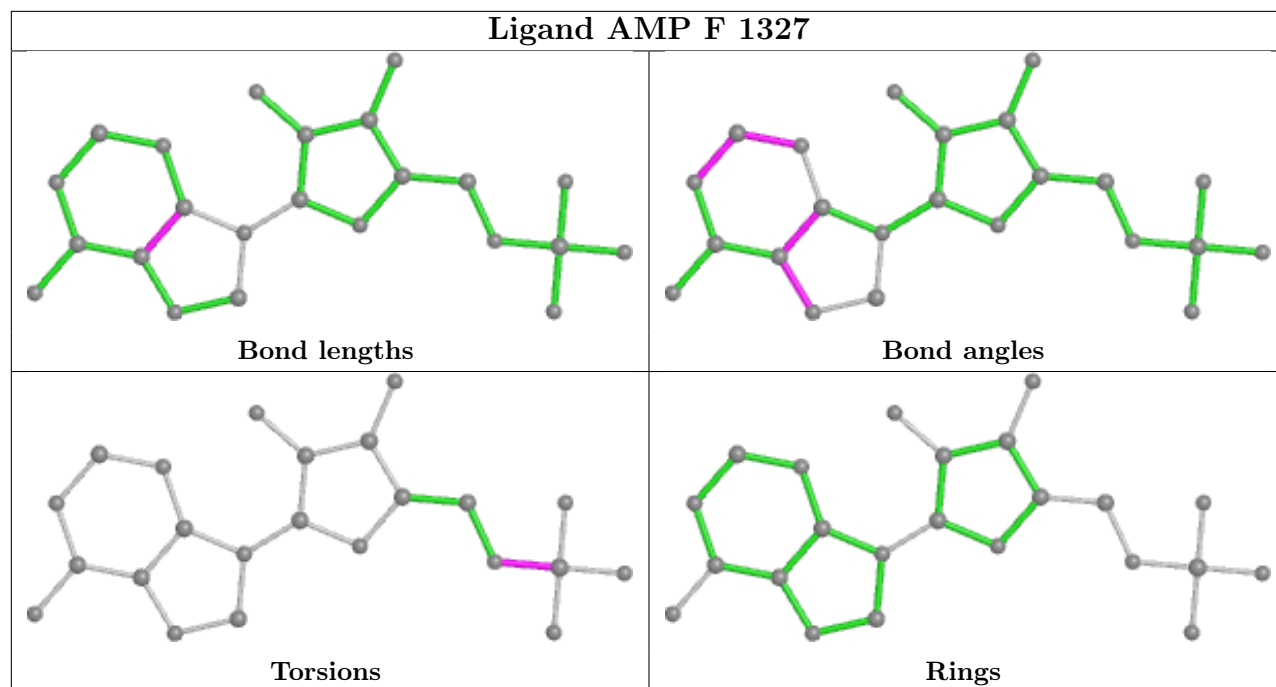
Mol	Chain	Res	Type	Atoms
6	E	1327	AMP	C5'-O5'-P-O1P
6	E	1327	AMP	C5'-O5'-P-O2P
6	E	1327	AMP	C5'-O5'-P-O3P
6	E	1328	AMP	C5'-O5'-P-O2P
6	E	1328	AMP	C5'-O5'-P-O3P

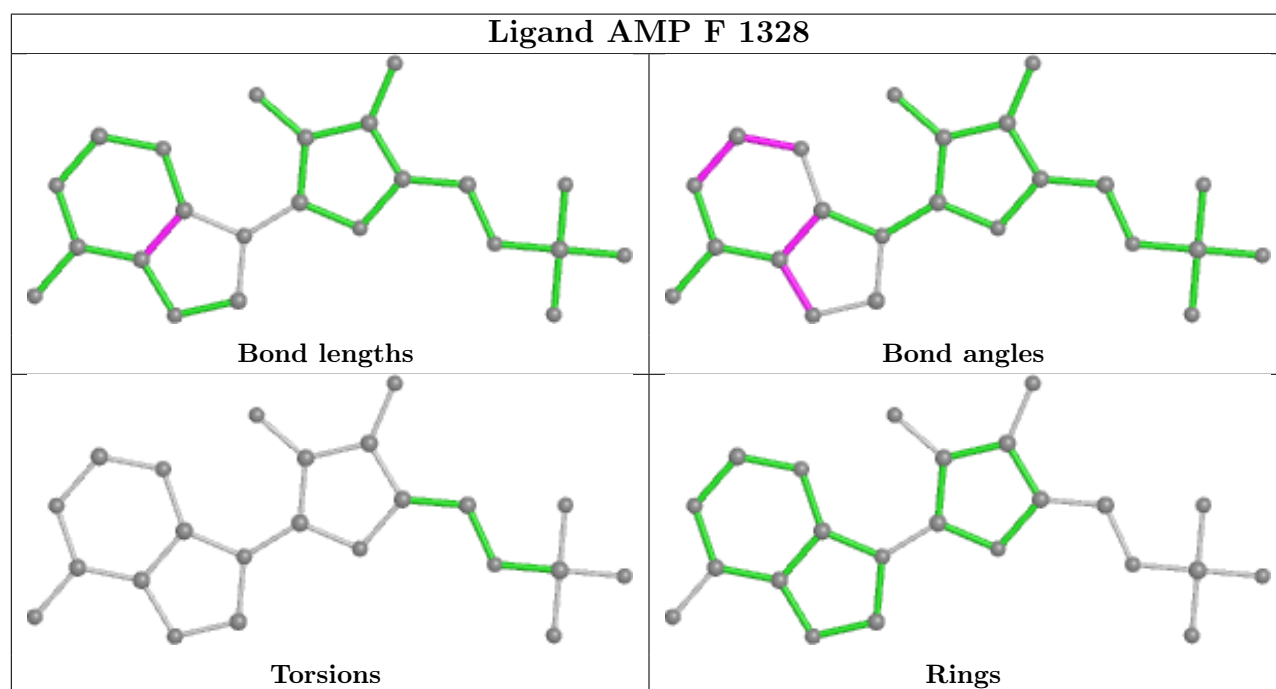
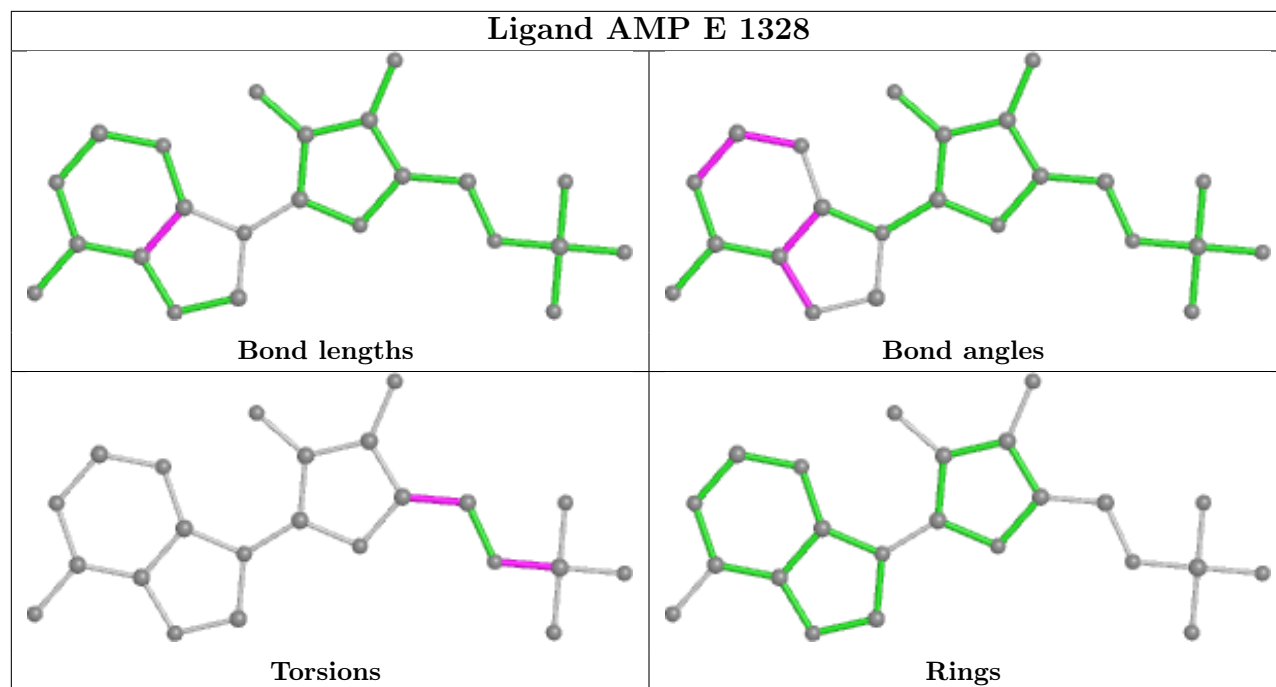
There are no ring outliers.

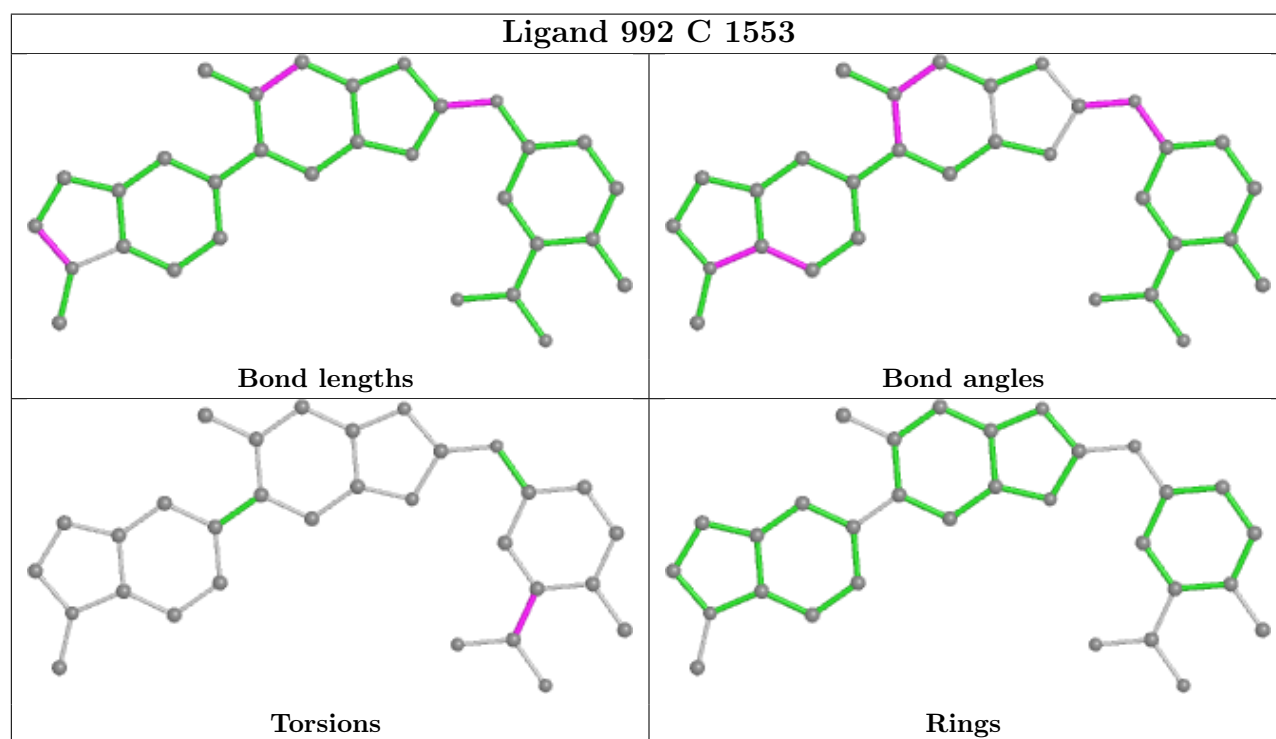
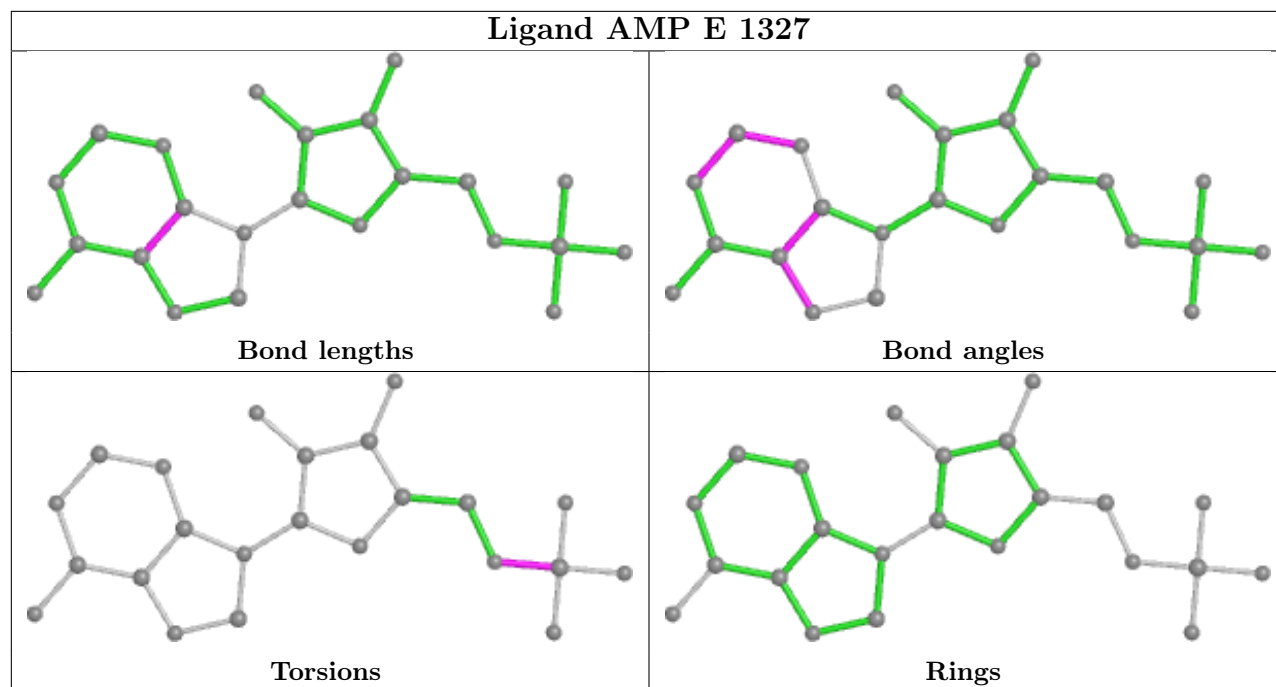
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1326	AMP	1	0
6	E	1327	AMP	1	0
5	C	1553	992	2	0
4	C	1552	STU	1	0
5	A	1553	992	2	0
4	A	1552	STU	2	0

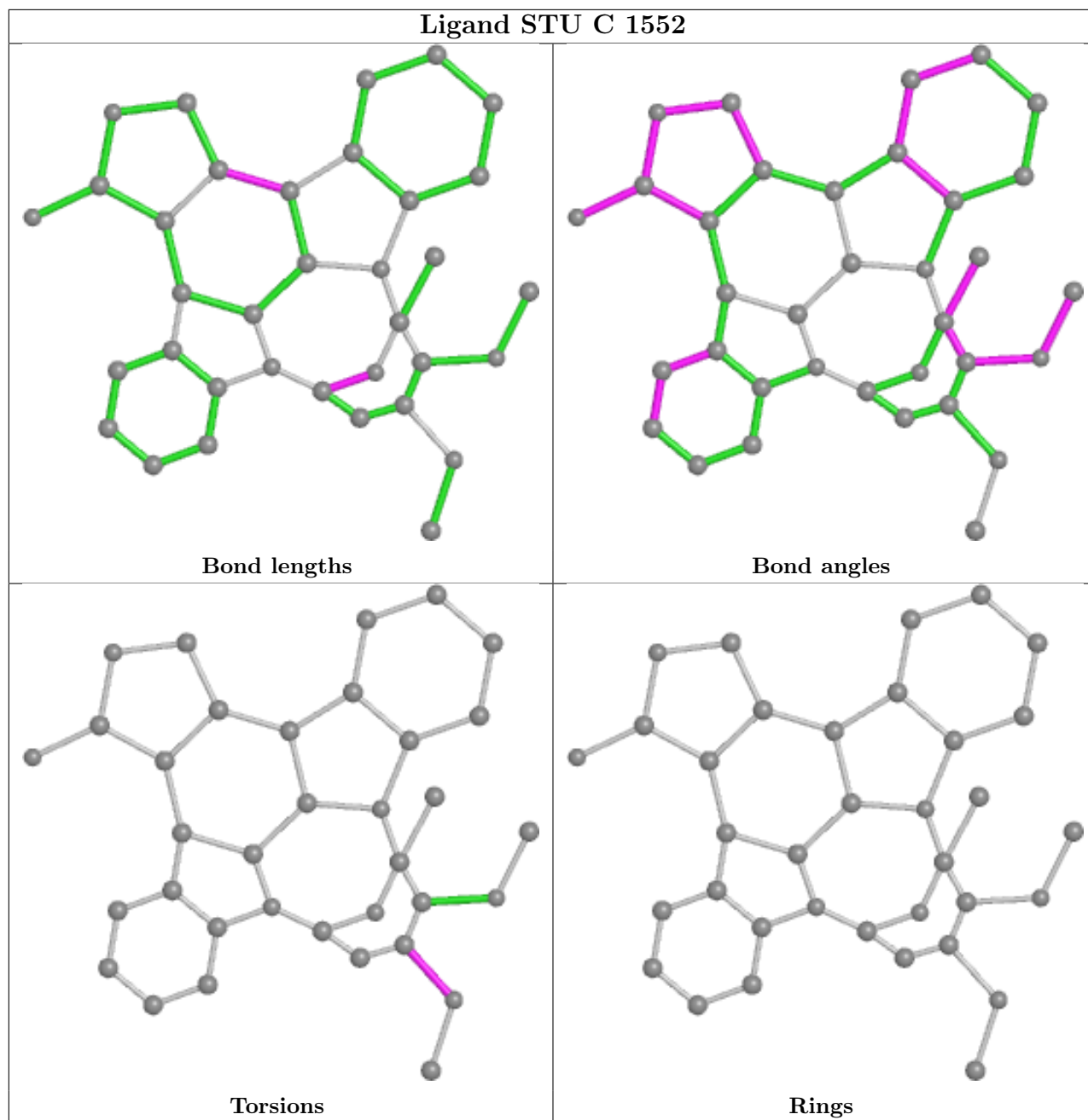
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

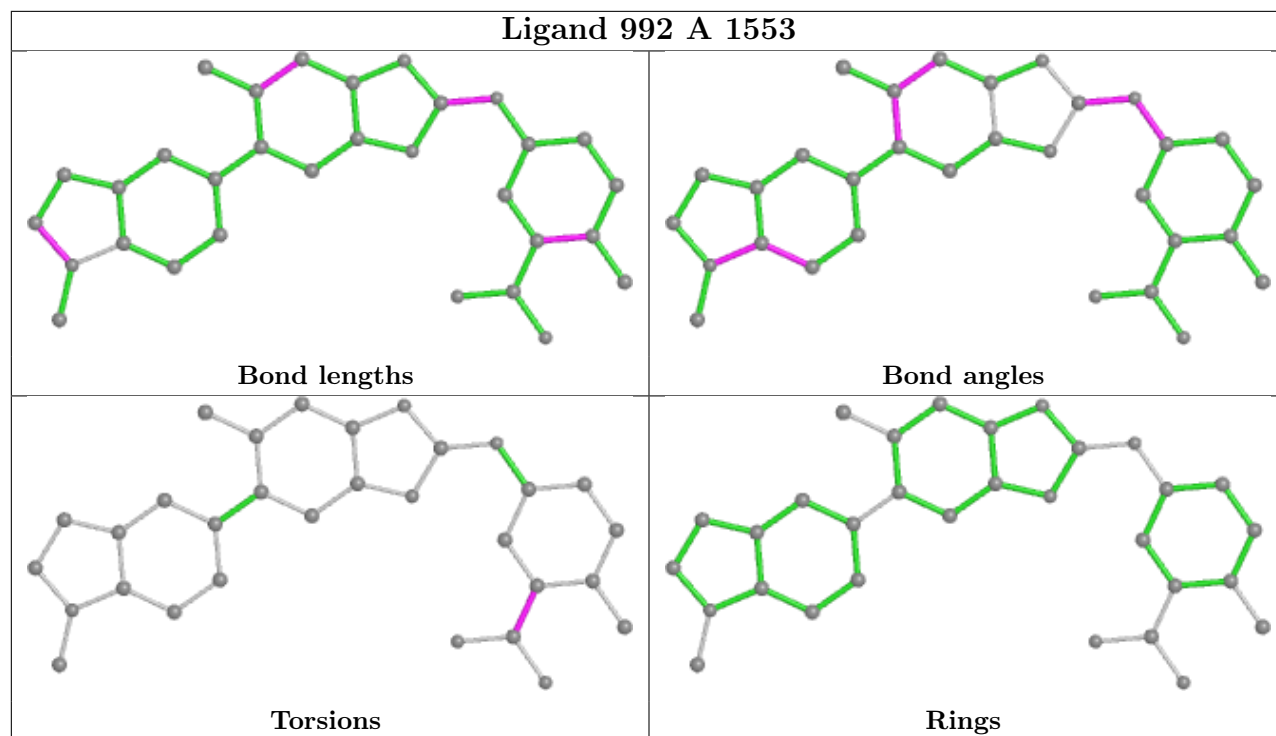


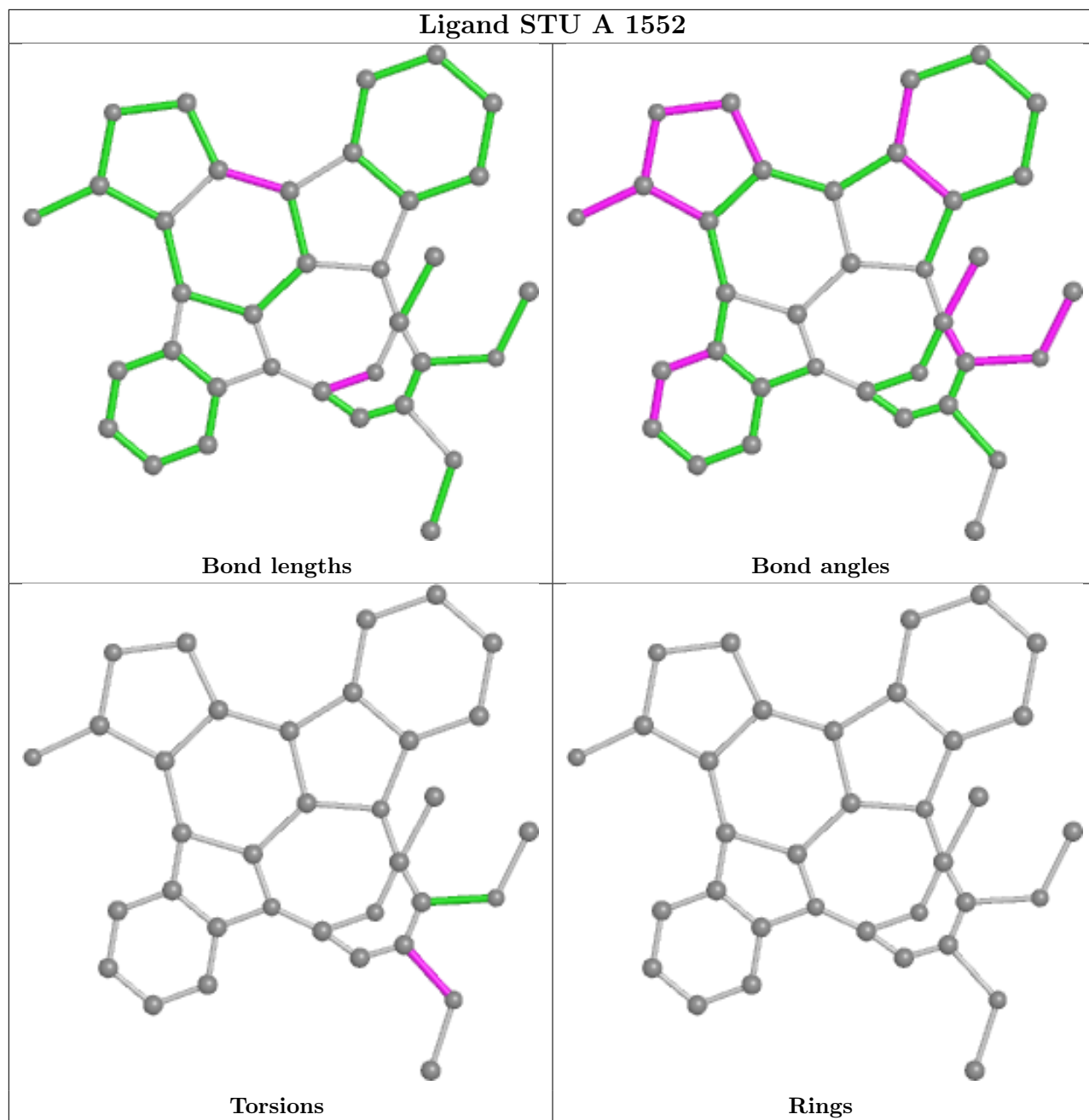


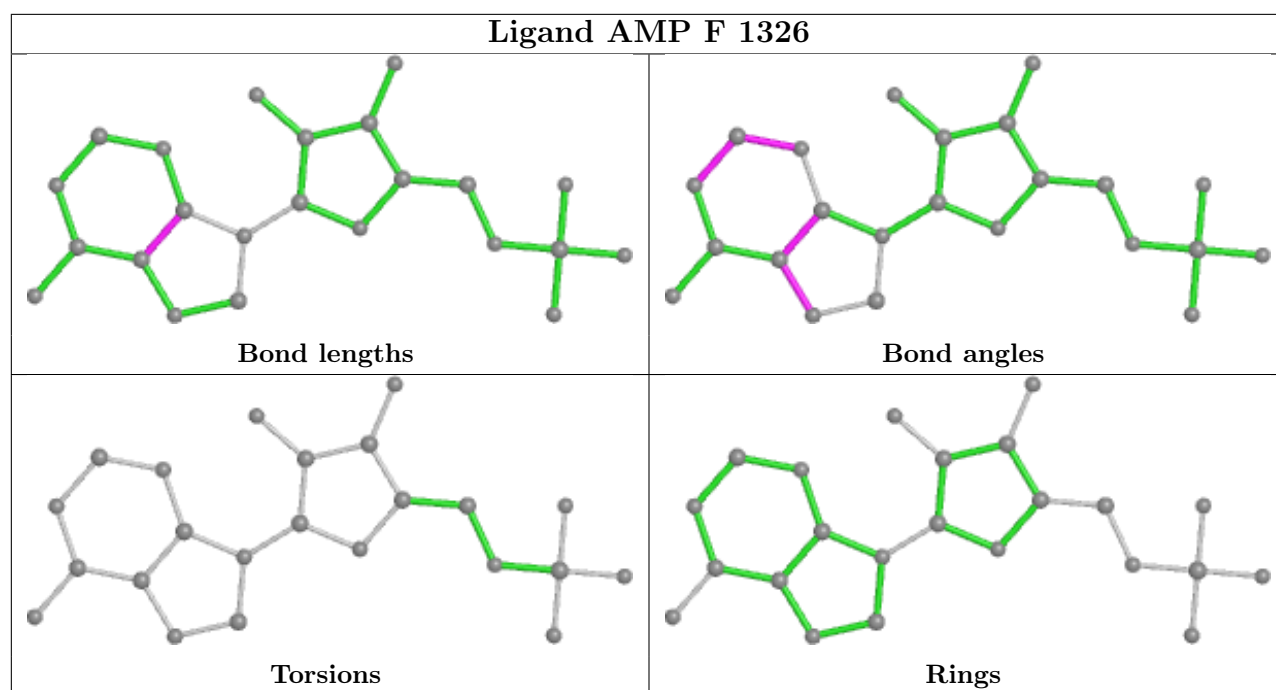












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	425/571 (74%)	-0.13	7 (1%) 72 43	39, 77, 122, 161	1 (0%)
1	C	403/571 (70%)	-0.01	10 (2%) 57 28	44, 75, 134, 171	2 (0%)
2	B	167/286 (58%)	-0.18	4 (2%) 59 30	50, 71, 122, 146	0
2	D	166/286 (58%)	0.10	9 (5%) 25 9	41, 91, 149, 173	0
3	E	294/331 (88%)	-0.26	7 (2%) 59 30	43, 66, 117, 161	2 (0%)
3	F	288/331 (87%)	-0.26	5 (1%) 70 41	39, 64, 117, 160	3 (1%)
All	All	1743/2376 (73%)	-0.13	42 (2%) 59 30	39, 72, 130, 173	8 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	148	THR	5.6
3	E	236	ARG	4.5
2	D	119	PRO	4.4
1	C	396	ALA	4.0
1	C	413	TYR	3.8

### 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
2	SEP	D	108	10/11	0.93	0.19	80,88,111,113	0
2	SEP	B	108	10/11	0.94	0.18	73,84,88,92	0
1	TPO	C	172	11/12	0.97	0.12	55,62,67,68	0
1	TPO	A	172	11/12	0.97	0.10	68,70,72,73	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

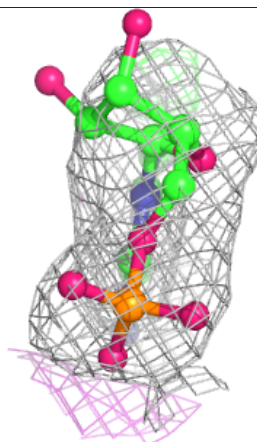
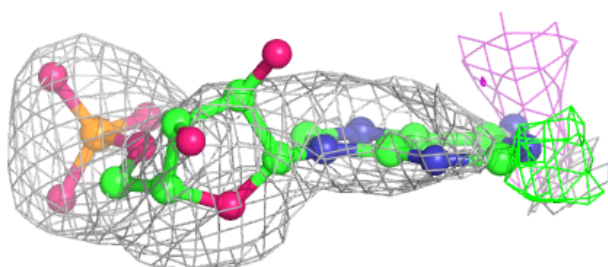
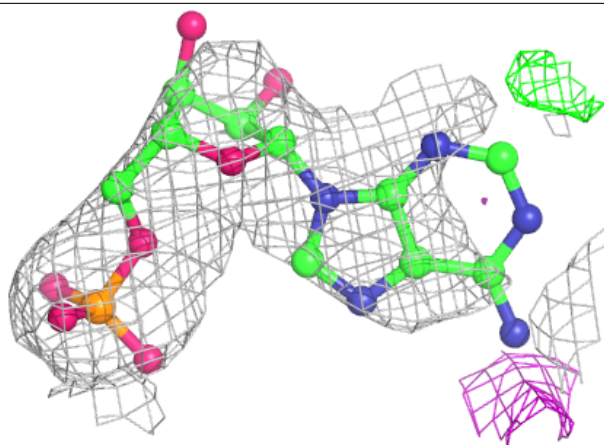
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	AMP	E	1326	23/23	0.82	0.29	127,147,161,165	0
5	992	C	1553	31/31	0.91	0.21	73,75,80,82	0
5	992	A	1553	31/31	0.91	0.24	61,67,84,88	0
6	AMP	F	1326	23/23	0.91	0.20	120,134,147,151	0
4	STU	A	1552	35/35	0.96	0.19	37,44,48,87	0
6	AMP	E	1327	23/23	0.96	0.18	49,57,71,79	0
4	STU	C	1552	35/35	0.96	0.18	36,43,51,52	0
6	AMP	F	1328	23/23	0.96	0.16	57,62,67,69	0
6	AMP	F	1327	23/23	0.97	0.14	74,84,90,101	0
6	AMP	E	1328	23/23	0.97	0.14	53,68,75,77	0

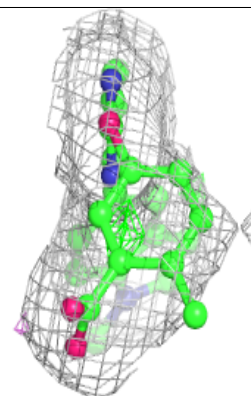
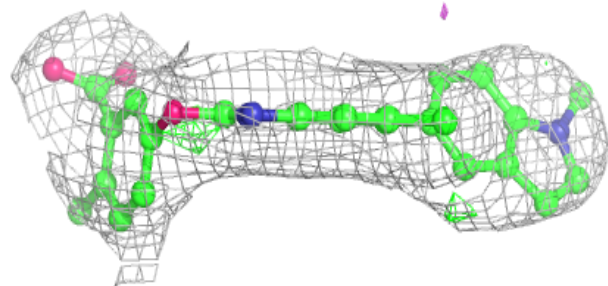
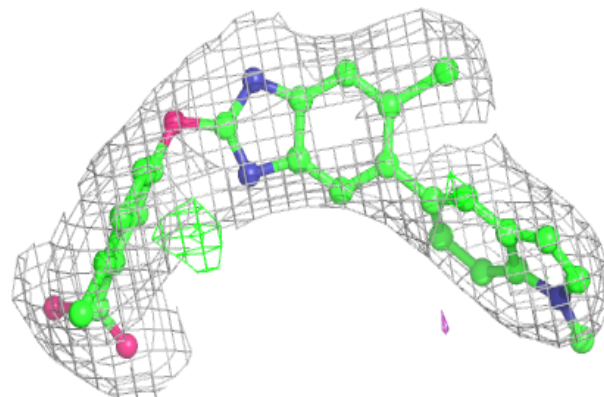
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AMP E 1326:**

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

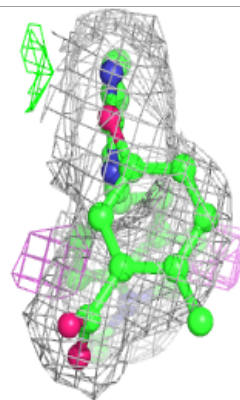
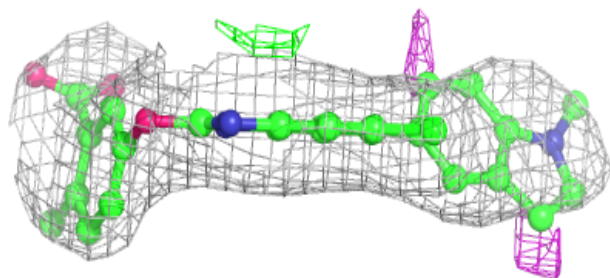
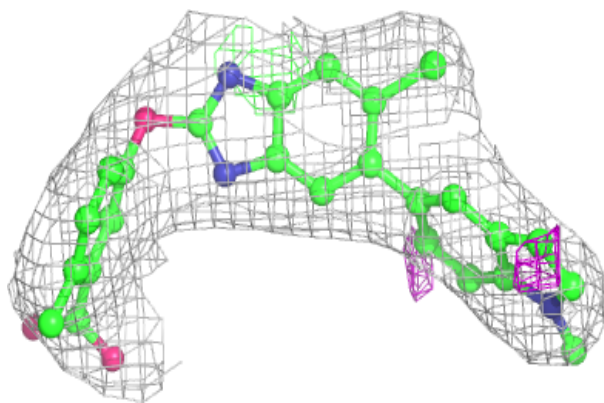
**Electron density around 992 C 1553:**

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

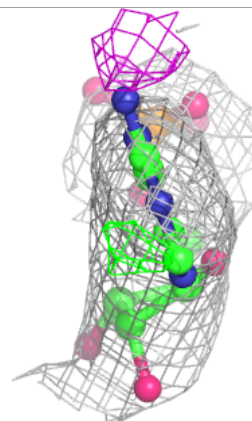
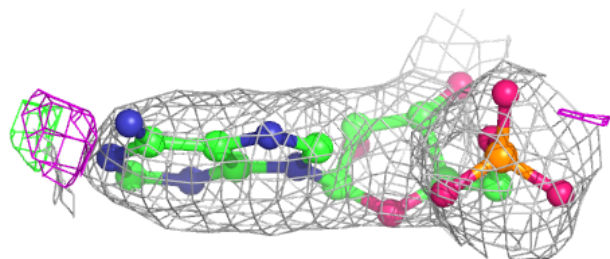
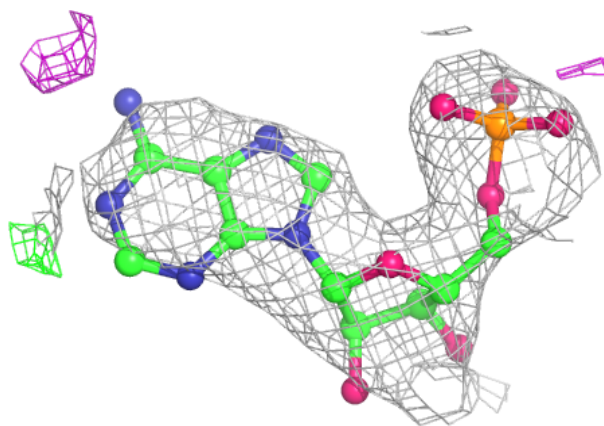


**Electron density around 992 A 1553:**

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

**Electron density around AMP F 1326:**

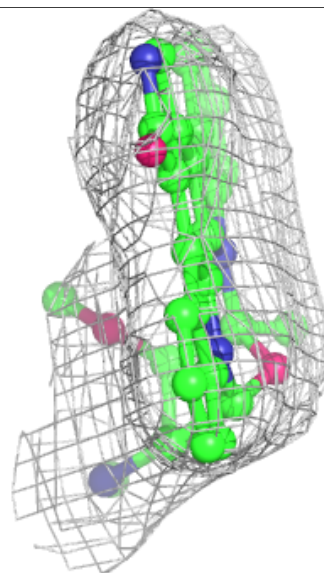
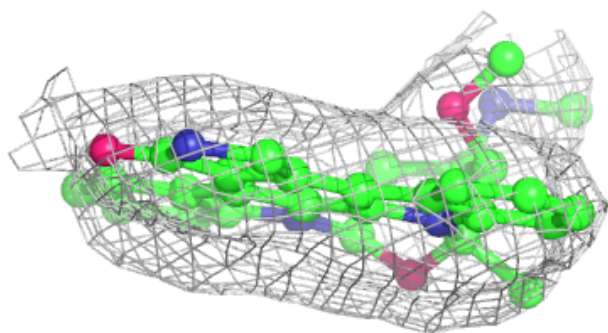
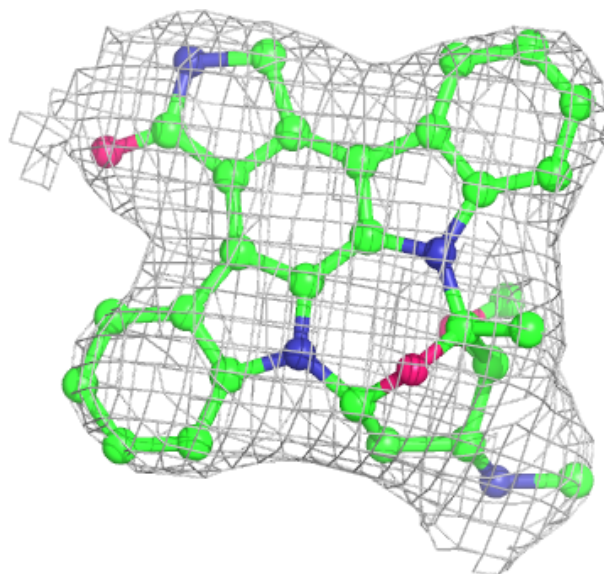
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





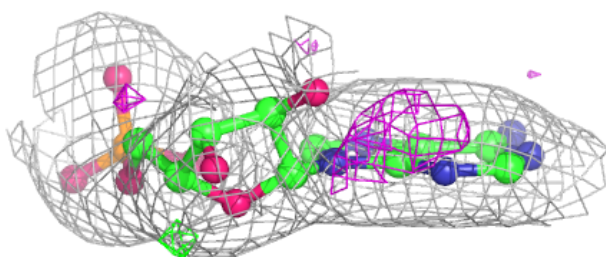
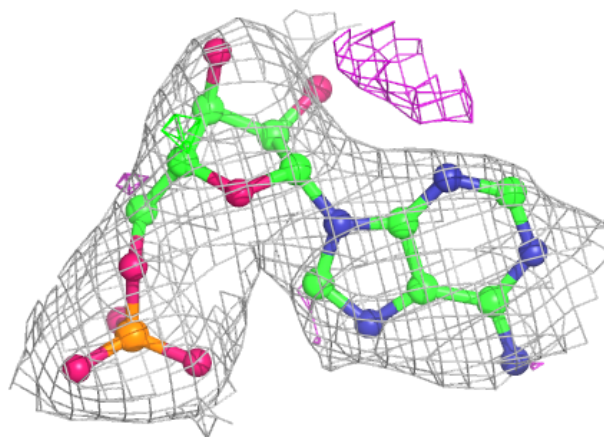
**Electron density around STU A 1552:**

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



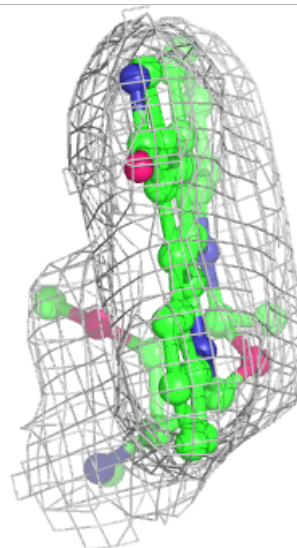
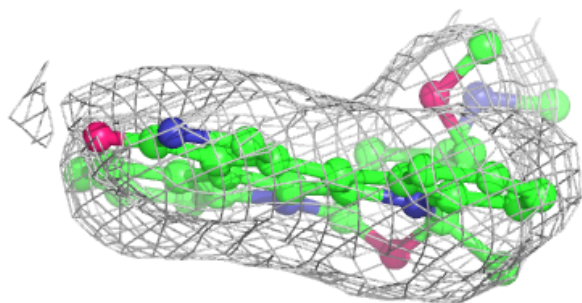
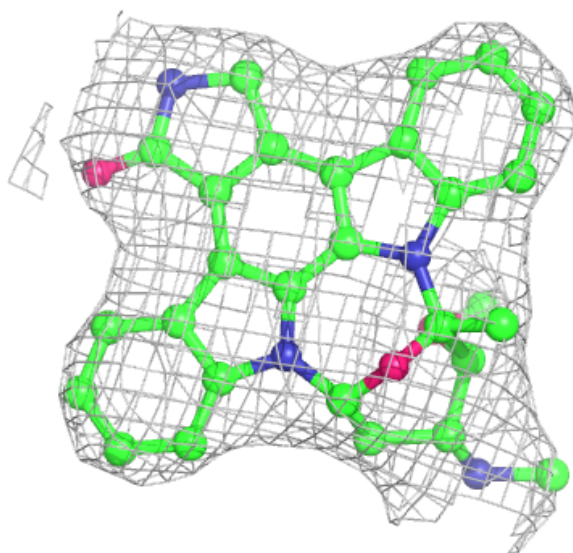
**Electron density around AMP E 1327:**

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



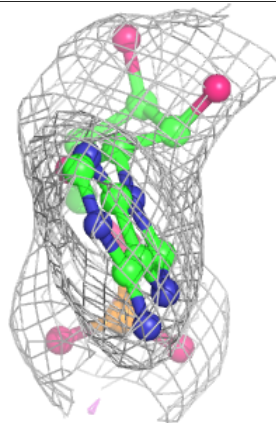
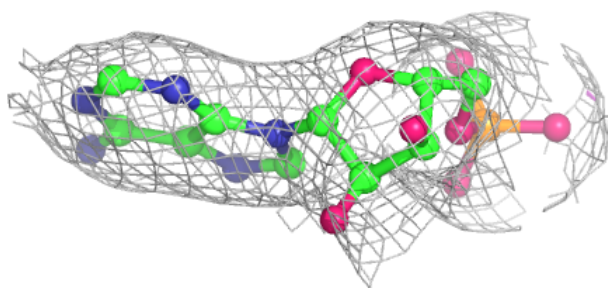
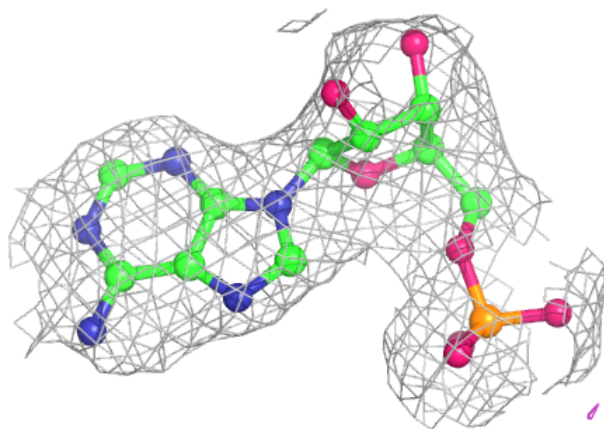
**Electron density around STU C 1552:**

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

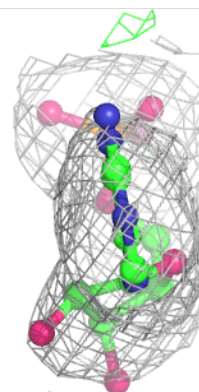
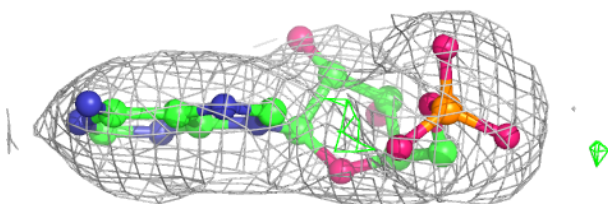
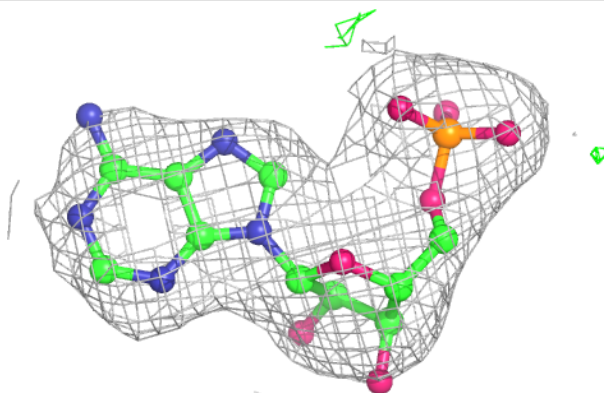


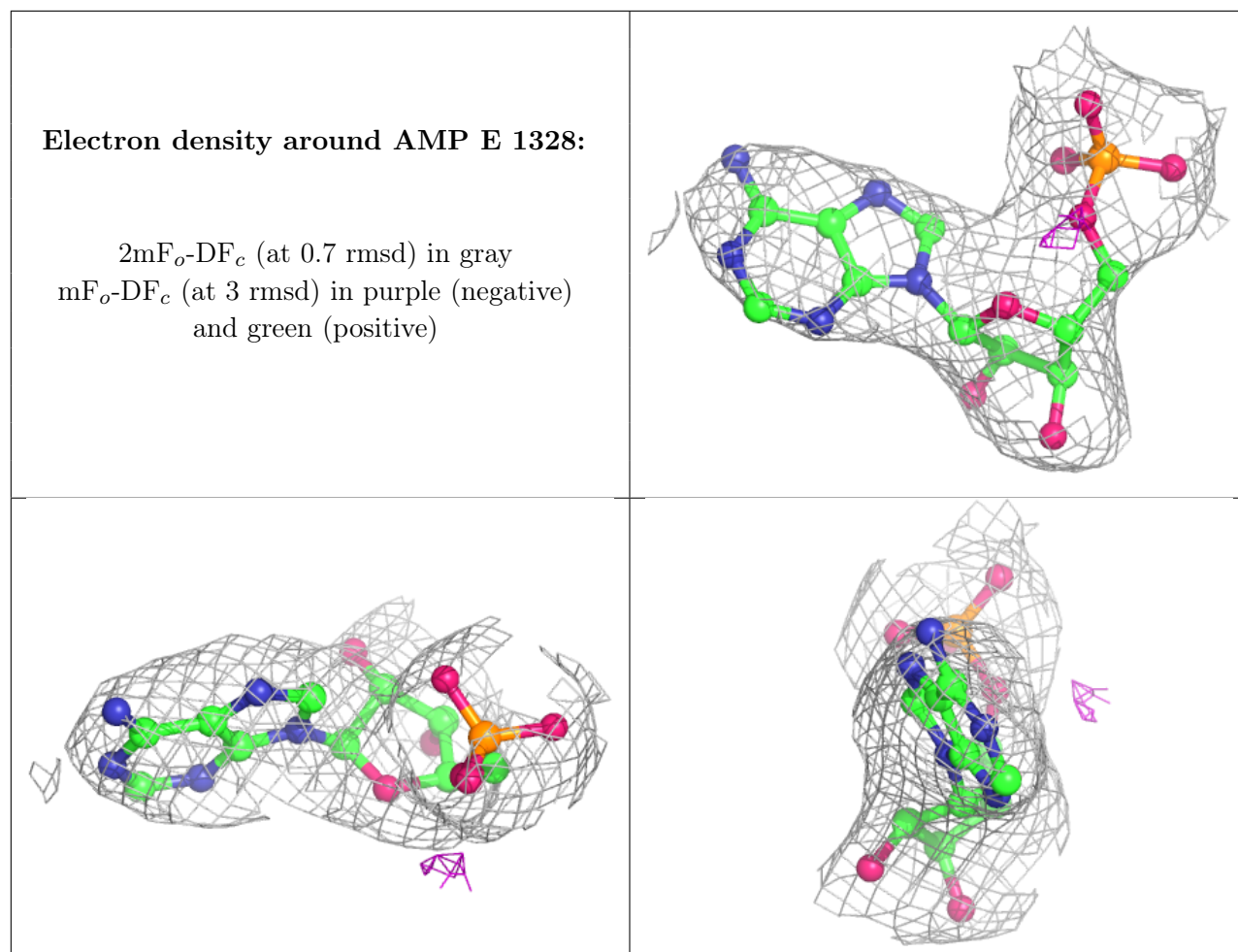
**Electron density around AMP F 1328:**

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

**Electron density around AMP F 1327:**

$2mF_o-DF_c$  (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.