



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:40 AM UTC

PDB ID : 6C9F / pdb_00006c9f
Title : AMP-activated protein kinase bound to pharmacological activator R734
Authors : Yan, Y.; Zhou, X.E.; Novick, S.; Shaw, S.J.; Li, Y.; Hitoshi, Y.; Brunzelle, J.S.; Griffin, P.R.; Xu, H.E.; Melcher, K.
Deposited on : 2018-01-26
Resolution : 2.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

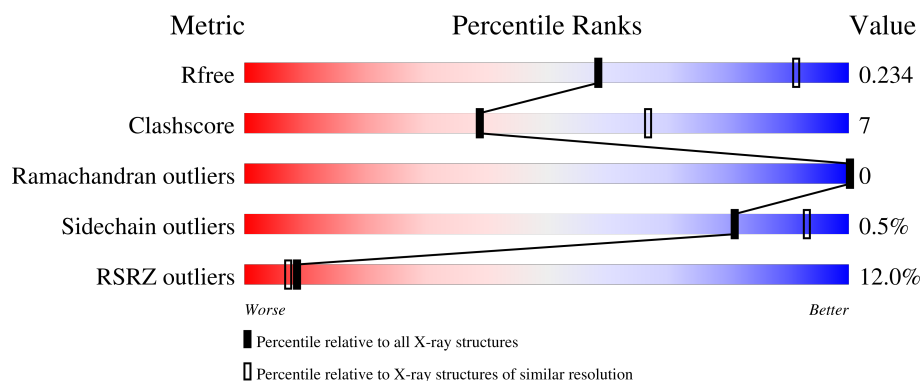
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	494	6% 62%13%24%
2	B	204	19% 74%12%14%
3	C	331	9% 75%15%9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6991 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-1,5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	P	S	0	0	0
			3025	1939	526	541	1	18			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	expression tag	UNP Q13131
A	4	GLY	-	expression tag	UNP Q13131
A	5	HIS	-	expression tag	UNP Q13131
A	6	HIS	-	expression tag	UNP Q13131
A	7	HIS	-	expression tag	UNP Q13131
A	8	HIS	-	expression tag	UNP Q13131
A	9	HIS	-	expression tag	UNP Q13131
A	10	HIS	-	expression tag	UNP Q13131
A	11	GLY	-	expression tag	UNP Q13131
A	12	SER	-	expression tag	UNP Q13131

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1410	912	239	254	5			

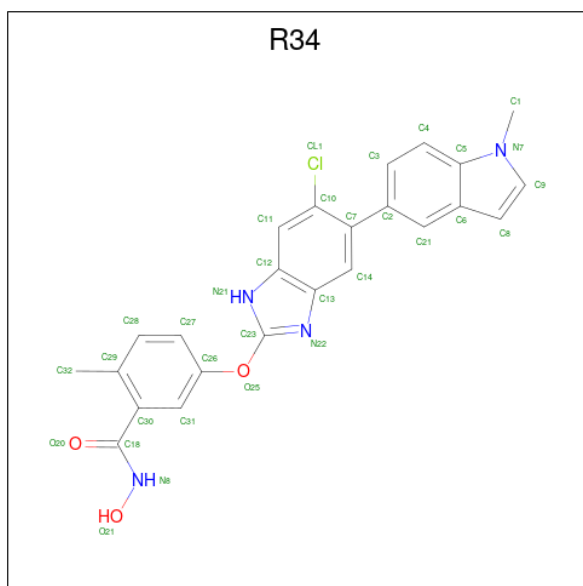
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	expression tag	UNP Q9Y478
B	108	ASP	SER	conflict	UNP Q9Y478

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

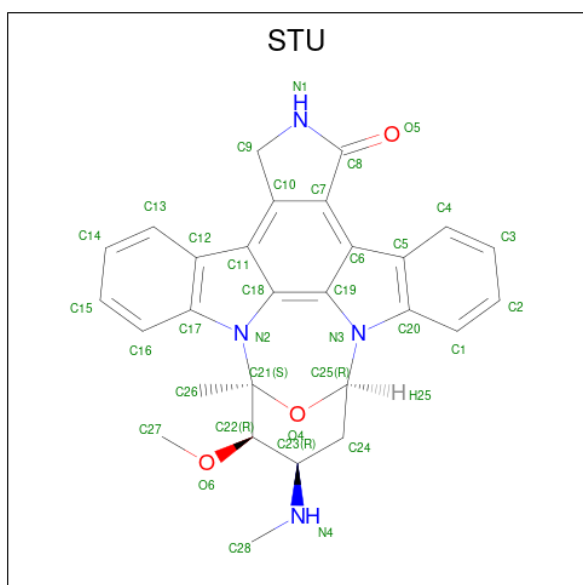
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	300	Total	C	N	O	S	0	0	0
			2420	1572	402	439	7			

- Molecule 4 is 5-{{6-chloro-5-(1-methyl-1H-indol-5-yl)-1H-benzimidazol-2-yl}oxy}-N-hydroxy-2-methylbenzamide (CCD ID: R34) (formula: C₂₄H₁₉ClN₄O₃).



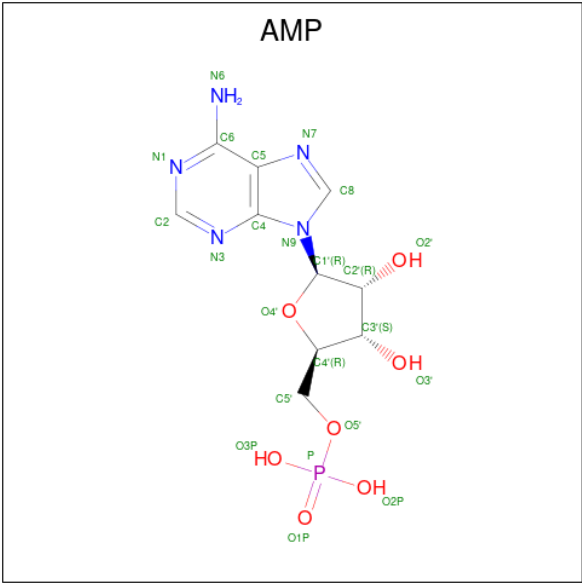
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			32	24	1	4	3		

- Molecule 5 is STAUROSPORINE (CCD ID: STU) (formula: C₂₈H₂₆N₄O₃).



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

- Molecule 6 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).

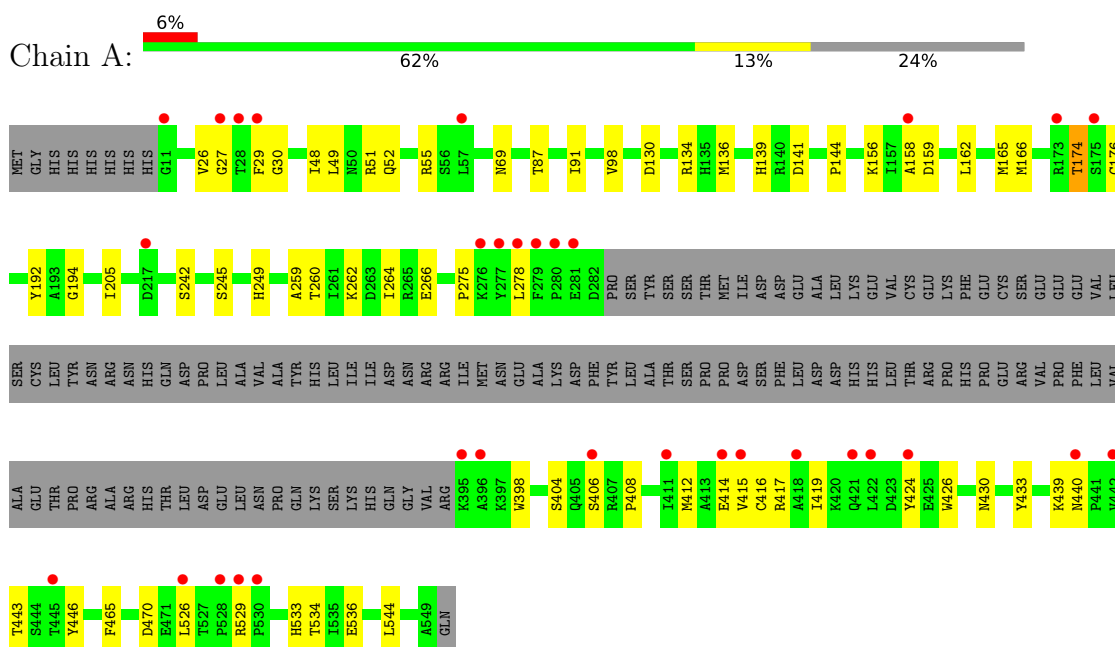


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

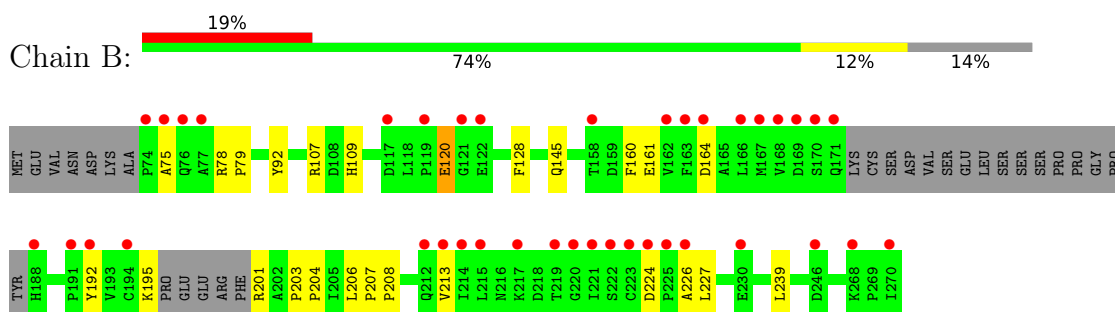
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

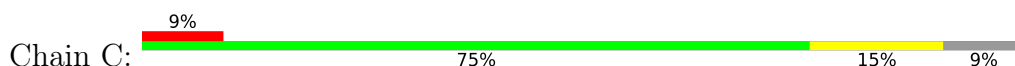
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1,5'-AMP-activated protein kinase catalytic subunit alpha-1

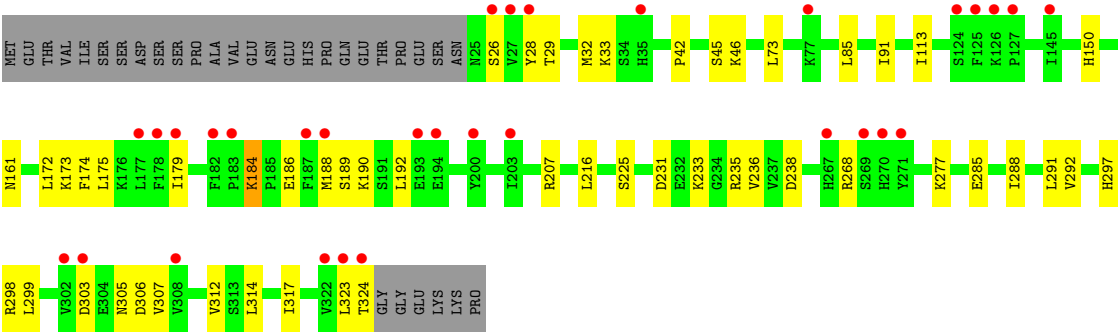


- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.29Å 123.29Å 406.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.67 – 2.92 49.67 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.67-2.92) 100.0 (49.67-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.228 , 0.245 (Not available) , 0.234	Depositor DCC
R_{free} test set	2918 reflections (7.18%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6991	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: STU, TPO, R34, AMP

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	0.27	0/3083	0.71	2/4160 (0.0%)
2	B	0.28	0/1450	0.71	0/1975
3	C	0.28	0/2471	0.71	0/3355
All	All	0.28	0/7004	0.71	2/9490 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLY	CA-C-N	-5.31	113.56	119.19
1	A	194	GLY	C-N-CA	-5.31	113.56	119.19

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	3025	0	3059	44	0
2	B	1410	0	1405	20	0
3	C	2420	0	2489	38	0
4	A	32	0	0	1	0
5	A	35	0	26	2	0
6	C	69	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6991	0	7015	95	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 7.

All (95) 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:A:430:ASN:HB3	1:A:433:TYR:HB3	1.61	0.81
1:A:136:MET:HA	1:A:166:MET:HE3	1.70	0.73
3:C:268:ARG:NH1	6:C:1102:AMP:O2'	2.23	0.72
1:A:69:ASN:ND2	1:A:165:MET:SD	2.64	0.71
1:A:440:ASN:ND2	1:A:443:THR:OG1	2.27	0.67
3:C:188:MET:HB3	3:C:285:GLU:HB3	1.77	0.67
3:C:238:ASP:OD1	3:C:268:ARG:NH2	2.28	0.66
1:A:30:GLY:H	4:A:601:R34:C18	2.09	0.65
3:C:73:LEU:HD21	3:C:85:LEU:HB2	1.81	0.63
1:A:398:TRP:HB2	2:B:213:VAL:HG11	1.80	0.61
1:A:470:ASP:HB2	1:A:526:LEU:HD23	1.83	0.61
1:A:534:THR:OG1	3:C:161:ASN:ND2	2.33	0.61
3:C:188:MET:HE1	3:C:288:ILE:HD12	1.84	0.59
1:A:430:ASN:HD21	2:B:201:ARG:NH2	2.00	0.59
1:A:415:VAL:O	1:A:419:ILE:HG13	2.03	0.59
1:A:98:VAL:HG11	1:A:156:LYS:HG3	1.85	0.58
3:C:303:ASP:OD2	3:C:307:VAL:HB	2.02	0.58
1:A:414:GLU:OE2	1:A:417:ARG:NH1	2.36	0.58
3:C:192:LEU:HD21	3:C:312:VAL:HG21	1.86	0.58
1:A:439:LYS:HB2	1:A:446:TYR:CE2	2.39	0.58
3:C:225:SER:OG	3:C:298:ARG:HD3	2.04	0.57
1:A:30:GLY:HA3	1:A:48:ILE:O	2.05	0.56
1:A:29:PHE:CE1	1:A:49:LEU:HD22	2.41	0.56
3:C:233:LYS:HD2	3:C:235:ARG:CZ	2.35	0.56
1:A:130:ASP:OD2	1:A:134:ARG:NH1	2.40	0.55
1:A:416:CYS:SG	2:B:195:LYS:HD3	2.47	0.55
1:A:275:PRO:HD2	1:A:278:LEU:HD12	1.88	0.54
3:C:277:LYS:NZ	3:C:306:ASP:OD1	2.37	0.54
1:A:415:VAL:HG12	1:A:419:ILE:HD11	1.89	0.54
2:B:78:ARG:HB3	2:B:160:PHE:CZ	2.43	0.54
3:C:32:MET:SD	3:C:175:LEU:HD11	2.48	0.53
2:B:145:GLN:OE1	2:B:145:GLN:N	2.38	0.53
2:B:107:ARG:NH2	2:B:109:HIS:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:HG	1:A:406:SER:HG	1.54	0.53
2:B:224:ASP:HB3	2:B:227:LEU:HG	1.91	0.52
3:C:305:ASN:O	3:C:306:ASP:HB2	2.10	0.51
1:A:51:ARG:NH1	1:A:87:THR:O	2.40	0.51
2:B:226:ALA:O	3:C:46:LYS:N	2.43	0.51
1:A:174:TPO:O	1:A:192:TYR:OH	2.21	0.51
3:C:150:HIS:NE2	6:C:1103:AMP:O1P	2.36	0.51
3:C:29:THR:O	3:C:33:LYS:HG3	2.12	0.50
1:A:426:TRP:CZ3	2:B:192:TYR:HB2	2.48	0.49
1:A:465:PHE:HB2	2:B:239:LEU:HB3	1.93	0.49
1:A:139:HIS:NE2	1:A:159:ASP:O	2.46	0.49
1:A:139:HIS:CE1	1:A:141:ASP:HB3	2.49	0.48
3:C:288:ILE:HG12	3:C:317:ILE:HD13	1.96	0.48
1:A:465:PHE:HE2	1:A:544:LEU:HD23	1.79	0.48
3:C:91:ILE:HG23	3:C:216:LEU:HD22	1.95	0.47
1:A:430:ASN:HD21	2:B:201:ARG:HH22	1.63	0.47
2:B:161:GLU:HB3	2:B:164:ASP:HB2	1.96	0.46
3:C:291:LEU:HD21	3:C:299:LEU:HG	1.98	0.46
1:A:158:ALA:HB3	5:A:602:STU:H271	1.98	0.46
3:C:26:SER:HB3	3:C:324:THR:HG22	1.96	0.46
5:A:602:STU:H16	5:A:602:STU:H261	1.98	0.46
1:A:52:GLN:OE1	1:A:55:ARG:NH1	2.49	0.46
1:A:408:PRO:O	1:A:412:MET:HB2	2.15	0.46
3:C:32:MET:SD	3:C:175:LEU:HD21	2.56	0.46
1:A:29:PHE:HE1	1:A:49:LEU:HD22	1.82	0.45
2:B:79:PRO:O	2:B:160:PHE:HE1	2.00	0.45
2:B:78:ARG:HB3	2:B:160:PHE:CE1	2.52	0.45
2:B:206:LEU:HD12	2:B:207:PRO:HD2	1.99	0.45
2:B:207:PRO:HA	2:B:208:PRO:HD3	1.78	0.44
3:C:174:PHE:HD2	3:C:175:LEU:HD12	1.81	0.44
1:A:242:SER:O	1:A:245:SER:OG	2.31	0.44
1:A:144:PRO:HD3	1:A:205:ILE:HG12	2.00	0.44
3:C:28:TYR:CE2	3:C:179:ILE:HG12	2.53	0.43
1:A:249:HIS:CG	1:A:259:ALA:HB2	2.53	0.43
1:A:262:LYS:HE2	1:A:266:GLU:OE2	2.18	0.43
3:C:186:GLU:O	3:C:190:LYS:HG2	2.18	0.43
1:A:529:ARG:NH2	1:A:536:GLU:OE2	2.51	0.43
1:A:419:ILE:HG22	1:A:424:TYR:HB2	1.99	0.43
1:A:529:ARG:HH12	1:A:533:HIS:HA	1.83	0.43
3:C:28:TYR:HE2	3:C:179:ILE:HG12	1.84	0.43
3:C:42:PRO:HG2	3:C:45:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:ARG:NH1	3:C:231:ASP:O	2.53	0.42
2:B:78:ARG:CZ	2:B:120:GLU:HG3	2.49	0.42
3:C:233:LYS:HD2	3:C:235:ARG:NH2	2.34	0.42
3:C:225:SER:OG	6:C:1103:AMP:O2P	2.32	0.42
3:C:73:LEU:HD22	3:C:113:ILE:HG21	2.01	0.42
2:B:75:ALA:HB1	2:B:78:ARG:HH21	1.84	0.42
3:C:172:LEU:HD22	3:C:314:LEU:HD22	2.01	0.42
1:A:162:LEU:HD13	1:A:176:CYS:HB3	2.01	0.42
3:C:186:GLU:O	3:C:189:SER:OG	2.35	0.41
1:A:174:TPO:HG21	1:A:174:TPO:O2P	2.20	0.41
2:B:203:PRO:HA	2:B:204:PRO:HD3	1.97	0.41
1:A:26:VAL:HG12	1:A:27:GLY:N	2.36	0.41
3:C:291:LEU:HD13	3:C:314:LEU:HD23	2.03	0.41
1:A:260:THR:O	1:A:264:ILE:HG13	2.20	0.41
2:B:92:TYR:HB2	2:B:128:PHE:HB3	2.03	0.41
3:C:175:LEU:O	3:C:179:ILE:HG13	2.21	0.41
3:C:297:HIS:HB2	3:C:298:ARG:NH2	2.36	0.41
3:C:173:LYS:HG3	3:C:292:VAL:HG13	2.03	0.41
3:C:303:ASP:OD1	3:C:305:ASN:N	2.54	0.40
1:A:49:LEU:HB2	1:A:91:ILE:HB	2.04	0.40
3:C:184:LYS:H	3:C:184:LYS:HG3	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/494 (74%)	363 (99%)	5 (1%)	0	100	100
2	B	170/204 (83%)	167 (98%)	3 (2%)	0	100	100
3	C	298/331 (90%)	292 (98%)	6 (2%)	0	100	100
All	All	836/1029 (81%)	822 (98%)	14 (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	335/447 (75%)	335 (100%)	0	100	100
2	B	159/185 (86%)	158 (99%)	1 (1%)	78	92
3	C	276/304 (91%)	273 (99%)	3 (1%)	65	86
All	All	770/936 (82%)	766 (100%)	4 (0%)	81	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	120	GLU
3	C	184	LYS
3	C	236	VAL
3	C	323	LEU

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

Mol	Chain	Res	Type
1	A	399	HIS
1	A	440	ASN
2	B	135	HIS
3	C	95	HIS
3	C	255	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	174	1	8,10,11	1.53	1 (12%)	10,14,16	1.61	2 (20%)

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
1	TPO	A	174	1	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	TPO	P-O1P	3.40	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	TPO	P-OG1-CB	-3.52	113.76	123.33
1	A	174	TPO	CG2-CB-CA	-2.37	108.64	113.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	174	TPO	O-C-CA-CB
1	A	174	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	174	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	STU	A	602	-	39,42,42	3.45	13 (33%)	50,68,68	1.67	8 (16%)
6	AMP	C	1103	-	25,25,25	1.42	4 (16%)	37,38,38	1.87	8 (21%)
6	AMP	C	1101	-	25,25,25	1.40	4 (16%)	37,38,38	1.88	7 (18%)
4	R34	A	601	-	34,36,36	2.00	5 (14%)	50,53,53	1.44	8 (16%)
6	AMP	C	1102	-	25,25,25	1.43	4 (16%)	37,38,38	1.86	8 (21%)

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	STU	A	602	-	-	1/4/42/42	-
6	AMP	C	1103	-	-	0/10/26/26	0/3/3/3
6	AMP	C	1101	-	-	2/10/26/26	0/3/3/3
4	R34	A	601	-	-	4/12/14/14	0/5/5/5
6	AMP	C	1102	-	-	3/10/26/26	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	STU	C8-N1	12.93	1.45	1.35
5	A	602	STU	C25-N3	-10.27	1.37	1.45
4	A	601	R34	C18-N8	7.93	1.42	1.32
5	A	602	STU	O5-C8	7.73	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	R34	C9-N7	-5.20	1.32	1.37
6	C	1102	AMP	C5-C4	4.77	1.47	1.39
6	C	1103	AMP	C5-C4	4.77	1.47	1.39
6	C	1101	AMP	C5-C4	4.77	1.47	1.39
5	A	602	STU	C18-N2	4.28	1.44	1.40
5	A	602	STU	C17-N2	3.87	1.45	1.40
5	A	602	STU	C22-C23	-3.87	1.49	1.53
5	A	602	STU	C20-N3	3.78	1.45	1.40
5	A	602	STU	C9-C10	3.53	1.53	1.50
4	A	601	R34	C7-C2	3.10	1.55	1.49
4	A	601	R34	C5-N7	-3.04	1.33	1.38
6	C	1102	AMP	C5-C6	2.75	1.48	1.41
6	C	1103	AMP	C5-C6	2.74	1.48	1.41
6	C	1101	AMP	C5-C6	2.72	1.48	1.41
5	A	602	STU	C12-C11	2.71	1.53	1.46
5	A	602	STU	C5-C6	2.62	1.53	1.46
5	A	602	STU	C26-C21	2.59	1.54	1.51
5	A	602	STU	C24-C25	2.52	1.56	1.51
6	C	1102	AMP	C8-N7	2.41	1.36	1.31
6	C	1103	AMP	C8-N7	2.41	1.36	1.31
6	C	1101	AMP	C8-N7	2.31	1.36	1.31
4	A	601	R34	C23-N22	2.26	1.34	1.30
6	C	1102	AMP	C5-N7	-2.25	1.35	1.39
6	C	1103	AMP	C5-N7	-2.22	1.35	1.39
6	C	1101	AMP	C5-N7	-2.18	1.35	1.39
5	A	602	STU	C19-N3	2.03	1.42	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1101	AMP	C5-C4-N3	-5.92	118.57	126.72
6	C	1102	AMP	C5-C4-N3	-5.75	118.80	126.72
6	C	1103	AMP	C5-C4-N3	-5.73	118.83	126.72
5	A	602	STU	C9-N1-C8	-5.61	108.74	113.86
5	A	602	STU	C9-C10-C7	4.90	111.68	109.88
6	C	1101	AMP	N3-C4-N9	4.71	135.17	127.17
6	C	1102	AMP	N3-C4-N9	4.57	134.94	127.17
6	C	1103	AMP	N3-C4-N9	4.50	134.82	127.17
4	A	601	R34	C5-N7-C9	4.15	110.95	108.35
4	A	601	R34	O21-N8-C18	-4.13	109.39	119.73
6	C	1101	AMP	C2-N3-C4	3.70	120.87	111.83
6	C	1103	AMP	C2-N3-C4	3.70	120.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1102	AMP	C2-N3-C4	3.64	120.73	111.83
5	A	602	STU	C28-N4-C23	-3.50	110.21	114.39
6	C	1103	AMP	C4-C5-N7	-3.46	106.62	110.58
6	C	1101	AMP	C4-C5-N7	-3.43	106.66	110.58
6	C	1102	AMP	C4-C5-N7	-3.41	106.68	110.58
6	C	1103	AMP	N3-C2-N1	-3.30	123.59	128.58
6	C	1101	AMP	N3-C2-N1	-3.17	123.78	128.58
6	C	1102	AMP	N3-C2-N1	-3.14	123.83	128.58
5	A	602	STU	C18-C19-N3	3.14	132.09	129.42
5	A	602	STU	C19-C18-N2	3.13	134.03	131.38
6	C	1102	AMP	C4-N9-C8	2.64	108.51	105.74
6	C	1103	AMP	C4-N9-C8	2.63	108.50	105.74
6	C	1101	AMP	C4-N9-C8	2.56	108.43	105.74
4	A	601	R34	C11-C10-C7	-2.55	119.99	121.97
6	C	1101	AMP	C5-N7-C8	2.53	107.43	103.45
6	C	1103	AMP	C5-N7-C8	2.51	107.40	103.45
6	C	1102	AMP	C5-N7-C8	2.48	107.34	103.45
5	A	602	STU	C11-C10-C7	-2.38	119.68	121.25
4	A	601	R34	C13-N22-C23	2.36	108.81	104.13
6	C	1103	AMP	C6-C5-N7	2.17	136.27	132.09
5	A	602	STU	C7-C8-N1	2.16	108.44	106.38
4	A	601	R34	C8-C9-N7	-2.16	108.35	110.39
4	A	601	R34	C26-O25-C23	2.08	122.31	118.13
4	A	601	R34	C12-C13-N22	-2.08	106.58	109.42
6	C	1102	AMP	C6-C5-N7	2.06	136.05	132.09
4	A	601	R34	C32-C29-C30	-2.05	119.77	122.81
5	A	602	STU	C10-C9-N1	2.01	103.71	101.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	R34	C30-C18-N8-O21
4	A	601	R34	O20-C18-N8-O21
6	C	1102	AMP	C5'-O5'-P-O1P
6	C	1102	AMP	C5'-O5'-P-O2P
6	C	1102	AMP	C5'-O5'-P-O3P
6	C	1101	AMP	O4'-C4'-C5'-O5'
5	A	602	STU	C24-C23-N4-C28
4	A	601	R34	O20-C18-C30-C31
4	A	601	R34	N8-C18-C30-C31
6	C	1101	AMP	C3'-C4'-C5'-O5'

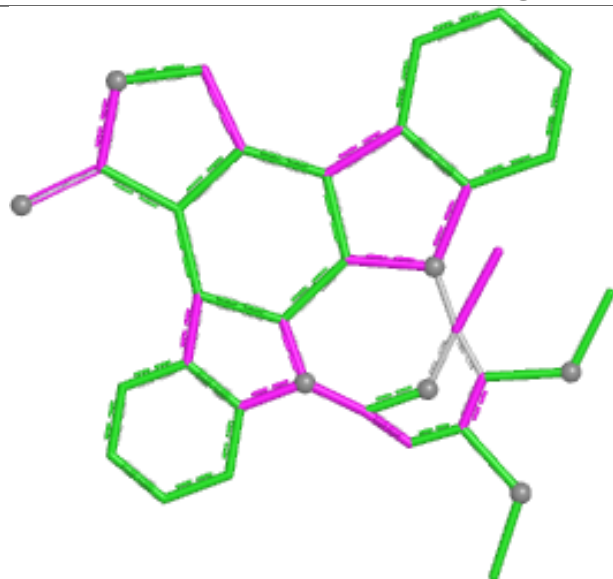
There are no ring outliers.

4 monomers are involved in 6 short contacts:

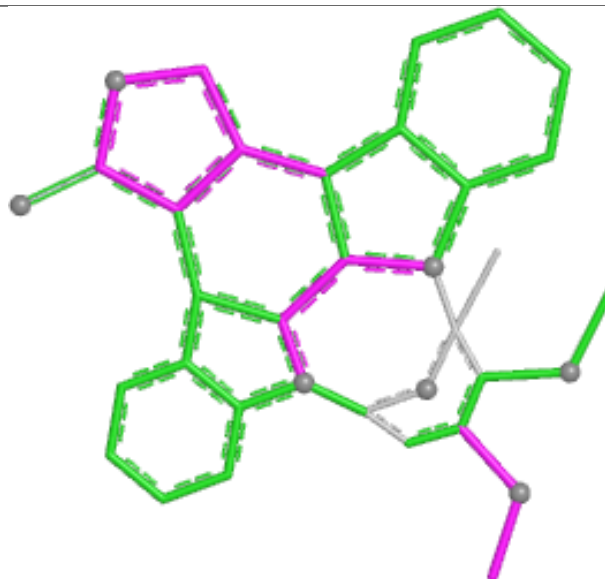
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	STU	2	0
6	C	1103	AMP	2	0
4	A	601	R34	1	0
6	C	1102	AMP	1	0

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

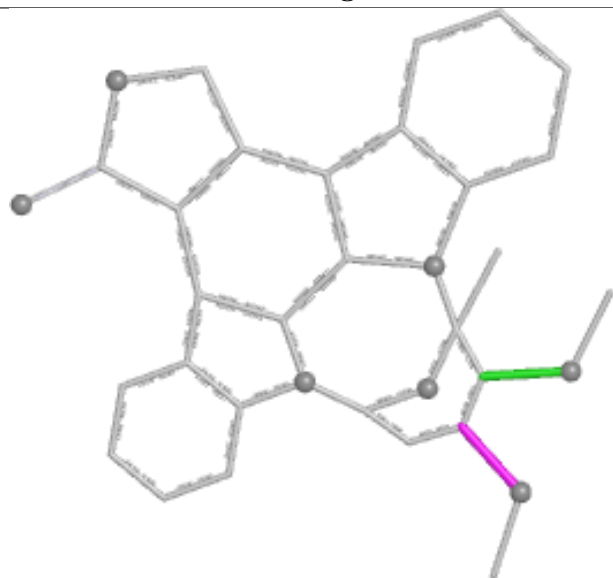
Ligand STU A 602



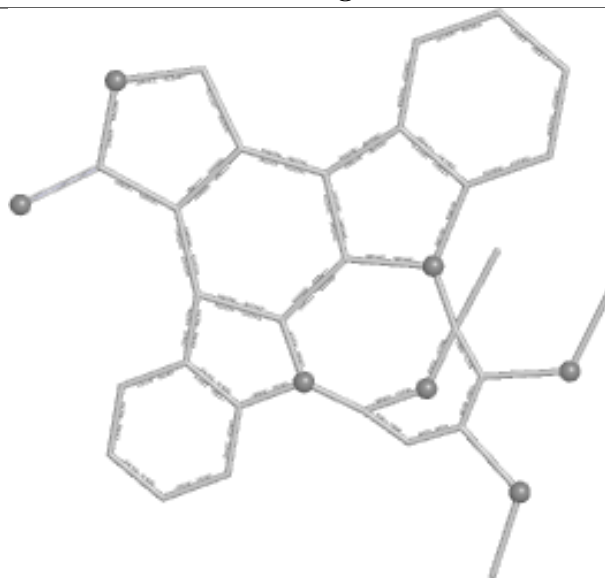
Bond lengths



Bond angles

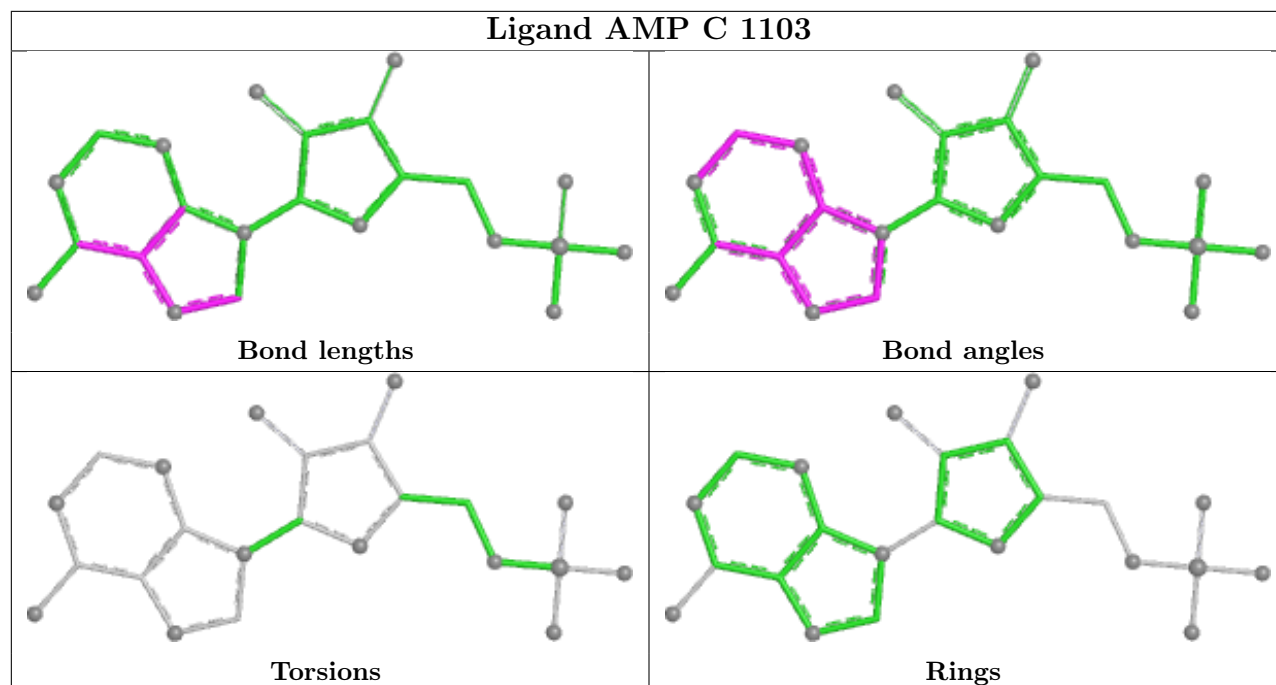


Torsions

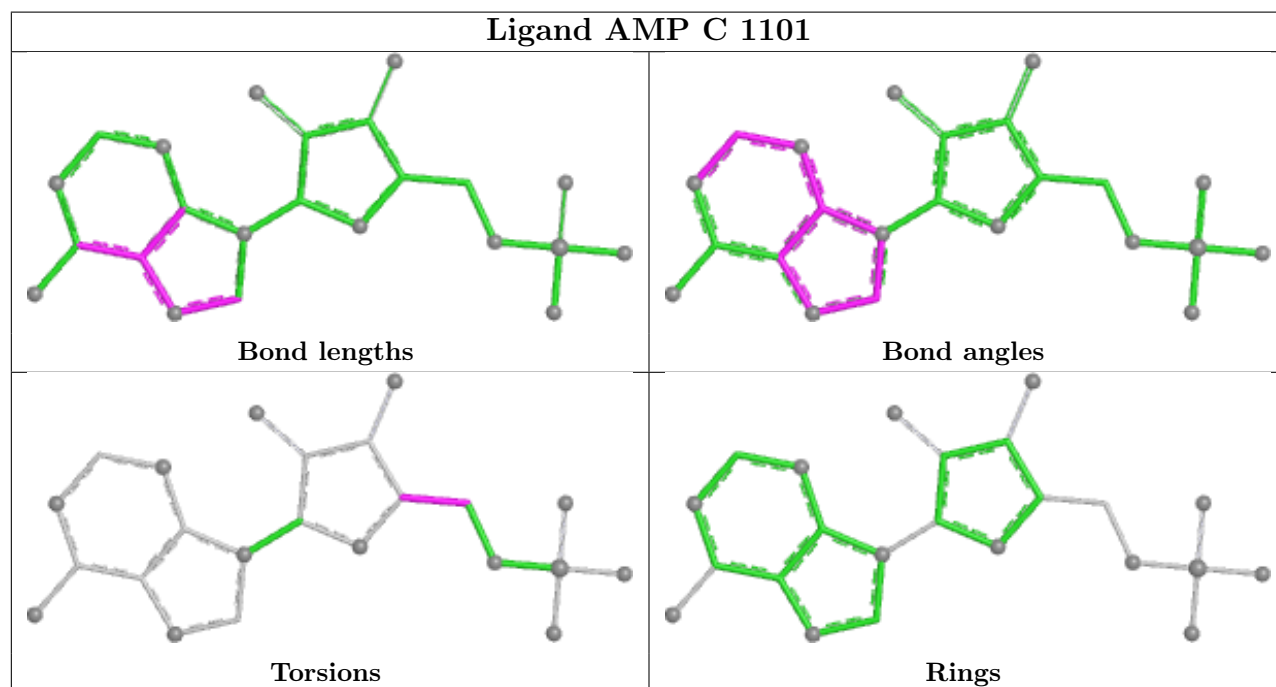


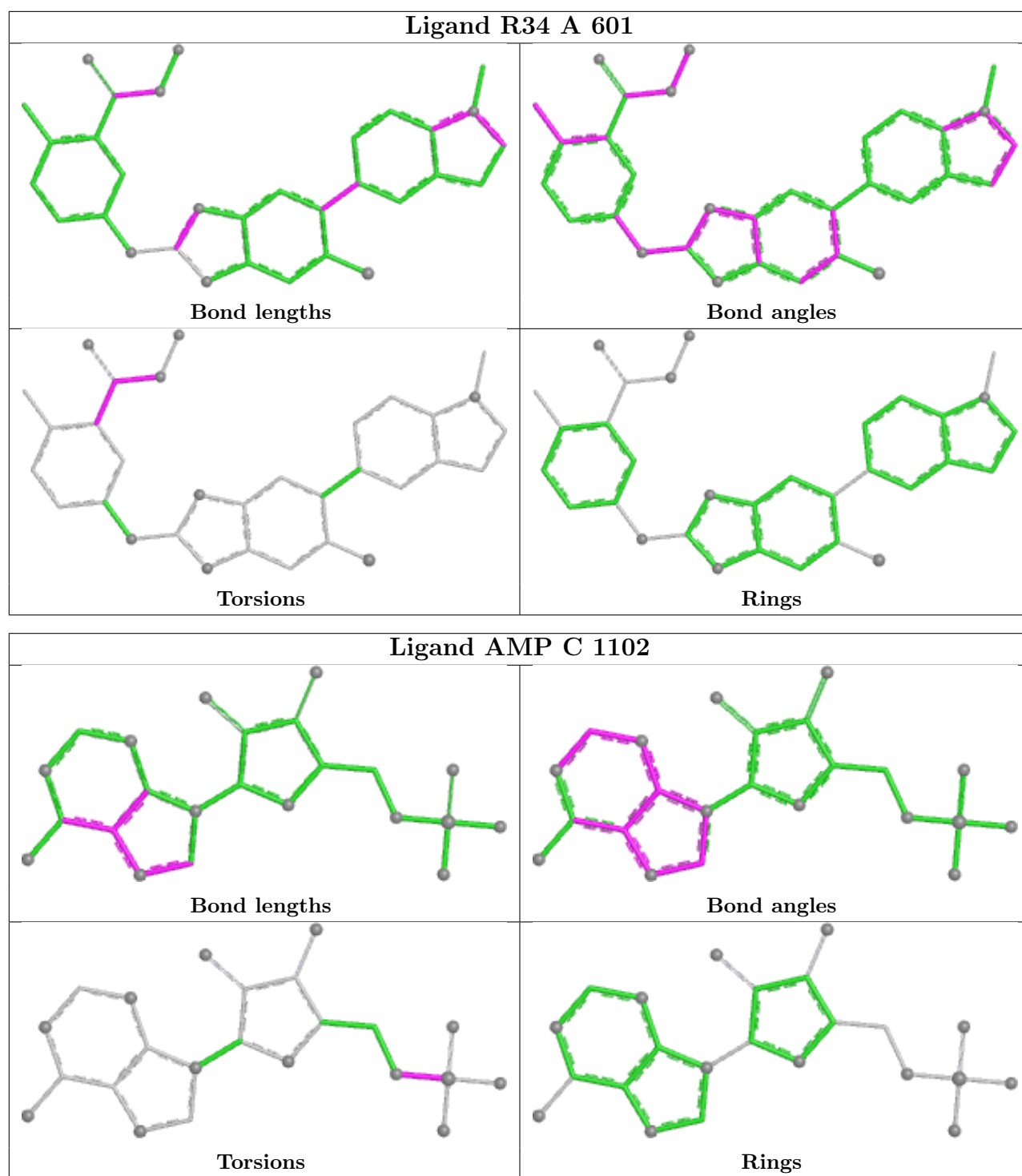
Rings

Ligand AMP C 1103



Ligand AMP C 1101





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	372/494 (75%)	0.39	32 (8%) 16 13	25, 53, 115, 219	0
2	B	176/204 (86%)	1.08	39 (22%) 2 2	31, 67, 142, 178	0
3	C	300/331 (90%)	0.86	31 (10%) 12 10	43, 78, 121, 146	0
All	All	848/1029 (82%)	0.70	102 (12%) 9 7	25, 67, 125, 219	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	224	ASP	6.9
3	C	187	PHE	6.9
2	B	221	ILE	6.5
2	B	194	CYS	6.3
2	B	222	SER	6.0
2	B	163	PHE	5.2
3	C	182	PHE	5.0
1	A	414	GLU	4.9
2	B	219	THR	4.8
3	C	178	PHE	4.8
2	B	74	PRO	4.8
3	C	177	LEU	4.7
3	C	323	LEU	4.7
1	A	277	TYR	4.6
3	C	271	TYR	4.6
2	B	223	CYS	4.6
1	A	28	THR	4.4
1	A	29	PHE	4.4
1	A	278	LEU	4.4
1	A	411	ILE	4.3
1	A	276	LYS	4.2
3	C	27	VAL	4.2
2	B	270	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	421	GLN	4.2
2	B	169	ASP	4.1
3	C	200	TYR	4.1
3	C	194	GLU	4.0
1	A	279	PHE	4.0
1	A	526	LEU	4.0
3	C	324	THR	3.9
2	B	162	VAL	3.9
3	C	269	SER	3.9
2	B	76	GLN	3.9
2	B	226	ALA	3.9
2	B	167	MET	3.8
1	A	175	SER	3.7
3	C	124	SER	3.7
1	A	395	LYS	3.7
2	B	215	LEU	3.6
3	C	183	PRO	3.6
2	B	77	ALA	3.5
2	B	220	GLY	3.5
2	B	117	ASP	3.5
2	B	170	SER	3.5
3	C	125	PHE	3.4
1	A	528	PRO	3.4
1	A	530	PRO	3.3
2	B	171	GLN	3.3
1	A	406	SER	3.3
2	B	188	HIS	3.2
3	C	193	GLU	3.2
1	A	280	PRO	3.1
1	A	11	GLY	3.1
2	B	192	TYR	3.0
3	C	322	VAL	3.0
2	B	217	LYS	3.0
3	C	179	ILE	2.9
1	A	27	GLY	2.9
2	B	75	ALA	2.9
2	B	213	VAL	2.8
2	B	166	LEU	2.7
1	A	418	ALA	2.7
3	C	28	TYR	2.7
2	B	225	PRO	2.7
1	A	424	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	230	GLU	2.6
3	C	203	ILE	2.6
2	B	168	VAL	2.5
2	B	122	GLU	2.5
3	C	77	LYS	2.5
2	B	214	ILE	2.5
1	A	158	ALA	2.4
3	C	270	HIS	2.4
3	C	267	HIS	2.4
3	C	26	SER	2.4
2	B	164	ASP	2.3
1	A	396	ALA	2.3
2	B	121	GLY	2.3
2	B	268	LYS	2.3
3	C	145	ILE	2.3
1	A	57	LEU	2.3
2	B	158	THR	2.3
1	A	442	VAL	2.3
3	C	127	PRO	2.3
3	C	188	MET	2.2
3	C	35	HIS	2.2
3	C	308	VAL	2.2
1	A	281	GLU	2.2
1	A	415	VAL	2.2
1	A	440	ASN	2.2
2	B	119	PRO	2.2
2	B	246	ASP	2.2
1	A	445	THR	2.2
1	A	173	ARG	2.1
1	A	422	LEU	2.1
1	A	529	ARG	2.1
2	B	191	PRO	2.1
1	A	217	ASP	2.1
2	B	212	GLN	2.0
3	C	126	LYS	2.0
3	C	302	VAL	2.0
3	C	303	ASP	2.0

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

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	A	174	11/12	0.89	0.10	31,44,63,72	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

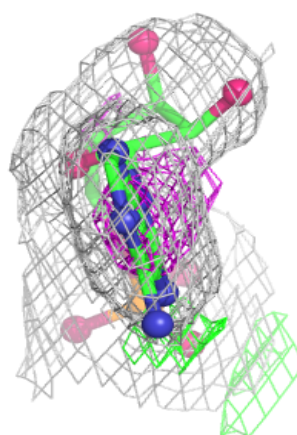
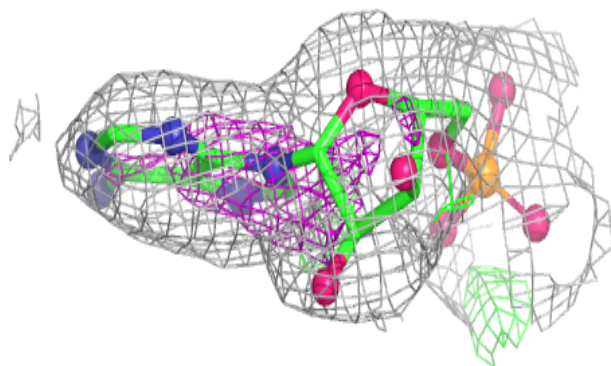
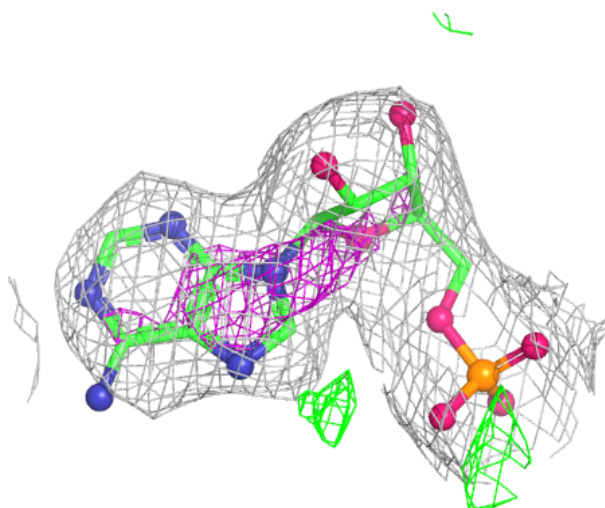
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	AMP	C	1101	23/23	0.86	0.12	40,54,67,77	0
6	AMP	C	1102	23/23	0.89	0.10	34,47,70,83	0
6	AMP	C	1103	23/23	0.90	0.09	42,52,62,70	0
4	R34	A	601	32/32	0.94	0.10	20,34,82,92	0
5	STU	A	602	35/35	0.95	0.09	11,24,32,37	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.

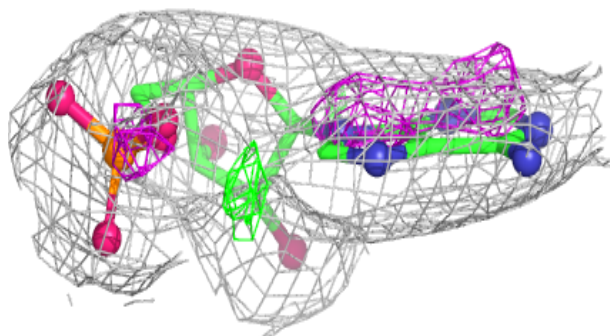
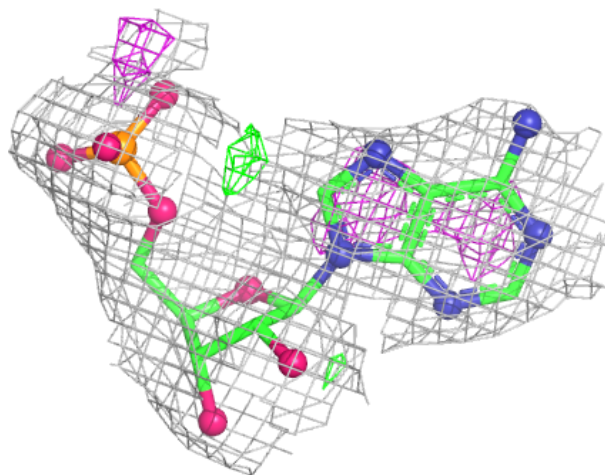
Electron density around AMP C 1101:

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



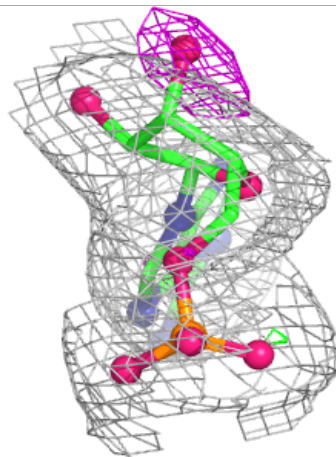
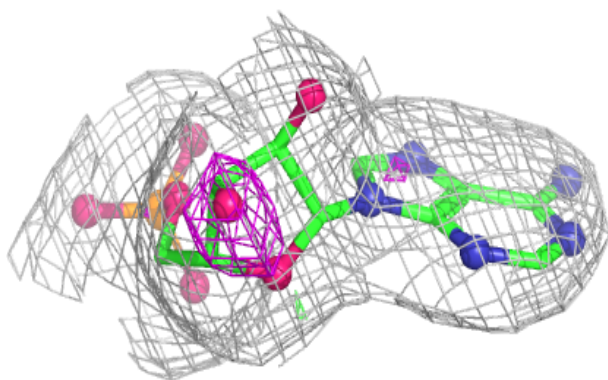
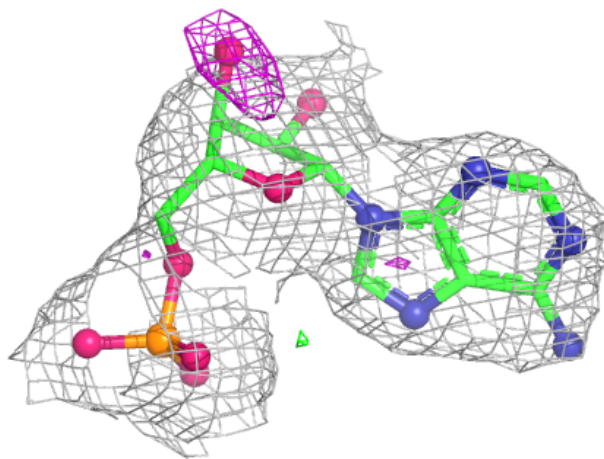
Electron density around AMP C 1102:

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



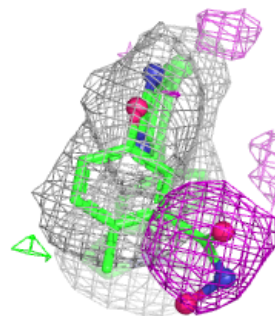
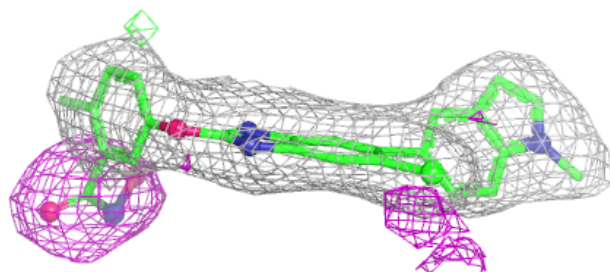
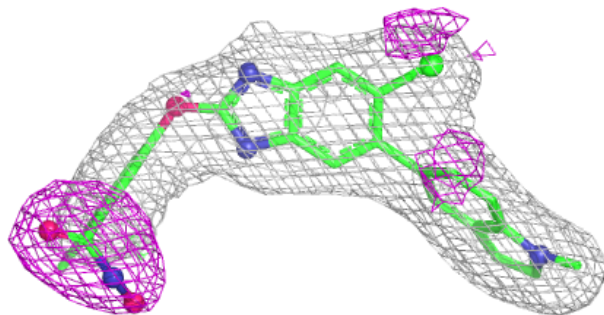
Electron density around AMP C 1103:

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



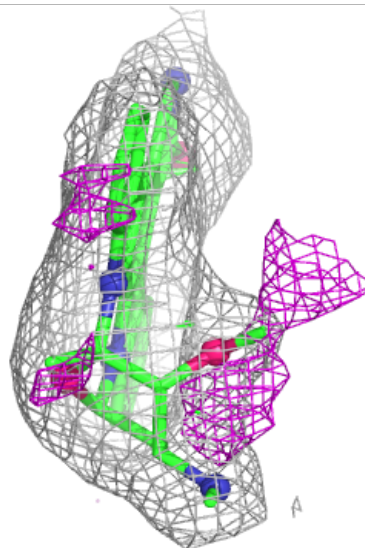
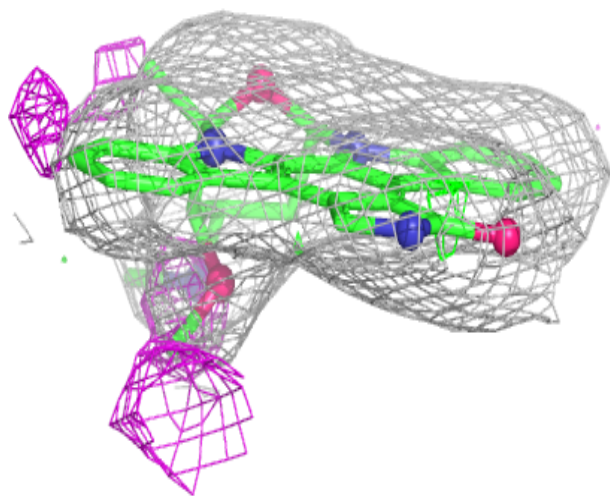
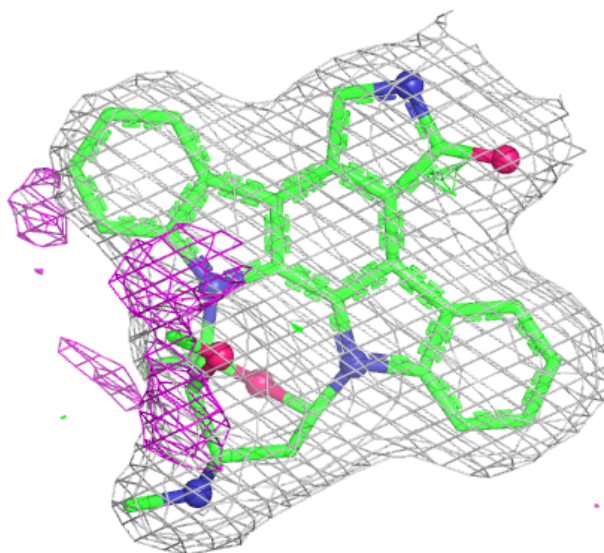
Electron density around R34 A 601:

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



Electron density around STU A 602:

$2mF_o-DF_c$ (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.