Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:19 am BST

PDB ID	:	4QFS
Title	:	Structure of AMPK in complex with Br2-A769662core activator and STAUROSPORINE inhibitor
Authors	:	Calabrese, M.F.; Kurumbail, R.G.
Deposited on	:	2014-05-21
Resolution	:	3.55 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 following versions of software and data (see references ⓘ) were used in the production of this report:

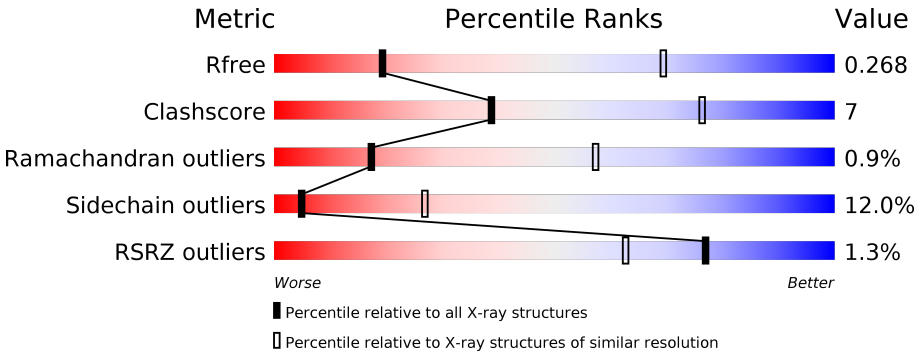
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	503	% 52% 18% • 28%
2	B	204	% 53% 22% • 23%
3	C	330	% 68% 12% • 19%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6128 atoms, of which 26 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	P	S	0	0	0
			2854	1826	493	516	1	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P54645
A	517	ALA	-	SEE REMARK 999	UNP P54645
A	518	SER	-	SEE REMARK 999	UNP P54645
A	519	GLY	-	SEE REMARK 999	UNP P54645
A	520	GLY	-	SEE REMARK 999	UNP P54645
A	521	PRO	-	SEE REMARK 999	UNP P54645
A	522	GLY	-	SEE REMARK 999	UNP P54645
A	523	GLY	-	SEE REMARK 999	UNP P54645
A	524	SER	-	SEE REMARK 999	UNP P54645

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	158	Total	C	N	O	S	0	0	0
			1214	790	203	218	3			

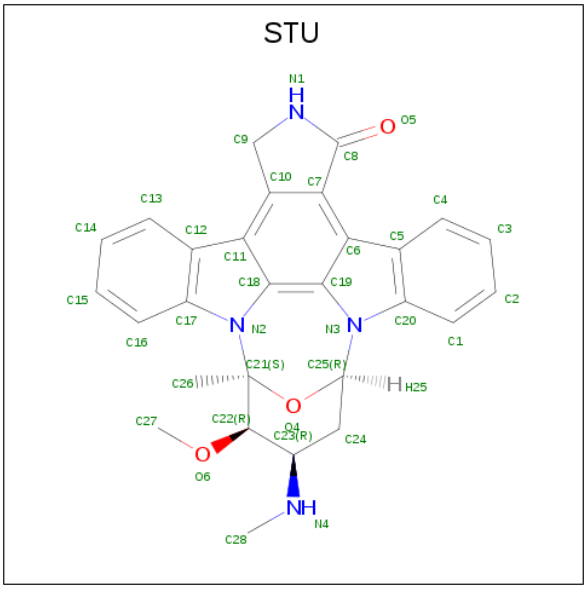
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	EXPRESSION TAG	UNP P80386
B	108	ASP	SER	ENGINEERED MUTATION	UNP P80386

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

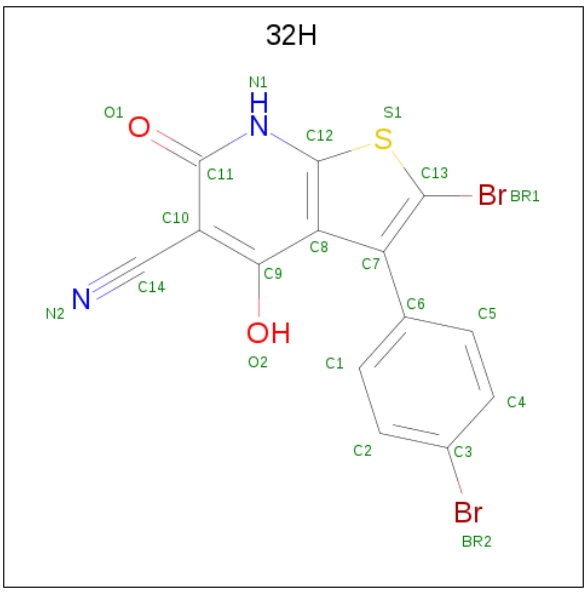
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			1940	1249	322	363	6			

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			61	28	26	4	3		

- Molecule 5 is 2-bromo-3-(4-bromophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine -5-carbonitrile (three-letter code: 32H) (formula: $C_{14}H_6Br_2N_2O_2S$).

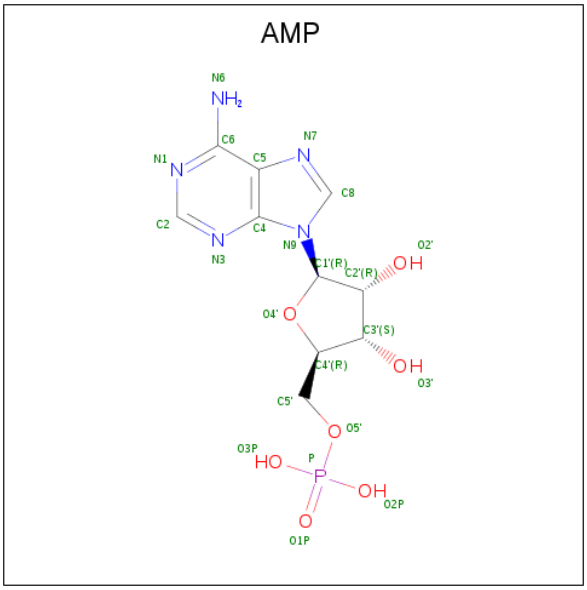


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	Br	C	N	O	S	0	0
			21	2	14	2	2	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

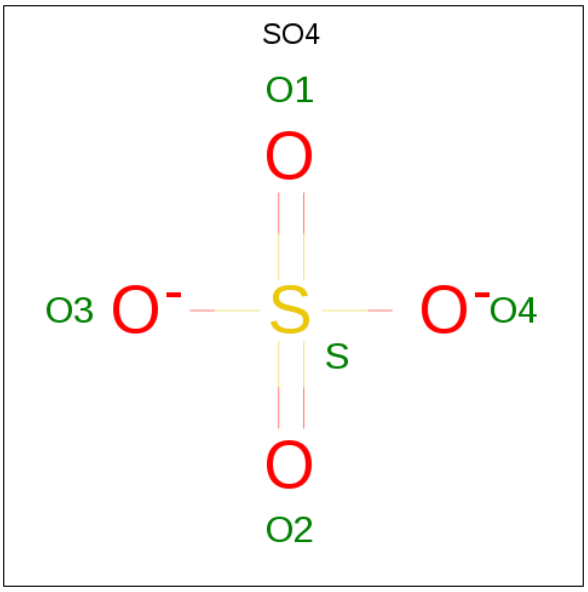
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	4	Total	Cl	0	0
			4	4		

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



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

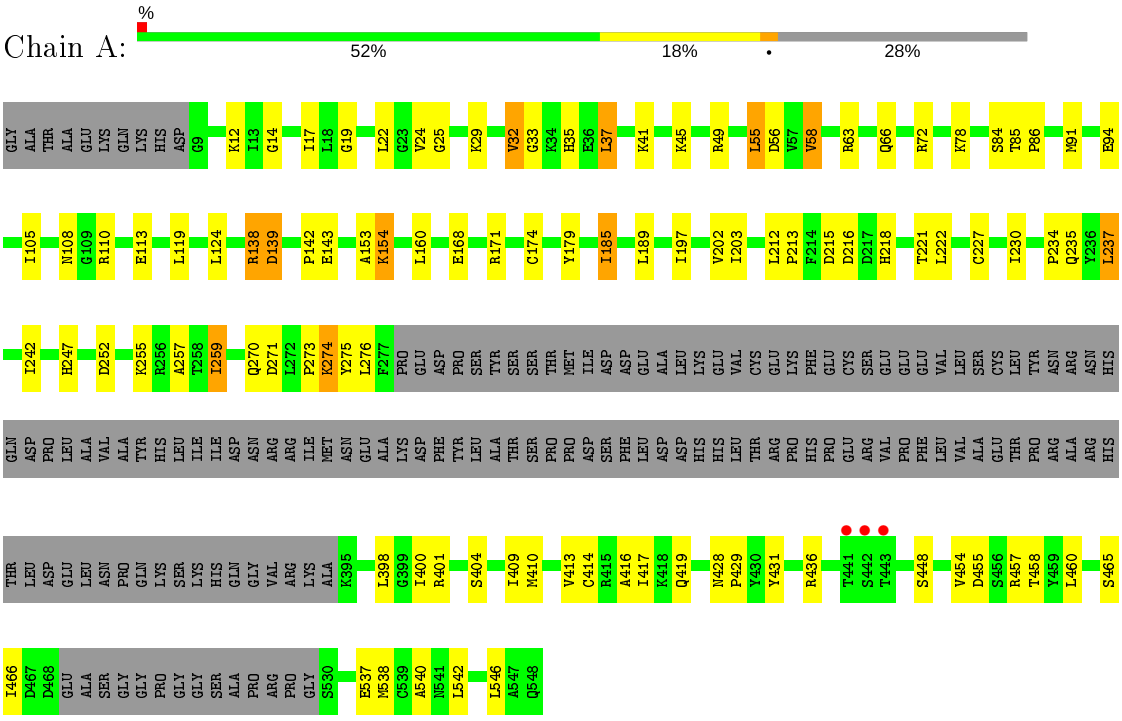


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0

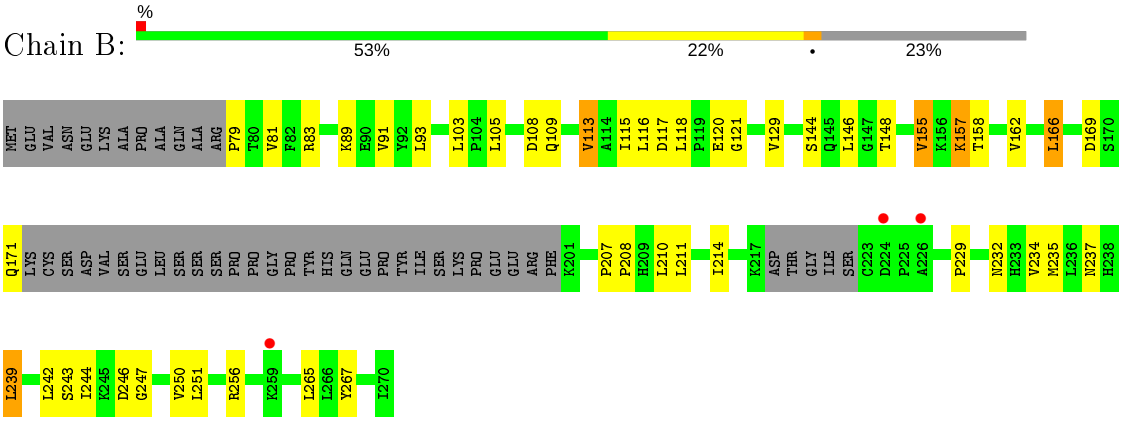
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

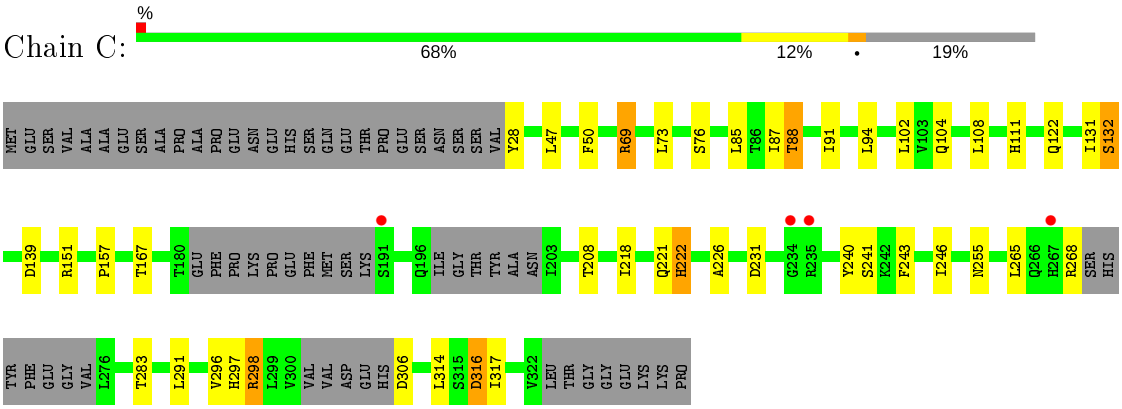


- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



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

Chain C:


%
68%
12%
19%
MET GLU SER VAL ALA ALA GLU SER ALA PRO ALA PRO GLU ASN GLU HIS SER GLN GLU THR PRO GLU SER ASN SER SER VAL Y28 L47 F50 R69 L73 S76 L85 T86 I87 T88 I91 L94 L102 V103 Q104 L108 H111 Q122 I131 S132
D139 R151 P157 T167 T180 GLU PHE PRO LYS PRO GLU PHE MET SER LYS S191 Q196 ILE GLY THR TYR ALA ASN I203 T208 I218 Q221 H222 A226 D231 G234 R235 Y240 S241 K242 F243 I246 N255 L265 Q266 H267 R268 SER HIS
TYR PHE GLU GLY VAL L276 T283 L291 V296 H297 R298 L299 V300 VAL VAL ASP GLU HIS D306 L314 S315 D316 I317 V322 LEU THR GLY GLY GLU LYS LYS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.88Å 123.88Å 401.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 3.55 29.59 – 3.55	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.59-3.55) 90.0 (29.59-3.55)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 3.55Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5, BUSTER 2.11.5	Depositor
R, R_{free}	0.226 , 0.269 0.221 , 0.268	Depositor DCC
R_{free} test set	1051 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	76.6	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 102.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6128	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, TPO, 32H, STU, SO4, 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	0.50	0/2905	0.76	2/3933 (0.1%)
2	B	0.49	0/1248	0.73	0/1711
3	C	0.47	0/1976	0.68	0/2710
All	All	0.49	0/6129	0.73	2/8354 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	GLY	N-CA-C	-6.69	96.37	113.10
1	A	55	LEU	N-CA-C	-5.21	96.92	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2854	0	2797	53	0
2	B	1214	0	1170	23	0
3	C	1940	0	1775	16	0
4	A	35	26	26	4	0
5	A	21	0	5	3	0
6	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	C	23	0	12	1	0
8	C	10	0	0	0	0
All	All	6102	26	5785	89	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 (89) 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:455:ASP:HB2	1:A:458:THR:HG22	1.58	0.84
4:A:601:STU:H16	4:A:601:STU:H261	1.60	0.80
2:B:79:PRO:HA	2:B:117:ASP:HA	1.68	0.74
1:A:185:ILE:HD11	1:A:227:CYS:SG	2.31	0.71
3:C:87:ILE:HG23	3:C:246:ILE:HG23	1.72	0.71
1:A:252:ASP:HB3	1:A:255:LYS:HB2	1.75	0.69
5:A:602:32H:H1	2:B:108:ASP:HB2	1.74	0.69
1:A:273:PRO:HD2	1:A:276:LEU:HD12	1.75	0.68
1:A:179:TYR:HA	1:A:202:VAL:HG21	1.80	0.63
1:A:465:SER:HB3	2:B:237:ASN:HB3	1.81	0.61
1:A:49:ARG:HH21	1:A:86:PRO:HA	1.65	0.60
1:A:160:LEU:HD13	1:A:174:CYS:HB2	1.84	0.60
1:A:12:LYS:HG2	1:A:17:ILE:HG22	1.83	0.59
1:A:237:LEU:HB3	1:A:242:ILE:HD11	1.85	0.59
1:A:35:HIS:HE1	1:A:37:LEU:HD12	1.69	0.58
1:A:398:LEU:HD22	2:B:210:LEU:HB3	1.87	0.56
1:A:218:HIS:HD2	1:A:221:THR:HG23	1.71	0.56
2:B:83:ARG:HG3	2:B:113:VAL:HG22	1.87	0.56
1:A:448:SER:HB3	1:A:466:ILE:HD11	1.88	0.55
1:A:413:VAL:O	1:A:417:ILE:HG13	2.06	0.54
3:C:87:ILE:HD12	3:C:246:ILE:HG21	1.90	0.53
2:B:208:PRO:HA	2:B:211:LEU:HD12	1.91	0.52
1:A:428:ASN:HB3	1:A:429:PRO:HD2	1.90	0.52
1:A:22:LEU:HD21	1:A:32:VAL:HG13	1.91	0.52
2:B:120:GLU:HA	2:B:155:VAL:HG13	1.92	0.51
2:B:144:SER:HB3	2:B:148:THR:HB	1.92	0.51
3:C:240:TYR:HD1	3:C:265:LEU:HG	1.75	0.51
1:A:58:VAL:HG23	2:B:166:LEU:HD12	1.92	0.51
1:A:212:LEU:HB2	1:A:215:ASP:HB2	1.94	0.50
1:A:436:ARG:HD3	1:A:538:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:HB2	1:A:409:ILE:HG13	1.94	0.50
1:A:431:TYR:HE1	1:A:448:SER:HB2	1.77	0.50
2:B:91:VAL:HG22	2:B:129:VAL:HG13	1.94	0.50
1:A:414:CYS:C	1:A:416:ALA:H	2.15	0.49
1:A:274:LYS:HD2	1:A:275:TYR:H	1.76	0.49
1:A:455:ASP:HB3	1:A:457:ARG:H	1.78	0.49
1:A:179:TYR:HD2	1:A:202:VAL:HG23	1.78	0.49
1:A:540:ALA:HB2	2:B:251:LEU:HD11	1.96	0.48
2:B:121:GLY:H	2:B:155:VAL:HG13	1.78	0.48
1:A:138:ARG:O	1:A:139:ASP:HB3	2.13	0.48
1:A:105:ILE:O	1:A:108:ASN:O	2.31	0.47
1:A:197:ILE:HD11	1:A:259:ILE:HG12	1.96	0.47
2:B:267:TYR:HB2	3:C:50:PHE:HD1	1.79	0.47
1:A:45:LYS:HB3	1:A:91:MET:HB2	1.96	0.47
1:A:189:LEU:HB2	2:B:207:PRO:HG3	1.97	0.47
1:A:202:VAL:HG12	1:A:213:PRO:HG2	1.97	0.47
4:A:601:STU:C16	4:A:601:STU:H261	2.30	0.47
5:A:602:32H:C5	2:B:113:VAL:HG21	2.46	0.46
2:B:239:LEU:HD11	2:B:251:LEU:HD22	1.98	0.46
3:C:291:LEU:HD23	3:C:296:VAL:HG23	1.97	0.46
2:B:91:VAL:HG13	2:B:129:VAL:HG22	1.99	0.45
1:A:142:PRO:HD2	1:A:179:TYR:CZ	2.51	0.45
2:B:93:LEU:HB2	2:B:105:LEU:HD21	1.98	0.45
3:C:132:SER:OG	3:C:157:PRO:HD3	2.16	0.45
2:B:242:LEU:HB2	2:B:250:VAL:HB	1.99	0.44
3:C:73:LEU:HD21	3:C:85:LEU:HB2	1.98	0.44
1:A:247:HIS:CG	1:A:257:ALA:HB2	2.52	0.44
1:A:85:THR:HB	1:A:86:PRO:HD2	1.98	0.44
1:A:138:ARG:O	1:A:139:ASP:CB	2.66	0.44
1:A:428:ASN:HB2	1:A:431:TYR:HB3	2.00	0.44
1:A:153:ALA:O	1:A:154:LYS:HD2	2.18	0.43
1:A:218:HIS:CD2	1:A:221:THR:HG23	2.50	0.43
1:A:398:LEU:O	1:A:460:LEU:HD11	2.19	0.43
3:C:226:ALA:HA	3:C:241:SER:HA	2.00	0.43
3:C:316:ASP:OD1	7:C:401:AMP:H3'	2.18	0.43
1:A:142:PRO:HD2	1:A:179:TYR:CE2	2.53	0.43
1:A:78:LYS:H	1:A:94:GLU:HG2	1.83	0.42
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.73	0.42
1:A:401:ARG:HG2	1:A:401:ARG:H	1.73	0.42
5:A:602:32H:BR1	5:A:602:32H:C1	3.23	0.42
1:A:84:SER:HB2	2:B:162:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:ILE:HG13	3:C:132:SER:H	1.85	0.42
3:C:314:LEU:HA	3:C:317:ILE:HD12	2.01	0.42
2:B:157:LYS:HE2	2:B:157:LYS:H	1.84	0.42
3:C:243:PHE:O	3:C:246:ILE:HG13	2.18	0.42
3:C:69:ARG:HG2	3:C:87:ILE:HD11	2.01	0.42
1:A:410:MET:O	1:A:413:VAL:HG22	2.19	0.42
3:C:218:ILE:O	3:C:222:HIS:HB2	2.20	0.42
1:A:19:GLY:HA3	1:A:32:VAL:HG23	2.01	0.42
1:A:142:PRO:HD3	1:A:203:ILE:HG12	2.02	0.42
3:C:297:HIS:HB3	3:C:298:ARG:CZ	2.49	0.42
1:A:33:GLY:O	1:A:41:LYS:HA	2.21	0.41
1:A:143:GLU:HB3	4:A:601:STU:H281	2.03	0.41
4:A:601:STU:C16	4:A:601:STU:C26	2.95	0.41
3:C:88:THR:HA	3:C:91:ILE:HD12	2.03	0.41
1:A:234:PRO:HD2	1:A:237:LEU:HD22	2.02	0.41
1:A:63:ARG:O	1:A:66:GLN:HB2	2.21	0.41
2:B:81:VAL:HG22	2:B:115:ILE:HG12	2.04	0.40
2:B:214:ILE:HB	2:B:229:PRO:HD2	2.02	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	355/503 (71%)	333 (94%)	20 (6%)	2 (1%)	25 64
2	B	152/204 (74%)	137 (90%)	12 (8%)	3 (2%)	7 42
3	C	257/330 (78%)	242 (94%)	13 (5%)	2 (1%)	19 59
All	All	764/1037 (74%)	712 (93%)	45 (6%)	7 (1%)	17 57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLY
1	A	139	ASP
3	C	122	GLN
3	C	231	ASP
2	B	246	ASP
2	B	247	GLY
2	B	244	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	306/448 (68%)	274 (90%)	32 (10%)	7 33
2	B	130/185 (70%)	110 (85%)	20 (15%)	2 18
3	C	189/299 (63%)	166 (88%)	23 (12%)	5 26
All	All	625/932 (67%)	550 (88%)	75 (12%)	5 27

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	29	LYS
1	A	32	VAL
1	A	37	LEU
1	A	55	LEU
1	A	56	ASP
1	A	58	VAL
1	A	72	ARG
1	A	110	ARG
1	A	113	GLU
1	A	119	LEU
1	A	124	LEU
1	A	138	ARG
1	A	154	LYS
1	A	168	GLU
1	A	171	ARG

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Mol	Chain	Res	Type
1	A	185	ILE
1	A	216	ASP
1	A	222	LEU
1	A	230	ILE
1	A	235	GLN
1	A	237	LEU
1	A	259	ILE
1	A	270	GLN
1	A	271	ASP
1	A	274	LYS
1	A	400	ILE
1	A	419	GLN
1	A	454	VAL
1	A	537	GLU
1	A	542	LEU
1	A	546	LEU
2	B	89	LYS
2	B	103	LEU
2	B	109	GLN
2	B	113	VAL
2	B	116	LEU
2	B	118	LEU
2	B	146	LEU
2	B	155	VAL
2	B	157	LYS
2	B	158	THR
2	B	166	LEU
2	B	169	ASP
2	B	171	GLN
2	B	232	ASN
2	B	234	VAL
2	B	235	MET
2	B	239	LEU
2	B	243	SER
2	B	256	ARG
2	B	265	LEU
3	C	28	TYR
3	C	47	LEU
3	C	69	ARG
3	C	76	SER
3	C	88	THR
3	C	94	LEU

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Mol	Chain	Res	Type
3	C	102	LEU
3	C	104	GLN
3	C	108	LEU
3	C	111	HIS
3	C	132	SER
3	C	139	ASP
3	C	151	ARG
3	C	167	THR
3	C	208	THR
3	C	221	GLN
3	C	222	HIS
3	C	255	ASN
3	C	268	ARG
3	C	283	THR
3	C	298	ARG
3	C	306	ASP
3	C	316	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
2	B	110	ASN
2	B	216	ASN
2	B	232	ASN
3	C	104	GLN
3	C	247	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)

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	172	1	8,10,11	1.53	1 (12%)	10,14,16	1.85	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	172	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-3.67	1.52	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	TPO	P-OG1-CB	-3.59	112.36	123.21
1	A	172	TPO	O3P-P-O2P	2.82	118.42	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	AMP	C	401	-	22,25,25	0.57	0	25,38,38	1.19	2 (8%)
8	SO4	C	403	-	4,4,4	0.30	0	6,6,6	0.25	0
8	SO4	C	402	-	4,4,4	0.29	0	6,6,6	0.32	0
4	STU	A	601	-	30,42,42	2.48	10 (33%)	31,68,68	2.09	11 (35%)
5	32H	A	602	-	19,23,23	1.04	2 (10%)	18,34,34	2.90	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AMP	C	401	-	-	2/6/26/26	0/3/3/3
4	STU	A	601	-	-	1/4/42/42	-
5	32H	A	602	-	-	0/5/6/6	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C9-C10	-5.86	1.46	1.50
4	A	601	STU	C12-C17	4.58	1.48	1.41
4	A	601	STU	C5-C20	4.51	1.48	1.41
4	A	601	STU	C10-C11	4.36	1.49	1.42
4	A	601	STU	C11-C18	4.18	1.47	1.42
4	A	601	STU	C7-C6	3.66	1.49	1.43
4	A	601	STU	C9-N1	3.46	1.49	1.45
4	A	601	STU	C6-C19	3.29	1.46	1.42
4	A	601	STU	C19-C18	3.21	1.49	1.42
5	A	602	32H	C11-N1	3.00	1.38	1.33
4	A	601	STU	O5-C8	2.79	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	32H	C8-C12	-2.15	1.39	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	602	32H	C10-C11-N1	-10.69	114.60	124.09
5	A	602	32H	C7-C8-C12	4.80	111.36	107.54
7	C	401	AMP	P-O5'-C5'	4.59	130.95	118.30
4	A	601	STU	C16-C17-N2	4.51	137.74	132.29
4	A	601	STU	C7-C10-C11	-4.34	116.58	122.42
4	A	601	STU	C7-C8-N1	3.74	110.15	106.37
4	A	601	STU	O5-C8-C7	-3.70	124.93	129.32
5	A	602	32H	C11-N1-C12	3.44	122.02	116.88
4	A	601	STU	C4-C5-C20	2.93	123.09	119.39
4	A	601	STU	C1-C20-C5	-2.84	116.64	120.73
4	A	601	STU	C16-C17-C12	-2.69	116.86	120.73
4	A	601	STU	C13-C12-C17	2.68	122.78	119.39
4	A	601	STU	C9-N1-C8	-2.59	111.36	113.85
7	C	401	AMP	C5-C6-N6	2.37	123.96	120.35
4	A	601	STU	C3-C4-C5	-2.08	117.37	120.86
4	A	601	STU	C1-C20-N3	2.02	134.66	132.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	401	AMP	C5'-O5'-P-O1P
7	C	401	AMP	C5'-O5'-P-O3P
4	A	601	STU	C24-C23-N4-C28

There are no ring outliers.

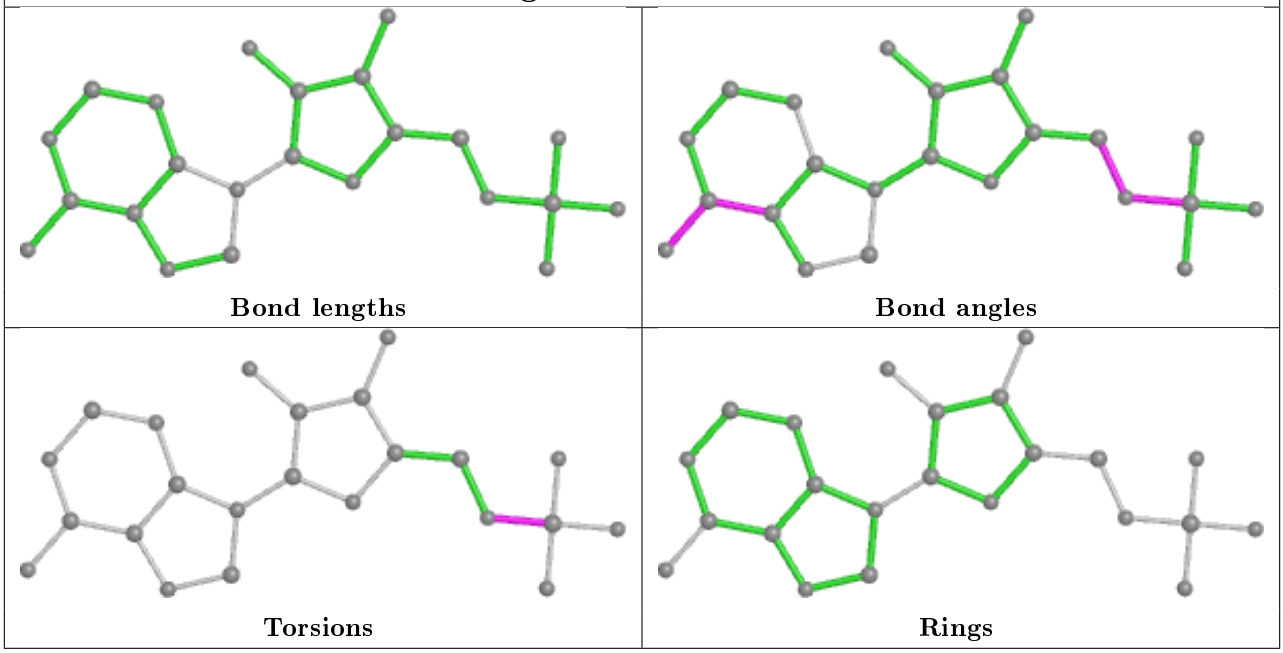
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	AMP	1	0
4	A	601	STU	4	0
5	A	602	32H	3	0

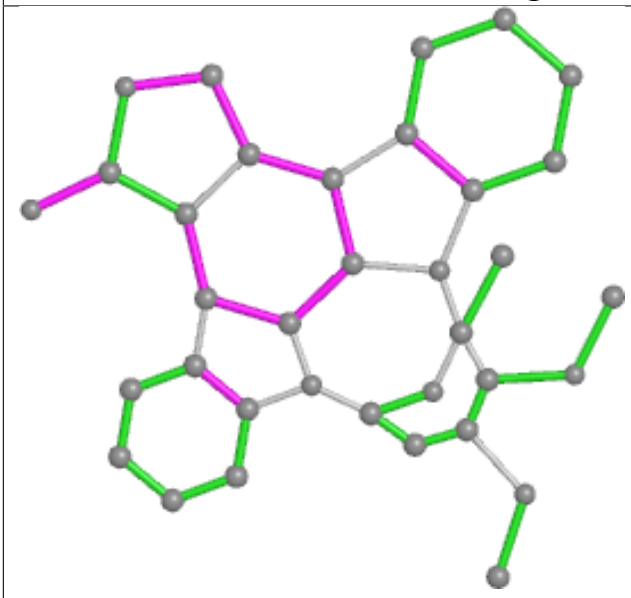
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

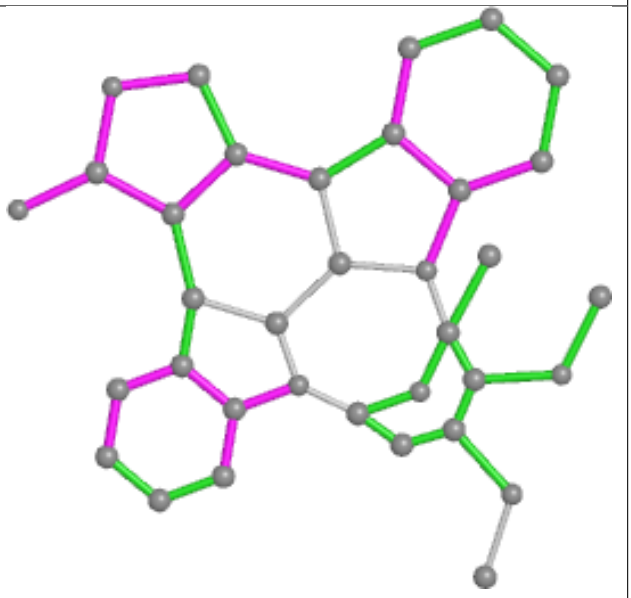
Ligand AMP C 401



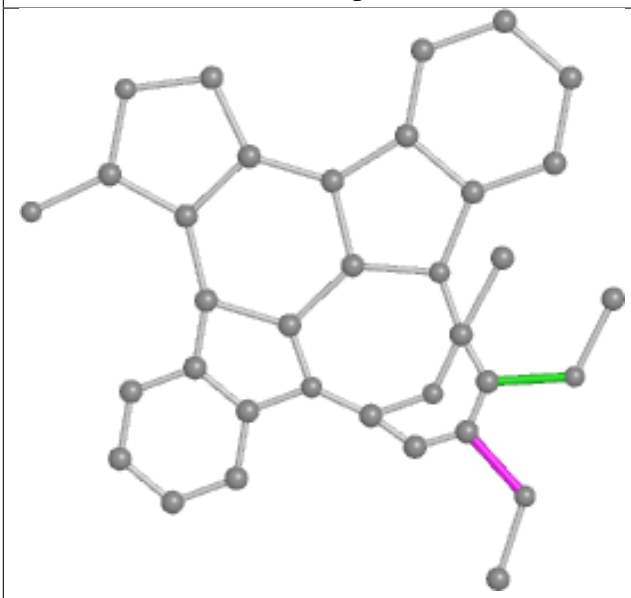
Ligand STU A 601



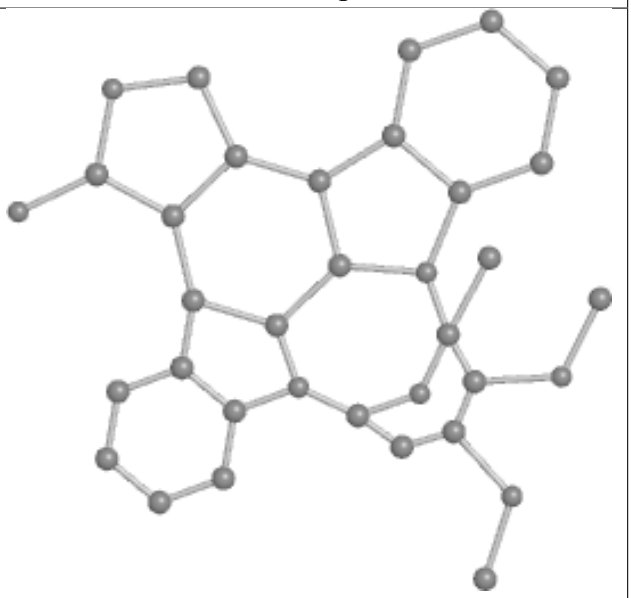
Bond lengths



Bond angles

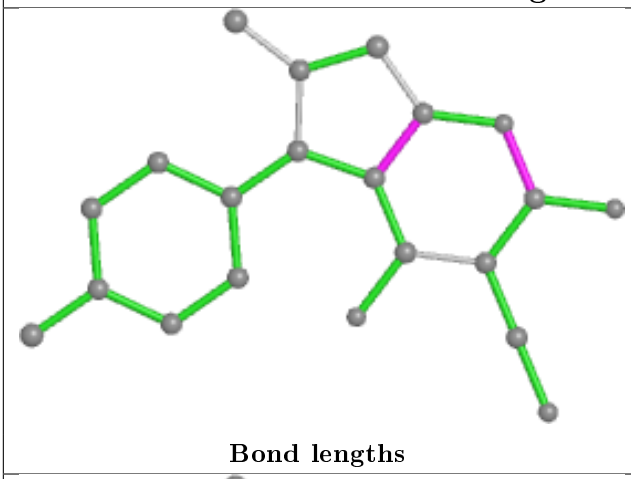


Torsions

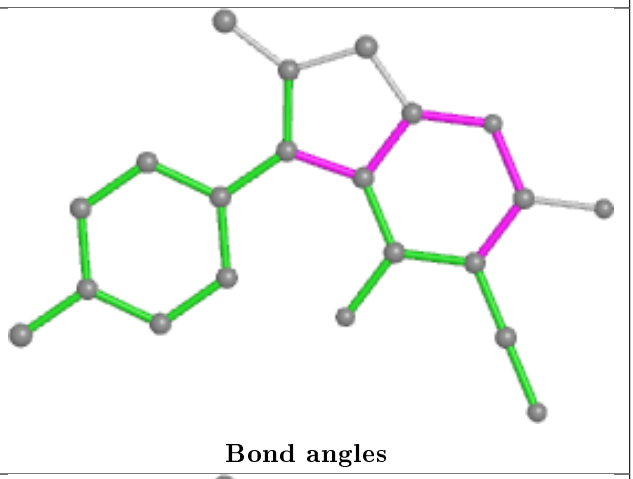


Rings

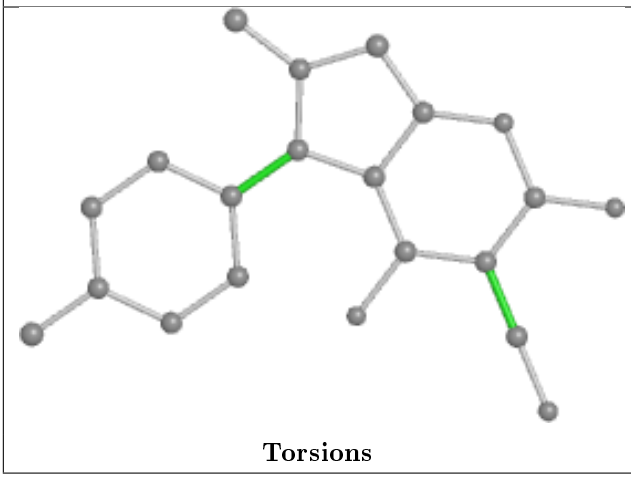
Ligand 32H A 602



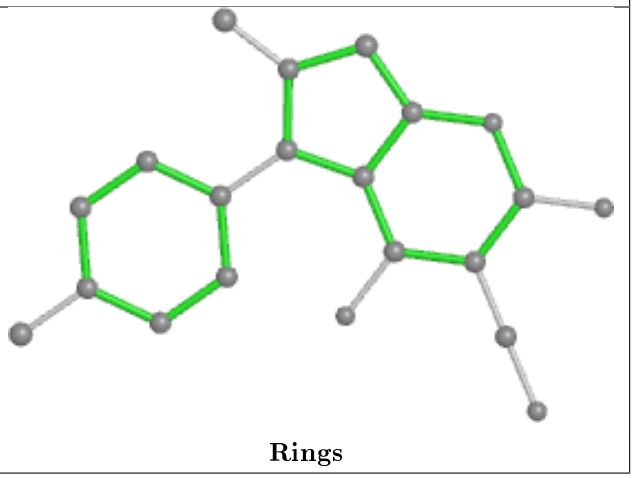
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	361/503 (71%)	-0.42	3 (0%)	86	74	44, 72, 170, 275	0
2	B	158/204 (77%)	-0.21	3 (1%)	66	50	54, 85, 123, 137	0
3	C	267/330 (80%)	-0.21	4 (1%)	73	59	63, 114, 234, 265	0
All	All	786/1037 (75%)	-0.30	10 (1%)	77	63	44, 90, 230, 275	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	SER	3.6
1	A	441	THR	2.8
3	C	267	HIS	2.7
3	C	191	SER	2.6
3	C	235	ARG	2.6
3	C	234	GLY	2.4
1	A	443	THR	2.3
2	B	226	ALA	2.1
2	B	224	ASP	2.1
2	B	259	LYS	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, 95^{th} 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	172	11/12	0.95	0.18	73,75,79,81	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

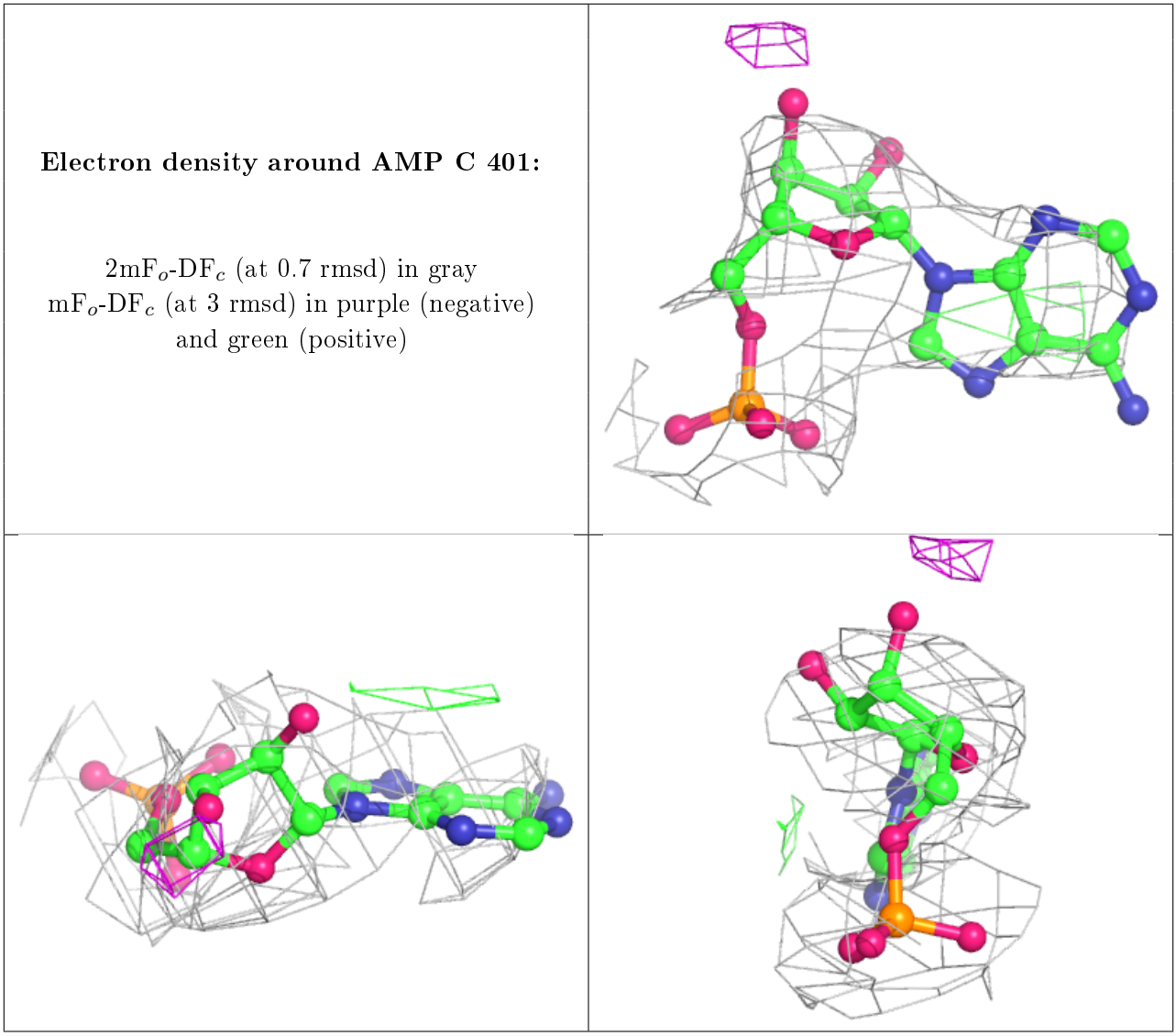
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	SO4	C	402	5/5	0.76	0.32	143,144,145,145	0
8	SO4	C	403	5/5	0.78	0.39	142,142,142,143	0
6	CL	A	604	1/1	0.82	0.12	117,117,117,117	0
6	CL	A	606	1/1	0.83	0.12	56,56,56,56	0
7	AMP	C	401	23/23	0.88	0.27	134,145,184,206	0
6	CL	B	301	1/1	0.89	0.56	89,89,89,89	0
5	32H	A	602	21/21	0.94	0.22	91,99,111,168	0
6	CL	A	603	1/1	0.95	0.14	69,69,69,69	0
4	STU	A	601	35/35	0.95	0.24	52,59,65,67	0
6	CL	A	605	1/1	0.97	0.28	50,50,50,50	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.

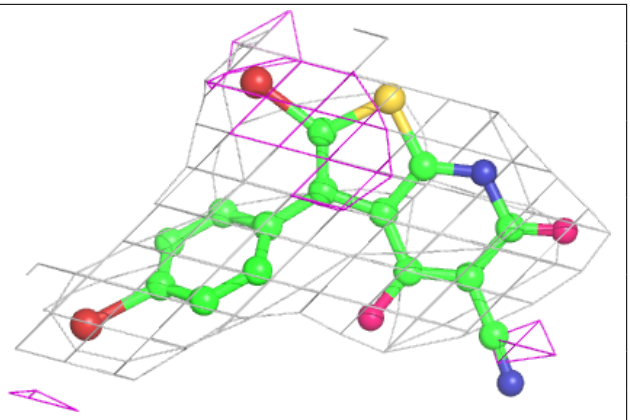
Electron density around AMP C 401:

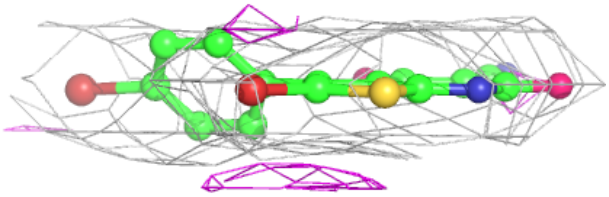
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

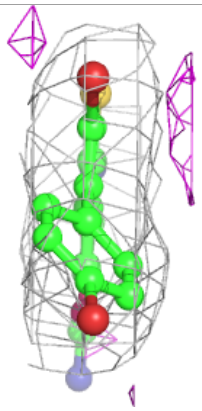


Electron density around 32H A 602:

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

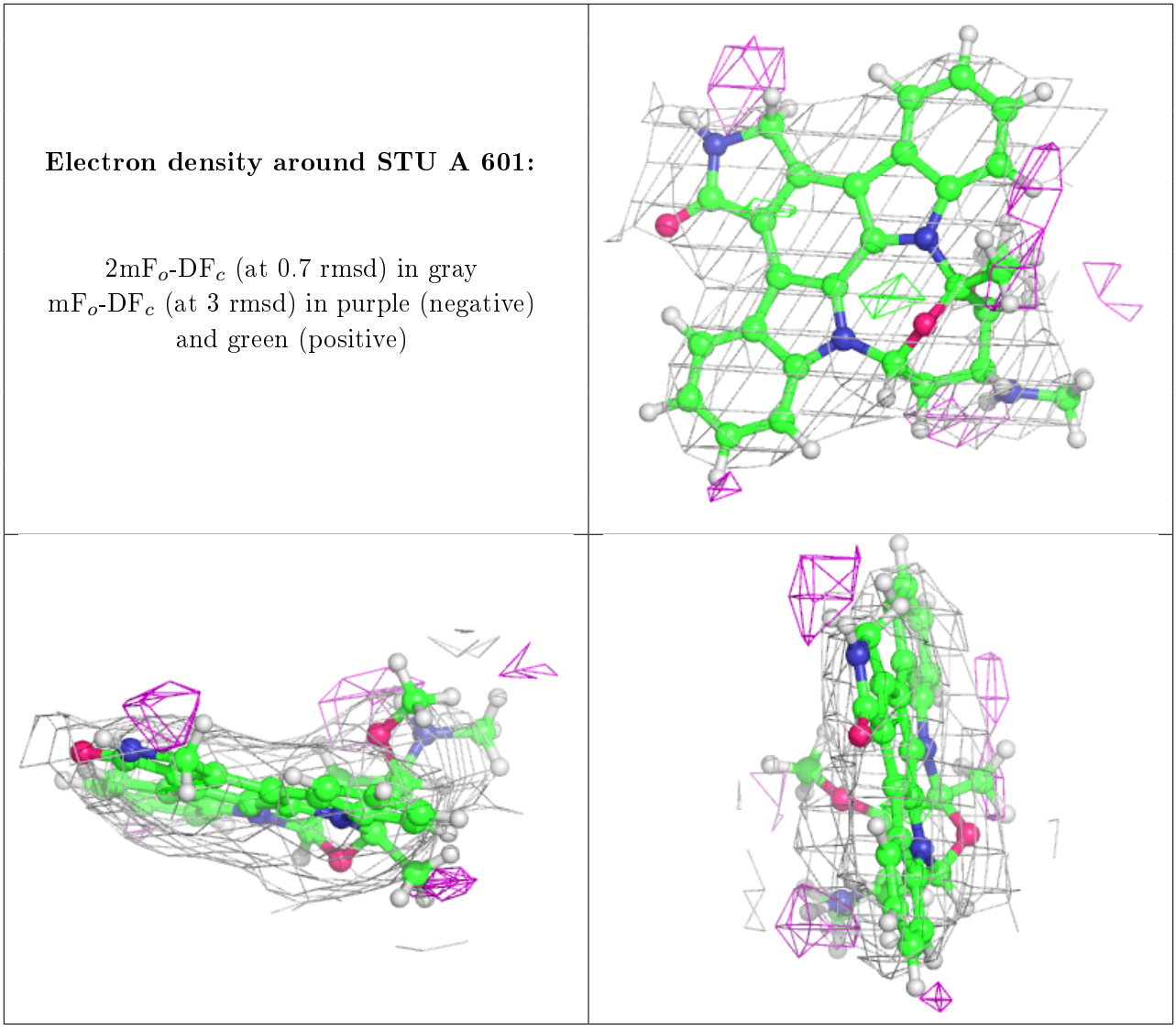






Electron density around STU A 601:

$2mF_o$-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.