Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 03:33 PM EDT

PDB ID	:	4ZHX
Title	:	Novel binding site for allosteric activation of AMPK
Authors	:	Langendorf, C.G.; Ngoei, K.R.; Issa, S.M.A.; Ling, N.; Gorman, M.A.; Parker, M.W.; Sakamoto, K.; Scott, J.W.; Oakhill, J.S.; Kemp, B.E.
Deposited on	:	2015-04-27
Resolution	:	2.99 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:

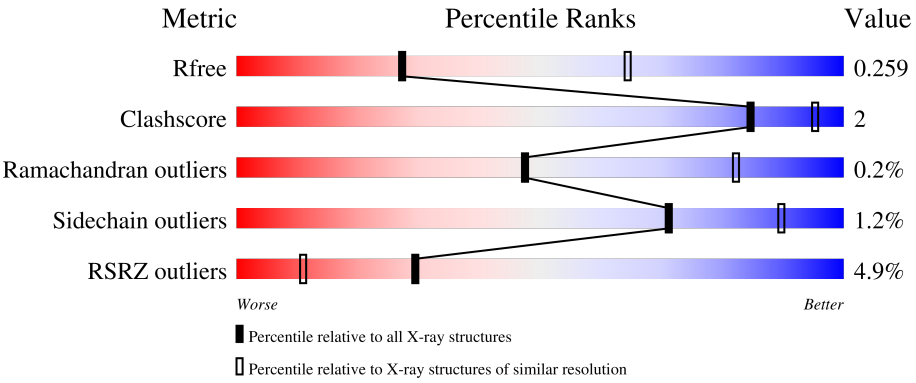
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 >=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	565	2% 69% · 28%
1	C	565	3% 74% 6% 20%
2	B	270	6% 56% 8% 36%
2	D	270	4% 56% 8% 35%
3	E	336	5% 79% 10% 11%

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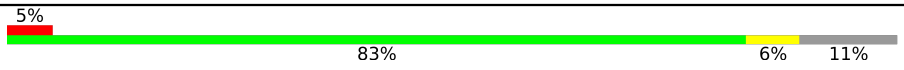
Mol	Chain	Length	Quality of chain
3	F	336	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14587 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	P	S	0	0	0
			3255	2092	563	577	1	22			
1	C	453	Total	C	N	O	P	S	0	0	0
			3567	2283	617	640	1	26			

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	P	S	0	0	0
			1310	845	221	240	1	3			
2	D	175	Total	C	N	O	P	S	0	0	0
			1373	884	230	252	1	6			

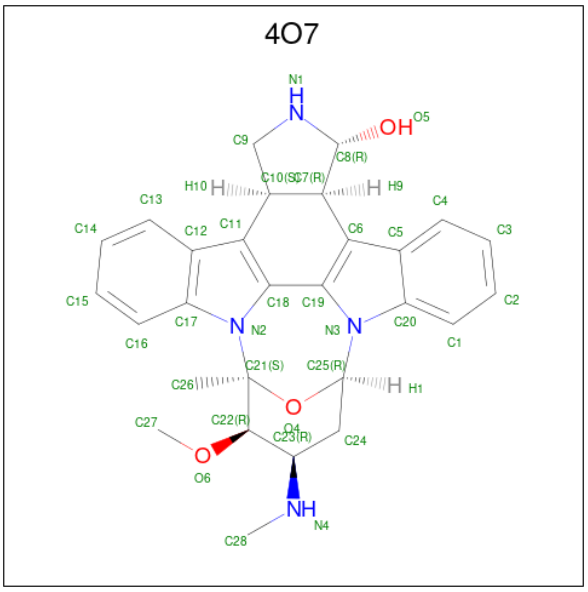
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	298	Total	C	N	O	S	0	2	0
			2381	1553	398	423	7			
3	F	300	Total	C	N	O	S	0	0	0
			2366	1535	396	428	7			

There are 12 discrepancies between the modelled and reference sequences:

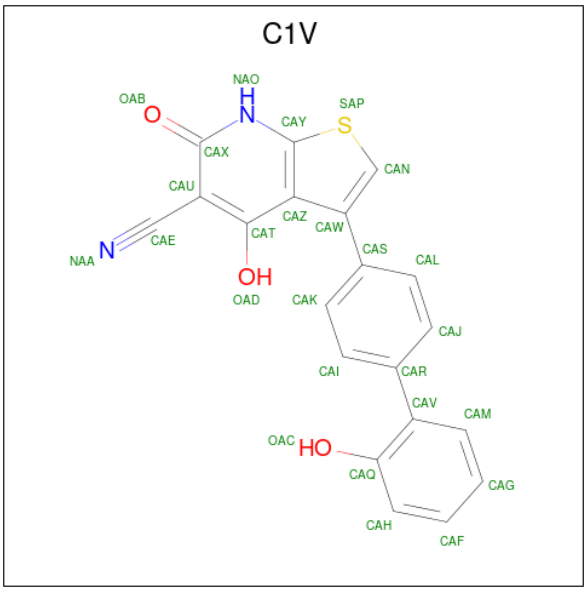
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine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

- Molecule 4 is (5S,6R,7R,9R,13cR,14R,16aS)-6-methoxy-5-methyl-7-(methylamino)-6,7,8,9,14,15,16,16a-octahydro-5H,13cH-5,9-epoxy-4b,9a,1 5-triazadibenzo[b,h]cyclonona[1,2,3,4-jkl]cyclopenta[e]-as-indacen-14-ol (three-letter code: 4O7) (formula: $C_{28}H_{30}N_4O_3$).



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

- Molecule 5 is 3-[4-(2-hydroxyphenyl)phenyl]-4-oxidanyl-6-oxidanylidene-7H-thieno[2,3-b]pyridine-5-carbonitrile (three-letter code: C1V) (formula: $C_{20}H_{12}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	26	20	2	3	1	0	0

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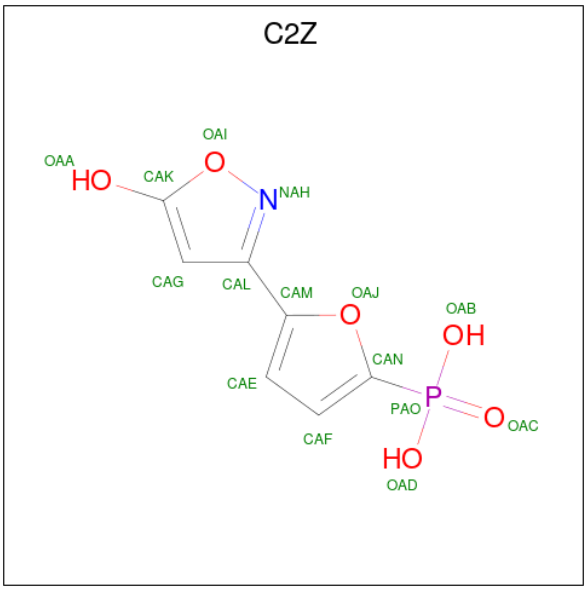
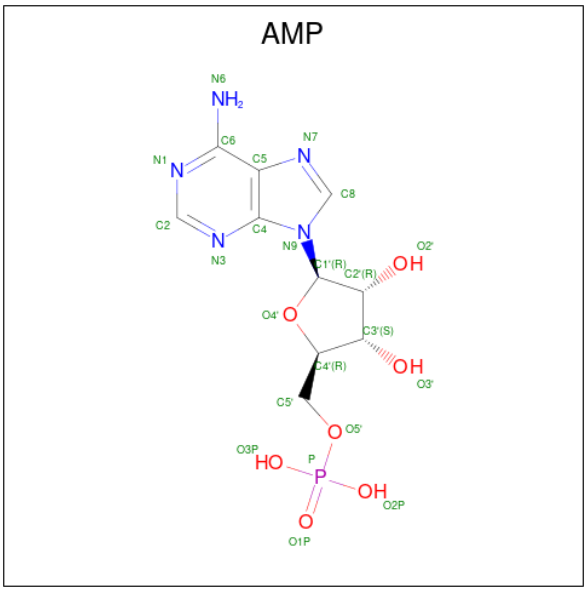
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

- Molecule 6 is 5-(5-hydroxyl-isoxazol-3-yl)-furan-2-phosphonic acid (three-letter code: C2Z) (formula: $C_7H_6NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
6	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

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



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

- Molecule 8 is water.

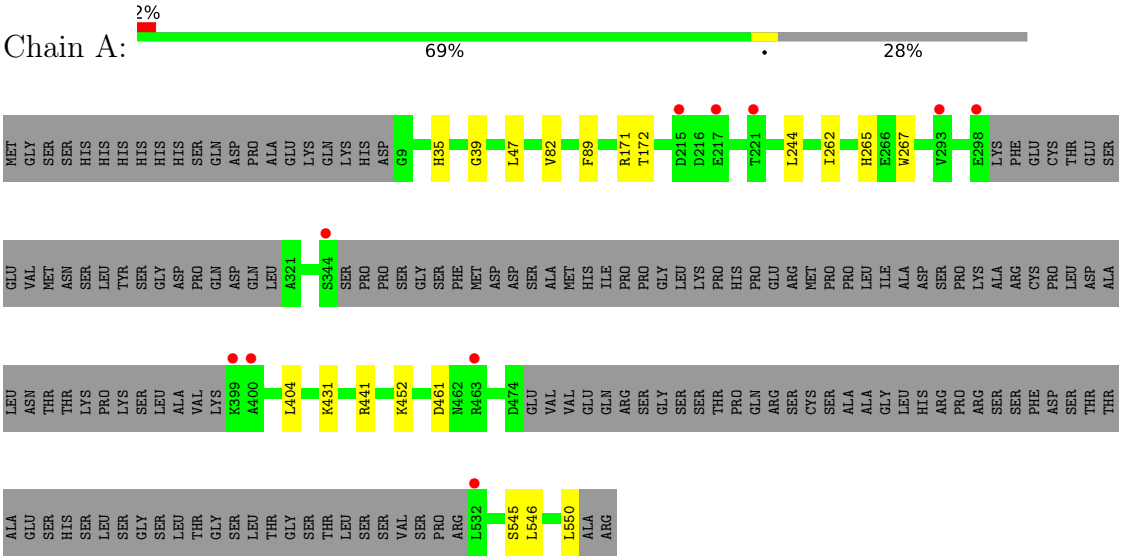
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	28	Total	O	0	0
			28	28		
8	B	13	Total	O	0	0
			13	13		
8	C	33	Total	O	0	0
			33	33		
8	D	16	Total	O	0	0
			16	16		
8	E	26	Total	O	0	0
			26	26		
8	F	21	Total	O	0	0
			21	21		

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.

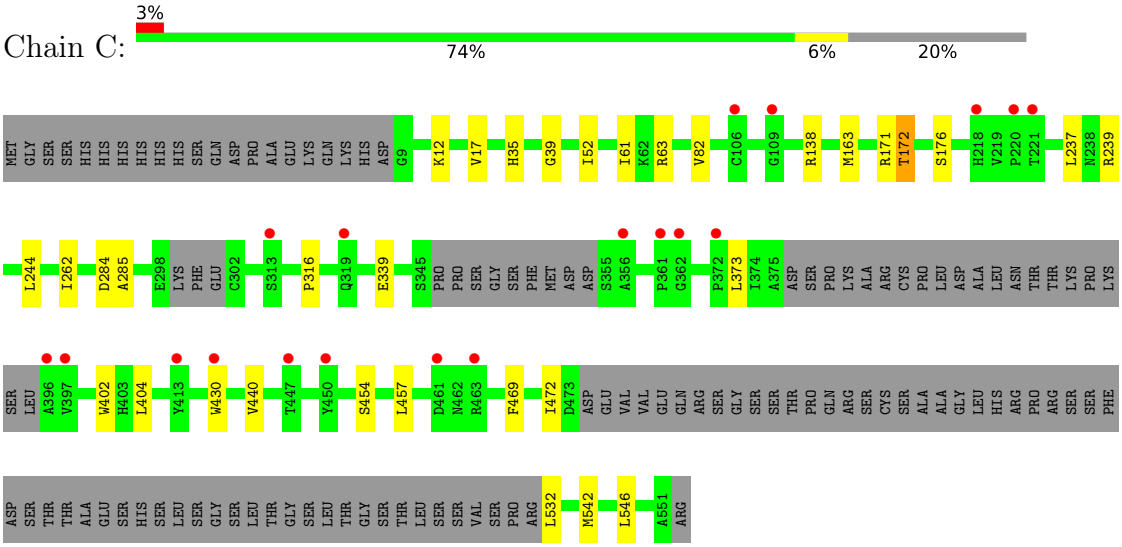
• Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2

Chain A:



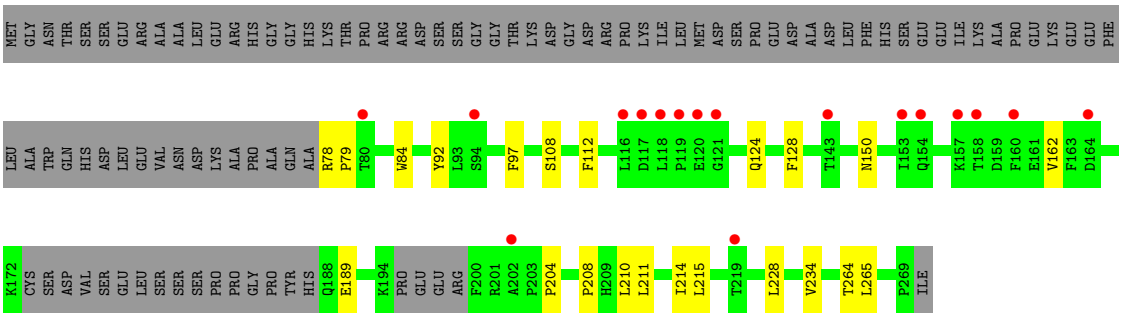
• Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2

Chain C:

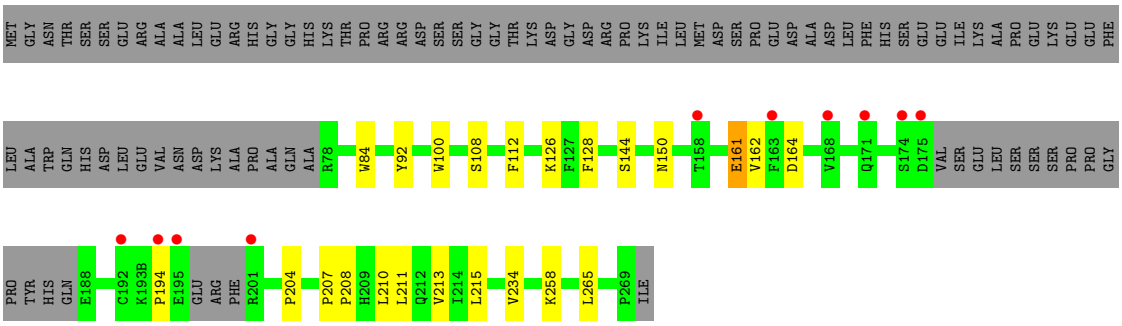


• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

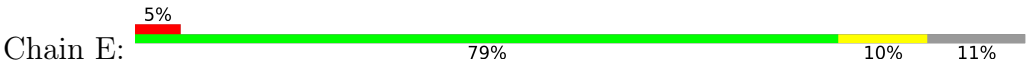
Chain B:

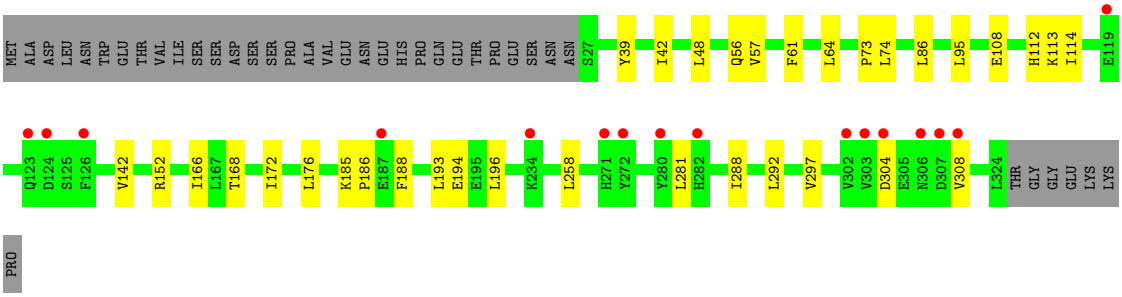


• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

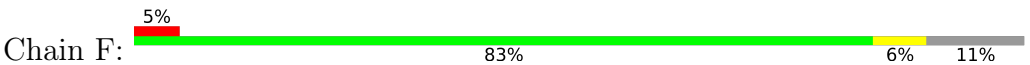


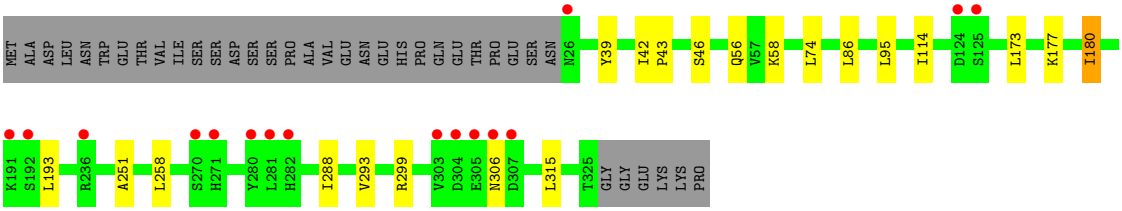
• Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1





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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.95Å 134.24Å 141.48Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	43.78 – 2.99 48.66 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.6 (43.78-2.99) 98.6 (48.66-2.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0	Depositor
R, R_{free}	0.225 , 0.243 0.240 , 0.259	Depositor DCC
R_{free} test set	2867 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14587	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: 4O7, C1V, TPO, AMP, C2Z, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/3316	0.55	0/4477
1	C	0.37	0/3637	0.56	0/4918
2	B	0.37	0/1335	0.55	0/1825
2	D	0.36	0/1400	0.55	0/1908
3	E	0.38	0/2437	0.56	0/3309
3	F	0.38	0/2414	0.56	0/3284
All	All	0.37	0/14539	0.55	0/19721

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3255	0	3224	9	0
1	C	3567	0	3505	16	1
2	B	1310	0	1239	12	0
2	D	1373	0	1342	12	1
3	E	2381	0	2443	17	0
3	F	2366	0	2400	11	0
4	A	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	0	0	0
5	B	26	0	12	0	0
5	C	26	0	12	0	0
6	E	30	0	0	0	0
7	F	46	0	24	0	0
8	A	28	0	0	0	0
8	B	13	0	0	0	0
8	C	33	0	0	1	0
8	D	16	0	0	0	0
8	E	26	0	0	0	0
8	F	21	0	0	0	0
All	All	14587	0	14201	67	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:43:PRO:HG2	3:F:46:SER:HB3	1.76	0.66
1:A:35:HIS:HB3	1:A:39:GLY:H	1.70	0.56
1:C:138:ARG:HH12	1:C:172:TPO:HB	1.73	0.54
3:F:177:LYS:HA	3:F:180:ILE:HD12	1.90	0.54
3:E:61:PHE:HA	3:E:64:LEU:HD12	1.90	0.53
2:B:78:ARG:CB	2:B:79:PRO:HD3	2.39	0.52
1:A:441:ARG:HG3	1:A:452:LYS:HB3	1.91	0.52
1:C:171:ARG:HH22	2:D:204:PRO:HB3	1.74	0.52
3:E:108:GLU:O	3:E:112:HIS:HB2	2.09	0.52
1:A:82:VAL:HG13	2:B:162:VAL:HG21	1.92	0.51
2:B:92:TYR:HB2	2:B:128:PHE:HB3	1.91	0.51
2:D:207:PRO:HD2	2:D:210:LEU:HD12	1.91	0.51
1:C:402:TRP:HB2	2:D:213:VAL:HG11	1.95	0.49
3:F:56:GLN:HE21	3:F:58:LYS:HB3	1.78	0.48
1:C:454:SER:HB2	1:C:472:ILE:HD11	1.96	0.48
1:C:82:VAL:HG13	2:D:162:VAL:HG21	1.96	0.48
2:B:264:THR:HG22	3:E:48:LEU:HD23	1.96	0.47
1:C:284:ASP:HB2	8:C:713:HOH:O	2.14	0.47
3:E:39:TYR:HA	3:E:42:ILE:HD12	1.95	0.47
1:A:404:LEU:HD22	2:B:210:LEU:HB3	1.95	0.47
2:D:208:PRO:HA	2:D:211:LEU:HD12	1.96	0.47
1:C:52:ILE:HD12	1:C:61:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:173:LEU:HD22	3:F:315:LEU:HD22	1.96	0.47
1:C:244:LEU:HD11	1:C:262:ILE:HG23	1.96	0.47
3:E:142:VAL:HG22	3:E:172:ILE:HD13	1.98	0.46
3:F:39:TYR:HA	3:F:42:ILE:HD12	1.96	0.46
3:E:56:GLN:HA	3:E:113:LYS:HA	1.97	0.46
3:E:188:PHE:HB2	3:E:196:LEU:HD21	1.96	0.46
1:C:469:PHE:HE2	1:C:546:LEU:HD23	1.81	0.46
2:B:208:PRO:HA	2:B:211:LEU:HD12	1.98	0.45
3:E:74:LEU:HD22	3:E:114:ILE:HG21	1.97	0.45
2:D:84:TRP:HB3	2:D:112:PHE:HB2	1.98	0.45
1:A:244:LEU:HD11	1:A:262:ILE:HG23	1.98	0.44
1:A:171:ARG:HH22	2:B:204:PRO:HB3	1.82	0.44
3:F:177:LYS:HG2	3:F:293:VAL:HG21	1.99	0.44
1:C:404:LEU:HD22	2:D:210:LEU:HB3	2.00	0.44
3:E:152:ARG:HG2	3:E:168:THR:HG22	2.00	0.44
3:E:292:LEU:HD23	3:E:297:VAL:HG23	2.00	0.44
2:D:161:GLU:HB3	2:D:164:ASP:HB2	1.99	0.43
2:D:100:TRP:HZ3	2:D:126:LYS:HB2	1.84	0.43
1:C:12:LYS:HG2	1:C:17:VAL:HG22	1.99	0.43
2:D:215:LEU:HD21	2:D:265:LEU:HD11	2.00	0.43
1:C:138:ARG:NH1	1:C:172:TPO:HB	2.34	0.43
3:E:193:LEU:HD13	3:E:288:ILE:HD13	2.01	0.43
3:F:74:LEU:HD22	3:F:114:ILE:HG21	2.01	0.43
1:C:35:HIS:HB3	1:C:39:GLY:H	1.84	0.42
1:A:265:HIS:HD2	1:A:267:TRP:H	1.66	0.42
3:E:95:LEU:HD22	3:E:258:LEU:HD11	2.01	0.42
2:B:214:ILE:HG12	2:B:228:LEU:HD22	2.02	0.42
2:B:124:GLN:HB3	2:B:150:ASN:HD22	1.85	0.42
2:B:215:LEU:HD21	2:B:265:LEU:HD11	2.01	0.42
3:E:194:GLU:HG3	3:E:281:LEU:HD22	2.02	0.42
3:F:95:LEU:HD22	3:F:258:LEU:HD11	2.02	0.41
3:F:193:LEU:HD13	3:F:288:ILE:HD13	2.02	0.41
3:F:74:LEU:HD21	3:F:86:LEU:HB2	2.02	0.41
1:C:373:LEU:HD12	3:F:251:ALA:HA	2.01	0.41
1:A:47:LEU:HB2	1:A:89:PHE:HB2	2.03	0.41
3:E:304:ASP:HB3	3:E:308:VAL:HB	2.03	0.41
1:A:431:LYS:HG3	2:B:189:GLU:HG2	2.02	0.41
1:C:430:TRP:HB3	1:C:440:VAL:HG12	2.03	0.41
2:D:126:LYS:HE2	2:D:150:ASN:HB3	2.02	0.41
3:E:73:PRO:HD3	3:E:166:ILE:HD11	2.03	0.41
2:B:84:TRP:HB3	2:B:112:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:LYS:HA	3:E:186:PRO:HD3	1.98	0.40
1:C:63:ARG:HH21	1:C:163:MET:HB2	1.87	0.40
2:D:92:TYR:HB2	2:D:128:PHE:HB3	2.04	0.40
3:E:74:LEU:HD21	3:E:86:LEU:HB2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ALA:O	2:D:144:SER:OG[2_946]	2.17	0.03

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	400/565 (71%)	388 (97%)	11 (3%)	1 (0%)	41 76
1	C	442/565 (78%)	423 (96%)	18 (4%)	1 (0%)	47 82
2	B	165/270 (61%)	156 (94%)	9 (6%)	0	100 100
2	D	168/270 (62%)	161 (96%)	5 (3%)	2 (1%)	13 48
3	E	298/336 (89%)	291 (98%)	7 (2%)	0	100 100
3	F	298/336 (89%)	290 (97%)	8 (3%)	0	100 100
All	All	1771/2342 (76%)	1709 (96%)	58 (3%)	4 (0%)	47 82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ASP
1	C	316	PRO
2	D	258	LYS
2	D	194	PRO

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	344/497 (69%)	341 (99%)	3 (1%)	78 92
1	C	378/497 (76%)	371 (98%)	7 (2%)	57 84
2	B	135/239 (56%)	133 (98%)	2 (2%)	65 87
2	D	152/239 (64%)	150 (99%)	2 (1%)	69 89
3	E	265/308 (86%)	263 (99%)	2 (1%)	81 93
3	F	262/308 (85%)	259 (99%)	3 (1%)	73 90
All	All	1536/2088 (74%)	1517 (99%)	19 (1%)	71 90

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	545	SER
1	A	546	LEU
1	A	550	LEU
2	B	97	PHE
2	B	234	VAL
1	C	176	SER
1	C	237	LEU
1	C	239	ARG
1	C	339	GLU
1	C	457	LEU
1	C	532	LEU
1	C	542	MET
2	D	161	GLU
2	D	234	VAL
3	E	57	VAL
3	E	176	LEU
3	F	180	ILE
3	F	299	ARG
3	F	306	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	132	GLN
2	D	237	ASN
3	E	93	ASN
3	F	56	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	C	172	1	8,10,11	1.21	1 (12%)	10,14,16	1.49	1 (10%)
2	SEP	B	108	2	8,9,10	0.98	1 (12%)	8,12,14	2.42	2 (25%)
1	TPO	A	172	1	8,10,11	1.25	1 (12%)	10,14,16	1.67	1 (10%)
2	SEP	D	108	2	8,9,10	0.96	0	8,12,14	1.78	2 (25%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-2.99	1.53	1.59
1	C	172	TPO	P-OG1	-2.77	1.54	1.59
2	B	108	SEP	P-OG	-2.16	1.53	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	108	SEP	OG-CB-CA	5.39	113.39	108.14
1	A	172	TPO	P-OG1-CB	-4.42	109.84	123.21
1	C	172	TPO	P-OG1-CB	-3.74	111.91	123.21
2	D	108	SEP	OG-CB-CA	3.53	111.58	108.14
2	B	108	SEP	P-OG-CB	-3.40	108.92	118.30
2	D	108	SEP	P-OG-CB	-2.33	111.87	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	172	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	C1V	C	602	-	29,29,29	3.66	10 (34%)	30,42,42	6.12	6 (20%)
6	C2Z	E	401	-	8,16,16	3.74	5 (62%)	8,24,24	2.00	3 (37%)
6	C2Z	E	402	-	8,16,16	3.74	5 (62%)	8,24,24	1.53	3 (37%)
4	4O7	C	601	-	30,42,42	2.53	8 (26%)	21,68,68	2.01	8 (38%)
4	4O7	A	601	-	30,42,42	2.54	8 (26%)	21,68,68	2.01	8 (38%)
7	AMP	F	402	-	22,25,25	0.56	0	25,38,38	0.98	2 (8%)
5	C1V	B	301	-	29,29,29	3.69	10 (34%)	30,42,42	5.84	6 (20%)
7	AMP	F	401	-	22,25,25	0.68	0	25,38,38	1.01	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
5	C1V	C	602	-	-	0/8/10/10	0/4/4/4
6	C2Z	E	401	-	-	0/0/10/10	0/2/2/2
6	C2Z	E	402	-	-	0/0/10/10	0/2/2/2
4	4O7	C	601	-	-	2/4/58/58	-
4	4O7	A	601	-	-	2/4/58/58	-
7	AMP	F	402	-	-	2/6/26/26	0/3/3/3
5	C1V	B	301	-	-	0/8/10/10	0/4/4/4
7	AMP	F	401	-	-	3/6/26/26	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	C1V	CAE-NAA	10.11	1.32	1.14
5	B	301	C1V	CAE-NAA	10.08	1.32	1.14
5	C	602	C1V	OAB-CAX	9.76	1.42	1.23
5	B	301	C1V	OAB-CAX	9.74	1.42	1.23
5	B	301	C1V	CAN-CAW	8.08	1.41	1.37
5	C	602	C1V	CAN-CAW	7.70	1.41	1.37
5	B	301	C1V	CAW-CAZ	6.91	1.49	1.41
5	C	602	C1V	CAW-CAZ	6.91	1.49	1.41
4	A	601	4O7	C8-N1	-6.78	1.35	1.45
4	C	601	4O7	C8-N1	-6.77	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	401	C2Z	CAL-CAM	-6.70	1.34	1.49
6	E	402	C2Z	CAL-CAM	-6.66	1.34	1.49
6	E	402	C2Z	PAO-OAC	6.18	1.61	1.49
6	E	401	C2Z	PAO-OAC	5.91	1.61	1.49
4	A	601	4O7	C11-C12	5.67	1.46	1.40
4	C	601	4O7	C11-C12	5.61	1.46	1.40
4	C	601	4O7	C10-C7	-5.38	1.48	1.55
4	A	601	4O7	C10-C7	-5.38	1.48	1.55
5	C	602	C1V	CAE-CAU	5.21	1.53	1.43
5	B	301	C1V	CAE-CAU	5.18	1.53	1.43
4	A	601	4O7	C6-C5	5.16	1.46	1.40
4	C	601	4O7	C6-C5	5.13	1.46	1.40
5	B	301	C1V	CAW-CAS	3.81	1.56	1.49
5	C	602	C1V	CAW-CAS	3.61	1.56	1.49
6	E	401	C2Z	CAG-CAL	-3.52	1.33	1.40
6	E	402	C2Z	CAG-CAL	-3.42	1.33	1.40
4	A	601	4O7	C18-C11	3.26	1.49	1.41
4	C	601	4O7	C18-C11	3.24	1.49	1.41
6	E	401	C2Z	PAO-OAD	2.95	1.61	1.54
6	E	402	C2Z	PAO-OAB	2.86	1.61	1.54
6	E	401	C2Z	PAO-OAB	2.85	1.61	1.54
4	A	601	4O7	C19-C6	2.84	1.48	1.41
4	C	601	4O7	C19-C6	2.82	1.48	1.41
5	B	301	C1V	CAU-CAT	2.64	1.43	1.38
6	E	402	C2Z	PAO-OAD	2.63	1.60	1.54
5	B	301	C1V	OAD-CAT	2.62	1.40	1.33
4	A	601	4O7	O5-C8	-2.61	1.28	1.40
5	C	602	C1V	CAU-CAT	2.60	1.43	1.38
5	C	602	C1V	OAD-CAT	2.58	1.40	1.33
4	C	601	4O7	O5-C8	-2.58	1.28	1.40
5	C	602	C1V	OAC-CAQ	2.51	1.41	1.36
4	C	601	4O7	C9-C10	-2.39	1.45	1.53
4	A	601	4O7	C9-C10	-2.38	1.45	1.53
5	B	301	C1V	OAC-CAQ	2.30	1.41	1.36
5	C	602	C1V	CAV-CAR	2.30	1.53	1.49
5	B	301	C1V	CAV-CAR	2.29	1.53	1.49

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301	C1V	CAU-CAE-NAA	-24.33	120.02	177.38
5	C	602	C1V	CAU-CAE-NAA	-24.24	120.24	177.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	602	C1V	CAW-CAN-SAP	-19.52	107.08	112.53
5	B	301	C1V	CAW-CAN-SAP	-17.44	107.66	112.53
5	C	602	C1V	CAN-CAW-CAZ	7.96	113.88	111.69
5	C	602	C1V	CAU-CAX-NAO	6.64	120.75	114.89
5	B	301	C1V	CAU-CAX-NAO	6.51	120.64	114.89
5	B	301	C1V	CAN-CAW-CAZ	6.07	113.36	111.69
4	A	601	4O7	C16-C17-N2	5.02	138.36	132.29
4	C	601	4O7	C16-C17-N2	4.95	138.28	132.29
5	B	301	C1V	CAN-CAW-CAS	-4.38	118.87	125.52
5	C	602	C1V	CAN-CAW-CAS	-3.93	119.56	125.52
6	E	401	C2Z	CAG-CAL-CAM	-3.53	124.17	129.32
7	F	402	AMP	P-O5'-C5'	3.52	128.00	118.30
4	C	601	4O7	C9-C10-C7	3.33	110.08	101.92
7	F	401	AMP	P-O5'-C5'	3.31	127.42	118.30
4	A	601	4O7	C9-C10-C7	3.31	110.04	101.92
5	C	602	C1V	CAE-CAU-CAX	3.30	120.35	115.80
5	B	301	C1V	CAE-CAU-CAX	3.19	120.19	115.80
4	A	601	4O7	C16-C17-C12	-3.06	116.78	120.94
4	C	601	4O7	C16-C17-C12	-3.05	116.79	120.94
4	C	601	4O7	C1-C20-C5	-2.82	117.11	120.94
4	A	601	4O7	C1-C20-C5	-2.78	117.16	120.94
4	A	601	4O7	C1-C20-N3	2.51	135.25	132.25
4	C	601	4O7	C26-C21-C22	-2.50	107.77	112.64
6	E	401	C2Z	OAD-PAO-OAC	-2.48	105.38	112.45
4	C	601	4O7	C1-C20-N3	2.47	135.21	132.25
4	A	601	4O7	C3-C4-C5	-2.45	117.50	120.89
6	E	401	C2Z	OAB-PAO-OAC	-2.44	105.49	112.45
4	C	601	4O7	C3-C4-C5	-2.44	117.51	120.89
6	E	402	C2Z	OAD-PAO-OAC	-2.39	105.65	112.45
7	F	402	AMP	C5-C6-N6	2.27	123.81	120.35
4	A	601	4O7	C26-C21-C22	-2.24	108.28	112.64
7	F	401	AMP	C5-C6-N6	2.23	123.74	120.35
6	E	402	C2Z	OAB-PAO-OAC	-2.19	106.20	112.45
6	E	402	C2Z	CAG-CAL-CAM	-2.09	126.28	129.32
4	A	601	4O7	C14-C13-C12	-2.08	118.01	120.89
4	C	601	4O7	C14-C13-C12	-2.02	118.09	120.89

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	4O7	C22-C23-N4-C28

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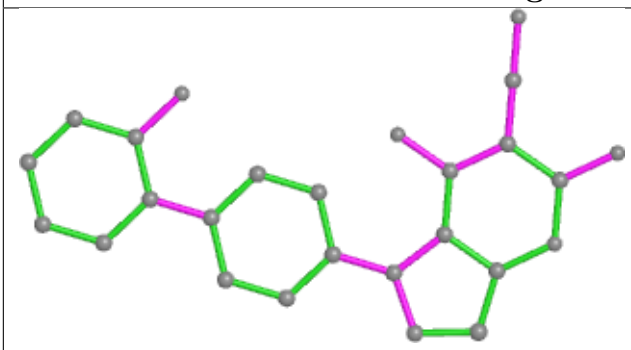
Mol	Chain	Res	Type	Atoms
4	C	601	4O7	C22-C23-N4-C28
7	F	401	AMP	C5'-O5'-P-O3P
7	F	402	AMP	C5'-O5'-P-O1P
7	F	402	AMP	C5'-O5'-P-O3P
4	C	601	4O7	C24-C23-N4-C28
4	A	601	4O7	C24-C23-N4-C28
7	F	401	AMP	C5'-O5'-P-O1P
7	F	401	AMP	C5'-O5'-P-O2P

There are no ring outliers.

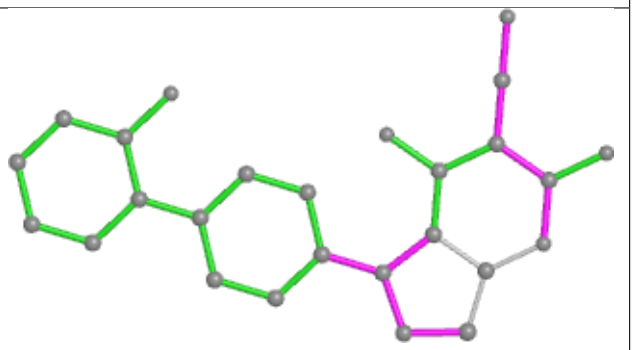
No monomer is involved in short contacts.

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

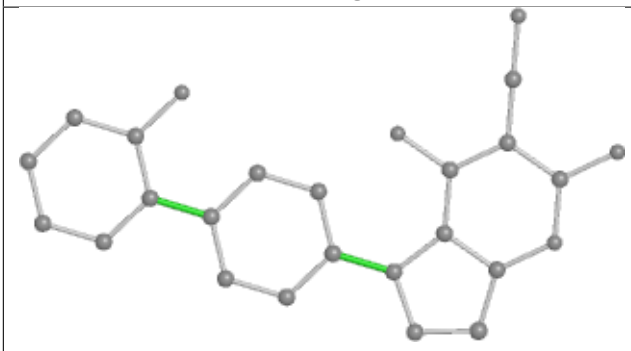
Ligand C1V C 602



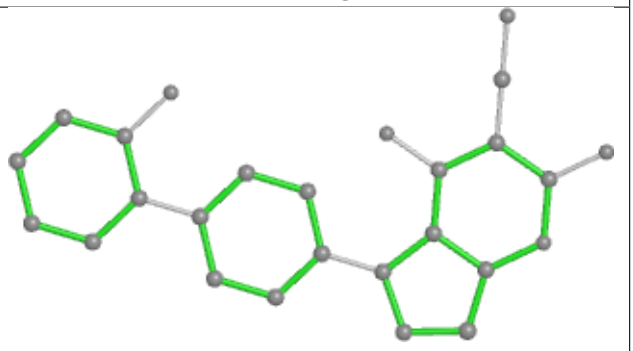
Bond lengths



Bond angles

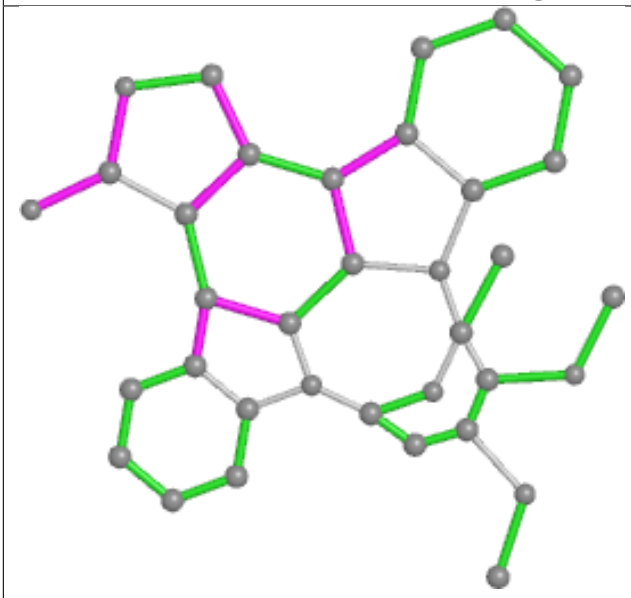


Torsions

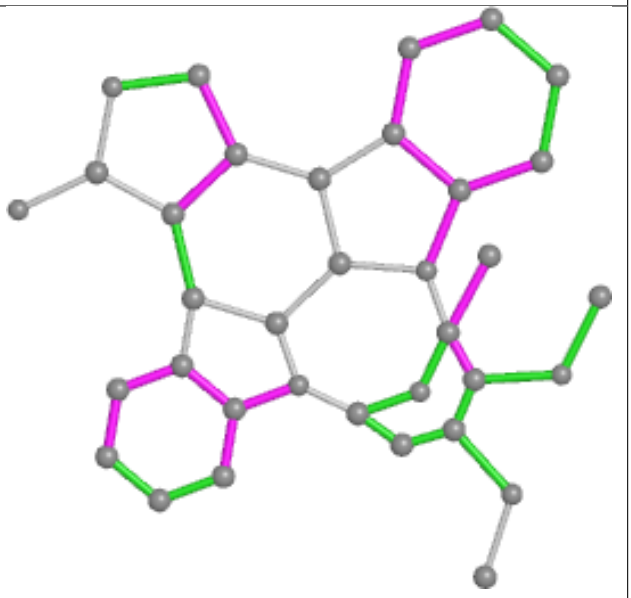


Rings

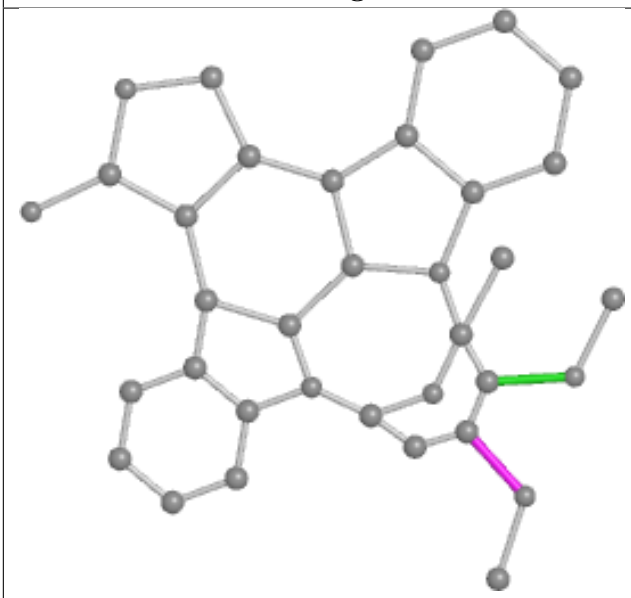
Ligand 4O7 C 601



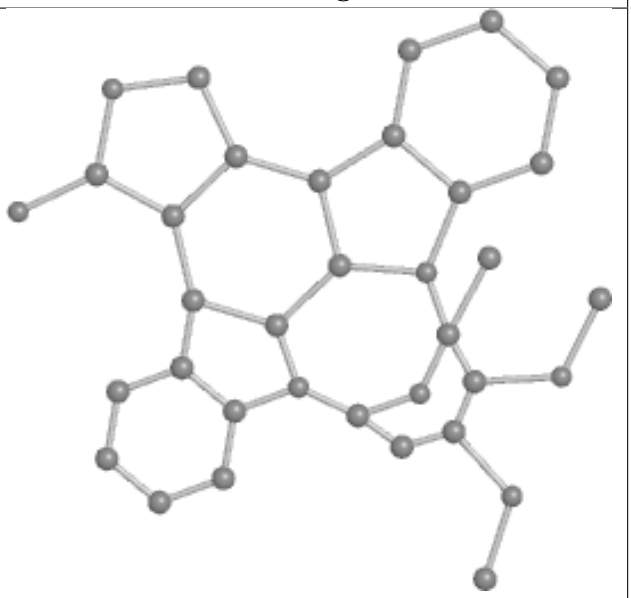
Bond lengths



Bond angles

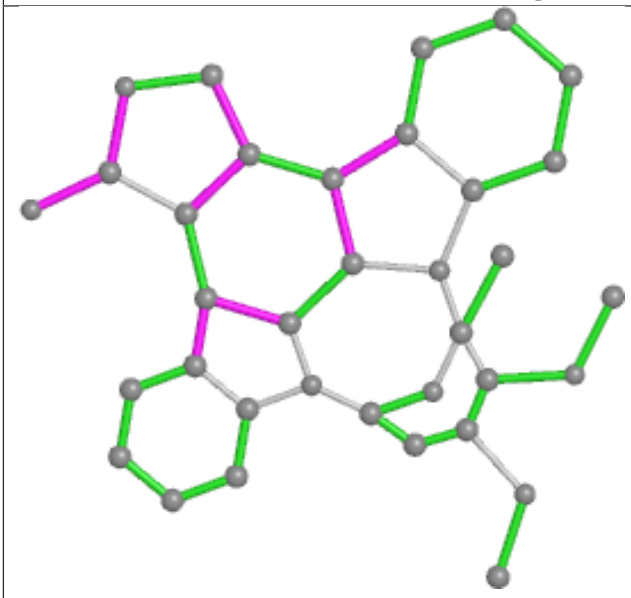


Torsions

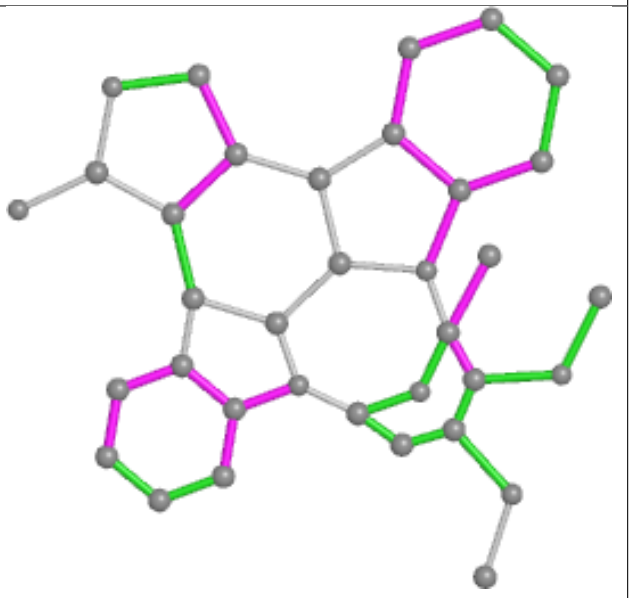


Rings

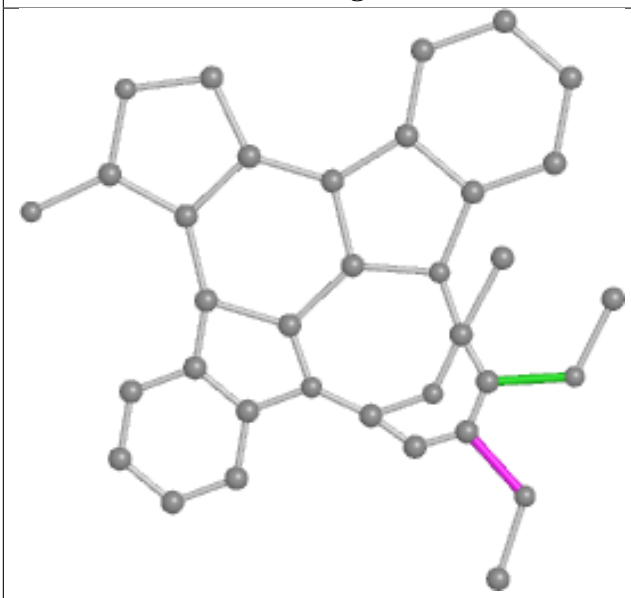
Ligand 4O7 A 601



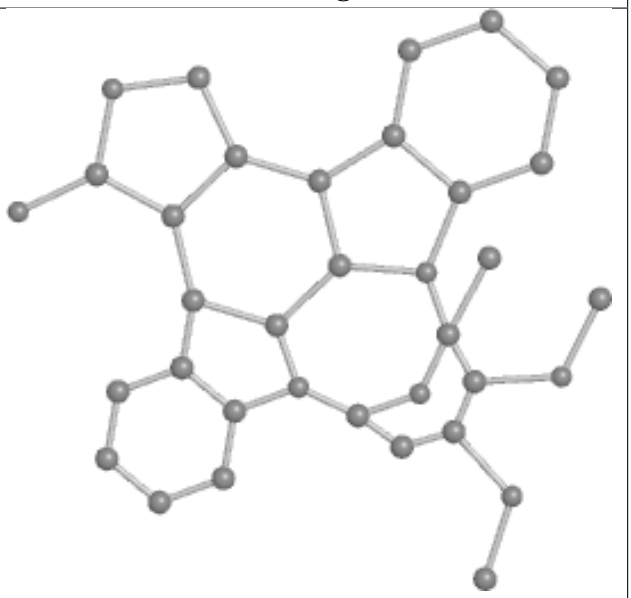
Bond lengths



Bond angles

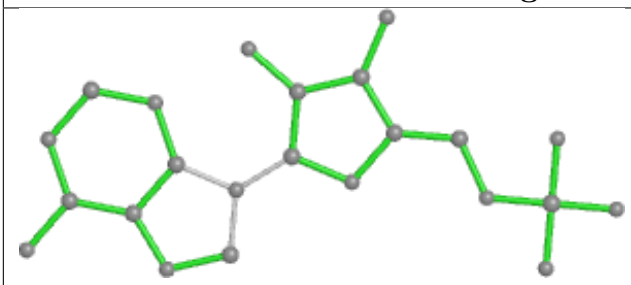


Torsions

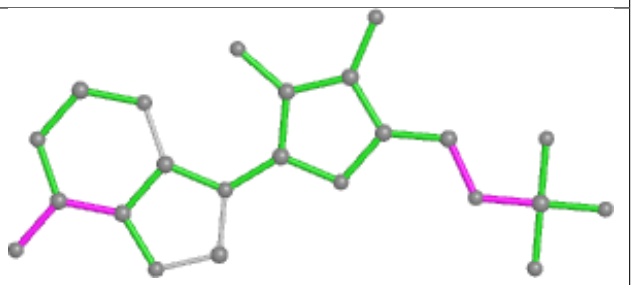


Rings

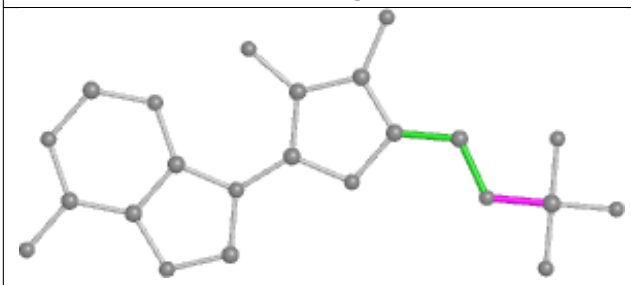
Ligand AMP F 402



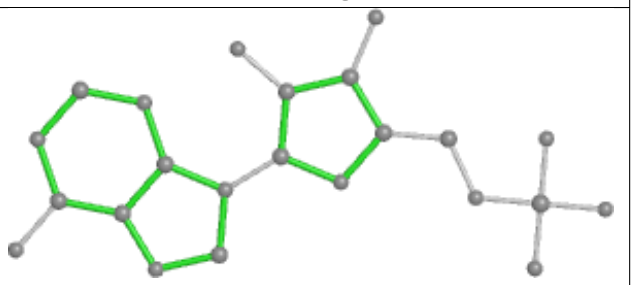
Bond lengths



Bond angles

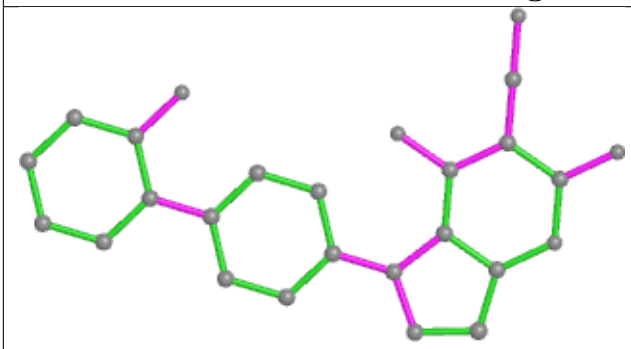


Torsions

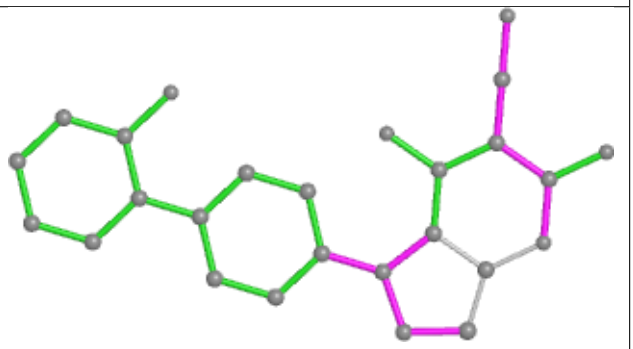


Rings

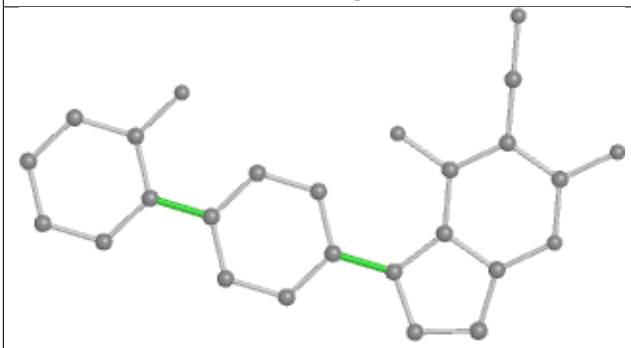
Ligand C1V B 301



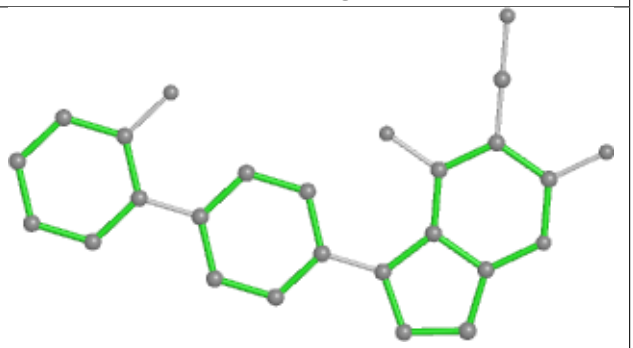
Bond lengths



Bond angles

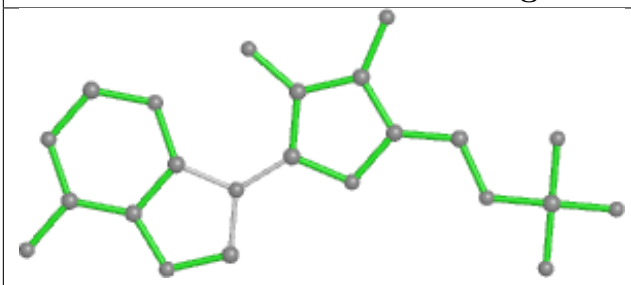


Torsions

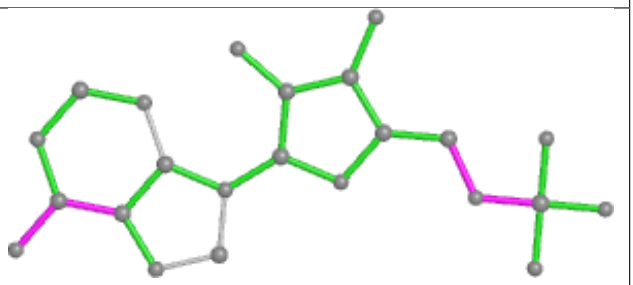


Rings

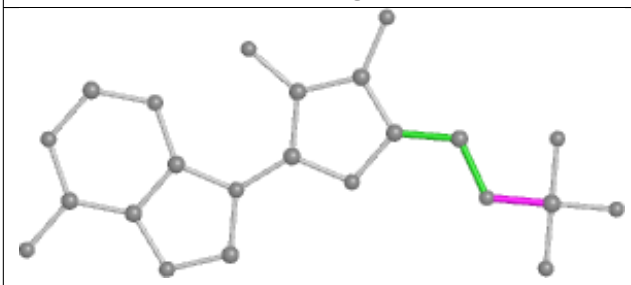
Ligand AMP F 401



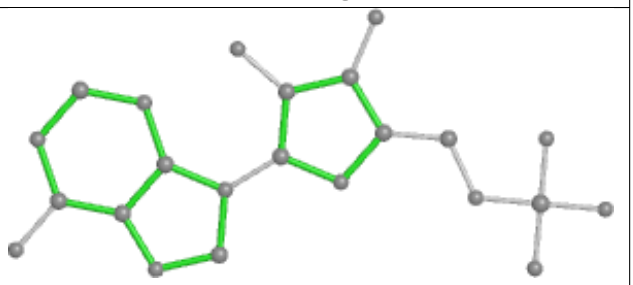
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 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	408/565 (72%)	0.45	10 (2%) 57 29	42, 69, 110, 163	0
1	C	452/565 (80%)	0.44	19 (4%) 36 14	33, 65, 108, 167	0
2	B	171/270 (63%)	0.74	17 (9%) 7 2	41, 85, 113, 142	0
2	D	174/270 (64%)	0.45	10 (5%) 23 8	43, 62, 103, 156	0
3	E	298/336 (88%)	0.43	16 (5%) 25 9	37, 62, 94, 113	0
3	F	300/336 (89%)	0.41	16 (5%) 26 10	36, 61, 93, 108	0
All	All	1803/2342 (76%)	0.47	88 (4%) 29 11	33, 66, 106, 167	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	GLN	6.3
3	E	306	ASN	5.8
3	F	304	ASP	5.6
3	E	272	TYR	4.4
3	E	123	GLN	4.0
2	D	194	PRO	4.0
1	C	413	TYR	3.8
3	F	303	VAL	3.8
2	D	175	ASP	3.7
3	E	124	ASP	3.7
2	B	94	SER	3.7
3	E	307	ASP	3.6
1	A	463	ARG	3.6
3	F	124	ASP	3.6
3	F	281	LEU	3.5
3	F	306	ASN	3.4
1	C	109	GLY	3.4
3	F	125	SER	3.3
2	B	160	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	174	SER	3.1
1	C	397	VAL	3.0
2	D	158	THR	3.0
3	E	303	VAL	2.9
2	D	195	GLU	2.9
1	A	293	VAL	2.8
1	A	298	GLU	2.8
3	E	126[A]	PHE	2.8
1	C	220	PRO	2.8
2	B	116	LEU	2.8
2	B	120	GLU	2.7
2	B	157	LYS	2.7
2	B	219	THR	2.7
3	E	302	VAL	2.7
3	E	304	ASP	2.7
1	C	430	TRP	2.6
2	B	164	ASP	2.6
1	A	399	LYS	2.6
1	C	313	SER	2.6
3	F	307	ASP	2.6
3	E	234	LYS	2.6
1	C	218	HIS	2.6
2	B	154	GLN	2.6
3	E	282	HIS	2.6
2	D	168	VAL	2.5
3	E	308	VAL	2.5
1	A	215	ASP	2.5
2	B	121	GLY	2.5
2	B	202	ALA	2.5
2	B	119	PRO	2.5
1	C	447	THR	2.5
1	C	461	ASP	2.4
1	C	372	PRO	2.4
3	E	271	HIS	2.4
3	F	280	TYR	2.4
2	D	192	CYS	2.4
3	F	236	ARG	2.4
3	F	305	GLU	2.4
2	B	80	THR	2.4
2	D	201	ARG	2.4
2	B	143	THR	2.4
1	C	463	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	26	ASN	2.3
3	F	270	SER	2.3
3	F	282	HIS	2.3
1	C	450	TYR	2.3
1	C	356	ALA	2.3
1	C	396	ALA	2.3
3	E	280	TYR	2.3
2	B	158	THR	2.2
2	B	153	ILE	2.2
3	F	191	LYS	2.2
2	D	163	PHE	2.2
3	E	187	GLU	2.2
1	C	361	PRO	2.2
1	C	106	CYS	2.2
1	C	362	GLY	2.2
2	B	118	LEU	2.2
1	A	400	ALA	2.2
2	D	171	GLN	2.2
3	F	271	HIS	2.1
1	A	532	LEU	2.1
3	F	192	SER	2.1
3	E	119	GLU	2.1
1	A	221	THR	2.1
1	A	217	GLU	2.1
1	A	344	SER	2.0
2	B	117	ASP	2.0
1	C	221	THR	2.0

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^{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	0.86	0.19	60,62,65,66	4
1	TPO	C	172	11/12	0.89	0.20	70,71,74,76	4
2	SEP	B	108	10/11	0.91	0.20	76,78,85,86	0
2	SEP	D	108	10/11	0.93	0.15	60,63,67,67	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

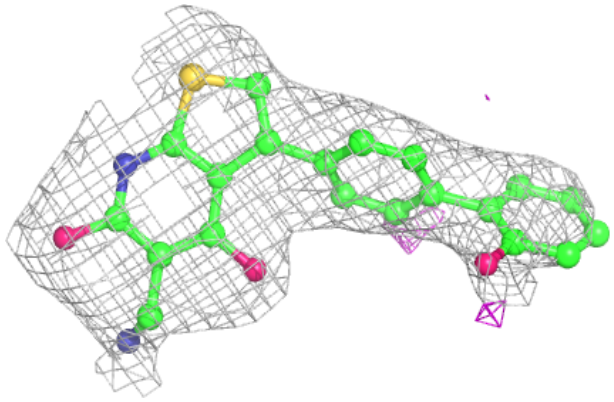
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

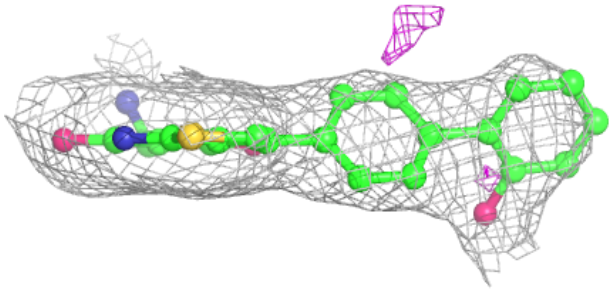
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	C2Z	E	402	15/15	0.86	0.26	95,95,95,95	0
6	C2Z	E	401	15/15	0.88	0.23	88,88,89,89	0
5	C1V	B	301	26/26	0.89	0.23	58,61,67,69	0
7	AMP	F	402	23/23	0.94	0.19	60,64,68,69	0
7	AMP	F	401	23/23	0.95	0.17	63,68,71,72	0
4	4O7	C	601	35/35	0.96	0.18	33,35,36,37	0
4	4O7	A	601	35/35	0.96	0.18	37,39,41,41	0
5	C1V	C	602	26/26	0.97	0.21	39,42,43,45	0

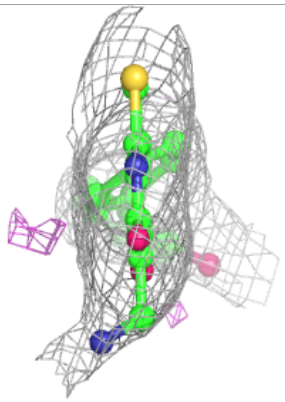
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C1V B 301:

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

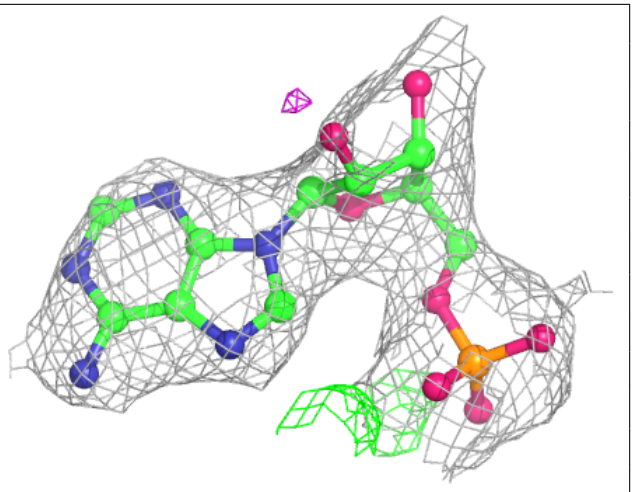


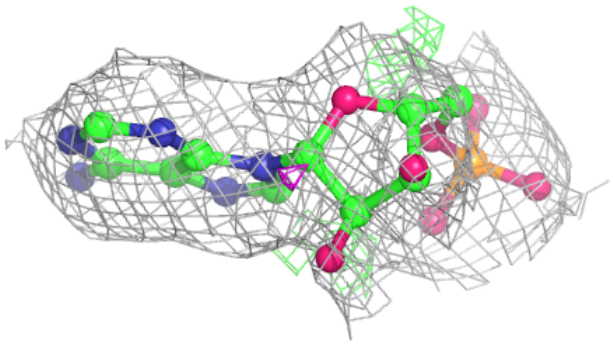


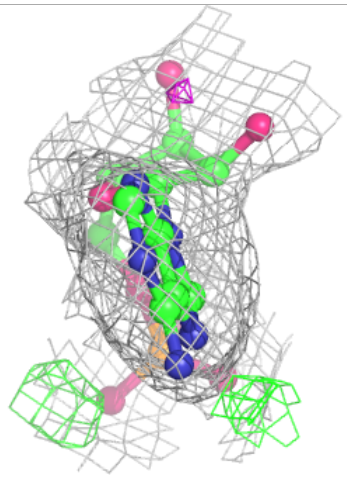


Electron density around AMP F 402:

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

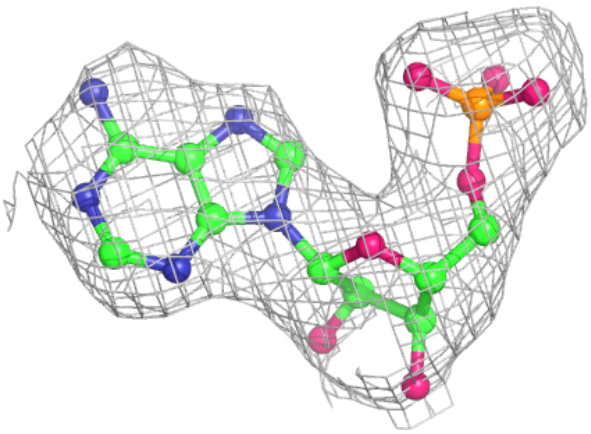


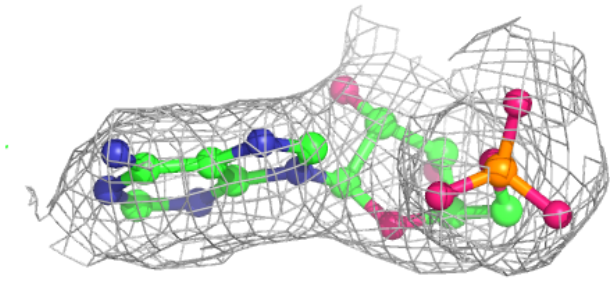


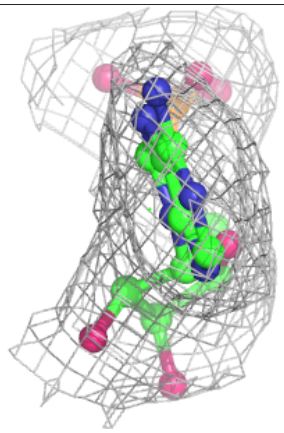


Electron density around AMP F 401:

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

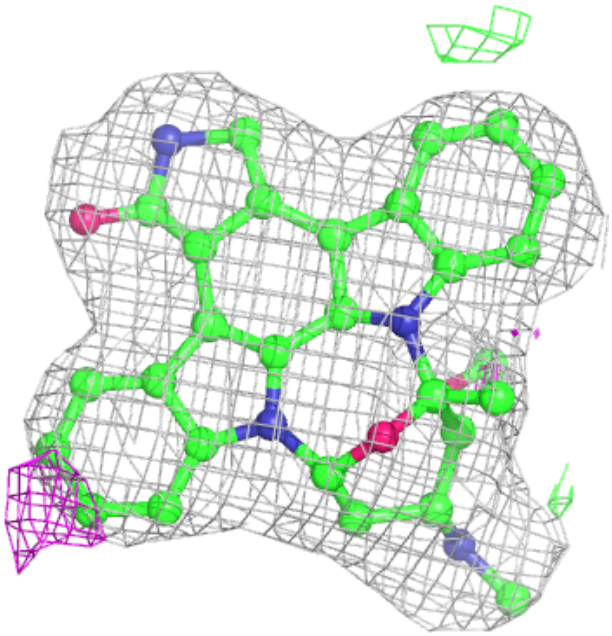


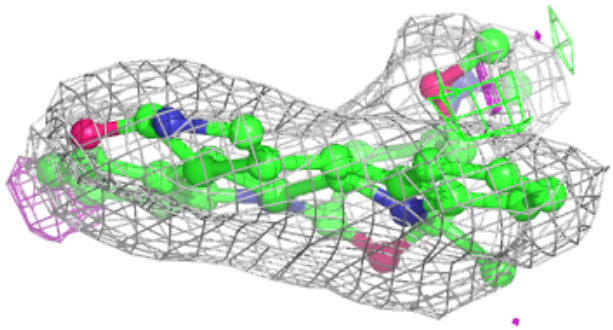


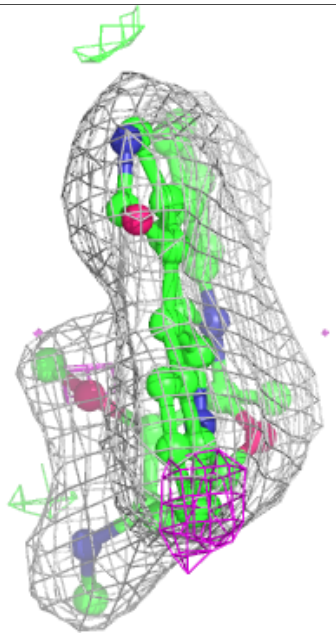


Electron density around 4O7 C 601:

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

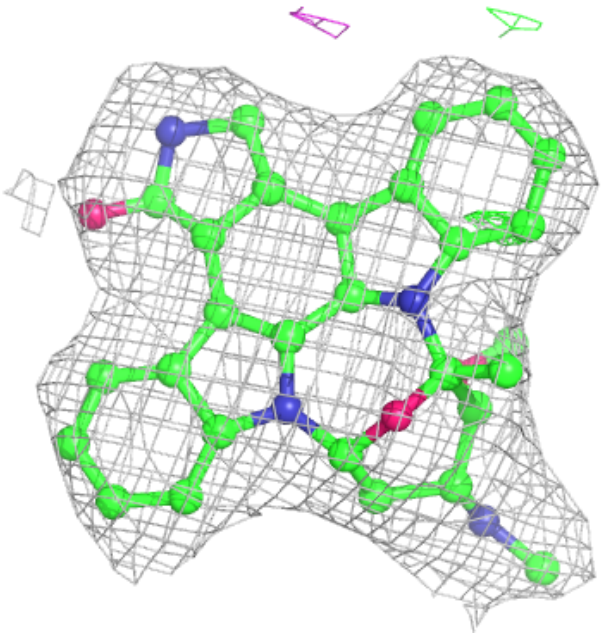


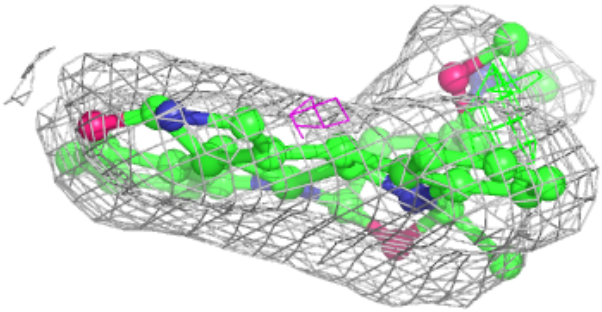


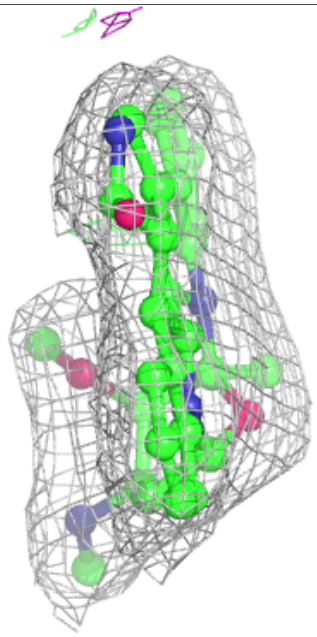


Electron density around 4O7 A 601:

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

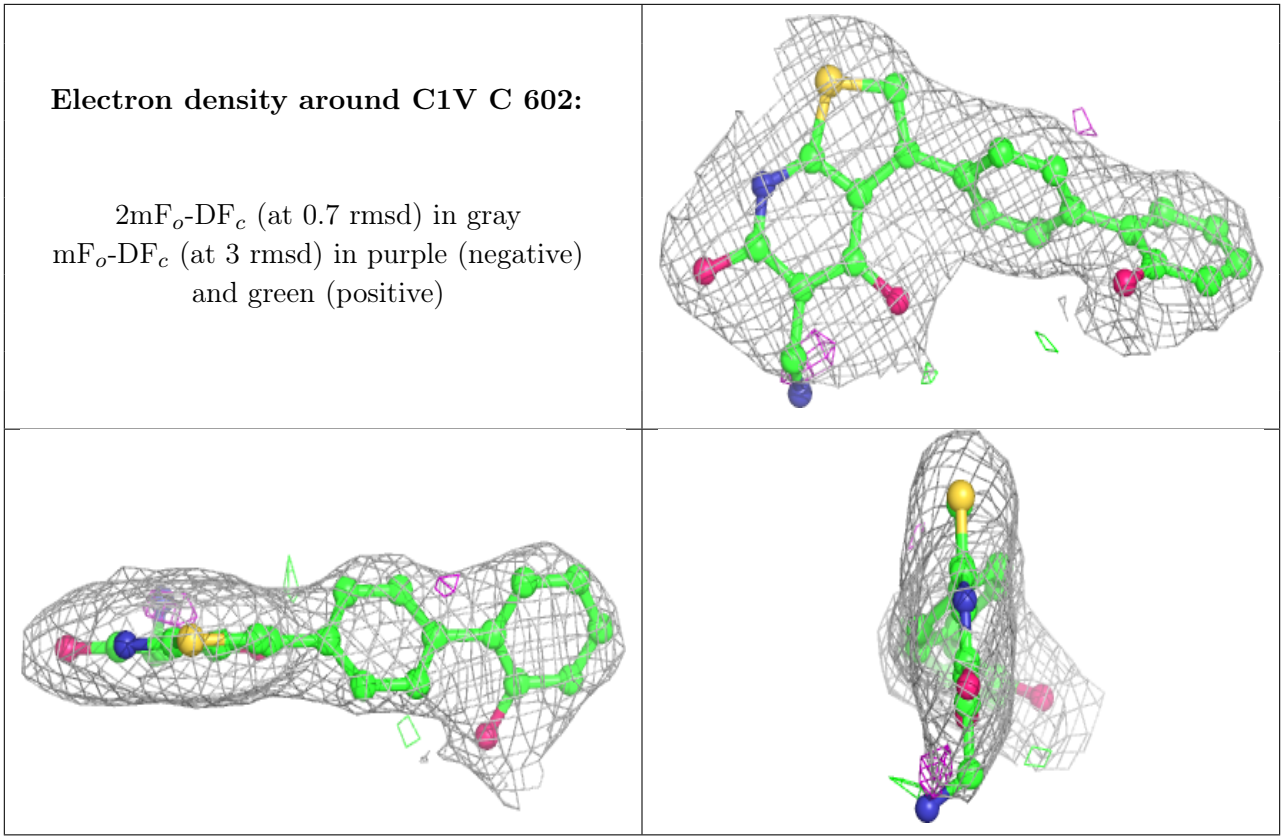






Electron density around C1V C 602:

$2mF_o$-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.