



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:05 PM BST

PDB ID : 5EZV  
Title : X-ray crystal structure of AMP-activated protein kinase alpha-2/alpha-1 RIM chimaera (alpha-2(1-347)/alpha-1(349-401)/alpha-2(397-end) beta-1 gamma-1) co-crystallized with C2 (5-(5-hydroxyl-isoxazol-3-yl)-furan-2-phosphonic acid)  
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Deposited on : 2015-11-26  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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	:	2.13.1
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)	:	2.13.1

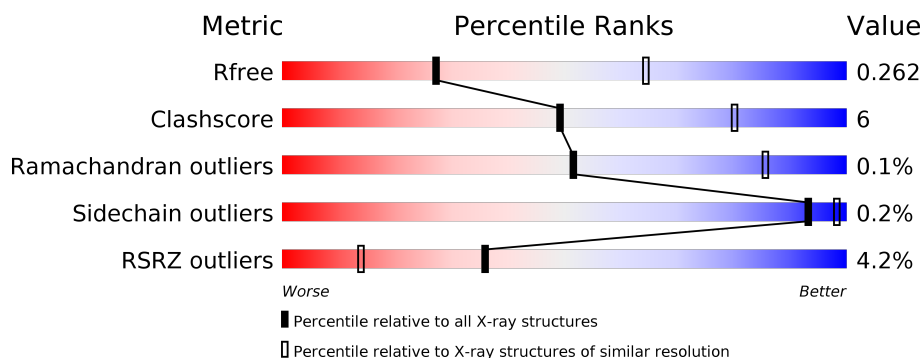
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	<div> <div>3%</div> <div>72% 7% 21%</div> </div>
1	C	560	<div> <div>3%</div> <div>71% 7% 21%</div> </div>
2	B	270	<div> <div>4%</div> <div>56% 12% 31%</div> </div>
2	D	270	<div> <div>2%</div> <div>60% 9% 31%</div> </div>
3	E	336	<div> <div>7%</div> <div>82% 7% 10%</div> </div>
3	F	336	<div> <div>4%</div> <div>76% 13% 11%</div> </div>

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

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

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14682 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/alpha-1 RIM SWAP chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	P	S	0	0	0
			3462	2214	589	634	1	24			
1	C	441	Total	C	N	O	P	S	0	0	0
			3419	2186	588	621	1	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P54646
A	-12	GLY	-	expression tag	UNP P54646
A	-11	SER	-	expression tag	UNP P54646
A	-10	SER	-	expression tag	UNP P54646
A	-9	HIS	-	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
C	-13	MET	-	initiating methionine	UNP P54646
C	-12	GLY	-	expression tag	UNP P54646
C	-11	SER	-	expression tag	UNP P54646
C	-10	SER	-	expression tag	UNP P54646
C	-9	HIS	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P54646
C	-3	HIS	-	expression tag	UNP P54646
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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	P	S	0	0	0
			1400	904	233	257	1	5			
2	D	186	Total	C	N	O	P	S	0	0	0
			1422	914	234	267	1	6			

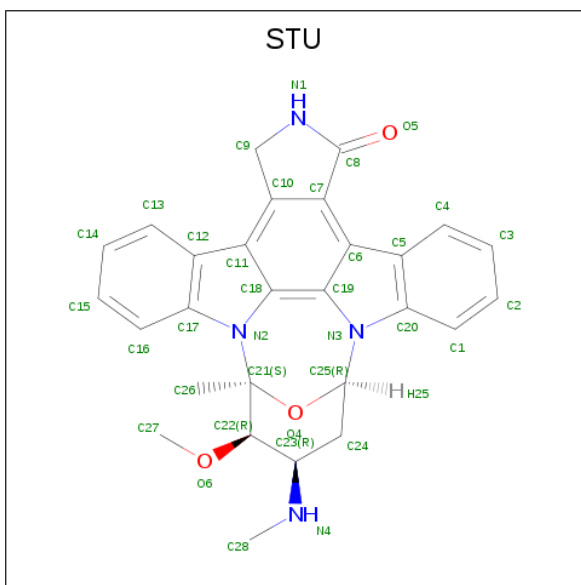
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	302	Total	C	N	O	S		0	0	0
			2362	1538	391	426	7				
3	F	300	Total	C	N	O	S		0	1	0
			2351	1529	393	422	7				

There are 12 discrepancies between the modelled and reference sequences:

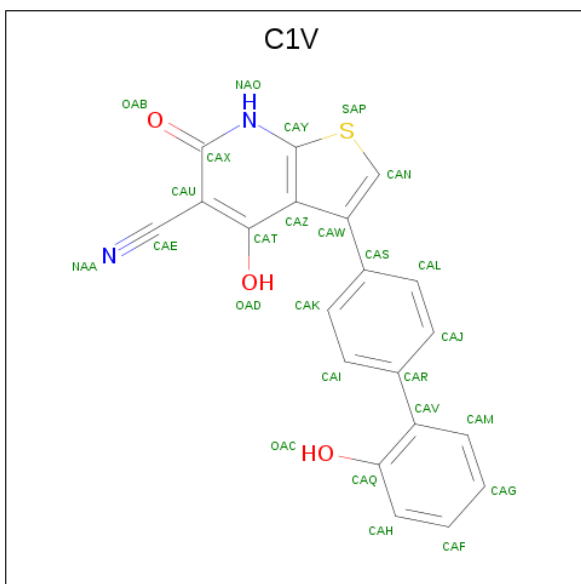
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine	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 STAUROSPORINE (three-letter code: STU) (formula: C<sub>28</sub>H<sub>26</sub>N<sub>4</sub>O<sub>3</sub>).



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

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



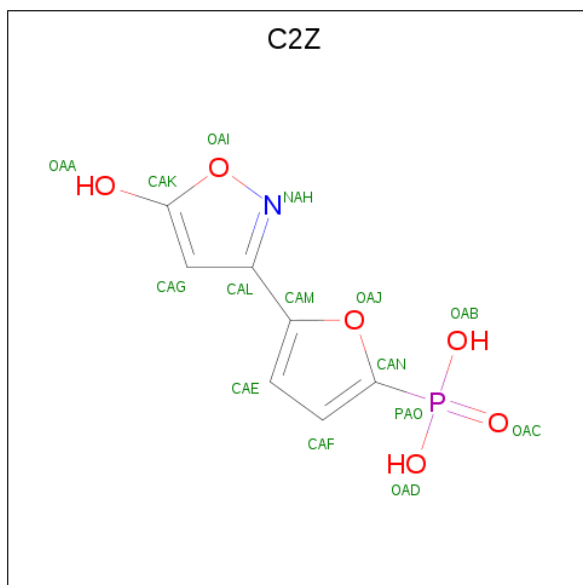
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

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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<sub>7</sub>H<sub>6</sub>NO<sub>6</sub>P).



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		
6	F	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
6	F	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total	O	0	0
			32	32		
7	B	8	Total	O	0	0
			8	8		
7	C	25	Total	O	0	0
			25	25		
7	D	7	Total	O	0	0
			7	7		

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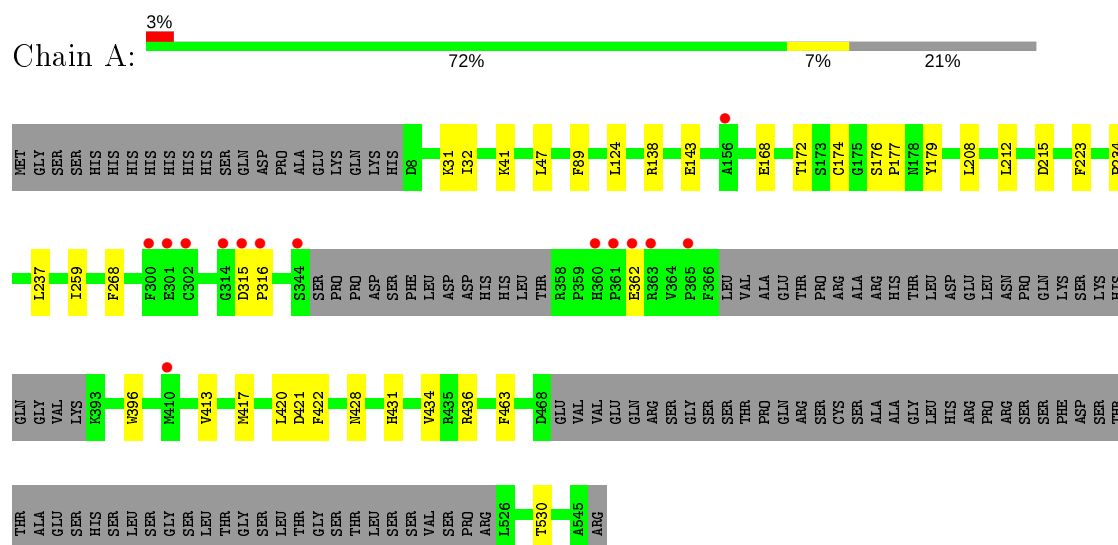
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	7	Total	O	0	0
			7	7		
7	F	5	Total	O	0	0
			5	5		



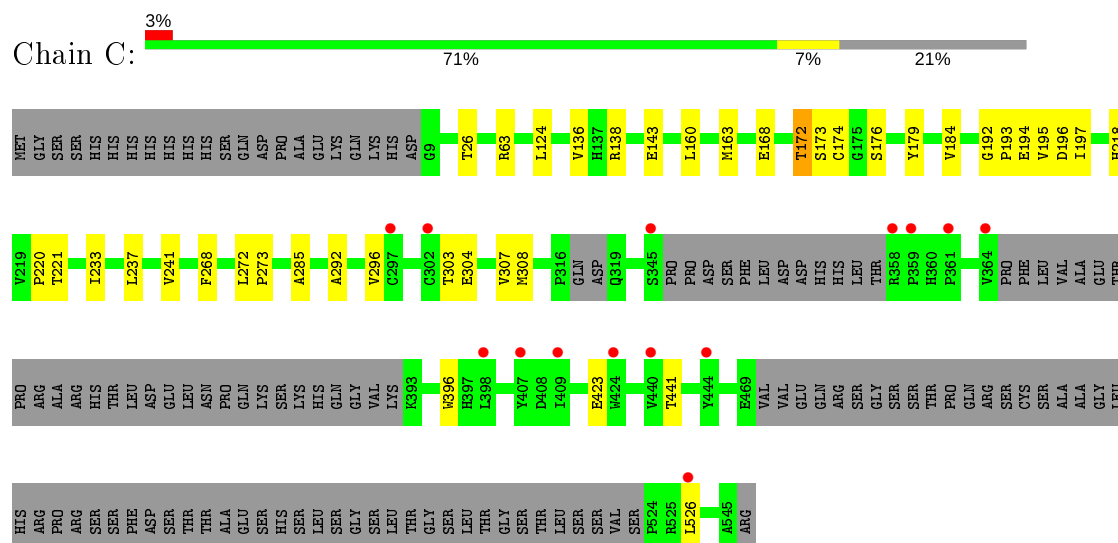
### 3 Residue-property plots [i](#)

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.

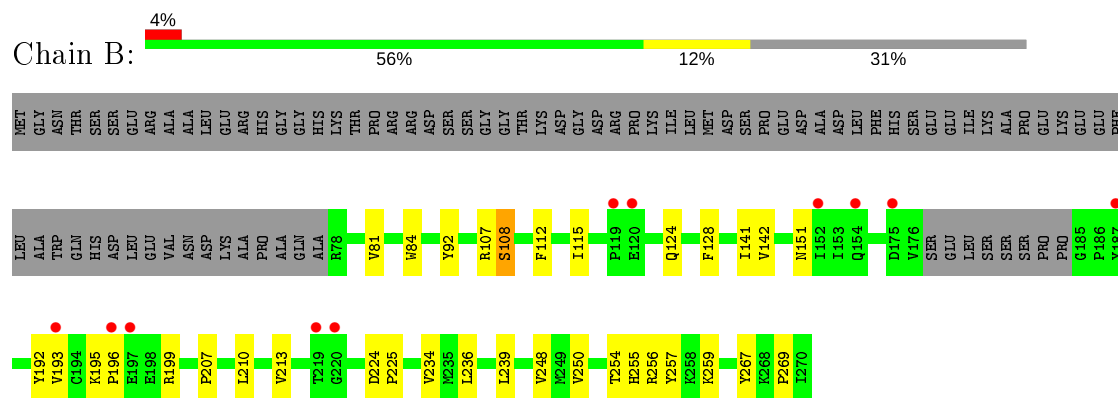
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2/alpha-1 RIM SWAP chimera



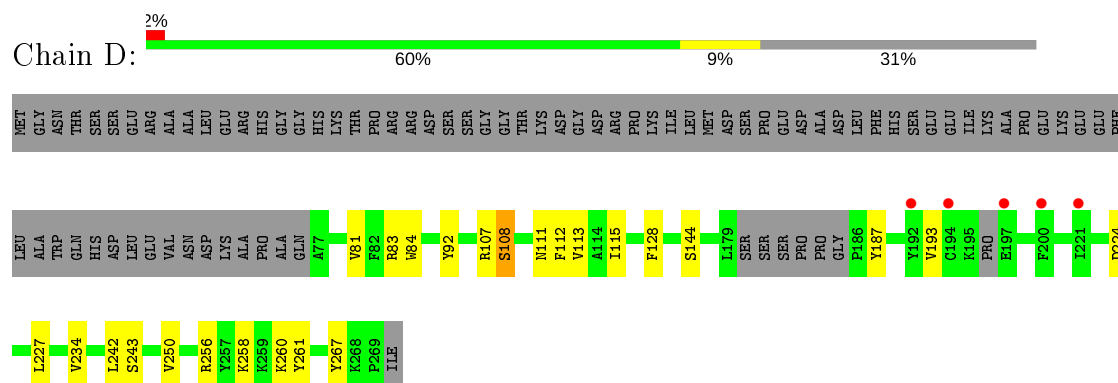
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2/alpha-1 RIM SWAP chimera



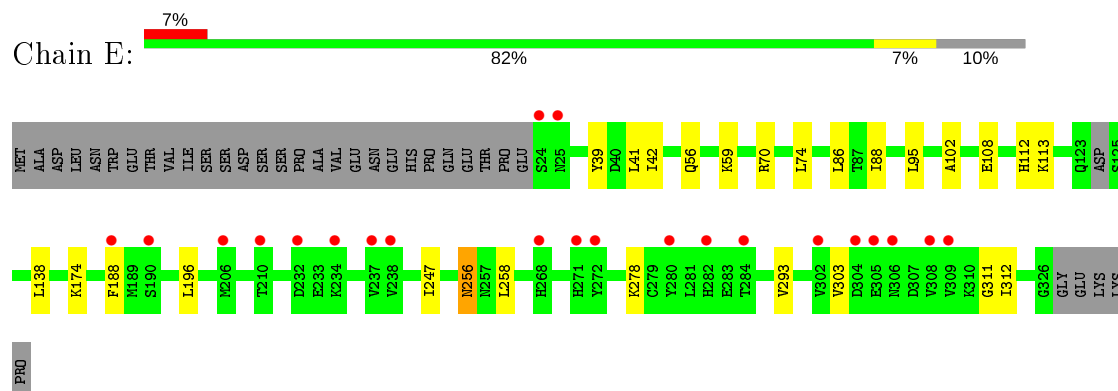
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



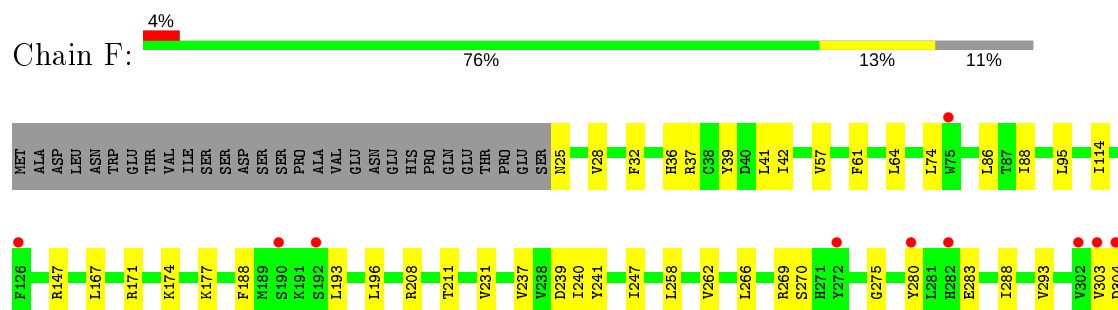
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.61Å 134.11Å 141.29Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	49.30 – 2.99 49.31 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.30-2.99) 99.3 (49.31-2.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT 1.10.0	Depositor
R, $R_{free}$	0.224 , 0.245 0.241 , 0.262	Depositor DCC
$R_{free}$ test set	2867 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, STU, C2Z, C1V, 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	0/3528	0.56	0/4778
1	C	0.38	0/3485	0.57	0/4724
2	B	0.38	0/1431	0.58	0/1964
2	D	0.38	0/1452	0.55	0/1989
3	E	0.38	0/2411	0.58	0/3281
3	F	0.38	0/2402	0.58	0/3269
All	All	0.38	0/14709	0.57	0/20005

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3462	0	3311	33	0
1	C	3419	0	3255	42	1
2	B	1400	0	1308	29	0
2	D	1422	0	1317	22	1
3	E	2362	0	2379	18	0
3	F	2351	0	2368	38	0
4	A	35	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	26	3	0
5	A	26	0	12	0	0
5	C	26	0	12	1	0
6	E	30	0	0	0	0
6	F	30	0	0	0	0
7	A	32	0	0	0	0
7	B	8	0	0	0	0
7	C	25	0	0	0	0
7	D	7	0	0	0	0
7	E	7	0	0	0	0
7	F	5	0	0	0	0
All	All	14682	0	14014	169	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 6.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ALA:O	1:C:296:VAL:HG23	1.55	1.06
1:A:138:ARG:NH2	1:A:172:TPO:O2P	1.89	1.05
3:E:256:ASN:O	3:E:256:ASN:ND2	1.92	1.03
3:F:262:VAL:O	3:F:266:LEU:HD13	1.60	1.00
1:C:296:VAL:CG1	1:C:303:THR:HA	1.94	0.97
2:D:107:ARG:HG2	2:D:108:SEP:O	1.64	0.96
2:B:224:ASP:OD1	2:B:225:PRO:HD2	1.67	0.92
1:C:237:LEU:HD11	1:C:241:VAL:CG1	2.02	0.89
1:A:124:LEU:HD11	1:A:259:ILE:HG12	1.53	0.89
1:A:138:ARG:HH22	1:A:172:TPO:HB	1.38	0.89
2:B:224:ASP:OD1	2:B:225:PRO:CD	2.24	0.84
1:C:296:VAL:HG13	1:C:303:THR:HA	1.60	0.84
3:F:240:ILE:HG22	3:F:275:GLY:HA3	1.57	0.84
1:C:296:VAL:HG11	1:C:303:THR:HA	1.59	0.81
1:C:396:TRP:CH2	2:D:250:VAL:HG12	2.15	0.81
1:A:138:ARG:NH2	1:A:172:TPO:HB	1.96	0.80
2:D:256:ARG:HG2	2:D:256:ARG:HH11	1.44	0.80
2:D:256:ARG:HG2	2:D:256:ARG:NH1	1.99	0.77
3:F:239:ASP:OD1	3:F:240:ILE:N	2.19	0.75
1:C:272:LEU:C	1:C:272:LEU:HD13	2.08	0.74
1:C:237:LEU:HD11	1:C:241:VAL:HG13	1.70	0.72
1:C:138:ARG:NH1	1:C:172:TPO:O2P	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:THR:HG22	1:C:526:LEU:HD22	1.71	0.72
1:C:192:GLY:O	1:C:195:VAL:HG22	1.90	0.71
2:B:256:ARG:HG2	2:B:257:TYR:O	1.91	0.70
1:C:396:TRP:HH2	2:D:250:VAL:HG12	1.57	0.69
1:C:304:GLU:O	1:C:307:VAL:HG12	1.92	0.69
1:A:124:LEU:HD23	1:A:268:PHE:CZ	2.31	0.66
4:C:601:STU:H16	4:C:601:STU:H261	1.78	0.65
3:F:57:VAL:HG22	3:F:61:PHE:CE2	2.32	0.65
3:F:241:TYR:HD1	3:F:266:LEU:HD11	1.62	0.64
1:A:422:PHE:CE2	1:A:436:ARG:HD3	2.33	0.64
1:A:422:PHE:HE2	1:A:436:ARG:HD3	1.62	0.64
4:A:601:STU:H16	4:A:601:STU:H261	1.79	0.64
1:A:138:ARG:CZ	1:A:172:TPO:O2P	2.47	0.63
1:A:396:TRP:CH2	2:B:250:VAL:HG12	2.33	0.63
3:E:41:LEU:HD13	3:E:138:LEU:HD21	1.82	0.62
1:A:168:GLU:O	2:B:234:VAL:HG12	1.98	0.62
1:C:233:ILE:HG23	1:C:237:LEU:HD23	1.81	0.62
3:F:241:TYR:CD1	3:F:266:LEU:HD11	2.35	0.61
2:B:259:LYS:HB2	3:E:39:TYR:OH	2.01	0.61
1:C:237:LEU:HD11	1:C:241:VAL:HG11	1.81	0.60
3:F:41:LEU:HD11	3:F:167:LEU:HD13	1.83	0.60
1:C:272:LEU:HD13	1:C:273:PRO:N	2.16	0.59
1:C:237:LEU:CD1	1:C:241:VAL:CG1	2.80	0.59
2:D:83:ARG:NE	2:D:111:ASN:OD1	2.33	0.58
2:B:195:LYS:CB	2:B:196:PRO:HD2	2.32	0.58
1:C:143:GLU:HB3	4:C:601:STU:H281	1.84	0.58
2:D:107:ARG:HD2	2:D:112:PHE:CZ	2.39	0.57
3:F:239:ASP:CG	3:F:240:ILE:H	2.06	0.57
1:A:143:GLU:HB3	4:A:601:STU:H281	1.86	0.57
1:A:413:VAL:O	1:A:417:MET:HG3	2.05	0.57
3:F:266:LEU:HD12	3:F:266:LEU:N	2.19	0.57
1:C:168:GLU:O	2:D:234:VAL:HG12	2.03	0.57
1:C:138:ARG:NH2	1:C:172:TPO:O2P	2.38	0.56
1:C:272:LEU:C	1:C:272:LEU:CD1	2.74	0.56
2:B:195:LYS:CB	2:B:199:ARG:CB	2.85	0.54
1:C:173:SER:HA	1:C:184:VAL:CG2	2.37	0.54
3:E:256:ASN:C	3:E:256:ASN:HD22	1.91	0.54
3:F:240:ILE:HG22	3:F:275:GLY:CA	2.36	0.54
1:A:428:ASN:HB3	1:A:431:HIS:HB3	1.89	0.54
1:C:176:SER:HB3	1:C:179:TYR:HD2	1.73	0.53
2:B:224:ASP:OD1	2:B:225:PRO:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PRO:O	1:C:197:ILE:HG12	2.10	0.51
3:E:88:ILE:HG23	3:E:247:ILE:HG23	1.93	0.51
3:F:266:LEU:O	3:F:270:SER:N	2.43	0.51
2:B:250:VAL:HG22	2:B:267:TYR:CD2	2.45	0.51
1:A:420:LEU:O	1:A:421:ASP:HB3	2.10	0.51
1:C:173:SER:HA	1:C:184:VAL:HG22	1.91	0.51
1:C:396:TRP:CH2	2:D:250:VAL:CG1	2.89	0.51
1:C:218:HIS:CE1	1:C:220:PRO:HD2	2.46	0.51
1:A:396:TRP:HH2	2:B:250:VAL:HG12	1.74	0.51
3:F:39:TYR:HA	3:F:42:ILE:HD12	1.93	0.51
1:A:234:PRO:HD2	1:A:237:LEU:HD12	1.93	0.50
3:F:266:LEU:N	3:F:266:LEU:CD1	2.74	0.50
1:A:362:GLU:HG2	3:E:70:ARG:HH21	1.76	0.50
1:A:396:TRP:HB2	2:B:213:VAL:HG11	1.94	0.50
1:A:47:LEU:HB2	1:A:89:PHE:HB2	1.93	0.50
2:B:124:GLN:HE21	2:B:142:VAL:HG11	1.77	0.49
2:B:107:ARG:HB2	2:B:112:PHE:CE2	2.47	0.49
3:F:41:LEU:HD11	3:F:167:LEU:CD1	2.41	0.49
3:E:174:LYS:HG2	3:E:293:VAL:HG13	1.94	0.49
1:A:138:ARG:NH1	1:A:172:TPO:O2P	2.45	0.49
2:D:258:LYS:NZ	3:F:37:ARG:HH12	2.11	0.48
2:B:84:TRP:HB3	2:B:112:PHE:HB2	1.94	0.48
2:D:242:LEU:HD23	2:D:243:SER:O	2.13	0.48
1:C:296:VAL:HG11	1:C:303:THR:CA	2.37	0.48
3:F:61:PHE:HA	3:F:64:LEU:HD12	1.96	0.48
2:D:260:LYS:NZ	3:F:39:TYR:O	2.47	0.48
2:B:92:TYR:HB2	2:B:128:PHE:HB3	1.93	0.48
3:E:108:GLU:O	3:E:112:HIS:HB2	2.14	0.48
3:F:262:VAL:O	3:F:266:LEU:CD1	2.48	0.48
2:B:195:LYS:CB	2:B:196:PRO:CD	2.92	0.48
1:C:307:VAL:HG13	1:C:308:MET:N	2.28	0.47
1:A:530:THR:HG23	2:B:255:HIS:CE1	2.49	0.47
3:E:56:GLN:HB2	3:E:59:LYS:HE3	1.96	0.47
2:B:248:VAL:HA	2:B:269:PRO:HA	1.97	0.47
3:E:74:LEU:HD21	3:E:86:LEU:HB2	1.97	0.47
3:F:25:ASN:O	3:F:28:VAL:HG23	2.15	0.47
3:E:56:GLN:HA	3:E:113:LYS:HA	1.96	0.47
2:B:124:GLN:NE2	2:B:142:VAL:HG11	2.30	0.47
2:D:250:VAL:HG22	2:D:267:TYR:CD2	2.50	0.46
1:A:212:LEU:HB2	1:A:215:ASP:HB2	1.97	0.46
1:A:463:PHE:HB2	2:B:239:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:TYR:HB2	2:D:128:PHE:HB3	1.98	0.46
3:F:303:VAL:HG13	3:F:307:ASP:O	2.16	0.46
1:C:441:THR:HG22	1:C:526:LEU:CD2	2.42	0.46
1:A:177:PRO:HB3	1:A:223:PHE:HE1	1.81	0.46
1:C:272:LEU:HD13	1:C:273:PRO:O	2.15	0.46
1:A:422:PHE:HB3	1:A:434:VAL:CG2	2.46	0.46
2:B:207:PRO:HD2	2:B:210:LEU:HD12	1.98	0.46
3:F:74:LEU:HD22	3:F:114:ILE:HG21	1.97	0.46
1:C:423:GLU:HB3	2:D:187:TYR:HB3	1.98	0.45
1:C:26:THR:HG21	1:C:160:LEU:HG	1.99	0.45
3:F:41:LEU:HD13	3:F:171:ARG:CG	2.47	0.45
1:C:63:ARG:HE	1:C:163:MET:HG3	1.82	0.45
1:C:138:ARG:CZ	1:C:172:TPO:O2P	2.65	0.45
2:B:81:VAL:HG22	2:B:115:ILE:HG12	1.97	0.45
2:B:192:TYR:CE1	2:B:193:VAL:O	2.70	0.45
1:A:172:TPO:HG23	1:A:174:CYS:SG	2.57	0.45
1:A:208:LEU:HB3	1:A:237:LEU:HD21	1.99	0.45
3:F:174:LYS:HG3	3:F:293:VAL:HG13	1.99	0.45
1:C:307:VAL:CG1	1:C:308:MET:N	2.80	0.44
3:E:256:ASN:C	3:E:256:ASN:ND2	2.61	0.44
3:F:88:ILE:HG23	3:F:247:ILE:HG23	2.00	0.44
3:F:25:ASN:HA	3:F:28:VAL:HG23	1.99	0.44
1:C:124:LEU:HD23	1:C:268:PHE:CZ	2.53	0.44
2:D:256:ARG:HH11	2:D:256:ARG:CG	2.15	0.44
1:C:218:HIS:NE2	1:C:220:PRO:HD2	2.33	0.43
2:B:192:TYR:CD1	2:B:193:VAL:O	2.70	0.43
3:E:311:GLY:O	3:E:312:ILE:HD13	2.17	0.43
1:C:160:LEU:HD13	1:C:174:CYS:HB3	1.99	0.43
3:F:74:LEU:HD21	3:F:86:LEU:HB2	2.01	0.43
5:C:602:C1V:HAM	2:D:113:VAL:HG12	2.00	0.43
2:D:256:ARG:HD3	2:D:261:TYR:HE1	1.84	0.43
3:F:188:PHE:HB2	3:F:196:LEU:HD21	2.00	0.43
3:E:188:PHE:HB2	3:E:196:LEU:HD21	2.02	0.42
3:F:208:ARG:HB2	3:F:211:THR:HG23	2.00	0.42
3:F:231:VAL:HG22	3:F:237:VAL:HG22	2.02	0.42
3:F:303:VAL:HG12	3:F:304:ASP:O	2.19	0.42
2:B:250:VAL:HG21	2:B:267:TYR:CE2	2.54	0.42
3:E:39:TYR:HA	3:E:42:ILE:HD12	2.02	0.42
3:F:177:LYS:HG2	3:F:293:VAL:HG11	2.01	0.42
3:F:303:VAL:CG1	3:F:304:ASP:N	2.83	0.42
2:D:81:VAL:HG22	2:D:115:ILE:HG12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:102:ALA:HA	3:E:256:ASN:ND2	2.35	0.41
2:D:224:ASP:HB3	2:D:227:LEU:HD12	2.01	0.41
3:E:278:LYS:HD2	3:E:303:VAL:HG21	2.01	0.41
3:F:280:TYR:HB2	3:F:283:GLU:HG3	2.02	0.41
1:A:421:ASP:CG	1:A:421:ASP:O	2.59	0.41
1:A:31:LYS:NZ	2:B:108:SEP:O2P	2.30	0.41
3:F:95:LEU:HD22	3:F:258:LEU:HD11	2.03	0.41
1:A:315:ASP:HA	1:A:316:PRO:HD3	1.98	0.41
3:F:193:LEU:HD13	3:F:288:ILE:HD13	2.02	0.41
1:A:32:ILE:HD11	1:A:41:LYS:HD3	2.02	0.41
1:C:136:VAL:HG23	1:C:196:ASP:OD2	2.21	0.41
2:B:141:ILE:HG22	2:B:151:ASN:ND2	2.35	0.41
2:B:236:LEU:HD23	2:B:254:THR:HG22	2.03	0.41
4:C:601:STU:H261	4:C:601:STU:C16	2.48	0.41
3:F:41:LEU:HD13	3:F:171:ARG:HG2	2.03	0.41
1:A:176:SER:HB2	1:A:179:TYR:HD2	1.85	0.41
2:D:107:ARG:CG	2:D:108:SEP:O	2.51	0.40
2:D:84:TRP:HB3	2:D:112:PHE:HB2	2.03	0.40
1:A:417:MET:HB3	1:A:422:PHE:HB2	2.03	0.40
1:C:194:GLU:HG2	1:C:195:VAL:N	2.36	0.40
1:C:218:HIS:ND1	1:C:221:THR:HG23	2.36	0.40
3:F:303:VAL:HG12	3:F:304:ASP:N	2.36	0.40
3:E:95:LEU:HD22	3:E:258:LEU:HD11	2.03	0.40
3:F:32:PHE:CE1	3:F:36:HIS:CD2	3.10	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]	2.16	0.04

## 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	433/560 (77%)	422 (98%)	11 (2%)	0	100	100
1	C	430/560 (77%)	413 (96%)	17 (4%)	0	100	100
2	B	180/270 (67%)	177 (98%)	3 (2%)	0	100	100
2	D	179/270 (66%)	174 (97%)	4 (2%)	1 (1%)	25	64
3	E	298/336 (89%)	293 (98%)	5 (2%)	0	100	100
3	F	299/336 (89%)	293 (98%)	6 (2%)	0	100	100
All	All	1819/2332 (78%)	1772 (97%)	46 (2%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	193	VAL

### 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	358/497 (72%)	358 (100%)	0	100	100
1	C	349/497 (70%)	349 (100%)	0	100	100
2	B	145/239 (61%)	145 (100%)	0	100	100
2	D	149/239 (62%)	149 (100%)	0	100	100
3	E	259/308 (84%)	258 (100%)	1 (0%)	91	97
3	F	255/308 (83%)	253 (99%)	2 (1%)	81	93
All	All	1515/2088 (73%)	1512 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	256	ASN
3	F	147	ARG

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Mol	Chain	Res	Type
3	F	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	124	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	TPO	A	172	1	8,10,11	0.85	0	10,14,16	1.21	0
2	SEP	D	108	2	8,9,10	0.92	0	8,12,14	1.17	1 (12%)
2	SEP	B	108	2	8,9,10	0.92	0	8,12,14	1.41	1 (12%)
1	TPO	C	172	1	8,10,11	0.80	0	10,14,16	1.28	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' 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	-
2	SEP	D	108	2	-	2/5/8/10	-
2	SEP	B	108	2	-	3/5/8/10	-
1	TPO	C	172	1	-	2/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	108	SEP	OG-CB-CA	2.89	110.96	108.14
2	D	108	SEP	O3P-P-O2P	2.08	115.57	107.64
1	C	172	TPO	O-C-CA	-2.06	119.39	124.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	6	0
2	D	108	SEP	2	0
2	B	108	SEP	1	0
1	C	172	TPO	3	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
4	STU	C	601	-	30,42,42	2.72	9 (30%)	31,68,68	3.86	13 (41%)
5	C1V	A	602	-	27,29,29	3.25	8 (29%)	30,42,42	6.68	7 (23%)
4	STU	A	601	-	30,42,42	2.73	10 (33%)	31,68,68	3.79	12 (38%)
5	C1V	C	602	-	27,29,29	3.28	8 (29%)	30,42,42	6.73	7 (23%)
6	C2Z	F	401	-	8,16,16	3.70	5 (62%)	8,24,24	2.07	2 (25%)
6	C2Z	F	402	-	8,16,16	3.66	5 (62%)	8,24,24	1.71	2 (25%)
6	C2Z	E	401	-	8,16,16	3.68	5 (62%)	8,24,24	2.10	2 (25%)
6	C2Z	E	402	-	8,16,16	3.08	4 (50%)	8,24,24	2.21	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
4	STU	C	601	-	-	2/4/42/42	-
5	C1V	A	602	-	-	0/9/10/10	0/4/4/4
4	STU	A	601	-	-	2/4/42/42	-
5	C1V	C	602	-	-	0/9/10/10	0/4/4/4
6	C2Z	F	401	-	-	0/0/10/10	0/2/2/2
6	C2Z	F	402	-	-	0/0/10/10	0/2/2/2
6	C2Z	E	401	-	-	0/0/10/10	0/2/2/2
6	C2Z	E	402	-	-	0/0/10/10	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	C1V	CAN-CAW	7.97	1.41	1.37
5	A	602	C1V	CAU-CAE	7.95	1.53	1.44
5	C	602	C1V	CAU-CAE	7.88	1.53	1.44
5	A	602	C1V	CAN-CAW	7.73	1.41	1.37
5	C	602	C1V	CAE-NAA	7.53	1.32	1.14
5	A	602	C1V	CAE-NAA	7.50	1.32	1.14
4	C	601	STU	C9-C10	-7.14	1.45	1.50
5	C	602	C1V	OAB-CAX	6.99	1.42	1.24
5	A	602	C1V	OAB-CAX	6.98	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C9-C10	-6.94	1.45	1.50
6	E	401	C2Z	CAM-CAL	-6.81	1.33	1.49
6	F	401	C2Z	CAM-CAL	-6.77	1.34	1.49
6	F	402	C2Z	CAM-CAL	-6.70	1.34	1.49
6	E	402	C2Z	CAM-CAL	-6.68	1.34	1.49
6	F	401	C2Z	PAO-OAC	5.92	1.61	1.49
6	F	402	C2Z	PAO-OAC	5.67	1.60	1.49
6	E	401	C2Z	PAO-OAC	5.58	1.60	1.49
4	A	601	STU	C11-C18	5.42	1.49	1.42
4	C	601	STU	C11-C18	5.35	1.49	1.42
4	A	601	STU	C12-C17	4.68	1.49	1.41
4	A	601	STU	C6-C19	4.67	1.48	1.42
4	A	601	STU	C5-C20	4.65	1.49	1.41
4	C	601	STU	C6-C19	4.62	1.48	1.42
4	C	601	STU	C5-C20	4.60	1.49	1.41
4	C	601	STU	C12-C17	4.59	1.48	1.41
4	A	601	STU	C10-C11	4.54	1.50	1.42
4	C	601	STU	C10-C11	4.45	1.50	1.42
5	C	602	C1V	CAW-CAZ	4.43	1.49	1.41
5	A	602	C1V	CAW-CAZ	4.43	1.49	1.41
4	A	601	STU	C7-C6	3.90	1.49	1.43
4	C	601	STU	C7-C6	3.82	1.49	1.43
5	C	602	C1V	CAW-CAS	3.72	1.56	1.49
5	A	602	C1V	CAW-CAS	3.70	1.56	1.49
4	A	601	STU	C19-C18	3.61	1.50	1.42
6	E	401	C2Z	CAG-CAL	-3.56	1.33	1.40
6	F	401	C2Z	CAG-CAL	-3.56	1.33	1.40
4	C	601	STU	C19-C18	3.56	1.50	1.42
6	E	402	C2Z	CAG-CAL	-3.50	1.33	1.40
6	F	402	C2Z	CAG-CAL	-3.43	1.33	1.40
6	F	402	C2Z	PAO-OAB	3.00	1.61	1.54
6	E	401	C2Z	PAO-OAB	2.98	1.61	1.54
6	E	402	C2Z	PAO-OAD	2.97	1.61	1.54
6	E	402	C2Z	PAO-OAB	2.63	1.60	1.54
4	C	601	STU	O5-C8	2.57	1.28	1.23
4	A	601	STU	O5-C8	2.57	1.28	1.23
6	F	402	C2Z	PAO-OAD	-2.57	1.48	1.54
6	F	401	C2Z	PAO-OAD	-2.56	1.48	1.54
5	C	602	C1V	OAC-CAQ	2.52	1.41	1.36
6	E	401	C2Z	PAO-OAD	-2.52	1.48	1.54
5	A	602	C1V	OAC-CAQ	2.51	1.41	1.36
6	F	401	C2Z	PAO-OAB	2.47	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	C1V	CAV-CAR	2.32	1.53	1.49
5	A	602	C1V	CAV-CAR	2.12	1.53	1.49
4	A	601	STU	C9-N1	2.06	1.47	1.45

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	C1V	CAU-CAE-NAA	-29.70	120.06	177.31
5	A	602	C1V	CAU-CAE-NAA	-29.03	121.36	177.31
5	A	602	C1V	CAW-CAN-SAP	-19.14	107.19	112.53
5	C	602	C1V	CAW-CAN-SAP	-18.66	107.32	112.53
4	C	601	STU	O5-C8-C7	-12.41	114.58	129.32
4	A	601	STU	O5-C8-C7	-12.06	115.00	129.32
4	C	601	STU	O5-C8-N1	-11.70	111.60	125.27
4	A	601	STU	O5-C8-N1	-11.28	112.10	125.27
5	A	602	C1V	CAN-SAP-CAY	6.80	99.32	91.12
5	C	602	C1V	CAN-SAP-CAY	6.80	99.32	91.12
4	C	601	STU	C6-C7-C8	-6.69	119.76	129.76
4	A	601	STU	C6-C7-C8	-6.57	119.94	129.76
4	A	601	STU	C9-N1-C8	-6.10	107.98	113.85
4	C	601	STU	C9-N1-C8	-5.83	108.24	113.85
4	A	601	STU	C16-C17-N2	5.01	138.35	132.29
6	E	402	C2Z	OAC-PAO-CAN	5.00	119.45	110.84
4	C	601	STU	C16-C17-N2	4.94	138.26	132.29
5	C	602	C1V	CAW-CAZ-CAY	4.90	111.44	107.54
5	A	602	C1V	CAW-CAZ-CAY	4.83	111.39	107.54
5	C	602	C1V	CAN-CAW-CAS	-4.49	118.71	125.52
5	A	602	C1V	CAN-CAW-CAS	-4.24	119.08	125.52
5	A	602	C1V	CAU-CAX-NAO	-4.06	120.49	124.09
5	C	602	C1V	CAU-CAX-NAO	-3.94	120.59	124.09
6	F	401	C2Z	OAB-PAO-OAC	-3.89	101.38	112.45
5	A	602	C1V	CAX-NAO-CAY	3.83	122.60	116.88
6	F	402	C2Z	OAB-PAO-OAC	-3.79	101.66	112.45
6	E	401	C2Z	CAG-CAL-CAM	-3.72	123.89	129.32
5	C	602	C1V	CAX-NAO-CAY	3.65	122.33	116.88
6	E	401	C2Z	OAB-PAO-OAC	-3.55	102.35	112.45
6	F	401	C2Z	CAG-CAL-CAM	-3.51	124.20	129.32
4	A	601	STU	C7-C10-C11	-2.77	118.68	122.42
4	C	601	STU	C16-C17-C12	-2.76	116.75	120.73
4	A	601	STU	C16-C17-C12	-2.75	116.76	120.73
4	C	601	STU	C1-C20-C5	-2.56	117.04	120.73
4	C	601	STU	C13-C12-C11	-2.55	127.35	134.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C13-C12-C11	-2.55	127.36	134.64
4	C	601	STU	C7-C10-C11	-2.54	119.00	122.42
4	C	601	STU	C1-C20-N3	2.51	135.24	132.25
4	A	601	STU	C1-C20-C5	-2.43	117.22	120.73
4	A	601	STU	C1-C20-N3	2.39	135.11	132.25
4	A	601	STU	C26-C21-C22	-2.35	108.06	112.64
4	C	601	STU	C4-C5-C20	2.27	122.27	119.39
6	E	402	C2Z	CAG-CAL-CAM	-2.25	126.03	129.32
4	C	601	STU	C26-C21-C22	-2.23	108.29	112.64
6	F	402	C2Z	CAG-CAL-CAM	-2.10	126.25	129.32
4	A	601	STU	C4-C5-C6	-2.10	128.63	134.64
4	C	601	STU	C3-C4-C5	-2.05	117.42	120.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	STU	C22-C23-N4-C28
4	C	601	STU	C24-C23-N4-C28
4	A	601	STU	C24-C23-N4-C28
4	A	601	STU	C22-C23-N4-C28

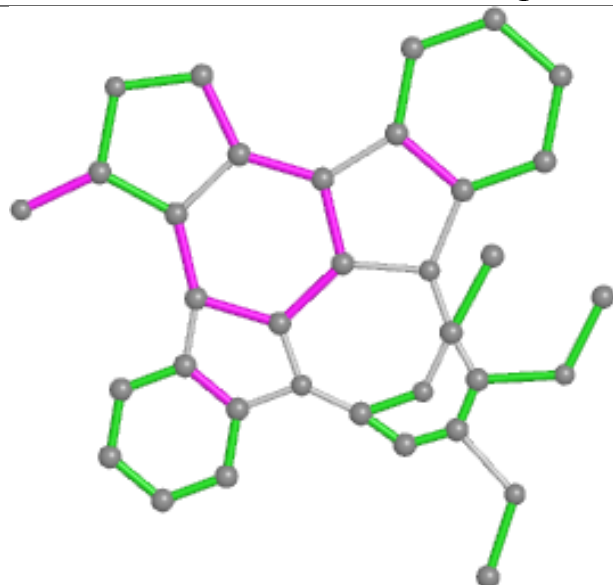
There are no ring outliers.

3 monomers are involved in 6 short contacts:

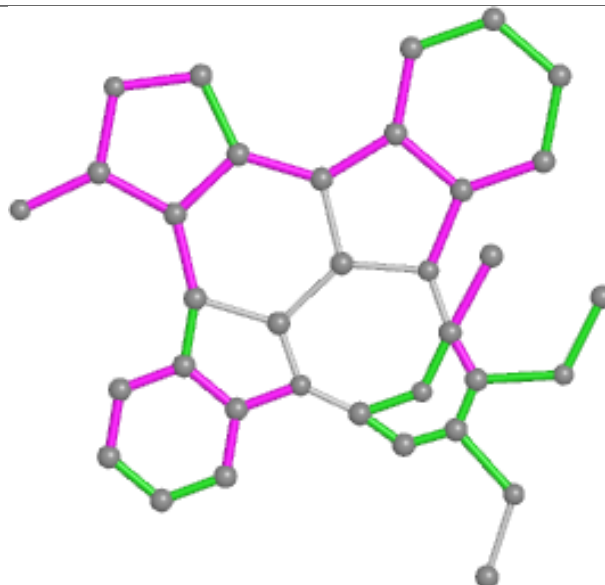
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	STU	3	0
4	A	601	STU	2	0
5	C	602	C1V	1	0

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.

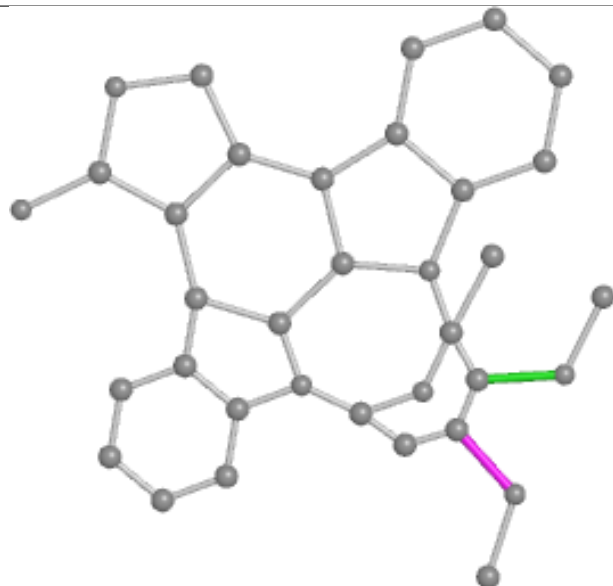
## Ligand STU C 601



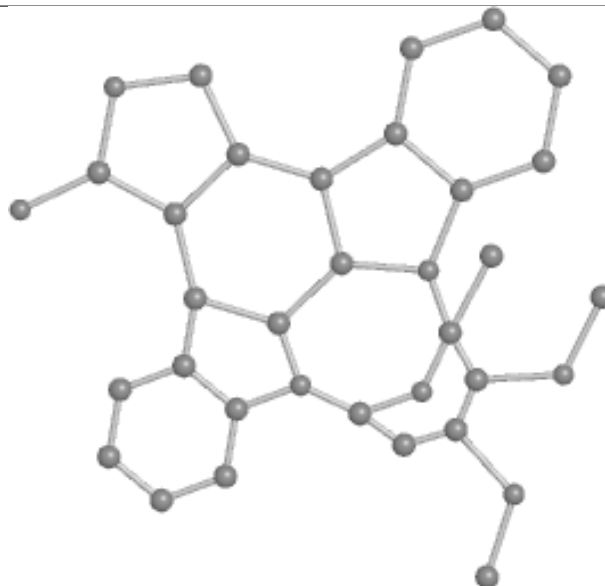
Bond lengths



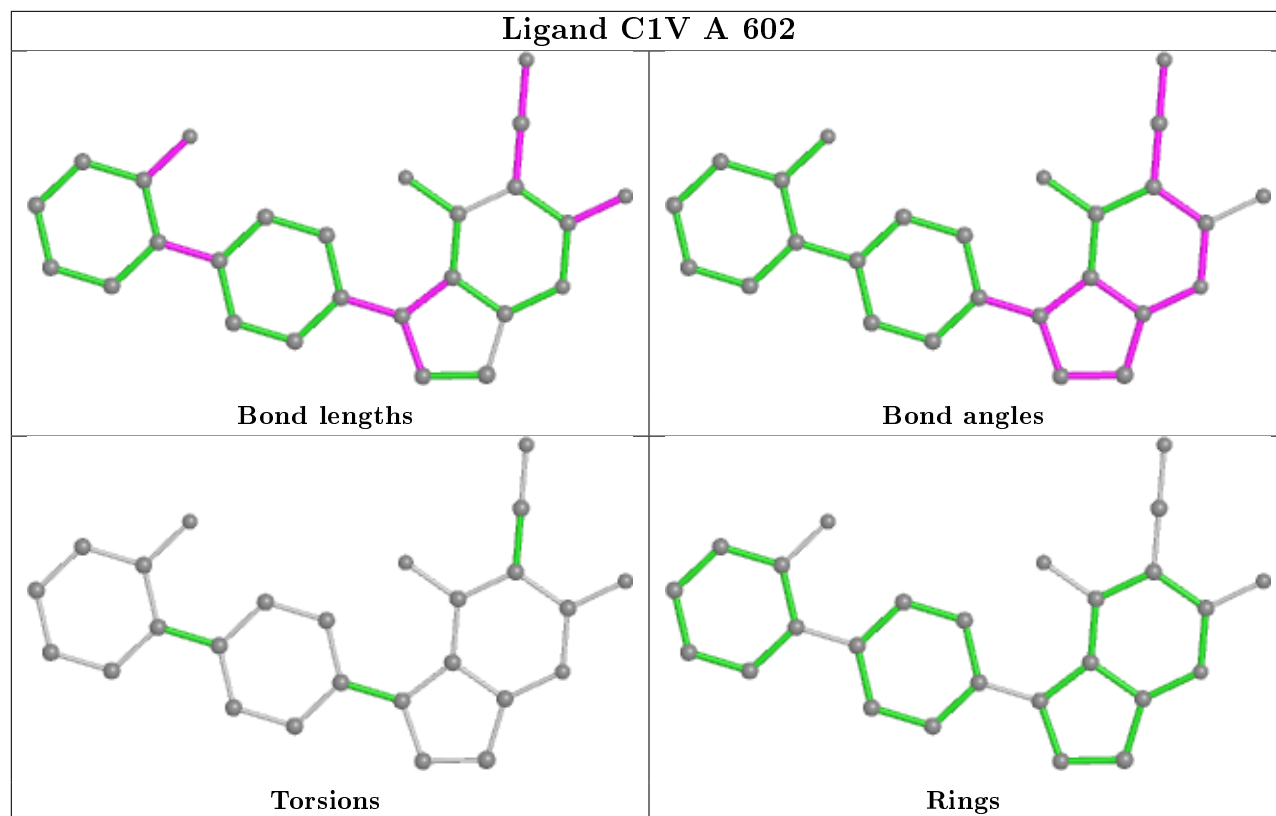
Bond angles



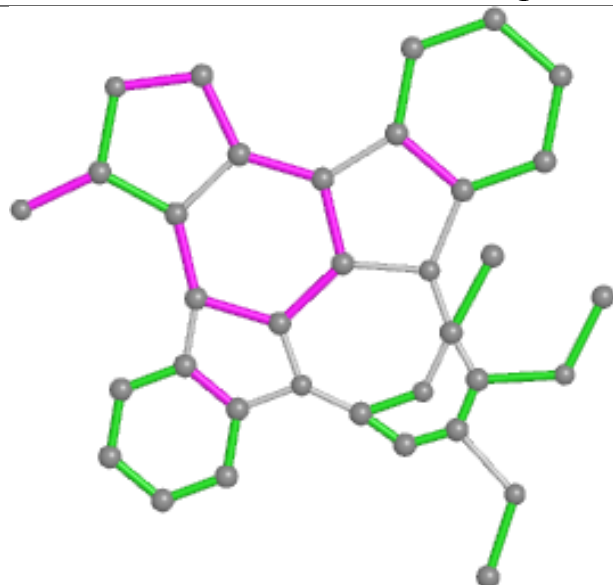
Torsions



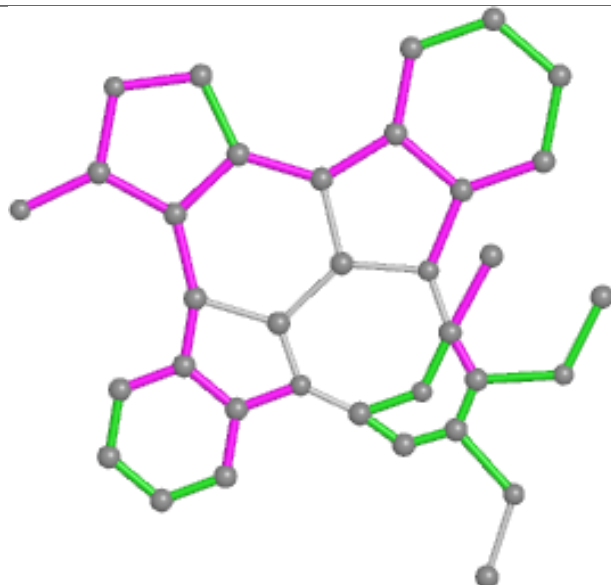
Rings



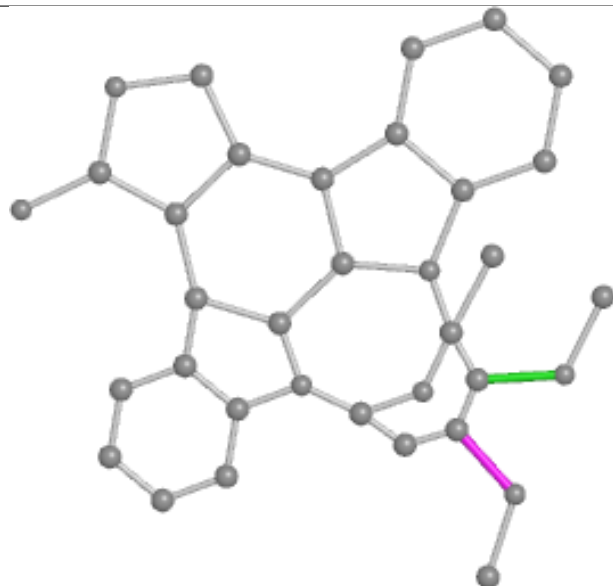
## Ligand STU A 601



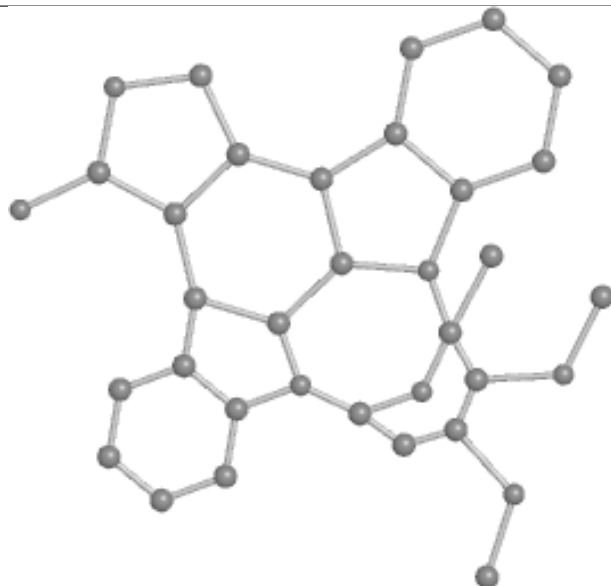
Bond lengths



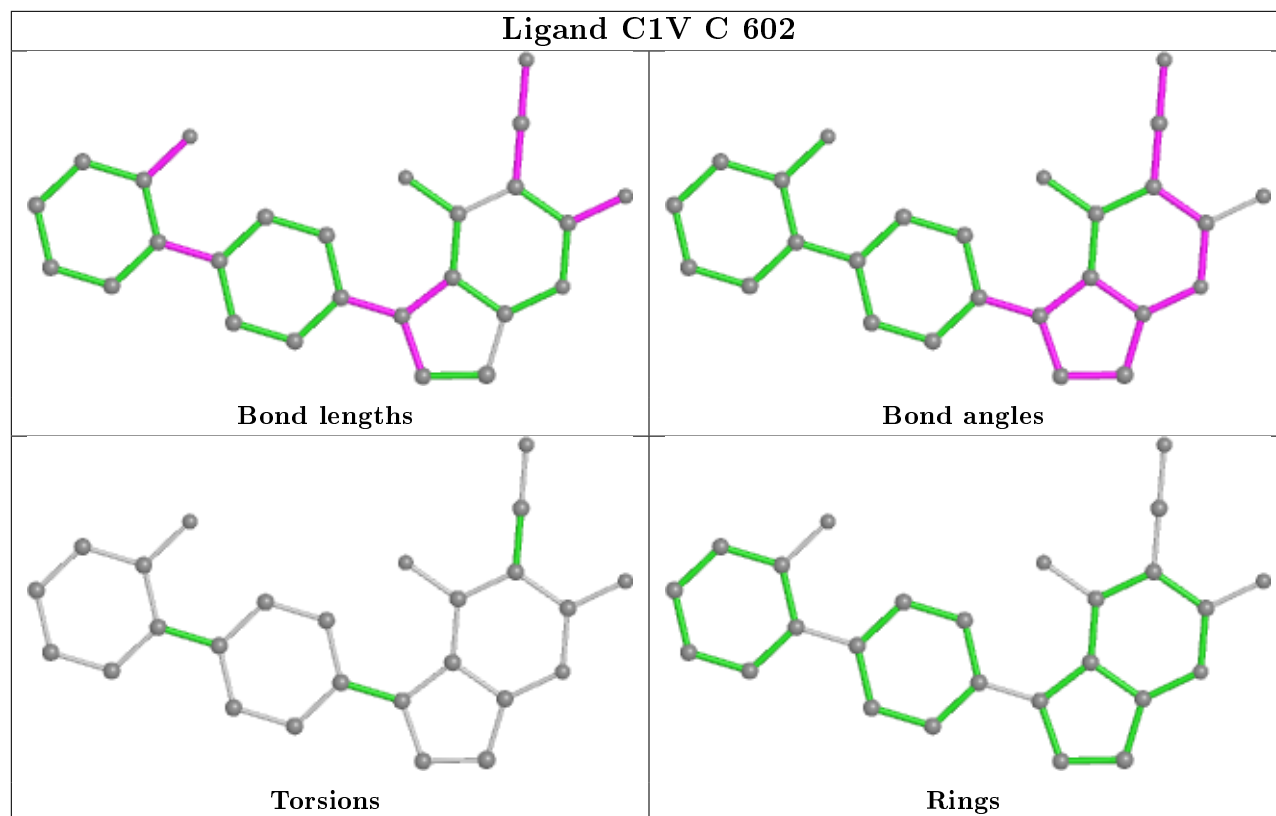
Bond angles



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	441/560 (78%)	0.23	14 (3%)	47 20	40, 63, 98, 142	0
1	C	440/560 (78%)	0.25	14 (3%)	47 20	38, 67, 105, 126	0
2	B	184/270 (68%)	0.41	11 (5%)	21 7	42, 71, 109, 131	0
2	D	185/270 (68%)	0.37	5 (2%)	54 26	51, 71, 115, 146	0
3	E	302/336 (89%)	0.44	22 (7%)	15 4	40, 65, 93, 113	0
3	F	300/336 (89%)	0.30	12 (4%)	38 15	43, 68, 93, 109	0
All	All	1852/2332 (79%)	0.31	78 (4%)	36 14	38, 67, 103, 146	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	GLY	6.7
1	A	361	PRO	4.5
3	F	304	ASP	4.3
2	B	120	GLU	4.2
1	A	300	PHE	4.2
3	F	303	VAL	4.0
3	F	280	TYR	4.0
3	E	280	TYR	3.8
1	A	302	CYS	3.8
1	A	362	GLU	3.7
2	D	194	CYS	3.7
3	E	306	ASN	3.6
1	C	302	CYS	3.5
3	E	268	HIS	3.4
2	B	154	GLN	3.3
3	E	25	ASN	3.2
3	F	126	PHE	3.2
3	E	282	HIS	3.2
1	A	360	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	197	GLU	3.1
3	E	271	HIS	3.1
1	A	363	ARG	3.1
2	D	197	GLU	3.1
3	E	24	SER	3.1
1	C	361	PRO	3.1
3	F	305	GLU	3.0
2	B	219	THR	3.0
1	A	410	MET	3.0
1	C	364	VAL	3.0
1	C	526	LEU	3.0
3	E	238	VAL	2.8
1	A	315	ASP	2.8
1	A	365	PRO	2.7
3	F	192	SER	2.7
1	C	359	PRO	2.7
3	E	304	ASP	2.7
3	E	190	SER	2.7
3	F	272	TYR	2.7
3	E	237	VAL	2.7
3	E	302	VAL	2.7
2	D	200	PHE	2.6
3	E	305	GLU	2.6
1	C	407	TYR	2.6
2	B	196	PRO	2.6
2	D	192	TYR	2.6
1	C	345	SER	2.6
1	A	301	GLU	2.4
3	E	234	LYS	2.4
3	E	309	VAL	2.4
3	F	190	SER	2.4
1	C	424	TRP	2.4
3	E	210	THR	2.4
2	B	119	PRO	2.4
1	A	156	ALA	2.3
3	F	302	VAL	2.3
1	C	409	ILE	2.3
3	E	308	VAL	2.3
2	B	187	TYR	2.3
2	D	221	ILE	2.3
3	E	206	MET	2.3
3	F	306	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	175	ASP	2.2
1	C	358	ARG	2.2
1	A	344	SER	2.2
1	A	316	PRO	2.1
3	F	282	HIS	2.1
2	B	193	VAL	2.1
1	C	297	CYS	2.1
3	E	188	PHE	2.1
1	C	440	VAL	2.1
1	C	398	LEU	2.1
2	B	152	ILE	2.1
3	E	232	ASP	2.1
3	E	272	TYR	2.1
3	E	284	THR	2.1
2	B	220	GLY	2.1
3	F	75	TRP	2.0
1	C	444	TYR	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	A	172	11/12	0.92	0.12	56,57,60,61	1
2	SEP	D	108	10/11	0.92	0.13	65,65,69,69	0
2	SEP	B	108	10/11	0.94	0.12	64,64,67,67	0
1	TPO	C	172	11/12	0.94	0.14	69,69,73,73	2

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

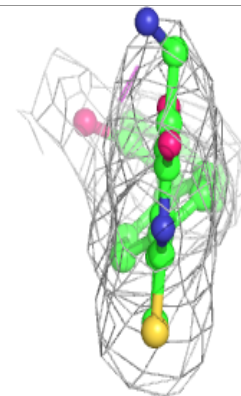
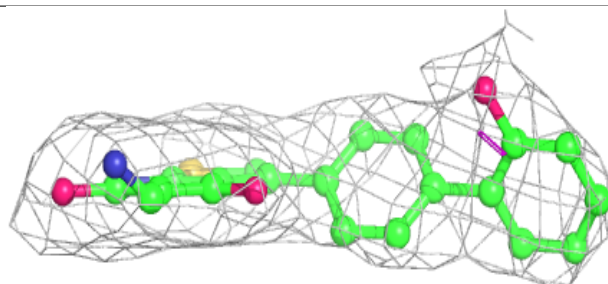
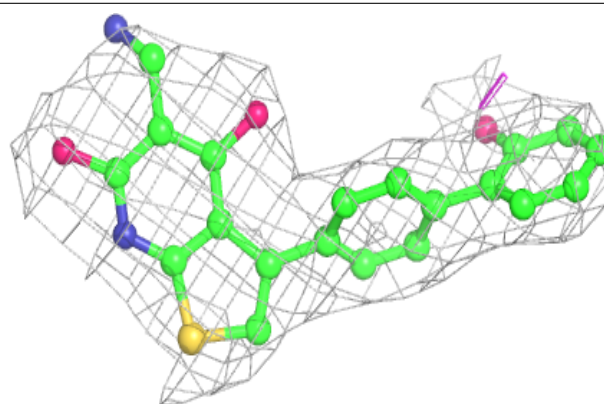


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	C2Z	E	401	15/15	0.83	0.24	100,100,101,101	0
6	C2Z	E	402	15/15	0.86	0.22	92,92,93,93	0
6	C2Z	F	402	15/15	0.91	0.20	88,88,88,88	0
6	C2Z	F	401	15/15	0.92	0.18	92,93,94,94	0
5	C1V	A	602	26/26	0.94	0.24	44,45,47,48	0
4	STU	A	601	35/35	0.96	0.18	38,39,40,40	0
5	C1V	C	602	26/26	0.96	0.21	42,44,45,45	0
4	STU	C	601	35/35	0.96	0.21	39,40,42,43	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.

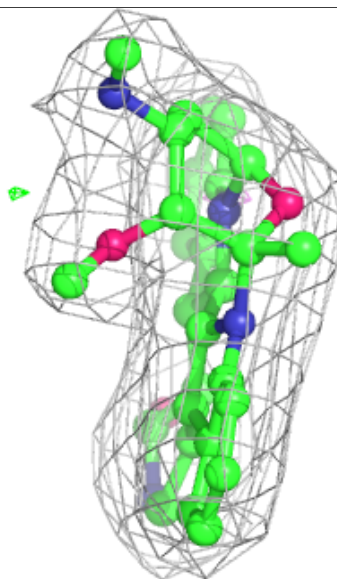
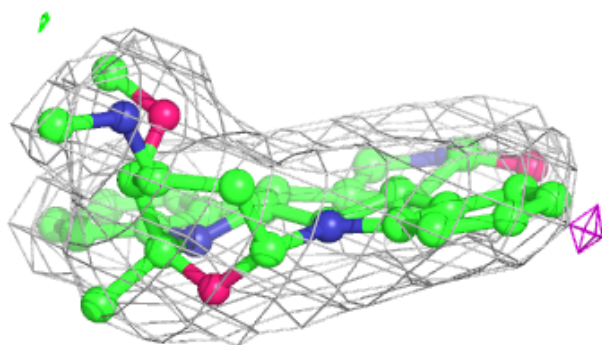
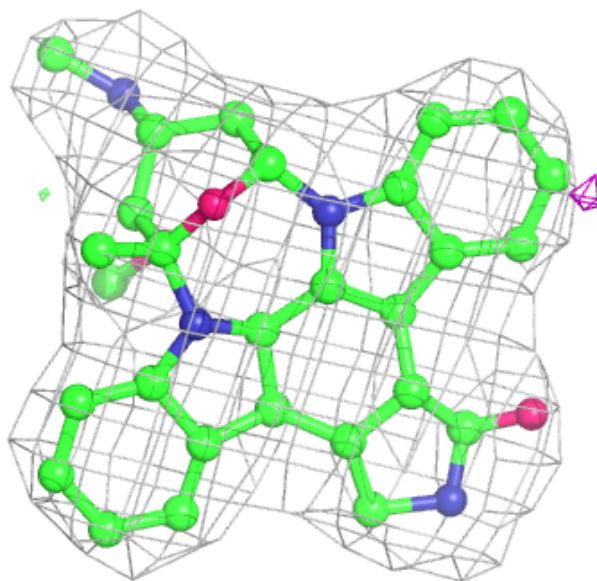
**Electron density around C1V A 602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



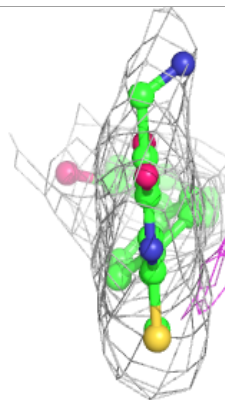
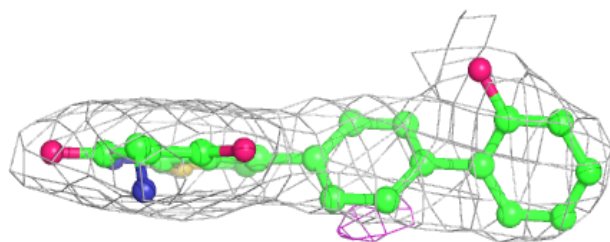
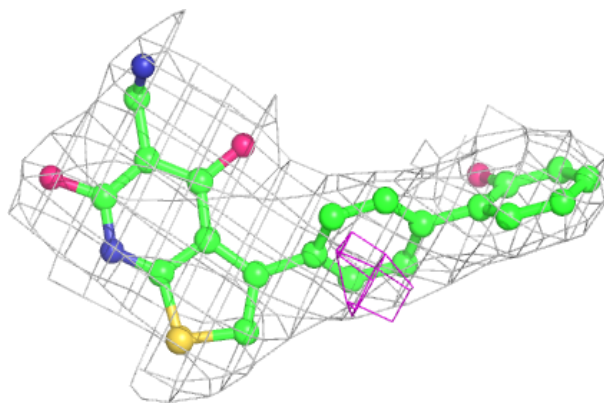
**Electron density around STU A 601:**

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



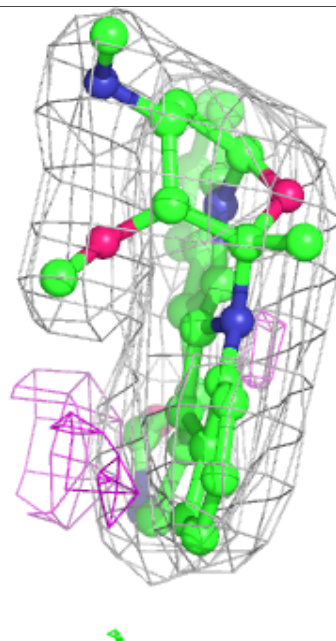
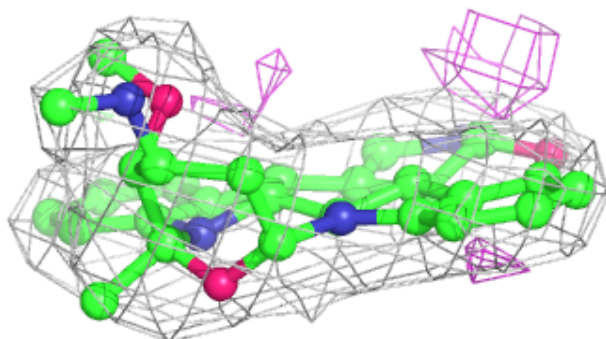
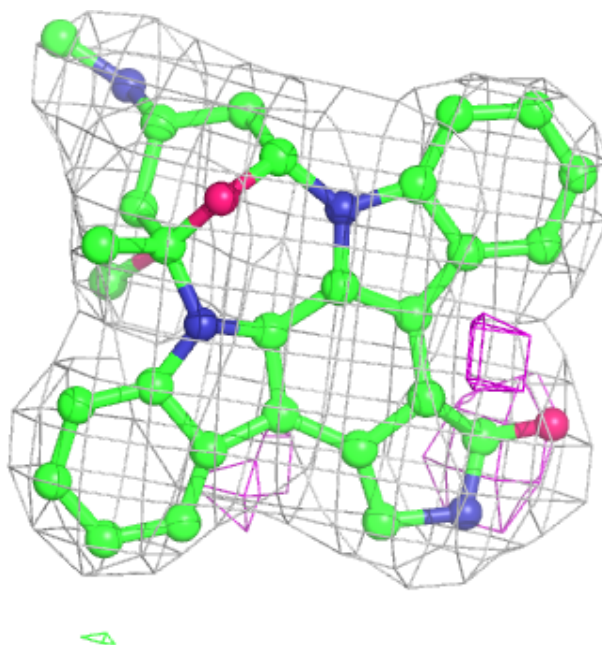
**Electron density around C1V C 602:**

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



**Electron density around STU 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.