Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 02:37 AM EDT

PDB ID	:	6B1U
Title	:	Structure of full-length human AMPK (a2b1g1) in complex with a small molecule activator SC4
Authors	:	Ngoei, K.R.W.; Langendorf, C.G.; Ling, N.X.Y.; Hoque, A.; Johnson, S.; Camerino, M.C.; Walker, S.R.; Bozikis, Y.E.; Dite, T.A.; Ovens, A.J.; Smiles, W.J.; Jacobs, R.; Huang, H.; Parker, M.W.; Scott, J.W.; Rider, M.H.; Kemp, B.E.; Foitzik, R.C.; Baell, J.B.; Oakhill, J.S.
Deposited on	:	2017-09-19
Resolution	:	2.77 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 (i) 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 (i)) were used in the production of this report:

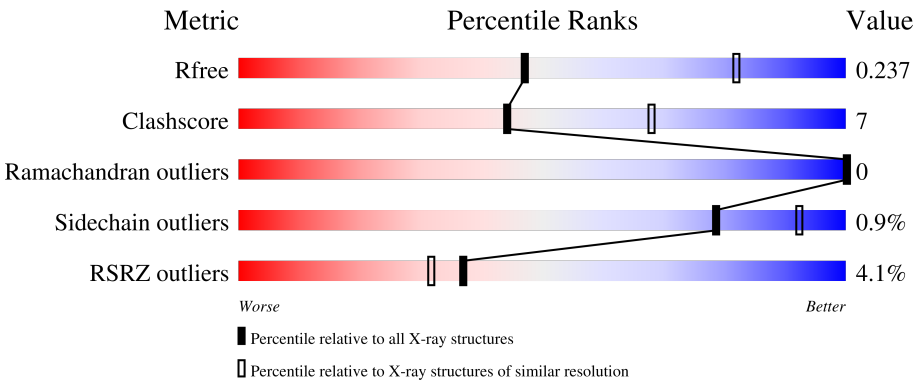
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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%, 72%, 6%, 22%
1	C	565	4%, 73%, 8%, 19%
2	B	270	6%, 59%, 9%, 32%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
2	D	270	2% 59% 9% 33%
3	E	336	3% 75% 13% 11%
3	F	336	3% 79% 10% • 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14977 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
			Total	C	N	O	P	S			
1	A	442	3456	2221	588	622	1	24	0	0	0
1	C	460	3585	2295	610	654	1	25	0	0	0

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	conflict	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	conflict	UNP P54646

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	184	1401	904	232	259	1	5	0	0	0
2	D	182	1423	916	235	265	1	6	0	0	0

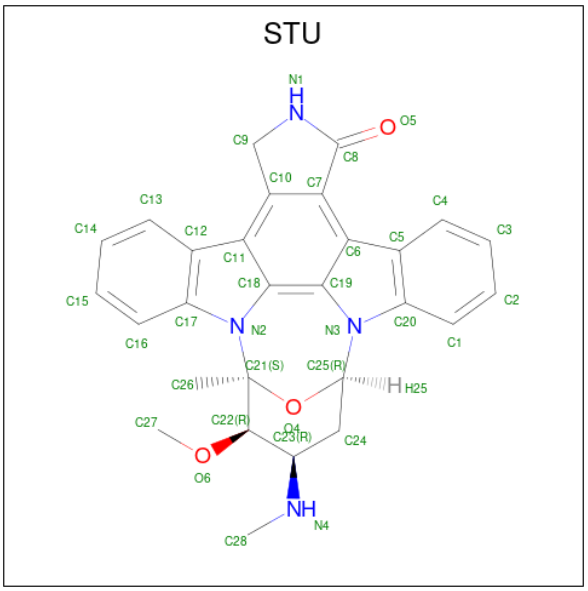
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	299	2332	1522	383	420	7	0	0	0
3	F	299	2340	1525	389	419	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

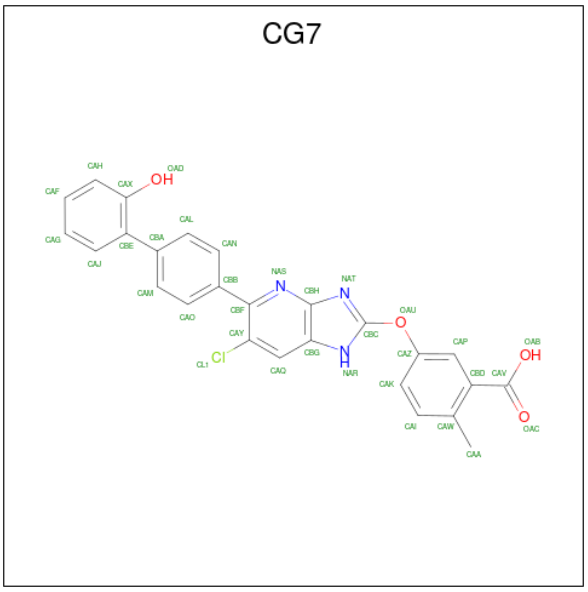
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine	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: $C_{28}H_{26}N_4O_3$).



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 5-{[6-chloro-5-(2'-hydroxy[1,1'-biphenyl]-4-yl)-1H-imidazo[4,5-b]pyridin-2-yl]oxy}-2-methylbenzoic acid (three-letter code: CG7) (formula: $C_{26}H_{18}ClN_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	A	1	68	52	2	6	8	0	1

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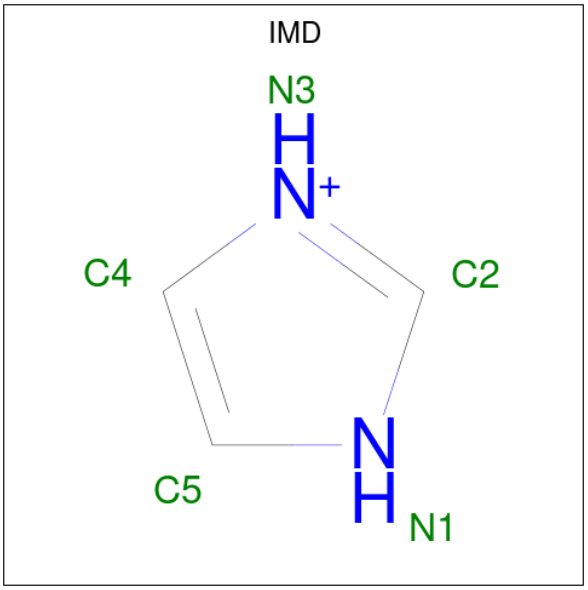
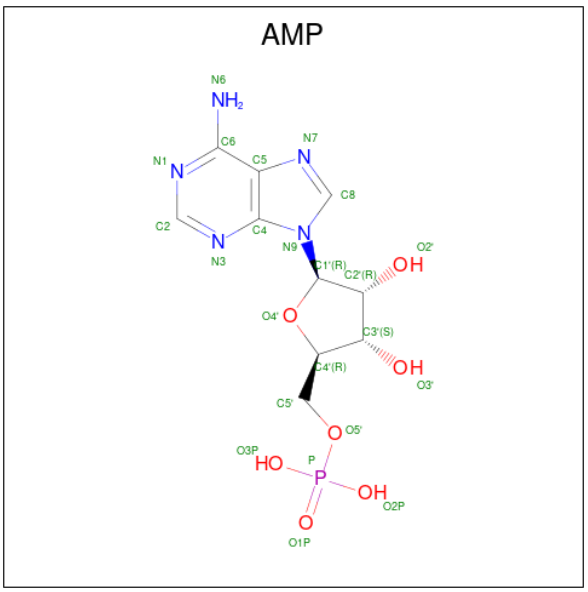
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	C	1	34	26	1	3	4	0	0

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
6	C	1	5	3	2	0	0

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



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

- Molecule 8 is water.

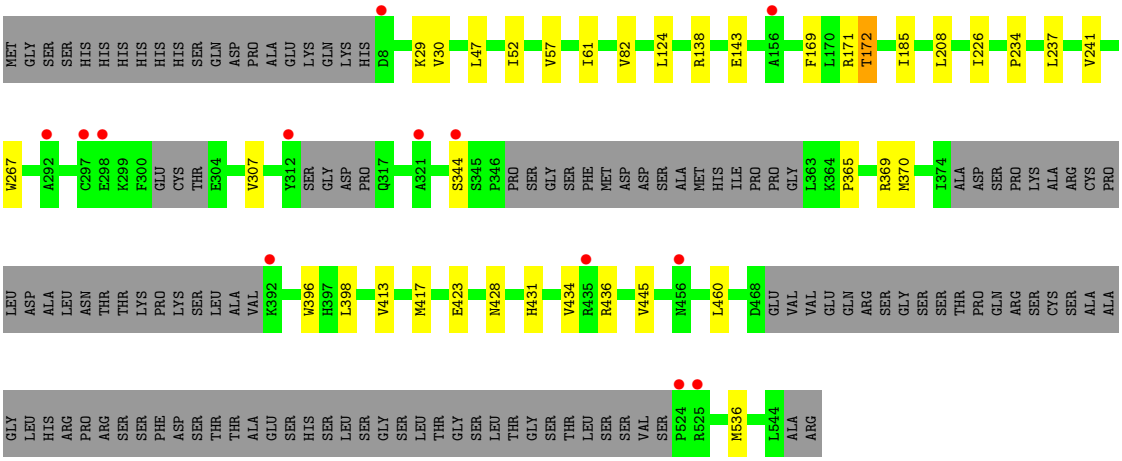
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	48	48	48	0	0
			Total	O		
8	B	5	5	5	0	0
			Total	O		
8	C	37	37	37	0	0
			Total	O		
8	D	22	22	22	0	0
			Total	O		
8	E	35	35	35	0	0
			Total	O		
8	F	24	24	24	0	0

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.

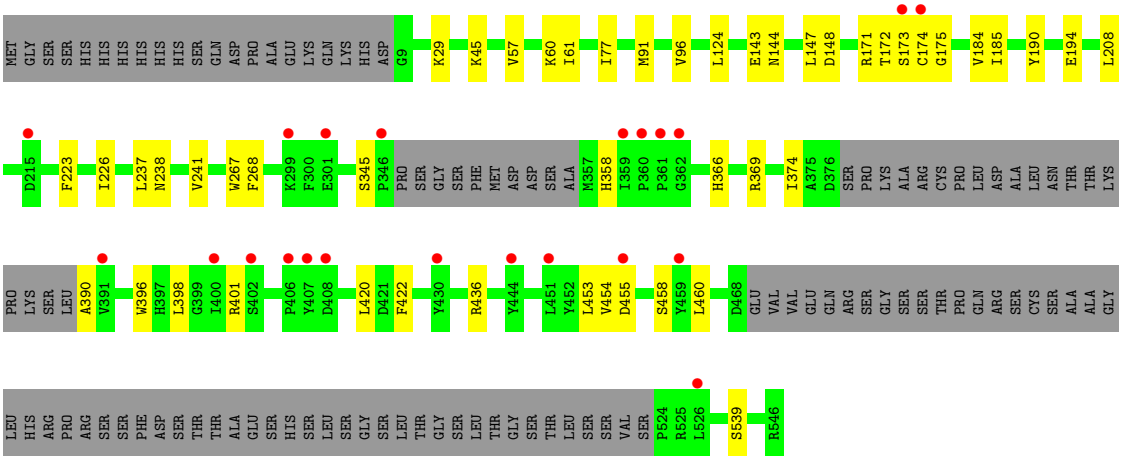
• Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2

Chain A:



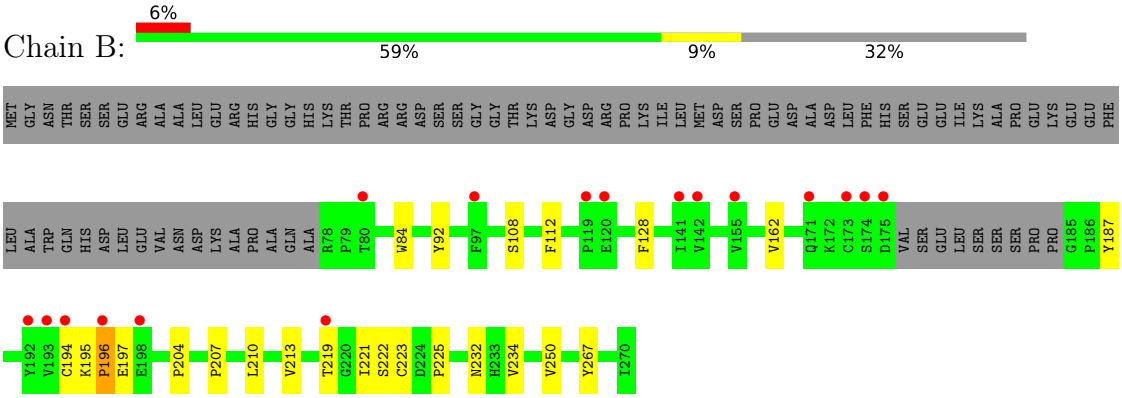
• Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2

Chain C:



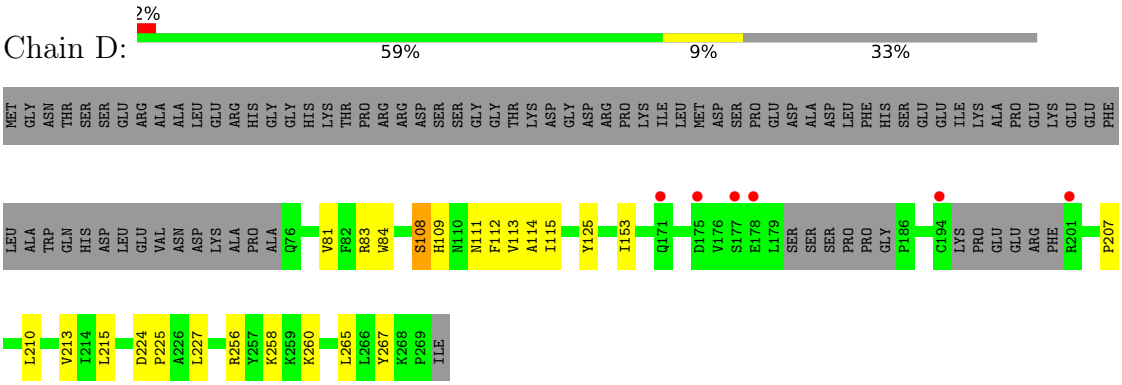
• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

Chain B:



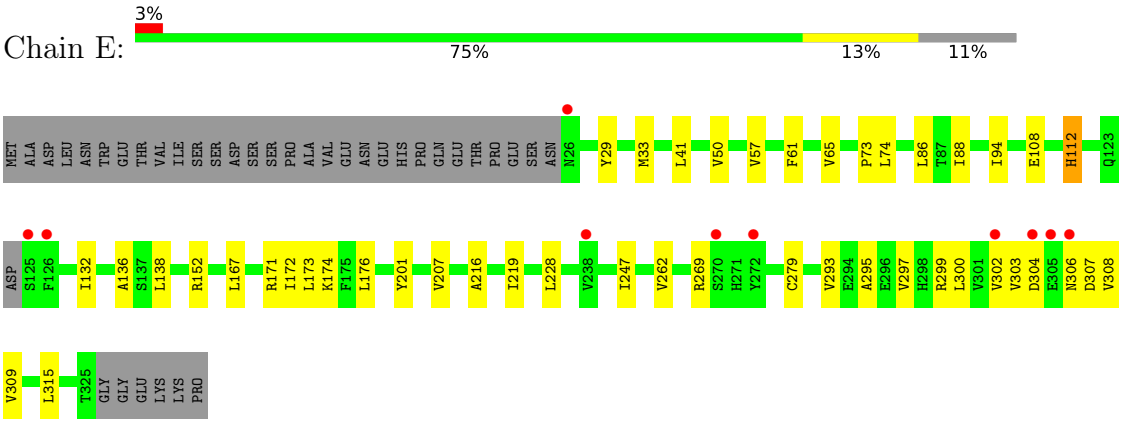
• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

Chain D:



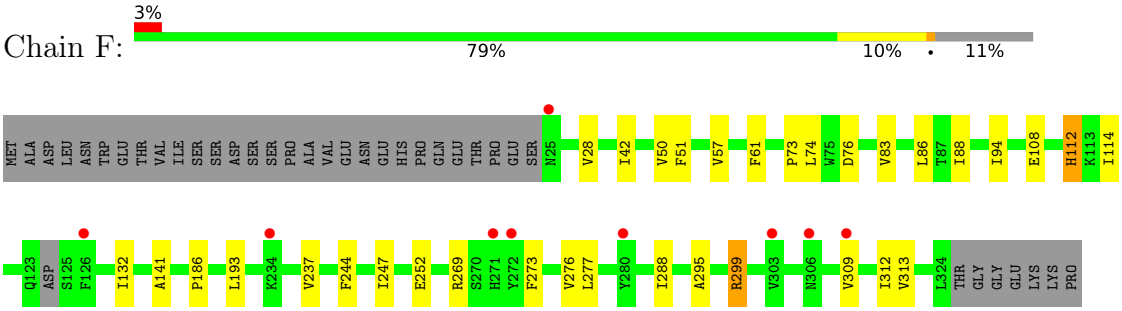
• Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.83Å 133.90Å 141.72Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	48.64 – 2.77 48.64 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.64-2.77) 99.8 (48.64-2.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.194 , 0.226 0.211 , 0.237	Depositor DCC
R_{free} test set	3627 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, IMD, STU, SEP, CG7, AMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.38	0/3523	0.57	0/4771
1	C	0.39	0/3659	0.58	0/4963
2	B	0.41	1/1432 (0.1%)	0.61	1/1965 (0.1%)
2	D	0.38	0/1453	0.58	0/1987
3	E	0.39	0/2381	0.57	0/3244
3	F	0.39	0/2388	0.57	0/3250
All	All	0.39	1/14836 (0.0%)	0.58	1/20180 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	196	PRO	N-CD	5.12	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	195	LYS	C-N-CD	5.64	140.25	128.40

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	3456	0	3339	48	0
1	C	3585	0	3440	38	1
2	B	1401	0	1310	30	0
2	D	1423	0	1351	16	0
3	E	2332	0	2339	41	1
3	F	2340	0	2358	30	0
4	A	35	0	26	12	0
4	C	35	0	26	5	0
5	A	68	0	0	4	0
5	C	34	0	0	2	0
6	C	5	0	5	0	0
7	E	46	0	24	4	0
7	F	46	0	24	1	0
8	A	48	0	0	0	0
8	B	5	0	0	0	0
8	C	37	0	0	0	0
8	D	22	0	0	0	0
8	E	35	0	0	0	0
8	F	24	0	0	0	0
All	All	14977	0	14242	192	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 7.

All (192) 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:185:ILE:CD1	1:C:226:ILE:HD12	1.66	1.24
1:C:185:ILE:HD13	1:C:226:ILE:CD1	1.76	1.15
3:E:303:VAL:HG11	3:E:307:ASP:HA	1.44	0.98
1:A:365:PRO:HB3	2:B:221:ILE:CG2	1.93	0.97
1:A:370:MET:HE2	3:E:65:VAL:HA	1.46	0.96
1:C:185:ILE:CD1	1:C:226:ILE:CD1	2.40	0.95
4:A:601:STU:H272	4:A:601:STU:C18	1.97	0.95
4:A:601:STU:H261	4:A:601:STU:H16	1.52	0.92
1:C:185:ILE:HD13	1:C:226:ILE:HD11	1.50	0.90
4:C:601:STU:H261	4:C:601:STU:H16	1.52	0.90
2:B:232:ASN:OD1	2:B:234:VAL:HG12	1.74	0.88
4:A:601:STU:H241	4:A:601:STU:H273	1.56	0.86
1:A:370:MET:CE	3:E:65:VAL:HA	2.07	0.84
3:F:57:VAL:CG1	3:F:61:PHE:CE2	2.61	0.83
3:F:57:VAL:HG12	3:F:61:PHE:CE2	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PRO:HB3	2:B:221:ILE:HG21	1.62	0.80
3:F:299:ARG:HG3	3:F:312:ILE:HD11	1.64	0.78
1:A:434:VAL:HG12	1:A:536:MET:HE1	1.67	0.76
4:A:601:STU:H272	4:A:601:STU:C19	2.16	0.76
1:C:185:ILE:HD11	1:C:226:ILE:HD12	1.66	0.76
3:E:303:VAL:HG13	3:E:308:VAL:N	2.03	0.74
3:E:297:VAL:HG13	7:E:401:AMP:C8	2.23	0.74
1:C:241:VAL:HG22	1:C:267:TRP:CD2	2.23	0.73
1:A:143:GLU:HB3	4:A:601:STU:H281	1.70	0.72
1:C:184:VAL:HG12	1:C:190:TYR:CE1	2.24	0.72
1:C:29:LYS:HB2	5:C:602:CG7:CAI	2.20	0.72
1:A:396:TRP:CH2	2:B:250:VAL:HG12	2.25	0.71
3:E:303:VAL:CG1	3:E:307:ASP:HA	2.19	0.71
1:C:241:VAL:HG22	1:C:267:TRP:CE2	2.26	0.71
1:A:434:VAL:HG12	1:A:536:MET:CE	2.21	0.70
3:E:201:TYR:HE1	3:E:302:VAL:HG11	1.56	0.70
1:A:241:VAL:HG22	1:A:267:TRP:CE2	2.27	0.69
1:C:241:VAL:CG2	1:C:267:TRP:CE2	2.75	0.69
1:A:169:PHE:CE1	2:B:234:VAL:HG21	2.28	0.69
1:A:241:VAL:HG22	1:A:267:TRP:CD2	2.28	0.69
1:A:169:PHE:CZ	2:B:234:VAL:HG22	2.30	0.67
4:A:601:STU:H261	4:A:601:STU:C16	2.23	0.66
1:C:143:GLU:HB3	4:C:601:STU:H281	1.76	0.66
1:A:169:PHE:CZ	2:B:234:VAL:CG2	2.79	0.65
3:F:237:VAL:HG11	3:F:276:VAL:HG11	1.78	0.65
1:C:124:LEU:HD23	1:C:268:PHE:CZ	2.31	0.65
1:A:307:VAL:HG12	1:A:307:VAL:O	1.96	0.65
4:A:601:STU:H241	4:A:601:STU:C27	2.25	0.64
1:A:365:PRO:HA	2:B:221:ILE:HG22	1.79	0.64
3:E:57:VAL:HG12	3:E:61:PHE:CE2	2.32	0.64
3:E:297:VAL:CG1	7:E:401:AMP:N7	2.62	0.63
1:C:185:ILE:HG23	1:C:223:PHE:CD2	2.33	0.63
3:E:303:VAL:HG11	3:E:307:ASP:CA	2.26	0.62
1:A:396:TRP:HH2	2:B:250:VAL:HG12	1.65	0.62
3:E:201:TYR:CE1	3:E:302:VAL:HG11	2.34	0.61
1:C:366:HIS:HB3	1:C:369:ARG:HG2	1.83	0.61
2:D:108:SEP:P	2:D:109:HIS:H	2.22	0.61
1:A:241:VAL:CG2	1:A:267:TRP:CE2	2.84	0.60
3:E:295:ALA:O	3:E:297:VAL:HG23	2.02	0.60
2:D:113:VAL:HG12	2:D:114:ALA:N	2.16	0.59
1:C:374:ILE:HA	1:C:390:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:VAL:CG1	2:D:114:ALA:N	2.65	0.59
3:E:41:LEU:HD12	3:E:138:LEU:HD22	1.85	0.59
3:F:74:LEU:HD21	3:F:86:LEU:HB2	1.86	0.58
1:A:396:TRP:HB2	2:B:213:VAL:HG11	1.85	0.58
3:E:207:VAL:HG23	3:E:228:LEU:HB3	1.86	0.58
2:B:232:ASN:CG	2:B:234:VAL:HG12	2.24	0.57
1:C:185:ILE:HG23	1:C:223:PHE:CE2	2.39	0.57
3:F:132:ILE:HD13	3:F:141:ALA:HB2	1.86	0.57
3:F:237:VAL:HG12	3:F:276:VAL:HG21	1.87	0.57
3:E:57:VAL:CG1	3:E:61:PHE:CE2	2.87	0.57
1:A:138:ARG:HH12	1:A:172:TPO:HB	1.68	0.57
4:C:601:STU:H261	4:C:601:STU:C16	2.24	0.56
3:E:297:VAL:HG11	7:E:401:AMP:C5	2.40	0.56
1:C:237:LEU:HD23	1:C:238:ASN:O	2.06	0.56
3:E:172:ILE:O	3:E:176:LEU:HD13	2.05	0.56
1:A:396:TRP:CH2	2:B:250:VAL:CG1	2.88	0.56
5:A:602[A]:CG7:CAN	5:A:602[A]:CG7:CL1	2.91	0.56
3:F:312:ILE:HD13	7:F:402:AMP:N7	2.21	0.56
1:C:57:VAL:HG12	1:C:61:ILE:HG12	1.87	0.55
5:C:602:CG7:CAO	5:C:602:CG7:CL1	2.92	0.55
3:E:41:LEU:HD22	3:E:171:ARG:HG3	1.89	0.55
1:A:29:LYS:HB2	5:A:602[B]:CG7:CAI	2.37	0.54
1:A:396:TRP:HH2	2:B:250:VAL:CG1	2.20	0.54
4:A:601:STU:H273	4:A:601:STU:C24	2.31	0.54
3:E:41:LEU:HD13	3:E:167:LEU:HD11	1.88	0.54
3:E:304:ASP:OD2	3:E:306:ASN:N	2.41	0.54
3:F:50:VAL:HG22	3:F:73:PRO:HG2	1.90	0.54
4:A:601:STU:C27	4:A:601:STU:C24	2.85	0.53
3:E:207:VAL:HG11	3:E:262:VAL:HG21	1.89	0.53
3:E:297:VAL:HG13	7:E:401:AMP:N7	2.24	0.53
3:E:108:GLU:O	3:E:112:HIS:HB2	2.08	0.53
3:F:277:LEU:CD1	3:F:295:ALA:HB1	2.39	0.53
1:C:194:GLU:OE1	1:C:194:GLU:N	2.32	0.52
3:E:303:VAL:HG13	3:E:308:VAL:H	1.74	0.52
5:A:602[B]:CG7:CAN	5:A:602[B]:CG7:CL1	2.95	0.52
2:D:260:LYS:NZ	3:F:42:ILE:O	2.34	0.52
3:E:57:VAL:HG11	3:E:94:ILE:HD13	1.92	0.51
3:E:88:ILE:HG12	3:E:247:ILE:HD13	1.91	0.51
1:A:169:PHE:CE1	2:B:234:VAL:CG2	2.94	0.51
1:A:208:LEU:HB3	1:A:237:LEU:HD21	1.92	0.51
2:B:84:TRP:HB3	2:B:112:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:SEP:OG	2:D:109:HIS:N	2.41	0.50
2:B:219:THR:HG22	2:B:223:CYS:SG	2.52	0.50
1:C:420:LEU:HD22	1:C:539:SER:HB3	1.94	0.50
1:A:47:LEU:HB3	1:A:52:ILE:HD11	1.93	0.50
1:A:365:PRO:CB	2:B:221:ILE:CG2	2.80	0.49
1:A:423:GLU:HB3	2:B:187:TYR:HB3	1.94	0.49
1:A:344:SER:O	2:B:219:THR:O	2.29	0.49
4:A:601:STU:C16	4:A:601:STU:C26	2.90	0.49
2:B:250:VAL:HG21	2:B:267:TYR:CE2	2.47	0.49
1:C:144:ASN:OD1	4:C:601:STU:H272	2.12	0.48
2:D:267:TYR:HB2	3:F:51:PHE:HD1	1.79	0.48
3:F:108:GLU:O	3:F:112:HIS:HB2	2.13	0.48
2:B:250:VAL:HG22	2:B:267:TYR:CD2	2.48	0.48
4:C:601:STU:C16	4:C:601:STU:C26	2.89	0.48
3:E:57:VAL:HG11	3:E:94:ILE:CD1	2.44	0.48
3:F:277:LEU:HD13	3:F:295:ALA:CB	2.43	0.48
3:E:29:TYR:O	3:E:33:MET:HG2	2.14	0.47
3:E:303:VAL:CG1	3:E:308:VAL:N	2.73	0.47
3:F:74:LEU:HD22	3:F:114:ILE:HG21	1.96	0.47
1:C:369:ARG:HD2	2:D:225:PRO:HG3	1.95	0.47
1:C:396:TRP:HB2	2:D:213:VAL:HG11	1.95	0.47
2:D:84:TRP:HB3	2:D:112:PHE:HB2	1.96	0.47
1:C:96:VAL:HG13	1:C:148:ASP:HA	1.96	0.47
2:D:207:PRO:HD2	2:D:210:LEU:HD12	1.95	0.47
3:E:207:VAL:CG2	3:E:228:LEU:HD13	2.44	0.47
1:A:307:VAL:O	1:A:307:VAL:CG1	2.62	0.47
3:F:57:VAL:HG11	3:F:94:ILE:CD1	2.44	0.47
1:C:422:PHE:HE1	1:C:436:ARG:HD3	1.80	0.46
1:A:428:ASN:HB3	1:A:431:HIS:HB3	1.97	0.46
1:A:398:LEU:O	1:A:460:LEU:HD11	2.16	0.46
2:B:196:PRO:HG2	2:B:197:GLU:H	1.82	0.45
1:C:208:LEU:CD1	1:C:241:VAL:HG11	2.46	0.45
1:C:374:ILE:HD12	3:F:252:GLU:HA	1.98	0.45
3:F:76:ASP:HB2	3:F:83:VAL:CG2	2.46	0.45
2:D:125:TYR:HE1	2:D:153:ILE:HG23	1.82	0.45
5:A:602[B]:CG7:CAK	5:A:602[B]:CG7:NAT	2.74	0.45
2:B:92:TYR:HB2	2:B:128:PHE:HB3	1.99	0.44
1:A:436:ARG:HH21	1:A:445:VAL:HG21	1.82	0.44
3:E:303:VAL:HG12	3:E:304:ASP:N	2.32	0.44
3:F:132:ILE:CD1	3:F:141:ALA:HB2	2.48	0.44
1:C:241:VAL:CG2	1:C:267:TRP:NE1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:VAL:HG22	2:D:115:ILE:HG12	1.99	0.44
2:D:83:ARG:HD2	2:D:111:ASN:ND2	2.32	0.44
2:B:219:THR:CG2	2:B:223:CYS:SG	3.06	0.44
3:E:50:VAL:HG22	3:E:73:PRO:HG2	2.00	0.44
4:A:601:STU:H272	4:A:601:STU:N2	2.29	0.44
3:F:193:LEU:HD21	3:F:313:VAL:HG21	2.00	0.43
3:F:237:VAL:CG1	3:F:276:VAL:HG21	2.48	0.43
1:A:434:VAL:CG1	1:A:536:MET:CE	2.96	0.43
3:F:193:LEU:HD13	3:F:288:ILE:HD13	1.99	0.43
1:A:185:ILE:HD11	1:A:226:ILE:HD13	2.01	0.43
1:A:365:PRO:CA	2:B:221:ILE:HG22	2.44	0.43
1:C:77:ILE:CD1	1:C:96:VAL:HG21	2.49	0.43
3:F:269:ARG:HG2	3:F:273:PHE:HB2	1.99	0.43
1:A:234:PRO:HD2	1:A:237:LEU:HD12	1.99	0.43
1:C:45:LYS:HB3	1:C:91:MET:HB2	2.01	0.43
1:A:208:LEU:CD1	1:A:241:VAL:HG11	2.49	0.43
1:C:185:ILE:CG2	1:C:223:PHE:CD2	3.01	0.43
1:C:174:CYS:HB3	1:C:175:GLY:H	1.65	0.42
3:E:173:LEU:HD22	3:E:315:LEU:HD22	2.00	0.42
3:F:244:PHE:O	3:F:247:ILE:HG22	2.19	0.42
1:C:57:VAL:HG13	1:C:60:LYS:HB3	2.01	0.42
1:A:208:LEU:HD13	1:A:241:VAL:HG11	2.01	0.42
1:A:57:VAL:HG12	1:A:61:ILE:HG12	2.00	0.42
2:D:256:ARG:HD3	2:D:258:LYS:O	2.20	0.42
1:C:398:LEU:O	1:C:460:LEU:HD11	2.19	0.42
2:B:207:PRO:HD2	2:B:210:LEU:HD12	2.02	0.42
1:C:454:VAL:O	1:C:458:SER:HB3	2.20	0.42
3:E:41:LEU:CD1	3:E:138:LEU:HD22	2.50	0.42
3:E:279:CYS:HB3	3:E:300:LEU:HD13	2.02	0.42
1:C:401:ARG:HG3	1:C:460:LEU:HD13	2.02	0.42
3:F:28:VAL:HG22	3:F:186:PRO:HG3	2.02	0.41
1:A:370:MET:CE	3:E:65:VAL:HG22	2.50	0.41
1:A:57:VAL:HG12	1:A:57:VAL:O	2.20	0.41
3:E:174:LYS:HG3	3:E:293:VAL:HG13	2.02	0.41
2:D:215:LEU:HD11	2:D:265:LEU:HD11	2.02	0.41
3:F:237:VAL:HG23	3:F:309:VAL:HG22	2.02	0.41
3:F:57:VAL:CG1	3:F:61:PHE:HE2	2.25	0.41
1:C:77:ILE:HD11	1:C:96:VAL:HG21	2.03	0.41
1:C:96:VAL:HG12	1:C:147:LEU:O	2.21	0.41
3:E:57:VAL:HG12	3:E:61:PHE:HE2	1.82	0.41
1:A:241:VAL:CG2	1:A:267:TRP:NE1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:57:VAL:HG11	3:F:94:ILE:HD13	2.03	0.40
3:F:88:ILE:HG12	3:F:247:ILE:HD13	2.03	0.40
1:A:82:VAL:HB	2:B:162:VAL:HG21	2.03	0.40
1:A:171:ARG:HH22	2:B:204:PRO:HB3	1.85	0.40
3:E:74:LEU:HD21	3:E:86:LEU:HB2	2.02	0.40
1:A:30:VAL:HG21	4:A:601:STU:C17	2.50	0.40
1:A:413:VAL:HG12	1:A:417:MET:HE2	2.03	0.40
2:D:224:ASP:HB3	2:D:227:LEU:HG	2.03	0.40
1:A:369:ARG:HD2	2:B:225:PRO:HG3	2.03	0.40
3:E:132:ILE:HD11	3:E:136:ALA:CB	2.52	0.40
1:A:365:PRO:HB3	2:B:221:ILE:HG22	1.90	0.40
3:E:216:ALA:HA	3:E:219:ILE:HD12	2.02	0.40
3:F:277:LEU:HD13	3:F:295:ALA:HB1	2.03	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:358:HIS:O	3:E:309:VAL:N[1_445]	2.01	0.19

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	429/565 (76%)	420 (98%)	9 (2%)	0	100	100
1	C	451/565 (80%)	442 (98%)	9 (2%)	0	100	100
2	B	179/270 (66%)	175 (98%)	4 (2%)	0	100	100
2	D	175/270 (65%)	171 (98%)	4 (2%)	0	100	100
3	E	295/336 (88%)	289 (98%)	6 (2%)	0	100	100
3	F	295/336 (88%)	290 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1824/2342 (78%)	1787 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	358/497 (72%)	357 (100%)	1 (0%)	92	97
1	C	373/497 (75%)	368 (99%)	5 (1%)	69	89
2	B	146/239 (61%)	144 (99%)	2 (1%)	67	87
2	D	154/239 (64%)	154 (100%)	0	100	100
3	E	254/308 (82%)	250 (98%)	4 (2%)	62	86
3	F	255/308 (83%)	253 (99%)	2 (1%)	81	93
All	All	1540/2088 (74%)	1526 (99%)	14 (1%)	78	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
2	B	194	CYS
2	B	222	SER
1	C	171	ARG
1	C	173	SER
1	C	345	SER
1	C	453	LEU
1	C	455	ASP
3	E	112	HIS
3	E	152	ARG
3	E	269	ARG
3	E	299	ARG
3	F	112	HIS
3	F	299	ARG

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

Mol	Chain	Res	Type
1	A	431	HIS
1	A	450	GLN
1	C	335	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SEP	B	108	2	8,9,10	0.86	0	8,12,14	1.51	1 (12%)
1	TPO	A	172	1	8,10,11	1.09	0	10,14,16	1.41	1 (10%)
2	SEP	D	108	2	8,9,10	1.01	0	8,12,14	1.60	1 (12%)
1	TPO	C	172	1	8,10,11	0.85	0	10,14,16	1.02	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
2	SEP	B	108	2	-	0/5/8/10	-
1	TPO	A	172	1	-	0/9/11/13	-
2	SEP	D	108	2	-	1/5/8/10	-
1	TPO	C	172	1	-	2/9/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	108	SEP	OG-CB-CA	3.49	111.55	108.14
2	B	108	SEP	O3P-P-OG	2.75	114.04	106.73
1	A	172	TPO	O2P-P-O1P	-2.10	102.45	110.68
1	C	172	TPO	O-C-CA	-2.04	119.42	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	172	TPO	C-CA-CB-CG2
1	C	172	TPO	O-C-CA-CB
2	D	108	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	1	0
2	D	108	SEP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	AMP	E	401	-	22,25,25	1.09	2 (9%)	25,38,38	1.40	5 (20%)
7	AMP	E	402	-	22,25,25	1.05	1 (4%)	25,38,38	1.43	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CG7	A	602[A]	-	37,38,38	2.36	6 (16%)	44,55,55	1.32	5 (11%)
7	AMP	F	402	-	22,25,25	1.06	1 (4%)	25,38,38	1.56	6 (24%)
4	STU	C	601	-	30,42,42	2.53	10 (33%)	31,68,68	2.44	12 (38%)
4	STU	A	601	-	30,42,42	2.52	10 (33%)	31,68,68	2.45	13 (41%)
5	CG7	A	602[B]	-	37,38,38	2.37	6 (16%)	44,55,55	1.33	5 (11%)
6	IMD	C	603	-	3,5,5	0.39	0	4,5,5	0.72	0
7	AMP	F	401	-	22,25,25	1.09	2 (9%)	25,38,38	1.45	5 (20%)
5	CG7	C	602	-	37,38,38	2.37	6 (16%)	44,55,55	1.33	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AMP	E	401	-	-	1/6/26/26	0/3/3/3
7	AMP	E	402	-	-	3/6/26/26	0/3/3/3
5	CG7	A	602[A]	-	-	4/14/16/16	0/5/5/5
7	AMP	F	402	-	-	1/6/26/26	0/3/3/3
4	STU	C	601	-	-	2/4/42/42	-
4	STU	A	601	-	-	4/4/42/42	-
5	CG7	A	602[B]	-	-	5/14/16/16	0/5/5/5
6	IMD	C	603	-	-	-	0/1/1/1
7	AMP	F	401	-	-	3/6/26/26	0/3/3/3
5	CG7	C	602	-	-	4/14/16/16	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602[B]	CG7	CBB-CBF	-8.50	1.39	1.49
5	C	602	CG7	CBB-CBF	-8.44	1.39	1.49
5	A	602[A]	CG7	CBB-CBF	-8.42	1.39	1.49
4	C	601	STU	C9-C10	-6.02	1.45	1.50
4	A	601	STU	C9-C10	-5.99	1.45	1.50
5	A	602[B]	CG7	CAA-CAW	-5.57	1.39	1.51
5	A	602[A]	CG7	CAA-CAW	-5.55	1.39	1.51
5	C	602	CG7	CAA-CAW	-5.53	1.40	1.51
5	C	602	CG7	CBE-CBA	-5.49	1.39	1.49
5	A	602[B]	CG7	CBE-CBA	-5.49	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602[A]	CG7	CBE-CBA	-5.48	1.39	1.49
5	A	602[B]	CG7	CAQ-CBG	-5.32	1.33	1.41
5	C	602	CG7	CAQ-CBG	-5.30	1.33	1.41
5	A	602[A]	CG7	CAQ-CBG	-5.26	1.33	1.41
5	C	602	CG7	CBD-CAV	-4.67	1.39	1.49
5	A	602[A]	CG7	CBD-CAV	-4.61	1.39	1.49
5	A	602[B]	CG7	CBD-CAV	-4.60	1.39	1.49
4	C	601	STU	C5-C20	4.59	1.48	1.41
4	A	601	STU	C5-C20	4.56	1.48	1.41
4	C	601	STU	C12-C17	4.55	1.48	1.41
4	A	601	STU	C12-C17	4.52	1.48	1.41
4	A	601	STU	C10-C11	4.33	1.49	1.42
4	C	601	STU	C10-C11	4.32	1.49	1.42
4	A	601	STU	C11-C18	4.26	1.48	1.42
4	C	601	STU	C11-C18	4.24	1.48	1.42
4	A	601	STU	C9-N1	3.96	1.49	1.45
4	C	601	STU	C9-N1	3.92	1.49	1.45
4	C	601	STU	C7-C6	3.66	1.49	1.43
4	A	601	STU	C7-C6	3.61	1.49	1.43
4	C	601	STU	C6-C19	3.23	1.46	1.42
4	A	601	STU	C6-C19	3.22	1.46	1.42
4	C	601	STU	C19-C18	3.16	1.49	1.42
4	A	601	STU	C19-C18	3.15	1.49	1.42
7	E	401	AMP	C5-C4	2.85	1.48	1.40
4	C	601	STU	O5-C8	2.81	1.29	1.23
4	A	601	STU	O5-C8	2.80	1.29	1.23
7	F	401	AMP	C5-C4	2.80	1.48	1.40
7	F	402	AMP	C5-C4	2.78	1.48	1.40
7	E	402	AMP	C5-C4	2.72	1.48	1.40
5	A	602[A]	CG7	CBG-CBH	-2.52	1.34	1.40
5	A	602[B]	CG7	CBG-CBH	-2.48	1.34	1.40
5	C	602	CG7	CBG-CBH	-2.48	1.34	1.40
7	E	401	AMP	C2-N3	2.05	1.35	1.32
7	F	401	AMP	C2-N3	2.04	1.35	1.32

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	STU	C7-C8-N1	5.51	111.95	106.37
4	C	601	STU	C7-C8-N1	5.45	111.89	106.37
4	A	601	STU	C9-N1-C8	-5.09	108.95	113.85
4	C	601	STU	C9-N1-C8	-5.06	108.98	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	STU	O5-C8-C7	-4.46	124.02	129.32
4	C	601	STU	O5-C8-C7	-4.44	124.05	129.32
4	C	601	STU	C7-C10-C11	-4.29	116.64	122.42
4	A	601	STU	C7-C10-C11	-4.26	116.69	122.42
7	F	401	AMP	N3-C2-N1	-3.81	122.73	128.68
7	E	401	AMP	N3-C2-N1	-3.78	122.77	128.68
7	F	402	AMP	N3-C2-N1	-3.65	122.97	128.68
5	C	602	CG7	CBB-CBF-NAS	3.61	120.41	115.69
5	A	602[B]	CG7	CBB-CBF-NAS	3.61	120.40	115.69
5	A	602[A]	CG7	CBC-OAU-CAZ	-3.61	109.51	118.78
5	A	602[B]	CG7	CBC-OAU-CAZ	-3.60	109.52	118.78
5	A	602[A]	CG7	CBB-CBF-NAS	3.60	120.39	115.69
5	C	602	CG7	CBC-OAU-CAZ	-3.59	109.56	118.78
5	A	602[B]	CG7	CAQ-CAY-CBF	-3.52	118.81	122.00
5	A	602[A]	CG7	CAQ-CAY-CBF	-3.47	118.85	122.00
5	C	602	CG7	CAQ-CAY-CBF	-3.46	118.86	122.00
7	E	402	AMP	N3-C2-N1	-3.36	123.42	128.68
4	C	601	STU	C4-C5-C20	3.34	123.61	119.39
4	A	601	STU	C4-C5-C20	3.33	123.60	119.39
4	C	601	STU	C16-C17-N2	3.31	136.30	132.29
4	A	601	STU	C16-C17-N2	3.22	136.19	132.29
4	C	601	STU	C10-C9-N1	3.02	104.83	101.76
4	A	601	STU	C10-C9-N1	2.99	104.80	101.76
5	C	602	CG7	CBF-NAS-CBH	2.93	120.75	117.99
5	A	602[B]	CG7	CBF-NAS-CBH	2.87	120.70	117.99
5	A	602[A]	CG7	CBF-NAS-CBH	2.84	120.66	117.99
4	C	601	STU	C1-C20-C5	-2.78	116.73	120.73
4	A	601	STU	C1-C20-C5	-2.76	116.75	120.73
4	A	601	STU	C13-C12-C17	2.74	122.86	119.39
4	A	601	STU	C26-C21-C22	-2.70	107.38	112.64
7	E	402	AMP	C4-C5-N7	-2.70	106.59	109.40
7	F	401	AMP	C3'-C2'-C1'	2.62	104.93	100.98
4	C	601	STU	C13-C12-C17	2.62	122.71	119.39
4	C	601	STU	C3-C4-C5	-2.57	116.54	120.86
4	A	601	STU	C3-C4-C5	-2.56	116.55	120.86
7	F	402	AMP	C4-C5-N7	-2.54	106.75	109.40
7	E	401	AMP	C3'-C2'-C1'	2.54	104.80	100.98
4	A	601	STU	C14-C13-C12	-2.51	116.64	120.86
4	C	601	STU	C14-C13-C12	-2.46	116.72	120.86
4	C	601	STU	C26-C21-C22	-2.35	108.06	112.64
7	F	402	AMP	C3'-C2'-C1'	2.32	104.48	100.98
7	E	401	AMP	C2-N1-C6	2.28	122.65	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	401	AMP	C2-N1-C6	2.27	122.64	118.75
5	A	602[B]	CG7	CBA-CBE-CAX	-2.26	120.39	122.36
5	C	602	CG7	CBA-CBE-CAX	-2.24	120.40	122.36
7	E	401	AMP	C4-C5-N7	-2.22	107.08	109.40
7	F	402	AMP	P-O5'-C5'	2.22	124.42	118.30
7	F	402	AMP	C2-N1-C6	2.20	122.51	118.75
7	F	401	AMP	C4-C5-N7	-2.20	107.11	109.40
7	E	402	AMP	P-O5'-C5'	2.19	124.32	118.30
5	A	602[A]	CG7	CBA-CBE-CAX	-2.16	120.47	122.36
7	F	402	AMP	O3P-P-O2P	2.15	115.86	107.64
7	E	401	AMP	P-O5'-C5'	2.08	124.02	118.30
4	A	601	STU	C16-C17-C12	-2.06	117.76	120.73
7	F	401	AMP	P-O5'-C5'	2.02	123.85	118.30

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	STU	C23-C22-O6-C27
7	E	402	AMP	C5'-O5'-P-O1P
7	E	402	AMP	C5'-O5'-P-O2P
7	F	401	AMP	C5'-O5'-P-O1P
7	F	401	AMP	C5'-O5'-P-O2P
4	A	601	STU	C24-C23-N4-C28
4	A	601	STU	C21-C22-O6-C27
5	C	602	CG7	OAC-CAV-CBD-CAP
5	C	602	CG7	OAB-CAV-CBD-CAP
5	A	602[B]	CG7	OAB-CAV-CBD-CAP
5	A	602[A]	CG7	OAC-CAV-CBD-CAP
5	A	602[B]	CG7	OAC-CAV-CBD-CAP
5	A	602[A]	CG7	OAB-CAV-CBD-CAP
5	A	602[B]	CG7	OAB-CAV-CBD-CAW
5	A	602[B]	CG7	OAC-CAV-CBD-CAW
4	A	601	STU	C22-C23-N4-C28
4	C	601	STU	C22-C23-N4-C28
5	C	602	CG7	OAC-CAV-CBD-CAW
5	A	602[B]	CG7	CAK-CAZ-OAU-CBC
5	C	602	CG7	OAB-CAV-CBD-CAW
5	A	602[A]	CG7	OAC-CAV-CBD-CAW
5	A	602[A]	CG7	OAB-CAV-CBD-CAW
4	C	601	STU	C24-C23-N4-C28
7	E	402	AMP	C5'-O5'-P-O3P

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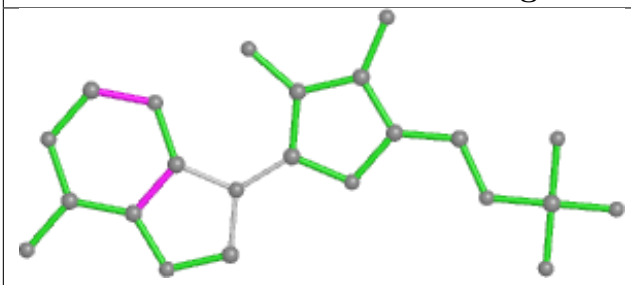
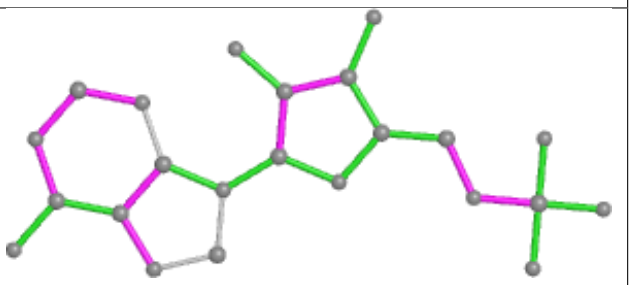
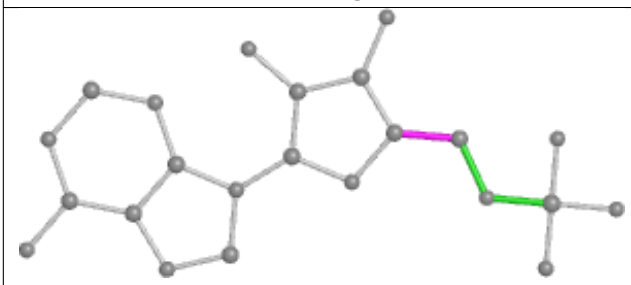
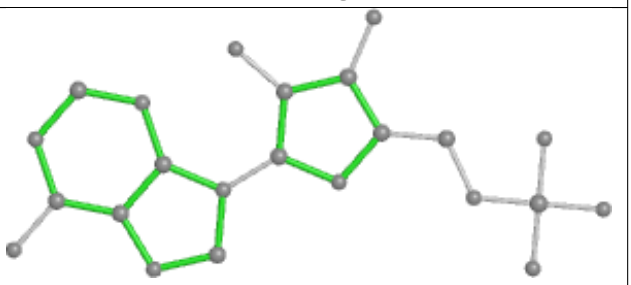
Mol	Chain	Res	Type	Atoms
7	F	401	AMP	C5'-O5'-P-O3P
7	F	402	AMP	C5'-O5'-P-O2P
7	E	401	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	401	AMP	4	0
5	A	602[A]	CG7	1	0
7	F	402	AMP	1	0
4	C	601	STU	5	0
4	A	601	STU	12	0
5	A	602[B]	CG7	3	0
5	C	602	CG7	2	0

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

Ligand AMP E 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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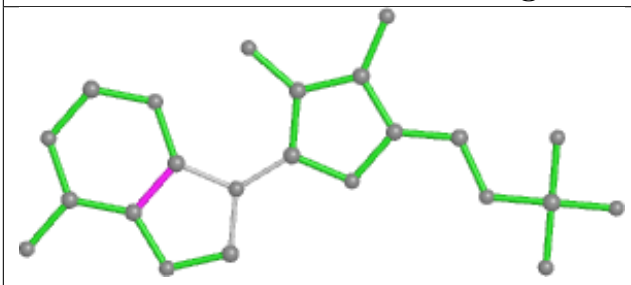
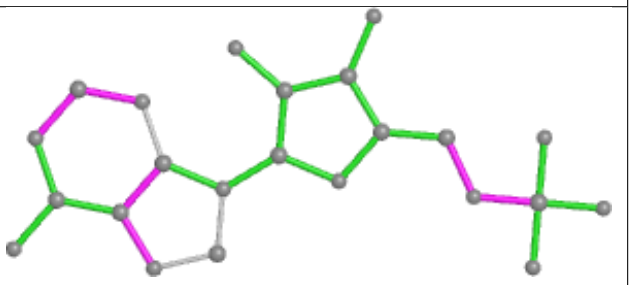
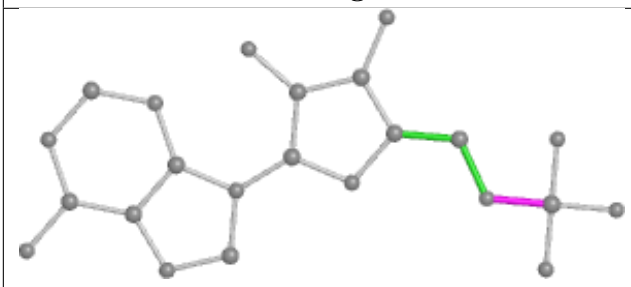
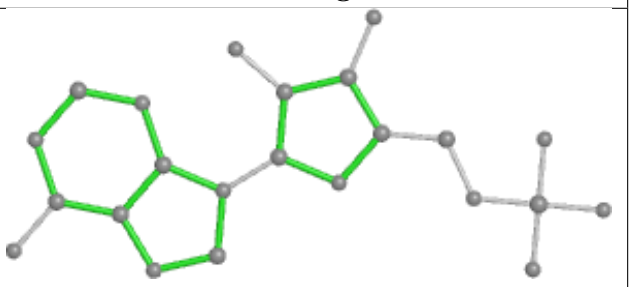
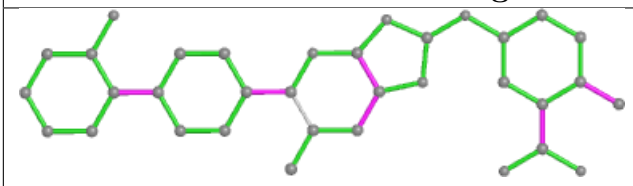
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CG7 A 602 (A)



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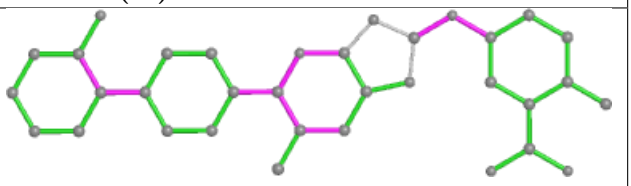

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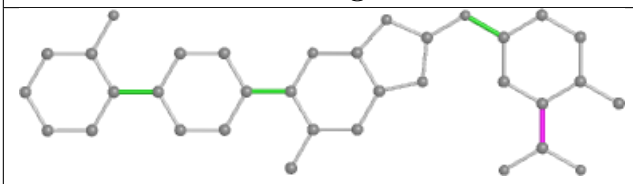

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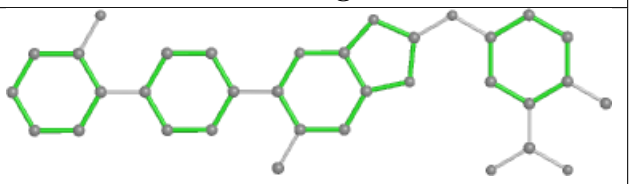

Rings

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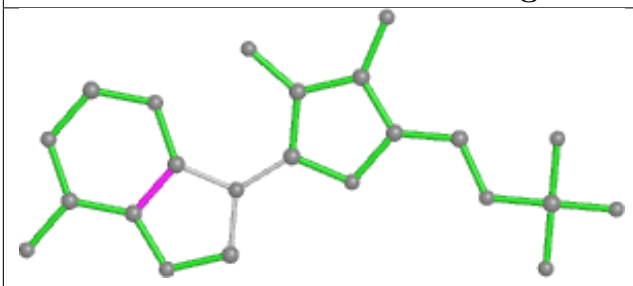

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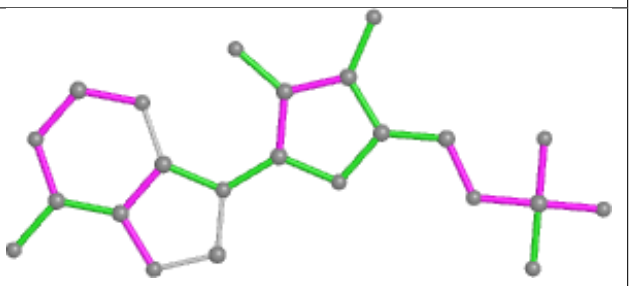

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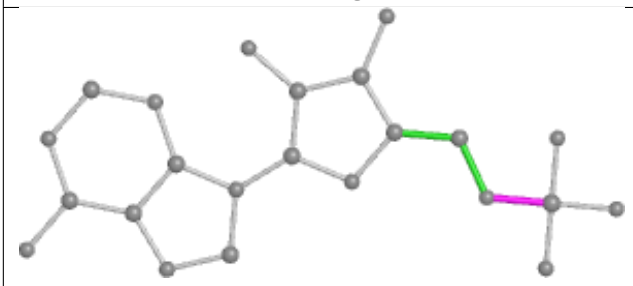

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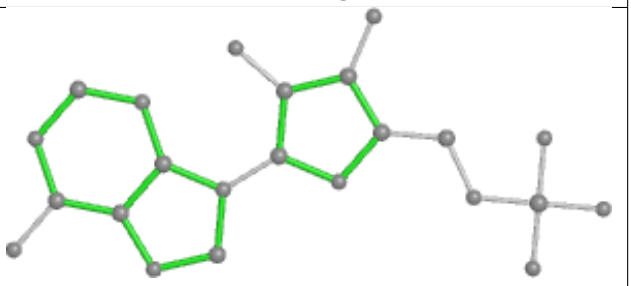
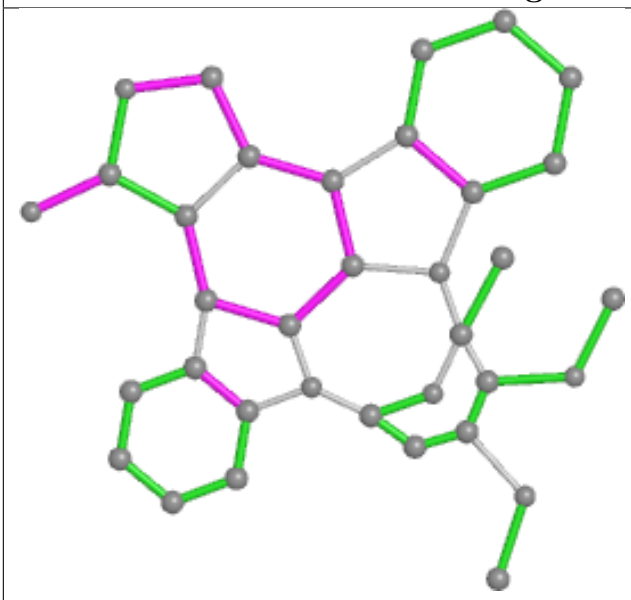


Rings

Ligand STU C 601



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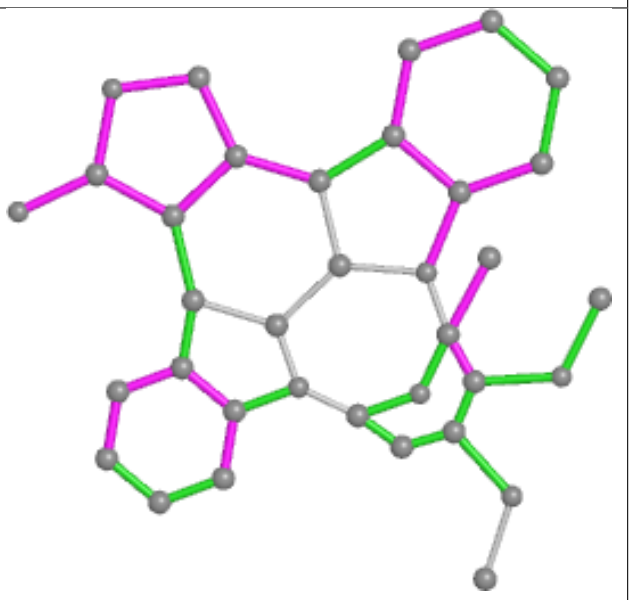

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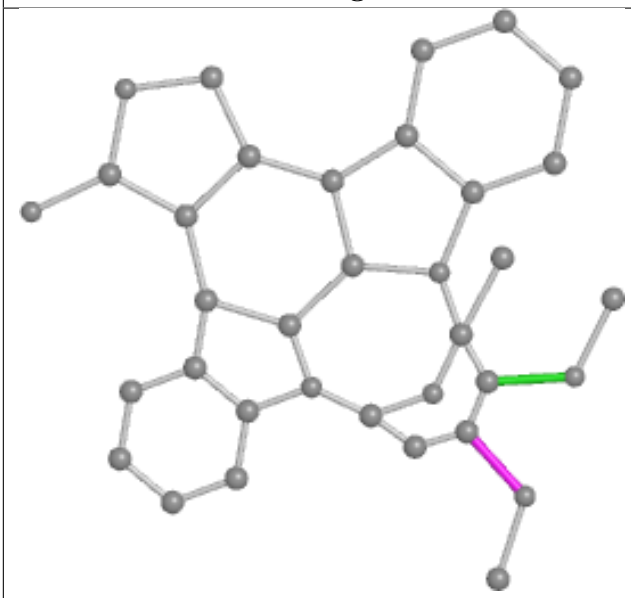

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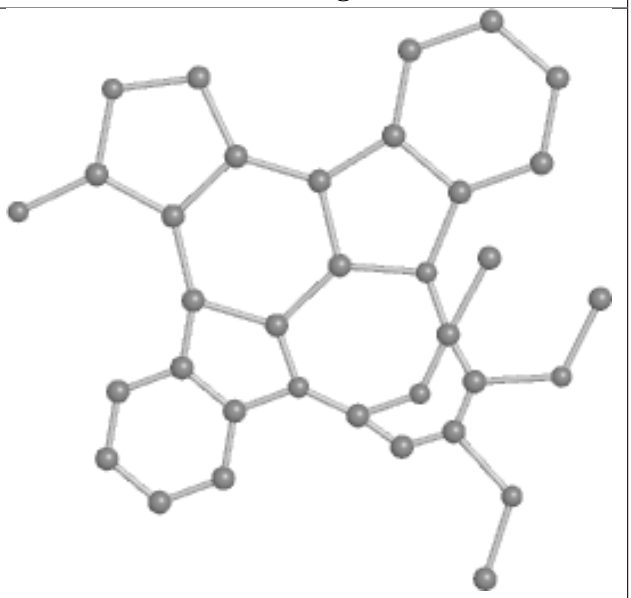
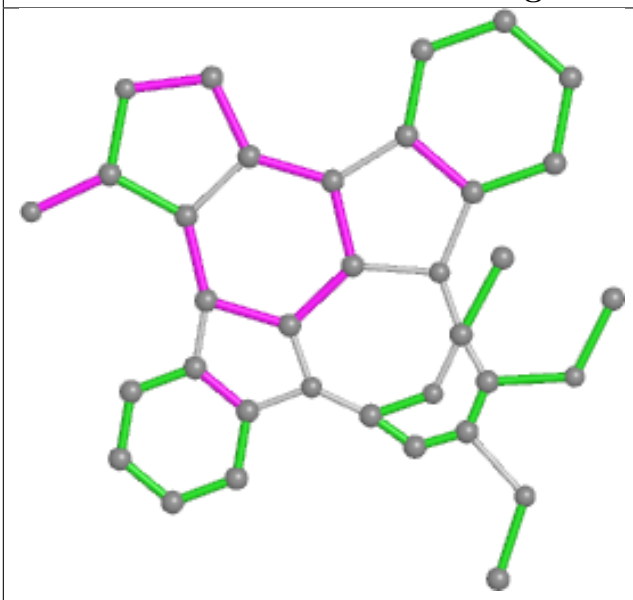


Rings

Ligand STU A 601



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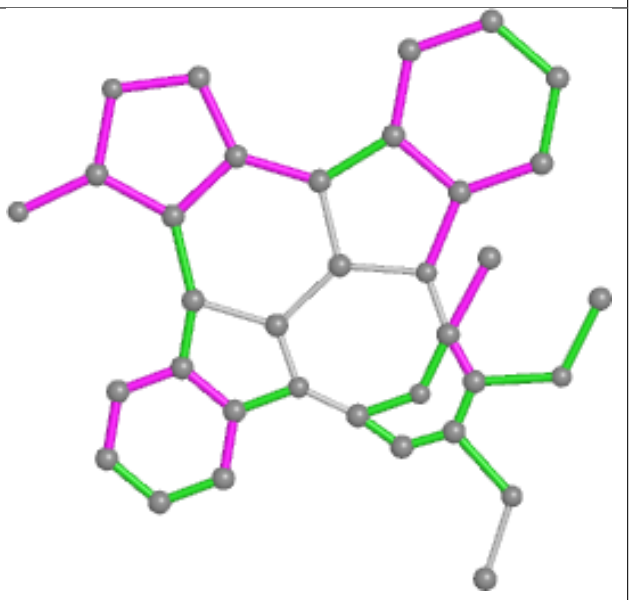

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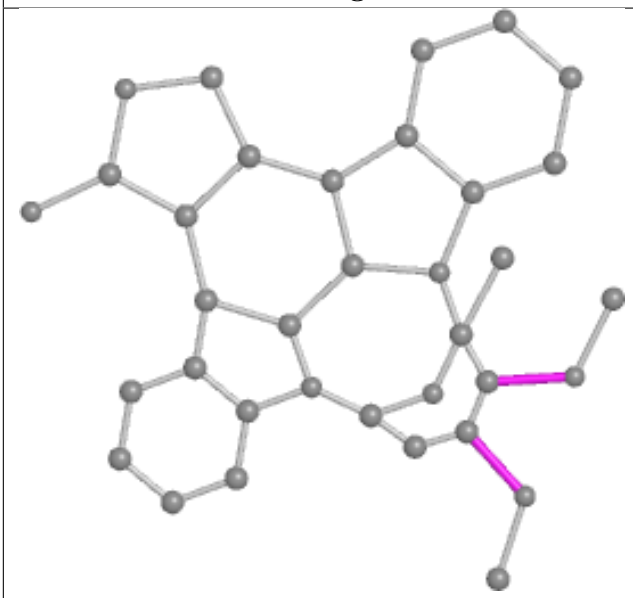

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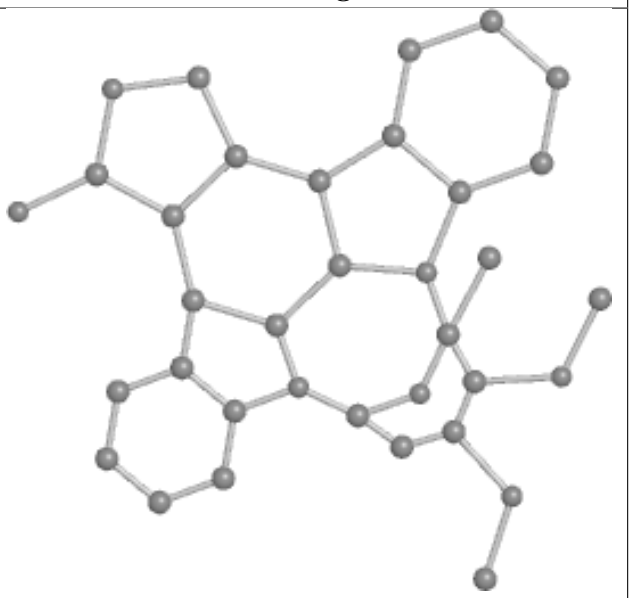
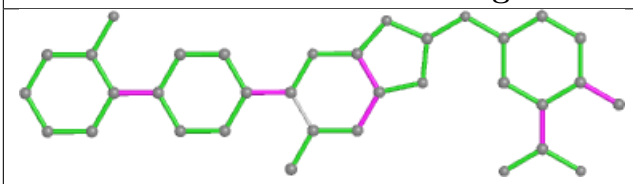


Rings

Ligand CG7 A 602 (B)



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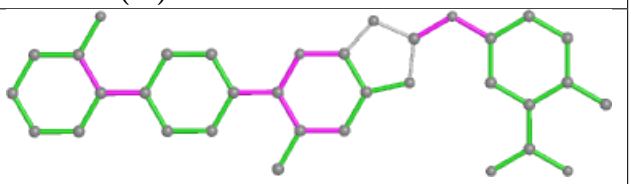
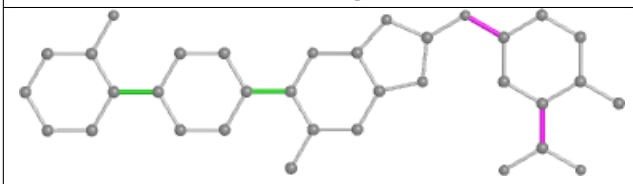
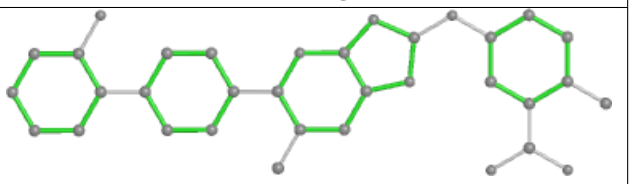


Bond angles

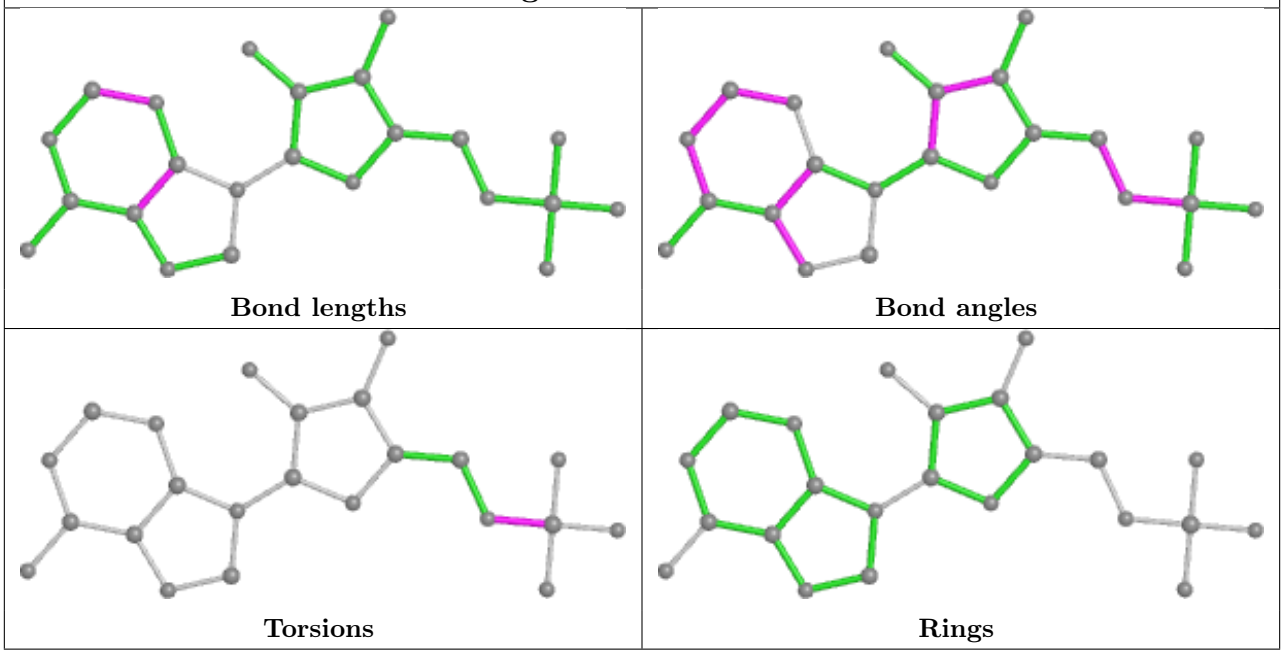


Torsions

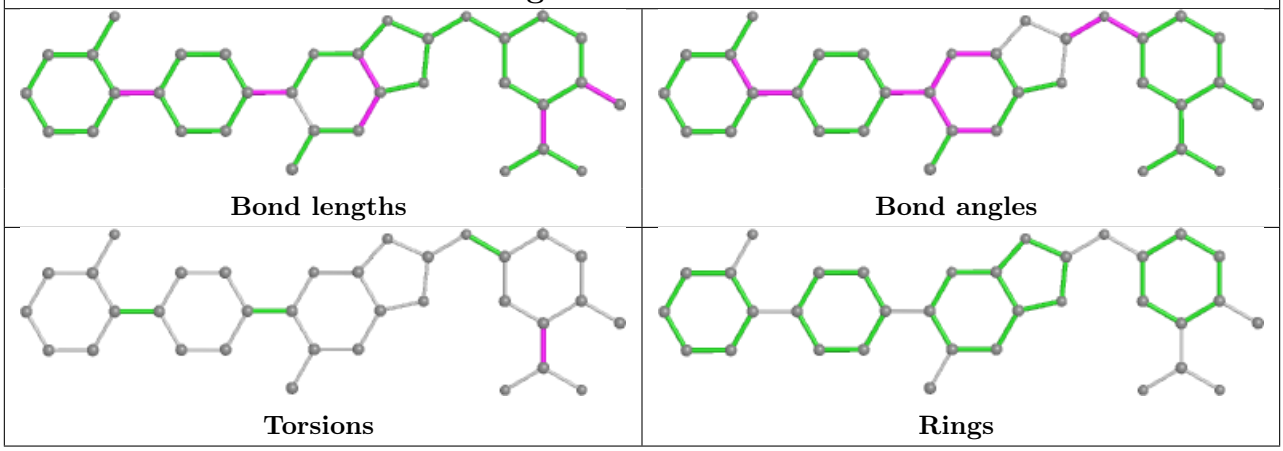


Rings

Ligand AMP F 401



Ligand CG7 C 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	441/565 (78%)	0.16	13 (2%)	51	46	39, 66, 111, 144	0
1	C	459/565 (81%)	0.17	22 (4%)	30	24	35, 63, 105, 128	0
2	B	183/270 (67%)	0.56	17 (9%)	8	6	38, 76, 121, 149	0
2	D	181/270 (67%)	0.19	6 (3%)	46	41	41, 60, 106, 151	0
3	E	299/336 (88%)	0.12	10 (3%)	46	41	37, 56, 94, 129	0
3	F	299/336 (88%)	0.06	9 (3%)	50	45	37, 59, 89, 134	0
All	All	1862/2342 (79%)	0.18	77 (4%)	37	32	35, 63, 106, 151	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	407	TYR	5.7
1	A	524	PRO	5.1
3	E	304	ASP	5.0
2	B	175	ASP	4.7
2	B	196	PRO	4.6
2	B	192	TYR	3.9
2	B	194	CYS	3.7
1	C	526	LEU	3.6
3	E	272	TYR	3.6
3	F	126	PHE	3.6
2	D	194	CYS	3.6
1	C	360	PRO	3.5
3	E	305	GLU	3.4
2	B	141	ILE	3.4
1	C	362	GLY	3.4
3	F	234	LYS	3.3
2	D	171	GLN	3.2
2	B	174	SER	3.2
2	B	171	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	525	ARG	3.1
3	E	306	ASN	3.0
2	B	97	PHE	3.0
3	F	280	TYR	2.9
2	B	120	GLU	2.9
2	B	193	VAL	2.9
1	A	344	SER	2.8
3	E	302	VAL	2.8
2	B	80	THR	2.8
1	C	402	SER	2.7
1	C	346	PRO	2.7
1	C	455	ASP	2.7
1	A	297	CYS	2.7
2	B	173	CYS	2.7
1	C	391	VAL	2.7
1	A	312	TYR	2.7
1	C	430	TYR	2.7
2	B	119	PRO	2.6
1	A	456	ASN	2.6
3	E	26	ASN	2.6
3	F	303	VAL	2.6
2	D	177	SER	2.6
1	C	301	GLU	2.5
3	E	125	SER	2.5
1	A	8	ASP	2.5
3	F	271	HIS	2.5
1	C	215	ASP	2.4
3	F	309	VAL	2.4
2	D	175	ASP	2.4
2	D	201	ARG	2.3
1	C	408	ASP	2.3
2	B	155	VAL	2.3
1	C	459	TYR	2.3
3	E	126	PHE	2.3
1	C	451	LEU	2.3
1	C	173	SER	2.3
1	C	406	PRO	2.2
1	A	321	ALA	2.2
1	C	400	ILE	2.2
1	A	298	GLU	2.2
2	B	198	GLU	2.2
3	F	272	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	174	CYS	2.1
2	B	219	THR	2.1
2	B	142	VAL	2.1
1	A	392	LYS	2.1
3	F	306	ASN	2.1
3	E	238	VAL	2.1
1	C	361	PRO	2.1
1	C	299	LYS	2.1
1	A	292	ALA	2.1
1	A	435	ARG	2.1
3	F	25	ASN	2.1
1	C	359	ILE	2.0
1	A	156	ALA	2.0
2	D	178	GLU	2.0
1	C	444	TYR	2.0
3	E	270	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	C	172	11/12	0.85	0.22	76,79,85,86	4
1	TPO	A	172	11/12	0.87	0.22	67,69,75,76	4
2	SEP	B	108	10/11	0.95	0.14	63,64,71,71	0
2	SEP	D	108	10/11	0.97	0.12	57,59,66,66	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

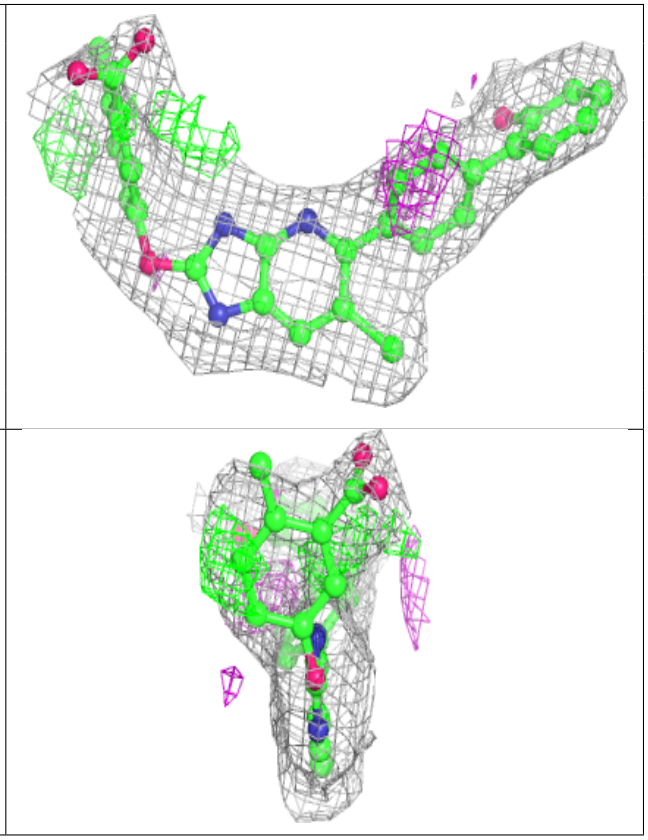
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CG7	A	602[A]	34/34	0.89	0.22	54,62,66,66	34
5	CG7	A	602[B]	34/34	0.89	0.22	49,56,58,58	34
6	IMD	C	603	5/5	0.89	0.33	86,87,87,87	0
5	CG7	C	602	34/34	0.94	0.21	41,45,67,69	0
4	STU	A	601	35/35	0.96	0.18	40,41,43,44	0
4	STU	C	601	35/35	0.96	0.18	36,38,43,43	0
7	AMP	E	401	23/23	0.97	0.16	49,52,57,58	0
7	AMP	F	402	23/23	0.97	0.16	47,52,56,57	0
7	AMP	F	401	23/23	0.98	0.17	46,48,50,51	0
7	AMP	E	402	23/23	0.98	0.14	48,51,54,55	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.

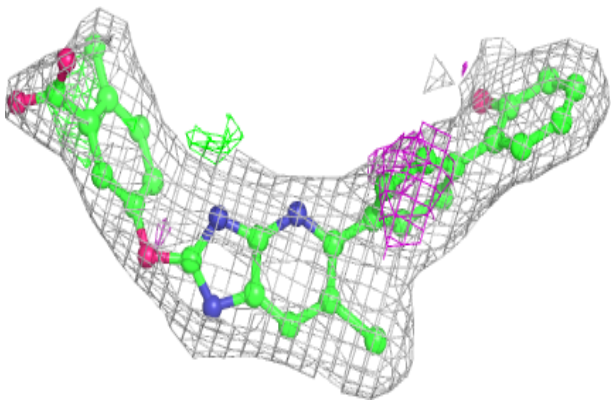
Electron density around CG7 A 602 (A):

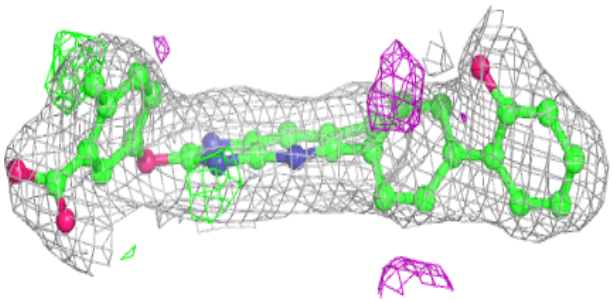
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

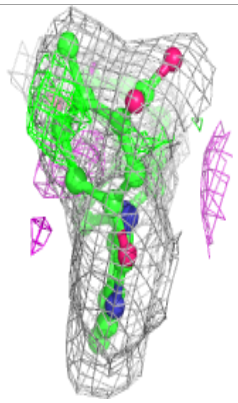


Electron density around CG7 A 602 (B):

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

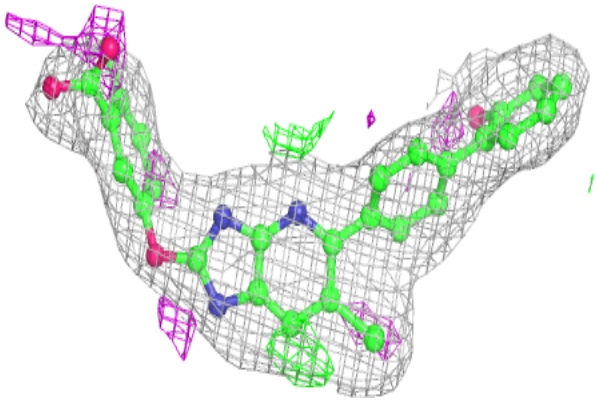


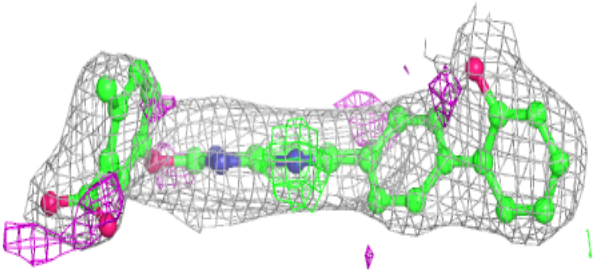


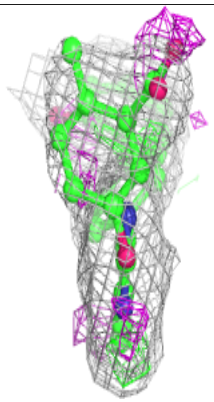


Electron density around CG7 C 602:

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







Electron density around STU A 601:

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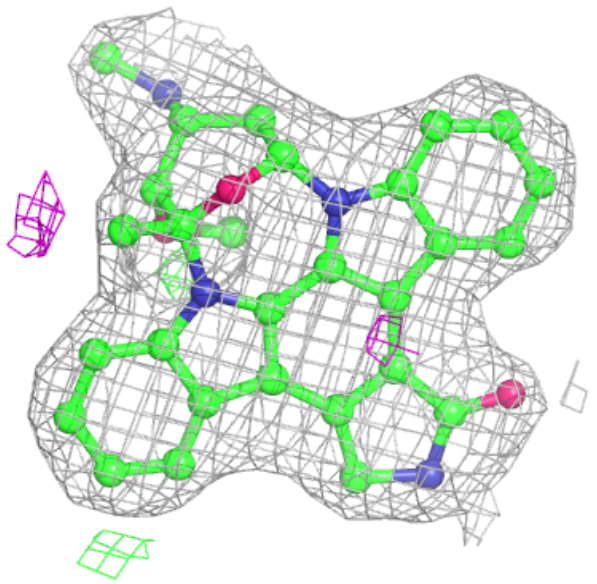
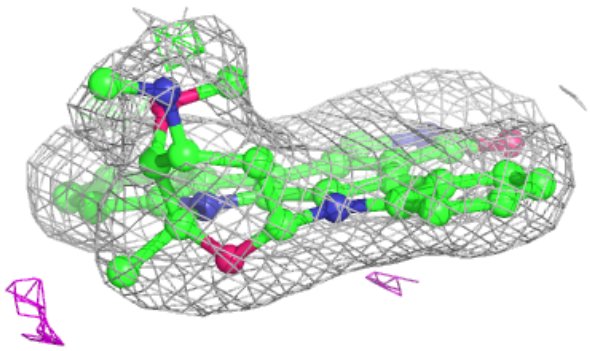
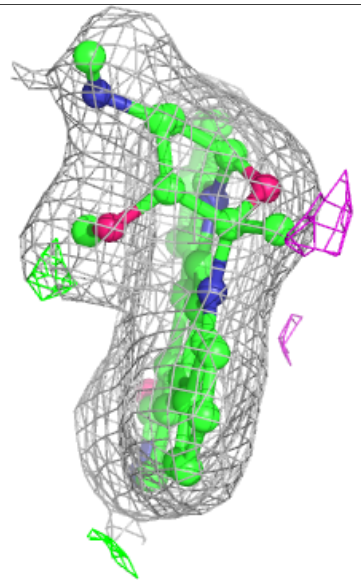
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around STU C 601:

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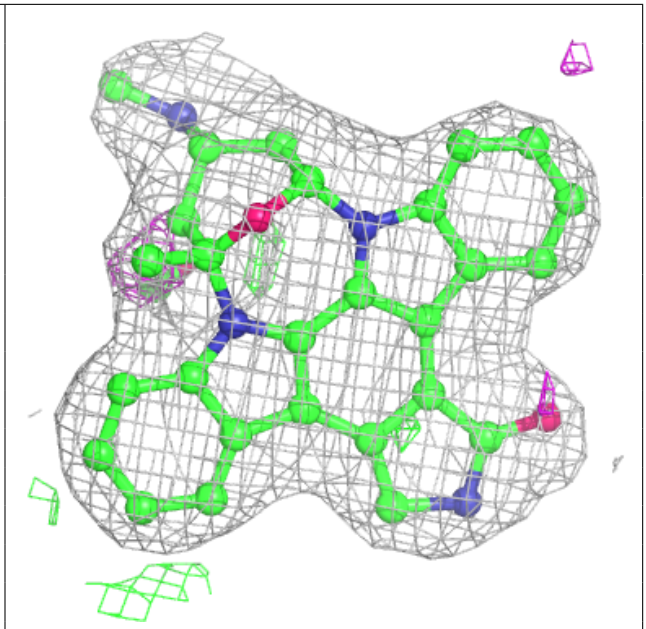
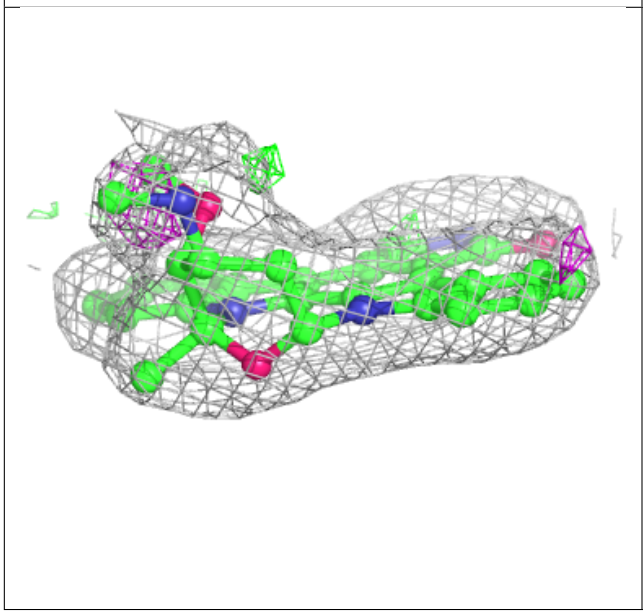
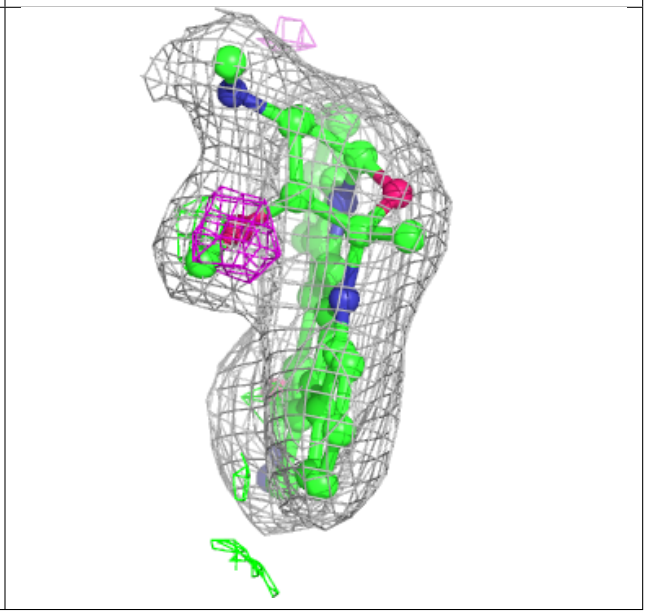
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

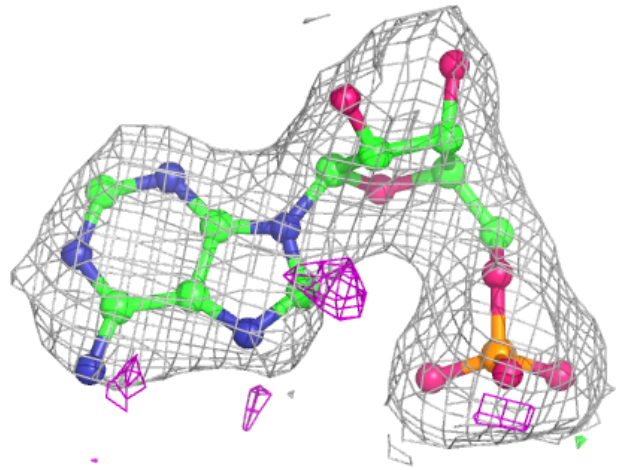


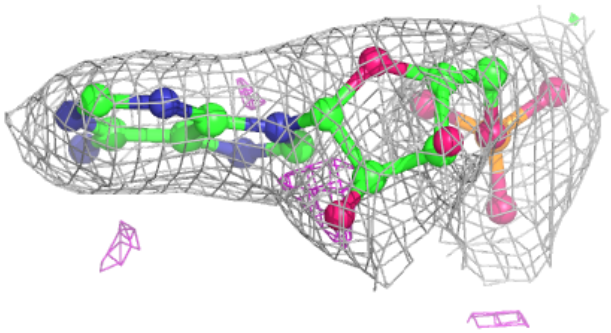


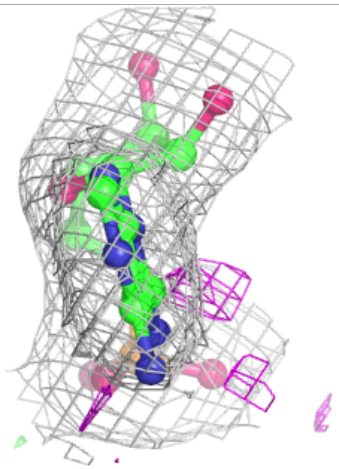


Electron density around AMP E 401:

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







Electron density around AMP F 402:

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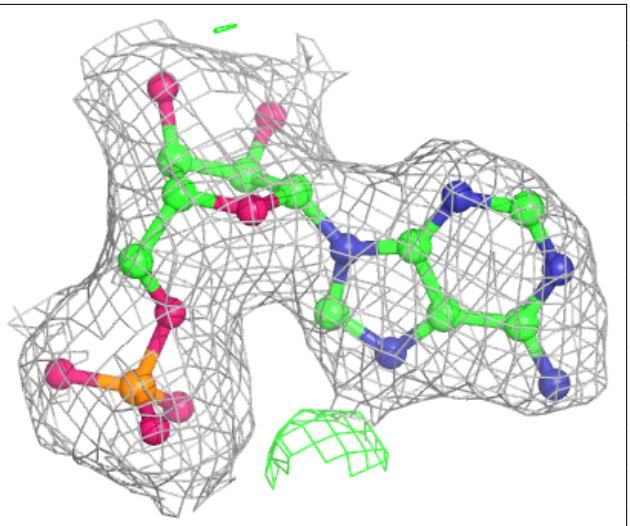
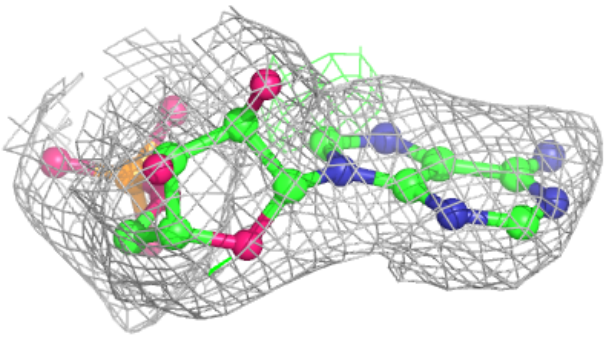
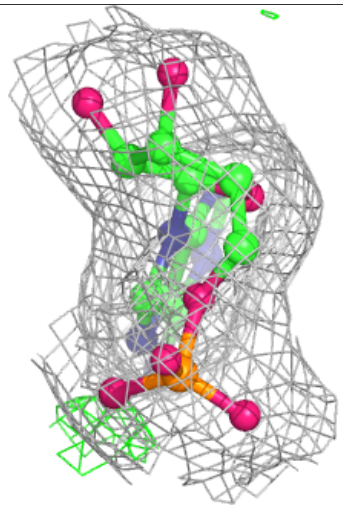
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

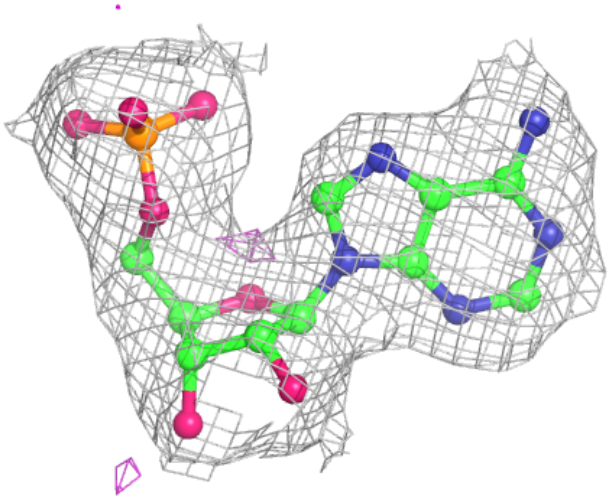


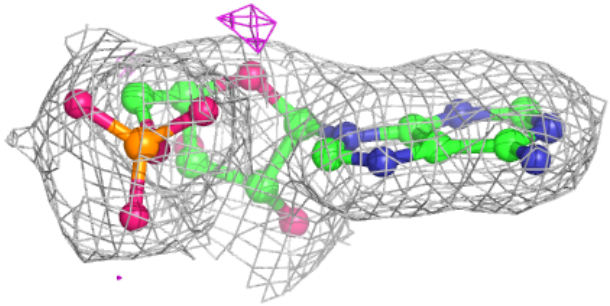


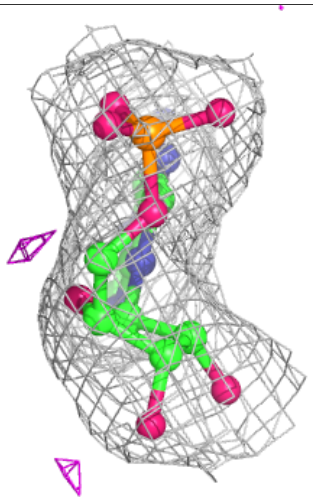


Electron density around AMP F 401:

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







Electron density around AMP E 402:

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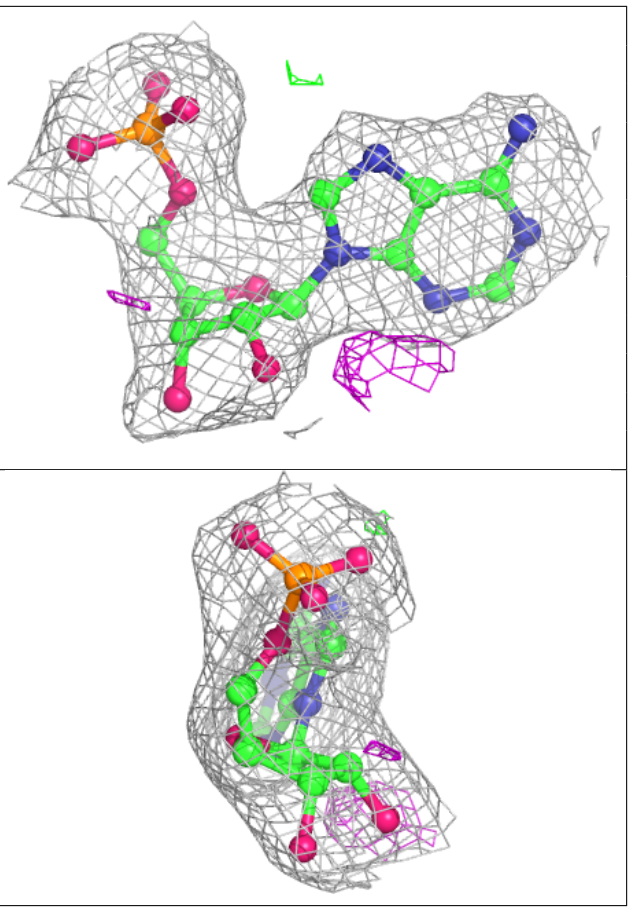
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.