



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:48 pm BST

PDB ID : 4LEZ  
Title : Structure of mouse cGAS bound to an 18bp DNA and cGAS product  
Authors : Li, P.  
Deposited on : 2013-06-26  
Resolution : 2.36 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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

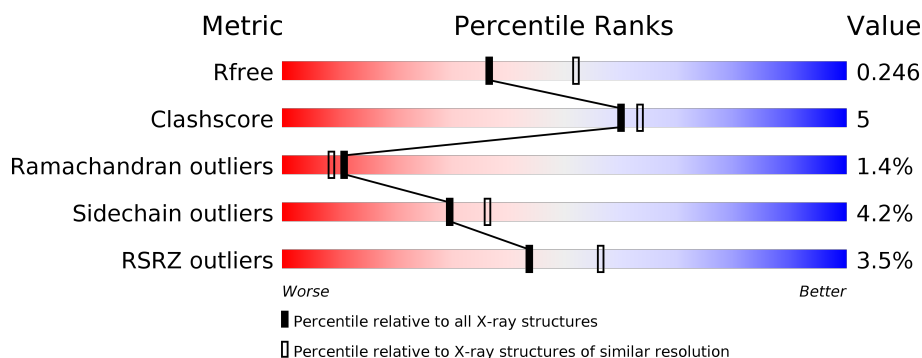
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	366	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>••</div> </div> </div>
1	C	366	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
2	E	18	<div> <div></div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
2	F	18	<div> <div></div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
2	I	18	<div> <div></div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
2	J	18	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7645 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2969	1910	506	540	13			
1	C	359	Total	C	N	O	S	0	0	0
			2969	1910	506	540	13			

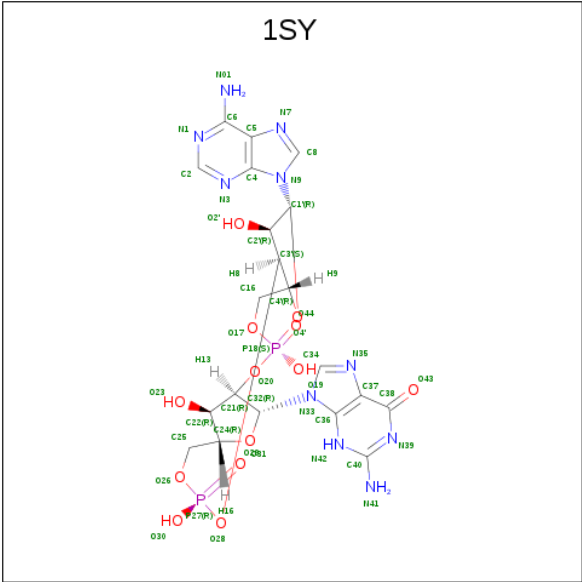
- Molecule 2 is a DNA chain called 18bp dsDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	F	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	I	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			
2	J	18	Total	C	N	O	P	0	0	0
			366	177	66	106	17			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is cGAMP (three-letter code: 1SY) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			45	20	10	13	2		
4	C	1	Total	C	N	O	P	0	0
			45	20	10	13	2		

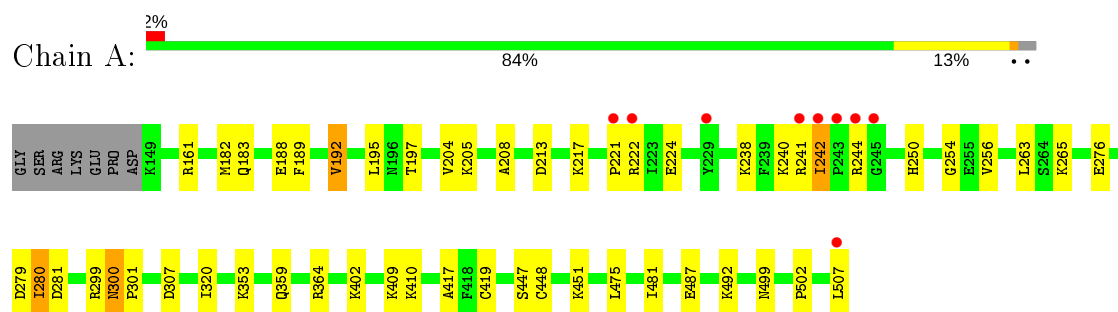
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	C	51	Total	O	0	0
			51	51		
5	E	16	Total	O	0	0
			16	16		
5	F	7	Total	O	0	0
			7	7		
5	I	7	Total	O	0	0
			7	7		
5	J	4	Total	O	0	0
			4	4		

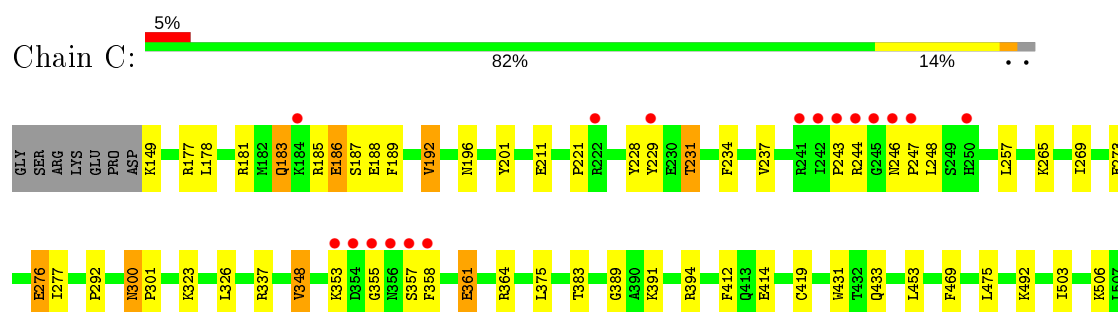
### 3 Residue-property plots [i](#)

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

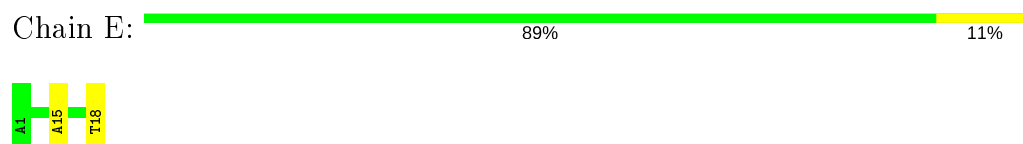
- Molecule 1: Cyclic GMP-AMP synthase



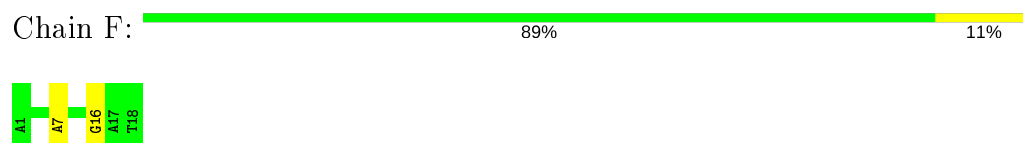
- Molecule 1: Cyclic GMP-AMP synthase



- Molecule 2: 18bp dsDNA

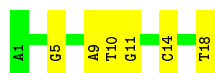


- Molecule 2: 18bp dsDNA




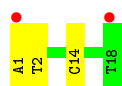
- Molecule 2: 18bp dsDNA

Chain I:  67% 33%



● Molecule 2: 18bp dsDNA

Chain J:  11% 83% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.21Å 99.03Å 142.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.55 – 2.36 33.55 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.6 (33.55-2.36) 87.8 (33.55-2.36)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.36Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.192 , 0.247 0.192 , 0.246	Depositor DCC
$R_{free}$ test set	2000 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 37.5	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	0.96	EDS
Total number of atoms	7645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5663e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1SY

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	0.42	0/3033	0.56	0/4071
1	C	0.40	0/3033	0.57	0/4071
2	E	0.69	0/410	1.30	1/631 (0.2%)
2	F	0.74	0/410	1.32	2/631 (0.3%)
2	I	0.64	0/410	1.28	3/631 (0.5%)
2	J	0.69	0/410	1.31	4/631 (0.6%)
All	All	0.48	0/7706	0.80	10/10666 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	15	DA	O4'-C1'-N9	9.91	114.94	108.00
2	F	7	DA	O4'-C1'-N9	-8.20	102.26	108.00
2	I	14	DC	O4'-C1'-N1	6.59	112.62	108.00
2	I	5	DG	O4'-C1'-N9	-5.94	103.84	108.00
2	J	14	DC	O4'-C1'-N1	5.80	112.06	108.00
2	J	14	DC	C3'-C2'-C1'	-5.47	95.94	102.50
2	F	16	DG	C3'-C2'-C1'	-5.24	96.22	102.50
2	J	2	DT	N3-C4-O4	5.19	123.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	14	DC	C1'-O4'-C4'	-5.06	105.04	110.10
2	I	14	DC	C3'-C2'-C1'	-5.06	96.43	102.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	ASN	Peptide
1	C	300	ASN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2969	0	3022	24	0
1	C	2969	0	3022	33	0
2	E	366	0	206	1	0
2	F	366	0	206	0	0
2	I	366	0	206	3	0
2	J	366	0	206	2	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	45	0	22	5	0
4	C	45	0	22	5	0
5	A	66	0	0	1	0
5	C	51	0	0	5	0
5	E	16	0	0	1	0
5	F	7	0	0	0	0
5	I	7	0	0	1	0
5	J	4	0	0	0	0
All	All	7645	0	6912	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (65) 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:364:ARG:HH21	4:C:602:1SY:H3	1.28	0.82
2:E:18:DT:OP2	5:E:110:HOH:O	2.00	0.80
2:I:11:DG:N7	5:I:104:HOH:O	2.16	0.79
4:A:602:1SY:O19	5:A:760:HOH:O	2.02	0.78
1:C:188:GLU:O	5:C:733:HOH:O	2.05	0.72
1:C:177:ARG:NH2	1:C:276:GLU:O	2.24	0.70
1:A:419:CYS:HB2	4:A:602:1SY:H16	1.80	0.62
4:A:602:1SY:H4	4:A:602:1SY:O17	2.03	0.59
1:A:364:ARG:HH21	4:A:602:1SY:H3	1.50	0.58
1:C:237:VAL:HG13	1:C:257:LEU:HB3	1.85	0.58
1:C:149:LYS:N	5:C:731:HOH:O	2.37	0.58
1:C:211:GLU:O	5:C:730:HOH:O	2.18	0.57
1:C:231:THR:HG21	1:C:234:PHE:HB2	1.86	0.57
4:C:602:1SY:O17	4:C:602:1SY:H4	2.06	0.56
1:A:238:LYS:HD3	1:A:256:VAL:HG12	1.88	0.56
1:A:205:LYS:HE2	1:A:208:ALA:O	2.05	0.56
1:C:181:ARG:O	1:C:185:ARG:HB3	2.07	0.55
1:A:242:ILE:HG22	1:A:244:ARG:HG2	1.89	0.55
1:C:419:CYS:HB2	4:C:602:1SY:H16	1.88	0.55
1:C:181:ARG:HH11	1:C:185:ARG:HH11	1.55	0.55
1:A:281:ASP:HB3	1:A:299:ARG:HB2	1.90	0.54
1:A:279:ASP:HB3	1:A:280:ILE:HD13	1.90	0.53
1:C:358:PHE:HB3	1:C:361:GLU:HG2	1.91	0.53
1:C:243:PRO:HB2	1:C:246:ASN:HD21	1.74	0.52
1:A:224:GLU:OE2	1:A:240:LYS:HG3	2.09	0.52
1:C:188:GLU:HA	1:C:247:PRO:HB3	1.92	0.52
1:C:433:GLN:NE2	5:C:718:HOH:O	2.43	0.51
1:C:364:ARG:NH2	4:C:602:1SY:H3	2.05	0.50
1:C:185:ARG:O	1:C:187:SER:N	2.38	0.50
1:C:181:ARG:NE	1:C:273:GLU:OE1	2.45	0.50
1:C:503:ILE:HG13	1:C:506:LYS:HD2	1.95	0.49
1:A:353:LYS:HA	1:A:359:GLN:NE2	2.28	0.49
1:A:195:LEU:HD12	1:A:217:LYS:HD3	1.96	0.47
1:A:188:GLU:OE1	1:A:265:LYS:NZ	2.46	0.47
1:C:337:ARG:NH1	5:C:751:HOH:O	2.34	0.46
2:I:18:DT:H3	2:J:1:DA:H61	1.62	0.46
1:C:228:TYR:OH	1:C:357:SER:HB3	2.15	0.46
1:A:410:LYS:HZ1	1:A:507:LEU:HD13	1.80	0.46
1:C:188:GLU:OE1	1:C:265:LYS:NZ	2.49	0.45
1:C:383:THR:O	1:C:389:GLY:HA3	2.16	0.45
1:C:364:ARG:NH2	4:C:602:1SY:N7	2.65	0.45
1:A:183:GLN:HE22	1:A:192:VAL:HG12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:MET:HG3	1:A:189:PHE:HB2	1.98	0.44
1:C:183:GLN:HB2	1:C:183:GLN:HE21	1.54	0.44
1:C:189:PHE:O	1:C:192:VAL:HB	2.18	0.44
1:A:417:ALA:HB1	1:A:481:ILE:HG12	2.00	0.43
1:C:394:ARG:HB3	1:C:431:TRP:CZ2	2.53	0.43
2:J:1:DA:H2'	2:J:1:DA:N3	2.33	0.43
1:A:204:VAL:O	1:A:402:LYS:HE2	2.19	0.42
1:A:448:CYS:O	1:A:451:LYS:HG2	2.19	0.42
1:C:326:LEU:HD13	1:C:469:PHE:CE2	2.53	0.42
1:A:492:LYS:HA	1:A:492:LYS:HD3	1.86	0.42
1:A:222:ARG:HH21	1:A:241:ARG:NH1	2.17	0.41
1:A:222:ARG:HE	1:A:241:ARG:HD3	1.85	0.41
1:A:197:THR:O	1:A:213:ASP:HB2	2.20	0.41
1:C:181:ARG:HD2	1:C:185:ARG:HD2	2.01	0.41
1:A:189:PHE:O	1:A:192:VAL:HB	2.21	0.41
1:C:196:ASN:HB3	1:C:201:TYR:CD2	2.56	0.41
1:C:292:PRO:HB3	1:C:348:VAL:HG13	2.03	0.41
1:C:353:LYS:C	1:C:355:GLY:H	2.24	0.41
1:A:307:ASP:OD2	4:A:602:1SY:H9	2.21	0.40
1:A:499:ASN:O	1:A:502:PRO:HD3	2.21	0.40
1:C:412:PHE:CZ	1:C:492:LYS:HE3	2.57	0.40
2:I:9:DA:H2'	2:I:10:DT:C6	2.57	0.40
1:C:185:ARG:CZ	1:C:269:ILE:HG12	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	357/366 (98%)	341 (96%)	12 (3%)	4 (1%)	14	13
1	C	357/366 (98%)	333 (93%)	18 (5%)	6 (2%)	9	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	714/732 (98%)	674 (94%)	30 (4%)	10 (1%)	11	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	301	PRO
1	C	186	GLU
1	C	300	ASN
1	C	229	TYR
1	C	301	PRO
1	C	221	PRO
1	C	244	ARG
1	A	254	GLY
1	A	300	ASN

### 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	332/338 (98%)	320 (96%)	12 (4%)	35	43
1	C	332/338 (98%)	316 (95%)	16 (5%)	25	30
All	All	664/676 (98%)	636 (96%)	28 (4%)	30	36

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ARG
1	A	192	VAL
1	A	242	ILE
1	A	250	HIS
1	A	263	LEU
1	A	276	GLU
1	A	280	ILE
1	A	320	ILE

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Mol	Chain	Res	Type
1	A	409	LYS
1	A	447	SER
1	A	475	LEU
1	A	487	GLU
1	C	178	LEU
1	C	183	GLN
1	C	186	GLU
1	C	192	VAL
1	C	231	THR
1	C	248	LEU
1	C	276	GLU
1	C	277	ILE
1	C	323	LYS
1	C	348	VAL
1	C	361	GLU
1	C	375	LEU
1	C	391	LYS
1	C	414	GLU
1	C	453	LEU
1	C	475	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	C	246	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1SY	A	602	-	43,51,51	1.79	11 (25%)	52,80,80	1.85	10 (19%)
4	1SY	C	602	-	43,51,51	1.78	11 (25%)	52,80,80	1.83	9 (17%)

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	1SY	A	602	-	-	6/22/62/62	0/6/7/7
4	1SY	C	602	-	-	7/22/62/62	0/6/7/7

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	1SY	O43-C38	6.33	1.40	1.24
4	C	602	1SY	O43-C38	6.02	1.39	1.24
4	C	602	1SY	C40-N41	3.64	1.41	1.33
4	C	602	1SY	C22-C21	-3.30	1.45	1.52
4	A	602	1SY	C40-N41	3.29	1.40	1.33
4	A	602	1SY	C6-N01	3.22	1.45	1.34
4	C	602	1SY	C6-N01	3.20	1.45	1.34
4	A	602	1SY	O4'-C1'	3.16	1.45	1.41
4	C	602	1SY	O4'-C1'	3.07	1.45	1.41
4	A	602	1SY	C22-C21	-2.83	1.46	1.52
4	A	602	1SY	C2'-C3'	-2.79	1.46	1.52
4	A	602	1SY	O31-C32	2.78	1.45	1.41
4	C	602	1SY	C2'-C1'	-2.65	1.49	1.53
4	C	602	1SY	C3'-C4'	-2.64	1.45	1.52
4	C	602	1SY	C22-C24	-2.56	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	1SY	C2'-C1'	-2.54	1.49	1.53
4	C	602	1SY	C2'-C3'	-2.53	1.47	1.52
4	C	602	1SY	O31-C24	2.46	1.50	1.45
4	A	602	1SY	C22-C24	-2.42	1.46	1.53
4	C	602	1SY	O31-C32	2.40	1.44	1.41
4	A	602	1SY	O31-C24	2.36	1.50	1.45
4	A	602	1SY	C3'-C4'	-2.12	1.47	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	1SY	C40-N42-C36	6.65	122.95	115.36
4	C	602	1SY	C40-N42-C36	6.41	122.67	115.36
4	A	602	1SY	N3-C2-N1	-4.94	120.96	128.68
4	C	602	1SY	N3-C2-N1	-4.64	121.43	128.68
4	C	602	1SY	N42-C40-N39	-4.48	121.24	127.22
4	A	602	1SY	N42-C40-N39	-4.35	121.42	127.22
4	A	602	1SY	C36-C37-N35	-3.78	105.46	109.40
4	C	602	1SY	C38-C37-C36	-3.55	117.40	120.80
4	C	602	1SY	C36-C37-N35	-3.51	105.74	109.40
4	A	602	1SY	C38-C37-C36	-3.47	117.48	120.80
4	C	602	1SY	C4-C5-N7	-3.29	105.97	109.40
4	A	602	1SY	C38-N39-C40	2.79	120.35	115.93
4	C	602	1SY	C38-N39-C40	2.69	120.21	115.93
4	A	602	1SY	C37-C38-N39	-2.52	119.98	123.43
4	A	602	1SY	C4-C5-N7	-2.43	106.86	109.40
4	A	602	1SY	O31-C32-C21	-2.33	102.55	106.59
4	C	602	1SY	C37-C38-N39	-2.31	120.28	123.43
4	A	602	1SY	C2-N1-C6	2.18	122.49	118.75
4	C	602	1SY	C2-N1-C6	2.11	122.36	118.75

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	1SY	C21-O20-P18-O17
4	A	602	1SY	C21-O20-P18-O44
4	C	602	1SY	C21-O20-P18-O17
4	C	602	1SY	C21-O20-P18-O44
4	C	602	1SY	C25-O26-P27-O28
4	A	602	1SY	C25-O26-P27-O28
4	C	602	1SY	C16-O17-P18-O20

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Mol	Chain	Res	Type	Atoms
4	A	602	1SY	C16-O17-P18-O20
4	A	602	1SY	C16-O17-P18-O44
4	A	602	1SY	C25-O26-P27-O30
4	C	602	1SY	C16-O17-P18-O44
4	C	602	1SY	C25-O26-P27-O29
4	C	602	1SY	C25-O26-P27-O30

There are no ring outliers.

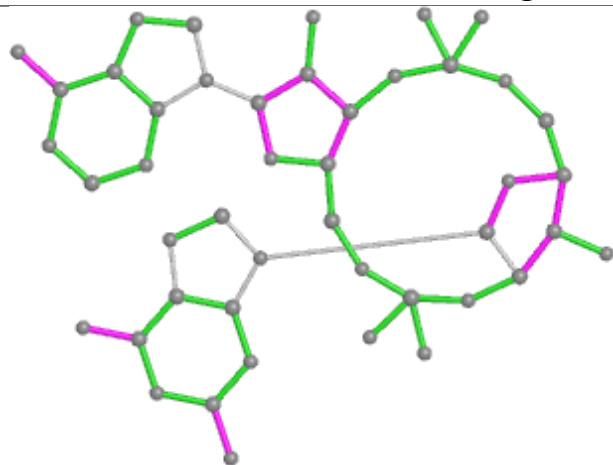
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	1SY	5	0
4	C	602	1SY	5	0

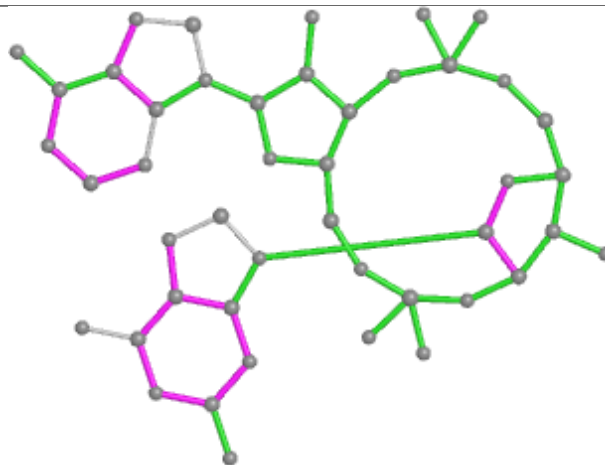
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



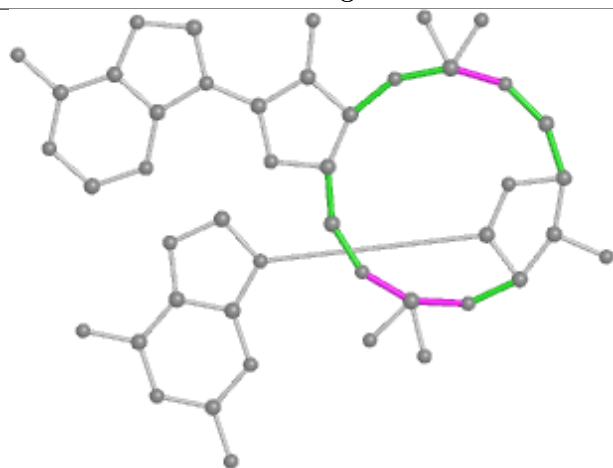
## Ligand 1SY A 602



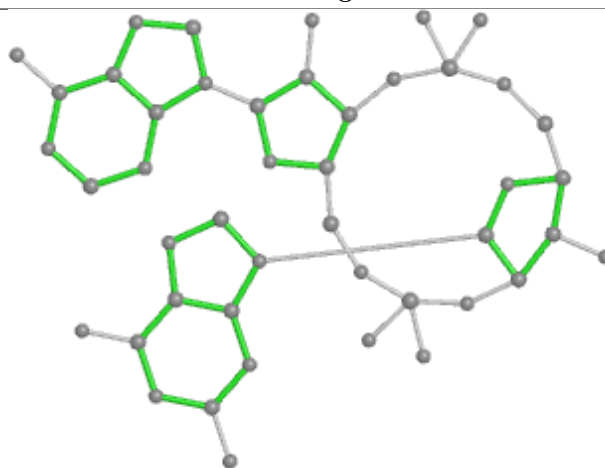
Bond lengths



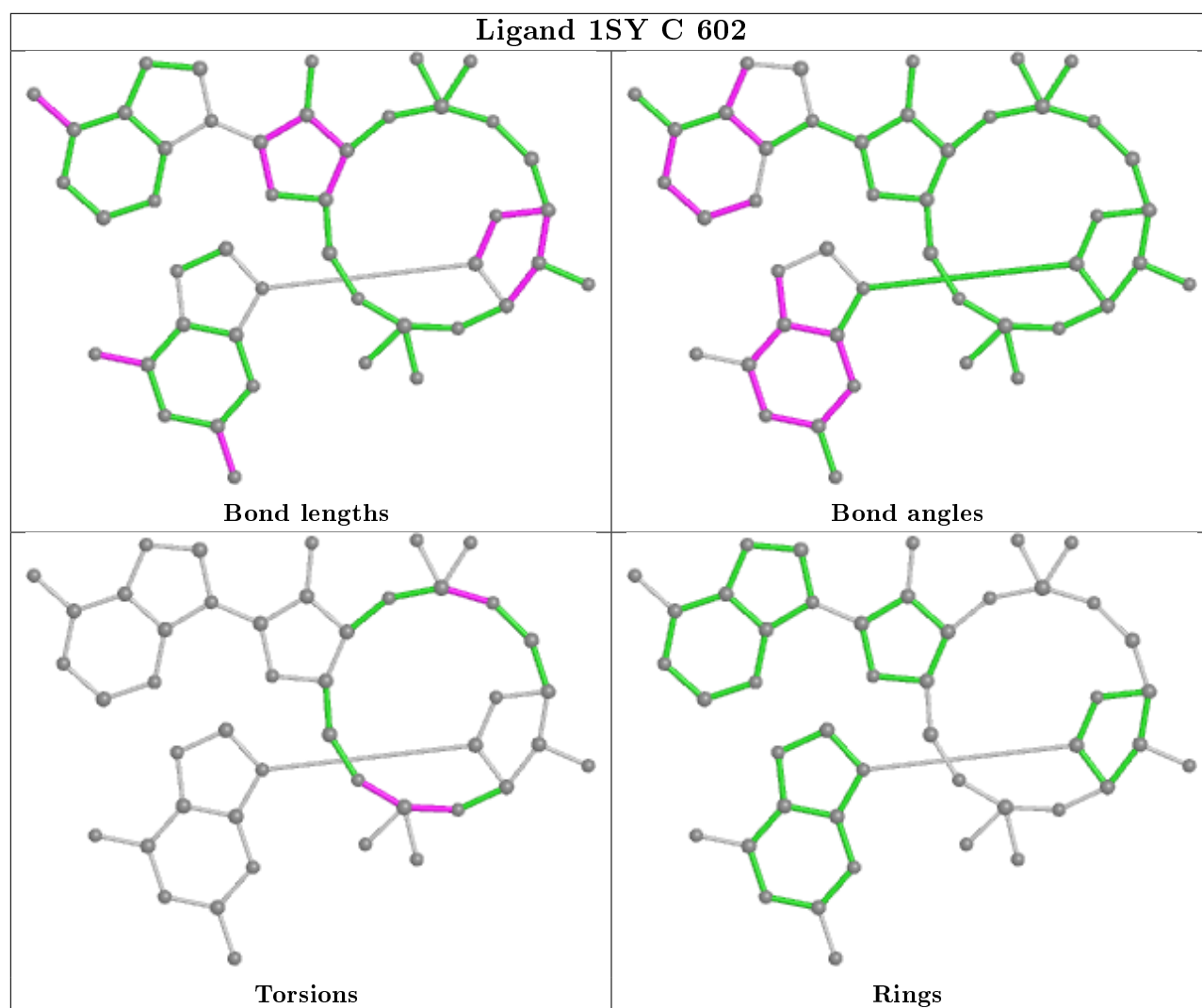
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	359/366 (98%)	-0.09	9 (2%) 57 67	36, 59, 106, 161	0
1	C	359/366 (98%)	0.03	17 (4%) 31 44	35, 64, 130, 167	0
2	E	18/18 (100%)	-0.36	0 100 100	43, 73, 140, 142	0
2	F	18/18 (100%)	-0.45	0 100 100	49, 79, 127, 145	0
2	I	18/18 (100%)	-0.14	0 100 100	47, 76, 138, 139	0
2	J	18/18 (100%)	0.03	2 (11%) 5 8	51, 87, 158, 159	0
All	All	790/804 (98%)	-0.05	28 (3%) 44 56	35, 62, 130, 167	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	ILE	8.3
1	C	245	GLY	6.0
1	A	243	PRO	5.4
1	C	244	ARG	4.8
1	C	358	PHE	4.4
1	A	245	GLY	4.3
1	C	241	ARG	4.3
1	C	356	ASN	4.1
1	C	247	PRO	4.0
1	C	357	SER	4.0
1	C	354	ASP	3.9
1	C	184	LYS	3.8
1	A	222	ARG	3.7
1	A	244	ARG	3.7
1	A	242	ILE	3.6
1	A	507	LEU	3.5
1	C	243	PRO	3.4
1	A	241	ARG	3.3
1	C	355	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	18	DT	3.0
1	C	353	LYS	2.6
1	C	229	TYR	2.5
1	C	246	ASN	2.4
1	C	222	ARG	2.4
1	C	250	HIS	2.2
2	J	1	DA	2.2
1	A	229	TYR	2.1
1	A	221	PRO	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

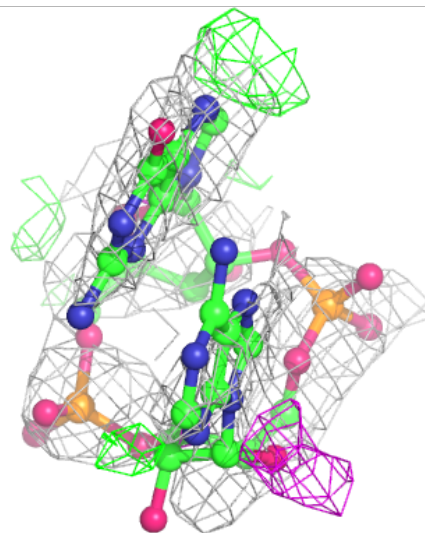
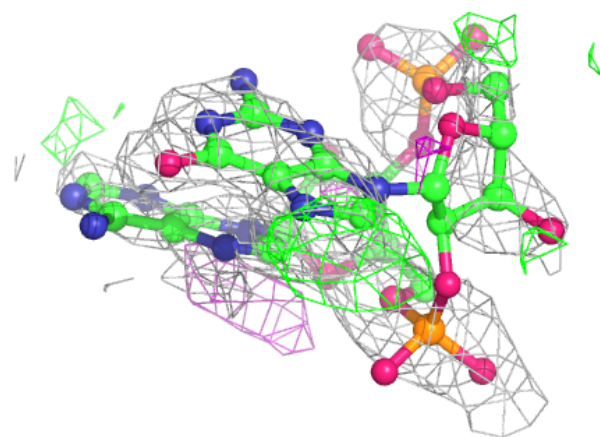
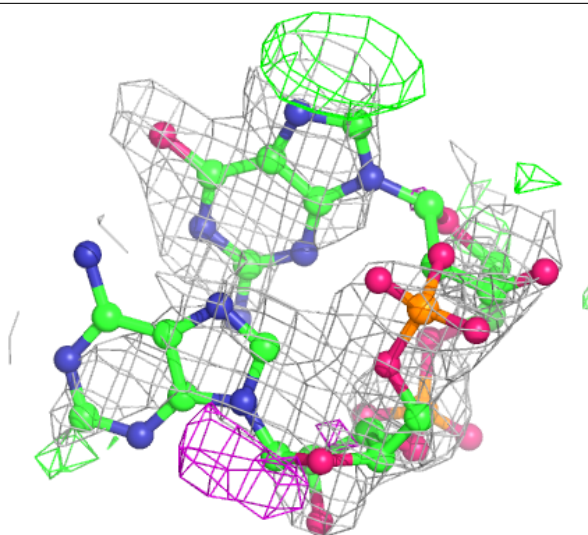
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	1SY	A	602	45/45	0.71	0.33	62,89,117,141	45
4	1SY	C	602	45/45	0.89	0.25	43,61,76,84	45
3	ZN	A	601	1/1	0.99	0.13	44,44,44,44	0
3	ZN	C	601	1/1	0.99	0.12	43,43,43,43	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.

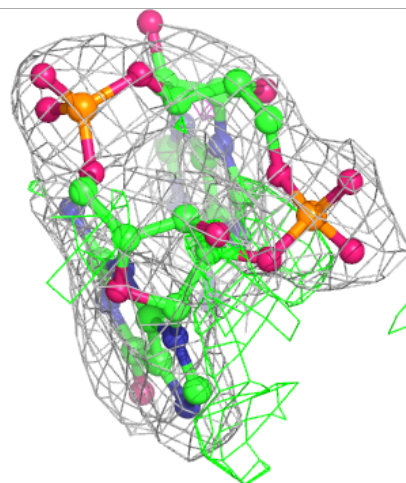
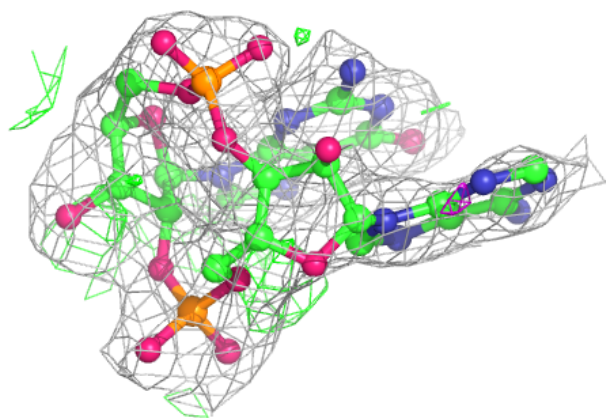
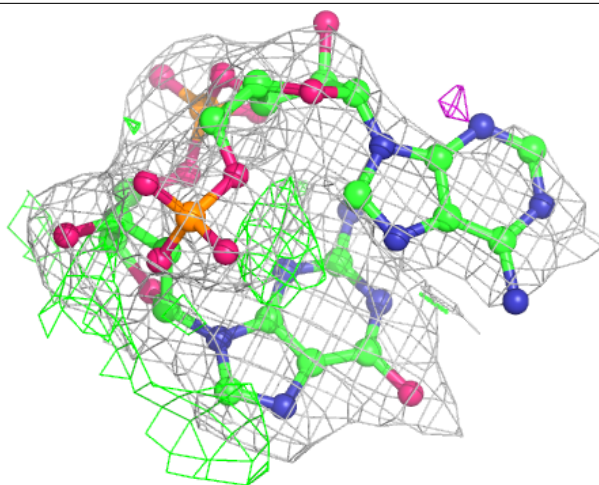
**Electron density around 1SY A 602:**

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 1SY C 602:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.