



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:21 PM EDT

PDB ID : 6HYQ  
Title : Regulatory subunit of a cAMP-independent protein kinase A from Trypanosoma cruzi bound to guanosine  
Authors : Volpato Santos, Y.; Lorentzen, E.; Basquin, J.; Boshart, M.  
Deposited on : 2018-10-22  
Resolution : 2.08 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

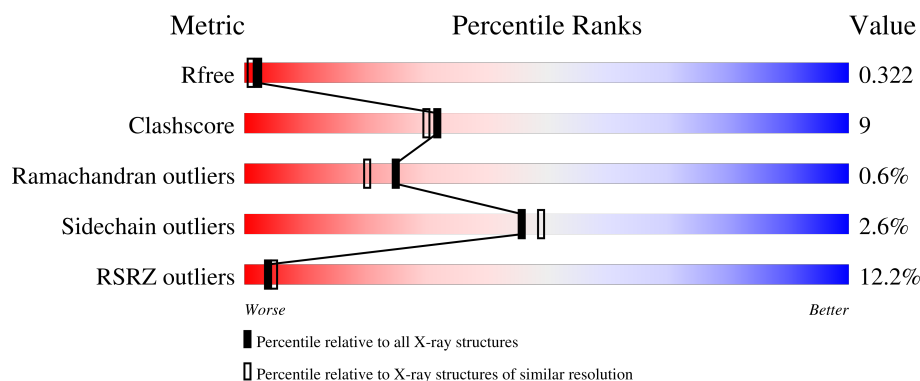
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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  $\geq 3$ , 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	304	
1	B	304	
1	C	304	
1	D	304	

## 2 Entry composition [i](#)

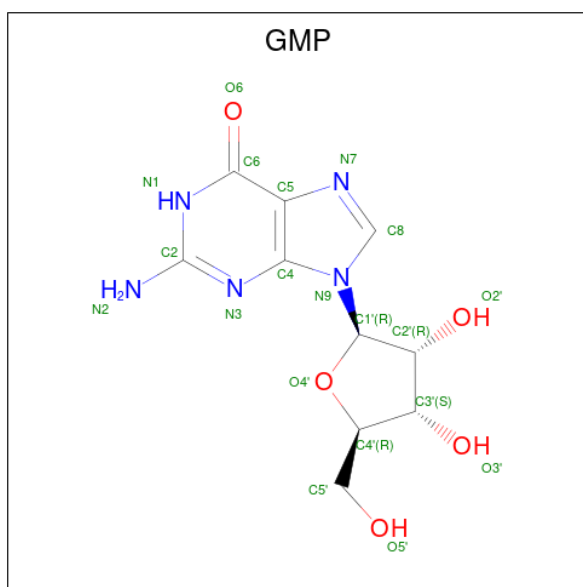
There are 4 unique types of molecules in this entry. The entry contains 18613 atoms, of which 9167 are hydrogens and 0 are deuteriums.

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 Protein kinase A regulatory subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	280	Total	C	H	N	O	S	21	13	0
			4510	1441	2255	369	430	15			
1	B	282	Total	C	H	N	O	S	6	13	0
			4553	1461	2265	374	438	15			
1	C	284	Total	C	H	N	O	S	16	13	0
			4591	1465	2295	377	439	15			
1	D	279	Total	C	H	N	O	S	1	14	0
			4522	1451	2252	371	433	15			

- Molecule 2 is GUANOSINE (three-letter code: GMP) (formula:  $C_{10}H_{13}N_5O_5$ ) (labeled as "Ligand of Interest" by depositor).



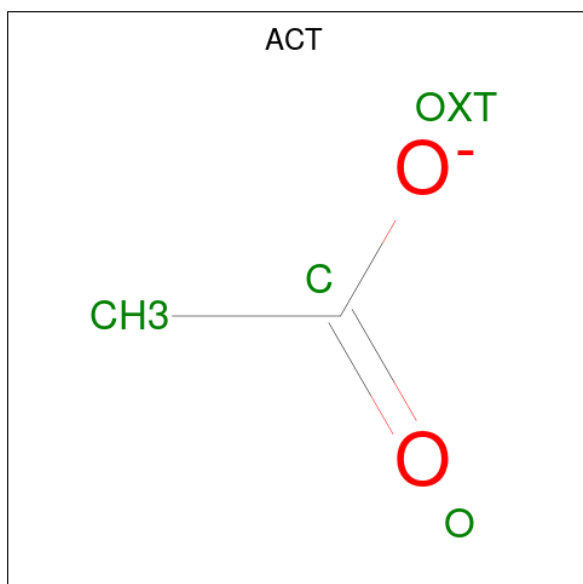
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			32	10	12	5	5		
2	A	1	Total	C	H	N	O	0	0
			32	10	12	5	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			32	10	12	5	5		
2	B	1	Total	C	H	N	O	0	0
			32	10	12	5	5		
2	C	1	Total	C	H	N	O	0	0
			32	10	12	5	5		
2	C	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
2	D	1	Total	C	H	N	O	0	0
			32	10	12	5	5		
2	D	1	Total	C	H	N	O	0	0
			32	10	12	5	5		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	41	Total	O	0	0
			41	41		

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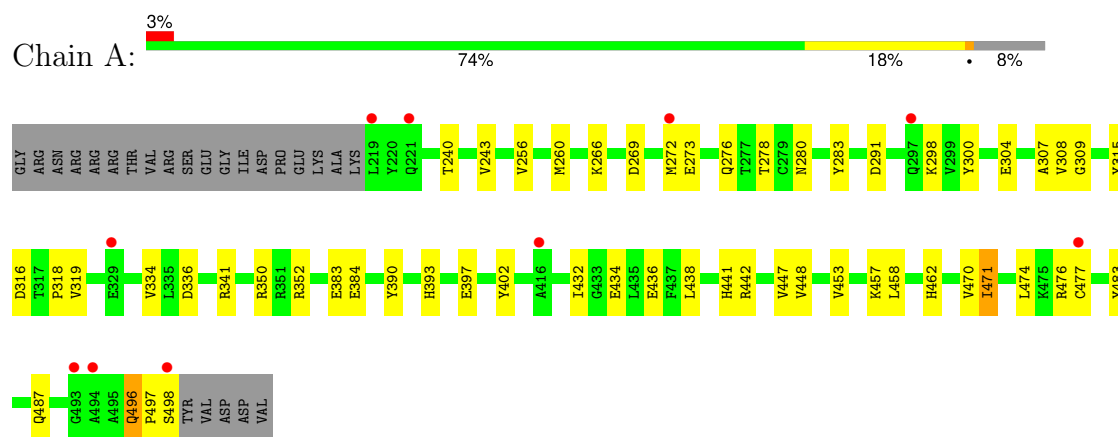
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	45	Total 45	O 45	0	0
4	D	39	Total 39	O 39	0	0

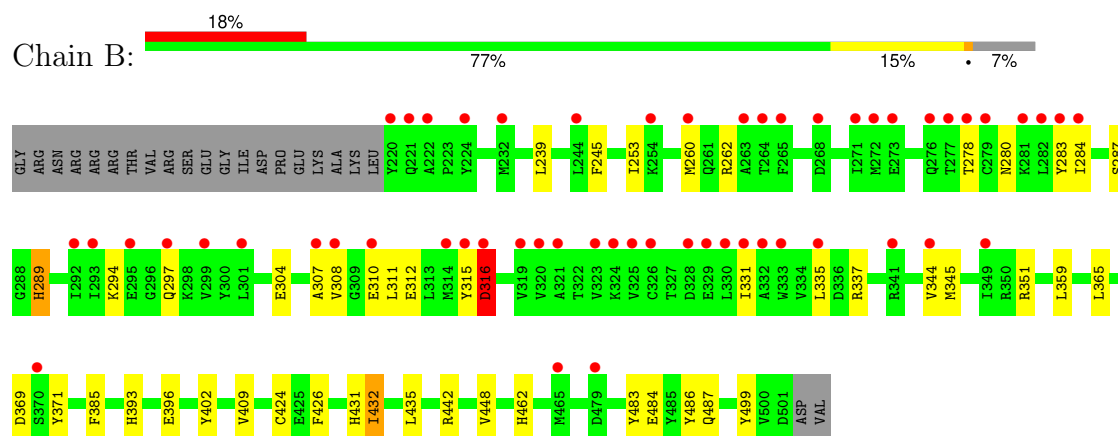
### 3 Residue-property plots [i](#)

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.

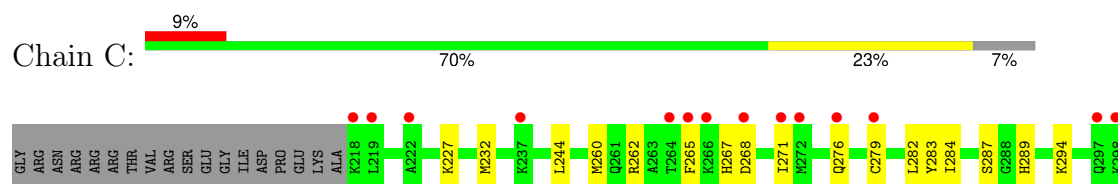
#### • Molecule 1: Protein kinase A regulatory subunit

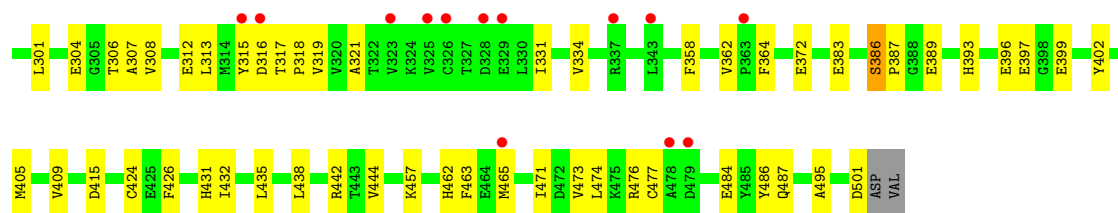


#### • Molecule 1: Protein kinase A regulatory subunit

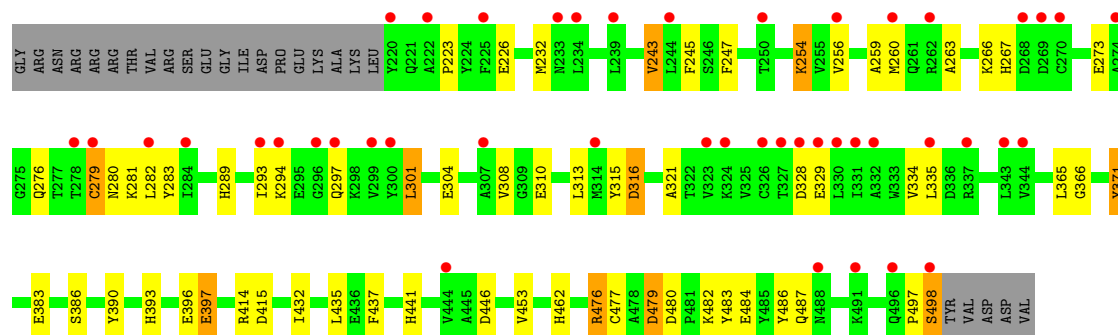


#### • Molecule 1: Protein kinase A regulatory subunit





● Molecule 1: Protein kinase A regulatory subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.91Å 80.82Å 149.34Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	59.84 – 2.08 59.84 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.7 (59.84-2.08) 85.8 (59.84-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.260 , 0.319 0.264 , 0.322	Depositor DCC
$R_{free}$ test set	4281 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: ACT, GMP

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	0.96	8/2351 (0.3%)	0.95	6/3188 (0.2%)
1	B	0.88	2/2379 (0.1%)	0.89	3/3225 (0.1%)
1	C	0.85	2/2385 (0.1%)	0.89	3/3227 (0.1%)
1	D	0.88	5/2359 (0.2%)	0.92	6/3197 (0.2%)
All	All	0.89	17/9474 (0.2%)	0.91	18/12837 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	477	CYS	CB-SG	6.75	1.93	1.82
1	D	243	VAL	CB-CG2	6.39	1.66	1.52
1	A	447	VAL	CB-CG1	6.16	1.65	1.52
1	B	385	PHE	CE2-CZ	5.95	1.48	1.37
1	A	243	VAL	CB-CG2	5.86	1.65	1.52
1	A	315	TYR	CD2-CE2	5.86	1.48	1.39
1	A	448	VAL	CB-CG1	-5.71	1.40	1.52
1	A	397	GLU	CB-CG	5.56	1.62	1.52
1	A	397	GLU	CG-CD	5.54	1.60	1.51
1	C	397	GLU	CB-CG	5.50	1.62	1.52
1	D	453	VAL	CB-CG2	5.46	1.64	1.52
1	D	247	PHE	CE2-CZ	5.39	1.47	1.37
1	D	486	TYR	CB-CG	-5.35	1.43	1.51
1	B	448	VAL	CB-CG2	5.25	1.63	1.52
1	D	371	TYR	CD1-CE1	5.14	1.47	1.39
1	A	483	TYR	CD1-CE1	5.09	1.47	1.39
1	A	436	GLU	CG-CD	5.02	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ARG	NE-CZ-NH1	-13.21	113.70	120.30
1	D	476[A]	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	D	476[B]	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	B	442	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	B	351	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	C	415	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	476	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	B	351	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	415	ASP	CB-CG-OD1	5.55	123.30	118.30
1	D	476[A]	ARG	CG-CD-NE	-5.51	100.23	111.80
1	D	476[B]	ARG	CG-CD-NE	-5.51	100.23	111.80
1	A	240	THR	CA-CB-CG2	-5.48	104.72	112.40
1	D	414	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	476	ARG	CG-CD-NE	-5.19	100.90	111.80
1	C	442	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	336	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	244	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	A	352	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2255	2255	2240	32	2
1	B	2288	2265	2267	33	0
1	C	2296	2295	2272	56	1
1	D	2270	2252	2263	41	3
2	A	40	24	26	4	0
2	B	40	24	26	2	0
2	C	40	25	26	1	0
2	D	40	24	26	2	0
3	B	4	3	3	1	0
4	A	48	0	0	5	0
4	B	41	0	0	3	0
4	C	45	0	0	6	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	39	0	0	6	0
All	All	9446	9167	9149	163	5

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 9.

All (163) 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:B:262:ARG:NH2	4:B:701:HOH:O	1.99	0.94
1:C:501:ASP:OD1	4:C:701:HOH:O	1.94	0.85
1:D:477:CYS:O	1:D:487:GLN:NE2	2.12	0.83
1:D:498:SER:O	4:D:701:HOH:O	1.98	0.81
1:C:393:HIS:HB2	1:C:396[A]:GLU:OE2	1.82	0.79
1:C:431:HIS:NE2	1:C:431:HIS:ND1	2.32	0.78
1:D:310:GLU:OE1	1:D:371:TYR:OH	2.02	0.77
1:C:426:PHE:CE2	1:C:426:PHE:CE1	2.66	0.75
1:C:484:GLU:HA	1:C:487:GLN:HG2	1.70	0.74
1:A:273:GLU:N	1:A:276[A]:GLN:OE1	2.22	0.73
1:D:397:GLU:O	4:D:702:HOH:O	2.08	0.72
1:C:396[B]:GLU:OE1	4:C:702:HOH:O	2.11	0.69
1:A:383:GLU:OE1	1:A:457:LYS:HD3	1.92	0.69
1:B:310:GLU:HG2	1:B:311:LEU:N	2.09	0.68
1:C:364:PHE:CG	1:C:364:PHE:CE1	2.80	0.66
1:A:496:GLN:NE2	4:A:701:HOH:O	2.09	0.66
1:D:279:CYS:SG	1:D:280:ASN:N	2.69	0.65
1:C:424:CYS:SG	2:C:602:GMP:N2	2.70	0.65
1:A:383:GLU:OE2	4:A:702:HOH:O	2.14	0.64
1:A:341:ARG:NE	4:A:703:HOH:O	2.24	0.64
1:C:431:HIS:ND1	1:C:431:HIS:CB	2.60	0.64
1:B:393:HIS:HB2	1:B:396[A]:GLU:CD	2.18	0.63
1:C:462:HIS:HD2	4:C:730:HOH:O	1.81	0.63
1:C:474:LEU:N	1:C:474:LEU:HG	2.14	0.62
1:C:431:HIS:NE2	1:C:431:HIS:CB	2.64	0.60
1:D:480:ASP:OD2	1:D:482:LYS:N	2.35	0.60
1:B:280:ASN:O	1:B:337:ARG:HB2	2.01	0.59
1:D:479:ASP:OD1	1:D:479:ASP:N	2.35	0.59
1:D:281:LYS:HE3	1:D:283:TYR:OH	2.04	0.57
1:A:384:GLU:HA	1:A:453:VAL:O	2.04	0.57
1:D:483:TYR:O	1:D:487:GLN:HG2	2.05	0.56
1:B:369:ASP:OD1	1:B:371:TYR:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:CG	1:B:311:LEU:N	2.68	0.55
1:D:282:LEU:HB2	1:D:313:LEU:CD1	2.37	0.55
1:A:383:GLU:OE1	1:A:457:LYS:CD	2.54	0.54
1:B:409:VAL:CG2	1:B:426:PHE:HB2	2.37	0.54
1:A:477:CYS:O	1:A:487:GLN:OE1	2.25	0.54
1:B:284[B]:ILE:CD1	1:B:307:ALA:HB2	2.37	0.54
1:D:476[A]:ARG:HD2	1:D:479:ASP:OD2	2.08	0.54
1:B:462:HIS:HD2	4:B:729:HOH:O	1.90	0.53
1:C:473:VAL:O	1:C:476[B]:ARG:HG2	2.09	0.53
1:D:308:VAL:HA	2:D:601:GMP:O2'	2.08	0.53
1:B:260[B]:MET:SD	1:B:335:LEU:HB2	2.49	0.53
1:A:276[B]:GLN:NE2	1:A:278:THR:OG1	2.37	0.52
1:C:474:LEU:C	1:C:474:LEU:CB	2.77	0.52
1:D:441:HIS:HA	1:D:497:PRO:HA	1.91	0.52
1:A:383:GLU:HB2	1:A:457:LYS:HD3	1.92	0.52
1:C:484:GLU:O	1:C:487:GLN:HB2	2.10	0.52
1:D:267:HIS:HB2	1:D:328:ASP:HA	1.92	0.52
1:C:265:PHE:CD2	1:C:271:ILE:HG12	2.45	0.51
1:D:446:ASP:OD1	4:D:703:HOH:O	2.18	0.51
1:D:289:HIS:HB3	1:D:301:LEU:HD11	1.92	0.51
1:B:499:TYR:O	3:B:603:ACT:H1	2.10	0.50
1:B:402:TYR:O	1:B:431:HIS:HA	2.11	0.50
1:C:389:GLU:OE1	4:C:703:HOH:O	2.18	0.50
1:A:383:GLU:OE1	1:A:402:TYR:HE2	1.94	0.50
1:B:483:TYR:O	1:B:487:GLN:HG2	2.12	0.50
1:D:260[B]:MET:SD	1:D:335:LEU:HB2	2.50	0.50
1:D:273:GLU:N	1:D:276[A]:GLN:OE1	2.43	0.50
1:C:364:PHE:CD2	1:C:474:LEU:HD21	2.47	0.50
1:C:283:TYR:HB2	1:C:308:VAL:CG2	2.42	0.50
1:D:437:PHE:CD1	1:D:437:PHE:N	2.79	0.49
1:A:383:GLU:OE1	1:A:402:TYR:CE2	2.64	0.49
1:A:442:ARG:N	1:A:496:GLN:O	2.42	0.49
1:B:424:CYS:SG	2:B:602:GMP:N2	2.86	0.49
1:C:484:GLU:HB2	4:C:711:HOH:O	2.11	0.49
1:A:272:MET:HA	1:A:276[A]:GLN:OE1	2.13	0.49
1:C:386:SER:HB3	1:C:387:PRO:HD2	1.93	0.49
1:B:409:VAL:HG22	1:B:426:PHE:HB2	1.94	0.48
1:C:438:LEU:HD11	1:C:474:LEU:CB	2.42	0.48
1:D:383:GLU:OE1	4:D:704:HOH:O	2.20	0.48
1:C:283:TYR:HB2	1:C:308:VAL:HG22	1.96	0.48
1:C:306:THR:HG22	1:C:465:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LEU:N	1:C:474:LEU:C	2.67	0.47
1:A:283:TYR:CD2	1:A:334:VAL:HG22	2.49	0.47
1:C:294:LYS:HG2	1:C:321:ALA:HB2	1.97	0.47
1:C:289:HIS:HB3	1:C:301:LEU:HD11	1.96	0.47
1:C:312:GLU:HA	1:C:317:THR:HG22	1.96	0.47
2:B:601:GMP:N2	4:B:703:HOH:O	2.18	0.46
1:A:300:TYR:CD1	2:A:601:GMP:N2	2.83	0.46
1:A:438:LEU:HD11	1:A:474:LEU:HB3	1.97	0.46
1:D:435:LEU:HD12	2:D:602:GMP:C8	2.50	0.46
1:C:265:PHE:CE2	1:C:271:ILE:HG12	2.51	0.46
1:A:256:VAL:O	1:A:260[A]:MET:HG3	2.16	0.45
1:C:435:LEU:HD13	1:C:486:TYR:CG	2.50	0.45
1:C:284[B]:ILE:CD1	1:C:307:ALA:HB2	2.46	0.45
1:D:281:LYS:CE	1:D:283:TYR:OH	2.65	0.45
1:C:399:GLU:HG2	1:C:399:GLU:O	2.17	0.44
1:C:462:HIS:HE1	4:C:708:HOH:O	1.98	0.44
1:C:282:LEU:HB2	1:C:313:LEU:CD1	2.47	0.44
1:C:383:GLU:OE1	1:C:457:LYS:HD3	2.17	0.44
1:B:294:LYS:O	1:B:297[A]:GLN:HG2	2.18	0.44
1:D:223:PRO:HG2	1:D:259:ALA:HB1	1.99	0.44
1:C:409:VAL:HG22	1:C:426:PHE:HB2	1.98	0.44
1:A:470:VAL:O	1:A:471:ILE:C	2.55	0.44
1:B:284[B]:ILE:CD1	1:B:307:ALA:CB	2.95	0.44
1:C:284[B]:ILE:HD13	1:C:307:ALA:CB	2.48	0.44
1:A:462:HIS:HE1	4:A:727:HOH:O	2.00	0.43
1:B:287:SER:OG	1:B:331:ILE:HD12	2.18	0.43
1:A:318:PRO:O	1:A:319:VAL:C	2.57	0.43
1:A:441:HIS:HA	1:A:497:PRO:HA	2.00	0.43
1:B:304:GLU:H	1:B:304:GLU:CD	2.22	0.43
1:C:312:GLU:HG3	1:C:317:THR:HG23	2.00	0.43
1:D:232:MET:HE2	1:D:254:LYS:HE2	2.00	0.43
1:A:309:GLY:N	2:A:601:GMP:O3'	2.45	0.43
1:C:312:GLU:HG2	1:C:319:VAL:HA	1.99	0.43
1:D:393:HIS:HD2	4:D:703:HOH:O	2.01	0.43
1:C:386:SER:HB3	1:C:387:PRO:CD	2.49	0.43
1:D:282:LEU:HB2	1:D:313:LEU:HD12	2.00	0.43
1:D:462:HIS:HE1	4:D:722:HOH:O	2.01	0.43
1:A:434:GLU:HG3	1:A:474:LEU:HD22	2.00	0.43
1:D:266:LYS:HD3	1:D:329:GLU:HG3	2.00	0.43
1:B:284[B]:ILE:HD12	1:B:307:ALA:HB2	1.99	0.43
1:C:260[A]:MET:HA	1:C:334:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260[B]:MET:HA	1:C:334:VAL:O	2.18	0.43
1:D:294:LYS:O	1:D:297[A]:GLN:HG2	2.18	0.43
1:A:390:TYR:CG	1:A:393:HIS:CE1	3.07	0.43
1:A:283:TYR:O	1:A:307:ALA:HA	2.18	0.43
1:D:267:HIS:N	1:D:328:ASP:O	2.53	0.42
1:A:300:TYR:CG	2:A:601:GMP:N2	2.87	0.42
1:D:329:GLU:N	1:D:329:GLU:OE1	2.52	0.42
1:A:458:LEU:HD11	1:A:462:HIS:HB2	2.02	0.42
1:D:365:LEU:O	1:D:366:GLY:C	2.58	0.42
1:C:267:HIS:CE1	1:C:268:ASP:OD1	2.73	0.42
1:C:386:SER:CB	1:C:387:PRO:CD	2.97	0.42
1:B:369:ASP:OD1	1:B:369:ASP:C	2.57	0.42
1:C:435:LEU:HD13	1:C:486:TYR:CD1	2.55	0.42
1:C:282:LEU:HB2	1:C:313:LEU:HD12	2.02	0.42
1:D:263:ALA:HB2	1:D:334:VAL:HG21	2.01	0.42
1:D:390:TYR:CD2	1:D:393:HIS:CD2	3.08	0.42
1:B:312:GLU:O	1:B:316[B]:ASP:HA	2.19	0.42
1:B:312:GLU:O	1:B:316[A]:ASP:HA	2.19	0.42
1:C:318:PRO:O	1:C:319:VAL:C	2.56	0.42
1:D:484:GLU:HA	1:D:487:GLN:HG2	2.01	0.42
1:C:358:PHE:O	1:C:362:VAL:HG23	2.20	0.41
1:A:462:HIS:HD2	4:A:717:HOH:O	2.02	0.41
1:B:359:LEU:HD22	1:B:365:LEU:CD1	2.50	0.41
1:D:294:LYS:HG2	1:D:321:ALA:HB2	2.03	0.41
1:A:308:VAL:HA	2:A:601:GMP:O2'	2.20	0.41
1:C:409:VAL:CG2	1:C:426:PHE:HB2	2.50	0.41
1:C:444:VAL:CG1	1:C:495:ALA:HB2	2.51	0.41
1:B:283:TYR:HB2	1:B:308:VAL:CG2	2.51	0.41
1:D:245:PHE:CD1	1:D:245:PHE:N	2.88	0.41
1:B:432:ILE:N	1:B:432:ILE:HD13	2.36	0.41
1:C:287:SER:OG	1:C:331:ILE:HD12	2.21	0.41
1:D:256:VAL:O	1:D:260[A]:MET:HG3	2.20	0.41
1:B:289:HIS:HE1	1:B:304:GLU:OE2	2.03	0.41
1:B:435:LEU:HD13	1:B:486:TYR:CD1	2.55	0.41
1:A:291:ASP:OD2	1:A:298:LYS:HD3	2.22	0.40
1:B:239:LEU:HD23	1:B:245:PHE:CE2	2.56	0.40
1:B:484:GLU:HA	1:B:487:GLN:HG2	2.02	0.40
1:C:227:LYS:HB2	1:C:232:MET:HG2	2.03	0.40
1:A:266:LYS:H	1:A:269:ASP:CG	2.25	0.40
1:C:358:PHE:CZ	1:C:405:MET:HG2	2.56	0.40
1:B:344:VAL:O	1:B:345:MET:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:PHE:CE2	1:C:471:ILE:HD11	2.57	0.40
1:B:435:LEU:HD13	1:B:486:TYR:CG	2.56	0.40
1:C:402:TYR:O	1:C:431:HIS:HA	2.22	0.40

All (5) 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:D:396[B]:GLU:OE1	4:C:727:HOH:O[2_746]	1.82	0.38
1:D:397:GLU:OE2	4:C:727:HOH:O[2_746]	1.90	0.30
1:A:350:ARG:NH1	1:A:496:GLN:OE1[2_747]	2.04	0.16
1:C:372:GLU:OE1	1:D:476[A]:ARG:HH22[2_656]	1.48	0.12
1:A:350:ARG:HH11	1:A:496:GLN:OE1[2_747]	1.54	0.06

## 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	291/304 (96%)	277 (95%)	12 (4%)	2 (1%)	22	17
1	B	293/304 (96%)	270 (92%)	20 (7%)	3 (1%)	15	10
1	C	294/304 (97%)	274 (93%)	16 (5%)	4 (1%)	11	6
1	D	291/304 (96%)	270 (93%)	18 (6%)	3 (1%)	15	10
All	All	1169/1216 (96%)	1091 (93%)	66 (6%)	12 (1%)	25	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	316[A]	ASP
1	B	316[B]	ASP
1	C	276[A]	GLN

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Mol	Chain	Res	Type
1	C	276[B]	GLN
1	C	316[A]	ASP
1	C	316[B]	ASP
1	A	316[A]	ASP
1	A	316[B]	ASP
1	D	397	GLU
1	D	316[A]	ASP
1	D	316[B]	ASP
1	B	253	ILE

### 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	250/262 (95%)	244 (98%)	6 (2%)	49	52
1	B	253/262 (97%)	248 (98%)	5 (2%)	55	59
1	C	252/262 (96%)	247 (98%)	5 (2%)	55	59
1	D	251/262 (96%)	239 (95%)	12 (5%)	25	23
All	All	1006/1048 (96%)	978 (97%)	28 (3%)	46	46

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

Mol	Chain	Res	Type
1	A	280	ASN
1	A	304	GLU
1	A	432	ILE
1	A	471	ILE
1	A	496	GLN
1	A	498	SER
1	B	278	THR
1	B	289	HIS
1	B	316[A]	ASP
1	B	316[B]	ASP
1	B	432	ILE
1	C	262	ARG

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Mol	Chain	Res	Type
1	C	279	CYS
1	C	304	GLU
1	C	386	SER
1	C	432	ILE
1	D	226	GLU
1	D	254	LYS
1	D	279	CYS
1	D	301	LEU
1	D	304	GLU
1	D	316[A]	ASP
1	D	316[B]	ASP
1	D	386[A]	SER
1	D	386[B]	SER
1	D	432	ILE
1	D	479	ASP
1	D	498	SER

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

Mol	Chain	Res	Type
1	A	487	GLN
1	B	267	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

9 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$
2	GMP	A	602	-	18,22,22	2.27	6 (33%)	18,33,33	1.41	2 (11%)
3	ACT	B	603	-	3,3,3	0.87	0	3,3,3	1.49	0
2	GMP	D	602	-	18,22,22	2.77	7 (38%)	18,33,33	1.78	5 (27%)
2	GMP	D	601	-	18,22,22	2.69	7 (38%)	18,33,33	1.46	5 (27%)
2	GMP	C	601	-	18,22,22	2.78	7 (38%)	18,33,33	2.21	6 (33%)
2	GMP	B	601	-	18,22,22	2.57	7 (38%)	18,33,33	2.15	4 (22%)
2	GMP	C	602	-	18,22,22	2.71	7 (38%)	18,33,33	1.58	6 (33%)
2	GMP	A	601	-	18,22,22	2.44	7 (38%)	18,33,33	1.42	4 (22%)
2	GMP	B	602	-	18,22,22	2.75	5 (27%)	18,33,33	2.09	5 (27%)

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	GMP	A	602	-	-	0/2/22/22	0/3/3/3
2	GMP	D	602	-	-	0/2/22/22	0/3/3/3
2	GMP	D	601	-	-	1/2/22/22	0/3/3/3
2	GMP	C	601	-	-	0/2/22/22	0/3/3/3
2	GMP	B	601	-	-	0/2/22/22	0/3/3/3
2	GMP	C	602	-	-	0/2/22/22	0/3/3/3
2	GMP	A	601	-	-	0/2/22/22	0/3/3/3
2	GMP	B	602	-	-	0/2/22/22	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	GMP	C2-N2	6.64	1.49	1.34
2	C	602	GMP	C2-N2	6.54	1.49	1.34
2	D	602	GMP	C2-N2	6.38	1.49	1.34
2	A	602	GMP	C2-N2	6.19	1.48	1.34
2	B	602	GMP	C4-N3	6.07	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	GMP	C2-N2	5.97	1.48	1.34
2	C	601	GMP	C4-N3	5.92	1.51	1.37
2	B	602	GMP	C2-N2	5.92	1.48	1.34
2	B	602	GMP	C5-C6	5.71	1.58	1.47
2	B	601	GMP	C2-N2	5.67	1.47	1.34
2	C	602	GMP	C4-N3	5.42	1.50	1.37
2	A	601	GMP	C4-N3	5.24	1.49	1.37
2	D	601	GMP	C4-N3	5.08	1.49	1.37
2	A	601	GMP	C2-N2	5.07	1.46	1.34
2	B	601	GMP	C4-N3	4.97	1.49	1.37
2	C	601	GMP	C2-N3	4.78	1.44	1.33
2	B	601	GMP	C2-N3	4.62	1.44	1.33
2	D	602	GMP	C2-N3	4.57	1.44	1.33
2	D	601	GMP	C2-N3	4.48	1.44	1.33
2	D	602	GMP	C5-C6	4.38	1.56	1.47
2	B	601	GMP	C5-C6	4.38	1.56	1.47
2	D	602	GMP	C4-N3	4.25	1.47	1.37
2	A	601	GMP	C6-N1	4.04	1.44	1.37
2	C	602	GMP	C5-C6	3.88	1.55	1.47
2	A	602	GMP	C4-N3	3.87	1.46	1.37
2	C	601	GMP	C6-N1	3.86	1.43	1.37
2	C	602	GMP	C2-N3	3.78	1.42	1.33
2	D	601	GMP	C6-N1	3.77	1.43	1.37
2	B	602	GMP	C2-N3	3.58	1.41	1.33
2	D	602	GMP	C5-C4	-3.56	1.34	1.43
2	A	601	GMP	C2-N3	3.55	1.41	1.33
2	A	602	GMP	C2-N3	3.53	1.41	1.33
2	D	602	GMP	C6-N1	3.48	1.43	1.37
2	C	601	GMP	C5-C4	-3.30	1.34	1.43
2	C	602	GMP	C5-C4	-3.11	1.35	1.43
2	C	601	GMP	C2-N1	3.01	1.44	1.37
2	B	602	GMP	C2-N1	2.95	1.44	1.37
2	D	601	GMP	C2-N1	2.83	1.44	1.37
2	D	601	GMP	C5-C4	-2.74	1.36	1.43
2	C	602	GMP	C2-N1	2.70	1.44	1.37
2	C	602	GMP	C6-N1	2.63	1.41	1.37
2	B	601	GMP	C5-C4	-2.62	1.36	1.43
2	A	601	GMP	C5-C4	-2.60	1.36	1.43
2	D	601	GMP	C5-C6	2.60	1.52	1.47
2	A	602	GMP	C6-N1	2.51	1.41	1.37
2	A	602	GMP	C5-C4	-2.42	1.37	1.43
2	C	601	GMP	C5-C6	2.32	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GMP	C6-N1	2.28	1.41	1.37
2	A	602	GMP	C2-N1	2.22	1.43	1.37
2	D	602	GMP	C2-N1	2.16	1.42	1.37
2	A	601	GMP	C5-C6	2.16	1.51	1.47
2	B	601	GMP	C2-N1	2.16	1.42	1.37
2	A	601	GMP	C2-N1	2.16	1.42	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	GMP	O6-C6-N1	-6.73	112.64	120.62
2	B	601	GMP	O6-C6-N1	-5.63	113.94	120.62
2	C	601	GMP	O6-C6-C5	-5.10	114.21	124.32
2	C	601	GMP	C5-C6-N1	4.37	122.41	114.07
2	C	601	GMP	C2-N1-C6	-4.30	117.25	125.11
2	B	601	GMP	C8-N7-C5	4.24	109.76	102.55
2	B	601	GMP	C2-N1-C6	-3.78	118.19	125.11
2	D	602	GMP	C8-N7-C5	3.66	108.78	102.55
2	B	601	GMP	C5-C6-N1	3.48	120.70	114.07
2	A	602	GMP	N1-C2-N3	-3.35	117.19	123.32
2	C	602	GMP	C8-N7-C5	3.23	108.04	102.55
2	D	602	GMP	O6-C6-N1	-3.01	117.05	120.62
2	D	602	GMP	C2-N1-C6	-2.99	119.64	125.11
2	C	602	GMP	C5-C6-N1	2.97	119.74	114.07
2	D	602	GMP	C5-C6-N1	2.97	119.74	114.07
2	D	601	GMP	N1-C2-N3	-2.94	117.94	123.32
2	B	602	GMP	C8-N7-C5	2.88	107.45	102.55
2	C	601	GMP	C8-N7-C5	2.78	107.28	102.55
2	A	602	GMP	N2-C2-N1	2.74	122.54	116.76
2	A	601	GMP	N2-C2-N3	2.73	125.00	119.67
2	B	602	GMP	O6-C6-C5	2.68	129.63	124.32
2	B	602	GMP	N2-C2-N3	2.65	124.84	119.67
2	C	602	GMP	N2-C2-N1	2.58	122.21	116.76
2	A	601	GMP	O4'-C1'-N9	-2.55	105.36	108.75
2	A	601	GMP	N1-C2-N3	-2.45	118.83	123.32
2	C	601	GMP	N2-C2-N1	2.40	121.83	116.76
2	C	602	GMP	N1-C2-N3	-2.38	118.96	123.32
2	D	601	GMP	O4'-C1'-N9	-2.37	105.60	108.75
2	D	601	GMP	O6-C6-C5	-2.33	119.71	124.32
2	C	601	GMP	O6-C6-N1	2.32	123.38	120.62
2	D	602	GMP	N1-C2-N3	-2.30	119.11	123.32
2	C	602	GMP	O6-C6-N1	-2.29	117.90	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	GMP	C5-C6-N1	2.21	118.28	114.07
2	A	601	GMP	O6-C6-C5	-2.18	119.99	124.32
2	C	602	GMP	C2-N1-C6	-2.14	121.19	125.11
2	D	601	GMP	C8-N7-C5	2.08	106.10	102.55
2	B	602	GMP	N1-C2-N3	-2.04	119.58	123.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

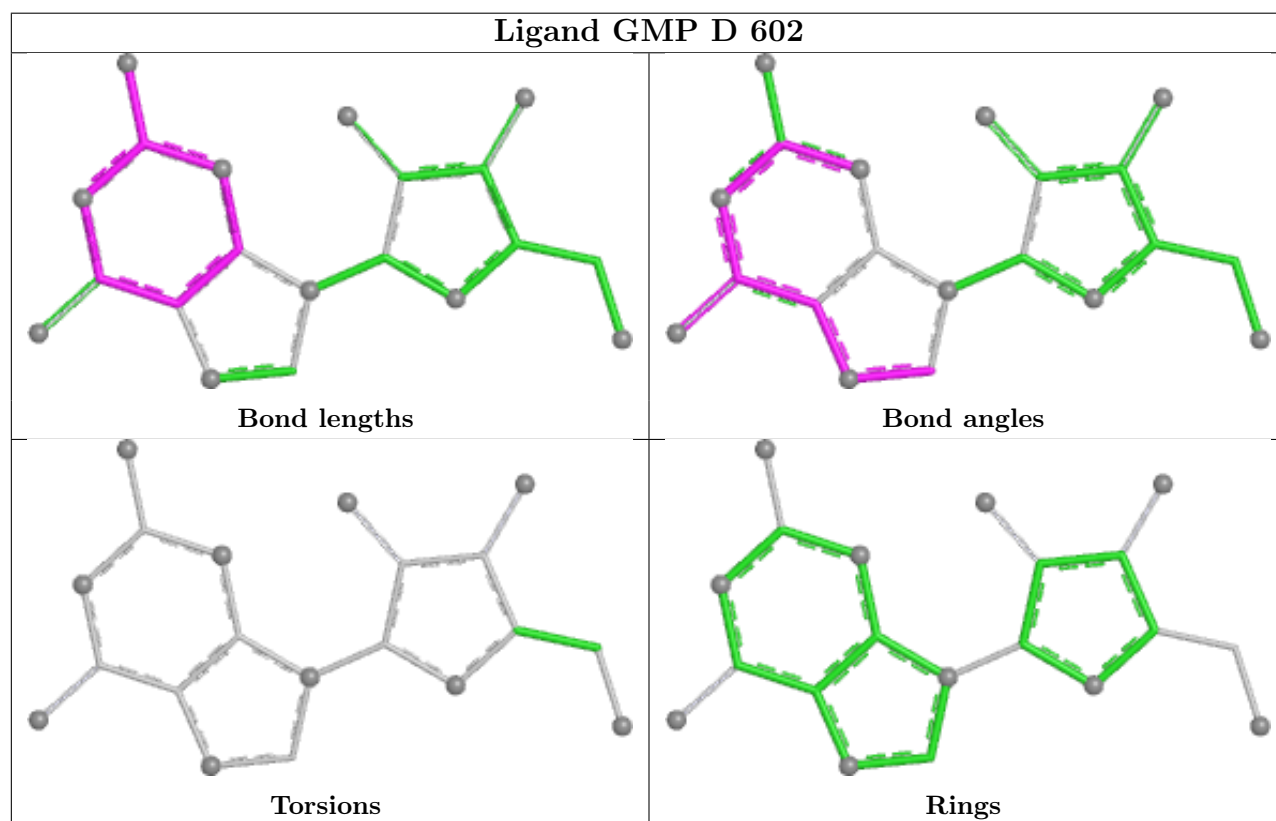
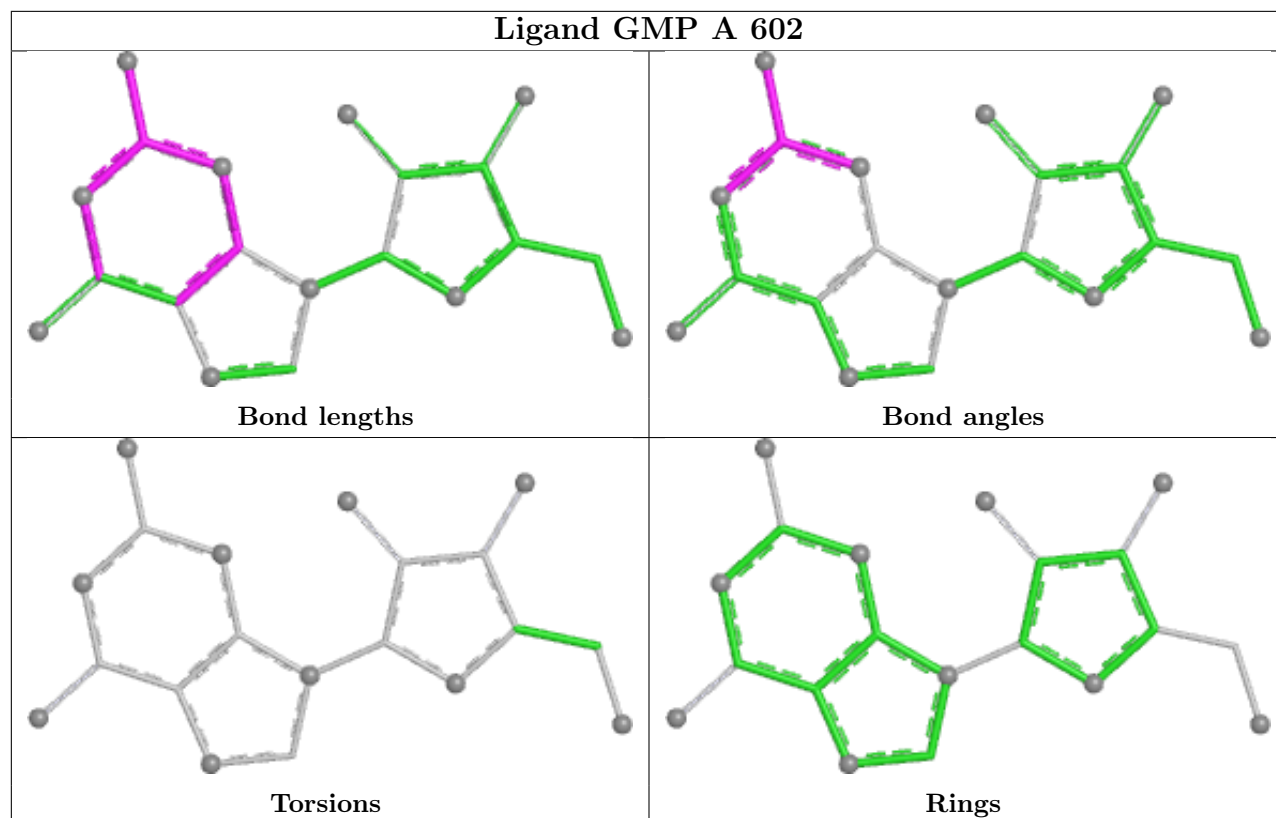
Mol	Chain	Res	Type	Atoms
2	D	601	GMP	O4'-C4'-C5'-O5'

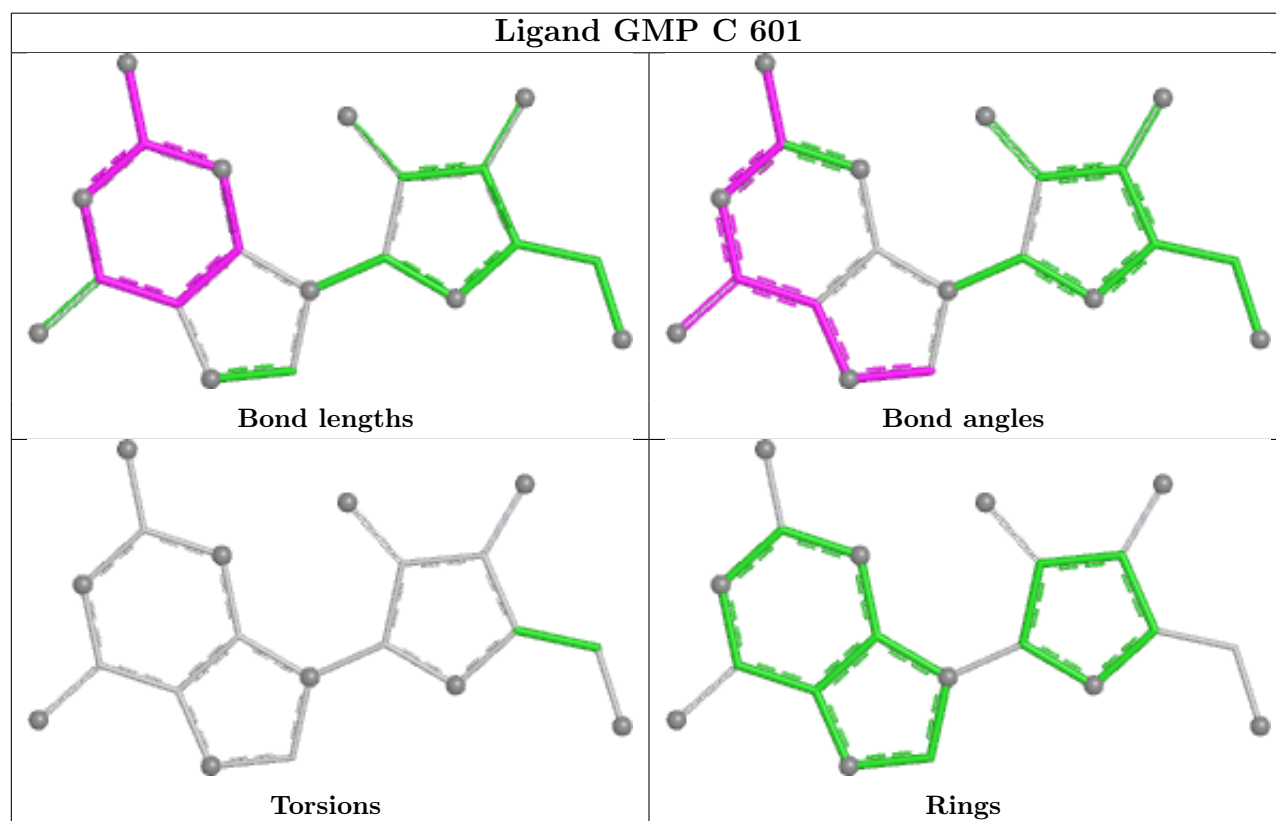
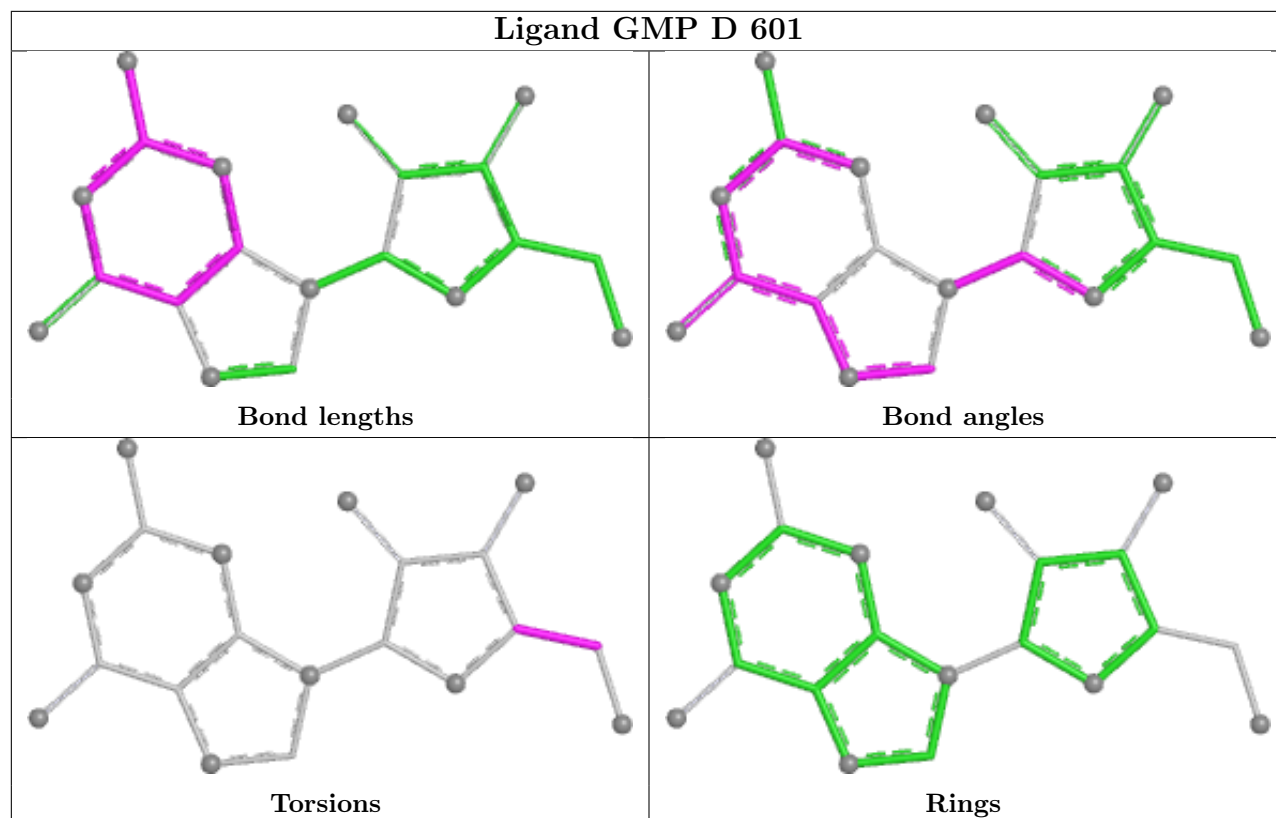
There are no ring outliers.

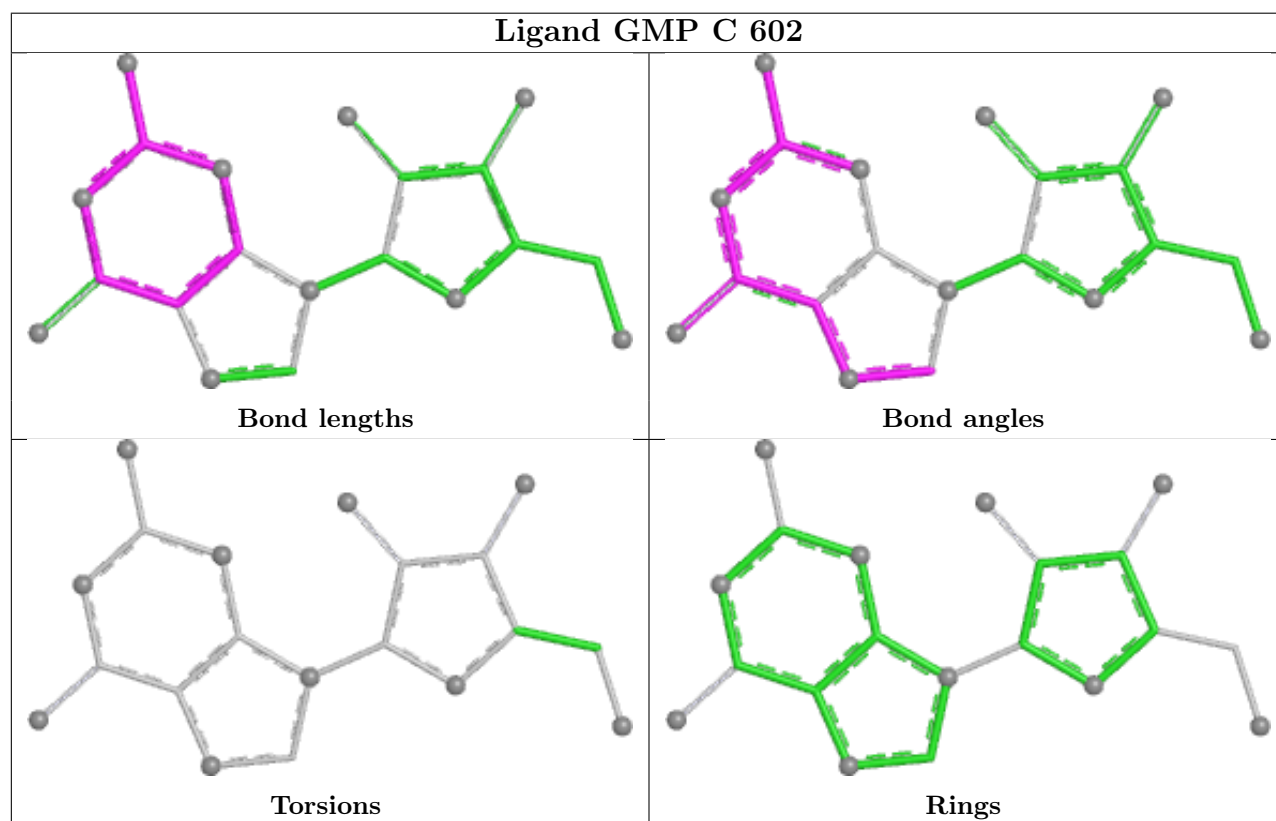
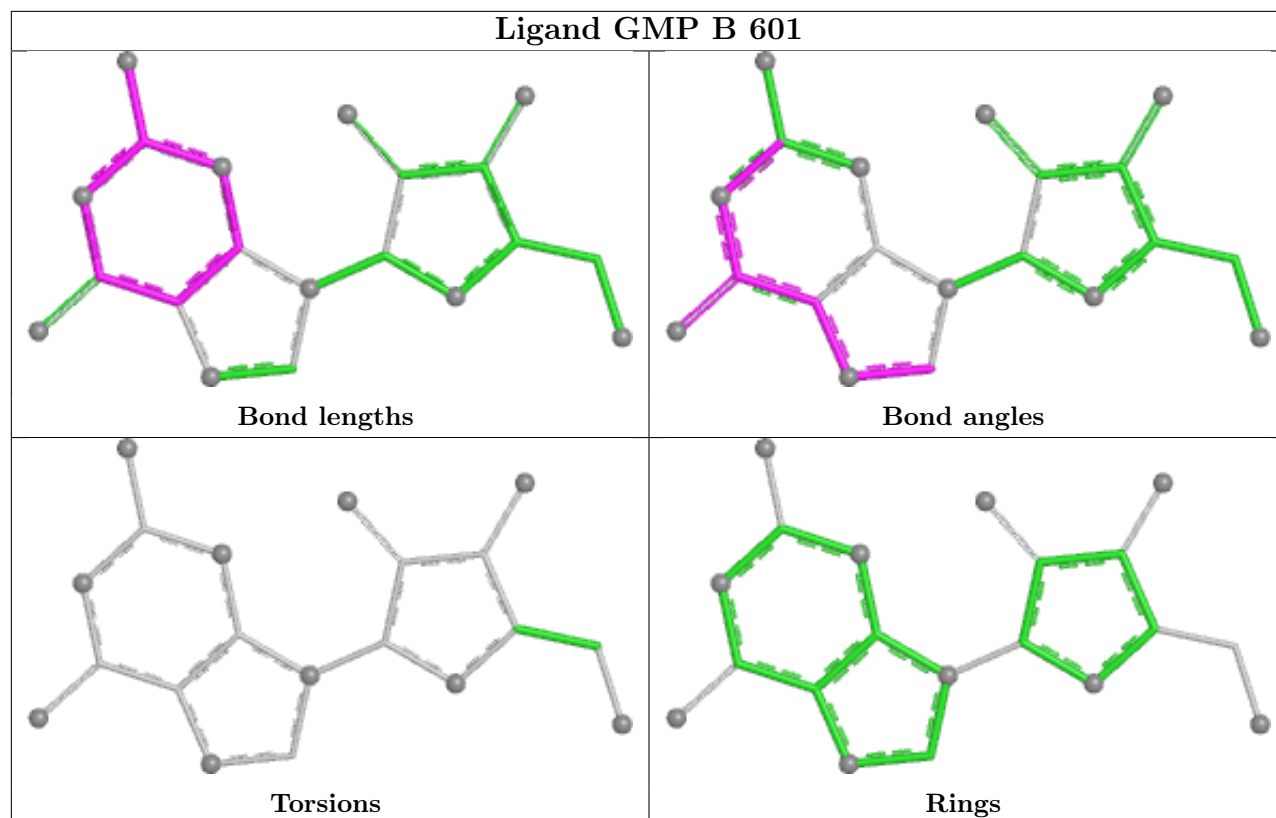
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	ACT	1	0
2	D	602	GMP	1	0
2	D	601	GMP	1	0
2	B	601	GMP	1	0
2	C	602	GMP	1	0
2	A	601	GMP	4	0
2	B	602	GMP	1	0

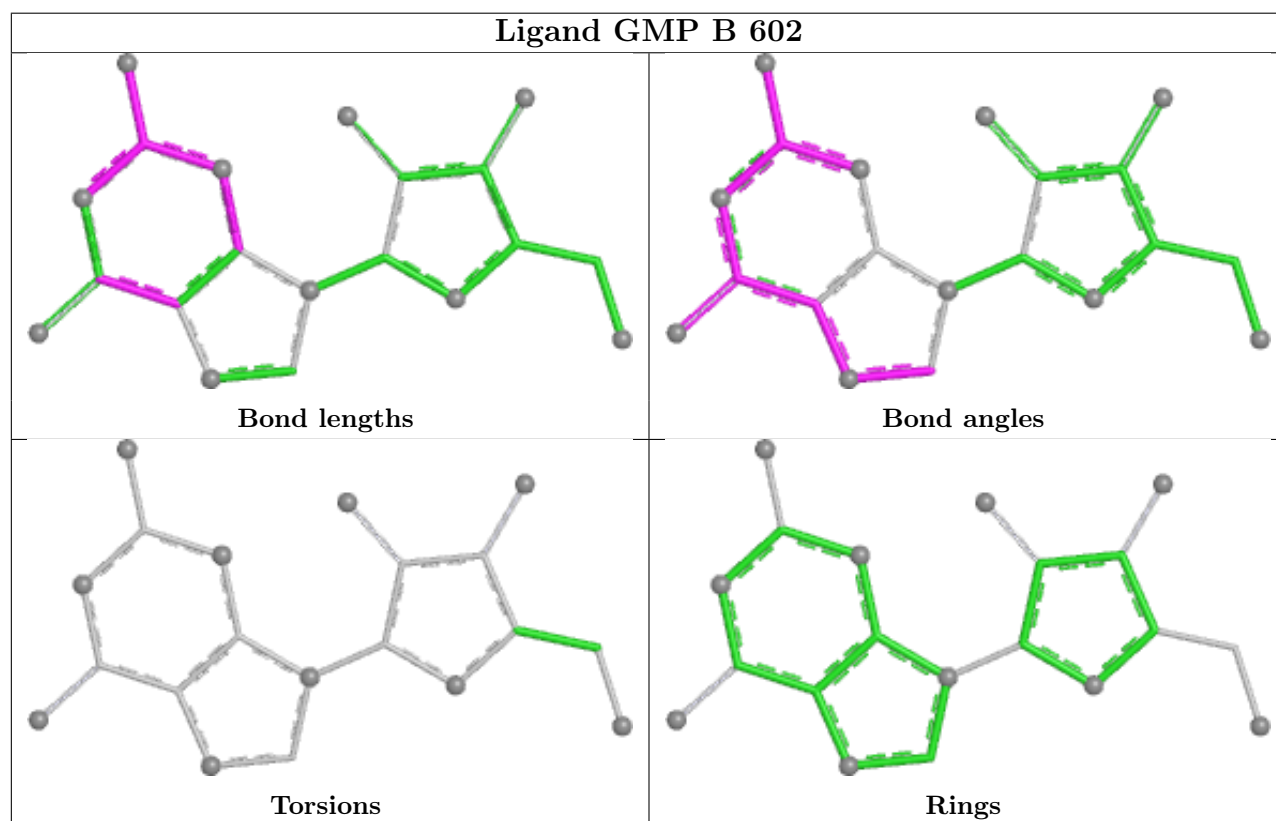
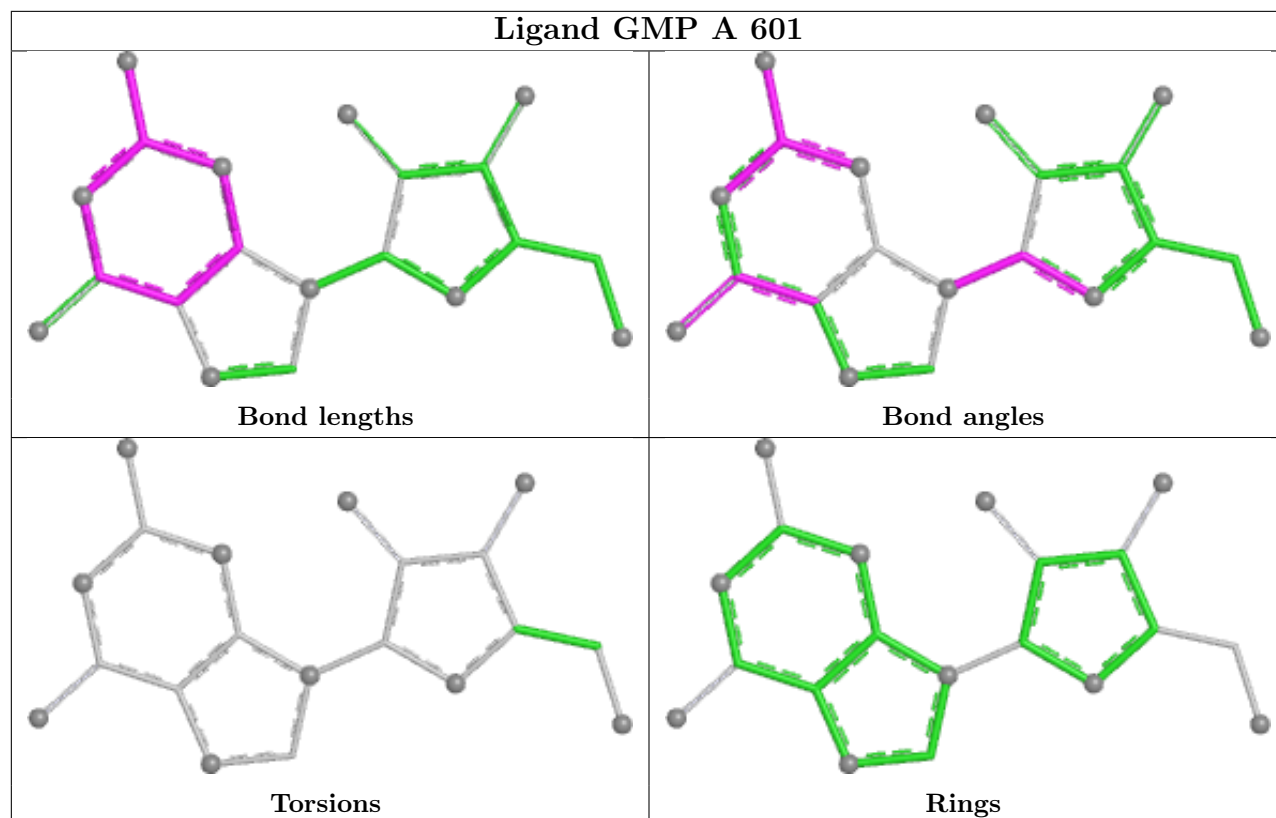
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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	280/304 (92%)	0.44	10 (3%) 42 48	51, 76, 124, 151	0
1	B	282/304 (92%)	1.03	55 (19%) 1 1	47, 94, 141, 184	0
1	C	284/304 (93%)	0.64	27 (9%) 8 10	52, 83, 129, 155	0
1	D	279/304 (91%)	0.89	45 (16%) 1 2	52, 91, 132, 157	0
All	All	1125/1216 (92%)	0.75	137 (12%) 4 5	47, 83, 135, 184	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	LYS	7.0
1	B	263	ALA	6.4
1	D	328	ASP	6.2
1	B	278	THR	6.1
1	D	343[A]	LEU	6.0
1	C	323	VAL	5.4
1	B	232	MET	5.4
1	B	282	LEU	5.4
1	A	477	CYS	4.9
1	B	308	VAL	4.7
1	D	278	THR	4.5
1	C	479	ASP	4.4
1	D	496	GLN	4.4
1	D	256	VAL	4.3
1	C	279	CYS	4.3
1	A	221	GLN	4.2
1	B	331	ILE	4.2
1	B	320	VAL	4.2
1	D	299	VAL	4.1
1	D	329	GLU	4.1
1	D	239	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	297[A]	GLN	3.9
1	D	284[A]	ILE	3.8
1	B	330	LEU	3.8
1	D	331	ILE	3.7
1	B	335	LEU	3.7
1	A	329	GLU	3.6
1	B	220	TYR	3.6
1	B	332	ALA	3.6
1	C	237	LYS	3.5
1	C	298	LYS	3.5
1	B	315	TYR	3.5
1	B	284[A]	ILE	3.4
1	B	273	GLU	3.3
1	D	250	THR	3.3
1	B	479	ASP	3.3
1	B	301	LEU	3.3
1	D	324	LYS	3.3
1	C	297[A]	GLN	3.2
1	B	323	VAL	3.2
1	B	260[A]	MET	3.1
1	B	279	CYS	3.1
1	B	264	THR	3.1
1	B	319	VAL	3.1
1	B	221	GLN	3.1
1	D	330	LEU	3.1
1	D	270	CYS	3.1
1	B	321	ALA	3.0
1	D	234	LEU	3.0
1	B	224	TYR	3.0
1	B	329	GLU	3.0
1	D	220	TYR	2.9
1	D	268	ASP	2.9
1	B	244	LEU	2.9
1	D	326	CYS	2.9
1	B	292	ILE	2.9
1	B	333	TRP	2.8
1	B	314[A]	MET	2.8
1	B	328	ASP	2.8
1	B	295	GLU	2.8
1	B	222	ALA	2.7
1	B	349	ILE	2.7
1	C	343[A]	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	THR	2.7
1	A	272	MET	2.7
1	D	444	VAL	2.6
1	B	281	LYS	2.6
1	D	337	ARG	2.6
1	D	293	ILE	2.6
1	A	416	ALA	2.6
1	D	279	CYS	2.6
1	D	323	VAL	2.6
1	C	315	TYR	2.6
1	A	297[A]	GLN	2.6
1	D	307	ALA	2.6
1	B	271	ILE	2.6
1	B	293	ILE	2.6
1	B	265	PHE	2.6
1	C	266	LYS	2.5
1	B	307	ALA	2.5
1	D	498	SER	2.5
1	D	262	ARG	2.5
1	C	271	ILE	2.5
1	D	294	LYS	2.5
1	D	344	VAL	2.5
1	D	269	ASP	2.4
1	B	465	MET	2.4
1	C	329	GLU	2.4
1	C	325	VAL	2.4
1	B	326	CYS	2.4
1	D	327	THR	2.4
1	B	283	TYR	2.4
1	A	493	GLY	2.4
1	D	296	GLY	2.4
1	B	268	ASP	2.4
1	C	478	ALA	2.4
1	C	328	ASP	2.4
1	C	465	MET	2.3
1	D	332	ALA	2.3
1	A	219	LEU	2.3
1	D	244	LEU	2.3
1	D	222	ALA	2.3
1	D	274	ALA	2.3
1	D	491	LYS	2.3
1	B	310	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	316[A]	ASP	2.3
1	B	325	VAL	2.3
1	D	300	TYR	2.3
1	B	272	MET	2.2
1	B	254	LYS	2.2
1	B	276[A]	GLN	2.2
1	C	276[A]	GLN	2.2
1	D	233	ASN	2.2
1	D	225	PHE	2.2
1	C	265	PHE	2.2
1	A	494	ALA	2.2
1	D	282	LEU	2.2
1	B	299	VAL	2.2
1	C	268	ASP	2.2
1	B	370	SER	2.2
1	C	222	ALA	2.1
1	C	264	THR	2.1
1	B	341	ARG	2.1
1	A	498	SER	2.1
1	D	297[A]	GLN	2.1
1	D	314[A]	MET	2.1
1	C	326	CYS	2.1
1	D	488	ASN	2.0
1	C	219	LEU	2.0
1	C	363	PRO	2.0
1	B	344	VAL	2.0
1	D	260[A]	MET	2.0
1	C	316[A]	ASP	2.0
1	C	337	ARG	2.0
1	C	272	MET	2.0
1	D	335	LEU	2.0
1	B	324	LYS	2.0

## 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](#)

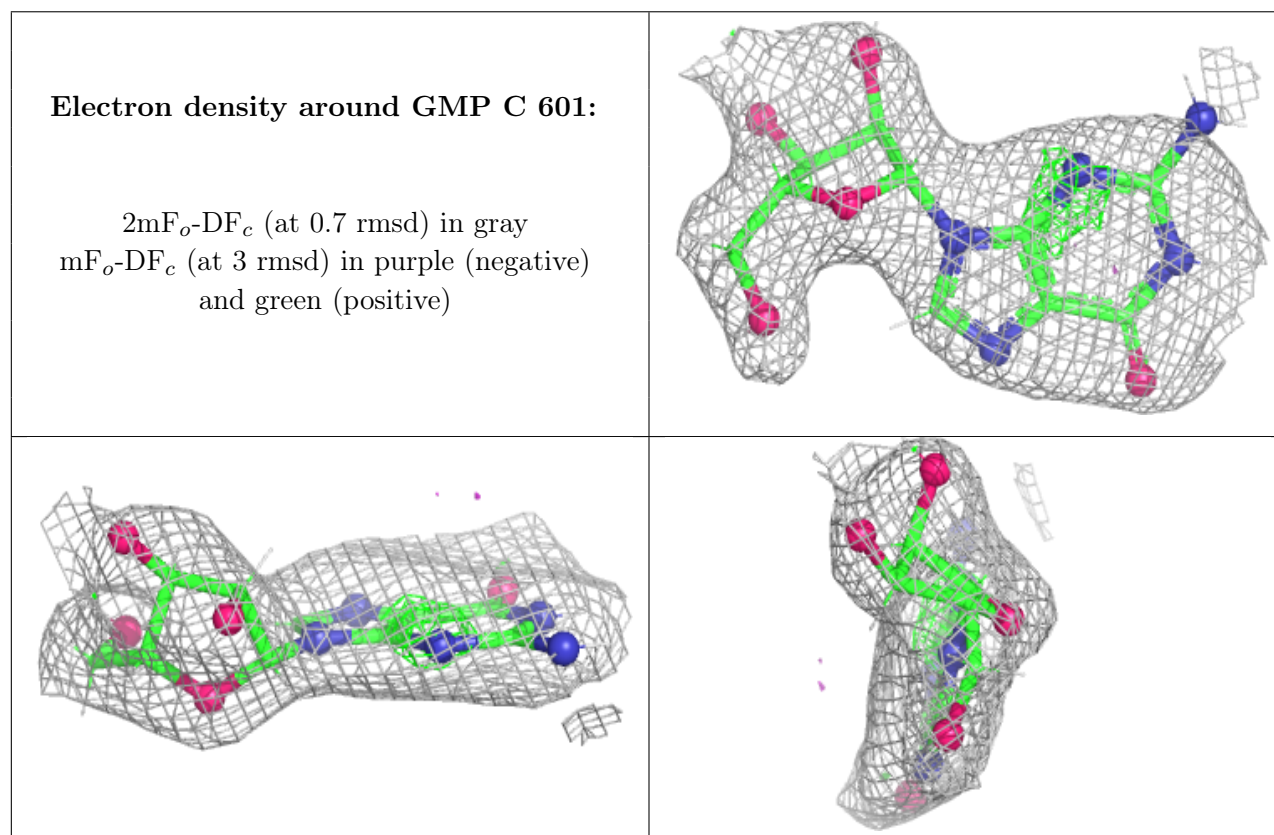
There are no monosaccharides in this entry.

## 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.

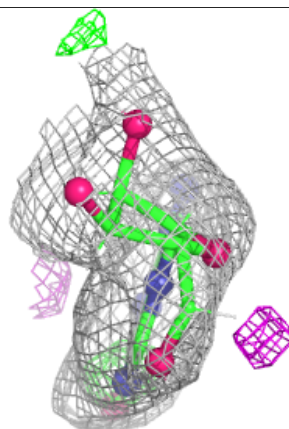
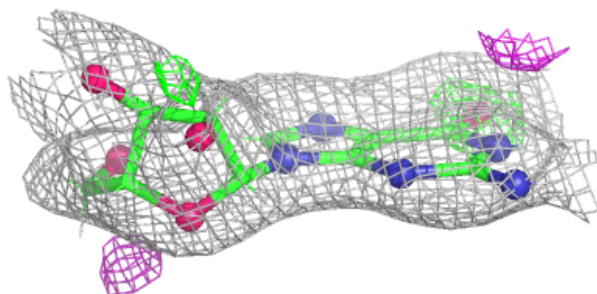
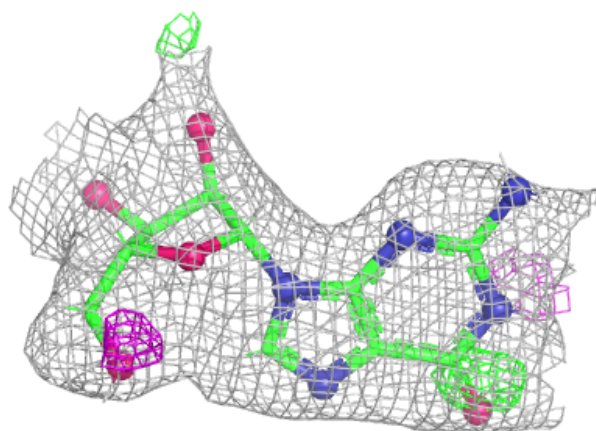
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GMP	C	601	20/20	0.78	0.21	67,101,141,204	0
2	GMP	B	601	20/20	0.84	0.16	71,111,151,171	0
3	ACT	B	603	4/4	0.91	0.11	67,93,95,127	0
2	GMP	D	601	20/20	0.92	0.13	65,86,127,150	0
2	GMP	A	601	20/20	0.92	0.12	49,75,105,126	0
2	GMP	B	602	20/20	0.93	0.13	43,59,107,111	0
2	GMP	A	602	20/20	0.94	0.14	45,70,121,136	0
2	GMP	D	602	20/20	0.95	0.15	48,73,122,139	0
2	GMP	C	602	20/20	0.95	0.13	49,68,186,223	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 GMP B 601:**

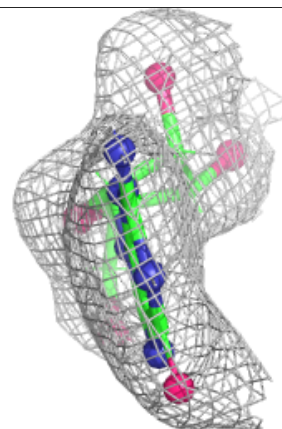
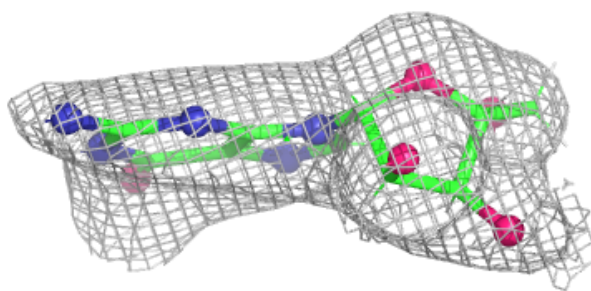
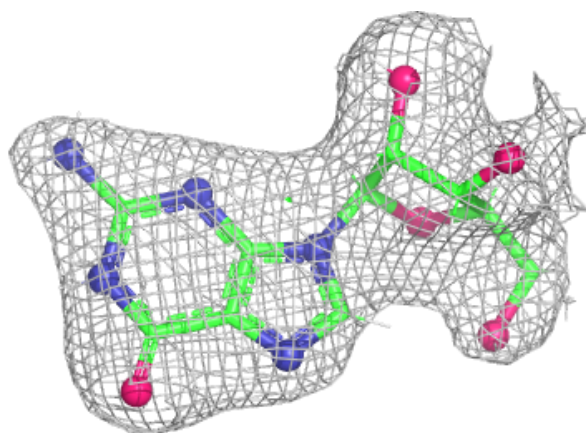
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





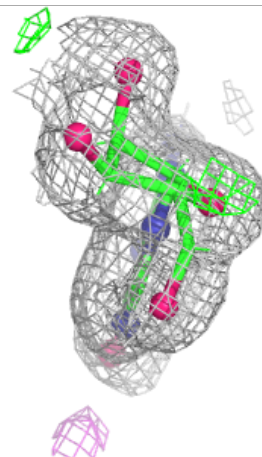
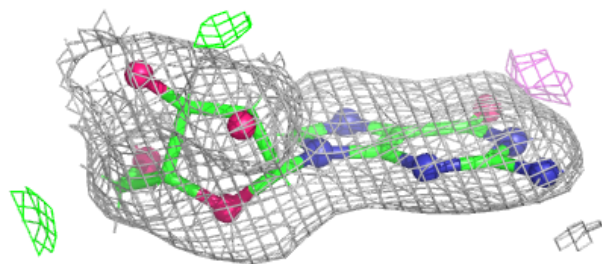
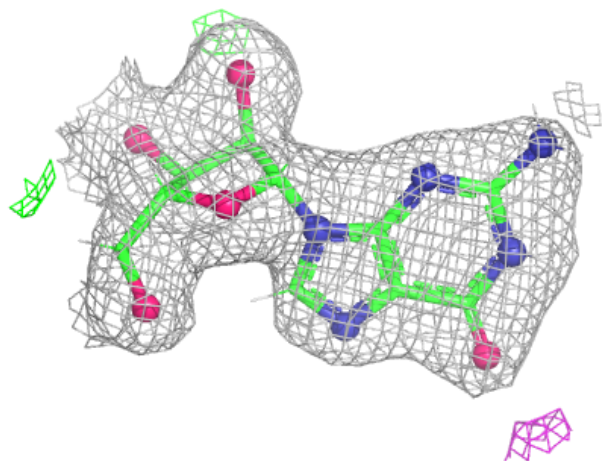
**Electron density around GMP D 601:**

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



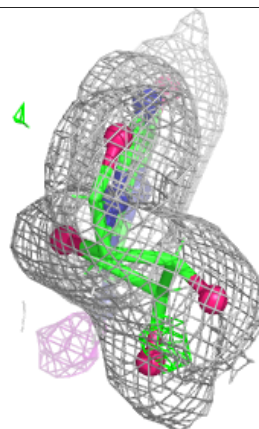
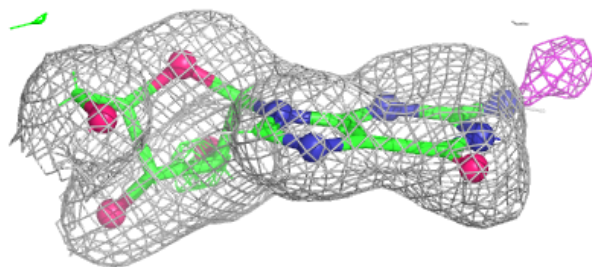
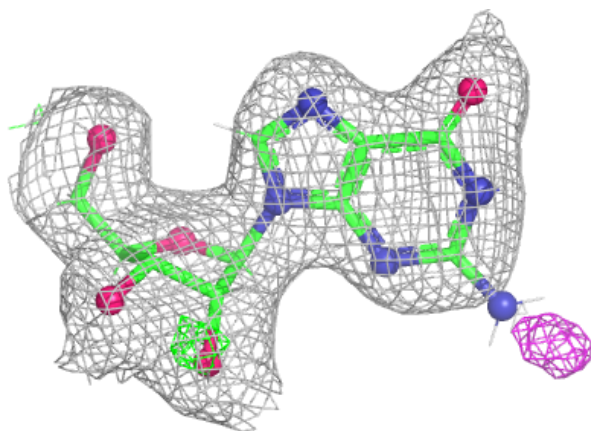
**Electron density around GMP A 601:**

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



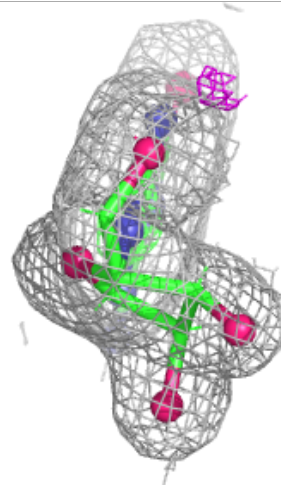
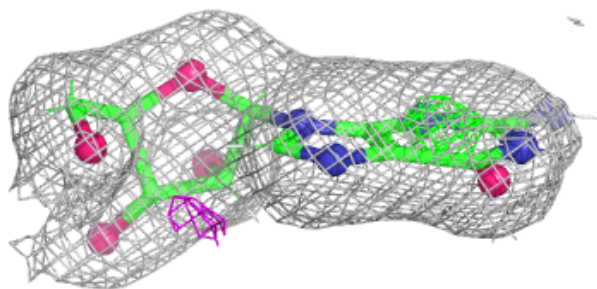
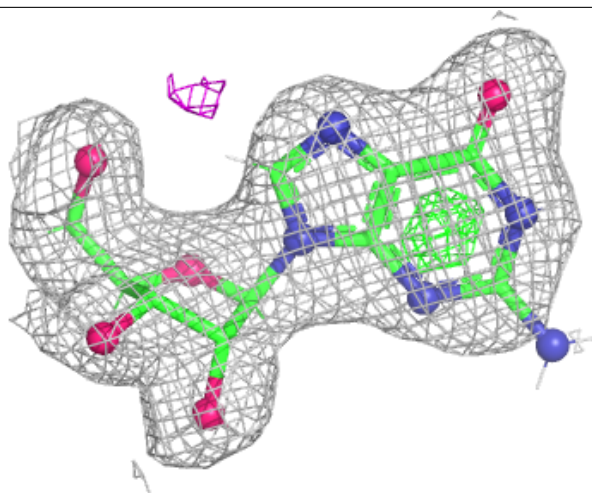
**Electron density around GMP B 602:**

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



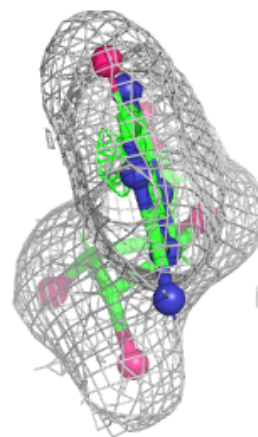
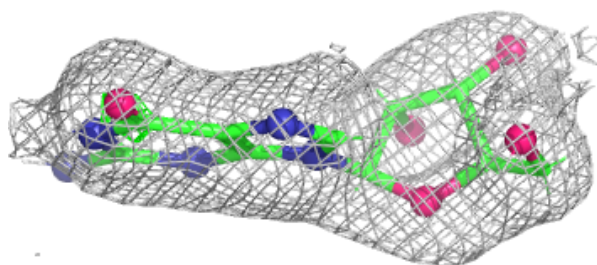
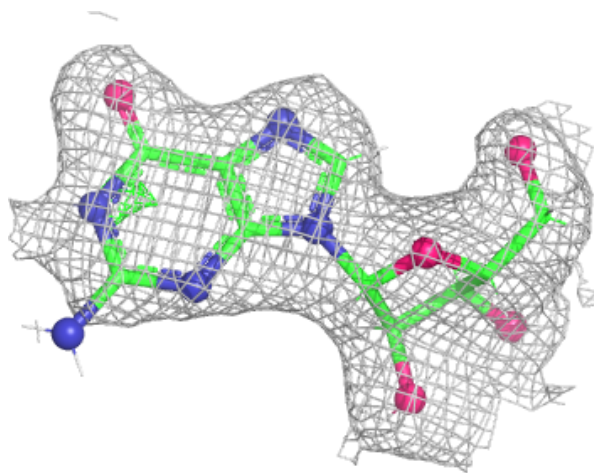
**Electron density around GMP A 602:**

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



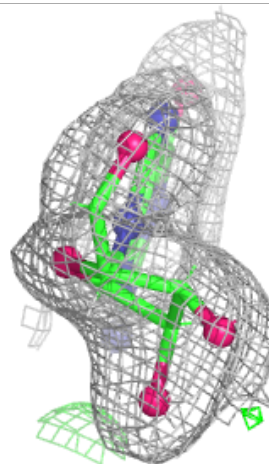
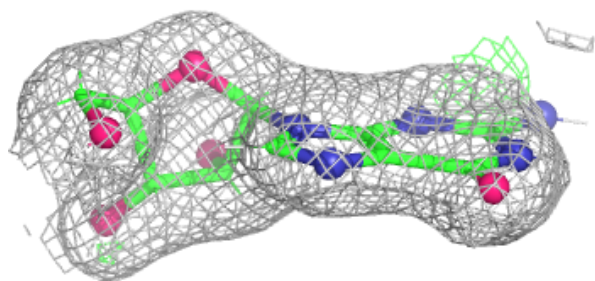
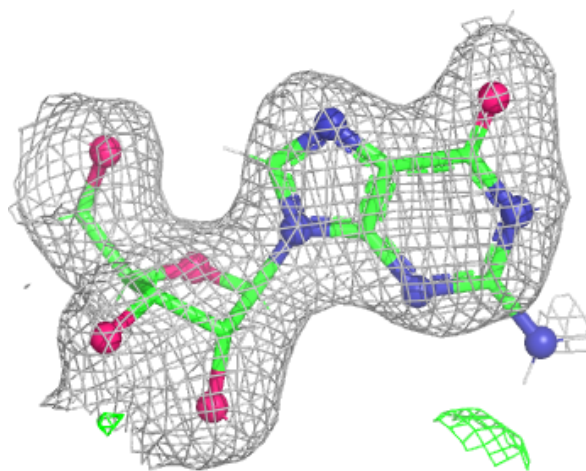
**Electron density around GMP D 602:**

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



**Electron density around GMP C 602:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.