



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:29 PM UTC

PDB ID : 6HYQ / pdb_00006hyq
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

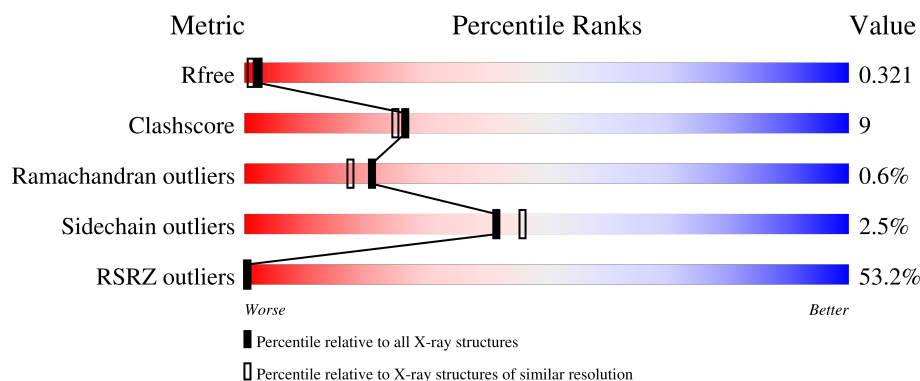
1 Overall quality at a glance

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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (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 ≥ 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	40% 76% 15% 8%
1	B	304	55% 76% 15% 7%
1	C	304	48% 72% 21% 7%
1	D	304	54% 72% 18% 8%

2 Entry composition [i](#)

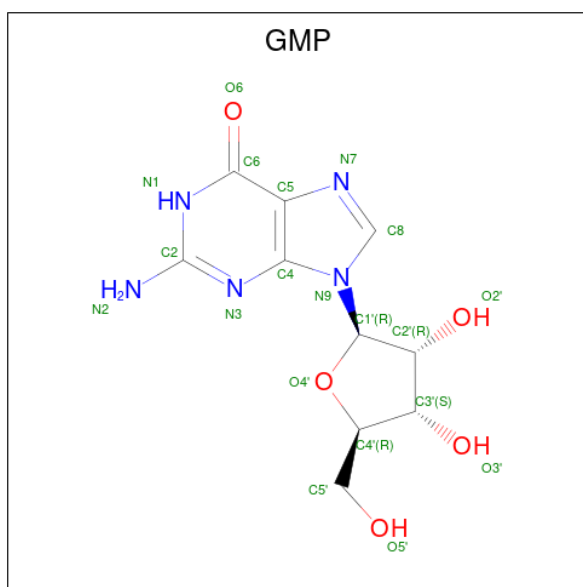
There are 4 unique types of molecules in this entry. The entry contains 18613 atoms, of which 9167 are hydrogens and 0 are deuteriums.

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 (CCD ID: GMP) (formula: C₁₀H₁₃N₅O₅) (labeled as "Ligand of Interest" by depositor).



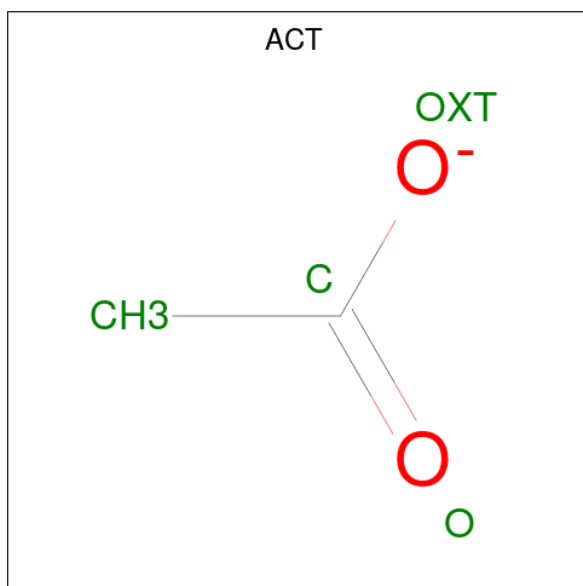
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			32	10	12	5	5		
2	A	1	Total	C	H	N	O	0	0
			32	10	12	5	5		

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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 (CCD ID: 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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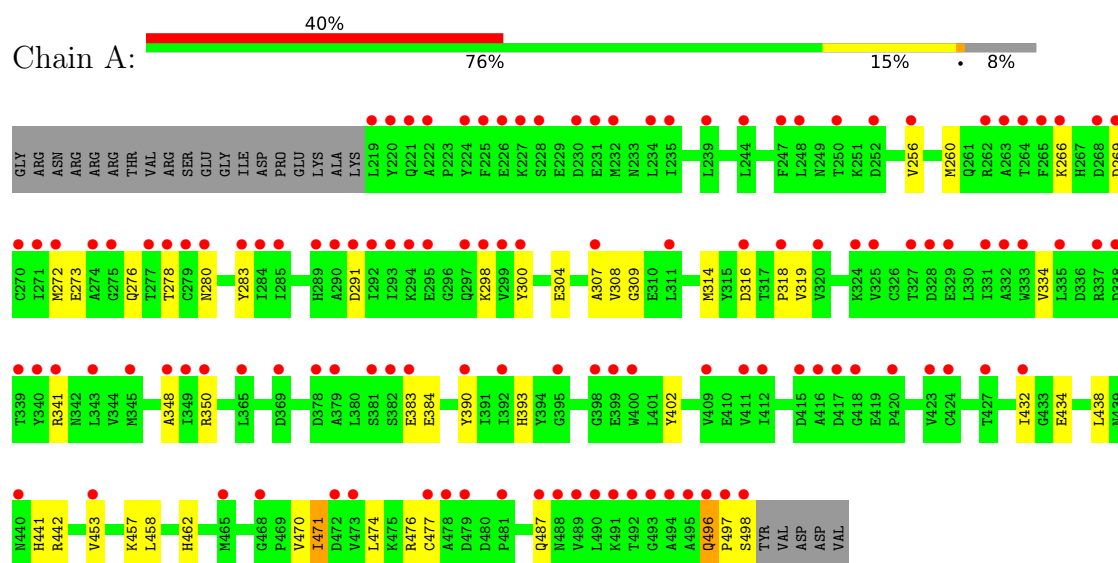
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	45	Total 45	O 45	0	0
4	D	39	Total 39	O 39	0	0

3 Residue-property plots [i](#)

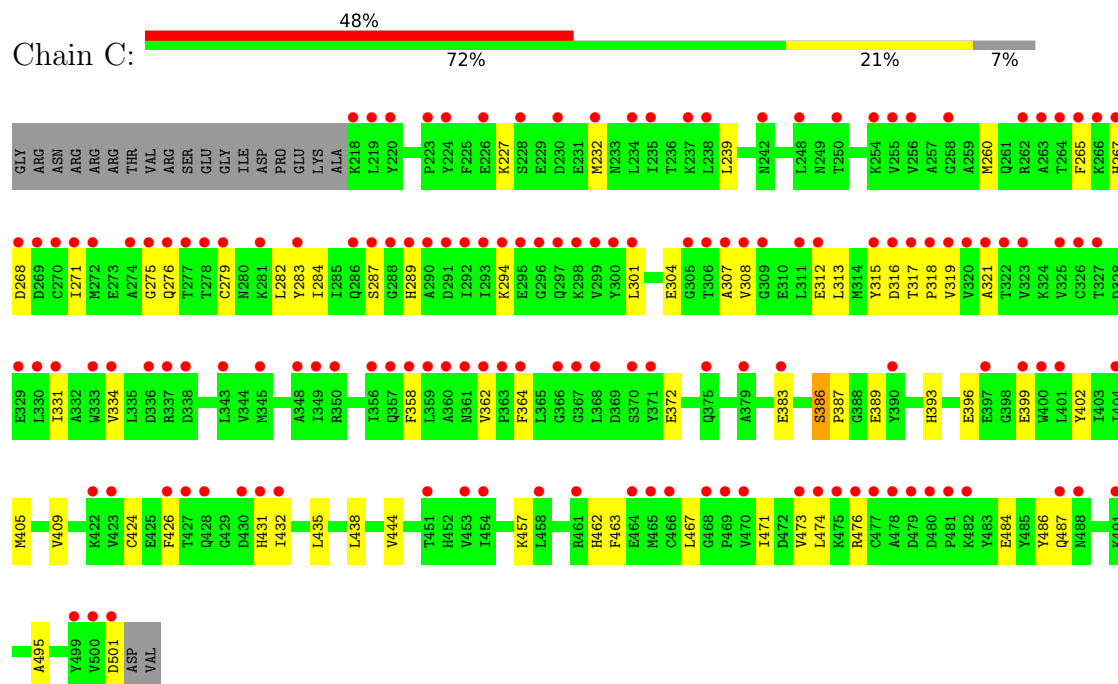
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



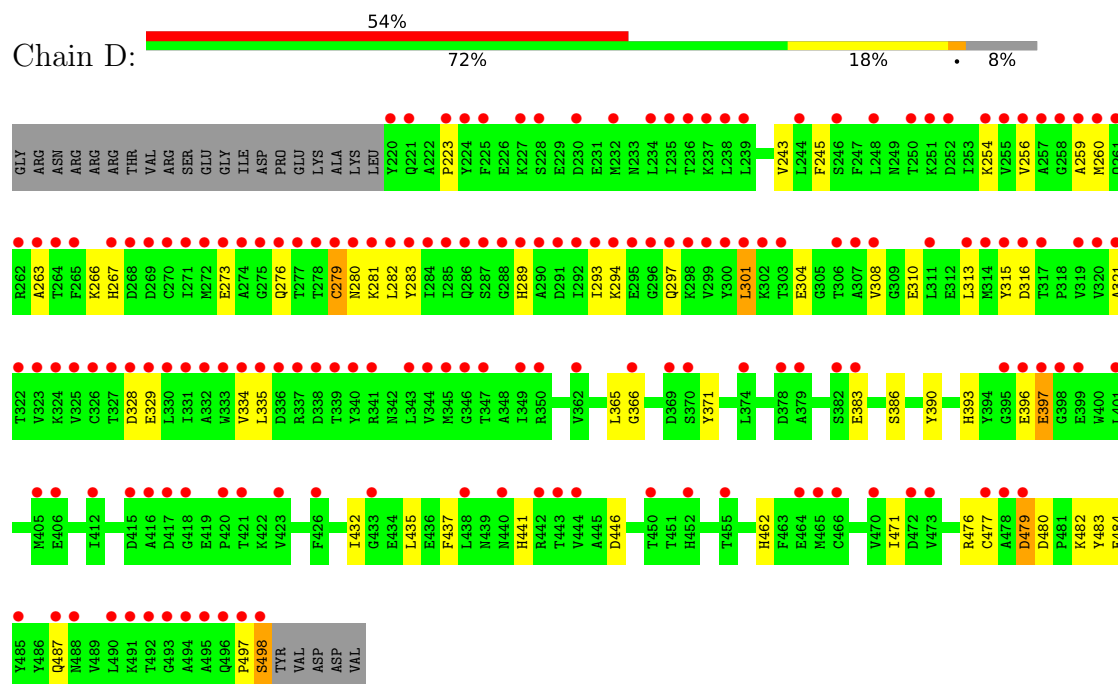
• Molecule 1: Protein kinase A regulatory subunit

Chain C:



• Molecule 1: Protein kinase A regulatory subunit

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 99.1 (59.84-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.260 , 0.319 0.264 , 0.321	Depositor DCC
R_{free} test set	4294 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 87.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18613	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.93	0/2351	0.96	2/3188 (0.1%)
1	B	0.84	0/2379	0.88	0/3225
1	C	0.80	0/2385	0.91	0/3227
1	D	0.81	0/2359	0.88	0/3197
All	All	0.85	0/9474	0.91	2/12837 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ARG	NE-CZ-NH1	-7.80	113.70	121.50
1	A	476	ARG	CG-CD-NE	-5.05	100.90	112.00

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	2255	2255	2240	34	2
1	B	2288	2265	2267	37	0
1	C	2296	2295	2272	59	1
1	D	2270	2252	2263	40	3
2	A	40	24	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	D	39	0	0	6	0
All	All	9446	9167	9149	171	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 (171) 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:393:HIS:HB2	1:B:396[A]:GLU:CD	2.18	0.68
1:B:310:GLU:HG2	1:B:311:LEU:N	2.09	0.66
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:474:LEU:C	1:C:474:LEU:CB	2.77	0.57
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
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:N	1:C:474:LEU:C	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:470:VAL:O	1:A:471:ILE:C	2.55	0.48
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:A:318:PRO:O	1:A:319:VAL:C	2.57	0.48
1:B:304:GLU:H	1:B:304:GLU:CD	2.22	0.48
1:C:283:TYR:HB2	1:C:308:VAL:HG22	1.96	0.48
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:B:369:ASP:OD1	1:B:369:ASP:C	2.57	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:C:318:PRO:O	1:C:319:VAL:C	2.56	0.46
1:A:314[B]:MET:HE3	1:A:348:ALA:HB1	1.96	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:D:365:LEU:O	1:D:366:GLY:C	2.58	0.45
1:A:266:LYS:H	1:A:269:ASP:CG	2.25	0.45
1:B:344:VAL:O	1:B:345:MET:C	2.59	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: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:441:HIS:HA	1:A:497:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:C	1:B:234:LEU:HD23	2.43	0.43
1:C:312:GLU:HG3	1:C:317:THR:HG23	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
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:B:264:THR:C	1:B:265:PHE:CD1	2.97	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:A:383:GLU:CD	1:A:402:TYR:HE2	2.27	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: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: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:C:386:SER:O	1:C:387:PRO:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:239:LEU:HD21	1:C:260[B]:MET:HE3	2.02	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:C:358:PHE:CZ	1:C:405:MET:HG2	2.56	0.40
1:B:318:PRO:O	1:B:319:VAL:C	2.62	0.40
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 [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	291/304 (96%)	277 (95%)	12 (4%)	2 (1%)	18 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	293/304 (96%)	270 (92%)	20 (7%)	3 (1%)	12	8
1	C	294/304 (97%)	274 (93%)	16 (5%)	4 (1%)	9	5
1	D	291/304 (96%)	270 (93%)	18 (6%)	3 (1%)	12	8
All	All	1169/1216 (96%)	1091 (93%)	66 (6%)	12 (1%)	21	8

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
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%)	43	47
1	B	253/262 (97%)	247 (98%)	6 (2%)	43	47
1	C	252/262 (96%)	248 (98%)	4 (2%)	55	62
1	D	251/262 (96%)	241 (96%)	10 (4%)	28	28
All	All	1006/1048 (96%)	980 (97%)	26 (3%)	42	45

All (26) 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	304	GLU
1	B	316[A]	ASP
1	B	316[B]	ASP
1	B	432	ILE
1	C	279	CYS
1	C	304	GLU
1	C	386	SER
1	C	432	ILE
1	D	254	LYS
1	D	279	CYS
1	D	301	LEU
1	D	304	GLU
1	D	386[A]	SER
1	D	386[B]	SER
1	D	432	ILE
1	D	471	ILE
1	D	479	ASP
1	D	498	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	HIS
1	A	487	GLN
1	B	261	GLN
1	B	267	HIS
1	C	393	HIS
1	C	496	GLN
1	D	462	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	601	-	22,22,22	2.63	8 (36%)	33,33,33	1.69	6 (18%)
3	ACT	B	603	-	3,3,3	0.87	0	3,3,3	1.50	0
2	GMP	C	601	-	22,22,22	2.68	8 (36%)	33,33,33	2.25	8 (24%)
2	GMP	A	602	-	22,22,22	2.24	6 (27%)	33,33,33	1.69	6 (18%)
2	GMP	A	601	-	22,22,22	2.38	7 (31%)	33,33,33	1.44	8 (24%)
2	GMP	B	601	-	22,22,22	2.44	6 (27%)	33,33,33	2.22	11 (33%)
2	GMP	B	602	-	22,22,22	2.63	8 (36%)	33,33,33	1.73	8 (24%)
2	GMP	C	602	-	22,22,22	2.61	7 (31%)	33,33,33	1.86	11 (33%)
2	GMP	D	602	-	22,22,22	2.51	8 (36%)	33,33,33	2.08	9 (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	D	601	-	-	1/6/22/22	0/3/3/3
2	GMP	C	601	-	-	0/6/22/22	0/3/3/3
2	GMP	A	602	-	-	0/6/22/22	0/3/3/3
2	GMP	A	601	-	-	0/6/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GMP	B	601	-	-	0/6/22/22	0/3/3/3
2	GMP	B	602	-	-	0/6/22/22	0/3/3/3
2	GMP	C	602	-	-	0/6/22/22	0/3/3/3
2	GMP	D	602	-	-	0/6/22/22	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	GMP	C4-N3	7.69	1.51	1.34
2	C	601	GMP	C4-N3	7.54	1.51	1.34
2	C	602	GMP	C4-N3	7.01	1.50	1.34
2	A	601	GMP	C4-N3	6.81	1.49	1.34
2	D	601	GMP	C4-N3	6.65	1.49	1.34
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	B	601	GMP	C4-N3	6.53	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	C	601	GMP	C2-N2	5.97	1.48	1.34
2	B	602	GMP	C2-N2	5.92	1.48	1.34
2	D	602	GMP	C4-N3	5.78	1.47	1.34
2	B	601	GMP	C2-N2	5.67	1.47	1.34
2	A	602	GMP	C4-N3	5.37	1.46	1.34
2	A	601	GMP	C2-N2	5.08	1.46	1.34
2	C	601	GMP	C2-N3	4.81	1.44	1.33
2	B	601	GMP	C2-N3	4.66	1.44	1.33
2	D	602	GMP	C2-N3	4.61	1.44	1.33
2	D	601	GMP	C2-N3	4.52	1.44	1.33
2	B	602	GMP	C5-C6	3.85	1.58	1.44
2	C	602	GMP	C2-N3	3.81	1.42	1.33
2	B	602	GMP	C2-N3	3.61	1.41	1.33
2	A	601	GMP	C2-N3	3.57	1.41	1.33
2	A	602	GMP	C2-N3	3.56	1.41	1.33
2	A	601	GMP	C4-N9	-3.37	1.29	1.38
2	C	601	GMP	C5-N7	-3.29	1.32	1.39
2	D	602	GMP	C5-C6	3.14	1.56	1.44
2	B	601	GMP	C5-C6	3.14	1.56	1.44
2	C	602	GMP	C4-N9	-3.03	1.30	1.38
2	C	601	GMP	C2-N1	3.01	1.44	1.37
2	D	601	GMP	C5-N7	-2.96	1.33	1.39
2	B	602	GMP	C2-N1	2.95	1.44	1.37
2	D	601	GMP	C4-N9	-2.92	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	GMP	C5-C6	2.87	1.55	1.44
2	D	601	GMP	C2-N1	2.83	1.44	1.37
2	B	601	GMP	C5-N7	-2.83	1.33	1.39
2	A	602	GMP	C4-N9	-2.80	1.30	1.38
2	A	601	GMP	C6-N1	2.74	1.44	1.38
2	C	602	GMP	C2-N1	2.70	1.44	1.37
2	B	602	GMP	C4-N9	-2.68	1.31	1.38
2	A	602	GMP	C5-N7	-2.62	1.33	1.39
2	A	601	GMP	C5-N7	-2.61	1.33	1.39
2	C	602	GMP	C5-N7	-2.60	1.33	1.39
2	C	601	GMP	C6-N1	2.60	1.43	1.38
2	D	602	GMP	C5-N7	-2.57	1.33	1.39
2	D	601	GMP	C6-N1	2.52	1.43	1.38
2	D	602	GMP	C4-N9	-2.41	1.31	1.38
2	B	602	GMP	C5-N7	-2.30	1.34	1.39
2	D	602	GMP	C6-N1	2.28	1.43	1.38
2	C	601	GMP	O6-C6	-2.25	1.19	1.23
2	A	602	GMP	C2-N1	2.22	1.43	1.37
2	D	601	GMP	C5-C6	2.18	1.52	1.44
2	D	602	GMP	C2-N1	2.16	1.42	1.37
2	B	601	GMP	C2-N1	2.16	1.42	1.37
2	A	601	GMP	C2-N1	2.16	1.42	1.37
2	B	602	GMP	O6-C6	-2.08	1.19	1.23
2	C	601	GMP	C5-C6	2.03	1.52	1.44

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GMP	C5-C4-N3	-6.47	118.09	128.39
2	C	601	GMP	C5-C4-N3	-6.14	118.61	128.39
2	D	602	GMP	C2-N3-C4	5.90	122.46	112.30
2	D	602	GMP	C5-C4-N3	-5.47	119.69	128.39
2	C	601	GMP	C2-N3-C4	5.26	121.36	112.30
2	B	601	GMP	C2-N3-C4	5.23	121.30	112.30
2	A	602	GMP	C2-N3-C4	5.19	121.24	112.30
2	C	602	GMP	C2-N3-C4	4.88	120.70	112.30
2	C	601	GMP	O6-C6-C5	-4.67	114.21	126.53
2	D	601	GMP	C2-N3-C4	4.61	120.24	112.30
2	A	602	GMP	C5-C4-N3	-4.38	121.41	128.39
2	C	602	GMP	C5-C4-N3	-4.38	121.42	128.39
2	C	601	GMP	N9-C4-N3	4.38	134.71	125.95
2	C	601	GMP	C2-N1-C6	-4.34	117.25	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	GMP	C5-C4-N3	-4.15	121.78	128.39
2	B	602	GMP	O6-C6-N1	-3.98	112.64	120.11
2	B	601	GMP	C2-N1-C6	-3.82	118.19	125.11
2	B	601	GMP	C4-C5-N7	-3.63	104.92	110.67
2	C	601	GMP	C5-C6-N1	3.60	122.41	113.25
2	C	602	GMP	N9-C8-N7	-3.51	106.89	113.40
2	B	602	GMP	C2-N3-C4	3.51	118.34	112.30
2	D	602	GMP	N9-C8-N7	-3.46	106.98	113.40
2	B	602	GMP	C6-C5-N7	3.38	136.44	130.29
2	A	602	GMP	N1-C2-N3	-3.35	117.19	123.32
2	B	601	GMP	O6-C6-N1	-3.28	113.94	120.11
2	A	601	GMP	C2-N3-C4	3.23	117.87	112.30
2	B	601	GMP	C5-C4-N9	3.19	111.37	105.66
2	B	602	GMP	C5-C4-N3	-3.11	123.44	128.39
2	B	601	GMP	C8-N7-C5	3.09	109.76	104.26
2	D	602	GMP	N9-C4-N3	3.07	132.10	125.95
2	D	602	GMP	C2-N1-C6	-3.01	119.64	125.11
2	D	601	GMP	N1-C2-N3	-2.94	117.94	123.32
2	A	601	GMP	N9-C8-N7	-2.93	107.97	113.40
2	B	601	GMP	C5-C6-N1	2.93	120.70	113.25
2	D	601	GMP	N9-C4-N3	2.88	131.71	125.95
2	B	602	GMP	N9-C8-N7	-2.78	108.24	113.40
2	C	601	GMP	N9-C8-N7	-2.78	108.24	113.40
2	A	602	GMP	N2-C2-N1	2.74	122.54	116.76
2	D	601	GMP	N9-C8-N7	-2.74	108.33	113.40
2	B	601	GMP	N9-C8-N7	-2.73	108.33	113.40
2	A	601	GMP	N2-C2-N3	2.73	125.00	119.67
2	B	602	GMP	N2-C2-N3	2.65	124.84	119.67
2	D	601	GMP	O6-C6-C5	-2.58	119.71	126.53
2	C	602	GMP	N2-C2-N1	2.58	122.21	116.76
2	B	601	GMP	C6-C5-N7	2.56	134.94	130.29
2	A	602	GMP	N9-C4-N3	2.55	131.06	125.95
2	C	602	GMP	C5-C6-N1	2.55	119.74	113.25
2	D	602	GMP	C5-C6-N1	2.55	119.74	113.25
2	D	602	GMP	C8-N7-C5	2.54	108.78	104.26
2	A	601	GMP	O6-C6-C5	-2.48	119.99	126.53
2	A	601	GMP	N1-C2-N3	-2.45	118.84	123.32
2	C	601	GMP	N2-C2-N1	2.40	121.83	116.76
2	A	601	GMP	C8-N9-C4	2.40	110.53	106.03
2	C	602	GMP	N1-C2-N3	-2.38	118.97	123.32
2	C	602	GMP	C6-C5-N7	2.37	134.59	130.29
2	C	602	GMP	N9-C4-N3	2.33	130.61	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	GMP	N1-C2-N3	-2.30	119.11	123.32
2	B	601	GMP	N9-C4-N3	2.29	130.53	125.95
2	A	601	GMP	C5-C4-N3	-2.28	124.76	128.39
2	B	602	GMP	C4-C5-N7	-2.19	107.20	110.67
2	A	602	GMP	N9-C8-N7	-2.18	109.35	113.40
2	C	602	GMP	C2-N1-C6	-2.16	121.19	125.11
2	C	602	GMP	C8-N7-C5	2.12	108.04	104.26
2	D	602	GMP	C4-C5-N7	-2.08	107.37	110.67
2	A	601	GMP	N9-C4-N3	2.05	130.05	125.95
2	C	602	GMP	C4-C5-N7	-2.04	107.43	110.67
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:

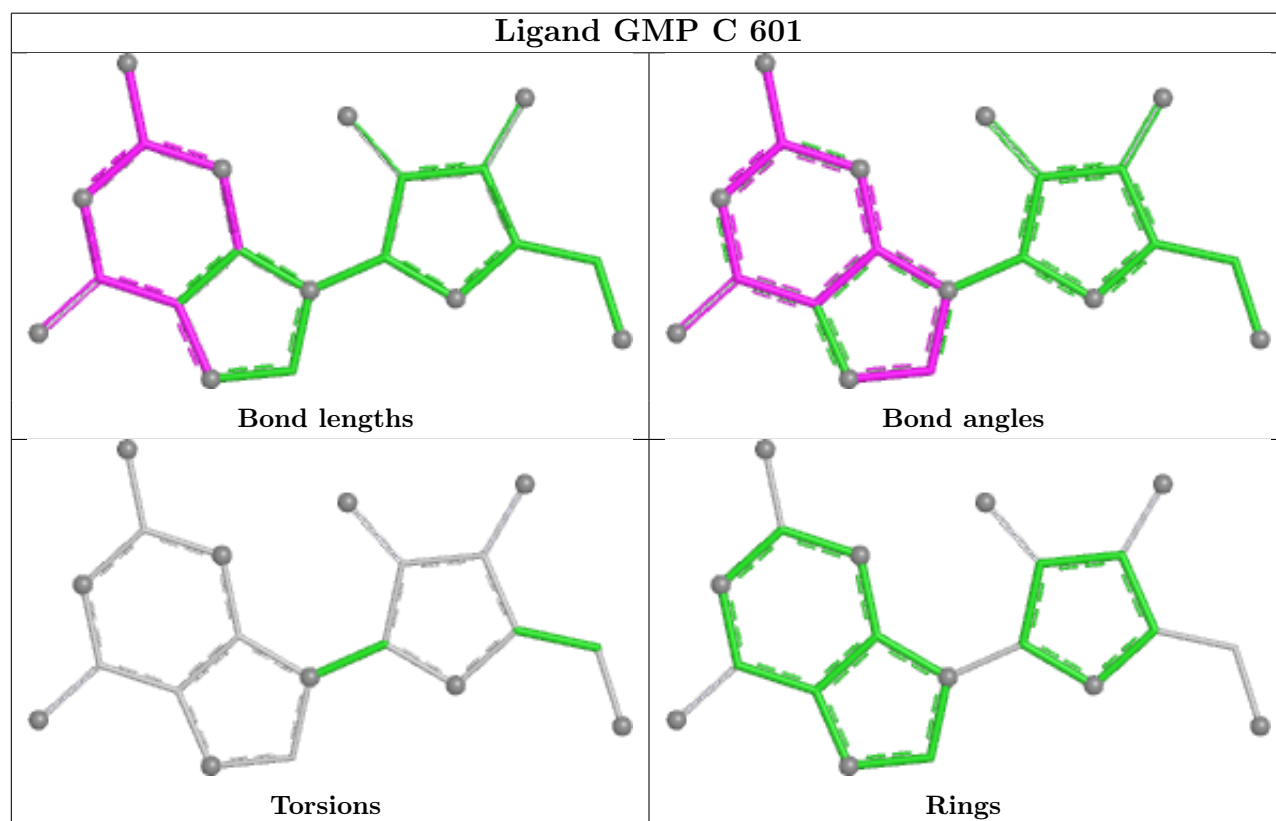
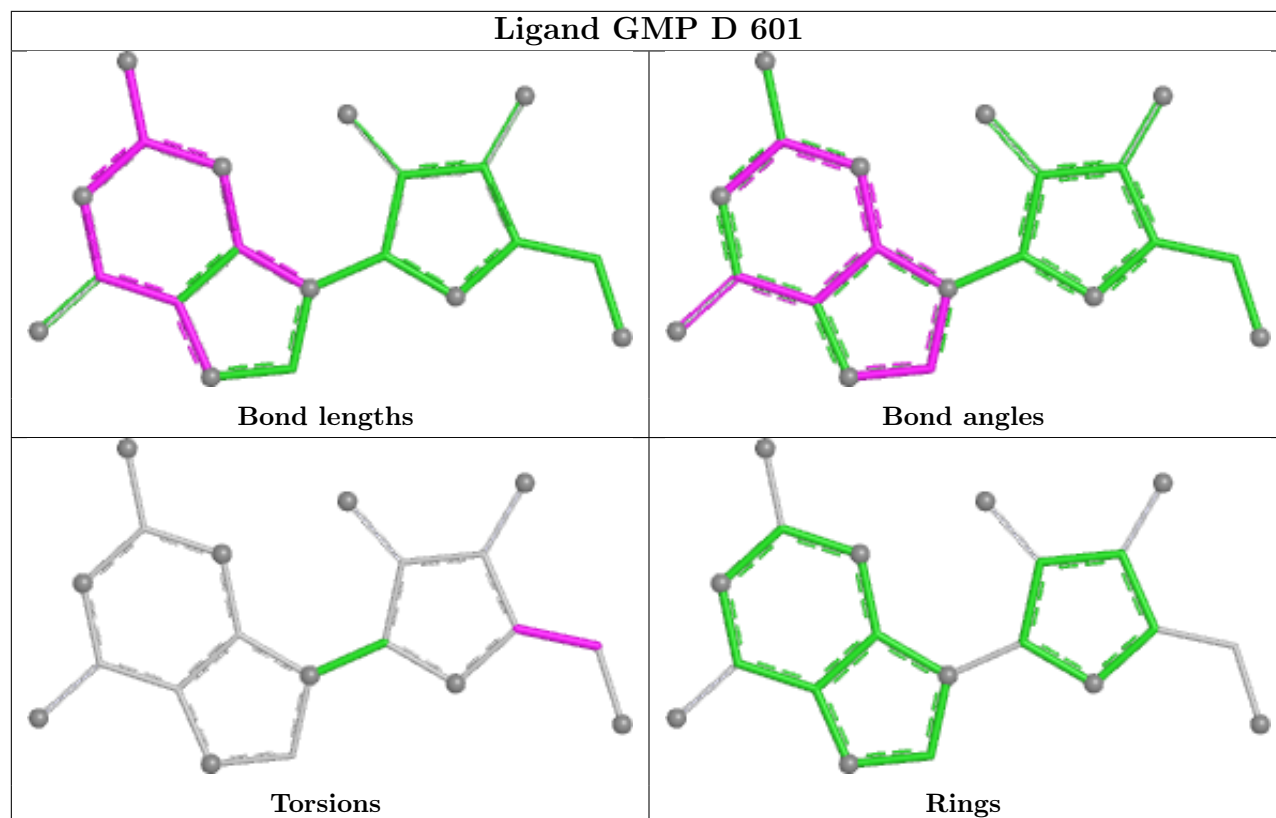
Mol	Chain	Res	Type	Atoms
2	D	601	GMP	O4'-C4'-C5'-O5'

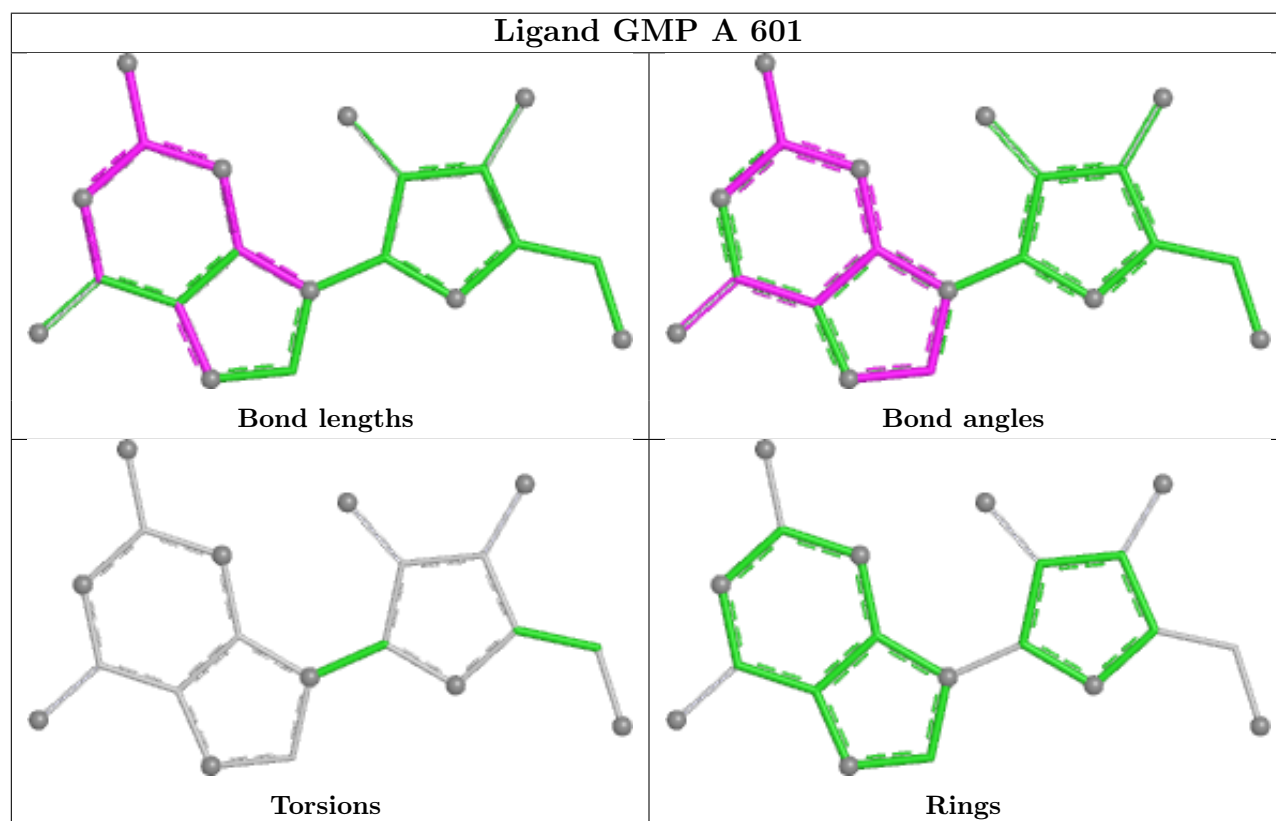
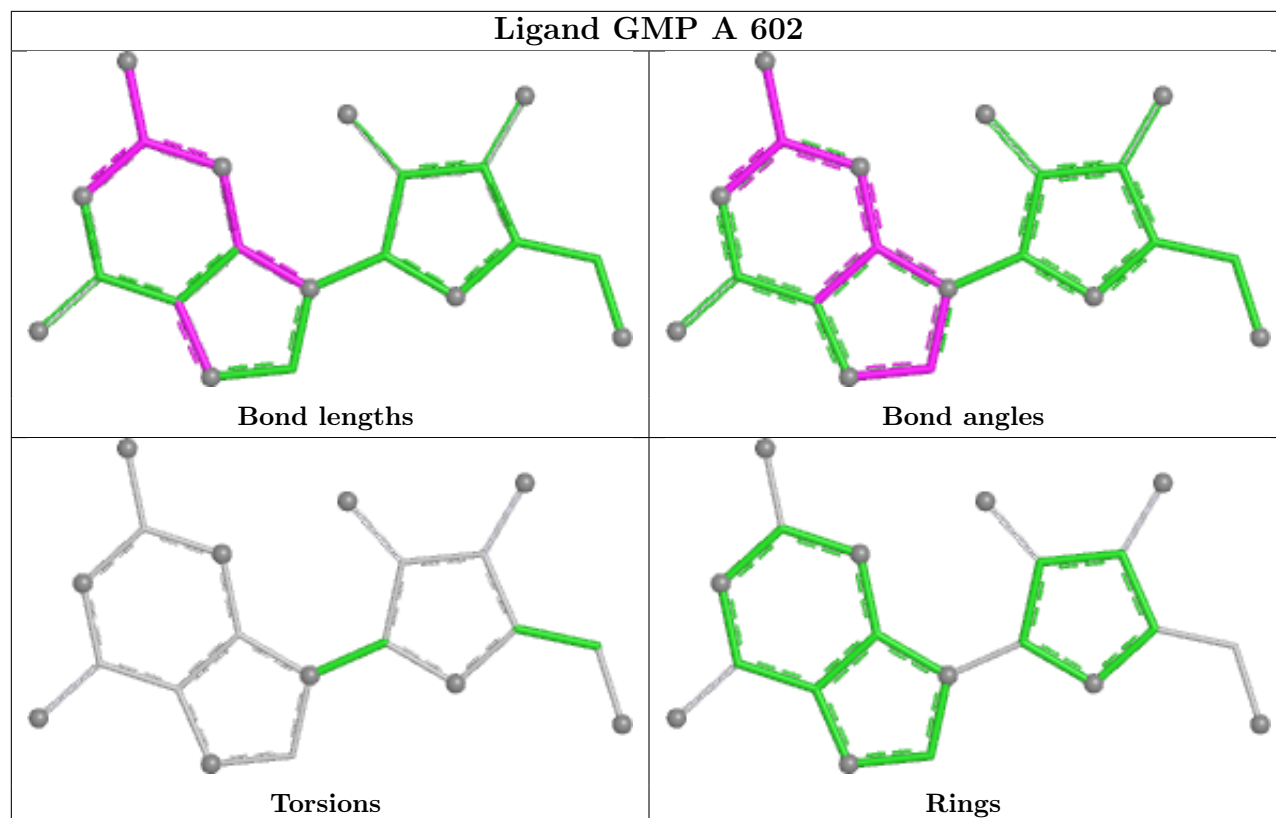
There are no ring outliers.

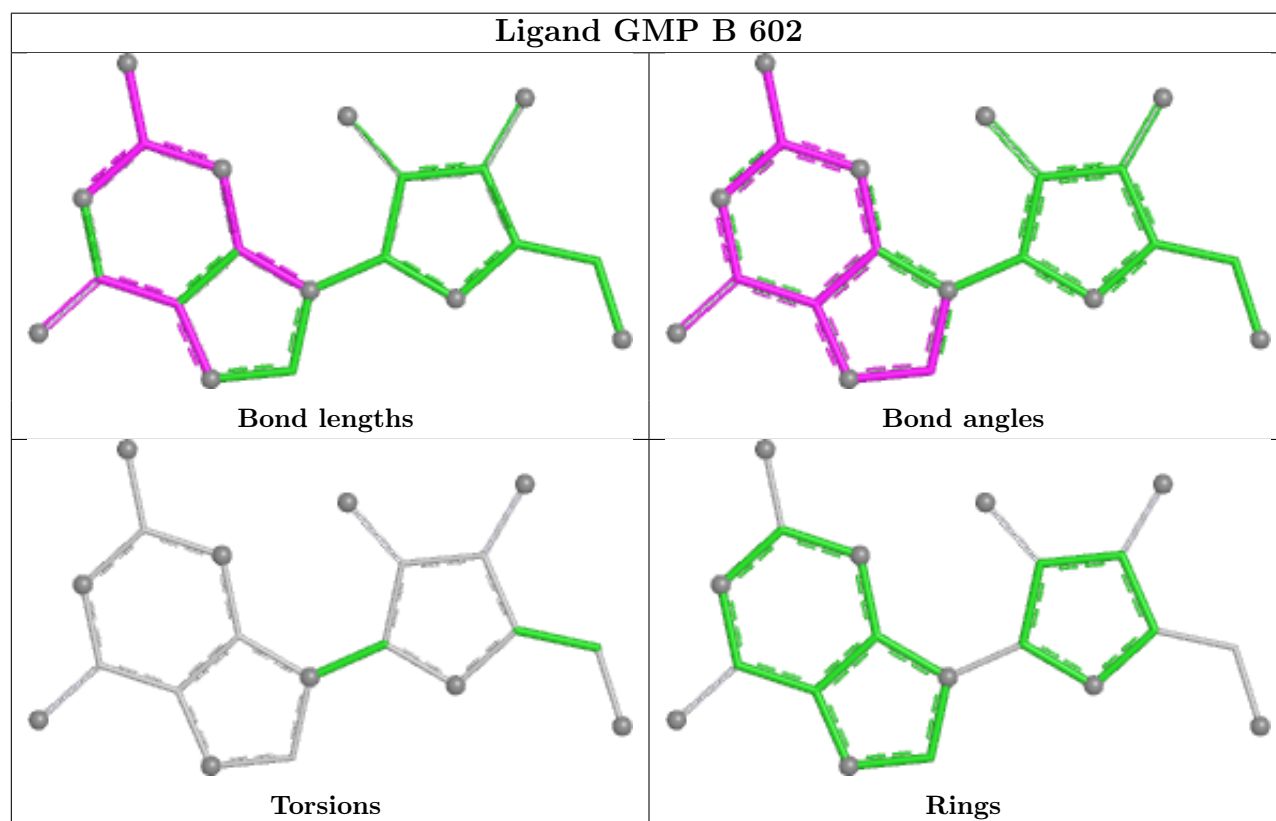
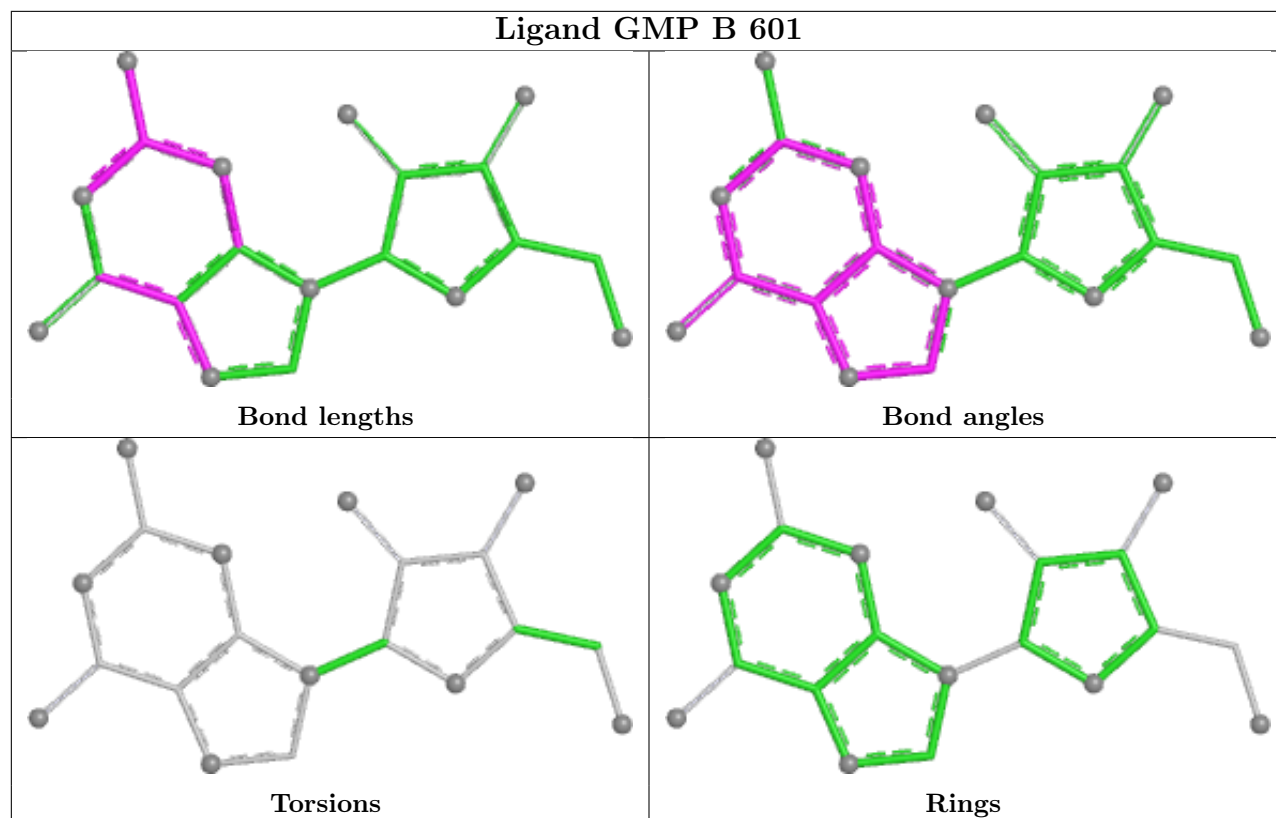
7 monomers are involved in 10 short contacts:

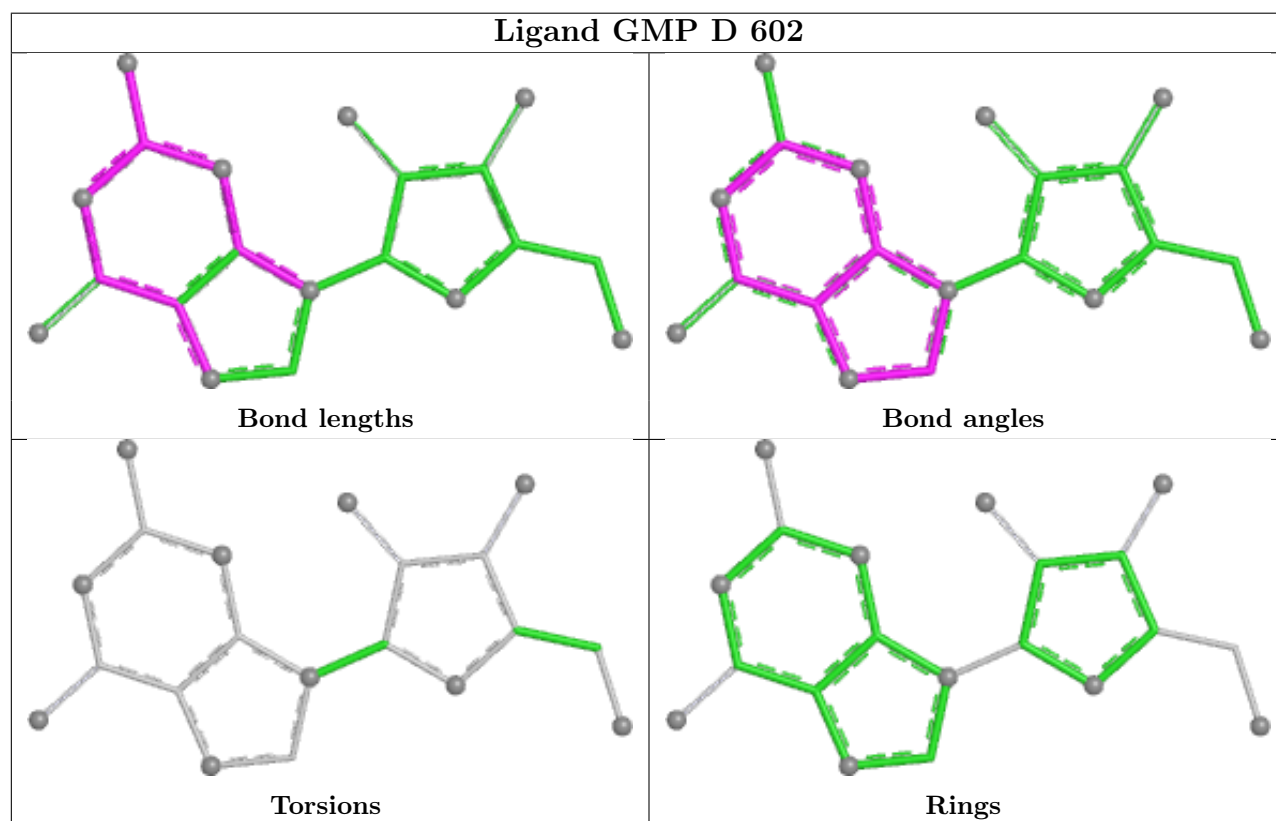
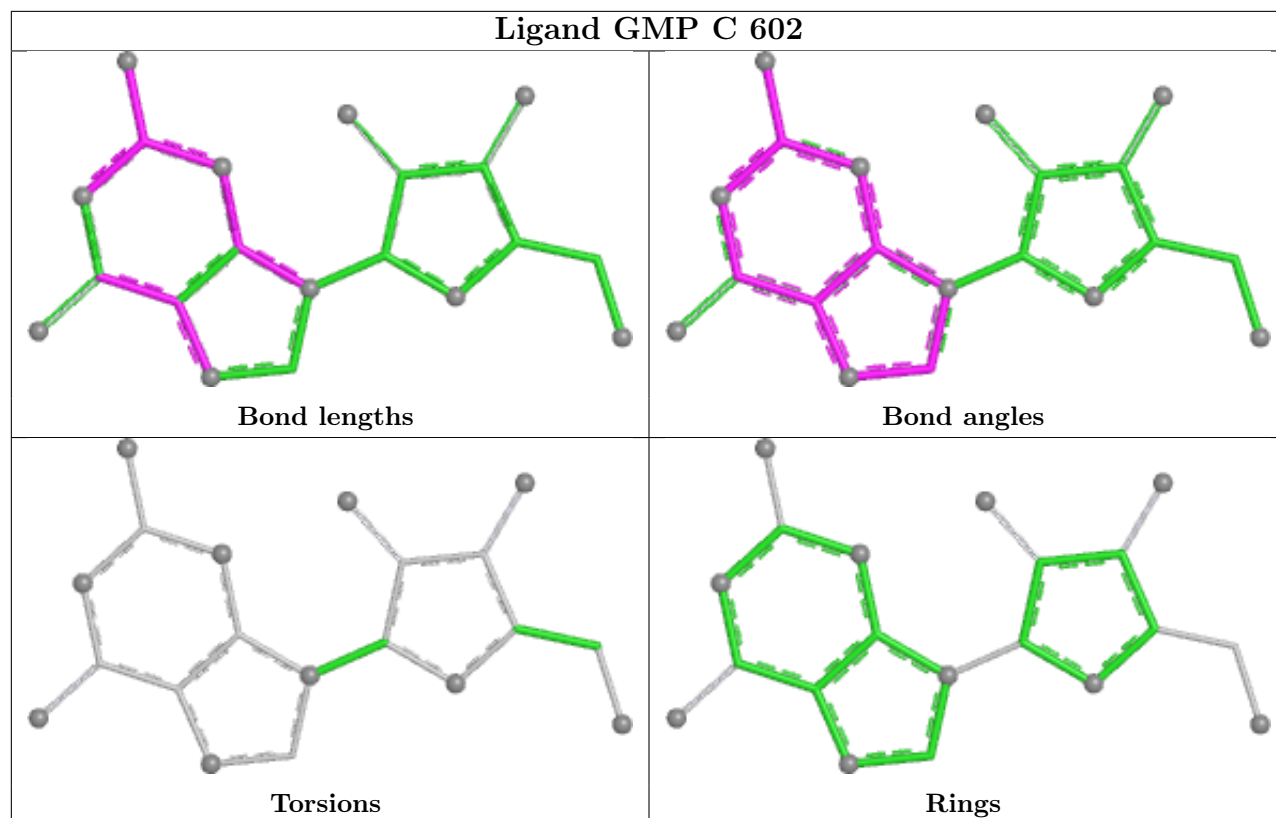
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	GMP	1	0
3	B	603	ACT	1	0
2	A	601	GMP	4	0
2	B	601	GMP	1	0
2	B	602	GMP	1	0
2	C	602	GMP	1	0
2	D	602	GMP	1	0

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, 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	280/304 (92%)	1.95	122 (43%) 0 1	37, 82, 137, 180	9 (3%)
1	B	282/304 (92%)	2.43	167 (59%) 0 0	36, 96, 154, 238	10 (3%)
1	C	284/304 (93%)	2.18	145 (51%) 0 0	36, 88, 144, 180	9 (3%)
1	D	279/304 (91%)	2.40	165 (59%) 0 0	39, 95, 145, 166	12 (4%)
All	All	1125/1216 (92%)	2.24	599 (53%) 0 0	36, 89, 147, 238	40 (3%)

All (599) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	CYS	9.0
1	B	465	MET	6.8
1	B	282	LEU	6.1
1	D	239	LEU	5.9
1	B	308	VAL	5.9
1	D	284[A]	ILE	5.8
1	B	320	VAL	5.8
1	D	308	VAL	5.8
1	A	272	MET	5.7
1	B	263	ALA	5.5
1	B	332	ALA	5.4
1	C	274	ALA	5.4
1	C	271	ILE	5.3
1	D	299	VAL	5.2
1	D	300	TYR	5.2
1	D	225	PHE	5.2
1	A	498	SER	5.2
1	A	495	ALA	5.2
1	B	265	PHE	5.2
1	C	323	VAL	5.2
1	B	370	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	301	LEU	5.0
1	A	383	GLU	5.0
1	B	283	TYR	4.9
1	D	325	VAL	4.9
1	D	307	ALA	4.9
1	D	494	ALA	4.9
1	D	244	LEU	4.9
1	C	426	PHE	4.9
1	C	383	GLU	4.8
1	C	465	MET	4.8
1	B	348	ALA	4.8
1	D	250	THR	4.8
1	B	224	TYR	4.7
1	B	232	MET	4.7
1	B	245	PHE	4.6
1	C	264	THR	4.6
1	B	244	LEU	4.6
1	B	299	VAL	4.6
1	B	356	ILE	4.6
1	D	293	ILE	4.6
1	D	256	VAL	4.6
1	C	290	ALA	4.6
1	B	235	ILE	4.6
1	B	284[A]	ILE	4.5
1	B	321	ALA	4.5
1	A	219	LEU	4.5
1	A	497	PRO	4.5
1	D	279	CYS	4.5
1	D	277	THR	4.4
1	B	323	VAL	4.4
1	C	370	SER	4.4
1	C	300	TYR	4.4
1	B	501	ASP	4.4
1	C	283	TYR	4.4
1	B	307	ALA	4.4
1	D	311	LEU	4.4
1	B	293	ILE	4.4
1	B	225	PHE	4.3
1	A	423	VAL	4.3
1	A	294	LYS	4.3
1	D	238	LEU	4.3
1	B	300	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	371	TYR	4.3
1	B	333	TRP	4.3
1	B	331	ILE	4.3
1	C	296	GLY	4.3
1	C	469	PRO	4.3
1	B	476[A]	ARG	4.2
1	C	343[A]	LEU	4.2
1	D	220	TYR	4.2
1	D	335	LEU	4.2
1	D	438	LEU	4.2
1	C	325	VAL	4.2
1	C	363	PRO	4.2
1	A	343[A]	LEU	4.2
1	B	335	LEU	4.2
1	C	320	VAL	4.2
1	D	255	VAL	4.2
1	D	497	PRO	4.1
1	B	256	VAL	4.1
1	B	271	ILE	4.1
1	D	326	CYS	4.1
1	D	294	LYS	4.1
1	D	496	GLN	4.1
1	B	319	VAL	4.1
1	D	416	ALA	4.1
1	C	270	CYS	4.0
1	A	494	ALA	4.0
1	B	295	GLU	4.0
1	C	305	GLY	4.0
1	A	224	TYR	4.0
1	A	299	VAL	4.0
1	D	270	CYS	4.0
1	D	465	MET	4.0
1	C	295	GLU	4.0
1	D	343[A]	LEU	3.9
1	B	250	THR	3.9
1	B	257	ALA	3.9
1	C	478	ALA	3.9
1	D	322	THR	3.9
1	C	237	LYS	3.9
1	D	285	ILE	3.9
1	A	472	ASP	3.9
1	C	279	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	343	LEU	3.9
1	B	264	THR	3.9
1	A	220	TYR	3.9
1	D	498	SER	3.9
1	D	248	LEU	3.9
1	A	479	ASP	3.8
1	C	292	ILE	3.8
1	C	293	ILE	3.8
1	D	271	ILE	3.8
1	B	326	CYS	3.8
1	B	297[A]	GLN	3.8
1	B	342	ASN	3.8
1	C	327	THR	3.8
1	C	349	ILE	3.8
1	D	331	ILE	3.8
1	D	259	ALA	3.8
1	D	263	ALA	3.8
1	C	501	ASP	3.8
1	D	320	VAL	3.8
1	B	220	TYR	3.8
1	B	315	TYR	3.8
1	B	274	ALA	3.8
1	D	330	LEU	3.8
1	A	275	GLY	3.8
1	D	440	ASN	3.7
1	D	283	TYR	3.7
1	C	291	ASP	3.7
1	B	491	LYS	3.7
1	B	292	ILE	3.7
1	A	274	ALA	3.7
1	A	478	ALA	3.7
1	C	360	ALA	3.7
1	C	479	ASP	3.7
1	D	275	GLY	3.7
1	A	316[A]	ASP	3.7
1	B	421	THR	3.7
1	B	469	PRO	3.7
1	D	223	PRO	3.7
1	B	260[A]	MET	3.7
1	B	479	ASP	3.7
1	B	487	GLN	3.7
1	D	333	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	255	VAL	3.6
1	A	225	PHE	3.6
1	D	236[A]	THR	3.6
1	D	421	THR	3.6
1	D	274	ALA	3.6
1	D	405	MET	3.6
1	D	323	VAL	3.6
1	D	268	ASP	3.6
1	A	492	THR	3.6
1	D	478	ALA	3.6
1	D	280	ASN	3.6
1	B	310	GLU	3.6
1	C	476[A]	ARG	3.6
1	D	251	LYS	3.6
1	C	333	TRP	3.6
1	D	292	ILE	3.6
1	D	301	LEU	3.6
1	A	493	GLY	3.6
1	C	220	TYR	3.6
1	B	311	LEU	3.5
1	D	466[A]	CYS	3.5
1	C	319	VAL	3.5
1	D	334	VAL	3.5
1	A	481	PRO	3.5
1	B	239	LEU	3.5
1	A	340	TYR	3.5
1	A	277	THR	3.5
1	B	318	PRO	3.5
1	D	332	ALA	3.5
1	D	258	GLY	3.5
1	B	314[A]	MET	3.5
1	C	482	LYS	3.5
1	A	297[A]	GLN	3.5
1	A	440	ASN	3.5
1	D	303	THR	3.5
1	B	481	PRO	3.4
1	D	349	ILE	3.4
1	B	324	LYS	3.4
1	C	475	LYS	3.4
1	D	224	TYR	3.4
1	B	500	VAL	3.4
1	D	278	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	269	ASP	3.4
1	D	479	ASP	3.4
1	B	330	LEU	3.4
1	B	298	LYS	3.4
1	B	278	THR	3.4
1	B	334	VAL	3.4
1	C	250	THR	3.4
1	C	322	THR	3.4
1	A	311	LEU	3.4
1	B	359	LEU	3.4
1	C	474	LEU	3.4
1	A	496	GLN	3.4
1	A	398	GLY	3.4
1	D	234	LEU	3.4
1	C	315	TYR	3.3
1	B	344	VAL	3.3
1	C	337	ARG	3.3
1	A	339	THR	3.3
1	B	303	THR	3.3
1	D	287	SER	3.3
1	C	308	VAL	3.3
1	A	416	ALA	3.3
1	A	432	ILE	3.3
1	A	239	LEU	3.3
1	B	474	LEU	3.3
1	C	272	MET	3.3
1	C	397	GLU	3.3
1	C	298	LYS	3.3
1	C	297[A]	GLN	3.3
1	D	369	ASP	3.3
1	B	289	HIS	3.2
1	D	420	PRO	3.2
1	C	334	VAL	3.2
1	D	495	ALA	3.2
1	A	293	ILE	3.2
1	B	233	ASN	3.2
1	B	272	MET	3.2
1	C	358	PHE	3.2
1	D	264	THR	3.2
1	C	488	ASN	3.2
1	A	327	THR	3.2
1	B	279	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	361	ASN	3.2
1	D	321	ALA	3.2
1	B	349	ILE	3.2
1	D	262	ARG	3.2
1	C	326	CYS	3.2
1	C	269	ASP	3.1
1	D	316[A]	ASP	3.1
1	C	224	TYR	3.1
1	D	485	TYR	3.1
1	A	250	THR	3.1
1	D	272	MET	3.1
1	D	378	ASP	3.1
1	D	442	ARG	3.1
1	B	454	ILE	3.1
1	B	340	TYR	3.1
1	D	298	LYS	3.1
1	D	345	MET	3.1
1	B	317	THR	3.1
1	B	222	ALA	3.1
1	C	348	ALA	3.1
1	D	418	GLY	3.1
1	C	223	PRO	3.1
1	A	415	ASP	3.1
1	D	267	HIS	3.1
1	B	325	VAL	3.1
1	B	473	VAL	3.1
1	C	500	VAL	3.1
1	C	311	LEU	3.1
1	B	285	ILE	3.1
1	C	331	ILE	3.1
1	C	345	MET	3.1
1	D	296	GLY	3.0
1	B	475	LYS	3.0
1	B	482	LYS	3.0
1	B	466[A]	CYS	3.0
1	C	321	ALA	3.0
1	D	401	LEU	3.0
1	B	327	THR	3.0
1	B	229	GLU	3.0
1	D	291	ASP	3.0
1	A	228	SER	3.0
1	D	490	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	418	GLY	3.0
1	D	395	GLY	3.0
1	D	383	GLU	3.0
1	A	264	THR	3.0
1	B	277	THR	3.0
1	C	318	PRO	3.0
1	A	283	TYR	3.0
1	D	328	ASP	3.0
1	C	254	LYS	3.0
1	B	357	GLN	3.0
1	A	222	ALA	3.0
1	B	270	CYS	3.0
1	A	473	VAL	3.0
1	B	238	LEU	3.0
1	B	361	ASN	3.0
1	A	331	ILE	3.0
1	B	254	LYS	3.0
1	C	491	LYS	3.0
1	B	358	PHE	3.0
1	D	337	ARG	2.9
1	D	444	VAL	2.9
1	B	236[A]	THR	2.9
1	B	368	LEU	2.9
1	C	238	LEU	2.9
1	D	423	VAL	2.9
1	B	253	ILE	2.9
1	C	268	ASP	2.9
1	A	341	ARG	2.9
1	C	400	TRP	2.9
1	A	234	LEU	2.9
1	B	258	GLY	2.9
1	C	219	LEU	2.9
1	A	338	ASP	2.9
1	C	473	VAL	2.9
1	D	336	ASP	2.9
1	B	488	ASN	2.9
1	D	257	ALA	2.9
1	B	472	ASP	2.8
1	D	282	LEU	2.8
1	D	344	VAL	2.8
1	B	397	GLU	2.8
1	A	269	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	374	LEU	2.8
1	A	329	GLU	2.8
1	C	399	GLU	2.8
1	B	223	PRO	2.8
1	C	404	ILE	2.8
1	C	294	LYS	2.8
1	B	230	ASP	2.8
1	C	265	PHE	2.8
1	D	232	MET	2.8
1	C	288	GLY	2.8
1	D	366	GLY	2.8
1	A	490	LEU	2.8
1	C	301	LEU	2.8
1	D	374	LEU	2.8
1	D	492	THR	2.8
1	A	270	CYS	2.8
1	B	243	VAL	2.8
1	B	477	CYS	2.8
1	A	491	LYS	2.8
1	B	281	LYS	2.8
1	D	324	LYS	2.8
1	C	228	SER	2.8
1	D	297[A]	GLN	2.8
1	A	268	ASP	2.8
1	B	366	GLY	2.8
1	B	385	PHE	2.8
1	C	266	LYS	2.8
1	D	306	THR	2.8
1	D	339	THR	2.8
1	A	221	GLN	2.7
1	C	357	GLN	2.7
1	C	431	HIS	2.7
1	B	336	ASP	2.7
1	B	346	GLY	2.7
1	C	366	GLY	2.7
1	D	346	GLY	2.7
1	D	265	PHE	2.7
1	A	453	VAL	2.7
1	C	299	VAL	2.7
1	C	423	VAL	2.7
1	D	273	GLU	2.7
1	D	370	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	268	ASP	2.7
1	D	472	ASP	2.7
1	B	294	LYS	2.7
1	A	262	ARG	2.7
1	B	262	ARG	2.7
1	B	350	ARG	2.7
1	D	276[A]	GLN	2.7
1	D	488	ASN	2.7
1	A	349	ILE	2.7
1	A	424	CYS	2.7
1	D	350	ARG	2.7
1	B	360	ALA	2.7
1	A	465	MET	2.7
1	B	480	ASP	2.7
1	D	252	ASP	2.7
1	D	237	LYS	2.7
1	B	461	ARG	2.7
1	A	487	GLN	2.6
1	C	226	GLU	2.6
1	A	335	LEU	2.6
1	A	382	SER	2.6
1	A	325	VAL	2.6
1	C	218	LYS	2.6
1	D	288	GLY	2.6
1	D	433	GLY	2.6
1	A	332	ALA	2.6
1	A	278	THR	2.6
1	B	240	THR	2.6
1	C	277	THR	2.6
1	C	317	THR	2.6
1	D	443	THR	2.6
1	A	365	LEU	2.6
1	A	420	PRO	2.6
1	C	248	LEU	2.6
1	D	491	LYS	2.6
1	D	340	TYR	2.6
1	C	356	ILE	2.6
1	B	296	GLY	2.6
1	C	232	MET	2.6
1	B	449	ALA	2.6
1	A	248	LEU	2.6
1	B	252	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	316[A]	ASP	2.6
1	C	364	PHE	2.6
1	D	286	GLN	2.6
1	C	267	HIS	2.6
1	C	289	HIS	2.6
1	B	478	ALA	2.6
1	D	327	THR	2.6
1	B	261	GLN	2.5
1	C	329	GLU	2.5
1	C	464	GLU	2.5
1	D	406	GLU	2.5
1	A	271	ILE	2.5
1	B	275	GLY	2.5
1	C	309	GLY	2.5
1	A	279	CYS	2.5
1	B	440	ASN	2.5
1	A	369	ASP	2.5
1	D	221	GLN	2.5
1	A	468[A]	GLY	2.5
1	B	288	GLY	2.5
1	B	309	GLY	2.5
1	D	473	VAL	2.5
1	C	390	TYR	2.5
1	A	291	ASP	2.5
1	B	427	THR	2.5
1	C	451	THR	2.5
1	B	363	PRO	2.5
1	D	261	GLN	2.5
1	D	399	GLU	2.5
1	C	458	LEU	2.5
1	B	345	MET	2.5
1	B	227	LYS	2.5
1	C	275	GLY	2.5
1	A	292	ILE	2.5
1	B	255	VAL	2.5
1	B	341	ARG	2.5
1	A	390	TYR	2.5
1	D	290	ALA	2.5
1	D	452	HIS	2.5
1	A	320	VAL	2.4
1	D	412[A]	ILE	2.5
1	D	295	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	260[A]	MET	2.4
1	C	262	ARG	2.4
1	C	461	ARG	2.4
1	B	468[A]	GLY	2.4
1	C	276[A]	GLN	2.4
1	C	375	GLN	2.4
1	C	428	GLN	2.4
1	D	470	VAL	2.4
1	B	424	CYS	2.4
1	B	339	THR	2.4
1	A	298	LYS	2.4
1	A	348	ALA	2.4
1	B	251	LYS	2.4
1	A	244	LEU	2.4
1	C	242	ASN	2.4
1	D	464	GLU	2.4
1	A	284[A]	ILE	2.4
1	D	319	VAL	2.4
1	A	333	TRP	2.4
1	A	350	ARG	2.4
1	C	477	CYS	2.4
1	C	499	TYR	2.4
1	A	379	ALA	2.4
1	D	379	ALA	2.4
1	B	396[A]	GLU	2.4
1	C	286	GLN	2.4
1	D	487	GLN	2.4
1	B	422	LYS	2.4
1	D	341	ARG	2.4
1	C	427	THR	2.4
1	B	420	PRO	2.4
1	A	300	TYR	2.3
1	A	295	GLU	2.3
1	B	248	LEU	2.3
1	B	401	LEU	2.3
1	A	417	ASP	2.3
1	B	316[A]	ASP	2.3
1	C	230	ASP	2.3
1	A	324	LYS	2.3
1	C	454	ILE	2.3
1	B	409	VAL	2.3
1	A	289	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	278	THR	2.3
1	B	312	GLU	2.3
1	D	329	GLU	2.3
1	A	290	ALA	2.3
1	D	493	GLY	2.3
1	A	252	ASP	2.3
1	A	328	ASP	2.3
1	A	345	MET	2.3
1	D	281	LYS	2.3
1	A	285	ILE	2.3
1	B	267	HIS	2.3
1	C	432	ILE	2.3
1	A	226	GLU	2.3
1	A	409	VAL	2.3
1	C	306	THR	2.3
1	C	466[A]	CYS	2.3
1	C	263	ALA	2.3
1	B	467	LEU	2.3
1	C	234	LEU	2.3
1	C	480	ASP	2.3
1	B	381	SER	2.3
1	B	286	GLN	2.3
1	B	347	THR	2.3
1	A	378	ASP	2.3
1	B	290	ALA	2.3
1	D	415	ASP	2.3
1	B	313	LEU	2.3
1	C	401	LEU	2.3
1	D	289	HIS	2.2
1	C	487	GLN	2.2
1	B	306	THR	2.2
1	B	249	ASN	2.2
1	C	422	LYS	2.2
1	A	230	ASP	2.2
1	C	258	GLY	2.2
1	B	234	LEU	2.2
1	C	371	TYR	2.2
1	D	315	TYR	2.2
1	A	427	THR	2.2
1	C	281	LYS	2.2
1	D	338	ASP	2.2
1	C	330	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	318	PRO	2.2
1	D	347	THR	2.2
1	D	455	THR	2.2
1	C	453	VAL	2.2
1	D	362	VAL	2.2
1	A	231	GLU	2.2
1	A	307	ALA	2.2
1	C	359	LEU	2.2
1	C	338	ASP	2.2
1	A	399	GLU	2.1
1	A	256	VAL	2.1
1	C	468[A]	GLY	2.1
1	C	307	ALA	2.1
1	D	246	SER	2.1
1	D	382	SER	2.1
1	A	227	LYS	2.1
1	D	254	LYS	2.1
1	D	302	LYS	2.1
1	D	397	GLU	2.1
1	C	481	PRO	2.1
1	D	450	THR	2.1
1	C	235	ILE	2.1
1	D	235	ILE	2.1
1	D	426	PHE	2.1
1	C	362	VAL	2.1
1	A	263	ALA	2.1
1	A	266	LYS	2.1
1	B	266	LYS	2.1
1	C	368	LEU	2.1
1	D	227	LYS	2.1
1	A	381	SER	2.1
1	B	287	SER	2.1
1	A	232	MET	2.1
1	A	280	ASN	2.1
1	B	338	ASP	2.1
1	C	336	ASP	2.1
1	D	230	ASP	2.1
1	D	317	THR	2.1
1	A	395	GLY	2.1
1	A	265	PHE	2.1
1	A	489	VAL	2.1
1	C	312	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	430	ASP	2.1
1	A	337	ARG	2.1
1	B	241	HIS	2.1
1	C	350	ARG	2.1
1	A	235	ILE	2.1
1	A	392	ILE	2.1
1	A	412[A]	ILE	2.1
1	A	247	PHE	2.1
1	A	411	VAL	2.1
1	B	411	VAL	2.1
1	C	470	VAL	2.1
1	A	400	TRP	2.1
1	B	226	GLU	2.0
1	B	372	GLU	2.0
1	C	287	SER	2.1
1	C	379	ALA	2.1
1	D	228	SER	2.1
1	B	490	LEU	2.0
1	A	488	ASN	2.0
1	B	237	LYS	2.0
1	D	398	GLY	2.0
1	B	353	GLU	2.0
1	B	464	GLU	2.0
1	C	256	VAL	2.0
1	D	396[A]	GLU	2.0
1	D	314[A]	MET	2.0
1	D	313	LEU	2.0
1	B	291	ASP	2.0
1	B	378	ASP	2.0
1	D	417	ASP	2.0
1	D	477	CYS	2.0
1	C	367	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

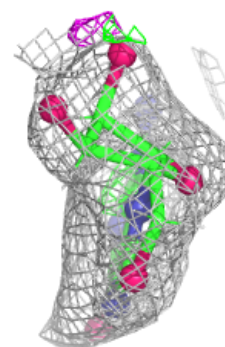
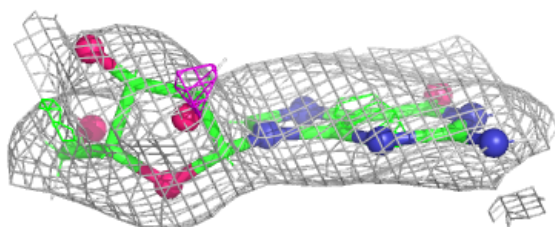
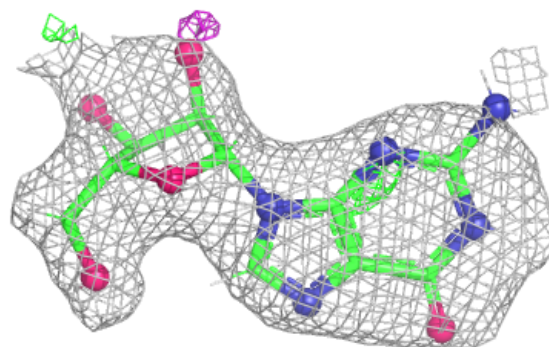
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GMP	C	601	20/20	0.86	0.21	67,101,141,204	0
2	GMP	B	601	20/20	0.87	0.18	71,111,151,171	0
3	ACT	B	603	4/4	0.90	0.13	67,93,95,127	0
2	GMP	A	601	20/20	0.93	0.13	49,75,105,126	0
2	GMP	D	601	20/20	0.94	0.12	65,86,127,150	0
2	GMP	D	602	20/20	0.94	0.14	48,73,122,139	0
2	GMP	C	602	20/20	0.94	0.13	49,68,186,223	0
2	GMP	B	602	20/20	0.95	0.11	43,59,107,111	0
2	GMP	A	602	20/20	0.95	0.14	45,70,121,136	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.

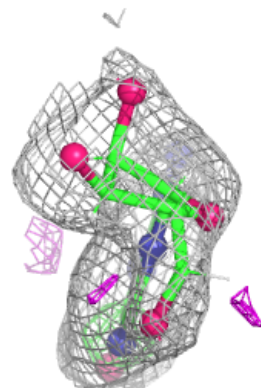
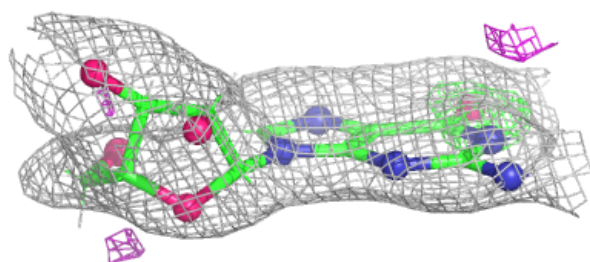
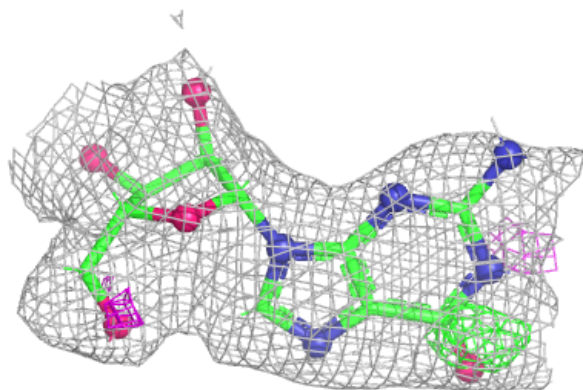
Electron density around GMP C 601:

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



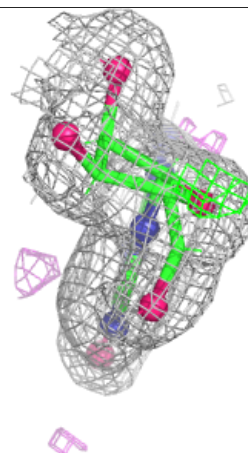
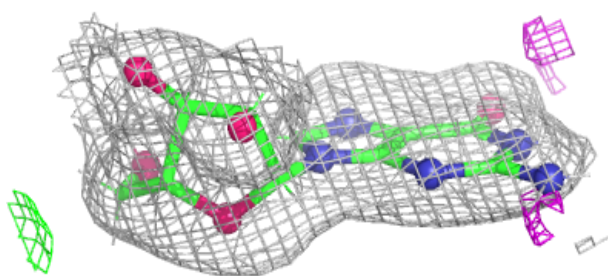
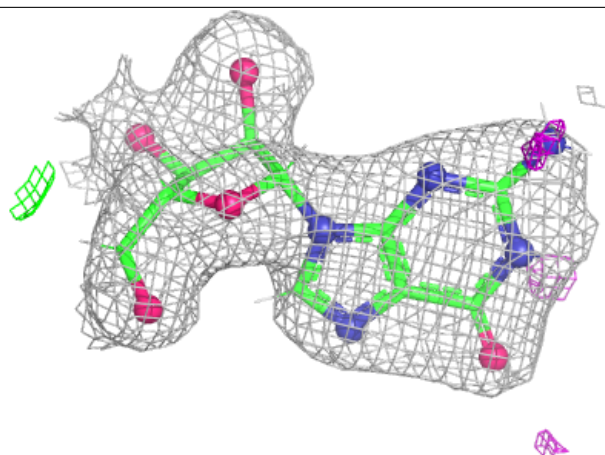
Electron density around GMP B 601:

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



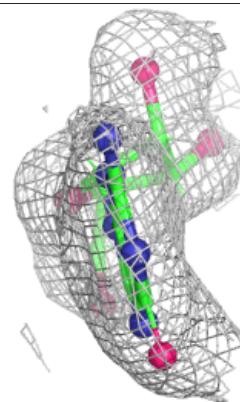
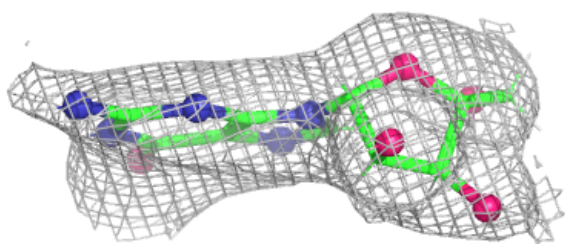
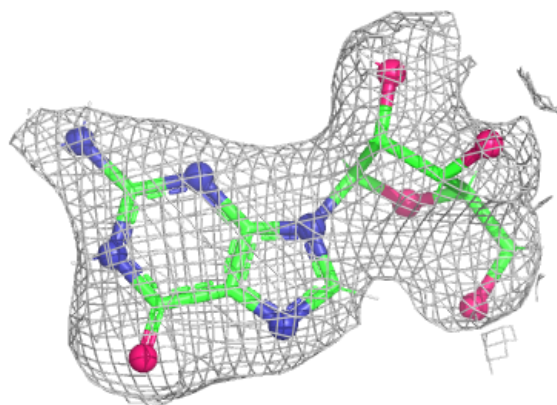
Electron density around GMP A 601:

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

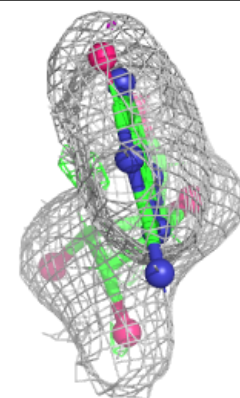
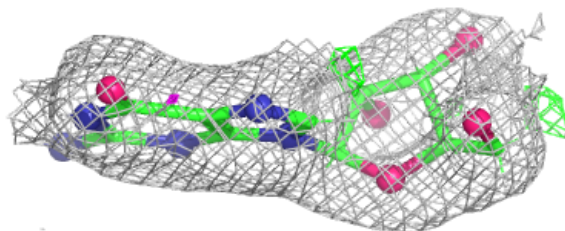
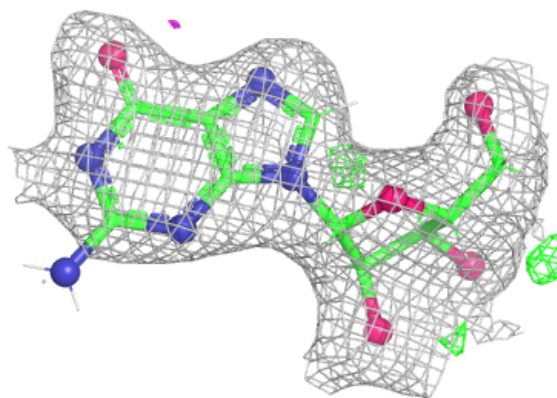


Electron density around GMP D 601:

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

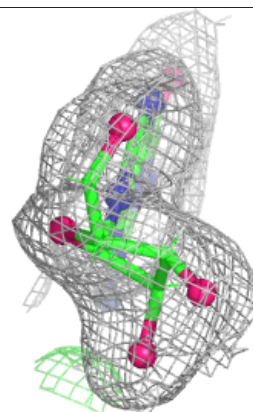
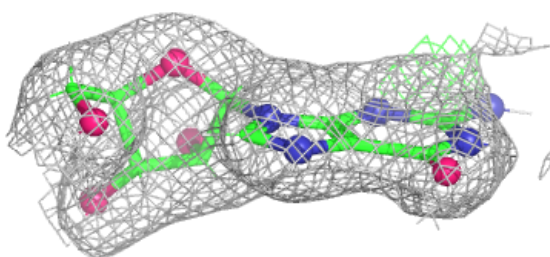
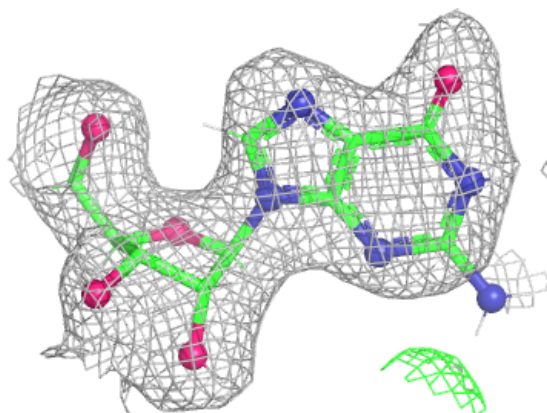
**Electron density around GMP D 602:**

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

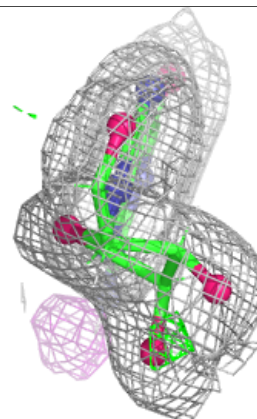
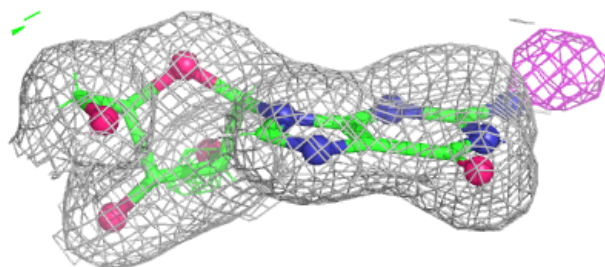
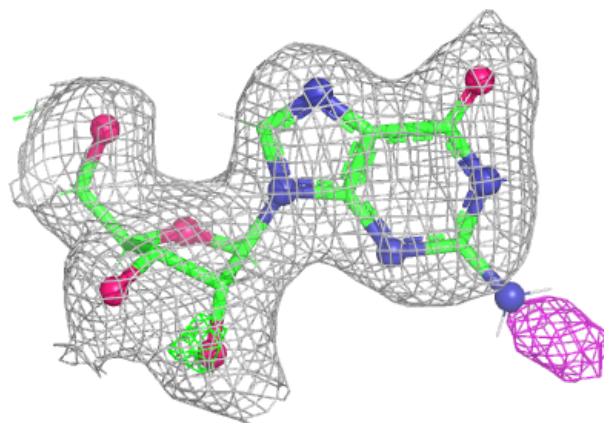


Electron density around GMP C 602:

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

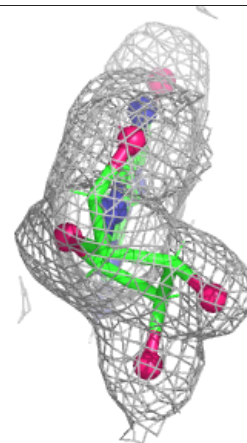
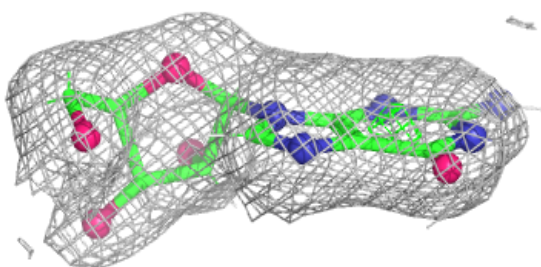
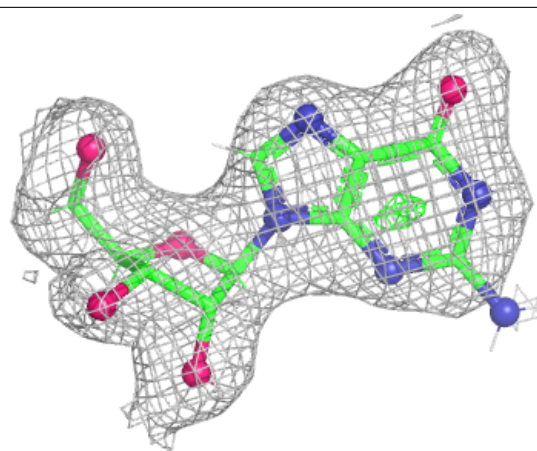
**Electron density around GMP B 602:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.