



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:37 PM UTC

PDB ID : 5X6Z / pdb_00005x6z
Title : Crystal structure of Rice Dwarf Virus P5 in complex with GTP and GDP
Authors : Nakamichi, Y.; Higashiura, A.; Nakagawa, A.
Deposited on : 2017-02-23
Resolution : 2.10 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

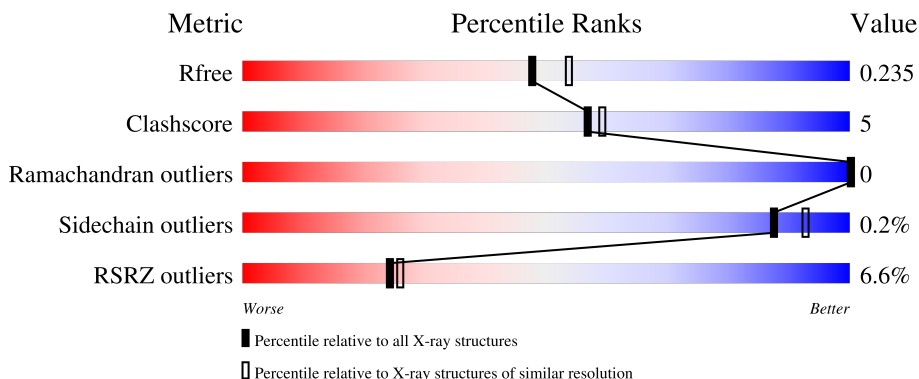
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

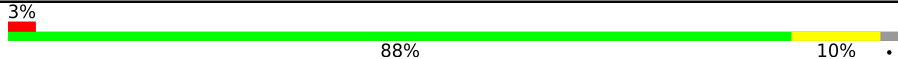
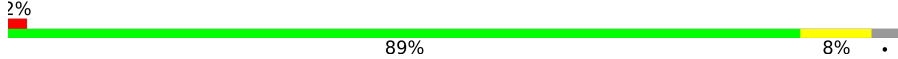
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	804	
1	B	804	
1	C	804	
1	D	804	

2 Entry composition [i](#)

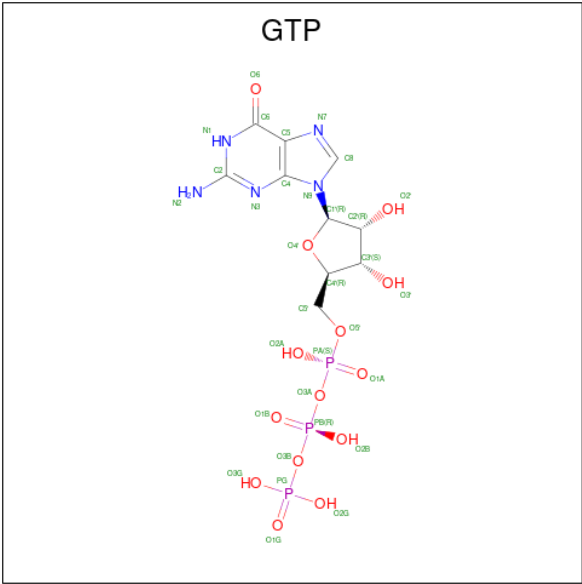
There are 4 unique types of molecules in this entry. The entry contains 26421 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called mRNA capping enzyme P5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	777	Total	C	N	O	S	0	0	0
			6171	3975	1022	1137	37			
1	A	784	Total	C	N	O	S	0	0	0
			6233	4013	1033	1149	38			
1	D	791	Total	C	N	O	S	0	1	0
			6297	4053	1047	1158	39			
1	B	776	Total	C	N	O	S	0	2	0
			6180	3978	1027	1137	38			

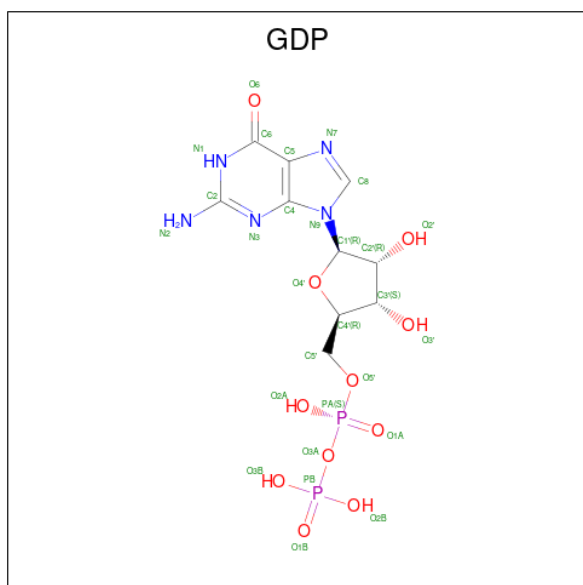
- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	B	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	D	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	330	Total O 330 330	0	0
4	A	395	Total O 395 395	0	0
4	D	320	Total O 320 320	0	0

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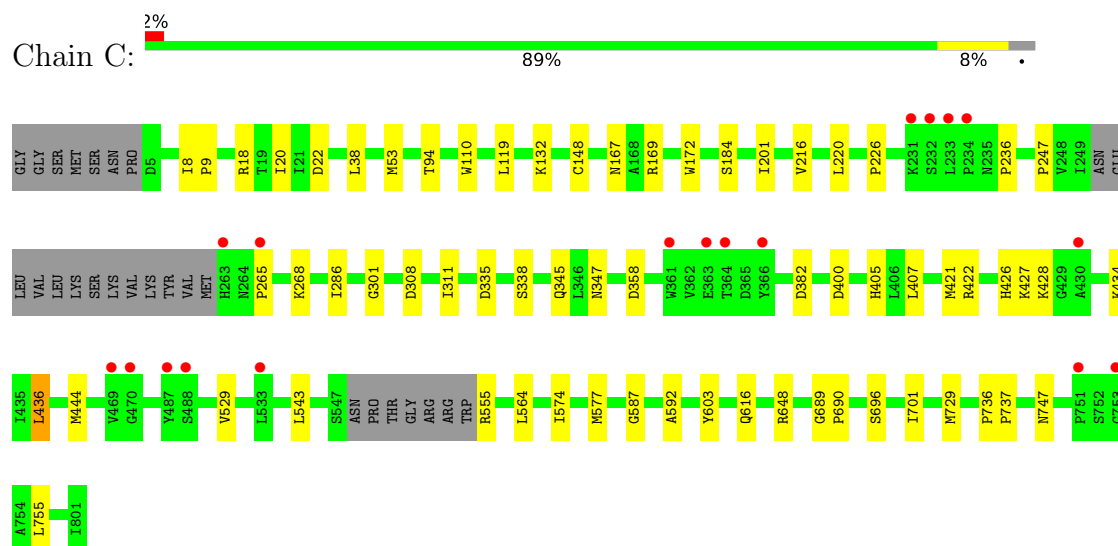
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	255	Total 255	O 255	0	0

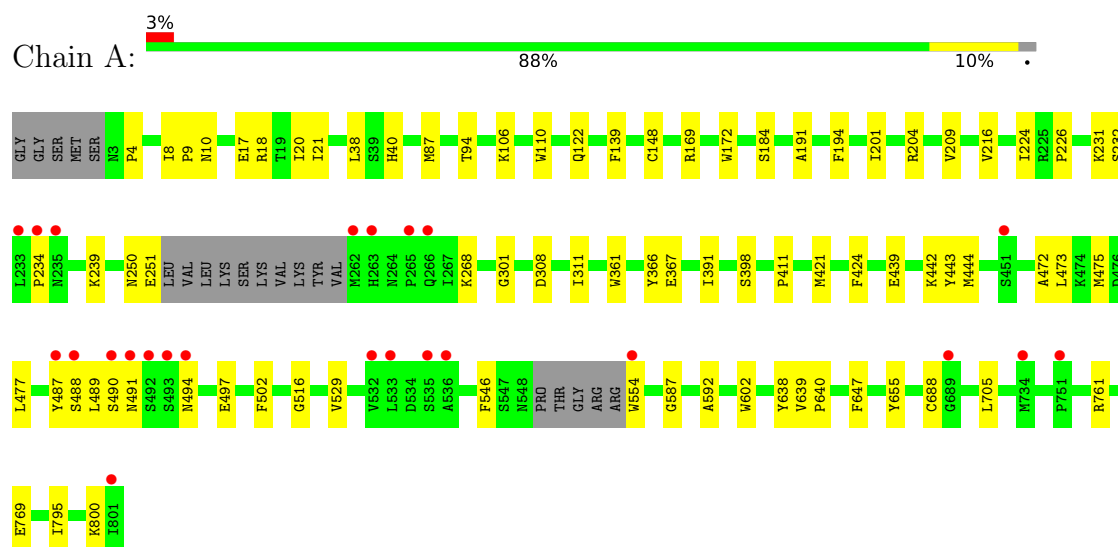
3 Residue-property plots [i](#)

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.

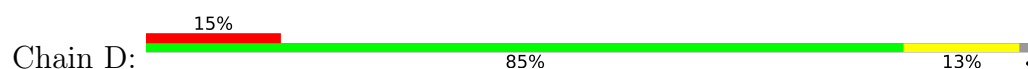
• Molecule 1: mRNA capping enzyme P5

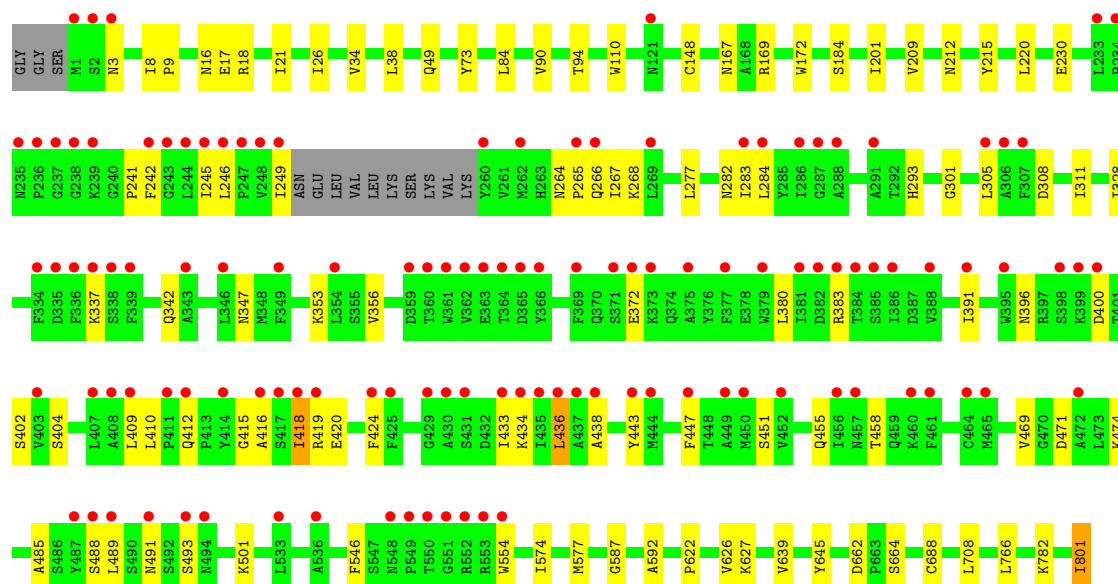


• Molecule 1: mRNA capping enzyme P5

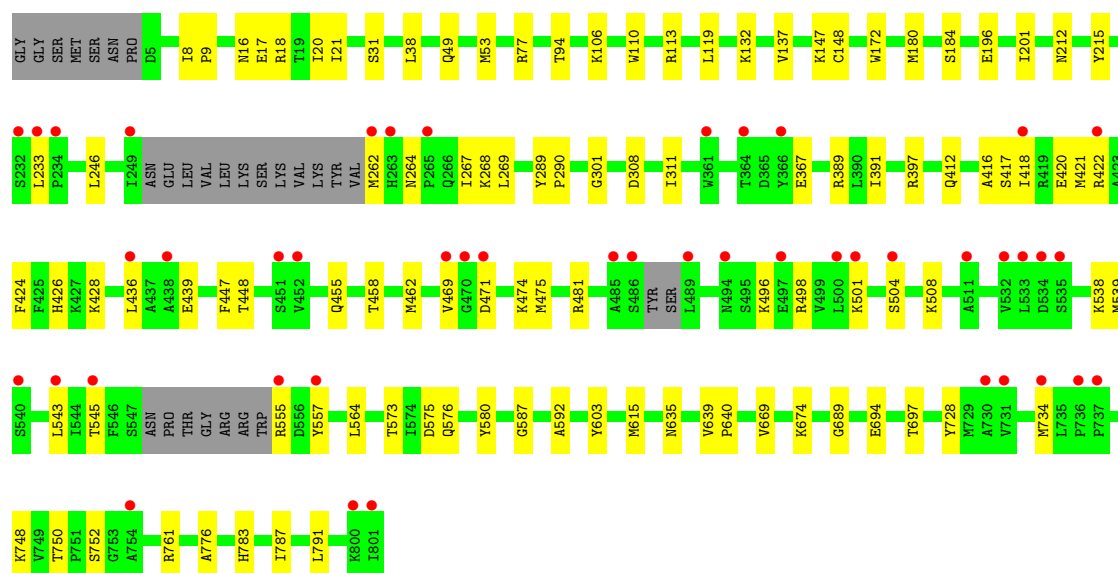
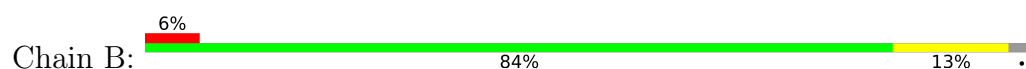


• Molecule 1: mRNA capping enzyme P5





• Molecule 1: mRNA capping enzyme P5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.39Å 83.45Å 141.98Å 103.10° 101.98° 95.69°	Depositor
Resolution (Å)	37.66 – 2.10 37.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.66-2.10) 95.4 (37.66-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.184 , 0.235 0.185 , 0.235	Depositor DCC
R_{free} test set	9116 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26421	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: GDP, GTP

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	0.35	0/6384	0.51	0/8664
1	B	0.31	0/6326	0.47	0/8580
1	C	0.35	0/6319	0.51	0/8574
1	D	0.37	0/6451	0.53	0/8756
All	All	0.35	0/25480	0.50	0/34574

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6233	0	6219	48	0
1	B	6180	0	6180	67	0
1	C	6171	0	6169	44	0
1	D	6297	0	6291	78	0
2	A	32	0	12	0	0
2	B	32	0	12	0	0
2	C	32	0	12	3	0
2	D	32	0	12	2	0
3	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	1	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	395	0	0	0	0
4	B	255	0	0	4	0
4	C	330	0	0	2	0
4	D	320	0	0	2	0
All	All	26421	0	24955	228	0

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

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:747:ASN:HB3	2:C:901:GTP:HN22	1.37	0.89
1:B:233:LEU:HD23	1:B:469:VAL:HG11	1.55	0.88
1:C:434:LYS:HE2	1:C:436:LEU:HD11	1.61	0.82
1:A:411:PRO:HB3	1:A:444:MET:HE1	1.66	0.78
1:D:416:ALA:HA	1:D:455:GLN:HE22	1.51	0.76
1:A:18:ARG:HH12	1:B:21:ILE:HB	1.52	0.74
1:C:543:LEU:HD11	1:C:555:ARG:NH1	2.02	0.74
1:C:747:ASN:HB3	2:C:901:GTP:N2	2.03	0.74
1:B:538:LYS:HE3	1:B:539:MET:H	1.52	0.73
1:B:418:ILE:HG22	1:B:420:GLU:H	1.56	0.70
1:B:543:LEU:HD12	1:B:557:TYR:HE1	1.57	0.70
1:A:494:ASN:HB3	1:A:497:GLU:HB3	1.72	0.69
1:A:688:CYS:O	1:A:761:ARG:NH2	2.25	0.69
1:C:201:ILE:HG21	1:C:301:GLY:HA3	1.76	0.67
1:B:669:VAL:HG21	1:B:674:LYS:HD2	1.78	0.66
1:D:249:ILE:CD1	1:D:443:TYR:HE1	2.07	0.66
1:C:265:PRO:O	1:C:268:LYS:NZ	2.29	0.66
1:B:615:MET:HE2	1:B:728:TYR:HE2	1.61	0.66
1:D:284:LEU:HD12	1:D:305:LEU:HD12	1.77	0.65
1:C:616:GLN:OE1	2:C:901:GTP:N1	2.25	0.65
1:D:418:ILE:HG12	1:D:419:ARG:H	1.61	0.65
1:B:264:ASN:HB3	1:B:267:ILE:HB	1.79	0.65
1:D:266:GLN:HG2	1:D:293:HIS:HB3	1.79	0.64
1:C:543:LEU:HD11	1:C:555:ARG:CZ	2.28	0.63
1:B:697:THR:HG21	4:B:1067:HOH:O	1.99	0.63
1:A:231:LYS:HE3	1:A:491:ASN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:MET:HG2	1:C:444:MET:HE3	1.81	0.62
1:C:308:ASP:HB3	1:C:311:ILE:HG13	1.80	0.62
1:D:308:ASP:HB3	1:D:311:ILE:HG13	1.81	0.62
2:D:901:GTP:N3	2:D:901:GTP:H2'	2.14	0.61
1:D:249:ILE:CD1	1:D:443:TYR:CE1	2.84	0.60
1:B:49:GLN:HB3	1:B:53:MET:HE2	1.83	0.60
1:D:249:ILE:HD13	1:D:443:TYR:CE1	2.36	0.60
1:A:473:LEU:HD11	1:A:490:SER:HB2	1.83	0.60
1:B:545:THR:HA	1:B:555:ARG:HD3	1.83	0.60
1:B:17:GLU:H	1:B:17:GLU:CD	2.10	0.60
1:C:20:ILE:HG21	1:C:529:VAL:HG11	1.83	0.59
1:D:201:ILE:HG21	1:D:301:GLY:HA3	1.84	0.59
1:D:16:ASN:HA	1:D:782:LYS:HE3	1.85	0.59
1:C:172:TRP:CZ2	1:C:592:ALA:HB2	2.37	0.58
1:D:245:ILE:HA	1:D:409:LEU:H	1.68	0.58
1:D:266:GLN:CG	1:D:293:HIS:HB3	2.32	0.58
1:D:209:VAL:HG12	1:D:488:SER:HB2	1.85	0.58
1:D:485:ALA:HB1	1:D:489:LEU:HB2	1.85	0.58
1:B:428:LYS:H	1:B:428:LYS:HD2	1.67	0.58
1:D:230:GLU:O	1:D:469:VAL:HA	2.04	0.57
1:D:284:LEU:HB3	1:D:356:VAL:HG22	1.86	0.57
1:B:184:SER:OG	1:B:587:GLY:HA3	2.05	0.57
1:B:436:LEU:HB2	1:B:439:GLU:HG3	1.86	0.57
1:B:212:ASN:HB3	1:B:215:TYR:HD2	1.70	0.57
1:D:451:SER:O	1:D:455:GLN:HG3	2.04	0.56
1:B:416:ALA:O	1:B:455:GLN:NE2	2.33	0.56
1:D:447:PHE:HE2	1:D:458:THR:HG21	1.70	0.56
1:D:337:LYS:NZ	1:D:372:GLU:OE2	2.36	0.56
1:B:475:MET:SD	1:B:481:ARG:NH2	2.78	0.56
1:D:400:ASP:OD2	1:D:436:LEU:HA	2.06	0.56
1:D:416:ALA:HA	1:D:455:GLN:NE2	2.19	0.55
1:B:119:LEU:HD11	1:B:132:LYS:HD2	1.88	0.55
1:D:172:TRP:CZ2	1:D:592:ALA:HB2	2.42	0.54
1:A:239:LYS:NZ	1:A:439:GLU:OE2	2.38	0.54
1:B:77:ARG:HG2	4:B:1083:HOH:O	2.06	0.54
1:A:367:GLU:OE2	1:A:398:SER:OG	2.21	0.54
1:D:284:LEU:CD1	1:D:305:LEU:HD12	2.37	0.54
1:B:9:PRO:HB3	1:B:639:VAL:HG22	1.90	0.54
1:A:421:MET:HE3	1:A:444:MET:HE3	1.89	0.53
1:D:412:GLN:CD	1:D:412:GLN:H	2.16	0.53
1:B:106:LYS:HD2	1:B:110:TRP:CH2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HH12	1:B:21:ILE:CB	2.22	0.53
1:D:8:ILE:HA	1:D:9:PRO:C	2.34	0.53
1:C:8:ILE:HA	1:C:9:PRO:C	2.33	0.53
1:A:191:ALA:HA	1:A:224:ILE:HD11	1.91	0.53
1:C:382:ASP:OD2	1:C:405:HIS:NE2	2.42	0.52
1:C:38:LEU:O	1:C:94:THR:HA	2.10	0.52
1:C:335:ASP:OD2	1:C:338:SER:OG	2.27	0.52
1:C:426:HIS:CE1	1:C:428:LYS:HG2	2.44	0.52
1:D:418:ILE:HG12	1:D:419:ARG:N	2.25	0.52
1:D:574:ILE:HD13	1:D:577:MET:HE3	1.92	0.52
1:C:53:MET:HE1	1:D:73:TYR:CE2	2.45	0.51
1:D:305:LEU:HD23	1:D:328:ILE:HB	1.92	0.51
1:A:184:SER:OG	1:A:587:GLY:HA3	2.09	0.51
1:A:201:ILE:HG21	1:A:301:GLY:HA3	1.91	0.51
1:B:417:SER:HA	1:B:448:THR:HG22	1.93	0.51
1:B:504:SER:O	1:B:508:LYS:HG3	2.11	0.51
1:C:18:ARG:HG2	1:D:18:ARG:CZ	2.40	0.51
1:C:110:TRP:CD1	1:C:148:CYS:HA	2.46	0.51
1:C:119:LEU:HD11	1:C:132:LYS:HD2	1.93	0.51
1:D:471:ASP:HB3	1:D:474:LYS:HG3	1.93	0.50
1:A:8:ILE:HA	1:A:9:PRO:C	2.35	0.50
1:B:8:ILE:HA	1:B:9:PRO:C	2.37	0.50
1:B:172:TRP:CZ2	1:B:592:ALA:HB2	2.45	0.50
1:D:9:PRO:HB3	1:D:639:VAL:HG22	1.92	0.50
1:B:776:ALA:HB2	1:B:783:HIS:CE1	2.46	0.50
1:A:472:ALA:O	1:A:475:MET:HG2	2.12	0.50
1:D:246:LEU:HD11	1:D:443:TYR:CG	2.47	0.49
1:C:648:ARG:HG3	1:C:701:ILE:HD11	1.93	0.49
1:B:246:LEU:HD21	1:B:421:MET:HE1	1.94	0.49
1:D:241:PRO:HB2	1:D:242:PHE:HD1	1.77	0.49
1:B:268:LYS:HG2	1:B:269:LEU:HD12	1.94	0.49
1:B:308:ASP:HB3	1:B:311:ILE:HG13	1.94	0.49
1:D:34:VAL:HB	1:D:90:VAL:HG22	1.94	0.49
1:C:747:ASN:CG	1:C:755:LEU:HD11	2.38	0.49
1:D:664:SER:HB3	1:B:734:MET:SD	2.53	0.48
1:B:389:ARG:O	1:B:426:HIS:ND1	2.46	0.48
1:B:689:GLY:O	1:B:761:ARG:NH2	2.41	0.48
1:A:705:LEU:HD11	1:A:795:ILE:HD13	1.94	0.48
1:B:694:GLU:O	1:B:697:THR:HG22	2.13	0.48
1:B:196:GLU:OE1	1:B:580:TYR:OH	2.23	0.48
1:A:172:TRP:CZ2	1:A:592:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:LEU:HD22	1:D:438:ALA:H	1.78	0.48
1:A:139:PHE:HA	1:B:640:PRO:HB3	1.95	0.47
1:D:626:VAL:HG23	1:D:627:LYS:HG2	1.96	0.47
1:B:201:ILE:HG21	1:B:301:GLY:HA3	1.95	0.47
1:B:564:LEU:HD13	1:B:603:TYR:CZ	2.50	0.47
1:D:249:ILE:HD11	1:D:443:TYR:CE1	2.49	0.47
1:C:426:HIS:HE1	1:C:428:LYS:HG2	1.80	0.47
1:A:18:ARG:CZ	1:B:18:ARG:HG2	2.44	0.47
1:D:110:TRP:CD1	1:D:148:CYS:HA	2.50	0.47
1:D:212:ASN:HB3	1:D:215:TYR:HD2	1.79	0.47
1:B:496:LYS:HG3	1:B:557:TYR:HD2	1.80	0.47
1:C:407:LEU:HB2	1:C:426:HIS:HB3	1.96	0.46
1:D:249:ILE:HD11	1:D:443:TYR:HE1	1.77	0.46
1:B:462:MET:HB2	1:B:462:MET:HE3	1.77	0.46
1:B:180:MET:HE3	1:B:180:MET:O	2.16	0.46
1:B:573:THR:OG1	1:B:576:GLN:HG3	2.15	0.46
1:B:787:ILE:O	1:B:791:LEU:HG	2.16	0.46
1:A:194:PHE:CG	1:A:204:ARG:HG2	2.50	0.46
1:B:38:LEU:O	1:B:94:THR:HA	2.14	0.46
1:C:236:PRO:HB2	1:C:247:PRO:HB3	1.96	0.46
1:B:501:LYS:N	1:B:501:LYS:HD2	2.31	0.46
1:B:474:LYS:HD2	1:B:474:LYS:HA	1.81	0.46
1:B:748:LYS:HG2	4:B:1145:HOH:O	2.16	0.45
1:B:262:MET:HE3	1:B:264:ASN:HD22	1.82	0.45
1:D:249:ILE:N	1:D:249:ILE:HD12	2.31	0.45
1:A:477:LEU:HD11	1:A:502:PHE:CE1	2.51	0.45
1:D:342:GLN:OE1	1:D:347:ASN:ND2	2.50	0.45
1:D:396:ASN:HB2	1:D:420:GLU:OE2	2.17	0.45
1:C:184:SER:OG	1:C:587:GLY:HA3	2.15	0.45
1:B:110:TRP:CD1	1:B:148:CYS:HA	2.51	0.45
1:D:49:GLN:HG2	4:D:1308:HOH:O	2.16	0.45
1:A:87:MET:HE3	1:B:635:ASN:HD21	1.81	0.45
1:D:265:PRO:HG2	1:D:266:GLN:NE2	2.32	0.45
1:A:38:LEU:O	1:A:94:THR:HA	2.16	0.45
1:D:268:LYS:NZ	1:D:415:GLY:HA2	2.32	0.44
1:D:264:ASN:HB2	1:D:267:ILE:HD13	2.00	0.44
1:D:282:ASN:HB2	1:D:353:LYS:O	2.16	0.44
1:C:167:ASN:O	1:C:169:ARG:HG3	2.18	0.44
1:D:662:ASP:OD2	1:D:664:SER:OG	2.23	0.44
1:C:574:ILE:HA	1:C:577:MET:HE3	1.99	0.44
1:D:184:SER:OG	1:D:587:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:SER:HA	1:D:434:LYS:HA	2.00	0.44
1:B:391:ILE:O	1:B:424:PHE:HA	2.17	0.44
1:C:216:VAL:HA	1:C:226:PRO:HG3	2.00	0.44
1:A:308:ASP:HB3	1:A:311:ILE:HG13	1.99	0.44
1:B:471:ASP:OD1	1:B:498:ARG:NH2	2.51	0.44
1:C:564:LEU:HD13	1:C:603:TYR:CZ	2.53	0.43
1:D:38:LEU:O	1:D:94:THR:HA	2.18	0.43
1:D:645:TYR:OH	2:D:901:GTP:O2G	2.29	0.43
1:D:17:GLU:O	1:D:21:ILE:HG12	2.18	0.43
1:A:250:ASN:O	1:A:251:GLU:HB2	2.18	0.43
1:B:113:ARG:HD3	1:B:575:ASP:OD2	2.18	0.43
1:D:245:ILE:HD13	1:D:433:ILE:HD13	2.00	0.43
1:C:729:MET:CE	1:C:755:LEU:HD23	2.48	0.43
1:D:3:ASN:OD1	1:D:3:ASN:N	2.52	0.43
1:C:22:ASP:OD2	1:D:18:ARG:NH2	2.37	0.43
1:A:110:TRP:CD1	1:A:148:CYS:HA	2.54	0.43
1:D:241:PRO:HB2	1:D:242:PHE:CD1	2.54	0.43
1:A:9:PRO:HB3	1:A:639:VAL:HG22	2.01	0.43
1:D:491:ASN:HB3	1:D:493:SER:O	2.19	0.43
1:B:137:VAL:HG11	3:B:902:GDP:C2	2.54	0.43
1:B:575:ASP:HB3	4:B:1107:HOH:O	2.19	0.42
1:C:268:LYS:H	1:C:268:LYS:HD2	1.83	0.42
1:C:427:LYS:NZ	4:C:1028:HOH:O	2.52	0.42
1:A:268:LYS:H	1:A:268:LYS:HG2	1.58	0.42
1:A:638:TYR:O	1:A:640:PRO:HD3	2.19	0.42
1:C:345:GLN:C	1:C:347:ASN:H	2.28	0.42
1:B:31:SER:O	1:B:147:LYS:HE3	2.19	0.42
1:A:516:GLY:HA3	1:A:602:TRP:CE3	2.54	0.42
1:A:20:ILE:HG21	1:A:529:VAL:HG11	2.02	0.42
1:B:447:PHE:HE1	1:B:458:THR:HG21	1.85	0.42
1:C:696:SER:O	1:C:696:SER:OG	2.34	0.42
1:A:17:GLU:O	1:A:21:ILE:HG12	2.19	0.42
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.71	0.42
1:D:220:LEU:HD13	1:D:220:LEU:HA	1.90	0.42
1:D:356:VAL:HB	1:D:391:ILE:HG12	2.00	0.42
1:A:443:TYR:HD1	1:A:444:MET:HE2	1.84	0.42
1:D:380:LEU:O	1:D:383:ARG:HG2	2.19	0.42
1:A:9:PRO:HG2	1:A:647:PHE:CZ	2.55	0.42
1:B:750:THR:OG1	1:B:752:SER:HB3	2.19	0.42
1:D:167:ASN:O	1:D:169:ARG:HG3	2.20	0.42
1:C:422:ARG:HD2	4:C:1154:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:MET:SD	1:C:755:LEU:HD23	2.60	0.41
1:D:284:LEU:HD23	1:D:356:VAL:HG13	2.02	0.41
1:D:546:PHE:HB2	1:D:554:TRP:CE2	2.55	0.41
1:D:688:CYS:O	1:D:801:ILE:HG12	2.20	0.41
1:B:615:MET:HE2	1:B:728:TYR:CE2	2.47	0.41
1:C:400:ASP:OD2	1:C:436:LEU:HD12	2.20	0.41
1:A:169:ARG:HG2	1:B:9:PRO:HD2	2.02	0.41
1:A:216:VAL:HA	1:A:226:PRO:HG3	2.03	0.41
1:D:574:ILE:HD13	1:D:577:MET:CE	2.50	0.41
1:A:391:ILE:O	1:A:424:PHE:HA	2.20	0.41
1:B:16:ASN:O	1:B:20:ILE:HG12	2.21	0.41
1:B:543:LEU:HD12	1:B:557:TYR:CE1	2.46	0.41
1:D:26:ILE:HG22	1:D:84:LEU:HD22	2.02	0.41
1:A:361:TRP:HB2	1:A:366:TYR:CZ	2.55	0.41
1:C:689:GLY:HA3	1:C:690:PRO:HA	1.95	0.41
1:A:4:PRO:O	1:A:10:ASN:ND2	2.52	0.41
1:A:232:SER:O	1:A:234:PRO:HD3	2.21	0.41
1:D:277:LEU:HD23	1:D:283:ILE:HG13	2.02	0.41
1:D:801:ILE:HD13	1:D:801:ILE:HA	1.74	0.41
1:B:367:GLU:HG2	1:B:397:ARG:HD2	2.03	0.41
1:C:220:LEU:HD13	1:C:220:LEU:HA	1.93	0.41
1:C:286:ILE:HB	1:C:358:ASP:HA	2.02	0.41
1:D:622:PRO:HB2	1:D:626:VAL:HG13	2.04	0.41
1:C:736:PRO:HA	1:C:737:PRO:HD3	1.89	0.40
1:B:412:GLN:NE2	1:B:420:GLU:OE2	2.34	0.40
1:A:209:VAL:HG11	1:A:489:LEU:HD23	2.03	0.40
1:A:800:LYS:H	1:A:800:LYS:HG3	1.77	0.40
1:D:404:SER:HB2	4:D:1193:HOH:O	2.21	0.40
1:D:766:LEU:HD12	1:D:766:LEU:HA	1.91	0.40
1:A:487:TYR:HD2	1:A:488:SER:HB3	1.87	0.40
1:D:410:LEU:HD12	1:D:424:PHE:CE2	2.56	0.40
1:D:626:VAL:HG12	1:D:708:LEU:HG	2.04	0.40
1:B:289:TYR:HA	1:B:290:PRO:HA	1.90	0.40
1:A:40:HIS:NE2	1:A:122:GLN:O	2.52	0.40
1:A:106:LYS:HD2	1:A:110:TRP:CH2	2.57	0.40
1:A:546:PHE:HB2	1:A:554:TRP:CE2	2.56	0.40
1:A:655:TYR:CE1	1:A:769:GLU:HB3	2.56	0.40
1:D:501:LYS:HE2	1:D:501:LYS:HB2	1.83	0.40

There are no symmetry-related clashes.

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	778/804 (97%)	760 (98%)	18 (2%)	0	100	100
1	B	770/804 (96%)	748 (97%)	22 (3%)	0	100	100
1	C	771/804 (96%)	755 (98%)	16 (2%)	0	100	100
1	D	788/804 (98%)	764 (97%)	24 (3%)	0	100	100
All	All	3107/3216 (97%)	3027 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	694/711 (98%)	693 (100%)	1 (0%)	88	93
1	B	688/711 (97%)	686 (100%)	2 (0%)	86	91
1	C	687/711 (97%)	686 (100%)	1 (0%)	88	93
1	D	701/711 (99%)	698 (100%)	3 (0%)	84	89
All	All	2770/2844 (97%)	2763 (100%)	7 (0%)	87	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	436	LEU
1	A	442	LYS

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Mol	Chain	Res	Type
1	D	418	ILE
1	D	436	LEU
1	D	801	ILE
1	B	422[A]	ARG
1	B	422[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	491	ASN
1	C	597	ASN
1	C	704	HIS
1	A	345	GLN
1	A	597	ASN
1	A	796	ASN
1	D	121	ASN
1	D	347	ASN
1	D	350	GLN
1	D	455	GLN
1	B	13	GLN
1	B	350	GLN
1	B	459	GLN
1	B	681	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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GDP	B	902	-	29,30,30	1.17	4 (13%)	45,47,47	1.87	9 (20%)
2	GTP	A	901	-	33,34,34	1.03	2 (6%)	50,54,54	1.51	11 (22%)
2	GTP	C	901	-	33,34,34	1.05	3 (9%)	50,54,54	1.70	11 (22%)
3	GDP	A	902	-	29,30,30	1.13	2 (6%)	45,47,47	1.86	8 (17%)
3	GDP	D	902	-	29,30,30	1.15	2 (6%)	45,47,47	1.89	9 (20%)
2	GTP	B	901	-	33,34,34	1.08	4 (12%)	50,54,54	1.62	10 (20%)
2	GTP	D	901	-	33,34,34	1.00	2 (6%)	50,54,54	2.04	15 (30%)
3	GDP	C	902	-	29,30,30	1.12	3 (10%)	45,47,47	1.89	11 (24%)

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
3	GDP	B	902	-	-	6/16/32/32	0/3/3/3
2	GTP	A	901	-	-	3/22/38/38	0/3/3/3
2	GTP	C	901	-	-	8/22/38/38	0/3/3/3
3	GDP	A	902	-	-	0/16/32/32	0/3/3/3
3	GDP	D	902	-	-	4/16/32/32	0/3/3/3
2	GTP	B	901	-	-	5/22/38/38	0/3/3/3
2	GTP	D	901	-	-	6/22/38/38	0/3/3/3
3	GDP	C	902	-	-	3/16/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	GDP	C5-C4	3.28	1.47	1.38
3	D	902	GDP	C5-C4	3.23	1.47	1.38
2	A	901	GTP	PB-O3A	3.22	1.63	1.59
3	B	902	GDP	C5-C4	3.14	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GDP	C5-C4	3.10	1.47	1.38
2	B	901	GTP	PB-O3A	3.04	1.62	1.59
2	C	901	GTP	PB-O3A	2.99	1.62	1.59
2	B	901	GTP	PB-O3B	2.72	1.62	1.59
3	D	902	GDP	PA-O3A	2.65	1.62	1.59
3	B	902	GDP	PA-O3A	2.59	1.62	1.59
2	D	901	GTP	PA-O3A	2.44	1.62	1.59
2	C	901	GTP	PA-O3A	2.36	1.62	1.59
3	C	902	GDP	PA-O3A	2.32	1.62	1.59
3	A	902	GDP	PA-O3A	2.30	1.62	1.59
2	C	901	GTP	C2-N3	2.19	1.38	1.33
2	B	901	GTP	C2-N3	2.19	1.38	1.33
2	A	901	GTP	PA-O3A	2.15	1.61	1.59
2	D	901	GTP	C2-N3	2.13	1.38	1.33
3	B	902	GDP	C4-N9	-2.11	1.32	1.38
2	B	901	GTP	PA-O3A	2.06	1.61	1.59
3	B	902	GDP	C5-N7	-2.03	1.35	1.39
3	C	902	GDP	C4-N9	-2.02	1.32	1.38

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	GDP	C5-C4-N3	-5.93	118.96	128.39
3	A	902	GDP	C5-C4-N3	-5.84	119.10	128.39
3	B	902	GDP	C5-C4-N3	-5.77	119.21	128.39
2	D	901	GTP	C5-C4-N3	-5.61	119.46	128.39
3	B	902	GDP	C2-N3-C4	5.47	121.72	112.30
3	D	902	GDP	C2-N3-C4	5.46	121.71	112.30
2	C	901	GTP	C2-N3-C4	5.46	121.70	112.30
3	A	902	GDP	C2-N3-C4	5.46	121.70	112.30
2	C	901	GTP	C5-C4-N3	-5.19	120.12	128.39
2	D	901	GTP	C2-N3-C4	5.08	121.05	112.30
2	B	901	GTP	C5-C4-N3	-5.00	120.44	128.39
3	C	902	GDP	C2-N3-C4	4.93	120.78	112.30
3	C	902	GDP	C5-C4-N3	-4.89	120.61	128.39
3	D	902	GDP	N9-C4-N3	4.82	135.60	125.95
2	A	901	GTP	C2-N3-C4	4.76	120.50	112.30
2	B	901	GTP	C2-N3-C4	4.65	120.31	112.30
3	A	902	GDP	N9-C4-N3	4.46	134.86	125.95
2	A	901	GTP	C5-C4-N3	-4.41	121.36	128.39
3	B	902	GDP	N9-C4-N3	4.39	134.73	125.95
2	D	901	GTP	N9-C4-N3	4.34	134.64	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	GDP	C6-C5-N7	4.18	137.90	130.29
3	C	902	GDP	C2'-C1'-N9	-3.70	102.95	113.25
3	A	902	GDP	C6-C5-N7	3.62	136.87	130.29
3	C	902	GDP	N9-C4-N3	3.57	133.09	125.95
2	D	901	GTP	O2A-PA-O3A	3.47	116.66	107.27
3	D	902	GDP	C6-C5-N7	3.46	136.59	130.29
3	B	902	GDP	C6-C5-N7	3.35	136.39	130.29
2	D	901	GTP	C2-N1-C6	-3.22	119.27	125.11
2	D	901	GTP	C2'-C1'-N9	-3.19	104.37	113.25
2	D	901	GTP	O6-C6-C5	-3.13	118.28	126.53
2	D	901	GTP	O5'-C5'-C4'	2.99	119.18	108.99
2	B	901	GTP	C2-N1-C6	-2.96	119.74	125.11
3	B	902	GDP	O6-C6-C5	-2.91	118.84	126.53
3	D	902	GDP	O6-C6-C5	-2.87	118.94	126.53
2	B	901	GTP	N9-C4-N3	2.84	131.64	125.95
2	B	901	GTP	N9-C8-N7	-2.81	108.19	113.40
2	D	901	GTP	C5-C6-N1	2.76	120.27	113.25
2	D	901	GTP	O2B-PB-O3A	2.75	114.71	107.27
2	B	901	GTP	C8-N7-C5	2.75	109.15	104.26
2	D	901	GTP	O4'-C1'-N9	-2.67	102.30	108.36
3	C	902	GDP	C4-C5-N7	-2.67	106.44	110.67
2	A	901	GTP	C2-N1-C6	-2.67	120.27	125.11
2	C	901	GTP	C2-N1-C6	-2.64	120.33	125.11
2	B	901	GTP	O2B-PB-O3B	2.64	114.40	107.27
2	D	901	GTP	N9-C8-N7	-2.61	108.56	113.40
3	A	902	GDP	C4-C5-N7	-2.59	106.56	110.67
2	A	901	GTP	N9-C8-N7	-2.58	108.61	113.40
2	B	901	GTP	C5-C6-N1	2.55	119.75	113.25
2	D	901	GTP	C3'-C2'-C1'	2.55	106.29	101.46
2	C	901	GTP	C4-C5-N7	-2.54	106.65	110.67
3	A	902	GDP	O6-C6-C5	-2.53	119.84	126.53
2	A	901	GTP	C5-C6-N1	2.53	119.70	113.25
3	C	902	GDP	O6-C6-C5	-2.50	119.93	126.53
3	B	902	GDP	O2A-PA-O3A	2.45	113.91	107.27
2	C	901	GTP	C8-N7-C5	2.45	108.62	104.26
3	D	902	GDP	C4-C5-N7	-2.37	106.91	110.67
2	C	901	GTP	N9-C4-N3	2.34	130.64	125.95
3	B	902	GDP	O3B-PB-O3A	2.30	112.36	104.64
3	B	902	GDP	C4-C5-N7	-2.29	107.04	110.67
2	D	901	GTP	O2B-PB-O3B	2.29	113.47	107.27
2	C	901	GTP	C3'-C2'-C1'	2.28	105.78	101.46
2	C	901	GTP	C5-C6-N1	2.27	119.02	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	GTP	C8-N7-C5	2.23	108.24	104.26
2	A	901	GTP	C8-N7-C5	2.22	108.22	104.26
2	A	901	GTP	N2-C2-N1	2.21	121.43	116.76
2	A	901	GTP	N9-C4-N3	2.21	130.36	125.95
2	B	901	GTP	C4-C5-N7	-2.20	107.18	110.67
3	C	902	GDP	C3'-C2'-C1'	2.20	105.62	101.46
3	D	902	GDP	C5-C6-N1	2.17	118.78	113.25
2	C	901	GTP	C6-C5-N7	2.16	134.22	130.29
2	B	901	GTP	O6-C6-C5	-2.14	120.89	126.53
3	C	902	GDP	N2-C2-N1	2.11	121.22	116.76
3	C	902	GDP	C6-C5-C4	-2.11	115.66	118.83
3	D	902	GDP	C3'-C2'-C1'	2.10	105.44	101.46
2	A	901	GTP	C2'-C1'-N9	-2.06	107.51	113.25
3	B	902	GDP	N2-C2-N1	2.05	121.09	116.76
3	A	902	GDP	C5-C6-N1	2.04	118.45	113.25
2	A	901	GTP	O6-C6-C5	-2.04	121.15	126.53
3	C	902	GDP	O4'-C1'-N9	2.04	112.97	108.36
2	C	901	GTP	N9-C8-N7	-2.03	109.64	113.40
2	A	901	GTP	C6-C5-N7	2.03	133.98	130.29
3	A	902	GDP	C8-N7-C5	2.02	107.86	104.26
3	D	902	GDP	C8-N9-C4	2.00	109.78	106.03
2	C	901	GTP	C5-C4-N9	2.00	109.24	105.66

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	GTP	PB-O3B-PG-O3G
2	C	901	GTP	PB-O3A-PA-O5'
2	C	901	GTP	C5'-O5'-PA-O3A
2	C	901	GTP	C5'-O5'-PA-O1A
2	C	901	GTP	C5'-O5'-PA-O2A
2	D	901	GTP	C5'-O5'-PA-O3A
2	D	901	GTP	O4'-C4'-C5'-O5'
3	C	902	GDP	PA-O3A-PB-O2B
3	D	902	GDP	C5'-O5'-PA-O3A
3	D	902	GDP	C5'-O5'-PA-O2A
3	B	902	GDP	PA-O3A-PB-O2B
3	B	902	GDP	PA-O3A-PB-O3B
3	B	902	GDP	C5'-O5'-PA-O3A
3	B	902	GDP	C5'-O5'-PA-O2A
2	D	901	GTP	C3'-C4'-C5'-O5'

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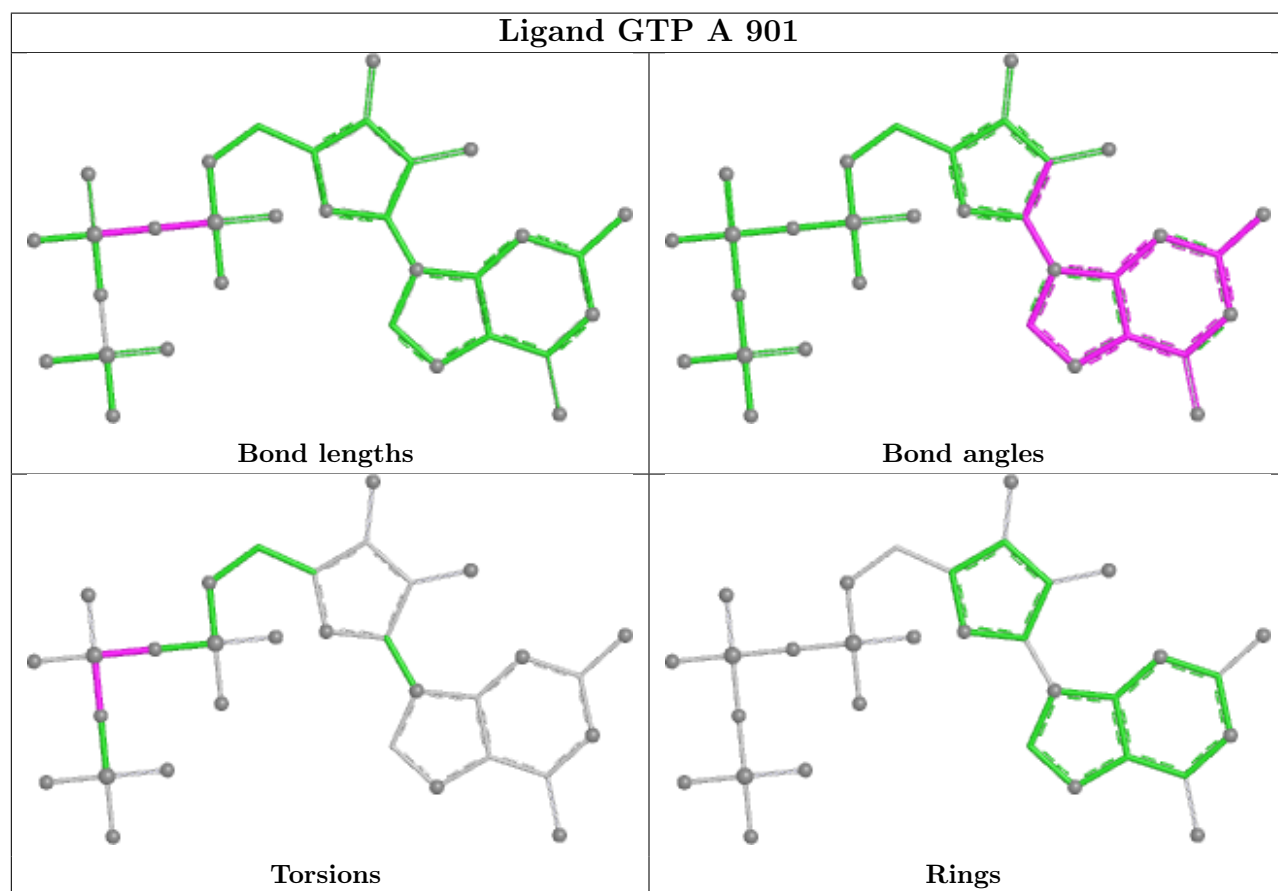
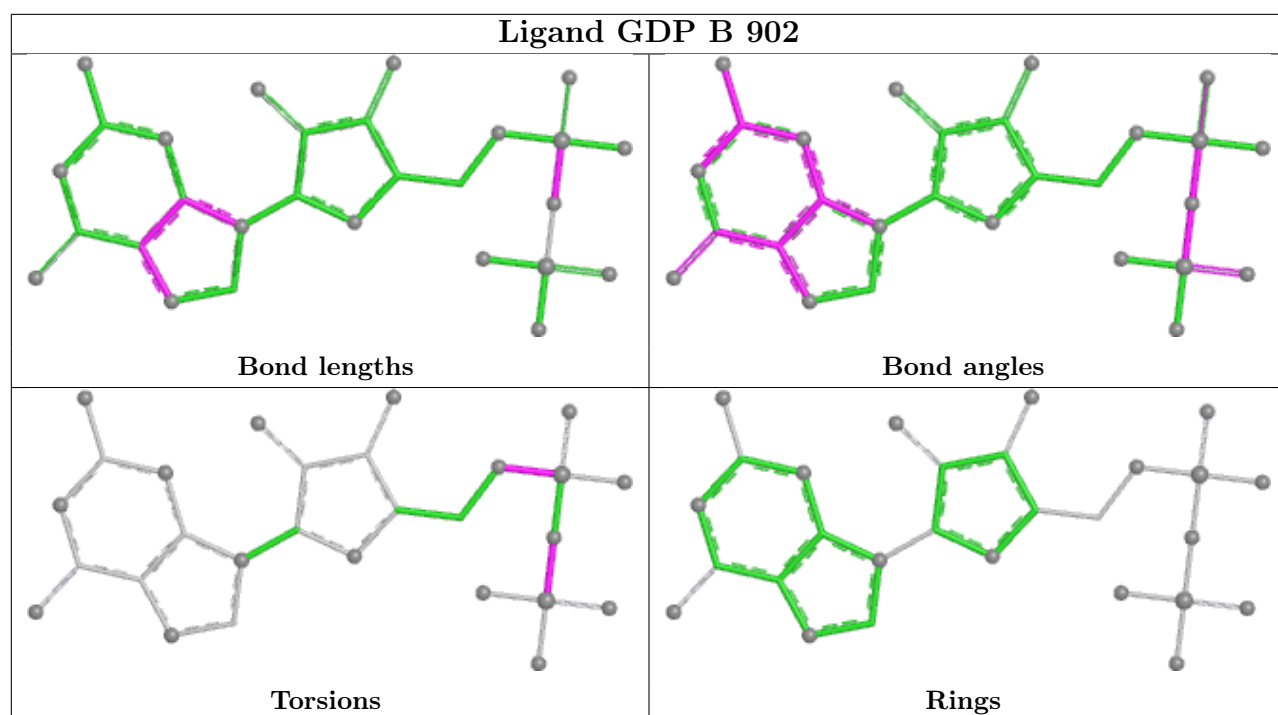
Mol	Chain	Res	Type	Atoms
2	B	901	GTP	PB-O3B-PG-O1G
2	B	901	GTP	PG-O3B-PB-O1B
2	A	901	GTP	PA-O3A-PB-O1B
2	D	901	GTP	C5'-O5'-PA-O1A
2	D	901	GTP	C5'-O5'-PA-O2A
3	B	902	GDP	C5'-O5'-PA-O1A
2	B	901	GTP	PA-O3A-PB-O2B
3	D	902	GDP	O4'-C4'-C5'-O5'
3	D	902	GDP	PB-O3A-PA-O1A
3	B	902	GDP	PA-O3A-PB-O1B
3	C	902	GDP	PA-O3A-PB-O3B
2	C	901	GTP	PA-O3A-PB-O1B
2	C	901	GTP	PA-O3A-PB-O2B
2	A	901	GTP	PG-O3B-PB-O2B
2	B	901	GTP	PA-O3A-PB-O1B
2	C	901	GTP	PB-O3B-PG-O1G
3	C	902	GDP	PA-O3A-PB-O1B
2	D	901	GTP	C2'-C1'-N9-C4
2	A	901	GTP	PA-O3A-PB-O2B
2	B	901	GTP	PG-O3B-PB-O2B

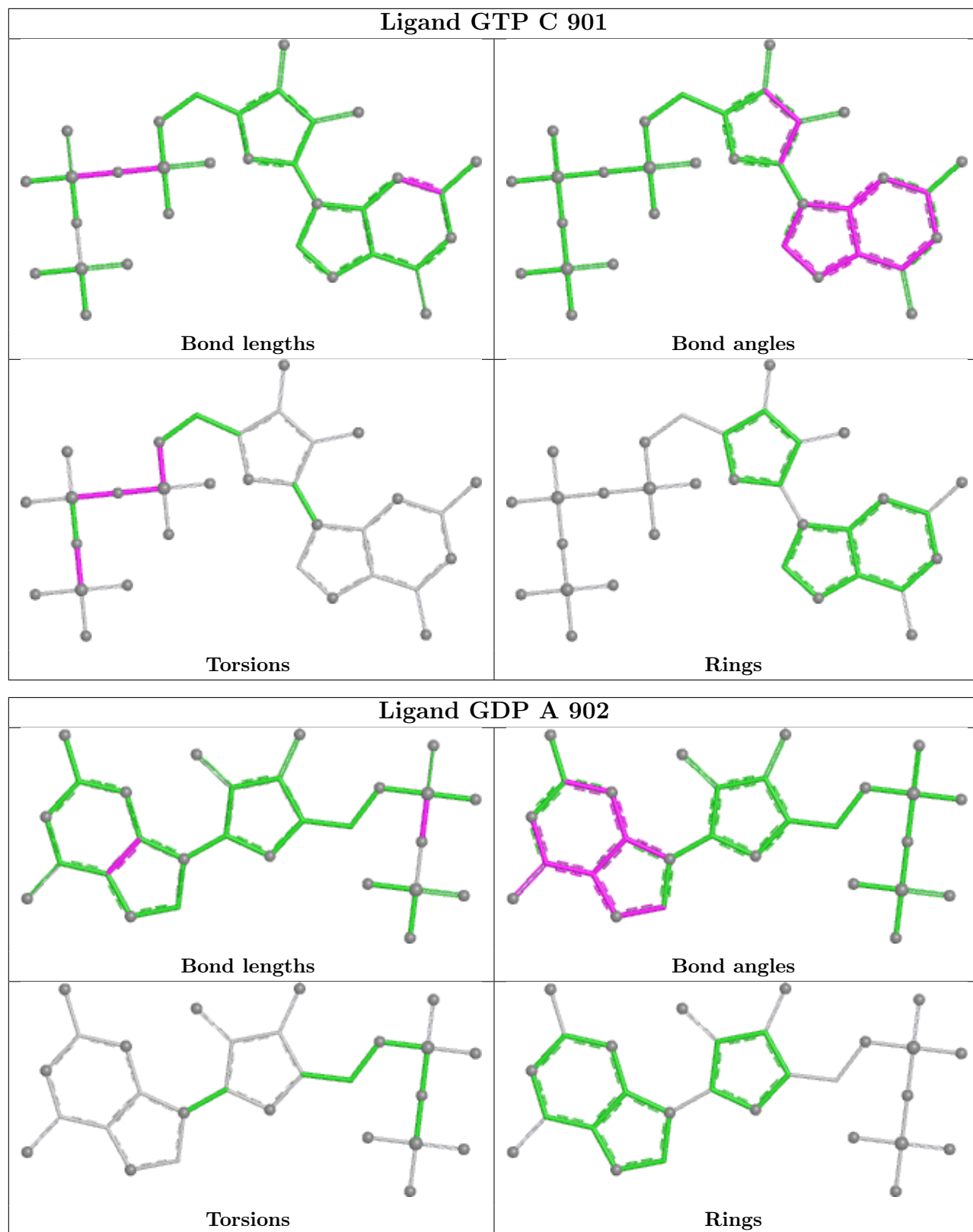
There are no ring outliers.

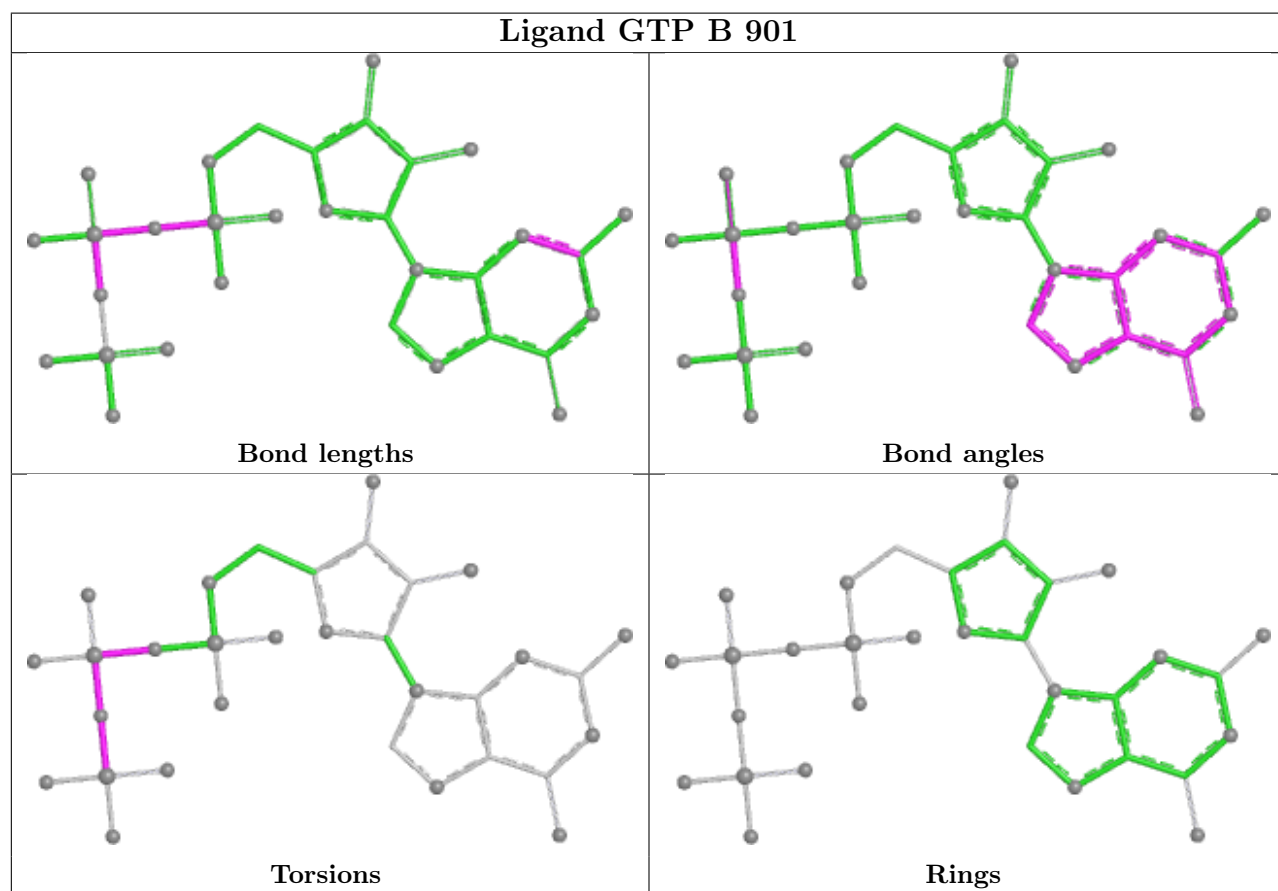
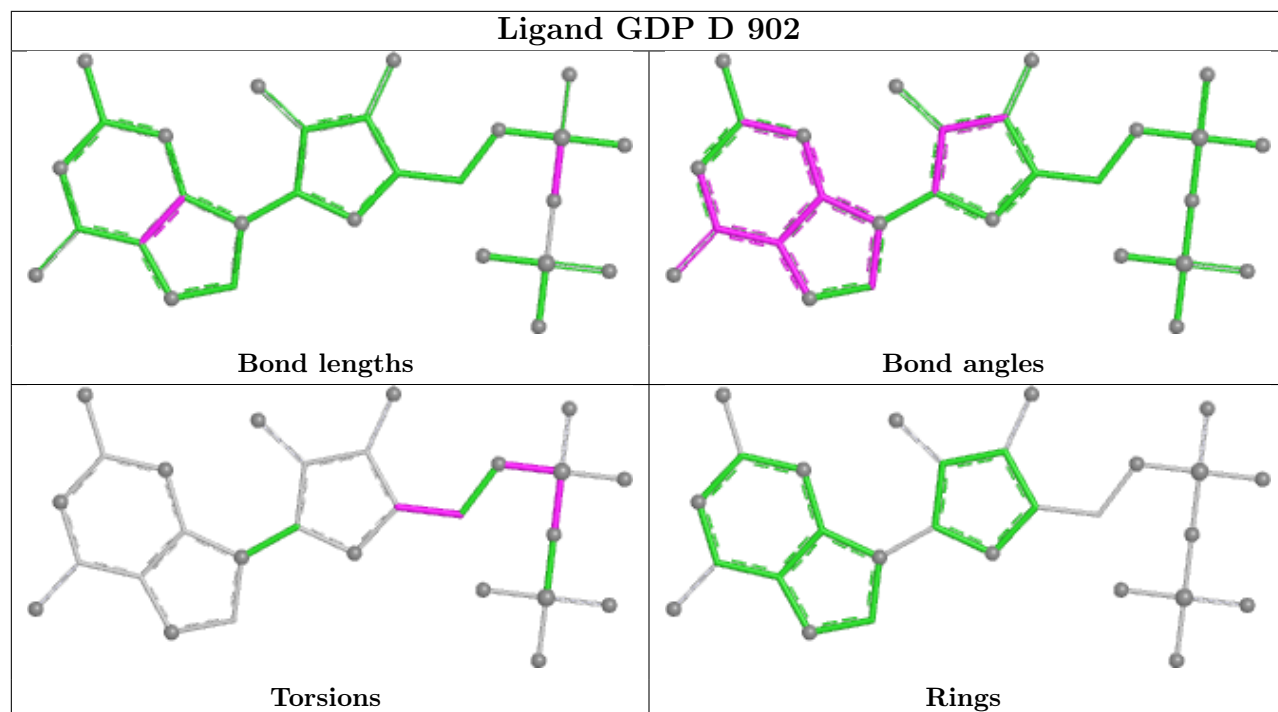
3 monomers are involved in 6 short contacts:

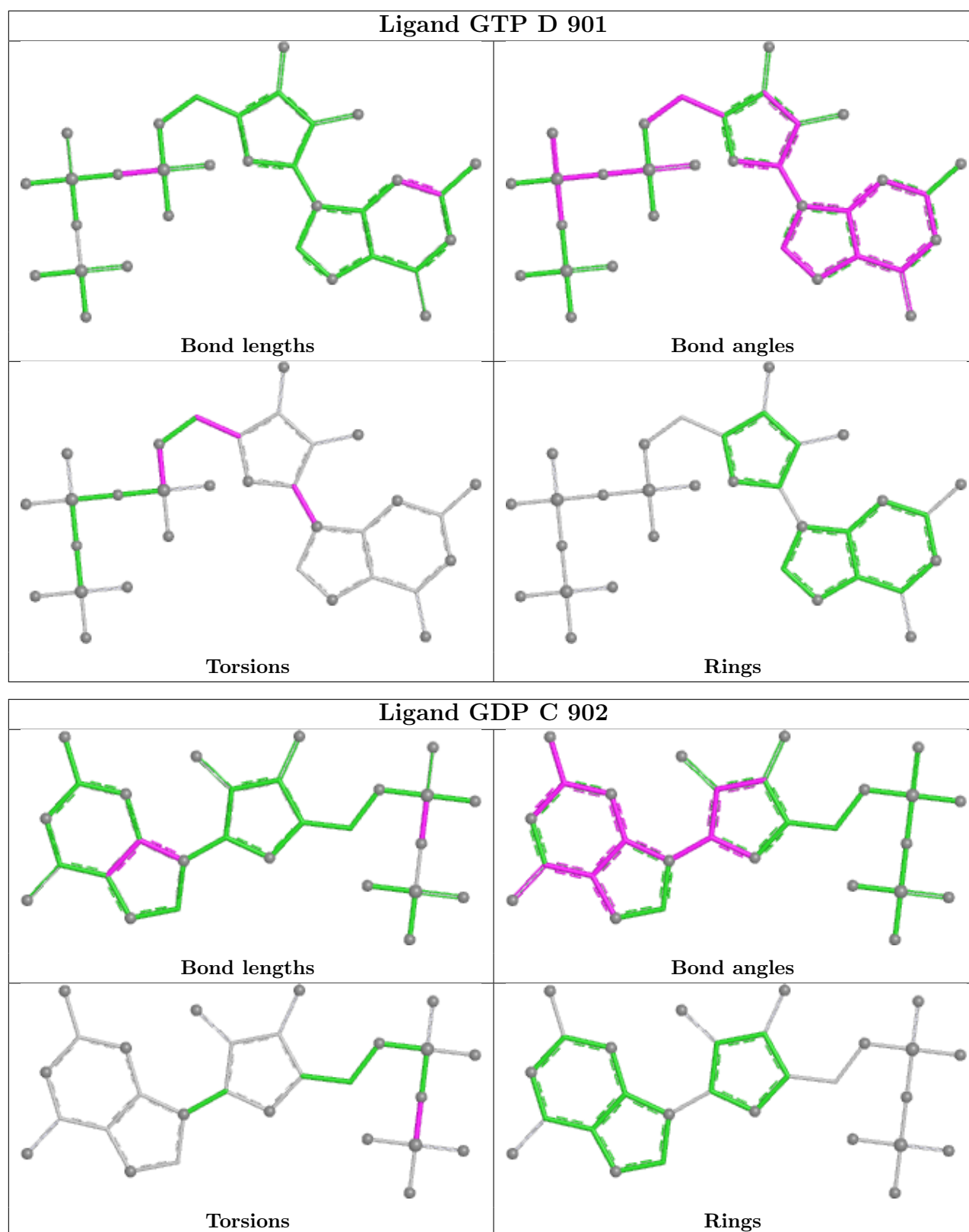
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	GDP	1	0
2	C	901	GTP	3	0
2	D	901	GTP	2	0

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

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	784/804 (97%)	-0.10	24 (3%) 51 54	11, 23, 47, 71	0
1	B	776/804 (96%)	0.35	45 (5%) 29 30	12, 30, 59, 83	2 (0%)
1	C	777/804 (96%)	0.08	18 (2%) 61 64	8, 26, 48, 72	0
1	D	791/804 (98%)	0.44	120 (15%) 5 5	8, 25, 70, 83	1 (0%)
All	All	3128/3216 (97%)	0.19	207 (6%) 24 26	8, 26, 58, 83	3 (0%)

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	TRP	6.8
1	D	361	TRP	5.7
1	A	494	ASN	5.2
1	D	436	LEU	5.0
1	C	233	LEU	5.0
1	D	362	VAL	4.8
1	D	384	THR	4.5
1	D	430	ALA	4.4
1	D	386	ILE	4.3
1	A	234	PRO	4.3
1	A	493	SER	4.3
1	D	371	SER	4.3
1	D	418	ILE	4.2
1	D	489	LEU	4.2
1	D	435	ILE	4.1
1	B	801	ILE	4.1
1	D	452	VAL	4.1
1	D	412	GLN	4.1
1	D	456	ILE	4.0
1	D	339	PHE	4.0
1	D	366	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	234	PRO	3.9
1	B	233	LEU	3.9
1	D	403	VAL	3.9
1	B	485	ALA	3.9
1	D	409	LEU	3.9
1	D	334	PHE	3.8
1	B	557	TYR	3.7
1	D	260	TYR	3.7
1	B	543	LEU	3.6
1	A	233	LEU	3.6
1	D	239	LYS	3.5
1	D	443	TYR	3.5
1	D	494	ASN	3.5
1	D	438	ALA	3.4
1	D	385	SER	3.4
1	B	438	ALA	3.4
1	D	307	PHE	3.4
1	C	487	TYR	3.4
1	D	552	ARG	3.4
1	D	433	ILE	3.3
1	D	246	LEU	3.3
1	D	266	GLN	3.3
1	D	269	LEU	3.3
1	D	336	PHE	3.3
1	C	469	VAL	3.3
1	D	338	SER	3.2
1	D	416	ALA	3.2
1	D	233	LEU	3.2
1	C	232	SER	3.2
1	B	734	MET	3.2
1	B	534	ASP	3.1
1	D	242	PHE	3.1
1	B	249	ILE	3.1
1	D	488	SER	3.1
1	D	491	ASN	3.1
1	D	244	LEU	3.1
1	D	1	MET	3.1
1	D	335	ASP	3.0
1	D	306	ALA	3.0
1	D	411	PRO	3.0
1	D	549	PRO	3.0
1	D	343	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	379	TRP	3.0
1	D	429	GLY	2.9
1	D	400	ASP	2.9
1	D	284	LEU	2.9
1	B	500	LEU	2.9
1	A	801	ILE	2.9
1	D	245	ILE	2.9
1	A	488	SER	2.9
1	D	2	SER	2.9
1	D	287	GLY	2.9
1	B	452	VAL	2.8
1	C	234	PRO	2.8
1	D	265	PRO	2.8
1	D	349	PHE	2.8
1	C	430	ALA	2.8
1	A	262	MET	2.8
1	A	734	MET	2.8
1	C	470	GLY	2.8
1	D	249	ILE	2.8
1	A	491	ASN	2.8
1	D	408	ALA	2.8
1	A	751	PRO	2.8
1	D	363	GLU	2.7
1	D	243	GLY	2.7
1	B	366	TYR	2.7
1	B	533	LEU	2.7
1	C	751	PRO	2.7
1	A	535	SER	2.7
1	B	451	SER	2.7
1	D	419	ARG	2.7
1	D	365	ASP	2.7
1	D	553	ARG	2.7
1	D	346	LEU	2.7
1	B	265	PRO	2.7
1	D	377	PHE	2.6
1	A	265	PRO	2.6
1	D	493	SER	2.6
1	B	535	SER	2.6
1	B	418	ILE	2.6
1	D	551	GLY	2.6
1	D	550	THR	2.6
1	D	247	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	234	PRO	2.6
1	D	487	TYR	2.6
1	D	395	TRP	2.6
1	A	533	LEU	2.6
1	B	540	SER	2.6
1	D	414	TYR	2.6
1	D	288	ALA	2.6
1	D	554	TRP	2.6
1	D	425	PHE	2.5
1	D	372	GLU	2.5
1	D	121	ASN	2.5
1	A	490	SER	2.5
1	D	286	ILE	2.5
1	C	265	PRO	2.5
1	C	361	TRP	2.5
1	A	554	TRP	2.5
1	B	555	ARG	2.5
1	D	450	MET	2.5
1	C	488	SER	2.4
1	D	364	THR	2.4
1	A	451	SER	2.4
1	D	417	SER	2.4
1	B	486	SER	2.4
1	B	364	THR	2.4
1	D	449	ALA	2.4
1	B	511	ALA	2.4
1	D	235	ASN	2.4
1	A	266	GLN	2.4
1	C	231	LYS	2.4
1	D	373	LYS	2.4
1	B	545	THR	2.4
1	D	236	PRO	2.4
1	B	436	LEU	2.4
1	D	399	LYS	2.4
1	A	263	HIS	2.4
1	A	487	TYR	2.3
1	B	489	LEU	2.3
1	D	359	ASP	2.3
1	D	248	VAL	2.3
1	B	737	PRO	2.3
1	D	369	PHE	2.3
1	C	364	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	291	ALA	2.3
1	B	471	ASP	2.3
1	B	497	GLU	2.3
1	D	381	ILE	2.3
1	D	383	ARG	2.3
1	D	337	LYS	2.3
1	D	382	ASP	2.3
1	D	354	LEU	2.3
1	B	736	PRO	2.2
1	B	800	LYS	2.2
1	A	536	ALA	2.2
1	C	263	HIS	2.2
1	D	431	SER	2.2
1	B	504	SER	2.2
1	B	262	MET	2.2
1	D	437	ALA	2.2
1	C	533	LEU	2.2
1	B	232	SER	2.2
1	D	461	PHE	2.2
1	D	388	VAL	2.2
1	B	532	VAL	2.2
1	D	305	LEU	2.2
1	A	492	SER	2.2
1	D	424	PHE	2.1
1	C	753	GLY	2.1
1	B	754	ALA	2.1
1	D	533	LEU	2.1
1	C	366	TYR	2.1
1	D	548	ASN	2.1
1	D	434	LYS	2.1
1	D	262	MET	2.1
1	D	465	MET	2.1
1	D	360	THR	2.1
1	D	391	ILE	2.1
1	D	460	LYS	2.1
1	D	472	ALA	2.1
1	D	536	ALA	2.1
1	B	730	ALA	2.1
1	D	407	LEU	2.1
1	D	464	CYS	2.1
1	B	422[A]	ARG	2.1
1	D	237	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	238	GLY	2.1
1	D	447	PHE	2.1
1	B	731	VAL	2.1
1	D	375	ALA	2.1
1	D	398	SER	2.1
1	B	501	LYS	2.0
1	D	283	ILE	2.0
1	C	363	GLU	2.0
1	A	532	VAL	2.0
1	B	469	VAL	2.0
1	D	444	MET	2.0
1	A	235	ASN	2.0
1	D	3	ASN	2.0
1	D	457	ASN	2.0
1	B	494	ASN	2.0
1	B	263	HIS	2.0
1	A	689	GLY	2.0
1	B	470	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GDP	D	902	28/28	0.78	0.12	25,37,68,84	0
3	GDP	A	902	28/28	0.83	0.10	24,36,68,77	0
3	GDP	C	902	28/28	0.83	0.11	13,35,67,79	0
3	GDP	B	902	28/28	0.83	0.11	26,37,69,78	0
2	GTP	C	901	32/32	0.85	0.11	22,37,48,50	0

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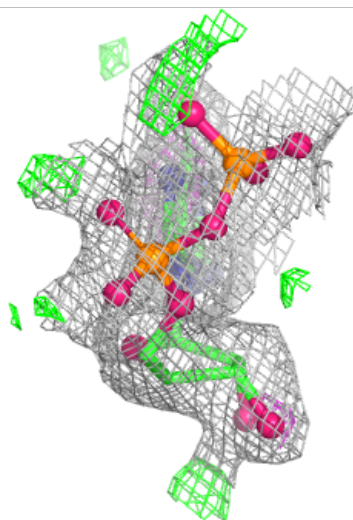
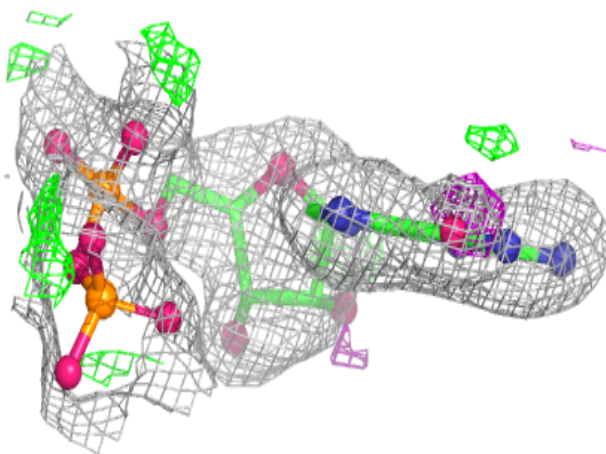
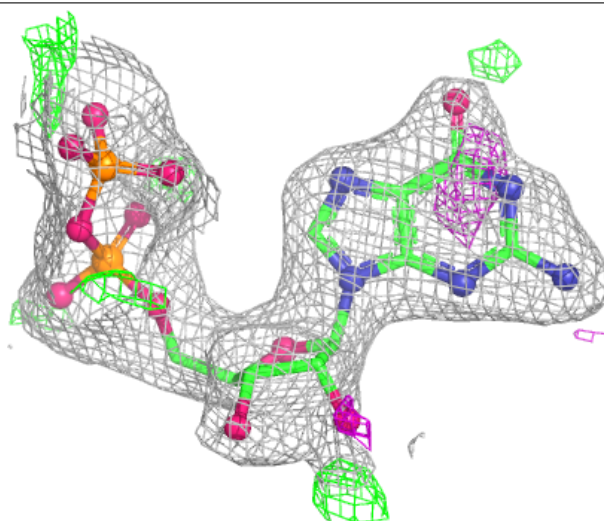
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GTP	D	901	32/32	0.86	0.11	20,41,54,62	0
2	GTP	B	901	32/32	0.91	0.10	25,36,48,55	0
2	GTP	A	901	32/32	0.92	0.09	18,27,44,47	0

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.

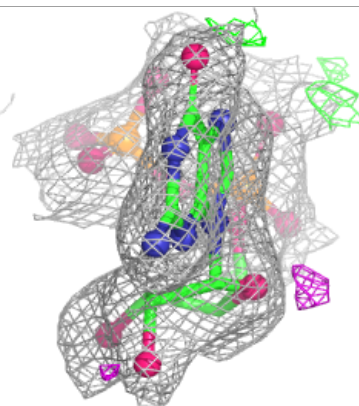
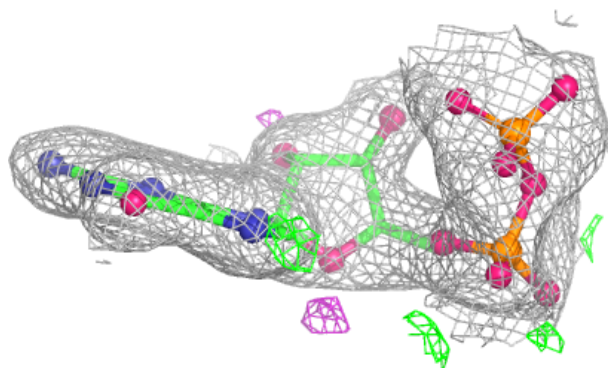
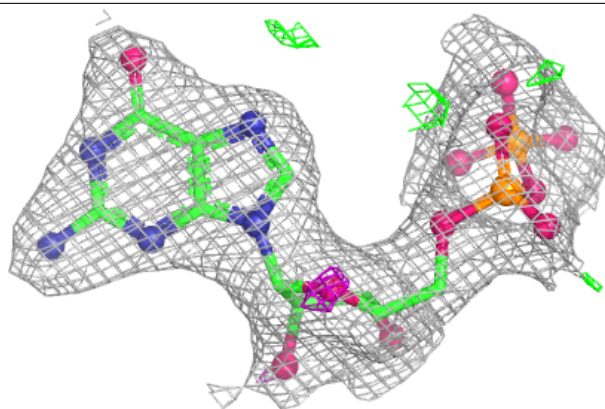
Electron density around GDP D 902:

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

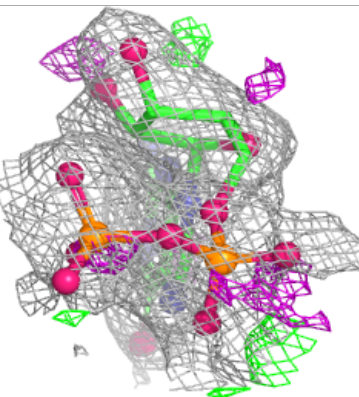
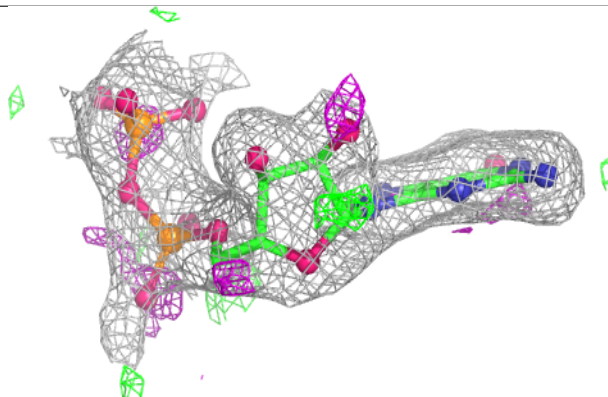
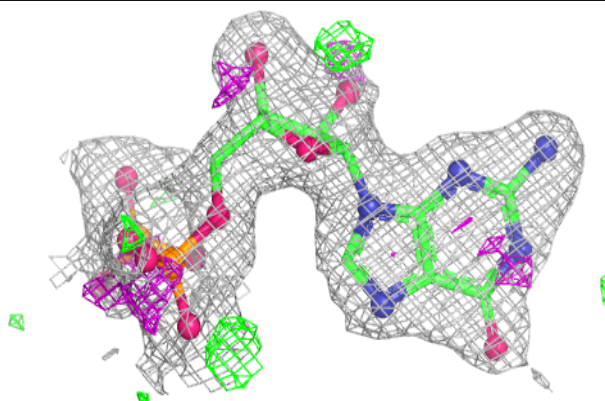


Electron density around GDP A 902:

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

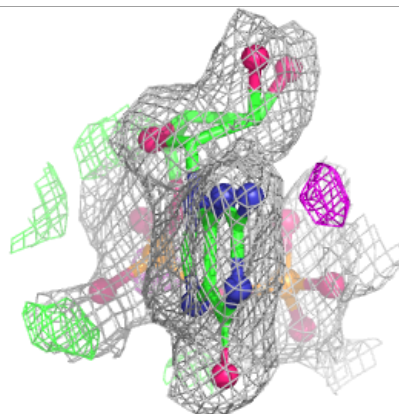
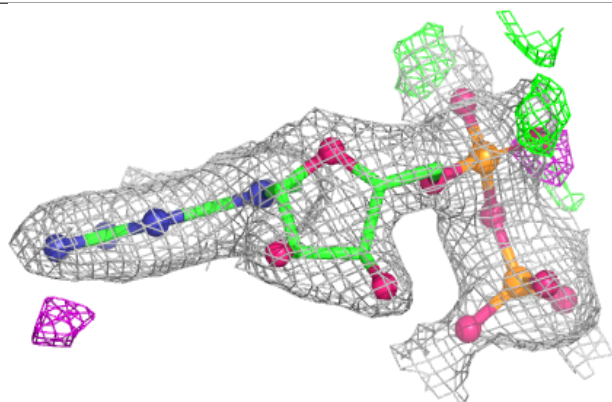
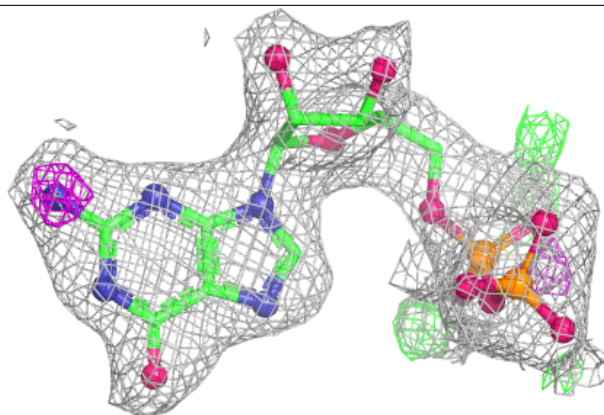
**Electron density around GDP C 902:**

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

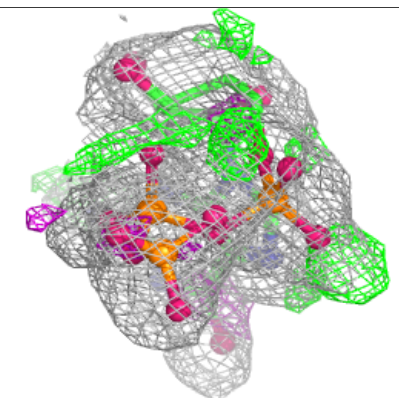
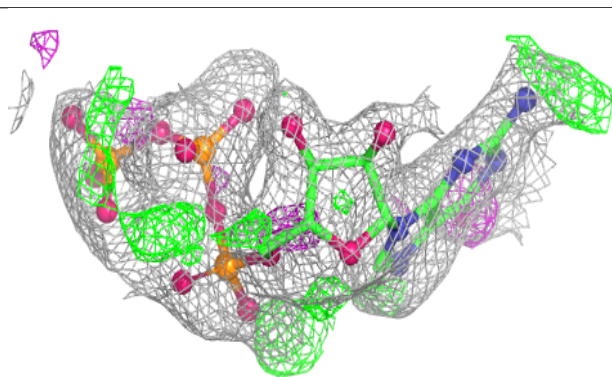
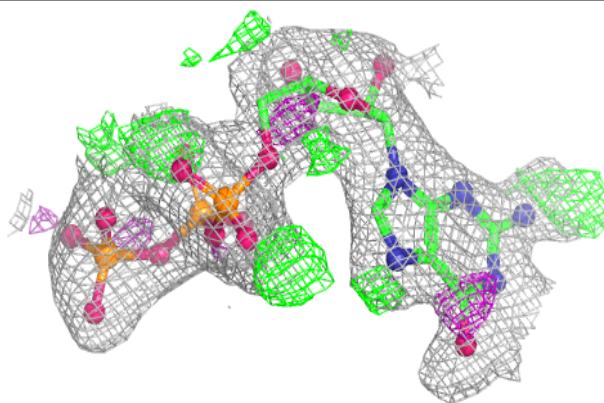


Electron density around GDP B 902:

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

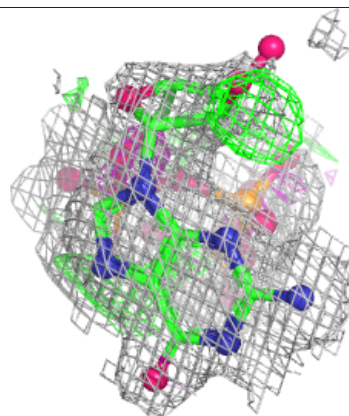
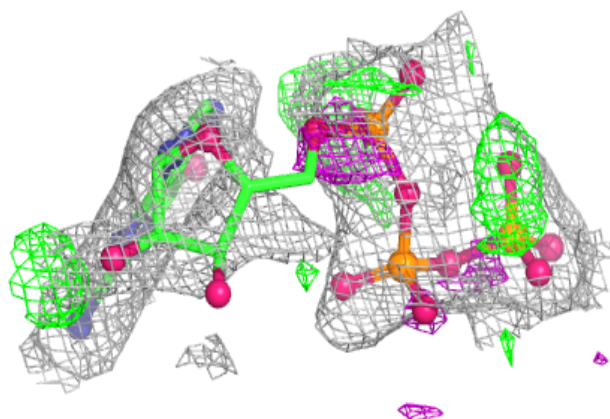
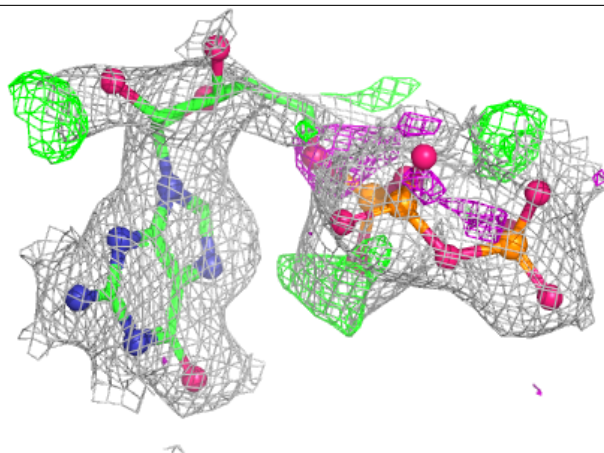
**Electron density around GTP C 901:**

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

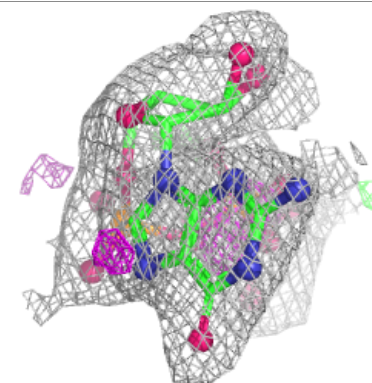
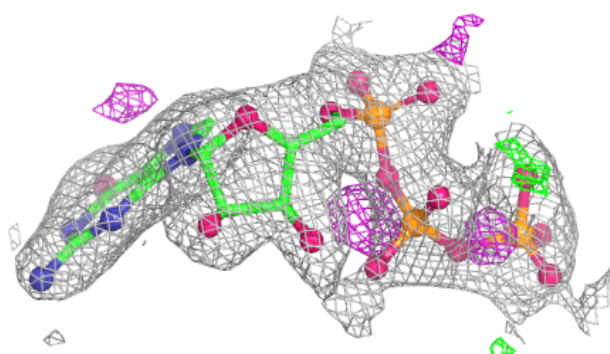
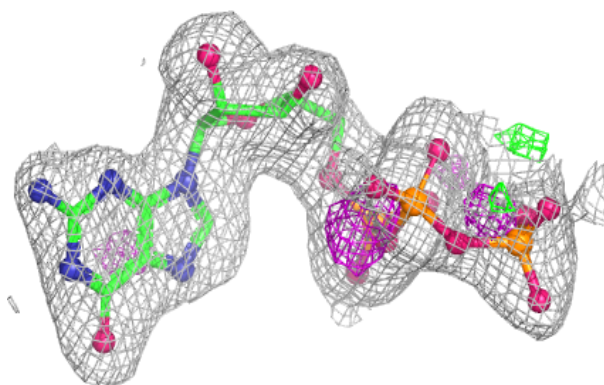


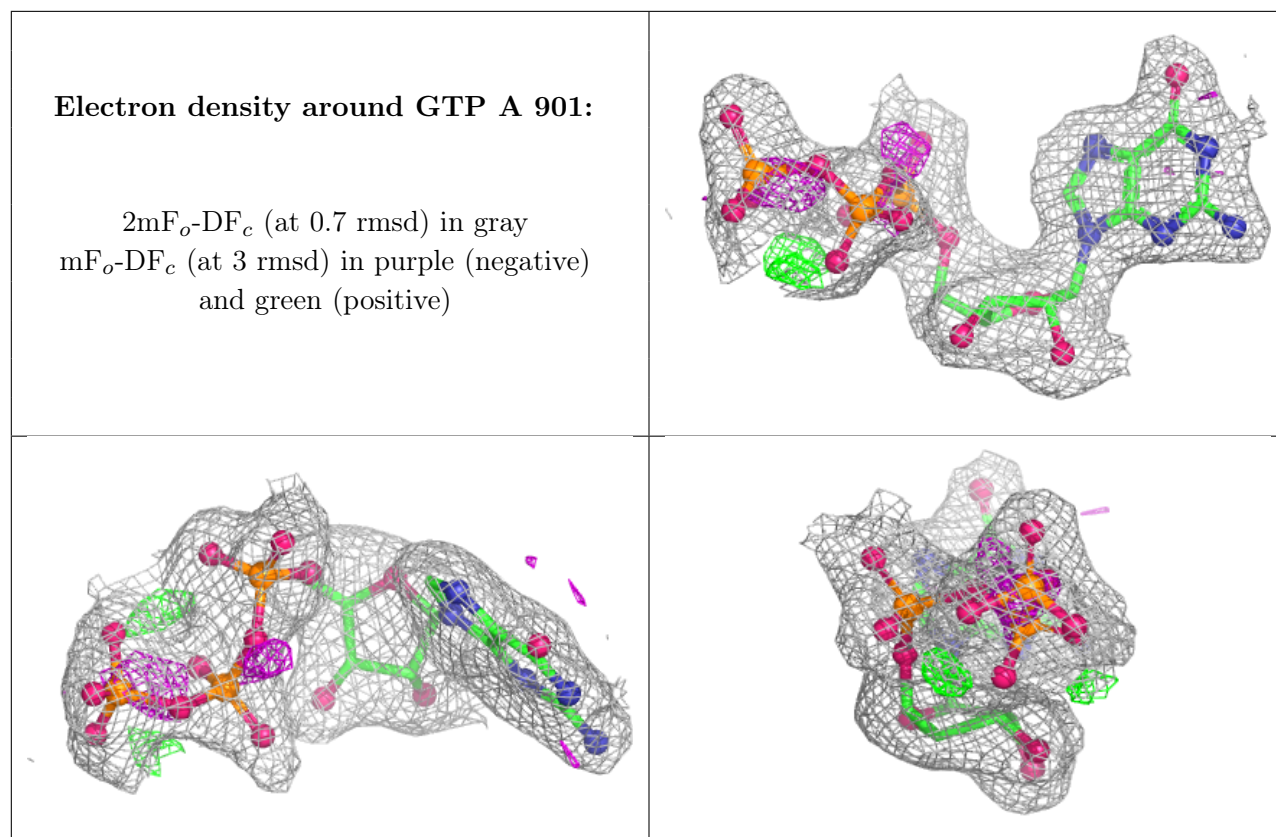
Electron density around GTP D 901:

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

**Electron density around GTP B 901:**

$2mF_o-DF_c$ (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.