



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 06:21 PM EDT

PDB ID : 4TO0
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP-dCTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

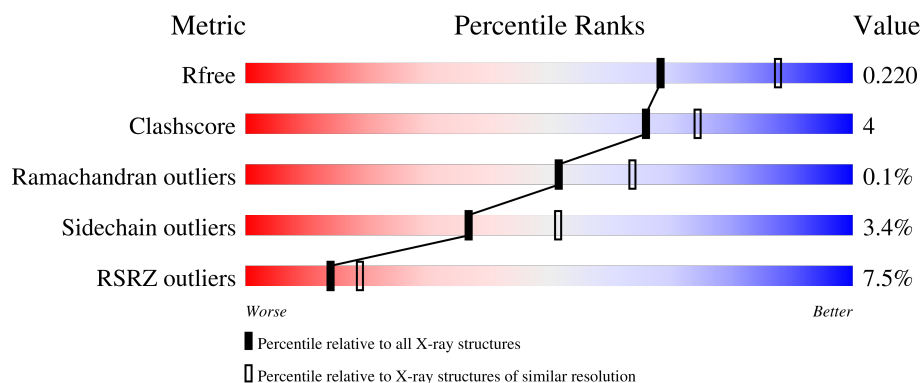
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	514	<div> <div>8%</div> <div>85% 8% • 7%</div> </div>
1	B	514	<div> <div>4%</div> <div>84% 8% • 7%</div> </div>
1	C	514	<div> <div>6%</div> <div>82% 10% • 6%</div> </div>
1	D	514	<div> <div>10%</div> <div>83% 10% • 6%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16246 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.

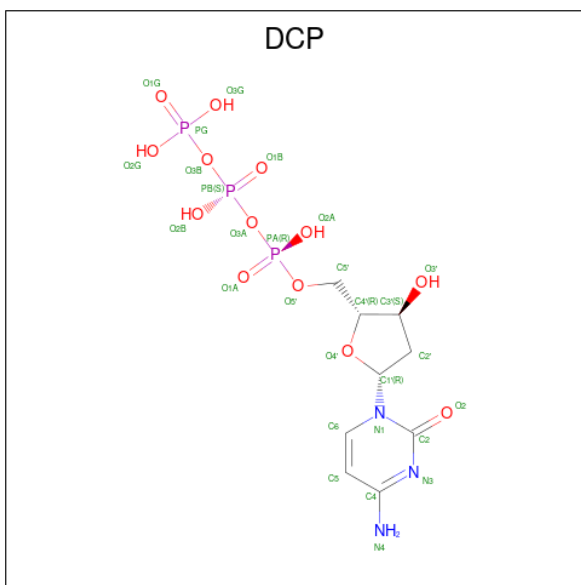
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	1	0
			3922	2511	684	706	21			
1	B	480	Total	C	N	O	S	0	0	0
			3924	2512	684	708	20			
1	C	481	Total	C	N	O	S	0	2	0
			3944	2522	687	715	20			
1	D	484	Total	C	N	O	S	0	0	0
			3953	2530	688	715	20			

There are 8 discrepancies between the modelled and reference sequences:

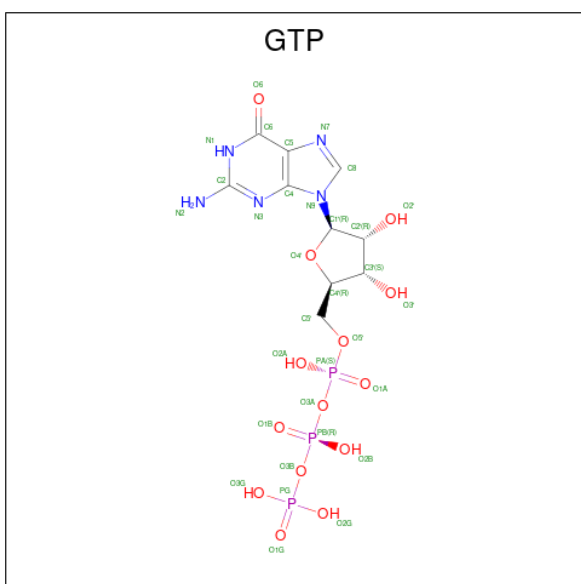
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



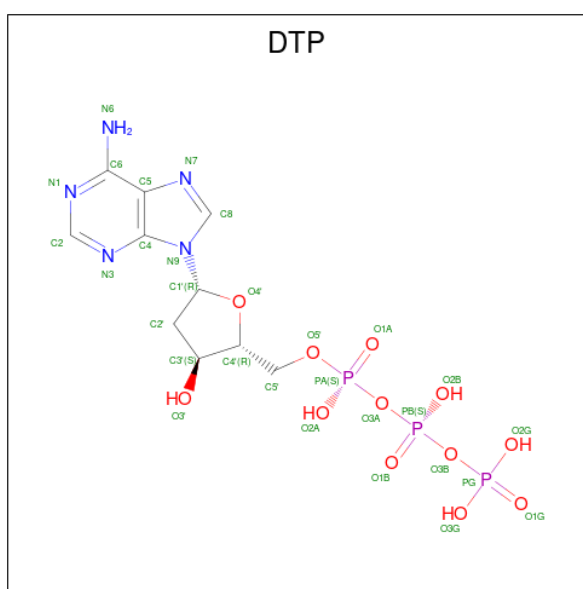
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	B	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	C	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	D	1	Total 28	C 9	N 3	O 13	P 3	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0

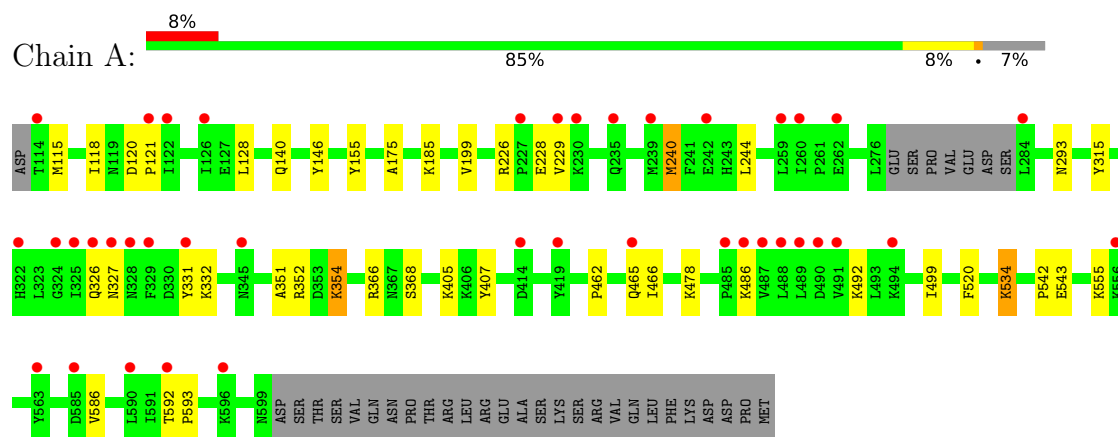
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	42	Total 42	O 42	0	0
6	C	38	Total 38	O 38	0	0
6	D	27	Total 27	O 27	0	0

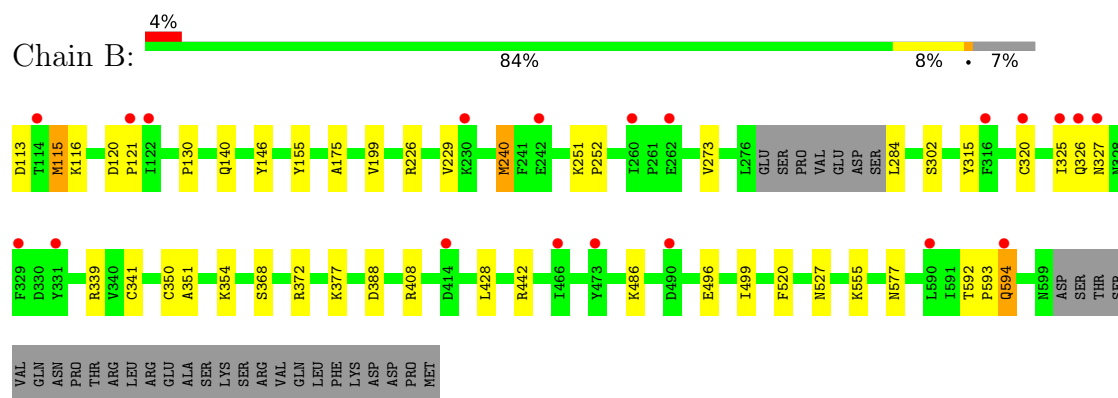
3 Residue-property plots [i](#)

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.

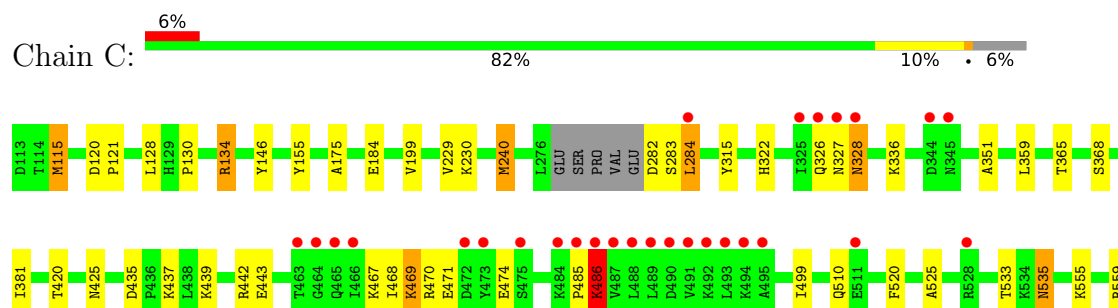
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

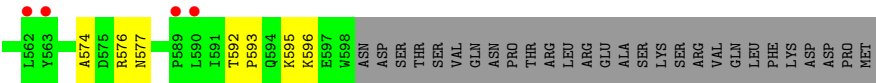


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

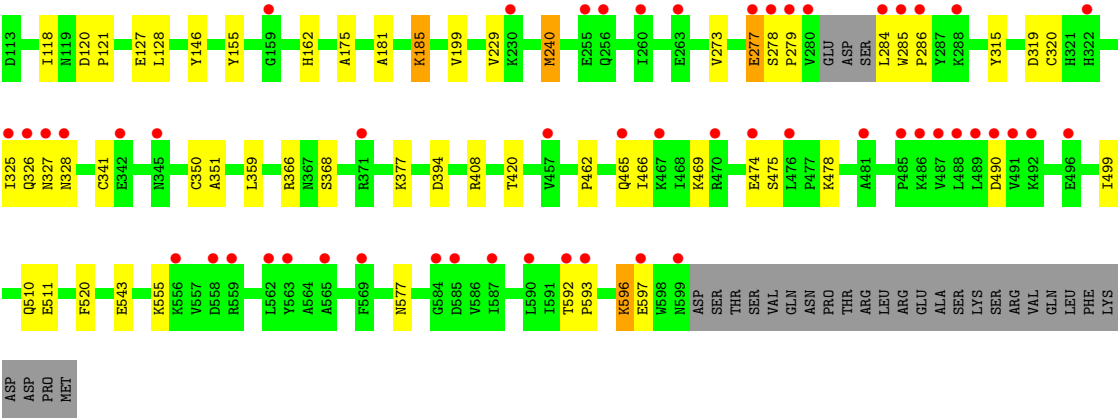
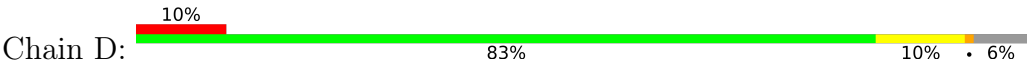


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.42Å 141.33Å 97.52Å 90.00° 114.58° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 47.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.30) 97.9 (47.88-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.191 , 0.222 0.194 , 0.220	Depositor DCC
R_{free} test set	4490 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16246	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: MG, DCP, GTP, DTP

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	0.64	0/4014	0.77	2/5418 (0.0%)
1	B	0.71	0/4016	0.78	2/5421 (0.0%)
1	C	0.71	0/4036	0.80	4/5448 (0.1%)
1	D	0.64	0/4046	0.75	1/5463 (0.0%)
All	All	0.68	0/16112	0.78	9/21750 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	576	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	C	359	LEU	CB-CG-CD1	5.93	121.09	111.00
1	B	442	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	442	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	366	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	D	366	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	226	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	C	284	LEU	CB-CG-CD1	5.05	119.59	111.00
1	B	226	ARG	NE-CZ-NH2	5.04	122.82	120.30

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	3922	0	3915	28	2
1	B	3924	0	3915	33	0
1	C	3944	0	3927	49	0
1	D	3953	0	3942	29	2
2	A	28	0	12	1	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	1	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	1	0
3	D	32	0	12	0	0
4	A	30	0	12	0	0
4	B	30	0	12	0	0
4	C	30	0	12	0	0
4	D	30	0	12	0	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	32	0	0	1	0
6	B	42	0	0	1	0
6	C	38	0	0	4	0
6	D	27	0	0	2	0
All	All	16246	0	15843	129	2

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 4.

All (129) 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:574:ALA:O	1:C:595:LYS:NZ	1.67	1.23
1:B:115:MET:HE2	1:B:116:LYS:N	1.73	1.03
1:C:328:ASN:ND2	1:C:365:THR:OG1	1.94	0.98
1:C:439:LYS:O	1:C:443:GLU:HG3	1.62	0.98
1:B:115:MET:HE2	1:B:115:MET:C	1.84	0.96
1:B:115:MET:HE2	1:B:116:LYS:CA	1.99	0.92
1:B:372:ARG:HH22	1:D:328:ASN:HD21	1.19	0.91
1:B:115:MET:HE1	1:B:116:LYS:O	1.72	0.90
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:H	1.20	0.88
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:N	1.70	0.87
1:C:533:THR:OG1	1:C:535[A]:ASN:ND2	2.09	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ASP:OD2	1:C:437:LYS:HD2	1.75	0.85
1:C:435:ASP:OD1	1:C:437:LYS:HG2	1.77	0.84
1:B:115:MET:CE	1:B:116:LYS:C	2.45	0.84
1:A:326:GLN:HB2	1:C:327:ASN:O	1.78	0.84
1:B:115:MET:CE	1:B:116:LYS:N	2.41	0.83
1:B:115:MET:C	1:B:115:MET:CE	2.49	0.80
1:B:115:MET:CE	1:B:116:LYS:O	2.31	0.78
1:A:140:GLN:HG3	1:A:240:MET:CE	2.15	0.76
1:A:327:ASN:O	1:C:326:GLN:HB2	1.86	0.76
1:B:327:ASN:O	1:D:326:GLN:HB2	1.86	0.75
1:C:435:ASP:CG	1:C:437:LYS:HG3	2.08	0.73
2:D:702:DCP:O1B	6:D:827:HOH:O	2.05	0.73
1:B:140:GLN:HG3	1:B:240:MET:CE	2.17	0.73
1:B:115:MET:HE2	1:B:116:LYS:C	2.08	0.72
1:C:435:ASP:CG	1:C:437:LYS:CG	2.58	0.72
1:C:470:ARG:HB2	1:C:470:ARG:CZ	2.20	0.71
1:A:492:LYS:NZ	6:A:801:HOH:O	2.22	0.71
1:B:115:MET:HE1	1:B:116:LYS:C	2.07	0.71
1:C:435:ASP:OD1	1:C:437:LYS:CG	2.39	0.71
1:D:596:LYS:HE2	1:D:597:GLU:OE1	1.91	0.69
1:B:326:GLN:HB2	1:D:327:ASN:O	1.92	0.69
1:C:435:ASP:OD2	1:C:437:LYS:CD	2.42	0.67
3:C:704:GTP:O2B	6:C:819:HOH:O	2.11	0.67
1:C:322:HIS:CE1	6:C:818:HOH:O	2.48	0.66
1:C:535[A]:ASN:H	1:C:535[A]:ASN:ND2	1.94	0.64
1:A:155:TYR:HH	1:D:146:TYR:HH	1.46	0.63
1:C:574:ALA:C	1:C:595:LYS:NZ	2.51	0.62
1:C:468:ILE:HG23	6:C:801:HOH:O	2.01	0.61
1:B:594:GLN:N	1:B:594:GLN:OE1	2.33	0.61
1:A:405:LYS:HD3	1:A:407:TYR:OH	2.03	0.58
1:C:435:ASP:OD2	1:C:437:LYS:CG	2.51	0.58
1:D:499:ILE:HD11	1:D:555:LYS:HE2	1.86	0.58
1:C:499:ILE:HD11	1:C:555:LYS:HE2	1.86	0.57
1:C:535[A]:ASN:N	1:C:535[A]:ASN:ND2	2.45	0.57
1:A:140:GLN:CG	1:A:240:MET:CE	2.83	0.56
1:A:331:TYR:C	1:A:331:TYR:CD1	2.78	0.56
1:C:467:LYS:HG2	1:C:469:LYS:HE3	1.87	0.56
1:A:499:ILE:HD11	1:A:555:LYS:HE2	1.86	0.55
1:A:534:LYS:HE2	1:A:542:PRO:O	2.06	0.55
1:B:499:ILE:HD11	1:B:555:LYS:HE2	1.87	0.55
1:B:140:GLN:CG	1:B:240:MET:CE	2.84	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:OE1	1:A:228:GLU:N	2.38	0.54
1:B:146:TYR:HH	1:C:155:TYR:HH	1.55	0.54
1:D:162:HIS:HE1	1:D:319:ASP:OD1	1.92	0.53
1:B:339:ARG:HH11	1:B:527:ASN:ND2	2.06	0.53
1:B:339:ARG:HH11	1:B:527:ASN:HD21	1.57	0.52
1:D:181:ALA:O	1:D:185:LYS:HD2	2.10	0.51
1:A:140:GLN:CG	1:A:240:MET:HE3	2.41	0.51
1:C:120:ASP:OD2	1:C:121:PRO:HD2	2.11	0.51
1:B:140:GLN:CG	1:B:240:MET:HE3	2.41	0.50
1:D:162:HIS:H	1:D:162:HIS:CD2	2.29	0.50
1:C:469:LYS:HB3	1:C:471:GLU:OE1	2.12	0.49
1:C:574:ALA:C	1:C:595:LYS:HZ2	2.13	0.49
1:C:336:LYS:CE	1:D:127:GLU:HG3	2.43	0.49
1:C:485:PRO:O	1:C:486:LYS:HB2	2.12	0.49
1:D:120:ASP:OD2	1:D:121:PRO:HD2	2.12	0.49
1:D:377:LYS:HE2	6:D:816:HOH:O	2.13	0.49
1:A:120:ASP:OD2	1:A:121:PRO:HD2	2.13	0.48
1:A:146:TYR:HH	1:D:155:TYR:HH	1.60	0.48
1:A:293:ASN:OD1	1:A:293:ASN:N	2.46	0.48
1:B:377:LYS:HE2	6:B:806:HOH:O	2.13	0.48
1:D:279:PRO:HG3	1:D:286:PRO:HB3	1.96	0.48
1:D:511:GLU:H	1:D:511:GLU:CD	2.17	0.47
2:A:701:DCP:O2G	2:A:701:DCP:O2B	2.31	0.47
1:C:467:LYS:CE	1:C:469:LYS:CE	2.92	0.47
1:D:474:GLU:O	1:D:478:LYS:NZ	2.38	0.47
1:A:331:TYR:CD1	1:A:332:LYS:N	2.83	0.47
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.46
1:A:592:THR:N	1:A:593:PRO:CD	2.79	0.46
1:D:592:THR:N	1:D:593:PRO:CD	2.79	0.46
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.46
1:C:134:ARG:NE	1:C:134:ARG:HA	2.30	0.46
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.16	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.46
1:C:485:PRO:O	1:C:486:LYS:CB	2.64	0.46
1:A:118:ILE:HD12	1:A:128:LEU:HD11	1.97	0.45
1:B:155:TYR:HH	1:C:146:TYR:HH	1.61	0.45
1:C:328:ASN:HD21	1:C:365:THR:HG1	1.48	0.45
1:D:118:ILE:HD12	1:D:128:LEU:HD11	1.98	0.45
1:C:240:MET:HE3	1:C:420:THR:HA	1.99	0.45
1:D:175:ALA:HB1	1:D:199:VAL:HG12	1.99	0.45
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:SER:HA	1:D:478:LYS:HE2	1.98	0.44
1:A:352:ARG:HG2	1:A:354:LYS:HD3	1.98	0.44
1:A:586:VAL:HG11	1:C:525:ALA:HB3	1.99	0.44
1:C:115:MET:HG3	1:C:128:LEU:O	2.17	0.44
1:B:115:MET:HB2	1:B:115:MET:HE3	1.72	0.44
1:D:462:PRO:HB3	1:D:466:ILE:HB	1.99	0.44
1:B:320:CYS:HB3	1:B:325:ILE:O	2.18	0.44
1:B:592:THR:N	1:B:593:PRO:CD	2.81	0.44
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.00	0.44
1:A:140:GLN:HG3	1:A:240:MET:HE2	2.00	0.43
1:B:341:CYS:HB2	1:B:350:CYS:SG	2.59	0.43
1:C:592:THR:N	1:C:593:PRO:CD	2.81	0.43
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.01	0.43
1:D:240:MET:HE3	1:D:420:THR:HA	2.01	0.43
1:B:175:ALA:HB1	1:B:199:VAL:HG12	2.00	0.43
1:A:462:PRO:HB3	1:A:466:ILE:HB	2.00	0.43
1:C:437:LYS:HB3	1:C:437:LYS:HE2	1.90	0.43
1:A:405:LYS:HD3	1:A:407:TYR:CZ	2.54	0.42
1:C:467:LYS:CE	1:C:469:LYS:HE3	2.49	0.42
1:D:320:CYS:HB3	1:D:325:ILE:O	2.19	0.42
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.02	0.42
1:C:577:ASN:HA	6:C:826:HOH:O	2.19	0.42
1:B:113:ASP:HB3	1:B:130:PRO:HB3	2.01	0.42
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.02	0.41
1:C:435:ASP:OD2	1:C:437:LYS:HG3	2.20	0.41
1:D:284:LEU:HD13	1:D:285:TRP:N	2.35	0.41
1:A:118:ILE:HD13	1:A:118:ILE:HG21	1.81	0.41
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.95	0.41
1:D:394:ASP:O	1:D:408:ARG:HD2	2.21	0.41
1:A:146:TYR:OH	1:D:155:TYR:OH	2.35	0.41
1:C:467:LYS:HE3	1:C:469:LYS:CE	2.50	0.41
1:D:277:GLU:HG2	1:D:278:SER:N	2.36	0.41
1:A:244:LEU:HD23	1:A:244:LEU:C	2.41	0.40
1:C:471:GLU:OE1	1:C:471:GLU:N	2.32	0.40
1:C:467:LYS:HE2	1:C:469:LYS:CE	2.51	0.40
1:D:341:CYS:HB2	1:D:350:CYS:SG	2.62	0.40

All (2) 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:A:465:GLN:O	1:D:469:LYS:CD[1_655]	1.90	0.30
1:A:543:GLU:O	1:D:465:GLN:OE1[1_655]	2.09	0.11

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	476/514 (93%)	471 (99%)	5 (1%)	0	100	100
1	B	476/514 (93%)	466 (98%)	10 (2%)	0	100	100
1	C	479/514 (93%)	470 (98%)	8 (2%)	1 (0%)	47	58
1	D	480/514 (93%)	472 (98%)	8 (2%)	0	100	100
All	All	1911/2056 (93%)	1879 (98%)	31 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	LYS

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	426/459 (93%)	416 (98%)	10 (2%)	50	67
1	B	426/459 (93%)	411 (96%)	15 (4%)	36	50
1	C	429/459 (94%)	407 (95%)	22 (5%)	24	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	430/459 (94%)	417 (97%)	13 (3%)	41 57
All	All	1711/1836 (93%)	1651 (96%)	60 (4%)	37 50

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	185	LYS
1	A	229	VAL
1	A	240	MET
1	A	315	TYR
1	A	354	LYS
1	A	368	SER
1	A	478	LYS
1	A	486	LYS
1	A	534	LYS
1	B	115	MET
1	B	229	VAL
1	B	240	MET
1	B	273	VAL
1	B	284	LEU
1	B	302	SER
1	B	315	TYR
1	B	354	LYS
1	B	368	SER
1	B	388	ASP
1	B	408	ARG
1	B	486	LYS
1	B	496	GLU
1	B	577	ASN
1	B	594	GLN
1	C	115	MET
1	C	130	PRO
1	C	134	ARG
1	C	184	GLU
1	C	229	VAL
1	C	230	LYS
1	C	240	MET
1	C	282	ASP
1	C	283	SER
1	C	284	LEU
1	C	315	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	328	ASN
1	C	368[A]	SER
1	C	368[B]	SER
1	C	469	LYS
1	C	474	GLU
1	C	486	LYS
1	C	510	GLN
1	C	535[A]	ASN
1	C	535[B]	ASN
1	C	559	ARG
1	C	596	LYS
1	D	185	LYS
1	D	229	VAL
1	D	240	MET
1	D	273	VAL
1	D	277	GLU
1	D	315	TYR
1	D	359	LEU
1	D	368	SER
1	D	490	ASP
1	D	510	GLN
1	D	543	GLU
1	D	577	ASN
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	326	GLN
1	A	328	ASN
1	B	322	HIS
1	B	425	ASN
1	B	527	ASN
1	B	577	ASN
1	C	321	HIS
1	C	322	HIS
1	C	326	GLN
1	C	328	ASN
1	D	162	HIS
1	D	235	GLN
1	D	321	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	322	HIS
1	D	326	GLN
1	D	328	ASN
1	D	535	ASN
1	D	539	GLN
1	D	594	GLN
1	D	599	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	D	704	5	26,34,34	1.23	2 (7%)	33,54,54	2.09	13 (39%)
4	DTP	B	702	5	26,32,32	1.45	5 (19%)	30,50,50	1.37	5 (16%)
4	DTP	D	703	5	26,32,32	1.21	3 (11%)	30,50,50	1.37	4 (13%)
2	DCP	D	702	-	23,29,29	0.71	0	30,45,45	1.47	3 (10%)
3	GTP	C	704	5	26,34,34	2.00	4 (15%)	33,54,54	2.15	11 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DTP	A	703	5	26,32,32	1.35	4 (15%)	30,50,50	1.44	4 (13%)
4	DTP	C	701	5	26,32,32	1.31	2 (7%)	30,50,50	1.59	9 (30%)
2	DCP	C	703	-	23,29,29	0.87	0	30,45,45	1.35	4 (13%)
3	GTP	A	702	5	26,34,34	1.26	4 (15%)	33,54,54	2.10	11 (33%)
2	DCP	B	701	-	23,29,29	1.02	1 (4%)	30,45,45	1.42	4 (13%)
3	GTP	B	703	5	26,34,34	1.30	2 (7%)	33,54,54	2.16	10 (30%)
2	DCP	A	701	-	23,29,29	0.71	0	30,45,45	1.56	5 (16%)

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	GTP	D	704	5	-	2/18/38/38	0/3/3/3
4	DTP	B	702	5	-	6/18/34/34	0/3/3/3
4	DTP	D	703	5	-	4/18/34/34	0/3/3/3
2	DCP	D	702	-	-	6/19/34/34	0/2/2/2
3	GTP	C	704	5	-	3/18/38/38	0/3/3/3
4	DTP	A	703	5	-	6/18/34/34	0/3/3/3
4	DTP	C	701	5	-	5/18/34/34	0/3/3/3
2	DCP	C	703	-	-	3/19/34/34	0/2/2/2
3	GTP	A	702	5	-	4/18/38/38	0/3/3/3
2	DCP	B	701	-	-	6/19/34/34	0/2/2/2
3	GTP	B	703	5	-	2/18/38/38	0/3/3/3
2	DCP	A	701	-	-	9/19/34/34	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	GTP	O4'-C1'	7.47	1.51	1.41
3	C	704	GTP	C2'-C1'	-4.56	1.46	1.53
4	C	701	DTP	C2-N3	3.94	1.38	1.32
3	D	704	GTP	O4'-C1'	3.76	1.46	1.41
3	A	702	GTP	C5-C6	3.31	1.47	1.41
3	B	703	GTP	C5-C6	2.94	1.46	1.41
3	D	704	GTP	C5-C6	2.85	1.46	1.41
4	B	702	DTP	C2-N3	2.81	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	DTP	O4'-C4'	-2.75	1.38	1.45
3	B	703	GTP	C5-C4	2.66	1.48	1.40
4	A	703	DTP	C2-N3	2.66	1.36	1.32
4	D	703	DTP	C8-N7	2.64	1.39	1.34
4	A	703	DTP	PG-O2G	-2.63	1.44	1.54
4	D	703	DTP	C2-N3	2.60	1.36	1.32
4	A	703	DTP	C5-C4	2.58	1.47	1.40
4	B	702	DTP	C5-C4	2.46	1.47	1.40
4	B	702	DTP	O3'-C3'	2.46	1.48	1.43
4	C	701	DTP	C2-N1	2.39	1.38	1.33
2	B	701	DCP	C2-N3	-2.38	1.33	1.38
3	A	702	GTP	C5-C4	2.37	1.47	1.40
3	C	704	GTP	C4-N3	-2.12	1.32	1.35
3	A	702	GTP	PG-O2G	-2.11	1.46	1.54
4	D	703	DTP	C5-C4	2.10	1.46	1.40
3	A	702	GTP	C2'-C1'	-2.10	1.50	1.53
4	A	703	DTP	C2-N1	2.09	1.37	1.33
3	C	704	GTP	C5-C4	2.04	1.46	1.40
4	B	702	DTP	C2-N1	2.03	1.37	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	704	GTP	C2-N3-C4	4.97	121.03	115.36
3	D	704	GTP	C5-C6-N1	-4.94	116.68	123.43
3	A	702	GTP	C2-N1-C6	4.65	123.33	115.93
2	D	702	DCP	C4-N3-C2	4.61	121.01	116.34
3	D	704	GTP	C2-N1-C6	4.51	123.10	115.93
3	B	703	GTP	C2-N1-C6	4.46	123.01	115.93
3	B	703	GTP	C5-C6-N1	-4.44	117.35	123.43
3	A	702	GTP	C4-C5-C6	-4.34	116.65	120.80
2	A	701	DCP	C4-N3-C2	4.20	120.59	116.34
3	A	702	GTP	C5-C6-N1	-4.13	117.78	123.43
3	B	703	GTP	C2-N3-C4	4.06	120.00	115.36
3	C	704	GTP	C3'-C2'-C1'	4.04	107.07	100.98
2	B	701	DCP	PB-O3B-PG	-4.04	118.96	132.83
3	D	704	GTP	C3'-C2'-C1'	4.03	107.05	100.98
3	C	704	GTP	C5-C6-N1	-3.88	118.13	123.43
2	A	701	DCP	PB-O3B-PG	-3.86	119.56	132.83
3	B	703	GTP	C3'-C2'-C1'	3.80	106.70	100.98
3	B	703	GTP	C4-C5-C6	-3.76	117.21	120.80
3	B	703	GTP	N3-C2-N1	-3.74	122.24	127.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	DTP	N3-C2-N1	-3.69	122.92	128.68
3	A	702	GTP	C3'-C2'-C1'	3.68	106.51	100.98
3	A	702	GTP	PA-O3A-PB	-3.67	120.23	132.83
2	C	703	DCP	PB-O3B-PG	-3.65	120.30	132.83
4	A	703	DTP	N6-C6-N1	3.63	126.11	118.57
3	A	702	GTP	C2-N3-C4	3.57	119.43	115.36
3	C	704	GTP	O2'-C2'-C1'	-3.55	97.73	110.85
4	C	701	DTP	O3B-PG-O1G	-3.53	91.62	111.19
3	B	703	GTP	O2B-PB-O1B	3.45	129.28	112.24
3	C	704	GTP	C4-C5-C6	-3.34	117.61	120.80
3	D	704	GTP	PA-O3A-PB	-3.30	121.51	132.83
3	A	702	GTP	N3-C2-N1	-3.27	122.86	127.22
4	B	702	DTP	N3-C2-N1	-3.25	123.60	128.68
3	D	704	GTP	C2-N3-C4	3.25	119.07	115.36
3	D	704	GTP	C4-C5-C6	-3.24	117.71	120.80
3	C	704	GTP	C2-N1-C6	3.17	120.97	115.93
3	C	704	GTP	PA-O3A-PB	-3.17	121.94	132.83
3	C	704	GTP	C4-C5-N7	-3.09	106.18	109.40
2	D	702	DCP	PB-O3B-PG	-3.08	122.27	132.83
3	B	703	GTP	PB-O3B-PG	-3.07	122.28	132.83
2	B	701	DCP	C4-N3-C2	3.05	119.43	116.34
4	C	701	DTP	C5-C6-N6	-3.04	115.73	120.35
4	B	702	DTP	PB-O3B-PG	-2.95	122.70	132.83
2	D	702	DCP	PB-O3A-PA	-2.92	122.81	132.83
4	C	701	DTP	O2G-PG-O1G	2.87	121.90	110.68
2	C	703	DCP	PB-O3A-PA	-2.81	123.17	132.83
3	C	704	GTP	N3-C2-N1	-2.77	123.53	127.22
3	B	703	GTP	O2'-C2'-C1'	-2.75	100.71	110.85
2	A	701	DCP	PB-O3A-PA	-2.75	123.40	132.83
4	B	702	DTP	O3G-PG-O1G	2.75	121.44	110.68
4	A	703	DTP	O3B-PG-O1G	-2.74	96.02	111.19
4	A	703	DTP	N3-C2-N1	-2.73	124.42	128.68
3	B	703	GTP	PA-O3A-PB	-2.72	123.48	132.83
4	A	703	DTP	C5-C6-N6	-2.70	116.25	120.35
2	B	701	DCP	PB-O3A-PA	-2.63	123.80	132.83
3	A	702	GTP	PB-O3B-PG	-2.61	123.85	132.83
3	D	704	GTP	O3G-PG-O2G	2.61	117.60	107.64
3	D	704	GTP	O2A-PA-O1A	2.59	125.06	112.24
4	C	701	DTP	N6-C6-N1	2.58	123.94	118.57
3	D	704	GTP	N3-C2-N1	-2.54	123.83	127.22
4	B	702	DTP	O3B-PG-O1G	-2.51	97.28	111.19
3	A	702	GTP	O3G-PG-O2G	2.50	117.18	107.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	704	GTP	O5'-PA-O1A	-2.49	99.33	109.07
4	B	702	DTP	O2A-PA-O1A	2.47	124.45	112.24
3	A	702	GTP	O2B-PB-O1B	2.45	124.35	112.24
3	C	704	GTP	N2-C2-N1	2.39	120.98	117.25
2	A	701	DCP	O3B-PG-O1G	-2.36	98.10	111.19
4	C	701	DTP	O2B-PB-O1B	2.30	123.61	112.24
4	C	701	DTP	N3-C2-N1	-2.30	125.09	128.68
3	D	704	GTP	PB-O3B-PG	-2.29	124.96	132.83
4	D	703	DTP	O3G-PG-O2G	2.20	116.03	107.64
3	D	704	GTP	C4-C5-N7	-2.19	107.12	109.40
4	C	701	DTP	O2A-PA-O1A	2.16	122.94	112.24
4	C	701	DTP	O3G-PG-O2G	2.14	115.83	107.64
3	A	702	GTP	O2'-C2'-C1'	-2.09	103.13	110.85
2	C	703	DCP	O2B-PB-O1B	2.07	122.49	112.24
2	A	701	DCP	O3G-PG-O2G	2.07	115.53	107.64
4	D	703	DTP	PB-O3B-PG	-2.06	125.77	132.83
4	C	701	DTP	C4-C5-N7	-2.05	107.26	109.40
3	C	704	GTP	O3G-PG-O2G	2.03	115.41	107.64
2	B	701	DCP	O3B-PG-O1G	-2.01	100.02	111.19
3	D	704	GTP	O2'-C2'-C1'	-2.01	103.43	110.85
4	D	703	DTP	N6-C6-N1	2.01	122.74	118.57
2	C	703	DCP	O2A-PA-O1A	2.00	122.15	112.24

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DCP	C5'-O5'-PA-O2A
2	B	701	DCP	C5'-O5'-PA-O1A
2	D	702	DCP	C5'-O5'-PA-O2A
4	C	701	DTP	PB-O3B-PG-O2G
4	D	703	DTP	PB-O3B-PG-O2G
4	D	703	DTP	PB-O3B-PG-O3G
2	A	701	DCP	C3'-C4'-C5'-O5'
2	D	702	DCP	C4'-C5'-O5'-PA
2	B	701	DCP	C3'-C4'-C5'-O5'
3	A	702	GTP	PB-O3B-PG-O1G
4	A	703	DTP	PB-O3B-PG-O1G
4	C	701	DTP	PB-O3B-PG-O1G
2	A	701	DCP	C4'-C5'-O5'-PA
2	C	703	DCP	C4'-C5'-O5'-PA
2	A	701	DCP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

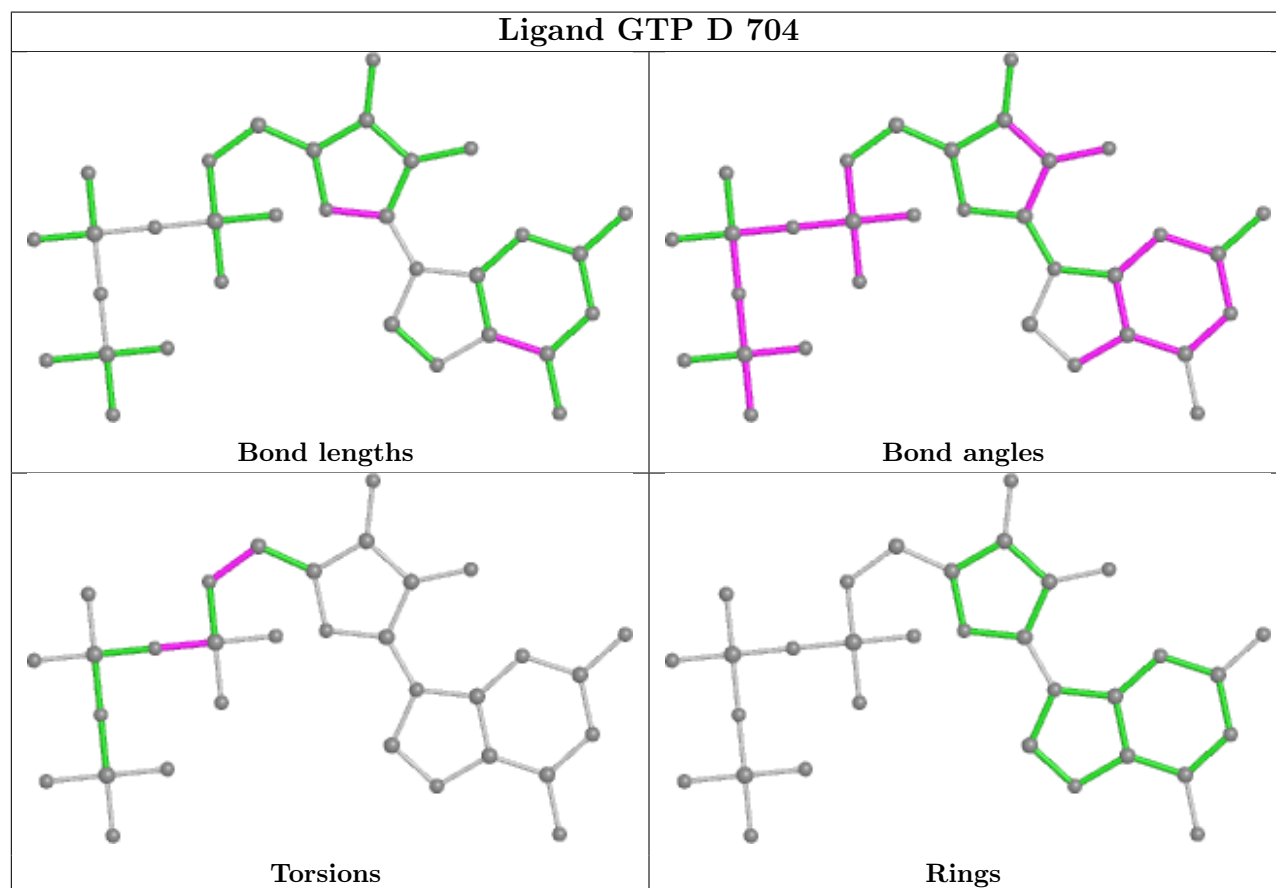
Mol	Chain	Res	Type	Atoms
2	B	701	DCP	C4'-C5'-O5'-PA
2	A	701	DCP	PB-O3A-PA-O5'
2	B	701	DCP	PB-O3A-PA-O5'
2	C	703	DCP	PB-O3A-PA-O5'
2	D	702	DCP	PB-O3A-PA-O5'
4	A	703	DTP	PB-O3B-PG-O3G
4	B	702	DTP	PB-O3B-PG-O3G
2	A	701	DCP	C5'-O5'-PA-O3A
2	B	701	DCP	C5'-O5'-PA-O3A
2	D	702	DCP	C5'-O5'-PA-O3A
2	B	701	DCP	O4'-C4'-C5'-O5'
3	A	702	GTP	PG-O3B-PB-O2B
4	A	703	DTP	PG-O3B-PB-O1B
4	A	703	DTP	PB-O3A-PA-O2A
4	B	702	DTP	PG-O3B-PB-O1B
4	B	702	DTP	PB-O3A-PA-O2A
4	C	701	DTP	PG-O3B-PB-O2B
2	D	702	DCP	C5'-O5'-PA-O1A
2	C	703	DCP	C3'-C4'-C5'-O5'
4	B	702	DTP	PB-O3B-PG-O1G
3	A	702	GTP	PG-O3B-PB-O1B
3	C	704	GTP	PG-O3B-PB-O2B
4	B	702	DTP	PB-O3A-PA-O1A
4	C	701	DTP	PB-O3A-PA-O2A
2	D	702	DCP	C3'-C4'-C5'-O5'
3	D	704	GTP	C4'-C5'-O5'-PA
3	A	702	GTP	C4'-C5'-O5'-PA
3	B	703	GTP	C4'-C5'-O5'-PA
2	A	701	DCP	PG-O3B-PB-O1B
3	C	704	GTP	C4'-C5'-O5'-PA
4	D	703	DTP	PB-O3B-PG-O1G
2	A	701	DCP	PG-O3B-PB-O2B
3	B	703	GTP	PG-O3B-PB-O2B
3	C	704	GTP	PG-O3B-PB-O1B
3	D	704	GTP	PB-O3A-PA-O2A
4	A	703	DTP	PG-O3B-PB-O2B
4	A	703	DTP	PB-O3A-PA-O1A
4	B	702	DTP	PG-O3B-PB-O2B
4	C	701	DTP	PB-O3A-PA-O1A
4	D	703	DTP	PB-O3A-PA-O2A
2	A	701	DCP	C5'-O5'-PA-O1A

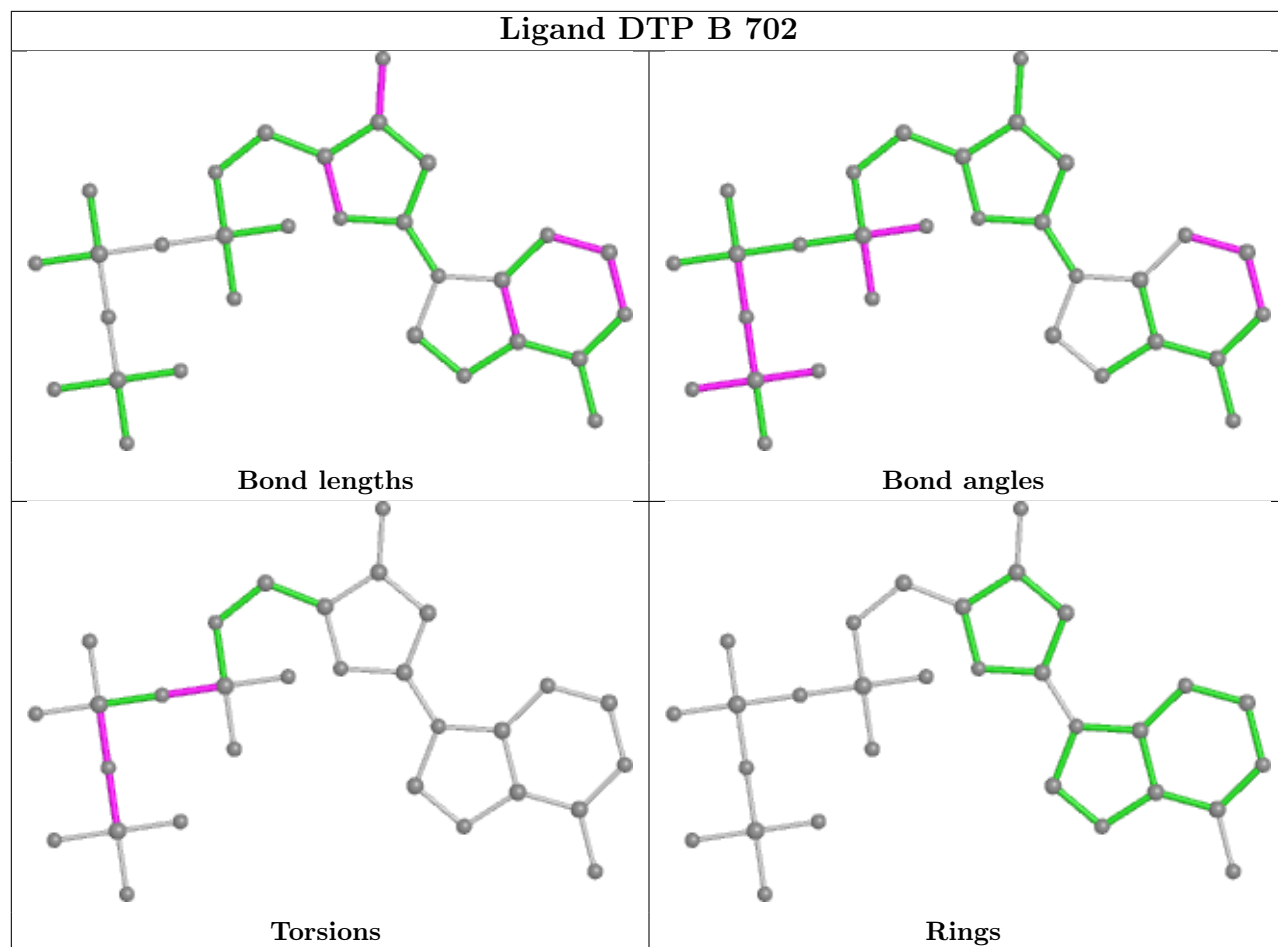
There are no ring outliers.

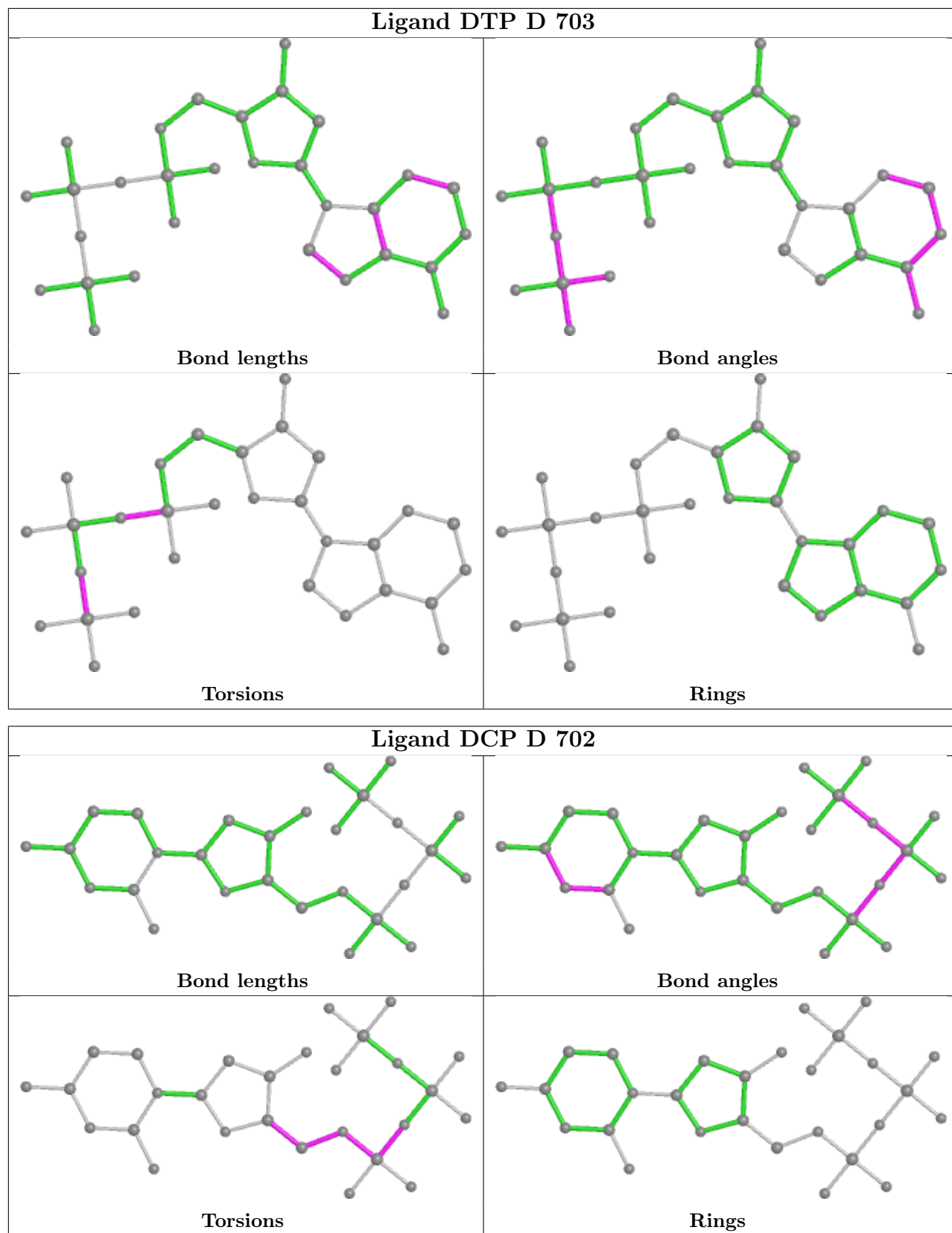
3 monomers are involved in 3 short contacts:

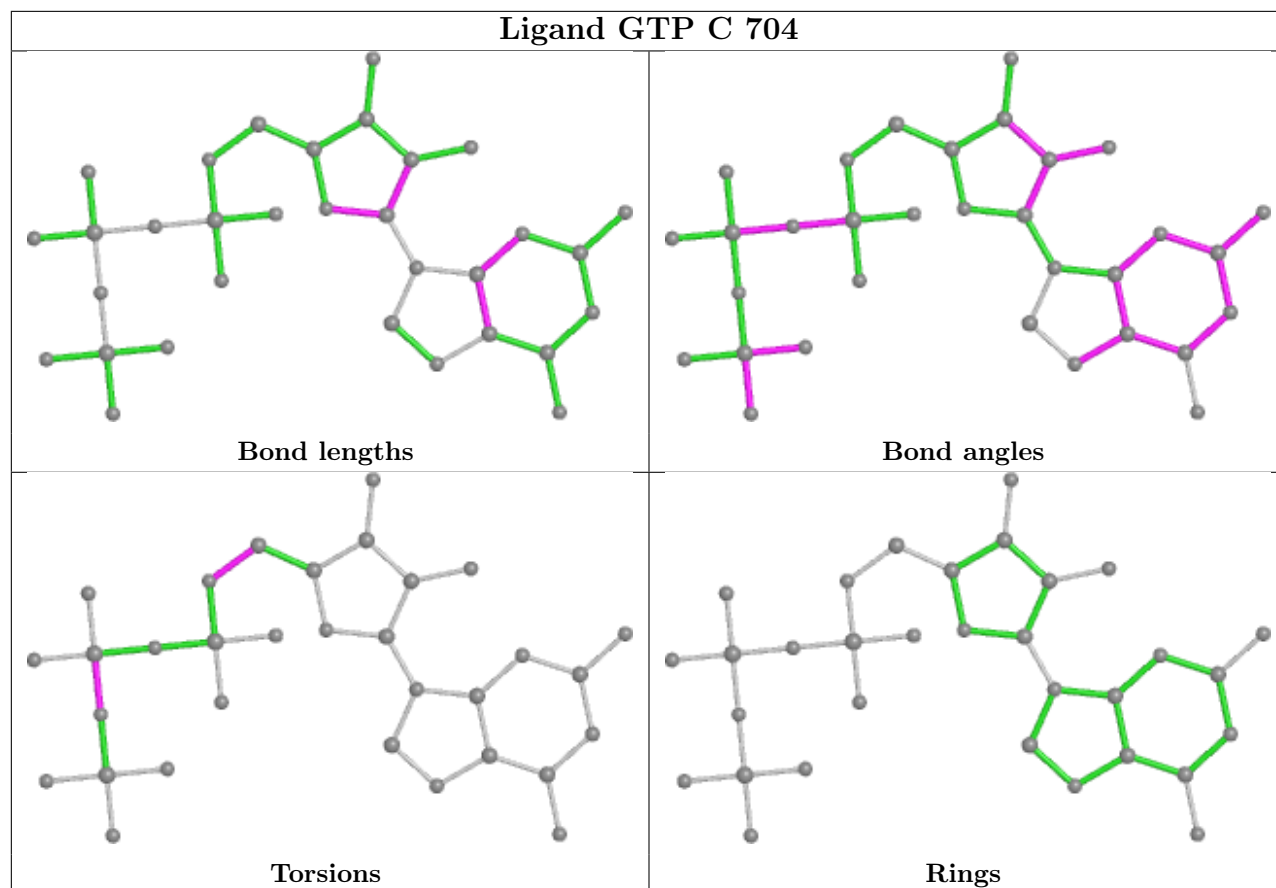
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	DCP	1	0
3	C	704	GTP	1	0
2	A	701	DCP	1	0

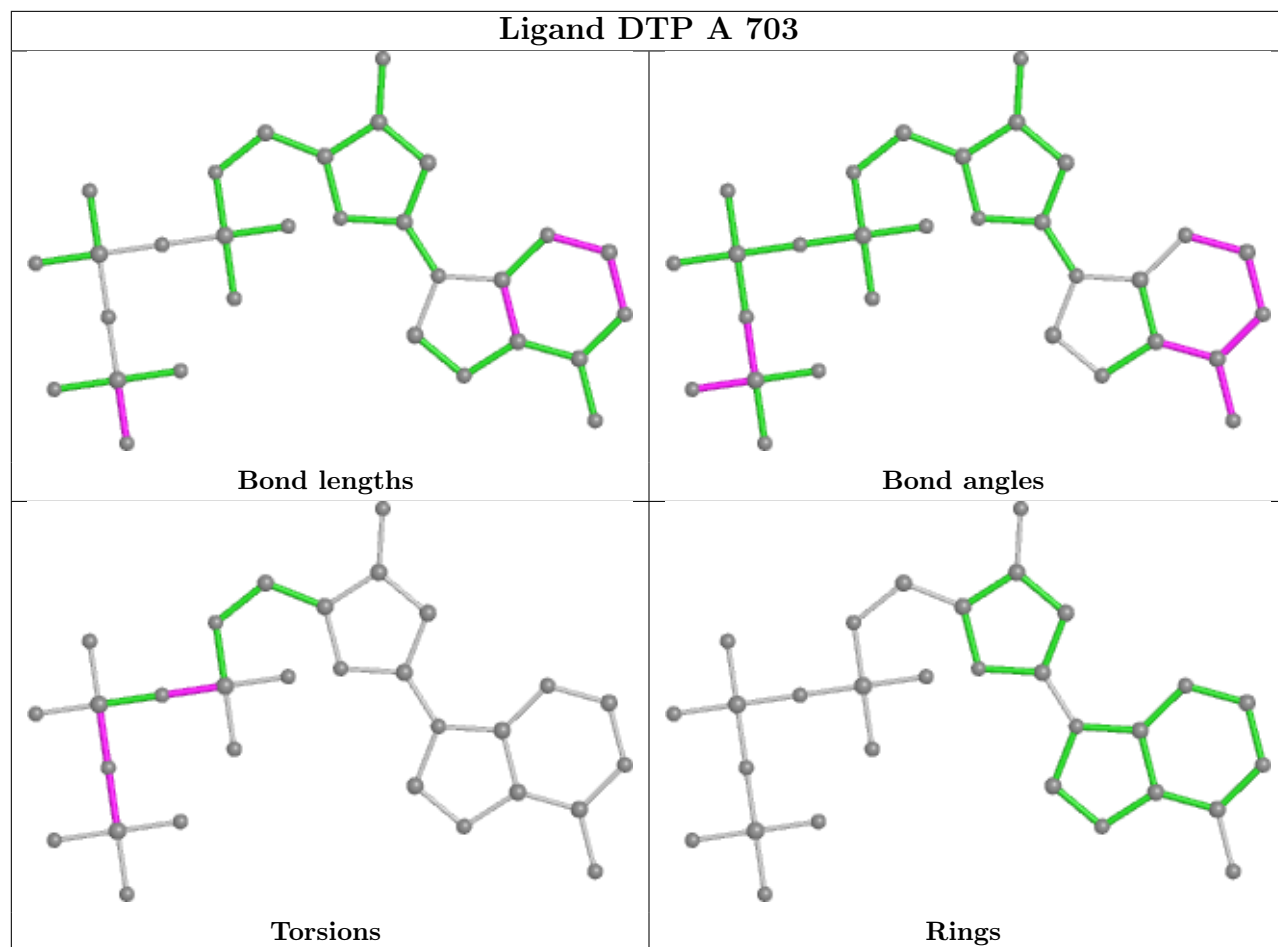
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



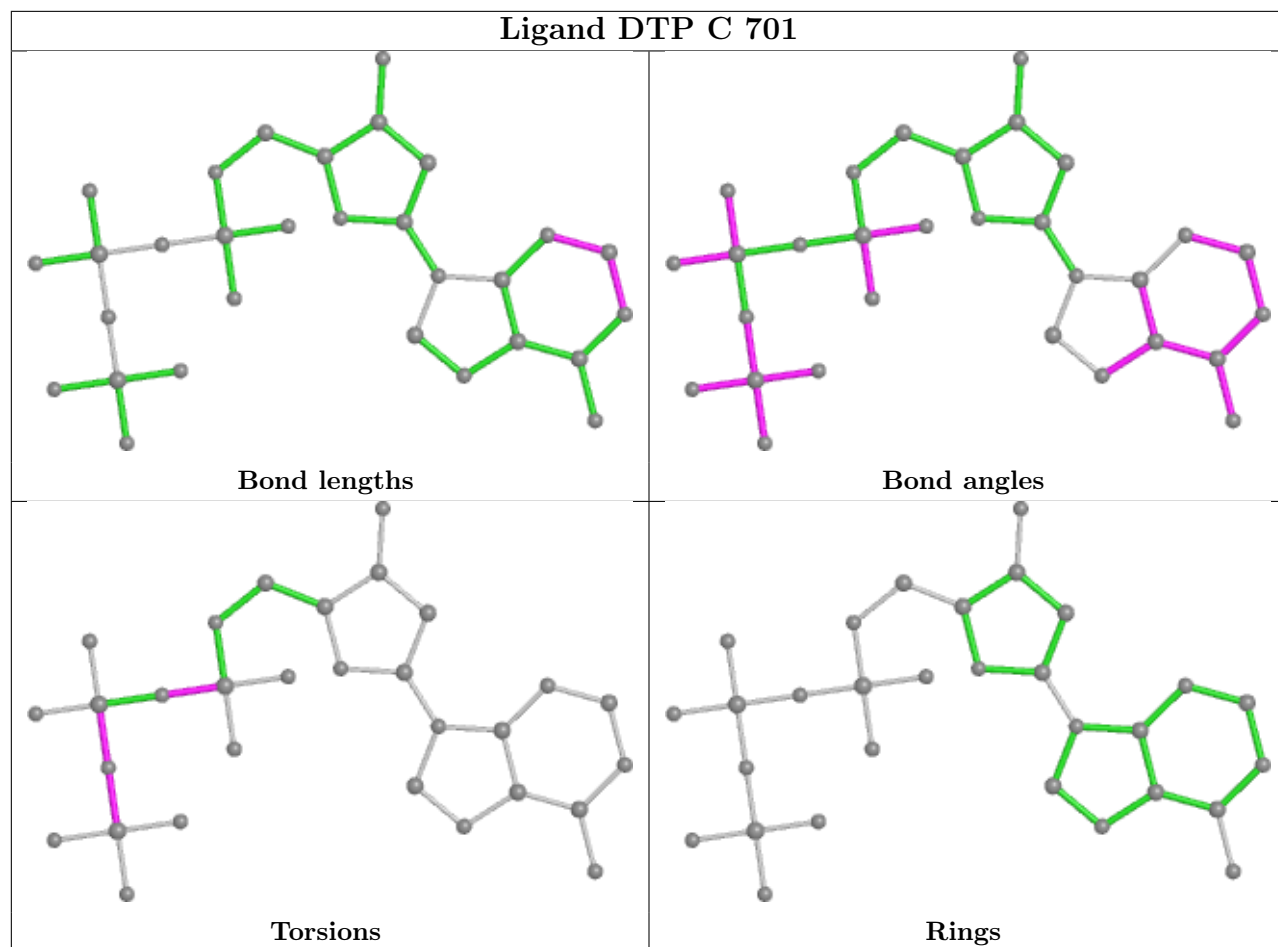




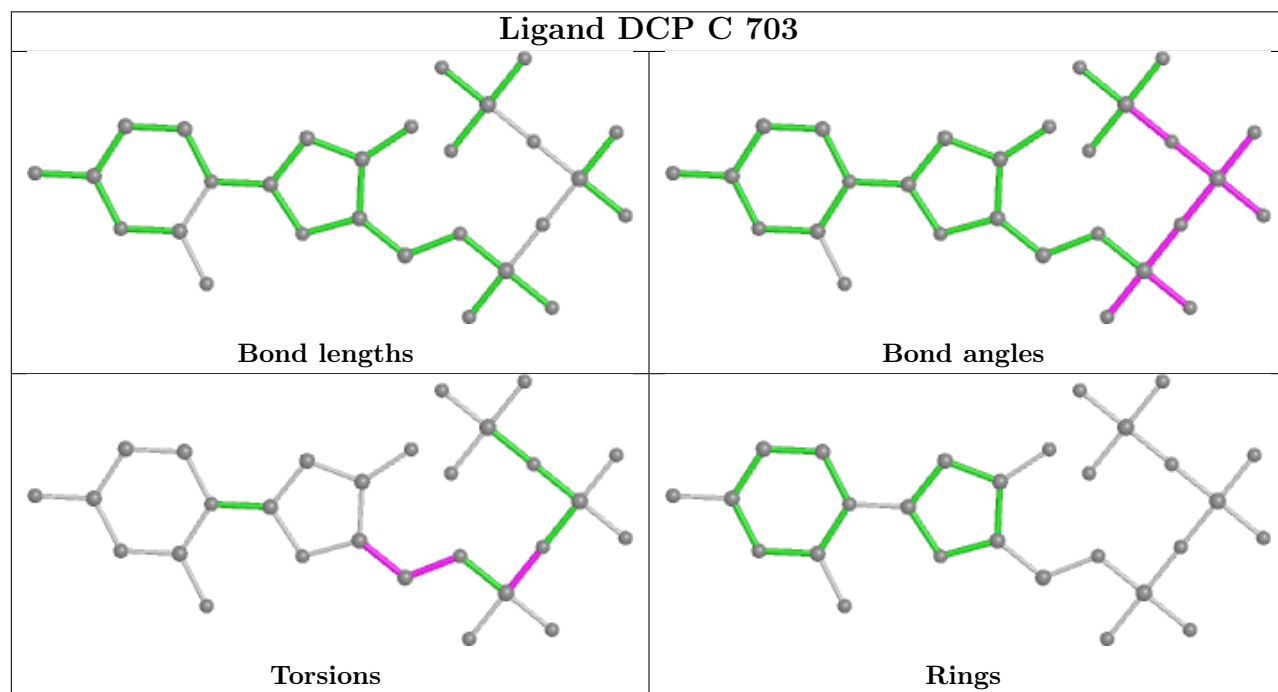


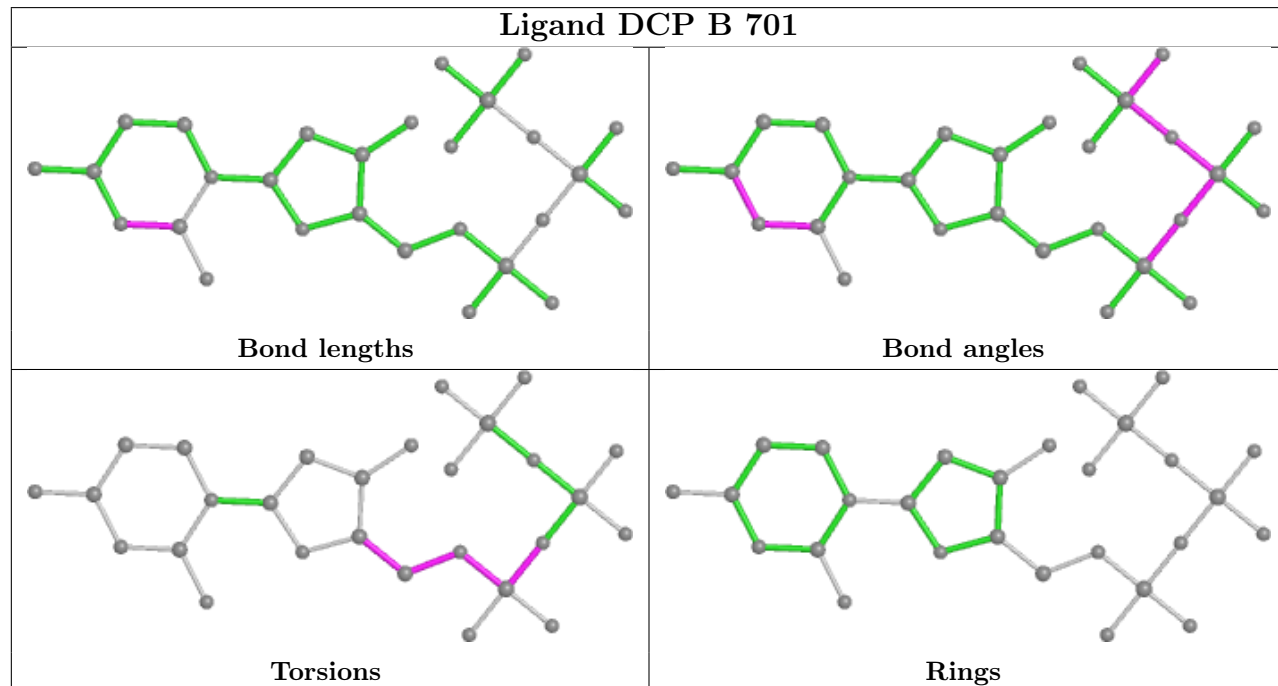
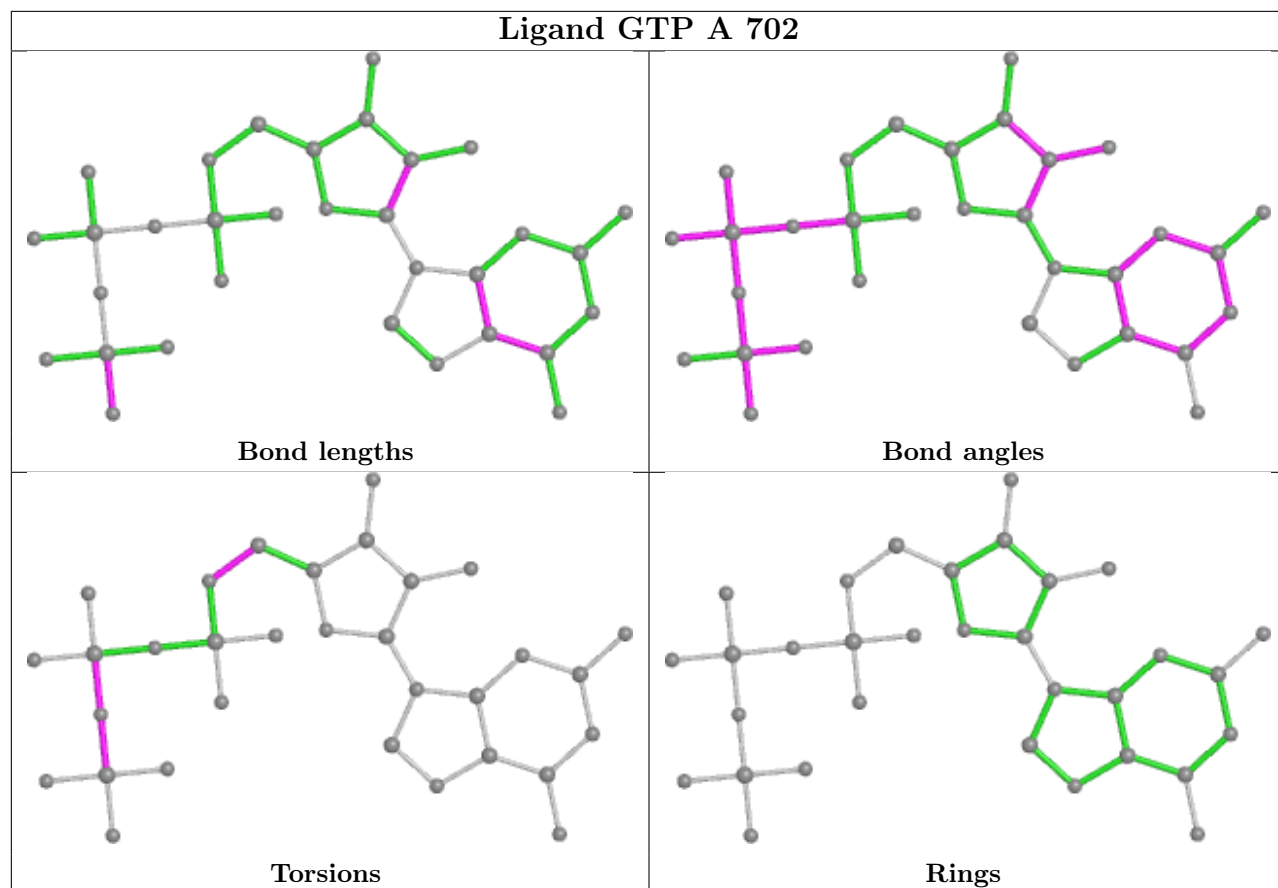


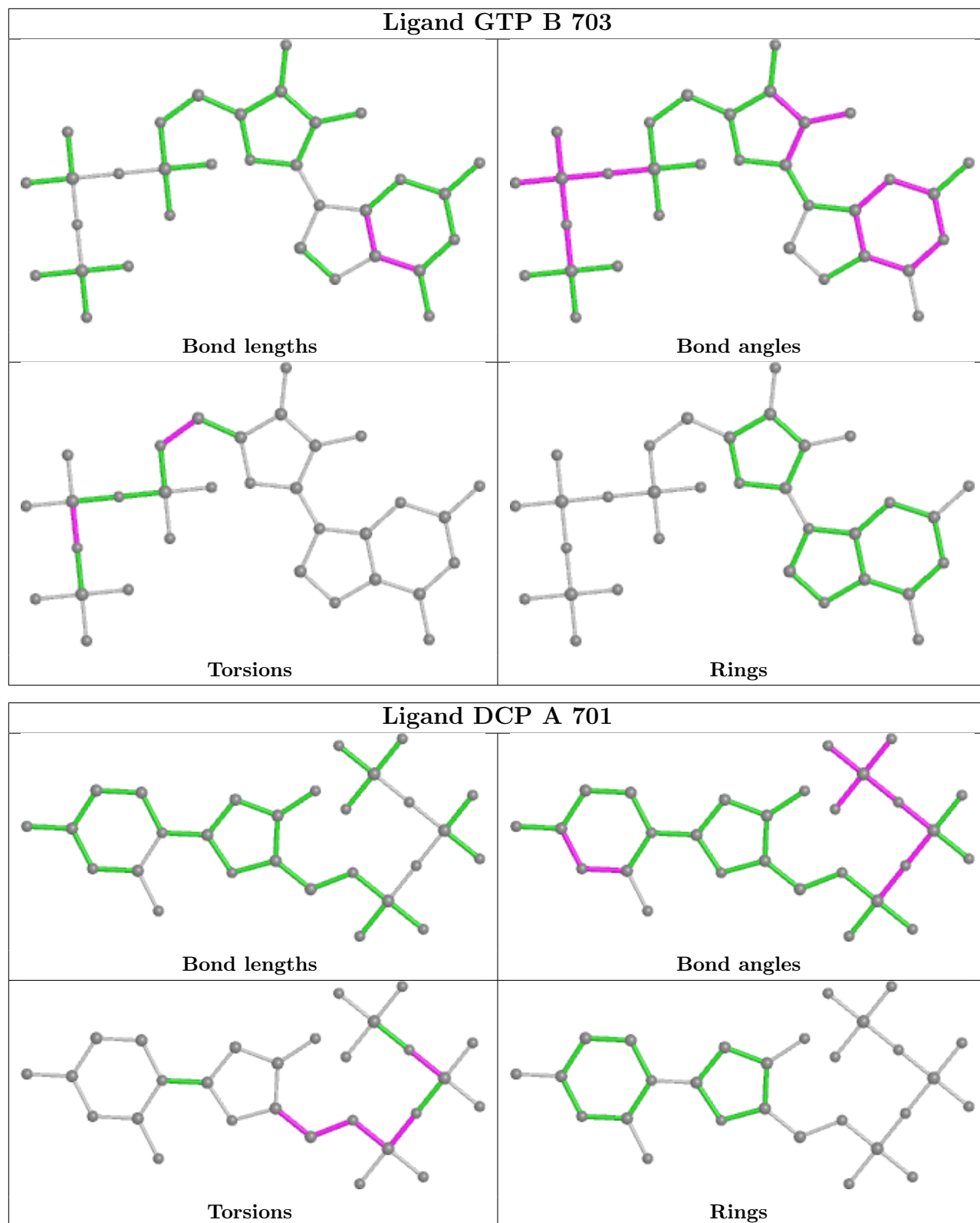
Ligand DTP C 701



Ligand DCP C 703







5.7 Other polymers ⓘ

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	479/514 (93%)	0.47	40 (8%) 11 15	33, 56, 90, 128	0
1	B	480/514 (93%)	0.28	20 (4%) 36 43	27, 48, 87, 108	0
1	C	481/514 (93%)	0.36	32 (6%) 17 23	29, 51, 95, 137	0
1	D	484/514 (94%)	0.67	53 (10%) 5 7	32, 58, 98, 168	0
All	All	1924/2056 (93%)	0.44	145 (7%) 14 19	27, 54, 91, 168	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	VAL	16.1
1	D	489	LEU	7.3
1	A	465	GLN	7.2
1	C	472	ASP	6.8
1	C	490	ASP	6.3
1	A	490	ASP	6.3
1	D	487	VAL	6.1
1	D	488	LEU	6.0
1	D	277	GLU	5.8
1	D	485	PRO	5.8
1	D	279	PRO	5.4
1	A	284	LEU	5.3
1	C	463	THR	5.2
1	A	488	LEU	5.0
1	A	326	GLN	5.0
1	D	486	LYS	4.9
1	C	486	LYS	4.9
1	B	490	ASP	4.8
1	A	327	ASN	4.8
1	A	262	GLU	4.8
1	C	489	LEU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	490	ASP	4.6
1	A	556	LYS	4.4
1	D	563	TYR	4.3
1	D	284	LEU	4.2
1	D	326	GLN	4.2
1	C	487	VAL	4.1
1	D	491	VAL	4.0
1	C	326	GLN	3.9
1	C	484	LYS	3.9
1	D	278	SER	3.8
1	D	255	GLU	3.8
1	B	327	ASN	3.7
1	C	344	ASP	3.7
1	C	491	VAL	3.7
1	C	488	LEU	3.6
1	C	485	PRO	3.5
1	C	473	TYR	3.5
1	D	325	ILE	3.4
1	C	328	ASN	3.4
1	D	590	LEU	3.4
1	D	562	LEU	3.3
1	A	230	LYS	3.3
1	D	496	GLU	3.3
1	A	489	LEU	3.2
1	D	569	PHE	3.2
1	B	262	GLU	3.2
1	D	263	GLU	3.2
1	C	528	ARG	3.2
1	D	285	TRP	3.1
1	A	596	LYS	3.1
1	B	473	TYR	3.0
1	A	590	LEU	3.0
1	D	597	GLU	3.0
1	B	466	ILE	3.0
1	A	235	GLN	3.0
1	B	114	THR	3.0
1	C	345	ASN	3.0
1	D	328	ASN	3.0
1	B	326	GLN	3.0
1	C	327	ASN	3.0
1	C	475	SER	2.9
1	B	230	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	345	ASN	2.9
1	D	592	THR	2.8
1	D	465	GLN	2.8
1	A	345	ASN	2.8
1	D	558	ASP	2.8
1	D	492	LYS	2.8
1	A	260	ILE	2.8
1	A	242	GLU	2.8
1	D	481	ALA	2.7
1	B	260	ILE	2.7
1	A	487	VAL	2.7
1	C	494	LYS	2.7
1	C	563	TYR	2.7
1	D	470	ARG	2.7
1	A	126	ILE	2.7
1	A	325	ILE	2.7
1	A	121	PRO	2.7
1	C	284	LEU	2.6
1	A	414	ASP	2.6
1	D	556	LYS	2.6
1	A	229	VAL	2.6
1	D	585	ASP	2.6
1	B	331	TYR	2.5
1	A	328	ASN	2.5
1	D	476	LEU	2.5
1	A	491	VAL	2.5
1	D	260	ILE	2.5
1	B	325	ILE	2.5
1	D	559	ARG	2.5
1	D	474	GLU	2.5
1	D	457	VAL	2.4
1	D	593	PRO	2.4
1	D	342	GLU	2.4
1	D	565	ALA	2.4
1	C	325	ILE	2.4
1	C	590	LEU	2.4
1	A	329	PHE	2.4
1	A	592	THR	2.4
1	B	594	GLN	2.4
1	C	464	GLY	2.3
1	A	322	HIS	2.3
1	C	589	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	288	LYS	2.3
1	D	230	LYS	2.3
1	D	327	ASN	2.3
1	C	562	LEU	2.3
1	C	511	GLU	2.3
1	C	492	LYS	2.2
1	B	121	PRO	2.2
1	B	329	PHE	2.2
1	C	465	GLN	2.2
1	B	122	ILE	2.2
1	A	259	LEU	2.2
1	C	493	LEU	2.2
1	A	585	ASP	2.2
1	D	371	ARG	2.2
1	D	587	ILE	2.2
1	A	324	GLY	2.2
1	A	494	LYS	2.1
1	A	331	TYR	2.1
1	A	122	ILE	2.1
1	B	242	GLU	2.1
1	B	316	PHE	2.1
1	C	495	ALA	2.1
1	A	486	LYS	2.1
1	D	256	GLN	2.1
1	A	239	MET	2.1
1	A	563	TYR	2.1
1	D	467	LYS	2.1
1	D	322	HIS	2.1
1	D	159	GLY	2.1
1	D	286	PRO	2.1
1	C	466	ILE	2.1
1	A	114	THR	2.1
1	B	320	CYS	2.1
1	A	227	PRO	2.1
1	A	485	PRO	2.1
1	D	584	GLY	2.0
1	B	414	ASP	2.0
1	B	590	LEU	2.0
1	A	419	TYR	2.0
1	D	599	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

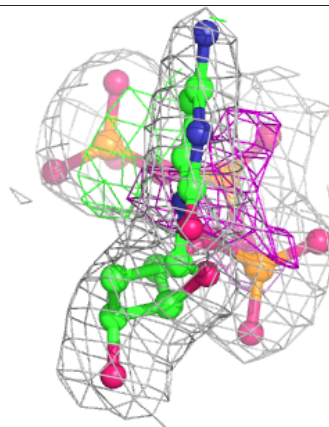
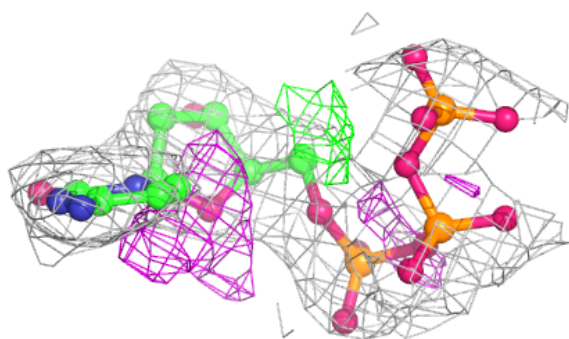
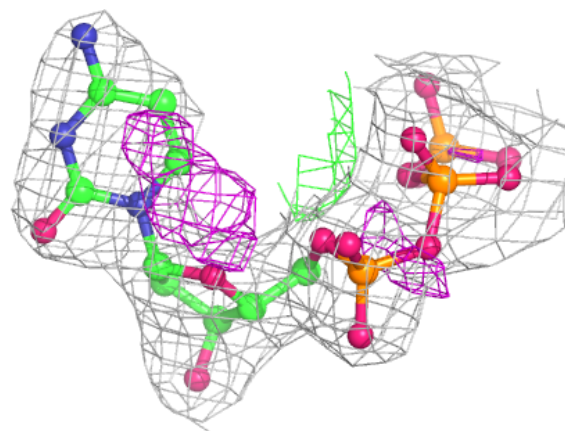
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DCP	A	701	28/28	0.90	0.13	48,61,84,86	0
5	MG	A	705	1/1	0.91	0.11	44,44,44,44	0
2	DCP	D	702	28/28	0.93	0.13	45,59,81,83	0
2	DCP	B	701	28/28	0.94	0.11	35,48,72,76	0
2	DCP	C	703	28/28	0.95	0.12	38,45,74,76	0
5	MG	A	704	1/1	0.96	0.12	32,32,32,32	0
5	MG	C	702	1/1	0.96	0.11	35,35,35,35	0
5	MG	D	701	1/1	0.96	0.11	38,38,38,38	0
4	DTP	B	702	30/30	0.98	0.15	28,33,50,56	0
4	DTP	D	703	30/30	0.98	0.16	32,38,54,56	0
3	GTP	A	702	32/32	0.98	0.11	34,37,41,42	0
3	GTP	B	703	32/32	0.98	0.13	28,33,38,41	0
3	GTP	D	704	32/32	0.98	0.12	32,37,46,49	0
4	DTP	A	703	30/30	0.98	0.15	26,30,52,54	0
4	DTP	C	701	30/30	0.99	0.16	32,38,52,56	0
3	GTP	C	704	32/32	0.99	0.12	22,30,37,39	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.

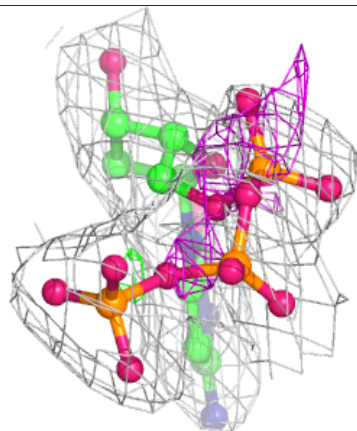
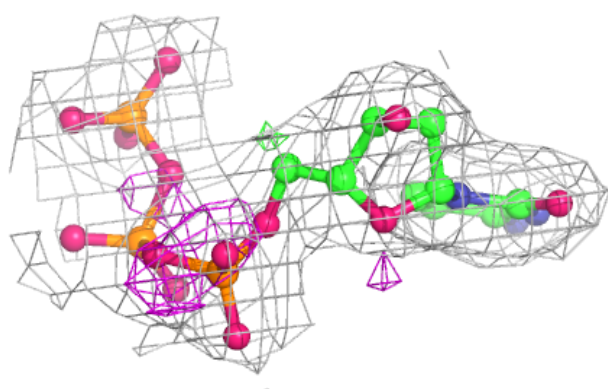
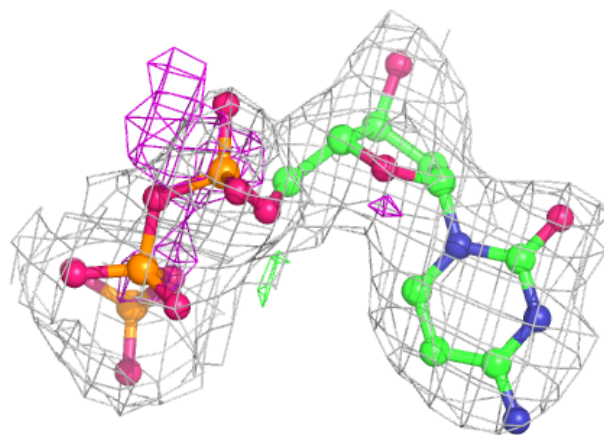
Electron density around DCP A 701:

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



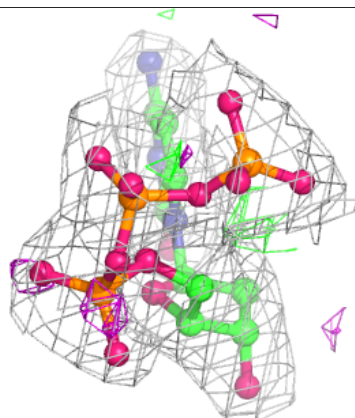
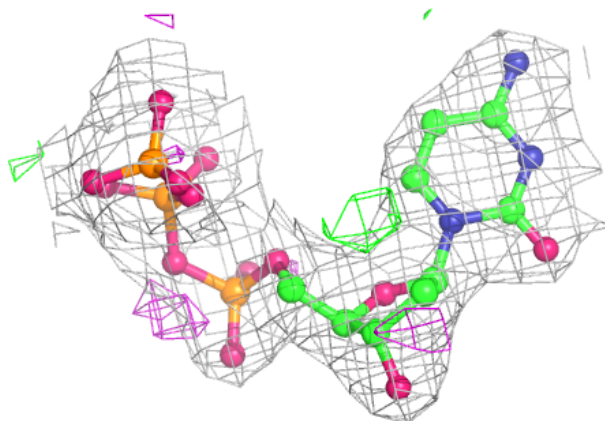
Electron density around DCP D 702:

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



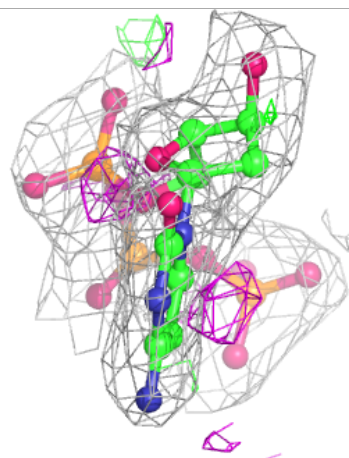
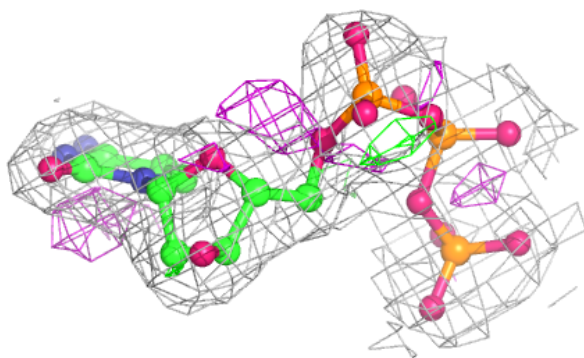
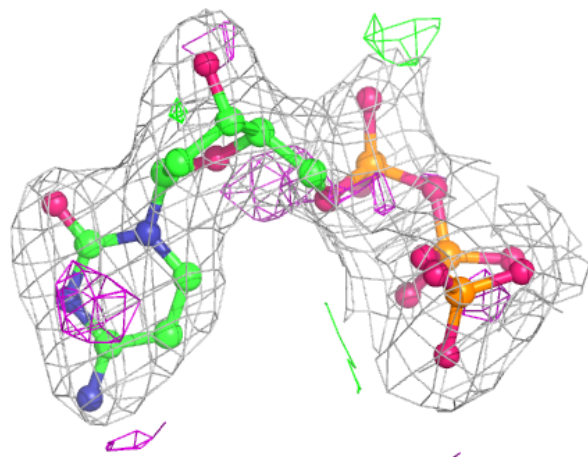
Electron density around DCP B 701:

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



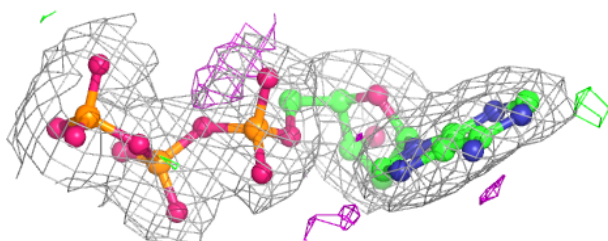
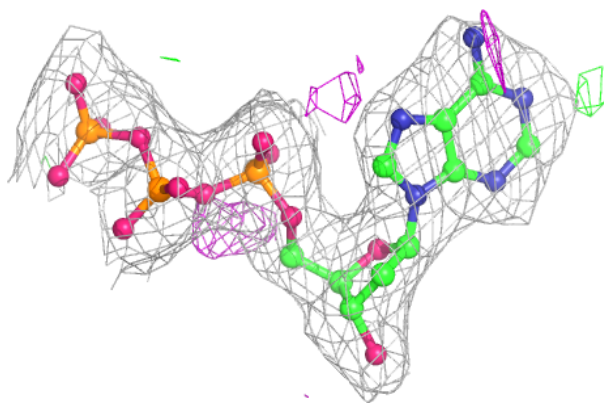
Electron density around DCP C 703:

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

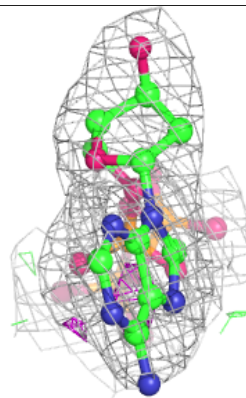
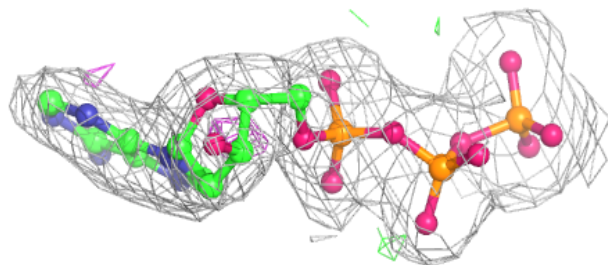
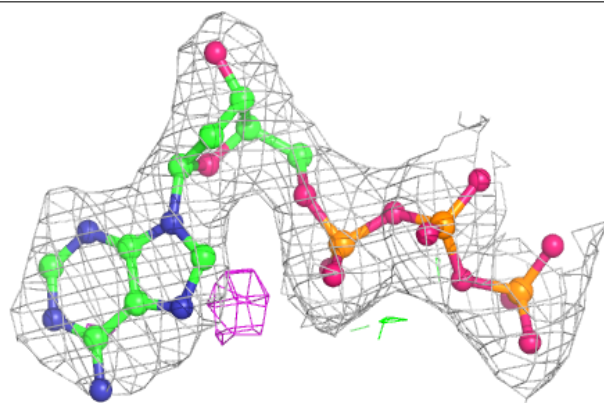


Electron density around DTP B 702:

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

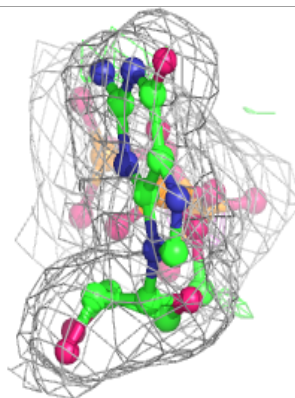
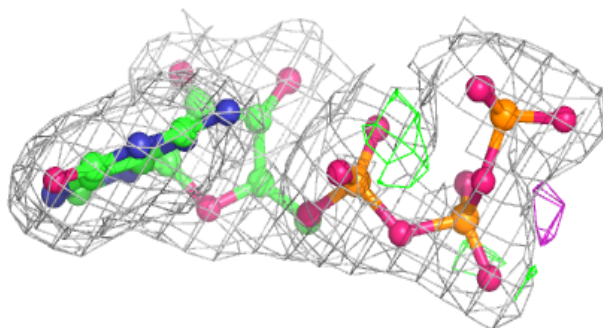
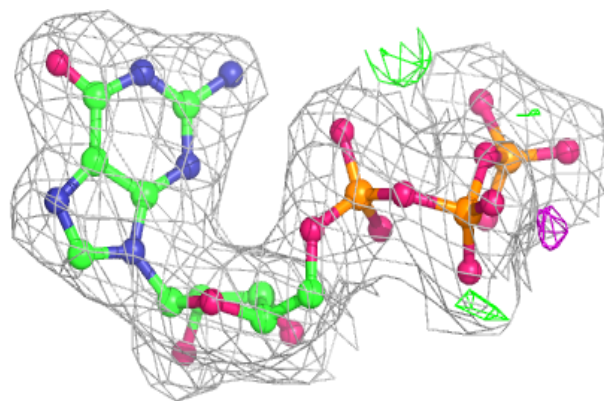
**Electron density around DTP D 703:**

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

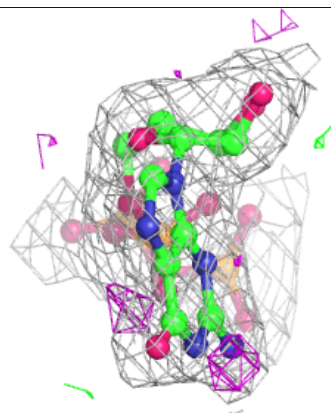
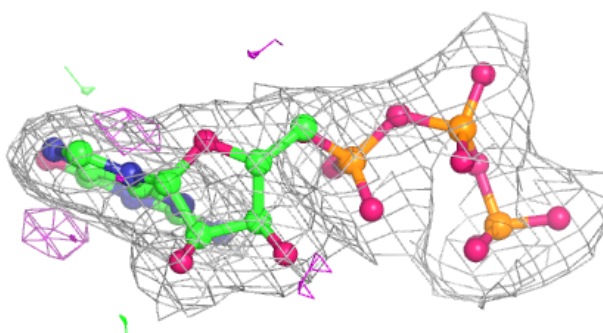
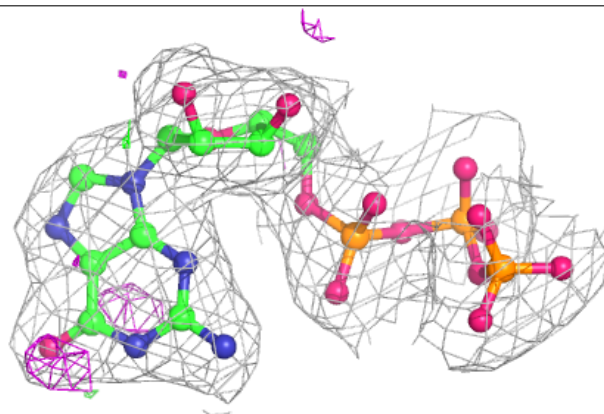


Electron density around GTP A 702:

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

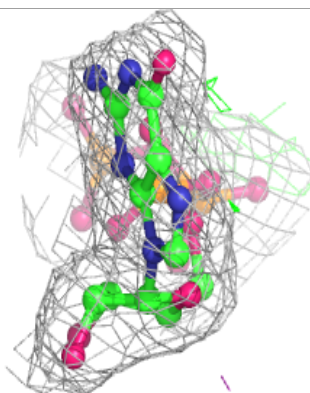
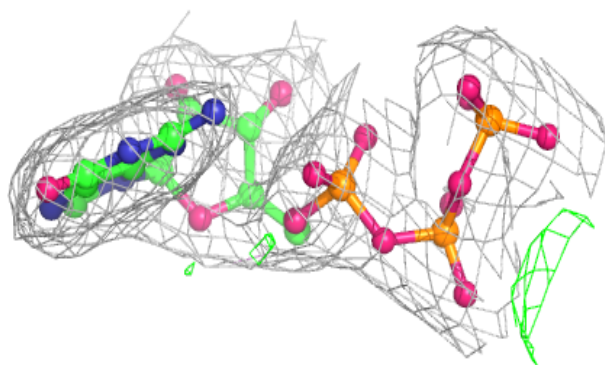
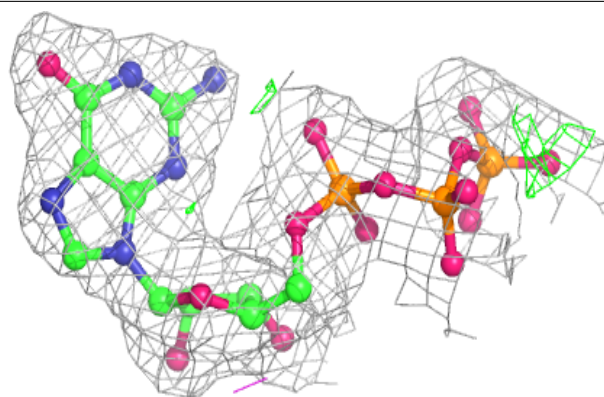
**Electron density around GTP B 703:**

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

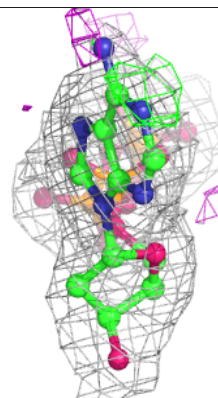
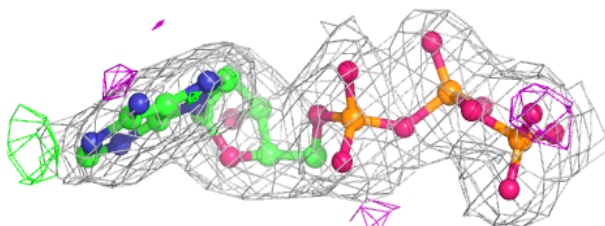
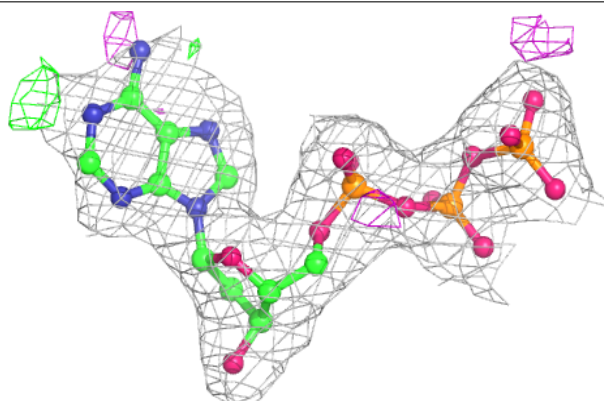


Electron density around GTP D 704:

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

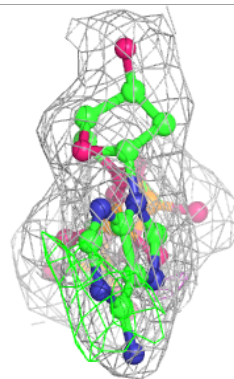
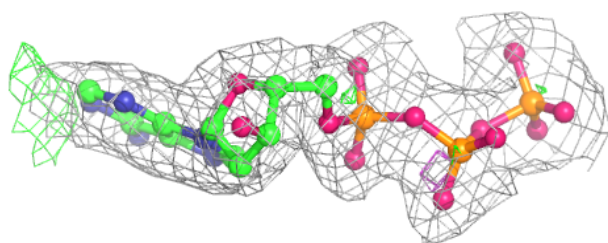
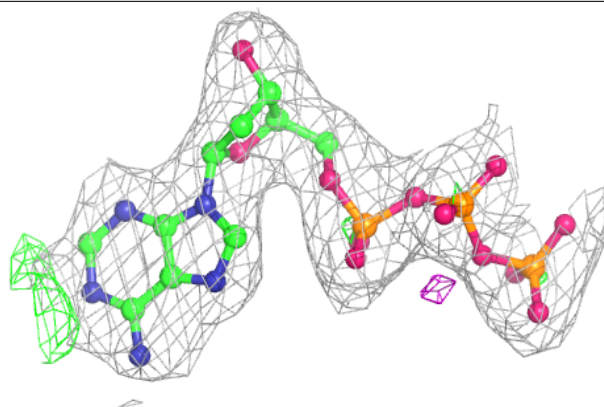
**Electron density around DTP A 703:**

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

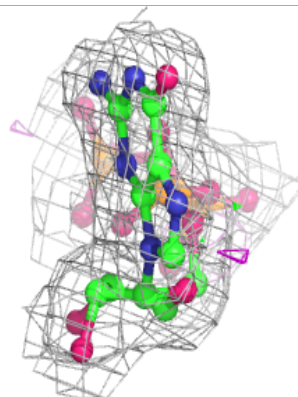
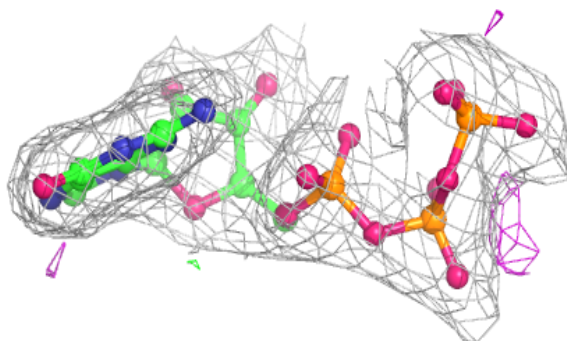
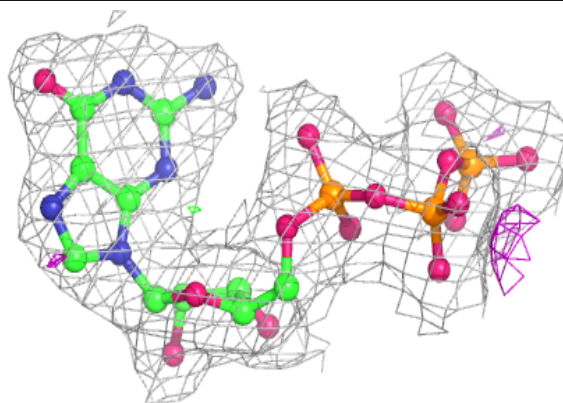


Electron density around DTP C 701:

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

**Electron density around GTP C 704:**

$2mF_o - DF_c$ (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.