



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 06:37 PM EDT

PDB ID : 4TO1
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP/dCTP-dCTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.55 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

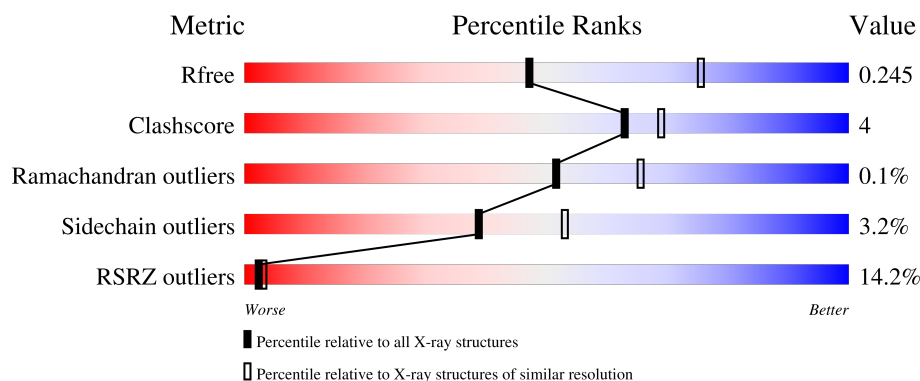
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	
1	B	514	
1	C	514	
1	D	514	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16149 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.

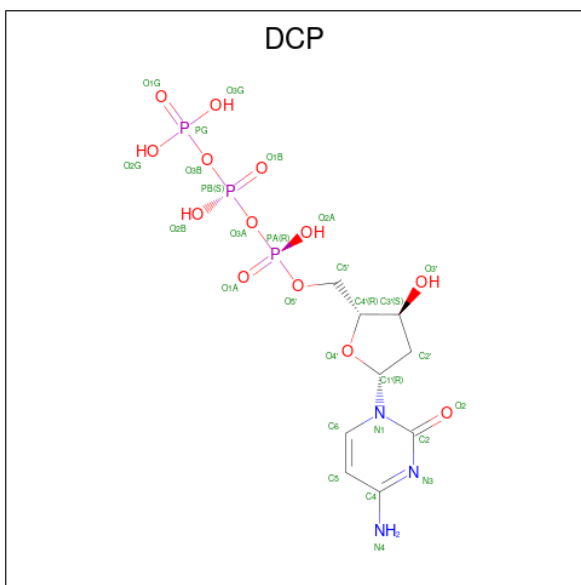
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

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	1	0
			3961	2535	689	716	21			

There are 8 discrepancies between the modelled and reference sequences:

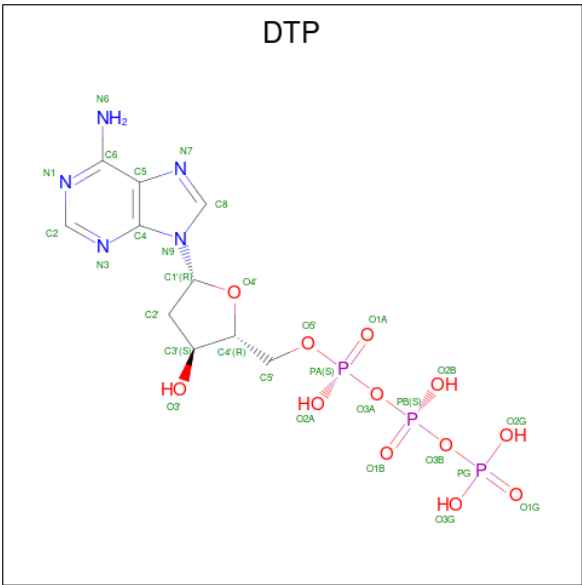
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	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	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
2	D	1	Total 28	C 9	N 3	O 13	P 3	0	0

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3$).

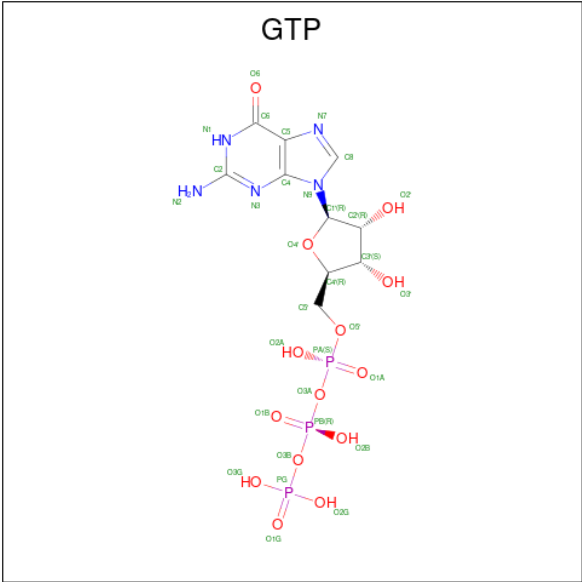


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

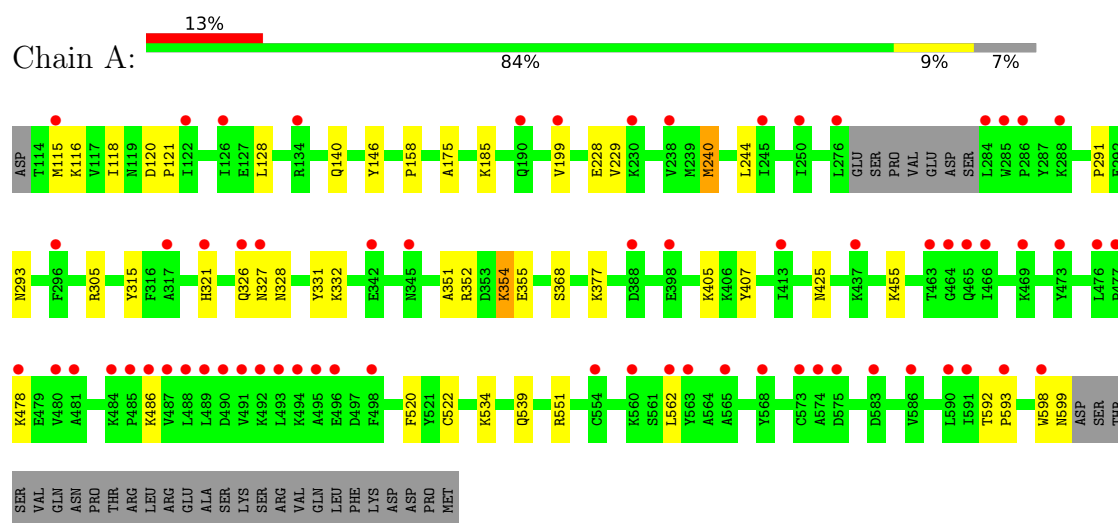
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	6	Total	O	0	0
			6	6		
6	C	22	Total	O	0	0
			22	22		
6	D	3	Total	O	0	0
			3	3		

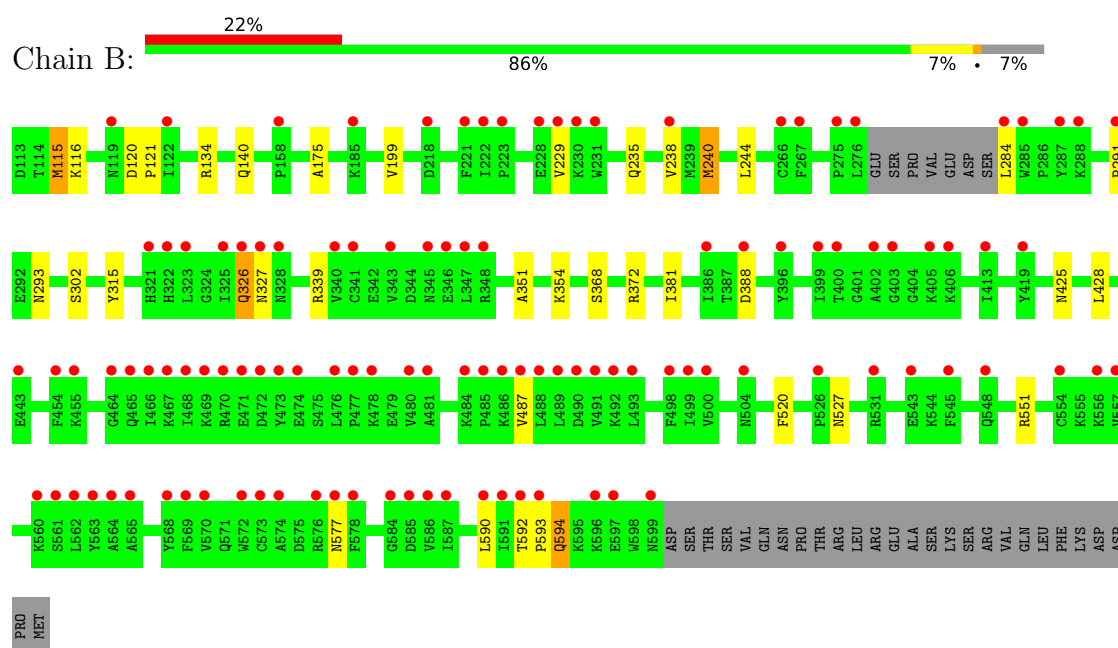
3 Residue-property plots

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

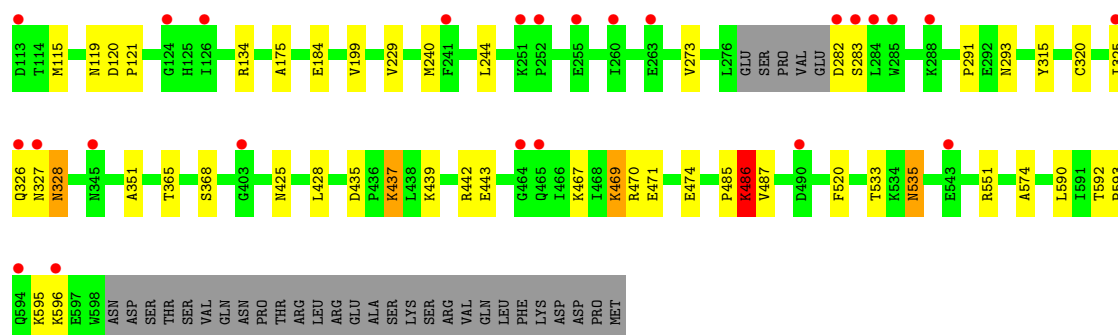


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1




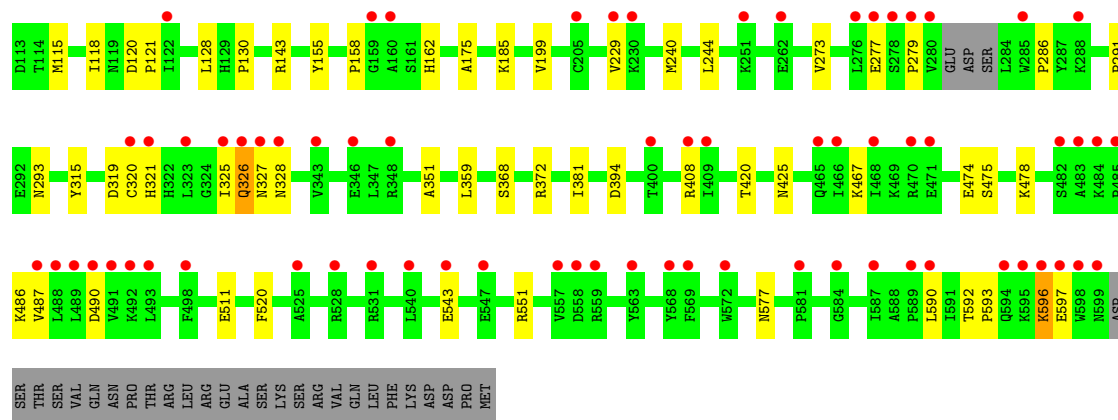
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:  5% 84% 9% 6%



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:  13% 83% 11% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.20Å 141.59Å 98.19Å 90.00° 115.79° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 48.75 – 2.54	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.55) 95.1 (48.75-2.54)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.221 , 0.235 0.233 , 0.245	Depositor DCC
R_{free} test set	3179 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.877	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16149	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: DCP, DTP, MG, 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	0.54	0/4014	0.72	3/5418 (0.1%)
1	B	0.52	0/4016	0.70	2/5421 (0.0%)
1	C	0.63	0/4036	0.74	2/5448 (0.0%)
1	D	0.55	0/4054	0.71	3/5473 (0.1%)
All	All	0.56	0/16120	0.72	10/21760 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	551	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	B	134	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	551	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	C	551	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	305	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	551	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	305	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	C	442	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	115[A]	MET	CG-SD-CE	5.01	108.22	100.20
1	D	115[B]	MET	CG-SD-CE	5.01	108.22	100.20

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	39	0
1	B	3924	0	3915	37	0
1	C	3944	0	3927	47	0
1	D	3961	0	3950	31	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
2	C	56	0	24	1	0
2	D	56	0	24	1	0
3	A	30	0	12	0	0
3	B	30	0	12	1	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	C	64	0	24	0	0
5	D	64	0	24	0	0
6	A	7	0	0	4	0
6	B	6	0	0	1	0
6	C	22	0	0	1	0
6	D	3	0	0	1	0
All	All	16149	0	15851	137	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 4.

All (137) 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	1.26
2:B:701:DCP:N3	6:B:801:HOH:O	1.91	1.01
1:B:115:MET:HE2	1:B:116:LYS:N	1.75	1.00
1:C:328:ASN:ND2	1:C:365:THR:OG1	1.96	0.99
1:B:115:MET:HE2	1:B:116:LYS:CA	1.94	0.96
1:C:439:LYS:O	1:C:443:GLU:HG3	1.63	0.96
1:C:435:ASP:OD1	1:C:437:LYS:HG2	1.69	0.93
1:B:115:MET:HE2	1:B:115:MET:C	1.90	0.92
1:C:533:THR:OG1	1:C:535[A]:ASN:ND2	2.03	0.92
1:B:115:MET:HE1	1:B:116:LYS:O	1.70	0.90
1:B:115:MET:CE	1:B:116:LYS:N	2.35	0.88
1:B:115:MET:CE	1:B:116:LYS:C	2.41	0.88
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:H	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:C	1:B:115:MET:CE	2.44	0.85
1:C:435:ASP:CG	1:C:437:LYS:HG3	1.98	0.83
1:B:115:MET:CE	1:B:116:LYS:O	2.28	0.82
1:C:467:LYS:CE	1:C:469:LYS:HE3	2.12	0.80
1:B:115:MET:HE2	1:B:116:LYS:C	1.99	0.79
1:C:485:PRO:O	1:C:486:LYS:HB2	1.81	0.79
1:C:435:ASP:CG	1:C:437:LYS:CG	2.52	0.78
1:A:326:GLN:NE2	1:C:326:GLN:HE21	1.81	0.77
1:C:435:ASP:OD2	1:C:437:LYS:HD2	1.85	0.76
1:A:326:GLN:NE2	1:C:326:GLN:NE2	2.33	0.75
1:C:435:ASP:OD1	1:C:437:LYS:CG	2.33	0.75
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:N	1.86	0.73
1:A:326:GLN:HE22	1:C:326:GLN:NE2	1.86	0.72
1:A:326:GLN:HE22	1:C:326:GLN:HE21	1.37	0.72
1:C:467:LYS:HE2	1:C:469:LYS:HE3	1.70	0.72
1:A:327:ASN:O	1:C:326:GLN:HB2	1.92	0.70
1:A:140:GLN:HG3	1:A:240:MET:CE	2.21	0.70
1:B:594:GLN:N	1:B:594:GLN:OE1	2.25	0.70
1:B:372:ARG:HH22	1:D:328:ASN:HD21	1.39	0.69
1:B:115:MET:HE1	1:B:116:LYS:C	2.09	0.68
1:D:596:LYS:HE2	1:D:597:GLU:OE1	1.93	0.68
1:B:140:GLN:HG3	1:B:240:MET:CE	2.25	0.67
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.30	0.64
1:C:470:ARG:HB2	1:C:470:ARG:CZ	2.27	0.64
1:B:327:ASN:O	1:D:326:GLN:HB2	1.96	0.64
1:B:326:GLN:HB2	1:D:327:ASN:O	2.01	0.61
1:A:331:TYR:OH	6:A:801:HOH:O	2.13	0.60
1:B:339:ARG:HH11	1:B:527:ASN:HD21	1.47	0.60
1:A:425:ASN:OD1	1:D:425:ASN:ND2	2.34	0.60
1:C:435:ASP:OD2	1:C:437:LYS:CD	2.49	0.59
1:C:435:ASP:OD2	1:C:437:LYS:CG	2.51	0.58
1:A:405:LYS:HD3	1:A:407:TYR:OH	2.04	0.58
1:A:146:TYR:HH	1:D:155:TYR:HH	1.53	0.56
1:B:115:MET:HE3	1:B:116:LYS:N	2.19	0.56
1:A:140:GLN:CG	1:A:240:MET:CE	2.84	0.56
1:B:487:VAL:HG23	1:B:590:LEU:HD12	1.89	0.55
1:D:487:VAL:HG23	1:D:590:LEU:HD12	1.89	0.54
1:A:326:GLN:HE21	1:A:327:ASN:H	1.55	0.54
1:C:487:VAL:HG23	1:C:590:LEU:HD12	1.89	0.54
1:A:326:GLN:HE21	1:A:327:ASN:N	2.05	0.53
1:B:339:ARG:HH11	1:B:527:ASN:ND2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:PRO:O	1:C:486:LYS:CB	2.51	0.53
1:C:535[A]:ASN:ND2	1:C:535[A]:ASN:H	2.01	0.53
1:D:162:HIS:HE1	1:D:319:ASP:OD1	1.91	0.53
1:A:140:GLN:CG	1:A:240:MET:HE3	2.39	0.52
1:B:140:GLN:CG	1:B:240:MET:CE	2.87	0.52
1:A:331:TYR:C	1:A:331:TYR:CD1	2.83	0.52
1:C:535[A]:ASN:ND2	1:C:535[A]:ASN:N	2.56	0.52
1:A:228:GLU:OE1	1:A:228:GLU:N	2.41	0.51
1:A:355:GLU:OE1	6:A:806:HOH:O	2.19	0.51
1:C:469:LYS:HB3	1:C:471:GLU:OE1	2.11	0.51
1:C:435:ASP:OD2	1:C:437:LYS:HG3	2.10	0.51
1:A:377:LYS:HE2	6:D:801:HOH:O	2.10	0.51
1:B:235:GLN:O	1:B:238:VAL:HG22	2.11	0.50
1:A:116:LYS:NZ	6:A:805:HOH:O	2.44	0.50
1:B:140:GLN:CG	1:B:240:MET:HE3	2.42	0.49
1:C:467:LYS:HE3	1:C:469:LYS:HE3	1.93	0.49
1:A:352:ARG:CZ	1:A:354:LYS:HD3	2.43	0.49
1:C:574:ALA:C	1:C:595:LYS:NZ	2.56	0.49
1:D:394:ASP:O	1:D:408:ARG:HD2	2.14	0.48
1:C:467:LYS:CE	1:C:469:LYS:CE	2.90	0.47
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.15	0.47
1:D:474:GLU:O	1:D:478:LYS:NZ	2.37	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:C:592:THR:N	1:C:593:PRO:CD	2.78	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.47
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.03	0.46
1:A:405:LYS:HD3	1:A:407:TYR:CZ	2.50	0.46
1:A:522:CYS:HB3	6:A:804:HOH:O	2.16	0.46
1:C:467:LYS:HE3	1:C:469:LYS:CE	2.46	0.46
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:D:475:SER:HA	1:D:478:LYS:HE2	1.98	0.45
1:B:326:GLN:O	1:D:328:ASN:ND2	2.49	0.45
1:A:592:THR:N	1:A:593:PRO:CD	2.79	0.45
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.90	0.45
1:B:592:THR:N	1:B:593:PRO:CD	2.79	0.45
1:D:279:PRO:HG3	1:D:286:PRO:HB3	1.99	0.45
1:A:293:ASN:OD1	1:A:293:ASN:N	2.47	0.44
1:D:118:ILE:HD12	1:D:128:LEU:HD11	1.98	0.44
1:A:118:ILE:HD12	1:A:128:LEU:HD11	2.00	0.44
1:B:115:MET:HE3	1:B:115:MET:HB2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ILE:HD13	1:D:118:ILE:HG21	1.79	0.44
1:D:511:GLU:H	1:D:511:GLU:CD	2.22	0.44
1:A:328:ASN:ND2	1:C:326:GLN:O	2.51	0.44
1:B:327:ASN:O	1:D:326:GLN:CB	2.63	0.44
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.00	0.44
1:D:120:ASP:OD2	1:D:121:PRO:HD2	2.17	0.44
1:A:598:TRP:O	1:A:599:ASN:HB2	2.18	0.43
1:B:115:MET:C	1:B:115:MET:HE3	2.33	0.43
1:C:244:LEU:C	1:C:244:LEU:HD23	2.39	0.43
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.17	0.43
1:A:118:ILE:HG21	1:A:118:ILE:HD13	1.80	0.43
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.19	0.43
1:B:175:ALA:HB1	1:B:199:VAL:HG12	2.00	0.43
1:C:437:LYS:HB3	1:C:437:LYS:HE2	1.82	0.43
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.19	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.43
2:A:701:DCP:O2G	2:A:701:DCP:O2B	2.36	0.43
1:C:119:ASN:HB2	2:D:702:DCP:H1'	2.00	0.43
1:C:120:ASP:OD2	1:C:121:PRO:HD2	2.17	0.43
1:A:158:PRO:HG3	1:D:118:ILE:HG21	2.00	0.42
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.18	0.42
1:A:120:ASP:OD2	1:A:121:PRO:HD2	2.18	0.42
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.92	0.42
1:A:326:GLN:CG	1:C:327:ASN:O	2.68	0.42
1:A:455:LYS:CB	1:A:562:LEU:HD21	2.50	0.42
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.02	0.42
1:C:320:CYS:HB3	1:C:325:ILE:O	2.19	0.42
1:D:244:LEU:C	1:D:244:LEU:HD23	2.39	0.42
1:B:425:ASN:HB2	1:C:428:LEU:HD13	2.01	0.42
1:A:118:ILE:HG21	1:D:158:PRO:HG3	2.02	0.42
1:D:467:LYS:HD3	1:D:467:LYS:HA	1.91	0.41
1:A:244:LEU:C	1:A:244:LEU:HD23	2.40	0.41
1:B:244:LEU:C	1:B:244:LEU:HD23	2.41	0.41
2:C:705:DCP:H5'1	6:C:816:HOH:O	2.20	0.41
1:D:143:ARG:HD2	1:D:420:THR:HA	2.03	0.41
3:B:702:DTP:N6	1:D:372:ARG:HG2	2.36	0.41
1:D:320:CYS:HB3	1:D:325:ILE:O	2.21	0.41
1:B:115:MET:CE	1:B:116:LYS:CA	2.75	0.41
1:A:331:TYR:CD1	1:A:332:LYS:N	2.89	0.40
1:C:467:LYS:HG2	1:C:469:LYS:CD	2.52	0.40
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.02	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	476/514 (93%)	469 (98%)	7 (2%)	0	100	100
1	B	476/514 (93%)	465 (98%)	11 (2%)	0	100	100
1	C	479/514 (93%)	467 (98%)	11 (2%)	1 (0%)	47	60
1	D	481/514 (94%)	470 (98%)	11 (2%)	0	100	100
All	All	1912/2056 (93%)	1871 (98%)	40 (2%)	1 (0%)	51	65

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%)	415 (97%)	11 (3%)	46	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	426/459 (93%)	414 (97%)	12 (3%)	43	58
1	C	429/459 (94%)	410 (96%)	19 (4%)	28	38
1	D	431/459 (94%)	416 (96%)	15 (4%)	36	49
All	All	1712/1836 (93%)	1655 (97%)	57 (3%)	39	51

All (57) 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	A	539	GLN
1	B	115	MET
1	B	229	VAL
1	B	240	MET
1	B	284	LEU
1	B	302	SER
1	B	315	TYR
1	B	326	GLN
1	B	354	LYS
1	B	368	SER
1	B	388	ASP
1	B	577	ASN
1	B	594	GLN
1	C	115	MET
1	C	134	ARG
1	C	184	GLU
1	C	229	VAL
1	C	240	MET
1	C	273	VAL
1	C	282	ASP
1	C	283	SER
1	C	315	TYR
1	C	328	ASN

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Mol	Chain	Res	Type
1	C	368[A]	SER
1	C	368[B]	SER
1	C	437	LYS
1	C	469	LYS
1	C	474	GLU
1	C	486	LYS
1	C	535[A]	ASN
1	C	535[B]	ASN
1	C	596	LYS
1	D	130	PRO
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	326	GLN
1	D	359	LEU
1	D	368	SER
1	D	486	LYS
1	D	490	ASP
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 (17) 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	599	ASN
1	C	322	HIS
1	C	326	GLN
1	C	328	ASN
1	D	162	HIS
1	D	322	HIS
1	D	328	ASN
1	D	425	ASN

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Mol	Chain	Res	Type
1	D	535	ASN
1	D	594	GLN
1	D	599	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
5	GTP	C	704	4	26,34,34	0.98	2 (7%)	33,54,54	1.82	8 (24%)
3	DTP	A	702	4	26,32,32	1.46	7 (26%)	30,50,50	1.51	3 (10%)
2	DCP	C	701	4	23,29,29	1.06	1 (4%)	30,45,45	1.40	7 (23%)
2	DCP	D	702	4	23,29,29	0.86	0	30,45,45	1.55	4 (13%)
5	GTP	D	704	4	26,34,34	1.21	2 (7%)	33,54,54	2.01	10 (30%)
5	GTP	D	701	4	26,34,34	1.20	3 (11%)	33,54,54	1.92	12 (36%)
5	GTP	C	706	4	26,34,34	1.25	3 (11%)	33,54,54	1.99	11 (33%)
3	DTP	B	702	4	26,32,32	1.20	2 (7%)	30,50,50	1.42	4 (13%)
2	DCP	A	701	-	23,29,29	0.72	0	30,45,45	1.53	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DCP	B	701	-	23,29,29	0.61	0	30,45,45	1.50	5 (16%)
2	DCP	D	703	-	23,29,29	0.75	0	30,45,45	1.44	4 (13%)
2	DCP	C	705	-	23,29,29	0.79	0	30,45,45	1.61	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
5	GTP	C	704	4	-	2/18/38/38	0/3/3/3
3	DTP	A	702	4	-	5/18/34/34	0/3/3/3
2	DCP	C	701	4	-	2/19/34/34	0/2/2/2
2	DCP	D	702	4	-	5/19/34/34	0/2/2/2
5	GTP	D	704	4	-	3/18/38/38	0/3/3/3
5	GTP	D	701	4	-	4/18/38/38	0/3/3/3
5	GTP	C	706	4	-	2/18/38/38	0/3/3/3
3	DTP	B	702	4	-	3/18/34/34	0/3/3/3
2	DCP	A	701	-	-	8/19/34/34	0/2/2/2
2	DCP	B	701	-	-	7/19/34/34	0/2/2/2
2	DCP	D	703	-	-	5/19/34/34	0/2/2/2
2	DCP	C	705	-	-	3/19/34/34	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	704	GTP	C5-C6	3.99	1.48	1.41
5	D	701	GTP	O4'-C1'	3.54	1.46	1.41
5	C	704	GTP	C5-C6	3.29	1.47	1.41
3	A	702	DTP	C2-N3	3.24	1.37	1.32
3	A	702	DTP	C5-C4	2.99	1.48	1.40
5	C	706	GTP	O4'-C1'	2.87	1.45	1.41
3	B	702	DTP	C5-C4	2.85	1.48	1.40
3	B	702	DTP	C2-N3	2.84	1.36	1.32
5	D	701	GTP	C5-C6	2.68	1.46	1.41
5	D	704	GTP	C5-C4	2.63	1.47	1.40
3	A	702	DTP	C2-N1	2.56	1.38	1.33
5	C	706	GTP	C5-C6	2.47	1.45	1.41
5	C	706	GTP	C5-C4	2.34	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	701	GTP	C5-C4	2.34	1.47	1.40
2	C	701	DCP	O4'-C4'	-2.26	1.39	1.45
3	A	702	DTP	C4-N3	-2.22	1.32	1.35
5	C	704	GTP	C5-C4	2.19	1.46	1.40
3	A	702	DTP	C5-N7	-2.11	1.32	1.39
3	A	702	DTP	C8-N7	2.03	1.38	1.34
3	A	702	DTP	O4'-C4'	-2.01	1.40	1.45

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	GTP	C5-C6-N1	-4.83	116.82	123.43
3	A	702	DTP	N6-C6-N1	4.72	128.37	118.57
2	A	701	DCP	C4-N3-C2	4.61	121.01	116.34
5	D	704	GTP	C5-C6-N1	-4.56	117.19	123.43
2	C	705	DCP	C4-N3-C2	4.44	120.84	116.34
5	C	704	GTP	C4-C5-C6	-4.33	116.66	120.80
5	D	704	GTP	C2-N1-C6	4.33	122.80	115.93
5	D	704	GTP	C4-C5-C6	-4.30	116.69	120.80
5	C	706	GTP	C2-N1-C6	4.20	122.60	115.93
2	B	701	DCP	C4-N3-C2	4.11	120.51	116.34
5	D	704	GTP	C2-N3-C4	4.02	119.95	115.36
2	D	702	DCP	C4-N3-C2	3.93	120.32	116.34
2	A	701	DCP	PB-O3B-PG	-3.82	119.71	132.83
2	B	701	DCP	PB-O3B-PG	-3.79	119.83	132.83
5	C	704	GTP	C2-N1-C6	3.76	121.90	115.93
5	D	704	GTP	C3'-C2'-C1'	3.74	106.61	100.98
3	B	702	DTP	N3-C2-N1	-3.67	122.94	128.68
5	C	704	GTP	C2-N3-C4	3.66	119.54	115.36
5	D	701	GTP	C5-C6-N1	-3.65	118.44	123.43
5	D	701	GTP	C4-C5-C6	-3.64	117.32	120.80
2	C	705	DCP	N4-C4-N3	3.64	122.25	116.49
5	C	706	GTP	C3'-C2'-C1'	3.58	106.38	100.98
3	A	702	DTP	C5-C6-N6	-3.56	114.94	120.35
5	D	701	GTP	N2-C2-N1	3.51	122.72	117.25
2	D	703	DCP	C4-N3-C2	3.41	119.80	116.34
5	D	701	GTP	C2-N3-C4	3.36	119.20	115.36
5	C	704	GTP	C5-C6-N1	-3.35	118.85	123.43
2	D	703	DCP	PB-O3B-PG	-3.28	121.57	132.83
5	D	701	GTP	C2-N1-C6	3.20	121.01	115.93
2	D	702	DCP	PB-O3A-PA	-3.19	121.88	132.83
2	D	703	DCP	N4-C4-N3	3.16	121.48	116.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	DTP	N6-C6-N1	3.08	124.97	118.57
2	D	702	DCP	PB-O3B-PG	-3.01	122.48	132.83
5	D	701	GTP	PA-O3A-PB	-3.01	122.51	132.83
2	C	705	DCP	PB-O3A-PA	-2.96	122.66	132.83
2	C	701	DCP	N4-C4-N3	2.94	121.14	116.49
5	C	706	GTP	PA-O3A-PB	-2.93	122.77	132.83
5	C	706	GTP	C4-C5-C6	-2.92	118.01	120.80
5	C	706	GTP	C2-N3-C4	2.89	118.66	115.36
2	C	705	DCP	PB-O3B-PG	-2.86	123.01	132.83
5	C	704	GTP	N3-C2-N1	-2.84	123.43	127.22
5	D	704	GTP	N3-C2-N1	-2.83	123.44	127.22
2	D	703	DCP	PB-O3A-PA	-2.81	123.19	132.83
5	D	704	GTP	PA-O3A-PB	-2.80	123.22	132.83
5	D	701	GTP	N2-C2-N3	-2.77	113.28	117.79
5	C	704	GTP	C3'-C2'-C1'	2.77	105.14	100.98
5	C	706	GTP	N3-C2-N1	-2.76	123.54	127.22
5	C	706	GTP	C4-C5-N7	-2.75	106.54	109.40
2	C	705	DCP	C5-C4-N4	-2.72	116.42	121.14
2	C	701	DCP	C4-N3-C2	2.72	119.10	116.34
2	B	701	DCP	PB-O3A-PA	-2.71	123.53	132.83
2	B	701	DCP	O3G-PG-O2G	2.68	117.90	107.64
3	A	702	DTP	O3G-PG-O1G	2.63	120.96	110.68
2	C	701	DCP	PB-O3B-PG	-2.61	123.86	132.83
5	C	706	GTP	PB-O3B-PG	-2.56	124.03	132.83
5	C	704	GTP	PA-O3A-PB	-2.55	124.08	132.83
2	C	701	DCP	O3G-PG-O2G	2.53	117.31	107.64
5	D	701	GTP	O2B-PB-O1B	2.52	124.70	112.24
2	A	701	DCP	PB-O3A-PA	-2.50	124.24	132.83
2	D	702	DCP	O2A-PA-O1A	2.46	124.41	112.24
5	D	701	GTP	PB-O3B-PG	-2.46	124.40	132.83
5	D	701	GTP	C3'-C2'-C1'	2.44	104.65	100.98
2	C	701	DCP	PB-O3A-PA	-2.42	124.53	132.83
5	D	701	GTP	N3-C2-N1	-2.41	124.00	127.22
5	D	704	GTP	PB-O3B-PG	-2.31	124.88	132.83
5	C	704	GTP	C4-C5-N7	-2.29	107.02	109.40
2	C	701	DCP	C2'-C3'-C4'	2.28	107.51	102.76
2	C	701	DCP	C5-C4-N4	-2.28	117.18	121.14
3	B	702	DTP	PB-O3B-PG	-2.27	125.03	132.83
5	D	704	GTP	C4-C5-N7	-2.26	107.04	109.40
5	D	704	GTP	O2A-PA-O1A	2.19	123.05	112.24
5	D	701	GTP	O3G-PG-O2G	2.16	115.89	107.64
5	C	706	GTP	O4'-C1'-C2'	-2.14	103.80	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	GTP	O2A-PA-O1A	2.14	122.80	112.24
2	B	701	DCP	C2'-C1'-N1	-2.12	109.37	114.27
3	B	702	DTP	C5-C6-N6	-2.07	117.20	120.35
2	A	701	DCP	N4-C4-N3	2.02	119.69	116.49

There are no chirality outliers.

All (49) 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	C	701	DCP	O4'-C1'-N1-C6
2	D	702	DCP	O4'-C1'-N1-C6
2	D	702	DCP	PB-O3B-PG-O2G
2	D	702	DCP	PB-O3B-PG-O3G
2	D	703	DCP	C5'-O5'-PA-O2A
3	A	702	DTP	PB-O3B-PG-O3G
3	B	702	DTP	PB-O3B-PG-O2G
3	B	702	DTP	PB-O3B-PG-O3G
2	A	701	DCP	C3'-C4'-C5'-O5'
2	A	701	DCP	O4'-C4'-C5'-O5'
2	B	701	DCP	C3'-C4'-C5'-O5'
2	B	701	DCP	O4'-C4'-C5'-O5'
3	A	702	DTP	PB-O3B-PG-O1G
2	A	701	DCP	C4'-C5'-O5'-PA
2	C	705	DCP	C4'-C5'-O5'-PA
2	D	703	DCP	C4'-C5'-O5'-PA
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	705	DCP	PB-O3A-PA-O5'
2	D	703	DCP	PB-O3A-PA-O5'
5	D	701	GTP	PB-O3B-PG-O1G
2	A	701	DCP	C5'-O5'-PA-O3A
2	B	701	DCP	C5'-O5'-PA-O3A
2	D	703	DCP	C5'-O5'-PA-O3A
3	A	702	DTP	PG-O3B-PB-O1B
2	B	701	DCP	C5'-O5'-PA-O2A
2	D	702	DCP	PG-O3B-PB-O1B
3	A	702	DTP	PB-O3A-PA-O2A
3	B	702	DTP	PB-O3A-PA-O2A
5	C	706	GTP	PG-O3B-PB-O2B

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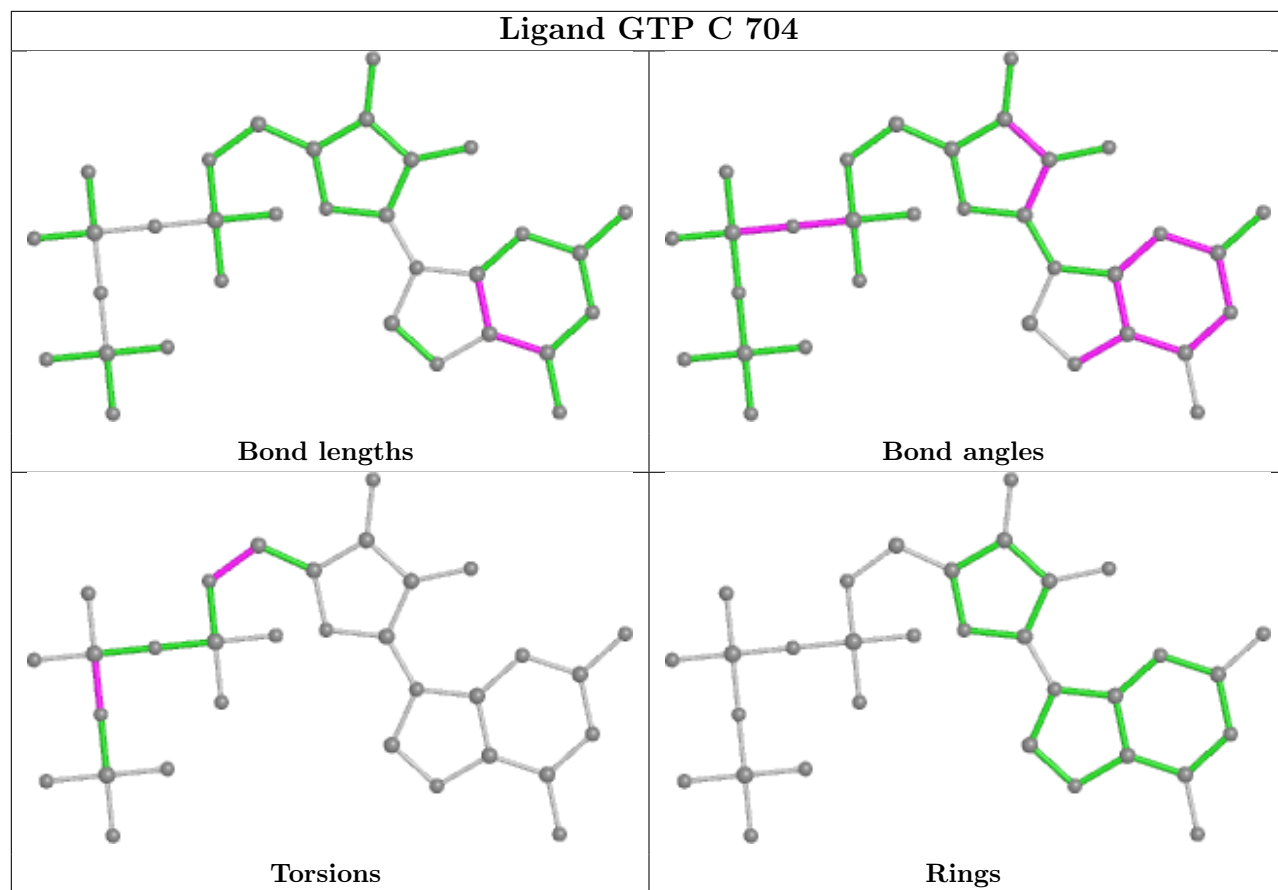
Mol	Chain	Res	Type	Atoms
5	D	701	GTP	PG-O3B-PB-O2B
2	C	705	DCP	C3'-C4'-C5'-O5'
5	D	704	GTP	C4'-C5'-O5'-PA
5	D	704	GTP	PG-O3B-PB-O1B
5	C	704	GTP	C4'-C5'-O5'-PA
5	C	706	GTP	C4'-C5'-O5'-PA
5	D	701	GTP	C4'-C5'-O5'-PA
2	A	701	DCP	PG-O3B-PB-O1B
2	C	701	DCP	PA-O3A-PB-O2B
3	A	702	DTP	PB-O3A-PA-O1A
5	C	704	GTP	PG-O3B-PB-O1B
5	D	701	GTP	PG-O3B-PB-O1B
5	D	704	GTP	PB-O3A-PA-O2A
2	A	701	DCP	C5'-O5'-PA-O1A
2	D	703	DCP	C5'-O5'-PA-O1A
2	D	702	DCP	PB-O3B-PG-O1G

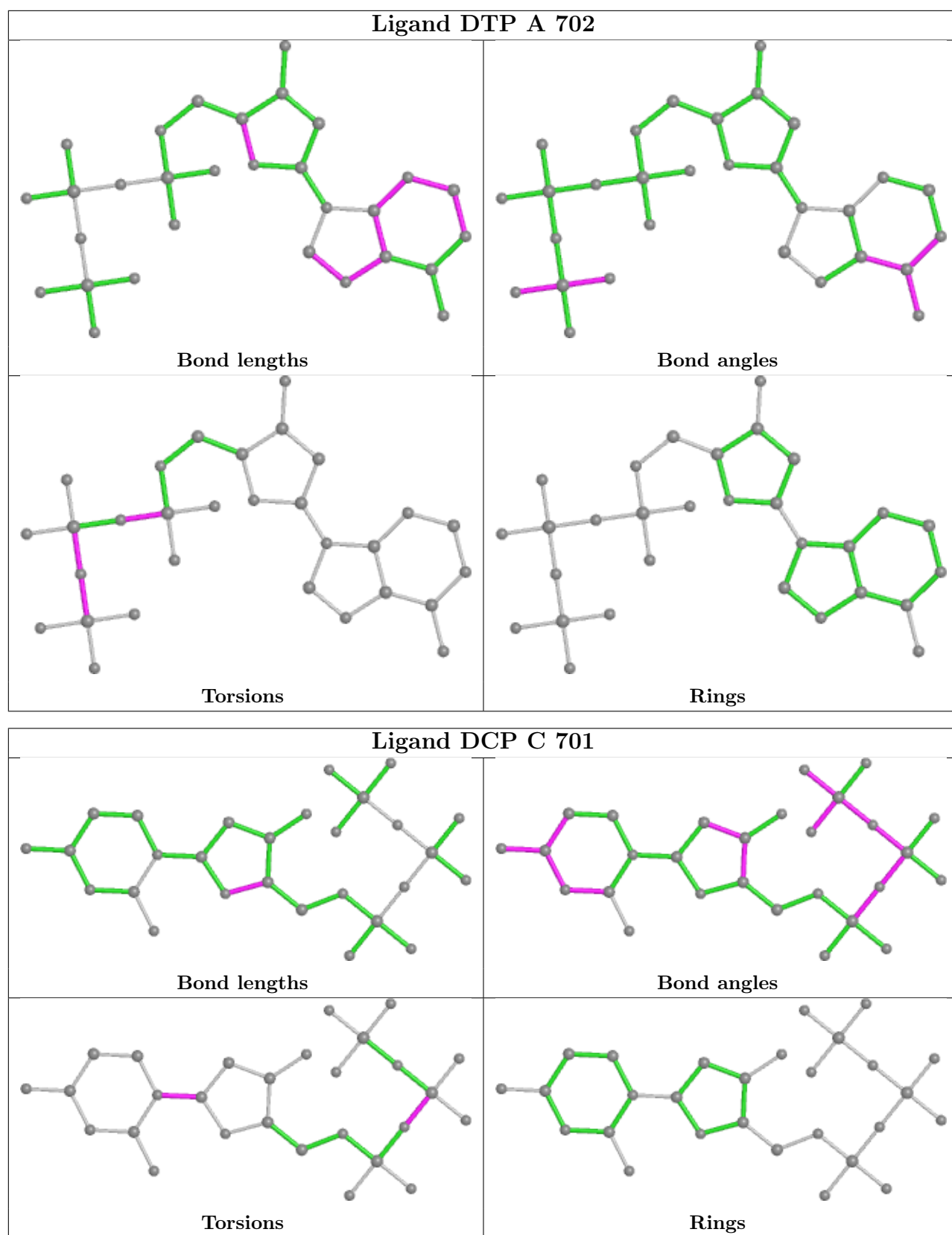
There are no ring outliers.

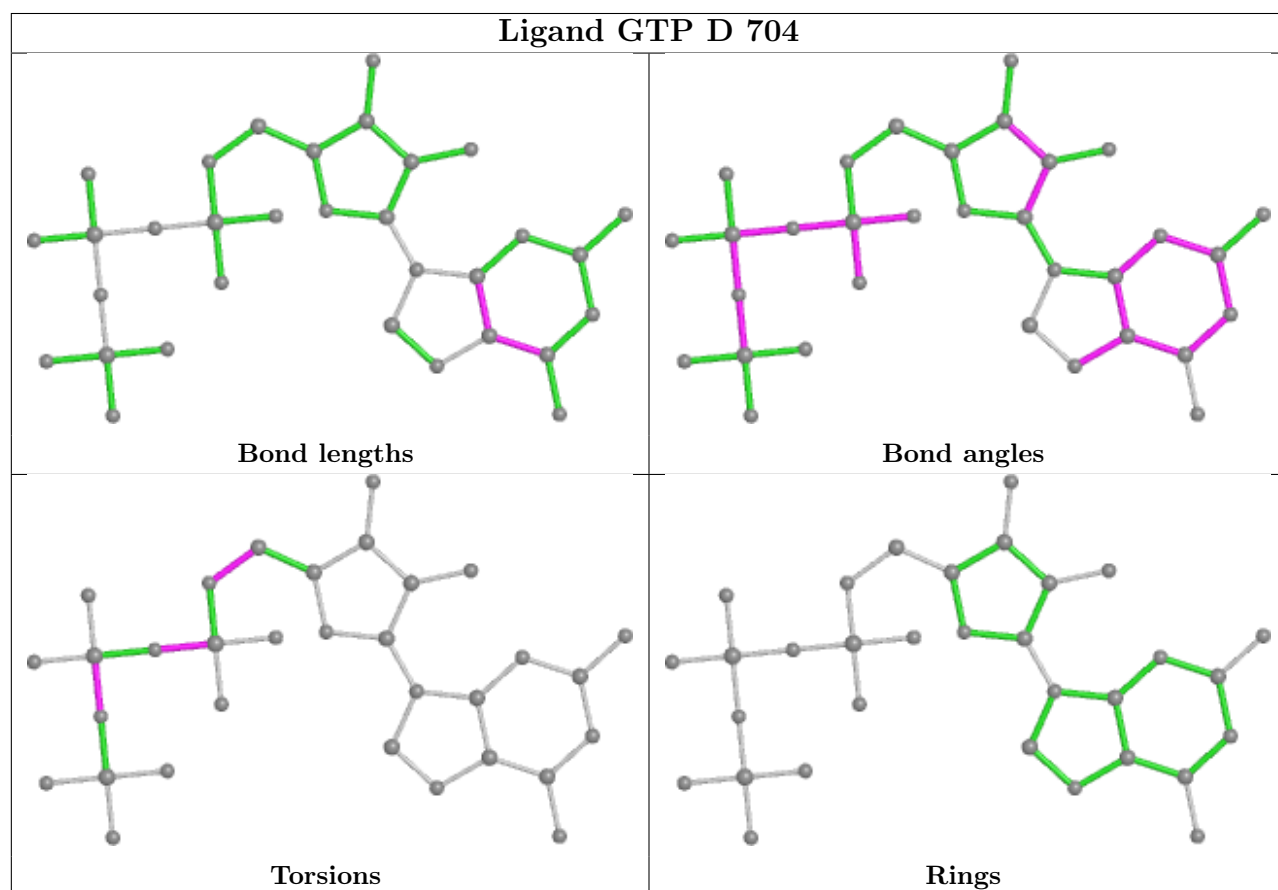
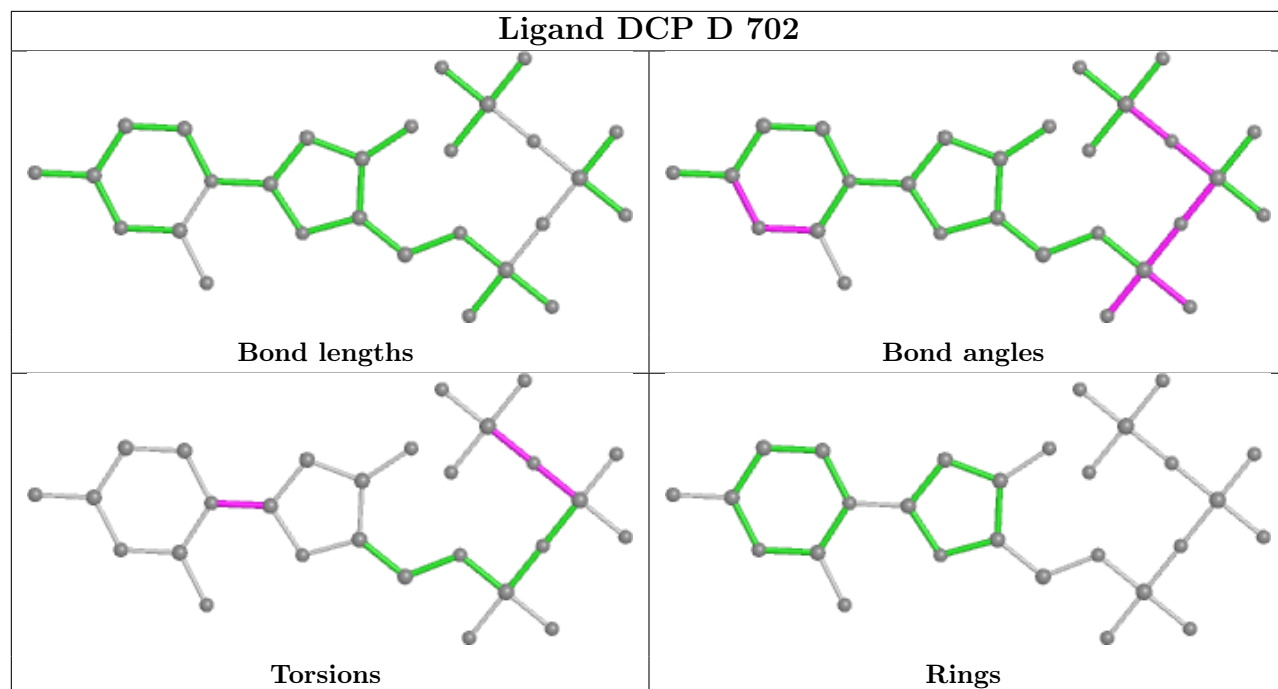
5 monomers are involved in 5 short contacts:

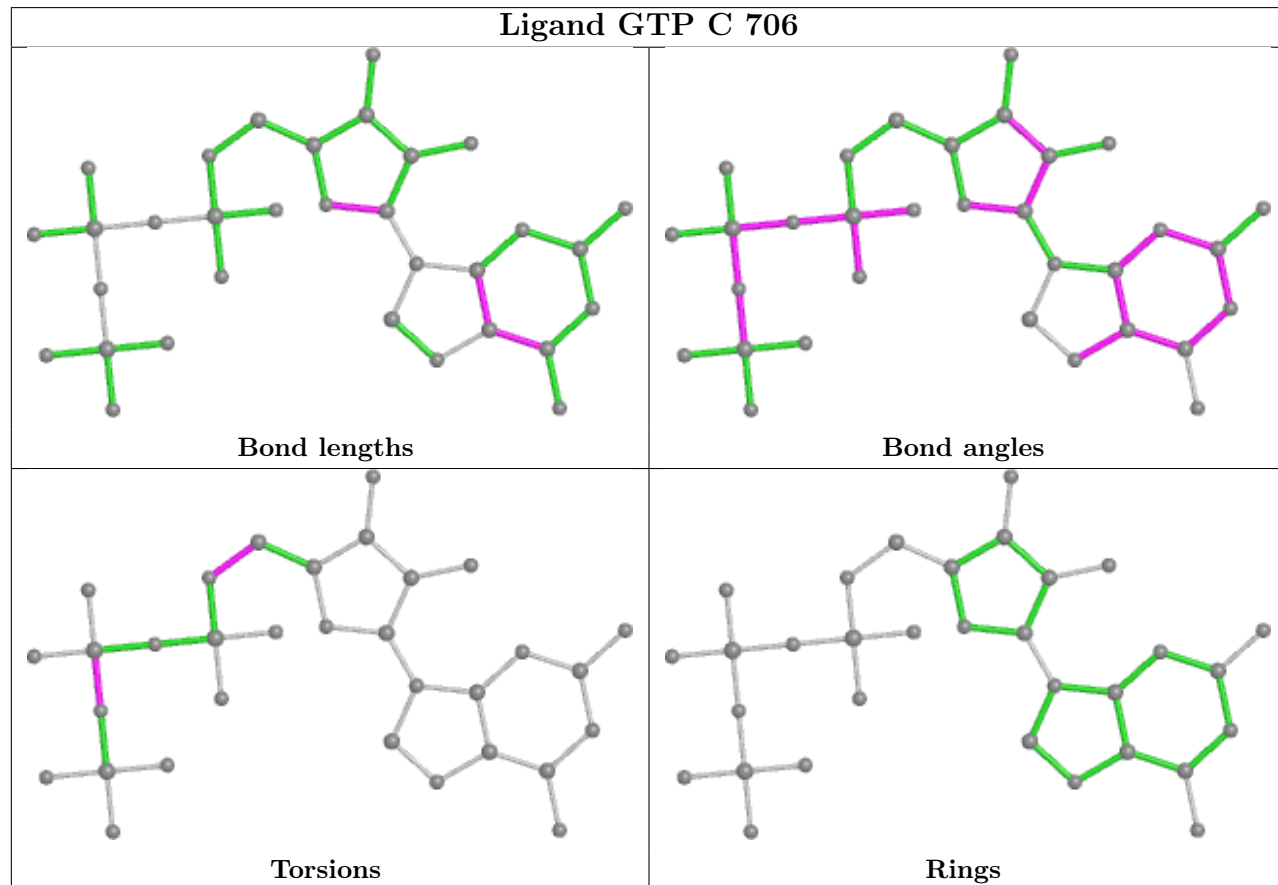
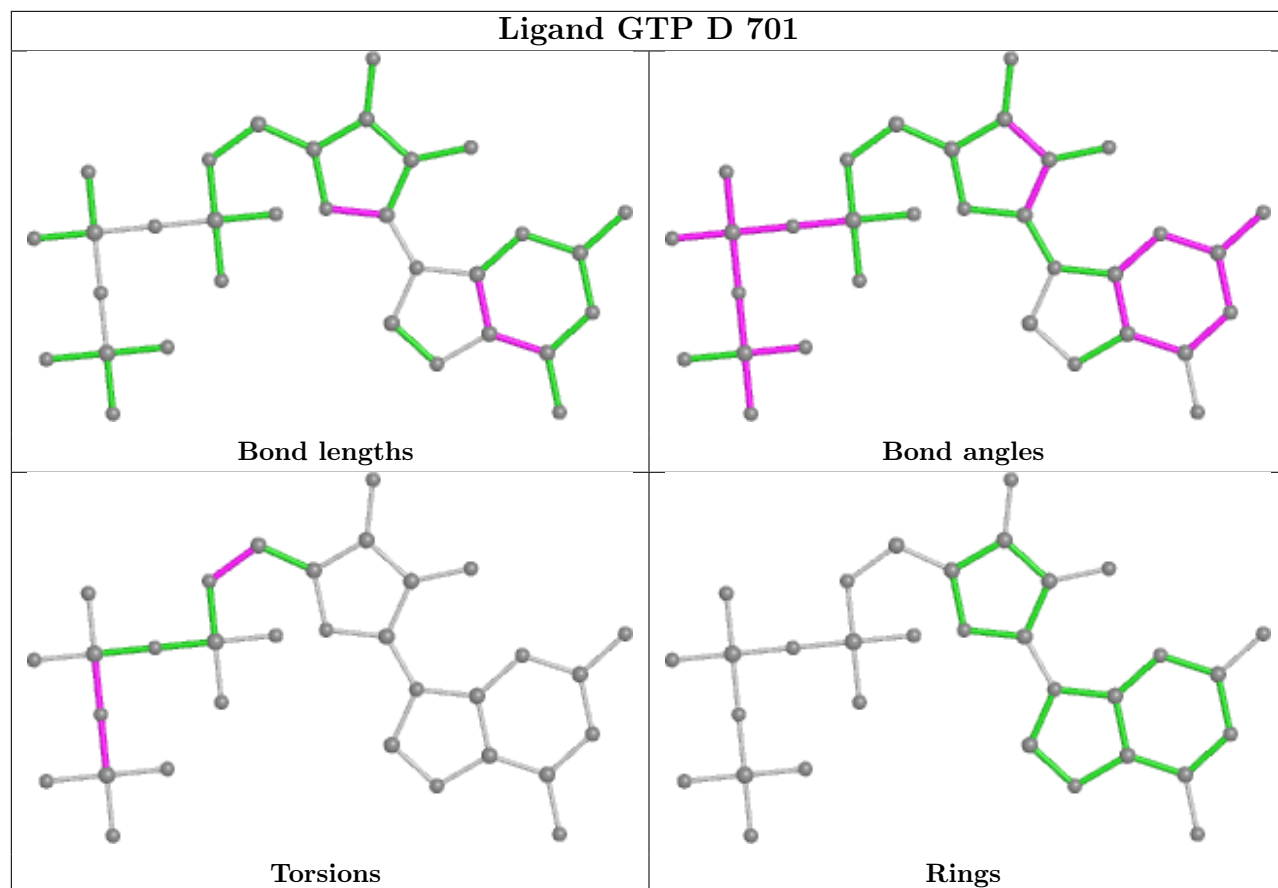
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	DCP	1	0
3	B	702	DTP	1	0
2	A	701	DCP	1	0
2	B	701	DCP	1	0
2	C	705	DCP	1	0

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.

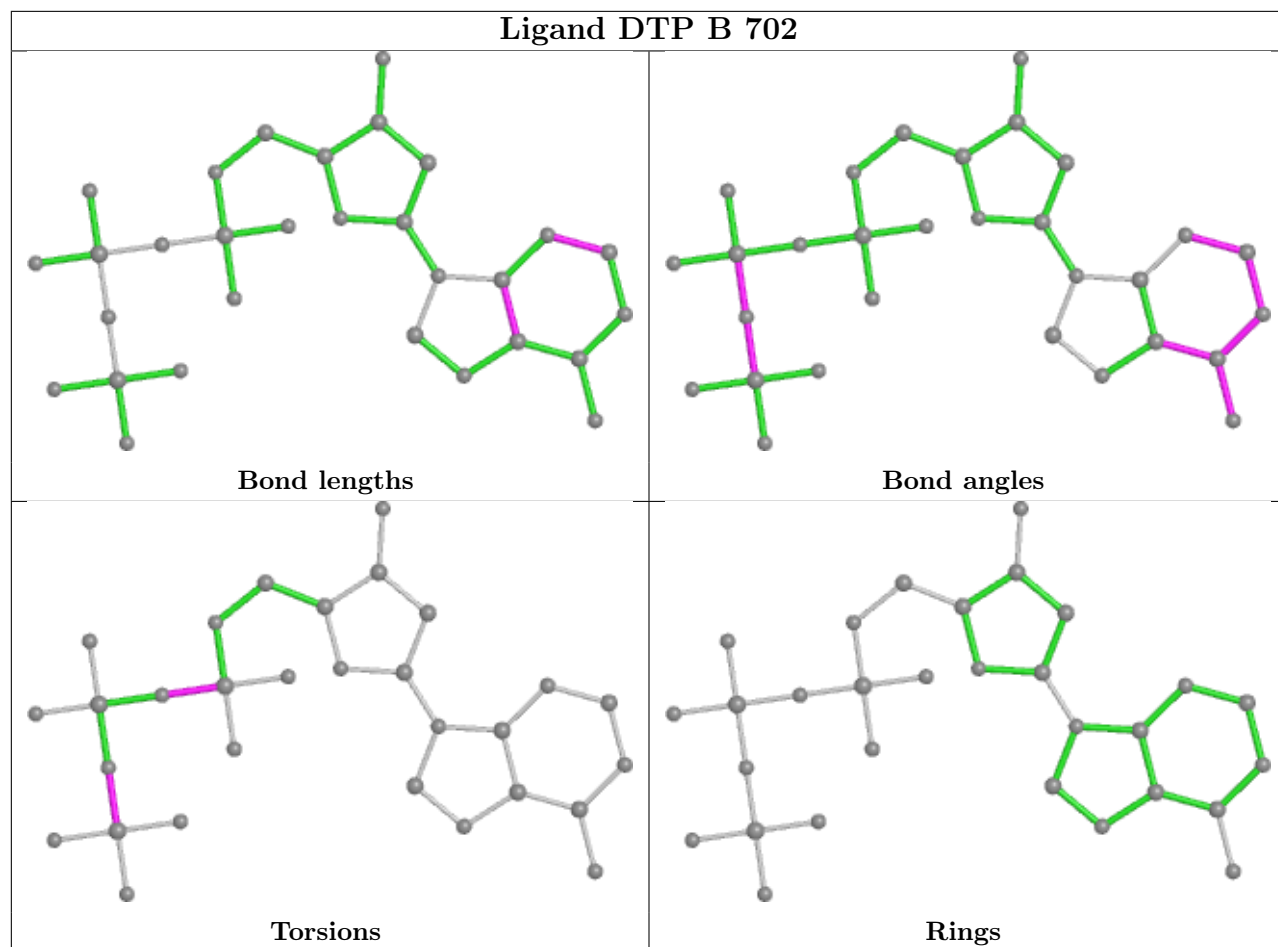




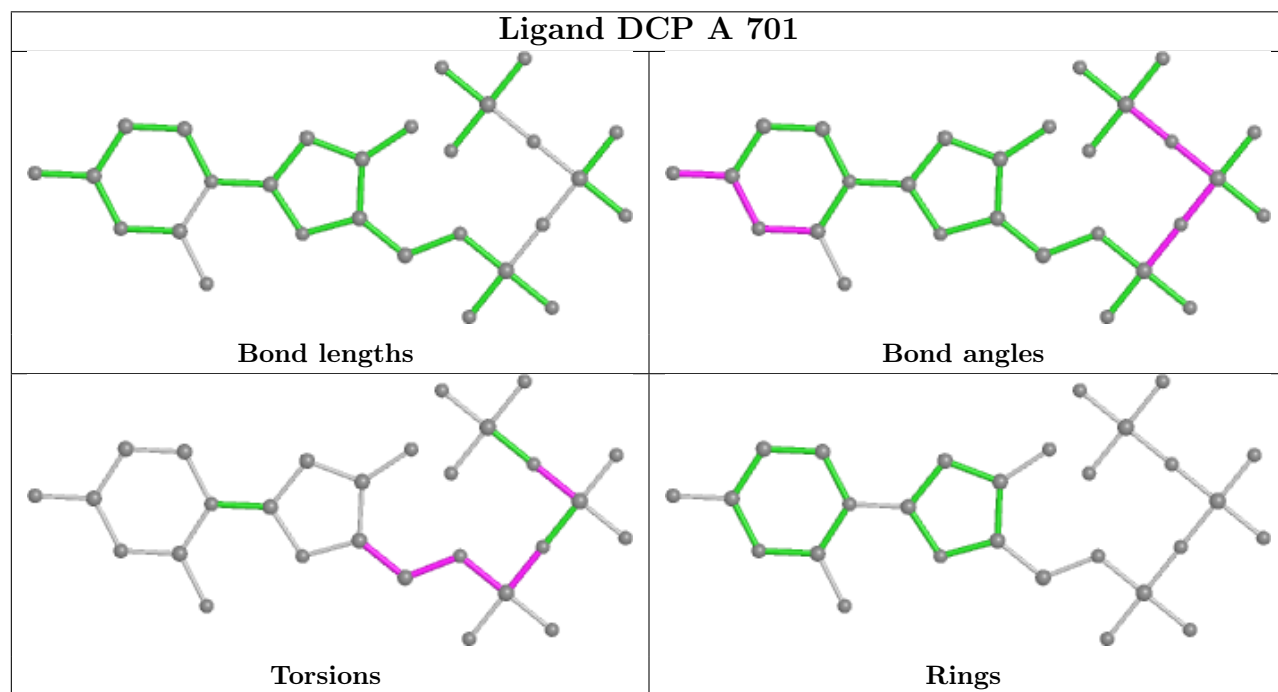


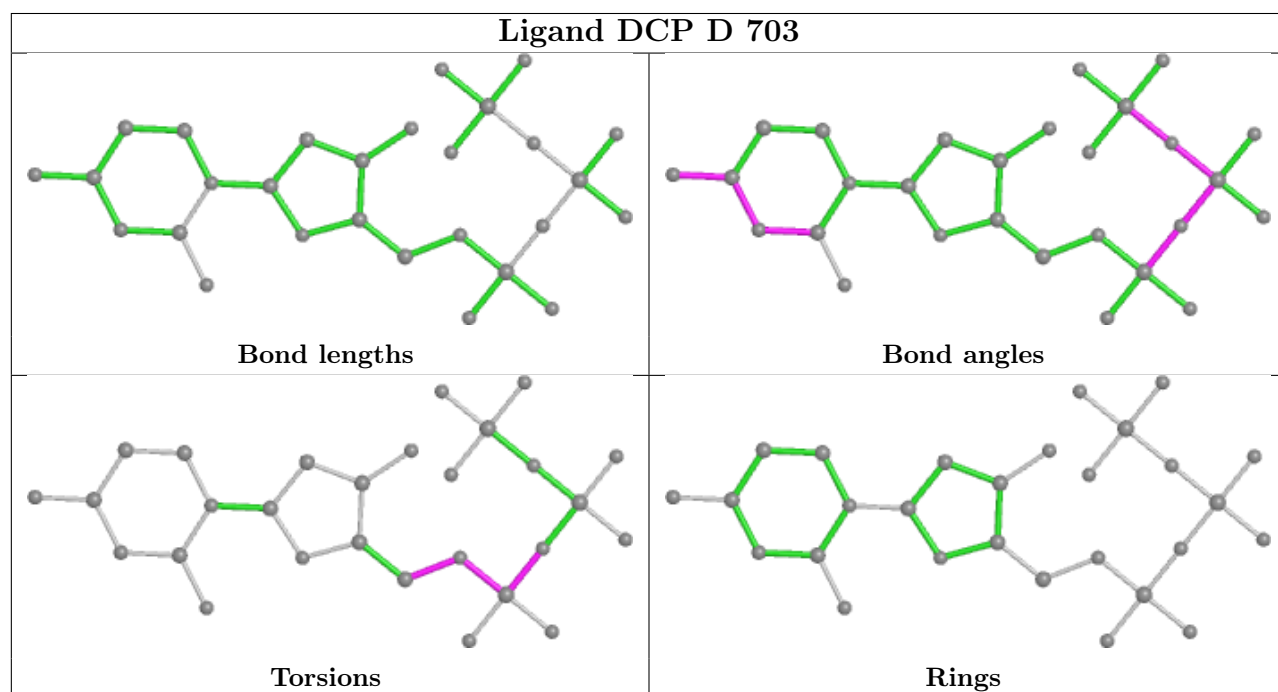
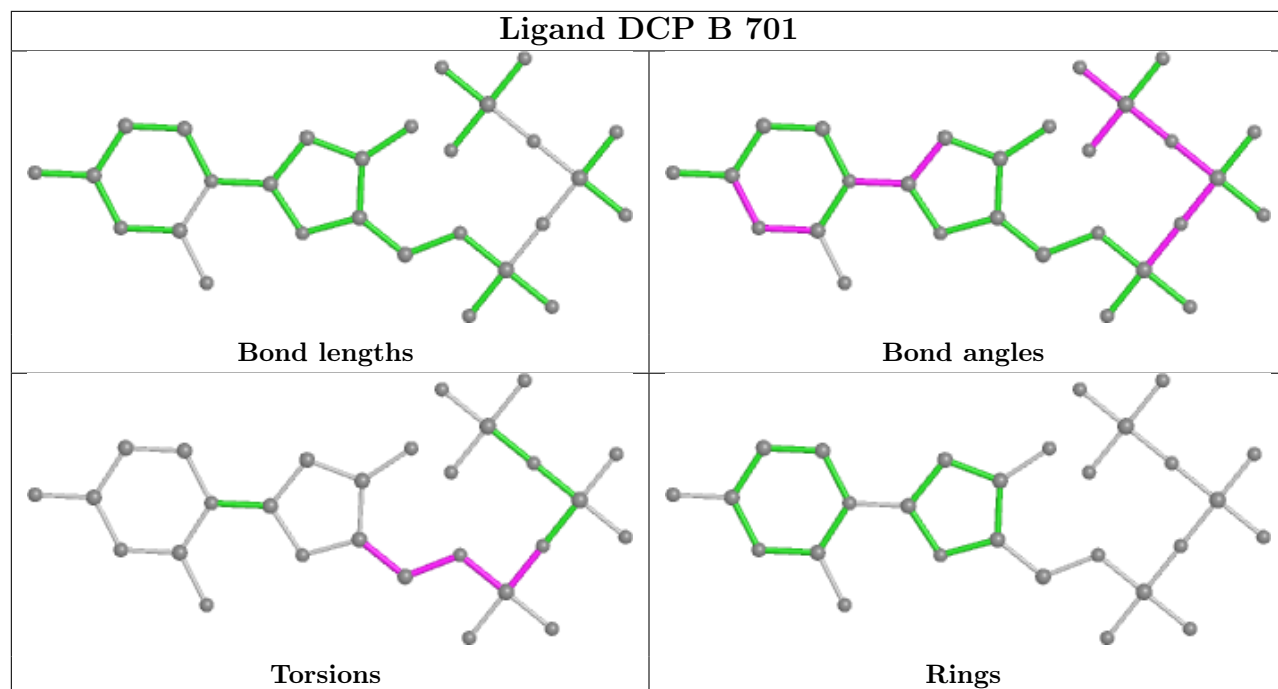


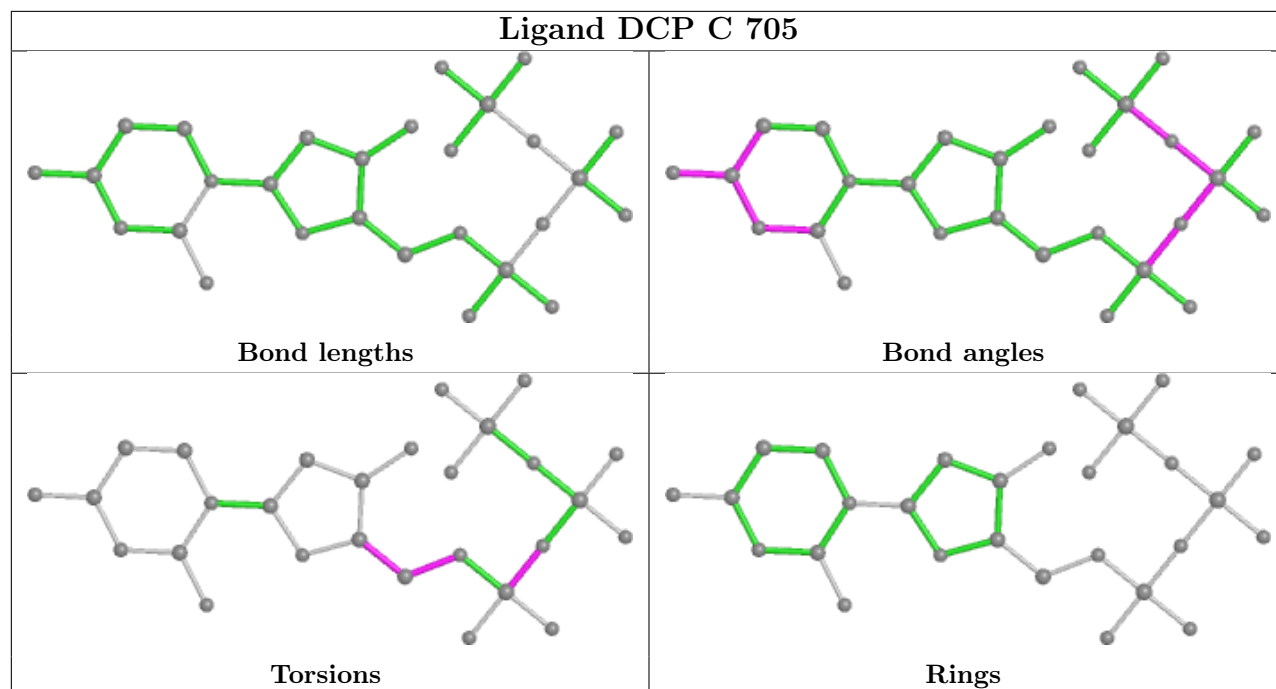
Ligand DTP B 702



Ligand DCP A 701







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	479/514 (93%)	0.83	66 (13%) 2 3	32, 74, 123, 162	0
1	B	480/514 (93%)	1.38	114 (23%) 0 0	38, 99, 174, 214	0
1	C	481/514 (93%)	0.46	25 (5%) 27 32	28, 62, 104, 153	0
1	D	484/514 (94%)	0.89	69 (14%) 2 3	35, 76, 126, 181	0
All	All	1924/2056 (93%)	0.89	274 (14%) 2 3	28, 76, 143, 214	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	VAL	10.9
1	B	487	VAL	10.2
1	B	489	LEU	9.3
1	B	466	ILE	9.2
1	A	489	LEU	8.6
1	D	279	PRO	8.6
1	A	490	ASP	8.3
1	D	490	ASP	8.1
1	B	230	LYS	6.9
1	B	493	LEU	6.8
1	B	345	ASN	6.7
1	B	486	LYS	6.7
1	A	493	LEU	6.5
1	B	573	CYS	6.5
1	B	402	ALA	6.4
1	A	491	VAL	6.3
1	A	492	LYS	6.1
1	B	488	LEU	6.0
1	A	488	LEU	5.9
1	B	223	PRO	5.9
1	D	590	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	563	TYR	5.7
1	B	572	TRP	5.6
1	B	591	ILE	5.6
1	B	276	LEU	5.5
1	B	491	VAL	5.5
1	B	585	ASP	5.4
1	D	599	ASN	5.4
1	A	487	VAL	5.4
1	B	467	LYS	5.3
1	D	489	LEU	5.3
1	D	488	LEU	5.1
1	B	229	VAL	5.1
1	A	484	LYS	5.0
1	D	484	LYS	5.0
1	D	491	VAL	4.9
1	B	288	LYS	4.9
1	B	481	ALA	4.9
1	B	490	ASP	4.8
1	D	595	LYS	4.8
1	B	578	PHE	4.8
1	A	284	LEU	4.8
1	B	484	LYS	4.7
1	A	463	THR	4.7
1	B	554	CYS	4.7
1	B	287	TYR	4.7
1	B	592	THR	4.6
1	B	569	PHE	4.6
1	D	557	VAL	4.6
1	B	347	LEU	4.5
1	D	589	PRO	4.5
1	B	565	ALA	4.4
1	B	480	VAL	4.3
1	B	284	LEU	4.3
1	A	554	CYS	4.3
1	D	598	TRP	4.3
1	B	599	ASN	4.3
1	B	403	GLY	4.2
1	A	498	PHE	4.2
1	B	526	PRO	4.2
1	D	543	GLU	4.2
1	A	486	LYS	4.1
1	B	485	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	597	GLU	4.1
1	B	341	CYS	4.1
1	B	285	TRP	4.1
1	C	284	LEU	4.0
1	A	464	GLY	4.0
1	D	483	ALA	4.0
1	B	556	LYS	3.9
1	D	466	ILE	3.9
1	B	593	PRO	3.9
1	B	275	PRO	3.9
1	C	283	SER	3.9
1	A	568	TYR	3.9
1	C	464	GLY	3.8
1	A	276	LEU	3.8
1	B	574	ALA	3.8
1	B	492	LYS	3.8
1	D	596	LYS	3.8
1	B	476	LEU	3.8
1	D	326	GLN	3.8
1	B	326	GLN	3.7
1	B	570	VAL	3.7
1	C	113	ASP	3.7
1	D	568	TYR	3.7
1	B	465	GLN	3.7
1	C	490	ASP	3.7
1	D	230	LYS	3.7
1	C	327	ASN	3.7
1	B	562	LEU	3.6
1	B	557	VAL	3.6
1	D	229	VAL	3.6
1	D	563	TYR	3.6
1	D	540	LEU	3.5
1	B	472	ASP	3.5
1	A	480	VAL	3.5
1	C	594	GLN	3.4
1	C	255	GLU	3.4
1	B	221	PHE	3.4
1	B	478	LYS	3.4
1	B	413	ILE	3.3
1	D	597	GLU	3.3
1	A	494	LYS	3.3
1	D	482	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	498	PHE	3.3
1	A	473	TYR	3.3
1	B	346	GLU	3.3
1	A	478	LYS	3.3
1	A	573	CYS	3.2
1	B	477	PRO	3.2
1	D	278	SER	3.2
1	B	560	LYS	3.2
1	D	498	PHE	3.1
1	C	288	LYS	3.1
1	A	326	GLN	3.1
1	D	528	ARG	3.1
1	B	500	VAL	3.1
1	D	485	PRO	3.1
1	A	565	ALA	3.0
1	B	470	ARG	3.0
1	A	285	TRP	3.0
1	B	348	ARG	3.0
1	A	286	PRO	3.0
1	A	238	VAL	3.0
1	B	531	ARG	3.0
1	A	496	GLU	2.9
1	A	245	ILE	2.9
1	B	185	LYS	2.9
1	A	481	ALA	2.9
1	B	576	ARG	2.9
1	D	328	ASN	2.9
1	D	493	LEU	2.9
1	D	531	ARG	2.9
1	D	327	ASN	2.9
1	B	471	GLU	2.9
1	B	222	ILE	2.9
1	A	342	GLU	2.9
1	D	470	ARG	2.9
1	D	492	LYS	2.9
1	A	562	LEU	2.9
1	A	560	LYS	2.8
1	D	277	GLU	2.8
1	A	591	ILE	2.8
1	B	454	PHE	2.8
1	B	587	ILE	2.8
1	B	548	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	465	GLN	2.7
1	A	477	PRO	2.7
1	D	346	GLU	2.7
1	A	476	LEU	2.7
1	C	596	LYS	2.7
1	B	464	GLY	2.7
1	D	487	VAL	2.7
1	D	288	LYS	2.7
1	A	321	HIS	2.7
1	B	328	ASN	2.7
1	D	594	GLN	2.7
1	A	469	LYS	2.7
1	D	343	VAL	2.6
1	C	345	ASN	2.6
1	A	437	LYS	2.6
1	B	596	LYS	2.6
1	B	400	THR	2.6
1	D	408	ARG	2.6
1	B	473	TYR	2.6
1	B	474	GLU	2.6
1	D	572	TRP	2.6
1	A	563	TYR	2.6
1	D	262	GLU	2.6
1	B	238	VAL	2.6
1	C	282	ASP	2.6
1	D	160	ALA	2.6
1	A	345	ASN	2.6
1	B	340	VAL	2.6
1	A	593	PRO	2.5
1	B	396	TYR	2.5
1	B	469	LYS	2.5
1	A	296	PHE	2.5
1	A	466	ILE	2.5
1	D	409	ILE	2.5
1	C	326	GLN	2.5
1	A	575	ASP	2.5
1	D	584	GLY	2.5
1	D	323	LEU	2.4
1	B	568	TYR	2.4
1	B	406	LYS	2.4
1	D	251	LYS	2.4
1	A	465	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	231	TRP	2.4
1	C	124	GLY	2.4
1	B	218	ASP	2.4
1	A	413	ILE	2.4
1	A	230	LYS	2.4
1	A	134	ARG	2.4
1	A	590	LEU	2.4
1	B	327	ASN	2.4
1	B	419	TYR	2.4
1	A	388	ASP	2.3
1	B	543	GLU	2.3
1	A	190	GLN	2.3
1	A	199	VAL	2.3
1	B	325	ILE	2.3
1	B	504	ASN	2.3
1	B	586	VAL	2.3
1	A	495	ALA	2.3
1	D	205	CYS	2.3
1	D	400	THR	2.3
1	B	158	PRO	2.3
1	D	285	TRP	2.3
1	A	122	ILE	2.3
1	A	126	ILE	2.3
1	A	598	TRP	2.3
1	B	545	PHE	2.3
1	C	251	LYS	2.2
1	D	581	PRO	2.2
1	B	388	ASP	2.2
1	D	122	ILE	2.2
1	B	322	HIS	2.2
1	C	285	TRP	2.2
1	D	471	GLU	2.2
1	A	288	LYS	2.2
1	B	455	LYS	2.2
1	B	590	LEU	2.2
1	C	252	PRO	2.2
1	A	583	ASP	2.2
1	B	119	ASN	2.2
1	B	561	SER	2.2
1	D	320	CYS	2.2
1	A	250	ILE	2.2
1	B	468	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	525	ALA	2.2
1	B	343	VAL	2.2
1	B	266	CYS	2.2
1	B	399	ILE	2.2
1	D	468	ILE	2.2
1	A	398	GLU	2.2
1	D	465	GLN	2.2
1	B	323	LEU	2.2
1	B	584	GLY	2.2
1	A	485	PRO	2.2
1	B	443	GLU	2.2
1	B	564	ALA	2.2
1	B	386	ILE	2.2
1	D	325	ILE	2.2
1	D	587	ILE	2.2
1	B	267	PHE	2.2
1	D	276	LEU	2.2
1	A	586	VAL	2.1
1	D	558	ASP	2.1
1	A	327	ASN	2.1
1	B	122	ILE	2.1
1	C	241	PHE	2.1
1	C	543	GLU	2.1
1	C	403	GLY	2.1
1	A	317	ALA	2.1
1	B	228	GLU	2.1
1	A	574	ALA	2.1
1	B	499	ILE	2.1
1	C	260	ILE	2.1
1	B	321	HIS	2.1
1	B	291	PRO	2.1
1	D	348	ARG	2.1
1	C	126	ILE	2.0
1	C	325	ILE	2.0
1	D	547	GLU	2.0
1	D	321	HIS	2.0
1	B	577	ASN	2.0
1	D	159	GLY	2.0
1	D	559	ARG	2.0
1	D	569	PHE	2.0
1	C	263	GLU	2.0
1	B	405	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	115	MET	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](#)

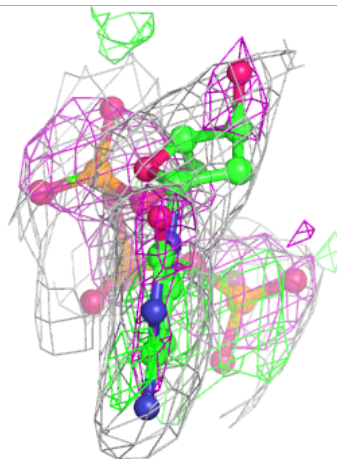
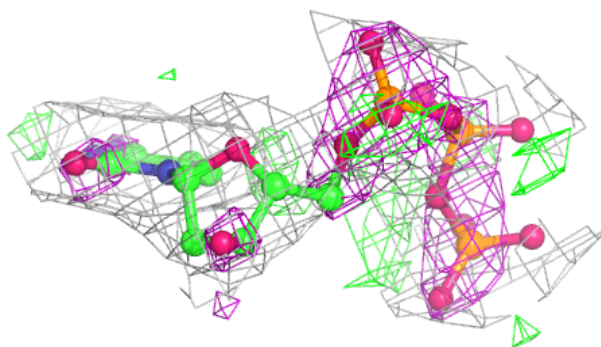
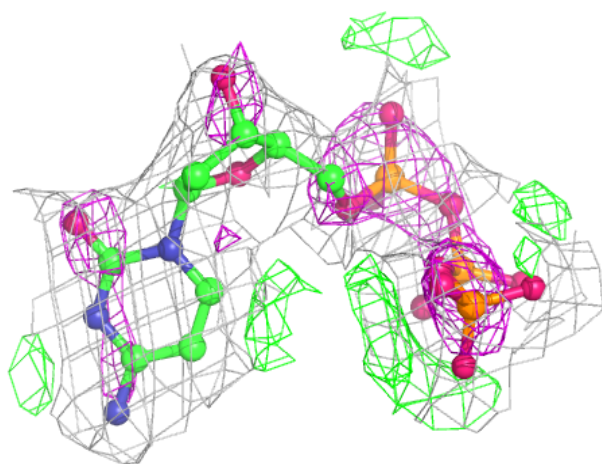
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	C	703	1/1	0.77	0.12	15,15,15,15	0
4	MG	A	704	1/1	0.80	0.11	48,48,48,48	0
4	MG	C	702	1/1	0.87	0.12	32,32,32,32	0
2	DCP	B	701	28/28	0.89	0.15	28,40,55,57	0
5	GTP	C	704	32/32	0.89	0.16	20,23,28,31	0
2	DCP	D	703	28/28	0.93	0.12	32,39,58,64	0
4	MG	A	703	1/1	0.93	0.05	28,28,28,28	0
2	DCP	A	701	28/28	0.93	0.12	38,46,67,75	0
3	DTP	B	702	30/30	0.94	0.13	16,20,33,36	0
2	DCP	D	702	28/28	0.94	0.13	16,20,34,35	0
5	GTP	D	704	32/32	0.94	0.12	16,20,26,26	0
2	DCP	C	705	28/28	0.95	0.11	27,35,65,72	0
2	DCP	C	701	28/28	0.95	0.12	19,25,37,51	0
5	GTP	D	701	32/32	0.96	0.10	22,26,29,30	0
3	DTP	A	702	30/30	0.97	0.14	15,21,37,42	0
5	GTP	C	706	32/32	0.97	0.10	16,22,25,26	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.

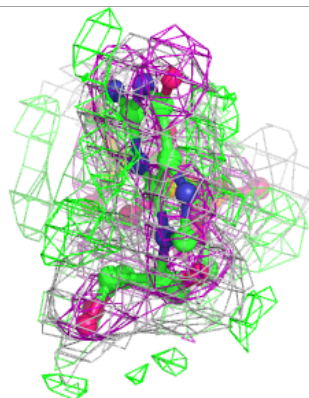
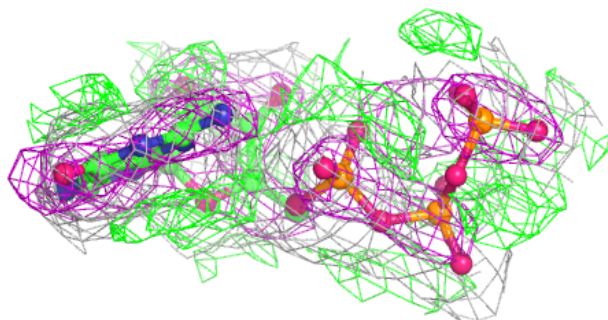
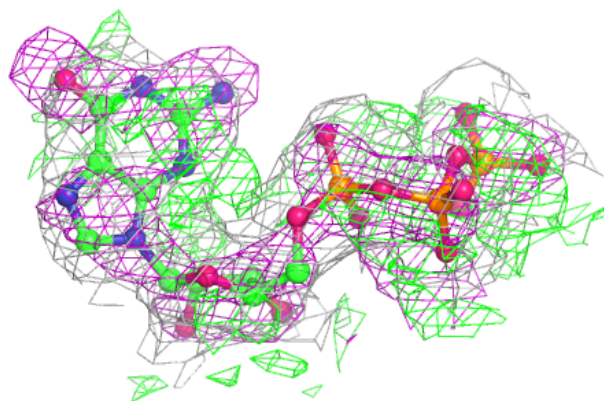
Electron density around DCP B 701:

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

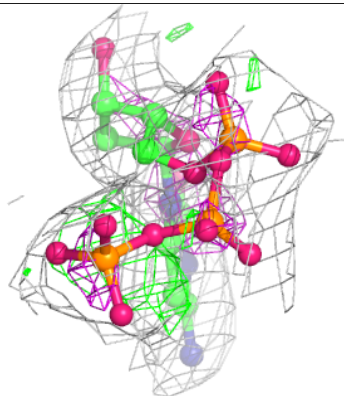
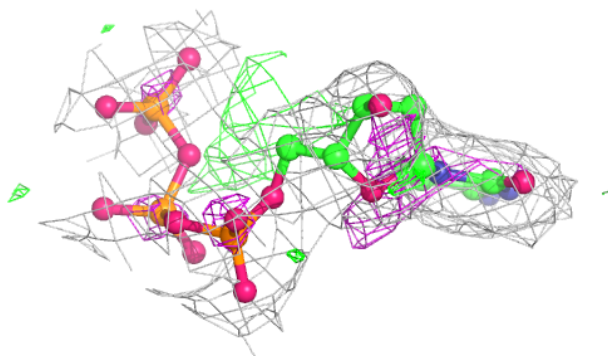
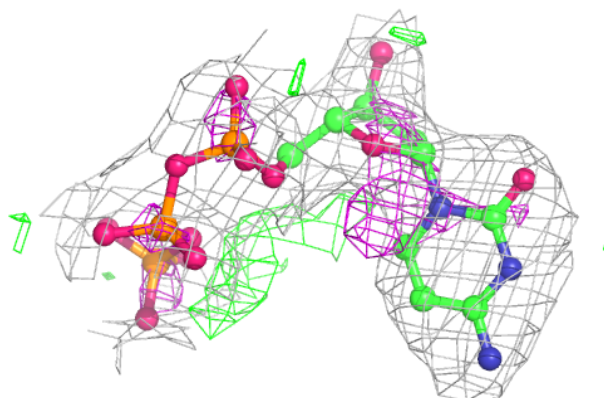


Electron density around GTP C 704:

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

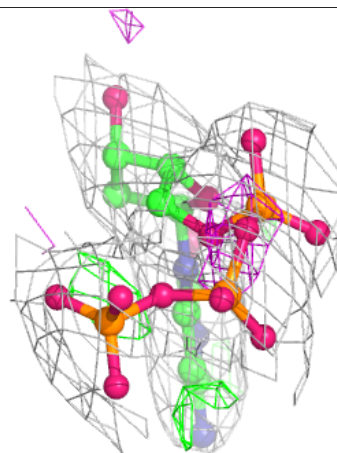
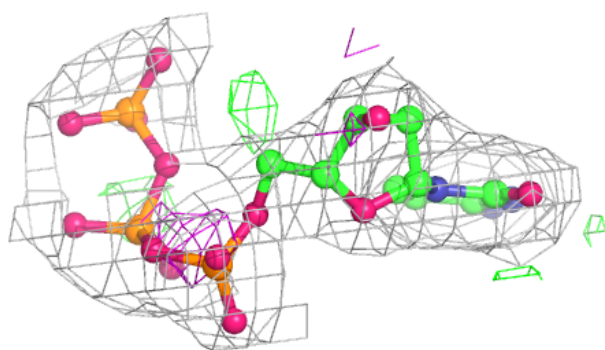
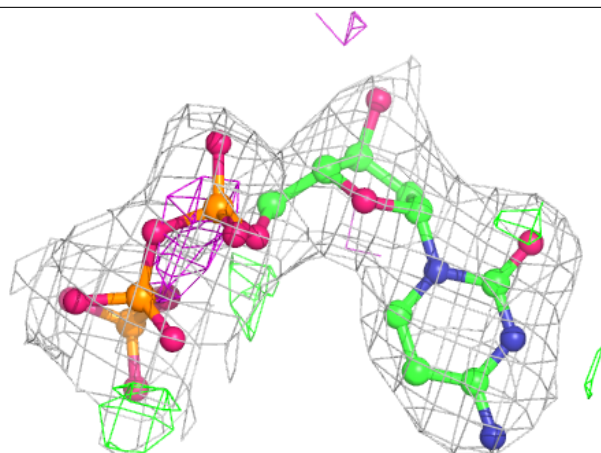
**Electron density around DCP D 703:**

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

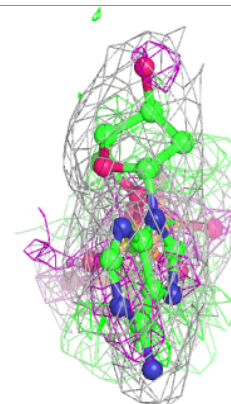
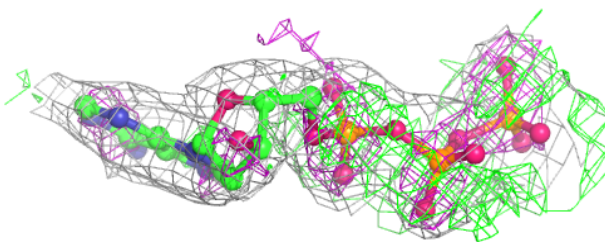
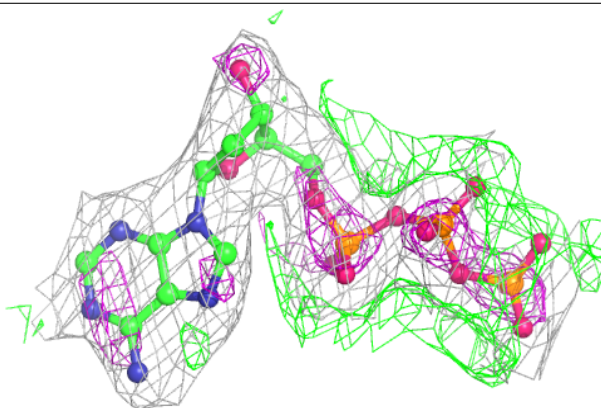


Electron density around DCP A 701:

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

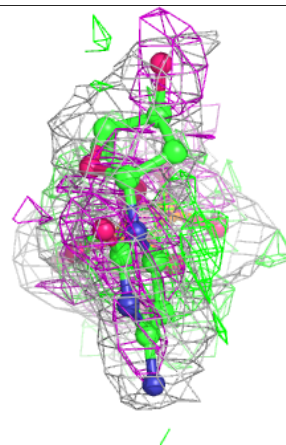
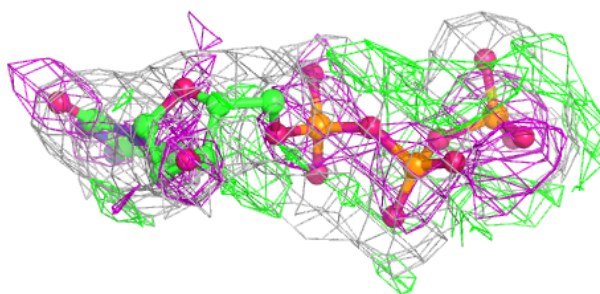
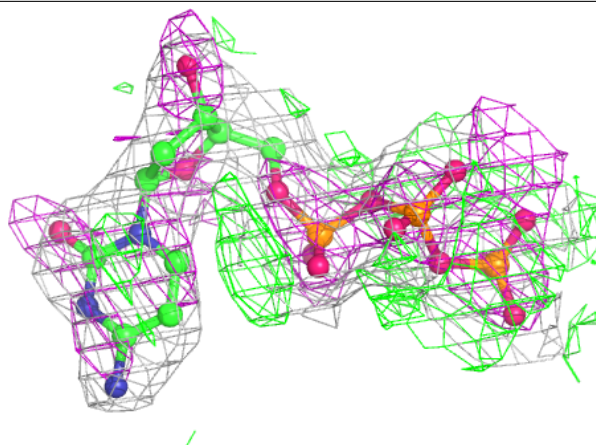
**Electron density around DTP B 702:**

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

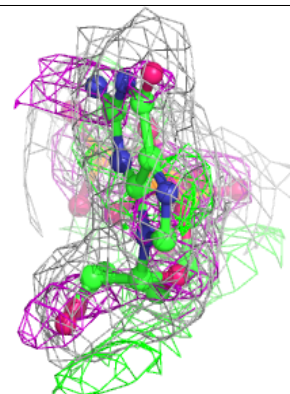
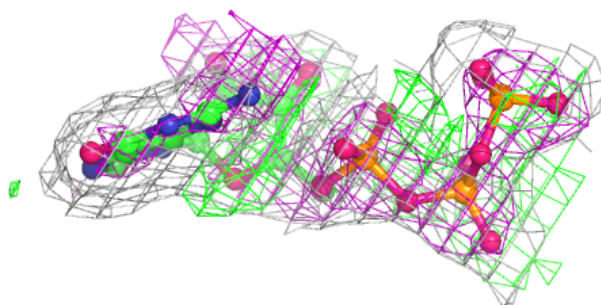
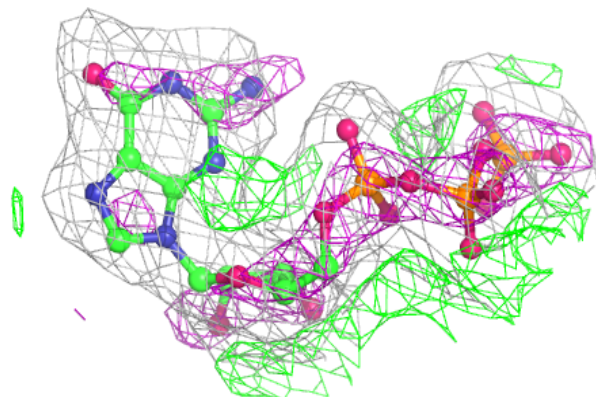


Electron density around DCP D 702:

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

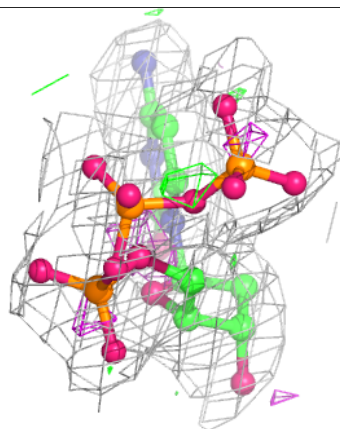
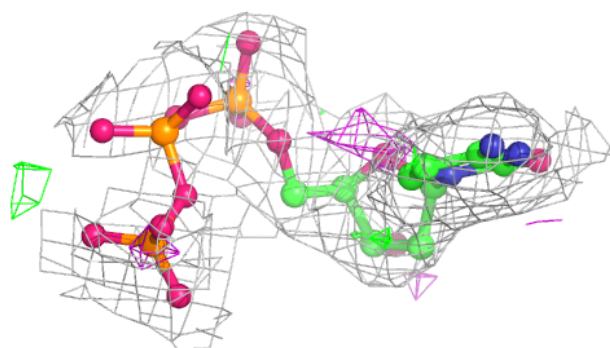
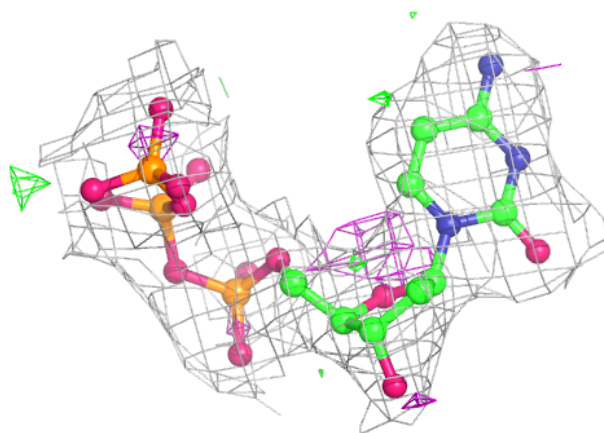
**Electron density around GTP D 704:**

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

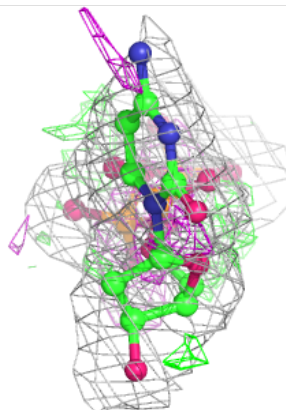
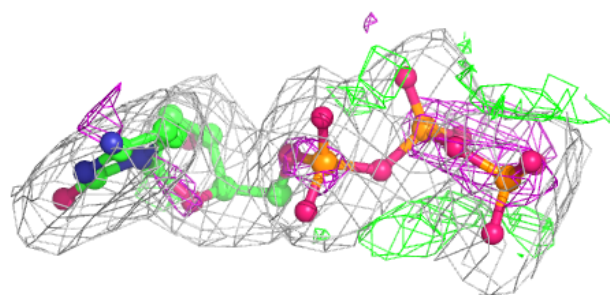
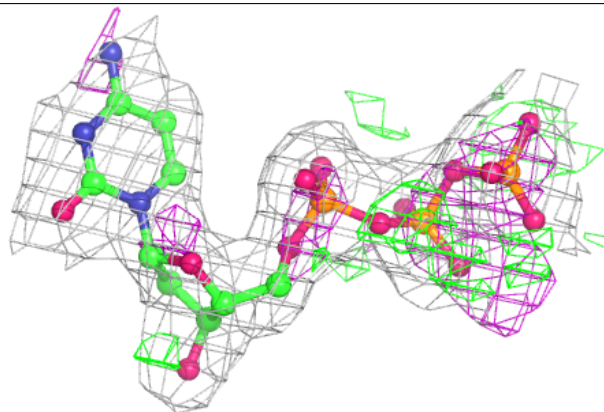


Electron density around DCP C 705:

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

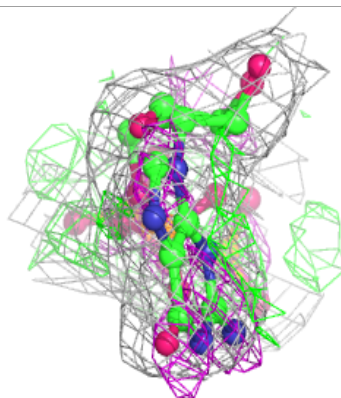
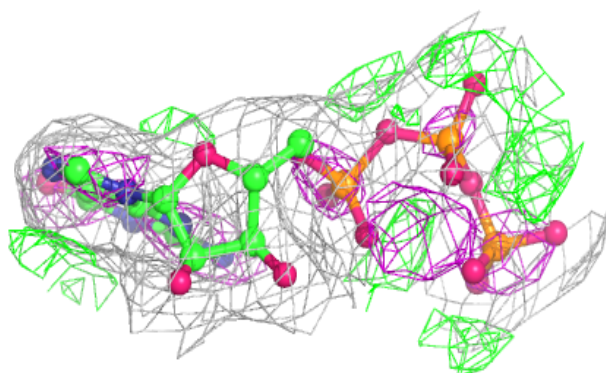
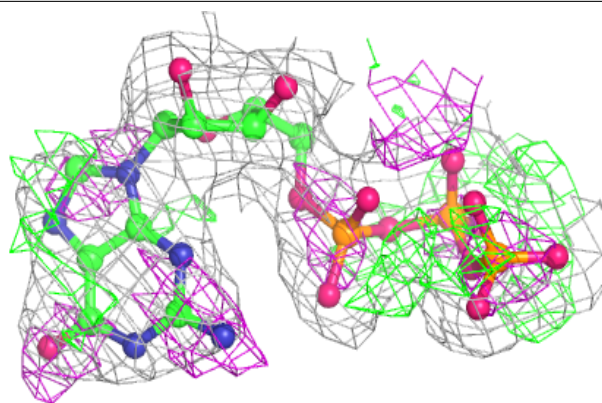
**Electron density around DCP C 701:**

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

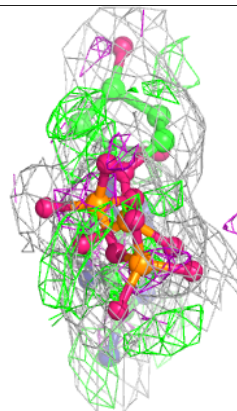
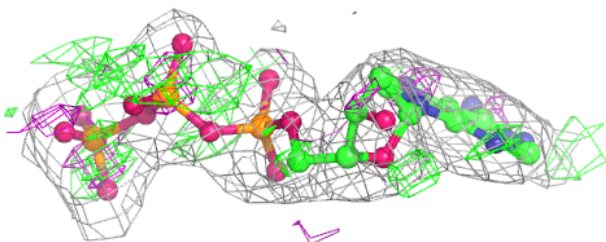
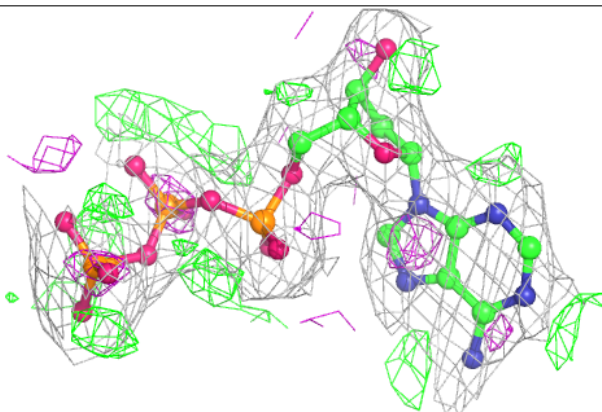


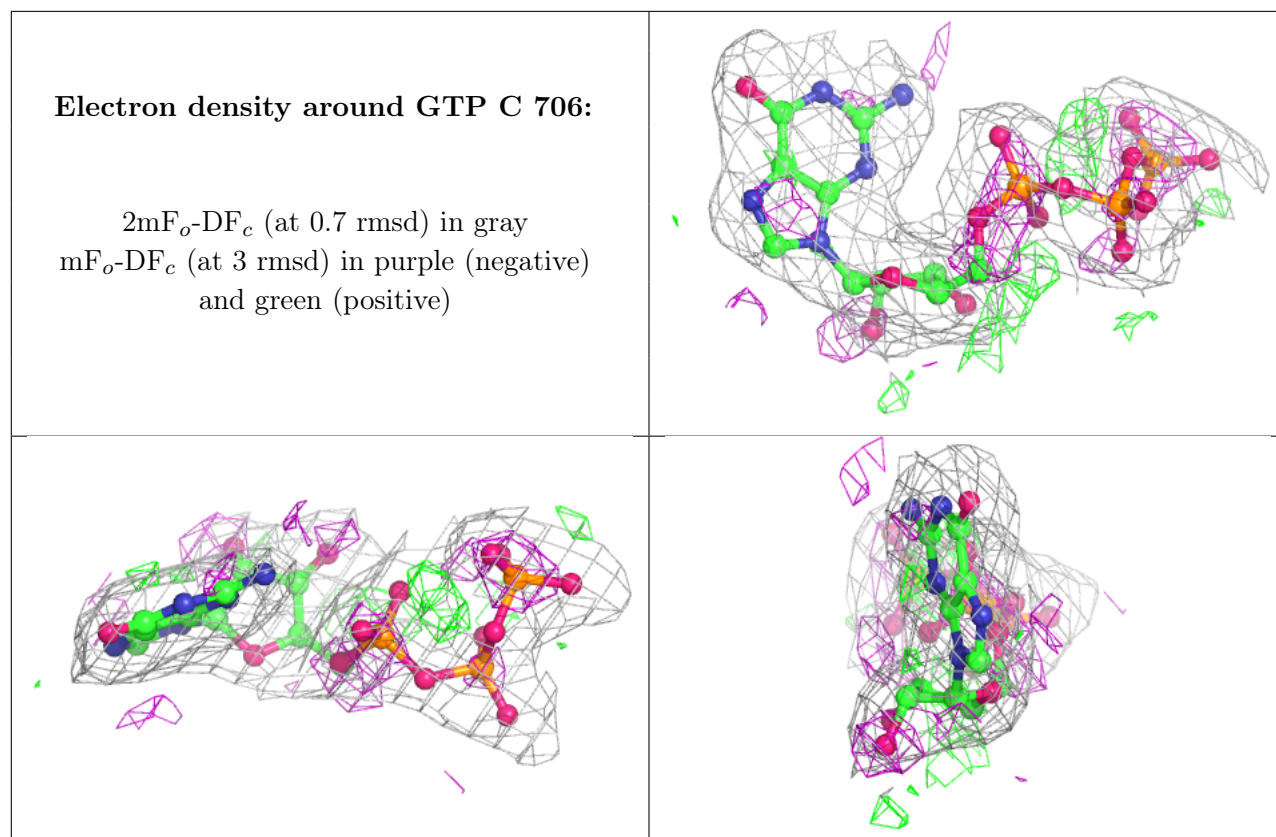
Electron density around GTP D 701:

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

**Electron density around DTP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.