Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 05:18 PM EDT

PDB ID	:	4TO4
Title	:	Structure basis of cellular dNTP regulation, SAMHD1-GTP-dGTP-dCTP complex
Authors	:	Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on	:	2014-06-05
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

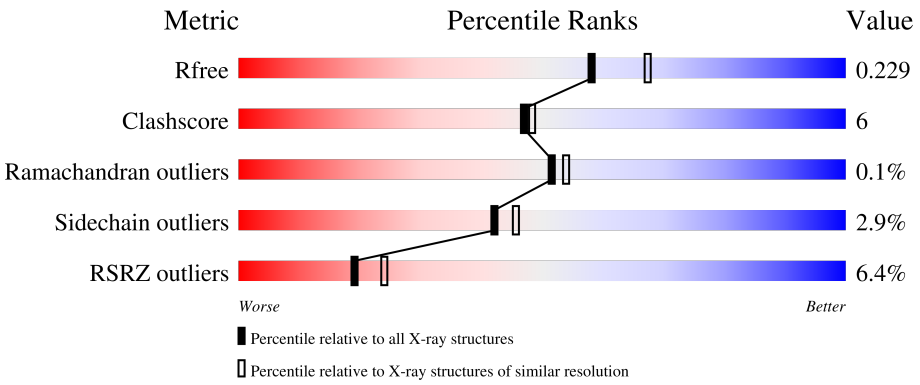
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	8% 83% 10% • 6%
1	B	514	7% 80% 12% • 6%
1	C	514	2% 80% 12% • 6%
1	D	514	7% 81% 12% • 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16513 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.

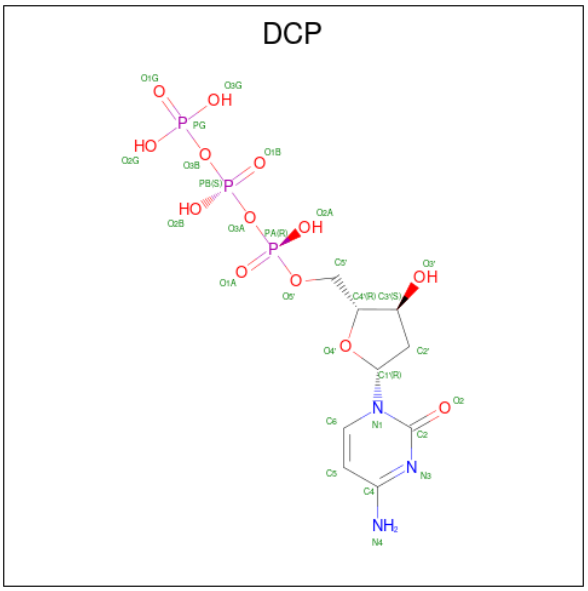
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	481	3933	2517	685	711	20	0	0	0
1	B	481	3933	2517	685	711	20	0	0	0
1	C	481	3945	2523	687	715	20	0	2	0
1	D	484	3963	2536	691	716	20	0	1	0

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: $C_9H_{16}N_3O_{13}P_3$).



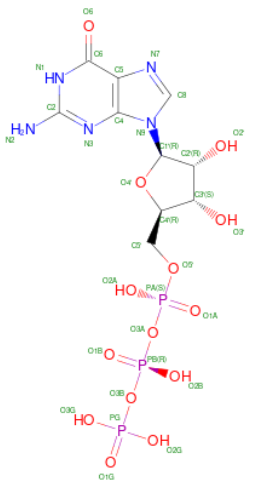
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	B	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	C	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	D	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

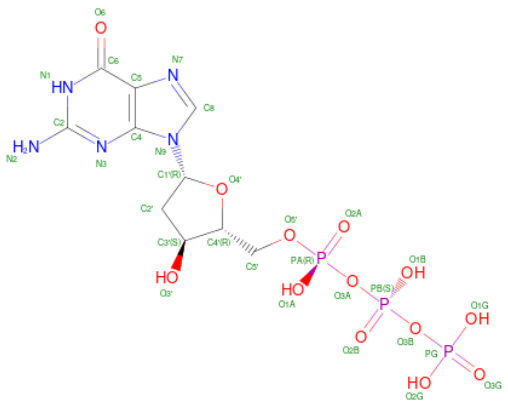
GTP



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

- Molecule 5 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

DGT



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0
5	B	1	31	10	5	13	3	0	0
5	C	1	31	10	5	13	3	0	0
5	D	1	31	10	5	13	3	0	0

- Molecule 6 is water.

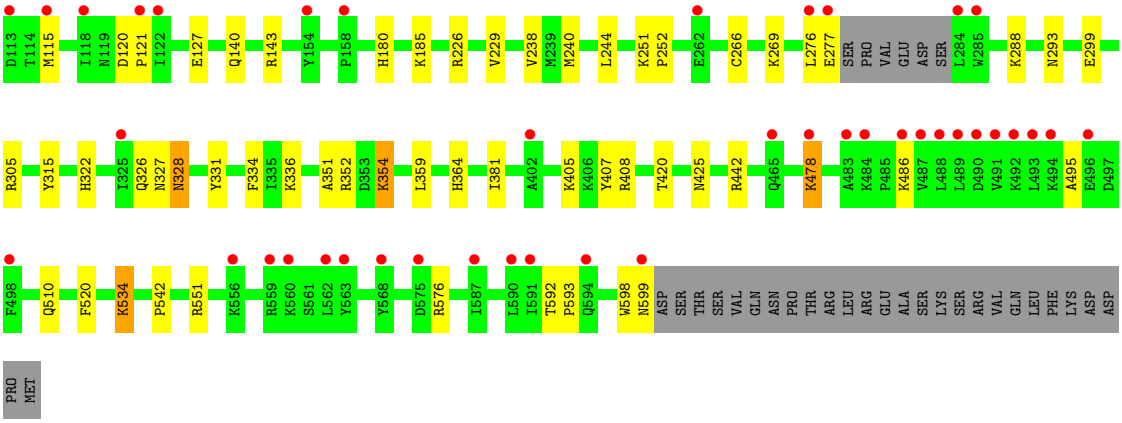
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	93	93	93	0	0
6	B	86	86	86	0	0
6	C	117	117	117	0	0
6	D	71	71	71	0	0

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.

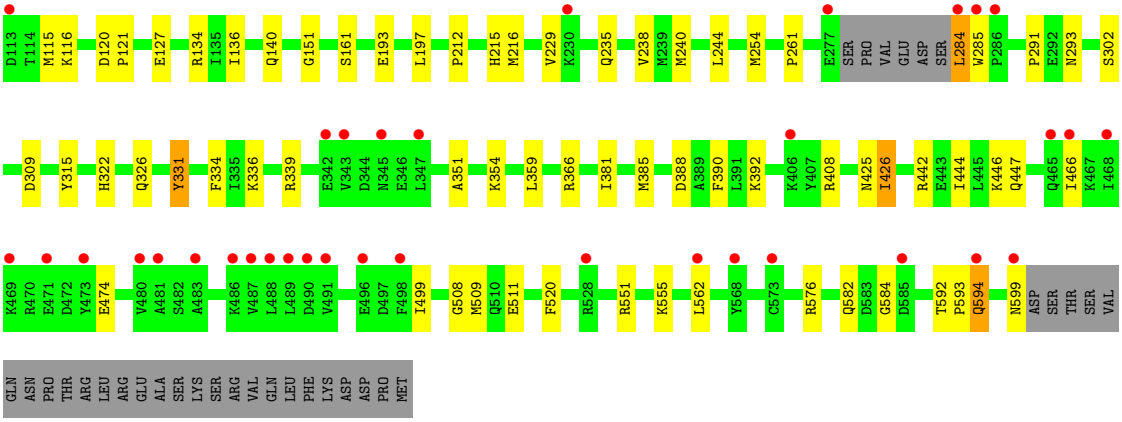
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



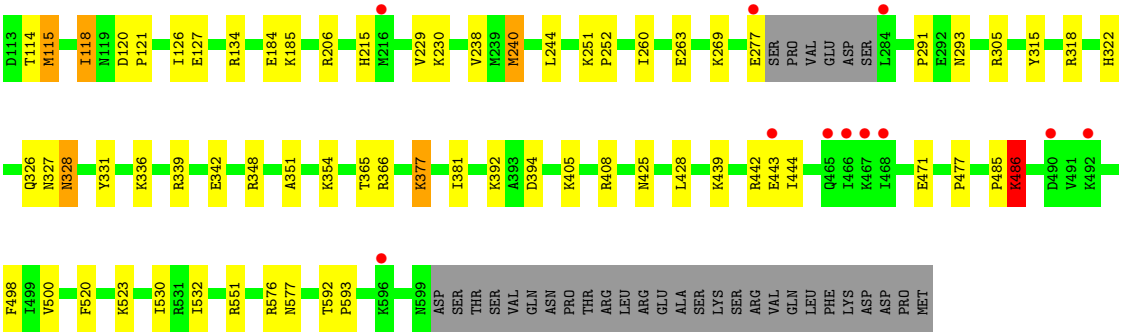
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:



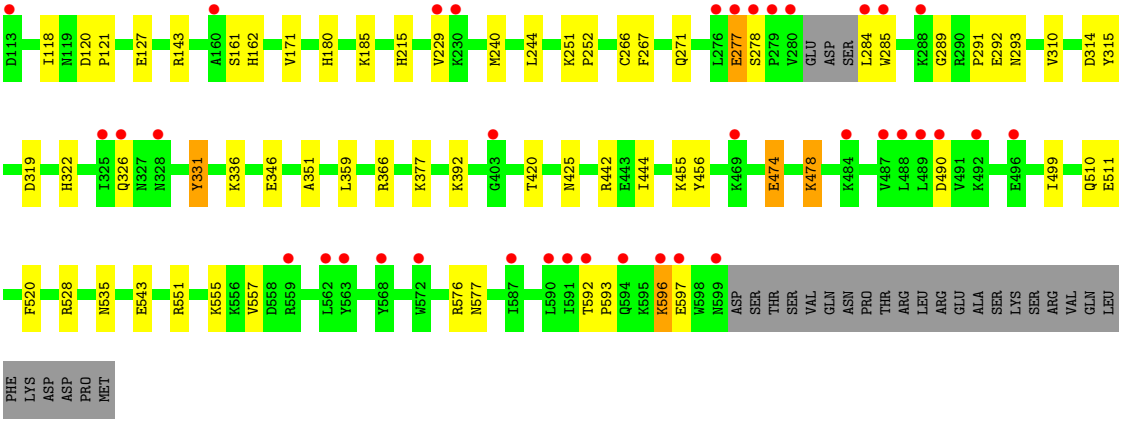
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.71Å 145.84Å 98.65Å 90.00° 114.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 47.06 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.10) 99.1 (47.06-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.197 , 0.225 0.202 , 0.229	Depositor DCC
R_{free} test set	6470 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16513	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GTP, MG, DGT, DCP

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	0.72	0/4025	0.81	6/5433 (0.1%)
1	B	0.70	1/4025 (0.0%)	0.80	7/5433 (0.1%)
1	C	0.77	2/4037 (0.0%)	0.83	7/5449 (0.1%)
1	D	0.69	1/4057 (0.0%)	0.77	6/5478 (0.1%)
All	All	0.72	4/16144 (0.0%)	0.80	26/21793 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	SER	CB-OG	5.83	1.49	1.42
1	D	161	SER	CB-OG	5.77	1.49	1.42
1	C	342	GLU	CD-OE2	5.39	1.31	1.25
1	C	318	ARG	CZ-NH1	5.09	1.39	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	442	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	366	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	318	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	C	551	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	442	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	551	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	D	442	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	442	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	134	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	576	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	D	366	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	576	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	B	134	ARG	NE-CZ-NH2	5.64	123.12	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	551	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	A	293	ASN	N-CA-CB	-5.60	100.53	110.60
1	B	551	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	534	LYS	CD-CE-NZ	5.32	123.93	111.70
1	D	576	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	C	366	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	551	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	D	528	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	442	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	551	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	206	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	339	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	D	551	ARG	NE-CZ-NH1	-5.01	117.80	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	3933	0	3921	43	0
1	B	3933	0	3921	53	0
1	C	3945	0	3929	60	0
1	D	3963	0	3948	49	0
2	A	28	0	12	0	0
2	B	28	0	12	2	0
2	C	28	0	12	2	0
2	D	28	0	12	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	12	1	0
4	B	64	0	24	1	0
4	D	32	0	12	0	0
5	A	31	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	31	0	12	2	0
5	C	31	0	12	0	0
5	D	31	0	12	0	0
6	A	93	0	0	12	0
6	B	86	0	0	22	0
6	C	117	0	0	31	0
6	D	71	0	0	25	0
All	All	16513	0	15863	199	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 6.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:MET:HE2	6:B:853:HOH:O	1.44	1.16
1:D:331:TYR:HE2	6:D:831:HOH:O	1.38	1.05
1:C:240:MET:SD	6:C:838:HOH:O	2.16	1.01
4:A:703:GTP:O3'	6:A:893:HOH:O	1.77	1.01
1:D:266:CYS:HB3	6:D:860:HOH:O	1.60	1.01
1:C:260:ILE:HB	6:C:844:HOH:O	1.57	1.00
1:A:276:LEU:HD11	6:A:836:HOH:O	1.62	0.99
1:C:439:LYS:O	1:C:443:GLU:HG3	1.65	0.96
1:C:471:GLU:HB2	6:C:824:HOH:O	1.66	0.95
1:C:115:MET:HE2	1:C:127:GLU:HG2	1.49	0.93
1:D:271:GLN:NE2	6:D:836:HOH:O	1.97	0.93
1:B:212:PRO:O	6:B:853:HOH:O	1.87	0.93
1:B:408:ARG:HD2	6:B:869:HOH:O	1.69	0.91
1:C:328:ASN:ND2	1:C:365:THR:OG1	2.03	0.91
1:C:485:PRO:O	1:C:486:LYS:HB2	1.71	0.90
1:B:115:MET:HB2	6:B:825:HOH:O	1.71	0.89
1:C:118:ILE:HD12	1:C:126:ILE:HB	1.55	0.88
1:B:584:GLY:HA3	6:B:836:HOH:O	1.75	0.87
1:D:171:VAL:HG22	6:D:834:HOH:O	1.77	0.83
1:C:348:ARG:HD3	6:C:856:HOH:O	1.78	0.82
1:C:118:ILE:CD1	1:C:126:ILE:HB	2.12	0.80
1:C:305:ARG:HD2	6:C:856:HOH:O	1.82	0.80
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.15	0.80
1:B:115:MET:CB	6:B:825:HOH:O	2.27	0.79
1:A:238:VAL:HG13	1:A:269:LYS:HE3	1.63	0.79
1:D:596:LYS:HE2	1:D:597:GLU:OE1	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:PRO:HB3	6:C:865:HOH:O	1.84	0.76
1:D:346:GLU:HA	6:D:816:HOH:O	1.85	0.75
1:D:292:GLU:O	6:D:816:HOH:O	2.04	0.75
1:B:385:MET:HE1	6:B:839:HOH:O	1.87	0.75
1:B:140:GLN:HG3	1:B:240:MET:CE	2.16	0.74
1:C:114:THR:HA	6:C:898:HOH:O	1.86	0.74
1:D:331:TYR:HD2	6:D:824:HOH:O	1.70	0.74
1:B:594:GLN:N	1:B:594:GLN:OE1	2.20	0.74
1:D:289:GLY:HA2	6:D:860:HOH:O	1.85	0.74
1:A:140:GLN:HG3	1:A:240:MET:CE	2.18	0.73
1:A:288:LYS:NZ	6:A:833:HOH:O	2.22	0.73
1:A:425:ASN:OD1	1:D:425:ASN:ND2	2.21	0.73
1:B:446:LYS:HE2	6:B:874:HOH:O	1.87	0.72
1:C:260:ILE:CB	6:C:844:HOH:O	2.27	0.72
1:B:466:ILE:HD12	6:B:870:HOH:O	1.88	0.71
1:D:331:TYR:CE2	6:D:831:HOH:O	2.24	0.70
1:B:447:GLN:C	6:B:839:HOH:O	2.29	0.70
1:D:535:ASN:HA	6:D:856:HOH:O	1.91	0.69
1:C:322:HIS:CE1	6:C:842:HOH:O	2.46	0.68
1:C:115:MET:SD	1:C:115:MET:C	2.73	0.67
1:C:260:ILE:CG2	6:C:844:HOH:O	2.42	0.66
1:B:193:GLU:O	6:B:847:HOH:O	2.13	0.66
1:D:267:PHE:CE2	6:D:836:HOH:O	2.49	0.66
1:D:310:VAL:O	6:D:834:HOH:O	2.14	0.66
1:C:485:PRO:O	1:C:486:LYS:CB	2.40	0.65
1:C:498:PHE:CB	6:C:865:HOH:O	2.45	0.65
1:C:405:LYS:HE2	6:C:906:HOH:O	1.95	0.65
1:C:115:MET:O	6:C:912:HOH:O	2.14	0.64
1:D:266:CYS:CB	6:D:860:HOH:O	2.28	0.64
1:B:140:GLN:CG	1:B:240:MET:CE	2.76	0.64
1:B:216:MET:HB3	6:B:853:HOH:O	1.97	0.64
1:A:326:GLN:HE21	1:A:327:ASN:H	1.46	0.63
5:B:706:DGT:O3G	6:B:886:HOH:O	2.15	0.63
1:C:498:PHE:HB3	6:C:865:HOH:O	1.99	0.63
1:D:180[B]:HIS:CD2	6:D:815:HOH:O	2.52	0.63
1:D:180[B]:HIS:HD2	6:D:815:HOH:O	1.81	0.63
1:A:328:ASN:OD1	1:A:328:ASN:C	2.37	0.63
1:D:266:CYS:SG	6:D:860:HOH:O	2.55	0.62
1:C:269:LYS:NZ	6:C:853:HOH:O	2.32	0.61
1:B:562:LEU:HB2	6:B:852:HOH:O	2.00	0.60
1:A:140:GLN:CG	1:A:240:MET:CE	2.78	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:MET:SD	1:C:115:MET:O	2.60	0.60
1:A:405:LYS:HD3	1:A:407:TYR:OH	2.02	0.60
1:C:532:ILE:HG13	6:C:874:HOH:O	2.01	0.60
1:C:326:GLN:O	6:C:854:HOH:O	2.16	0.59
1:A:326:GLN:HE21	1:A:327:ASN:N	2.00	0.59
1:B:322:HIS:CE1	6:C:821:HOH:O	2.55	0.59
1:B:254:MET:HE2	1:B:261:PRO:HG3	1.85	0.58
1:B:390:PHE:CZ	1:B:426:ILE:HG22	2.37	0.58
1:A:592:THR:O	6:A:860:HOH:O	2.16	0.58
1:A:276:LEU:CD1	6:A:836:HOH:O	2.35	0.58
1:A:180:HIS:CD2	6:A:808:HOH:O	2.56	0.58
1:B:582:GLN:HB2	6:D:850:HOH:O	2.05	0.57
1:A:140:GLN:HG3	1:A:240:MET:HE1	1.87	0.56
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.05	0.55
1:A:238:VAL:CG1	1:A:269:LYS:HE3	2.34	0.55
1:A:352:ARG:CZ	1:A:354:LYS:HD3	2.37	0.55
1:D:289:GLY:CA	6:D:860:HOH:O	2.47	0.55
1:C:336:LYS:HE3	1:D:127:GLU:HG3	1.89	0.54
1:D:577:ASN:HA	6:D:839:HOH:O	2.07	0.54
1:A:299:GLU:HG2	6:A:829:HOH:O	2.06	0.54
1:A:305:ARG:HB3	6:A:829:HOH:O	2.07	0.54
1:D:284:LEU:HD13	1:D:285:TRP:N	2.24	0.53
1:B:599:ASN:C	6:B:848:HOH:O	2.47	0.53
1:A:180:HIS:HD2	6:A:808:HOH:O	1.89	0.53
1:B:392:LYS:HE2	1:B:444:ILE:HD11	1.91	0.53
1:C:392:LYS:HE2	1:C:444:ILE:HD11	1.92	0.52
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.09	0.52
1:B:254:MET:HE1	1:B:261:PRO:HA	1.91	0.52
1:C:477:PRO:CB	6:C:865:HOH:O	2.52	0.52
1:D:392:LYS:HE2	1:D:444:ILE:HD11	1.91	0.52
1:B:331:TYR:CD1	1:B:331:TYR:C	2.82	0.52
1:C:185:LYS:HE2	6:C:877:HOH:O	2.09	0.52
1:C:305:ARG:CD	6:C:856:HOH:O	2.50	0.52
1:A:478:LYS:HE2	1:A:495:ALA:HB2	1.92	0.51
1:D:162:HIS:H	1:D:162:HIS:CD2	2.29	0.51
1:A:598:TRP:O	1:A:599:ASN:HB2	2.11	0.51
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.11	0.51
1:A:127:GLU:HG3	1:B:336:LYS:HE3	1.92	0.50
1:A:326:GLN:HG2	1:C:327:ASN:O	2.11	0.50
1:D:455:LYS:C	6:D:838:HOH:O	2.50	0.50
1:B:140:GLN:HG3	1:B:240:MET:HE2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.12	0.50
1:D:162:HIS:HE1	1:D:319:ASP:OD1	1.94	0.49
1:C:520:PHE:HB2	6:C:874:HOH:O	2.12	0.49
1:D:314:ASP:HB2	6:D:834:HOH:O	2.13	0.49
1:B:140:GLN:HG3	1:B:240:MET:HE1	1.93	0.48
1:A:336:LYS:HE3	1:B:127:GLU:HG3	1.95	0.48
1:C:331:TYR:C	1:C:331:TYR:CD1	2.86	0.48
1:A:226:ARG:HB3	1:A:229:VAL:HG23	1.95	0.48
1:B:390:PHE:CZ	1:B:426:ILE:CG2	2.97	0.48
1:C:127:GLU:HG3	1:D:336:LYS:HE3	1.95	0.48
1:D:331:TYR:CD2	6:D:824:HOH:O	2.54	0.48
1:A:266:CYS:HA	6:A:836:HOH:O	2.14	0.48
1:A:405:LYS:HD3	1:A:407:TYR:CZ	2.48	0.48
1:C:520:PHE:HD2	6:C:874:HOH:O	1.96	0.48
1:D:331:TYR:C	1:D:331:TYR:CD1	2.86	0.48
1:C:530:ILE:HG13	6:C:874:HOH:O	2.13	0.48
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.14	0.48
1:D:351:ALA:O	1:D:520:PHE:HA	2.14	0.47
1:D:511:GLU:H	1:D:511:GLU:CD	2.17	0.47
1:B:215:HIS:CD2	2:B:701:DCP:C6	2.97	0.47
1:D:474:GLU:O	1:D:478:LYS:NZ	2.39	0.47
1:A:352:ARG:NH2	1:A:354:LYS:HD3	2.29	0.47
1:B:511:GLU:H	1:B:511:GLU:CD	2.18	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.15	0.47
1:A:351:ALA:O	1:A:520:PHE:HA	2.13	0.47
1:B:508:GLY:C	6:B:840:HOH:O	2.53	0.47
1:D:215:HIS:NE2	2:D:703:DCP:O1A	2.47	0.47
1:A:331:TYR:C	1:A:331:TYR:CD1	2.87	0.47
2:B:701:DCP:H5'1	6:B:818:HOH:O	2.15	0.46
1:D:277:GLU:HG2	1:D:278:SER:N	2.30	0.46
1:A:326:GLN:NE2	1:C:326:GLN:HE21	2.14	0.46
1:B:115:MET:CE	1:B:127:GLU:OE1	2.64	0.46
2:C:703:DCP:H5'1	6:C:889:HOH:O	2.15	0.46
1:B:116:LYS:NZ	4:B:705:GTP:O2G	2.44	0.46
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.16	0.45
1:C:500:VAL:HG23	6:C:865:HOH:O	2.16	0.45
1:D:456:TYR:C	6:D:838:HOH:O	2.53	0.45
1:C:118:ILE:HD11	1:C:126:ILE:HB	1.95	0.45
1:A:322:HIS:NE2	6:A:859:HOH:O	2.36	0.45
1:C:523:LYS:HD2	6:C:911:HOH:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ALA:O	1:B:520:PHE:HA	2.17	0.45
1:C:215:HIS:CE1	2:C:703:DCP:O2A	2.70	0.45
1:B:254:MET:CE	1:B:261:PRO:HA	2.46	0.45
1:A:244:LEU:C	1:A:244:LEU:HD23	2.37	0.44
1:B:235:GLN:O	1:B:238:VAL:HG22	2.17	0.44
1:D:244:LEU:C	1:D:244:LEU:HD23	2.37	0.44
1:D:215:HIS:CE1	2:D:703:DCP:O1A	2.70	0.44
1:A:592:THR:N	1:A:593:PRO:CD	2.80	0.44
1:A:326:GLN:CG	1:C:327:ASN:O	2.65	0.44
1:C:115:MET:CE	1:C:127:GLU:HG2	2.33	0.44
1:B:284:LEU:HD13	1:B:285:TRP:N	2.32	0.44
1:D:314:ASP:CB	6:D:834:HOH:O	2.66	0.44
1:D:322:HIS:CE1	6:D:814:HOH:O	2.70	0.44
5:A:704:DGT:O2B	1:C:377:LYS:NZ	2.48	0.44
1:B:115:MET:C	6:B:825:HOH:O	2.56	0.44
1:C:244:LEU:C	1:C:244:LEU:HD23	2.38	0.43
1:C:351:ALA:O	1:C:520:PHE:HA	2.18	0.43
1:B:244:LEU:C	1:B:244:LEU:HD23	2.38	0.43
1:C:576:ARG:O	1:C:577:ASN:HB2	2.18	0.43
1:D:143:ARG:HD2	1:D:420:THR:HA	2.00	0.43
1:D:592:THR:N	1:D:593:PRO:CD	2.81	0.43
1:C:263:GLU:HB2	6:C:844:HOH:O	2.17	0.43
1:C:238:VAL:HG13	1:C:269:LYS:HD2	2.00	0.43
1:C:592:THR:N	1:C:593:PRO:CD	2.82	0.42
1:B:509:MET:N	6:B:840:HOH:O	2.52	0.42
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.01	0.42
1:A:334:PHE:CE2	1:A:359:LEU:HD21	2.54	0.42
1:B:309:ASP:HB3	6:B:842:HOH:O	2.18	0.42
1:B:594:GLN:OE1	1:B:594:GLN:CA	2.68	0.42
1:B:151:GLY:O	6:B:830:HOH:O	2.21	0.42
1:D:118:ILE:HD13	1:D:118:ILE:HG21	1.78	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.88	0.42
1:A:534:LYS:HE3	1:A:542:PRO:O	2.20	0.41
1:D:499:ILE:HD11	1:D:555:LYS:HE2	2.02	0.41
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.87	0.41
1:B:425:ASN:HB2	1:C:428:LEU:CD1	2.51	0.41
1:A:251:LYS:HB2	1:A:252:PRO:HD3	2.02	0.41
1:A:599:ASN:C	6:A:860:HOH:O	2.58	0.41
1:B:334:PHE:CE2	1:B:359:LEU:HD21	2.56	0.41
1:C:394:ASP:O	1:C:408:ARG:HD3	2.21	0.41
1:D:455:LYS:HG2	1:D:557:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:HIS:HE1	6:C:864:HOH:O	2.04	0.41
1:B:197:LEU:HG	6:B:847:HOH:O	2.20	0.41
5:B:706:DGT:O2B	1:D:377:LYS:NZ	2.52	0.41
1:C:498:PHE:HB2	6:C:865:HOH:O	2.17	0.41
1:D:251:LYS:HB2	1:D:252:PRO:HD3	2.02	0.41
1:A:143:ARG:HD2	1:A:420:THR:HA	2.03	0.40
1:C:263:GLU:CD	6:C:844:HOH:O	2.60	0.40
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.87	0.40
1:B:499:ILE:HD11	1:B:555:LYS:HE2	2.04	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	477/514 (93%)	467 (98%)	10 (2%)	0	100	100
1	B	477/514 (93%)	468 (98%)	9 (2%)	0	100	100
1	C	479/514 (93%)	469 (98%)	9 (2%)	1 (0%)	47	49
1	D	481/514 (94%)	471 (98%)	10 (2%)	0	100	100
All	All	1914/2056 (93%)	1875 (98%)	38 (2%)	1 (0%)	51	54

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	427/459 (93%)	417 (98%)	10 (2%)	50	55
1	B	427/459 (93%)	414 (97%)	13 (3%)	41	44
1	C	429/459 (94%)	416 (97%)	13 (3%)	41	44
1	D	431/459 (94%)	417 (97%)	14 (3%)	39	41
All	All	1714/1836 (93%)	1664 (97%)	50 (3%)	42	46

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	185	LYS
1	A	277	GLU
1	A	315	TYR
1	A	328	ASN
1	A	354	LYS
1	A	408	ARG
1	A	478	LYS
1	A	486	LYS
1	A	510	GLN
1	B	136	ILE
1	B	229	VAL
1	B	284	LEU
1	B	302	SER
1	B	315	TYR
1	B	326	GLN
1	B	331	TYR
1	B	339	ARG
1	B	354	LYS
1	B	388	ASP
1	B	426	ILE
1	B	474	GLU
1	B	594	GLN
1	C	115	MET
1	C	118	ILE
1	C	134	ARG
1	C	184	GLU
1	C	229	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	230	LYS
1	C	240	MET
1	C	277	GLU
1	C	315	TYR
1	C	328	ASN
1	C	354	LYS
1	C	377	LYS
1	C	486	LYS
1	D	185	LYS
1	D	229	VAL
1	D	240	MET
1	D	277	GLU
1	D	315	TYR
1	D	326	GLN
1	D	331	TYR
1	D	359	LEU
1	D	474	GLU
1	D	478	LYS
1	D	490	ASP
1	D	510	GLN
1	D	543	GLU
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	243	HIS
1	A	326	GLN
1	B	425	ASN
1	B	527	ASN
1	C	235	GLN
1	C	326	GLN
1	C	328	ASN
1	D	162	HIS
1	D	233	HIS
1	D	328	ASN
1	D	535	ASN
1	D	594	GLN

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 20 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
2	DCP	A	701	3	25,29,29	1.26	4 (16%)	37,45,45	1.42	6 (16%)
4	GTP	A	703	3	26,34,34	1.13	1 (3%)	32,54,54	1.68	6 (18%)
2	DCP	C	703	3	25,29,29	1.21	3 (12%)	37,45,45	1.46	5 (13%)
5	DGT	C	701	3	26,33,33	1.34	4 (15%)	32,52,52	1.56	7 (21%)
5	DGT	D	702	3	26,33,33	0.97	2 (7%)	32,52,52	1.32	6 (18%)
2	DCP	B	701	3	25,29,29	0.99	1 (4%)	37,45,45	1.37	4 (10%)
4	GTP	D	705	3	26,34,34	1.63	4 (15%)	32,54,54	1.73	7 (21%)
2	DCP	D	703	-	25,29,29	1.08	1 (4%)	37,45,45	1.40	5 (13%)
4	GTP	B	703	3	26,34,34	1.21	3 (11%)	32,54,54	1.64	5 (15%)
5	DGT	B	706	3	26,33,33	1.18	1 (3%)	32,52,52	1.79	11 (34%)
4	GTP	B	705	3	26,34,34	1.22	3 (11%)	32,54,54	1.69	11 (34%)
5	DGT	A	704	3	26,33,33	1.06	1 (3%)	32,52,52	1.74	9 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DCP	A	701	3	-	6/22/34/34	0/2/2/2
4	GTP	A	703	3	-	4/18/38/38	0/3/3/3
2	DCP	C	703	3	-	3/22/34/34	0/2/2/2
5	DGT	C	701	3	-	3/18/34/34	0/3/3/3
5	DGT	D	702	3	-	3/18/34/34	0/3/3/3
2	DCP	B	701	3	-	5/22/34/34	0/2/2/2
4	GTP	D	705	3	-	3/18/38/38	0/3/3/3
2	DCP	D	703	-	-	4/22/34/34	0/2/2/2
4	GTP	B	703	3	-	1/18/38/38	0/3/3/3
5	DGT	B	706	3	-	5/18/34/34	0/3/3/3
4	GTP	B	705	3	-	5/18/38/38	0/3/3/3
5	DGT	A	704	3	-	2/18/34/34	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	705	GTP	O4'-C1'	4.44	1.47	1.41
4	D	705	GTP	PA-O1A	-3.35	1.39	1.50
4	D	705	GTP	C2'-C1'	-3.13	1.49	1.53
4	B	703	GTP	C6-N1	-3.12	1.33	1.37
2	A	701	DCP	O3'-C3'	3.01	1.49	1.43
4	B	705	GTP	PA-O2A	-2.94	1.41	1.55
5	C	701	DGT	PG-O2G	-2.77	1.44	1.54
4	D	705	GTP	PG-O2G	-2.62	1.44	1.54
4	B	703	GTP	C5-C4	2.60	1.49	1.43
2	A	701	DCP	C2-N3	-2.54	1.31	1.36
5	B	706	DGT	C5-C4	2.49	1.49	1.43
2	D	703	DCP	C6-C5	2.49	1.40	1.35
2	C	703	DCP	C5-C4	-2.43	1.37	1.42
5	D	702	DGT	C5-C4	2.40	1.49	1.43
5	C	701	DGT	C6-N1	-2.38	1.34	1.37
2	B	701	DCP	C6-C5	2.35	1.40	1.35
5	A	704	DGT	O6-C6	2.28	1.27	1.23
4	B	705	GTP	C2'-C1'	-2.25	1.50	1.53
2	A	701	DCP	C4-N3	2.24	1.39	1.34
2	A	701	DCP	C6-C5	2.20	1.40	1.35
4	B	705	GTP	PB-O1B	-2.15	1.43	1.50
4	B	703	GTP	PG-O2G	-2.15	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	701	DGT	O4'-C4'	-2.12	1.40	1.45
4	A	703	GTP	PA-O2A	-2.12	1.45	1.55
5	D	702	DGT	C6-N1	-2.11	1.34	1.37
2	C	703	DCP	O2-C2	2.08	1.27	1.23
2	C	703	DCP	PA-O5'	2.02	1.67	1.59
5	C	701	DGT	O3'-C3'	2.01	1.47	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	705	GTP	C3'-C2'-C1'	5.36	109.05	100.98
4	B	703	GTP	C3'-C2'-C1'	4.90	108.35	100.98
4	A	703	GTP	C3'-C2'-C1'	4.65	107.98	100.98
2	D	703	DCP	PB-O3B-PG	-4.38	117.81	132.83
2	B	701	DCP	PB-O3B-PG	-4.30	118.07	132.83
2	C	703	DCP	O4'-C1'-N1	4.17	115.31	107.86
5	A	704	DGT	O2G-PG-O1G	3.99	122.88	107.64
2	A	701	DCP	PB-O3B-PG	-3.95	119.26	132.83
4	B	703	GTP	PA-O3A-PB	-3.81	119.75	132.83
4	D	705	GTP	PA-O3A-PB	-3.74	120.00	132.83
5	B	706	DGT	N2-C2-N1	3.72	124.64	116.71
5	B	706	DGT	N2-C2-N3	-3.58	112.76	119.74
2	C	703	DCP	PB-O3A-PA	-3.55	120.64	132.83
4	B	705	GTP	C3'-C2'-C1'	3.55	106.32	100.98
4	A	703	GTP	PA-O3A-PB	-3.51	120.80	132.83
5	A	704	DGT	O6-C6-N1	3.40	124.66	120.65
5	C	701	DGT	N2-C2-N3	-3.39	113.14	119.74
2	C	703	DCP	PB-O3B-PG	-3.31	121.48	132.83
2	A	701	DCP	PB-O3A-PA	-3.24	121.71	132.83
4	B	705	GTP	PA-O3A-PB	-3.20	121.85	132.83
2	B	701	DCP	PB-O3A-PA	-3.19	121.86	132.83
5	A	704	DGT	O6-C6-C5	-3.18	118.16	124.37
5	C	701	DGT	O6-C6-C5	-3.13	118.26	124.37
2	B	701	DCP	O3G-PG-O2G	3.06	119.35	107.64
5	A	704	DGT	N2-C2-N3	-3.02	113.85	119.74
5	B	706	DGT	O6-C6-C5	-3.01	118.50	124.37
4	B	705	GTP	O3G-PG-O1G	2.89	122.01	110.68
5	C	701	DGT	O6-C6-N1	2.88	124.05	120.65
5	B	706	DGT	O2G-PG-O1G	2.80	118.33	107.64
2	D	703	DCP	PB-O3A-PA	-2.76	123.37	132.83
2	A	701	DCP	O2B-PB-O1B	2.75	125.84	112.24
4	D	705	GTP	PB-O3B-PG	-2.75	123.39	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	701	DGT	N2-C2-N1	2.71	122.48	116.71
5	B	706	DGT	C5-C6-N1	2.70	118.72	113.95
4	A	703	GTP	O3B-PG-O1G	-2.68	96.33	111.19
4	A	703	GTP	O2B-PB-O1B	2.67	125.44	112.24
4	B	705	GTP	O3B-PG-O1G	-2.67	96.39	111.19
4	D	705	GTP	O2B-PB-O1B	2.62	125.20	112.24
2	D	703	DCP	C2'-C1'-N1	-2.60	107.77	113.77
5	C	701	DGT	PB-O3B-PG	-2.60	123.92	132.83
5	D	702	DGT	O2G-PG-O3B	-2.54	96.12	104.64
4	B	703	GTP	C5-C6-N1	2.54	118.43	113.95
5	A	704	DGT	O1B-PB-O2B	2.52	124.68	112.24
5	B	706	DGT	O3B-PG-O3G	-2.51	97.25	111.19
5	D	702	DGT	C8-N7-C5	2.48	107.72	102.99
5	B	706	DGT	C2'-C3'-C4'	2.48	107.92	102.76
4	B	703	GTP	PB-O3B-PG	-2.41	124.56	132.83
4	B	705	GTP	O6-C6-C5	-2.39	119.70	124.37
5	B	706	DGT	O1B-PB-O2B	2.38	123.99	112.24
5	D	702	DGT	C5-C6-N1	2.38	118.15	113.95
4	A	703	GTP	C8-N7-C5	2.37	107.51	102.99
5	D	702	DGT	O1A-PA-O2A	2.36	123.93	112.24
2	D	703	DCP	O4'-C1'-N1	2.36	112.09	107.86
4	B	705	GTP	C5-C6-N1	2.35	118.11	113.95
2	C	703	DCP	O3G-PG-O2G	2.34	116.59	107.64
4	B	705	GTP	O2B-PB-O1B	2.32	123.72	112.24
5	A	704	DGT	PB-O3B-PG	-2.32	124.86	132.83
4	B	705	GTP	N2-C2-N3	-2.31	115.24	119.74
2	B	701	DCP	C2'-C1'-N1	-2.29	108.50	113.77
4	D	705	GTP	O3G-PG-O2G	2.27	116.31	107.64
4	B	703	GTP	O2'-C2'-C1'	-2.24	102.59	110.85
4	D	705	GTP	C8-N7-C5	2.23	107.24	102.99
5	D	702	DGT	PB-O3B-PG	-2.22	125.20	132.83
2	A	701	DCP	O4'-C1'-N1	2.19	111.78	107.86
4	B	705	GTP	O2G-PG-O1G	2.18	119.22	110.68
2	C	703	DCP	C2'-C1'-N1	-2.14	108.84	113.77
5	D	702	DGT	C2'-C3'-C4'	2.13	107.20	102.76
5	B	706	DGT	O1A-PA-O2A	2.11	122.66	112.24
5	C	701	DGT	C5-C6-N1	2.11	117.67	113.95
4	A	703	GTP	O6-C6-C5	-2.10	120.28	124.37
5	C	701	DGT	O2G-PG-O3G	2.08	118.83	110.68
4	B	705	GTP	N2-C2-N1	2.08	121.14	116.71
5	B	706	DGT	C8-N7-C5	2.07	106.93	102.99
4	D	705	GTP	O2'-C2'-C1'	-2.06	103.26	110.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704	DGT	O2G-PG-O3B	-2.05	97.77	104.64
5	A	704	DGT	C2-N1-C6	-2.05	121.33	125.10
5	B	706	DGT	O1G-PG-O3B	-2.04	97.78	104.64
2	A	701	DCP	O3B-PG-O1G	-2.02	99.97	111.19
4	B	705	GTP	O2A-PA-O1A	2.02	122.22	112.24
5	A	704	DGT	O3B-PG-O3G	-2.02	99.99	111.19
2	A	701	DCP	O2-C2-N3	-2.01	119.06	122.33
2	D	703	DCP	O3G-PG-O2G	2.01	115.31	107.64

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DCP	C5'-O5'-PA-O1A
2	A	701	DCP	C5'-O5'-PA-O2A
4	B	705	GTP	PB-O3B-PG-O2G
5	B	706	DGT	PB-O3B-PG-O2G
5	C	701	DGT	PB-O3B-PG-O1G
5	D	702	DGT	PB-O3B-PG-O2G
2	C	703	DCP	C3'-C4'-C5'-O5'
2	C	703	DCP	O4'-C4'-C5'-O5'
2	D	703	DCP	O4'-C4'-C5'-O5'
2	B	701	DCP	C4'-C5'-O5'-PA
2	D	703	DCP	C4'-C5'-O5'-PA
2	D	703	DCP	C3'-C4'-C5'-O5'
2	A	701	DCP	C3'-C4'-C5'-O5'
2	C	703	DCP	C4'-C5'-O5'-PA
4	A	703	GTP	PB-O3B-PG-O1G
2	A	701	DCP	O4'-C4'-C5'-O5'
2	B	701	DCP	C3'-C4'-C5'-O5'
2	B	701	DCP	PB-O3A-PA-O5'
2	D	703	DCP	PB-O3A-PA-O5'
2	A	701	DCP	C4'-C5'-O5'-PA
4	B	705	GTP	PB-O3B-PG-O3G
2	A	701	DCP	C5'-O5'-PA-O3A
4	A	703	GTP	PG-O3B-PB-O1B
4	A	703	GTP	PG-O3B-PB-O2B
4	B	705	GTP	PG-O3B-PB-O2B
4	D	705	GTP	PG-O3B-PB-O1B
5	A	704	DGT	PG-O3B-PB-O1B
4	A	703	GTP	C4'-C5'-O5'-PA
2	B	701	DCP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	703	GTP	C4'-C5'-O5'-PA
4	D	705	GTP	C4'-C5'-O5'-PA
5	C	701	DGT	PG-O3B-PB-O1B
5	D	702	DGT	PG-O3B-PB-O1B
4	B	705	GTP	PG-O3B-PB-O1B
4	B	705	GTP	C4'-C5'-O5'-PA
5	A	704	DGT	PB-O3A-PA-O2A
5	C	701	DGT	PB-O3A-PA-O1A
2	B	701	DCP	C5'-O5'-PA-O3A
4	D	705	GTP	PG-O3B-PB-O2B
5	B	706	DGT	PG-O3B-PB-O1B
5	B	706	DGT	PG-O3B-PB-O2B
5	B	706	DGT	PB-O3A-PA-O1A
5	D	702	DGT	PG-O3B-PB-O2B
5	B	706	DGT	PB-O3B-PG-O3G

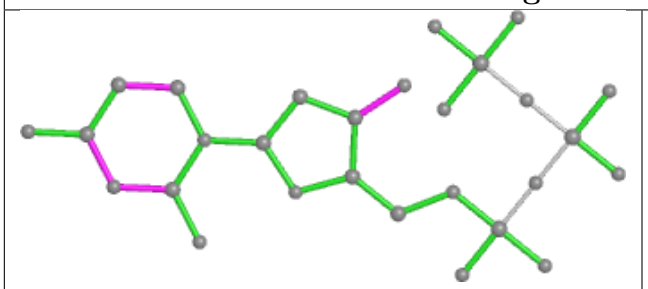
There are no ring outliers.

7 monomers are involved in 11 short contacts:

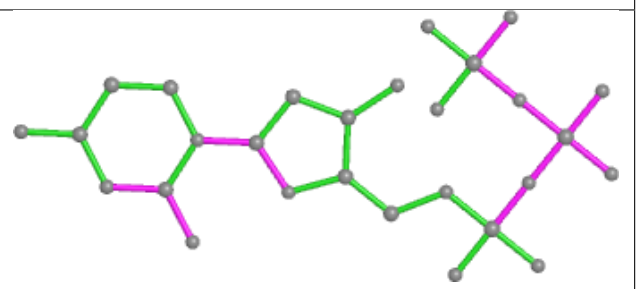
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	GTP	1	0
2	C	703	DCP	2	0
2	B	701	DCP	2	0
2	D	703	DCP	2	0
5	B	706	DGT	2	0
4	B	705	GTP	1	0
5	A	704	DGT	1	0

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 then 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.

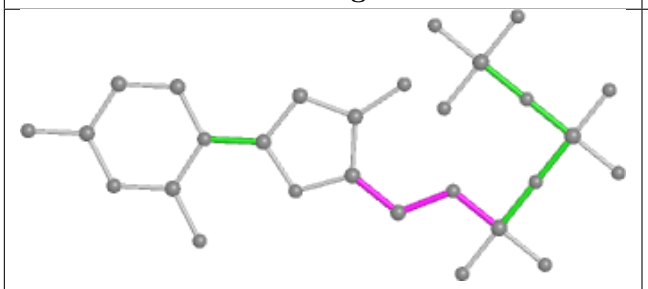
Ligand DCP A 701



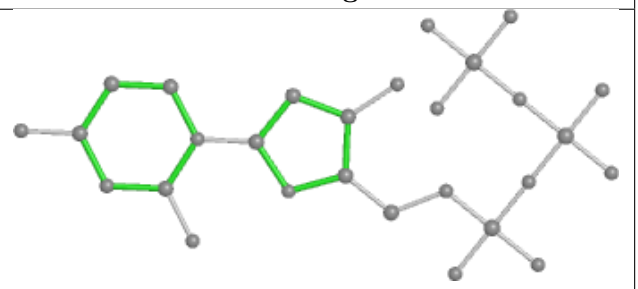
Bond lengths



Bond angles

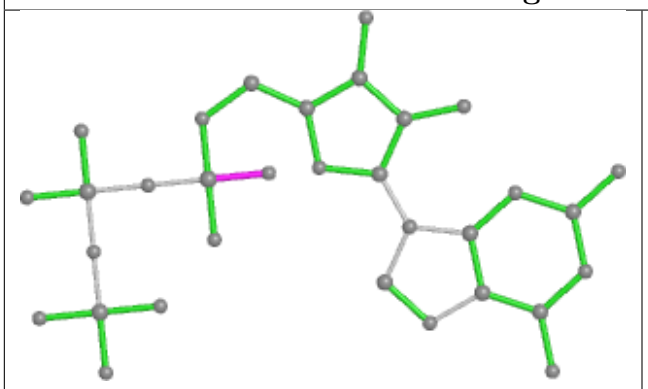


Torsions

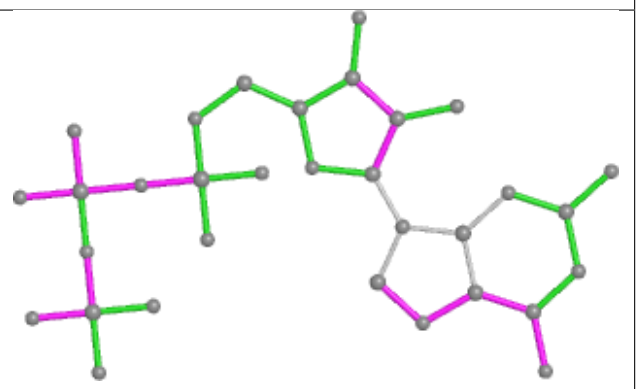


Rings

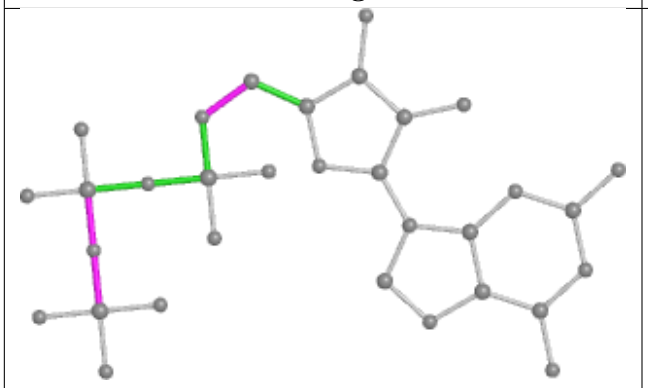
Ligand GTP A 703



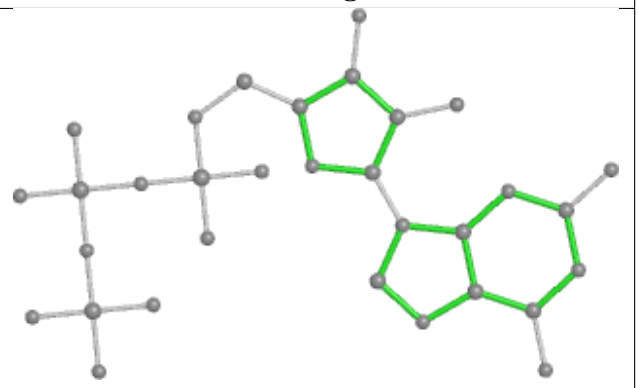
Bond lengths



Bond angles

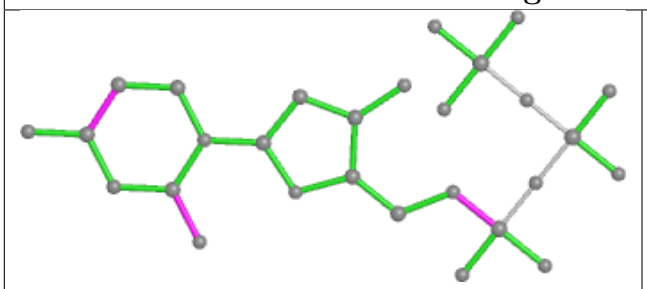


Torsions

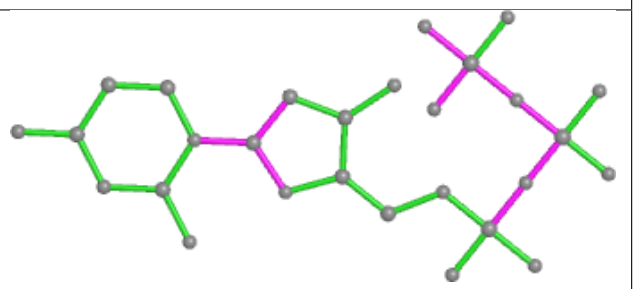


Rings

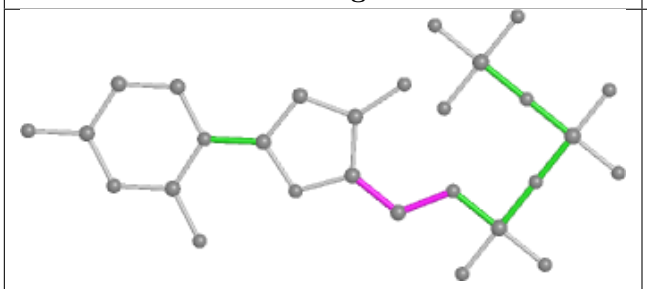
Ligand DCP C 703



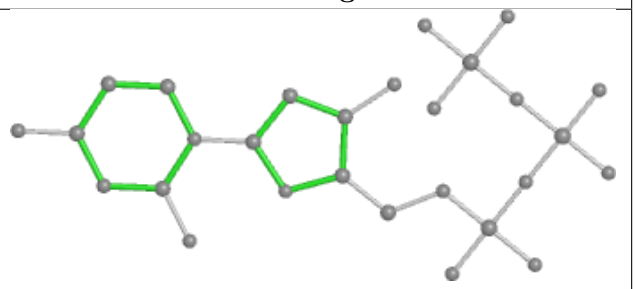
Bond lengths



Bond angles

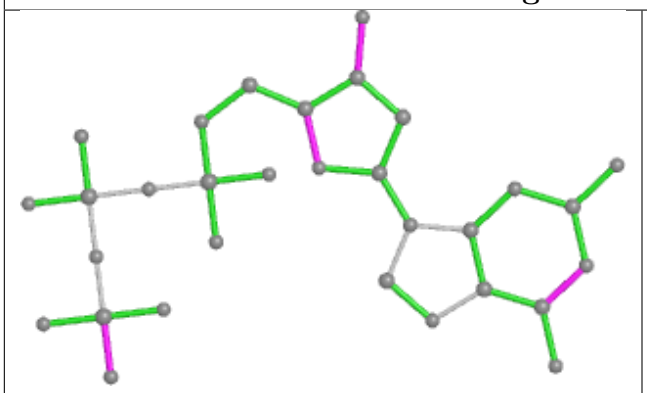


Torsions

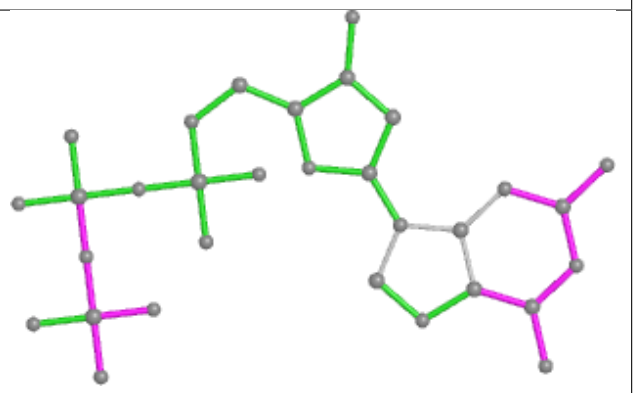


Rings

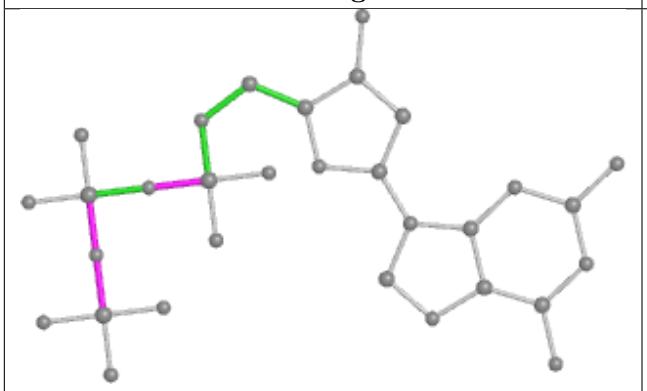
Ligand DGT C 701



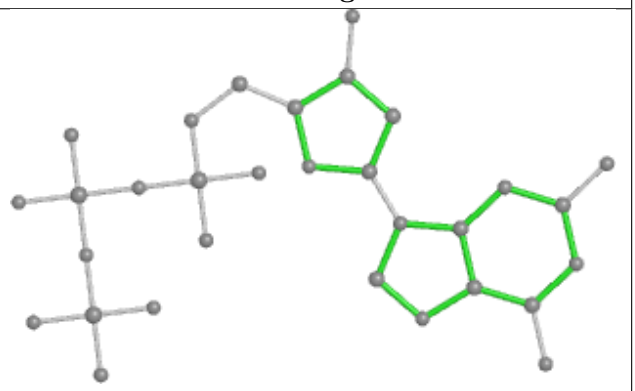
Bond lengths



Bond angles

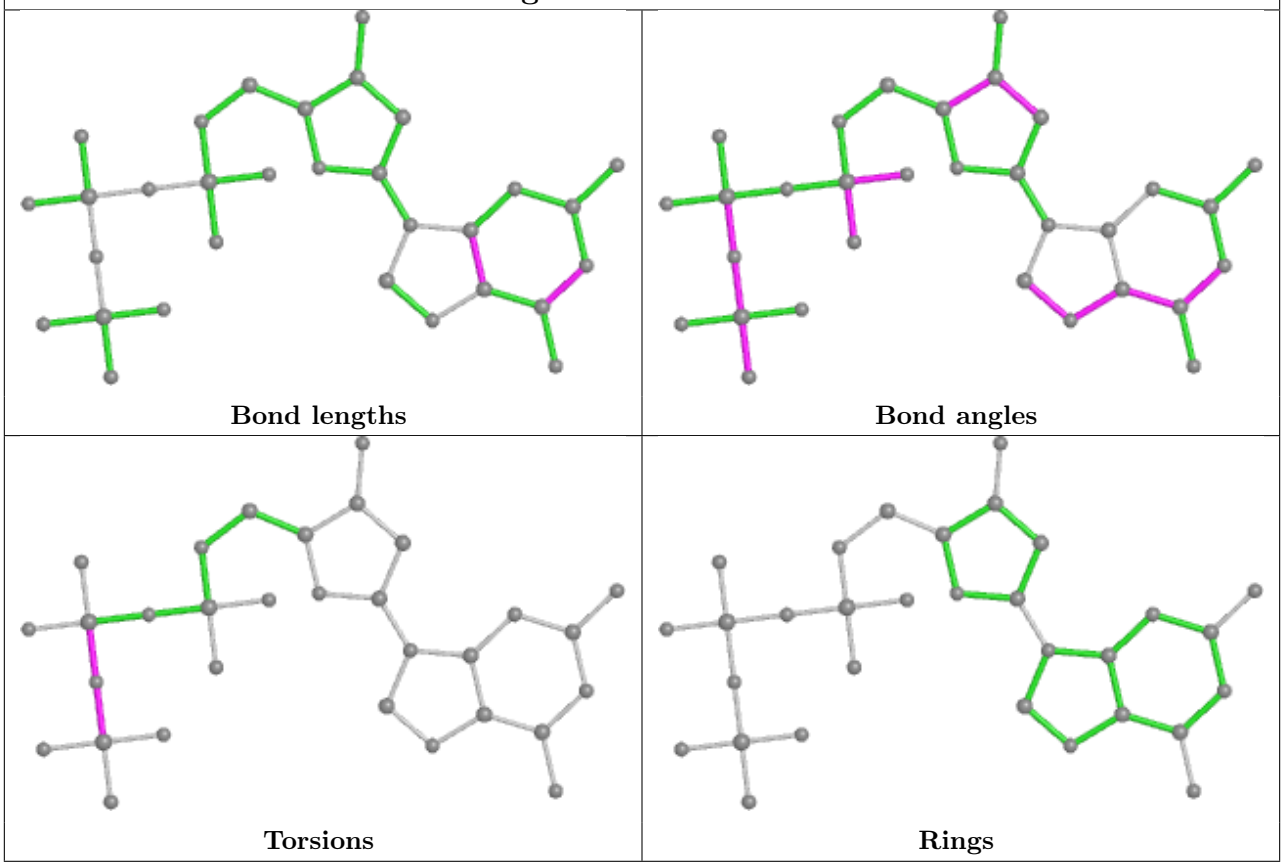


Torsions

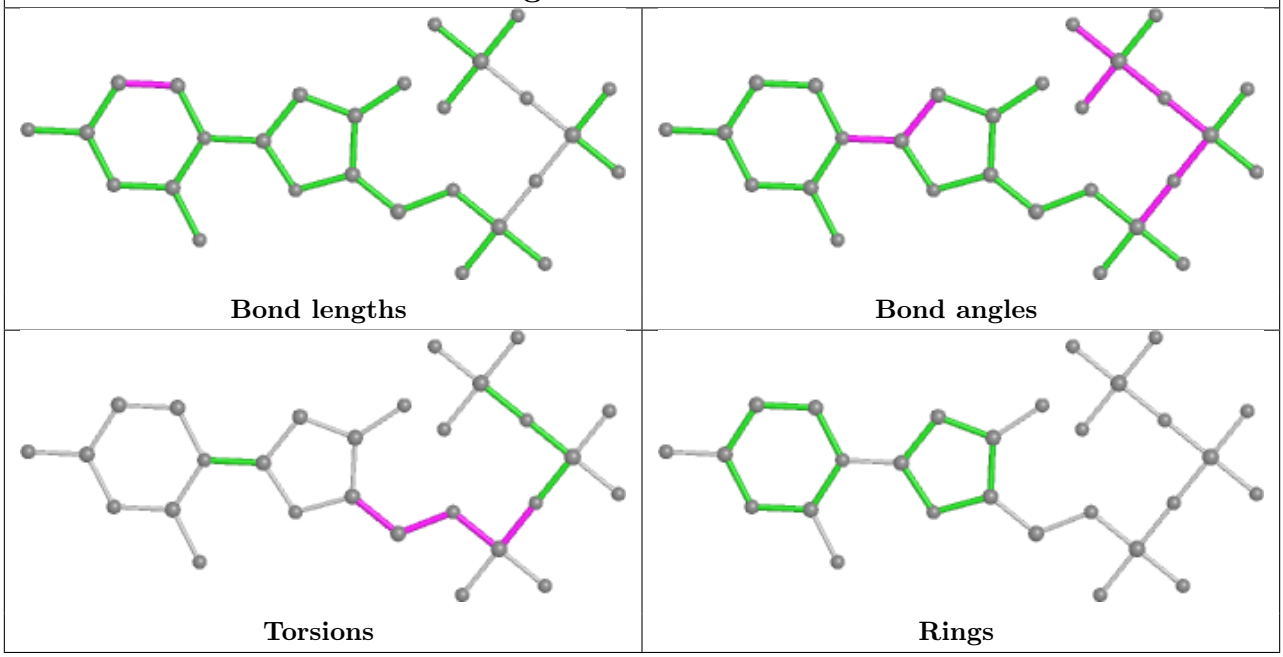


Rings

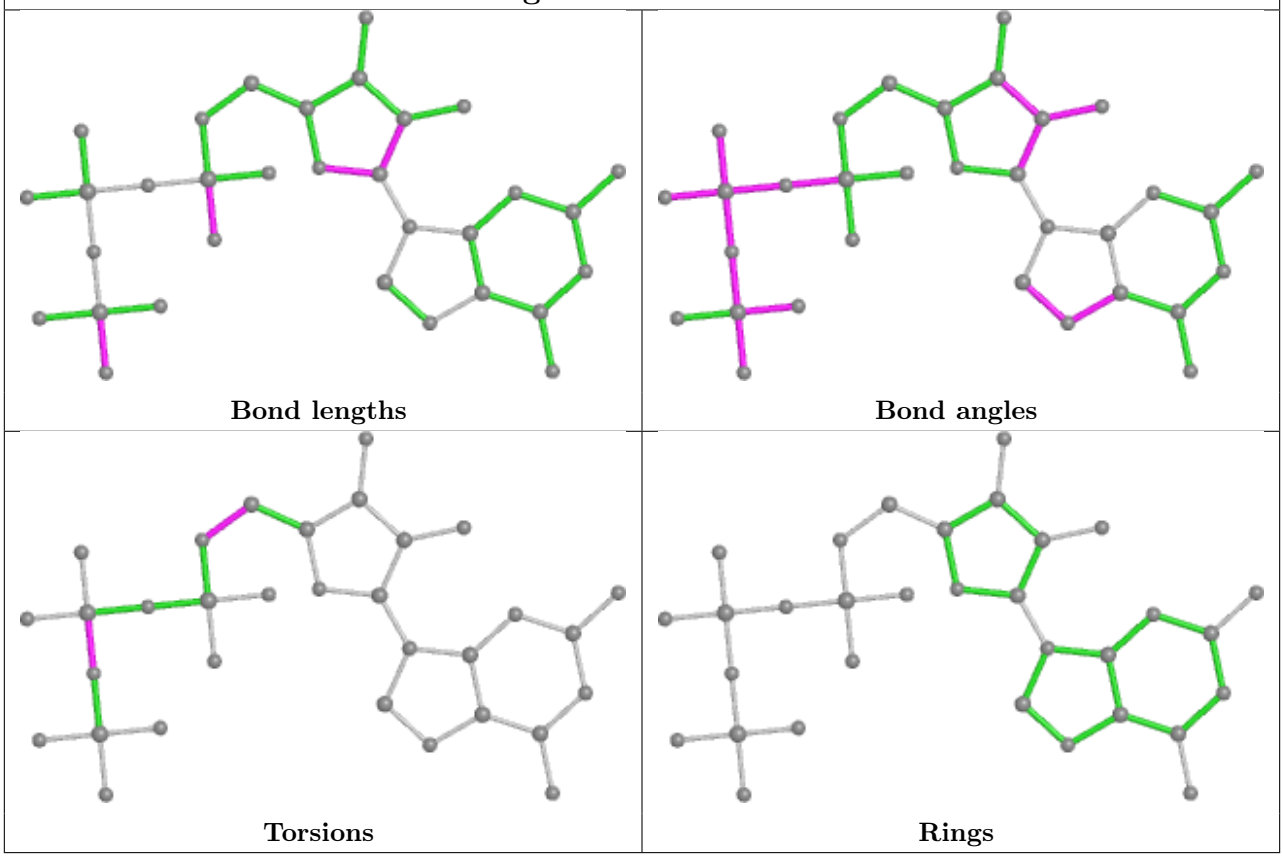
Ligand DGT D 702



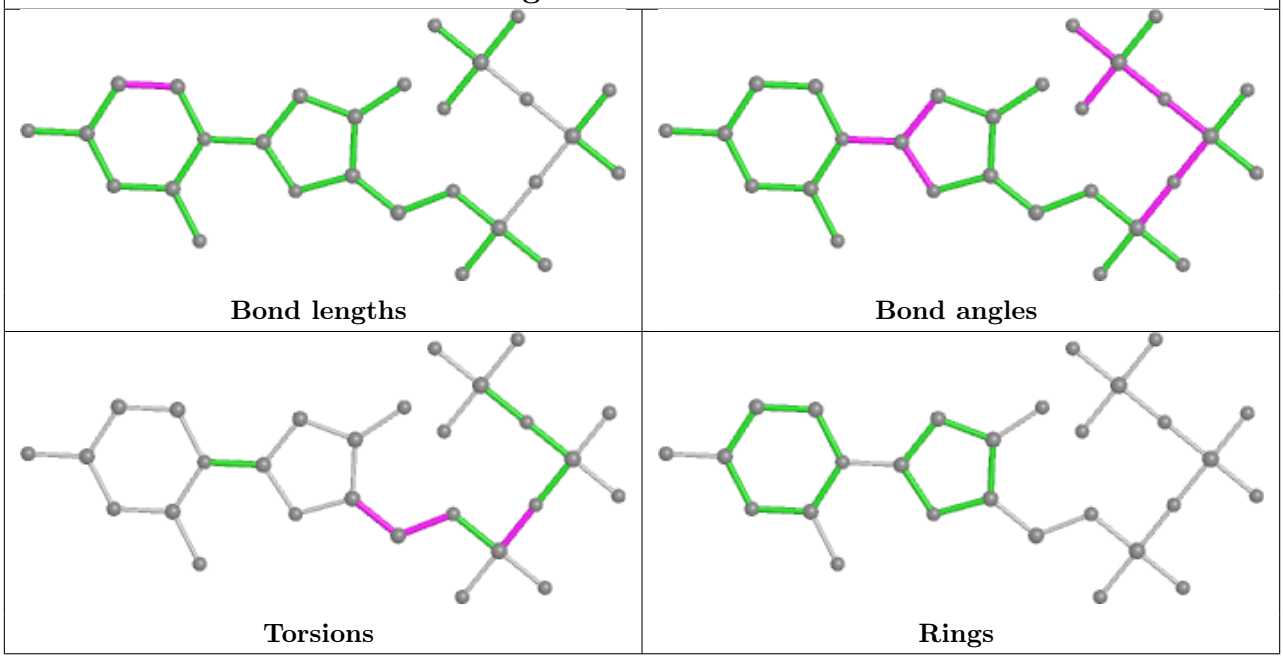
Ligand DCP B 701



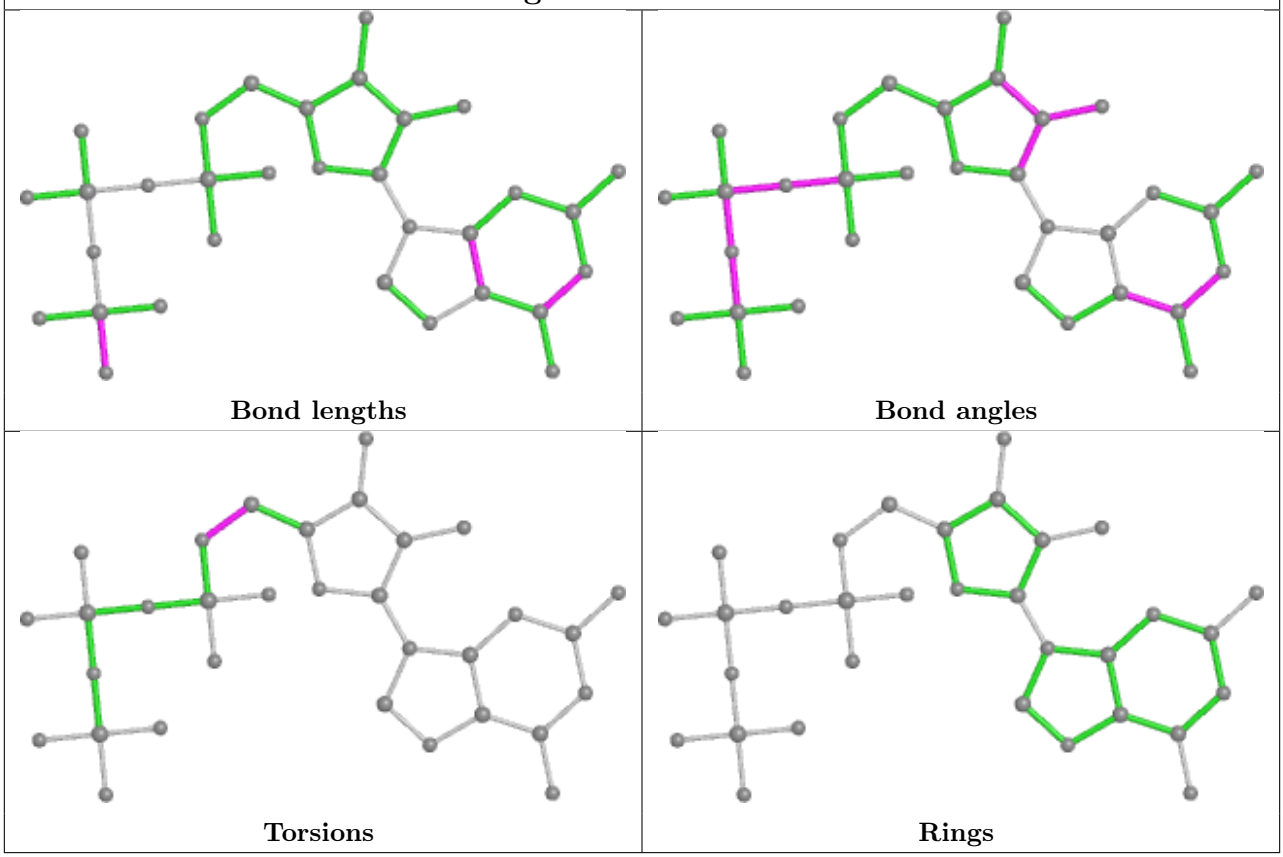
Ligand GTP D 705



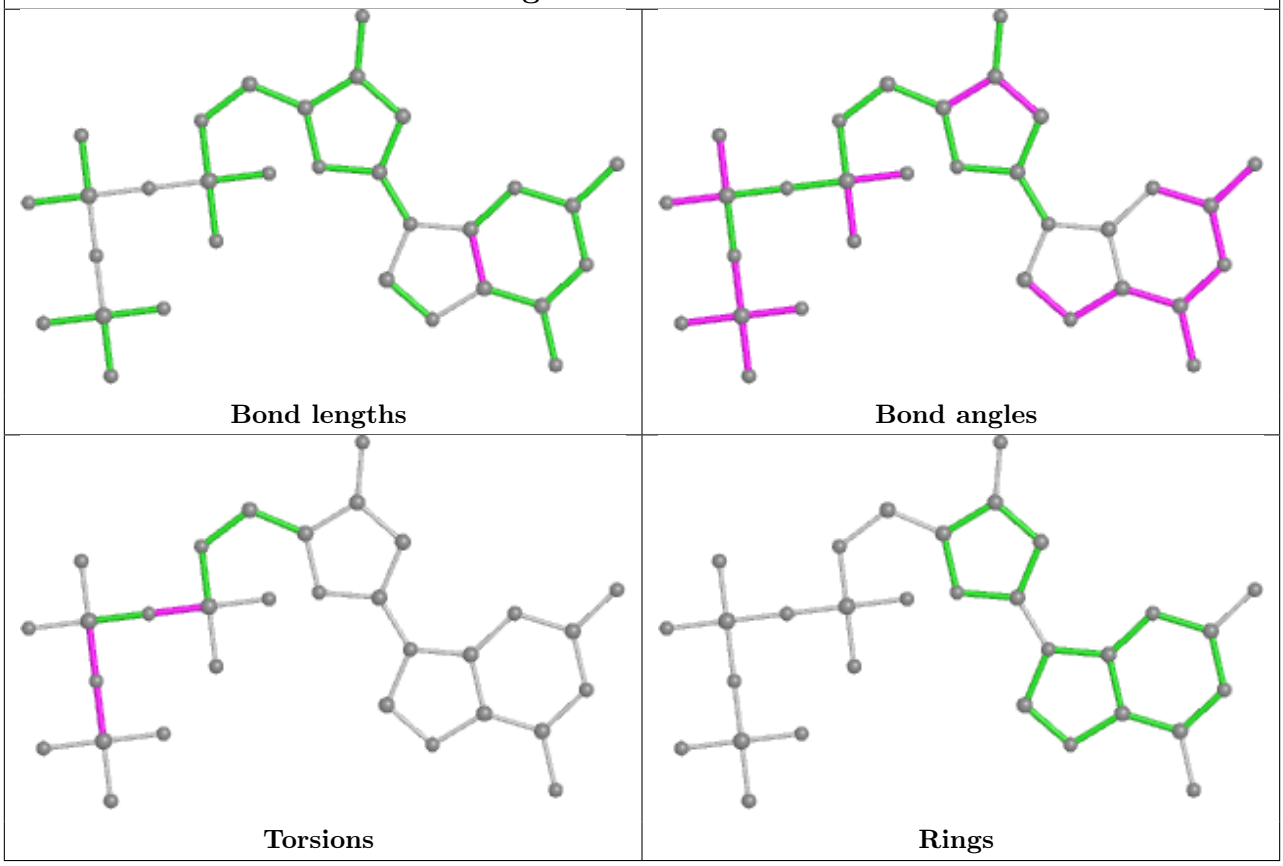
Ligand DCP D 703



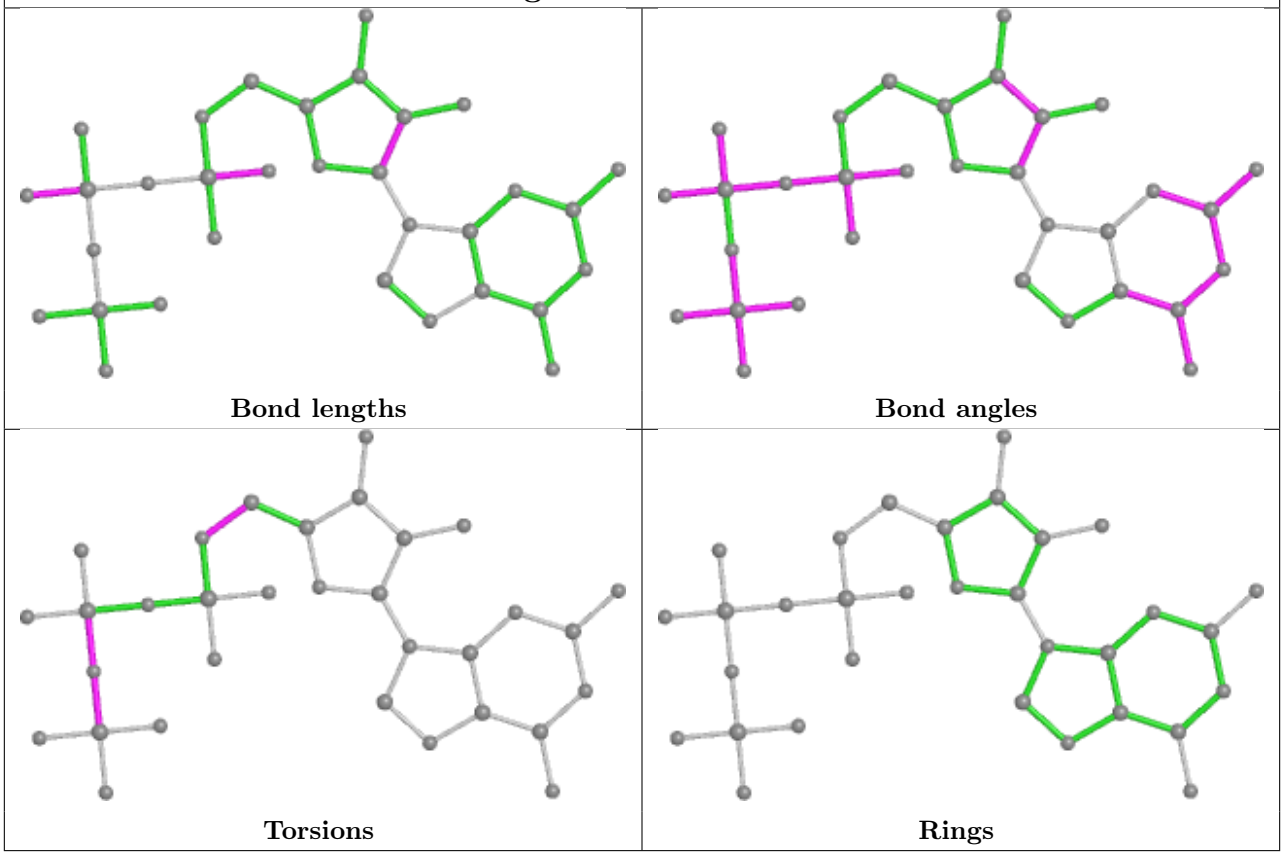
Ligand GTP B 703



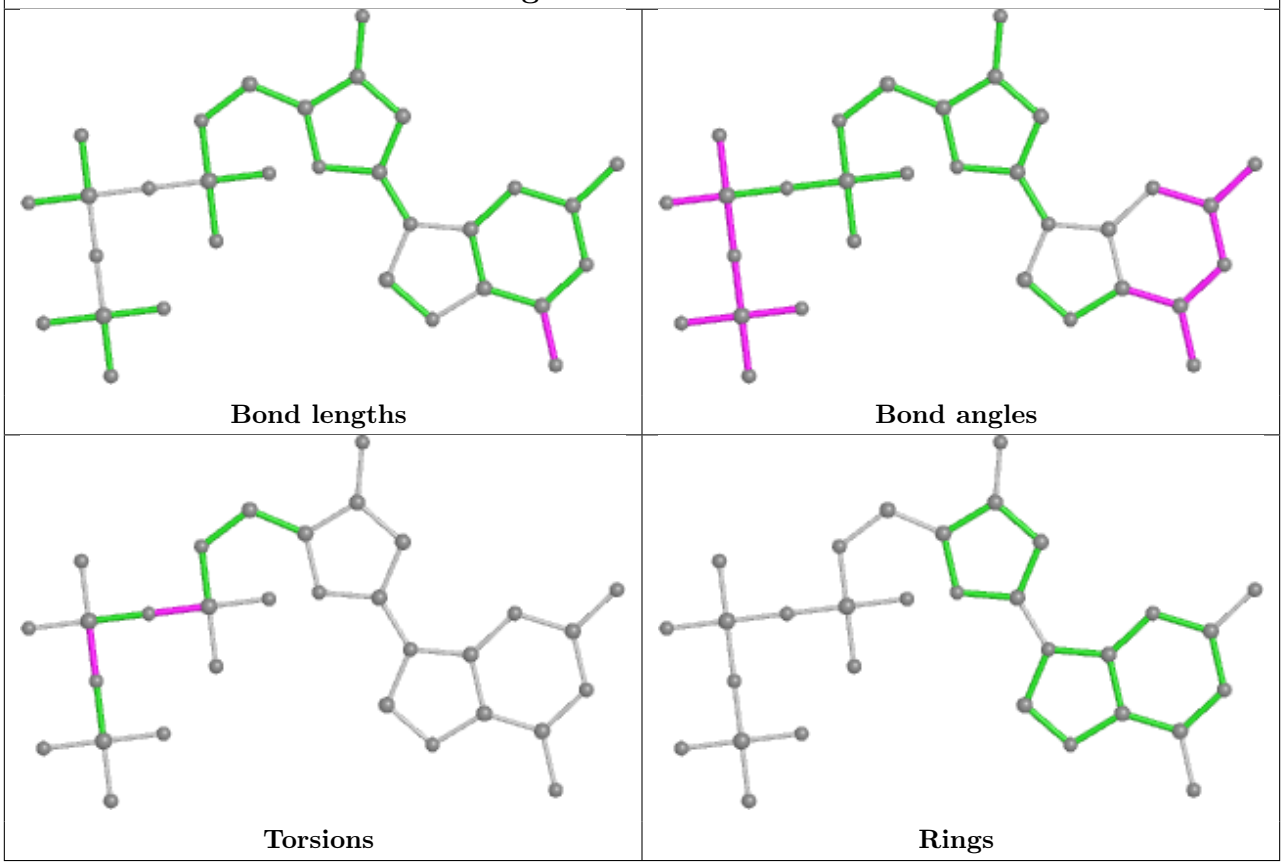
Ligand DGT B 706



Ligand GTP B 705



Ligand DGT A 704



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	481/514 (93%)	0.31	41 (8%)	10	13	25, 48, 81, 111	0
1	B	481/514 (93%)	0.36	35 (7%)	15	19	26, 52, 87, 123	0
1	C	481/514 (93%)	0.04	11 (2%)	60	65	22, 41, 71, 99	1 (0%)
1	D	484/514 (94%)	0.45	37 (7%)	13	18	27, 53, 84, 161	0
All	All	1927/2056 (93%)	0.29	124 (6%)	19	24	22, 48, 82, 161	1 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	VAL	15.2
1	D	279	PRO	12.5
1	A	488	LEU	8.3
1	D	488	LEU	7.0
1	A	490	ASP	6.6
1	C	284	LEU	6.5
1	A	284	LEU	6.1
1	B	277	GLU	5.3
1	D	590	LEU	5.2
1	B	488	LEU	5.1
1	A	487	VAL	5.0
1	D	599	ASN	5.0
1	B	599	ASN	4.8
1	C	490	ASP	4.7
1	B	466	ILE	4.7
1	B	487	VAL	4.6
1	D	591	ILE	4.6
1	D	490	ASP	4.5
1	A	486	LYS	4.4
1	A	489	LEU	4.3
1	B	489	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	468	ILE	4.3
1	D	276	LEU	4.3
1	D	113	ASP	4.2
1	A	491	VAL	4.1
1	B	491	VAL	4.0
1	A	599	ASN	3.8
1	A	113	ASP	3.7
1	B	498	PHE	3.7
1	A	492	LYS	3.6
1	D	403	GLY	3.5
1	B	284	LEU	3.5
1	B	480	VAL	3.5
1	A	262	GLU	3.4
1	C	216	MET	3.4
1	A	591	ILE	3.4
1	A	562	LEU	3.4
1	D	489	LEU	3.4
1	A	285	TRP	3.3
1	A	568	TYR	3.3
1	B	486	LYS	3.3
1	D	594	GLN	3.3
1	A	483	ALA	3.2
1	A	594	GLN	3.2
1	A	590	LEU	3.2
1	A	277	GLU	3.2
1	A	493	LEU	3.1
1	B	230	LYS	3.1
1	D	562	LEU	3.1
1	A	478	LYS	3.1
1	D	496	GLU	3.1
1	B	562	LEU	3.0
1	D	284	LEU	3.0
1	D	278	SER	3.0
1	B	568	TYR	2.9
1	B	286	PRO	2.9
1	B	406	LYS	2.9
1	D	572	TRP	2.9
1	A	494	LYS	2.9
1	D	587	ILE	2.8
1	B	465	GLN	2.8
1	B	490	ASP	2.8
1	C	465	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	568	TYR	2.8
1	D	229	VAL	2.7
1	D	160	ALA	2.7
1	A	560	LYS	2.7
1	B	285	TRP	2.7
1	C	467	LYS	2.7
1	B	585	ASP	2.7
1	D	285	TRP	2.6
1	B	473	TYR	2.6
1	A	465	GLN	2.6
1	B	113	ASP	2.6
1	B	496	GLU	2.6
1	A	556	LYS	2.6
1	D	492	LYS	2.5
1	D	487	VAL	2.5
1	A	118	ILE	2.5
1	C	466	ILE	2.5
1	B	471	GLU	2.5
1	D	563	TYR	2.5
1	C	443	GLU	2.5
1	A	276	LEU	2.4
1	D	559	ARG	2.4
1	C	468	ILE	2.4
1	D	597	GLU	2.4
1	D	328	ASN	2.4
1	D	596	LYS	2.4
1	A	121	PRO	2.3
1	B	481	ALA	2.3
1	A	484	LYS	2.3
1	C	492	LYS	2.3
1	D	288	LYS	2.3
1	A	325	ILE	2.3
1	A	496	GLU	2.3
1	B	342	GLU	2.3
1	C	277	GLU	2.3
1	A	563	TYR	2.2
1	D	469	LYS	2.2
1	A	402	ALA	2.2
1	D	277	GLU	2.2
1	C	596	LYS	2.2
1	D	230	LYS	2.2
1	B	573	CYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	484	LYS	2.2
1	A	122	ILE	2.2
1	B	483	ALA	2.2
1	D	325	ILE	2.2
1	B	594	GLN	2.1
1	A	158	PRO	2.1
1	B	469	LYS	2.1
1	A	559	ARG	2.1
1	B	347	LEU	2.1
1	A	498	PHE	2.1
1	A	115	MET	2.1
1	D	592	THR	2.1
1	A	154	TYR	2.1
1	B	528	ARG	2.0
1	D	326	GLN	2.0
1	B	343	VAL	2.0
1	A	575	ASP	2.0
1	B	345	ASN	2.0
1	A	587	ILE	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
3	MG	D	704	1/1	0.82	0.09	111,111,111,111	0
3	MG	C	702	1/1	0.83	0.08	37,37,37,37	0
3	MG	B	702	1/1	0.87	0.14	123,123,123,123	0
3	MG	A	702	1/1	0.89	0.06	73,73,73,73	0

Continued on next page...

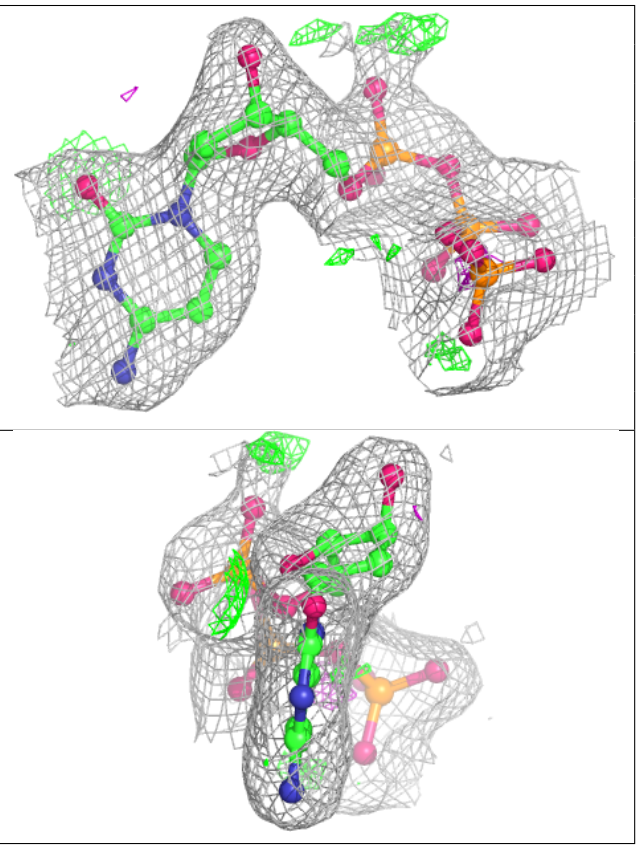
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DCP	B	701	28/28	0.91	0.11	37,43,71,73	0
2	DCP	A	701	28/28	0.92	0.12	31,40,72,78	0
2	DCP	D	703	28/28	0.92	0.11	35,42,76,80	0
3	MG	D	701	1/1	0.94	0.04	37,37,37,37	0
2	DCP	C	703	28/28	0.95	0.10	26,30,59,62	0
3	MG	C	704	1/1	0.96	0.03	60,60,60,60	0
3	MG	B	704	1/1	0.97	0.03	30,30,30,30	0
4	GTP	D	705	32/32	0.97	0.10	33,38,43,47	0
5	DGT	A	704	31/31	0.97	0.14	25,29,37,37	0
5	DGT	B	706	31/31	0.97	0.11	29,34,42,45	0
4	GTP	A	703	32/32	0.98	0.11	31,36,40,45	0
4	GTP	B	703	32/32	0.98	0.10	30,36,40,45	0
4	GTP	B	705	32/32	0.98	0.11	27,31,36,37	0
5	DGT	C	701	31/31	0.98	0.13	29,32,42,44	0
5	DGT	D	702	31/31	0.98	0.11	29,33,41,42	0
3	MG	A	705	1/1	0.99	0.05	41,41,41,41	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.

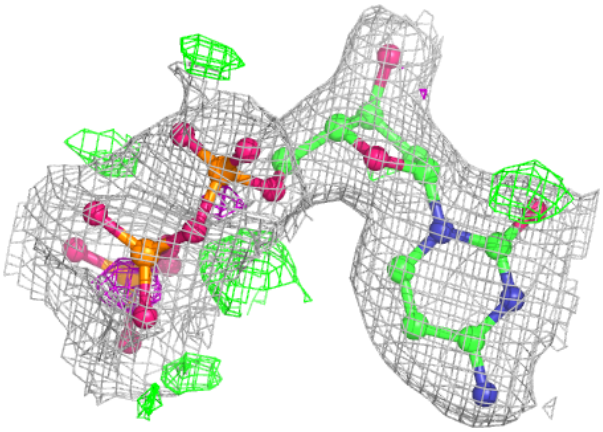
Electron density around DCP B 701:

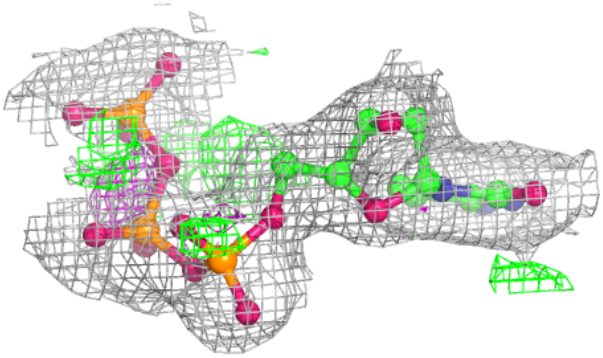
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

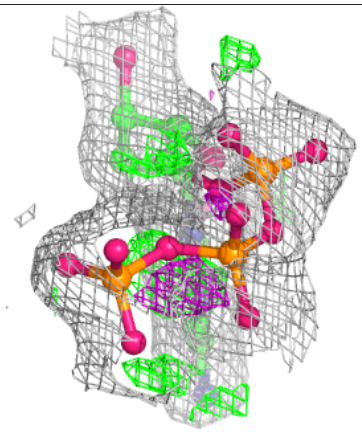


Electron density around DCP A 701:

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

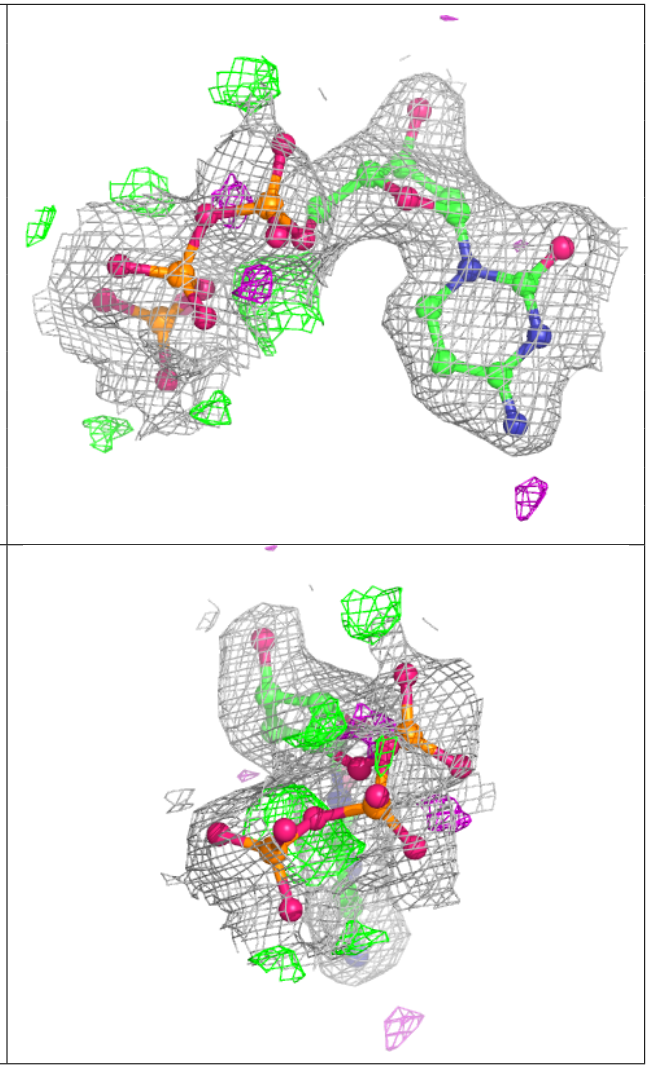






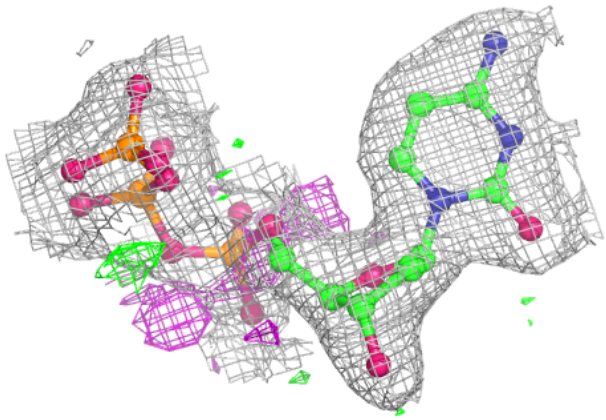
Electron density around DCP D 703:

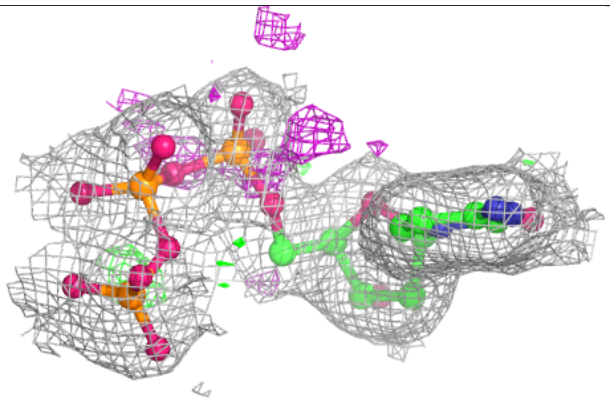
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

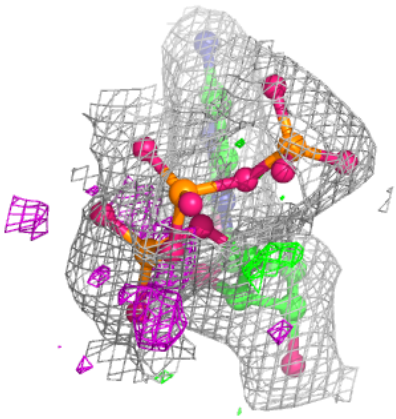


Electron density around DCP C 703:

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

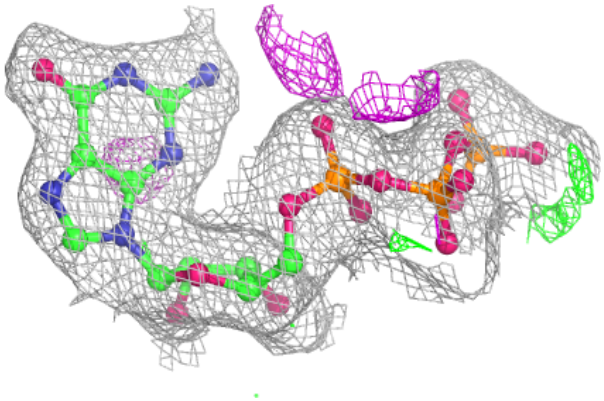


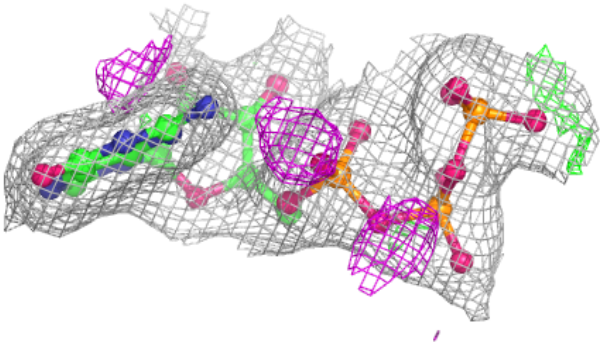


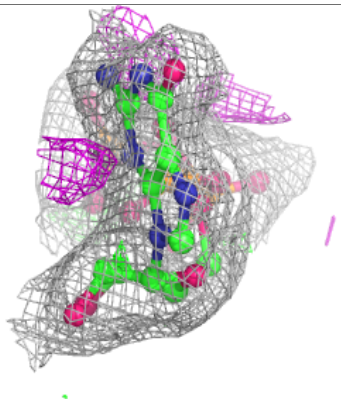


Electron density around GTP D 705:

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

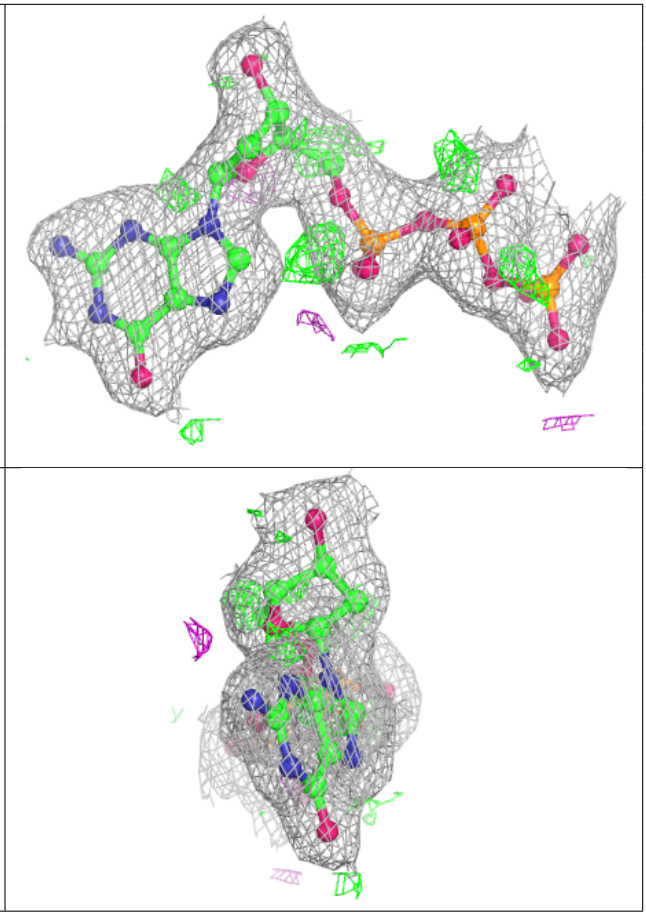






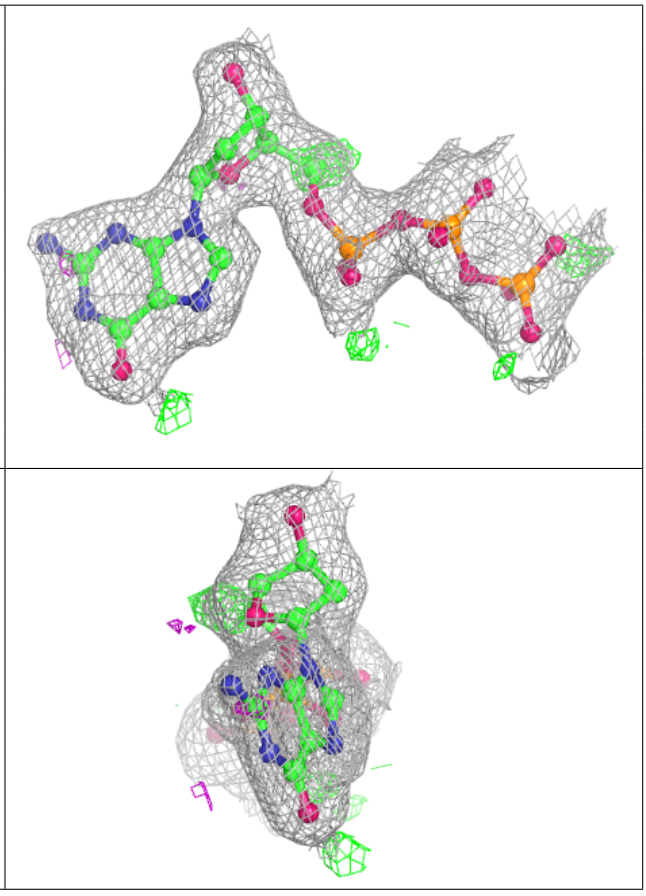
Electron density around DGT A 704:

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



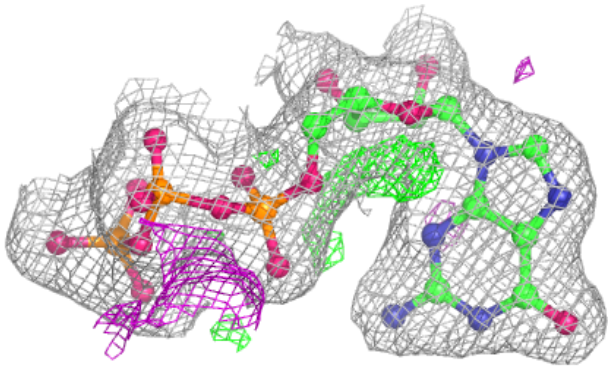
Electron density around DGT B 706:

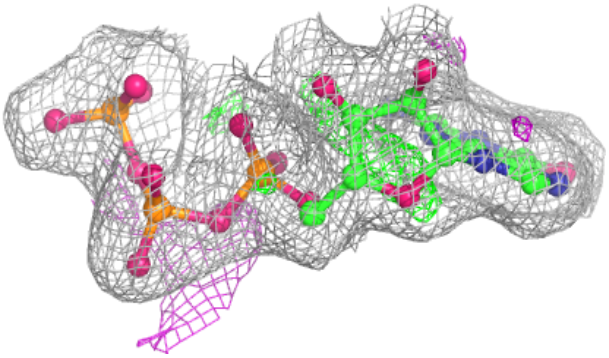
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

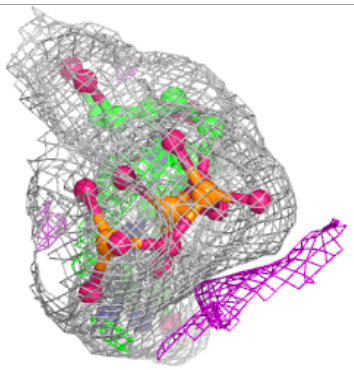


Electron density around GTP A 703:

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

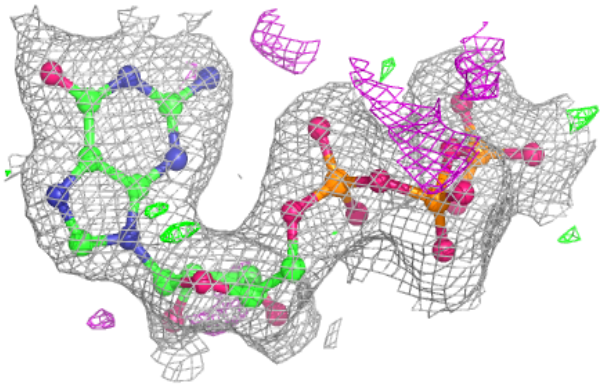


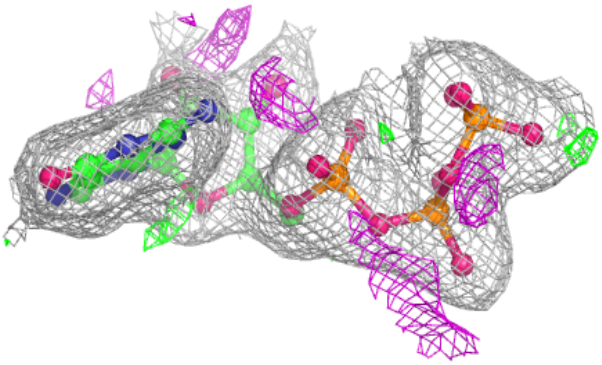


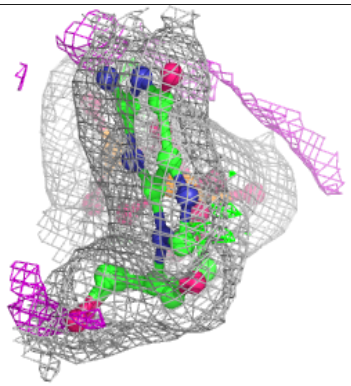


Electron density around GTP B 703:

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

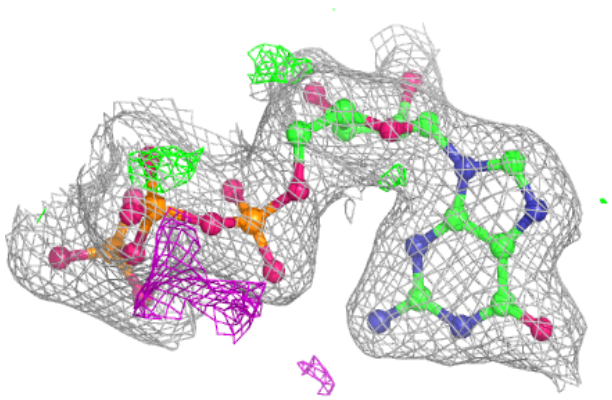


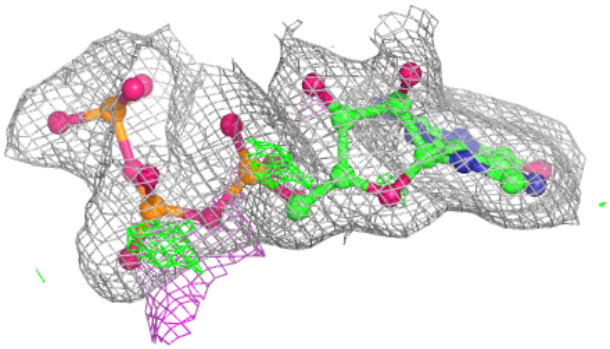


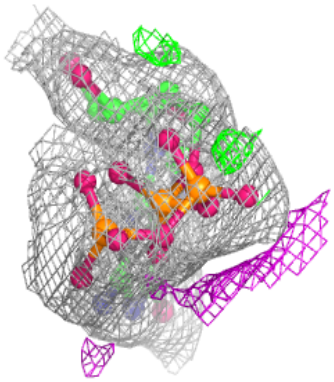


Electron density around GTP B 705:

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

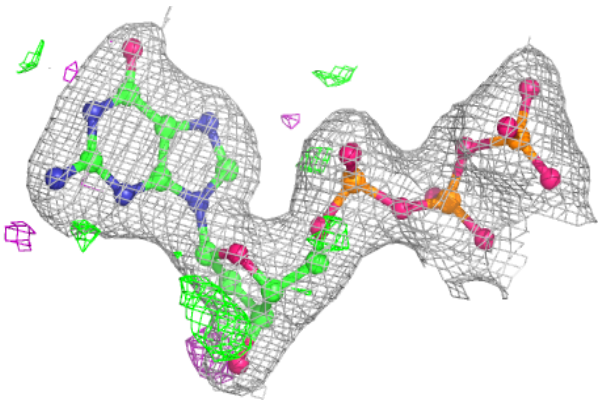


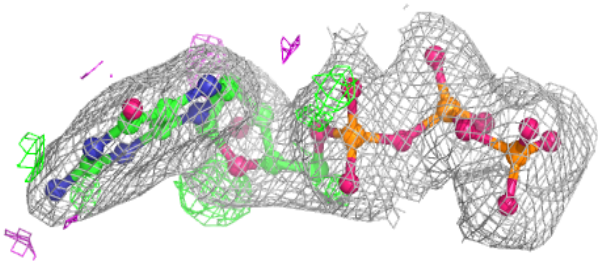


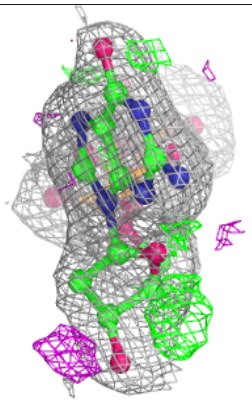


Electron density around DGT C 701:

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

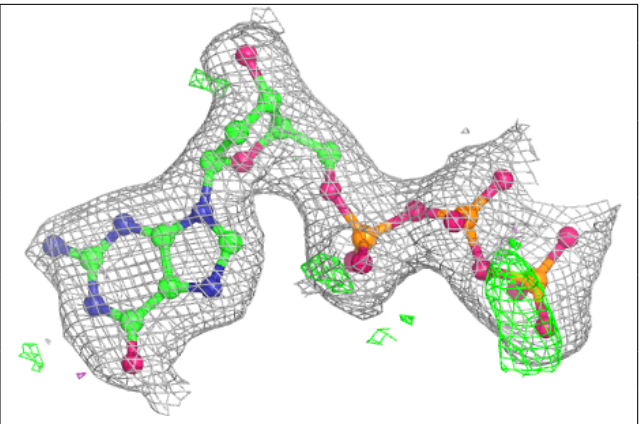


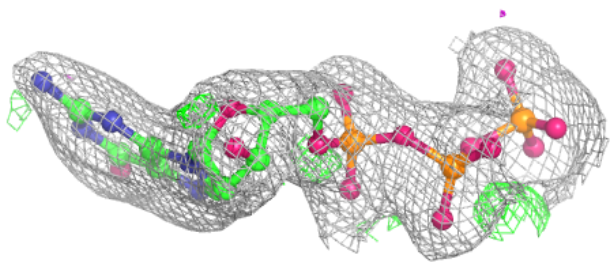


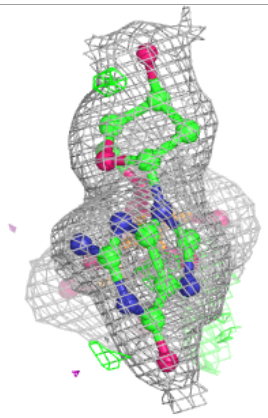


Electron density around DGT D 702:

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







6.5 Other polymers (i)

There are no such residues in this entry.