



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:09 PM UTC

PDB ID : 4TO4 / pdb_00004to4
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

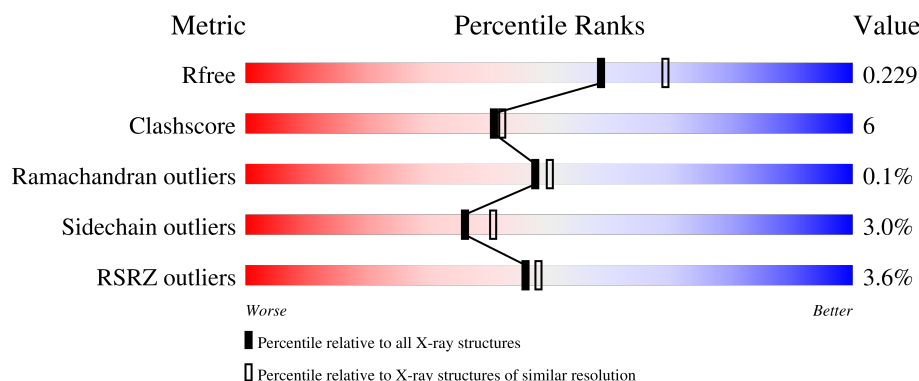
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

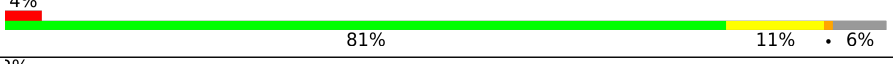
The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	 4% 83% 10% • 6%
1	B	514	 4% 81% 11% • 6%
1	C	514	 2% 81% 11% • 6%
1	D	514	 5% 82% 11% • 6%

2 Entry composition

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.

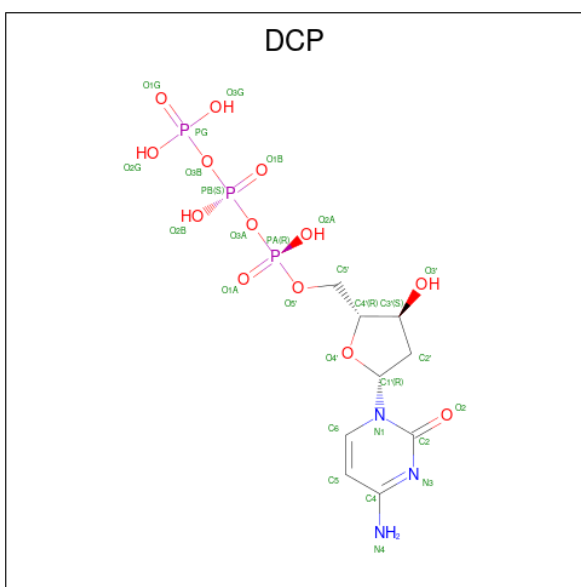
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).

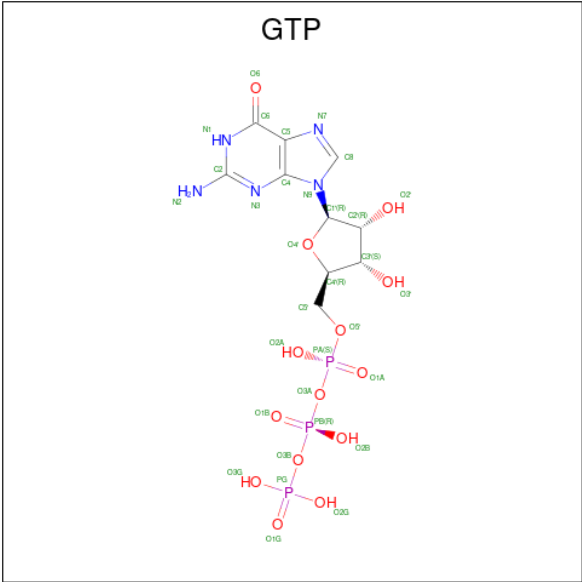


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	B	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	C	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
2	D	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

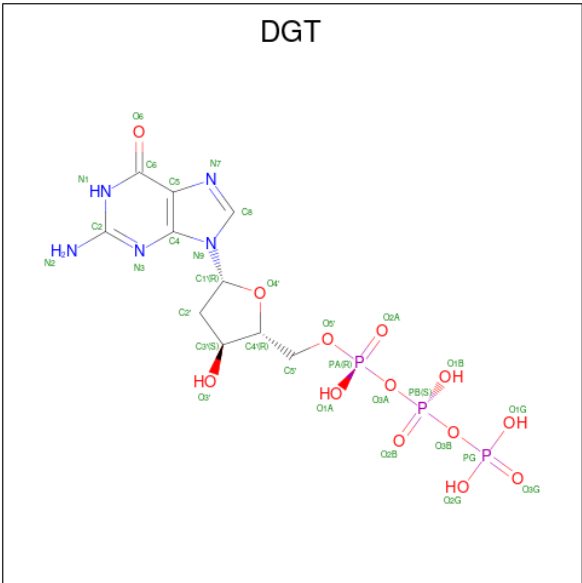
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

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



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

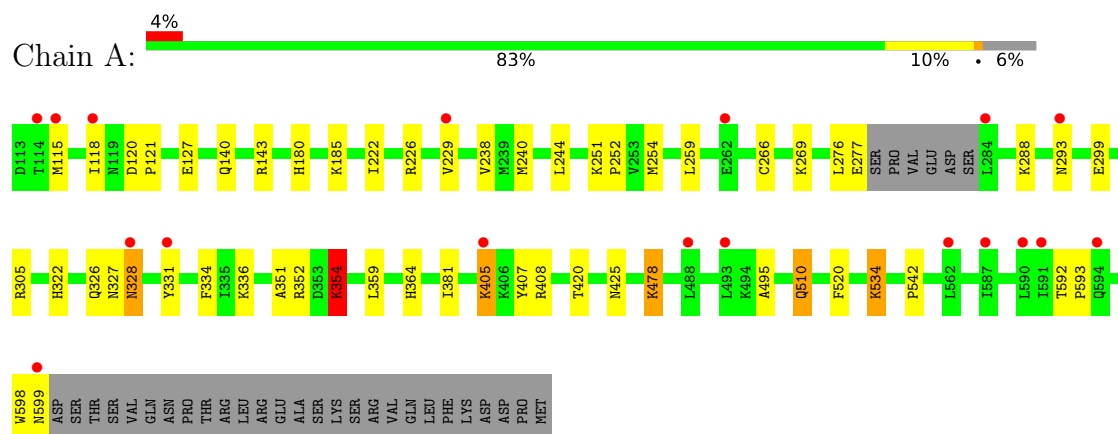
- Molecule 6 is water.

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

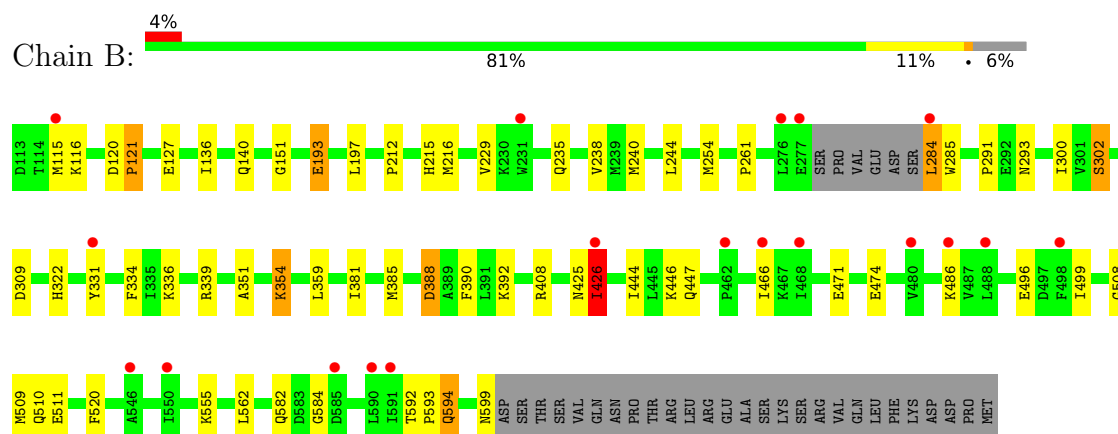
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

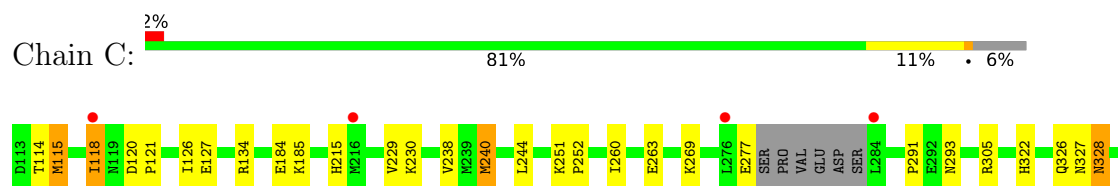
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

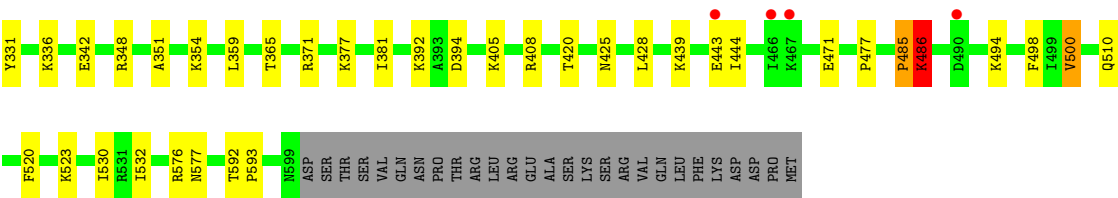


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

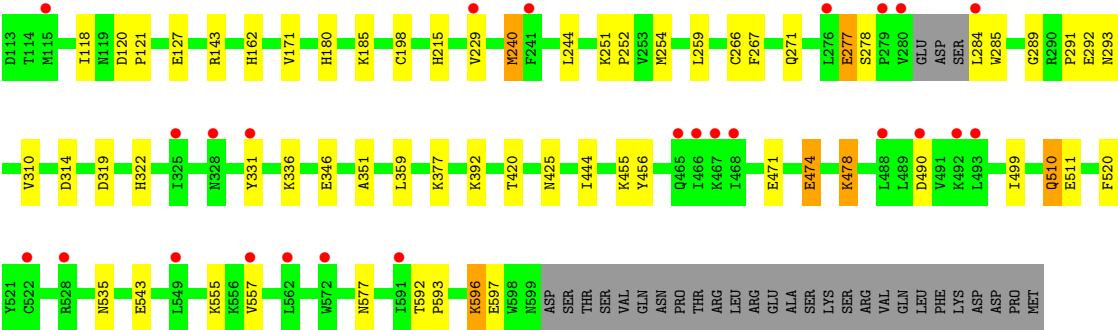
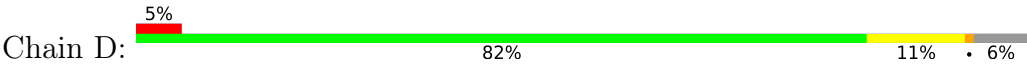


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.71Å 145.84Å 98.65Å 90.00° 114.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.10) 99.2 (50.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	6476 reflections (4.99%)	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 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DGT, GTP, 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	0.97	2/4025 (0.0%)	0.95	2/5433 (0.0%)
1	B	0.93	1/4025 (0.0%)	0.94	5/5433 (0.1%)
1	C	1.01	2/4037 (0.0%)	0.96	2/5449 (0.0%)
1	D	0.92	0/4057	0.90	1/5478 (0.0%)
All	All	0.96	5/16144 (0.0%)	0.94	10/21793 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	371	ARG	C-O	-5.70	1.17	1.24
1	B	121	PRO	C-O	-5.48	1.17	1.24
1	A	354	LYS	C-O	-5.24	1.17	1.24
1	C	500	VAL	C-O	-5.15	1.18	1.24
1	A	222	ILE	CA-C	5.12	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	GLN	CB-CA-C	-7.33	108.12	116.63
1	C	510	GLN	CB-CA-C	-6.13	109.52	116.63
1	D	510	GLN	CB-CA-C	-6.11	109.54	116.63
1	A	293	ASN	N-CA-CB	-5.90	100.53	110.49
1	B	426	ILE	CB-CA-C	5.67	119.79	112.14
1	B	510	GLN	CB-CA-C	-5.59	110.14	116.63
1	B	388	ASP	CB-CA-C	-5.41	102.39	110.88
1	C	485	PRO	N-CA-C	5.39	123.57	112.47
1	B	354	LYS	CG-CD-CE	5.36	123.63	111.30
1	B	302	SER	CB-CA-C	-5.19	103.86	111.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	45	0
1	B	3933	0	3921	55	0
1	C	3945	0	3929	63	0
1	D	3963	0	3948	52	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
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	23	0
6	C	117	0	0	32	0
6	D	71	0	0	26	0
All	All	16513	0	15863	208	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 (208) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.47	0.94
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
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:447:GLN:C	6:B:839:HOH:O	2.29	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:B:385:MET:HE1	6:B:839:HOH:O	1.90	0.72
1:C:260:ILE:CB	6:C:844:HOH:O	2.27	0.72
1:C:115:MET:SD	1:C:115:MET:C	2.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:328:ASN:OD1	1:A:328:ASN:C	2.37	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:B:254:MET:HE2	1:B:261:PRO:HG3	1.80	0.62
1:D:266:CYS:SG	6:D:860:HOH:O	2.55	0.62
1:B:115:MET:HE2	1:B:127:GLU:OE1	2.00	0.61
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
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:A:140:GLN:HG3	1:A:240:MET:HE1	1.85	0.59
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: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:B:140:GLN:HG3	1:B:240:MET:HE1	1.84	0.58
1:A:180:HIS:CD2	6:A:808:HOH:O	2.56	0.58
1:B:599:ASN:C	6:B:848:HOH:O	2.47	0.58
1:B:582:GLN:HB2	6:D:850:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:TYR:CD1	1:B:331:TYR:C	2.82	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:B:115:MET:HE3	1:B:127:GLU:HB3	1.88	0.55
1:D:455:LYS:C	6:D:838:HOH:O	2.50	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:C:331:TYR:C	1:C:331:TYR:CD1	2.86	0.53
1:D:284:LEU:HD13	1:D:285:TRP:N	2.24	0.53
1:D:511:GLU:H	1:D:511:GLU:CD	2.17	0.53
1:D:331:TYR:C	1:D:331:TYR:CD1	2.86	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: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: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:B:511:GLU:H	1:B:511:GLU:CD	2.18	0.52
1:A:478:LYS:HE2	1:A:495:ALA:HB2	1.92	0.51
1:B:508:GLY:C	6:B:840:HOH:O	2.53	0.51
1:D:474:GLU:O	1:D:478:LYS:NZ	2.39	0.51
1:A:331:TYR:C	1:A:331:TYR:CD1	2.87	0.51
1:B:116:LYS:NZ	4:B:705:GTP:O2G	2.44	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:D:456:TYR:C	6:D:838:HOH:O	2.53	0.50
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: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:244:LEU:C	1:D:244:LEU:HD23	2.37	0.49
1:A:244:LEU:C	1:A:244:LEU:HD23	2.37	0.49
1:D:314:ASP:HB2	6:D:834:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HE3	1:B:127:GLU:HG3	1.95	0.48
1:A:226:ARG:HB3	1:A:229:VAL:HG23	1.95	0.48
1:B:115:MET:C	6:B:825:HOH:O	2.56	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:C:244:LEU:C	1:C:244:LEU:HD23	2.38	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:B:244:LEU:C	1:B:244:LEU:HD23	2.38	0.48
1:B:254:MET:HE1	1:B:261:PRO:HA	1.94	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:B:215:HIS:CD2	2:B:701:DCP:C6	2.97	0.47
1:A:352:ARG:NH2	1:A:354:LYS:HD3	2.29	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:D:254:MET:HE3	1:D:259:LEU:HD23	1.97	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:D:215:HIS:NE2	2:D:703:DCP:O1A	2.47	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:A:254:MET:HE3	1:A:259:LEU:HD23	1.98	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:A:599:ASN:C	6:A:860:HOH:O	2.58	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:C:118:ILE:HD11	1:C:126:ILE:HB	1.95	0.45
1:C:263:GLU:CD	6:C:844:HOH:O	2.60	0.45
1:B:254:MET:CE	1:B:261:PRO:HA	2.46	0.45
1:D:240:MET:HE1	1:D:420:THR:OG1	2.16	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
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:235:GLN:O	1:B:238:VAL:HG22	2.17	0.44
1:D:215:HIS:CE1	2:D:703:DCP:O1A	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:THR:N	1:A:593:PRO:CD	2.80	0.44
1:A:326:GLN:CD	1:C:326:GLN:HE21	2.26	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:C:498:PHE:C	6:C:865:HOH:O	2.61	0.43
1:B:300:ILE:C	6:B:842:HOH:O	2.61	0.43
1:C:351:ALA:O	1:C:520:PHE:HA	2.18	0.43
1:C:240:MET:HE1	1:C:420:THR:OG1	2.18	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: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
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:D:198:CYS:C	6:D:836:HOH:O	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	44
1	D	481/514 (94%)	471 (98%)	10 (2%)	0	100	100
All	All	1914/2056 (93%)	1875 (98%)	38 (2%)	1 (0%)	48	50

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%)	416 (97%)	11 (3%)	40	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	427/459 (93%)	413 (97%)	14 (3%)	33	37
1	C	429/459 (94%)	415 (97%)	14 (3%)	33	37
1	D	431/459 (94%)	419 (97%)	12 (3%)	38	43
All	All	1714/1836 (93%)	1663 (97%)	51 (3%)	36	41

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	118	ILE
1	A	185	LYS
1	A	277	GLU
1	A	328	ASN
1	A	354	LYS
1	A	405	LYS
1	A	408	ARG
1	A	478	LYS
1	A	510	GLN
1	A	534	LYS
1	B	136	ILE
1	B	193	GLU
1	B	229	VAL
1	B	284	LEU
1	B	302	SER
1	B	339	ARG
1	B	354	LYS
1	B	388	ASP
1	B	426	ILE
1	B	471	GLU
1	B	474	GLU
1	B	486	LYS
1	B	496	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
1	C	230	LYS
1	C	240	MET
1	C	277	GLU

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Mol	Chain	Res	Type
1	C	328	ASN
1	C	342	GLU
1	C	354	LYS
1	C	359	LEU
1	C	486	LYS
1	C	494	LYS
1	D	185	LYS
1	D	229	VAL
1	D	240	MET
1	D	277	GLU
1	D	359	LEU
1	D	471	GLU
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 (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	200	GLN
1	A	233	HIS
1	A	243	HIS
1	A	248	ASN
1	A	326	GLN
1	A	364	HIS
1	A	370	HIS
1	A	375	GLN
1	A	380	ASN
1	A	425	ASN
1	A	510	GLN
1	A	567	GLN
1	A	571	GLN
1	A	594	GLN
1	B	149	GLN
1	B	200	GLN
1	B	233	HIS
1	B	235	GLN
1	B	364	HIS

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Mol	Chain	Res	Type
1	B	425	ASN
1	B	539	GLN
1	B	567	GLN
1	B	571	GLN
1	B	599	ASN
1	C	149	GLN
1	C	200	GLN
1	C	235	GLN
1	C	326	GLN
1	C	425	ASN
1	C	539	GLN
1	C	567	GLN
1	C	571	GLN
1	C	594	GLN
1	C	599	ASN
1	D	149	GLN
1	D	162	HIS
1	D	200	GLN
1	D	233	HIS
1	D	235	GLN
1	D	243	HIS
1	D	425	ASN
1	D	452	ASN
1	D	535	ASN
1	D	539	GLN
1	D	567	GLN
1	D	571	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 oligosaccharides in this entry.

5.6 Ligand geometry

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
5	DGT	A	704	3	32,33,33	1.34	5 (15%)	48,52,52	1.70	13 (27%)
2	DCP	C	703	3	28,29,29	1.85	5 (17%)	41,45,45	1.19	3 (7%)
2	DCP	B	701	3	28,29,29	1.66	3 (10%)	41,45,45	1.15	4 (9%)
5	DGT	B	706	3	32,33,33	1.42	6 (18%)	48,52,52	1.94	17 (35%)
4	GTP	D	705	3	33,34,34	1.64	8 (24%)	50,54,54	1.82	9 (18%)
5	DGT	C	701	3	32,33,33	1.41	6 (18%)	48,52,52	1.58	11 (22%)
5	DGT	D	702	3	32,33,33	1.36	4 (12%)	48,52,52	1.62	8 (16%)
4	GTP	A	703	3	33,34,34	1.36	5 (15%)	50,54,54	1.92	10 (20%)
4	GTP	B	703	3	33,34,34	1.59	7 (21%)	50,54,54	1.68	7 (14%)
2	DCP	A	701	3	28,29,29	1.70	5 (17%)	41,45,45	1.23	5 (12%)
4	GTP	B	705	3	33,34,34	1.28	4 (12%)	50,54,54	1.81	14 (28%)
2	DCP	D	703	-	28,29,29	1.78	4 (14%)	41,45,45	1.15	3 (7%)

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	DGT	A	704	3	-	3/22/34/34	0/3/3/3
2	DCP	C	703	3	-	3/22/34/34	0/2/2/2
2	DCP	B	701	3	-	4/22/34/34	0/2/2/2
5	DGT	B	706	3	-	6/22/34/34	0/3/3/3
4	GTP	D	705	3	-	4/22/38/38	0/3/3/3
5	DGT	C	701	3	-	4/22/34/34	0/3/3/3
5	DGT	D	702	3	-	4/22/34/34	0/3/3/3
4	GTP	A	703	3	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	B	703	3	-	3/22/38/38	0/3/3/3
2	DCP	A	701	3	-	7/22/34/34	0/2/2/2
4	GTP	B	705	3	-	6/22/38/38	0/3/3/3
2	DCP	D	703	-	-	4/22/34/34	0/2/2/2

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	703	DCP	PB-O3B	6.84	1.66	1.59
2	B	701	DCP	PB-O3B	6.67	1.66	1.59
2	A	701	DCP	PB-O3B	6.29	1.66	1.59
2	D	703	DCP	PB-O3B	5.53	1.65	1.59
2	D	703	DCP	PA-O3A	4.31	1.64	1.59
4	B	703	GTP	PB-O3A	4.07	1.63	1.59
4	B	703	GTP	C5-C4	3.98	1.49	1.38
4	D	705	GTP	PB-O3B	3.89	1.63	1.59
5	B	706	DGT	C5-C4	3.88	1.49	1.38
5	D	702	DGT	C5-C4	3.80	1.49	1.38
5	C	701	DGT	C5-C4	3.44	1.48	1.38
4	D	705	GTP	PA-O1A	-3.40	1.39	1.50
2	C	703	DCP	PA-O3A	3.39	1.63	1.59
4	D	705	GTP	C5-C4	3.22	1.47	1.38
4	A	703	GTP	C5-C4	3.21	1.47	1.38
5	A	704	DGT	C5-C4	3.14	1.47	1.38
2	D	703	DCP	PB-O3A	3.12	1.62	1.59
5	D	702	DGT	C5-N7	-3.10	1.32	1.39
2	A	701	DCP	O3'-C3'	3.05	1.49	1.43
4	B	703	GTP	C6-N1	-3.01	1.33	1.38
4	B	705	GTP	PA-O2A	-2.99	1.41	1.55
5	C	701	DGT	PG-O2G	-2.86	1.44	1.54
5	D	702	DGT	PB-O3A	2.83	1.62	1.59
5	A	704	DGT	C5-N7	-2.82	1.33	1.39
4	B	703	GTP	C4-N9	-2.78	1.31	1.38
4	A	703	GTP	C5-N7	-2.73	1.33	1.39
4	D	705	GTP	PG-O2G	-2.71	1.44	1.54
4	B	703	GTP	PA-O3A	2.70	1.62	1.59
4	B	705	GTP	C5-C4	2.70	1.46	1.38
5	A	704	DGT	C4-N9	-2.68	1.31	1.38
5	C	701	DGT	C4-N9	-2.64	1.31	1.38
2	A	701	DCP	C2-N3	-2.60	1.31	1.36
4	D	705	GTP	C5-N7	-2.52	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	DCP	C6-C5	2.47	1.40	1.35
5	C	701	DGT	C6-N1	-2.42	1.34	1.38
2	C	703	DCP	C5-C4	-2.38	1.37	1.42
5	B	706	DGT	PA-O3A	2.36	1.62	1.59
2	B	701	DCP	C6-C5	2.33	1.40	1.35
5	A	704	DGT	O6-C6	2.30	1.27	1.23
4	D	705	GTP	O4'-C1'	2.28	1.47	1.42
2	A	701	DCP	C4-N3	2.27	1.39	1.34
2	B	701	DCP	PA-O3A	2.24	1.61	1.59
5	A	704	DGT	PB-O3A	2.23	1.61	1.59
4	D	705	GTP	PA-O3A	2.23	1.61	1.59
4	A	703	GTP	PB-O3A	2.22	1.61	1.59
4	B	703	GTP	PG-O2G	-2.21	1.46	1.54
5	D	702	DGT	C6-N1	-2.20	1.34	1.38
4	B	705	GTP	PB-O1B	-2.18	1.43	1.50
2	A	701	DCP	C6-C5	2.17	1.40	1.35
4	A	703	GTP	PA-O2A	-2.15	1.45	1.55
5	B	706	DGT	C4-N9	-2.15	1.32	1.38
5	B	706	DGT	PB-O3B	2.14	1.61	1.59
5	C	701	DGT	O4'-C4'	-2.13	1.40	1.45
4	B	703	GTP	C5-N7	-2.10	1.34	1.39
4	A	703	GTP	C4-N9	-2.08	1.32	1.38
5	B	706	DGT	C5-N7	-2.08	1.34	1.39
2	C	703	DCP	PA-O5'	2.07	1.67	1.59
2	C	703	DCP	O2-C2	2.06	1.27	1.23
4	B	705	GTP	C6-N1	-2.04	1.35	1.38
5	C	701	DGT	O3'-C3'	2.04	1.47	1.43
5	B	706	DGT	PG-O1G	-2.04	1.47	1.54
4	D	705	GTP	C6-N1	-2.02	1.35	1.38

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	GTP	C5-C4-N3	-5.83	119.11	128.39
4	D	705	GTP	C5-C4-N3	-5.79	119.17	128.39
4	B	703	GTP	C5-C4-N3	-5.61	119.46	128.39
4	B	705	GTP	C5-C4-N3	-5.46	119.69	128.39
4	D	705	GTP	C2-N3-C4	4.77	120.51	112.30
4	D	705	GTP	N9-C4-N3	4.76	135.47	125.95
4	A	703	GTP	O3A-PB-O1B	-4.74	96.45	110.70
4	A	703	GTP	N9-C4-N3	4.64	135.23	125.95
5	D	702	DGT	C5-C4-N3	-4.61	121.06	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	GTP	C2-N3-C4	4.59	120.20	112.30
4	B	703	GTP	N9-C4-N3	4.53	135.01	125.95
4	B	705	GTP	C2-N3-C4	4.42	119.91	112.30
5	B	706	DGT	C6-C5-N7	4.29	138.10	130.29
4	B	705	GTP	N9-C4-N3	4.24	134.44	125.95
2	C	703	DCP	O4'-C1'-N1	4.20	115.31	107.86
5	B	706	DGT	C2-N3-C4	4.07	119.31	112.30
5	A	704	DGT	O2G-PG-O1G	4.02	122.88	107.80
4	D	705	GTP	C3'-C2'-C1'	4.01	109.05	101.46
5	D	702	DGT	N9-C4-N3	3.78	133.50	125.95
5	B	706	DGT	N2-C2-N1	3.73	124.64	116.76
5	D	702	DGT	C2-N3-C4	3.70	118.67	112.30
5	D	702	DGT	C6-C5-N7	3.69	137.00	130.29
5	B	706	DGT	C5-C4-N3	-3.69	122.52	128.39
4	B	703	GTP	C3'-C2'-C1'	3.64	108.35	101.46
5	B	706	DGT	N2-C2-N3	-3.54	112.76	119.67
4	B	703	GTP	C2-N3-C4	3.49	118.31	112.30
4	A	703	GTP	C3'-C2'-C1'	3.44	107.98	101.46
5	A	704	DGT	O3B-PB-O2B	-3.41	100.46	110.70
5	C	701	DGT	N2-C2-N3	-3.35	113.14	119.67
5	C	701	DGT	C5-C4-N3	-3.34	123.07	128.39
5	A	704	DGT	O6-C6-C5	-3.17	118.16	126.53
5	C	701	DGT	O6-C6-C5	-3.14	118.26	126.53
2	A	701	DCP	O3A-PB-O1B	-3.13	101.28	110.70
2	B	701	DCP	O3G-PG-O2G	3.08	119.35	107.80
5	B	706	DGT	O6-C6-C5	-3.04	118.50	126.53
4	A	703	GTP	C6-C5-N7	2.99	135.74	130.29
4	D	705	GTP	C6-C5-N7	2.98	135.72	130.29
5	A	704	DGT	N2-C2-N3	-2.98	113.85	119.67
2	B	701	DCP	O3A-PB-O1B	-2.96	101.80	110.70
2	A	701	DCP	O2B-PB-O1B	2.88	125.84	112.44
4	B	705	GTP	O3G-PG-O1G	2.87	122.01	110.83
5	A	704	DGT	N9-C4-N3	2.84	131.62	125.95
5	C	701	DGT	O3A-PA-O2A	-2.81	102.25	110.70
5	B	706	DGT	O2G-PG-O1G	2.81	118.33	107.80
4	A	703	GTP	O3B-PG-O1G	-2.80	96.33	111.04
4	A	703	GTP	O2B-PB-O1B	2.79	125.44	112.44
4	B	705	GTP	O3B-PG-O1G	-2.78	96.39	111.04
5	B	706	DGT	C6-C5-C4	-2.78	114.65	118.83
4	D	705	GTP	O2B-PB-O3A	-2.78	99.77	107.27
4	B	703	GTP	C6-C5-N7	2.75	135.30	130.29
4	D	705	GTP	O2B-PB-O1B	2.74	125.20	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	701	DGT	N2-C2-N1	2.71	122.48	116.76
5	C	701	DGT	N9-C4-N3	2.71	131.37	125.95
5	A	704	DGT	C5-C4-N3	-2.70	124.09	128.39
5	B	706	DGT	N9-C4-N3	2.69	131.33	125.95
4	B	705	GTP	C6-C5-N7	2.63	135.08	130.29
5	A	704	DGT	O1B-PB-O2B	2.63	124.68	112.44
5	B	706	DGT	O3B-PG-O3G	-2.62	97.25	111.04
5	C	701	DGT	C6-C5-N7	2.61	135.03	130.29
4	B	705	GTP	O6-C6-C5	-2.59	119.70	126.53
5	C	701	DGT	C2-N3-C4	2.57	116.72	112.30
4	B	705	GTP	C3'-C2'-C1'	2.57	106.32	101.46
5	D	702	DGT	O2G-PG-O3B	-2.54	96.12	104.64
5	B	706	DGT	C2'-C3'-C4'	2.52	107.92	102.80
5	A	704	DGT	C6-C5-N7	2.48	134.81	130.29
5	B	706	DGT	O1B-PB-O2B	2.48	123.99	112.44
5	B	706	DGT	O3A-PA-O2A	-2.48	103.25	110.70
5	D	702	DGT	O1A-PA-O2A	2.47	123.93	112.44
4	B	705	GTP	O2B-PB-O1B	2.42	123.72	112.44
5	A	704	DGT	O6-C6-N1	2.42	124.66	120.11
2	D	703	DCP	C2'-C1'-N1	-2.42	107.77	113.81
2	D	703	DCP	O4'-C1'-N1	2.38	112.09	107.86
4	A	703	GTP	O6-C6-C5	-2.37	120.28	126.53
2	C	703	DCP	O3G-PG-O2G	2.34	116.59	107.80
4	A	703	GTP	C4-C5-N7	-2.33	106.98	110.67
5	D	702	DGT	C4-C5-N7	-2.30	107.03	110.67
4	B	705	GTP	N2-C2-N3	-2.27	115.24	119.67
4	D	705	GTP	O3G-PG-O2G	2.27	116.31	107.80
4	B	705	GTP	O3A-PB-O1B	-2.26	103.92	110.70
2	A	701	DCP	O4'-C1'-N1	2.21	111.78	107.86
5	B	706	DGT	O1A-PA-O2A	2.20	122.66	112.44
4	B	703	GTP	O2'-C2'-C1'	-2.18	102.59	110.10
5	D	702	DGT	C2'-C3'-C4'	2.17	107.20	102.80
5	B	706	DGT	C4-C5-N7	-2.16	107.25	110.67
4	B	705	GTP	O2G-PG-O1G	2.15	119.22	110.83
5	B	706	DGT	C5-C6-N1	2.15	118.72	113.25
2	B	701	DCP	C2'-C1'-N1	-2.12	108.50	113.81
2	A	701	DCP	O3B-PG-O1G	-2.10	99.97	111.04
4	B	705	GTP	O2A-PA-O1A	2.10	122.22	112.44
5	A	704	DGT	O3B-PG-O3G	-2.10	99.99	111.04
5	C	701	DGT	O6-C6-N1	2.09	124.05	120.11
5	A	704	DGT	C2-N1-C6	-2.09	121.33	125.11
5	A	704	DGT	O1A-PA-O2A	2.08	122.11	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	DCP	O2-C2-N3	-2.07	119.06	122.33
4	B	705	GTP	N2-C2-N1	2.07	121.14	116.76
4	D	705	GTP	C4-C5-N7	-2.07	107.38	110.67
5	C	701	DGT	O2G-PG-O3G	2.05	118.83	110.83
5	A	704	DGT	O2G-PG-O3B	-2.05	97.77	104.64
5	B	706	DGT	O1G-PG-O3B	-2.04	97.78	104.64
4	B	703	GTP	C5-C6-N1	2.03	118.43	113.25
2	B	701	DCP	C2'-C3'-C4'	2.03	106.91	102.80
5	C	701	DGT	O1A-PA-O2A	2.02	121.83	112.44
2	C	703	DCP	O4'-C4'-C5'	2.00	115.75	109.33
2	D	703	DCP	O3G-PG-O2G	2.00	115.31	107.80

There are no chirality outliers.

All (53) 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
2	A	701	DCP	C5'-O5'-PA-O3A
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'
4	B	705	GTP	PB-O3B-PG-O3G
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

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

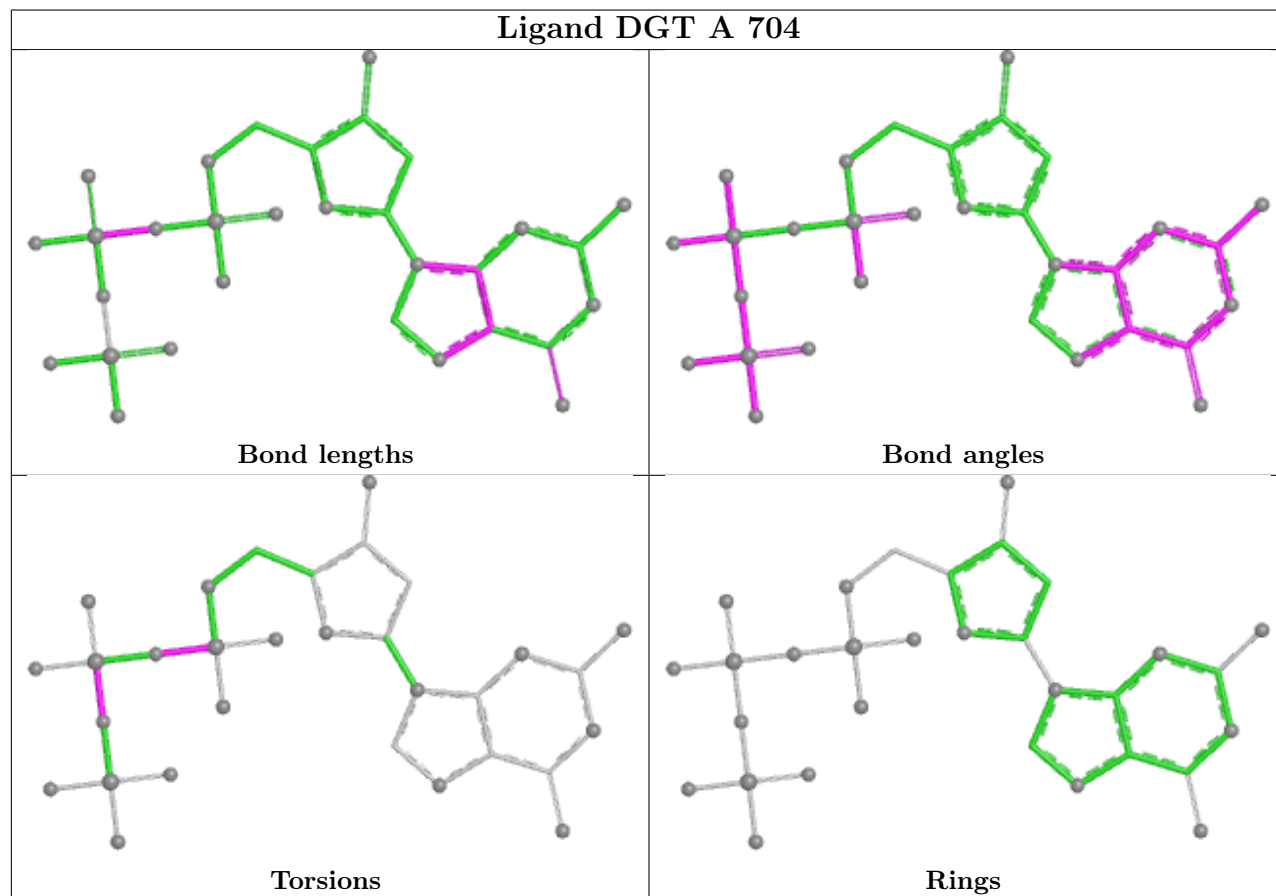
There are no ring outliers.

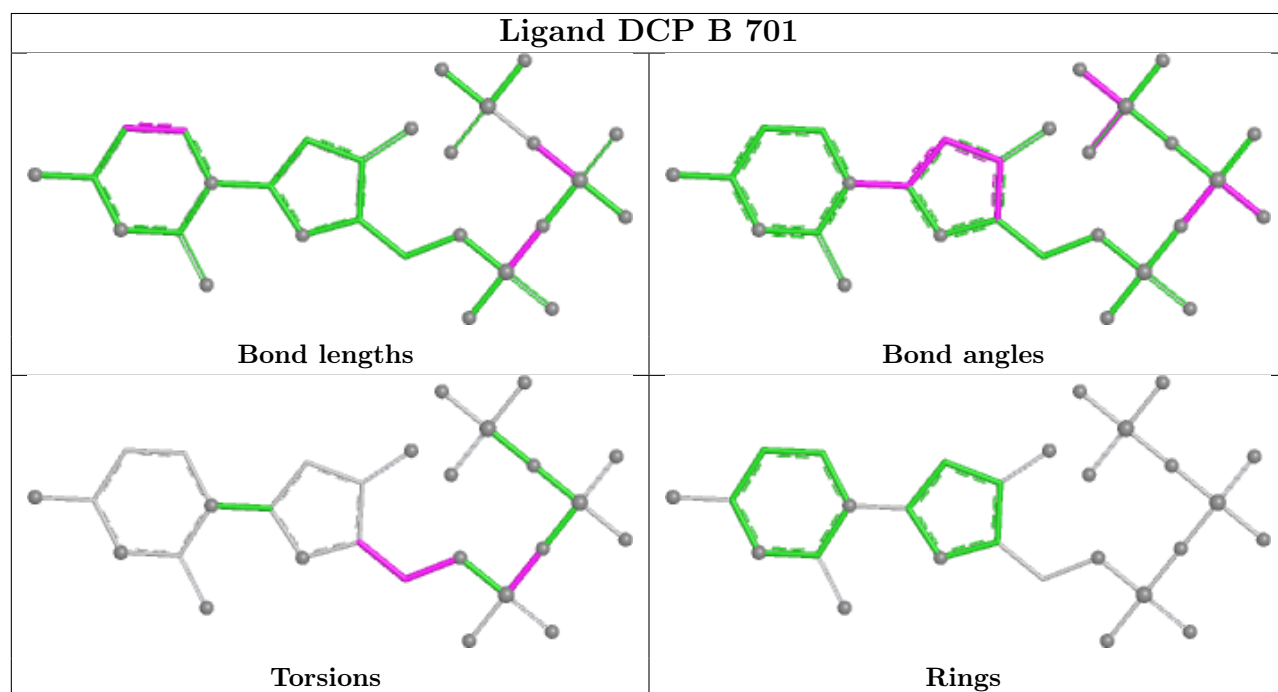
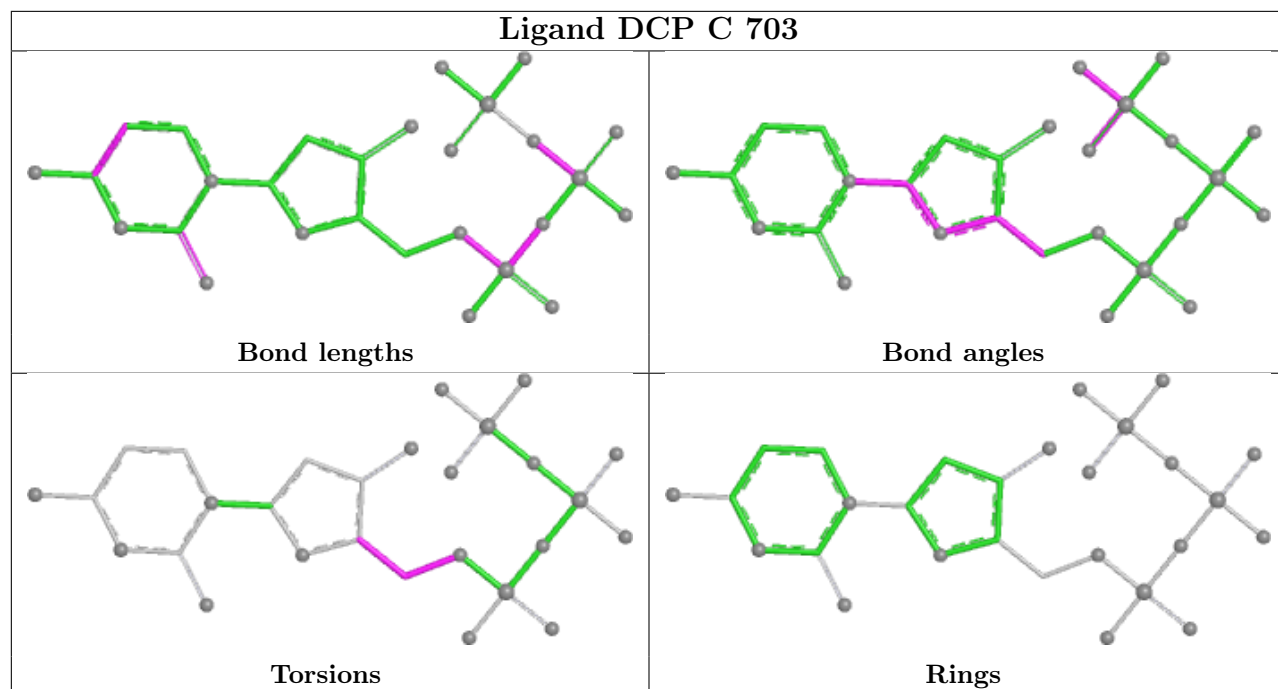
7 monomers are involved in 11 short contacts:

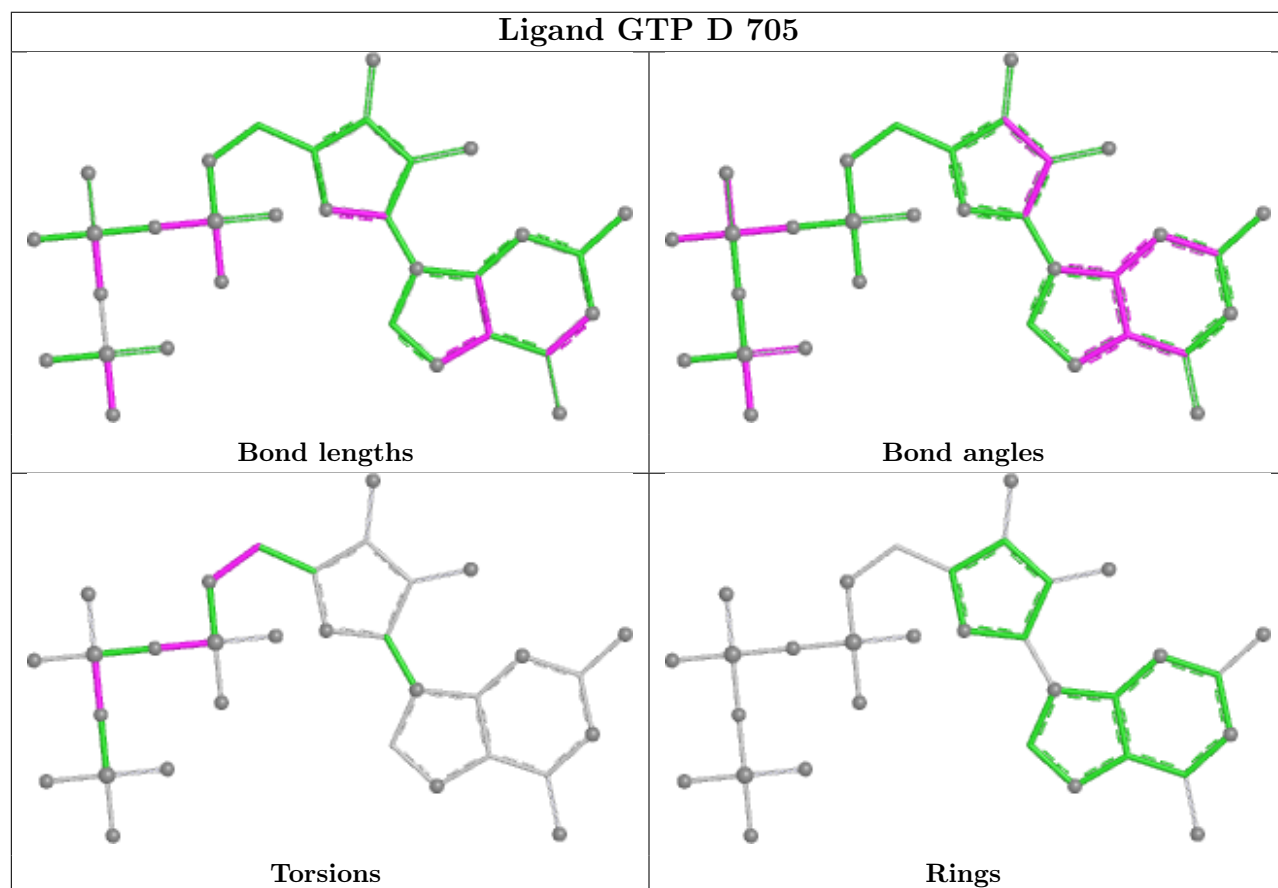
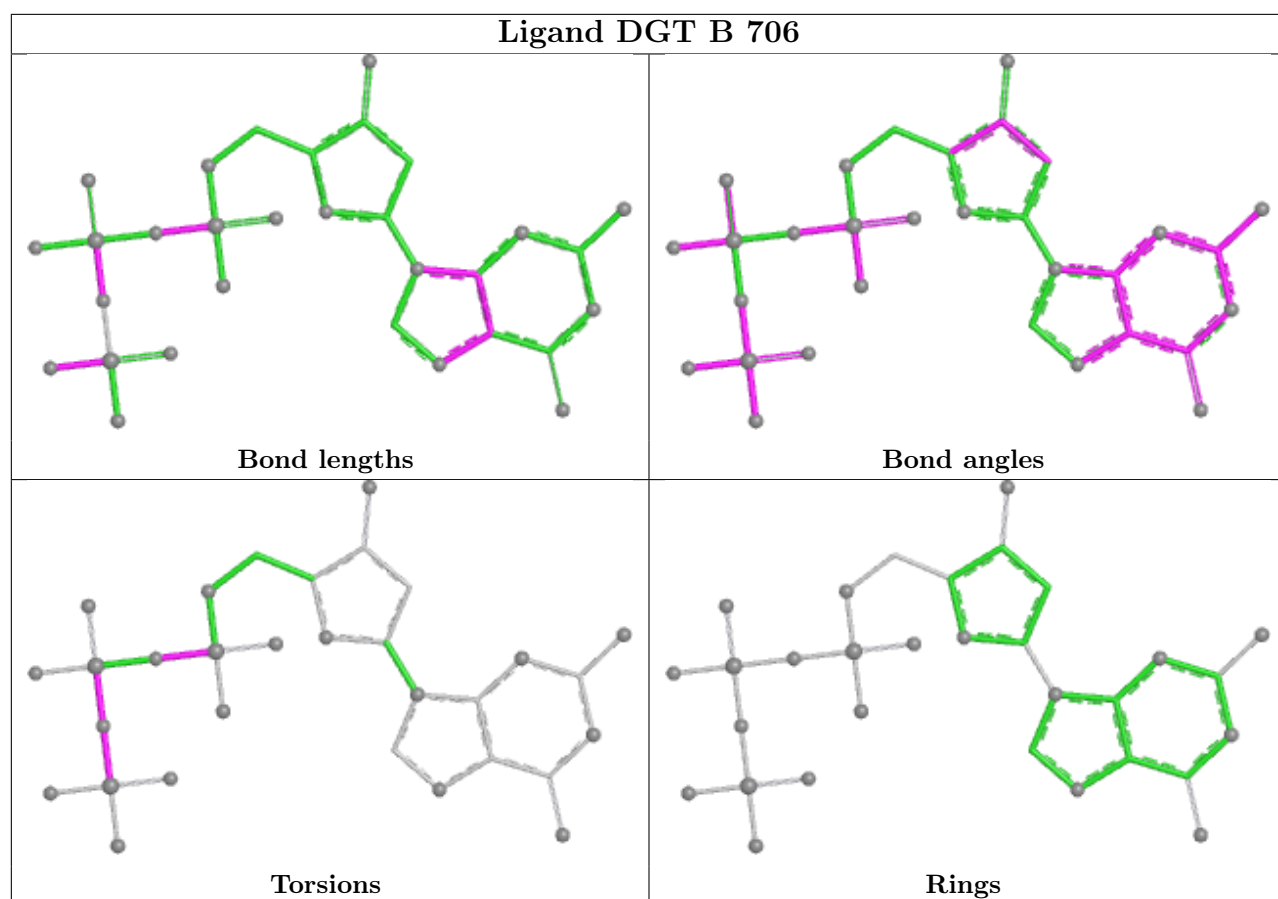
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	DGT	1	0
2	C	703	DCP	2	0
2	B	701	DCP	2	0
5	B	706	DGT	2	0
4	A	703	GTP	1	0
4	B	705	GTP	1	0
2	D	703	DCP	2	0

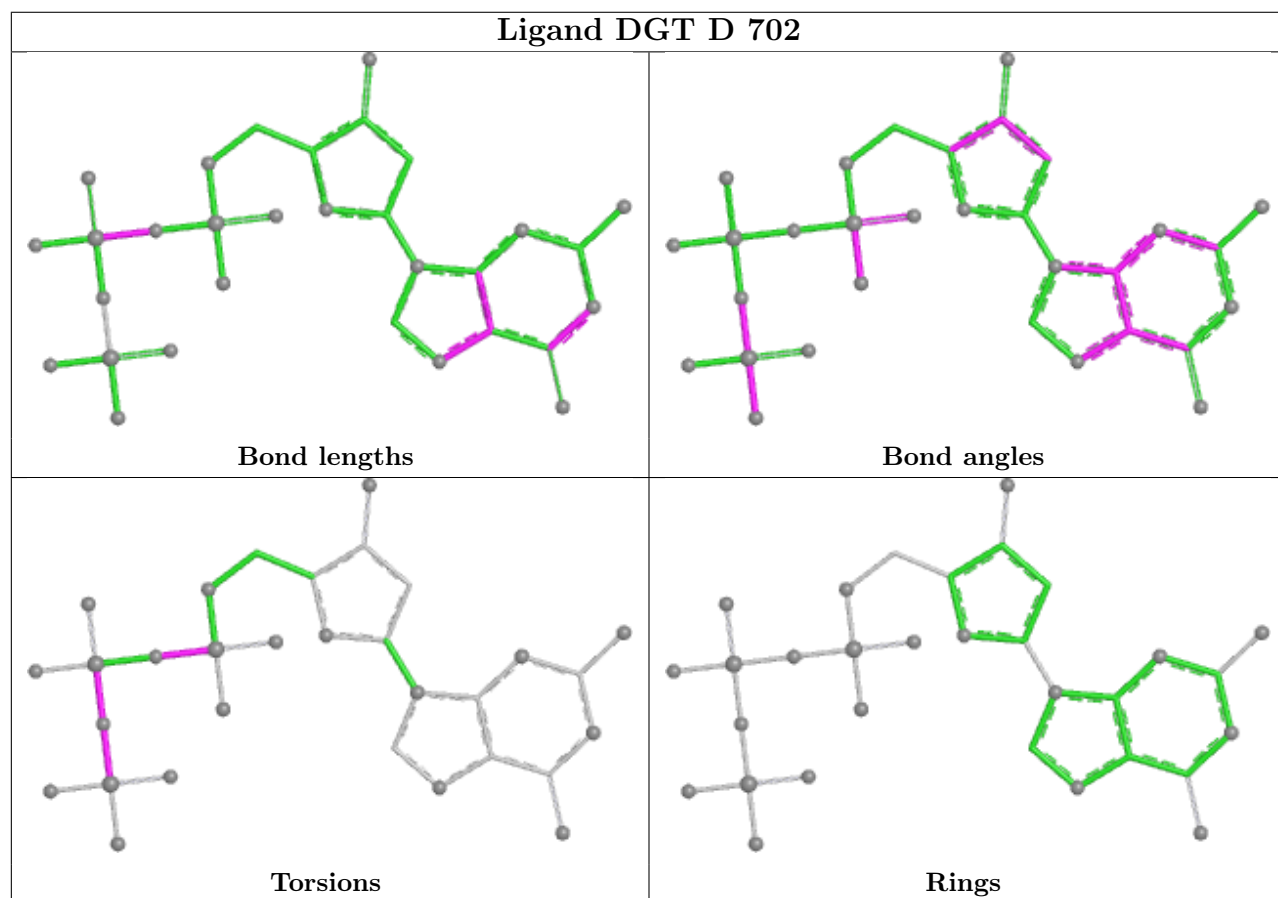
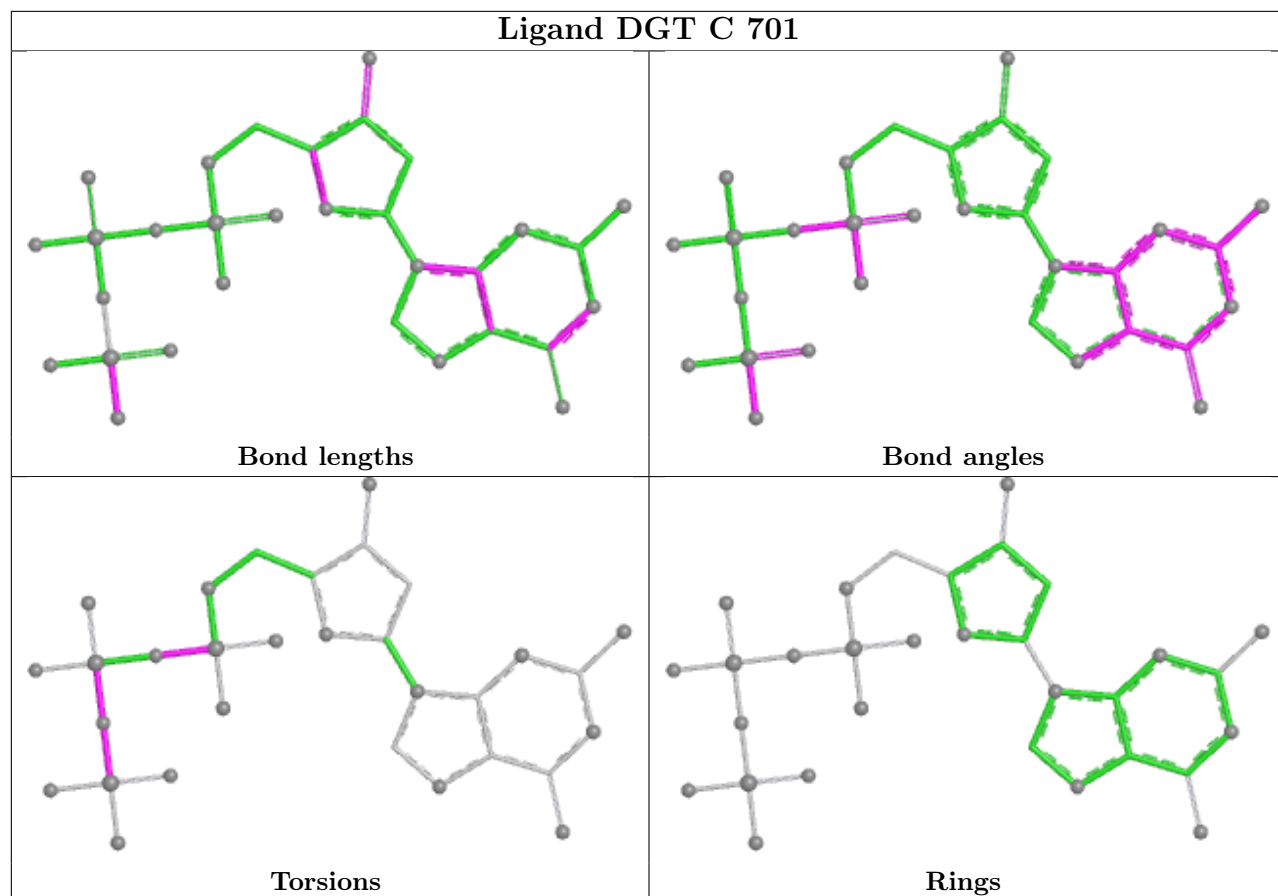
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

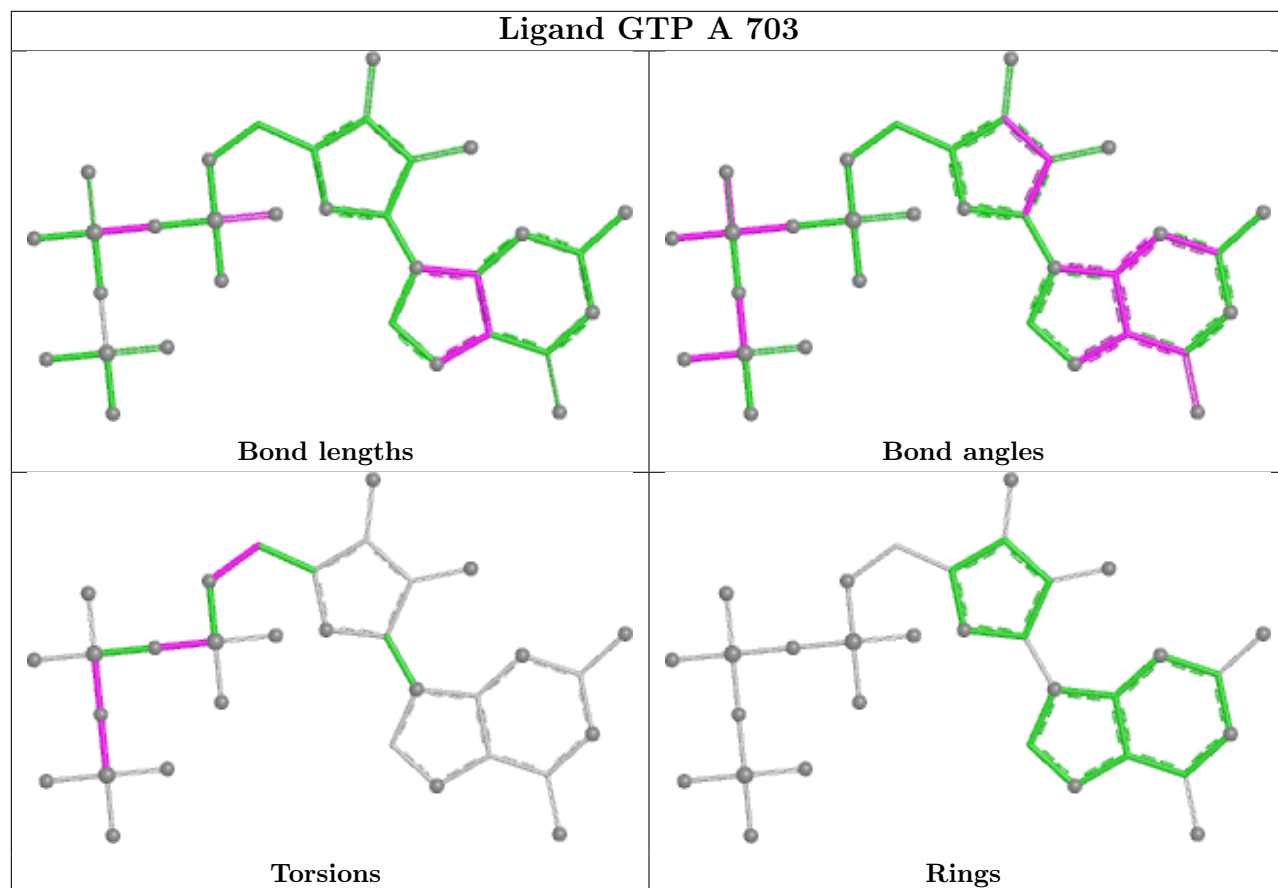




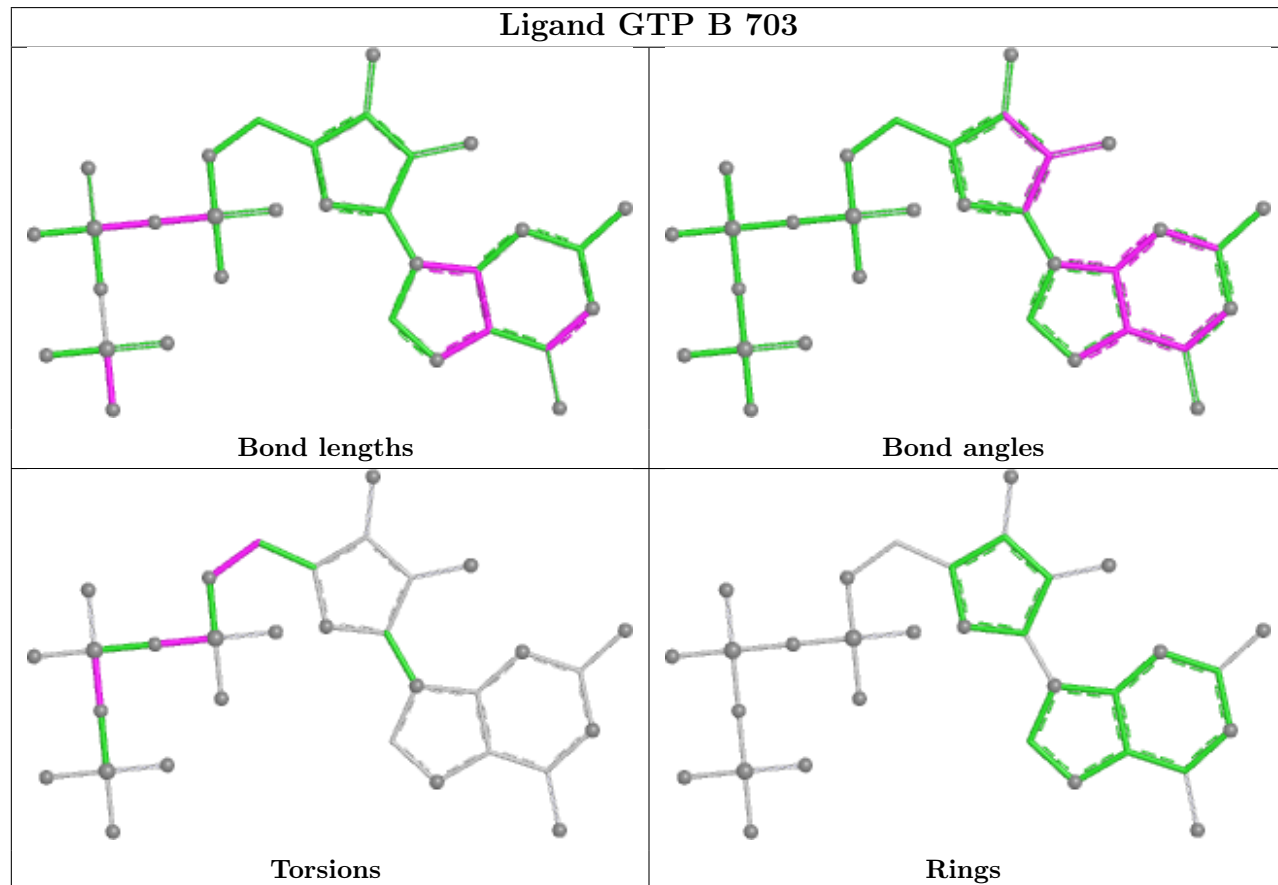


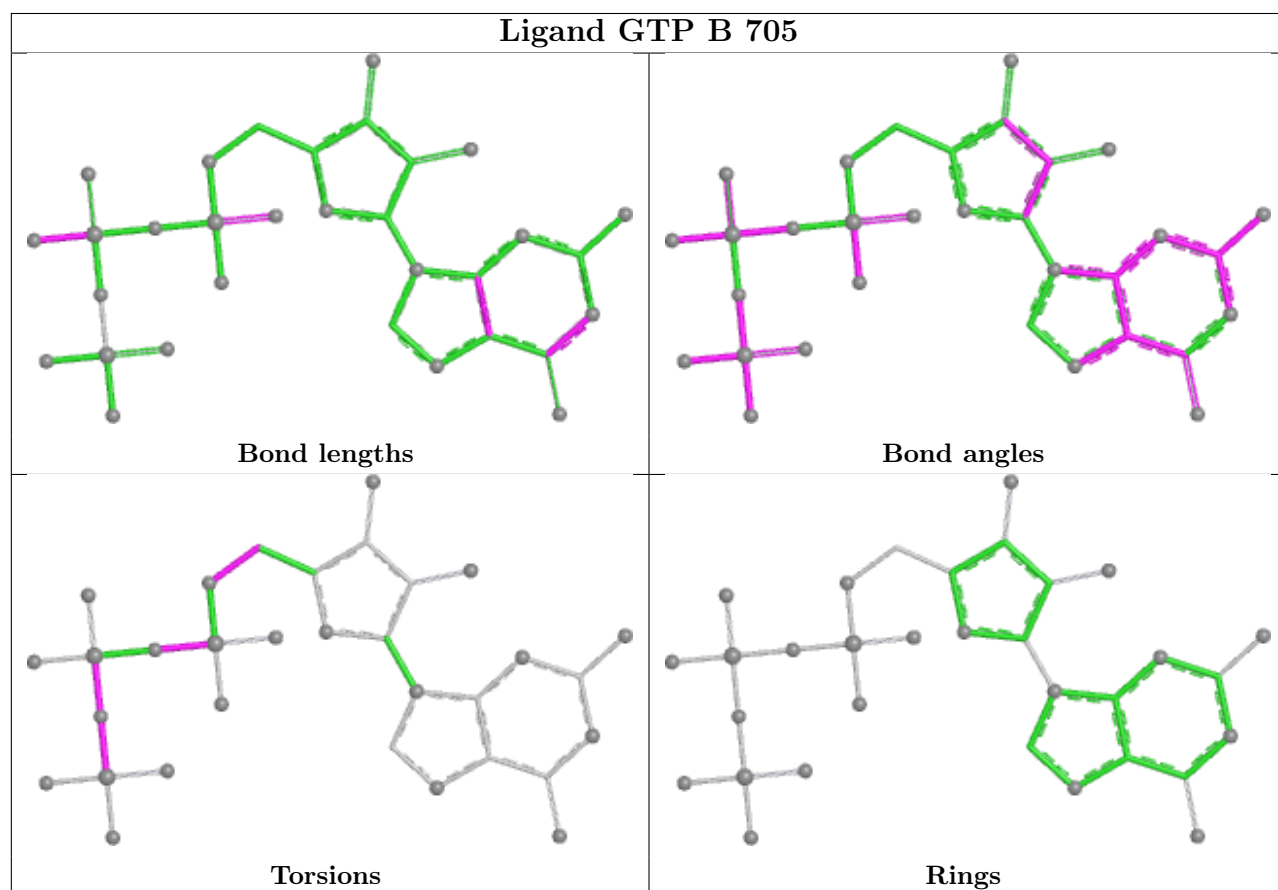
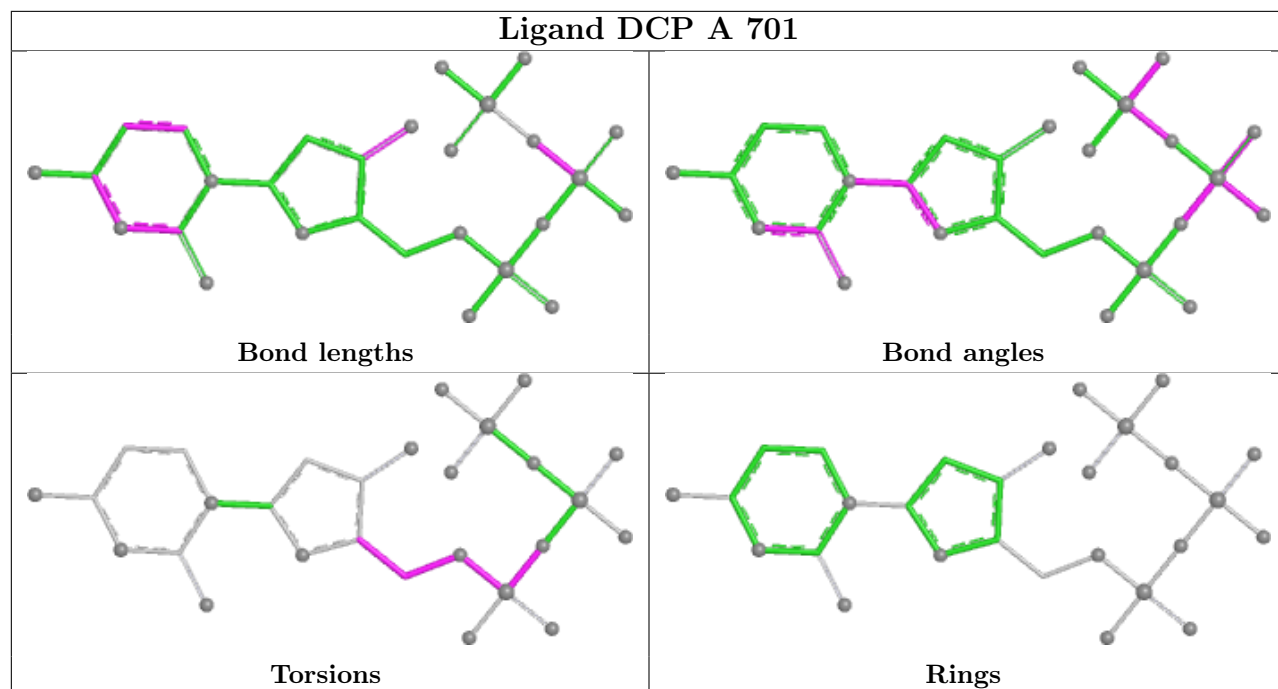


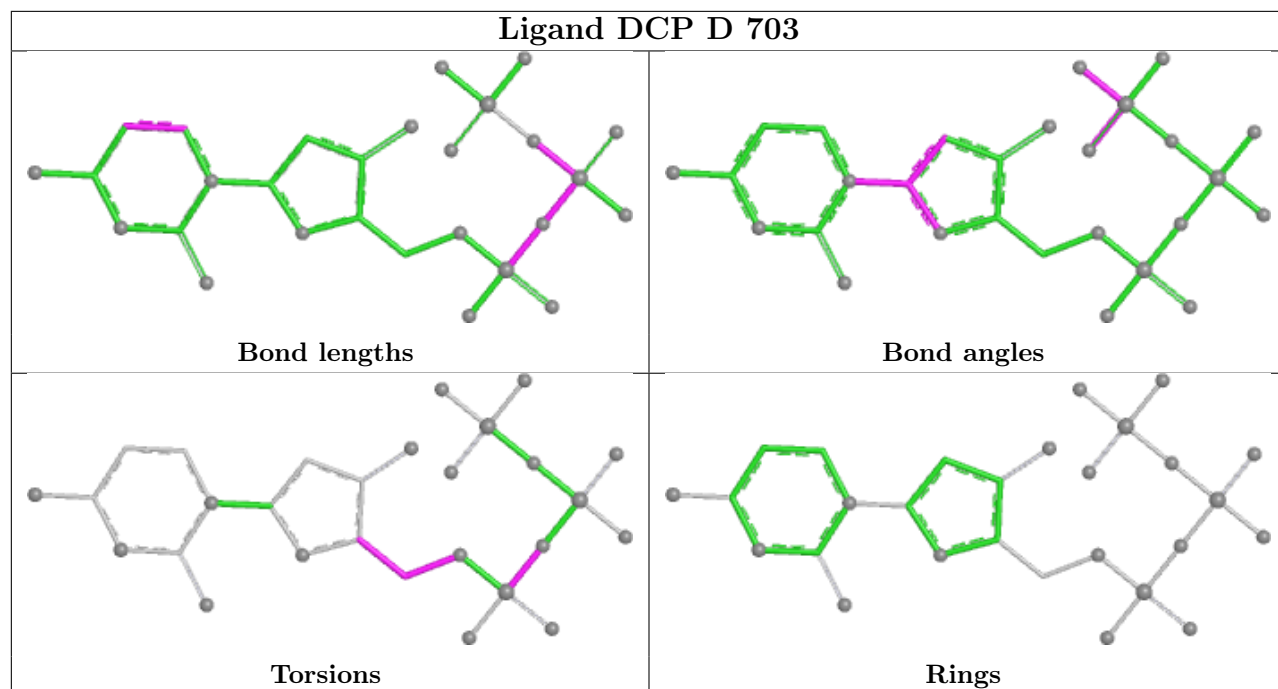
Ligand GTP A 703



Ligand GTP B 703







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	481/514 (93%)	0.48	18 (3%) 45 47	25, 48, 81, 111	0
1	B	481/514 (93%)	0.58	19 (3%) 42 44	26, 52, 87, 123	0
1	C	481/514 (93%)	0.27	8 (1%) 69 71	15, 41, 71, 99	3 (0%)
1	D	484/514 (94%)	0.62	25 (5%) 33 35	23, 53, 84, 161	1 (0%)
All	All	1927/2056 (93%)	0.49	70 (3%) 46 48	15, 48, 82, 161	4 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	LEU	4.0
1	D	280	VAL	4.0
1	C	284	LEU	3.9
1	D	284	LEU	3.9
1	B	284	LEU	3.5
1	A	118	ILE	3.5
1	C	216	MET	3.4
1	A	590	LEU	3.4
1	D	493	LEU	3.4
1	D	468	ILE	3.3
1	A	262	GLU	3.1
1	A	115	MET	3.1
1	D	488	LEU	3.0
1	A	328	ASN	3.0
1	B	466	ILE	2.9
1	C	466	ILE	2.8
1	C	467	LYS	2.8
1	C	118	ILE	2.8
1	D	328	ASN	2.8
1	B	488	LEU	2.7
1	D	229	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	585	ASP	2.7
1	D	331	TYR	2.7
1	D	572	TRP	2.7
1	D	115	MET	2.6
1	D	279	PRO	2.6
1	B	498	PHE	2.6
1	B	277	GLU	2.6
1	D	591	ILE	2.6
1	D	522	CYS	2.6
1	A	591	ILE	2.5
1	C	276	LEU	2.5
1	D	465	GLN	2.5
1	A	229	VAL	2.5
1	A	493	LEU	2.5
1	A	488	LEU	2.5
1	D	562	LEU	2.5
1	D	466	ILE	2.5
1	C	490	ASP	2.4
1	A	562	LEU	2.4
1	B	331	TYR	2.4
1	B	550	ILE	2.3
1	D	549	LEU	2.3
1	A	405	LYS	2.3
1	B	115	MET	2.3
1	A	293	ASN	2.3
1	B	590	LEU	2.3
1	A	599	ASN	2.2
1	D	490	ASP	2.2
1	A	114	THR	2.2
1	B	480	VAL	2.2
1	B	546	ALA	2.2
1	C	443	GLU	2.2
1	A	587	ILE	2.2
1	D	241	PHE	2.1
1	A	331	TYR	2.1
1	B	462	PRO	2.1
1	D	467	LYS	2.1
1	D	492	LYS	2.1
1	B	426	ILE	2.1
1	D	325	ILE	2.1
1	B	231	TRP	2.1
1	D	557	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	528	ARG	2.1
1	B	276	LEU	2.0
1	D	276	LEU	2.0
1	A	594	GLN	2.0
1	B	468	ILE	2.0
1	B	591	ILE	2.0
1	B	486	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	704	1/1	0.43	0.15	111,111,111,111	0
3	MG	B	702	1/1	0.75	0.13	123,123,123,123	0
2	DCP	D	703	28/28	0.85	0.12	35,42,76,80	0
3	MG	A	702	1/1	0.85	0.07	73,73,73,73	0
2	DCP	A	701	28/28	0.88	0.10	31,40,72,78	0
2	DCP	B	701	28/28	0.88	0.11	37,43,71,73	0
2	DCP	C	703	28/28	0.92	0.09	26,30,59,62	0
4	GTP	D	705	32/32	0.95	0.07	33,38,43,47	0
3	MG	C	702	1/1	0.96	0.05	37,37,37,37	0
4	GTP	A	703	32/32	0.97	0.06	31,36,40,45	0
4	GTP	B	703	32/32	0.97	0.06	30,36,40,45	0
4	GTP	B	705	32/32	0.97	0.05	27,31,36,37	0
3	MG	D	701	1/1	0.97	0.09	37,37,37,37	0
5	DGT	A	704	31/31	0.97	0.06	25,29,37,37	0
5	DGT	B	706	31/31	0.97	0.07	29,34,42,45	0
5	DGT	C	701	31/31	0.97	0.06	29,32,42,44	0

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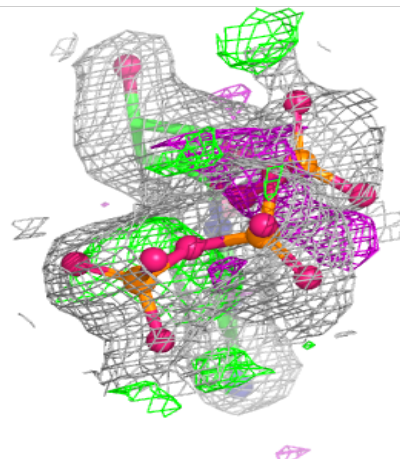
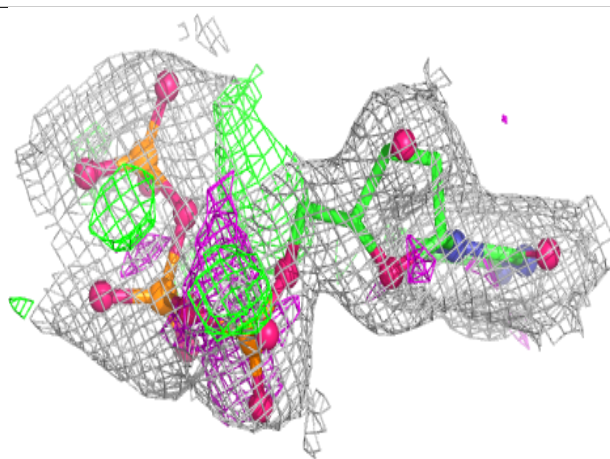
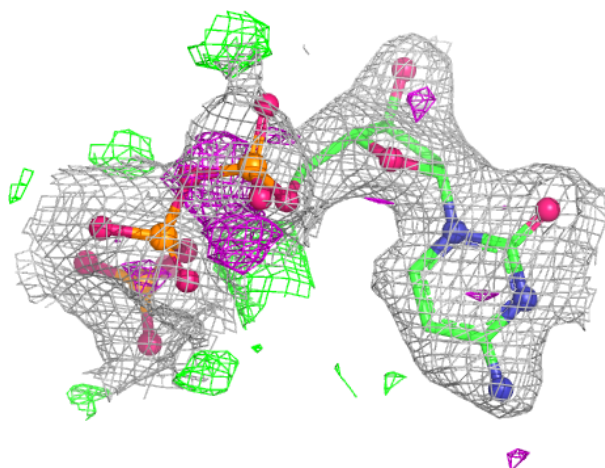
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DGT	D	702	31/31	0.97	0.06	29,33,41,42	0
3	MG	C	704	1/1	0.98	0.09	60,60,60,60	0
3	MG	A	705	1/1	0.99	0.07	41,41,41,41	0
3	MG	B	704	1/1	0.99	0.08	30,30,30,30	0

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.

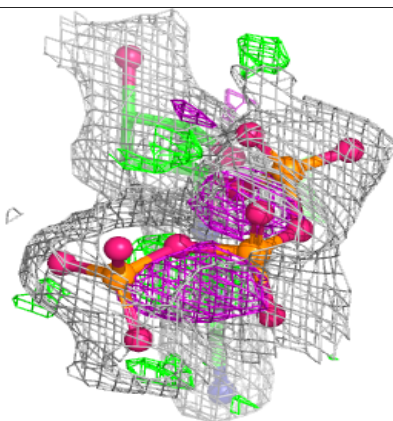
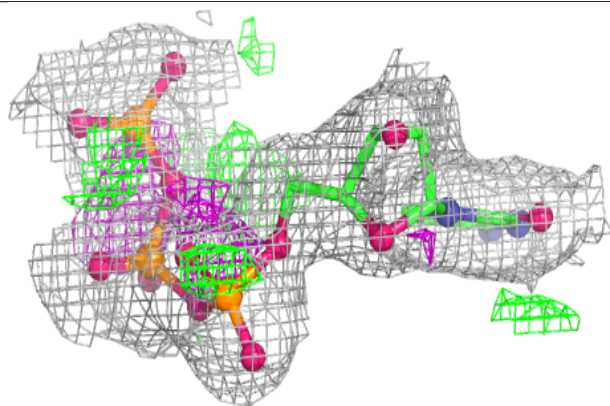
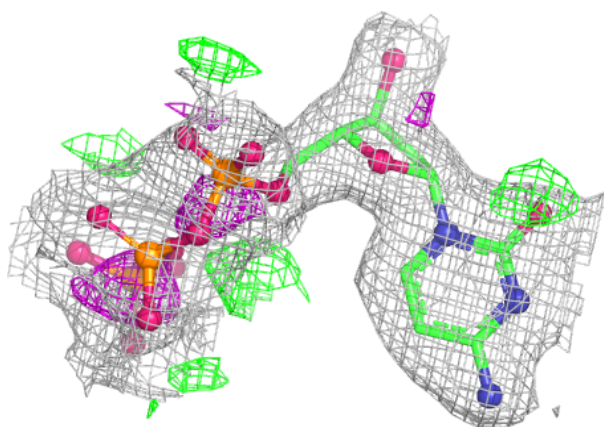
Electron density around DCP D 703:

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

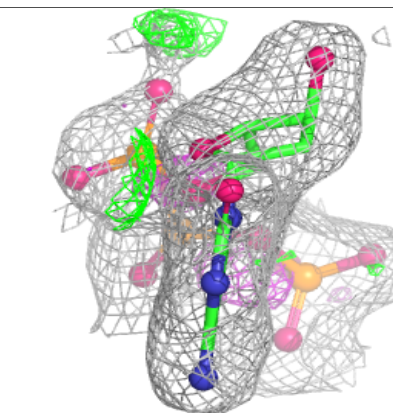
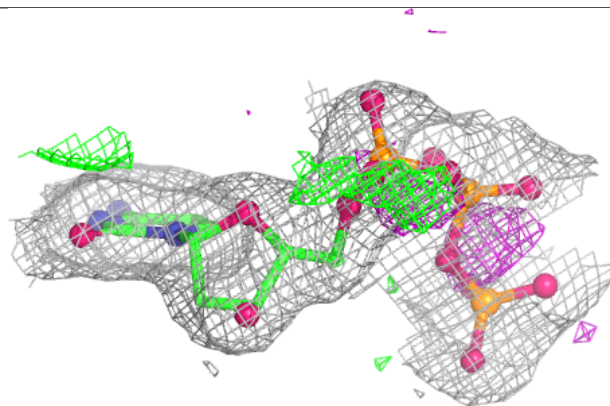
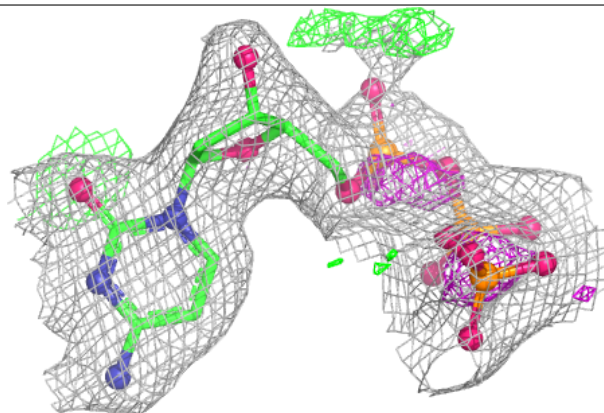


Electron density around DCP A 701:

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

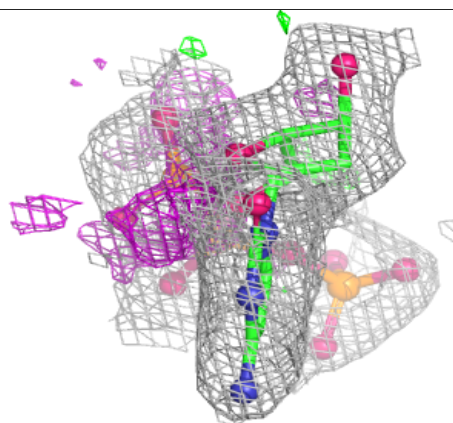
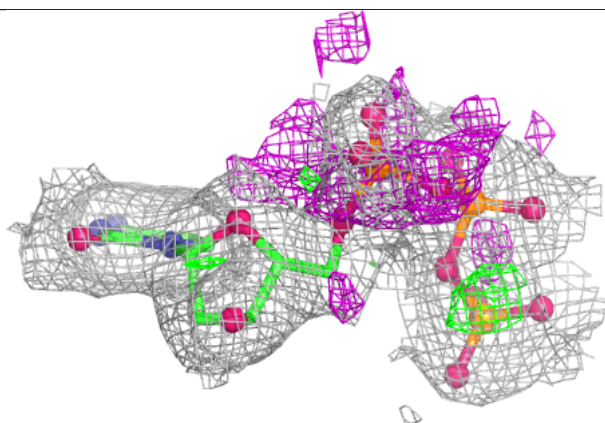
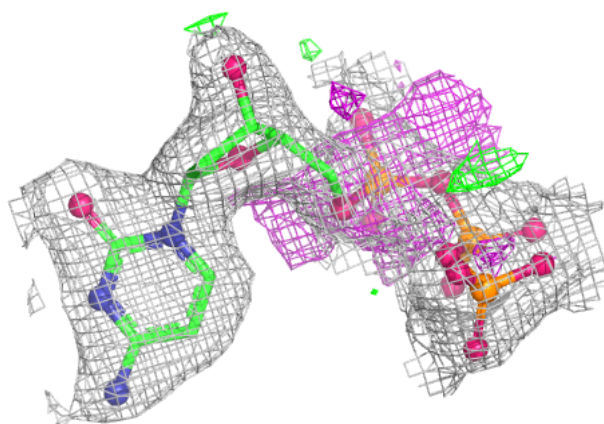
**Electron density around DCP B 701:**

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

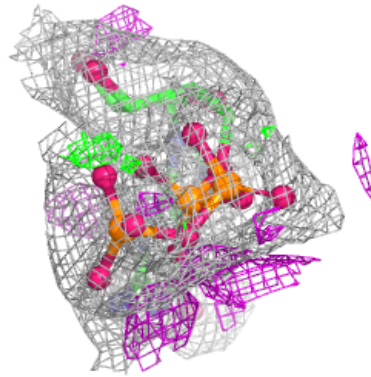
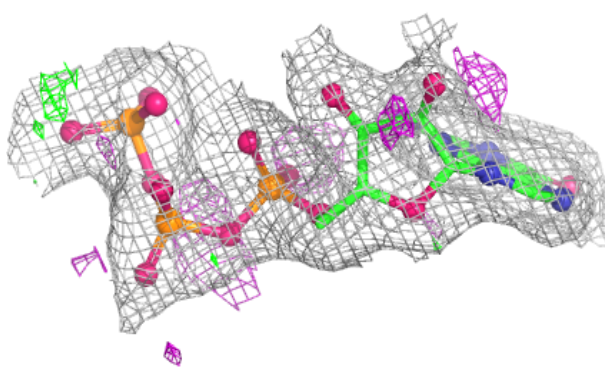
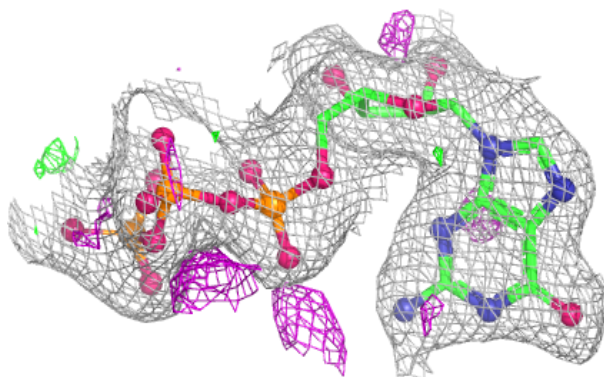


Electron density around DCP C 703:

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

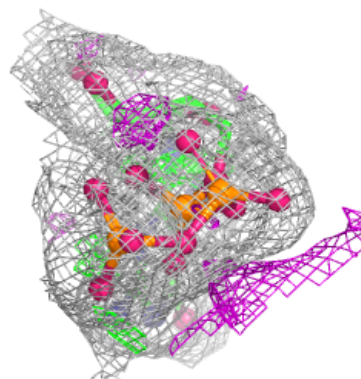
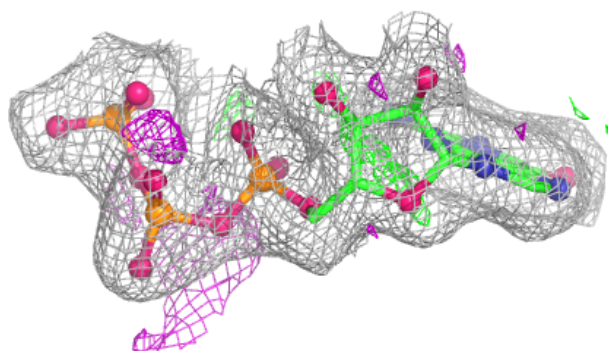
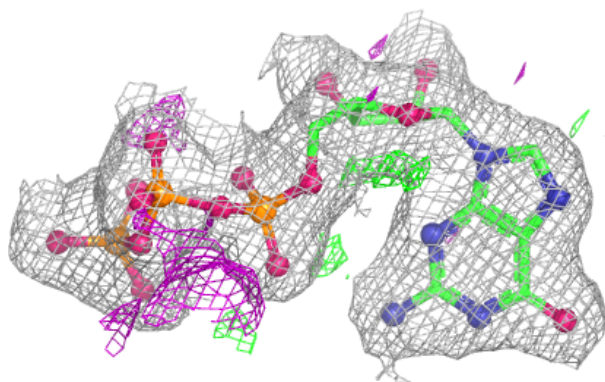
**Electron density around GTP D 705:**

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

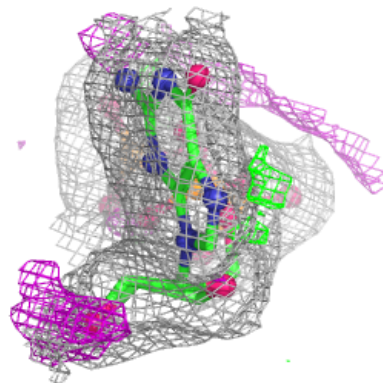
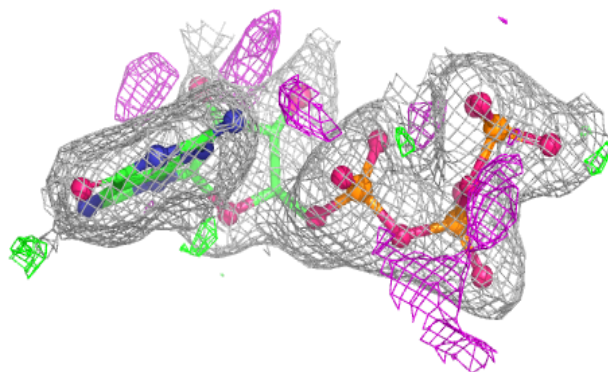
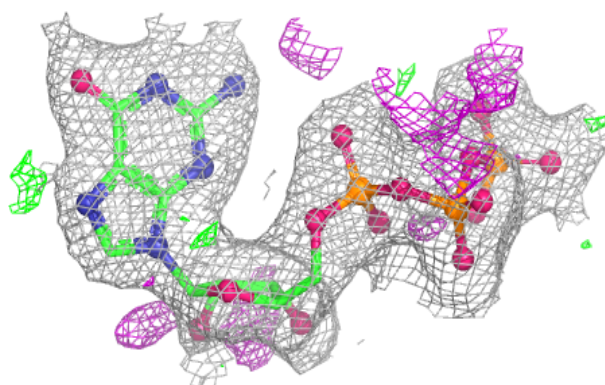


Electron density around GTP A 703:

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

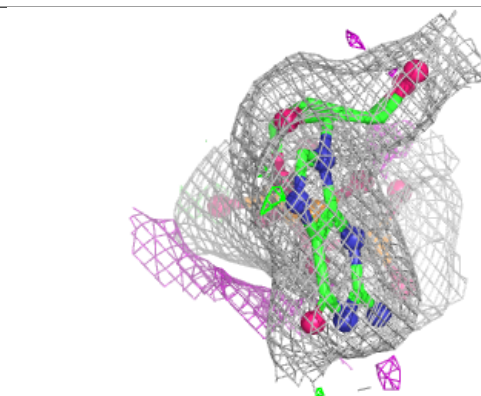
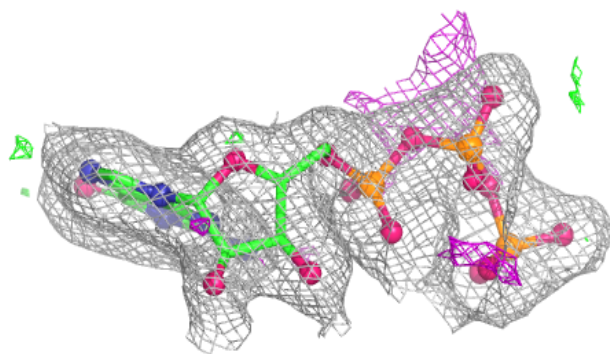
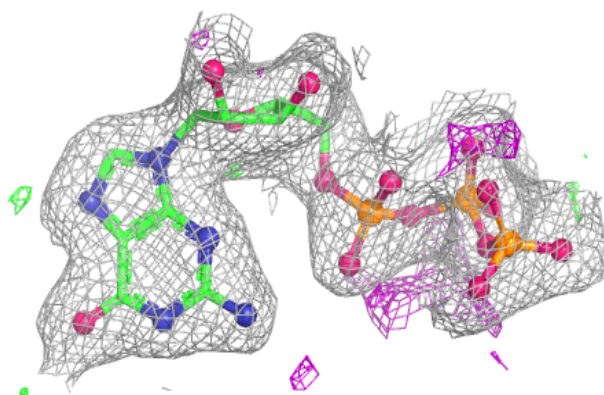
**Electron density around GTP B 703:**

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

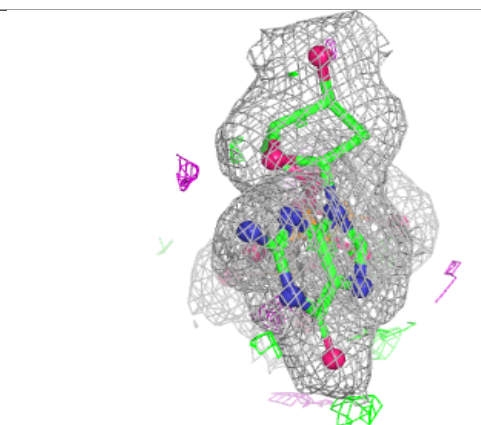
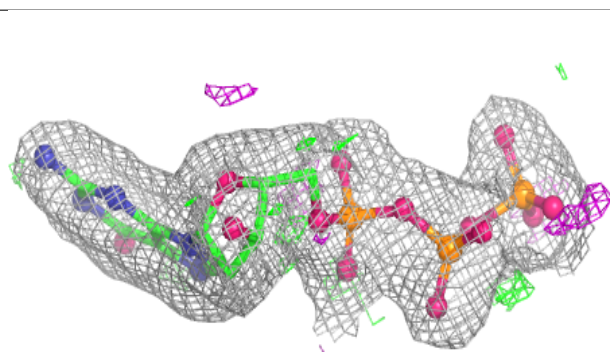
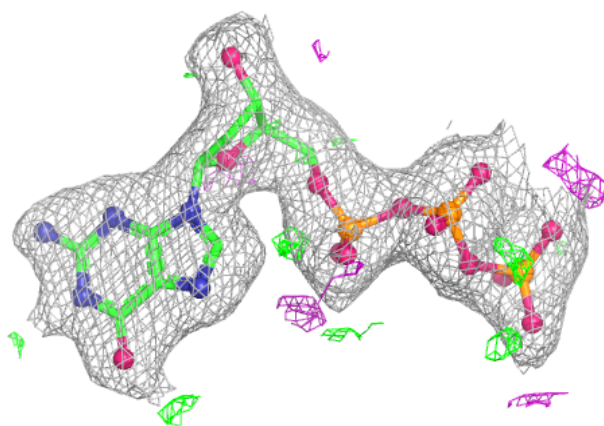


Electron density around GTP B 705:

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

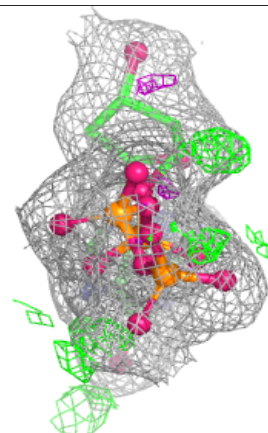
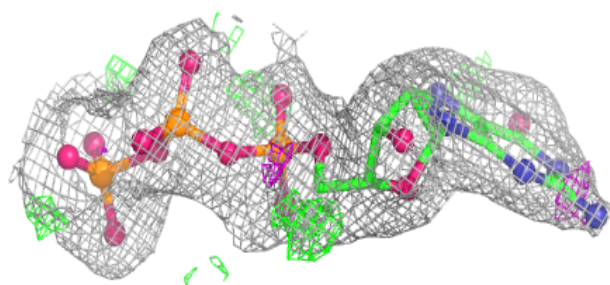
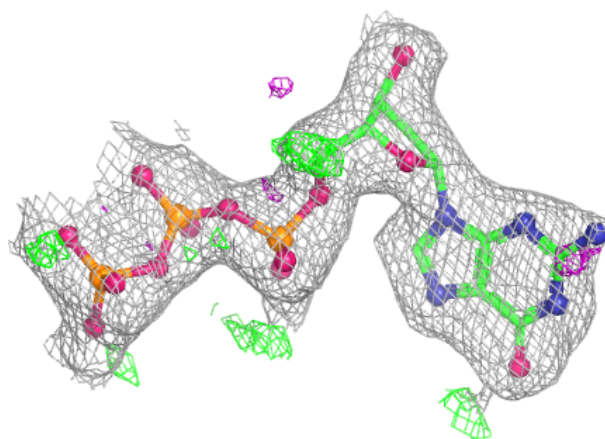
**Electron density around DGT A 704:**

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and green (positive)

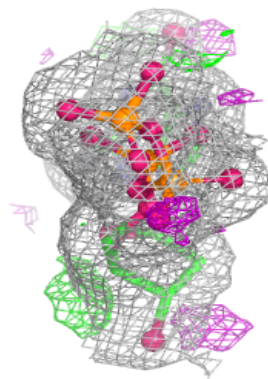
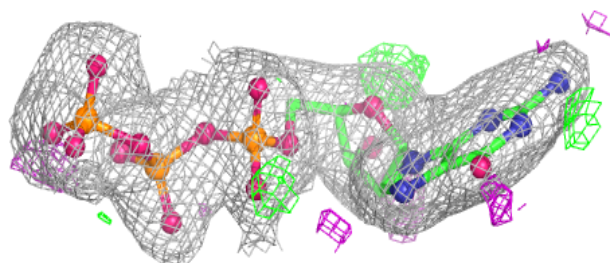
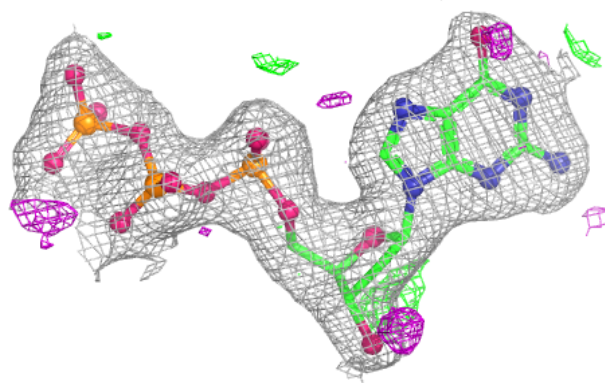


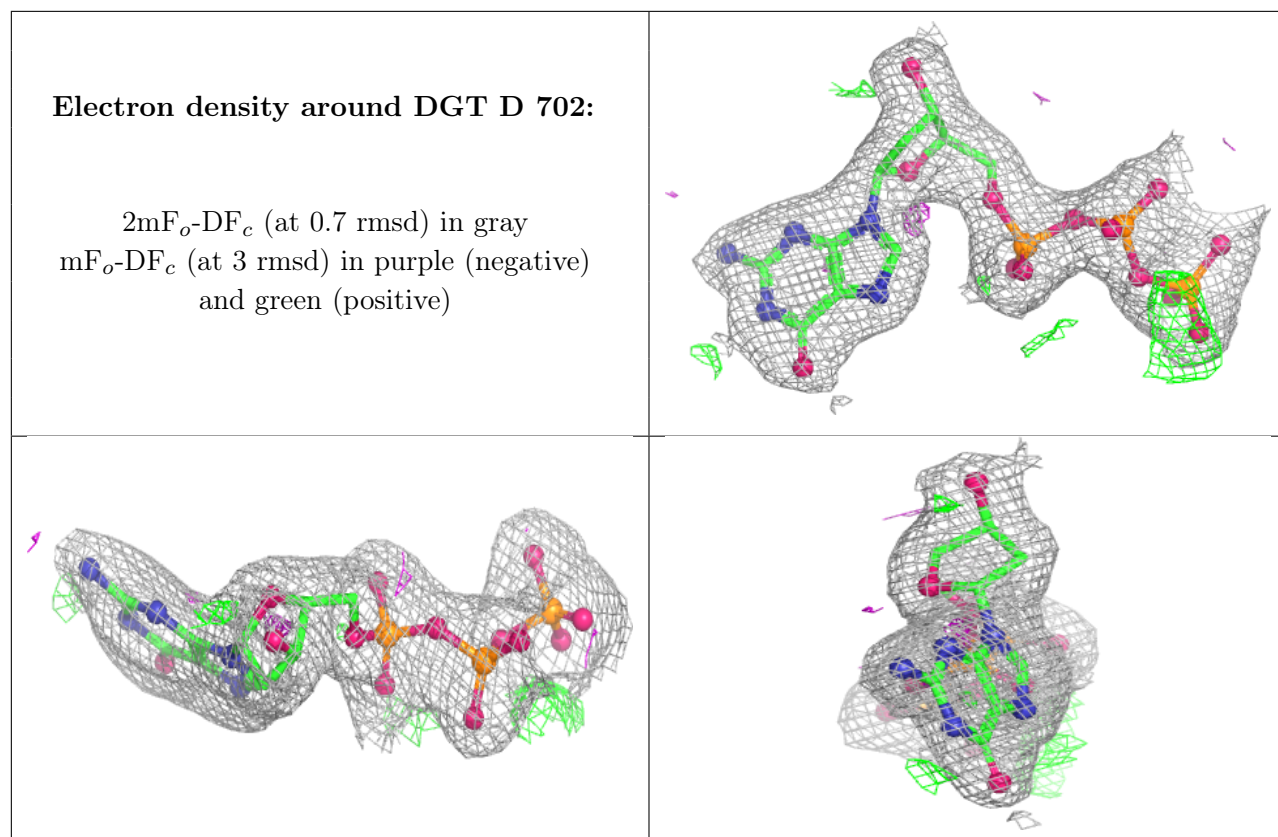
Electron density around DGT B 706:

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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)





6.5 Other polymers [i](#)

There are no such residues in this entry.