



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:47 AM UTC

PDB ID : 4TO6 / pdb_00004to6
Title : Structure basis of cellular dNTP regulation, SAMHD1-dGTP-dATP-dTTP/d
GTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.33 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

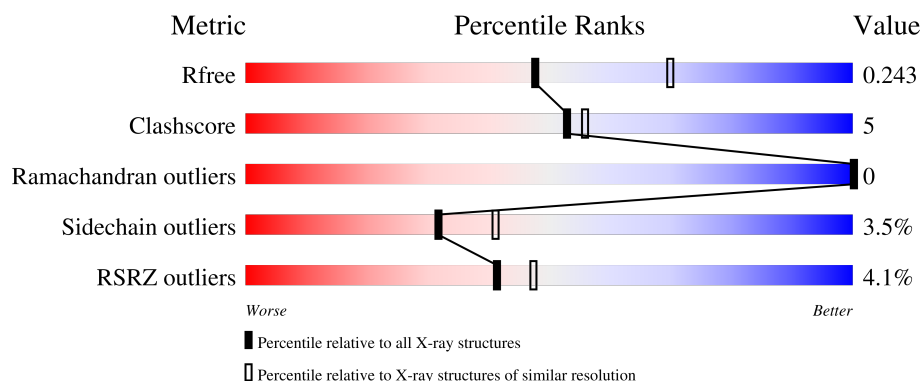
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	2% 82% 11% 7%
1	B	514	2% 82% 11% 7%
1	C	514	4% 82% 11% 7%
1	D	514	8% 82% 10% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16098 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.

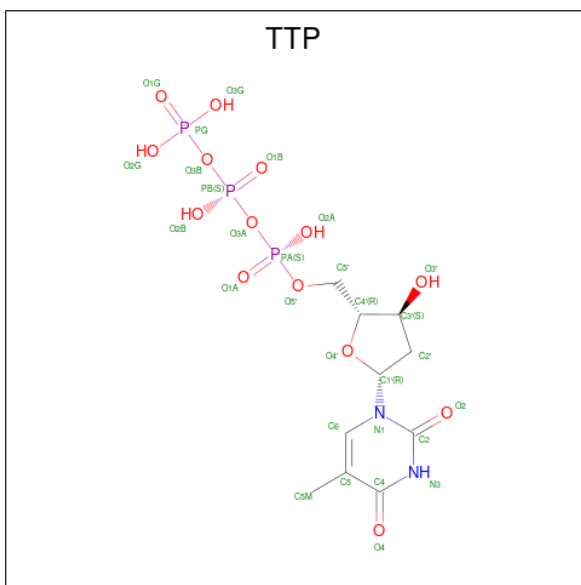
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	B	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	C	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	D	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			

There are 8 discrepancies between the modelled and reference sequences:

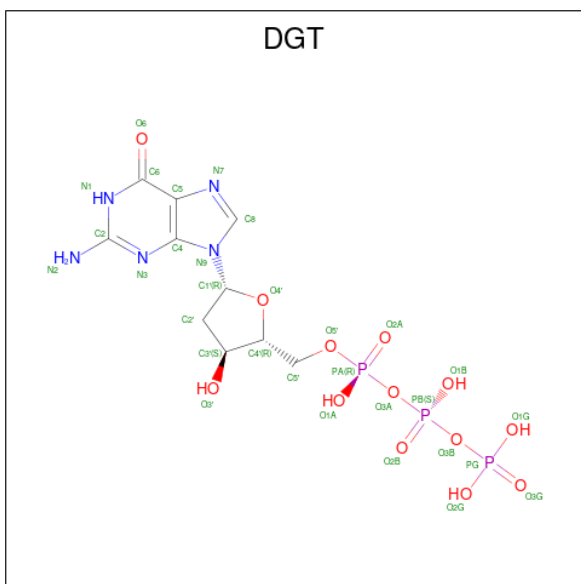
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation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

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



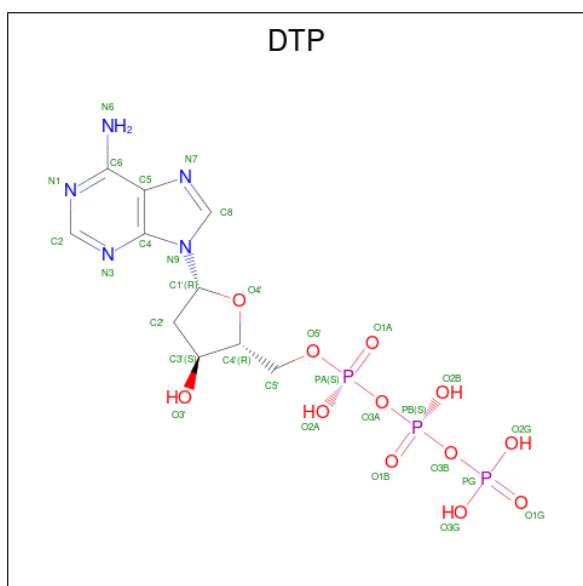
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	B	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	D	1	Total 29	C 10	N 2	O 14	P 3	0	0

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



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

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



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

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

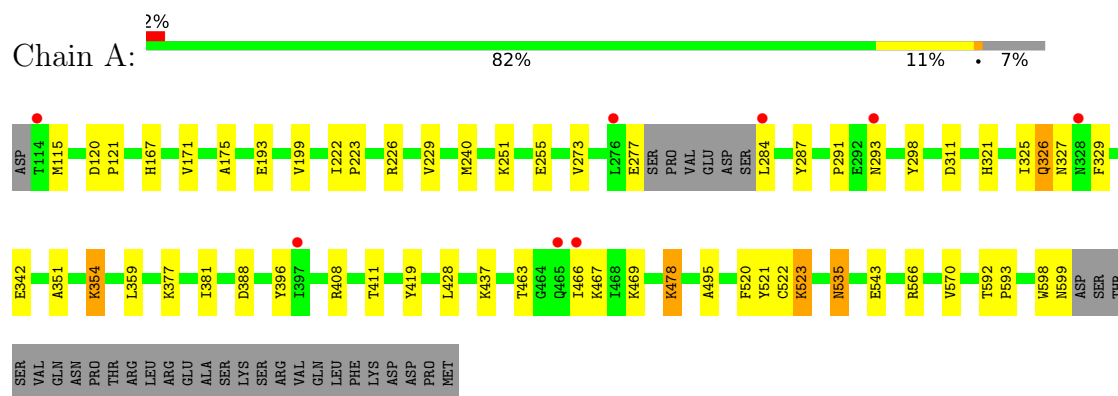
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total 16	O 16	0	0
6	B	4	Total 4	O 4	0	0
6	C	5	Total 5	O 5	0	0
6	D	7	Total 7	O 7	0	0

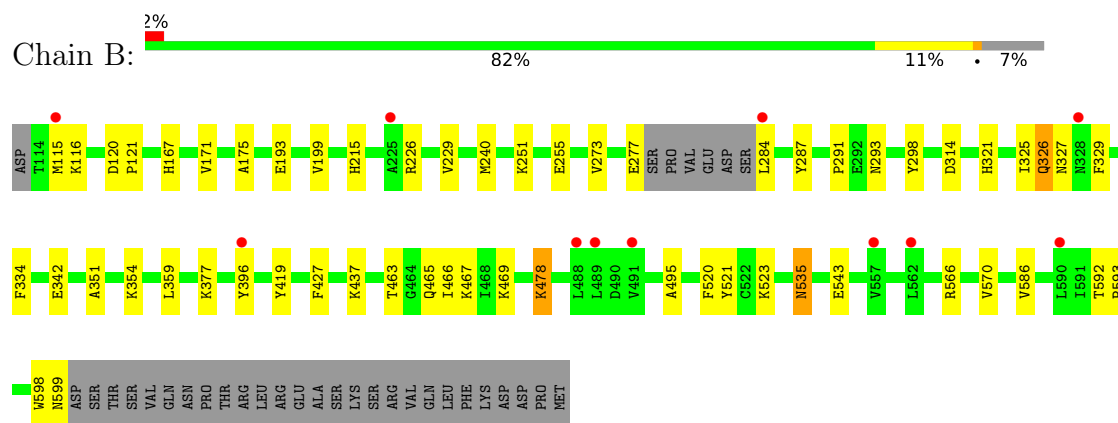
3 Residue-property plots

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

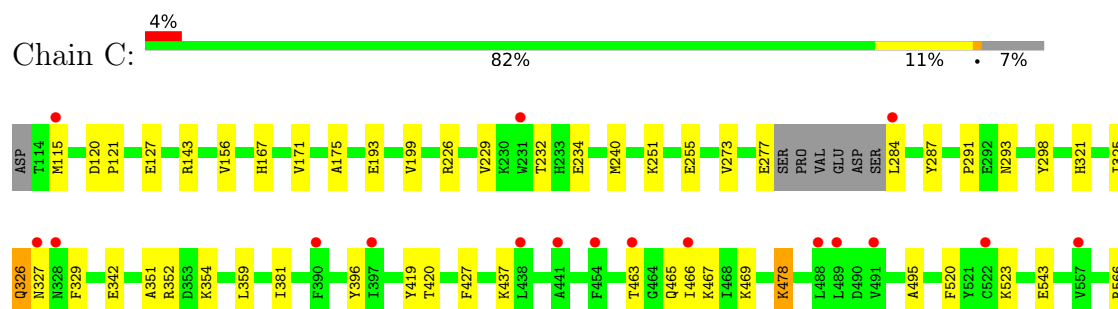
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

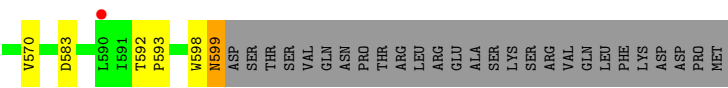


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

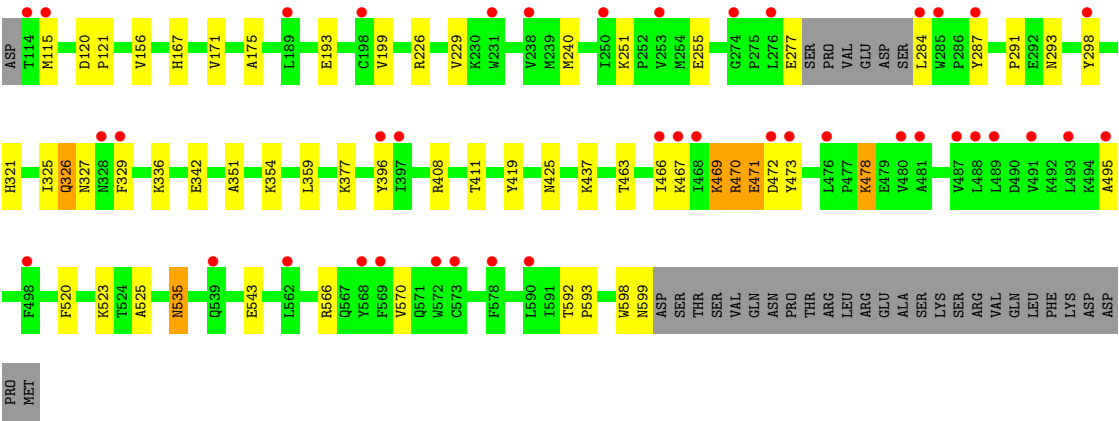
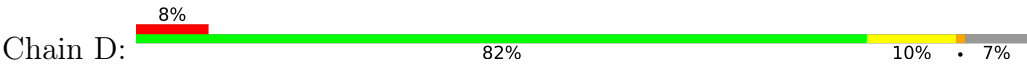


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● 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	82.59Å 140.81Å 96.90Å 90.00° 114.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.33 50.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.33) 99.4 (50.00-2.33)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.225 , 0.244 0.226 , 0.243	Depositor DCC
R_{free} test set	4268 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16098	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, DGT, TTP, MG

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	0.86	0/4017	0.92	1/5422 (0.0%)
1	B	0.79	1/4017 (0.0%)	0.88	1/5422 (0.0%)
1	C	0.78	0/4017	0.89	1/5422 (0.0%)
1	D	0.77	0/4017	0.89	1/5422 (0.0%)
All	All	0.80	1/16068 (0.0%)	0.89	4/21688 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	ASP	N-CA	-5.32	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	PHE	N-CA-C	6.51	119.03	108.41
1	B	329	PHE	N-CA-C	6.28	118.64	108.41
1	D	329	PHE	N-CA-C	6.11	118.36	108.41
1	C	329	PHE	N-CA-C	5.89	118.01	108.41

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	3925	0	3917	38	1
1	B	3925	0	3917	36	2
1	C	3925	0	3917	36	1
1	D	3925	0	3917	69	0
2	A	29	0	13	1	0
2	B	29	0	13	1	0
2	D	29	0	13	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	62	0	24	5	0
3	D	31	0	12	2	0
4	A	30	0	12	1	0
4	B	30	0	12	2	0
4	C	30	0	12	3	0
4	D	30	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	16	0	0	1	0
6	B	4	0	0	0	0
6	C	5	0	0	0	0
6	D	7	0	0	0	0
All	All	16098	0	15815	160	2

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

All (160) 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:D:469:LYS:HE3	1:D:470:ARG:N	1.62	1.15
1:C:598:TRP:O	1:C:599:ASN:HB2	1.49	1.10
1:D:469:LYS:NZ	1:D:469:LYS:HA	1.73	1.03
1:D:470:ARG:HA	1:D:473:TYR:CE2	1.94	1.03
1:D:469:LYS:HE3	1:D:470:ARG:H	0.86	1.02
1:B:116:LYS:NZ	3:C:704:DGT:O3G	2.02	0.92
1:D:470:ARG:NH1	1:D:471:GLU:HB3	1.87	0.90
1:D:469:LYS:HA	1:D:469:LYS:HZ2	1.38	0.86
1:D:470:ARG:HA	1:D:473:TYR:CZ	2.11	0.86
1:D:469:LYS:HB3	1:D:471:GLU:OE2	1.76	0.84
1:D:469:LYS:CE	1:D:470:ARG:H	1.82	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:NZ	3:C:704:DGT:O1G	2.10	0.83
1:D:470:ARG:NH1	1:D:471:GLU:CB	2.42	0.83
1:C:598:TRP:O	1:C:599:ASN:CB	2.31	0.78
1:D:470:ARG:NH1	1:D:471:GLU:CA	2.47	0.78
1:D:470:ARG:CZ	1:D:471:GLU:HB3	2.15	0.77
1:B:326:GLN:HG2	1:D:326:GLN:HE21	1.51	0.76
1:B:326:GLN:HE21	1:D:326:GLN:HG2	1.51	0.75
1:D:469:LYS:CE	1:D:470:ARG:HG3	2.21	0.69
1:D:470:ARG:HA	1:D:473:TYR:CD2	2.27	0.69
1:D:469:LYS:HA	1:D:469:LYS:CE	2.22	0.68
1:D:469:LYS:HE2	1:D:470:ARG:HG3	1.75	0.68
1:D:470:ARG:NH1	1:D:471:GLU:HA	2.11	0.65
1:D:470:ARG:CA	1:D:473:TYR:CE2	2.78	0.64
1:D:471:GLU:CD	1:D:472:ASP:OD1	2.41	0.63
1:A:354:LYS:NZ	4:A:703:DTP:O1A	2.30	0.63
1:A:521:TYR:CD1	1:A:521:TYR:O	2.52	0.63
1:D:469:LYS:HD3	1:D:470:ARG:HD3	1.79	0.63
1:D:470:ARG:HH11	1:D:471:GLU:HA	1.61	0.62
1:D:471:GLU:OE2	1:D:471:GLU:N	2.32	0.62
1:A:326:GLN:HE21	1:C:326:GLN:HG2	1.64	0.61
1:A:326:GLN:HG2	1:C:326:GLN:HE21	1.64	0.61
1:D:469:LYS:CE	1:D:469:LYS:CA	2.79	0.61
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.02	0.60
1:B:521:TYR:O	1:B:521:TYR:CD1	2.53	0.60
1:A:521:TYR:CD1	1:A:521:TYR:C	2.80	0.60
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.02	0.59
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.02	0.59
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.84	0.59
1:D:470:ARG:NE	1:D:471:GLU:N	2.50	0.59
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.02	0.59
1:B:521:TYR:CD1	1:B:521:TYR:C	2.80	0.59
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.01	0.59
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.03	0.59
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.03	0.58
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.03	0.58
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.86	0.57
1:C:463:THR:O	1:C:466:ILE:HG12	2.04	0.57
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.87	0.57
1:B:463:THR:O	1:B:466:ILE:HG12	2.05	0.56
1:A:463:THR:O	1:A:466:ILE:HG12	2.04	0.56
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ALA:HB1	1:D:199:VAL:HG12	1.87	0.56
1:D:463:THR:O	1:D:466:ILE:HG12	2.05	0.56
1:A:522:CYS:SG	1:C:583:ASP:HB3	2.47	0.55
1:A:298:TYR:O	6:A:812:HOH:O	2.18	0.54
1:D:469:LYS:HE3	1:D:470:ARG:HG3	1.89	0.54
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.44	0.53
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.43	0.53
1:B:226:ARG:O	1:B:229:VAL:HG12	2.09	0.53
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.44	0.52
1:C:226:ARG:O	1:C:229:VAL:HG12	2.10	0.52
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.44	0.52
1:A:377:LYS:NZ	4:C:701:DTP:O1B	2.43	0.52
1:D:226:ARG:O	1:D:229:VAL:HG12	2.09	0.52
1:C:566:ARG:O	1:C:570:VAL:HG23	2.10	0.51
1:D:470:ARG:CZ	1:D:471:GLU:N	2.73	0.51
1:D:470:ARG:HB3	1:D:473:TYR:CE2	2.45	0.51
1:B:566:ARG:O	1:B:570:VAL:HG23	2.10	0.51
1:A:226:ARG:O	1:A:229:VAL:HG12	2.11	0.50
1:D:566:ARG:O	1:D:570:VAL:HG23	2.11	0.50
1:A:566:ARG:O	1:A:570:VAL:HG23	2.11	0.50
1:B:543:GLU:HG2	1:D:543:GLU:HG2	1.92	0.50
1:C:156:VAL:O	3:C:704:DGT:H8	2.12	0.49
3:C:703:DGT:O1B	3:C:703:DGT:O1A	2.30	0.48
1:D:469:LYS:HB3	1:D:471:GLU:CD	2.39	0.48
1:C:325:ILE:HG22	1:C:326:GLN:N	2.29	0.48
1:A:251:LYS:O	1:A:255:GLU:HG3	2.14	0.48
4:B:704:DTP:O1B	3:D:704:DGT:H5'A	2.13	0.48
1:B:251:LYS:O	1:B:255:GLU:HG3	2.14	0.48
1:A:408:ARG:H	1:A:411:THR:HG1	1.61	0.47
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:C:167:HIS:O	1:C:171:VAL:HG23	2.14	0.47
1:A:167:HIS:O	1:A:171:VAL:HG23	2.14	0.47
1:A:535:ASN:OD1	1:A:535:ASN:N	2.46	0.47
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.47
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.97	0.47
1:D:251:LYS:O	1:D:255:GLU:HG3	2.15	0.47
1:D:287:TYR:CD1	1:D:298:TYR:CE1	3.02	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:A:327:ASN:O	1:C:326:GLN:HB3	2.14	0.47
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.96	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ARG:NH2	4:C:701:DTP:O1G	2.44	0.47
1:D:471:GLU:OE2	1:D:472:ASP:N	2.47	0.47
1:D:167:HIS:O	1:D:171:VAL:HG23	2.15	0.47
1:B:167:HIS:O	1:B:171:VAL:HG23	2.15	0.46
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.97	0.46
1:B:326:GLN:HB3	1:D:327:ASN:O	2.16	0.46
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.46
1:D:469:LYS:HA	1:D:469:LYS:HZ1	1.70	0.46
1:B:586:VAL:HG11	1:D:525:ALA:HB3	1.98	0.46
1:C:592:THR:N	1:C:593:PRO:CD	2.79	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.46
1:C:287:TYR:CD1	1:C:298:TYR:CE1	3.04	0.46
1:A:325:ILE:HG22	1:A:326:GLN:N	2.30	0.46
1:A:311:ASP:OD2	2:A:701:TTP:O1A	2.34	0.46
1:A:326:GLN:HG2	1:C:326:GLN:HG2	1.97	0.45
1:C:251:LYS:O	1:C:255:GLU:HG3	2.15	0.45
1:C:325:ILE:CG2	1:C:326:GLN:N	2.79	0.45
1:A:287:TYR:CD1	1:A:298:TYR:CE1	3.04	0.45
1:A:326:GLN:HB3	1:C:327:ASN:O	2.17	0.45
1:B:586:VAL:CG1	1:D:525:ALA:HB3	2.46	0.45
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.98	0.45
1:B:326:GLN:HG2	1:D:326:GLN:HG2	1.98	0.45
1:A:522:CYS:SG	1:C:583:ASP:CB	3.05	0.45
1:B:325:ILE:HG22	1:B:326:GLN:N	2.31	0.45
1:D:240:MET:CE	1:D:419:TYR:HD2	2.31	0.44
1:D:469:LYS:HE3	1:D:469:LYS:C	2.35	0.44
1:B:287:TYR:CD1	1:B:298:TYR:CE1	3.05	0.44
1:D:325:ILE:HG22	1:D:326:GLN:N	2.31	0.44
1:A:325:ILE:CG2	1:A:326:GLN:N	2.80	0.44
1:D:469:LYS:HE3	1:D:469:LYS:CA	2.47	0.44
1:B:325:ILE:CG2	1:B:326:GLN:N	2.81	0.44
1:B:535:ASN:OD1	1:B:535:ASN:N	2.47	0.44
1:D:469:LYS:HZ2	1:D:469:LYS:CA	2.22	0.44
1:C:352:ARG:HH22	4:C:701:DTP:PG	2.40	0.44
1:D:351:ALA:O	1:D:520:PHE:HA	2.18	0.43
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.06	0.43
1:A:598:TRP:O	1:A:599:ASN:HB2	2.19	0.43
1:C:351:ALA:O	1:C:520:PHE:HA	2.18	0.43
1:A:240:MET:CE	1:A:419:TYR:HD2	2.32	0.43
1:D:156:VAL:O	3:D:704:DGT:H8	2.18	0.43
1:C:143:ARG:HD2	1:C:420:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:HIS:CE1	1:C:321:HIS:CE1	3.06	0.43
1:C:240:MET:CE	1:C:419:TYR:HD2	2.32	0.42
1:C:427:PHE:C	1:C:427:PHE:CD1	2.96	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.87	0.42
1:D:325:ILE:CG2	1:D:326:GLN:N	2.82	0.42
1:B:327:ASN:O	1:D:326:GLN:HB3	2.20	0.42
1:D:470:ARG:CB	1:D:473:TYR:CE2	3.02	0.42
3:C:704:DGT:N3	3:C:704:DGT:H2'A	2.35	0.42
1:C:232:THR:HB	1:C:234:GLU:OE1	2.20	0.41
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.41
1:C:127:GLU:HG3	1:D:336:LYS:HE3	2.02	0.41
1:B:215:HIS:CD2	2:B:701:TTP:C6	3.08	0.41
1:D:408:ARG:H	1:D:411:THR:HG1	1.66	0.41
1:A:222:ILE:HB	1:A:223:PRO:HD3	2.03	0.41
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.88	0.41
1:B:598:TRP:O	1:B:599:ASN:HB2	2.20	0.41
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.02	0.41
1:B:334:PHE:CD1	1:B:334:PHE:C	2.99	0.41
1:D:535:ASN:OD1	1:D:535:ASN:N	2.47	0.41
1:C:478:LYS:H	1:C:478:LYS:HD2	1.85	0.41
1:B:427:PHE:CD1	1:B:427:PHE:C	2.99	0.40
4:B:704:DTP:O2B	1:D:377:LYS:NZ	2.54	0.40
1:B:543:GLU:CG	1:D:543:GLU:CG	2.99	0.40
1:D:478:LYS:HD2	1:D:478:LYS:H	1.86	0.40
1:B:240:MET:CE	1:B:419:TYR:HD2	2.34	0.40
1:B:377:LYS:NZ	4:D:702:DTP:O2B	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:NH2	1:B:478:LYS:CG[1_454]	1.86	0.34
1:B:543:GLU:O	1:C:465:GLN:OE1[1_655]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/514 (93%)	470 (99%)	6 (1%)	0	100	100
1	B	476/514 (93%)	469 (98%)	7 (2%)	0	100	100
1	C	476/514 (93%)	470 (99%)	6 (1%)	0	100	100
1	D	476/514 (93%)	471 (99%)	5 (1%)	0	100	100
All	All	1904/2056 (93%)	1880 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/459 (93%)	411 (96%)	15 (4%)	32	41
1	B	426/459 (93%)	411 (96%)	15 (4%)	32	41
1	C	426/459 (93%)	412 (97%)	14 (3%)	33	43
1	D	426/459 (93%)	411 (96%)	15 (4%)	32	41
All	All	1704/1836 (93%)	1645 (96%)	59 (4%)	32	41

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	193	GLU
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU
1	A	326	GLN
1	A	342	GLU
1	A	354	LYS

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Mol	Chain	Res	Type
1	A	359	LEU
1	A	388	ASP
1	A	467	LYS
1	A	469	LYS
1	A	478	LYS
1	A	523	LYS
1	A	535	ASN
1	B	115	MET
1	B	193	GLU
1	B	273	VAL
1	B	277	GLU
1	B	284	LEU
1	B	326	GLN
1	B	342	GLU
1	B	354	LYS
1	B	359	LEU
1	B	465	GLN
1	B	467	LYS
1	B	469	LYS
1	B	478	LYS
1	B	523	LYS
1	B	535	ASN
1	C	115	MET
1	C	193	GLU
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	326	GLN
1	C	342	GLU
1	C	354	LYS
1	C	359	LEU
1	C	467	LYS
1	C	469	LYS
1	C	478	LYS
1	C	523	LYS
1	C	599	ASN
1	D	115	MET
1	D	193	GLU
1	D	277	GLU
1	D	284	LEU
1	D	326	GLN
1	D	342	GLU

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Mol	Chain	Res	Type
1	D	354	LYS
1	D	359	LEU
1	D	467	LYS
1	D	469	LYS
1	D	470	ARG
1	D	471	GLU
1	D	478	LYS
1	D	523	LYS
1	D	535	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	149	GLN
1	A	210	HIS
1	A	235	GLN
1	A	243	HIS
1	A	248	ASN
1	A	326	GLN
1	A	447	GLN
1	A	567	GLN
1	B	140	GLN
1	B	149	GLN
1	B	210	HIS
1	B	235	GLN
1	B	243	HIS
1	B	248	ASN
1	B	326	GLN
1	B	447	GLN
1	B	567	GLN
1	C	140	GLN
1	C	149	GLN
1	C	200	GLN
1	C	210	HIS
1	C	215	HIS
1	C	235	GLN
1	C	243	HIS
1	C	248	ASN
1	C	322	HIS
1	C	326	GLN
1	C	447	GLN

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Mol	Chain	Res	Type
1	C	567	GLN
1	D	140	GLN
1	D	149	GLN
1	D	235	GLN
1	D	243	HIS
1	D	248	ASN
1	D	326	GLN
1	D	370	HIS
1	D	375	GLN
1	D	380	ASN
1	D	447	GLN
1	D	567	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DGT	B	702	5	32,33,33	1.46	5 (15%)	48,52,52	1.69	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DTP	A	703	5	31,32,32	1.67	8 (25%)	46,50,50	2.20	15 (32%)
3	DGT	C	704	5	32,33,33	1.38	6 (18%)	48,52,52	1.79	8 (16%)
2	TTP	B	701	-	29,30,30	1.57	7 (24%)	43,47,47	1.97	10 (23%)
2	TTP	A	701	-	29,30,30	1.70	8 (27%)	43,47,47	1.98	8 (18%)
3	DGT	C	703	-	32,33,33	1.35	3 (9%)	48,52,52	1.82	10 (20%)
3	DGT	A	702	5	32,33,33	1.69	6 (18%)	48,52,52	1.91	12 (25%)
2	TTP	D	703	-	29,30,30	1.47	4 (13%)	43,47,47	2.02	8 (18%)
4	DTP	B	704	5	31,32,32	1.84	5 (16%)	46,50,50	1.99	12 (26%)
4	DTP	C	701	5	31,32,32	1.54	6 (19%)	46,50,50	1.96	11 (23%)
3	DGT	D	704	5	32,33,33	1.71	6 (18%)	48,52,52	1.90	11 (22%)
4	DTP	D	702	5	31,32,32	1.69	6 (19%)	46,50,50	1.90	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DGT	B	702	5	-	5/22/34/34	0/3/3/3
4	DTP	A	703	5	-	8/22/34/34	0/3/3/3
3	DGT	C	704	5	-	6/22/34/34	0/3/3/3
2	TTP	B	701	-	-	4/22/34/34	0/2/2/2
2	TTP	A	701	-	-	4/22/34/34	0/2/2/2
3	DGT	C	703	-	-	11/22/34/34	0/3/3/3
3	DGT	A	702	5	-	7/22/34/34	0/3/3/3
2	TTP	D	703	-	-	4/22/34/34	0/2/2/2
4	DTP	B	704	5	-	4/22/34/34	0/3/3/3
4	DTP	C	701	5	-	6/22/34/34	0/3/3/3
3	DGT	D	704	5	-	5/22/34/34	0/3/3/3
4	DTP	D	702	5	-	5/22/34/34	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	704	DTP	PB-O3A	5.51	1.65	1.59
3	A	702	DGT	PB-O3B	4.69	1.64	1.59
4	B	704	DTP	PA-O3A	4.67	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	DTP	C5-C4	4.66	1.47	1.39
3	D	704	DGT	PA-O3A	4.19	1.64	1.59
4	B	704	DTP	C5-C4	4.16	1.46	1.39
3	A	702	DGT	C5-N7	-4.12	1.30	1.39
4	D	702	DTP	C8-N9	-3.85	1.31	1.37
2	B	701	TTP	C4-C5	3.84	1.51	1.44
3	C	703	DGT	C5-C4	3.78	1.49	1.38
2	A	701	TTP	PB-O3A	3.75	1.63	1.59
3	D	704	DGT	PB-O3B	3.67	1.63	1.59
2	D	703	TTP	C6-C5	3.59	1.40	1.34
4	D	702	DTP	PA-O3A	3.58	1.63	1.59
2	A	701	TTP	C4-C5	3.56	1.50	1.44
4	A	703	DTP	C5-C4	3.53	1.45	1.39
3	A	702	DGT	C6-N1	-3.52	1.32	1.38
4	A	703	DTP	PB-O3A	3.50	1.63	1.59
2	D	703	TTP	C4-C5	3.50	1.50	1.44
4	D	702	DTP	C5-N7	-3.47	1.32	1.39
3	B	702	DGT	C6-N1	-3.46	1.32	1.38
3	D	704	DGT	C5-N7	-3.44	1.32	1.39
2	D	703	TTP	C2-N1	3.42	1.43	1.38
4	D	702	DTP	C5-C4	3.40	1.45	1.39
3	D	704	DGT	C6-N1	-3.33	1.32	1.38
3	B	702	DGT	C4-N9	-3.29	1.29	1.38
3	D	704	DGT	C5-C4	3.29	1.47	1.38
4	C	701	DTP	PB-O3B	3.29	1.63	1.59
2	B	701	TTP	PB-O3B	3.26	1.63	1.59
3	C	704	DGT	C4-N9	-3.25	1.29	1.38
2	B	701	TTP	C2-N1	3.15	1.43	1.38
4	A	703	DTP	C8-N9	-3.15	1.32	1.37
3	A	702	DGT	C5-C4	3.08	1.47	1.38
3	C	704	DGT	C6-N1	-3.01	1.33	1.38
4	A	703	DTP	C5-N7	-2.94	1.33	1.39
3	B	702	DGT	PB-O3A	2.89	1.62	1.59
2	A	701	TTP	C6-C5	2.83	1.39	1.34
3	B	702	DGT	C5-N7	-2.83	1.33	1.39
2	A	701	TTP	C2-N1	2.81	1.42	1.38
3	B	702	DGT	C5-C4	2.78	1.46	1.38
4	B	704	DTP	C8-N7	2.73	1.36	1.31
2	A	701	TTP	PA-O3A	2.70	1.62	1.59
3	C	703	DGT	PB-O3B	2.69	1.62	1.59
4	C	701	DTP	C8-N7	2.64	1.36	1.31
4	D	702	DTP	C8-N7	2.61	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	TTP	C4-N3	-2.56	1.34	1.38
2	B	701	TTP	C6-C5	2.54	1.38	1.34
3	C	704	DGT	C5-C4	2.53	1.45	1.38
3	C	704	DGT	PB-O3B	2.52	1.62	1.59
3	A	702	DGT	C4-N9	-2.45	1.31	1.38
4	A	703	DTP	C8-N7	2.45	1.36	1.31
3	C	704	DGT	C5-N7	-2.45	1.34	1.39
4	C	701	DTP	C4-N9	-2.45	1.32	1.37
3	C	704	DGT	PB-O3A	2.43	1.62	1.59
2	A	701	TTP	C4-N3	-2.37	1.34	1.38
3	C	703	DGT	PB-O3A	2.26	1.61	1.59
4	D	702	DTP	C5-C6	2.21	1.47	1.41
2	A	701	TTP	PB-O3B	2.21	1.61	1.59
2	B	701	TTP	C4-N3	-2.21	1.34	1.38
2	A	701	TTP	C6-N1	-2.19	1.34	1.38
4	A	703	DTP	O4'-C4'	-2.18	1.40	1.45
4	C	701	DTP	C8-N9	-2.14	1.33	1.37
2	B	701	TTP	PA-O3A	2.10	1.61	1.59
2	B	701	TTP	PB-O3A	2.08	1.61	1.59
3	A	702	DGT	PB-O3A	2.08	1.61	1.59
4	C	701	DTP	C5-C6	2.08	1.46	1.41
3	D	704	DGT	C4-N9	-2.05	1.32	1.38
4	B	704	DTP	C5-N7	-2.02	1.35	1.39
4	A	703	DTP	PB-O3B	2.01	1.61	1.59
4	A	703	DTP	PA-O3A	2.01	1.61	1.59

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	704	DGT	C5-C4-N3	-6.03	118.79	128.39
3	A	702	DGT	C5-C4-N3	-6.02	118.81	128.39
3	C	704	DGT	C5-C4-N3	-5.94	118.94	128.39
2	D	703	TTP	C5-C4-N3	5.87	120.42	115.32
2	D	703	TTP	C4-N3-C2	-5.86	119.65	127.34
4	A	703	DTP	C5-C4-N3	-5.86	118.65	126.72
3	C	704	DGT	C2-N3-C4	5.78	122.25	112.30
2	A	701	TTP	C4-N3-C2	-5.78	119.76	127.34
4	D	702	DTP	C5-C4-N3	-5.64	118.95	126.72
3	C	703	DGT	C5-C4-N3	-5.64	119.42	128.39
3	B	702	DGT	C5-C4-N3	-5.49	119.66	128.39
2	A	701	TTP	N3-C2-N1	5.44	121.98	114.89
4	C	701	DTP	C5-C4-N3	-5.42	119.26	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	TTP	C4-N3-C2	-5.30	120.40	127.34
4	B	704	DTP	N3-C2-N1	-5.24	120.65	128.58
2	D	703	TTP	N3-C2-N1	5.22	121.68	114.89
3	B	702	DGT	C2-N3-C4	5.09	121.07	112.30
4	A	703	DTP	N3-C2-N1	-5.08	120.89	128.58
4	A	703	DTP	N3-C4-N9	5.04	135.74	127.17
2	B	701	TTP	N3-C2-N1	4.83	121.18	114.89
3	D	704	DGT	C2-N3-C4	4.70	120.40	112.30
3	C	703	DGT	C2-N3-C4	4.64	120.30	112.30
2	B	701	TTP	C5M-C5-C4	4.62	123.71	118.78
4	C	701	DTP	N3-C4-N9	4.54	134.90	127.17
2	B	701	TTP	C5-C4-N3	4.43	119.17	115.32
2	D	703	TTP	C5-C6-N1	-4.42	118.51	123.31
4	D	702	DTP	C4-C5-N7	-4.41	105.54	110.58
2	A	701	TTP	C5-C6-N1	-4.41	118.53	123.31
3	C	703	DGT	N9-C4-N3	4.40	134.75	125.95
4	C	701	DTP	N3-C2-N1	-4.39	121.94	128.58
2	A	701	TTP	C5-C4-N3	4.37	119.12	115.32
4	B	704	DTP	C5-C4-N3	-4.35	120.73	126.72
3	A	702	DGT	O1B-PB-O3A	4.34	118.99	107.27
4	A	703	DTP	C2-N3-C4	4.33	122.39	111.83
4	D	702	DTP	N3-C4-N9	4.31	134.49	127.17
4	A	703	DTP	C4-N9-C8	4.18	110.13	105.74
4	B	704	DTP	C4-N9-C8	4.17	110.12	105.74
3	D	704	DGT	O2G-PG-O1G	4.11	123.22	107.80
3	B	702	DGT	N9-C4-N3	4.04	134.03	125.95
2	B	701	TTP	C5M-C5-C6	-3.97	117.48	122.85
3	A	702	DGT	C2-N3-C4	3.92	119.06	112.30
4	B	704	DTP	N3-C4-N9	3.89	133.78	127.17
3	C	704	DGT	N9-C4-N3	3.85	133.66	125.95
4	A	703	DTP	C4-C5-N7	-3.71	106.34	110.58
4	C	701	DTP	C2-N3-C4	3.71	120.88	111.83
3	C	704	DGT	C6-C5-N7	3.70	137.03	130.29
3	C	703	DGT	C6-C5-N7	3.69	137.00	130.29
4	C	701	DTP	O3B-PG-O1G	-3.68	91.70	111.04
3	A	702	DGT	N9-C4-N3	3.65	133.25	125.95
2	B	701	TTP	C5-C6-N1	-3.62	119.38	123.31
4	B	704	DTP	C2-N1-C6	3.58	124.61	118.73
4	B	704	DTP	N9-C8-N7	-3.54	108.92	113.94
4	D	702	DTP	C5-N7-C8	3.49	108.94	103.45
4	B	704	DTP	C2-N3-C4	3.46	120.29	111.83
4	C	701	DTP	C4-N9-C8	3.42	109.33	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	DGT	O1G-PG-O3G	3.40	124.09	110.83
3	A	702	DGT	C4-C5-N7	-3.32	105.40	110.67
4	A	703	DTP	C5-N7-C8	3.29	108.62	103.45
3	D	704	DGT	N9-C4-N3	3.29	132.53	125.95
3	A	702	DGT	O5'-PA-O2A	-3.26	96.00	108.94
4	D	702	DTP	C4-N9-C8	3.25	109.15	105.74
4	A	703	DTP	N9-C8-N7	-3.25	109.32	113.94
4	D	702	DTP	C2-N3-C4	3.22	119.70	111.83
4	D	702	DTP	N3-C2-N1	-3.19	123.76	128.58
4	B	704	DTP	C5-N7-C8	3.18	108.45	103.45
3	D	704	DGT	C6-C5-N7	3.13	135.99	130.29
3	C	703	DGT	O2G-PG-O1G	3.13	119.53	107.80
4	B	704	DTP	C4-C5-N7	-3.09	107.05	110.58
2	D	703	TTP	O3G-PG-O2G	3.08	119.35	107.80
4	C	701	DTP	C4-C5-N7	-2.93	107.23	110.58
4	D	702	DTP	N9-C8-N7	-2.93	109.78	113.94
4	A	703	DTP	O2A-PA-O3A	2.92	115.17	107.27
3	D	704	DGT	O1A-PA-O3A	2.87	115.02	107.27
4	B	704	DTP	O3A-PB-O1B	-2.86	102.09	110.70
2	D	703	TTP	O4-C4-C5	-2.75	121.77	124.92
3	B	702	DGT	O6-C6-C5	-2.75	119.27	126.53
3	C	703	DGT	C2'-C3'-C4'	2.73	108.34	102.80
2	A	701	TTP	O3G-PG-O2G	2.73	118.05	107.80
4	A	703	DTP	O3G-PG-O2G	2.73	118.04	107.80
3	B	702	DGT	O2G-PG-O3G	2.71	121.41	110.83
4	C	701	DTP	O3B-PB-O1B	-2.71	102.55	110.70
4	A	703	DTP	C2'-C3'-C4'	2.68	108.23	102.80
3	C	703	DGT	O2G-PG-O3B	-2.65	95.74	104.64
3	C	704	DGT	C4-C5-N7	-2.63	106.50	110.67
3	A	702	DGT	C6-C5-N7	2.62	135.06	130.29
3	D	704	DGT	C4-C5-N7	-2.61	106.54	110.67
3	C	703	DGT	C4-C5-N7	-2.60	106.55	110.67
3	A	702	DGT	O1A-PA-O2A	2.59	124.49	112.44
4	C	701	DTP	C2-N1-C6	2.58	122.97	118.73
4	C	701	DTP	O2A-PA-O3A	2.54	114.13	107.27
3	C	704	DGT	O2G-PG-O1G	2.50	117.18	107.80
2	A	701	TTP	O2B-PB-O1B	2.40	123.60	112.44
3	D	704	DGT	O1A-PA-O2A	2.37	123.46	112.44
4	D	702	DTP	O3G-PG-O2G	2.34	116.58	107.80
2	D	703	TTP	O2B-PB-O1B	2.32	123.26	112.44
3	C	704	DGT	C5-C6-N1	2.32	119.16	113.25
3	A	702	DGT	C8-N7-C5	2.31	108.38	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	DTP	C6-C5-N7	2.31	136.55	132.09
2	B	701	TTP	C2'-C3'-C4'	2.31	107.48	102.80
3	D	704	DGT	O4'-C1'-N9	2.27	111.89	107.86
3	D	704	DGT	O4'-C1'-C2'	-2.22	102.09	106.25
3	B	702	DGT	C5-C6-N1	2.22	118.90	113.25
4	B	704	DTP	C2'-C3'-C4'	2.18	107.21	102.80
3	A	702	DGT	O3A-PA-O2A	2.15	117.16	110.70
2	B	701	TTP	O2A-PA-O1A	2.13	122.37	112.44
4	A	703	DTP	N6-C6-N1	2.13	123.11	118.38
4	C	701	DTP	N6-C6-N1	2.12	123.10	118.38
2	B	701	TTP	O3G-PG-O2G	2.12	115.74	107.80
4	A	703	DTP	C6-C5-N7	2.10	136.14	132.09
4	D	702	DTP	O3B-PG-O1G	-2.10	100.01	111.04
3	B	702	DGT	C6-C5-N7	2.09	134.09	130.29
3	A	702	DGT	O3B-PG-O3G	-2.07	100.16	111.04
3	D	704	DGT	O1B-PB-O3B	2.07	112.86	107.27
2	D	703	TTP	O2-C2-N3	-2.07	117.68	121.49
2	B	701	TTP	O2-C2-N1	-2.06	120.11	122.80
3	C	703	DGT	O6-C6-C5	-2.05	121.12	126.53
3	C	703	DGT	C5-C6-N1	2.05	118.46	113.25
4	A	703	DTP	O3A-PA-O1A	-2.04	104.56	110.70
3	C	704	DGT	C2-N1-C6	-2.04	121.41	125.11
2	A	701	TTP	O2-C2-N3	-2.02	117.76	121.49
2	A	701	TTP	O3A-PA-O1A	-2.01	104.65	110.70
4	A	703	DTP	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TTP	C5'-O5'-PA-O1A
2	A	701	TTP	C5'-O5'-PA-O2A
2	A	701	TTP	C5'-O5'-PA-O3A
2	B	701	TTP	PB-O3A-PA-O5'
2	D	703	TTP	C5'-O5'-PA-O1A
2	D	703	TTP	C5'-O5'-PA-O2A
2	D	703	TTP	C5'-O5'-PA-O3A
3	B	702	DGT	PB-O3B-PG-O1G
3	C	703	DGT	C5'-O5'-PA-O1A
3	D	704	DGT	C5'-O5'-PA-O2A
4	A	703	DTP	PB-O3B-PG-O3G
4	A	703	DTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	A	703	DTP	C5'-O5'-PA-O2A
4	A	703	DTP	O4'-C4'-C5'-O5'
4	C	701	DTP	PB-O3B-PG-O3G
4	D	702	DTP	PB-O3B-PG-O3G
4	A	703	DTP	C3'-C4'-C5'-O5'
3	C	703	DGT	C3'-C4'-C5'-O5'
3	C	703	DGT	PA-O3A-PB-O2B
2	A	701	TTP	PA-O3A-PB-O1B
4	B	704	DTP	PG-O3B-PB-O1B
4	C	701	DTP	PG-O3B-PB-O2B
4	C	701	DTP	PB-O3A-PA-O2A
3	D	704	DGT	C4'-C5'-O5'-PA
3	A	702	DGT	C2'-C1'-N9-C8
3	C	703	DGT	C5'-O5'-PA-O3A
3	C	703	DGT	C5'-O5'-PA-O2A
4	A	703	DTP	C5'-O5'-PA-O3A
2	B	701	TTP	C4'-C5'-O5'-PA
3	A	702	DGT	PB-O3B-PG-O3G
4	C	701	DTP	PB-O3B-PG-O1G
3	A	702	DGT	PG-O3B-PB-O1B
3	A	702	DGT	PB-O3A-PA-O1A
3	C	703	DGT	PA-O3A-PB-O1B
3	D	704	DGT	PG-O3B-PB-O1B
4	B	704	DTP	PB-O3A-PA-O2A
4	D	702	DTP	PB-O3A-PA-O2A
3	C	704	DGT	C4'-C5'-O5'-PA
3	A	702	DGT	C2'-C1'-N9-C4
3	C	704	DGT	C2'-C1'-N9-C4
2	D	703	TTP	C3'-C4'-C5'-O5'
3	C	703	DGT	O4'-C4'-C5'-O5'
2	B	701	TTP	PG-O3B-PB-O1B
3	C	703	DGT	PG-O3B-PB-O1B
4	B	704	DTP	PB-O3A-PA-O1A
3	A	702	DGT	C4'-C5'-O5'-PA
3	B	702	DGT	PB-O3B-PG-O3G
4	D	702	DTP	PB-O3B-PG-O1G
4	A	703	DTP	PB-O3B-PG-O2G
4	D	702	DTP	PB-O3B-PG-O2G
3	C	704	DGT	C2'-C1'-N9-C8
2	B	701	TTP	PG-O3B-PB-O2B
3	B	702	DGT	PG-O3B-PB-O1B
3	C	703	DGT	PB-O3A-PA-O1A

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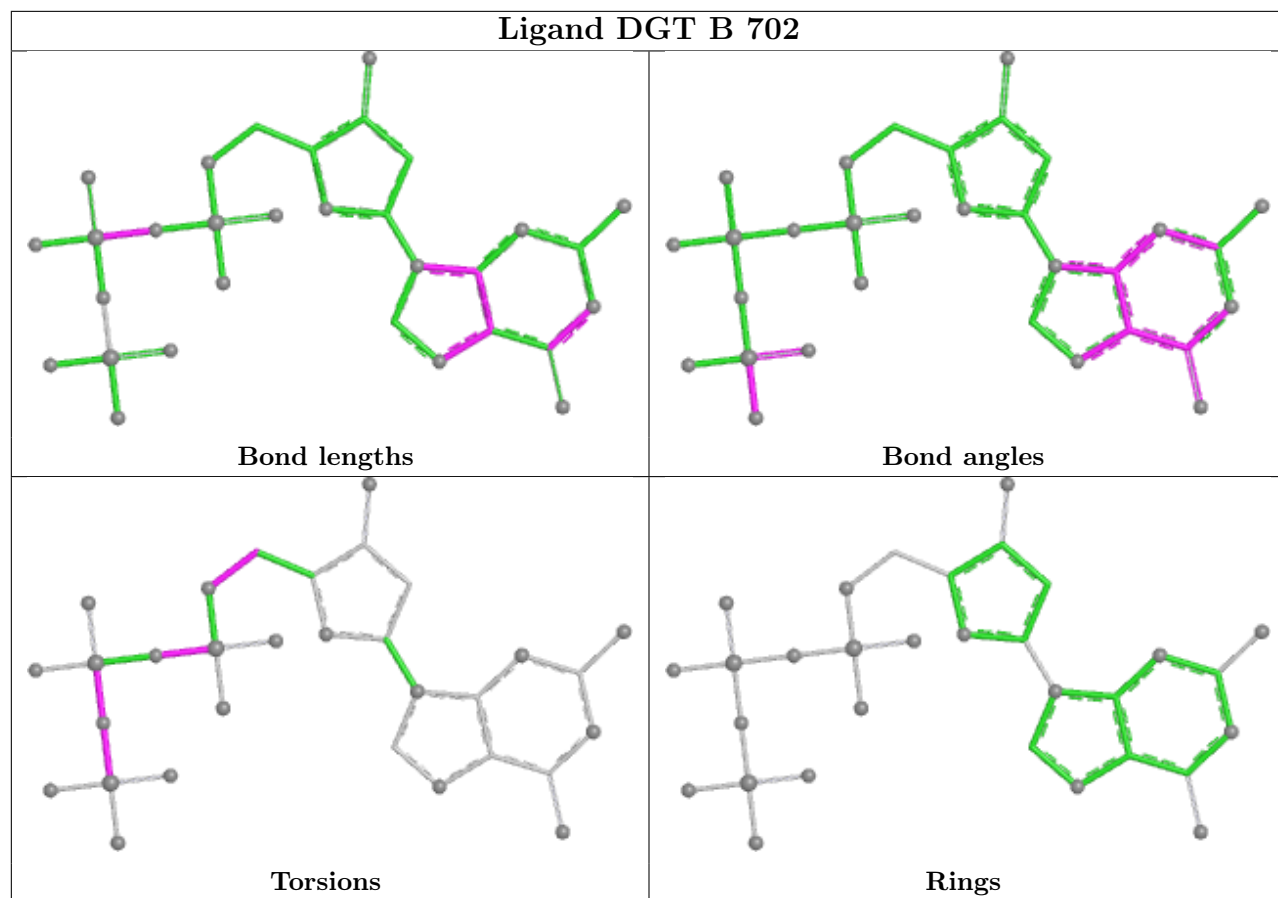
Mol	Chain	Res	Type	Atoms
3	C	703	DGT	PB-O3A-PA-O2A
3	C	704	DGT	PB-O3A-PA-O1A
3	C	704	DGT	PB-O3A-PA-O2A
3	D	704	DGT	PG-O3B-PB-O2B
4	A	703	DTP	PG-O3B-PB-O1B
4	C	701	DTP	PB-O3A-PA-O1A
3	B	702	DGT	C4'-C5'-O5'-PA
3	A	702	DGT	PB-O3A-PA-O2A
3	B	702	DGT	PB-O3A-PA-O1A
3	C	703	DGT	PG-O3B-PB-O2B
3	C	704	DGT	PG-O3B-PB-O1B
3	D	704	DGT	PB-O3A-PA-O1A
4	B	704	DTP	PG-O3B-PB-O2B
4	C	701	DTP	PG-O3B-PB-O1B
4	D	702	DTP	PG-O3B-PB-O2B

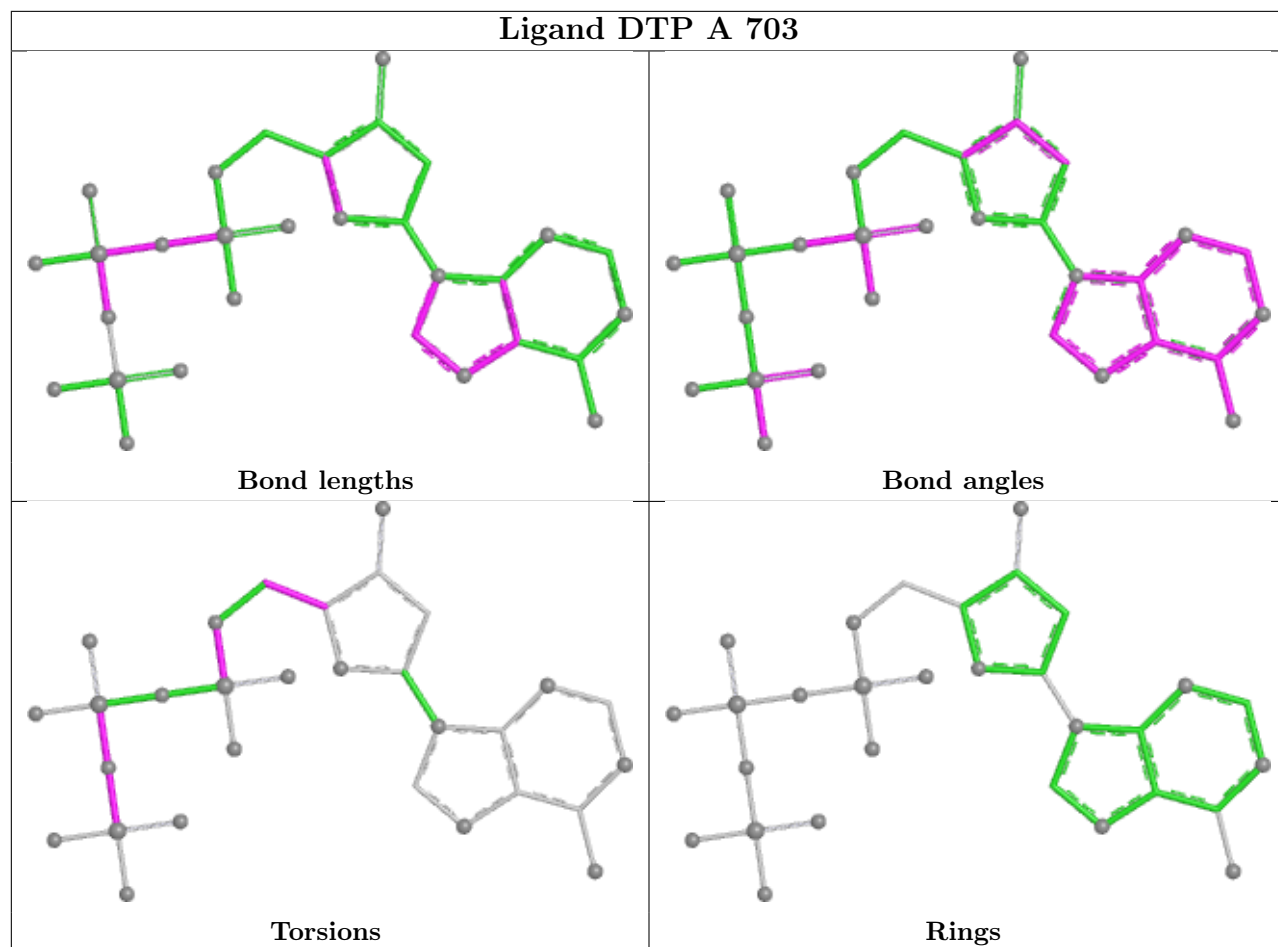
There are no ring outliers.

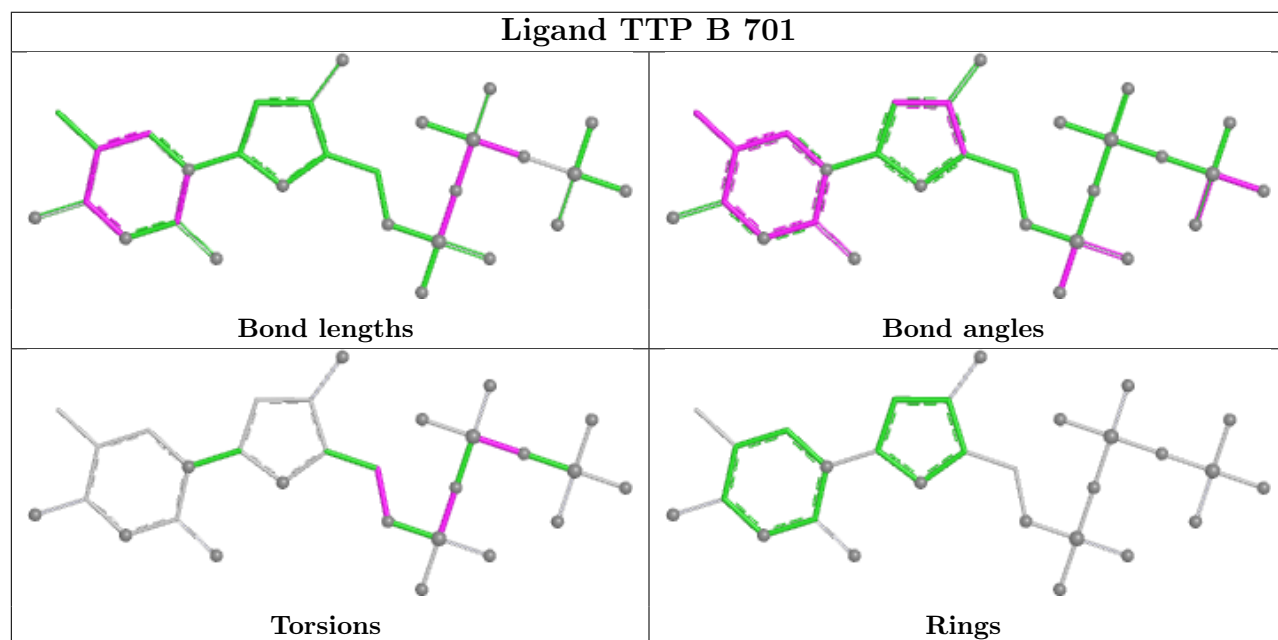
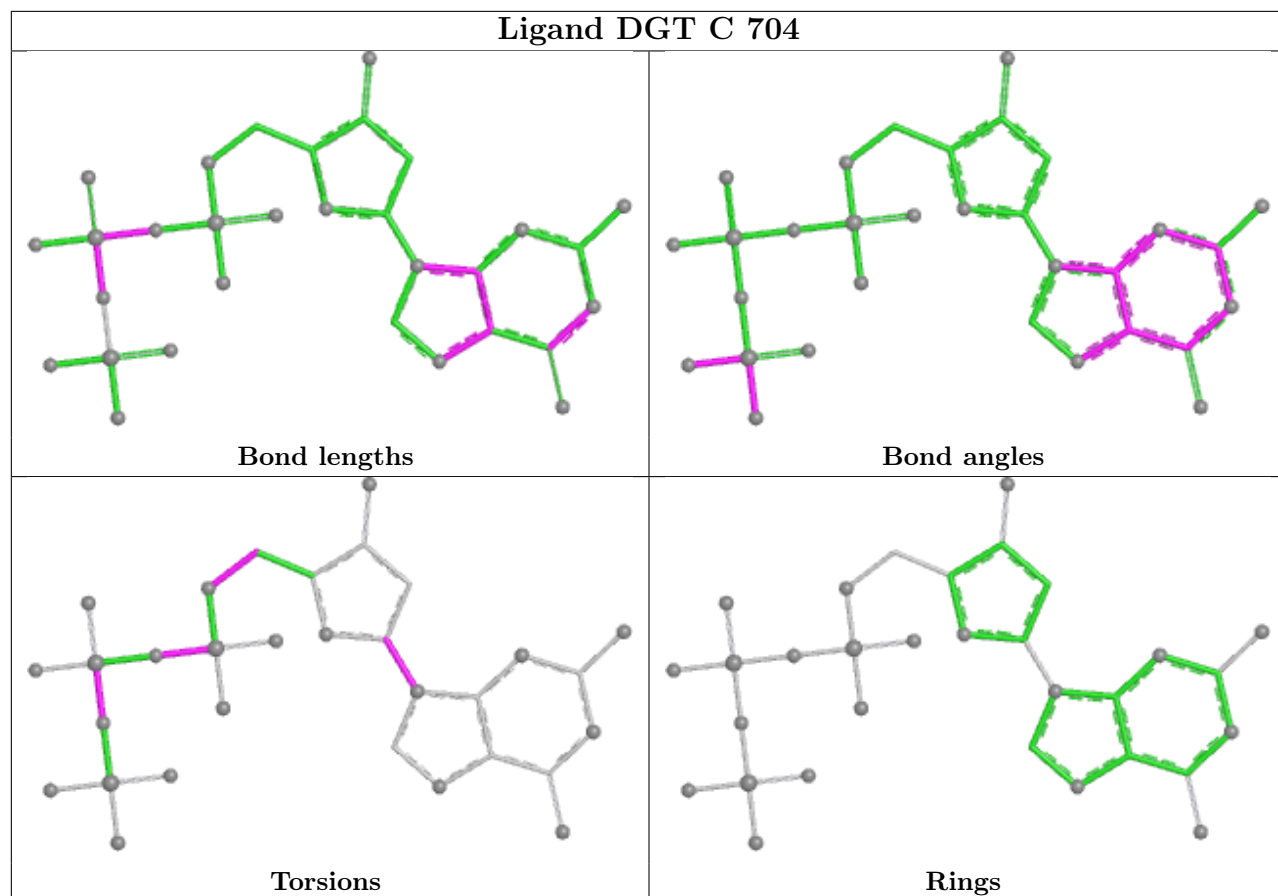
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	DTP	1	0
3	C	704	DGT	4	0
2	B	701	TTP	1	0
2	A	701	TTP	1	0
3	C	703	DGT	1	0
4	B	704	DTP	2	0
4	C	701	DTP	3	0
3	D	704	DGT	2	0
4	D	702	DTP	1	0

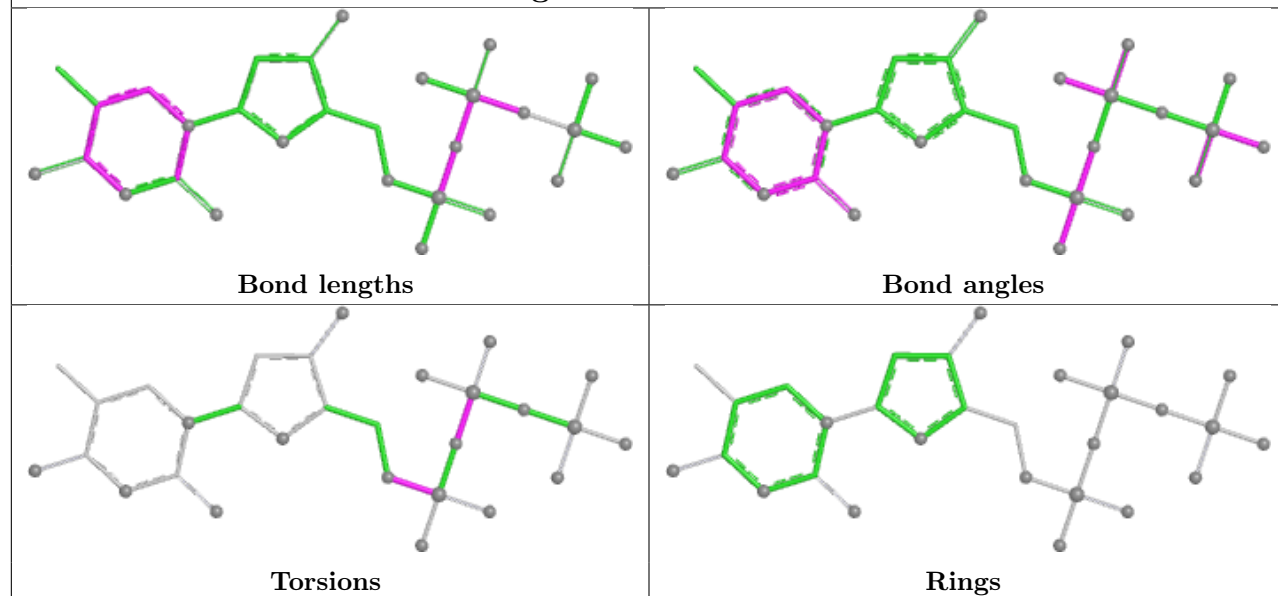
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



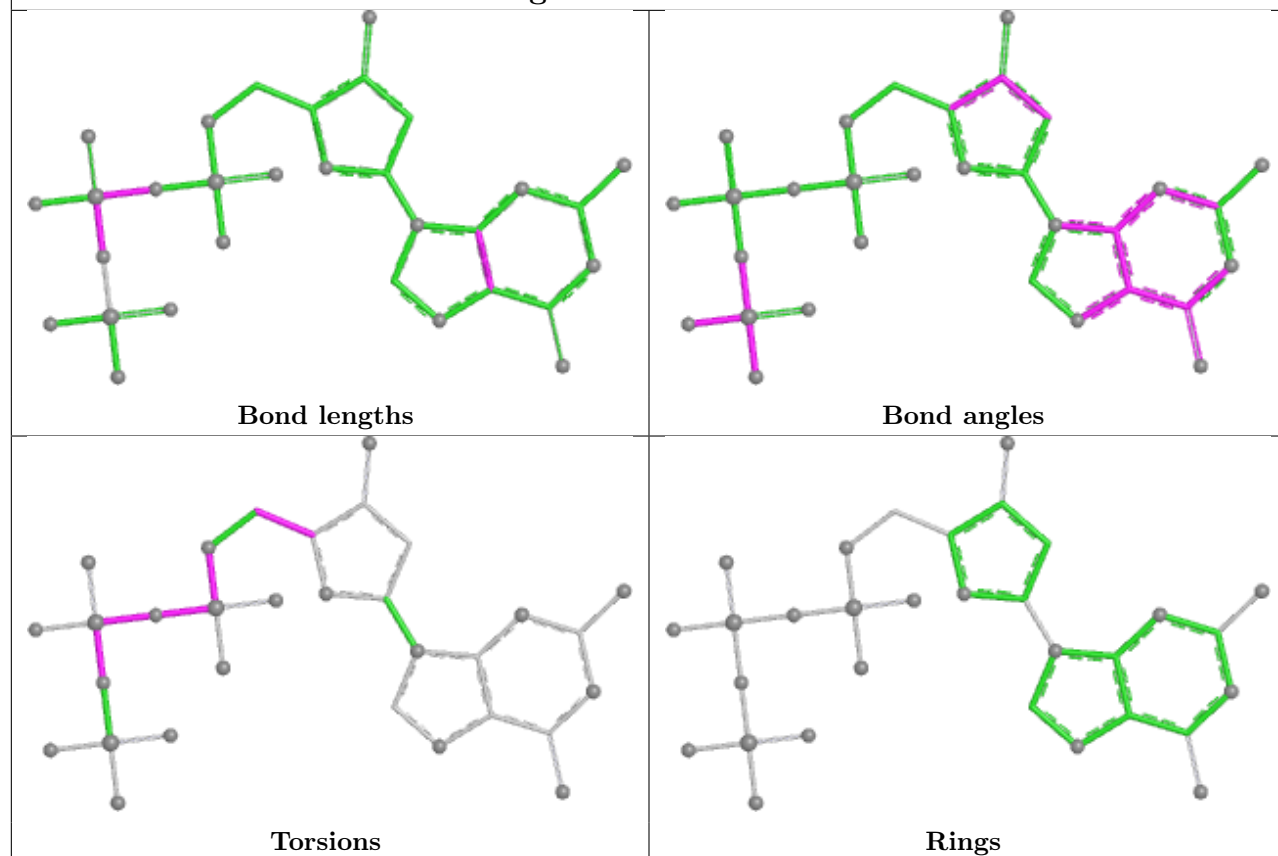


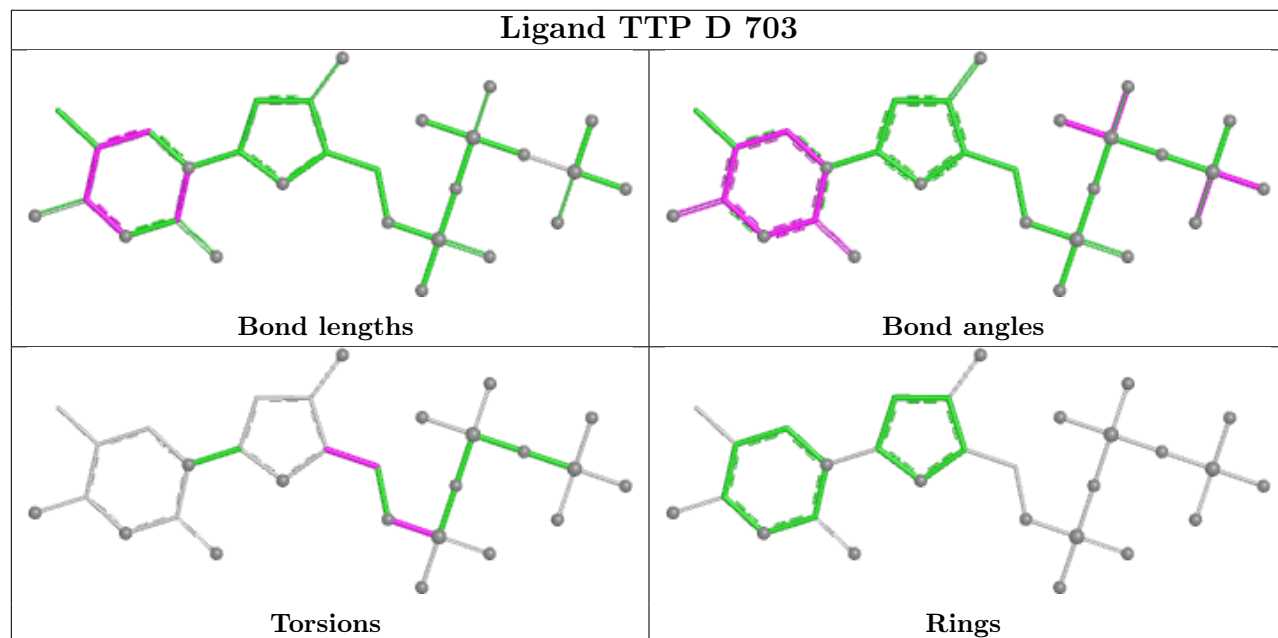
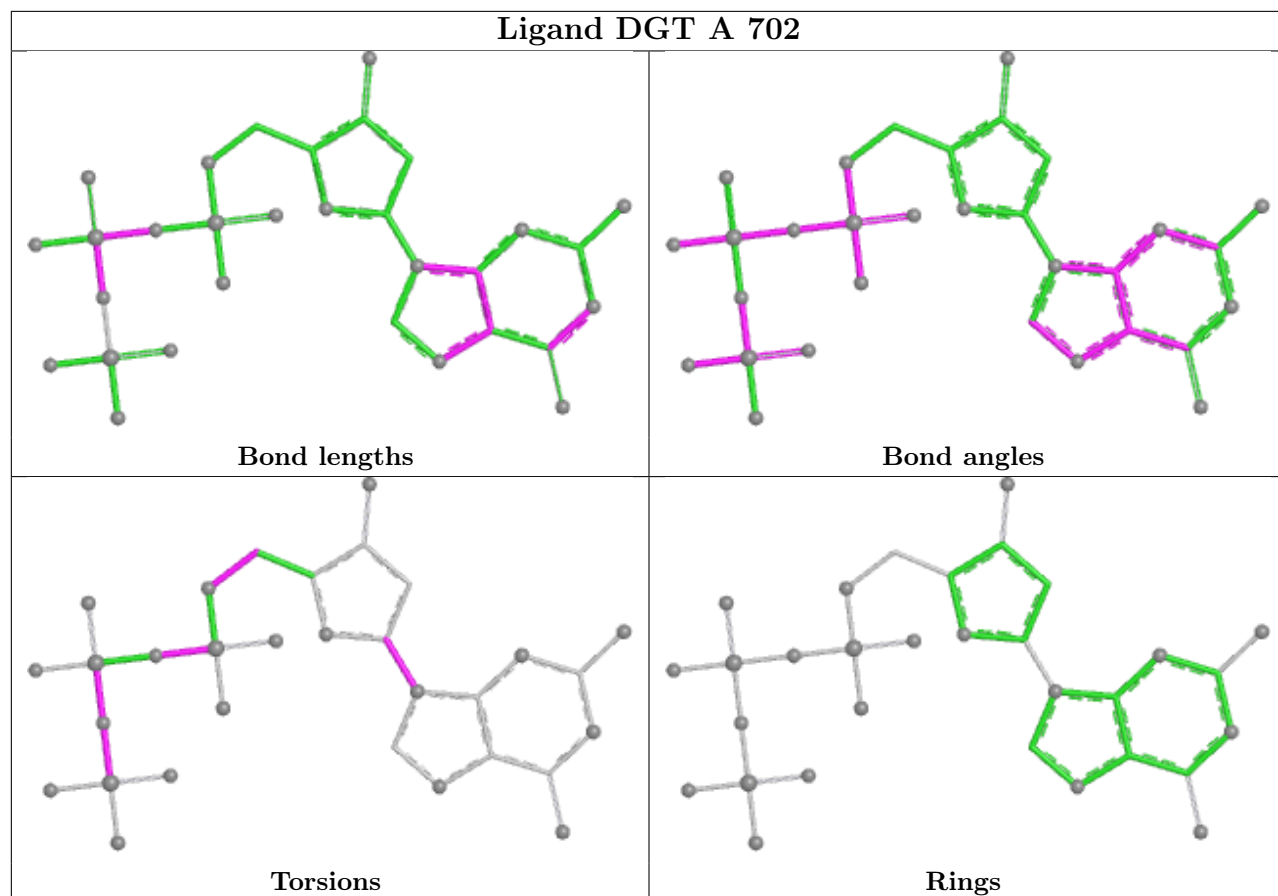


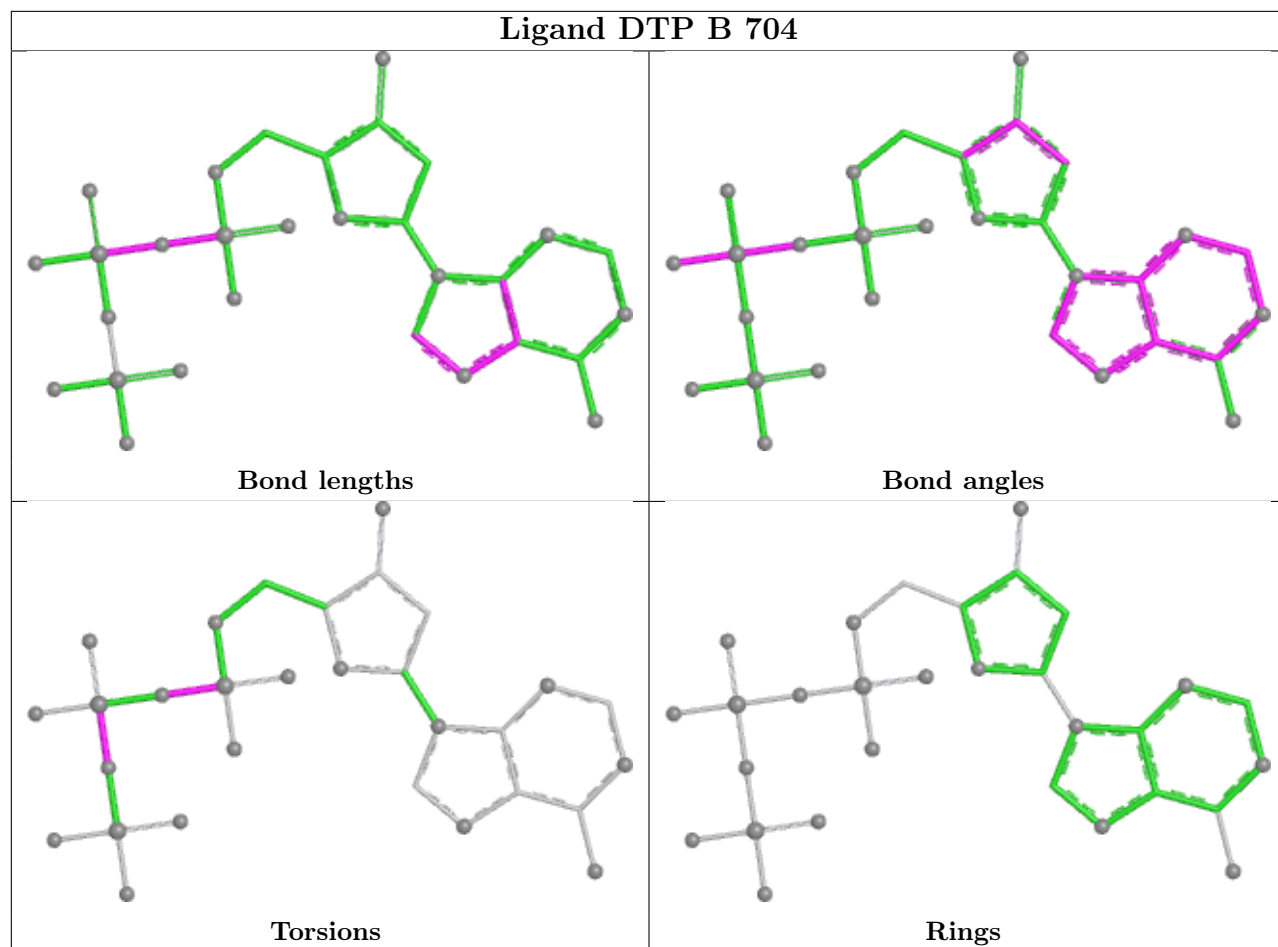
Ligand TTP A 701

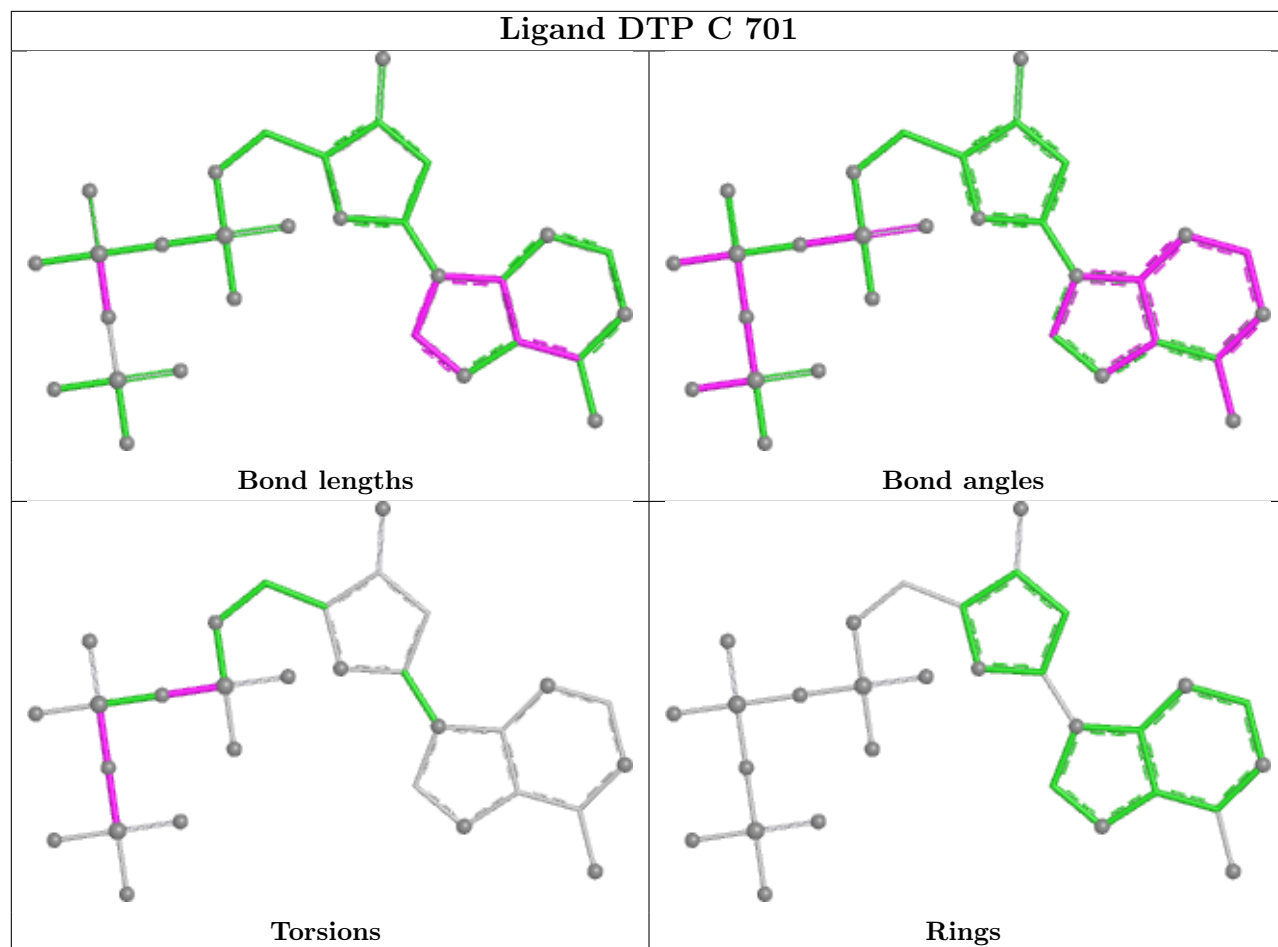


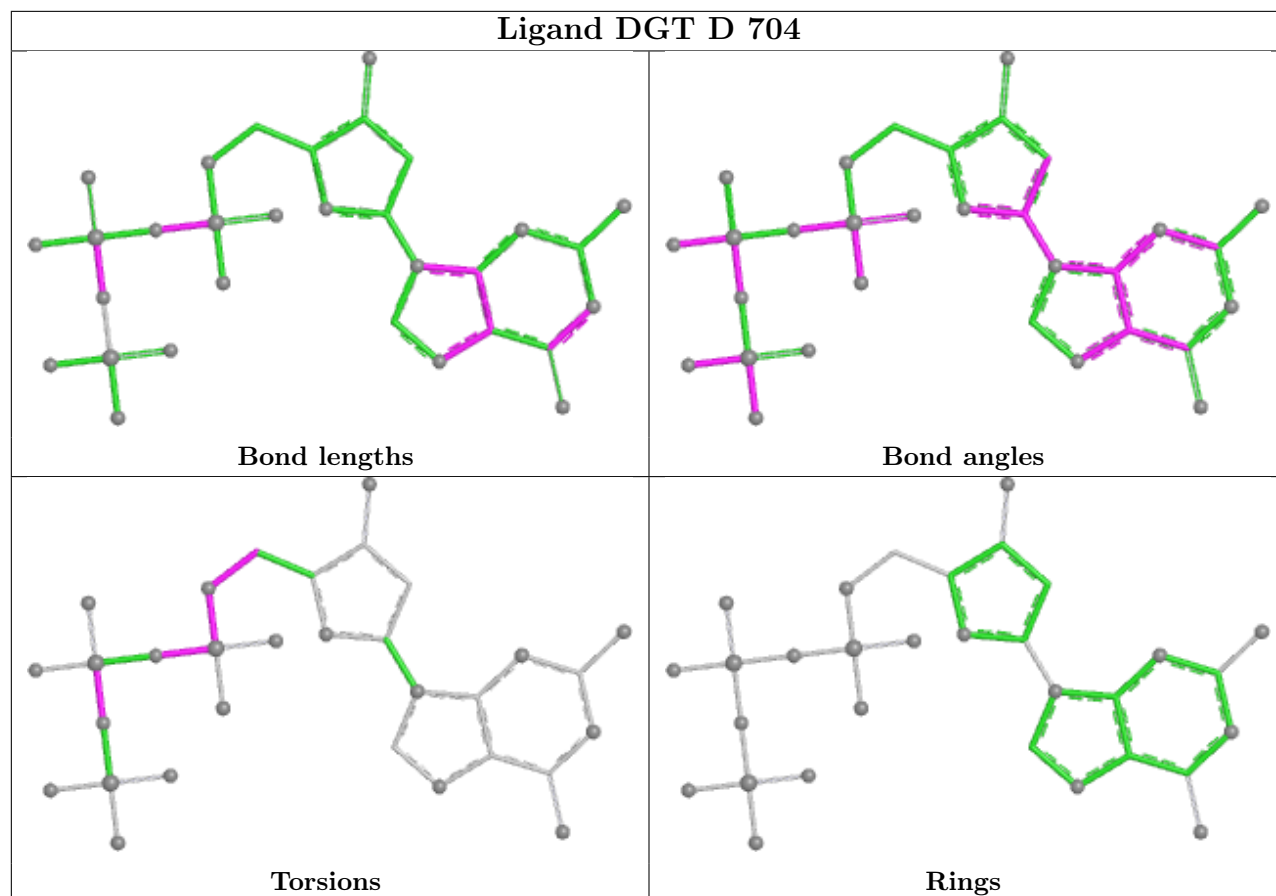
Ligand DGT C 703

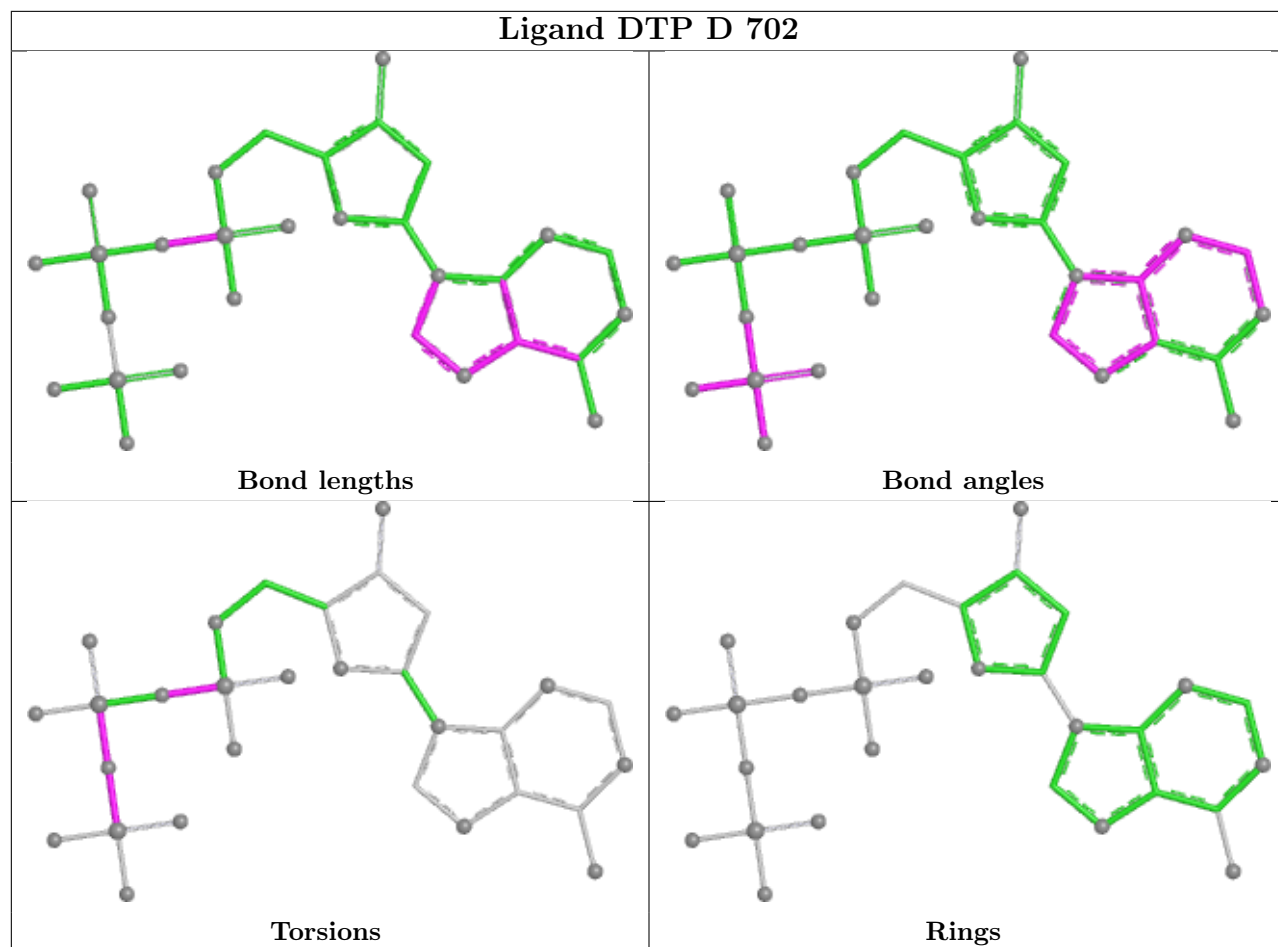












5.7 Other polymers [i](#)

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	480/514 (93%)	0.34	8 (1%) 69 73	29, 59, 94, 136	0
1	B	480/514 (93%)	0.48	11 (2%) 61 66	33, 66, 103, 133	0
1	C	480/514 (93%)	0.69	18 (3%) 44 50	35, 80, 129, 171	0
1	D	480/514 (93%)	0.81	41 (8%) 16 20	33, 77, 134, 176	0
All	All	1920/2056 (93%)	0.58	78 (4%) 41 47	29, 70, 119, 176	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	LEU	4.6
1	D	466	ILE	4.6
1	B	284	LEU	4.3
1	A	284	LEU	4.2
1	C	328	ASN	4.1
1	C	284	LEU	4.1
1	C	489	LEU	3.8
1	B	488	LEU	3.6
1	D	328	ASN	3.6
1	D	562	LEU	3.6
1	A	466	ILE	3.5
1	C	466	ILE	3.4
1	D	573	CYS	3.4
1	D	590	LEU	3.2
1	B	328	ASN	3.1
1	D	489	LEU	3.1
1	C	397	ILE	3.1
1	D	476	LEU	3.0
1	D	487	VAL	2.9
1	C	491	VAL	2.8
1	D	493	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	274	GLY	2.8
1	D	491	VAL	2.7
1	A	465	GLN	2.7
1	D	396	TYR	2.7
1	D	473	TYR	2.7
1	D	578	PHE	2.6
1	C	557	VAL	2.6
1	D	468	ILE	2.6
1	D	481	ALA	2.6
1	D	495	ALA	2.6
1	B	557	VAL	2.6
1	D	276	LEU	2.5
1	C	115	MET	2.5
1	D	572	TRP	2.5
1	A	114	THR	2.5
1	D	498	PHE	2.5
1	D	472	ASP	2.5
1	D	115	MET	2.4
1	B	225	ALA	2.4
1	C	463	THR	2.4
1	D	250	ILE	2.4
1	D	488	LEU	2.4
1	D	287	TYR	2.4
1	C	522	CYS	2.4
1	A	328	ASN	2.3
1	A	397	ILE	2.3
1	C	441	ALA	2.3
1	D	114	THR	2.3
1	D	285	TRP	2.3
1	D	397	ILE	2.2
1	D	329	PHE	2.2
1	B	115	MET	2.2
1	D	568	TYR	2.2
1	C	390	PHE	2.2
1	D	569	PHE	2.2
1	B	489	LEU	2.2
1	D	189	LEU	2.2
1	D	238	VAL	2.2
1	C	438	LEU	2.1
1	B	491	VAL	2.1
1	D	480	VAL	2.1
1	D	198	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	396	TYR	2.1
1	D	298	TYR	2.1
1	B	562	LEU	2.1
1	C	590	LEU	2.1
1	D	467	LYS	2.1
1	C	327	ASN	2.1
1	D	253	VAL	2.1
1	A	276	LEU	2.1
1	A	293	ASN	2.1
1	C	454	PHE	2.1
1	C	231	TRP	2.1
1	D	231	TRP	2.0
1	D	539	GLN	2.0
1	B	590	LEU	2.0
1	C	488	LEU	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.

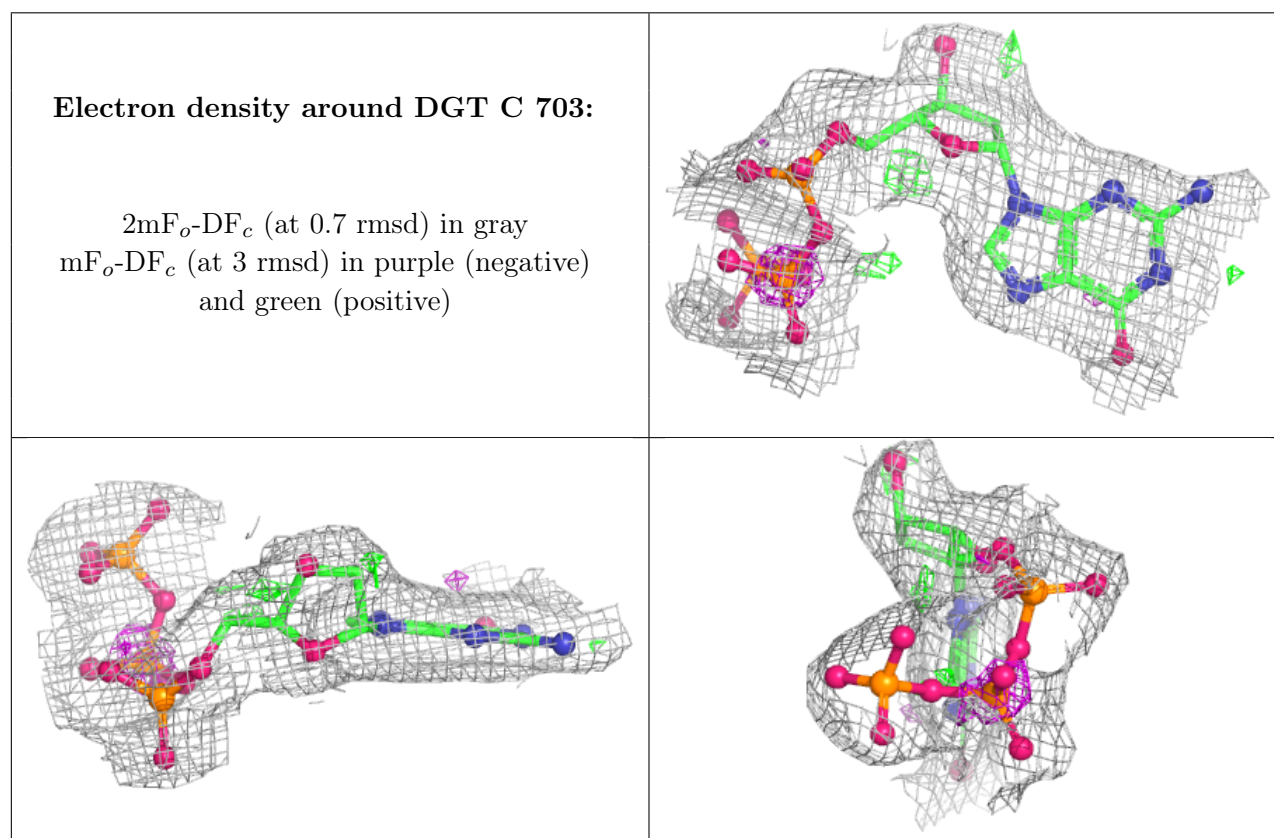
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DGT	C	703	31/31	0.85	0.11	66,83,98,110	0
2	TTP	A	701	29/29	0.87	0.10	37,55,81,89	0
2	TTP	D	703	29/29	0.88	0.10	58,73,91,100	0
2	TTP	B	701	29/29	0.91	0.08	58,68,79,81	0
3	DGT	B	702	31/31	0.97	0.06	39,44,49,49	0
3	DGT	A	702	31/31	0.97	0.05	38,43,49,52	0
3	DGT	C	704	31/31	0.97	0.06	47,54,69,71	0
3	DGT	D	704	31/31	0.97	0.05	37,41,50,51	0

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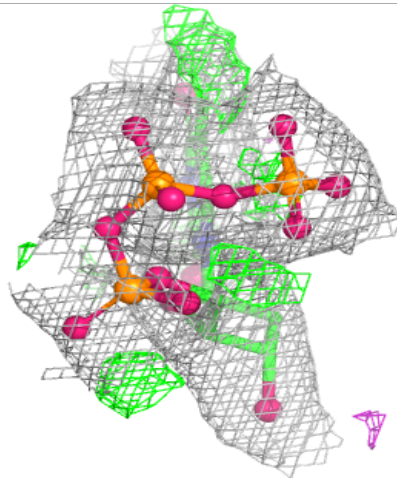
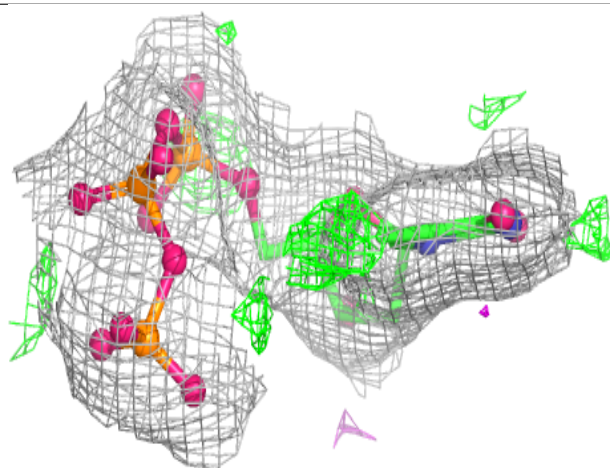
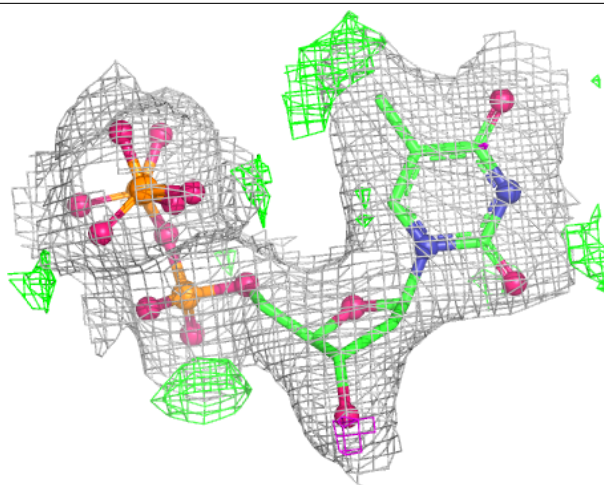
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DTP	A	703	30/30	0.97	0.05	42,45,56,56	0
4	DTP	B	704	30/30	0.97	0.05	34,39,46,49	0
4	DTP	D	702	30/30	0.97	0.05	32,39,42,44	0
4	DTP	C	701	30/30	0.98	0.04	33,36,39,41	0
5	MG	A	704	1/1	0.98	0.05	59,59,59,59	0
5	MG	D	701	1/1	0.99	0.04	50,50,50,50	0
5	MG	C	702	1/1	1.00	0.03	47,47,47,47	0
5	MG	B	703	1/1	1.00	0.03	55,55,55,55	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.



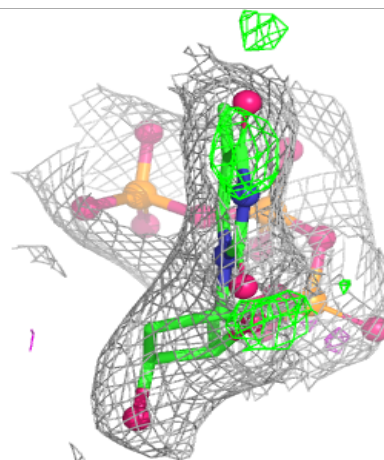
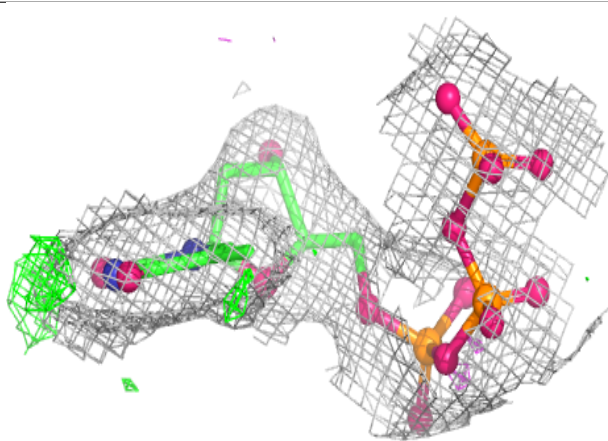
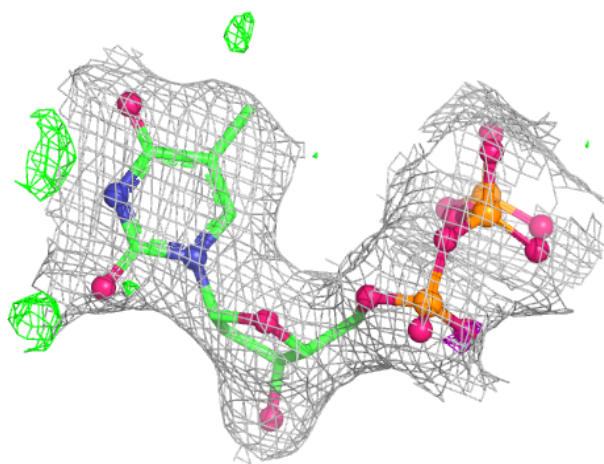
Electron density around TTP A 701:

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



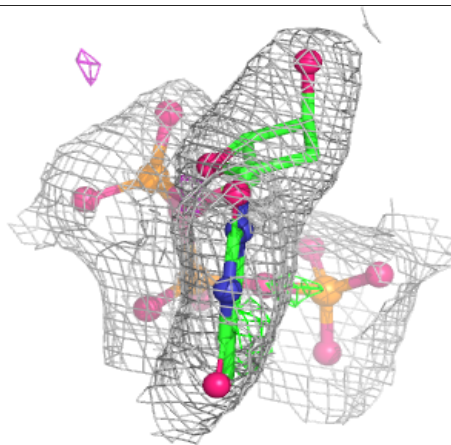
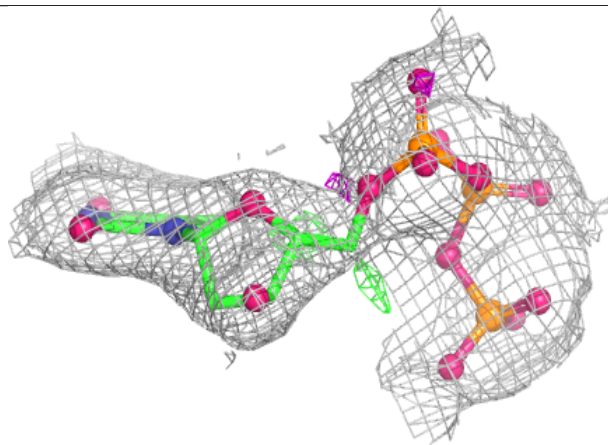
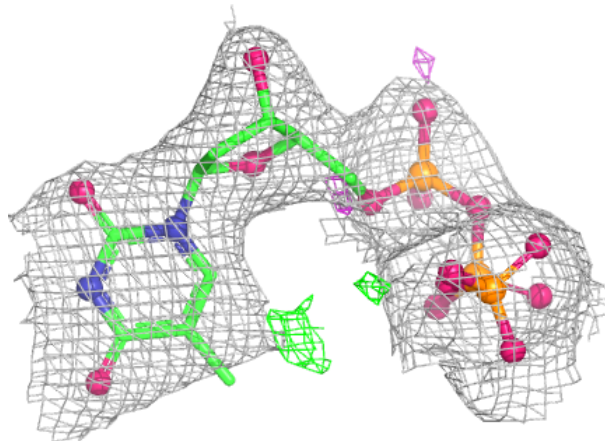
Electron density around TTP D 703:

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and green (positive)

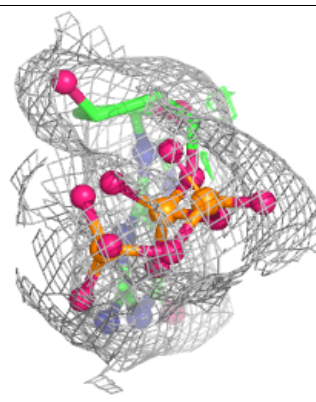
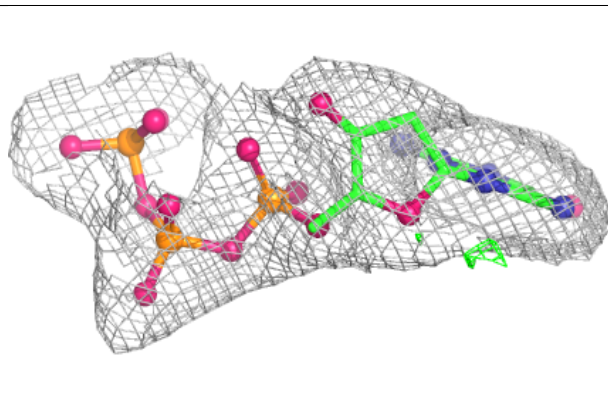
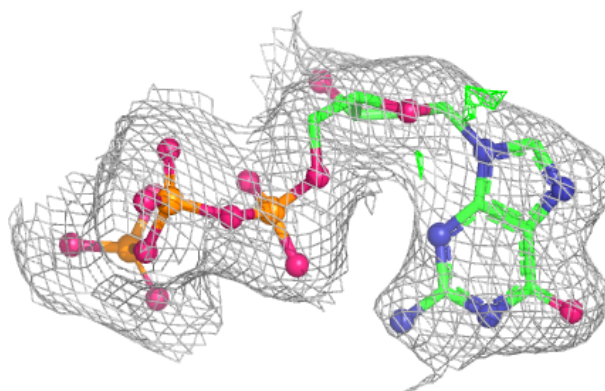


Electron density around TTP B 701:

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and green (positive)

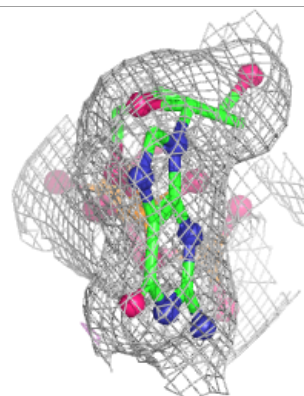
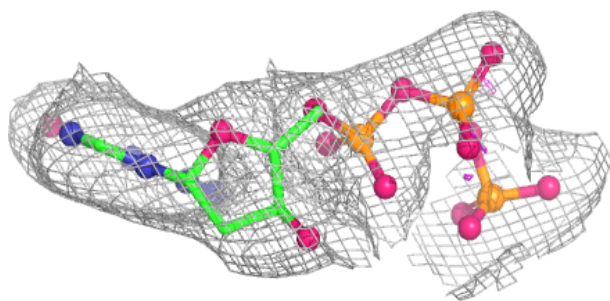
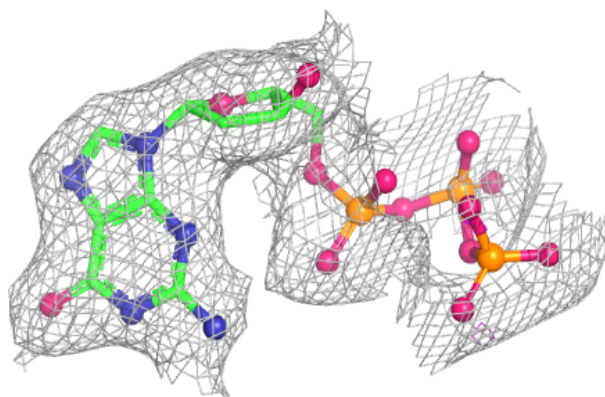
**Electron density around DGT B 702:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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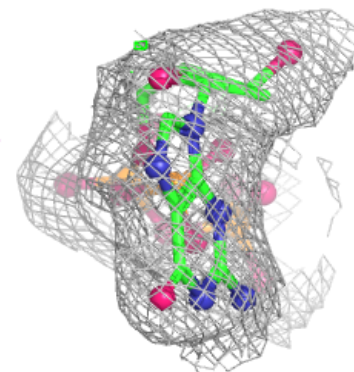
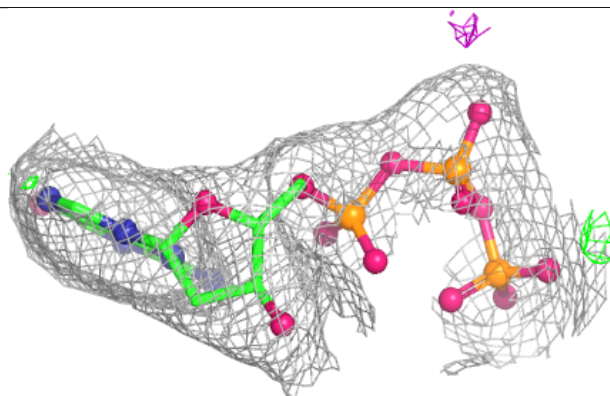
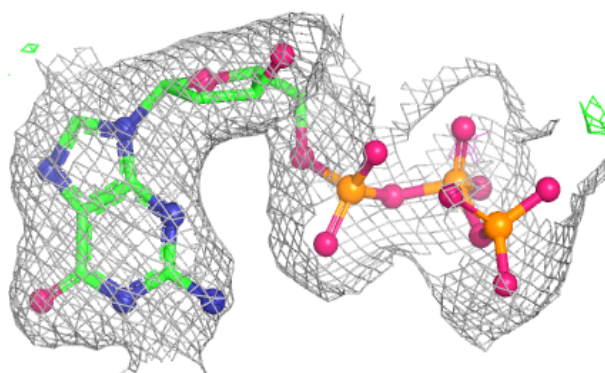


Electron density around DGT A 702:

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

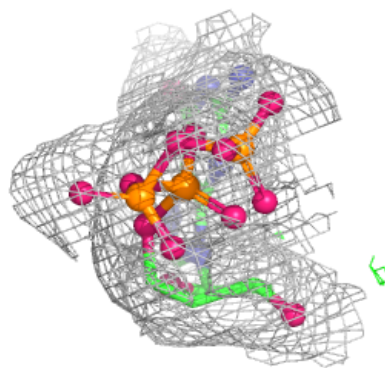
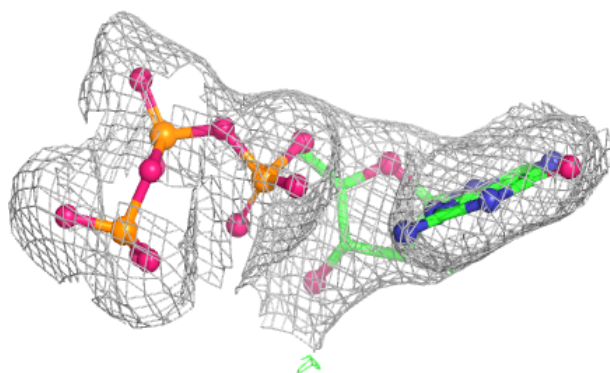
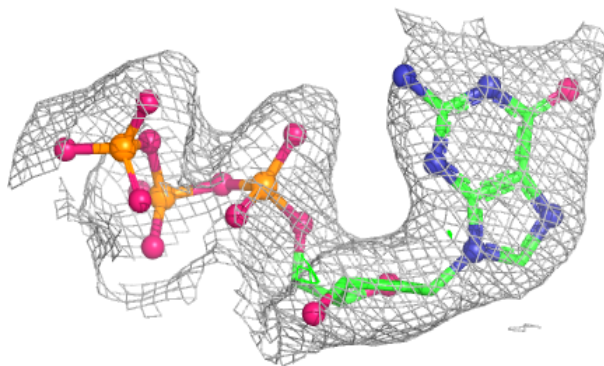
**Electron density around DGT C 704:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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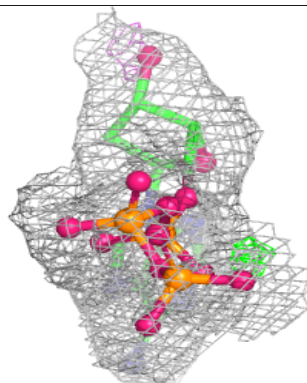
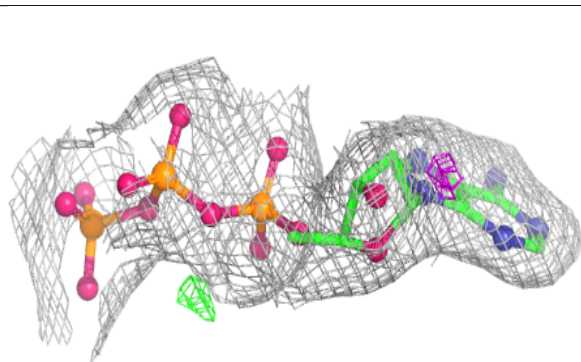
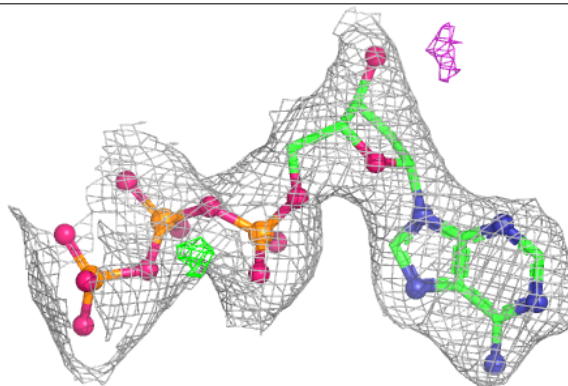


Electron density around DGT D 704:

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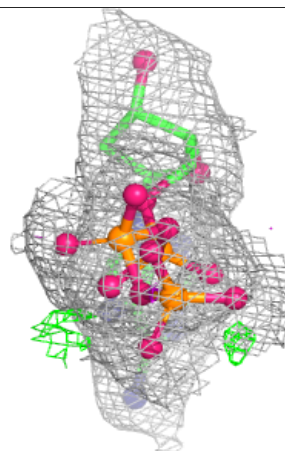
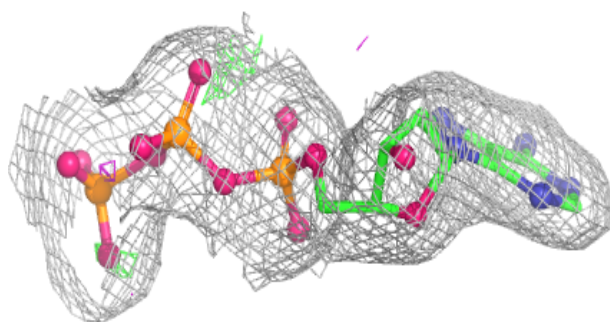
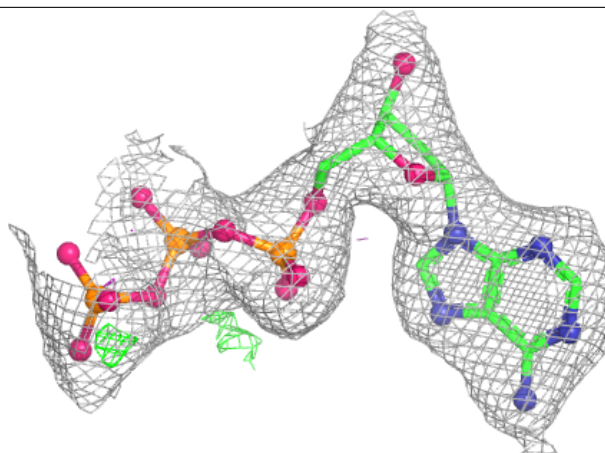
**Electron density around DTP A 703:**

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



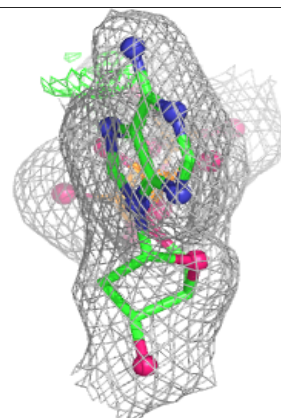
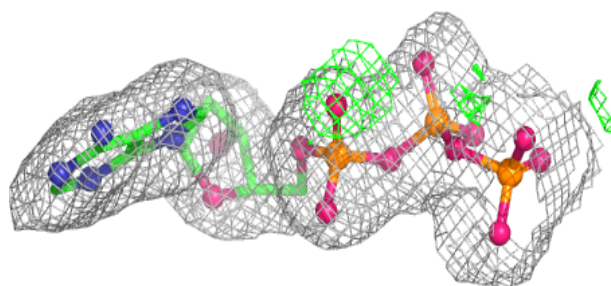
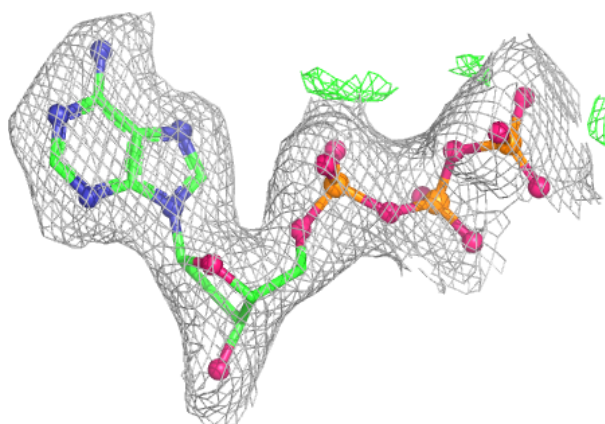
Electron density around DTP B 704:

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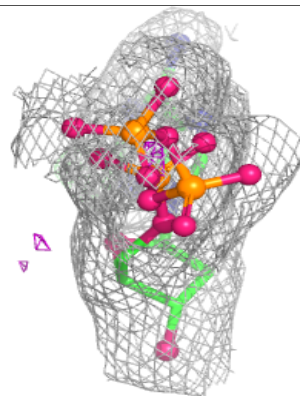
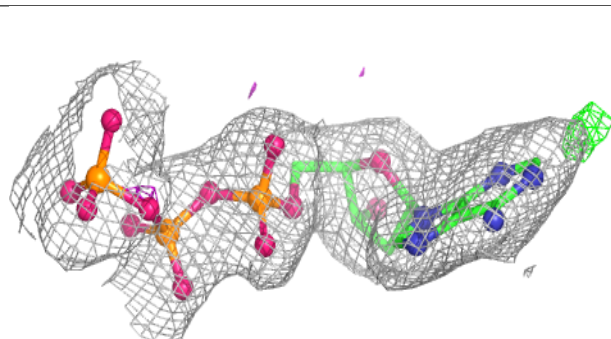
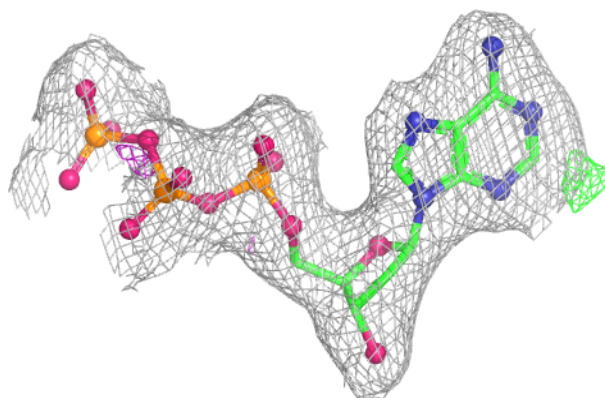


Electron density around DTP D 702:

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

**Electron density around DTP C 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.