



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:42 PM EDT

PDB ID : 4TO2 / pdb_00004to2
Title : Structure basis of cellular dNTP regulation, SAMHD1-dGTP-dGTP-dGTP/dTTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.27 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

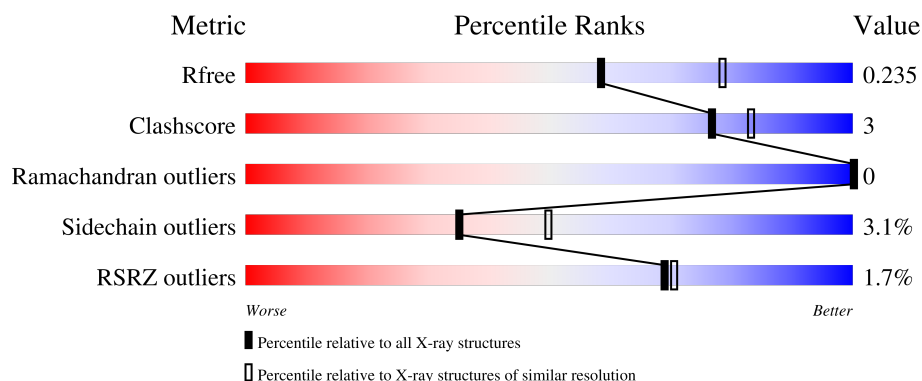
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	
1	C	514	
1	D	514	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16367 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	1	0
			3939	2520	686	712	21			
1	B	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			
1	C	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			
1	D	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			

There are 8 discrepancies between the modelled and reference sequences:

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

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



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

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

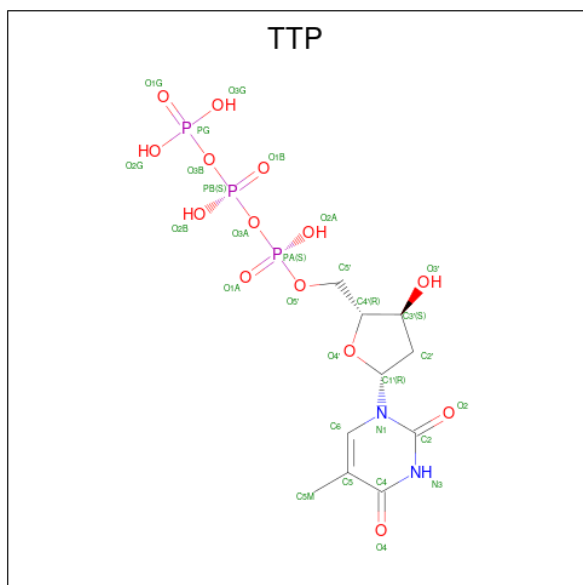
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	C	3	Total Mg 3 3	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



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

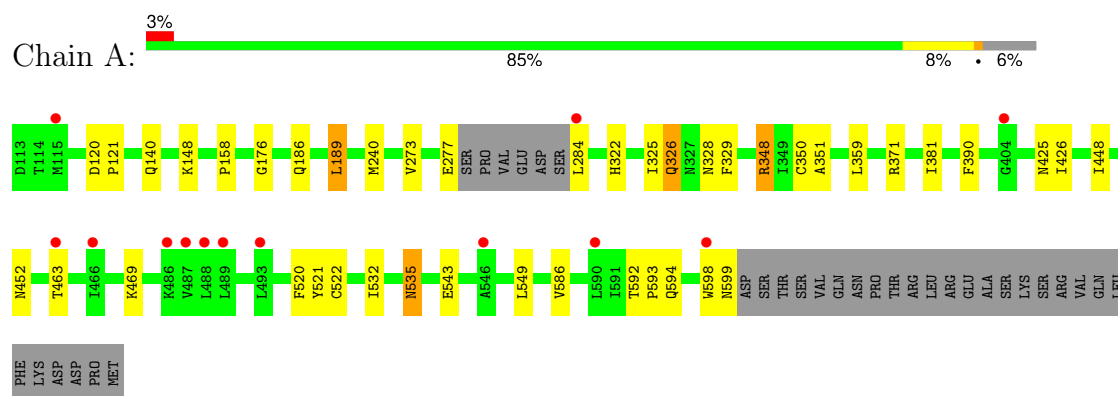
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	56	Total O 56 56	0	0
5	C	40	Total O 40 40	0	0
5	D	85	Total O 85 85	0	0

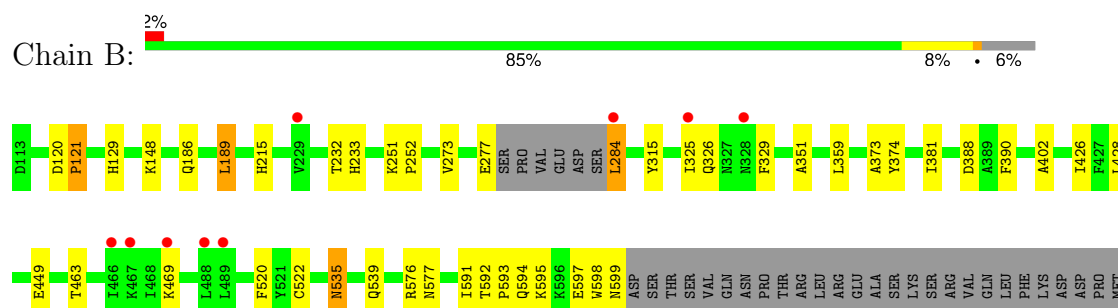
3 Residue-property plots

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.

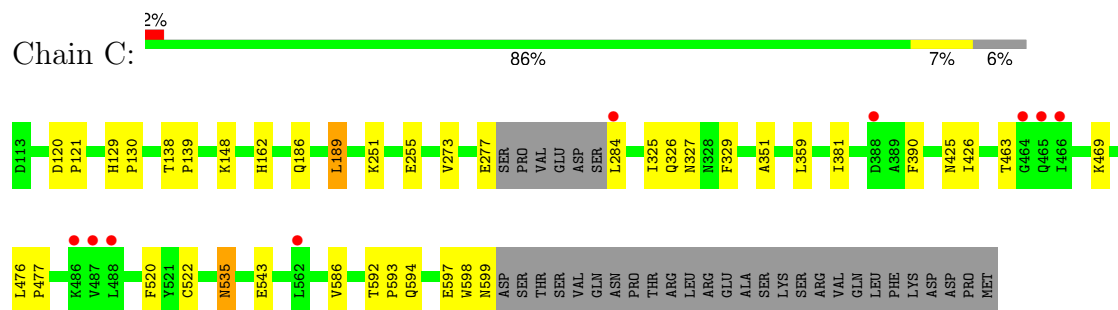
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



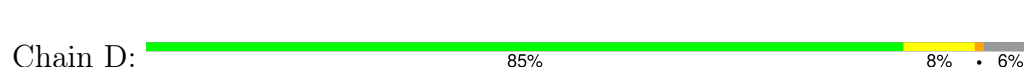
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

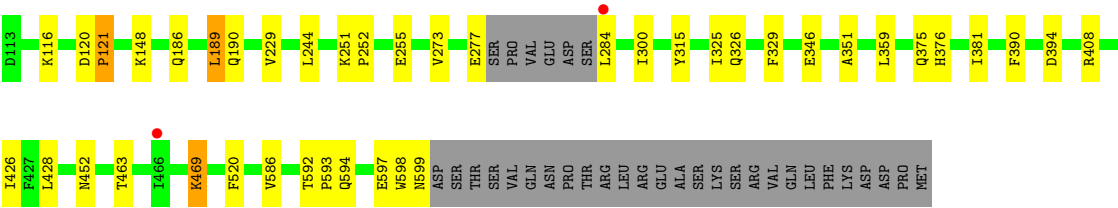


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• 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	85.31Å 145.80Å 98.26Å 90.00° 114.22° 90.00°	Depositor
Resolution (Å)	50.00 – 2.27 50.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.27) 98.3 (50.00-2.27)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.234 0.208 , 0.235	Depositor DCC
R_{free} test set	4973 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16367	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: DGT, MG, TTP

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	0.92	2/4031 (0.0%)	0.92	2/5441 (0.0%)
1	B	1.00	6/4031 (0.1%)	0.93	1/5441 (0.0%)
1	C	0.89	0/4031	0.91	2/5441 (0.0%)
1	D	1.08	1/4031 (0.0%)	0.95	2/5441 (0.0%)
All	All	0.97	9/16124 (0.1%)	0.93	7/21764 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	PRO	C-O	-7.61	1.14	1.24
1	D	121	PRO	C-O	-7.21	1.14	1.24
1	A	448	ILE	C-O	-7.04	1.16	1.24
1	B	374	TYR	N-CA	-5.71	1.39	1.46
1	B	402	ALA	CA-C	5.53	1.60	1.52
1	B	373	ALA	C-O	-5.28	1.17	1.24
1	A	532	ILE	C-O	-5.16	1.18	1.24
1	B	232	THR	N-CA	-5.02	1.39	1.45
1	B	129	HIS	CA-C	5.01	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	PHE	N-CA-C	8.45	122.51	108.73
1	B	329	PHE	N-CA-C	8.11	121.96	108.73
1	C	329	PHE	N-CA-C	7.89	121.58	108.73
1	A	329	PHE	N-CA-C	7.64	121.18	108.73
1	C	162	HIS	N-CA-C	5.13	117.33	110.35
1	A	348	ARG	CB-CG-CD	5.08	122.97	111.30
1	D	300	ILE	N-CA-C	5.06	115.73	110.82

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	3939	0	3925	33	0
1	B	3939	0	3925	23	0
1	C	3939	0	3925	21	0
1	D	3939	0	3925	20	0
2	A	93	0	36	2	0
2	B	93	0	36	2	0
2	C	62	0	24	0	0
2	D	93	0	36	2	0
3	A	3	0	0	1	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	C	29	0	13	1	0
5	A	52	0	0	10	0
5	B	56	0	0	3	0
5	C	40	0	0	5	0
5	D	85	0	0	2	0
All	All	16367	0	15845	93	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 3.

All (93) 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:A:350:CYS:HB3	5:A:850:HOH:O	1.49	1.09
1:B:449:GLU:HB3	5:C:829:HOH:O	1.53	1.08
1:A:140:GLN:CG	1:A:240:MET:HE1	1.95	0.97
1:D:346:GLU:HA	5:D:860:HOH:O	1.68	0.92
1:B:577:ASN:OD1	1:B:595:LYS:NZ	2.17	0.77
1:A:158:PRO:HG2	5:A:843:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLN:HB3	1:A:240:MET:CE	2.19	0.72
1:A:140:GLN:HG2	1:A:240:MET:HE1	1.72	0.70
1:A:140:GLN:CB	1:A:240:MET:HE1	2.22	0.69
1:A:140:GLN:HB3	1:A:240:MET:HE1	1.79	0.65
1:A:520:PHE:C	5:A:850:HOH:O	2.40	0.64
1:C:139:PRO:N	5:C:829:HOH:O	2.31	0.64
2:A:704:DGT:O1G	3:A:705:MG:MG	1.41	0.64
1:B:284:LEU:CD1	1:B:284:LEU:N	2.61	0.63
1:A:240:MET:HE3	1:A:240:MET:O	2.00	0.62
1:A:176:GLY:HA3	5:A:844:HOH:O	1.99	0.61
1:A:535:ASN:OD1	1:A:535:ASN:N	2.34	0.60
1:A:140:GLN:HG3	1:A:240:MET:HE1	1.84	0.60
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.42	0.59
1:D:469:LYS:HE2	5:D:881:HOH:O	2.02	0.59
1:B:535:ASN:N	1:B:535:ASN:OD1	2.32	0.58
1:A:350:CYS:CB	5:A:850:HOH:O	2.28	0.55
2:D:702:DGT:O3G	2:D:702:DGT:O1B	2.23	0.55
1:A:543:GLU:HG3	1:C:543:GLU:HG3	1.89	0.55
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.06	0.55
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.08	0.54
1:A:322:HIS:NE2	5:A:834:HOH:O	2.33	0.53
1:C:535:ASN:OD1	1:C:535:ASN:N	2.34	0.53
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.43	0.53
1:B:539:GLN:HG3	5:B:843:HOH:O	2.07	0.53
1:A:158:PRO:HB3	5:A:849:HOH:O	2.09	0.53
1:B:315:TYR:CE2	2:B:701:DGT:H5'	2.43	0.53
1:C:186:GLN:HB2	1:C:189:LEU:HD22	1.91	0.52
1:C:138:THR:C	5:C:829:HOH:O	2.52	0.52
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.46	0.51
4:C:704:TTP:O1G	4:C:704:TTP:O2B	2.28	0.51
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.11	0.50
1:D:390:PHE:CE2	1:D:426:ILE:HD11	2.46	0.50
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.94	0.50
1:A:371:ARG:NH1	1:A:549:LEU:HD21	2.27	0.49
1:B:233:HIS:HB2	5:B:849:HOH:O	2.11	0.49
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.95	0.49
1:A:140:GLN:HB3	1:A:240:MET:HE2	1.91	0.49
1:D:394:ASP:O	1:D:408:ARG:HD3	2.12	0.49
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.12	0.49
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.94	0.49
1:C:390:PHE:CE2	1:C:426:ILE:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522[A]:CYS:SG	1:C:586:VAL:HG11	2.54	0.48
1:B:284:LEU:N	1:B:284:LEU:HD12	2.29	0.48
1:A:322:HIS:CE1	5:A:834:HOH:O	2.66	0.47
1:D:597:GLU:OE1	1:D:597:GLU:N	2.33	0.47
1:A:521:TYR:HB3	5:A:850:HOH:O	2.14	0.47
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.97	0.46
1:C:139:PRO:CA	5:C:829:HOH:O	2.64	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.45
2:A:703:DGT:O3G	1:D:116:LYS:NZ	2.41	0.44
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.44
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.44
1:D:315:TYR:CE2	2:D:702:DGT:H5'	2.52	0.44
1:B:215:HIS:CE1	2:B:701:DGT:O2A	2.70	0.44
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.91	0.44
1:C:592:THR:N	1:C:593:PRO:CD	2.81	0.43
1:D:244:LEU:C	1:D:244:LEU:HD23	2.43	0.43
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.90	0.43
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.59	0.43
1:B:390:PHE:CE2	1:B:426:ILE:CD1	3.01	0.43
1:B:597:GLU:OE1	1:B:597:GLU:N	2.35	0.43
1:B:598:TRP:O	1:B:599:ASN:HB2	2.18	0.43
1:A:240:MET:HE3	1:A:240:MET:C	2.44	0.43
1:A:592:THR:N	1:A:593:PRO:CD	2.82	0.43
1:B:591:ILE:HG12	5:B:847:HOH:O	2.18	0.42
1:B:592:THR:N	1:B:593:PRO:CD	2.82	0.42
1:D:592:THR:N	1:D:593:PRO:CD	2.82	0.42
1:C:139:PRO:HA	5:C:829:HOH:O	2.20	0.42
1:B:576:ARG:O	1:B:577:ASN:HB2	2.20	0.42
1:A:598:TRP:O	1:A:599:ASN:HB2	2.19	0.42
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.42
1:D:251:LYS:HB2	1:D:252:PRO:HD3	2.02	0.42
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.01	0.41
1:D:375:GLN:O	1:D:376:HIS:C	2.63	0.41
1:A:326:GLN:HG2	1:C:327:ASN:O	2.21	0.41
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.87	0.41
1:C:476:LEU:N	1:C:477:PRO:CD	2.83	0.41
1:C:597:GLU:OE1	1:C:597:GLU:N	2.36	0.41
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.92	0.41
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LYS:O	1:C:255:GLU:HG2	2.22	0.40
1:D:390:PHE:CE2	1:D:426:ILE:CD1	3.04	0.40
1:A:328:ASN:HB3	5:A:830:HOH:O	2.21	0.40
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.57	0.40
1:D:251:LYS:O	1:D:255:GLU:HG2	2.21	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	478/514 (93%)	472 (99%)	6 (1%)	0	100	100
1	B	478/514 (93%)	471 (98%)	7 (2%)	0	100	100
1	C	478/514 (93%)	471 (98%)	7 (2%)	0	100	100
1	D	478/514 (93%)	471 (98%)	7 (2%)	0	100	100
All	All	1912/2056 (93%)	1885 (99%)	27 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	428/459 (93%)	414 (97%)	14 (3%)	33	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	428/459 (93%)	415 (97%)	13 (3%)	36	51
1	C	428/459 (93%)	416 (97%)	12 (3%)	38	53
1	D	428/459 (93%)	414 (97%)	14 (3%)	33	47
All	All	1712/1836 (93%)	1659 (97%)	53 (3%)	35	50

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LYS
1	A	189	LEU
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU
1	A	325	ILE
1	A	326	GLN
1	A	348	ARG
1	A	359	LEU
1	A	452	ASN
1	A	463	THR
1	A	469	LYS
1	A	535	ASN
1	A	594	GLN
1	B	148	LYS
1	B	189	LEU
1	B	273	VAL
1	B	277	GLU
1	B	284	LEU
1	B	325	ILE
1	B	326	GLN
1	B	359	LEU
1	B	388	ASP
1	B	463	THR
1	B	469	LYS
1	B	535	ASN
1	B	594	GLN
1	C	148	LYS
1	C	189	LEU
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	325	ILE

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Mol	Chain	Res	Type
1	C	326	GLN
1	C	359	LEU
1	C	463	THR
1	C	469	LYS
1	C	535	ASN
1	C	594	GLN
1	D	148	LYS
1	D	189	LEU
1	D	190	GLN
1	D	229	VAL
1	D	273	VAL
1	D	277	GLU
1	D	284	LEU
1	D	325	ILE
1	D	326	GLN
1	D	359	LEU
1	D	452	ASN
1	D	463	THR
1	D	469	LYS
1	D	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	210	HIS
1	A	235	GLN
1	A	243	HIS
1	A	364	HIS
1	A	370	HIS
1	A	375	GLN
1	A	380	ASN
1	A	425	ASN
1	A	447	GLN
1	A	567	GLN
1	A	571	GLN
1	A	594	GLN
1	B	149	GLN
1	B	200	GLN
1	B	210	HIS
1	B	215	HIS
1	B	235	GLN

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Mol	Chain	Res	Type
1	B	243	HIS
1	B	364	HIS
1	B	425	ASN
1	B	447	GLN
1	B	452	ASN
1	B	567	GLN
1	B	571	GLN
1	B	594	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	370	HIS
1	C	375	GLN
1	C	380	ASN
1	C	425	ASN
1	C	447	GLN
1	C	452	ASN
1	C	567	GLN
1	C	571	GLN
1	C	594	GLN
1	D	149	GLN
1	D	200	GLN
1	D	235	GLN
1	D	243	HIS
1	D	364	HIS
1	D	425	ASN
1	D	447	GLN
1	D	567	GLN
1	D	571	GLN
1	D	594	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DGT	D	702	3	32,33,33	2.00	6 (18%)	48,52,52	1.45	6 (12%)
2	DGT	D	704	3	32,33,33	1.45	6 (18%)	48,52,52	1.66	9 (18%)
4	TTP	C	704	3	29,30,30	1.62	8 (27%)	43,47,47	2.13	13 (30%)
2	DGT	A	704	3	32,33,33	1.74	7 (21%)	48,52,52	1.55	11 (22%)
2	DGT	A	703	3	32,33,33	1.42	5 (15%)	48,52,52	1.64	11 (22%)
2	DGT	B	701	3	32,33,33	1.80	7 (21%)	48,52,52	1.48	7 (14%)
2	DGT	C	701	3	32,33,33	1.39	3 (9%)	48,52,52	1.71	15 (31%)
2	DGT	B	704	3	32,33,33	1.54	7 (21%)	48,52,52	1.96	15 (31%)
2	DGT	C	706	3	32,33,33	1.77	7 (21%)	48,52,52	1.73	11 (22%)
2	DGT	A	701	3	32,33,33	1.40	5 (15%)	48,52,52	1.81	11 (22%)
2	DGT	D	701	3	32,33,33	1.32	3 (9%)	48,52,52	1.95	16 (33%)
2	DGT	B	703	3	32,33,33	1.52	5 (15%)	48,52,52	1.74	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	D	702	3	-	4/22/34/34	0/3/3/3
2	DGT	D	704	3	-	4/22/34/34	0/3/3/3
4	TTP	C	704	3	-	4/22/34/34	0/2/2/2
2	DGT	A	704	3	-	3/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	A	703	3	-	8/22/34/34	0/3/3/3
2	DGT	B	701	3	-	7/22/34/34	0/3/3/3
2	DGT	C	701	3	-	6/22/34/34	0/3/3/3
2	DGT	B	704	3	-	3/22/34/34	0/3/3/3
2	DGT	C	706	3	-	8/22/34/34	0/3/3/3
2	DGT	A	701	3	-	5/22/34/34	0/3/3/3
2	DGT	D	701	3	-	2/22/34/34	0/3/3/3
2	DGT	B	703	3	-	5/22/34/34	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	702	DGT	PB-O3B	5.71	1.65	1.59
2	D	702	DGT	PA-O3A	5.47	1.65	1.59
2	B	701	DGT	PA-O3A	5.06	1.65	1.59
2	C	706	DGT	PB-O3B	4.90	1.64	1.59
2	B	701	DGT	PB-O3B	4.29	1.64	1.59
2	A	704	DGT	C6-N1	-4.27	1.30	1.38
2	A	703	DGT	C6-N1	-4.26	1.30	1.38
2	C	701	DGT	PB-O3A	4.07	1.63	1.59
2	C	706	DGT	PA-O3A	-4.06	1.55	1.59
2	B	703	DGT	PA-O3A	-4.02	1.55	1.59
2	D	701	DGT	PB-O3A	3.97	1.63	1.59
2	B	704	DGT	C4-N9	-3.86	1.28	1.38
2	D	702	DGT	C5-C4	3.70	1.49	1.38
2	A	701	DGT	PA-O3A	3.70	1.63	1.59
2	B	701	DGT	C5-C4	3.68	1.48	1.38
4	C	704	TTP	PA-O3A	3.68	1.63	1.59
2	A	704	DGT	C5-N7	-3.61	1.31	1.39
2	A	703	DGT	C5-N7	-3.55	1.32	1.39
2	C	701	DGT	C6-N1	-3.54	1.32	1.38
4	C	704	TTP	C4-C5	3.52	1.50	1.44
2	B	703	DGT	C5-C4	3.49	1.48	1.38
2	B	704	DGT	C5-N7	-3.49	1.32	1.39
2	A	704	DGT	PB-O3A	3.47	1.63	1.59
2	A	704	DGT	C4-N9	-3.46	1.29	1.38
2	C	706	DGT	C5-N7	-3.46	1.32	1.39
2	A	704	DGT	PB-O3B	3.36	1.63	1.59
2	C	706	DGT	C5-C4	3.31	1.47	1.38
2	C	706	DGT	C6-N1	-3.27	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	DGT	PB-O3A	3.24	1.63	1.59
2	D	704	DGT	C4-N9	-3.23	1.29	1.38
2	A	701	DGT	C5-C4	3.15	1.47	1.38
2	B	703	DGT	C6-N1	-3.12	1.33	1.38
2	D	704	DGT	C5-N7	-3.10	1.32	1.39
2	D	704	DGT	C6-N1	-3.07	1.33	1.38
2	D	704	DGT	C5-C4	2.92	1.46	1.38
2	A	704	DGT	C5-C4	2.89	1.46	1.38
2	D	702	DGT	C4-N9	-2.85	1.30	1.38
4	C	704	TTP	C6-N1	-2.72	1.33	1.38
2	A	703	DGT	C4-N9	-2.71	1.31	1.38
2	C	701	DGT	C5-C4	2.67	1.46	1.38
2	D	702	DGT	C2-N2	2.62	1.40	1.34
2	D	702	DGT	PB-O3A	2.56	1.62	1.59
2	B	703	DGT	C5-N7	-2.53	1.34	1.39
2	A	701	DGT	PB-O3B	2.51	1.62	1.59
2	B	704	DGT	C6-N1	-2.49	1.34	1.38
2	C	706	DGT	C4-N9	-2.44	1.31	1.38
2	A	701	DGT	PB-O3A	2.37	1.62	1.59
2	D	701	DGT	C4-N9	-2.37	1.32	1.38
2	B	703	DGT	PB-O3A	-2.35	1.57	1.59
2	A	701	DGT	C4-N9	-2.35	1.32	1.38
4	C	704	TTP	O4'-C4'	-2.30	1.39	1.45
2	B	704	DGT	O4'-C4'	-2.25	1.40	1.45
2	B	704	DGT	O6-C6	2.25	1.27	1.23
2	B	701	DGT	C4-N9	-2.25	1.32	1.38
4	C	704	TTP	PB-O3B	2.21	1.61	1.59
2	A	703	DGT	C2-N3	2.19	1.38	1.33
4	C	704	TTP	C2-N1	2.16	1.41	1.38
2	D	704	DGT	PB-O3B	2.16	1.61	1.59
2	B	701	DGT	C2-N3	2.16	1.38	1.33
2	B	701	DGT	C8-N7	2.15	1.38	1.32
2	D	704	DGT	C8-N7	2.14	1.38	1.32
4	C	704	TTP	C2-N3	-2.13	1.34	1.38
4	C	704	TTP	PB-O3A	2.12	1.61	1.59
2	D	701	DGT	C5-C4	2.11	1.44	1.38
2	B	704	DGT	PA-O1A	-2.08	1.45	1.55
2	A	703	DGT	C5-C4	2.08	1.44	1.38
2	B	704	DGT	C5-C4	2.07	1.44	1.38
2	C	706	DGT	PG-O1G	-2.07	1.47	1.54
2	A	704	DGT	C8-N7	2.06	1.38	1.32

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	704	TTP	C5M-C5-C4	5.92	125.10	118.78
2	B	703	DGT	C5-C4-N3	-5.84	119.09	128.39
2	D	704	DGT	C5-C4-N3	-5.84	119.10	128.39
4	C	704	TTP	C4-N3-C2	-5.68	119.89	127.34
2	C	706	DGT	O3A-PB-O2B	-5.66	93.68	110.70
2	A	703	DGT	C5-C4-N3	-5.26	120.02	128.39
2	B	704	DGT	C5-C4-N3	-5.12	120.23	128.39
2	D	704	DGT	C2-N3-C4	4.84	120.64	112.30
4	C	704	TTP	N3-C2-N1	4.84	121.19	114.89
2	C	706	DGT	C5-C4-N3	-4.73	120.87	128.39
2	A	701	DGT	C5-C4-N3	-4.70	120.90	128.39
2	A	701	DGT	C2-N3-C4	4.67	120.35	112.30
2	B	703	DGT	C2-N3-C4	4.60	120.22	112.30
2	B	701	DGT	C5-C4-N3	-4.45	121.30	128.39
4	C	704	TTP	C5-C4-N3	4.45	119.19	115.32
4	C	704	TTP	C5M-C5-C6	-4.37	116.94	122.85
2	B	704	DGT	C2-N3-C4	4.30	119.71	112.30
2	B	701	DGT	C2-N3-C4	4.07	119.31	112.30
2	A	703	DGT	N9-C4-N3	4.05	134.06	125.95
2	D	701	DGT	O6-C6-C5	-4.03	115.89	126.53
2	D	702	DGT	O6-C6-C5	-4.03	115.89	126.53
2	B	704	DGT	O1A-PA-O3A	4.00	118.08	107.27
2	A	701	DGT	O2G-PG-O1G	3.90	122.42	107.80
2	B	704	DGT	N2-C2-N3	-3.84	112.18	119.67
2	D	701	DGT	O3B-PG-O3G	-3.82	90.95	111.04
2	C	701	DGT	C5-C4-N3	-3.79	122.36	128.39
2	A	701	DGT	N9-C4-N3	3.71	133.38	125.95
2	D	701	DGT	O1A-PA-O3A	3.69	117.24	107.27
2	C	706	DGT	N9-C4-N3	3.66	133.27	125.95
2	B	704	DGT	N2-C2-N1	3.63	124.42	116.76
2	B	703	DGT	N9-C4-N3	3.57	133.09	125.95
2	B	703	DGT	O1A-PA-O3A	3.57	116.91	107.27
2	C	701	DGT	C6-C5-N7	3.53	136.72	130.29
2	D	702	DGT	N9-C4-N3	3.49	132.94	125.95
2	D	702	DGT	C5-C4-N3	-3.48	122.86	128.39
2	A	701	DGT	O6-C6-C5	-3.44	117.45	126.53
2	A	704	DGT	O3A-PA-O2A	3.39	120.89	110.70
2	A	703	DGT	C2-N3-C4	3.36	118.08	112.30
2	C	706	DGT	C2-N3-C4	3.33	118.04	112.30
2	D	701	DGT	C5-C4-N3	-3.30	123.14	128.39
2	B	703	DGT	C6-C5-N7	3.27	136.25	130.29
2	A	704	DGT	O2G-PG-O1G	3.25	120.00	107.80
2	D	701	DGT	C2-N1-C6	-3.22	119.27	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	DGT	N9-C4-N3	3.20	132.35	125.95
2	A	701	DGT	C6-C5-N7	3.19	136.09	130.29
2	D	701	DGT	O6-C6-N1	3.18	126.09	120.11
4	C	704	TTP	O4-C4-C5	-3.17	121.29	124.92
2	D	704	DGT	N9-C4-N3	3.12	132.18	125.95
2	D	702	DGT	O6-C6-N1	3.08	125.91	120.11
2	B	704	DGT	C4-C5-N7	-3.05	105.84	110.67
2	D	701	DGT	C2-N3-C4	3.03	117.52	112.30
2	D	702	DGT	C2-N3-C4	3.01	117.49	112.30
2	C	701	DGT	C2-N3-C4	2.99	117.45	112.30
2	D	701	DGT	O1G-PG-O3G	2.97	122.42	110.83
2	B	704	DGT	O3A-PB-O2B	-2.97	101.77	110.70
2	D	701	DGT	O3A-PA-O2A	-2.93	101.88	110.70
2	B	704	DGT	O4'-C1'-N9	-2.86	102.78	107.86
2	A	704	DGT	C5-C4-N3	-2.86	123.84	128.39
2	B	701	DGT	C6-C5-N7	2.81	135.40	130.29
2	C	706	DGT	O3B-PG-O3G	-2.80	96.31	111.04
2	C	701	DGT	O1B-PB-O3A	2.79	114.80	107.27
2	A	704	DGT	O3A-PB-O2B	-2.79	102.33	110.70
2	C	701	DGT	N2-C2-N3	-2.78	114.24	119.67
2	D	701	DGT	O1B-PB-O3A	2.78	114.79	107.27
2	A	703	DGT	O1A-PA-O5'	2.74	119.98	107.57
2	D	701	DGT	N9-C4-N3	2.73	131.41	125.95
2	A	704	DGT	C6-C5-N7	2.72	135.24	130.29
2	C	701	DGT	C4-C5-N7	-2.65	106.47	110.67
2	B	704	DGT	O6-C6-N1	2.63	125.05	120.11
2	A	701	DGT	C5-C6-N1	2.62	119.93	113.25
2	A	703	DGT	O3A-PB-O2B	-2.61	102.86	110.70
4	C	704	TTP	O2B-PB-O1B	2.59	124.49	112.44
2	D	704	DGT	C6-C5-N7	2.56	134.95	130.29
2	D	701	DGT	O5'-PA-O2A	-2.56	98.79	108.94
2	A	701	DGT	O1A-PA-O2A	2.55	124.31	112.44
2	B	703	DGT	C4-C5-N7	-2.55	106.63	110.67
2	A	704	DGT	C2-N3-C4	2.55	116.69	112.30
2	A	703	DGT	O5'-PA-O2A	-2.49	99.07	108.94
2	C	706	DGT	O1B-PB-O2B	2.47	123.92	112.44
2	C	701	DGT	O1A-PA-O2A	2.46	123.89	112.44
2	A	704	DGT	O1A-PA-O3A	-2.46	100.63	107.27
2	C	706	DGT	O1B-PB-O3A	2.45	113.89	107.27
2	B	704	DGT	O6-C6-C5	-2.44	120.08	126.53
2	B	704	DGT	O2G-PG-O1G	2.44	116.96	107.80
2	A	704	DGT	O1B-PB-O2B	2.44	123.79	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	DGT	O4'-C1'-N9	-2.42	103.57	107.86
2	C	701	DGT	O3B-PG-O3G	-2.42	98.32	111.04
4	C	704	TTP	C5-C6-N1	-2.41	120.70	123.31
2	D	701	DGT	O1B-PB-O2B	2.40	123.63	112.44
2	C	701	DGT	O3A-PB-O2B	-2.40	103.48	110.70
2	A	703	DGT	O2G-PG-O3G	2.40	120.19	110.83
2	B	704	DGT	C6-C5-N7	2.39	134.64	130.29
2	B	701	DGT	O6-C6-C5	-2.38	120.24	126.53
2	A	701	DGT	C2-N1-C6	-2.37	120.82	125.11
4	C	704	TTP	O2G-PG-O1G	2.34	119.95	110.83
2	D	701	DGT	O1B-PB-O3B	-2.34	100.95	107.27
2	D	704	DGT	O1A-PA-O5'	2.32	118.08	107.57
2	D	701	DGT	O2G-PG-O3B	2.31	112.37	104.64
4	C	704	TTP	O4'-C1'-N1	2.30	111.95	107.86
2	A	703	DGT	O6-C6-C5	-2.29	120.49	126.53
2	A	703	DGT	C2-N1-C6	-2.28	120.98	125.11
2	D	702	DGT	C2-N1-C6	-2.27	120.99	125.11
2	A	701	DGT	C6-C5-C4	-2.27	115.42	118.83
2	C	706	DGT	O1B-PB-O3B	2.26	113.39	107.27
2	D	704	DGT	O1B-PB-O3B	2.26	113.39	107.27
2	C	701	DGT	O4'-C1'-N9	-2.26	103.86	107.86
2	C	706	DGT	O2G-PG-O3G	2.25	119.61	110.83
2	A	704	DGT	O2G-PG-O3G	2.24	119.55	110.83
2	C	706	DGT	O1G-PG-O3G	2.23	119.52	110.83
2	D	701	DGT	N2-C2-N3	-2.21	115.35	119.67
4	C	704	TTP	O2-C2-N1	-2.21	119.93	122.80
2	B	703	DGT	O2G-PG-O1G	2.18	115.99	107.80
2	C	701	DGT	O3A-PA-O2A	-2.18	104.16	110.70
2	A	703	DGT	O1B-PB-O3B	2.17	113.14	107.27
2	D	704	DGT	O2G-PG-O1G	2.14	115.83	107.80
2	B	704	DGT	N9-C4-N3	2.14	130.24	125.95
2	A	704	DGT	O1B-PB-O3A	2.14	113.04	107.27
2	B	701	DGT	C2-N1-C6	-2.13	121.25	125.11
2	B	704	DGT	O2G-PG-O3B	2.12	111.75	104.64
2	C	701	DGT	C2-N1-C6	-2.12	121.28	125.11
2	B	701	DGT	O1A-PA-O2A	2.10	122.23	112.44
2	B	704	DGT	C5-C4-N9	2.10	109.42	105.66
2	C	701	DGT	N9-C4-N3	2.10	130.15	125.95
4	C	704	TTP	O2A-PA-O1A	2.09	122.18	112.44
2	A	703	DGT	C6-C5-N7	2.08	134.07	130.29
4	C	704	TTP	O3B-PG-O1G	-2.06	100.22	111.04
2	C	701	DGT	C1'-N9-C4	-2.05	119.97	125.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	DGT	O1B-PB-O2B	2.05	121.98	112.44
2	B	703	DGT	O1B-PB-O3B	2.04	112.78	107.27
2	D	704	DGT	O5'-PA-O2A	-2.02	100.93	108.94
2	D	704	DGT	C4-C5-N7	-2.01	107.48	110.67
2	A	701	DGT	C8-N9-C4	2.01	109.80	106.03
2	C	706	DGT	C6-C5-N7	2.01	133.94	130.29

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DGT	PB-O3A-PA-O5'
2	A	703	DGT	PB-O3B-PG-O2G
2	B	701	DGT	C5'-O5'-PA-O1A
2	B	704	DGT	PB-O3B-PG-O1G
2	B	704	DGT	PB-O3B-PG-O2G
2	C	701	DGT	PB-O3B-PG-O1G
2	B	701	DGT	C4'-C5'-O5'-PA
4	C	704	TTP	C4'-C5'-O5'-PA
2	D	702	DGT	C4'-C5'-O5'-PA
2	A	704	DGT	PB-O3B-PG-O3G
2	C	701	DGT	PB-O3B-PG-O3G
2	C	706	DGT	PB-O3B-PG-O3G
2	A	701	DGT	C4'-C5'-O5'-PA
2	B	701	DGT	PB-O3A-PA-O5'
4	C	704	TTP	PB-O3A-PA-O5'
2	B	703	DGT	PB-O3B-PG-O2G
2	C	706	DGT	PB-O3B-PG-O1G
2	A	701	DGT	C3'-C4'-C5'-O5'
2	A	703	DGT	PB-O3A-PA-O1A
2	B	703	DGT	PG-O3B-PB-O1B
2	C	706	DGT	PG-O3B-PB-O2B
2	D	702	DGT	PG-O3B-PB-O1B
2	A	703	DGT	C4'-C5'-O5'-PA
2	A	701	DGT	O4'-C4'-C5'-O5'
2	A	703	DGT	C2'-C1'-N9-C8
2	C	706	DGT	PG-O3B-PB-O1B
2	D	704	DGT	PB-O3A-PA-O1A
2	A	703	DGT	C2'-C1'-N9-C4
2	C	706	DGT	C2'-C1'-N9-C4
2	D	704	DGT	C2'-C1'-N9-C4
2	B	703	DGT	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
2	B	701	DGT	O4'-C4'-C5'-O5'
2	C	701	DGT	PB-O3A-PA-O1A
2	C	701	DGT	PB-O3A-PA-O2A
2	D	701	DGT	PA-O3A-PB-O1B
2	D	702	DGT	PG-O3B-PB-O2B
2	D	704	DGT	PG-O3B-PB-O1B
2	C	706	DGT	C4'-C5'-O5'-PA
2	A	703	DGT	PB-O3B-PG-O1G
2	D	702	DGT	PB-O3B-PG-O2G
2	C	706	DGT	C2'-C1'-N9-C8
2	B	701	DGT	C3'-C4'-C5'-O5'
2	A	703	DGT	PG-O3B-PB-O1B
2	A	703	DGT	PB-O3A-PA-O2A
2	B	701	DGT	PG-O3B-PB-O1B
2	B	703	DGT	PG-O3B-PB-O2B
2	B	704	DGT	PB-O3A-PA-O1A
2	C	701	DGT	PA-O3A-PB-O1B
2	C	706	DGT	PB-O3A-PA-O1A
2	D	701	DGT	PB-O3A-PA-O1A
4	C	704	TTP	PG-O3B-PB-O2B
2	D	704	DGT	C4'-C5'-O5'-PA
2	A	701	DGT	PG-O3B-PB-O1B
2	A	704	DGT	PG-O3B-PB-O1B
2	A	704	DGT	PB-O3A-PA-O2A
2	B	701	DGT	PG-O3B-PB-O2B
2	B	703	DGT	PB-O3A-PA-O1A
2	C	701	DGT	PG-O3B-PB-O1B
4	C	704	TTP	C3'-C4'-C5'-O5'

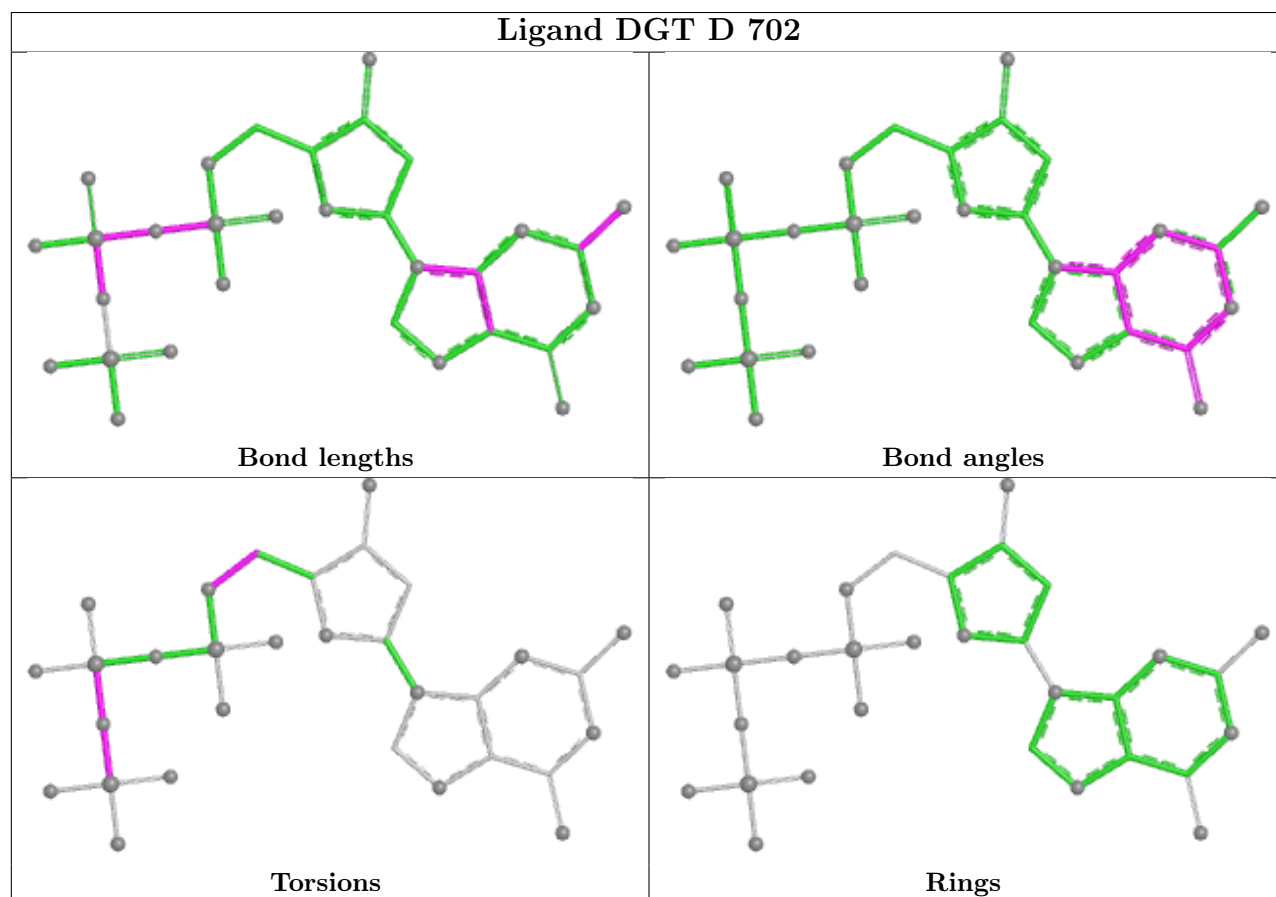
There are no ring outliers.

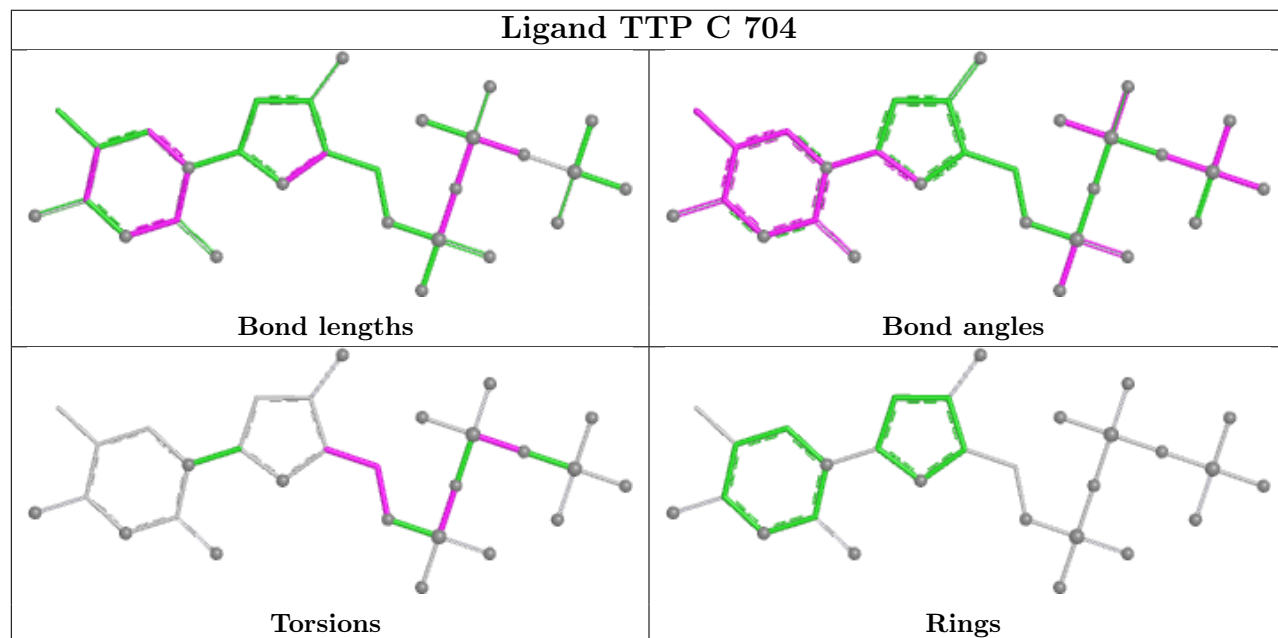
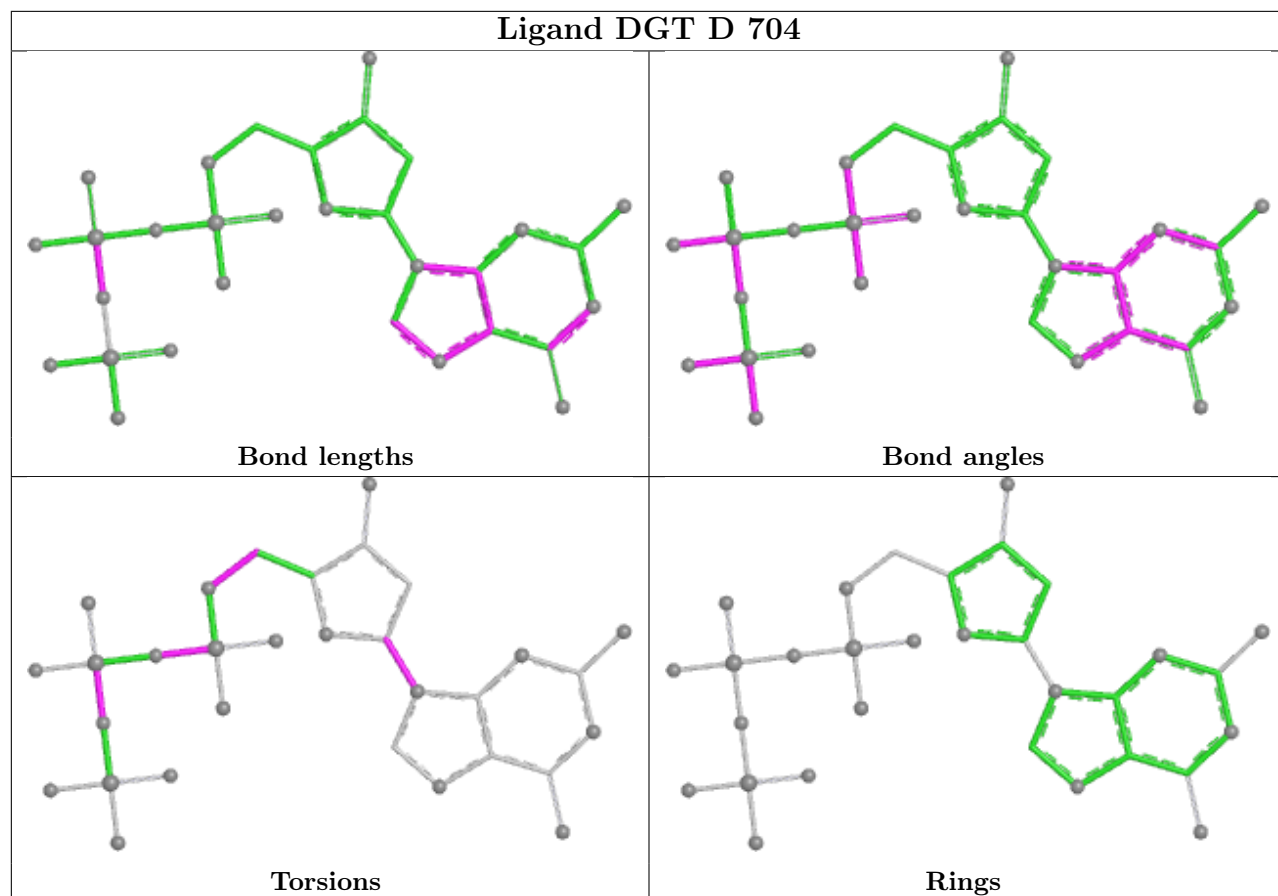
5 monomers are involved in 7 short contacts:

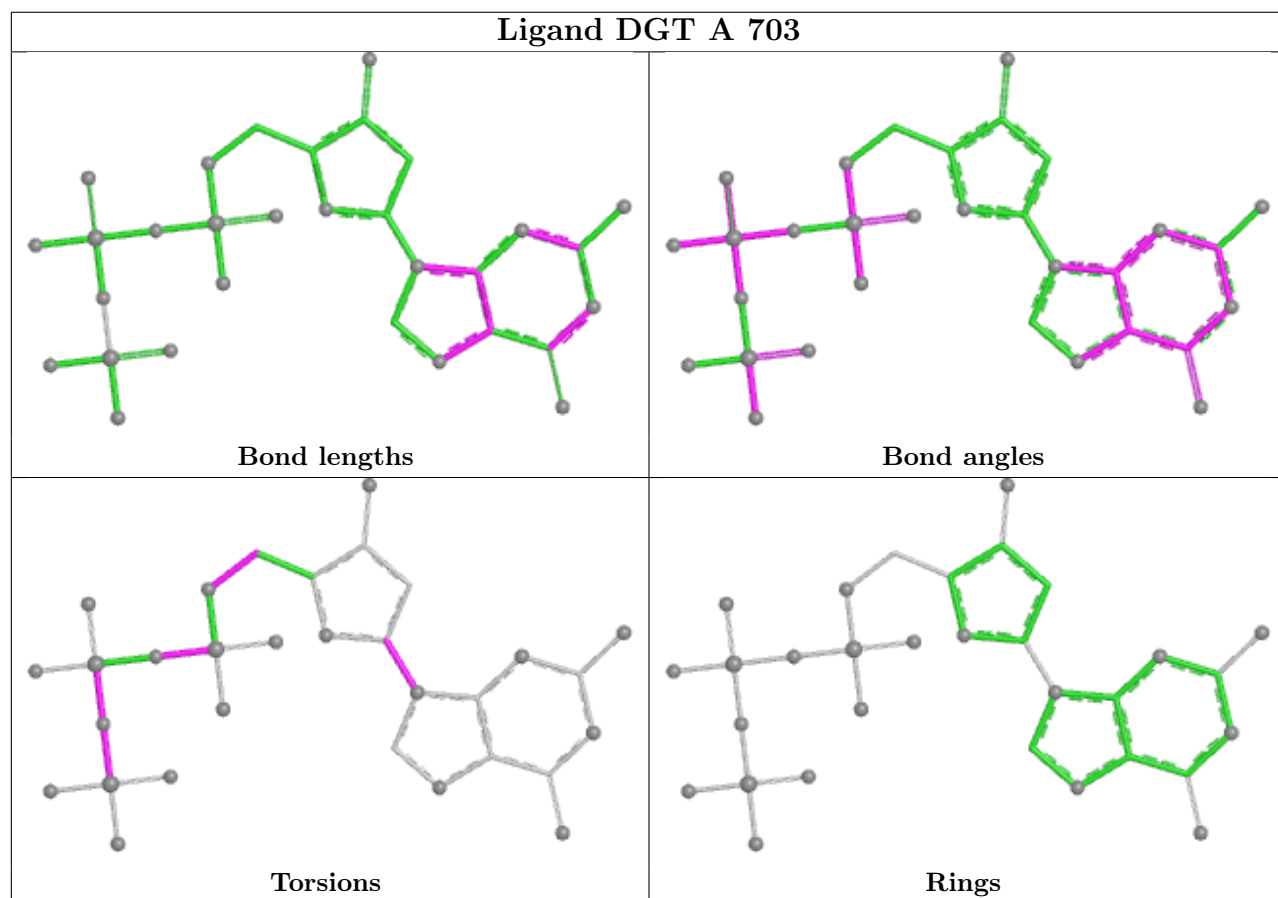
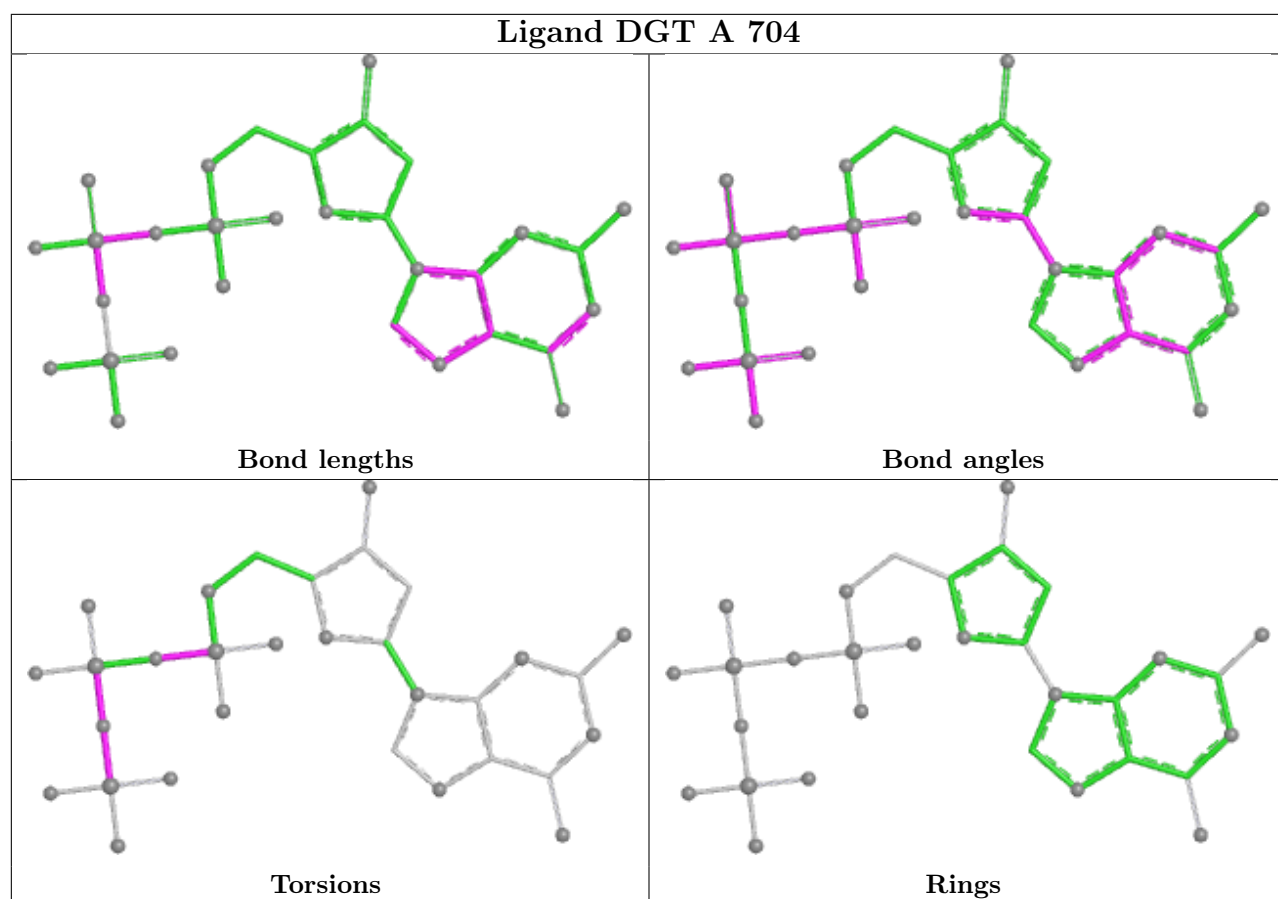
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	DGT	2	0
4	C	704	TTP	1	0
2	A	704	DGT	1	0
2	A	703	DGT	1	0
2	B	701	DGT	2	0

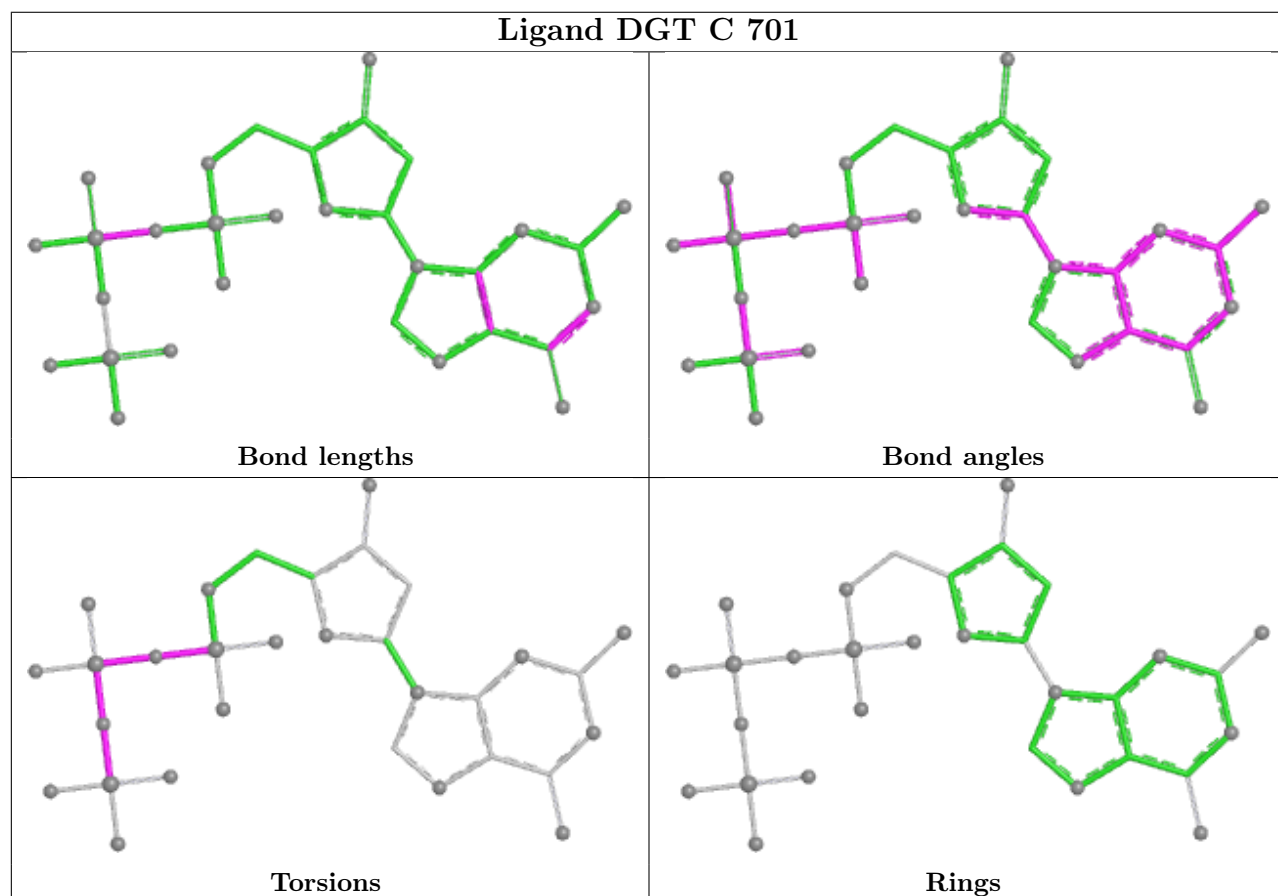
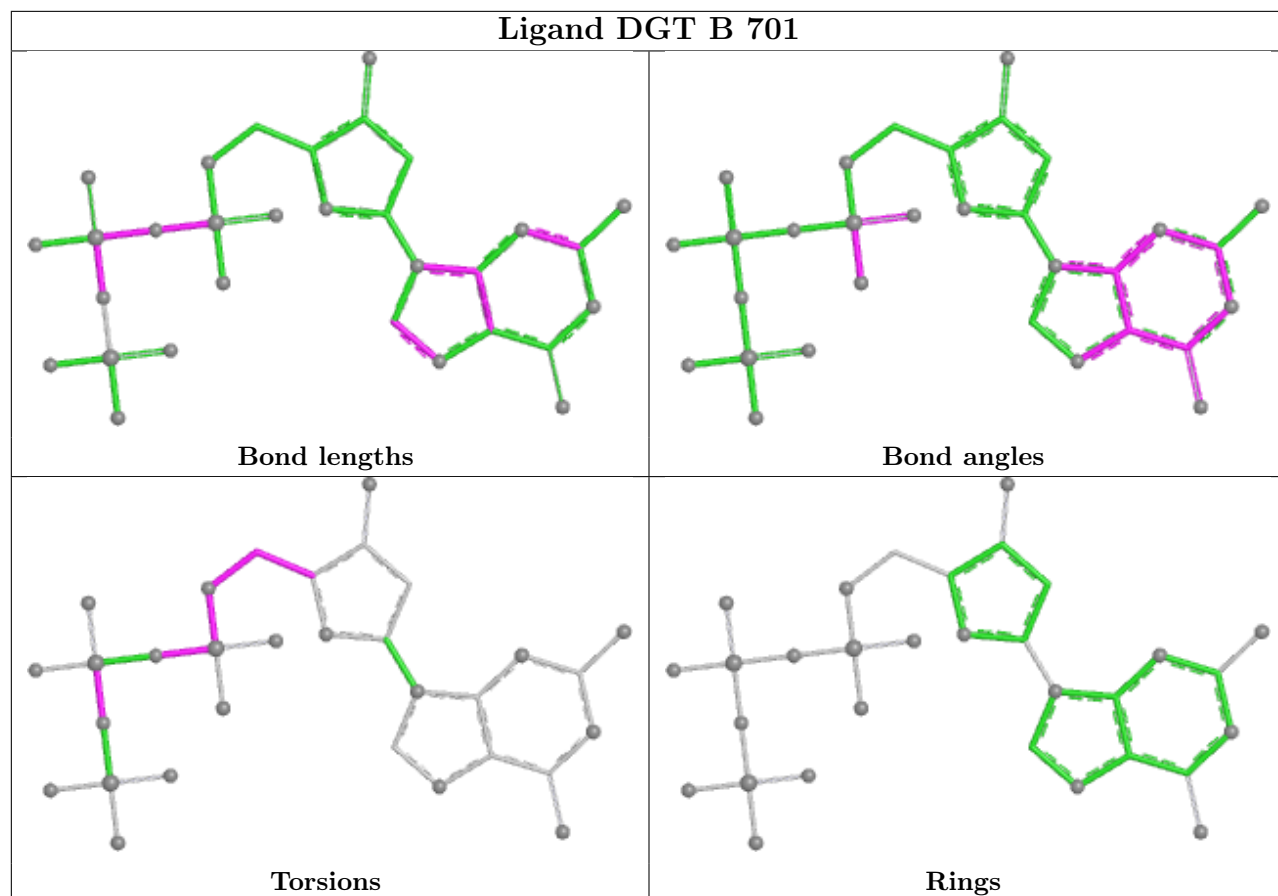
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

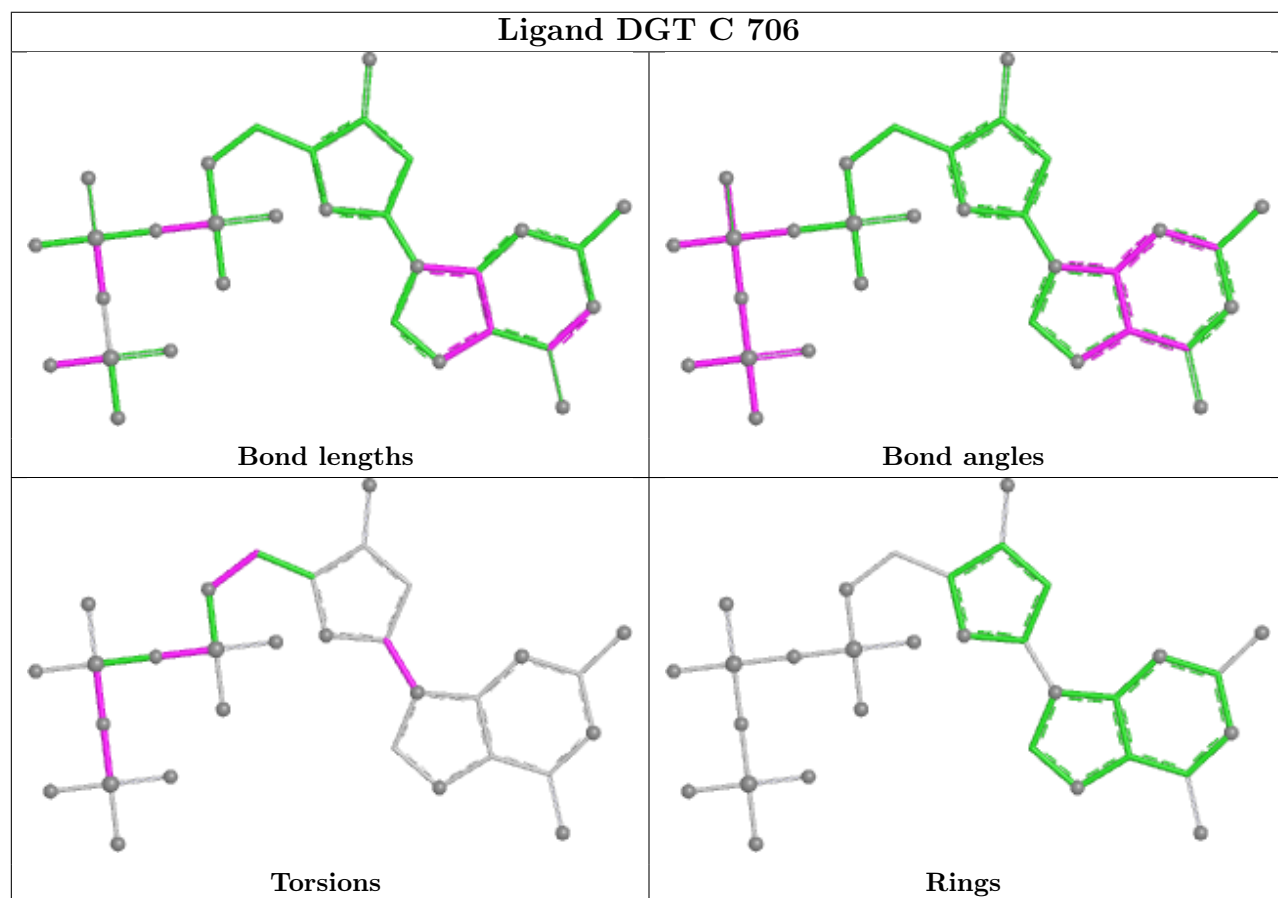
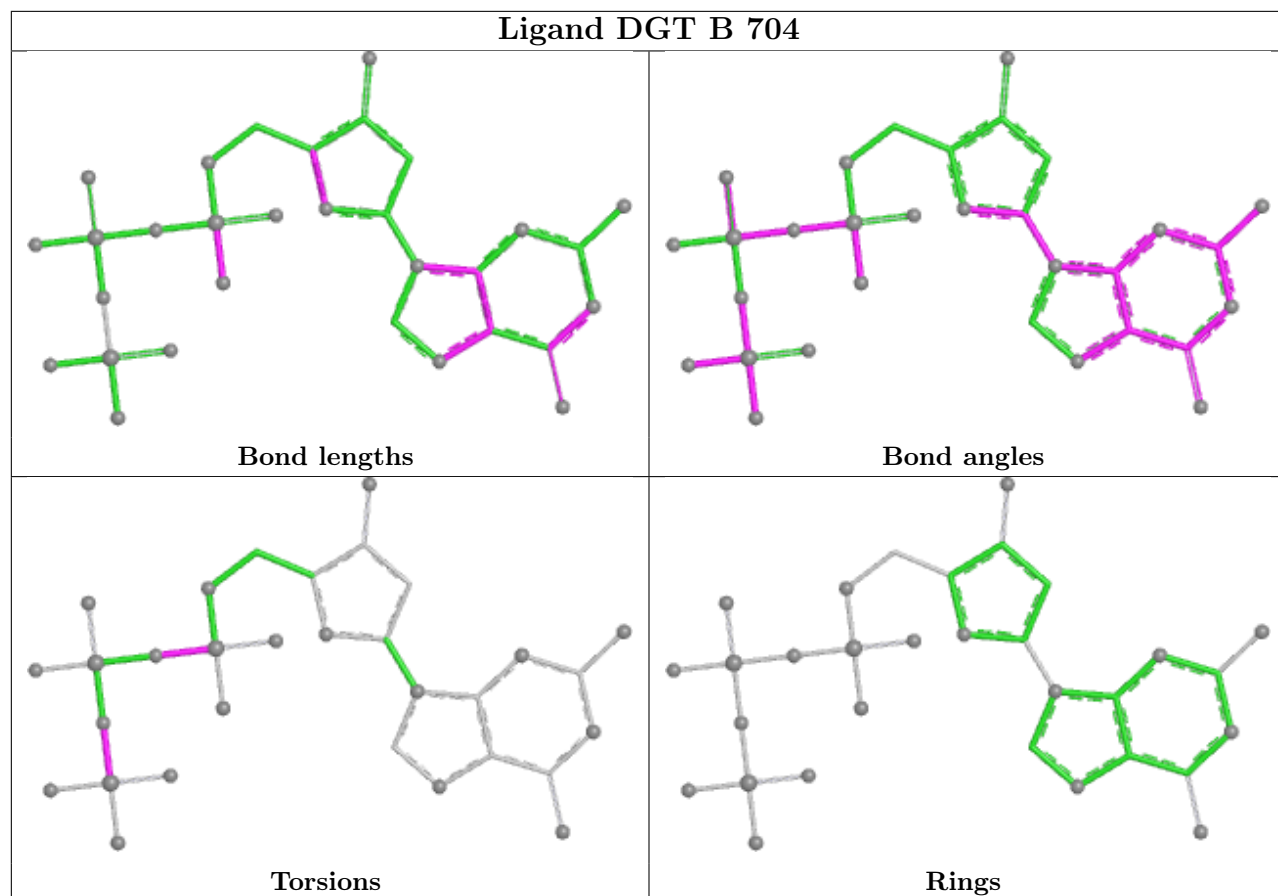
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

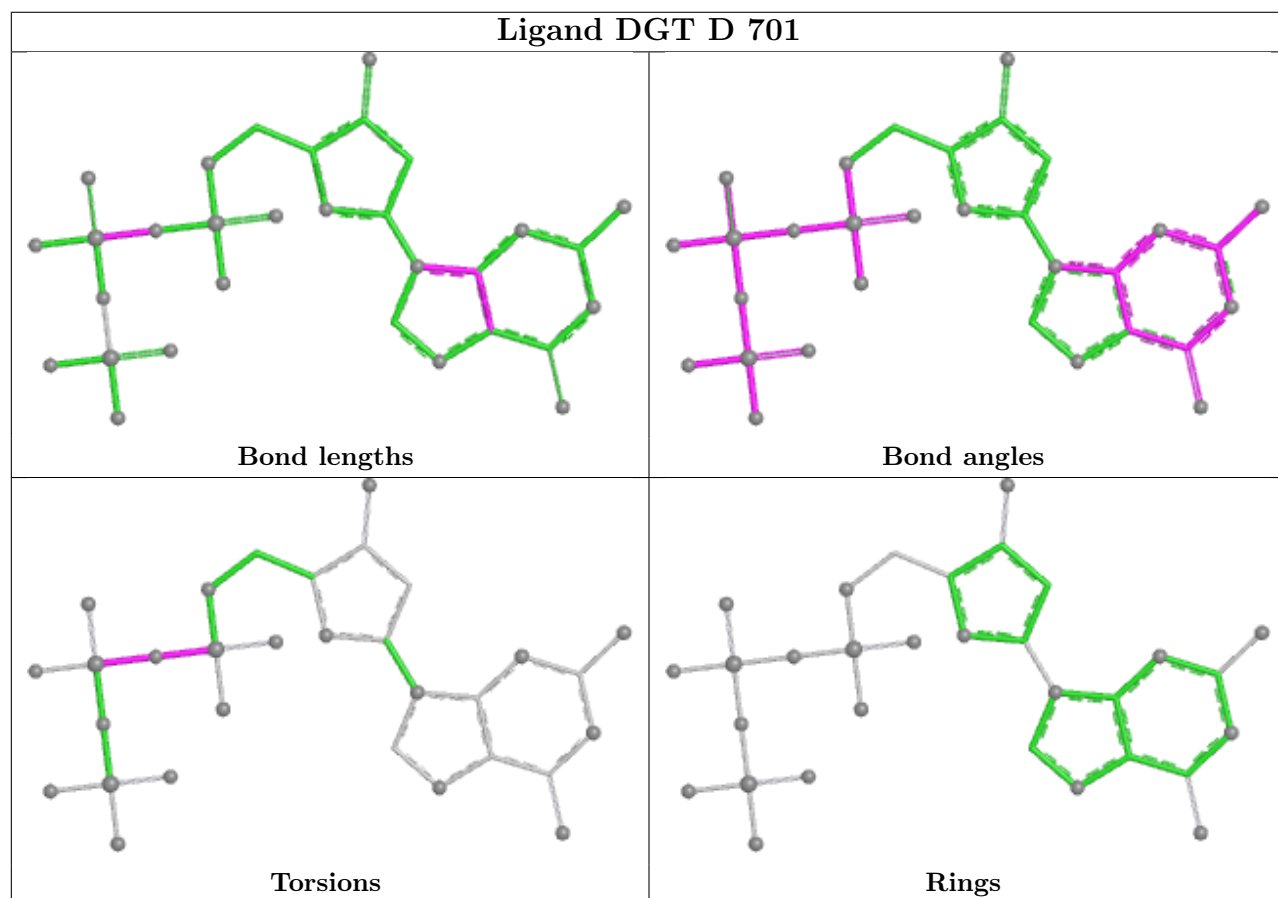
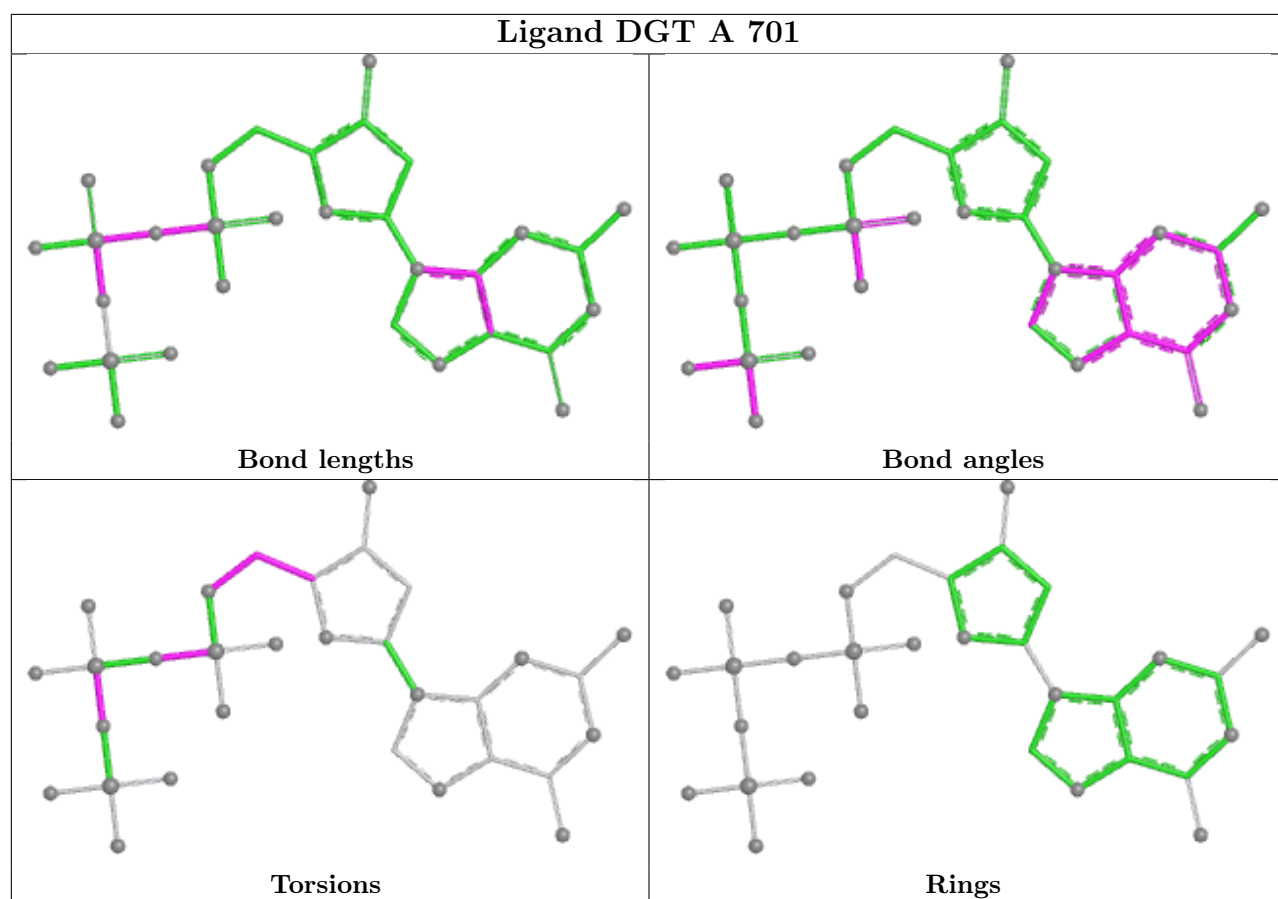


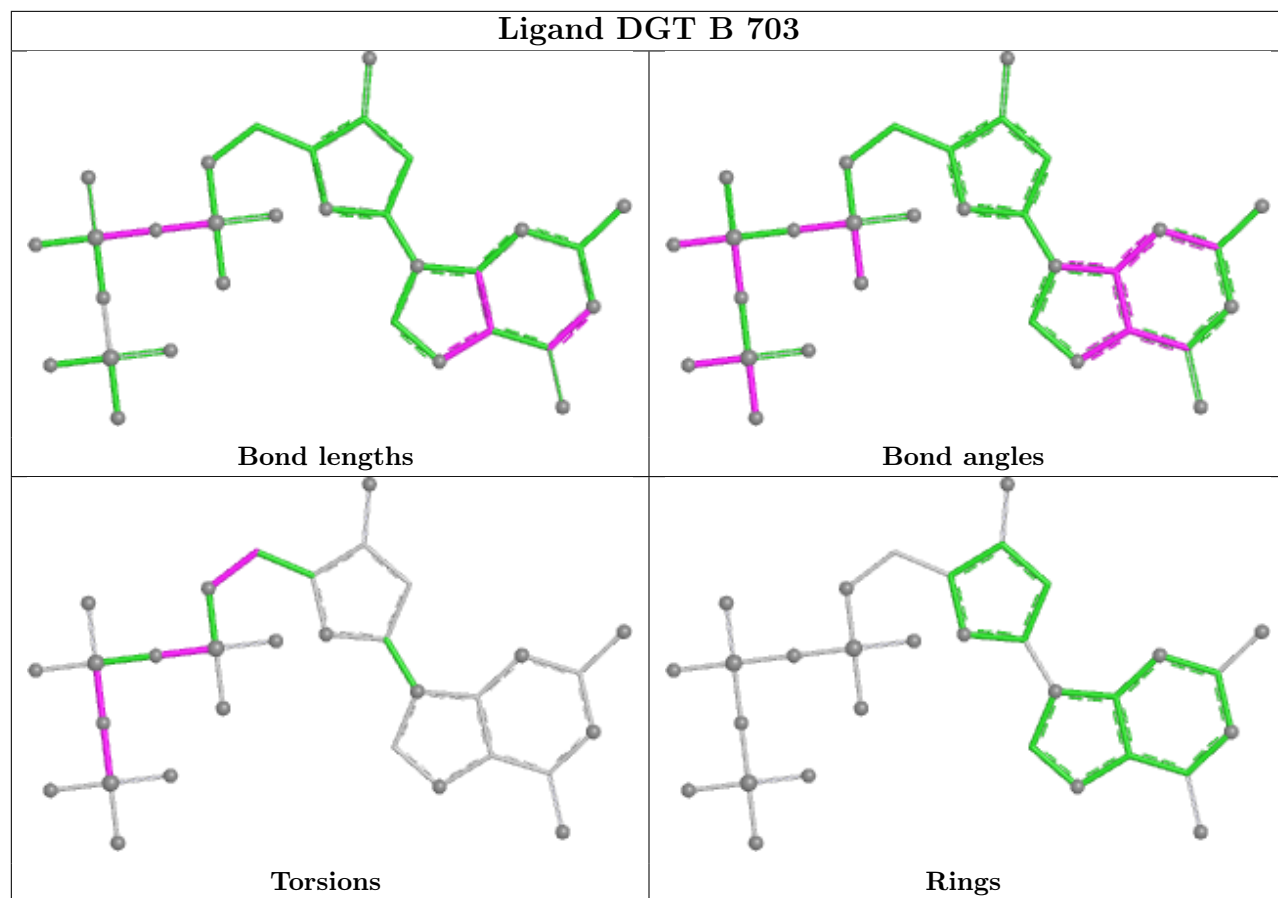












5.7 Other polymers [i](#)

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%)	0.43	13 (2%) 56 58	36, 72, 118, 145	1 (0%)
1	B	481/514 (93%)	0.23	9 (1%) 66 68	27, 61, 100, 130	1 (0%)
1	C	481/514 (93%)	0.39	9 (1%) 66 68	43, 75, 112, 148	1 (0%)
1	D	481/514 (93%)	0.18	2 (0%) 88 89	30, 54, 81, 108	1 (0%)
All	All	1924/2056 (93%)	0.31	33 (1%) 69 70	27, 64, 109, 148	4 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	LEU	5.2
1	C	284	LEU	4.9
1	D	284	LEU	4.8
1	A	466	ILE	4.2
1	A	488	LEU	3.4
1	B	328	ASN	3.4
1	C	562	LEU	3.2
1	C	466	ILE	3.1
1	A	489	LEU	2.9
1	B	284	LEU	2.8
1	C	465	GLN	2.6
1	A	487	VAL	2.5
1	C	488	LEU	2.5
1	B	229	VAL	2.4
1	B	467	LYS	2.4
1	A	486	LYS	2.4
1	B	488	LEU	2.3
1	D	466	ILE	2.3
1	A	463	THR	2.3
1	B	469	LYS	2.3
1	A	590	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	388	ASP	2.2
1	B	466	ILE	2.2
1	C	464	GLY	2.2
1	A	598	TRP	2.2
1	B	489	LEU	2.2
1	A	115	MET	2.1
1	C	486	LYS	2.1
1	C	487	VAL	2.1
1	A	404	GLY	2.1
1	A	546	ALA	2.0
1	B	325	ILE	2.0
1	A	493	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(Å ²)	Q<0.9
3	MG	C	705	1/1	0.81	0.28	92,92,92,92	0
2	DGT	D	702	31/31	0.87	0.12	49,59,84,86	0
2	DGT	A	701	31/31	0.88	0.11	58,75,92,93	0
4	TTP	C	704	29/29	0.89	0.12	59,72,97,101	0
3	MG	A	702	1/1	0.90	0.08	81,81,81,81	0
2	DGT	B	701	31/31	0.92	0.10	53,57,77,81	0
3	MG	B	702	1/1	0.92	0.06	74,74,74,74	0
3	MG	D	703	1/1	0.96	0.05	65,65,65,65	0
2	DGT	A	703	31/31	0.97	0.06	45,47,56,59	0
2	DGT	B	703	31/31	0.97	0.05	46,47,55,55	0
2	DGT	B	704	31/31	0.97	0.06	42,43,45,45	0

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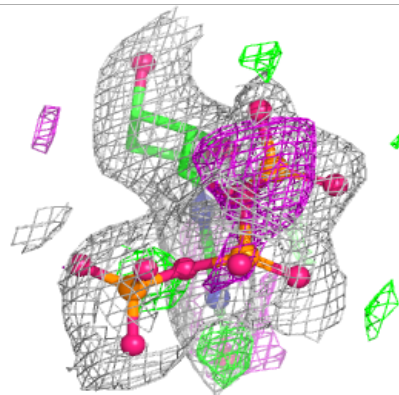
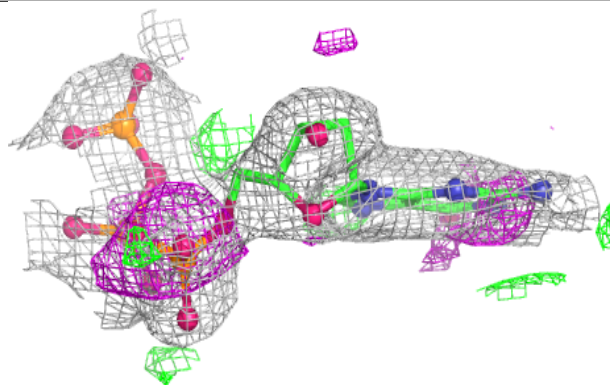
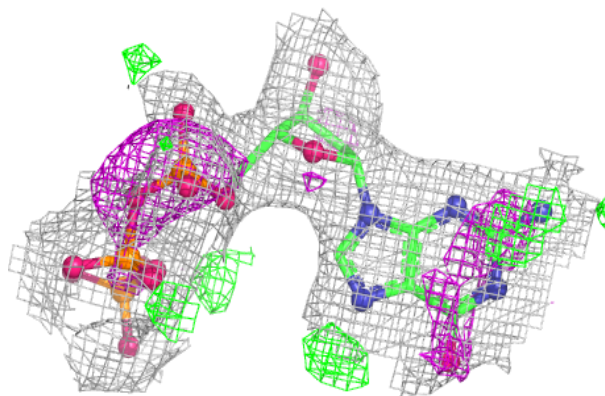
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DGT	C	701	31/31	0.97	0.06	44,46,53,53	0
2	DGT	A	704	31/31	0.97	0.06	47,49,54,55	0
2	DGT	D	704	31/31	0.98	0.05	44,45,47,47	0
2	DGT	D	701	31/31	0.98	0.05	41,42,45,46	0
2	DGT	C	706	31/31	0.98	0.04	49,50,58,60	0
3	MG	C	703	1/1	0.99	0.08	48,48,48,48	0
3	MG	A	706	1/1	0.99	0.07	45,45,45,45	0
3	MG	A	705	1/1	0.99	0.03	58,58,58,58	0
3	MG	C	702	1/1	0.99	0.06	50,50,50,50	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.

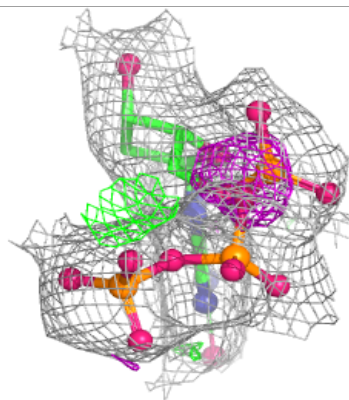
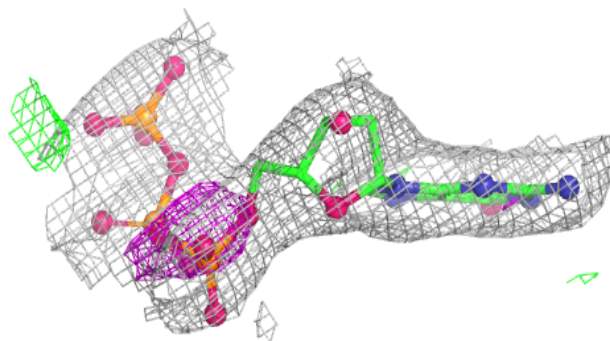
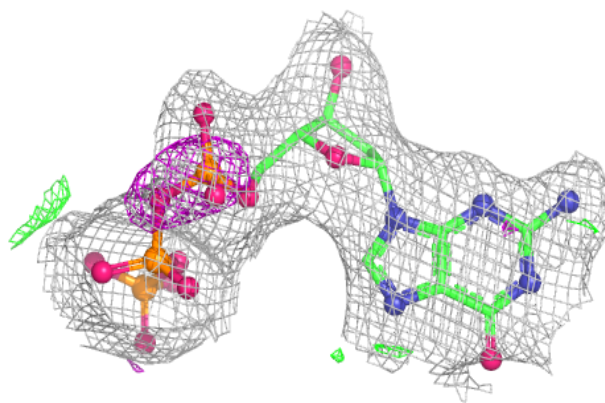
Electron density around DGT D 702:

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

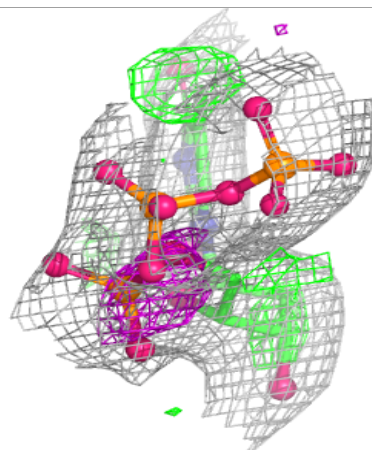
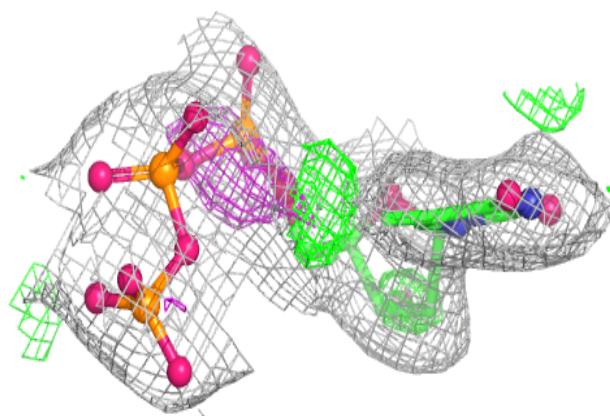
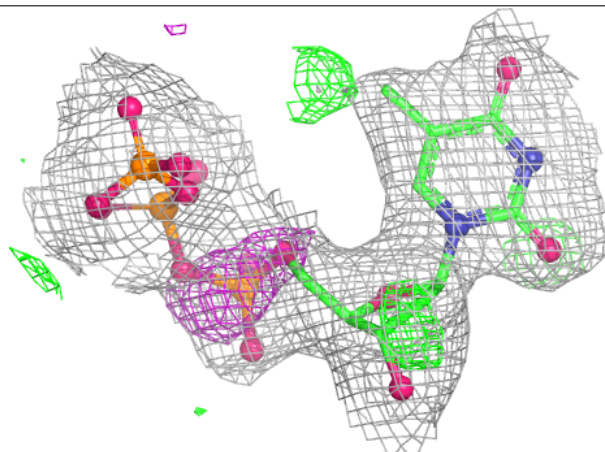


Electron density around DGT A 701:

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

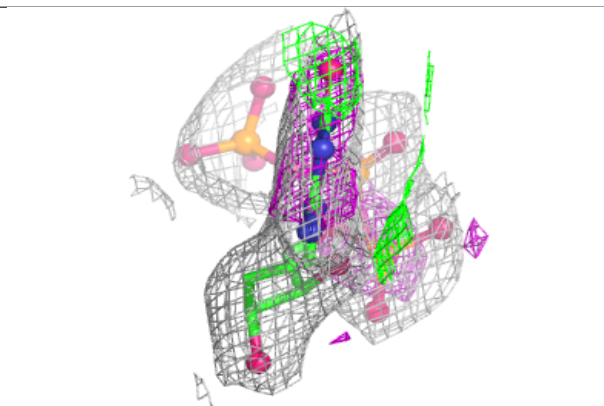
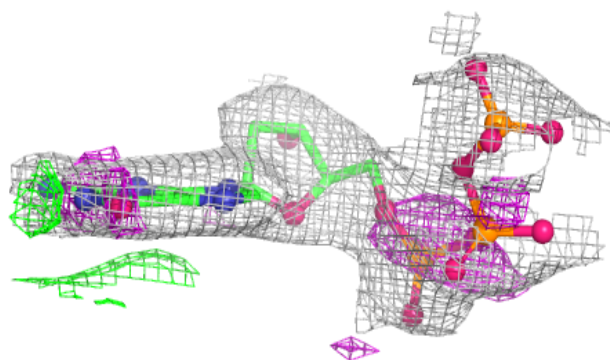
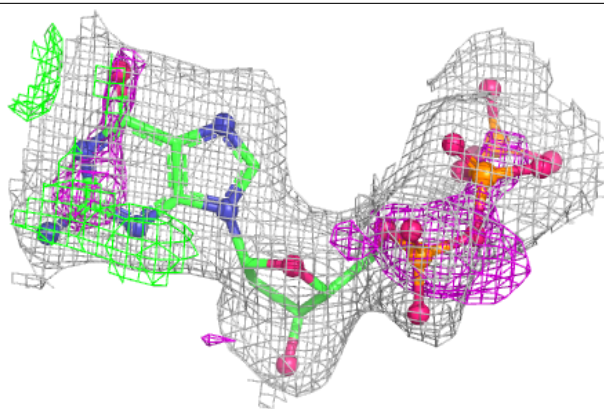
**Electron density around TTP C 704:**

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

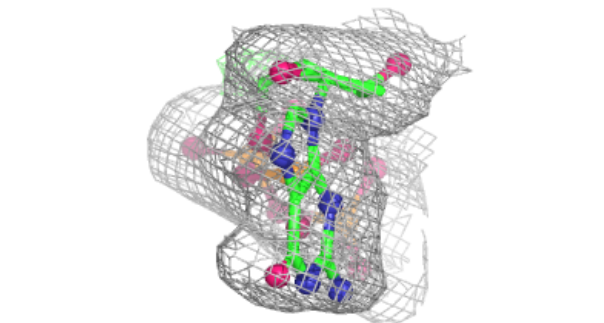
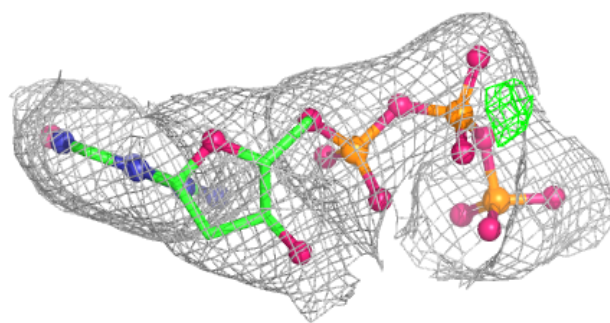
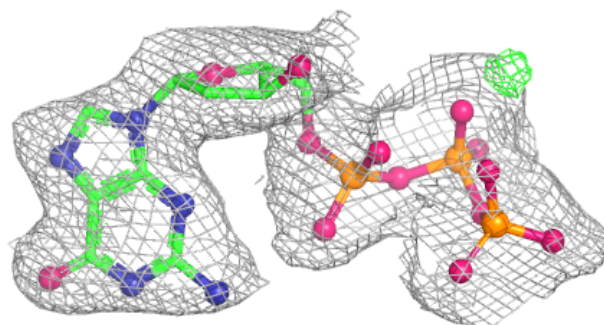


Electron density around DGT B 701:

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

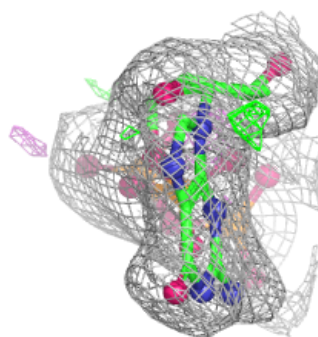
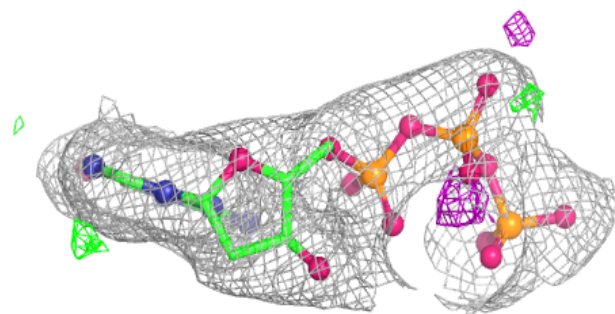
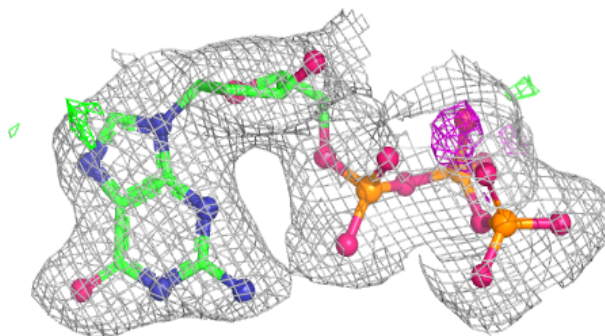
**Electron density around DGT A 703:**

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

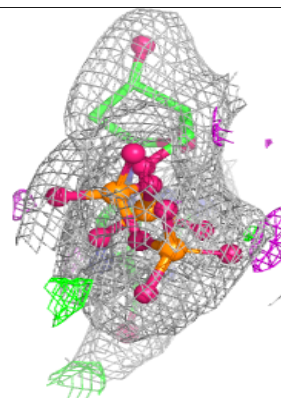
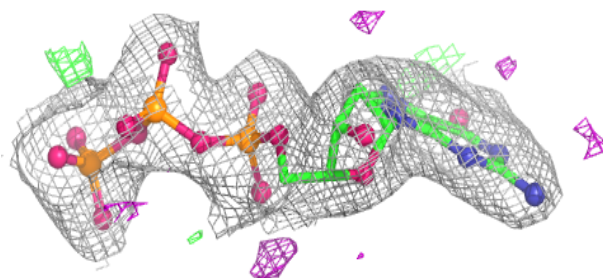
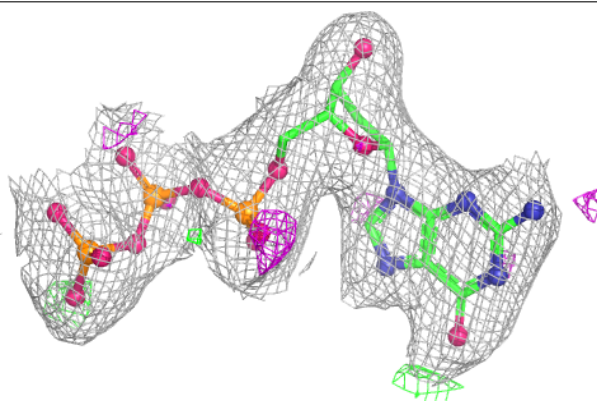


Electron density around DGT B 703:

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

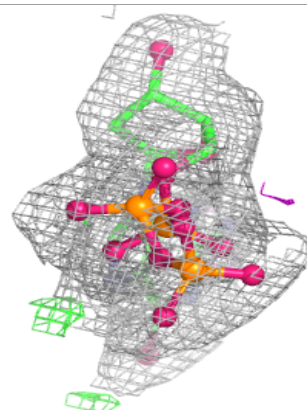
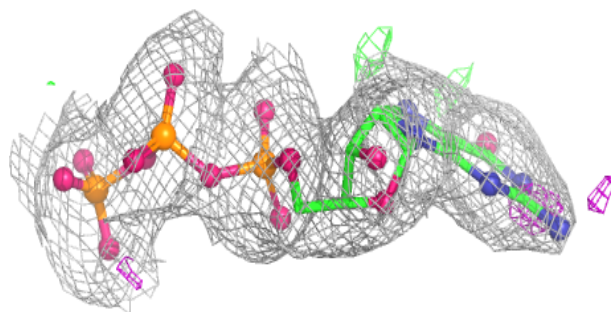
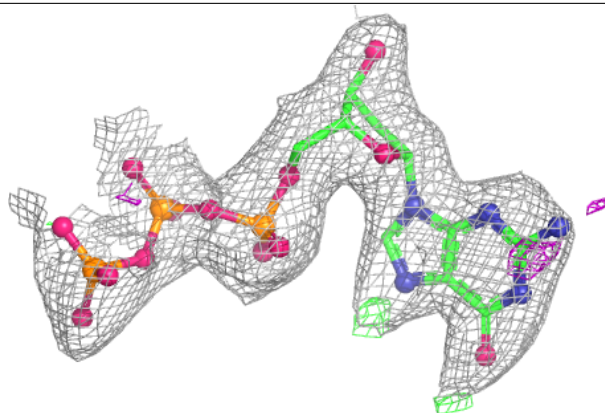
**Electron density around DGT B 704:**

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

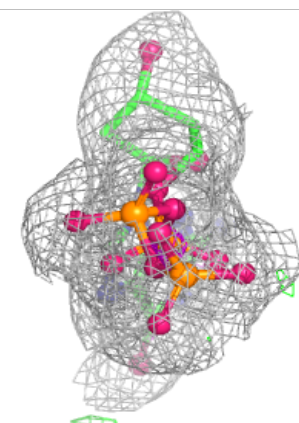
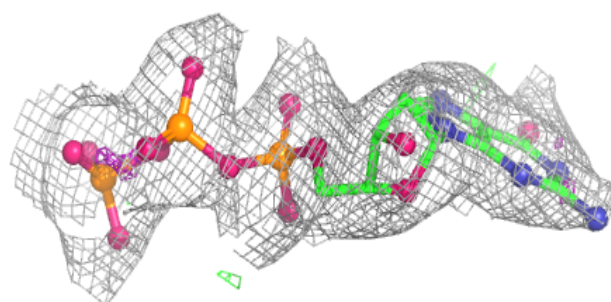
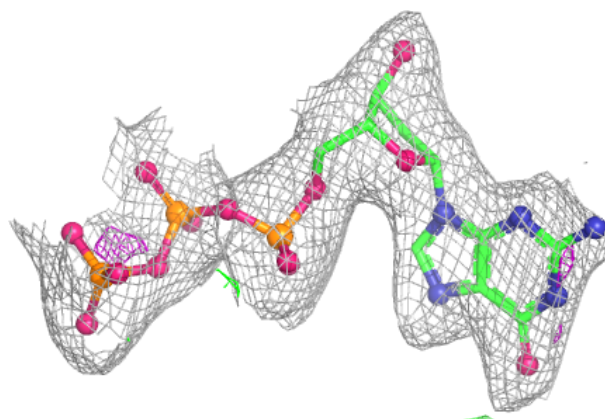


Electron density around DGT C 701:

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

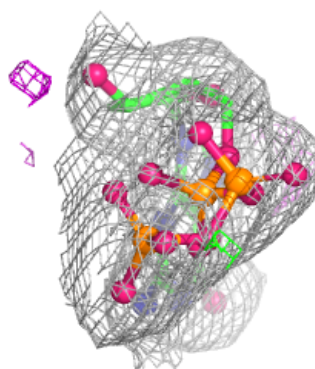
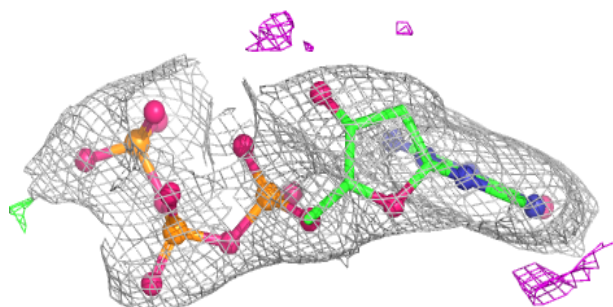
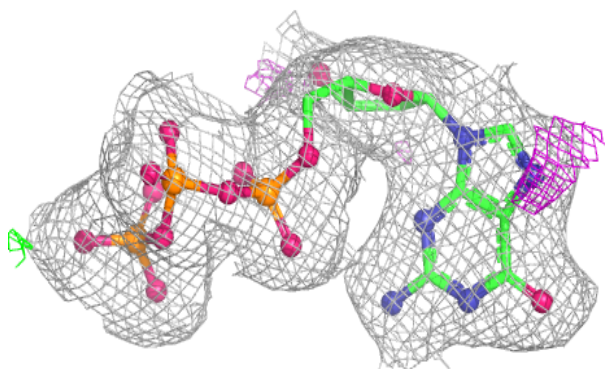
**Electron density around DGT A 704:**

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

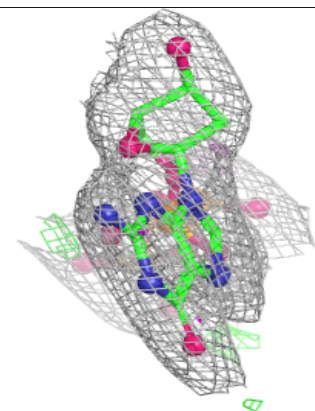
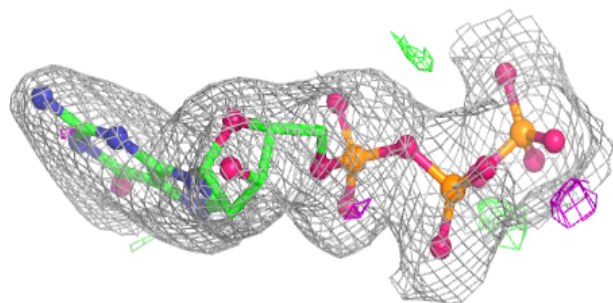
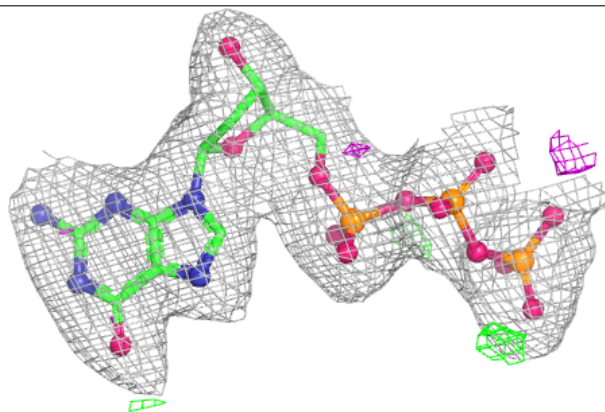


Electron density around DGT D 704:

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

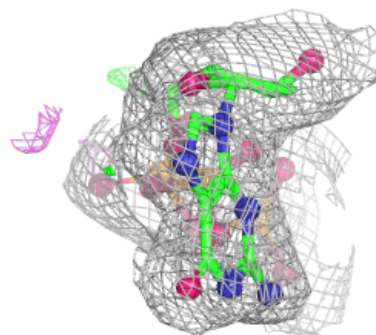
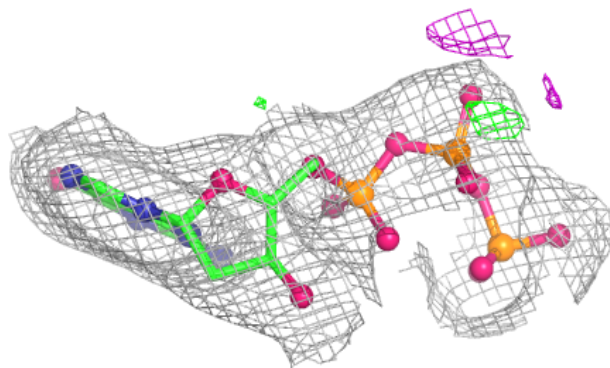
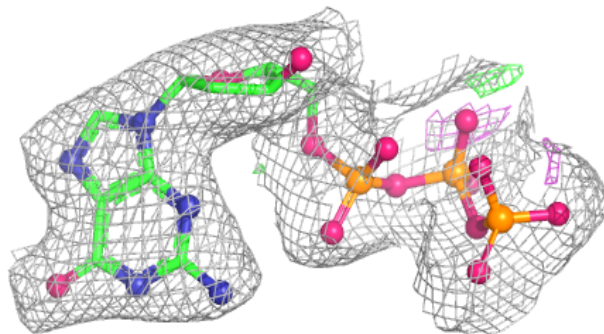
**Electron density around DGT D 701:**

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



Electron density around DGT C 706:

$2mF_o - DF_c$ (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.