



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:47 AM UTC

PDB ID : 4TNY / pdb_00004tny
Title : Structural basis of cellular dNTP regulation, SAMHD1-dGTP-dATP-dGTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.60 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

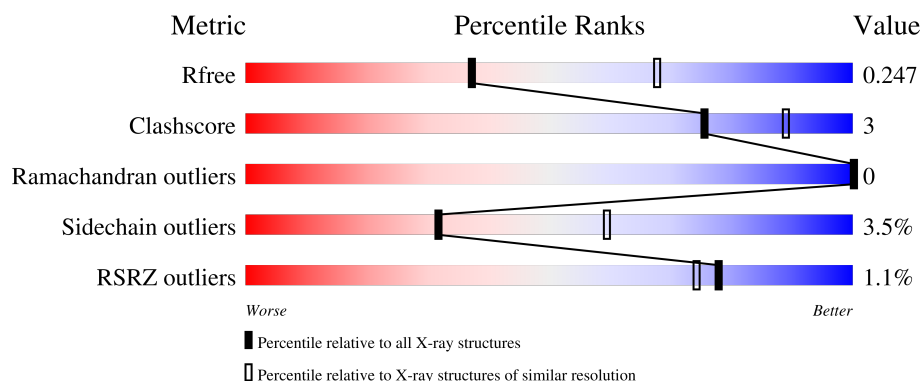
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	 85% 7% • 6%
1	B	514	 85% 7% • 6%
1	C	514	 84% 8% • 6%
1	D	514	 84% 8% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16275 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.

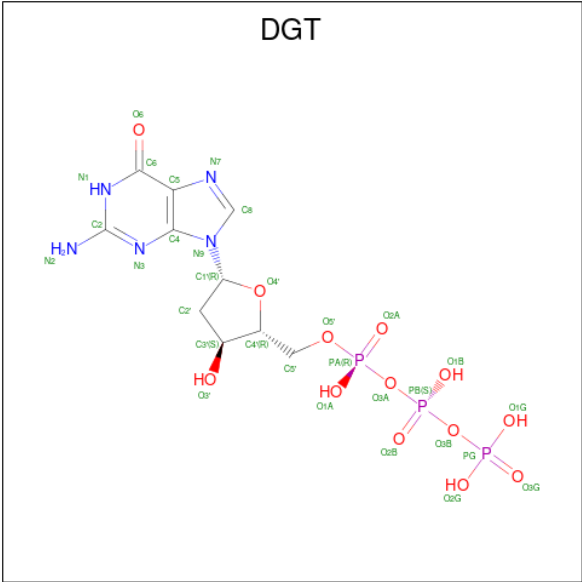
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	C	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	B	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	D	481	Total	C	N	O	S	0	4	0
			3966	2535	691	719	21			

There are 8 discrepancies between the modelled and reference sequences:

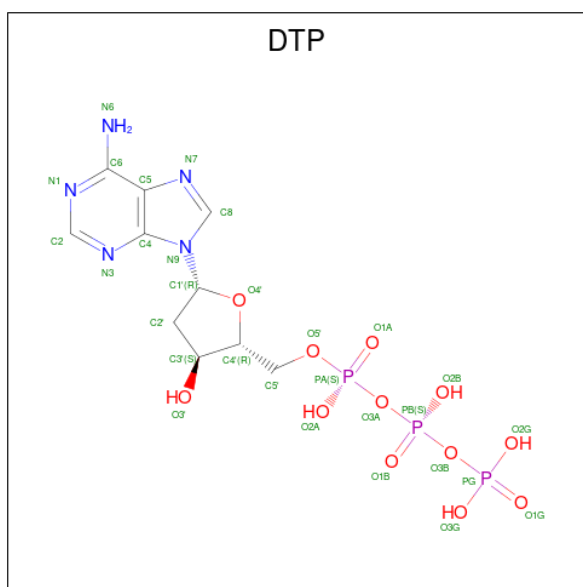
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	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	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	3	Total 3	O 3	0	0
5	B	1	Total 1	O 1	0	0
5	D	4	Total 4	O 4	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.

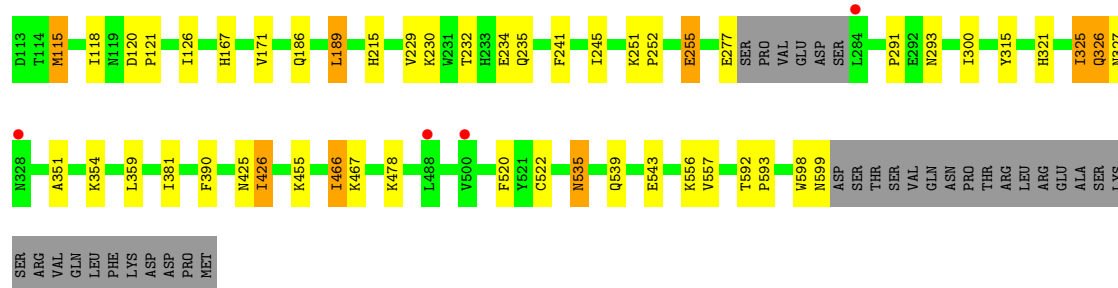
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A: 



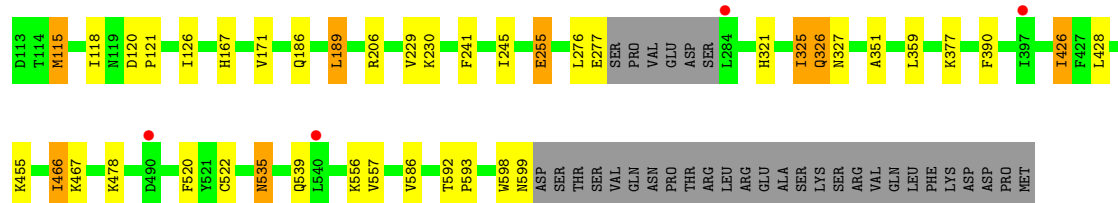
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C: 



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B: 



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.25Å 141.87Å 98.33Å 90.00° 116.38° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.60) 99.5 (50.00-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.214 , 0.244 0.220 , 0.247	Depositor DCC
R_{free} test set	3340 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16275	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, DTP, 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	0.89	0/4067	0.93	4/5490 (0.1%)
1	B	0.87	0/4067	0.92	4/5490 (0.1%)
1	C	0.87	0/4067	0.93	5/5490 (0.1%)
1	D	0.84	0/4059	0.92	4/5479 (0.1%)
All	All	0.87	0/16260	0.92	17/21949 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	ILE	N-CA-CB	6.81	118.98	110.47
1	C	126	ILE	CB-CA-C	-6.77	101.63	110.84
1	B	426	ILE	N-CA-CB	6.74	118.89	110.47
1	D	126	ILE	CB-CA-C	-6.62	101.84	110.84
1	D	426	ILE	N-CA-CB	6.28	118.32	110.47
1	A	426	ILE	N-CA-CB	6.22	118.24	110.47
1	A	126	ILE	CB-CA-C	-6.18	102.43	110.84
1	B	126	ILE	CB-CA-C	-6.17	102.44	110.84
1	B	255	GLU	N-CA-CB	5.58	118.33	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	GLU	N-CA-CB	5.55	118.28	110.12
1	A	255	GLU	N-CA-CB	5.36	117.99	110.12
1	C	255	GLU	N-CA-CB	5.27	117.86	110.12
1	B	325	ILE	CB-CA-C	5.19	118.49	110.50
1	C	325	ILE	CB-CA-C	5.16	118.45	110.50
1	A	325	ILE	CB-CA-C	5.15	118.43	110.50
1	D	325	ILE	CB-CA-C	5.13	118.41	110.50
1	C	300	ILE	N-CA-C	5.02	115.69	110.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Peptide
1	B	276	LEU	Peptide
1	D	276	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3974	0	3944	24	1
1	B	3974	0	3944	23	0
1	C	3974	0	3944	30	0
1	D	3966	0	3939	26	0
2	A	31	0	12	2	0
2	B	62	0	24	1	0
2	C	62	0	24	4	0
2	D	93	0	36	8	0
3	A	30	0	12	2	0
3	B	30	0	12	2	0
3	C	30	0	12	2	0
3	D	30	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	7	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	16275	0	15915	98	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LYS:NZ	3:D:703:DTP:O2B	2.09	0.85
1:A:535:ASN:OD1	1:A:535:ASN:N	2.21	0.71
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.32	0.68
1:B:535:ASN:OD1	1:B:535:ASN:N	2.22	0.66
1:C:535:ASN:OD1	1:C:535:ASN:N	2.21	0.66
2:D:704:DGT:PA	2:D:704:DGT:O3G	2.54	0.66
1:C:390:PHE:CE2	1:C:426:ILE:HD11	2.36	0.61
1:C:354:LYS:NZ	3:C:701:DTP:O1A	2.32	0.60
1:D:390:PHE:CE2	1:D:426:ILE:HD11	2.37	0.60
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.00	0.60
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.37	0.59
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.03	0.57
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.39	0.57
1:B:206:ARG:NH2	2:B:702:DGT:O2B	2.34	0.57
1:D:466:ILE:HD13	1:D:466:ILE:N	2.21	0.56
1:A:327:ASN:O	1:C:326:GLN:HG2	2.06	0.56
1:C:598:TRP:O	1:C:599:ASN:HB2	2.06	0.55
1:B:598:TRP:O	1:B:599:ASN:HB2	2.07	0.55
1:B:326:GLN:HG2	1:D:327:ASN:O	2.07	0.54
1:A:326:GLN:HG2	1:C:327:ASN:O	2.07	0.54
1:B:466:ILE:N	1:B:466:ILE:HD13	2.23	0.54
1:A:598:TRP:O	1:A:599:ASN:HB2	2.07	0.54
1:C:215:HIS:NE2	2:C:702:DGT:O2A	2.40	0.54
1:D:598:TRP:O	1:D:599:ASN:HB2	2.08	0.54
1:C:466:ILE:N	1:C:466:ILE:HD13	2.22	0.53
3:B:704:DTP:O2B	1:D:377:LYS:NZ	2.32	0.53
2:C:702:DGT:H4'	2:C:702:DGT:O1A	2.09	0.53
1:A:466:ILE:HD13	1:A:466:ILE:N	2.24	0.52
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.93	0.49
1:C:115:MET:SD	1:C:115:MET:C	2.96	0.49
1:B:115:MET:C	1:B:115:MET:SD	2.94	0.49
1:D:115:MET:C	1:D:115:MET:SD	2.96	0.49
1:A:115:MET:C	1:A:115:MET:SD	2.95	0.49
1:B:586:VAL:HG11	1:D:522[A]:CYS:SG	2.53	0.49
1:A:315:TYR:CD1	2:A:701:DGT:H3'	2.47	0.48
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.95	0.48
1:D:351:ALA:O	1:D:520:PHE:HA	2.13	0.48
1:D:598:TRP:O	1:D:599:ASN:CB	2.62	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.48
1:B:327:ASN:O	1:D:326:GLN:HG2	2.13	0.48
1:C:351:ALA:O	1:C:520:PHE:HA	2.14	0.48
1:A:598:TRP:O	1:A:599:ASN:CB	2.61	0.48
1:D:241:PHE:O	1:D:245:ILE:HG12	2.14	0.48
2:D:704:DGT:PG	2:D:704:DGT:O1A	2.72	0.47
1:C:241:PHE:O	1:C:245:ILE:HG12	2.14	0.47
1:C:598:TRP:O	1:C:599:ASN:CB	2.61	0.47
1:B:241:PHE:O	1:B:245:ILE:HG12	2.14	0.47
1:B:598:TRP:O	1:B:599:ASN:CB	2.61	0.47
1:A:354:LYS:NZ	3:A:702:DTP:O1A	2.42	0.47
1:A:315:TYR:CE2	2:A:701:DGT:H5'	2.48	0.47
1:A:241:PHE:O	1:A:245:ILE:HG12	2.14	0.47
1:D:167:HIS:O	1:D:171:VAL:HG23	2.15	0.47
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.14	0.47
1:A:167:HIS:O	1:A:171:VAL:HG23	2.16	0.46
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.46
1:C:167:HIS:O	1:C:171:VAL:HG23	2.16	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.46
1:B:167:HIS:O	1:B:171:VAL:HG23	2.15	0.46
1:D:156:VAL:O	2:D:705:DGT:H8	2.16	0.46
1:A:543:GLU:HG2	1:C:543:GLU:HG2	1.98	0.45
1:B:592:THR:N	1:B:593:PRO:CD	2.80	0.45
1:B:229:VAL:HG12	1:B:230:LYS:N	2.32	0.45
1:C:229:VAL:HG12	1:C:230:LYS:N	2.32	0.45
1:C:592:THR:N	1:C:593:PRO:CD	2.80	0.45
1:D:592:THR:N	1:D:593:PRO:CD	2.80	0.44
2:D:705:DGT:H3'	2:D:705:DGT:PA	2.57	0.44
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.89	0.44
1:A:229:VAL:HG12	1:A:230:LYS:N	2.33	0.44
1:D:229:VAL:HG12	1:D:230:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:701:DTP:O1B	2:D:702:DGT:H5'A	2.18	0.44
1:D:186:GLN:HB2	1:D:189:LEU:HD22	2.00	0.43
1:D:455:LYS:HG2	1:D:557:VAL:HG12	2.00	0.43
1:D:368:SER:HA	1:D:371:ARG:HD2	1.99	0.43
1:C:455:LYS:HG2	1:C:557:VAL:HG12	2.00	0.43
2:D:704:DGT:O1A	2:D:704:DGT:O1G	2.36	0.43
1:B:455:LYS:HG2	1:B:557:VAL:HG12	2.01	0.43
1:B:230:LYS:HA	1:B:230:LYS:HD2	1.88	0.43
1:C:230:LYS:HD2	1:C:230:LYS:HA	1.85	0.43
1:B:186:GLN:HB2	1:B:189:LEU:HD22	2.00	0.42
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.59	0.42
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.19	0.42
1:C:186:GLN:HB2	1:C:189:LEU:HD22	2.01	0.42
2:D:705:DGT:N3	2:D:705:DGT:H2'A	2.34	0.42
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.00	0.42
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.20	0.42
1:C:425:ASN:HB2	1:B:428:LEU:HD13	2.01	0.42
1:C:390:PHE:CE2	1:C:426:ILE:CD1	3.03	0.41
2:C:702:DGT:O1B	2:C:702:DGT:O3G	2.36	0.41
1:A:352:ARG:HH22	3:A:702:DTP:PG	2.44	0.41
3:B:704:DTP:H2'1	1:D:157:PHE:CE2	2.56	0.41
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.21	0.41
1:C:315:TYR:CE2	2:C:702:DGT:H5'	2.56	0.41
1:D:375:GLN:NE2	2:D:704:DGT:O6	2.45	0.41
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.09	0.40
1:D:354:LYS:NZ	3:D:703:DTP:O1A	2.53	0.40
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.03	0.40
1:C:232:THR:HB	1:C:234:GLU:OE1	2.21	0.40

All (1) 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:490:ASP:OD1	1:A:527:ASN:O[2_545]	2.17	0.03

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	482/514 (94%)	476 (99%)	6 (1%)	0	100	100
1	B	482/514 (94%)	477 (99%)	5 (1%)	0	100	100
1	C	482/514 (94%)	475 (98%)	7 (2%)	0	100	100
1	D	481/514 (94%)	476 (99%)	5 (1%)	0	100	100
All	All	1927/2056 (94%)	1904 (99%)	23 (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	432/459 (94%)	417 (96%)	15 (4%)	32	59
1	B	432/459 (94%)	418 (97%)	14 (3%)	34	62
1	C	432/459 (94%)	417 (96%)	15 (4%)	32	59
1	D	431/459 (94%)	416 (96%)	15 (4%)	32	59
All	All	1727/1836 (94%)	1668 (97%)	59 (3%)	32	60

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

Mol	Chain	Res	Type
1	A	115	MET
1	A	118	ILE

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	255	GLU
1	A	277	GLU
1	A	325	ILE
1	A	326	GLN
1	A	359	LEU
1	A	466	ILE
1	A	467	LYS
1	A	478	LYS
1	A	535	ASN
1	A	539	GLN
1	A	556	LYS
1	A	594	GLN
1	C	115	MET
1	C	118	ILE
1	C	189	LEU
1	C	235	GLN
1	C	255	GLU
1	C	277	GLU
1	C	325	ILE
1	C	326	GLN
1	C	359	LEU
1	C	466	ILE
1	C	467	LYS
1	C	478	LYS
1	C	535	ASN
1	C	539	GLN
1	C	556	LYS
1	B	115	MET
1	B	118	ILE
1	B	189	LEU
1	B	255	GLU
1	B	277	GLU
1	B	325	ILE
1	B	326	GLN
1	B	359	LEU
1	B	466	ILE
1	B	467	LYS
1	B	478	LYS
1	B	535	ASN
1	B	539	GLN
1	B	556	LYS

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Mol	Chain	Res	Type
1	D	115	MET
1	D	118	ILE
1	D	189	LEU
1	D	255	GLU
1	D	277	GLU
1	D	284	LEU
1	D	325	ILE
1	D	326	GLN
1	D	359	LEU
1	D	371	ARG
1	D	466	ILE
1	D	467	LYS
1	D	478	LYS
1	D	539	GLN
1	D	556	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	210	HIS
1	A	243	HIS
1	A	364	HIS
1	A	425	ASN
1	C	149	GLN
1	C	200	GLN
1	C	243	HIS
1	C	364	HIS
1	C	425	ASN
1	B	163	ASN
1	B	200	GLN
1	B	215	HIS
1	B	243	HIS
1	B	364	HIS
1	B	425	ASN
1	D	200	GLN
1	D	233	HIS
1	D	364	HIS
1	D	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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$
2	DGT	B	702	-	32,33,33	1.51	5 (15%)	48,52,52	1.74	9 (18%)
2	DGT	C	703	4	32,33,33	1.41	6 (18%)	48,52,52	1.58	8 (16%)
3	DTP	C	701	4	31,32,32	1.40	4 (12%)	46,50,50	2.30	13 (28%)
2	DGT	A	701	-	32,33,33	1.41	6 (18%)	48,52,52	1.58	9 (18%)
3	DTP	B	704	4	31,32,32	1.46	6 (19%)	46,50,50	2.15	13 (28%)
2	DGT	D	704	-	32,33,33	1.31	3 (9%)	48,52,52	1.88	8 (16%)
3	DTP	A	702	4	31,32,32	1.35	6 (19%)	46,50,50	2.35	18 (39%)
2	DGT	B	703	4	32,33,33	1.44	5 (15%)	48,52,52	1.84	7 (14%)
2	DGT	C	702	-	32,33,33	1.32	3 (9%)	48,52,52	1.73	6 (12%)
2	DGT	D	705	4	32,33,33	1.40	5 (15%)	48,52,52	1.66	7 (14%)
2	DGT	D	702	4	32,33,33	1.30	4 (12%)	48,52,52	1.78	12 (25%)
3	DTP	D	703	4	31,32,32	1.65	7 (22%)	46,50,50	2.13	13 (28%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	B	702	-	-	6/22/34/34	0/3/3/3
2	DGT	C	703	4	-	8/22/34/34	0/3/3/3
3	DTP	C	701	4	-	8/22/34/34	0/3/3/3
2	DGT	A	701	-	-	3/22/34/34	0/3/3/3
3	DTP	B	704	4	-	7/22/34/34	0/3/3/3
2	DGT	D	704	-	-	5/22/34/34	0/3/3/3
3	DTP	A	702	4	-	8/22/34/34	0/3/3/3
2	DGT	B	703	4	-	5/22/34/34	0/3/3/3
2	DGT	C	702	-	-	6/22/34/34	0/3/3/3
2	DGT	D	705	4	-	6/22/34/34	0/3/3/3
2	DGT	D	702	4	-	9/22/34/34	0/3/3/3
3	DTP	D	703	4	-	2/22/34/34	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	702	DGT	C6-N1	-4.22	1.31	1.38
2	B	703	DGT	C6-N1	-4.07	1.31	1.38
3	B	704	DTP	C5-C4	4.06	1.46	1.39
3	D	703	DTP	PA-O3A	4.00	1.63	1.59
3	A	702	DTP	C5-C4	3.83	1.45	1.39
2	A	701	DGT	C5-C4	3.83	1.49	1.38
2	C	703	DGT	C5-N7	-3.80	1.31	1.39
2	B	702	DGT	C5-C4	3.70	1.49	1.38
2	B	702	DGT	PB-O3B	3.67	1.63	1.59
3	D	703	DTP	C5-C4	3.56	1.45	1.39
2	D	705	DGT	C5-C4	3.52	1.48	1.38
2	B	703	DGT	C5-C4	3.46	1.48	1.38
2	C	702	DGT	C5-C4	3.40	1.48	1.38
2	D	704	DGT	C5-C4	3.40	1.48	1.38
2	D	705	DGT	PB-O3B	3.39	1.63	1.59
3	C	701	DTP	C5-C4	3.39	1.45	1.39
3	D	703	DTP	PB-O3A	3.32	1.63	1.59
3	B	704	DTP	C5-C6	3.25	1.50	1.41
3	C	701	DTP	C8-N9	-3.18	1.32	1.37
2	D	704	DGT	PB-O3B	3.14	1.62	1.59
2	C	703	DGT	C5-C4	3.03	1.47	1.38
2	D	705	DGT	C5-N7	-3.03	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	DTP	C5-N7	-2.96	1.33	1.39
2	C	703	DGT	C4-N9	-2.79	1.31	1.38
2	D	702	DGT	C5-N7	-2.78	1.33	1.39
2	B	703	DGT	C5-N7	-2.76	1.33	1.39
2	A	701	DGT	O4'-C4'	-2.73	1.38	1.45
2	B	702	DGT	PA-O3A	2.72	1.62	1.59
3	C	701	DTP	C5-N7	-2.71	1.34	1.39
2	D	705	DGT	C4-N9	-2.69	1.31	1.38
2	D	705	DGT	C6-N1	-2.61	1.34	1.38
3	D	703	DTP	C8-N9	-2.60	1.33	1.37
3	B	704	DTP	PB-O3B	2.59	1.62	1.59
2	C	703	DGT	C6-N1	-2.57	1.34	1.38
2	A	701	DGT	PA-O3A	2.46	1.62	1.59
3	D	703	DTP	O4'-C4'	-2.46	1.39	1.45
3	C	701	DTP	C5-C6	2.40	1.47	1.41
2	C	702	DGT	C6-N1	-2.40	1.34	1.38
2	C	703	DGT	PB-O3A	2.37	1.62	1.59
3	A	702	DTP	C8-N9	-2.31	1.33	1.37
3	D	703	DTP	C5-C6	2.31	1.47	1.41
2	D	702	DGT	C5-C4	2.28	1.45	1.38
2	C	702	DGT	PB-O3B	2.26	1.61	1.59
2	A	701	DGT	PB-O3A	2.24	1.61	1.59
2	A	701	DGT	C4-N9	-2.23	1.32	1.38
2	C	703	DGT	PA-O3A	2.22	1.61	1.59
3	B	704	DTP	C5-N7	-2.22	1.35	1.39
3	B	704	DTP	C8-N9	-2.20	1.33	1.37
3	A	702	DTP	C5-N7	-2.16	1.35	1.39
2	D	702	DGT	C4-N9	-2.15	1.32	1.38
2	B	702	DGT	C8-N7	2.13	1.38	1.32
2	B	703	DGT	PB-O3B	2.13	1.61	1.59
3	A	702	DTP	C8-N7	2.13	1.35	1.31
2	B	703	DGT	C4-N9	-2.08	1.32	1.38
3	A	702	DTP	PB-O3B	2.02	1.61	1.59
2	A	701	DGT	C5-N7	-2.01	1.35	1.39
2	D	704	DGT	C6-N1	-2.01	1.35	1.38
3	A	702	DTP	C5-C6	2.01	1.46	1.41
2	B	702	DGT	C5-N7	-2.01	1.35	1.39
3	B	704	DTP	C4-N9	-2.01	1.33	1.37

All (123) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	703	DGT	C5-C4-N3	-6.79	117.59	128.39
3	C	701	DTP	C5-C4-N3	-6.52	117.74	126.72
3	D	703	DTP	C5-C4-N3	-6.33	118.01	126.72
2	C	702	DGT	C5-C4-N3	-5.87	119.05	128.39
2	D	702	DGT	C5-C4-N3	-5.86	119.07	128.39
2	D	704	DGT	C5-C4-N3	-5.80	119.15	128.39
3	A	702	DTP	N3-C2-N1	-5.69	119.97	128.58
3	C	701	DTP	N3-C4-N9	5.59	136.67	127.17
3	A	702	DTP	C4-N9-C8	5.44	111.45	105.74
2	D	705	DGT	C5-C4-N3	-5.37	119.85	128.39
3	D	703	DTP	N3-C4-N9	5.23	136.06	127.17
2	C	703	DGT	C5-C4-N3	-5.22	120.08	128.39
2	B	702	DGT	C5-C4-N3	-5.08	120.31	128.39
3	B	704	DTP	N3-C2-N1	-5.02	120.98	128.58
2	D	704	DGT	C2-N3-C4	5.02	120.95	112.30
2	D	705	DGT	C2-N3-C4	4.87	120.69	112.30
2	B	703	DGT	C2-N3-C4	4.76	120.49	112.30
2	B	702	DGT	C2-N3-C4	4.73	120.44	112.30
3	B	704	DTP	C4-C5-N7	-4.66	105.25	110.58
2	C	702	DGT	C2-N3-C4	4.60	120.22	112.30
3	C	701	DTP	C4-C5-N7	-4.58	105.35	110.58
2	D	702	DGT	C2-N3-C4	4.45	119.96	112.30
3	C	701	DTP	C4-N9-C8	4.44	110.40	105.74
2	A	701	DGT	C5-C4-N3	-4.44	121.32	128.39
2	B	703	DGT	N9-C4-N3	4.43	134.82	125.95
3	A	702	DTP	C2-N1-C6	4.40	125.97	118.73
3	B	704	DTP	C5-C4-N3	-4.27	120.83	126.72
2	D	704	DGT	C6-C5-N7	4.24	138.00	130.29
2	C	702	DGT	N9-C4-N3	4.17	134.29	125.95
2	D	702	DGT	N9-C4-N3	4.14	134.24	125.95
3	C	701	DTP	C5-N7-C8	4.09	109.89	103.45
2	C	703	DGT	N9-C4-N3	4.09	134.13	125.95
3	B	704	DTP	C2-N1-C6	4.05	125.38	118.73
2	B	702	DGT	C6-C5-N7	4.02	137.60	130.29
3	D	703	DTP	C2-N3-C4	3.97	121.53	111.83
3	B	704	DTP	C2-N3-C4	3.90	121.35	111.83
3	B	704	DTP	C4-N9-C8	3.90	109.83	105.74
3	A	702	DTP	N3-C4-N9	3.86	133.74	127.17
2	D	704	DGT	N9-C4-N3	3.86	133.67	125.95
2	C	703	DGT	C2-N3-C4	3.80	118.85	112.30
3	A	702	DTP	N9-C8-N7	-3.80	108.54	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	DGT	C2-N3-C4	3.80	118.84	112.30
3	B	704	DTP	C6-C5-N7	3.76	139.34	132.09
2	D	705	DGT	N9-C4-N3	3.76	133.47	125.95
3	D	703	DTP	N3-C2-N1	-3.74	122.93	128.58
3	D	703	DTP	O3B-PG-O1G	-3.73	91.42	111.04
3	B	704	DTP	C5-N7-C8	3.72	109.30	103.45
3	A	702	DTP	C5-C4-N3	-3.71	121.61	126.72
3	D	703	DTP	C4-C5-N7	-3.69	106.36	110.58
3	C	701	DTP	C2-N3-C4	3.68	120.83	111.83
3	C	701	DTP	O5'-PA-O1A	-3.66	94.45	108.94
3	C	701	DTP	N9-C8-N7	-3.63	108.79	113.94
3	A	702	DTP	C2-N3-C4	3.62	120.68	111.83
2	C	702	DGT	C6-C5-N7	3.56	136.76	130.29
3	A	702	DTP	O5'-PA-O1A	-3.39	95.50	108.94
2	B	702	DGT	O4'-C1'-N9	3.38	113.87	107.86
2	A	701	DGT	C6-C5-N7	3.35	136.39	130.29
3	A	702	DTP	C4-C5-N7	-3.35	106.75	110.58
3	B	704	DTP	N9-C8-N7	-3.32	109.23	113.94
3	A	702	DTP	C6-C5-N7	3.31	138.47	132.09
3	B	704	DTP	N3-C4-N9	3.30	132.78	127.17
3	A	702	DTP	C5-N7-C8	3.28	108.61	103.45
3	D	703	DTP	C4-N9-C8	3.27	109.17	105.74
2	D	705	DGT	C6-C5-N7	3.24	136.19	130.29
3	D	703	DTP	C5-N7-C8	3.21	108.49	103.45
2	A	701	DGT	N9-C4-N3	3.15	132.26	125.95
3	C	701	DTP	N3-C2-N1	-3.08	123.92	128.58
2	D	704	DGT	C4-C5-N7	-3.01	105.90	110.67
2	B	702	DGT	N9-C4-N3	2.98	131.90	125.95
2	B	703	DGT	C4-C5-N7	-2.91	106.06	110.67
2	B	703	DGT	C6-C5-N7	2.87	135.51	130.29
2	C	703	DGT	O6-C6-C5	-2.85	119.02	126.53
3	D	703	DTP	C2'-C3'-C4'	2.80	108.47	102.80
2	D	702	DGT	C6-C5-N7	2.77	135.33	130.29
2	C	702	DGT	C4-C5-N7	-2.76	106.30	110.67
3	D	703	DTP	N9-C8-N7	-2.75	110.03	113.94
3	A	702	DTP	O3B-PG-O1G	-2.74	96.64	111.04
3	A	702	DTP	O2A-PA-O3A	2.71	114.59	107.27
3	B	704	DTP	O5'-PA-O1A	-2.70	98.22	108.94
2	D	704	DGT	O4'-C1'-N9	2.69	112.64	107.86
3	A	702	DTP	O3G-PG-O3B	2.66	113.55	104.64
2	B	703	DGT	O1B-PB-O3B	2.63	114.38	107.27
2	B	702	DGT	C4-C5-N7	-2.59	106.57	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	DGT	O1B-PB-O3A	2.58	114.24	107.27
3	A	702	DTP	O4'-C1'-N9	-2.57	103.35	107.96
2	D	705	DGT	O3A-PB-O2B	-2.54	103.07	110.70
3	C	701	DTP	O2A-PA-O3A	2.54	114.13	107.27
3	A	702	DTP	O2G-PG-O1G	2.48	120.49	110.83
3	D	703	DTP	O3G-PG-O1G	2.47	120.47	110.83
3	D	703	DTP	O2A-PA-O3A	2.41	113.78	107.27
3	D	703	DTP	O2B-PB-O1B	2.40	123.61	112.44
2	D	702	DGT	O3A-PB-O2B	-2.39	103.50	110.70
3	B	704	DTP	O2A-PA-O1A	2.39	123.56	112.44
2	D	705	DGT	C5-C6-N1	2.36	119.26	113.25
2	B	702	DGT	N2-C2-N1	2.32	121.65	116.76
2	A	701	DGT	O6-C6-C5	-2.31	120.43	126.53
3	A	702	DTP	O2A-PA-O1A	2.28	123.03	112.44
3	A	702	DTP	O3A-PA-O1A	-2.27	103.87	110.70
2	C	703	DGT	O3B-PG-O3G	-2.27	99.11	111.04
2	C	703	DGT	C6-C5-N7	2.26	134.40	130.29
2	D	702	DGT	O3B-PG-O3G	-2.25	99.20	111.04
2	D	704	DGT	C5-C6-N1	2.25	118.97	113.25
3	C	701	DTP	O3G-PG-O1G	2.24	119.56	110.83
2	D	702	DGT	O1A-PA-O2A	2.23	122.83	112.44
2	A	701	DGT	O4'-C1'-N9	2.23	111.82	107.86
2	A	701	DGT	N2-C2-N3	-2.21	115.36	119.67
2	A	701	DGT	O2G-PG-O1G	2.20	116.07	107.80
2	A	701	DGT	C4-C5-N7	-2.18	107.21	110.67
2	C	702	DGT	O4'-C1'-N9	2.18	111.73	107.86
3	C	701	DTP	O3'-C3'-C4'	-2.16	101.88	110.07
3	C	701	DTP	C6-C5-N7	2.16	136.25	132.09
2	D	702	DGT	O1G-PG-O3B	-2.12	97.52	104.64
2	D	702	DGT	C5-C6-N1	2.11	118.62	113.25
2	C	703	DGT	C5-C6-N1	2.09	118.58	113.25
2	D	702	DGT	O1G-PG-O3G	2.09	118.98	110.83
2	D	705	DGT	C6-C5-C4	-2.09	115.69	118.83
2	D	702	DGT	C4-C5-N7	-2.09	107.36	110.67
2	B	703	DGT	O6-C6-N1	-2.04	116.28	120.11
2	D	704	DGT	C8-N7-C5	2.04	107.89	104.26
2	B	702	DGT	N2-C2-N3	-2.03	115.70	119.67
2	B	702	DGT	O2G-PG-O3G	2.03	118.75	110.83
2	C	703	DGT	O3B-PB-O2B	-2.01	104.66	110.70
3	B	704	DTP	O3B-PG-O1G	-2.00	100.51	111.04

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	702	DGT	PB-O3B-PG-O2G
2	C	702	DGT	C5'-O5'-PA-O3A
2	C	702	DGT	C5'-O5'-PA-O1A
2	C	702	DGT	C4'-C5'-O5'-PA
2	C	703	DGT	PB-O3B-PG-O2G
2	B	702	DGT	C5'-O5'-PA-O3A
2	B	702	DGT	C5'-O5'-PA-O1A
2	D	702	DGT	PB-O3B-PG-O1G
2	D	702	DGT	PB-O3B-PG-O2G
2	D	704	DGT	C5'-O5'-PA-O3A
2	D	704	DGT	C5'-O5'-PA-O1A
2	D	705	DGT	C5'-O5'-PA-O2A
3	A	702	DTP	PB-O3B-PG-O3G
3	A	702	DTP	C5'-O5'-PA-O1A
3	A	702	DTP	C5'-O5'-PA-O2A
3	A	702	DTP	O4'-C4'-C5'-O5'
3	C	701	DTP	PB-O3B-PG-O3G
3	C	701	DTP	C5'-O5'-PA-O1A
3	C	701	DTP	C5'-O5'-PA-O2A
3	C	701	DTP	C5'-O5'-PA-O3A
3	C	701	DTP	O4'-C4'-C5'-O5'
3	B	704	DTP	PB-O3B-PG-O2G
3	B	704	DTP	PB-O3B-PG-O3G
3	B	704	DTP	C5'-O5'-PA-O1A
3	B	704	DTP	C5'-O5'-PA-O2A
3	B	704	DTP	O4'-C4'-C5'-O5'
3	B	704	DTP	C3'-C4'-C5'-O5'
3	D	703	DTP	PB-O3B-PG-O3G
3	A	702	DTP	C3'-C4'-C5'-O5'
3	C	701	DTP	C3'-C4'-C5'-O5'
2	B	702	DGT	C3'-C4'-C5'-O5'
2	A	701	DGT	C4'-C5'-O5'-PA
2	C	703	DGT	PG-O3B-PB-O2B
2	D	702	DGT	PG-O3B-PB-O2B
2	D	705	DGT	PG-O3B-PB-O2B
2	A	701	DGT	PB-O3A-PA-O5'
2	C	702	DGT	PB-O3A-PA-O5'
2	D	705	DGT	C2'-C1'-N9-C4
2	B	702	DGT	O4'-C4'-C5'-O5'
2	D	704	DGT	C3'-C4'-C5'-O5'
2	C	702	DGT	C5'-O5'-PA-O2A
2	B	703	DGT	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
2	D	704	DGT	C5'-O5'-PA-O2A
2	D	705	DGT	C2'-C1'-N9-C8
3	A	702	DTP	C5'-O5'-PA-O3A
3	B	704	DTP	C5'-O5'-PA-O3A
2	B	703	DGT	C4'-C5'-O5'-PA
2	D	705	DGT	C4'-C5'-O5'-PA
2	B	703	DGT	PG-O3B-PB-O1B
2	D	702	DGT	PG-O3B-PB-O1B
2	B	703	DGT	C2'-C1'-N9-C4
2	D	702	DGT	C2'-C1'-N9-C4
2	C	703	DGT	C4'-C5'-O5'-PA
2	D	704	DGT	O4'-C4'-C5'-O5'
2	D	702	DGT	C4'-C5'-O5'-PA
2	C	703	DGT	PB-O3B-PG-O1G
3	A	702	DTP	PB-O3B-PG-O2G
3	C	701	DTP	PB-O3B-PG-O2G
3	D	703	DTP	PB-O3B-PG-O2G
2	B	702	DGT	C4'-C5'-O5'-PA
2	D	702	DGT	C2'-C1'-N9-C8
2	A	701	DGT	PG-O3B-PB-O1B
2	C	703	DGT	PB-O3A-PA-O2A
2	D	705	DGT	PG-O3B-PB-O1B
3	A	702	DTP	PG-O3B-PB-O2B
3	C	701	DTP	PG-O3B-PB-O2B
2	C	703	DGT	PB-O3B-PG-O3G
2	D	702	DGT	PB-O3B-PG-O3G
2	C	703	DGT	PG-O3B-PB-O1B
2	C	703	DGT	PB-O3A-PA-O1A
2	B	702	DGT	PB-O3A-PA-O1A
2	B	703	DGT	PB-O3A-PA-O1A
2	D	702	DGT	PB-O3A-PA-O1A

There are no ring outliers.

10 monomers are involved in 22 short contacts:

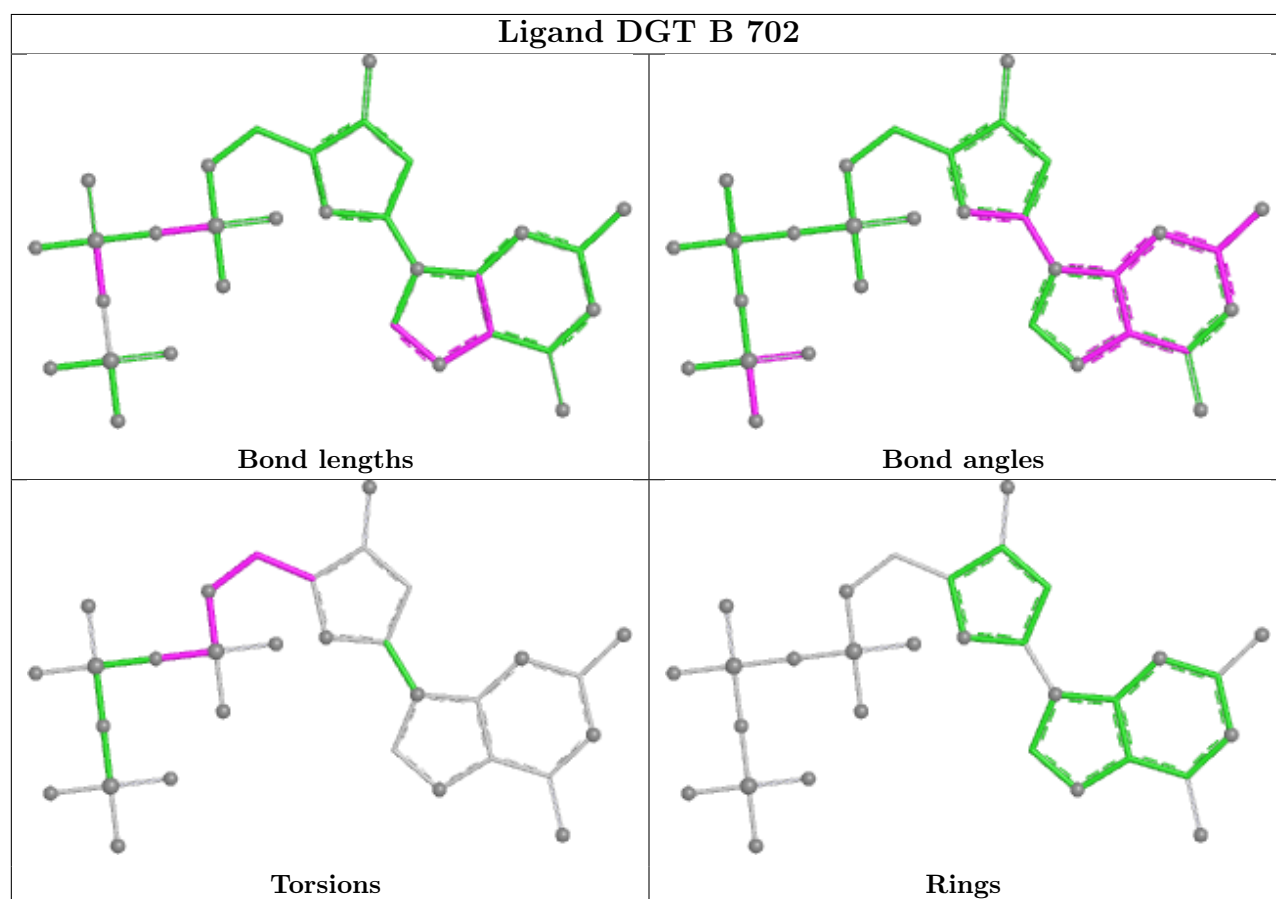
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	DGT	1	0
3	C	701	DTP	2	0
2	A	701	DGT	2	0
3	B	704	DTP	2	0
2	D	704	DGT	4	0
3	A	702	DTP	2	0

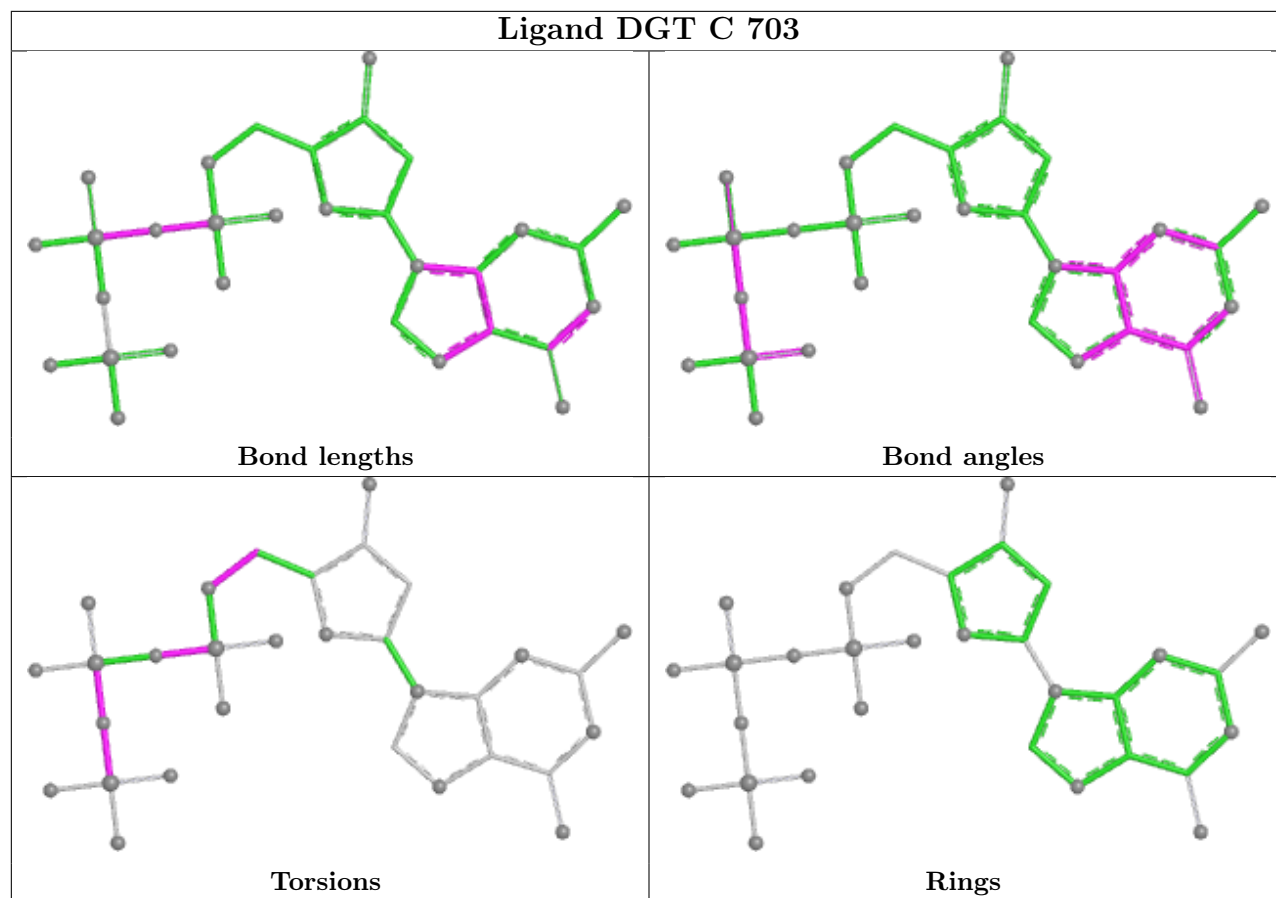
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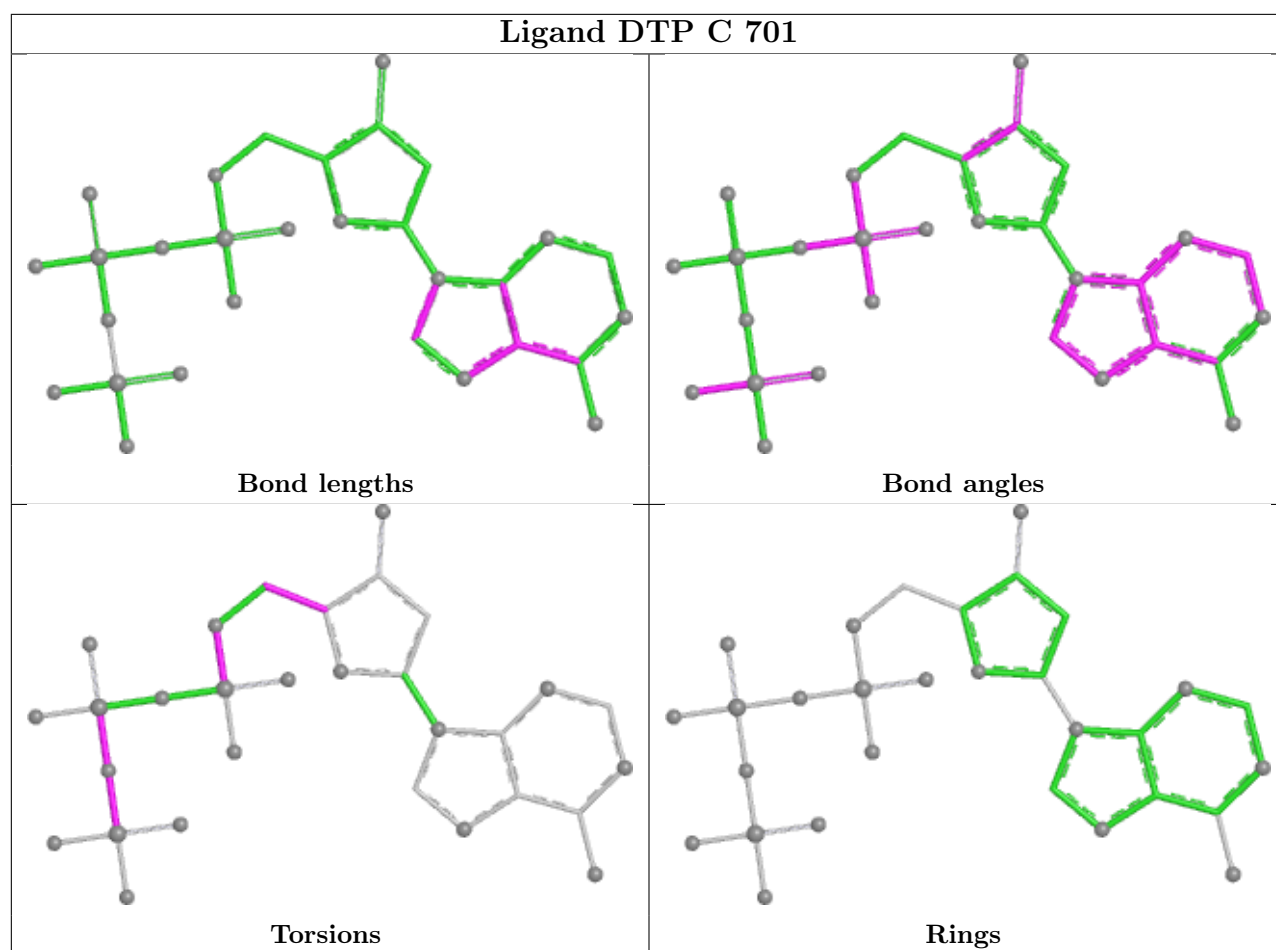
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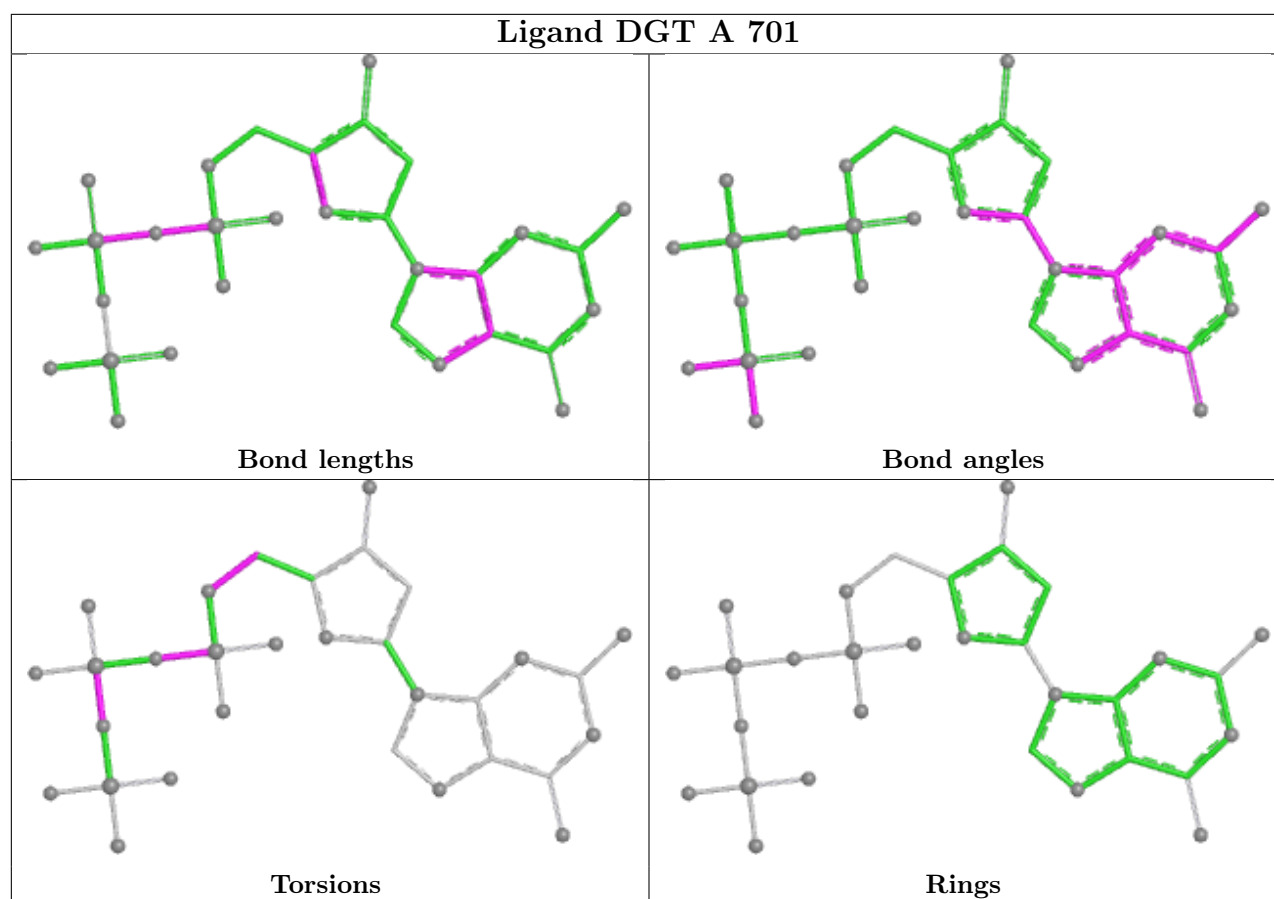
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	702	DGT	4	0
2	D	705	DGT	3	0
2	D	702	DGT	1	0
3	D	703	DTP	2	0

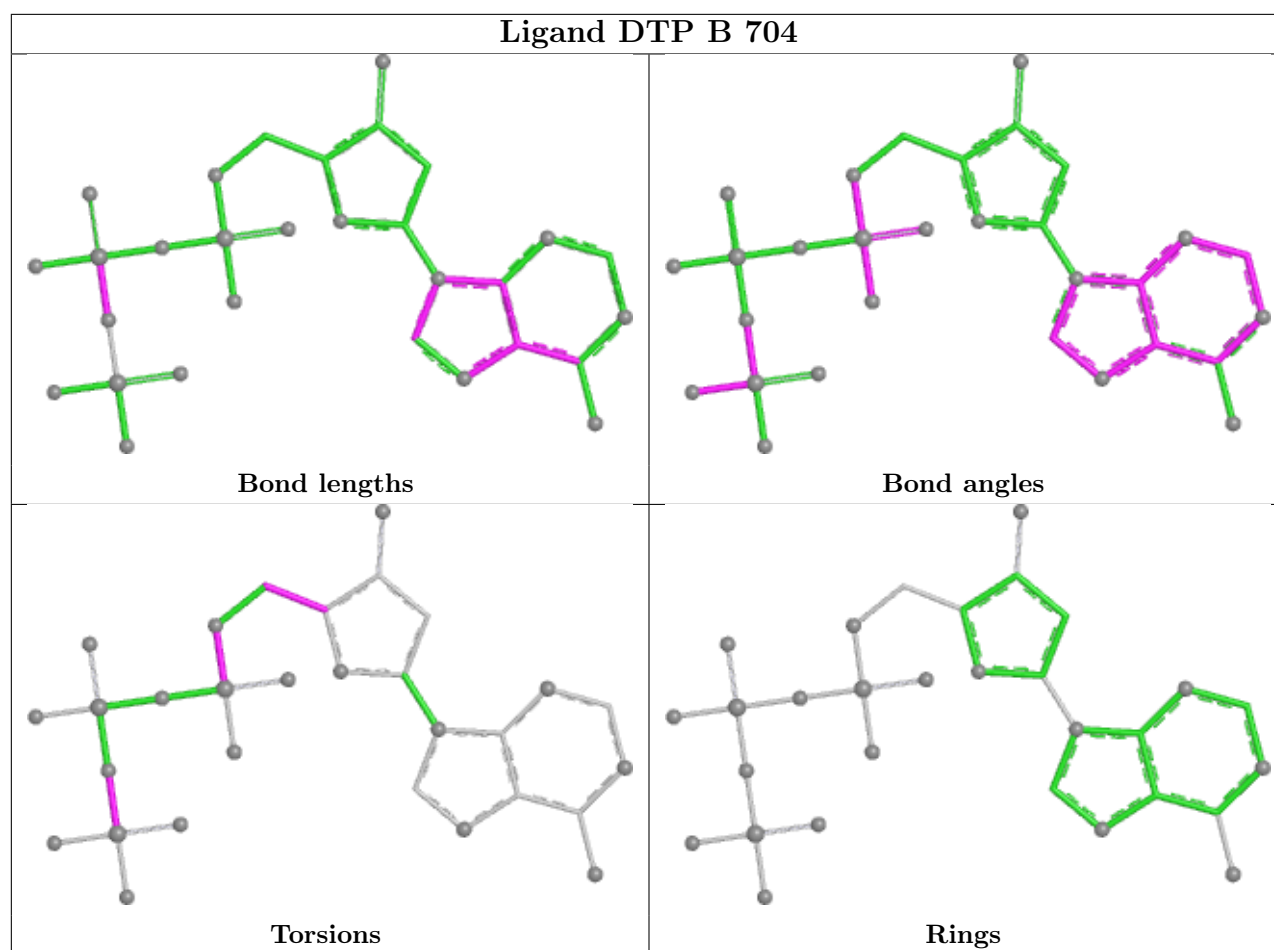
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

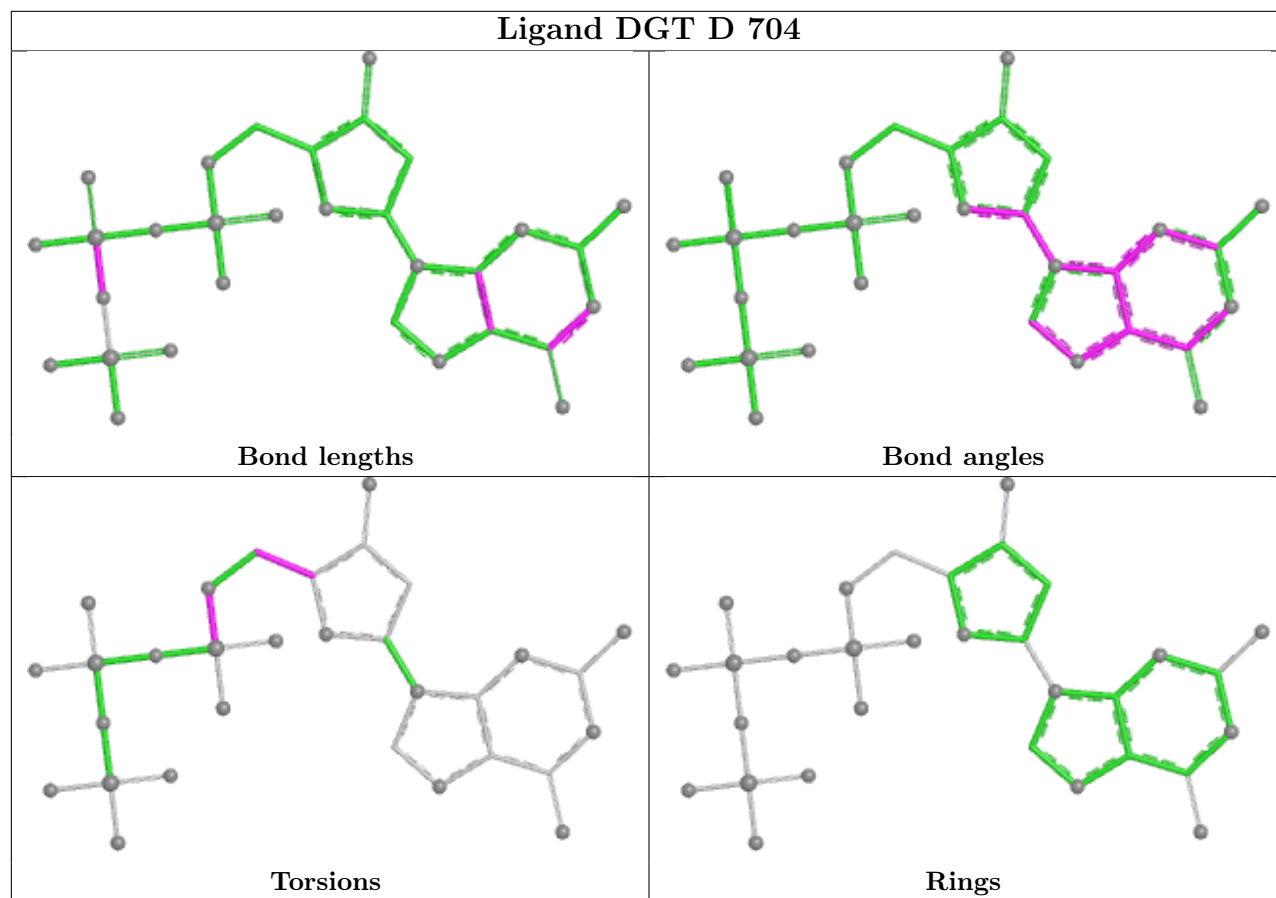


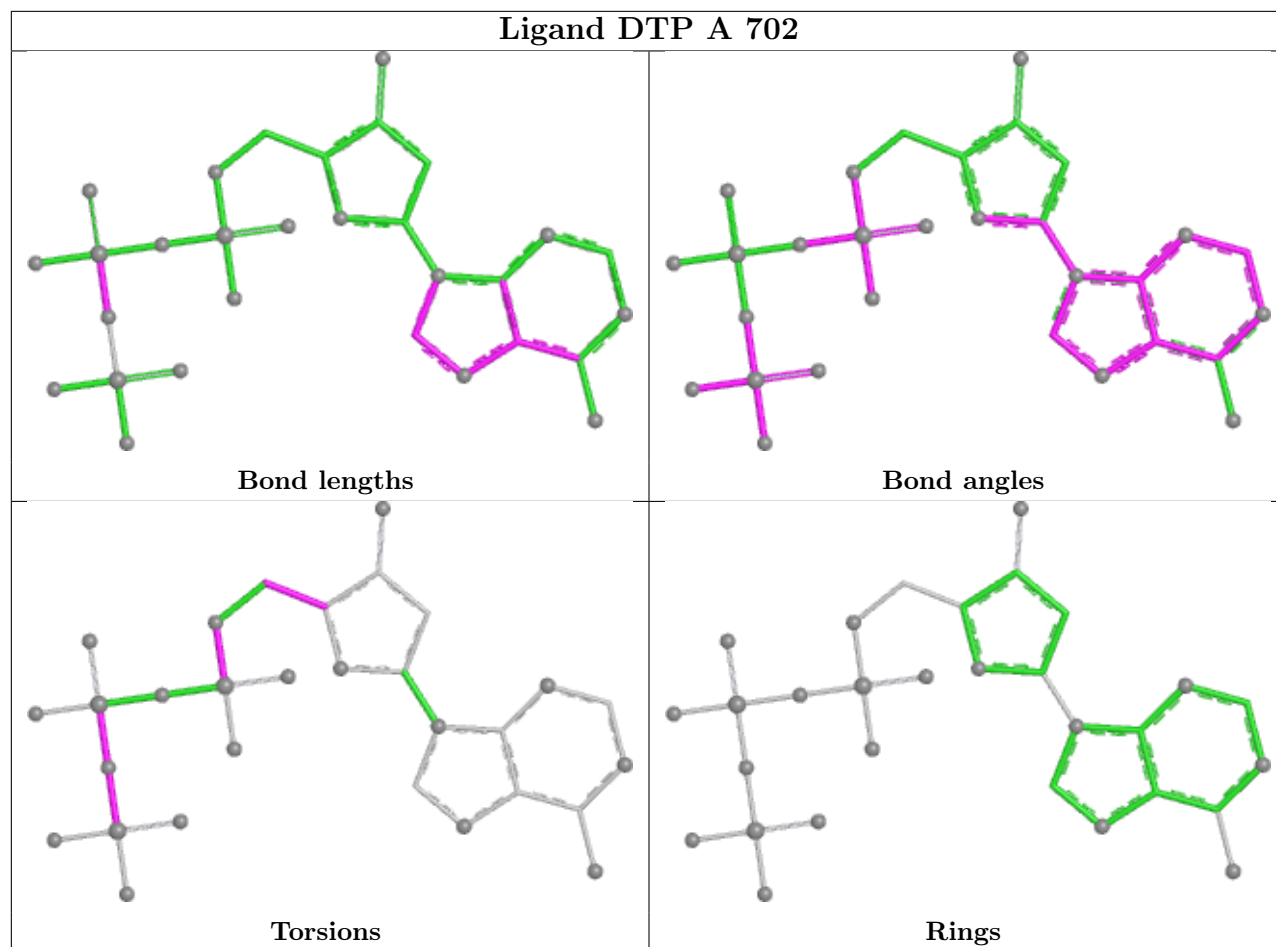


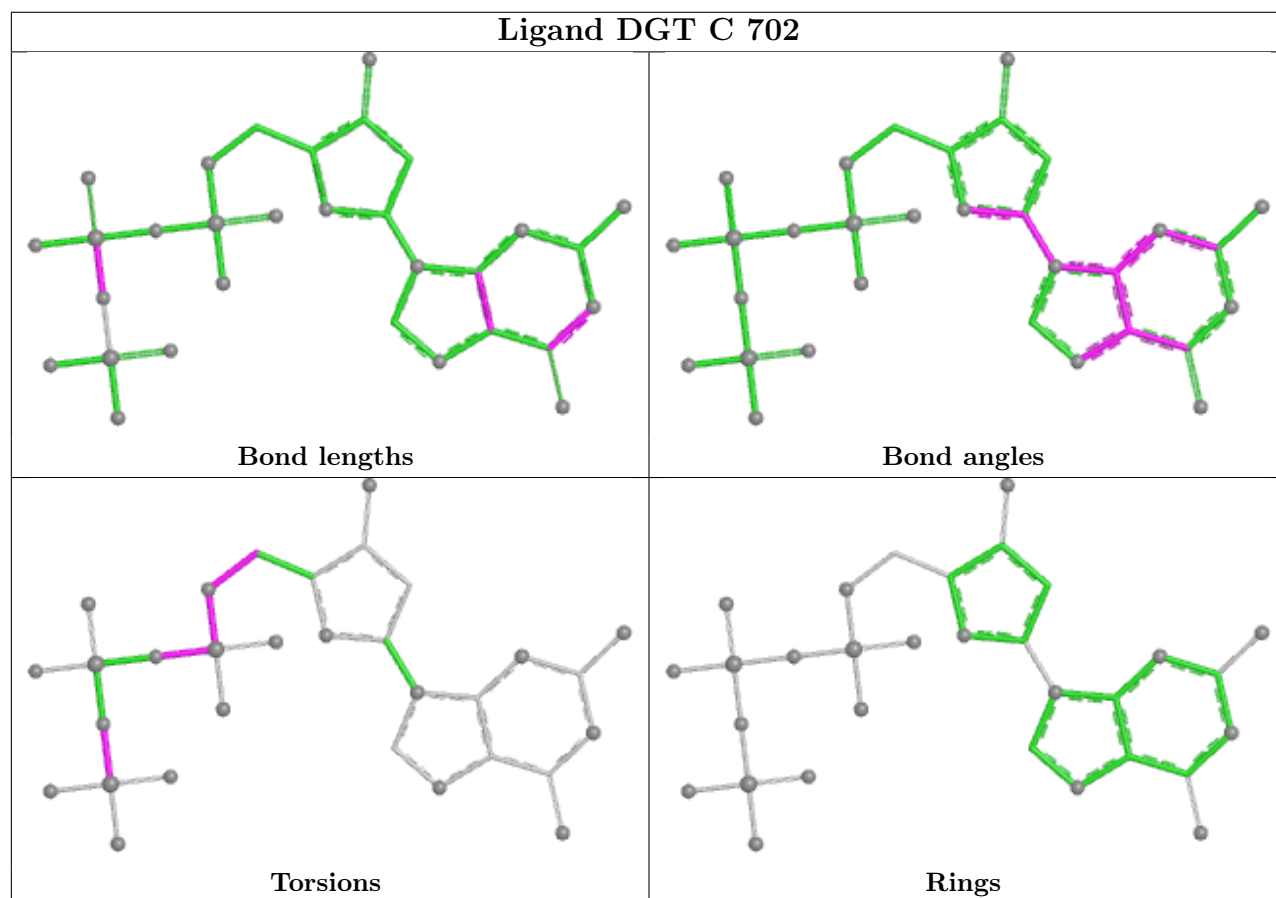
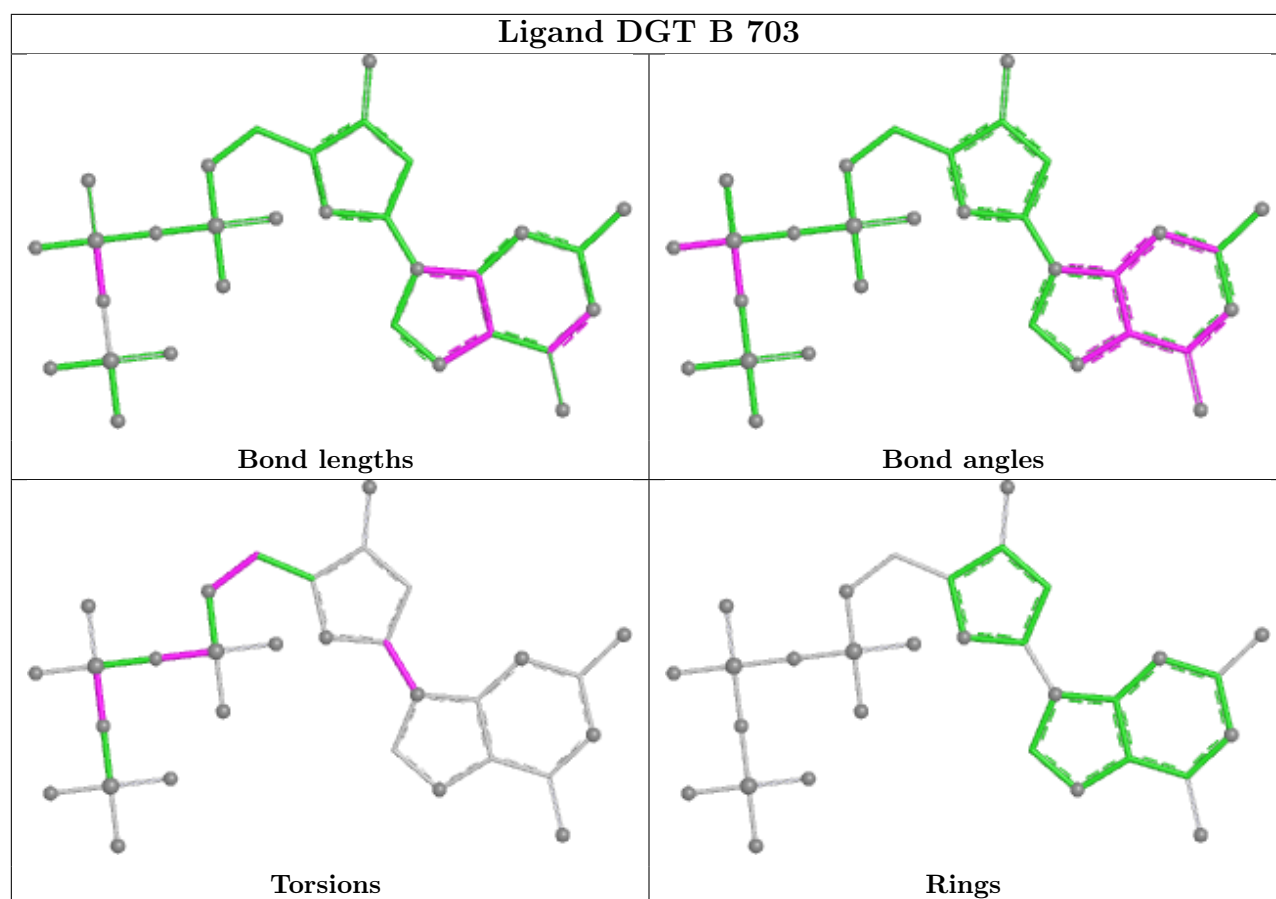


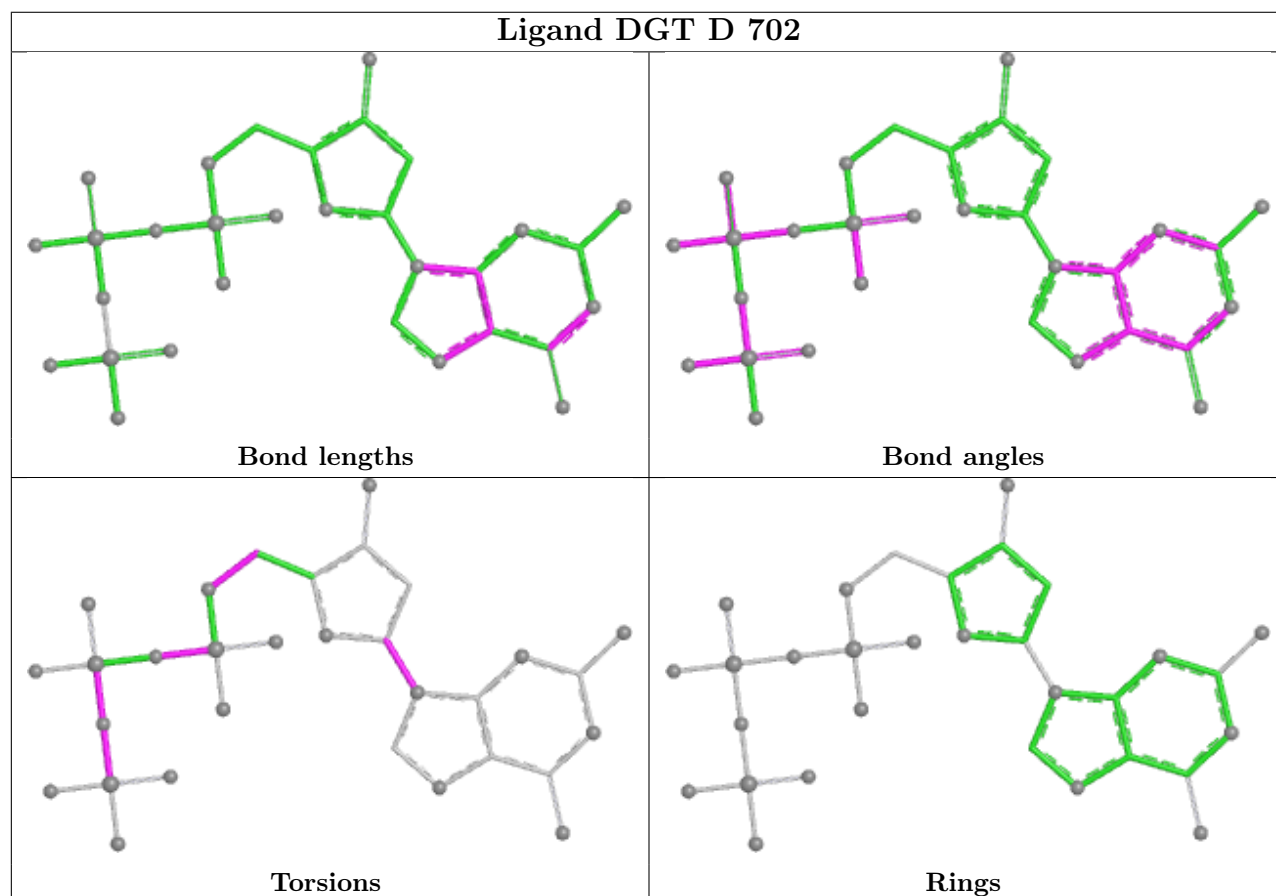
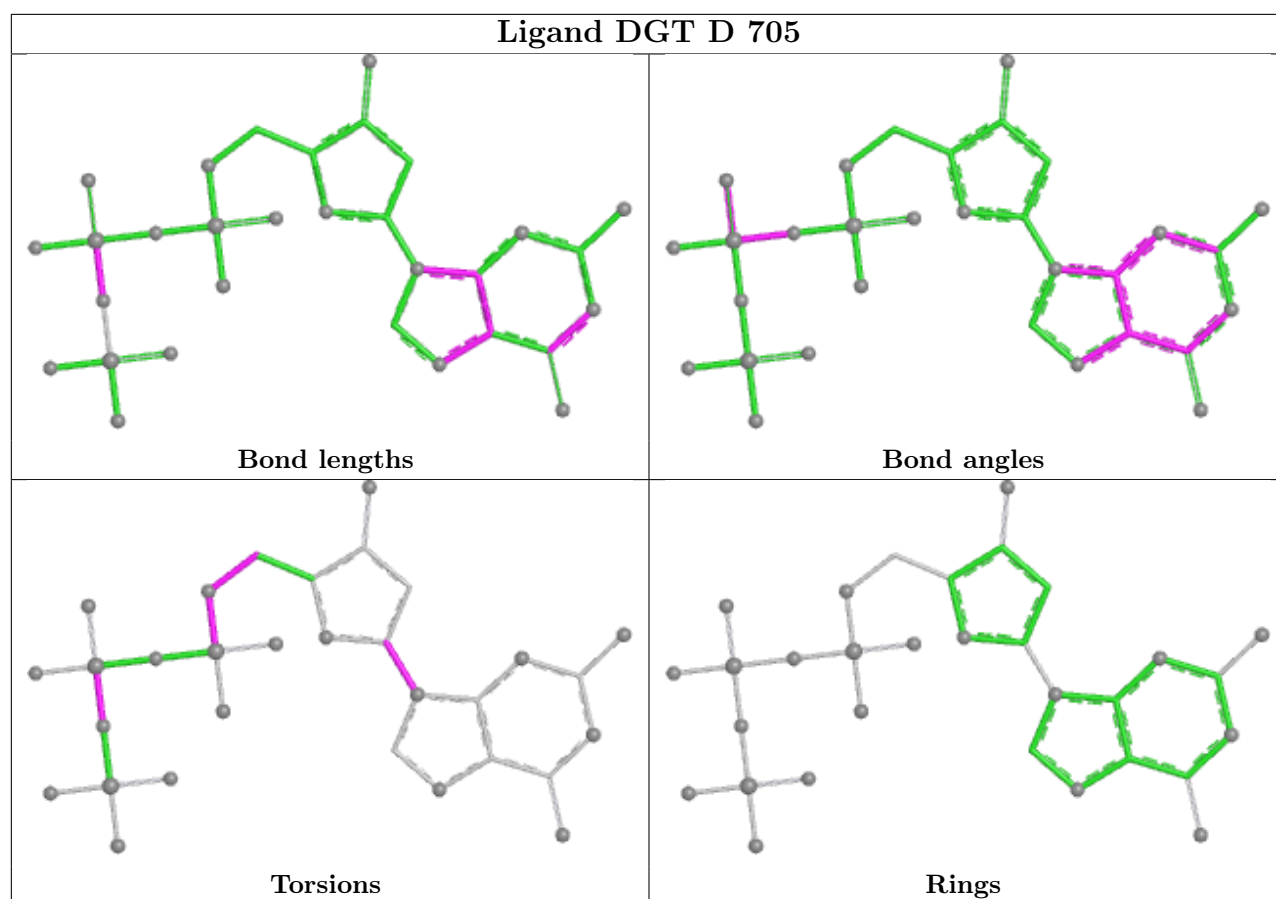


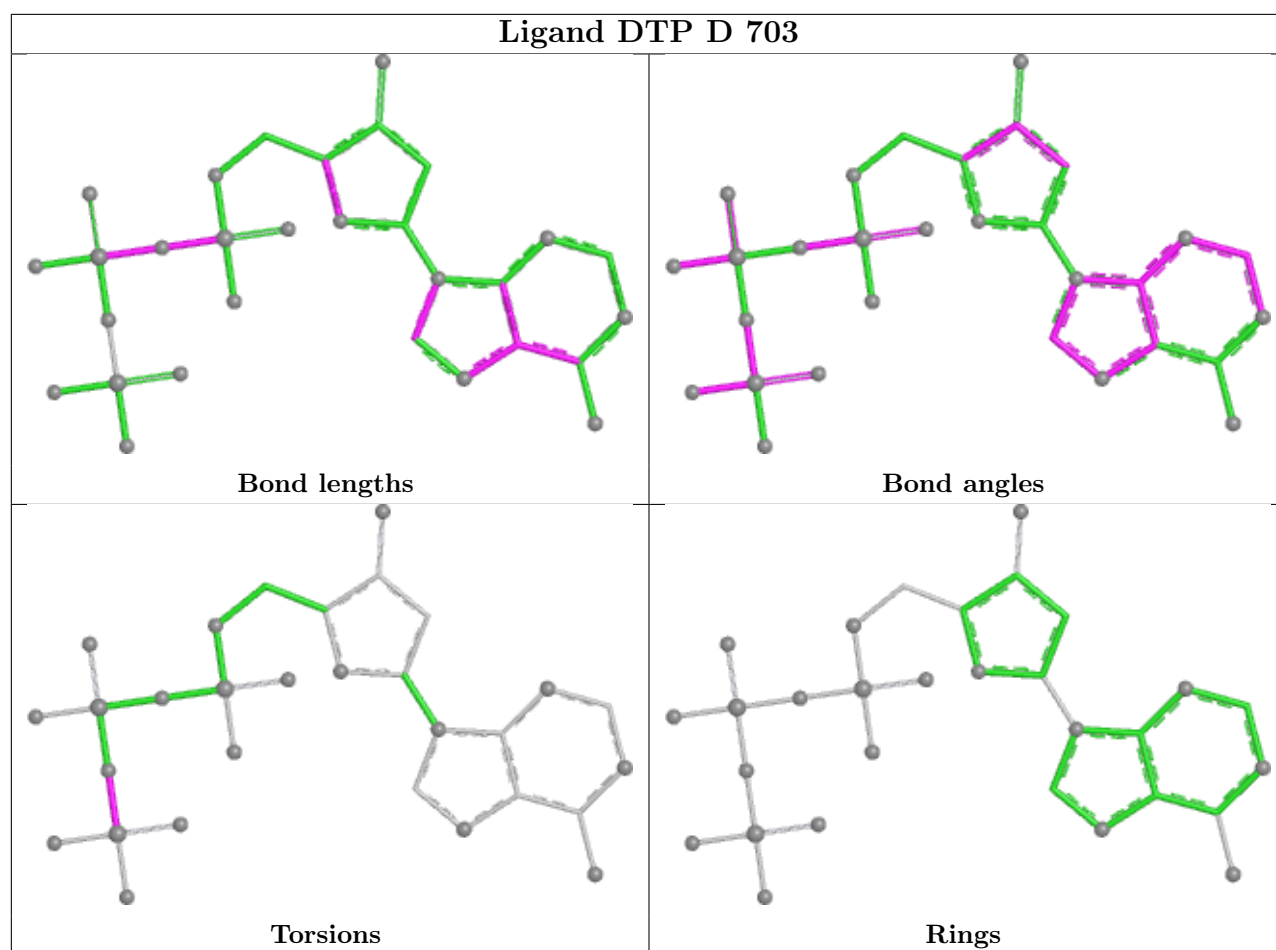












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/514 (93%)	-0.16	1 (0%) 91 90	28, 63, 104, 132	5 (1%)
1	B	481/514 (93%)	0.00	4 (0%) 82 80	31, 75, 119, 156	5 (1%)
1	C	481/514 (93%)	-0.01	4 (0%) 82 80	27, 73, 121, 156	5 (1%)
1	D	481/514 (93%)	0.35	12 (2%) 58 52	38, 100, 169, 208	4 (0%)
All	All	1924/2056 (93%)	0.05	21 (1%) 78 74	27, 76, 139, 208	19 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	LEU	4.4
1	D	569	PHE	3.9
1	B	284	LEU	3.3
1	D	480	VAL	3.1
1	B	540	LEU	2.9
1	D	562	LEU	2.9
1	D	476	LEU	2.8
1	C	284	LEU	2.7
1	D	388[A]	ASP	2.6
1	D	572	TRP	2.6
1	B	490	ASP	2.5
1	C	500	VAL	2.5
1	A	490	ASP	2.4
1	D	590	LEU	2.3
1	D	587	ILE	2.3
1	D	396	TYR	2.3
1	B	397	ILE	2.3
1	C	488	LEU	2.2
1	C	328	ASN	2.1
1	D	487	VAL	2.1
1	D	397	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

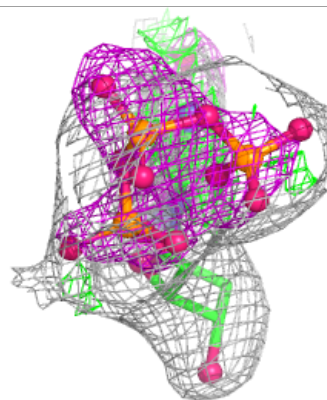
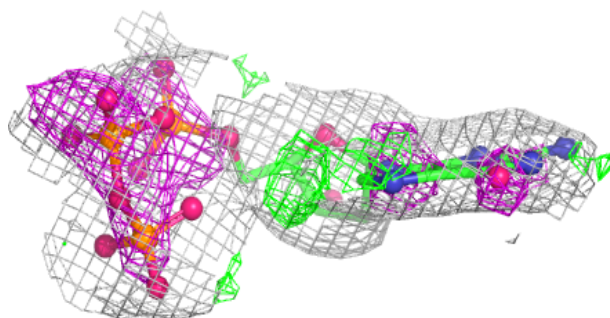
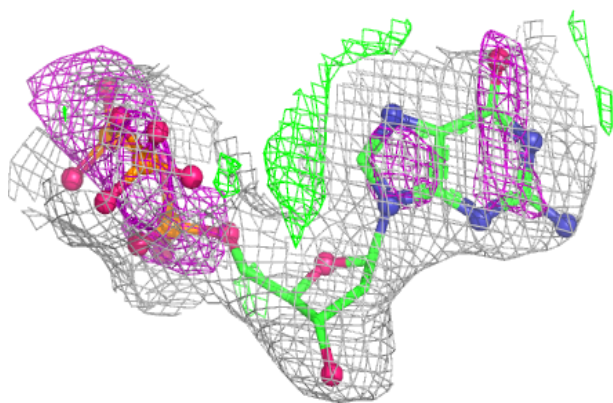
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	DGT	D	704	31/31	0.73	0.12	47,54,88,94	0
2	DGT	B	702	31/31	0.79	0.10	41,57,111,116	0
2	DGT	A	701	31/31	0.87	0.09	36,58,89,98	0
2	DGT	D	705	31/31	0.87	0.10	25,28,30,35	0
2	DGT	C	702	31/31	0.89	0.09	45,58,92,100	0
2	DGT	B	703	31/31	0.92	0.09	24,30,34,36	0
3	DTP	B	704	30/30	0.92	0.10	20,24,34,37	0
2	DGT	C	703	31/31	0.94	0.08	25,27,34,34	0
3	DTP	D	703	30/30	0.95	0.07	23,29,34,36	0
4	MG	C	704	1/1	0.95	0.06	45,45,45,45	0
4	MG	A	703	1/1	0.96	0.16	28,28,28,28	0
2	DGT	D	702	31/31	0.96	0.06	21,27,30,35	0
3	DTP	A	702	30/30	0.97	0.06	23,27,33,34	0
3	DTP	C	701	30/30	0.98	0.05	24,27,33,34	0
4	MG	B	701	1/1	0.99	0.07	32,32,32,32	0
4	MG	D	701	1/1	0.99	0.08	30,30,30,30	0

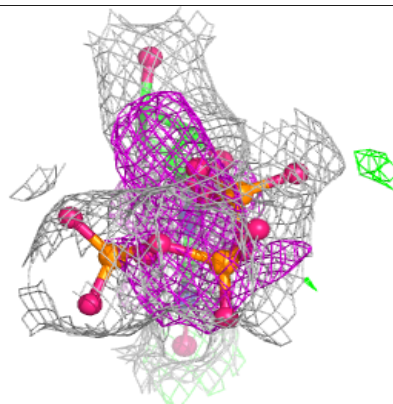
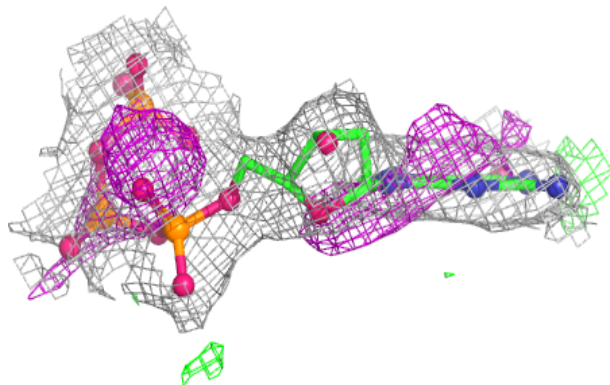
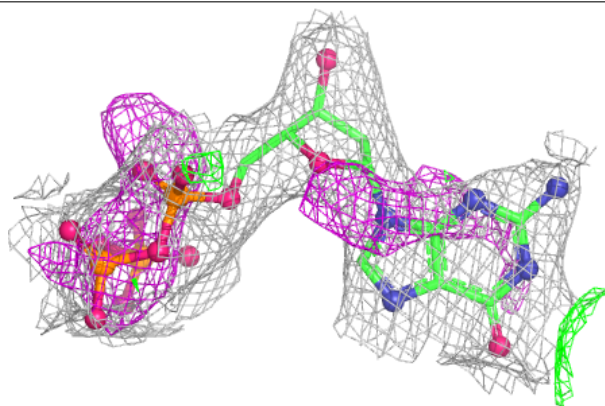
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

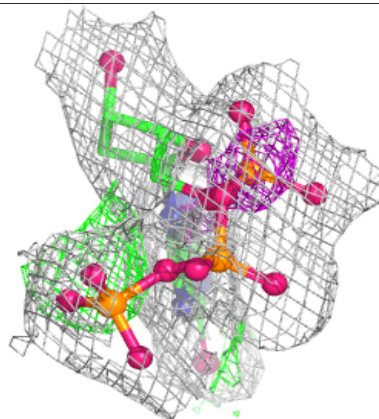
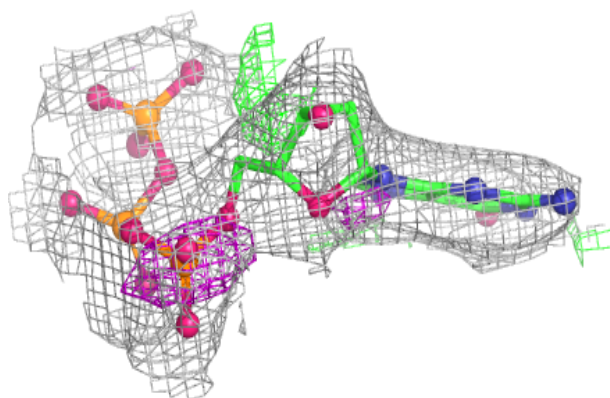
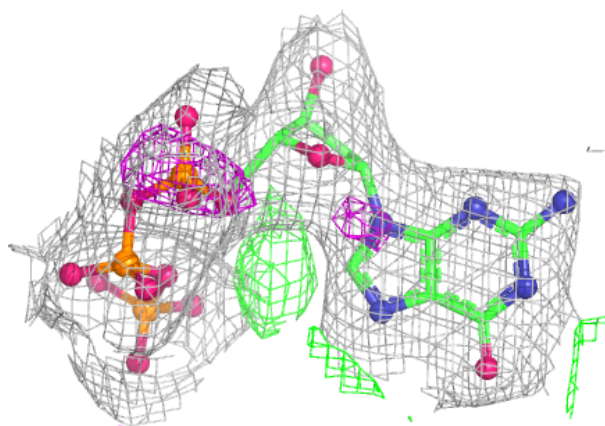
**Electron density around DGT B 702:**

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

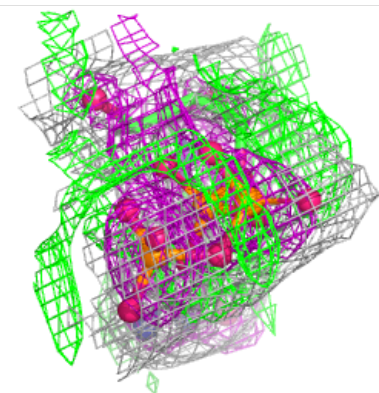
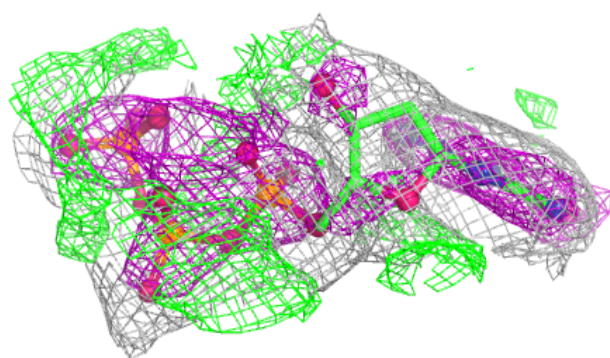
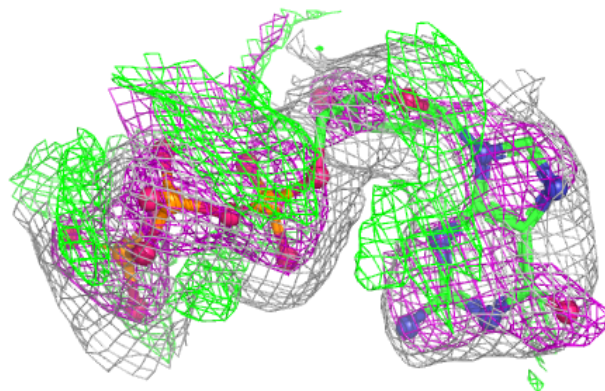


Electron density around DGT A 701:

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

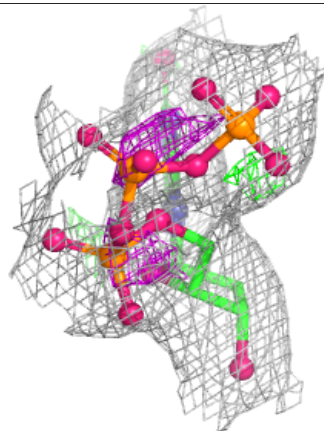
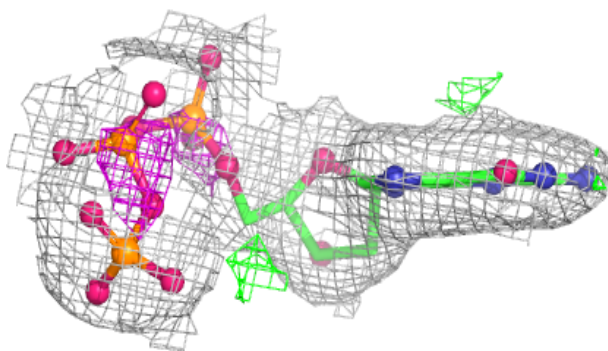
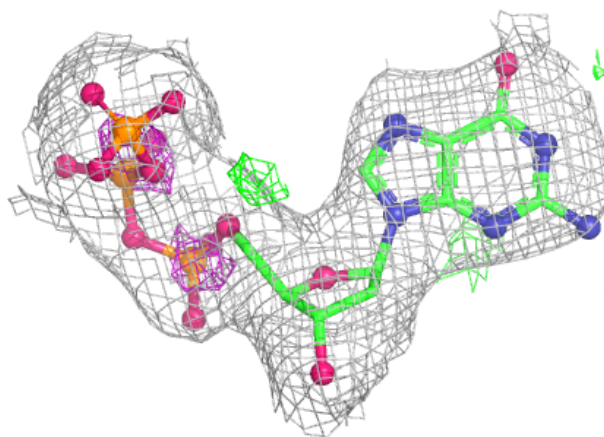
**Electron density around DGT D 705:**

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

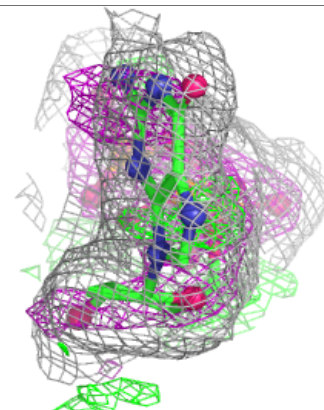
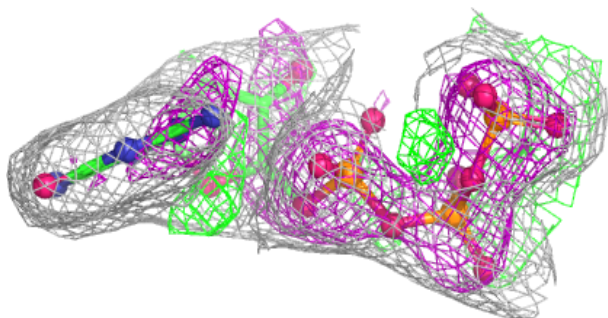
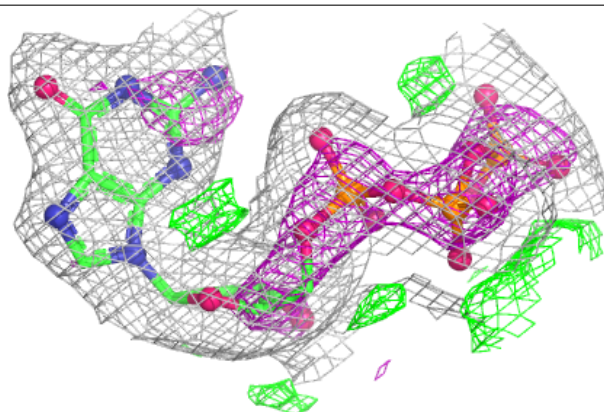


Electron density around DGT C 702:

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

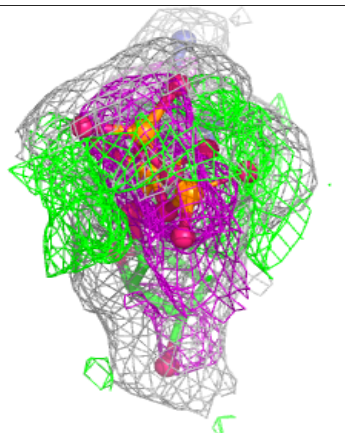
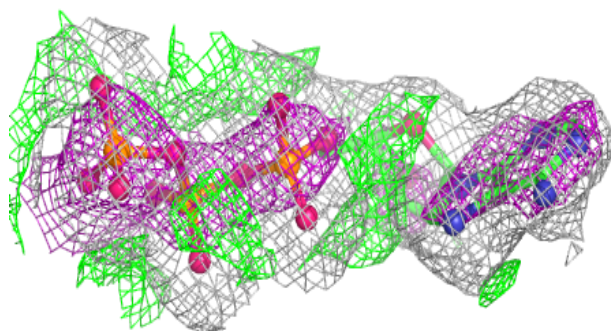
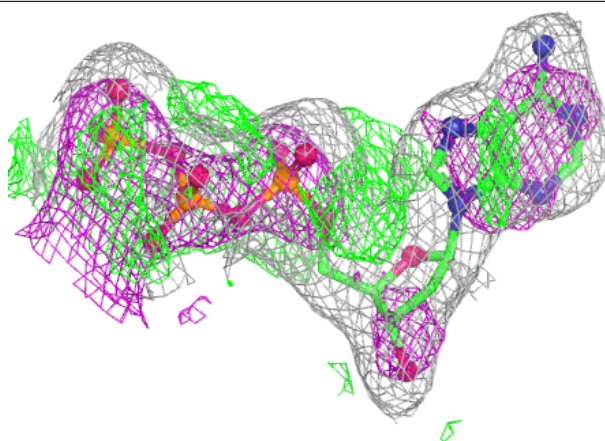
**Electron density around DGT B 703:**

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

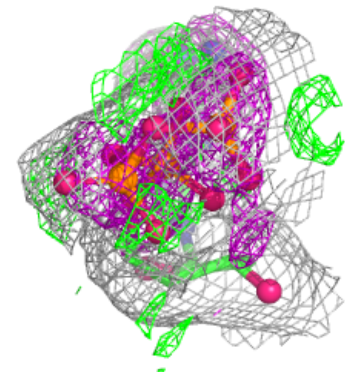
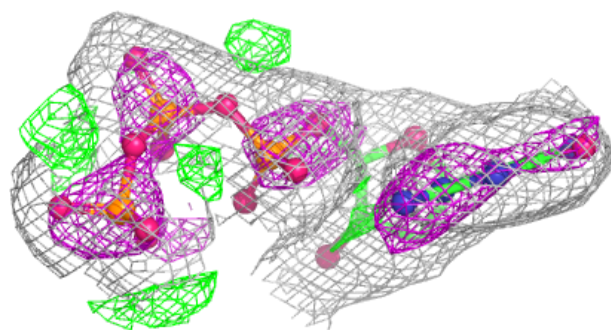
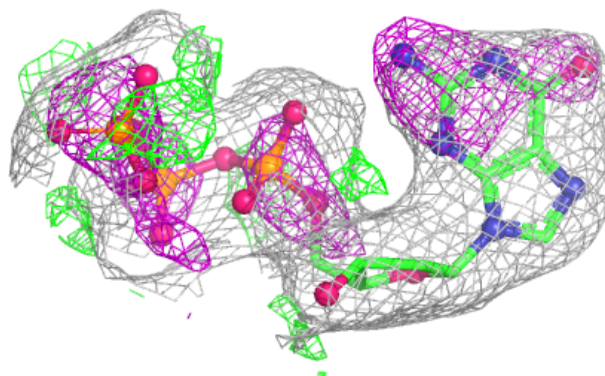


Electron density around DTP B 704:

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and green (positive)

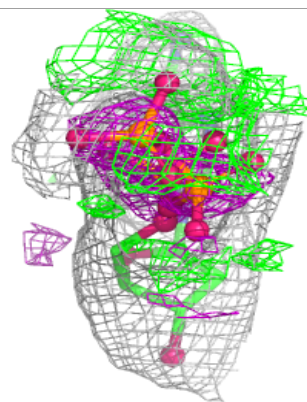
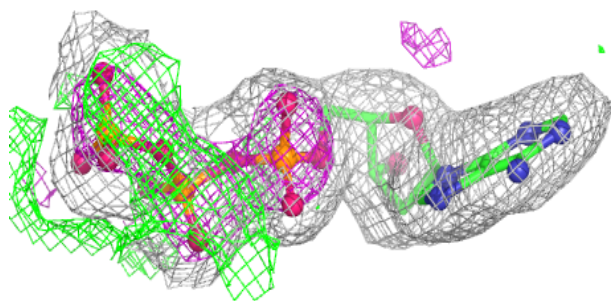
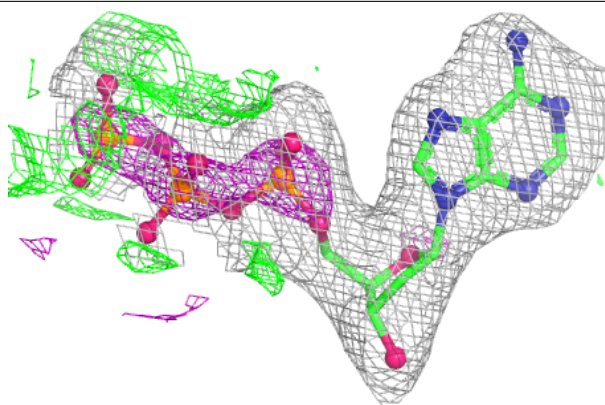
**Electron density around DGT C 703:**

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

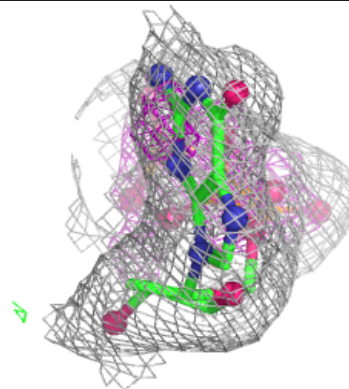
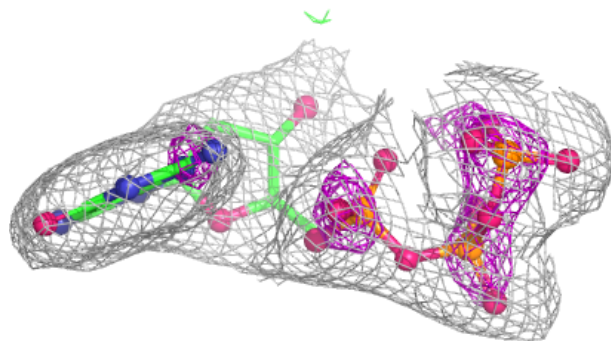
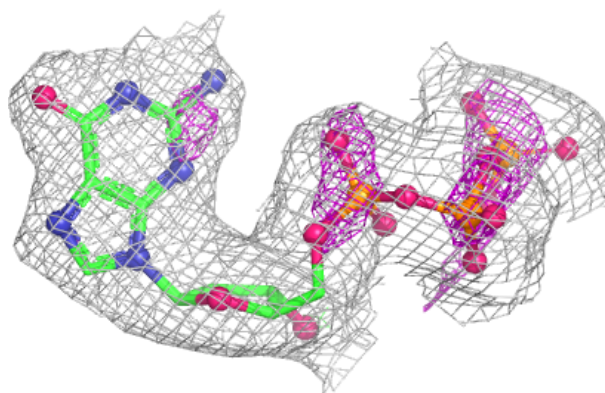


Electron density around DTP D 703:

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

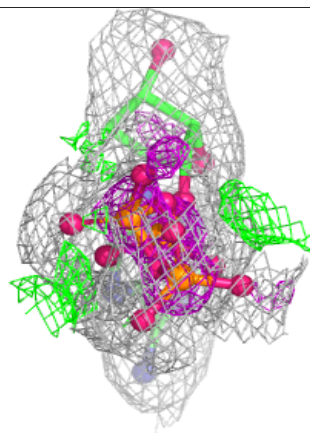
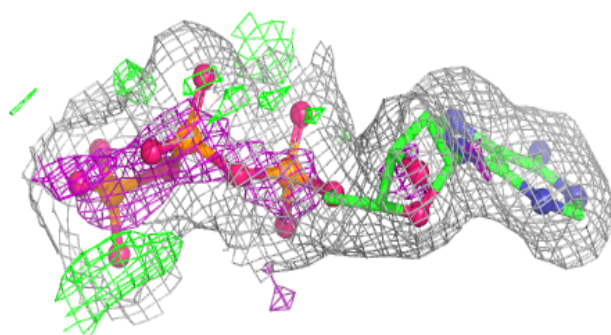
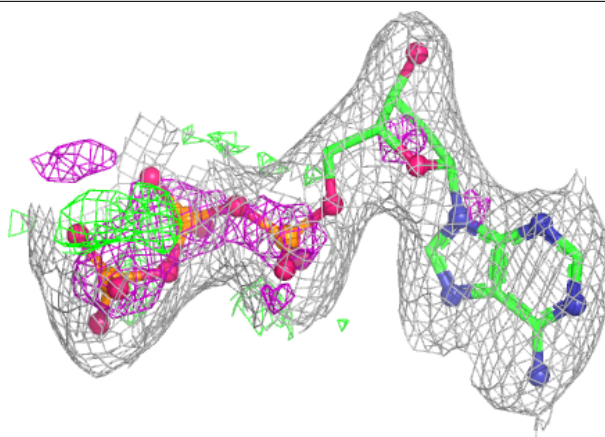
**Electron density around DGT D 702:**

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

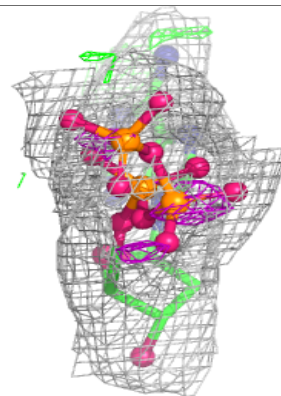
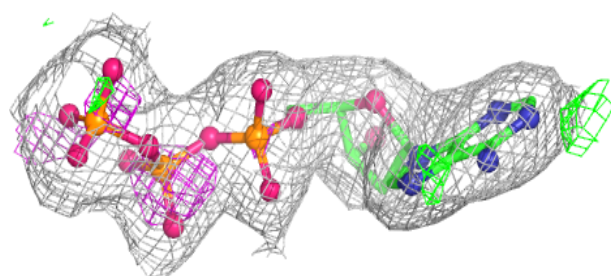
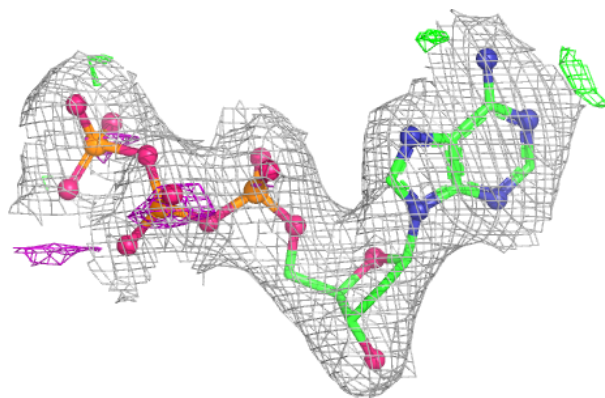


Electron density around DTP A 702:

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

**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.