



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:43 AM UTC

PDB ID : 4QFY / pdb_00004qfy
Title : Crystal structure of the tetrameric dGTP/dCTP-bound SAMHD1 (RN206) mutant catalytic core
Authors : Koharudin, L.M.I.; Wu, Y.; DeLucia, M.; Mehrens, J.; Gronenborn, A.M.; Ahn, J.
Deposited on : 2014-05-22
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

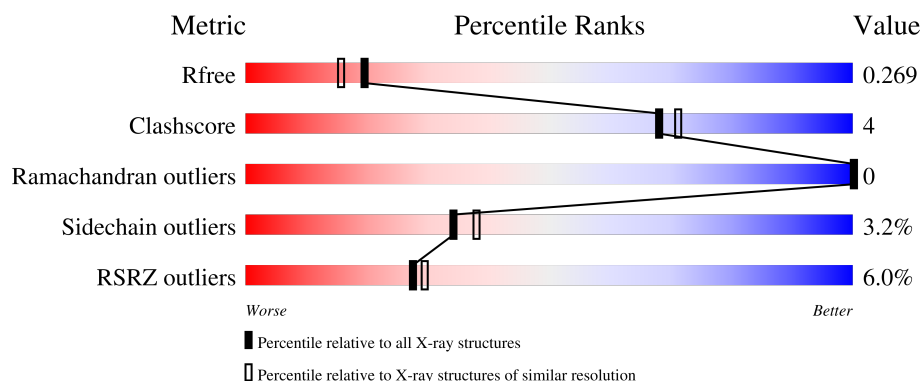
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	550	5% 75% 10% • 13%
1	B	550	3% 79% 8% • 13%
1	C	550	9% 78% 8% • 13%
1	D	550	3% 80% 7% • 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16518 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3934	2518	685	711	20			
1	B	481	Total	C	N	O	S	0	1	0
			3940	2522	687	711	20			
1	C	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	D	481	Total	C	N	O	S	0	2	0
			3949	2525	689	715	20			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	expression tag	UNP Q9Y3Z3
A	78	GLY	-	expression tag	UNP Q9Y3Z3
A	79	SER	-	expression tag	UNP Q9Y3Z3
A	80	SER	-	expression tag	UNP Q9Y3Z3
A	81	HIS	-	expression tag	UNP Q9Y3Z3
A	82	HIS	-	expression tag	UNP Q9Y3Z3
A	83	HIS	-	expression tag	UNP Q9Y3Z3
A	84	HIS	-	expression tag	UNP Q9Y3Z3
A	85	HIS	-	expression tag	UNP Q9Y3Z3
A	86	HIS	-	expression tag	UNP Q9Y3Z3
A	87	SER	-	expression tag	UNP Q9Y3Z3
A	88	SER	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	LEU	-	expression tag	UNP Q9Y3Z3
A	91	VAL	-	expression tag	UNP Q9Y3Z3
A	92	PRO	-	expression tag	UNP Q9Y3Z3
A	93	ARG	-	expression tag	UNP Q9Y3Z3
A	94	GLY	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
A	97	MET	-	expression tag	UNP Q9Y3Z3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ALA	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	MET	-	expression tag	UNP Q9Y3Z3
A	101	THR	-	expression tag	UNP Q9Y3Z3
A	102	GLY	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	GLN	-	expression tag	UNP Q9Y3Z3
A	105	GLN	-	expression tag	UNP Q9Y3Z3
A	106	MET	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	ARG	-	expression tag	UNP Q9Y3Z3
A	109	ASP	-	expression tag	UNP Q9Y3Z3
A	110	PRO	-	expression tag	UNP Q9Y3Z3
A	111	ASN	-	expression tag	UNP Q9Y3Z3
A	112	SER	-	expression tag	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	77	MET	-	expression tag	UNP Q9Y3Z3
B	78	GLY	-	expression tag	UNP Q9Y3Z3
B	79	SER	-	expression tag	UNP Q9Y3Z3
B	80	SER	-	expression tag	UNP Q9Y3Z3
B	81	HIS	-	expression tag	UNP Q9Y3Z3
B	82	HIS	-	expression tag	UNP Q9Y3Z3
B	83	HIS	-	expression tag	UNP Q9Y3Z3
B	84	HIS	-	expression tag	UNP Q9Y3Z3
B	85	HIS	-	expression tag	UNP Q9Y3Z3
B	86	HIS	-	expression tag	UNP Q9Y3Z3
B	87	SER	-	expression tag	UNP Q9Y3Z3
B	88	SER	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	LEU	-	expression tag	UNP Q9Y3Z3
B	91	VAL	-	expression tag	UNP Q9Y3Z3
B	92	PRO	-	expression tag	UNP Q9Y3Z3
B	93	ARG	-	expression tag	UNP Q9Y3Z3
B	94	GLY	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	MET	-	expression tag	UNP Q9Y3Z3
B	98	ALA	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	MET	-	expression tag	UNP Q9Y3Z3
B	101	THR	-	expression tag	UNP Q9Y3Z3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	102	GLY	-	expression tag	UNP Q9Y3Z3
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	GLN	-	expression tag	UNP Q9Y3Z3
B	105	GLN	-	expression tag	UNP Q9Y3Z3
B	106	MET	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	ASP	-	expression tag	UNP Q9Y3Z3
B	110	PRO	-	expression tag	UNP Q9Y3Z3
B	111	ASN	-	expression tag	UNP Q9Y3Z3
B	112	SER	-	expression tag	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	77	MET	-	expression tag	UNP Q9Y3Z3
C	78	GLY	-	expression tag	UNP Q9Y3Z3
C	79	SER	-	expression tag	UNP Q9Y3Z3
C	80	SER	-	expression tag	UNP Q9Y3Z3
C	81	HIS	-	expression tag	UNP Q9Y3Z3
C	82	HIS	-	expression tag	UNP Q9Y3Z3
C	83	HIS	-	expression tag	UNP Q9Y3Z3
C	84	HIS	-	expression tag	UNP Q9Y3Z3
C	85	HIS	-	expression tag	UNP Q9Y3Z3
C	86	HIS	-	expression tag	UNP Q9Y3Z3
C	87	SER	-	expression tag	UNP Q9Y3Z3
C	88	SER	-	expression tag	UNP Q9Y3Z3
C	89	GLY	-	expression tag	UNP Q9Y3Z3
C	90	LEU	-	expression tag	UNP Q9Y3Z3
C	91	VAL	-	expression tag	UNP Q9Y3Z3
C	92	PRO	-	expression tag	UNP Q9Y3Z3
C	93	ARG	-	expression tag	UNP Q9Y3Z3
C	94	GLY	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	MET	-	expression tag	UNP Q9Y3Z3
C	98	ALA	-	expression tag	UNP Q9Y3Z3
C	99	SER	-	expression tag	UNP Q9Y3Z3
C	100	MET	-	expression tag	UNP Q9Y3Z3
C	101	THR	-	expression tag	UNP Q9Y3Z3
C	102	GLY	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	GLN	-	expression tag	UNP Q9Y3Z3
C	105	GLN	-	expression tag	UNP Q9Y3Z3

Continued on next page...

Continued from previous page...

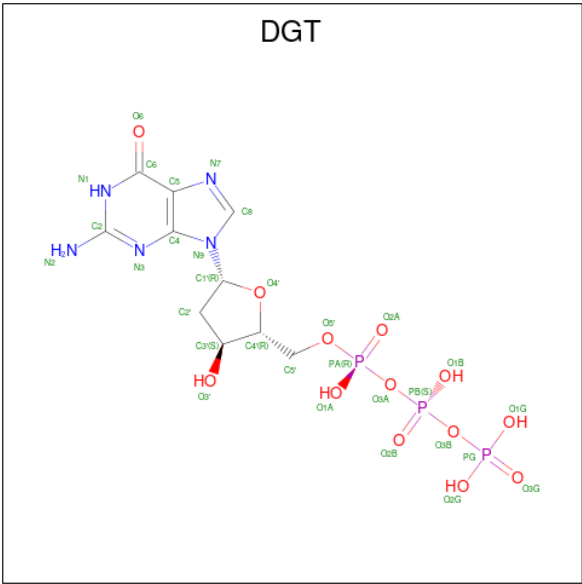
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	77	MET	-	expression tag	UNP Q9Y3Z3
D	78	GLY	-	expression tag	UNP Q9Y3Z3
D	79	SER	-	expression tag	UNP Q9Y3Z3
D	80	SER	-	expression tag	UNP Q9Y3Z3
D	81	HIS	-	expression tag	UNP Q9Y3Z3
D	82	HIS	-	expression tag	UNP Q9Y3Z3
D	83	HIS	-	expression tag	UNP Q9Y3Z3
D	84	HIS	-	expression tag	UNP Q9Y3Z3
D	85	HIS	-	expression tag	UNP Q9Y3Z3
D	86	HIS	-	expression tag	UNP Q9Y3Z3
D	87	SER	-	expression tag	UNP Q9Y3Z3
D	88	SER	-	expression tag	UNP Q9Y3Z3
D	89	GLY	-	expression tag	UNP Q9Y3Z3
D	90	LEU	-	expression tag	UNP Q9Y3Z3
D	91	VAL	-	expression tag	UNP Q9Y3Z3
D	92	PRO	-	expression tag	UNP Q9Y3Z3
D	93	ARG	-	expression tag	UNP Q9Y3Z3
D	94	GLY	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	MET	-	expression tag	UNP Q9Y3Z3
D	98	ALA	-	expression tag	UNP Q9Y3Z3
D	99	SER	-	expression tag	UNP Q9Y3Z3
D	100	MET	-	expression tag	UNP Q9Y3Z3
D	101	THR	-	expression tag	UNP Q9Y3Z3
D	102	GLY	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	GLN	-	expression tag	UNP Q9Y3Z3
D	105	GLN	-	expression tag	UNP Q9Y3Z3
D	106	MET	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	ARG	-	expression tag	UNP Q9Y3Z3
D	109	ASP	-	expression tag	UNP Q9Y3Z3

Continued on next page...

Continued from previous page...

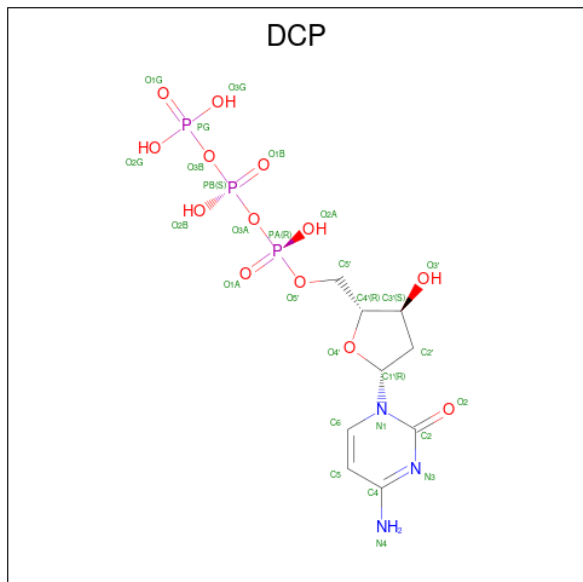
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	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	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	C	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'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	3	Total	Mg	0	0
			3	3		
4	D	1	Total	Mg	0	0
			1	1		

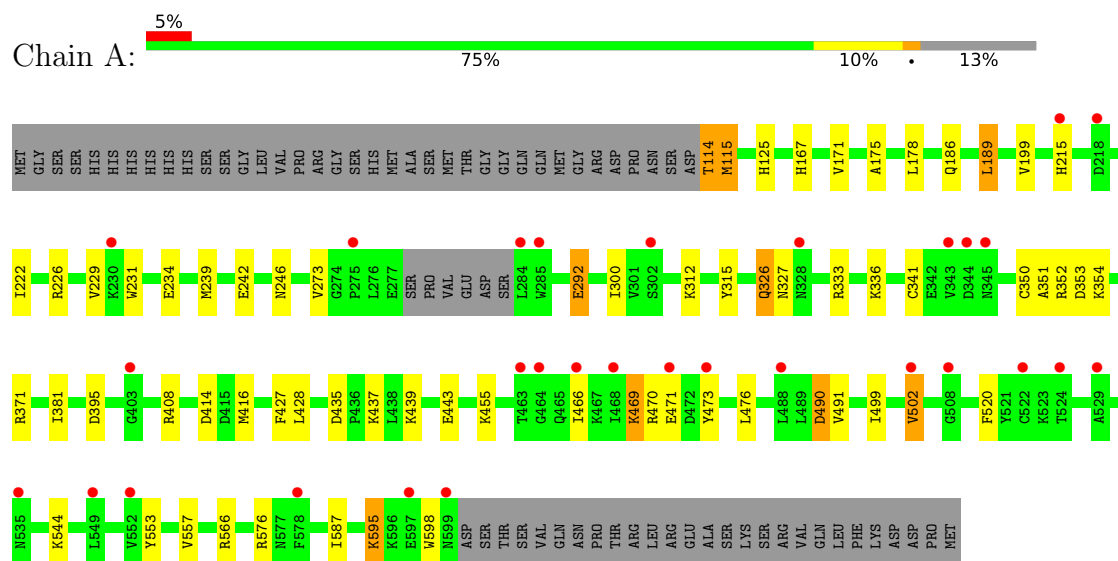
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total 74	O 74	0	0
5	B	124	Total 124	O 124	0	0
5	C	75	Total 75	O 75	0	0
5	D	121	Total 121	O 121	0	0

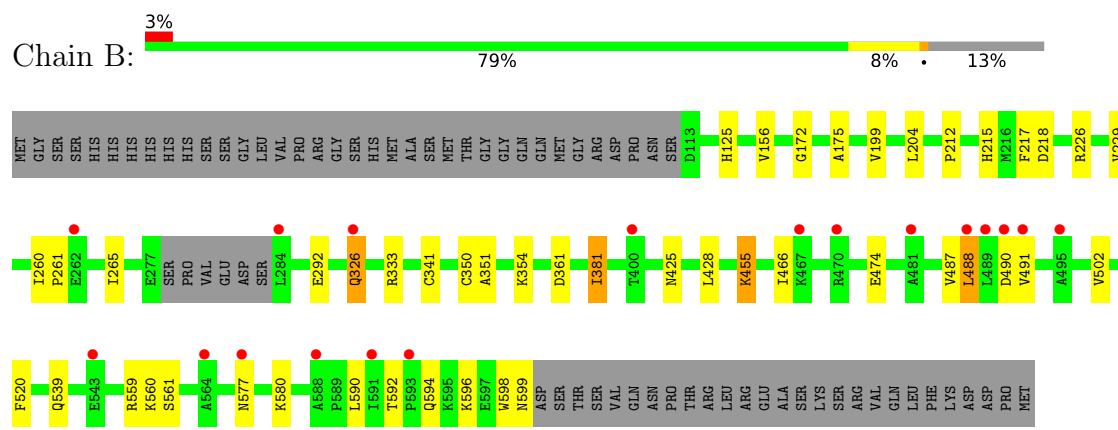
3 Residue-property plots [i](#)

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

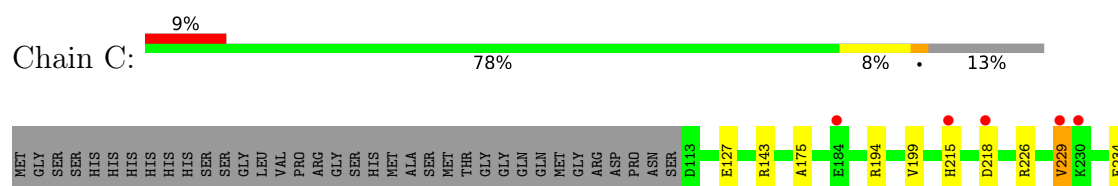
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

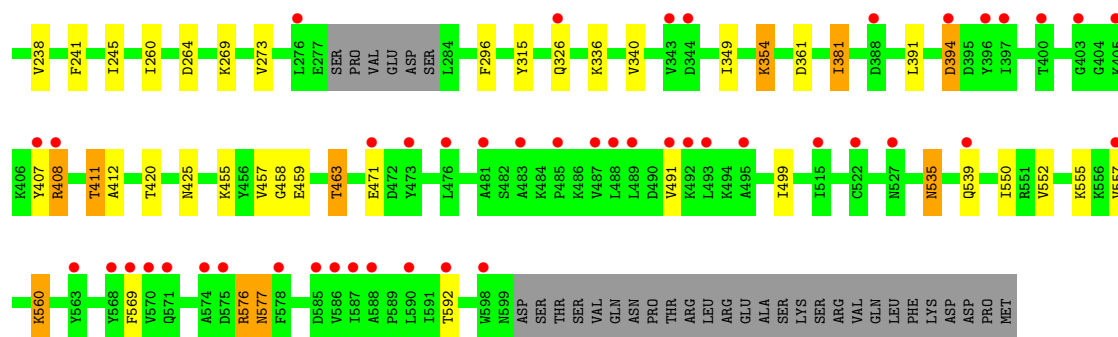


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

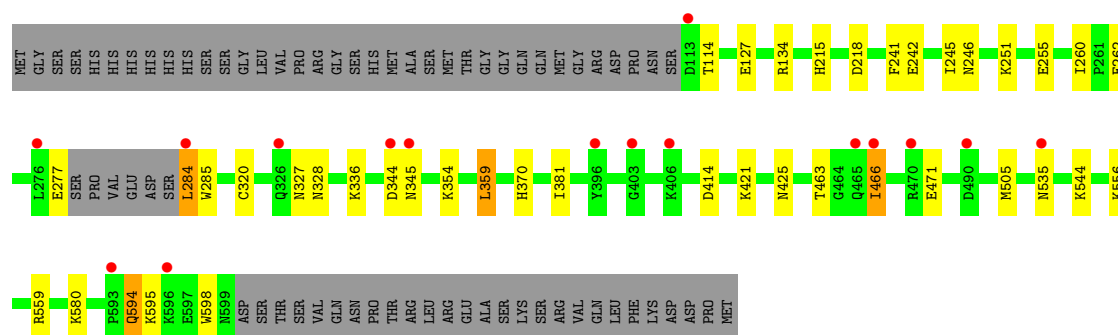
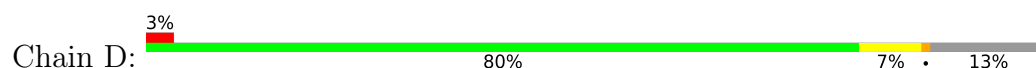


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● 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	87.97Å 147.02Å 98.87Å 90.00° 114.31° 90.00°	Depositor
Resolution (Å)	38.67 – 2.10 38.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.67-2.10) 99.8 (38.67-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.226 , 0.269 0.227 , 0.269	Depositor DCC
R_{free} test set	2011 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16518	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/4026	0.79	0/5434
1	B	0.38	0/4036	0.79	2/5448 (0.0%)
1	C	0.36	0/4025	0.81	5/5433 (0.1%)
1	D	0.38	0/4041	0.79	2/5455 (0.0%)
All	All	0.37	0/16128	0.79	9/21770 (0.0%)

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	C	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	592	THR	CA-C-N	-7.57	113.11	120.83
1	C	592	THR	C-N-CA	-7.57	113.11	120.83
1	D	260	ILE	CA-C-N	7.02	127.33	119.32
1	D	260	ILE	C-N-CA	7.02	127.33	119.32
1	C	458	GLY	N-CA-C	6.37	120.04	110.75
1	B	260	ILE	CA-C-N	6.07	126.24	119.32
1	B	260	ILE	C-N-CA	6.07	126.24	119.32
1	C	260	ILE	CA-C-N	6.04	126.21	119.32
1	C	260	ILE	C-N-CA	6.04	126.21	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	407	TYR	Peptide

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	3934	0	3922	41	0
1	B	3940	0	3928	28	0
1	C	3933	0	3921	35	0
1	D	3949	0	3932	23	0
2	A	93	0	36	1	0
2	B	31	0	12	0	0
2	C	93	0	36	3	0
2	D	31	0	12	1	0
3	A	28	0	12	2	0
3	B	28	0	12	1	0
3	C	28	0	12	2	0
3	D	28	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	A	74	0	0	0	0
5	B	124	0	0	1	0
5	C	75	0	0	0	0
5	D	121	0	0	1	0
All	All	16518	0	15847	116	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 4.

All (116) 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:C:336:LYS:HE3	1:D:127:GLU:HG3	1.63	0.79
1:B:425:ASN:OD1	1:C:425:ASN:ND2	2.14	0.78
1:A:544:LYS:NZ	1:C:539:GLN:OE1	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLU:OE2	1:A:246:ASN:ND2	2.24	0.70
1:C:455:LYS:HG2	1:C:557:VAL:HG12	1.75	0.68
1:A:439:LYS:HD2	1:A:443:GLU:HG2	1.77	0.66
1:C:127:GLU:HG3	1:D:336:LYS:HE3	1.75	0.66
1:A:215:HIS:NE2	3:A:702:DCP:O2A	2.31	0.64
1:B:490:ASP:OD2	1:B:560:LYS:NZ	2.32	0.63
1:A:239:MET:HE2	1:A:416:MET:HE3	1.81	0.62
1:A:371:ARG:NH2	1:C:361:ASP:OD2	2.31	0.62
1:C:234:GLU:HB3	1:C:273:VAL:HG23	1.84	0.59
1:A:326:GLN:OE1	1:C:326:GLN:NE2	2.27	0.58
1:B:215[A]:HIS:NE2	3:B:701:DCP:O1A	2.28	0.57
1:B:326:GLN:HG3	1:D:328[A]:ASN:HA	1.86	0.57
1:C:457:VAL:HB	1:C:552:VAL:HG13	1.87	0.56
1:D:535:ASN:OD1	1:D:535:ASN:N	2.38	0.56
1:C:552:VAL:HG11	1:C:569:PHE:CD1	2.42	0.55
1:A:490:ASP:N	1:A:490:ASP:OD1	2.30	0.54
1:C:296:PHE:HB2	1:C:349:ILE:HG13	1.89	0.54
1:C:215:HIS:HA	1:C:218:ASP:OD1	2.08	0.54
1:A:125:HIS:CE1	1:B:333:ARG:HB2	2.43	0.53
1:D:284:LEU:HD22	1:D:285:TRP:H	1.75	0.52
1:C:215:HIS:NE2	3:C:704:DCP:O1A	2.42	0.52
1:A:215:HIS:HE2	3:A:702:DCP:PA	2.32	0.52
1:A:435:ASP:OD2	1:A:437:LYS:HB2	2.10	0.51
1:B:354:LYS:NZ	5:B:840:HOH:O	2.28	0.51
1:C:391:LEU:O	1:C:394:ASP:HB2	2.10	0.51
1:D:215:HIS:NE2	3:D:702:DCP:O2A	2.43	0.51
1:A:326:GLN:HG3	1:A:327:ASN:N	2.26	0.50
1:C:408:ARG:HB2	1:C:411:THR:OG1	2.11	0.50
1:D:242:GLU:OE2	1:D:246:ASN:ND2	2.33	0.50
1:B:487:VAL:HG13	1:B:590:LEU:HD12	1.93	0.49
1:A:234:GLU:HB3	1:A:273:VAL:HG23	1.94	0.49
1:B:491:VAL:HG11	1:B:561:SER:HA	1.95	0.48
1:C:491:VAL:HG12	1:C:560:LYS:HG2	1.94	0.48
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.95	0.47
1:C:463:THR:OG1	1:C:577:ASN:O	2.30	0.47
1:D:327[A]:ASN:OD1	1:D:328[A]:ASN:N	2.47	0.47
1:D:215:HIS:HE2	3:D:702:DCP:PA	2.38	0.47
1:C:535:ASN:OD1	1:C:535:ASN:N	2.40	0.46
1:A:469:LYS:H	1:A:469:LYS:HG2	1.43	0.46
1:B:455:LYS:HE3	1:B:455:LYS:HA	1.98	0.46
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.97	0.46
1:A:470:ARG:HG3	1:A:473:TYR:CE2	2.51	0.46
1:D:215:HIS:HA	1:D:218:ASP:OD1	2.16	0.45
1:A:395:ASP:OD1	1:A:408:ARG:NH1	2.48	0.45
1:D:594:GLN:HG3	1:D:595:LYS:N	2.30	0.45
1:B:341:CYS:HB2	1:B:350:CYS:SG	2.56	0.45
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.98	0.45
1:A:167:HIS:O	1:A:171:VAL:HG23	2.17	0.45
1:A:473:TYR:CE1	1:A:502:VAL:HG11	2.52	0.45
1:C:499:ILE:HD11	1:C:555:LYS:HE2	1.97	0.45
1:A:292:GLU:H	1:A:292:GLU:HG3	1.54	0.45
1:C:394:ASP:CG	1:C:408:ARG:HH22	2.25	0.45
1:B:539:GLN:OE1	1:D:544:LYS:NZ	2.50	0.45
1:A:341:CYS:HB2	1:A:350:CYS:SG	2.56	0.44
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.75	0.44
1:B:596:LYS:NZ	1:B:599:ASN:O	2.34	0.44
1:A:428:LEU:HD12	1:D:425:ASN:HB2	1.98	0.44
1:C:560:LYS:HE3	1:C:560:LYS:HB3	1.53	0.44
1:A:595:LYS:HG2	1:A:598:TRP:CE2	2.53	0.44
1:B:172:GLY:HA3	1:B:204:LEU:HD13	2.00	0.44
1:B:156:VAL:O	2:C:702:DGT:H8	2.18	0.43
1:D:241:PHE:O	1:D:245:ILE:HG12	2.18	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:C:238:VAL:HG13	1:C:269:LYS:HD3	2.00	0.43
1:A:352:ARG:CZ	1:A:354:LYS:HD2	2.49	0.43
1:B:212:PRO:HD2	1:B:217:PHE:CD1	2.53	0.43
1:D:359:LEU:HD12	1:D:359:LEU:HA	1.80	0.43
1:C:394:ASP:O	1:C:408:ARG:CZ	2.66	0.43
1:D:370:HIS:HB3	1:D:505:MET:HE1	2.00	0.42
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.00	0.42
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.01	0.42
1:A:114:THR:HG22	1:A:115:MET:H	1.84	0.42
1:A:226:ARG:NH1	1:A:414:ASP:OD2	2.51	0.42
1:C:226:ARG:O	1:C:229:VAL:HG22	2.19	0.42
1:D:381:ILE:HA	1:D:381:ILE:HD12	1.85	0.42
2:C:702:DGT:H5'A	2:D:701:DGT:O1B	2.20	0.42
1:D:320:CYS:SG	1:D:327[B]:ASN:HB2	2.60	0.42
1:C:408:ARG:O	1:C:412:ALA:N	2.51	0.42
1:A:427:PHE:HD1	1:A:428:LEU:HD23	1.84	0.42
1:D:134:ARG:HD2	5:D:900:HOH:O	2.19	0.42
1:D:580:LYS:HB2	1:D:598:TRP:CG	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:HG21	1:A:231:TRP:HB3	2.01	0.42
1:A:499:ILE:HB	1:A:553:TYR:HB2	2.02	0.42
1:A:576:ARG:HE	1:A:576:ARG:HB3	1.71	0.42
2:A:701:DGT:H5'A	2:C:701:DGT:O1B	2.20	0.42
1:D:463:THR:O	1:D:466:ILE:HG22	2.20	0.42
1:A:333:ARG:HB2	1:B:125:HIS:CE1	2.54	0.42
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.91	0.42
1:B:580:LYS:HB2	1:B:598:TRP:CG	2.55	0.42
1:C:576:ARG:HE	1:C:576:ARG:HB3	1.62	0.41
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.41
1:B:488:LEU:H	1:B:488:LEU:HG	1.53	0.41
1:C:241:PHE:O	1:C:245:ILE:HG12	2.20	0.41
1:A:178:LEU:HD23	1:A:300:ILE:HG23	2.02	0.41
1:B:466:ILE:HD12	1:B:466:ILE:H	1.85	0.41
1:A:353:ASP:OD1	1:A:354:LYS:N	2.51	0.41
1:B:226:ARG:HB3	1:B:229:VAL:HG12	2.01	0.41
1:C:143:ARG:HD2	1:C:420:THR:HA	2.01	0.41
1:D:251:LYS:O	1:D:255:GLU:HG3	2.21	0.41
1:B:261:PRO:O	1:B:265:ILE:HB	2.20	0.41
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.81	0.41
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.56	0.41
1:B:215[A]:HIS:HA	1:B:218:ASP:OD1	2.21	0.41
1:C:354:LYS:HE2	1:C:354:LYS:HB3	1.78	0.41
1:A:566:ARG:HD3	1:A:587:ILE:HB	2.03	0.40
1:C:215:HIS:HE2	3:C:704:DCP:PA	2.43	0.40
1:A:336:LYS:HD2	1:B:125:HIS:HB3	2.04	0.40
1:B:596:LYS:HA	1:B:596:LYS:HD2	1.82	0.40
1:C:459:GLU:HA	1:C:550:ILE:O	2.21	0.40
1:A:471:GLU:N	1:A:471:GLU:CD	2.79	0.40
1:C:194:ARG:HE	1:C:264:ASP:CG	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/550 (87%)	466 (98%)	11 (2%)	0	100	100
1	B	478/550 (87%)	462 (97%)	16 (3%)	0	100	100
1	C	477/550 (87%)	458 (96%)	19 (4%)	0	100	100
1	D	479/550 (87%)	468 (98%)	11 (2%)	0	100	100
All	All	1911/2200 (87%)	1854 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/488 (88%)	414 (97%)	13 (3%)	36	41
1	B	428/488 (88%)	416 (97%)	12 (3%)	38	43
1	C	427/488 (88%)	413 (97%)	14 (3%)	33	37
1	D	429/488 (88%)	414 (96%)	15 (4%)	32	35
All	All	1711/1952 (88%)	1657 (97%)	54 (3%)	34	38

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	115	MET
1	A	189	LEU
1	A	229	VAL
1	A	292	GLU
1	A	326	GLN
1	A	466	ILE
1	A	469	LYS
1	A	476	LEU
1	A	490	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	491	VAL
1	A	502	VAL
1	A	595	LYS
1	B	292	GLU
1	B	326	GLN
1	B	361	ASP
1	B	381	ILE
1	B	455	LYS
1	B	474	GLU
1	B	488	LEU
1	B	502	VAL
1	B	559	ARG
1	B	577	ASN
1	B	592	THR
1	B	594	GLN
1	C	229	VAL
1	C	315	TYR
1	C	340	VAL
1	C	354	LYS
1	C	381	ILE
1	C	394	ASP
1	C	408	ARG
1	C	411	THR
1	C	463	THR
1	C	471	GLU
1	C	535	ASN
1	C	560	LYS
1	C	576	ARG
1	C	577	ASN
1	D	114	THR
1	D	262	GLU
1	D	277	GLU
1	D	284	LEU
1	D	344	ASP
1	D	345	ASN
1	D	354	LYS
1	D	359	LEU
1	D	414	ASP
1	D	421	LYS
1	D	466	ILE
1	D	471	GLU
1	D	556	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	559	ARG
1	D	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	235	GLN
1	A	243	HIS
1	A	248	ASN
1	A	321	HIS
1	A	364	HIS
1	A	425	ASN
1	A	517	HIS
1	B	140	GLN
1	B	163	ASN
1	B	235	GLN
1	B	248	ASN
1	B	567	GLN
1	C	567	GLN
1	D	235	GLN
1	D	243	HIS
1	D	248	ASN
1	D	539	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DGT	C	703	4	32,33,33	2.09	10 (31%)	48,52,52	1.69	11 (22%)
2	DGT	D	701	4	32,33,33	2.08	9 (28%)	48,52,52	1.57	10 (20%)
2	DGT	A	704	4	32,33,33	2.07	9 (28%)	48,52,52	1.61	9 (18%)
2	DGT	A	701	4	32,33,33	2.07	9 (28%)	48,52,52	1.61	8 (16%)
3	DCP	C	704	4	28,29,29	1.52	6 (21%)	41,45,45	1.13	4 (9%)
2	DGT	C	702	4	32,33,33	2.06	8 (25%)	48,52,52	1.75	12 (25%)
3	DCP	D	702	4	28,29,29	1.51	6 (21%)	41,45,45	1.12	5 (12%)
3	DCP	B	701	4	28,29,29	1.51	6 (21%)	41,45,45	1.07	4 (9%)
2	DGT	A	703	4	32,33,33	2.10	10 (31%)	48,52,52	1.58	9 (18%)
3	DCP	A	702	4	28,29,29	1.53	7 (25%)	41,45,45	1.07	3 (7%)
2	DGT	C	701	4	32,33,33	2.05	9 (28%)	48,52,52	1.64	10 (20%)
2	DGT	B	702	4	32,33,33	2.08	10 (31%)	48,52,52	1.62	9 (18%)

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	C	703	4	-	6/22/34/34	0/3/3/3
2	DGT	D	701	4	-	3/22/34/34	0/3/3/3
2	DGT	A	704	4	-	4/22/34/34	0/3/3/3
2	DGT	A	701	4	-	4/22/34/34	0/3/3/3
3	DCP	C	704	4	-	3/22/34/34	0/2/2/2
2	DGT	C	702	4	-	7/22/34/34	0/3/3/3
3	DCP	D	702	4	-	3/22/34/34	0/2/2/2
3	DCP	B	701	4	-	4/22/34/34	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	A	703	4	-	2/22/34/34	0/3/3/3
3	DCP	A	702	4	-	3/22/34/34	0/2/2/2
2	DGT	C	701	4	-	3/22/34/34	0/3/3/3
2	DGT	B	702	4	-	3/22/34/34	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	703	DGT	O6-C6	6.97	1.36	1.23
2	D	701	DGT	O6-C6	6.89	1.36	1.23
2	C	702	DGT	O6-C6	6.86	1.36	1.23
2	C	703	DGT	O6-C6	6.81	1.36	1.23
2	A	704	DGT	O6-C6	6.73	1.36	1.23
2	C	701	DGT	O6-C6	6.71	1.36	1.23
2	A	701	DGT	O6-C6	6.71	1.36	1.23
2	B	702	DGT	O6-C6	6.50	1.35	1.23
2	A	703	DGT	PB-O3B	-4.09	1.55	1.59
2	A	704	DGT	PB-O3A	-4.02	1.55	1.59
3	B	701	DCP	C4-N4	3.97	1.43	1.33
3	A	702	DCP	C4-N4	3.87	1.43	1.33
3	D	702	DCP	C4-N4	3.84	1.43	1.33
3	C	704	DCP	C4-N4	3.84	1.43	1.33
2	D	701	DGT	PB-O3B	-3.78	1.55	1.59
2	C	702	DGT	PB-O3A	-3.74	1.55	1.59
2	C	702	DGT	PB-O3B	-3.74	1.55	1.59
2	A	704	DGT	PB-O3B	-3.73	1.55	1.59
2	C	701	DGT	PB-O3B	-3.72	1.55	1.59
2	B	702	DGT	PB-O3B	-3.66	1.55	1.59
2	A	701	DGT	PB-O3B	-3.62	1.55	1.59
2	C	703	DGT	PB-O3B	-3.58	1.55	1.59
2	C	701	DGT	PB-O3A	-3.56	1.55	1.59
2	A	701	DGT	PB-O3A	-3.41	1.55	1.59
2	D	701	DGT	PB-O3A	-3.36	1.55	1.59
2	C	703	DGT	PB-O3A	-3.25	1.56	1.59
2	A	703	DGT	PB-O3A	-3.23	1.56	1.59
2	C	703	DGT	C5'-C4'	-3.02	1.42	1.51
2	A	701	DGT	C5'-C4'	-2.99	1.42	1.51
2	A	703	DGT	C2-N2	2.89	1.40	1.34
2	A	704	DGT	C5'-C4'	-2.84	1.43	1.51
2	A	701	DGT	C2-N2	2.84	1.40	1.34
2	B	702	DGT	C5'-C4'	-2.83	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	DGT	PG-O3G	2.81	1.59	1.50
2	C	702	DGT	C5'-C4'	-2.81	1.43	1.51
2	C	703	DGT	O3'-C3'	-2.78	1.37	1.43
2	C	701	DGT	C5'-C4'	-2.77	1.43	1.51
2	C	701	DGT	C2-N2	2.77	1.40	1.34
2	B	702	DGT	PA-O3A	2.77	1.62	1.59
2	B	702	DGT	C2-N2	2.76	1.40	1.34
2	C	703	DGT	C2-N2	2.75	1.40	1.34
2	D	701	DGT	O3'-C3'	-2.75	1.37	1.43
2	A	703	DGT	C5'-C4'	-2.74	1.43	1.51
2	B	702	DGT	PB-O3A	-2.74	1.56	1.59
2	A	703	DGT	O3'-C3'	-2.73	1.37	1.43
2	D	701	DGT	C5'-C4'	-2.72	1.43	1.51
2	A	704	DGT	C2-N2	2.69	1.40	1.34
2	D	701	DGT	C2-N2	2.69	1.40	1.34
2	C	702	DGT	O3'-C3'	-2.66	1.37	1.43
2	D	701	DGT	C6-N1	-2.66	1.33	1.38
3	C	704	DCP	O3'-C3'	-2.65	1.37	1.43
2	A	701	DGT	O3'-C3'	-2.64	1.37	1.43
3	D	702	DCP	C5'-C4'	-2.64	1.43	1.51
2	A	704	DGT	O3'-C3'	-2.64	1.37	1.43
3	A	702	DCP	O3'-C3'	-2.61	1.37	1.43
3	B	701	DCP	O3'-C3'	-2.60	1.37	1.43
3	D	702	DCP	O3'-C3'	-2.54	1.38	1.43
2	B	702	DGT	O3'-C3'	-2.54	1.38	1.43
3	C	704	DCP	C2-N1	-2.53	1.34	1.40
2	C	702	DGT	C2-N2	2.52	1.40	1.34
3	B	701	DCP	C5'-C4'	-2.51	1.44	1.51
2	C	703	DGT	C2'-C3'	-2.51	1.46	1.52
2	A	703	DGT	PA-O3A	2.51	1.62	1.59
2	C	701	DGT	C6-N1	-2.50	1.34	1.38
2	C	701	DGT	O3'-C3'	-2.50	1.38	1.43
2	B	702	DGT	C6-N1	-2.49	1.34	1.38
2	A	701	DGT	C2'-C3'	-2.48	1.46	1.52
2	D	701	DGT	C2'-C3'	-2.45	1.46	1.52
3	A	702	DCP	C5'-C4'	-2.45	1.44	1.51
2	A	704	DGT	C2'-C3'	-2.43	1.46	1.52
3	D	702	DCP	C2-N1	-2.42	1.35	1.40
3	B	701	DCP	C2-N1	-2.41	1.35	1.40
2	D	701	DGT	PA-O3A	2.41	1.62	1.59
3	C	704	DCP	C5'-C4'	-2.40	1.44	1.51
2	A	703	DGT	C2'-C3'	-2.39	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	DCP	C2-N1	-2.38	1.35	1.40
3	B	701	DCP	C2'-C3'	-2.35	1.46	1.52
2	B	702	DGT	C2'-C3'	-2.35	1.46	1.52
2	C	703	DGT	PA-O3A	2.34	1.62	1.59
2	C	703	DGT	C6-N1	-2.30	1.34	1.38
3	C	704	DCP	C2'-C3'	-2.28	1.47	1.52
2	C	701	DGT	PA-O3A	2.28	1.62	1.59
2	A	701	DGT	C6-N1	-2.28	1.34	1.38
2	A	703	DGT	C6-N1	-2.27	1.34	1.38
2	C	702	DGT	C2'-C3'	-2.27	1.47	1.52
2	A	704	DGT	C6-N1	-2.26	1.34	1.38
3	A	702	DCP	C2'-C3'	-2.25	1.47	1.52
2	C	702	DGT	PA-O3A	2.24	1.61	1.59
3	D	702	DCP	C2'-C3'	-2.17	1.47	1.52
2	A	701	DGT	C5-N7	-2.15	1.34	1.39
2	C	703	DGT	C5-N7	-2.14	1.34	1.39
2	C	701	DGT	C2'-C3'	-2.13	1.47	1.52
3	A	702	DCP	C6-C5	2.11	1.40	1.35
3	C	704	DCP	C6-C5	2.09	1.39	1.35
3	A	702	DCP	PB-O3B	-2.09	1.57	1.59
3	D	702	DCP	C6-C5	2.07	1.39	1.35
2	A	703	DGT	C5-N7	-2.03	1.35	1.39
3	B	701	DCP	C6-C5	2.03	1.39	1.35
2	A	704	DGT	C3'-C4'	-2.01	1.47	1.53

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	DGT	C5-C4-N3	-5.49	119.66	128.39
2	C	702	DGT	C5-C4-N3	-5.48	119.67	128.39
2	C	703	DGT	C5-C4-N3	-5.47	119.69	128.39
2	C	701	DGT	C5-C4-N3	-5.43	119.74	128.39
2	A	701	DGT	C5-C4-N3	-5.41	119.77	128.39
2	A	703	DGT	C5-C4-N3	-5.25	120.03	128.39
2	D	701	DGT	C5-C4-N3	-5.06	120.34	128.39
2	B	702	DGT	C5-C4-N3	-4.99	120.44	128.39
2	C	702	DGT	C2-N3-C4	4.77	120.52	112.30
2	A	704	DGT	C2-N3-C4	4.66	120.33	112.30
2	A	701	DGT	C2-N3-C4	4.64	120.30	112.30
2	C	703	DGT	C2-N3-C4	4.64	120.30	112.30
2	C	701	DGT	C2-N3-C4	4.55	120.14	112.30
2	A	703	DGT	C2-N3-C4	4.39	119.86	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	DGT	C2-N3-C4	4.35	119.80	112.30
2	D	701	DGT	C2-N3-C4	4.30	119.70	112.30
2	C	703	DGT	N9-C4-N3	3.87	133.69	125.95
2	A	701	DGT	N9-C4-N3	3.82	133.60	125.95
2	A	704	DGT	N9-C4-N3	3.71	133.37	125.95
2	C	702	DGT	N9-C4-N3	3.59	133.12	125.95
2	A	703	DGT	N9-C4-N3	3.57	133.10	125.95
2	C	701	DGT	N9-C4-N3	3.43	132.81	125.95
2	B	702	DGT	N9-C4-N3	3.24	132.43	125.95
2	D	701	DGT	N9-C4-N3	3.18	132.31	125.95
2	C	702	DGT	O1G-PG-O3B	2.80	114.02	104.64
3	D	702	DCP	O2-C2-N3	-2.61	118.21	122.33
2	A	703	DGT	O5'-C5'-C4'	2.61	117.89	108.99
2	D	701	DGT	N9-C8-N7	-2.54	108.69	113.40
3	A	702	DCP	O2-C2-N3	-2.54	118.33	122.33
3	B	701	DCP	O3G-PG-O3B	2.51	113.04	104.64
2	B	702	DGT	N9-C8-N7	-2.48	108.80	113.40
2	C	703	DGT	O2G-PG-O3B	2.47	112.92	104.64
2	B	702	DGT	O5'-C5'-C4'	2.46	117.38	108.99
3	C	704	DCP	O5'-C5'-C4'	2.45	117.34	108.99
2	D	701	DGT	C6-C5-N7	2.45	134.75	130.29
3	A	702	DCP	O5'-C5'-C4'	2.44	117.30	108.99
3	D	702	DCP	O4'-C1'-N1	2.43	112.17	107.86
2	B	702	DGT	C6-C5-N7	2.42	134.70	130.29
3	C	704	DCP	O4'-C1'-N1	2.41	112.13	107.86
3	C	704	DCP	C5-C6-N1	-2.40	117.93	121.84
2	C	701	DGT	O1A-PA-O3A	2.34	113.60	107.27
2	D	701	DGT	C4-C5-N7	-2.33	106.97	110.67
3	B	701	DCP	O2-C2-N3	-2.33	118.66	122.33
2	A	703	DGT	N9-C8-N7	-2.33	109.08	113.40
2	C	703	DGT	N9-C8-N7	-2.31	109.11	113.40
2	C	701	DGT	C6-C5-N7	2.29	134.45	130.29
2	C	701	DGT	O1B-PB-O3B	2.29	113.45	107.27
2	C	702	DGT	C2-N1-C6	-2.28	120.98	125.11
2	C	702	DGT	N9-C8-N7	-2.28	109.18	113.40
2	A	701	DGT	N9-C8-N7	-2.27	109.19	113.40
2	C	701	DGT	C4-C5-N7	-2.26	107.08	110.67
2	B	702	DGT	C5-C6-N1	2.26	119.00	113.25
2	A	704	DGT	O5'-C5'-C4'	2.25	116.66	108.99
2	D	701	DGT	C8-N7-C5	2.25	108.26	104.26
2	C	702	DGT	C4-C5-N7	-2.24	107.12	110.67
2	C	702	DGT	C5-C6-N1	2.24	118.95	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	DCP	O4'-C1'-N1	2.22	111.81	107.86
2	C	702	DGT	C6-C5-N7	2.21	134.31	130.29
3	C	704	DCP	O2-C2-N3	-2.20	118.86	122.33
2	C	701	DGT	N9-C8-N7	-2.19	109.34	113.40
2	C	701	DGT	C5-C6-N1	2.17	118.79	113.25
2	C	703	DGT	C8-N7-C5	2.17	108.13	104.26
2	C	702	DGT	C8-N7-C5	2.17	108.13	104.26
2	C	702	DGT	O5'-C5'-C4'	2.15	116.33	108.99
3	D	702	DCP	C5-C6-N1	-2.14	118.36	121.84
2	A	701	DGT	C5-C6-N1	2.13	118.68	113.25
2	A	704	DGT	C5-C6-N1	2.13	118.68	113.25
2	C	703	DGT	O5'-C5'-C4'	2.13	116.25	108.99
2	B	702	DGT	C4-C5-N7	-2.13	107.29	110.67
2	C	703	DGT	C5-C6-N1	2.12	118.65	113.25
2	D	701	DGT	O5'-C5'-C4'	2.12	116.19	108.99
2	C	702	DGT	O6-C6-C5	-2.11	120.95	126.53
3	B	701	DCP	C5-C6-N1	-2.11	118.41	121.84
2	A	701	DGT	C8-N7-C5	2.10	108.01	104.26
2	D	701	DGT	C5-C6-N1	2.10	118.60	113.25
2	A	703	DGT	C5-C6-N1	2.10	118.59	113.25
2	A	703	DGT	O6-C6-C5	-2.10	121.00	126.53
2	A	704	DGT	N9-C8-N7	-2.09	109.53	113.40
3	B	701	DCP	O5'-C5'-C4'	2.08	116.06	108.99
2	B	702	DGT	C8-N7-C5	2.08	107.96	104.26
2	C	701	DGT	C8-N7-C5	2.07	107.95	104.26
2	A	703	DGT	O1G-PG-O3B	2.07	111.57	104.64
3	D	702	DCP	O3G-PG-O3B	2.06	111.55	104.64
2	C	703	DGT	C4-C5-N7	-2.06	107.41	110.67
2	A	701	DGT	C6-C5-N7	2.04	134.00	130.29
2	A	704	DGT	C4-C5-N7	-2.04	107.44	110.67
2	D	701	DGT	O2G-PG-O3B	2.03	111.45	104.64
2	A	704	DGT	O6-C6-C5	-2.02	121.21	126.53
2	A	704	DGT	C6-C5-N7	2.01	133.96	130.29
2	A	703	DGT	C4-C5-N7	-2.01	107.48	110.67
3	D	702	DCP	O5'-C5'-C4'	2.01	115.83	108.99
2	A	701	DGT	C4-C5-N7	-2.01	107.49	110.67
2	C	703	DGT	C6-C5-N7	2.01	133.94	130.29
2	C	703	DGT	O6-C6-C5	-2.00	121.25	126.53

There are no chirality outliers.

All (45) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

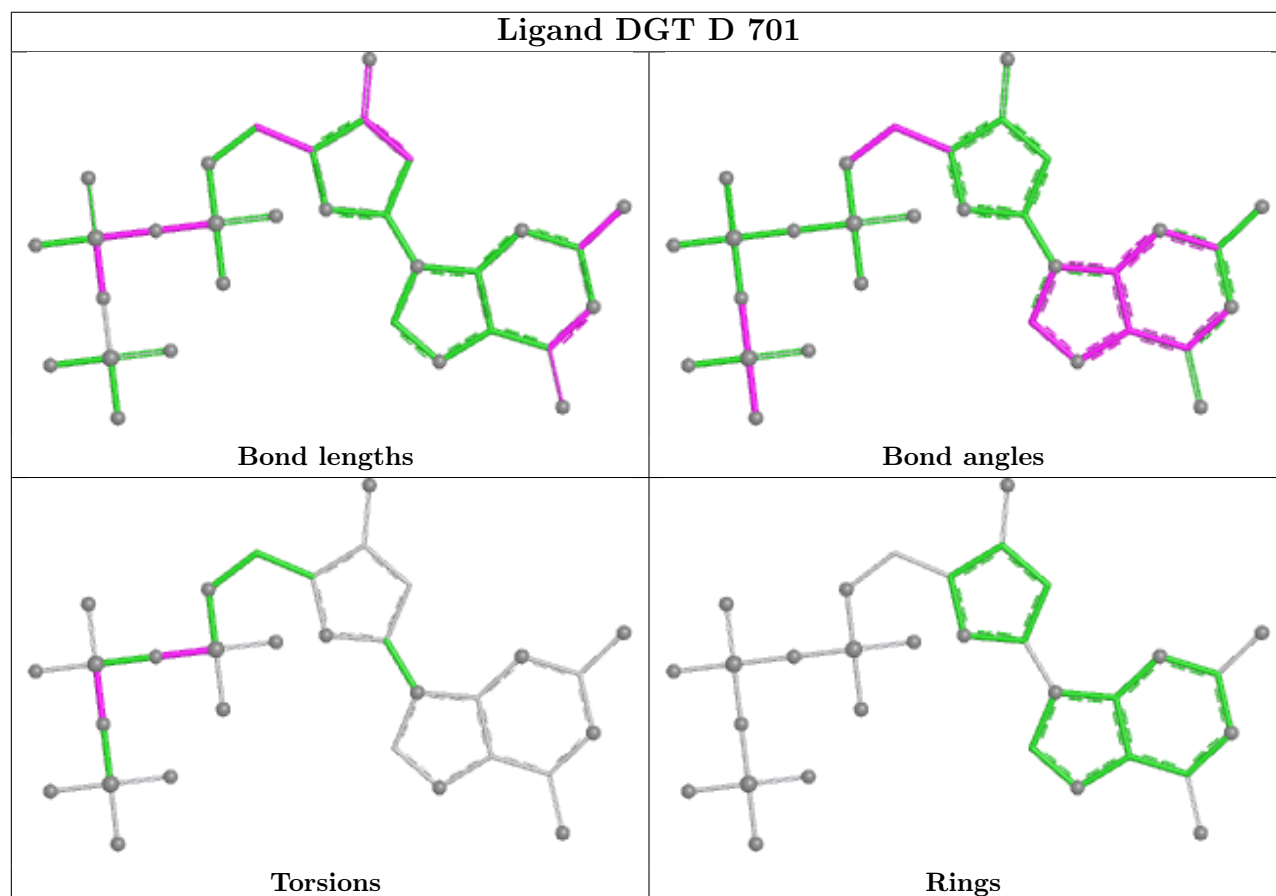
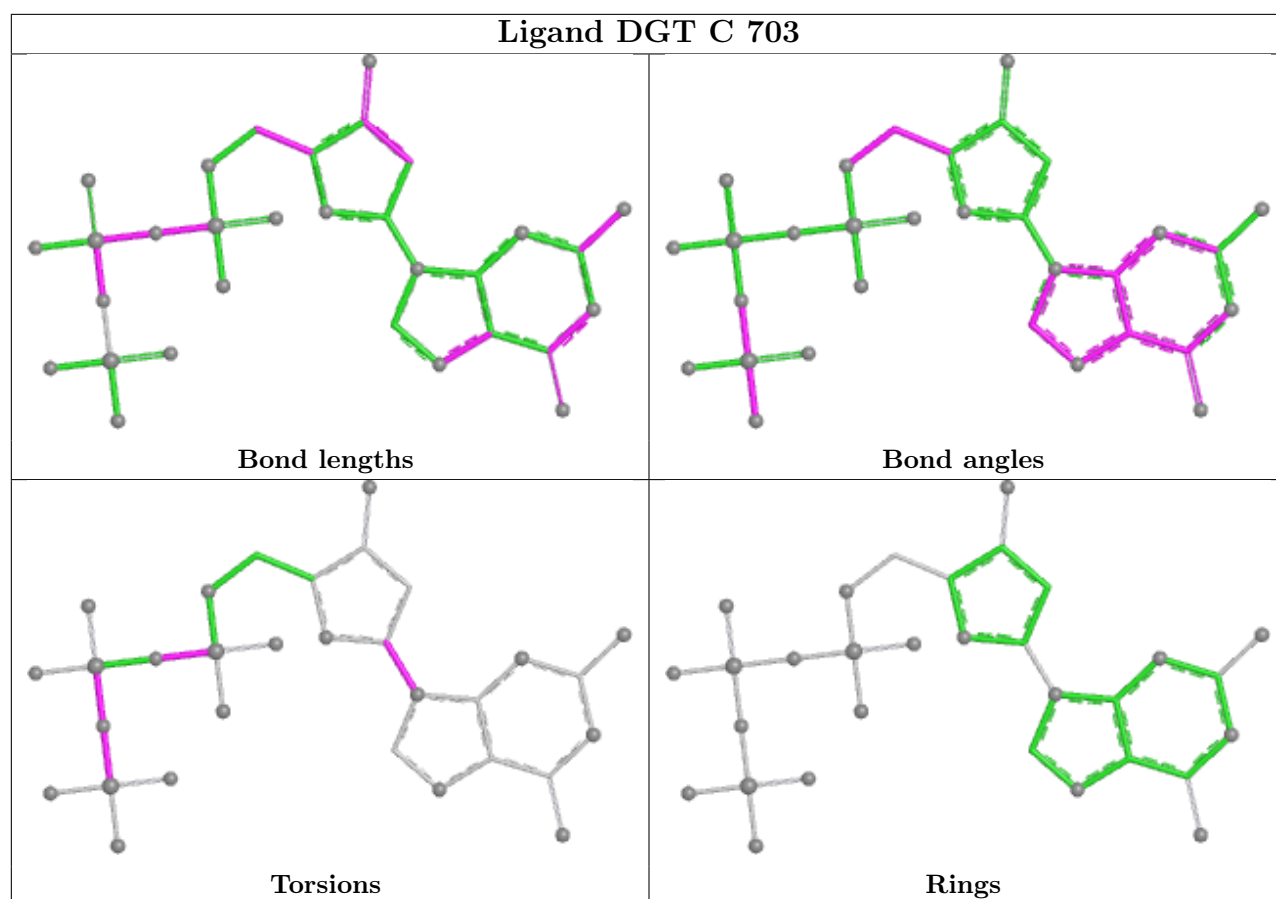
Mol	Chain	Res	Type	Atoms
2	A	704	DGT	PG-O3B-PB-O1B
2	D	701	DGT	PB-O3A-PA-O1A

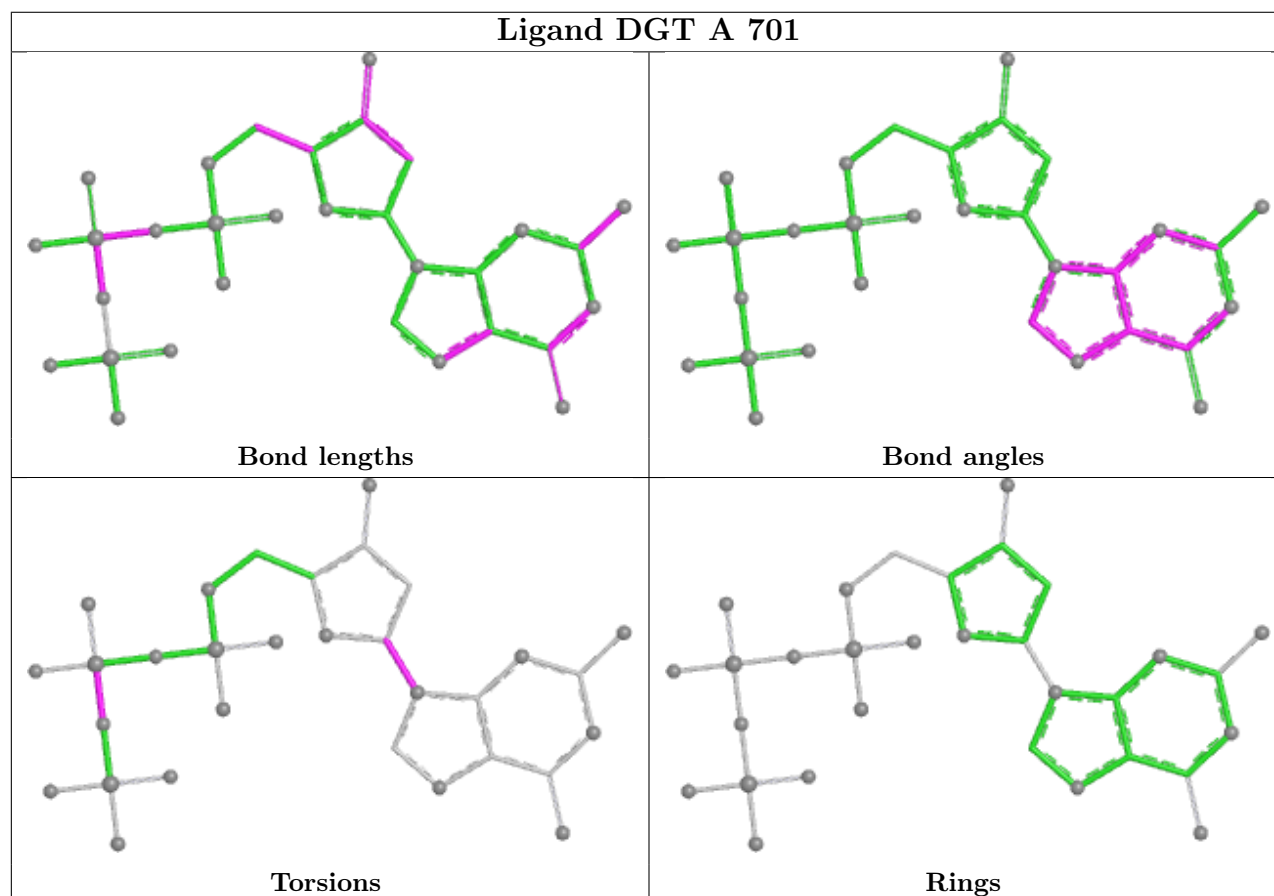
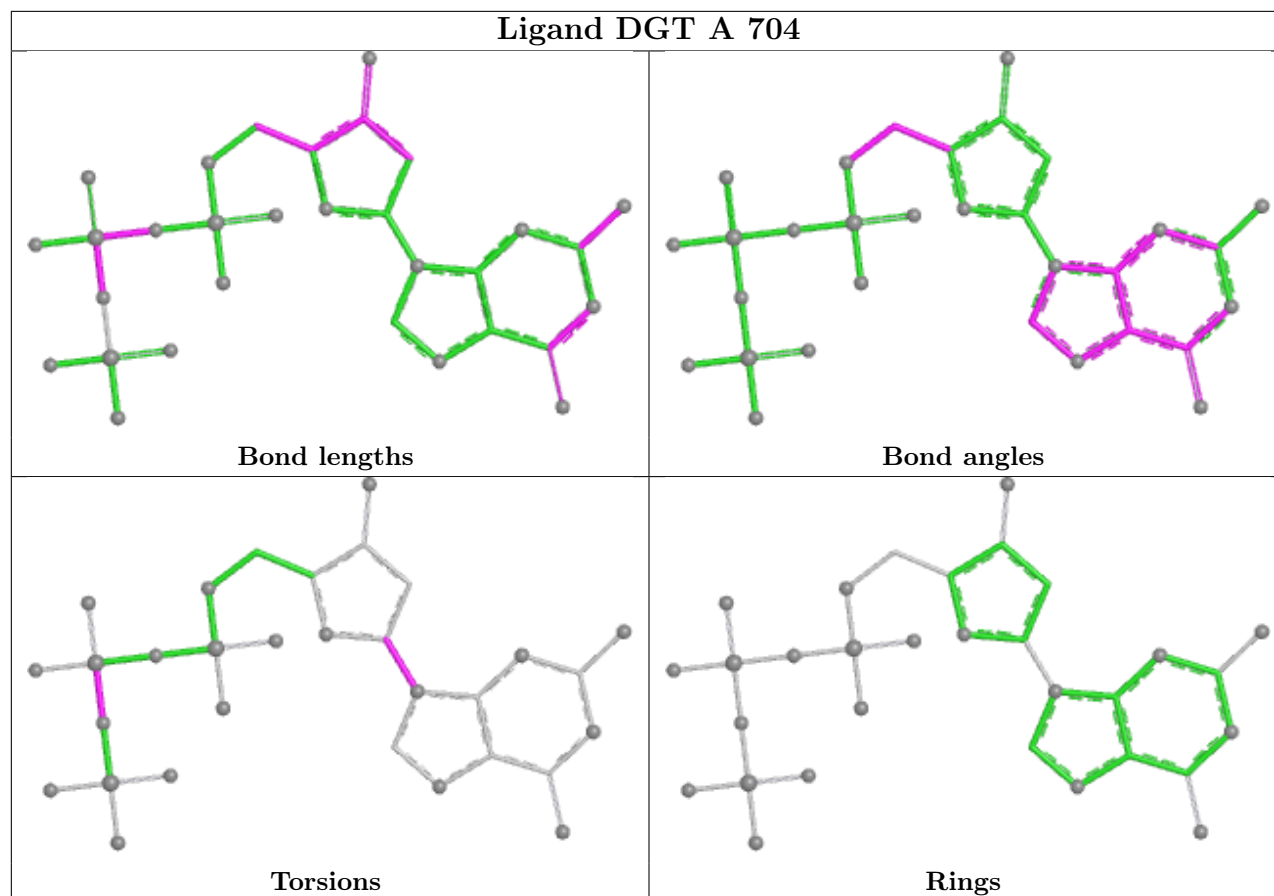
There are no ring outliers.

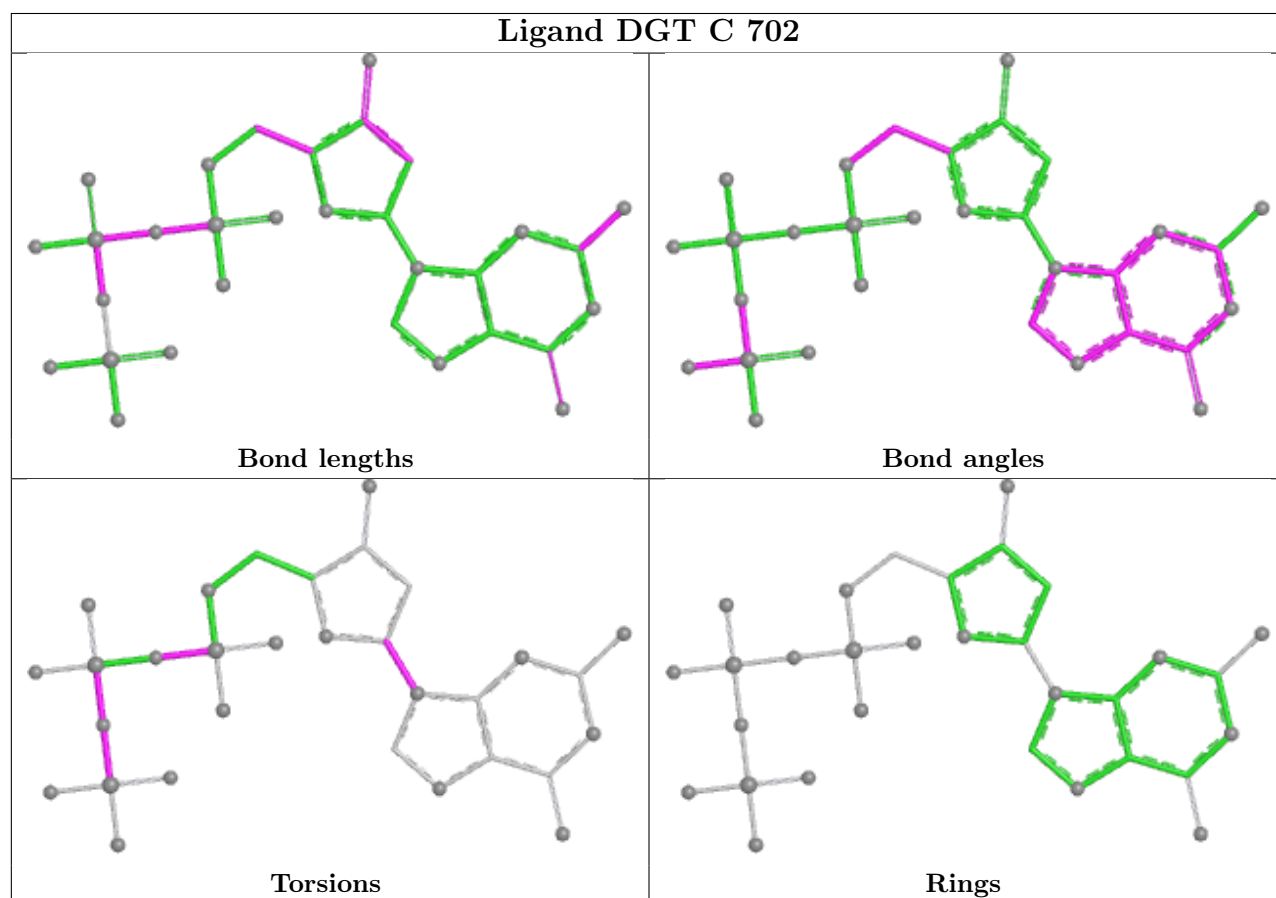
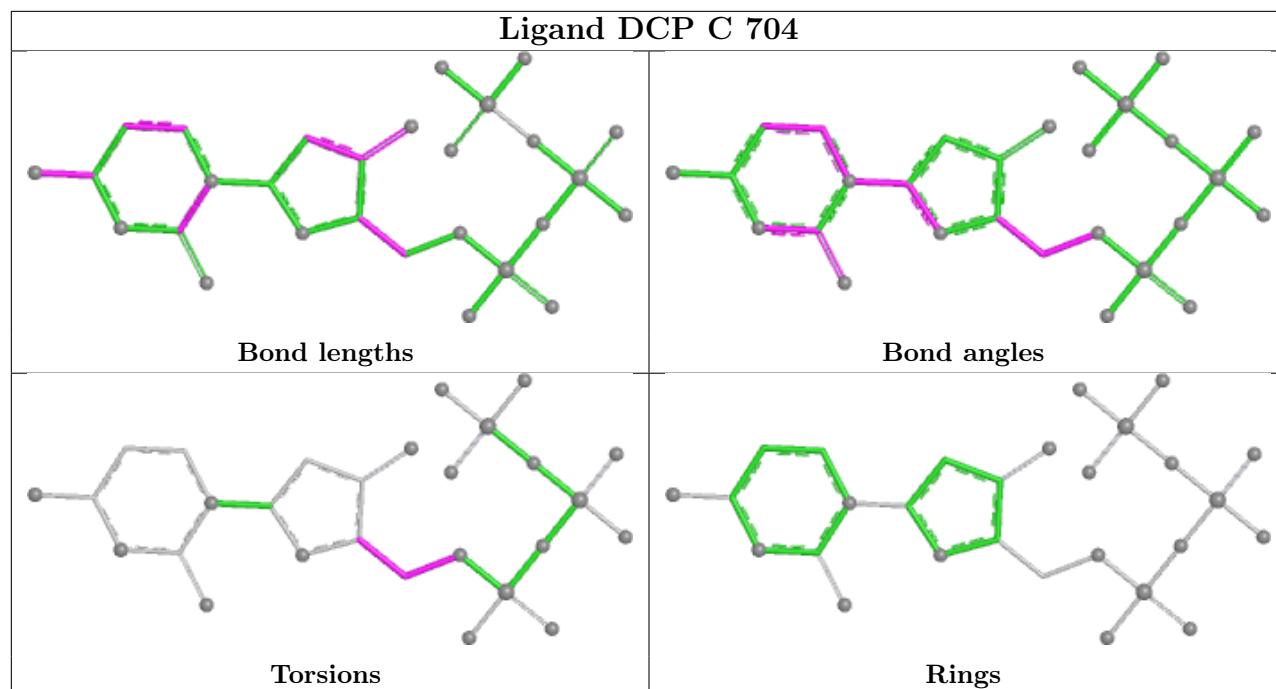
8 monomers are involved in 10 short contacts:

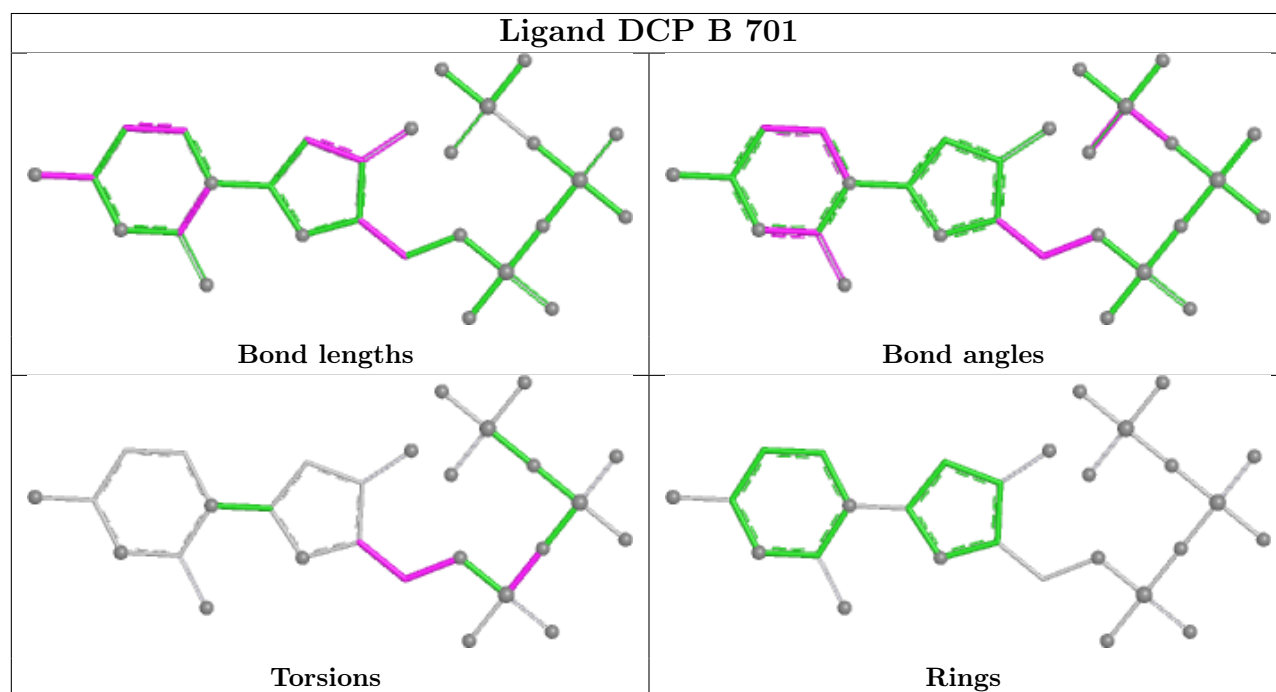
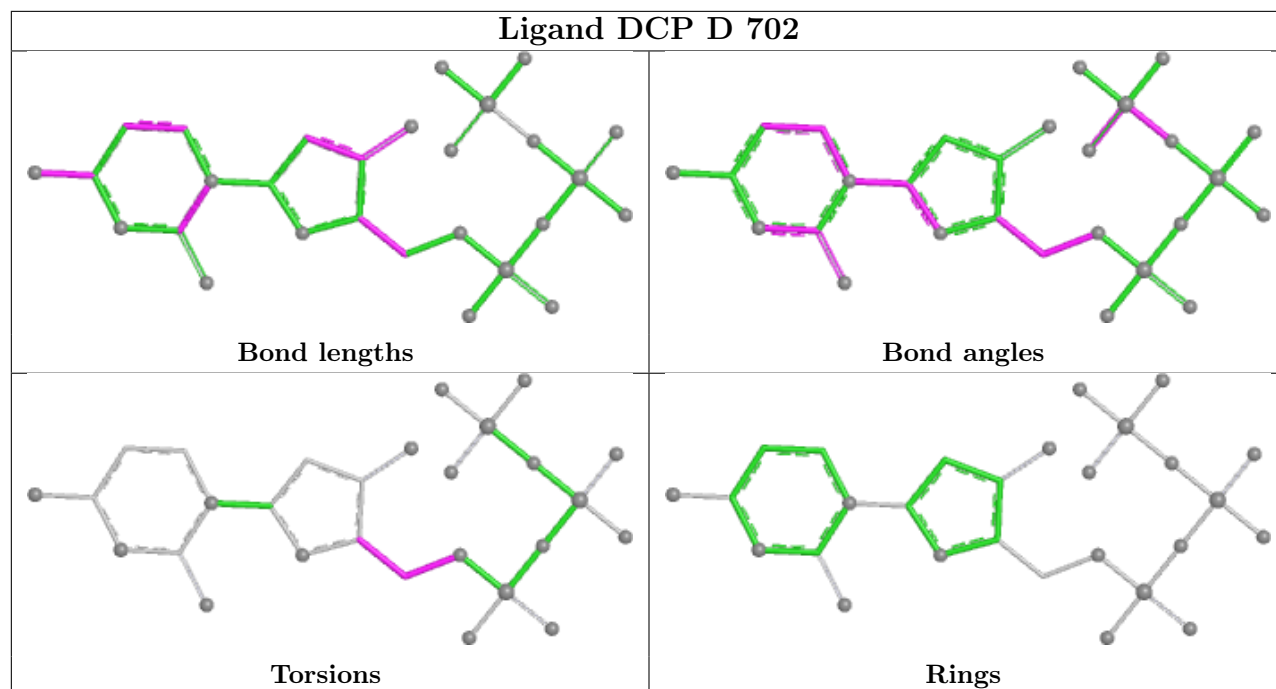
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	DGT	1	0
2	A	701	DGT	1	0
3	C	704	DCP	2	0
2	C	702	DGT	2	0
3	D	702	DCP	2	0
3	B	701	DCP	1	0
3	A	702	DCP	2	0
2	C	701	DGT	1	0

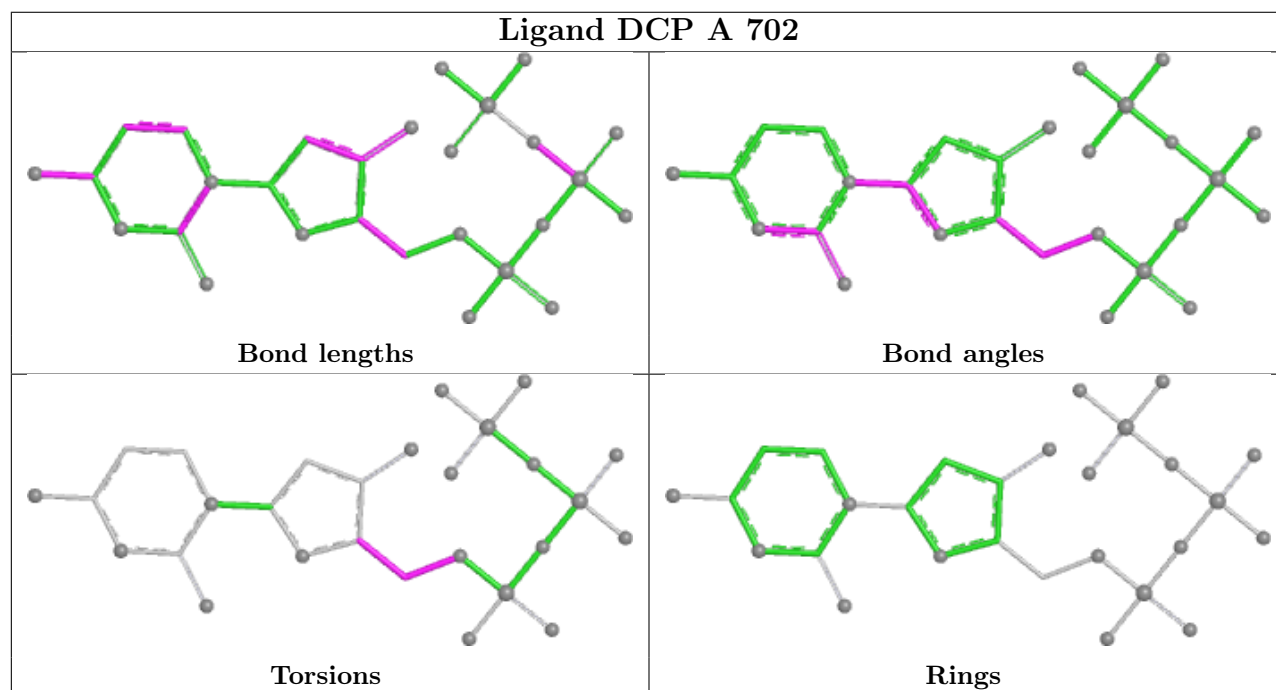
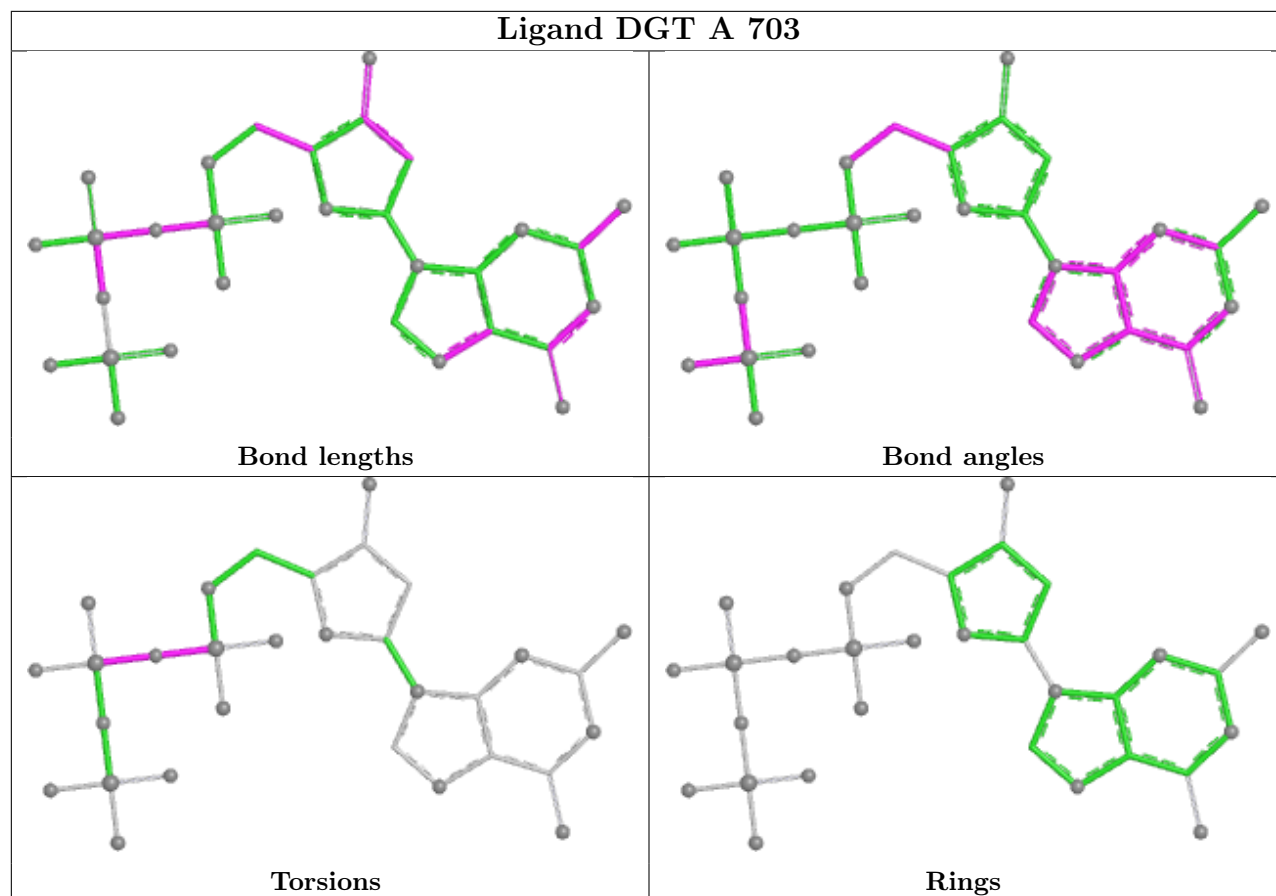
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

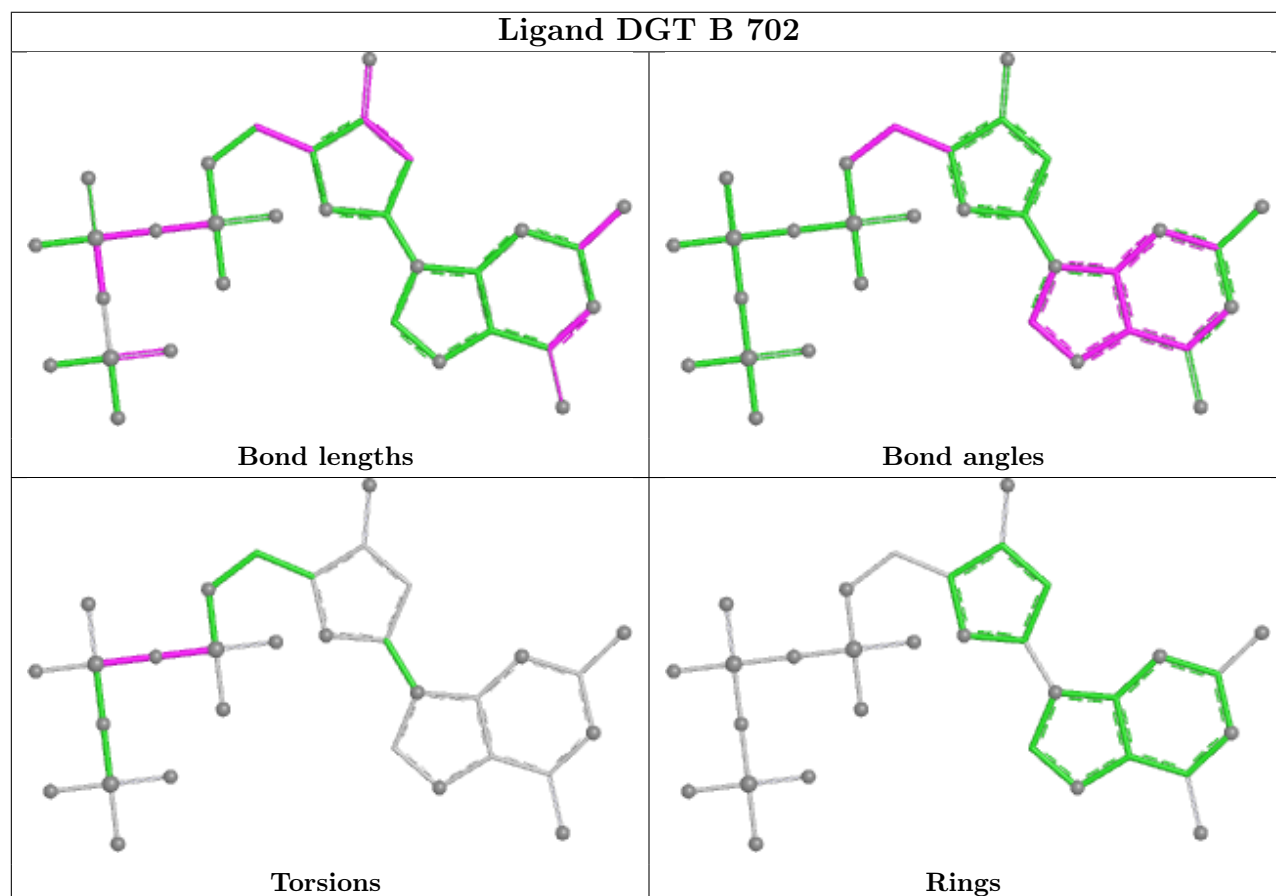
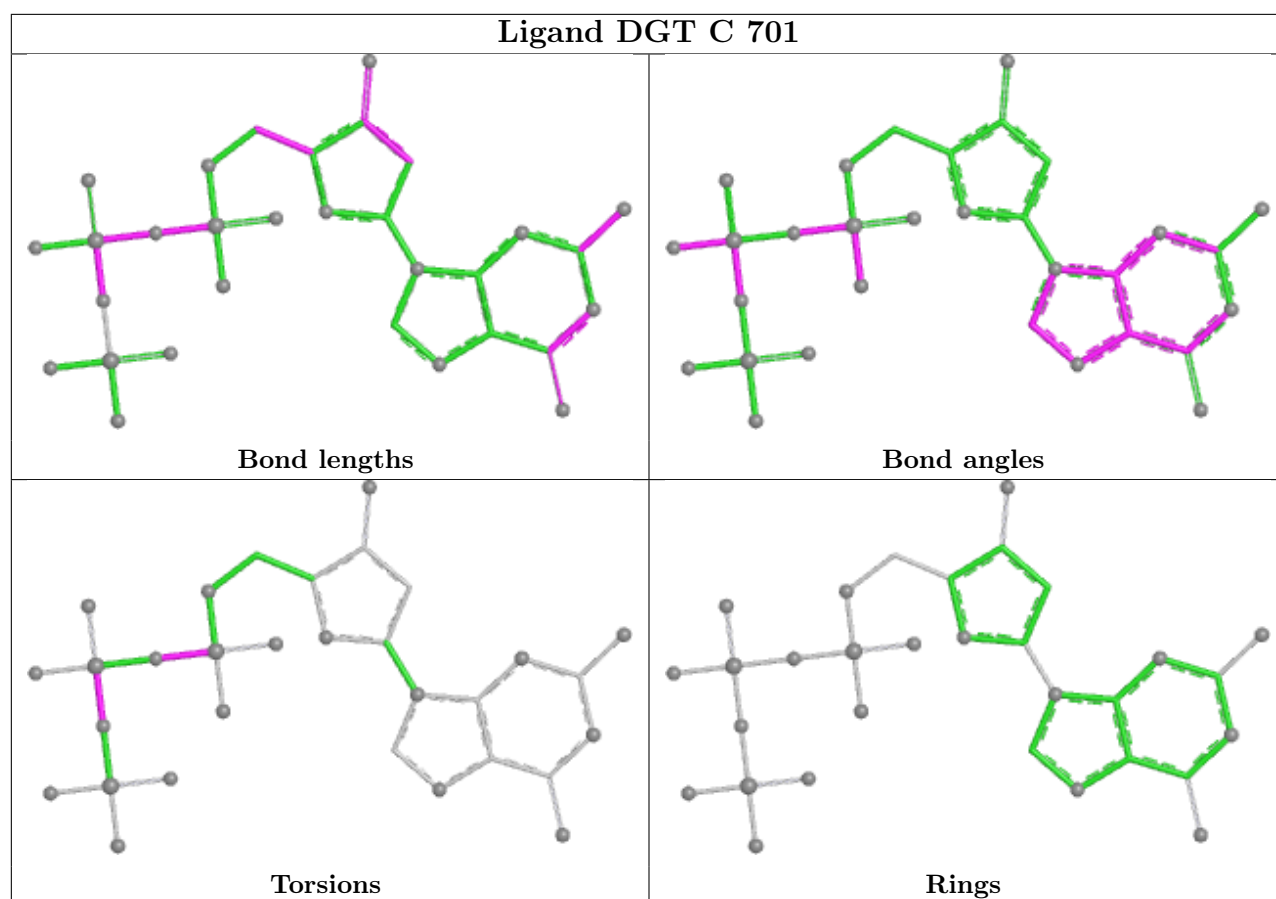












5.7 Other polymers [i](#)

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	480/550 (87%)	0.66	30 (6%) 26 27	17, 28, 42, 52	238 (49%)
1	B	481/550 (87%)	0.38	18 (3%) 45 47	13, 24, 40, 55	194 (40%)
1	C	481/550 (87%)	0.77	51 (10%) 11 12	17, 28, 51, 71	238 (49%)
1	D	481/550 (87%)	0.28	16 (3%) 49 51	13, 23, 34, 55	190 (39%)
All	All	1923/2200 (87%)	0.52	115 (5%) 27 29	13, 26, 43, 71	860 (44%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	408	ARG	4.4
1	B	488	LEU	4.3
1	A	535	ASN	4.3
1	A	343	VAL	4.1
1	C	394	ASP	4.0
1	C	574	ALA	3.9
1	D	466	ILE	3.7
1	D	396	TYR	3.7
1	D	345	ASN	3.6
1	C	488	LEU	3.5
1	A	284	LEU	3.5
1	C	592	THR	3.4
1	A	529	ALA	3.4
1	D	113	ASP	3.4
1	B	491	VAL	3.4
1	C	568	TYR	3.3
1	C	569	PHE	3.2
1	B	495	ALA	3.2
1	B	489	LEU	3.1
1	D	535	ASN	3.1
1	C	184	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	557	VAL	3.1
1	D	284	LEU	3.1
1	C	400	THR	3.0
1	C	388	ASP	3.0
1	C	473	TYR	3.0
1	A	328	ASN	2.9
1	C	343	VAL	2.9
1	A	473	TYR	2.9
1	A	549	LEU	2.9
1	D	593	PRO	2.9
1	C	491	VAL	2.9
1	A	468	ILE	2.9
1	C	578	PHE	2.8
1	C	575	ASP	2.8
1	C	590	LEU	2.8
1	A	215	HIS	2.8
1	B	467	LYS	2.8
1	B	326	GLN	2.7
1	C	588	ALA	2.7
1	C	570	VAL	2.7
1	B	400	THR	2.7
1	D	276	LEU	2.7
1	C	563	TYR	2.7
1	C	487	VAL	2.7
1	C	492	LYS	2.7
1	A	488	LEU	2.6
1	C	527	ASN	2.6
1	B	490	ASP	2.6
1	C	571	GLN	2.6
1	A	578	PHE	2.5
1	C	326	GLN	2.5
1	A	275	PRO	2.5
1	C	485	PRO	2.5
1	A	463	THR	2.5
1	A	524	THR	2.5
1	C	405	LYS	2.5
1	C	489	LEU	2.4
1	A	502	VAL	2.4
1	C	344	ASP	2.4
1	C	397	ILE	2.4
1	D	344	ASP	2.4
1	C	522	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	276	LEU	2.4
1	A	345	ASN	2.4
1	A	597	GLU	2.3
1	D	465	GLN	2.3
1	A	508	GLY	2.3
1	A	466	ILE	2.3
1	D	326	GLN	2.3
1	C	407	TYR	2.3
1	B	543	GLU	2.3
1	B	593	PRO	2.3
1	A	218	ASP	2.3
1	C	493	LEU	2.3
1	C	218	ASP	2.3
1	C	396	TYR	2.3
1	B	564	ALA	2.2
1	B	284	LEU	2.2
1	A	471	GLU	2.2
1	A	599	ASN	2.2
1	C	587	ILE	2.2
1	A	464	GLY	2.2
1	C	403	GLY	2.2
1	B	588	ALA	2.2
1	A	522	CYS	2.2
1	B	262	GLU	2.2
1	A	344	ASP	2.2
1	A	403	GLY	2.2
1	C	215	HIS	2.2
1	C	598	TRP	2.2
1	C	495	ALA	2.1
1	C	230	LYS	2.1
1	B	591	ILE	2.1
1	C	586	VAL	2.1
1	C	483	ALA	2.1
1	C	515	ILE	2.1
1	D	403	GLY	2.1
1	D	470	ARG	2.1
1	A	285	TRP	2.1
1	C	471	GLU	2.1
1	C	585	ASP	2.1
1	D	490	ASP	2.1
1	D	406	LYS	2.1
1	A	552	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	229	VAL	2.1
1	C	476	LEU	2.0
1	B	577	ASN	2.0
1	B	470	ARG	2.0
1	A	230	LYS	2.0
1	A	302	SER	2.0
1	B	481	ALA	2.0
1	C	481	ALA	2.0
1	C	539	GLN	2.0
1	D	596	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

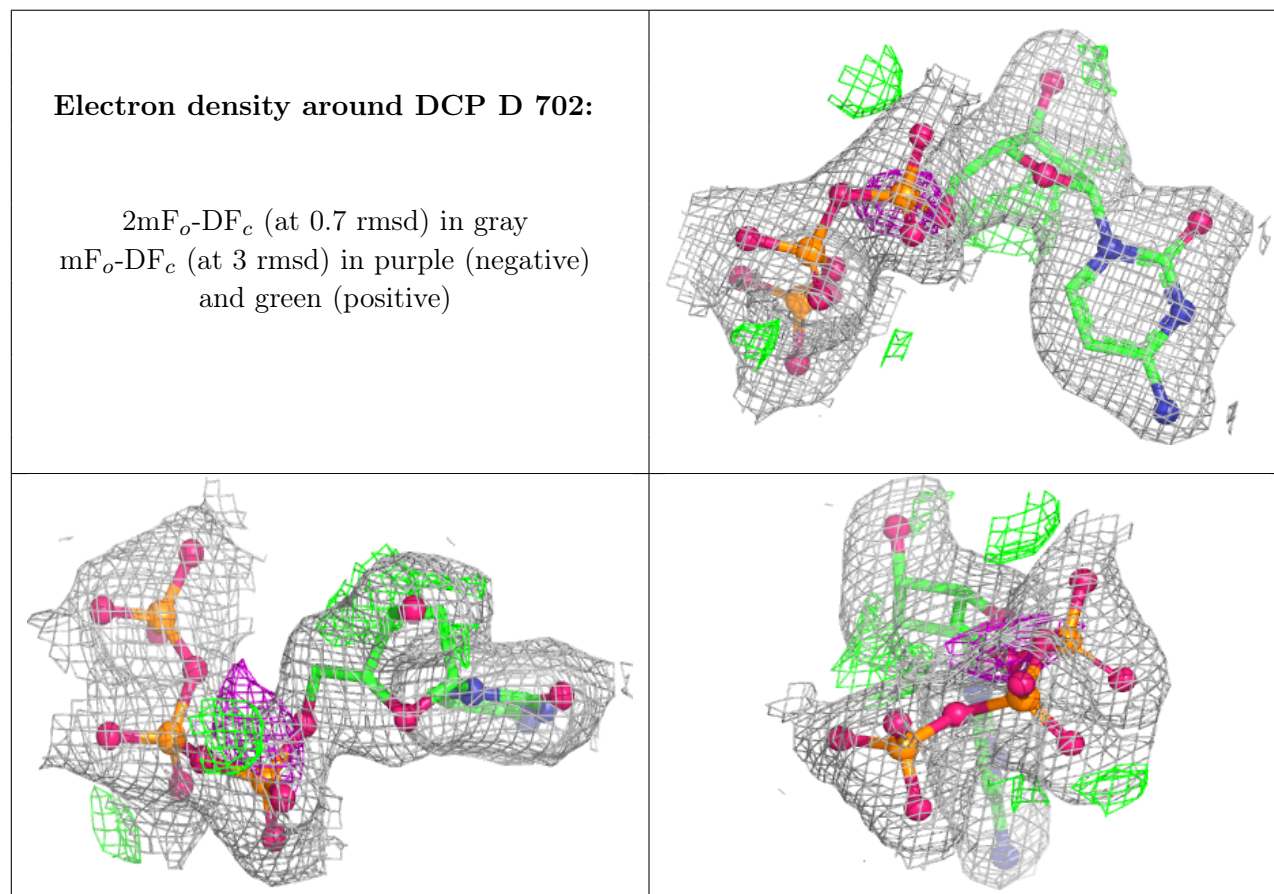
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	706	1/1	0.82	0.06	19,19,19,19	0
4	MG	B	704	1/1	0.91	0.06	23,23,23,23	1
4	MG	C	706	1/1	0.91	0.09	35,35,35,35	0
4	MG	A	705	1/1	0.92	0.11	34,34,34,34	0
3	DCP	D	702	28/28	0.93	0.08	13,18,22,24	28
3	DCP	C	704	28/28	0.94	0.07	19,27,30,34	28
4	MG	B	703	1/1	0.94	0.07	26,26,26,26	0
3	DCP	A	702	28/28	0.95	0.07	19,25,31,33	28
2	DGT	A	703	31/31	0.95	0.07	19,24,30,32	31
2	DGT	C	701	31/31	0.95	0.07	16,21,26,29	0
4	MG	C	705	1/1	0.95	0.04	22,22,22,22	1
2	DGT	C	703	31/31	0.95	0.06	17,22,27,30	31
2	DGT	C	702	31/31	0.96	0.06	16,20,25,28	0

Continued on next page...

Continued from previous page...

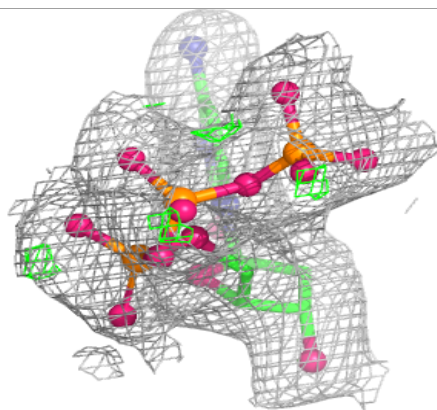
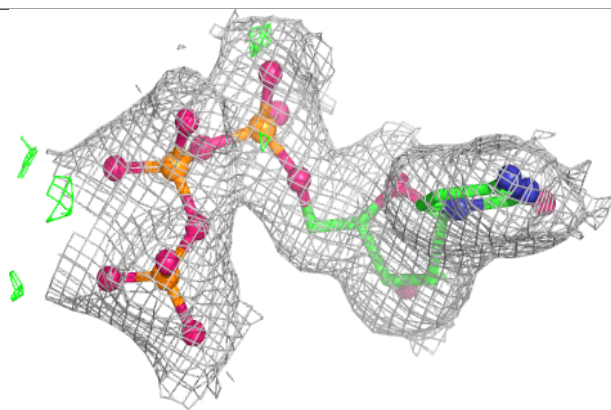
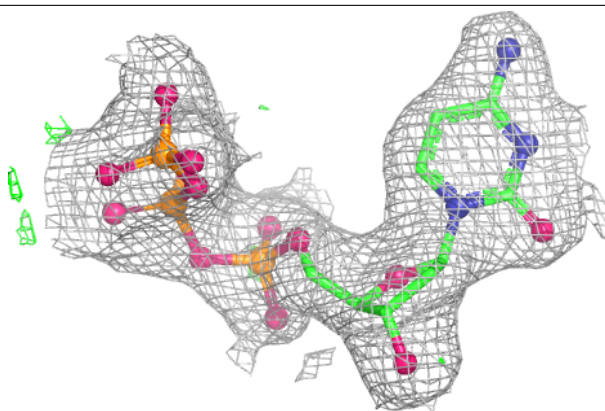
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DGT	B	702	31/31	0.96	0.06	15,17,21,22	0
2	DGT	A	701	31/31	0.96	0.06	17,21,28,30	0
3	DCP	B	701	28/28	0.96	0.06	14,19,23,28	28
2	DGT	A	704	31/31	0.97	0.06	13,17,22,25	0
2	DGT	D	701	31/31	0.97	0.05	15,19,26,27	0
4	MG	C	707	1/1	0.98	0.03	22,22,22,22	0
4	MG	D	703	1/1	0.98	0.06	17,17,17,17	1

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

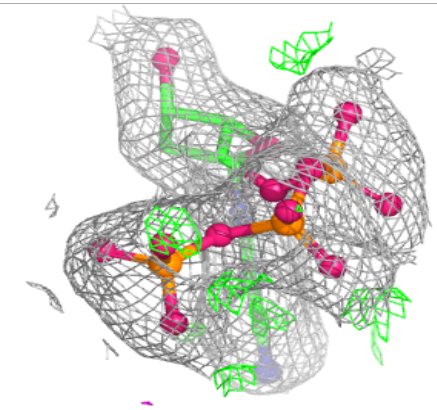
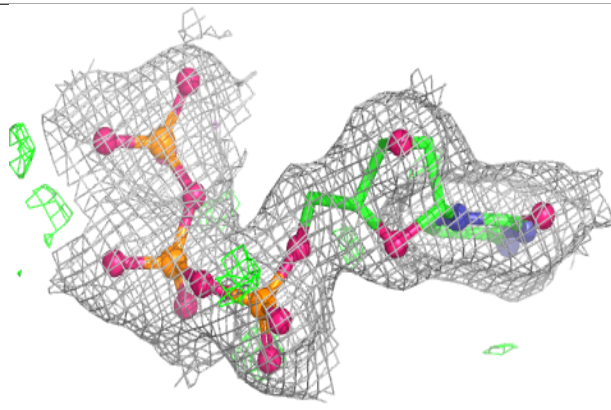
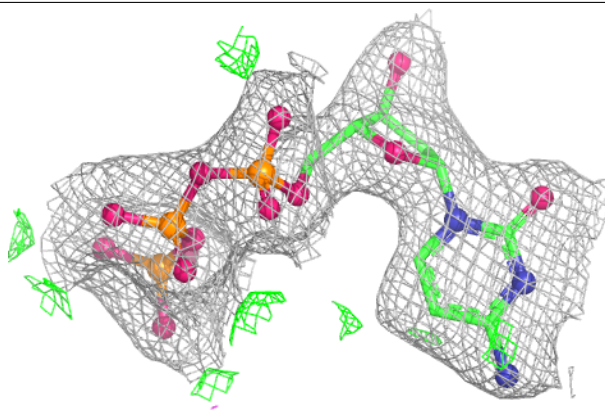


Electron density around DCP C 704:

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

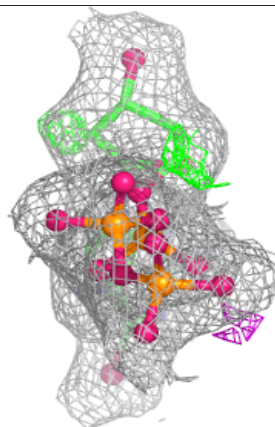
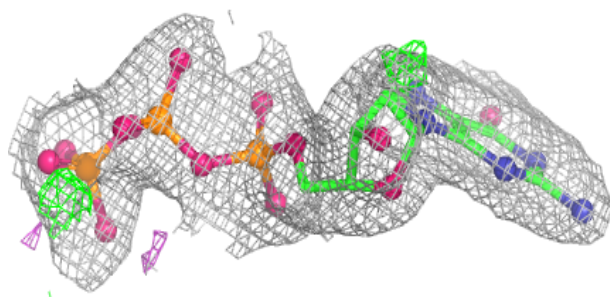
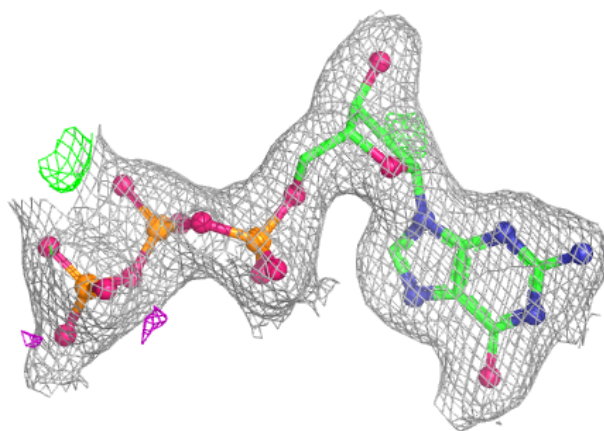
**Electron density around DCP A 702:**

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

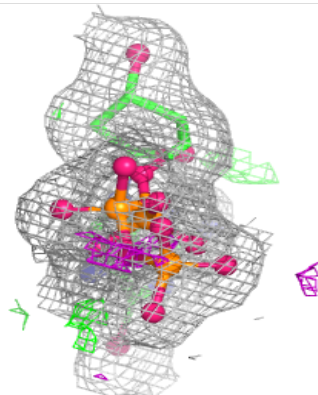
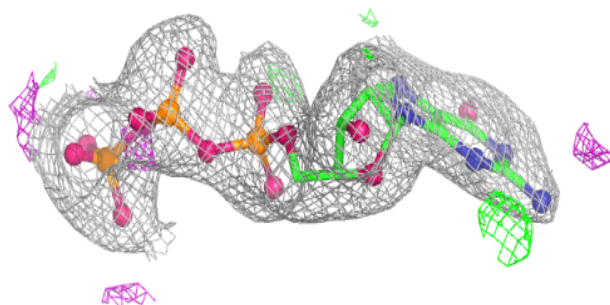
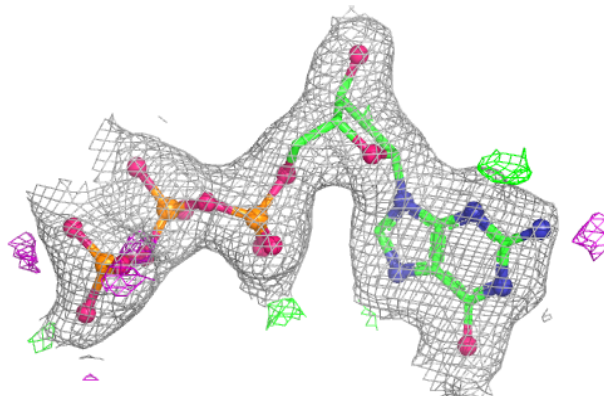


Electron density around DGT A 703:

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

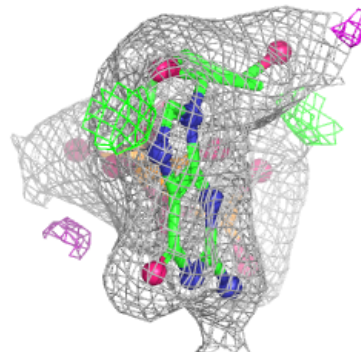
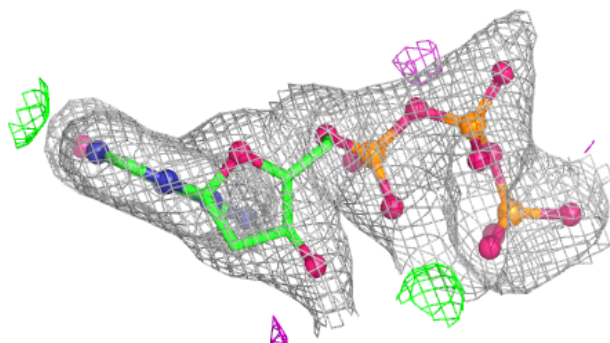
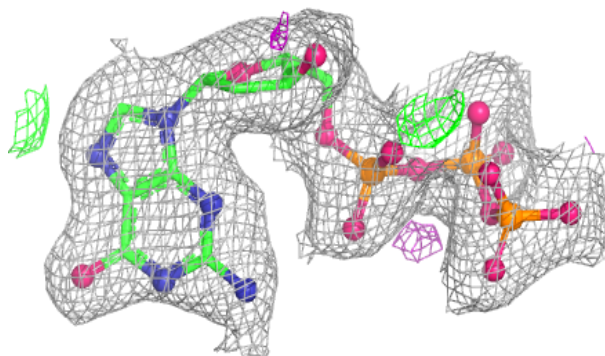
**Electron density around DGT C 701:**

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

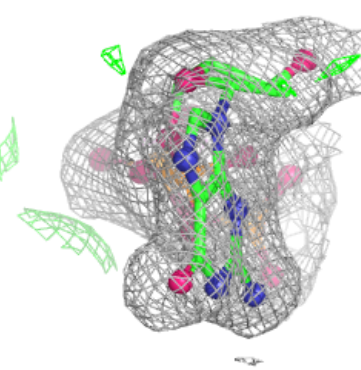
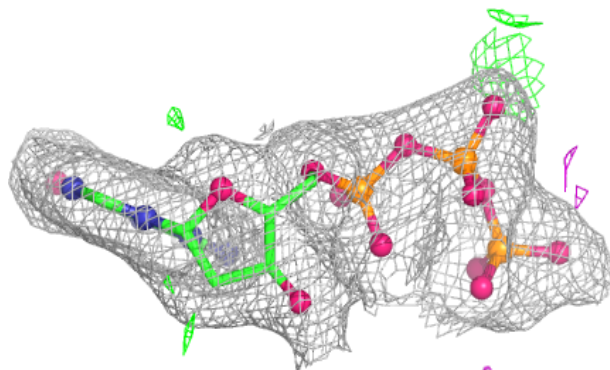
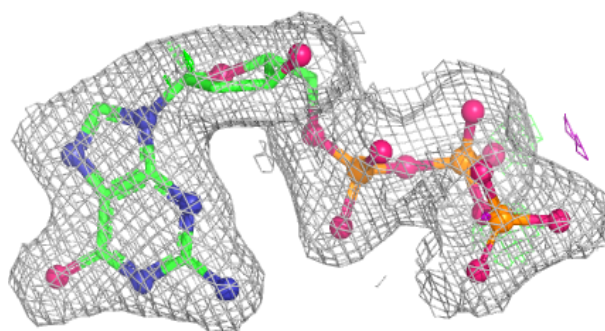


Electron density around DGT C 703:

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

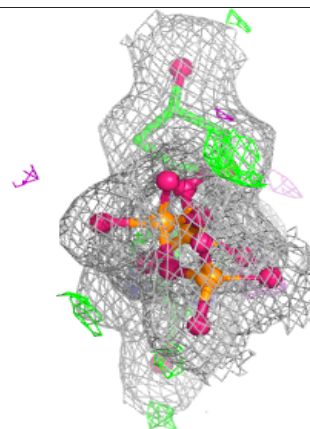
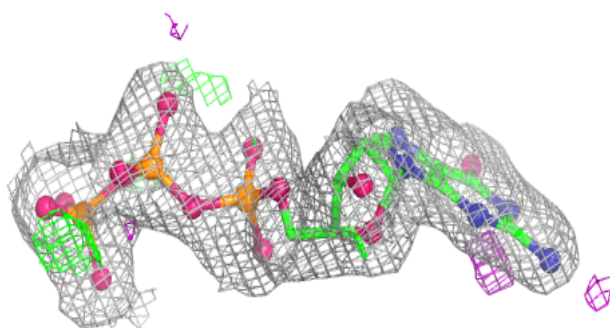
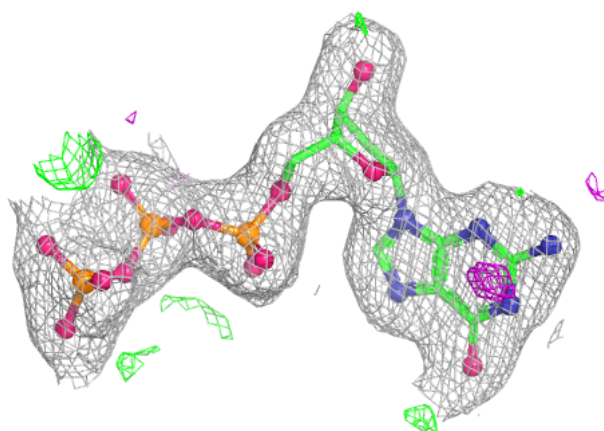
**Electron density around DGT C 702:**

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

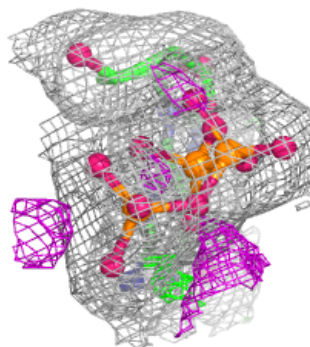
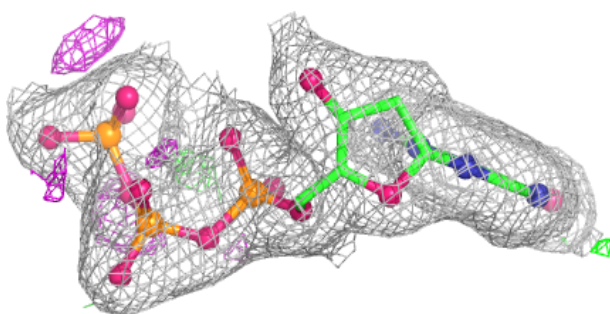
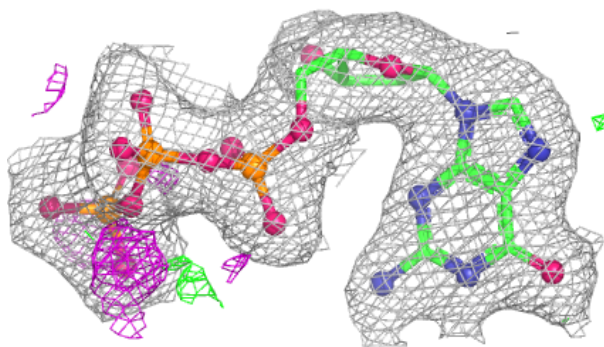


Electron density around DGT B 702:

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

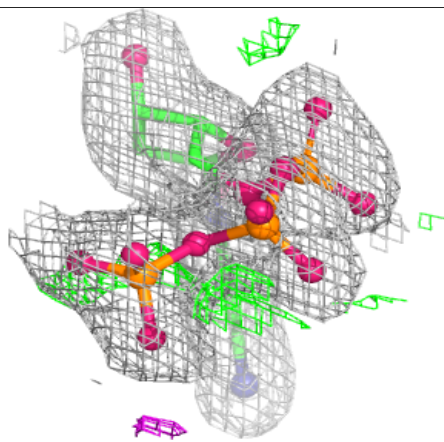
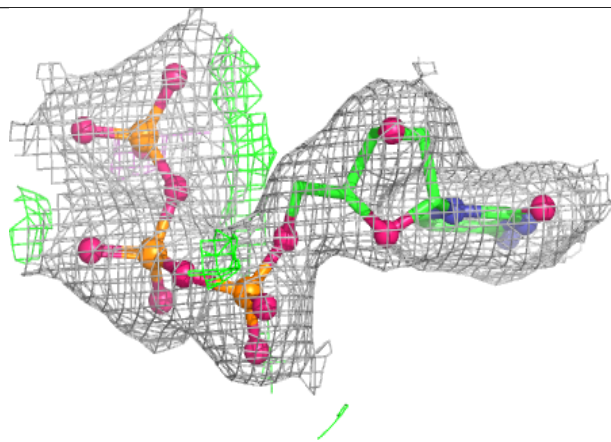
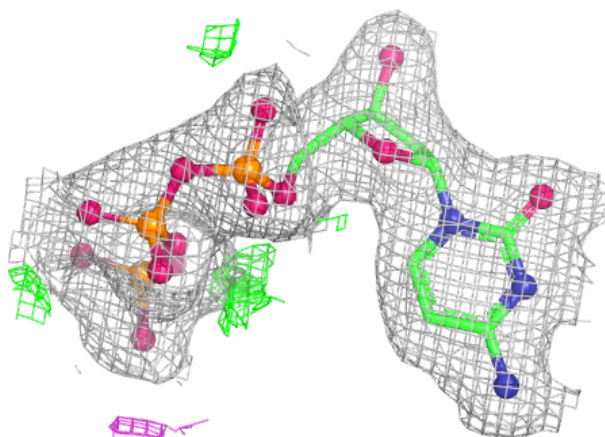
**Electron density around DGT A 701:**

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

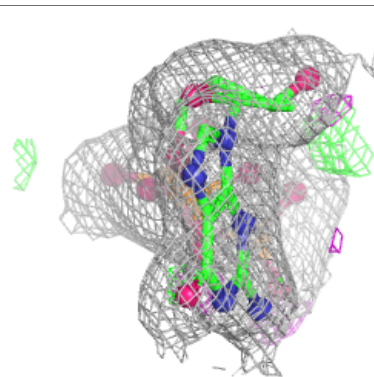
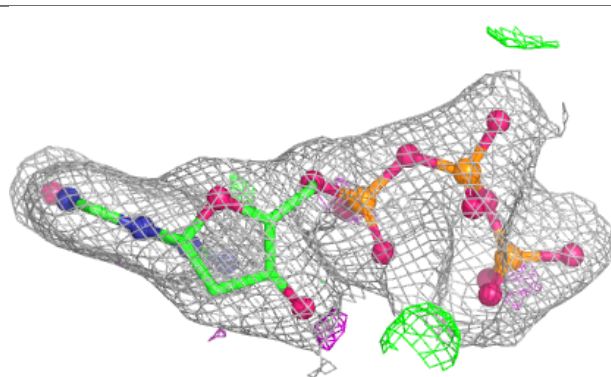
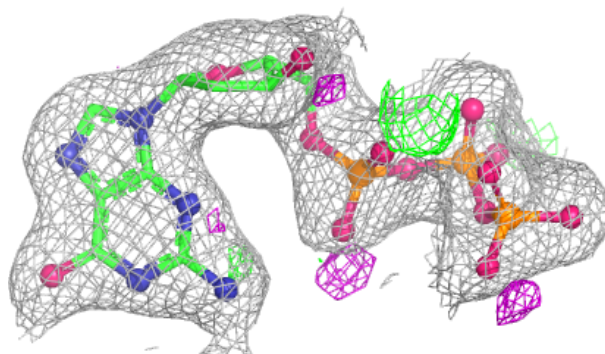


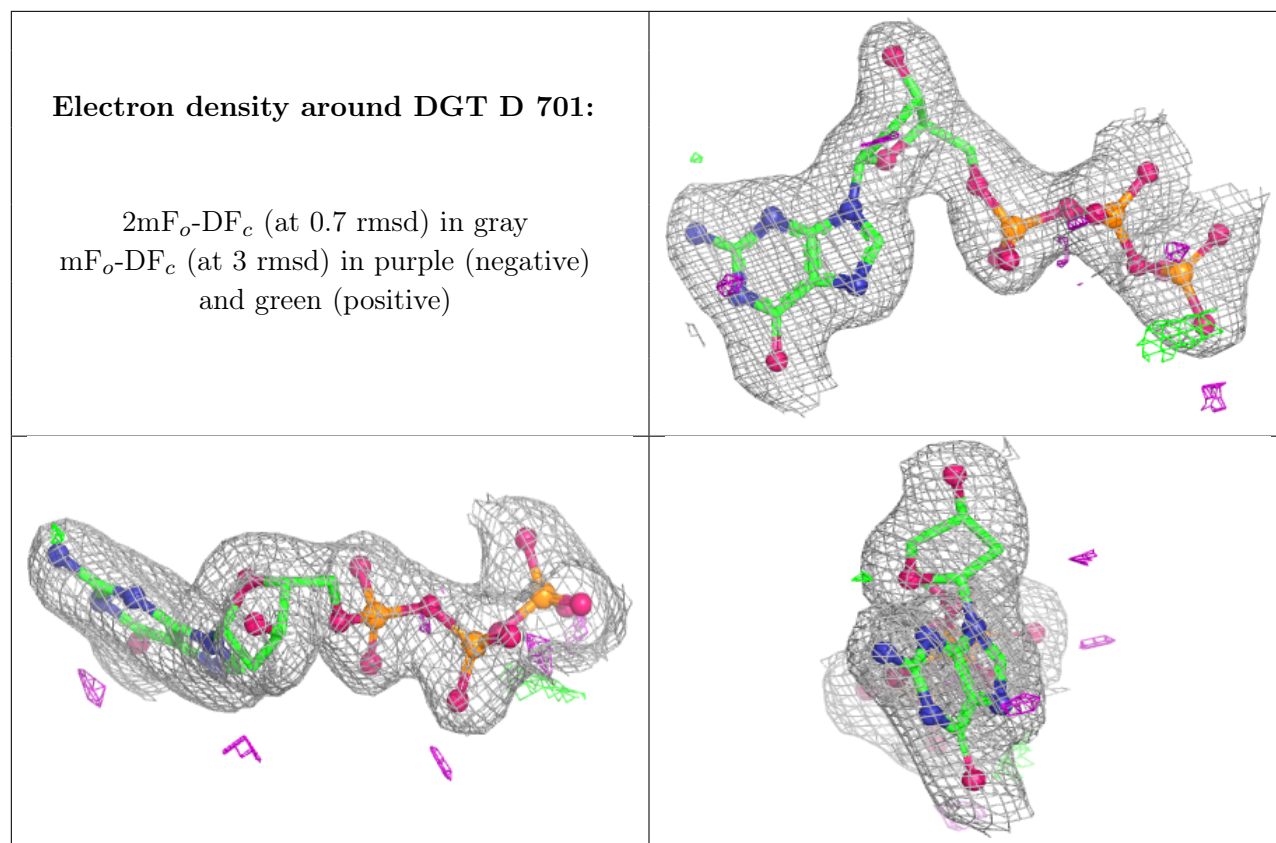
Electron density around DCP B 701:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.