



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:56 PM UTC

PDB ID : 7LTT / pdb_00007ltt
Title : SAMHD1(113-626) H206R D207N R366C
Authors : Temple, J.T.; Bowen, N.E.
Deposited on : 2021-02-20
Resolution : 1.90 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

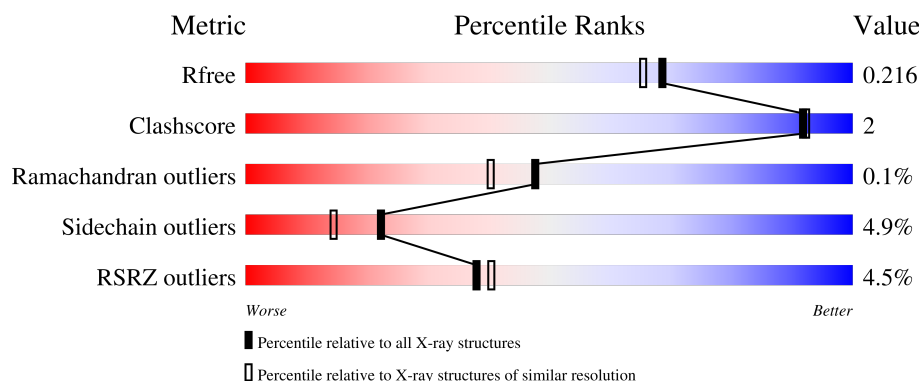
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	535	2% 83% 6% 10%
1	B	535	11% 81% 7% 10%
1	C	535	2% 82% 6% 10%
1	D	535	0% 83% 6% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16703 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
			3963	2533	689	718	23			
1	B	481	Total	C	N	O	S	0	4	0
			3954	2528	688	715	23			
1	C	481	Total	C	N	O	S	0	4	0
			3958	2530	686	719	23			
1	D	481	Total	C	N	O	S	0	5	0
			3965	2534	690	718	23			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	MET	-	initiating methionine	UNP Q9Y3Z3
A	93	GLY	-	expression tag	UNP Q9Y3Z3
A	94	SER	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
A	97	HIS	-	expression tag	UNP Q9Y3Z3
A	98	HIS	-	expression tag	UNP Q9Y3Z3
A	99	HIS	-	expression tag	UNP Q9Y3Z3
A	100	HIS	-	expression tag	UNP Q9Y3Z3
A	101	HIS	-	expression tag	UNP Q9Y3Z3
A	102	SER	-	expression tag	UNP Q9Y3Z3
A	103	SER	-	expression tag	UNP Q9Y3Z3
A	104	GLY	-	expression tag	UNP Q9Y3Z3
A	105	LEU	-	expression tag	UNP Q9Y3Z3
A	106	VAL	-	expression tag	UNP Q9Y3Z3
A	107	PRO	-	expression tag	UNP Q9Y3Z3
A	108	ARG	-	expression tag	UNP Q9Y3Z3
A	109	GLY	-	expression tag	UNP Q9Y3Z3
A	110	SER	-	expression tag	UNP Q9Y3Z3
A	111	HIS	-	expression tag	UNP Q9Y3Z3
A	112	MET	-	expression tag	UNP Q9Y3Z3

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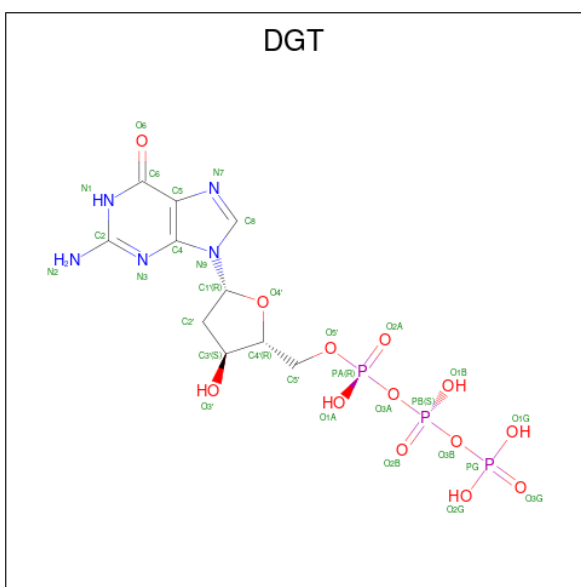
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
A	366	CYS	ARG	engineered mutation	UNP Q9Y3Z3
B	92	MET	-	initiating methionine	UNP Q9Y3Z3
B	93	GLY	-	expression tag	UNP Q9Y3Z3
B	94	SER	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	HIS	-	expression tag	UNP Q9Y3Z3
B	98	HIS	-	expression tag	UNP Q9Y3Z3
B	99	HIS	-	expression tag	UNP Q9Y3Z3
B	100	HIS	-	expression tag	UNP Q9Y3Z3
B	101	HIS	-	expression tag	UNP Q9Y3Z3
B	102	SER	-	expression tag	UNP Q9Y3Z3
B	103	SER	-	expression tag	UNP Q9Y3Z3
B	104	GLY	-	expression tag	UNP Q9Y3Z3
B	105	LEU	-	expression tag	UNP Q9Y3Z3
B	106	VAL	-	expression tag	UNP Q9Y3Z3
B	107	PRO	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	GLY	-	expression tag	UNP Q9Y3Z3
B	110	SER	-	expression tag	UNP Q9Y3Z3
B	111	HIS	-	expression tag	UNP Q9Y3Z3
B	112	MET	-	expression tag	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	366	CYS	ARG	engineered mutation	UNP Q9Y3Z3
C	92	MET	-	initiating methionine	UNP Q9Y3Z3
C	93	GLY	-	expression tag	UNP Q9Y3Z3
C	94	SER	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	HIS	-	expression tag	UNP Q9Y3Z3
C	98	HIS	-	expression tag	UNP Q9Y3Z3
C	99	HIS	-	expression tag	UNP Q9Y3Z3
C	100	HIS	-	expression tag	UNP Q9Y3Z3
C	101	HIS	-	expression tag	UNP Q9Y3Z3
C	102	SER	-	expression tag	UNP Q9Y3Z3
C	103	SER	-	expression tag	UNP Q9Y3Z3
C	104	GLY	-	expression tag	UNP Q9Y3Z3
C	105	LEU	-	expression tag	UNP Q9Y3Z3
C	106	VAL	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	107	PRO	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	GLY	-	expression tag	UNP Q9Y3Z3
C	110	SER	-	expression tag	UNP Q9Y3Z3
C	111	HIS	-	expression tag	UNP Q9Y3Z3
C	112	MET	-	expression tag	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	366	CYS	ARG	engineered mutation	UNP Q9Y3Z3
D	92	MET	-	initiating methionine	UNP Q9Y3Z3
D	93	GLY	-	expression tag	UNP Q9Y3Z3
D	94	SER	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	HIS	-	expression tag	UNP Q9Y3Z3
D	98	HIS	-	expression tag	UNP Q9Y3Z3
D	99	HIS	-	expression tag	UNP Q9Y3Z3
D	100	HIS	-	expression tag	UNP Q9Y3Z3
D	101	HIS	-	expression tag	UNP Q9Y3Z3
D	102	SER	-	expression tag	UNP Q9Y3Z3
D	103	SER	-	expression tag	UNP Q9Y3Z3
D	104	GLY	-	expression tag	UNP Q9Y3Z3
D	105	LEU	-	expression tag	UNP Q9Y3Z3
D	106	VAL	-	expression tag	UNP Q9Y3Z3
D	107	PRO	-	expression tag	UNP Q9Y3Z3
D	108	ARG	-	expression tag	UNP Q9Y3Z3
D	109	GLY	-	expression tag	UNP Q9Y3Z3
D	110	SER	-	expression tag	UNP Q9Y3Z3
D	111	HIS	-	expression tag	UNP Q9Y3Z3
D	112	MET	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	366	CYS	ARG	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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	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	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

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

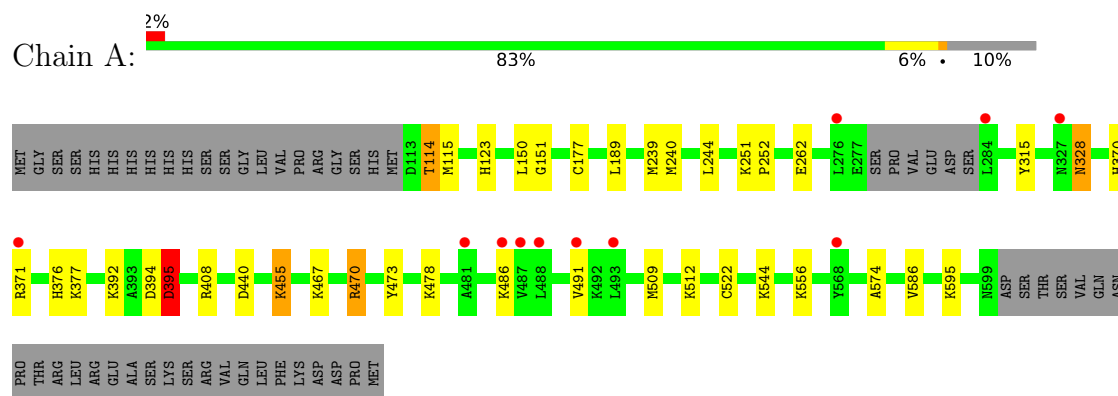
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total 169	O 169	0	0
4	B	133	Total 133	O 133	0	0
4	C	124	Total 124	O 124	0	0
4	D	185	Total 185	O 185	0	0

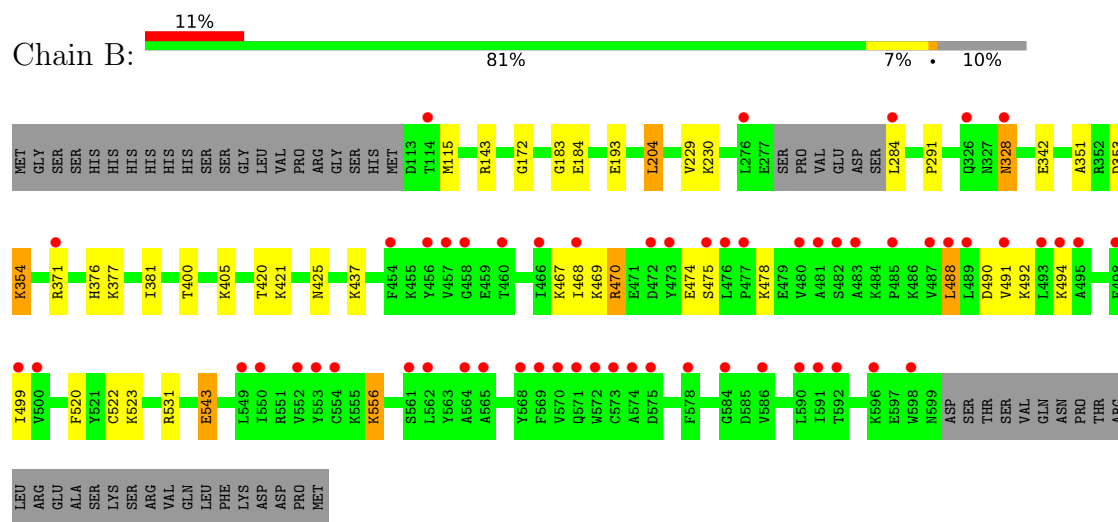
3 Residue-property plots

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

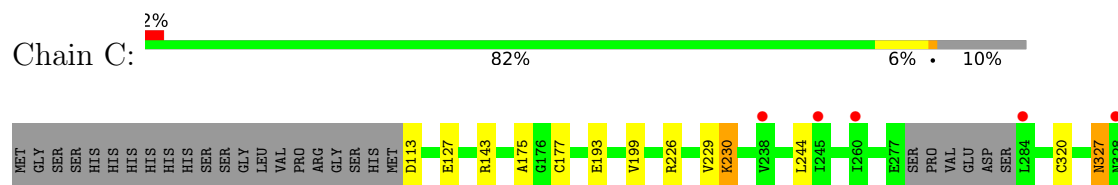
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

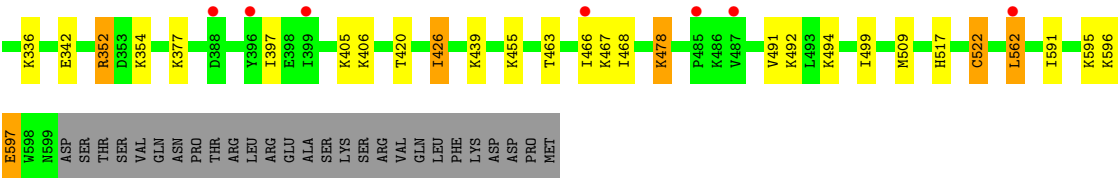


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

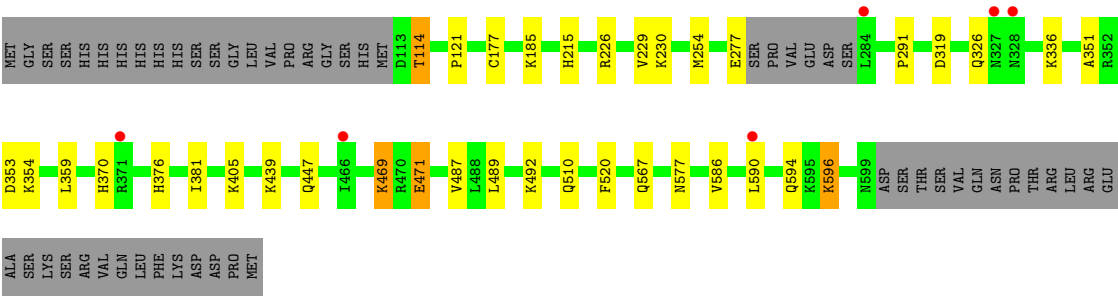
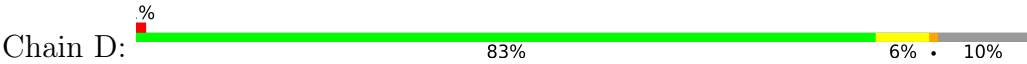


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.93Å 140.10Å 97.19Å 90.00° 114.18° 90.00°	Depositor
Resolution (Å)	39.38 – 1.90 39.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.38-1.90) 99.1 (39.38-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.212 0.189 , 0.216	Depositor DCC
R_{free} test set	7735 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16703	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.27	10/4058 (0.2%)	1.29	7/5477 (0.1%)
1	B	1.18	3/4049 (0.1%)	1.29	7/5465 (0.1%)
1	C	1.05	4/4053 (0.1%)	1.26	3/5471 (0.1%)
1	D	1.13	6/4060 (0.1%)	1.27	4/5480 (0.1%)
All	All	1.16	23/16220 (0.1%)	1.28	21/21893 (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	4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	394	ASP	C-N	-32.45	0.89	1.34
1	B	183	GLY	C-N	-30.08	0.93	1.33
1	B	184	GLU	C-N	-12.62	1.16	1.34
1	A	395	ASP	C-N	-11.79	1.17	1.33
1	D	353	ASP	C-N	-8.08	1.22	1.33
1	A	123	HIS	CE1-NE2	8.08	1.40	1.32
1	A	239	MET	C-N	-8.04	1.23	1.33
1	A	522[A]	CYS	C-O	7.84	1.32	1.23
1	A	522[B]	CYS	C-O	7.84	1.32	1.23
1	C	522[A]	CYS	C-O	7.37	1.33	1.23
1	C	522[B]	CYS	C-O	7.37	1.33	1.23
1	C	522[A]	CYS	CA-C	6.47	1.60	1.52
1	C	522[B]	CYS	CA-C	6.47	1.60	1.52
1	B	376	HIS	CE1-NE2	6.45	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	376	HIS	CE1-NE2	6.02	1.38	1.32
1	D	319	ASP	C-O	-5.94	1.17	1.24
1	A	522[A]	CYS	CA-C	5.76	1.60	1.52
1	A	522[B]	CYS	CA-C	5.76	1.60	1.52
1	A	240	MET	C-N	5.65	1.41	1.33
1	D	370	HIS	CE1-NE2	5.49	1.38	1.32
1	D	254	MET	C-O	5.19	1.30	1.24
1	D	215	HIS	CE1-NE2	5.07	1.37	1.32
1	A	376	HIS	CE1-NE2	5.06	1.37	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	GLY	CA-C-N	8.74	132.33	120.44
1	B	183	GLY	C-N-CA	8.74	132.33	120.44
1	A	522[A]	CYS	CA-C-O	7.11	129.66	121.28
1	A	522[B]	CYS	CA-C-O	7.11	129.66	121.28
1	A	114	THR	N-CA-C	-7.05	104.60	112.57
1	A	394	ASP	CA-C-N	6.27	129.84	120.31
1	A	394	ASP	C-N-CA	6.27	129.84	120.31
1	C	522[A]	CYS	CA-C-O	6.11	128.49	121.28
1	C	522[B]	CYS	CA-C-O	6.11	128.49	121.28
1	B	425	ASN	CA-CB-CG	-5.91	106.69	112.60
1	B	193	GLU	CB-CG-CD	5.85	122.55	112.60
1	D	291	PRO	CA-C-N	5.48	127.62	120.28
1	D	291	PRO	C-N-CA	5.48	127.62	120.28
1	B	353	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	352	ARG	CG-CD-NE	-5.33	100.28	112.00
1	D	114	THR	N-CA-C	-5.25	106.56	113.17
1	A	262	GLU	CB-CG-CD	5.21	121.45	112.60
1	D	353	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	315	TYR	CB-CA-C	5.05	119.17	110.79
1	B	291	PRO	N-CA-C	5.05	118.53	110.40
1	B	543	GLU	CB-CA-C	5.04	119.39	109.72

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	HIS	Mainchain
1	A	371[A]	ARG	Mainchain
1	A	395	ASP	Mainchain

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	3963	0	3940	13	0
1	B	3954	0	3935	11	0
1	C	3958	0	3934	18	0
1	D	3965	0	3942	12	0
2	A	93	0	36	0	0
2	B	62	0	24	0	0
2	C	62	0	24	0	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
4	A	169	0	0	4	0
4	B	133	0	0	1	0
4	C	124	0	0	3	0
4	D	185	0	0	2	0
All	All	16703	0	15847	50	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 2.

All (50) 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:177[B]:CYS:SG	4:C:924:HOH:O	2.32	0.88
1:A:177[B]:CYS:SG	4:A:969:HOH:O	2.32	0.87
1:D:177[B]:CYS:SG	4:D:1082:HOH:O	2.42	0.78
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.27	0.75
1:A:150:LEU:C	4:A:801:HOH:O	2.33	0.71
1:C:397:ILE:HG21	1:C:426:ILE:HD11	1.73	0.70
1:A:395:ASP:OD1	1:A:408:ARG:NH1	2.26	0.67
1:C:517:HIS:HE1	4:C:915:HOH:O	1.79	0.64
1:B:172:GLY:HA3	1:B:204:LEU:HD13	1.84	0.58
1:A:151:GLY:N	4:A:801:HOH:O	2.39	0.53
1:B:523:LYS:NZ	4:B:802:HOH:O	2.40	0.53
1:C:320:CYS:SG	1:C:327:ASN:HB3	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ALA:O	1:D:520:PHE:HA	2.10	0.52
1:C:127:GLU:HG3	1:D:336:LYS:HE3	1.94	0.49
1:C:595:LYS:HE3	1:C:597:GLU:HG3	1.93	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:C:352:ARG:HG2	1:C:354:LYS:HE2	1.97	0.47
1:D:487:VAL:HG22	1:D:590:LEU:HB2	1.95	0.47
1:A:392:LYS:HD3	1:A:440:ASP:HB3	1.97	0.47
1:C:517:HIS:CE1	4:C:915:HOH:O	2.61	0.46
1:A:328:ASN:OD1	1:A:328:ASN:N	2.49	0.45
1:C:463:THR:O	1:C:466:ILE:HD12	2.16	0.45
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.99	0.45
1:A:251:LYS:HB2	1:A:252:PRO:HD3	1.99	0.45
1:A:586:VAL:HG11	1:C:522[B]:CYS:SG	2.57	0.45
1:B:328:ASN:HA	1:D:326:GLN:HB2	1.98	0.44
1:A:455:LYS:HA	1:A:455:LYS:HD2	1.85	0.44
1:C:562:LEU:HD13	1:C:562:LEU:HA	1.81	0.44
1:A:509:MET:HE2	1:A:512:LYS:HE3	2.00	0.44
1:C:230:LYS:HA	1:C:230:LYS:HD3	1.80	0.44
1:C:143:ARG:HD2	1:C:420:THR:HA	2.00	0.43
1:C:597:GLU:H	1:C:597:GLU:HG2	1.35	0.43
1:C:478:LYS:H	1:C:478:LYS:HG2	1.46	0.43
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.86	0.43
1:A:470:ARG:HG2	1:A:473:TYR:CE2	2.53	0.43
1:B:556:LYS:HE2	1:B:556:LYS:HB3	1.39	0.42
1:B:143:ARG:HD2	1:B:420:THR:HA	2.01	0.42
1:D:596:LYS:HA	1:D:596:LYS:HD2	1.56	0.42
1:C:509:MET:HE1	1:C:517:HIS:ND1	2.35	0.42
1:D:447:GLN:HG3	4:D:1079:HOH:O	2.19	0.42
4:A:874:HOH:O	1:D:121:PRO:HG3	2.20	0.41
1:B:488:LEU:H	1:B:488:LEU:HG	1.44	0.41
1:D:471:GLU:H	1:D:471:GLU:HG3	1.34	0.41
1:C:244:LEU:C	1:C:244:LEU:HD23	2.45	0.41
1:A:244:LEU:C	1:A:244:LEU:HD23	2.46	0.41
1:B:354:LYS:HB2	1:B:354:LYS:HE3	1.80	0.41
1:A:574:ALA:HA	1:A:595:LYS:HD2	2.03	0.40
1:D:469:LYS:H	1:D:469:LYS:HG2	1.64	0.40
1:D:489:LEU:HD21	1:D:567:GLN:HG3	2.03	0.40
1:B:400:THR:O	1:B:421:LYS:HE2	2.21	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	482/535 (90%)	478 (99%)	4 (1%)	0	100	100
1	B	481/535 (90%)	469 (98%)	10 (2%)	2 (0%)	30	22
1	C	482/535 (90%)	477 (99%)	5 (1%)	0	100	100
1	D	482/535 (90%)	478 (99%)	4 (1%)	0	100	100
All	All	1927/2140 (90%)	1902 (99%)	23 (1%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	468	ILE
1	B	470	ARG

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	432/477 (91%)	419 (97%)	13 (3%)	36	30
1	B	431/477 (90%)	403 (94%)	28 (6%)	15	8
1	C	432/477 (91%)	407 (94%)	25 (6%)	18	10
1	D	432/477 (91%)	414 (96%)	18 (4%)	26	19
All	All	1727/1908 (90%)	1643 (95%)	84 (5%)	22	14

All (84) 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	328	ASN
1	A	377	LYS
1	A	455	LYS
1	A	467	LYS
1	A	470	ARG
1	A	478	LYS
1	A	486	LYS
1	A	491	VAL
1	A	544	LYS
1	A	556	LYS
1	B	115	MET
1	B	204	LEU
1	B	229	VAL
1	B	230	LYS
1	B	284	LEU
1	B	328	ASN
1	B	342	GLU
1	B	354	LYS
1	B	371[A]	ARG
1	B	371[B]	ARG
1	B	377	LYS
1	B	405	LYS
1	B	437	LYS
1	B	467	LYS
1	B	469	LYS
1	B	470	ARG
1	B	474	GLU
1	B	475	SER
1	B	478	LYS
1	B	488	LEU
1	B	490	ASP
1	B	491	VAL
1	B	492	LYS
1	B	494	LYS
1	B	499	ILE
1	B	531	ARG
1	B	543	GLU
1	B	556	LYS
1	C	113	ASP
1	C	193	GLU

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Mol	Chain	Res	Type
1	C	226	ARG
1	C	229	VAL
1	C	230	LYS
1	C	327	ASN
1	C	336	LYS
1	C	342	GLU
1	C	377	LYS
1	C	405	LYS
1	C	406	LYS
1	C	426	ILE
1	C	439	LYS
1	C	455	LYS
1	C	467	LYS
1	C	468	ILE
1	C	478	LYS
1	C	491	VAL
1	C	492	LYS
1	C	494	LYS
1	C	499	ILE
1	C	562	LEU
1	C	591	ILE
1	C	596	LYS
1	C	597	GLU
1	D	114	THR
1	D	185	LYS
1	D	226	ARG
1	D	229	VAL
1	D	230	LYS
1	D	277	GLU
1	D	354	LYS
1	D	359	LEU
1	D	381	ILE
1	D	405	LYS
1	D	439	LYS
1	D	469	LYS
1	D	471	GLU
1	D	492	LYS
1	D	510	GLN
1	D	577	ASN
1	D	594	GLN
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	149	GLN
1	A	200	GLN
1	A	235	GLN
1	A	243	HIS
1	A	326	GLN
1	A	517	HIS
1	B	149	GLN
1	B	180	HIS
1	B	200	GLN
1	B	248	ASN
1	B	567	GLN
1	C	149	GLN
1	C	180	HIS
1	C	190	GLN
1	C	200	GLN
1	C	210	HIS
1	C	235	GLN
1	C	248	ASN
1	C	321	HIS
1	C	364	HIS
1	C	539	GLN
1	C	567	GLN
1	C	571	GLN
1	C	594	GLN
1	D	140	GLN
1	D	149	GLN
1	D	200	GLN
1	D	215	HIS
1	D	243	HIS
1	D	248	ASN
1	D	321	HIS
1	D	535	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	703	3	32,33,33	1.01	2 (6%)	48,52,52	0.91	1 (2%)
2	DGT	C	701	3	32,33,33	0.57	0	48,52,52	0.56	0
2	DGT	A	702	3	32,33,33	0.74	1 (3%)	48,52,52	0.88	3 (6%)
2	DGT	B	702	3	32,33,33	0.79	0	48,52,52	0.86	3 (6%)
2	DGT	A	701	3	32,33,33	0.86	2 (6%)	48,52,52	0.96	4 (8%)
2	DGT	C	704	3	32,33,33	0.62	0	48,52,52	0.85	1 (2%)
2	DGT	A	704	3	32,33,33	1.13	3 (9%)	48,52,52	0.98	1 (2%)
2	DGT	D	800	3	32,33,33	0.64	0	48,52,52	0.79	3 (6%)

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	703	3	-	4/22/34/34	0/3/3/3
2	DGT	C	701	3	-	3/22/34/34	0/3/3/3
2	DGT	A	702	3	-	2/22/34/34	0/3/3/3
2	DGT	B	702	3	-	8/22/34/34	0/3/3/3
2	DGT	A	701	3	-	6/22/34/34	0/3/3/3
2	DGT	C	704	3	-	6/22/34/34	0/3/3/3
2	DGT	A	704	3	-	5/22/34/34	0/3/3/3
2	DGT	D	800	3	-	5/22/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	704	DGT	PG-O1G	-3.71	1.41	1.54
2	A	704	DGT	PB-O3A	3.41	1.63	1.59
2	B	703	DGT	PG-O2G	-2.93	1.43	1.54
2	B	703	DGT	PB-O3B	2.43	1.62	1.59
2	A	701	DGT	PG-O3G	2.21	1.57	1.50
2	A	702	DGT	PG-O1G	-2.15	1.46	1.54
2	A	704	DGT	PA-O3A	2.04	1.61	1.59
2	A	701	DGT	PG-O1G	-2.01	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	704	DGT	O3B-PG-O3G	-2.92	95.67	111.04
2	A	702	DGT	O1A-PA-O3A	-2.85	99.56	107.27
2	B	702	DGT	O2G-PG-O3B	2.60	113.35	104.64
2	A	701	DGT	C1'-N9-C8	-2.56	122.16	127.91
2	A	702	DGT	O1A-PA-O2A	2.51	124.12	112.44
2	D	800	DGT	O2G-PG-O1G	2.45	117.00	107.80
2	D	800	DGT	O1B-PB-O2B	2.38	123.52	112.44
2	B	702	DGT	O3B-PG-O3G	-2.23	99.33	111.04
2	D	800	DGT	O1A-PA-O2A	2.22	122.80	112.44
2	A	701	DGT	O1A-PA-O2A	2.18	122.58	112.44
2	A	701	DGT	C1'-N9-C4	2.16	131.34	125.50
2	A	701	DGT	O1B-PB-O3B	2.16	113.10	107.27
2	A	702	DGT	O2G-PG-O3G	2.14	119.18	110.83
2	B	702	DGT	O1B-PB-O2B	2.12	122.33	112.44
2	B	703	DGT	O2G-PG-O3G	2.12	119.08	110.83
2	A	704	DGT	O1A-PA-O2A	2.08	122.11	112.44

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	702	DGT	PB-O3B-PG-O2G
2	A	702	DGT	PG-O3B-PB-O2B
2	C	701	DGT	PA-O3A-PB-O2B
2	B	702	DGT	PB-O3B-PG-O3G
2	A	701	DGT	PG-O3B-PB-O2B
2	A	704	DGT	PG-O3B-PB-O2B
2	B	702	DGT	PG-O3B-PB-O1B
2	B	703	DGT	PG-O3B-PB-O1B

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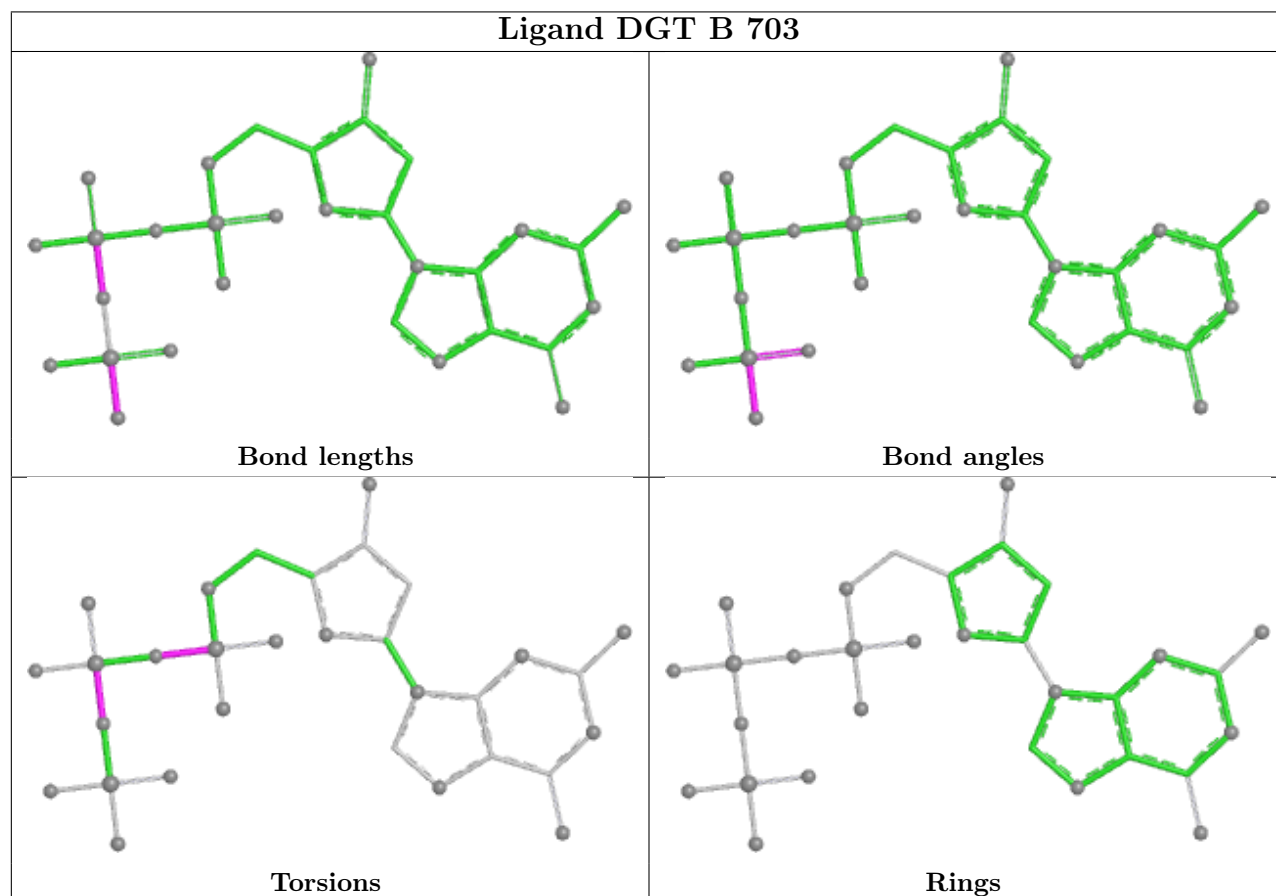
Mol	Chain	Res	Type	Atoms
2	B	703	DGT	PB-O3A-PA-O2A
2	D	800	DGT	PB-O3A-PA-O2A
2	A	704	DGT	C2'-C1'-N9-C8
2	C	704	DGT	C2'-C1'-N9-C8
2	D	800	DGT	C5'-O5'-PA-O1A
2	A	702	DGT	PG-O3B-PB-O1B
2	B	702	DGT	PG-O3B-PB-O2B
2	B	703	DGT	PG-O3B-PB-O2B
2	C	701	DGT	PA-O3A-PB-O1B
2	C	704	DGT	PG-O3B-PB-O1B
2	A	704	DGT	C4'-C5'-O5'-PA
2	B	702	DGT	C4'-C5'-O5'-PA
2	A	701	DGT	C4'-C5'-O5'-PA
2	A	701	DGT	PG-O3B-PB-O1B
2	C	704	DGT	PB-O3A-PA-O1A
2	D	800	DGT	PG-O3B-PB-O2B
2	A	704	DGT	C2'-C1'-N9-C4
2	C	704	DGT	C4'-C5'-O5'-PA
2	A	701	DGT	PB-O3B-PG-O1G
2	B	702	DGT	C2'-C1'-N9-C8
2	A	704	DGT	PG-O3B-PB-O1B
2	B	702	DGT	PB-O3A-PA-O2A
2	B	703	DGT	PB-O3A-PA-O1A
2	C	704	DGT	PG-O3B-PB-O2B
2	A	701	DGT	C2'-C1'-N9-C4
2	A	701	DGT	PB-O3A-PA-O1A
2	B	702	DGT	PB-O3A-PA-O1A
2	C	701	DGT	PG-O3B-PB-O1B
2	C	704	DGT	PB-O3A-PA-O2A
2	D	800	DGT	PG-O3B-PB-O1B
2	D	800	DGT	PB-O3A-PA-O1A

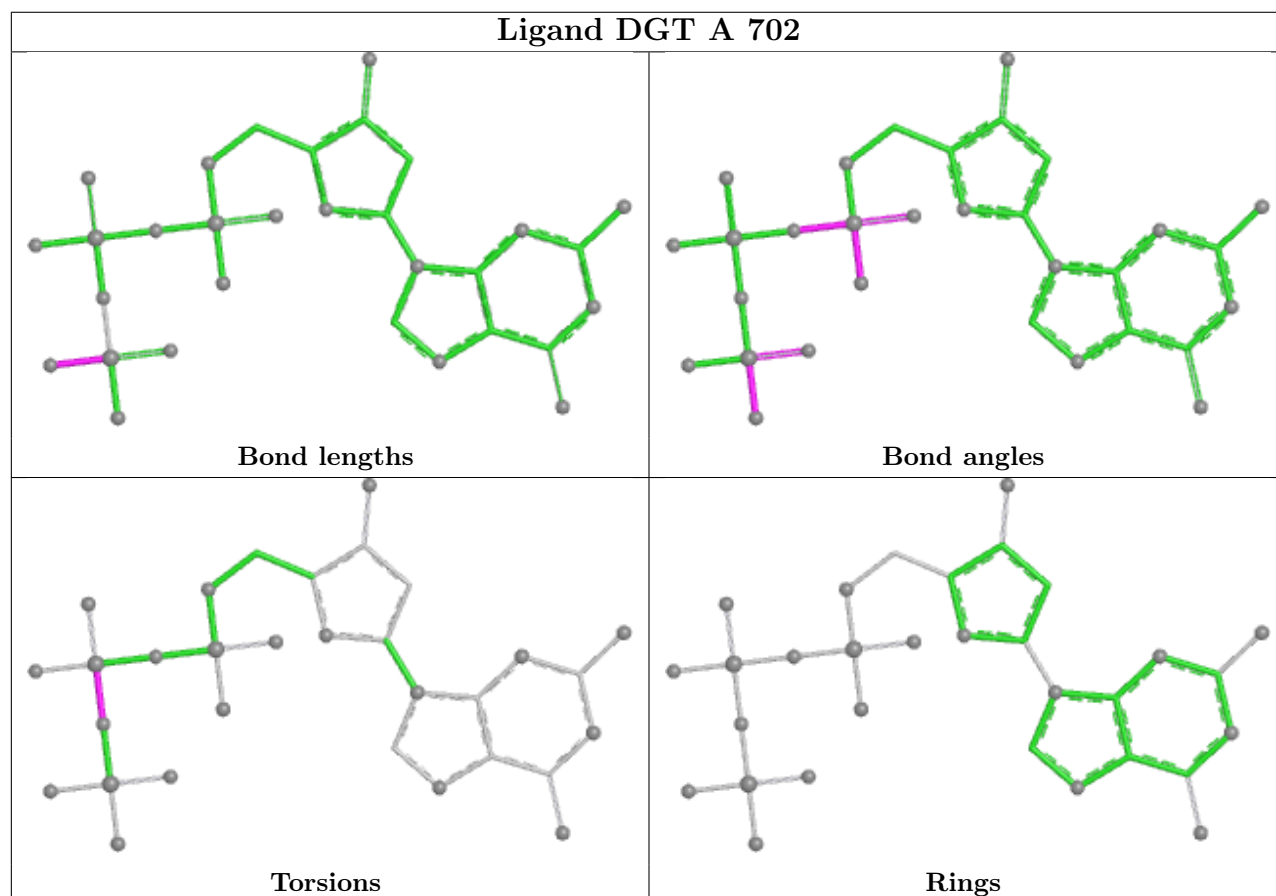
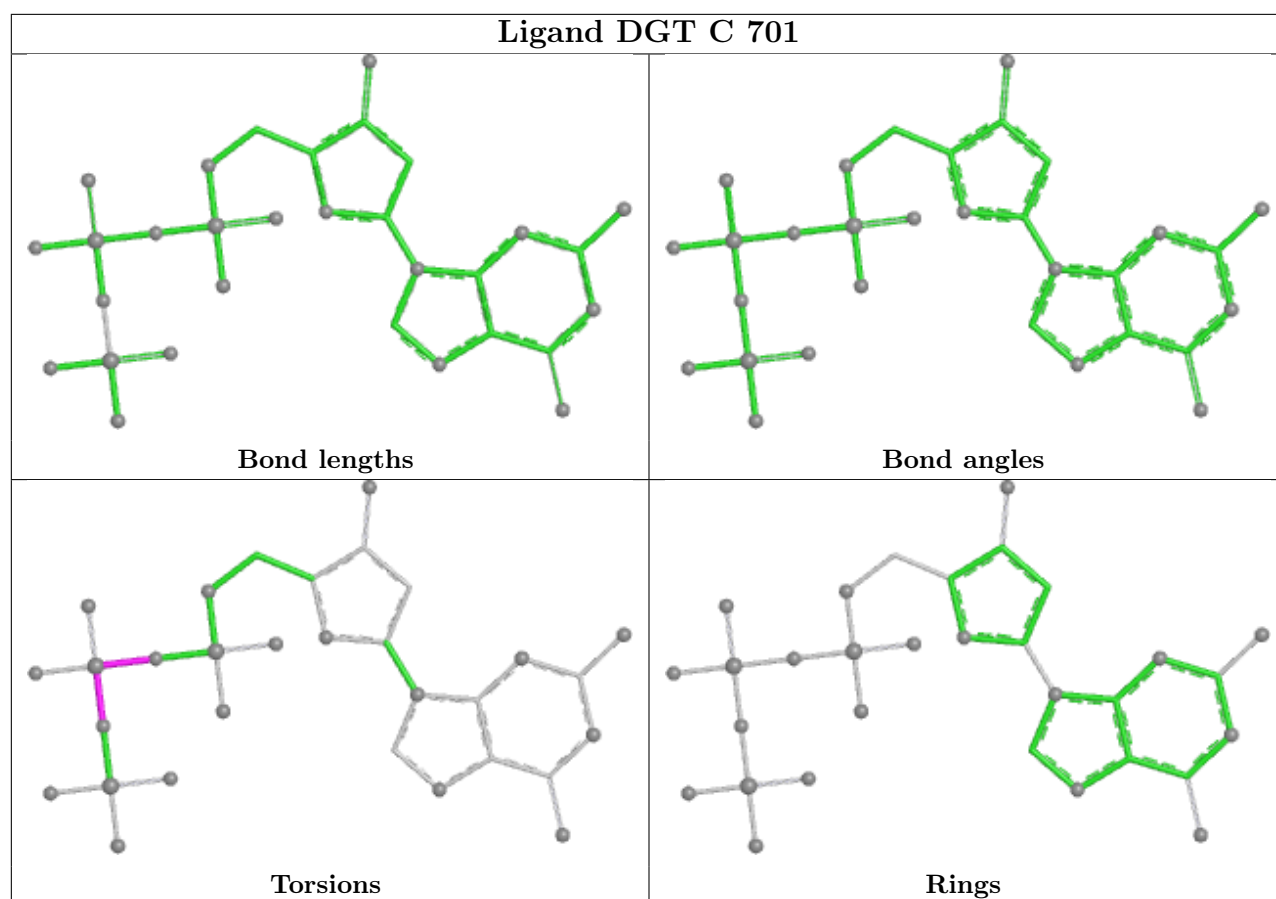
There are no ring outliers.

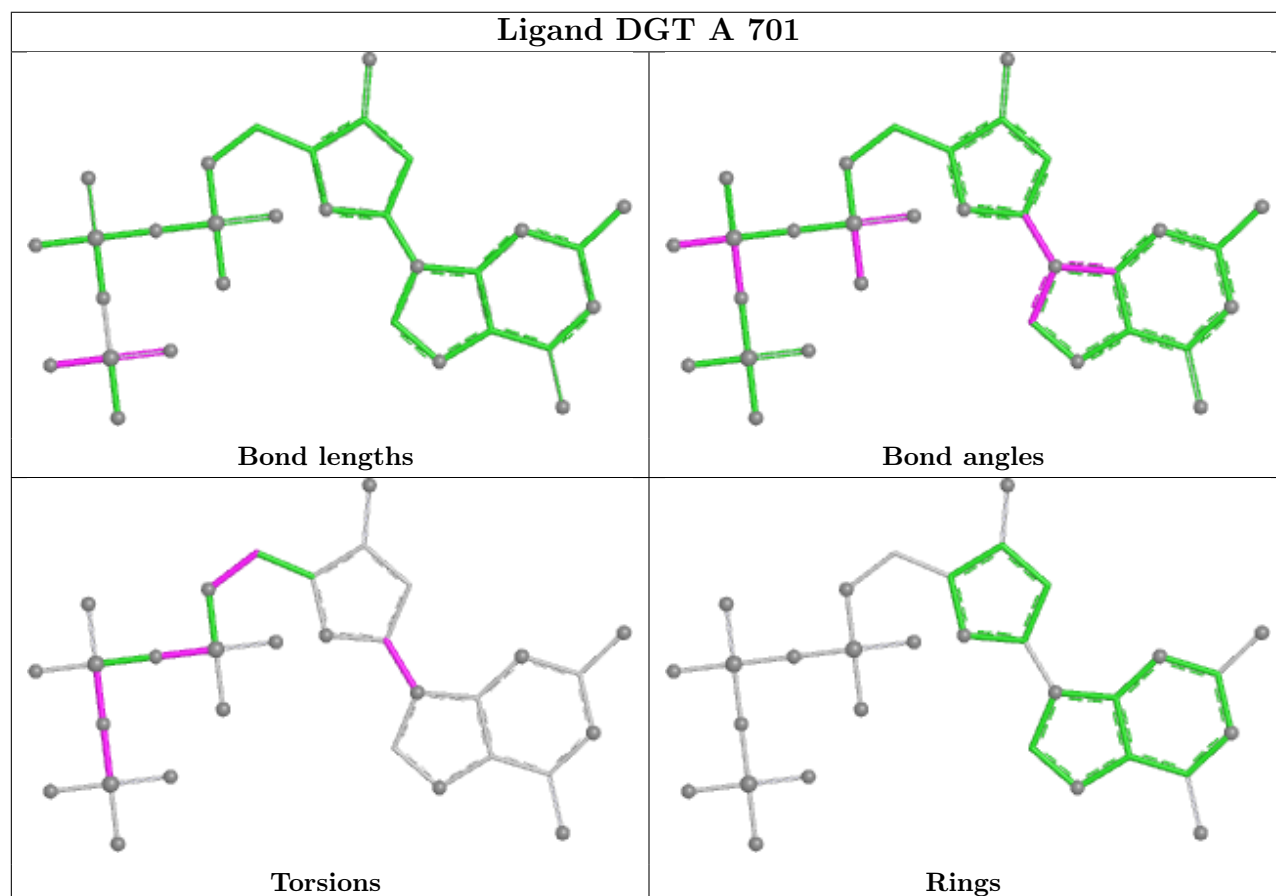
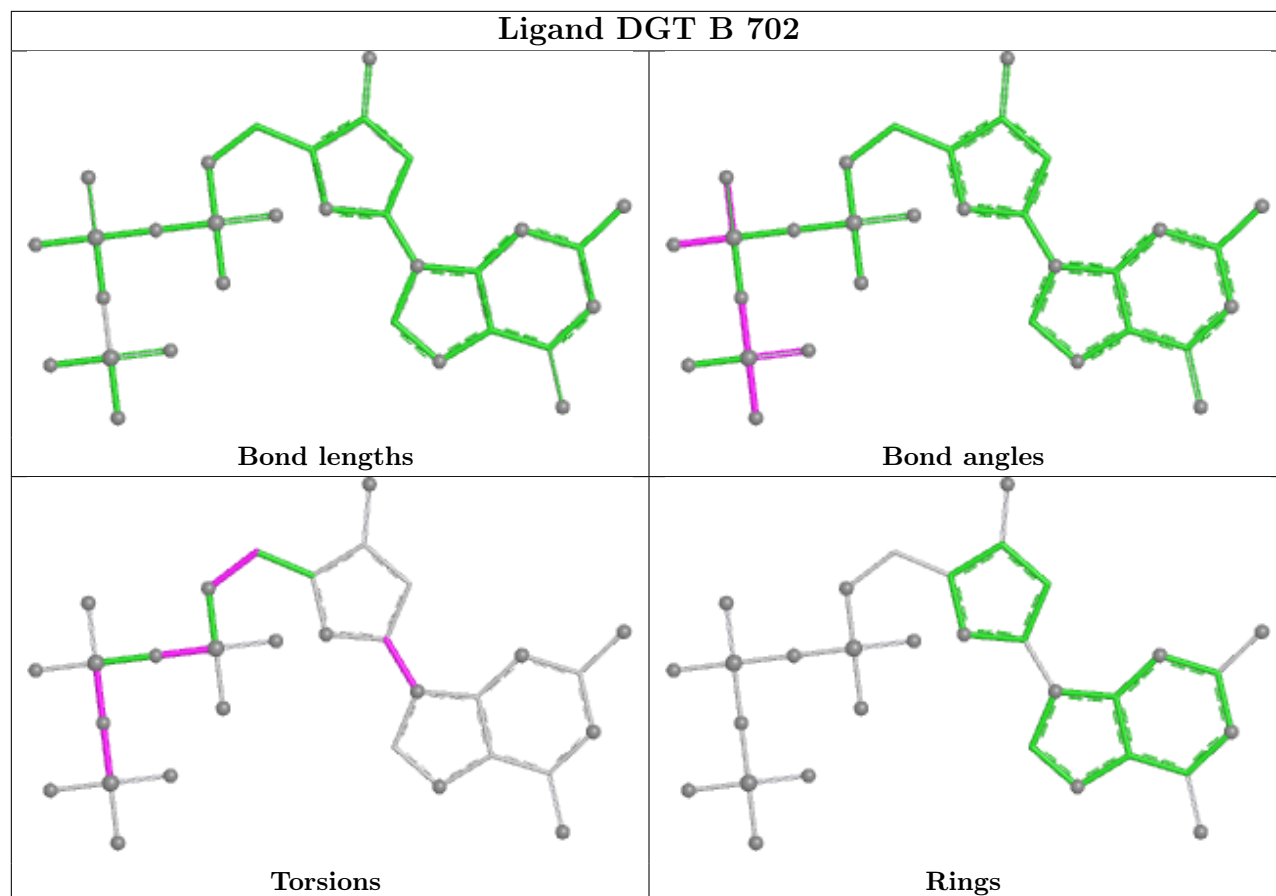
No monomer is involved in short contacts.

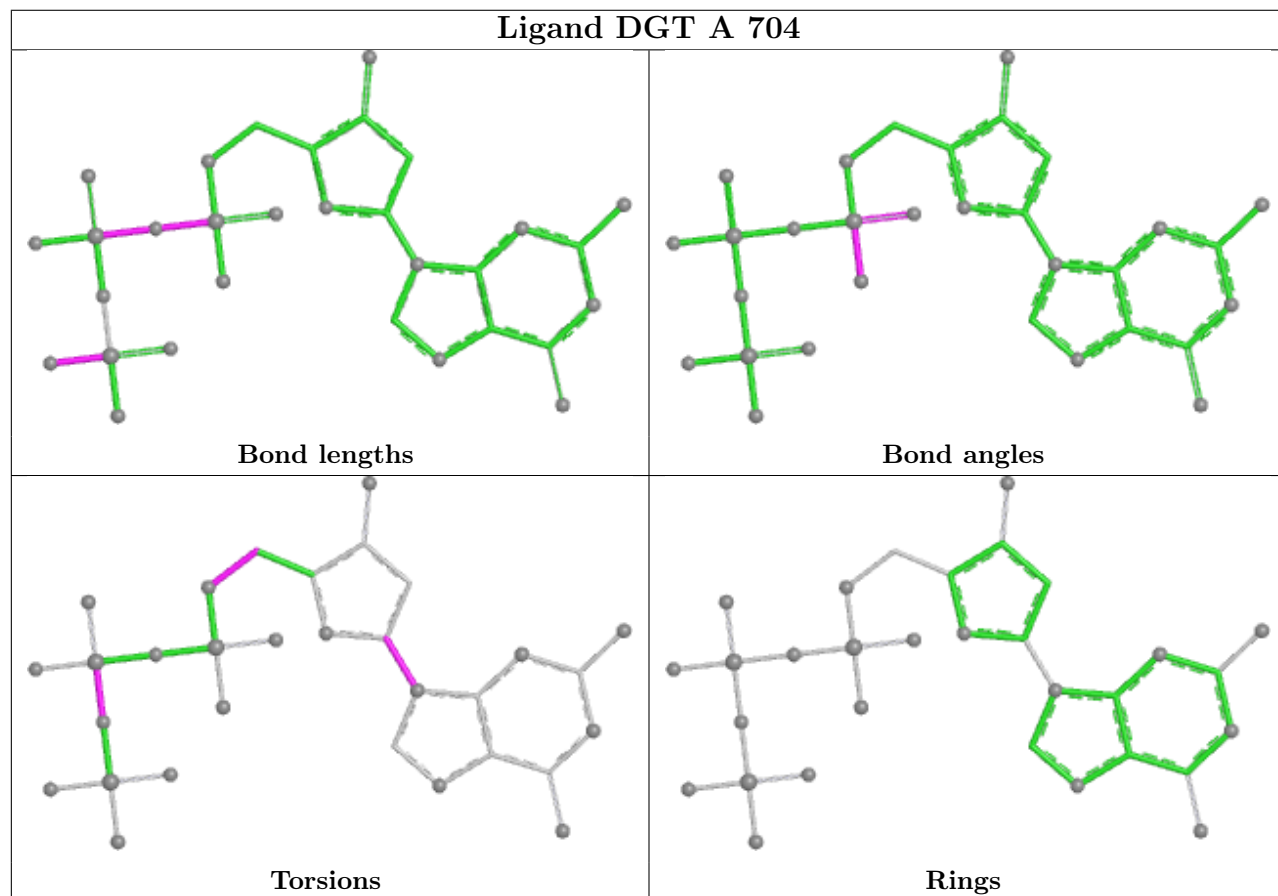
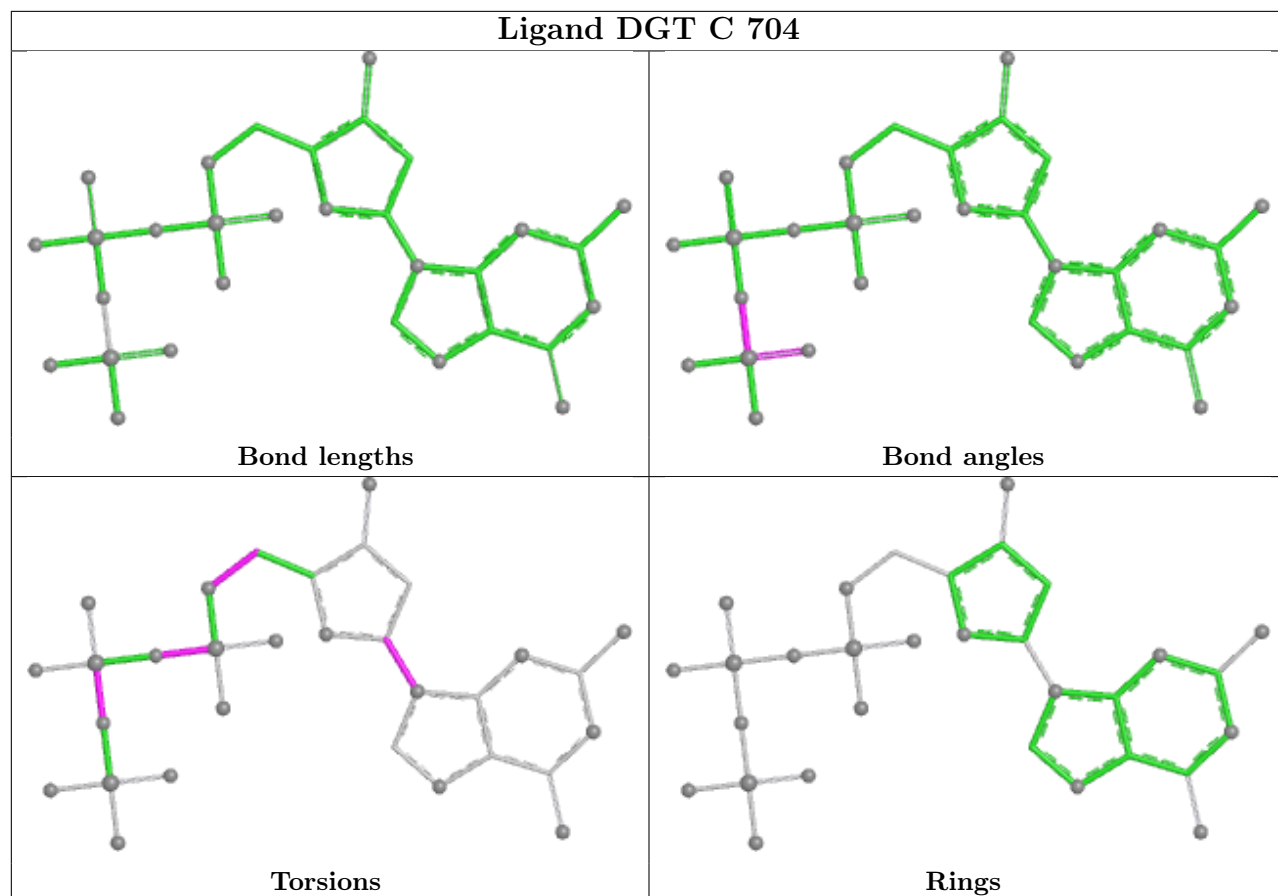
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

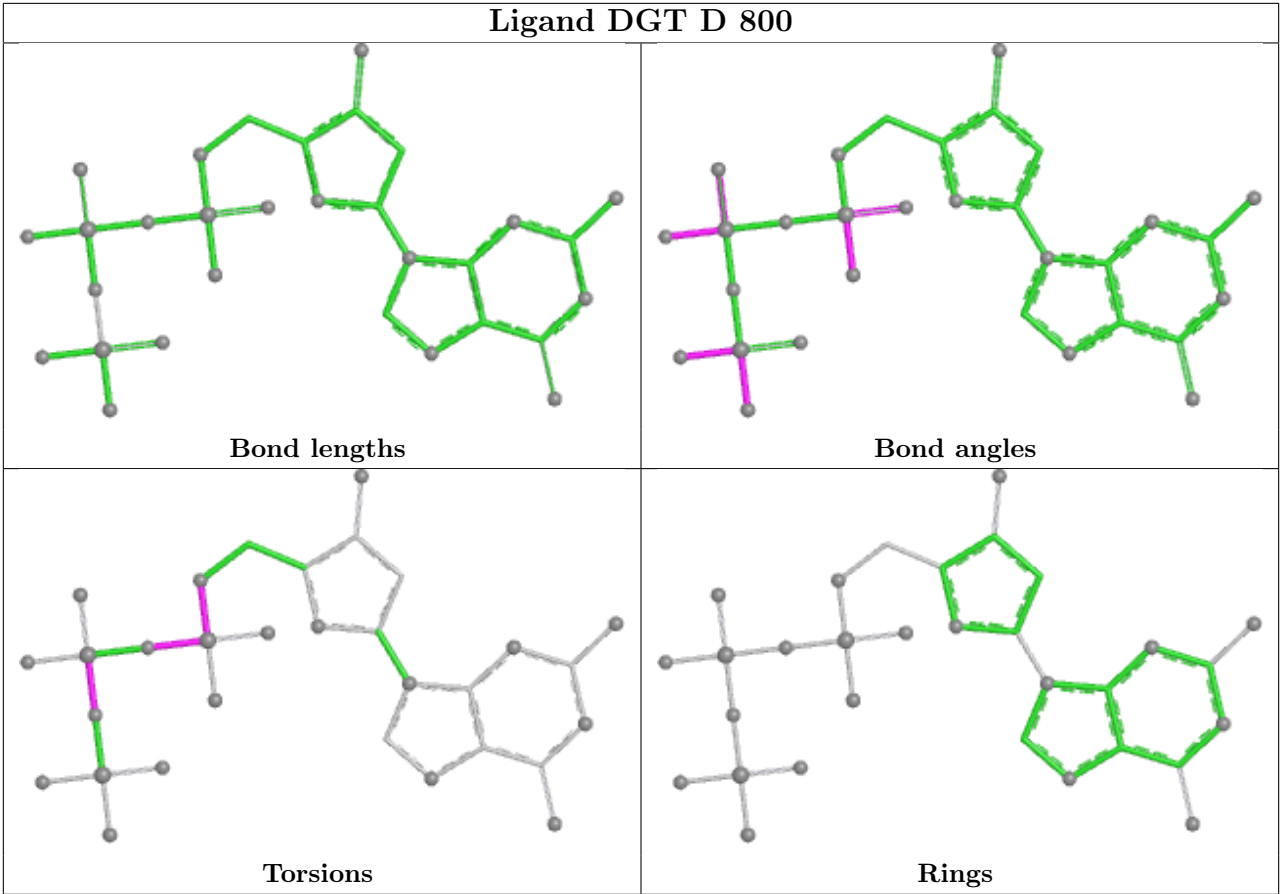
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	395:ASP	C	396:TYR	N	1.17
1	B	184:GLU	C	185:LYS	N	1.16
1	A	370:HIS	C	371[B]:ARG	N	1.14
1	B	183:GLY	C	184:GLU	N	0.93
1	A	394:ASP	C	395:ASP	N	0.89

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	481/535 (89%)	0.06	11 (2%) 61 65	15, 39, 68, 102	5 (1%)
1	B	481/535 (89%)	0.59	58 (12%) 8 9	18, 49, 113, 143	4 (0%)
1	C	481/535 (89%)	0.39	12 (2%) 58 62	18, 52, 88, 116	4 (0%)
1	D	481/535 (89%)	-0.12	6 (1%) 76 79	16, 37, 62, 95	5 (1%)
All	All	1924/2140 (89%)	0.23	87 (4%) 38 40	15, 44, 90, 143	18 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	LEU	6.1
1	B	498	PHE	5.3
1	B	468	ILE	5.0
1	C	466	ILE	5.0
1	B	495	ALA	4.9
1	B	480	VAL	4.8
1	C	284	LEU	4.4
1	B	569	PHE	4.3
1	B	488	LEU	4.3
1	B	570	VAL	4.2
1	B	572	TRP	4.2
1	B	493	LEU	4.1
1	B	483	ALA	4.1
1	B	466	ILE	4.0
1	B	574	ALA	4.0
1	B	562	LEU	3.9
1	B	550	ILE	3.8
1	B	491	VAL	3.8
1	A	284	LEU	3.7
1	B	477	PRO	3.6
1	B	568	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	284	LEU	3.6
1	B	499	ILE	3.5
1	B	457	VAL	3.5
1	B	460	THR	3.4
1	B	573	CYS	3.2
1	B	552	VAL	3.1
1	A	276	LEU	3.1
1	B	553	TYR	3.1
1	D	371[A]	ARG	3.1
1	C	562	LEU	3.0
1	B	591	ILE	3.0
1	B	554	CYS	3.0
1	B	489	LEU	3.0
1	B	590	LEU	3.0
1	A	487	VAL	2.9
1	B	578	PHE	2.9
1	C	388	ASP	2.9
1	B	500	VAL	2.9
1	C	485	PRO	2.8
1	B	481	ALA	2.8
1	D	328	ASN	2.8
1	B	456	TYR	2.7
1	B	458	GLY	2.7
1	B	584	GLY	2.7
1	B	564	ALA	2.7
1	B	371[A]	ARG	2.7
1	A	491	VAL	2.7
1	D	284	LEU	2.6
1	B	473	TYR	2.5
1	B	575	ASP	2.5
1	A	488	LEU	2.5
1	B	561	SER	2.5
1	D	466	ILE	2.4
1	B	494	LYS	2.4
1	B	565	ALA	2.4
1	B	592	THR	2.4
1	A	481	ALA	2.4
1	B	487	VAL	2.4
1	D	590	LEU	2.4
1	C	328	ASN	2.4
1	A	493	LEU	2.3
1	D	327	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	568	TYR	2.3
1	B	475	SER	2.3
1	B	571	GLN	2.3
1	A	371[A]	ARG	2.2
1	C	245	ILE	2.2
1	C	260	ILE	2.2
1	B	596	LYS	2.2
1	B	114	THR	2.2
1	B	328	ASN	2.2
1	B	454	PHE	2.2
1	B	586	VAL	2.2
1	B	549	LEU	2.2
1	B	485	PRO	2.2
1	A	327	ASN	2.1
1	C	396	TYR	2.1
1	B	326	GLN	2.1
1	B	598	TRP	2.1
1	B	472	ASP	2.1
1	C	487	VAL	2.1
1	B	276	LEU	2.1
1	C	399	ILE	2.1
1	A	486	LYS	2.1
1	B	482	SER	2.0
1	C	238	VAL	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](#)

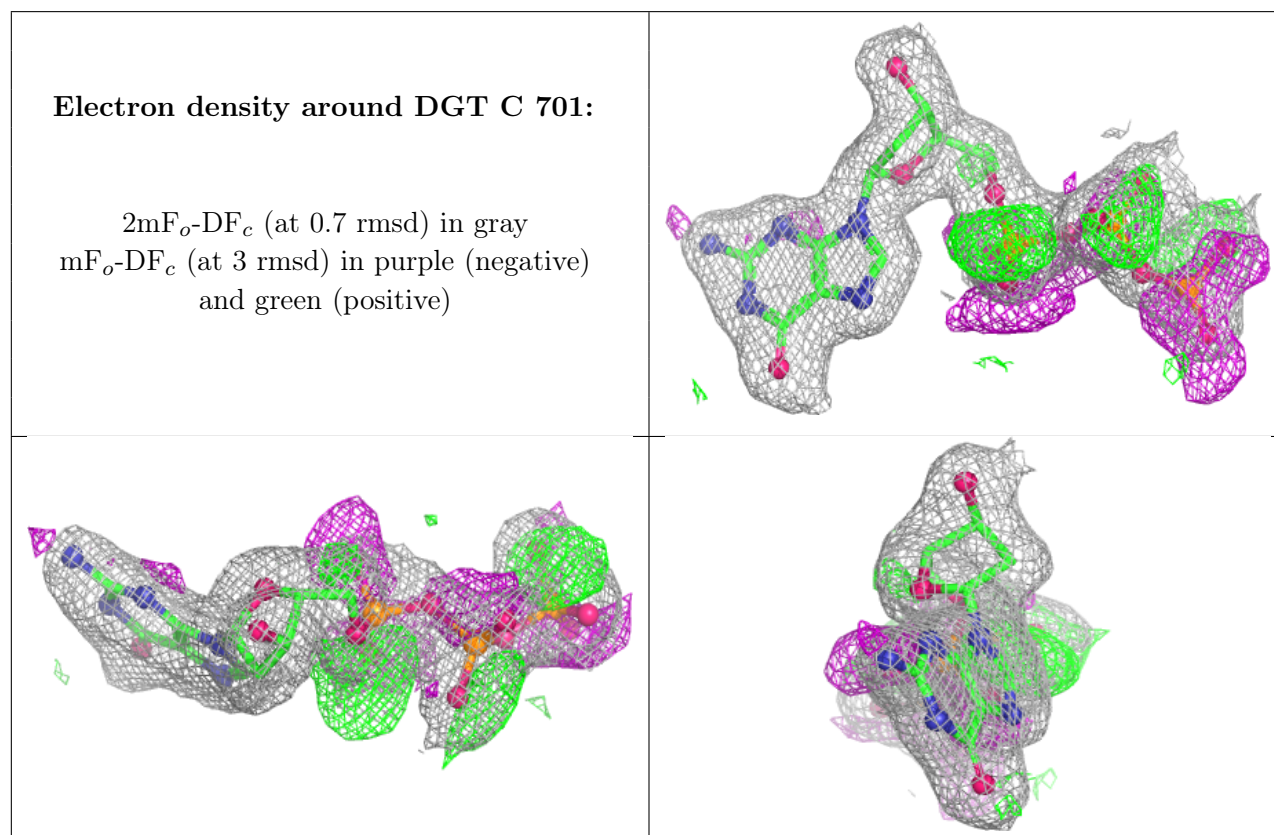
There are no oligosaccharides in this entry.

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.

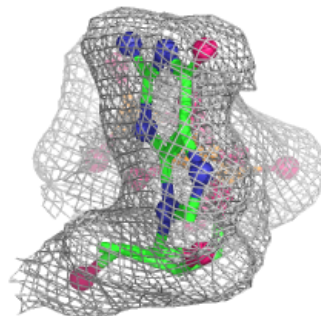
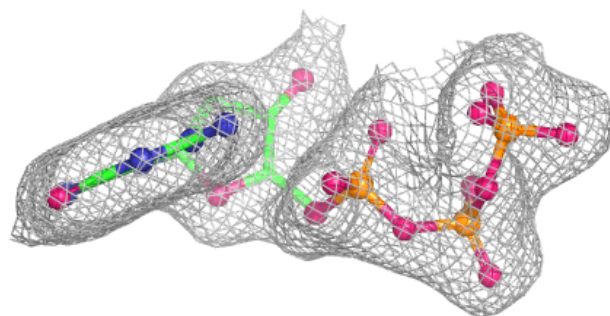
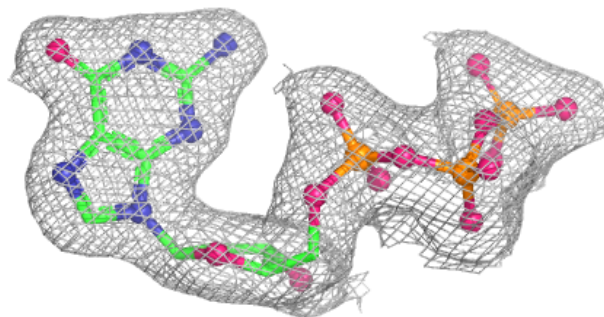
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DGT	C	701	31/31	0.92	0.08	20,24,26,27	0
2	DGT	B	702	31/31	0.98	0.04	31,34,38,43	0
2	DGT	A	704	31/31	0.98	0.04	22,25,31,34	0
2	DGT	C	704	31/31	0.98	0.05	34,40,47,49	0
2	DGT	D	800	31/31	0.98	0.04	31,34,42,45	0
3	MG	C	703	1/1	0.98	0.03	41,41,41,41	0
2	DGT	A	702	31/31	0.99	0.04	26,29,34,36	0
2	DGT	B	703	31/31	0.99	0.04	22,25,29,31	0
3	MG	C	702	1/1	0.99	0.02	25,25,25,25	0
2	DGT	A	701	31/31	0.99	0.03	20,23,30,33	0
3	MG	A	703	1/1	1.00	0.02	28,28,28,28	0
3	MG	B	701	1/1	1.00	0.02	33,33,33,33	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.

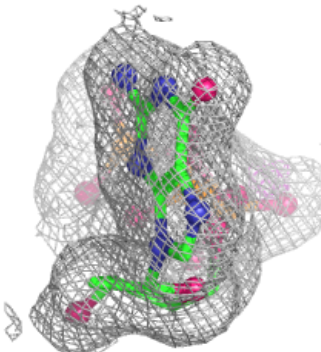
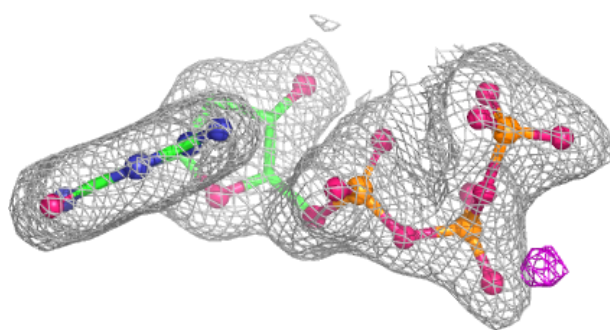
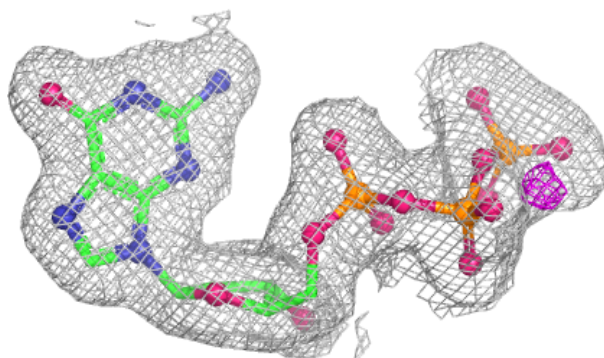


Electron density around DGT B 702:

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

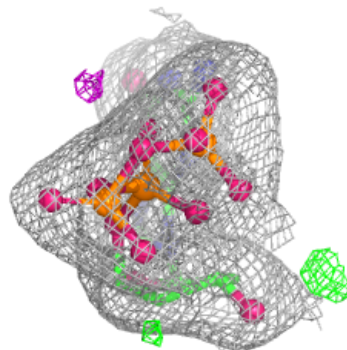
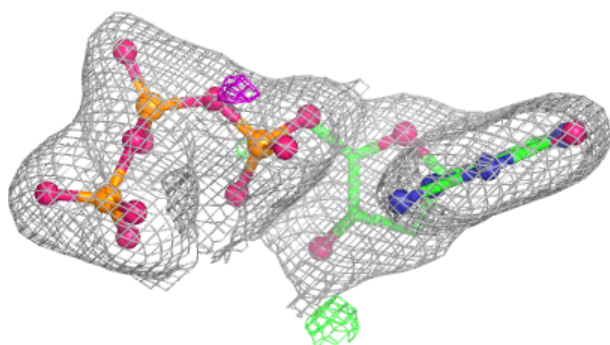
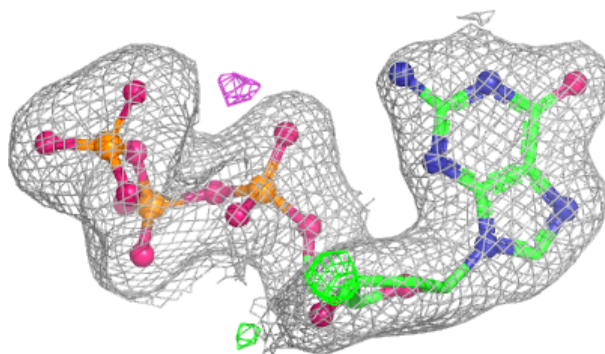
**Electron density around DGT A 704:**

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

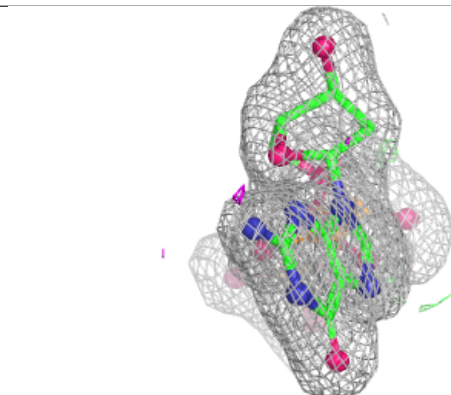
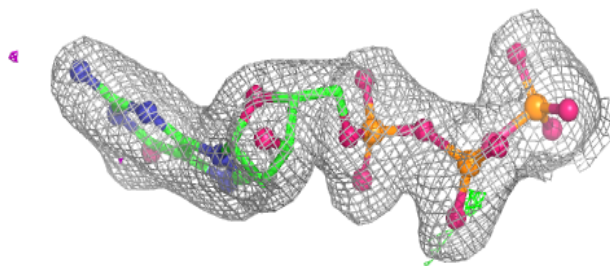
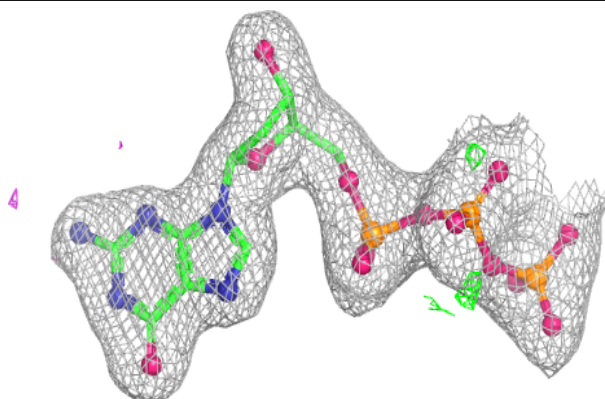


Electron density around DGT C 704:

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

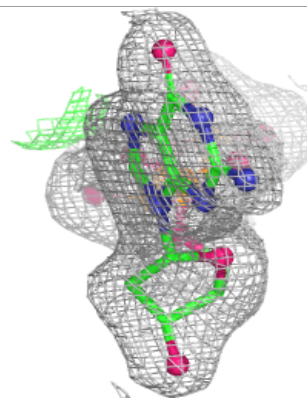
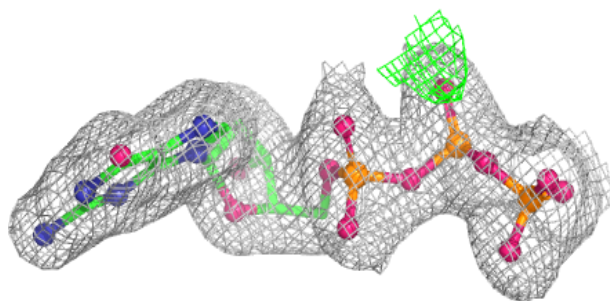
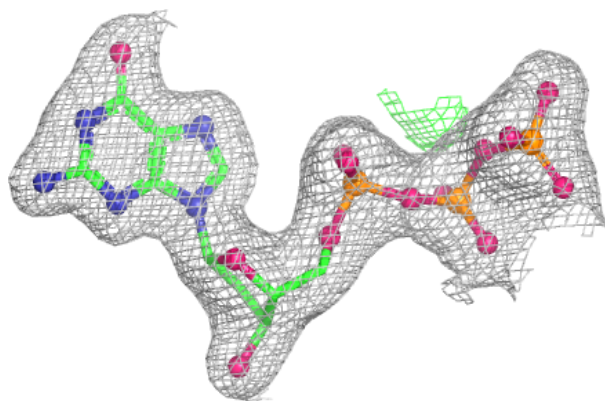
**Electron density around DGT D 800:**

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

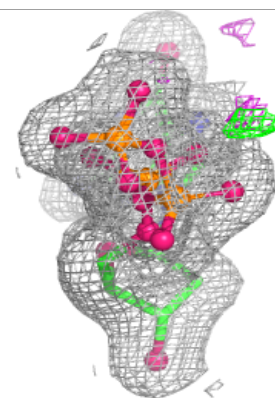
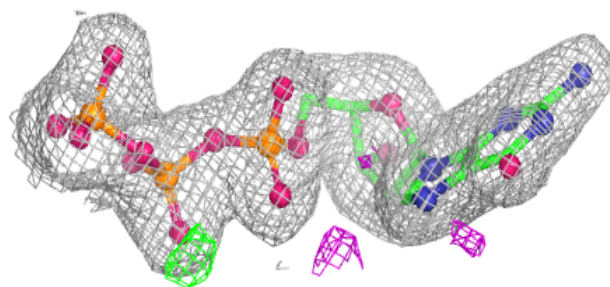
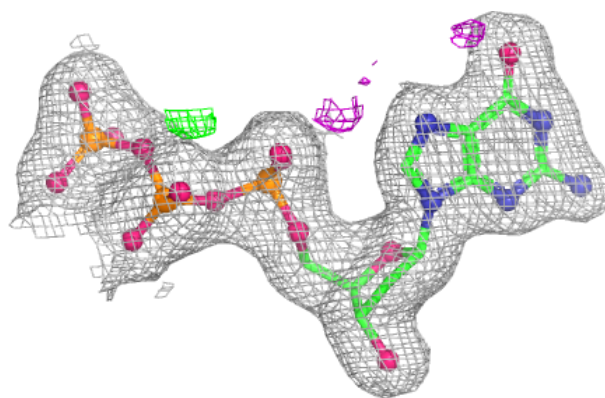


Electron density around DGT A 702:

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

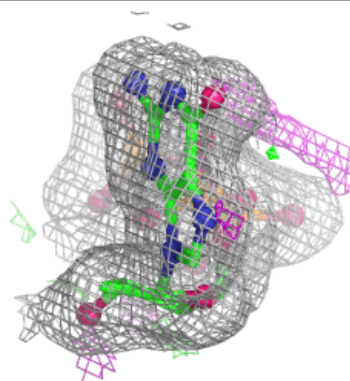
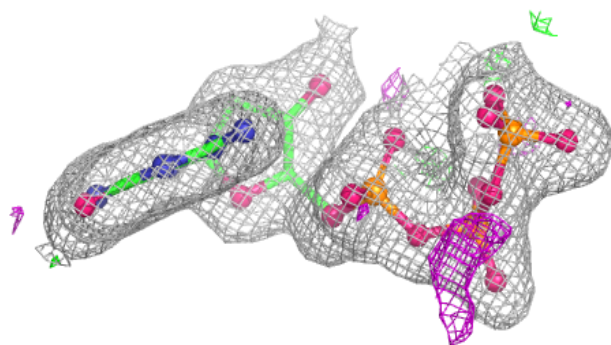
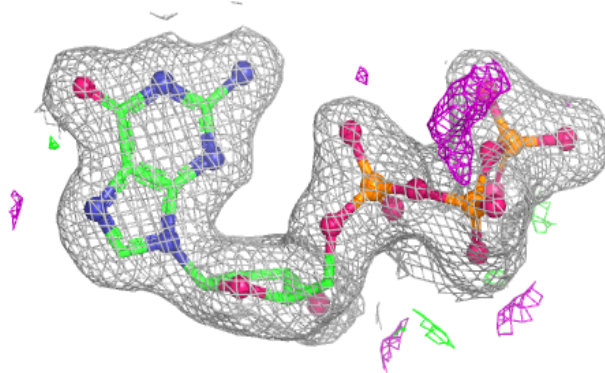
**Electron density around DGT B 703:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.