



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:28 AM UTC

PDB ID : 4BZB / pdb_00004bzb
Title : Crystal structure of the tetrameric dGTP-bound SAMHD1 mutant catalytic core
Authors : Ji, X.; Yang, H.; Wu, Y.; Yan, J.; Mehrens, J.; DeLucia, M.; Hao, C.; Gronenborn, A.M.; Skowronski, J.; Ahn, J.; Xiong, Y.
Deposited on : 2013-07-25
Resolution : 1.83 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

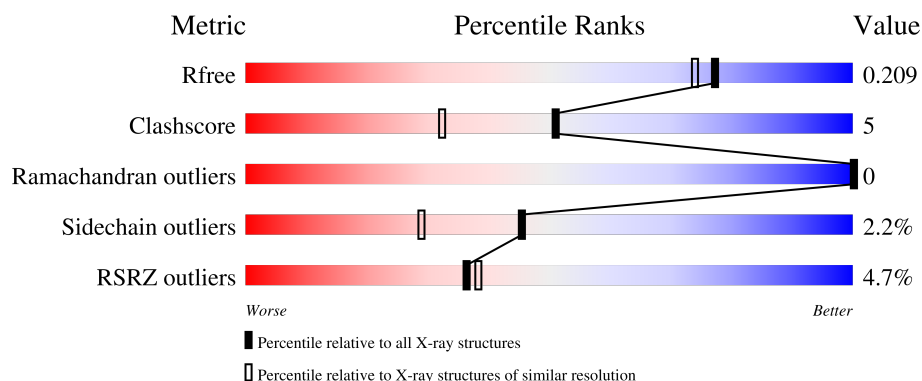
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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% 78% 9% • 13%
1	B	550	4% 79% 8% • 13%
1	C	550	4% 77% 10% • 13%
1	D	550	3% 79% 8% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17207 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 TRIPHOSPHO-HYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	7	0
			3997	2554	698	724	21			
1	B	481	Total	C	N	O	S	0	4	0
			3975	2543	694	718	20			
1	C	481	Total	C	N	O	S	0	5	0
			3981	2546	695	719	21			
1	D	481	Total	C	N	O	S	0	7	0
			3997	2554	698	724	21			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	expression tag	UNP Q9Y3Z3
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	101	THR	-	expression tag	UNP Q9Y3Z3
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

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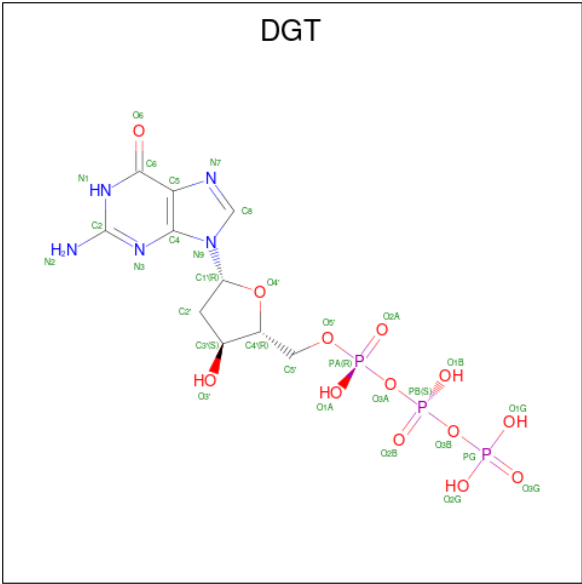
Chain	Residue	Modelled	Actual	Comment	Reference
C	105	GLN	-	expression tag	UNP Q9Y3Z3
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	109	ASP	-	expression tag	UNP Q9Y3Z3
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).



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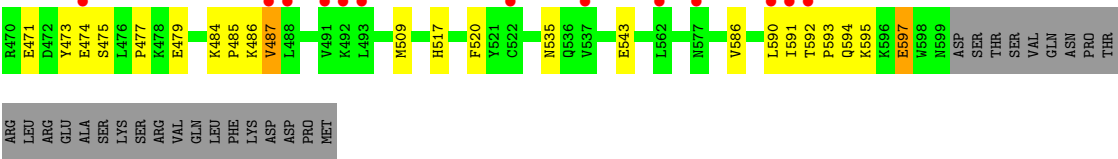
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

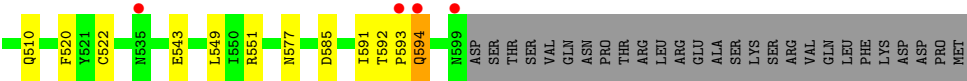
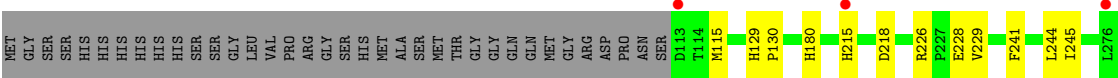
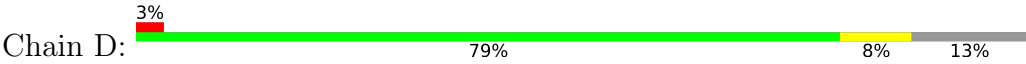
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	228	Total	O	0	0
			228	228		
4	B	271	Total	O	0	0
			271	271		
4	C	156	Total	O	0	0
			156	156		
4	D	222	Total	O	0	0
			222	222		



● 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	87.20Å 146.75Å 98.72Å 90.00° 114.42° 90.00°	Depositor
Resolution (Å)	48.73 – 1.83 48.73 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.73-1.83) 99.7 (48.73-1.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.206 0.193 , 0.209	Depositor DCC
R_{free} test set	9923 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17207	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: 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	0.43	0/4091	0.72	2/5522 (0.0%)
1	B	0.41	0/4069	0.71	4/5492 (0.1%)
1	C	0.42	0/4075	0.71	4/5500 (0.1%)
1	D	0.47	2/4091 (0.0%)	0.71	3/5522 (0.1%)
All	All	0.44	2/16326 (0.0%)	0.71	13/22036 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	354	LYS	N-CA	-8.47	1.34	1.46
1	D	405	LYS	N-CA	-5.53	1.38	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	354	LYS	N-CA-CB	-7.33	98.45	110.40
1	B	576	ARG	CA-C-N	-6.53	113.47	123.47
1	B	576	ARG	C-N-CA	-6.53	113.47	123.47
1	C	591	ILE	N-CA-C	6.00	116.78	110.72
1	A	575	ASP	CA-C-N	-5.80	113.38	122.65
1	A	575	ASP	C-N-CA	-5.80	113.38	122.65
1	B	575	ASP	CA-C-N	-5.48	113.50	122.54
1	B	575	ASP	C-N-CA	-5.48	113.50	122.54
1	C	484	LYS	CA-C-N	5.43	125.08	119.05
1	C	484	LYS	C-N-CA	5.43	125.08	119.05
1	D	353	ASP	CA-C-O	5.31	126.36	120.63
1	C	473	TYR	N-CA-C	5.29	117.05	111.28
1	D	510	GLN	CB-CA-C	-5.09	110.72	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3997	0	3964	42	0
1	B	3975	0	3952	42	0
1	C	3981	0	3956	57	0
1	D	3997	0	3964	35	0
2	A	93	0	36	0	0
2	B	93	0	36	0	0
2	C	93	0	36	0	0
2	D	93	0	36	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	228	0	0	3	0
4	B	271	0	0	9	0
4	C	156	0	0	1	0
4	D	222	0	0	5	0
All	All	17207	0	15980	169	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 5.

All (169) 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:439:LYS:HE2	1:C:443:GLU:HG2	1.28	1.14
1:C:439:LYS:NZ	1:C:443:GLU:HG3	1.62	1.12
1:D:585:ASP:OD1	1:D:592:THR:HG21	1.49	1.11
1:C:439:LYS:HE2	1:C:443:GLU:CG	1.89	1.03
1:C:439:LYS:HZ3	1:C:443:GLU:HG3	1.23	0.94
1:C:474:GLU:O	1:C:477:PRO:HD2	1.69	0.93
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.03	0.93
1:A:466:ILE:HD13	1:A:466:ILE:N	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:LYS:O	1:B:537:VAL:HG22	1.72	0.90
1:C:487:VAL:HG13	1:C:590:LEU:CD1	2.04	0.88
1:D:331[A]:TYR:CD1	4:D:2099:HOH:O	2.27	0.87
1:C:439:LYS:CE	1:C:443:GLU:CG	2.54	0.85
1:C:592:THR:OG1	1:C:593:PRO:HD3	1.78	0.84
1:B:331[A]:TYR:CD1	4:B:2113:HOH:O	2.32	0.82
1:B:355:GLU:OE2	4:B:2122:HOH:O	1.98	0.81
1:C:595:LYS:HE3	1:C:597:GLU:CG	2.11	0.81
1:C:439:LYS:CE	1:C:443:GLU:HG3	2.11	0.80
1:C:487:VAL:CG1	1:C:590:LEU:HD12	2.14	0.78
1:C:487:VAL:HG13	1:C:590:LEU:HD13	1.66	0.76
1:B:537:VAL:HG23	1:B:538:SER:H	1.50	0.76
1:B:355:GLU:OE1	4:B:2136:HOH:O	2.05	0.73
1:B:576:ARG:O	1:B:577:ASN:HB2	1.88	0.73
1:A:390:PHE:CE2	1:A:426:ILE:CD1	2.71	0.73
1:C:595:LYS:HG3	1:C:597:GLU:HG2	1.73	0.70
1:D:585:ASP:OD1	1:D:592:THR:CG2	2.37	0.70
1:C:331[A]:TYR:CD1	4:C:2079:HOH:O	2.44	0.69
1:A:466:ILE:N	1:A:466:ILE:CD1	2.55	0.69
1:A:465:GLN:CG	1:A:466:ILE:HD13	2.24	0.68
1:B:534:LYS:O	1:B:537:VAL:CG2	2.41	0.68
1:C:469:LYS:HD2	1:C:471:GLU:OE2	1.95	0.67
1:C:474:GLU:C	1:C:477:PRO:HD2	2.20	0.67
1:C:487:VAL:HG13	1:C:590:LEU:HD12	1.76	0.67
1:C:487:VAL:CG1	1:C:590:LEU:CD1	2.71	0.67
1:C:439:LYS:NZ	1:C:443:GLU:CG	2.48	0.67
1:B:326:GLN:HG3	1:D:326:GLN:OE1	1.96	0.66
1:B:576:ARG:O	1:B:577:ASN:CB	2.43	0.65
1:A:592:THR:OG1	1:A:593:PRO:HD3	1.97	0.65
1:A:465:GLN:CG	1:A:466:ILE:CD1	2.75	0.64
1:A:331[B]:TYR:CD2	4:A:2101:HOH:O	2.50	0.64
1:B:368:SER:HA	1:B:371[B]:ARG:HG2	1.80	0.64
1:C:487:VAL:HG11	1:C:590:LEU:HD12	1.79	0.63
1:B:592:THR:OG1	1:B:593:PRO:HD3	1.98	0.62
1:C:475:SER:O	1:C:479:GLU:HG3	2.00	0.62
1:D:284:LEU:HD13	1:D:285:TRP:N	2.14	0.62
1:A:115:MET:C	1:A:115:MET:SD	2.83	0.62
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.00	0.62
1:D:591:ILE:O	1:D:594:GLN:HG2	2.01	0.61
1:A:465:GLN:HG2	1:A:466:ILE:CD1	2.30	0.61
1:C:190:GLN:HA	1:C:190:GLN:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLN:HG3	1:A:466:ILE:CD1	2.31	0.60
1:A:331[A]:TYR:CD1	1:A:331[A]:TYR:C	2.80	0.60
1:C:439:LYS:HD3	1:C:439:LYS:C	2.27	0.59
1:B:535:ASN:N	1:B:535:ASN:OD1	2.34	0.59
1:A:465:GLN:HG2	1:A:466:ILE:HD13	1.84	0.59
1:C:595:LYS:HE3	1:C:597:GLU:HG3	1.82	0.59
1:C:535:ASN:N	1:C:535:ASN:OD1	2.36	0.58
1:B:470:ARG:O	1:B:470:ARG:HD2	2.04	0.58
1:A:535:ASN:N	1:A:535:ASN:OD1	2.32	0.57
1:A:466:ILE:HD13	1:A:466:ILE:H	1.67	0.57
1:C:390:PHE:CZ	1:C:426:ILE:CG2	2.88	0.57
1:C:485:PRO:O	1:C:486:LYS:CB	2.53	0.57
1:D:228:GLU:OE1	1:D:228:GLU:N	2.34	0.57
4:A:2224:HOH:O	1:C:354:LYS:HE2	2.05	0.57
1:B:276:LEU:O	1:B:277:GLU:C	2.47	0.57
1:D:284:LEU:HD13	1:D:284:LEU:C	2.28	0.57
1:D:331[B]:TYR:C	1:D:331[B]:TYR:CD1	2.84	0.56
1:C:485:PRO:O	1:C:486:LYS:HB2	2.05	0.56
1:A:597:GLU:OE1	1:A:597:GLU:N	2.31	0.56
1:B:172:GLY:HA3	1:B:204:LEU:HD13	1.88	0.56
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.06	0.55
1:A:390:PHE:CZ	1:A:426:ILE:CD1	2.89	0.55
1:C:331[B]:TYR:CD1	1:C:331[B]:TYR:C	2.85	0.54
1:A:352:ARG:HG3	1:A:354:LYS:HG2	1.89	0.54
1:A:592:THR:N	1:A:593:PRO:CD	2.71	0.54
1:C:595:LYS:HE3	1:C:597:GLU:CD	2.31	0.54
1:B:455:LYS:HA	1:B:455:LYS:HE2	1.89	0.53
1:A:594:GLN:HG2	1:A:595:LYS:N	2.23	0.53
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.45	0.52
1:C:455:LYS:HA	1:C:455:LYS:HE2	1.91	0.52
1:B:331[B]:TYR:CD1	1:B:331[B]:TYR:C	2.87	0.52
1:A:598:TRP:O	1:A:599:ASN:CB	2.58	0.51
1:B:537:VAL:HG23	1:B:541:LEU:HD12	1.93	0.51
1:C:543:GLU:HA	1:C:543:GLU:OE1	2.11	0.51
1:C:595:LYS:CE	1:C:597:GLU:HG3	2.40	0.51
1:C:277:GLU:O	1:C:277:GLU:HG2	2.11	0.51
1:C:392:LYS:HE2	1:C:444:ILE:HD11	1.92	0.51
4:B:2031:HOH:O	1:C:322:HIS:CE1	2.64	0.51
1:B:223:PRO:HB3	1:B:470:ARG:HH22	1.76	0.51
1:C:592:THR:N	1:C:593:PRO:CD	2.73	0.50
1:D:592:THR:N	1:D:593:PRO:HD2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:O	1:B:229:VAL:HG12	2.11	0.50
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.46	0.50
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.47	0.50
1:B:537:VAL:HG23	1:B:538:SER:N	2.22	0.49
1:A:465:GLN:HG3	1:A:466:ILE:HD13	1.92	0.49
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.47	0.49
1:C:485:PRO:CB	1:C:487:VAL:HG23	2.42	0.49
1:D:226:ARG:O	1:D:229:VAL:HG12	2.13	0.49
1:B:392:LYS:HE2	1:B:444:ILE:HD11	1.94	0.49
1:D:592:THR:N	1:D:593:PRO:CD	2.76	0.48
1:B:329:PHE:O	4:B:2113:HOH:O	2.20	0.48
1:B:326:GLN:CG	1:D:326:GLN:OE1	2.60	0.48
1:C:595:LYS:CE	1:C:597:GLU:CG	2.88	0.48
1:D:392:LYS:HE2	1:D:444:ILE:HD11	1.94	0.48
1:C:509:MET:HE1	1:C:517:HIS:ND1	2.29	0.48
1:D:371[A]:ARG:NH2	1:D:549:LEU:HD21	2.28	0.48
1:C:226:ARG:O	1:C:229:VAL:HG12	2.13	0.47
1:D:331[A]:TYR:HD1	4:D:2099:HOH:O	1.81	0.47
1:C:244:LEU:C	1:C:244:LEU:HD23	2.40	0.47
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.96	0.47
1:A:390:PHE:CZ	1:A:426:ILE:HD11	2.47	0.47
1:B:298:TYR:O	4:B:2087:HOH:O	2.20	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.77	0.47
1:C:277:GLU:O	1:C:277:GLU:CG	2.62	0.47
1:C:351:ALA:O	1:C:520:PHE:HA	2.14	0.47
1:A:522[A]:CYS:SG	1:C:586:VAL:HG11	2.55	0.47
1:D:298:TYR:O	4:D:2080:HOH:O	2.20	0.47
1:C:398:GLU:CD	1:C:406:LYS:HD2	2.40	0.47
1:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.46
1:A:244:LEU:C	1:A:244:LEU:HD23	2.40	0.46
1:B:244:LEU:C	1:B:244:LEU:HD23	2.40	0.46
1:D:326:GLN:HG3	1:D:327:ASN:N	2.31	0.46
1:B:534:LYS:C	1:B:537:VAL:HG22	2.38	0.46
1:C:398:GLU:OE1	1:C:406:LYS:HD2	2.16	0.46
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.46
1:B:496:GLU:H	1:B:496:GLU:CD	2.23	0.45
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:D:398:GLU:CD	1:D:406:LYS:HD2	2.42	0.45
1:D:244:LEU:C	1:D:244:LEU:HD23	2.42	0.45
1:D:398:GLU:OE1	1:D:406:LYS:HD2	2.17	0.45
1:D:215:HIS:HA	1:D:218:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:HA	1:A:218:ASP:OD1	2.17	0.44
1:A:454:PHE:CD2	1:A:499:ILE:CD1	3.01	0.44
1:B:331[A]:TYR:HD1	4:B:2113:HOH:O	1.87	0.44
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.89	0.44
1:C:215:HIS:HA	1:C:218:ASP:OD1	2.17	0.44
1:D:371[A]:ARG:HG2	1:D:505:MET:HE2	1.99	0.44
1:B:537:VAL:HB	4:B:2243:HOH:O	2.18	0.44
1:C:320:CYS:HB3	1:C:325:ILE:O	2.18	0.44
1:D:355:GLU:OE1	4:D:2116:HOH:O	2.21	0.43
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.54	0.43
1:A:326:GLN:HG3	1:A:327:ASN:N	2.34	0.43
1:A:598:TRP:O	1:A:599:ASN:HB2	2.18	0.43
1:D:503:ILE:HD12	1:D:551:ARG:HD3	2.00	0.42
1:D:284:LEU:C	1:D:284:LEU:CD1	2.92	0.42
1:D:591:ILE:O	1:D:594:GLN:CG	2.66	0.42
1:C:284:LEU:HD12	1:C:285:TRP:N	2.34	0.42
1:A:405:LYS:HD3	1:A:407:TYR:OH	2.19	0.42
1:A:533:THR:OG1	1:A:536:GLN:HG3	2.19	0.42
1:B:534:LYS:HG2	4:B:2241:HOH:O	2.19	0.42
1:B:223:PRO:CB	1:B:470:ARG:HH22	2.33	0.42
1:D:115:MET:C	1:D:115:MET:SD	3.03	0.42
1:D:592:THR:HB	1:D:593:PRO:HD3	2.01	0.42
1:A:331[B]:TYR:HD2	4:A:2101:HOH:O	1.98	0.42
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.89	0.41
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.02	0.41
1:C:592:THR:N	1:C:593:PRO:HD2	2.35	0.41
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.03	0.41
1:C:241:PHE:O	1:C:245:ILE:HG12	2.20	0.41
1:C:485:PRO:HB2	1:C:487:VAL:HG23	2.03	0.41
1:D:241:PHE:O	1:D:245:ILE:HG12	2.20	0.41
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.88	0.41
1:A:479:GLU:OE1	1:A:576:ARG:NH1	2.54	0.41
1:A:125:HIS:CE1	1:B:333:ARG:HB2	2.56	0.40
1:A:320:CYS:HB3	1:A:325:ILE:O	2.22	0.40
1:B:241:PHE:O	1:B:245:ILE:HG12	2.21	0.40
1:B:586:VAL:HG11	1:D:522[A]:CYS:SG	2.62	0.40
1:A:139:PRO:HG3	4:D:2156:HOH:O	2.20	0.40
1:B:284:LEU:HD12	1:B:285:TRP:N	2.36	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	484/550 (88%)	479 (99%)	5 (1%)	0	100	100
1	B	481/550 (88%)	475 (99%)	6 (1%)	0	100	100
1	C	482/550 (88%)	475 (98%)	7 (2%)	0	100	100
1	D	484/550 (88%)	478 (99%)	6 (1%)	0	100	100
All	All	1931/2200 (88%)	1907 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/488 (89%)	421 (97%)	13 (3%)	36	19
1	B	431/488 (88%)	425 (99%)	6 (1%)	59	45
1	C	432/488 (88%)	421 (98%)	11 (2%)	42	24
1	D	434/488 (89%)	424 (98%)	10 (2%)	44	27
All	All	1731/1952 (89%)	1691 (98%)	40 (2%)	45	27

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LEU
1	A	235	GLN

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Mol	Chain	Res	Type
1	A	255	GLU
1	A	331[A]	TYR
1	A	331[B]	TYR
1	A	361	ASP
1	A	398	GLU
1	A	463	THR
1	A	466	ILE
1	A	467	LYS
1	A	534	LYS
1	A	535	ASN
1	A	594	GLN
1	B	204	LEU
1	B	284	LEU
1	B	361	ASP
1	B	467	LYS
1	B	487	VAL
1	B	496	GLU
1	C	115	MET
1	C	180[A]	HIS
1	C	180[B]	HIS
1	C	284	LEU
1	C	354	LYS
1	C	361	ASP
1	C	425	ASN
1	C	426	ILE
1	C	487	VAL
1	C	594	GLN
1	C	597	GLU
1	D	180[A]	HIS
1	D	180[B]	HIS
1	D	326	GLN
1	D	361	ASP
1	D	377	LYS
1	D	425	ASN
1	D	465	GLN
1	D	467	LYS
1	D	577	ASN
1	D	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	233	HIS
1	A	248	ASN
1	A	321	HIS
1	A	326	GLN
1	A	375	GLN
1	A	380	ASN
1	B	149	GLN
1	B	233	HIS
1	B	235	GLN
1	B	248	ASN
1	B	375	GLN
1	B	380	ASN
1	B	447	GLN
1	B	452	ASN
1	C	149	GLN
1	C	235	GLN
1	C	243	HIS
1	C	248	ASN
1	C	321	HIS
1	C	322	HIS
1	C	375	GLN
1	C	380	ASN
1	C	447	GLN
1	C	452	ASN
1	D	149	GLN
1	D	235	GLN
1	D	248	ASN
1	D	375	GLN
1	D	380	ASN
1	D	577	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 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	800	3	32,33,33	1.22	5 (15%)	48,52,52	1.64	7 (14%)
2	DGT	A	900	3	32,33,33	1.19	4 (12%)	48,52,52	1.63	6 (12%)
2	DGT	A	800	3	32,33,33	1.32	7 (21%)	48,52,52	1.74	7 (14%)
2	DGT	B	900	3	32,33,33	1.15	3 (9%)	48,52,52	1.67	6 (12%)
2	DGT	C	900	3	32,33,33	1.19	4 (12%)	48,52,52	1.74	7 (14%)
2	DGT	D	900	3	32,33,33	1.20	4 (12%)	48,52,52	1.65	6 (12%)
2	DGT	D	700	3	32,33,33	1.29	5 (15%)	48,52,52	1.68	6 (12%)
2	DGT	B	800	3	32,33,33	1.28	5 (15%)	48,52,52	1.63	6 (12%)
2	DGT	B	700	3	32,33,33	1.28	5 (15%)	48,52,52	1.69	7 (14%)
2	DGT	D	800	3	32,33,33	1.22	5 (15%)	48,52,52	1.64	7 (14%)
2	DGT	A	700	3	32,33,33	1.27	5 (15%)	48,52,52	1.76	7 (14%)
2	DGT	C	700	3	32,33,33	1.28	6 (18%)	48,52,52	1.75	7 (14%)

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	800	3	-	4/22/34/34	0/3/3/3
2	DGT	A	900	3	-	4/22/34/34	0/3/3/3
2	DGT	A	800	3	-	3/22/34/34	0/3/3/3
2	DGT	B	900	3	-	8/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	C	900	3	-	7/22/34/34	0/3/3/3
2	DGT	D	900	3	-	6/22/34/34	0/3/3/3
2	DGT	D	700	3	-	3/22/34/34	0/3/3/3
2	DGT	B	800	3	-	3/22/34/34	0/3/3/3
2	DGT	B	700	3	-	3/22/34/34	0/3/3/3
2	DGT	D	800	3	-	3/22/34/34	0/3/3/3
2	DGT	A	700	3	-	3/22/34/34	0/3/3/3
2	DGT	C	700	3	-	3/22/34/34	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	DGT	C5-C4	3.21	1.47	1.38
2	D	900	DGT	C5-C4	3.20	1.47	1.38
2	A	900	DGT	C5-C4	3.18	1.47	1.38
2	C	900	DGT	C5-C4	3.15	1.47	1.38
2	C	700	DGT	C5-C4	3.14	1.47	1.38
2	D	700	DGT	C5-C4	3.06	1.47	1.38
2	B	700	DGT	C5-C4	3.06	1.47	1.38
2	B	900	DGT	C5-C4	3.01	1.47	1.38
2	B	800	DGT	C6-N1	-2.94	1.33	1.38
2	A	800	DGT	C5-C4	2.91	1.46	1.38
2	B	700	DGT	PB-O3B	2.88	1.62	1.59
2	C	800	DGT	C5-C4	2.87	1.46	1.38
2	D	800	DGT	C5-C4	2.86	1.46	1.38
2	B	800	DGT	C5-C4	2.75	1.46	1.38
2	A	800	DGT	PA-O3A	2.63	1.62	1.59
2	D	700	DGT	PB-O3B	2.61	1.62	1.59
2	A	800	DGT	C6-N1	-2.60	1.34	1.38
2	B	800	DGT	PA-O3A	2.58	1.62	1.59
2	A	700	DGT	PB-O3B	2.49	1.62	1.59
2	B	700	DGT	C6-N1	-2.47	1.34	1.38
2	D	900	DGT	C6-N1	-2.46	1.34	1.38
2	A	900	DGT	C5-N7	-2.46	1.34	1.39
2	A	800	DGT	PB-O3A	2.43	1.62	1.59
2	A	900	DGT	C6-N1	-2.40	1.34	1.38
2	D	800	DGT	C6-N1	-2.40	1.34	1.38
2	D	800	DGT	PB-O3A	2.39	1.62	1.59
2	D	700	DGT	C6-N1	-2.36	1.34	1.38
2	C	700	DGT	PB-O3A	2.36	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	DGT	C6-N1	-2.33	1.34	1.38
2	B	800	DGT	C5-N7	-2.30	1.34	1.39
2	B	700	DGT	PA-O3A	2.30	1.62	1.59
2	A	700	DGT	PA-O3A	2.29	1.62	1.59
2	A	800	DGT	PB-O3B	2.29	1.62	1.59
2	D	800	DGT	C4-N9	-2.28	1.32	1.38
2	B	900	DGT	C6-N1	-2.27	1.34	1.38
2	C	700	DGT	C6-N1	-2.23	1.34	1.38
2	C	700	DGT	C5-N7	-2.23	1.34	1.39
2	C	900	DGT	PB-O3A	2.22	1.61	1.59
2	D	700	DGT	C5-N7	-2.22	1.34	1.39
2	C	900	DGT	C5-N7	-2.21	1.34	1.39
2	C	800	DGT	C6-N1	-2.19	1.34	1.38
2	C	700	DGT	PB-O3B	2.18	1.61	1.59
2	B	700	DGT	C5-N7	-2.16	1.34	1.39
2	B	900	DGT	C5-N7	-2.16	1.34	1.39
2	C	700	DGT	PA-O3A	2.15	1.61	1.59
2	C	900	DGT	C6-N1	-2.14	1.34	1.38
2	D	700	DGT	PA-O3A	2.11	1.61	1.59
2	B	800	DGT	C4-N9	-2.09	1.32	1.38
2	C	800	DGT	C4-N9	-2.08	1.32	1.38
2	D	900	DGT	PB-O3A	2.07	1.61	1.59
2	C	800	DGT	PB-O3B	2.07	1.61	1.59
2	A	800	DGT	C5-N7	-2.07	1.34	1.39
2	D	900	DGT	C5-N7	-2.07	1.34	1.39
2	A	800	DGT	C4-N9	-2.06	1.32	1.38
2	C	800	DGT	PA-O3A	2.06	1.61	1.59
2	A	900	DGT	C4-N9	-2.05	1.32	1.38
2	D	800	DGT	C5-N7	-2.02	1.35	1.39
2	A	700	DGT	C5-N7	-2.01	1.35	1.39

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	DGT	C5-C4-N3	-5.94	118.93	128.39
2	C	700	DGT	C5-C4-N3	-5.93	118.95	128.39
2	D	900	DGT	C5-C4-N3	-5.86	119.06	128.39
2	C	900	DGT	C5-C4-N3	-5.83	119.11	128.39
2	B	900	DGT	C5-C4-N3	-5.75	119.24	128.39
2	A	900	DGT	C5-C4-N3	-5.70	119.32	128.39
2	A	800	DGT	C5-C4-N3	-5.69	119.33	128.39
2	B	700	DGT	C5-C4-N3	-5.63	119.42	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	DGT	C5-C4-N3	-5.52	119.60	128.39
2	C	800	DGT	C5-C4-N3	-5.32	119.93	128.39
2	B	800	DGT	C5-C4-N3	-5.07	120.31	128.39
2	D	800	DGT	C5-C4-N3	-4.95	120.51	128.39
2	C	900	DGT	C2-N3-C4	4.88	120.70	112.30
2	C	700	DGT	C2-N3-C4	4.87	120.69	112.30
2	A	800	DGT	C2-N3-C4	4.85	120.66	112.30
2	A	700	DGT	C2-N3-C4	4.79	120.55	112.30
2	D	900	DGT	C2-N3-C4	4.75	120.49	112.30
2	B	900	DGT	C2-N3-C4	4.65	120.31	112.30
2	A	900	DGT	C2-N3-C4	4.63	120.28	112.30
2	C	800	DGT	C2-N3-C4	4.54	120.12	112.30
2	C	700	DGT	N9-C4-N3	4.53	135.01	125.95
2	D	700	DGT	C2-N3-C4	4.49	120.04	112.30
2	D	700	DGT	N9-C4-N3	4.49	134.93	125.95
2	B	700	DGT	C2-N3-C4	4.46	119.99	112.30
2	A	700	DGT	N9-C4-N3	4.43	134.81	125.95
2	D	900	DGT	N9-C4-N3	4.41	134.78	125.95
2	B	700	DGT	N9-C4-N3	4.41	134.77	125.95
2	A	900	DGT	N9-C4-N3	4.24	134.43	125.95
2	B	800	DGT	C2-N3-C4	4.22	119.58	112.30
2	C	900	DGT	N9-C4-N3	4.18	134.31	125.95
2	A	800	DGT	N9-C4-N3	4.18	134.31	125.95
2	B	900	DGT	N9-C4-N3	4.18	134.30	125.95
2	D	800	DGT	C2-N3-C4	4.06	119.29	112.30
2	C	800	DGT	N9-C4-N3	4.04	134.04	125.95
2	D	800	DGT	N9-C4-N3	3.91	133.77	125.95
2	B	800	DGT	N9-C4-N3	3.74	133.44	125.95
2	B	800	DGT	C6-C5-N7	3.73	137.07	130.29
2	A	800	DGT	C6-C5-N7	3.68	136.99	130.29
2	D	800	DGT	C6-C5-N7	3.50	136.66	130.29
2	C	800	DGT	C6-C5-N7	3.50	136.66	130.29
2	C	900	DGT	C6-C5-N7	3.42	136.51	130.29
2	C	700	DGT	C6-C5-N7	3.32	136.34	130.29
2	A	700	DGT	C6-C5-N7	3.29	136.28	130.29
2	D	900	DGT	C6-C5-N7	3.19	136.09	130.29
2	B	900	DGT	C6-C5-N7	3.11	135.96	130.29
2	B	700	DGT	C6-C5-N7	3.10	135.94	130.29
2	A	900	DGT	C6-C5-N7	3.08	135.89	130.29
2	D	700	DGT	C6-C5-N7	3.00	135.75	130.29
2	C	900	DGT	C4-C5-N7	-2.72	106.37	110.67
2	A	800	DGT	C4-C5-N7	-2.59	106.56	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	DGT	C4-C5-N7	-2.59	106.56	110.67
2	A	700	DGT	C4-C5-N7	-2.58	106.59	110.67
2	B	800	DGT	C4-C5-N7	-2.55	106.64	110.67
2	B	700	DGT	O6-C6-C5	-2.53	119.85	126.53
2	D	800	DGT	O6-C6-C5	-2.49	119.95	126.53
2	B	900	DGT	C4-C5-N7	-2.45	106.79	110.67
2	D	700	DGT	O6-C6-C5	-2.44	120.08	126.53
2	D	800	DGT	C4-C5-N7	-2.39	106.88	110.67
2	C	800	DGT	O6-C6-C5	-2.39	120.23	126.53
2	D	900	DGT	C4-C5-N7	-2.38	106.90	110.67
2	C	800	DGT	C4-C5-N7	-2.35	106.94	110.67
2	B	700	DGT	C4-C5-N7	-2.32	107.00	110.67
2	C	700	DGT	O6-C6-C5	-2.28	120.51	126.53
2	A	900	DGT	C4-C5-N7	-2.27	107.06	110.67
2	C	900	DGT	O6-C6-C5	-2.26	120.58	126.53
2	C	900	DGT	O3A-PB-O2B	-2.23	103.99	110.70
2	A	900	DGT	O6-C6-C5	-2.22	120.68	126.53
2	A	700	DGT	O6-C6-C5	-2.21	120.71	126.53
2	B	700	DGT	O4'-C1'-N9	2.20	111.78	107.86
2	B	800	DGT	O6-C6-C5	-2.17	120.80	126.53
2	A	800	DGT	C5-C6-N1	2.14	118.71	113.25
2	A	800	DGT	O6-C6-C5	-2.14	120.88	126.53
2	D	900	DGT	O6-C6-C5	-2.14	120.89	126.53
2	D	700	DGT	C4-C5-N7	-2.12	107.31	110.67
2	A	700	DGT	O4'-C1'-N9	2.09	111.58	107.86
2	B	900	DGT	O6-C6-C5	-2.06	121.11	126.53
2	D	800	DGT	C8-N9-C4	2.03	109.83	106.03
2	C	700	DGT	C8-N7-C5	2.02	107.85	104.26
2	C	800	DGT	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	DGT	O4'-C4'-C5'-O5'
2	A	700	DGT	C3'-C4'-C5'-O5'
2	B	700	DGT	O4'-C4'-C5'-O5'
2	B	700	DGT	C3'-C4'-C5'-O5'
2	C	700	DGT	O4'-C4'-C5'-O5'
2	C	700	DGT	C3'-C4'-C5'-O5'
2	D	700	DGT	O4'-C4'-C5'-O5'
2	D	700	DGT	C3'-C4'-C5'-O5'

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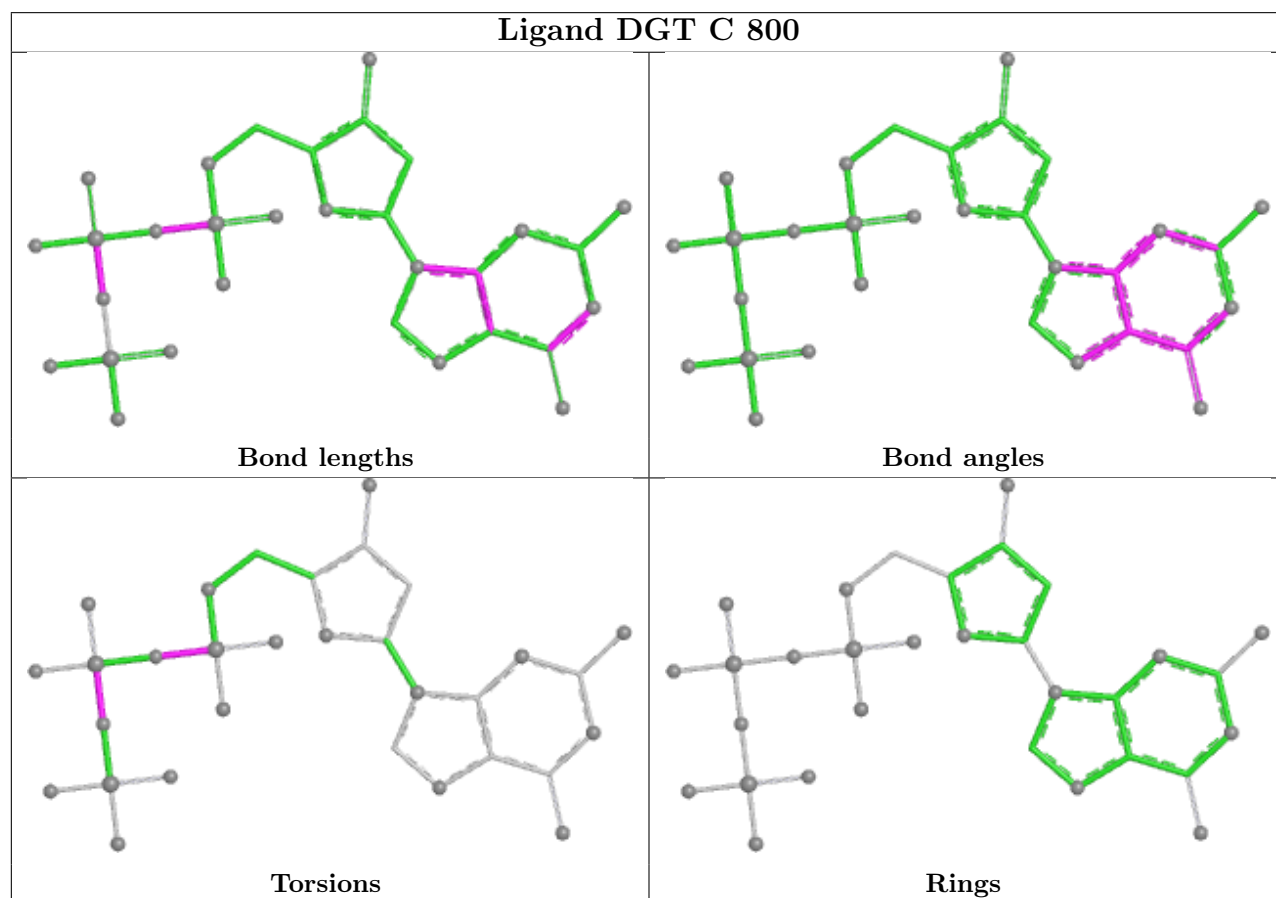
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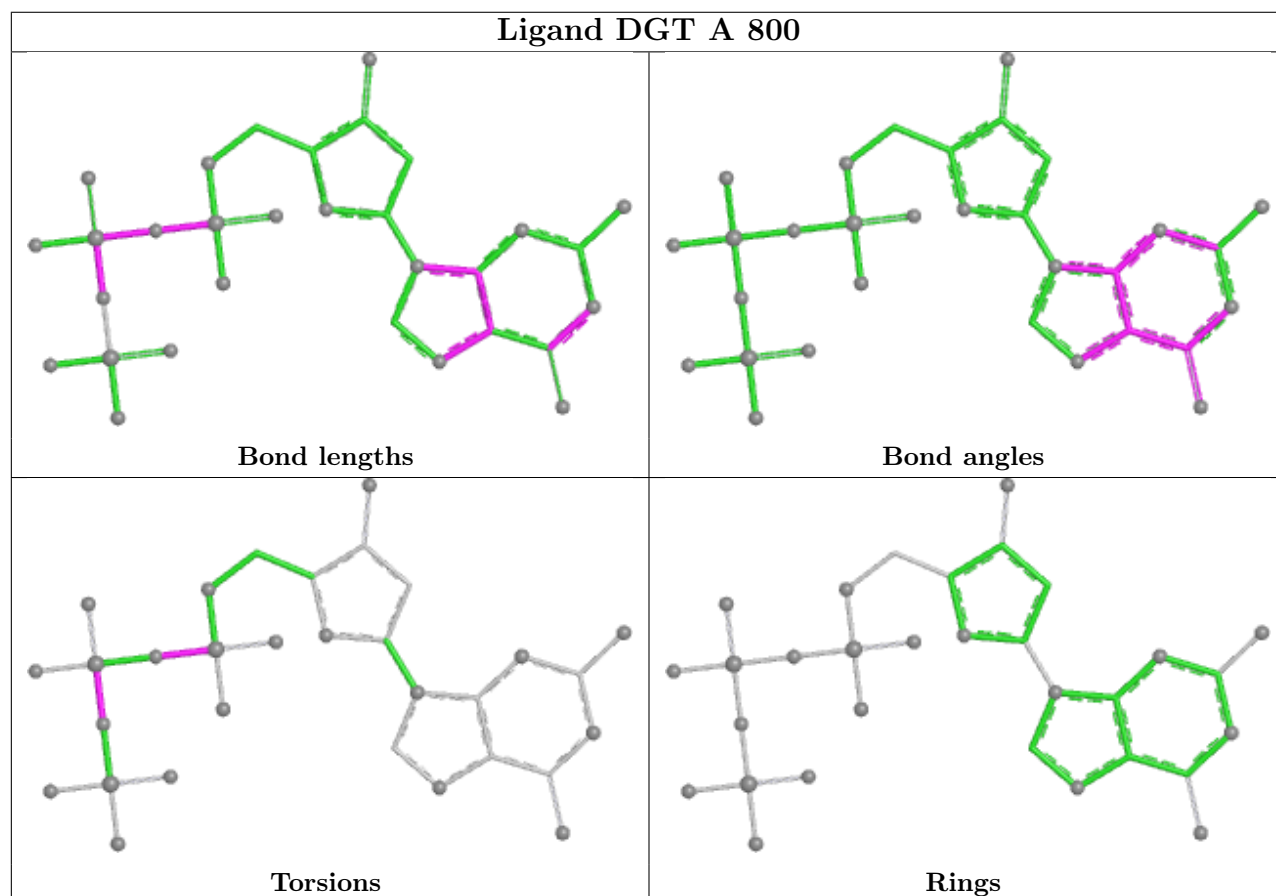
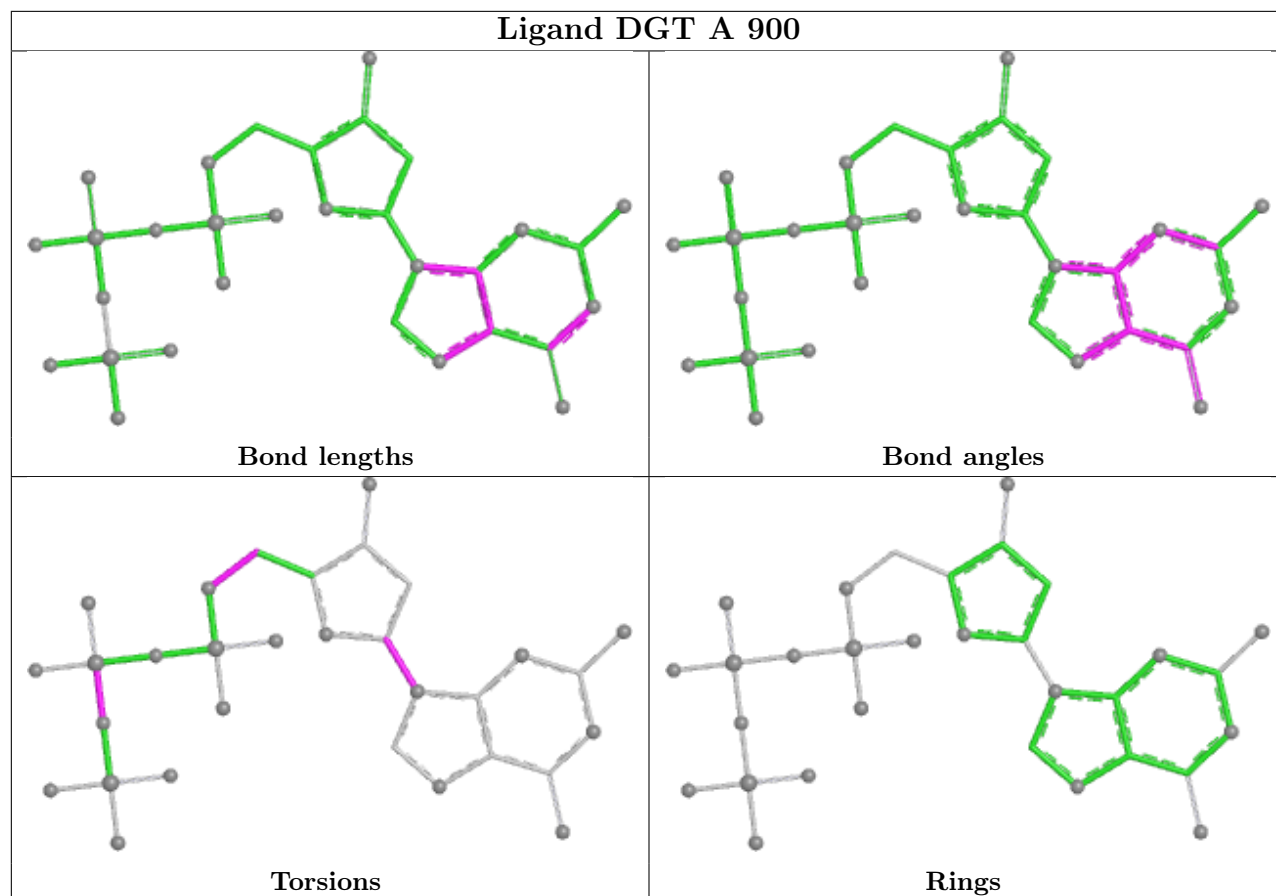
Mol	Chain	Res	Type	Atoms
2	D	700	DGT	C4'-C5'-O5'-PA
2	A	700	DGT	C4'-C5'-O5'-PA
2	B	700	DGT	C4'-C5'-O5'-PA
2	C	700	DGT	C4'-C5'-O5'-PA
2	B	900	DGT	PB-O3B-PG-O3G
2	A	800	DGT	PG-O3B-PB-O2B
2	B	800	DGT	PG-O3B-PB-O2B
2	B	900	DGT	PG-O3B-PB-O1B
2	C	800	DGT	PG-O3B-PB-O1B
2	C	900	DGT	PG-O3B-PB-O1B
2	D	800	DGT	PG-O3B-PB-O1B
2	D	900	DGT	PG-O3B-PB-O2B
2	A	900	DGT	C2'-C1'-N9-C4
2	B	900	DGT	C2'-C1'-N9-C8
2	D	900	DGT	C2'-C1'-N9-C8
2	C	900	DGT	PB-O3B-PG-O3G
2	C	800	DGT	PG-O3B-PB-O2B
2	B	900	DGT	C2'-C1'-N9-C4
2	C	900	DGT	C2'-C1'-N9-C4
2	D	900	DGT	C2'-C1'-N9-C4
2	A	900	DGT	C2'-C1'-N9-C8
2	C	900	DGT	C2'-C1'-N9-C8
2	A	900	DGT	C4'-C5'-O5'-PA
2	D	900	DGT	C4'-C5'-O5'-PA
2	D	800	DGT	PG-O3B-PB-O2B
2	D	900	DGT	PB-O3B-PG-O2G
2	B	900	DGT	C4'-C5'-O5'-PA
2	C	900	DGT	C4'-C5'-O5'-PA
2	A	800	DGT	PG-O3B-PB-O1B
2	B	800	DGT	PG-O3B-PB-O1B
2	B	900	DGT	PG-O3B-PB-O2B
2	C	800	DGT	PB-O3A-PA-O2A
2	C	900	DGT	PG-O3B-PB-O2B
2	C	900	DGT	PB-O3A-PA-O1A
2	A	800	DGT	PB-O3A-PA-O1A
2	A	900	DGT	PG-O3B-PB-O1B
2	B	800	DGT	PB-O3A-PA-O1A
2	B	900	DGT	PB-O3A-PA-O1A
2	B	900	DGT	PB-O3A-PA-O2A
2	C	800	DGT	PB-O3A-PA-O1A
2	D	800	DGT	PB-O3A-PA-O1A
2	D	900	DGT	PG-O3B-PB-O1B

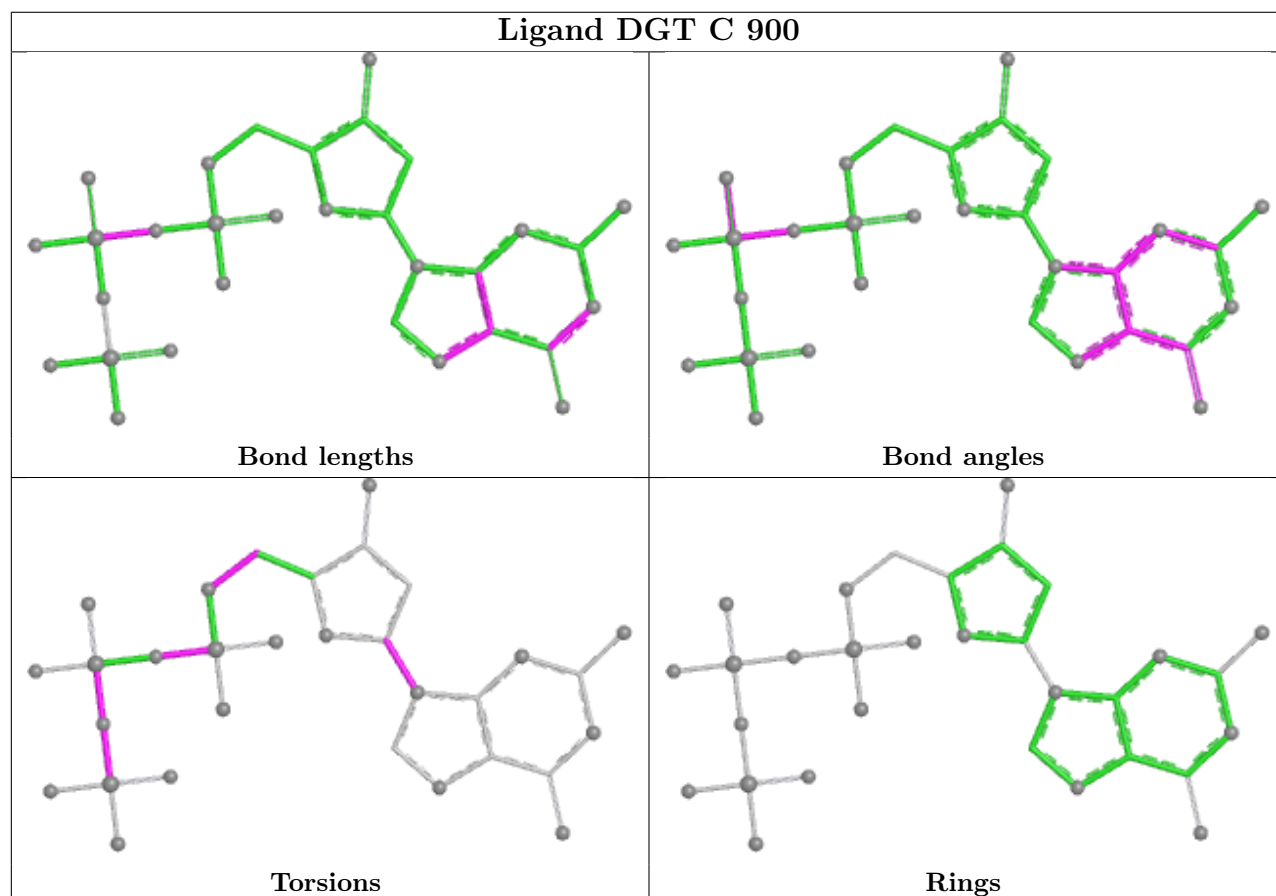
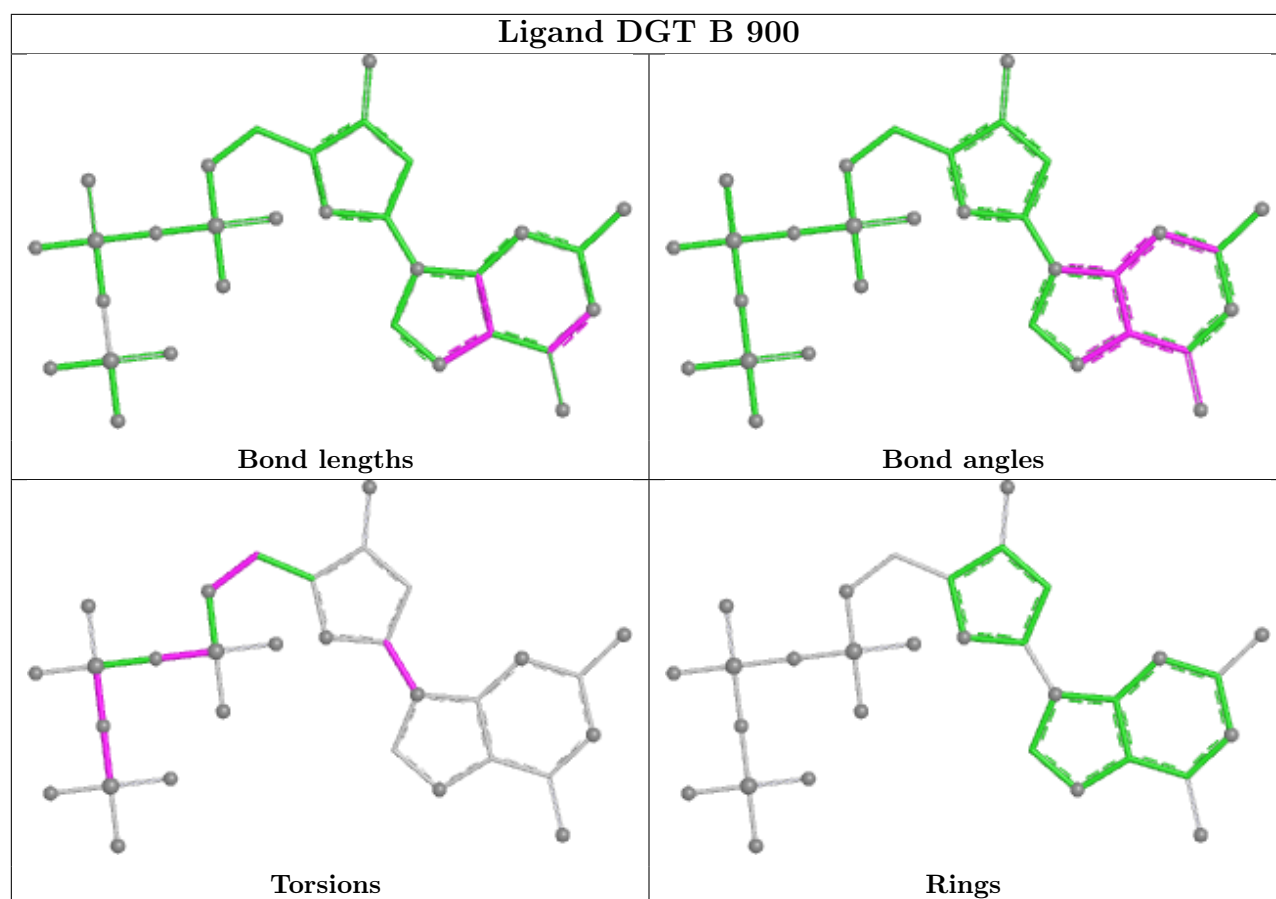
There are no ring outliers.

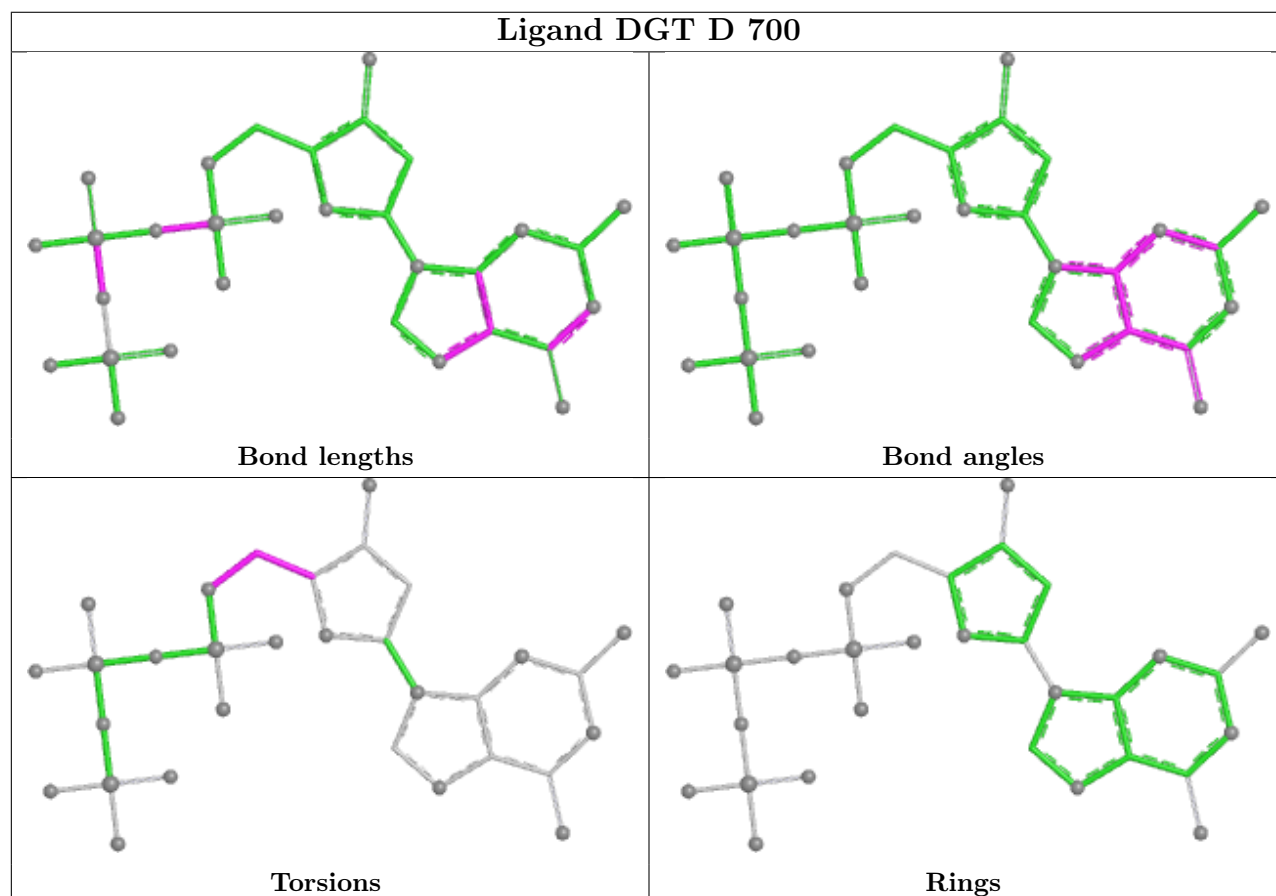
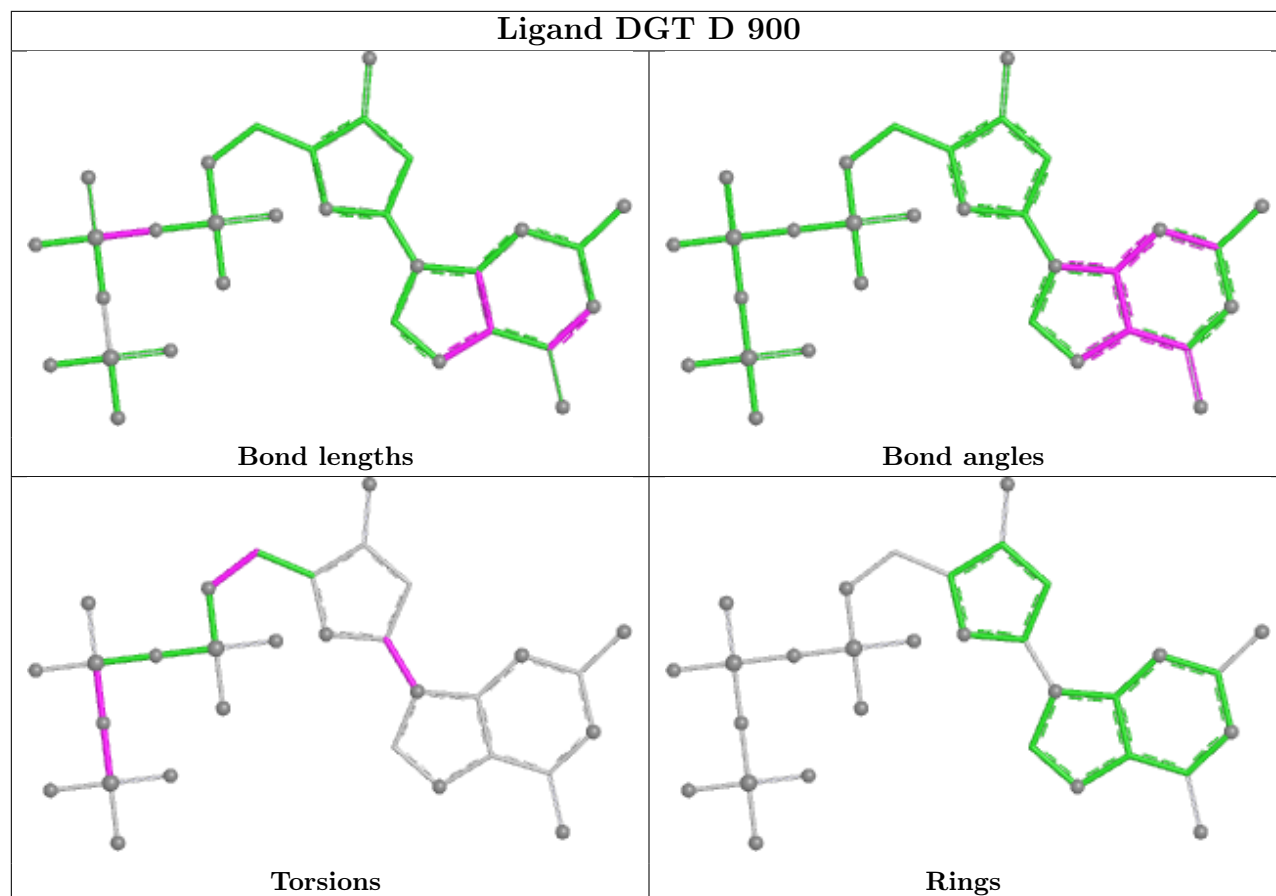
No monomer is involved in short contacts.

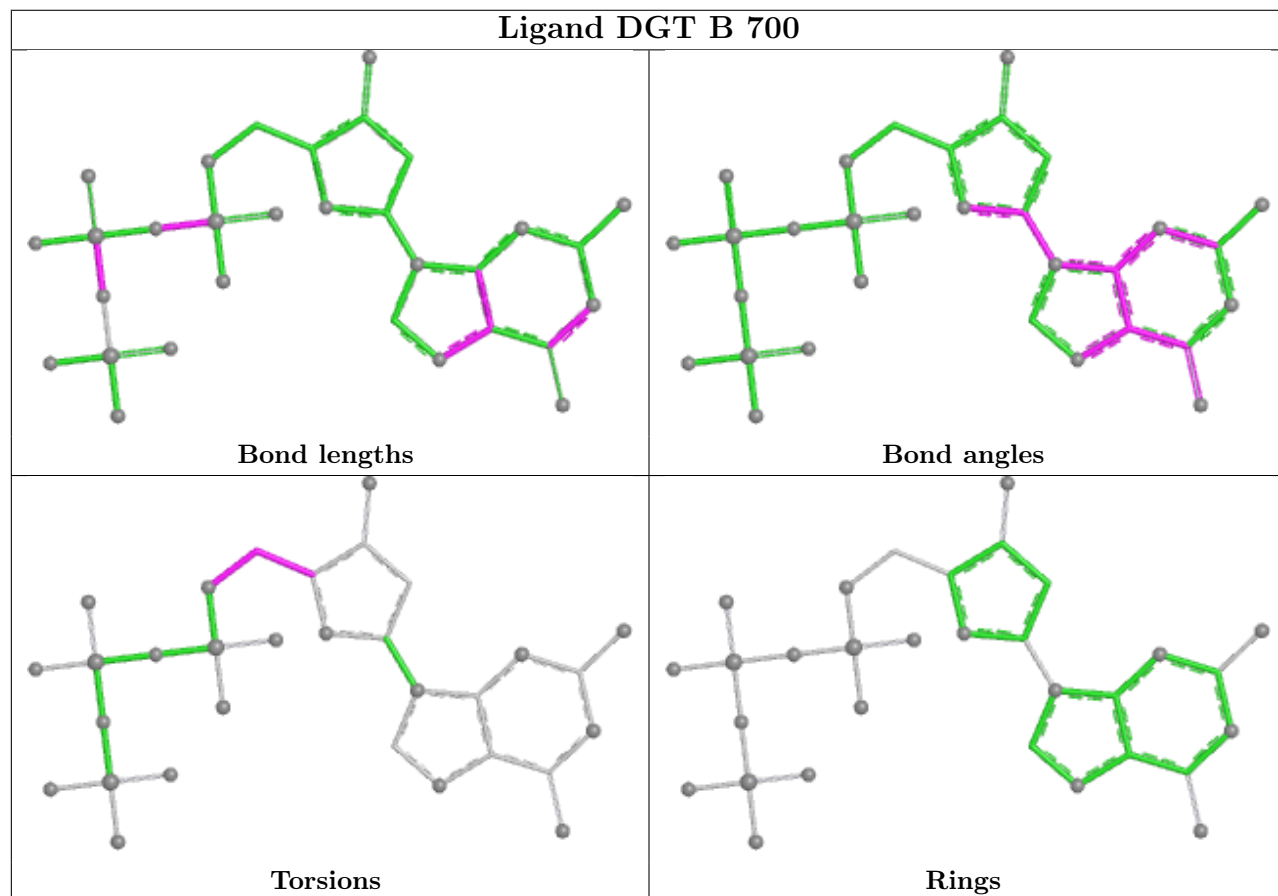
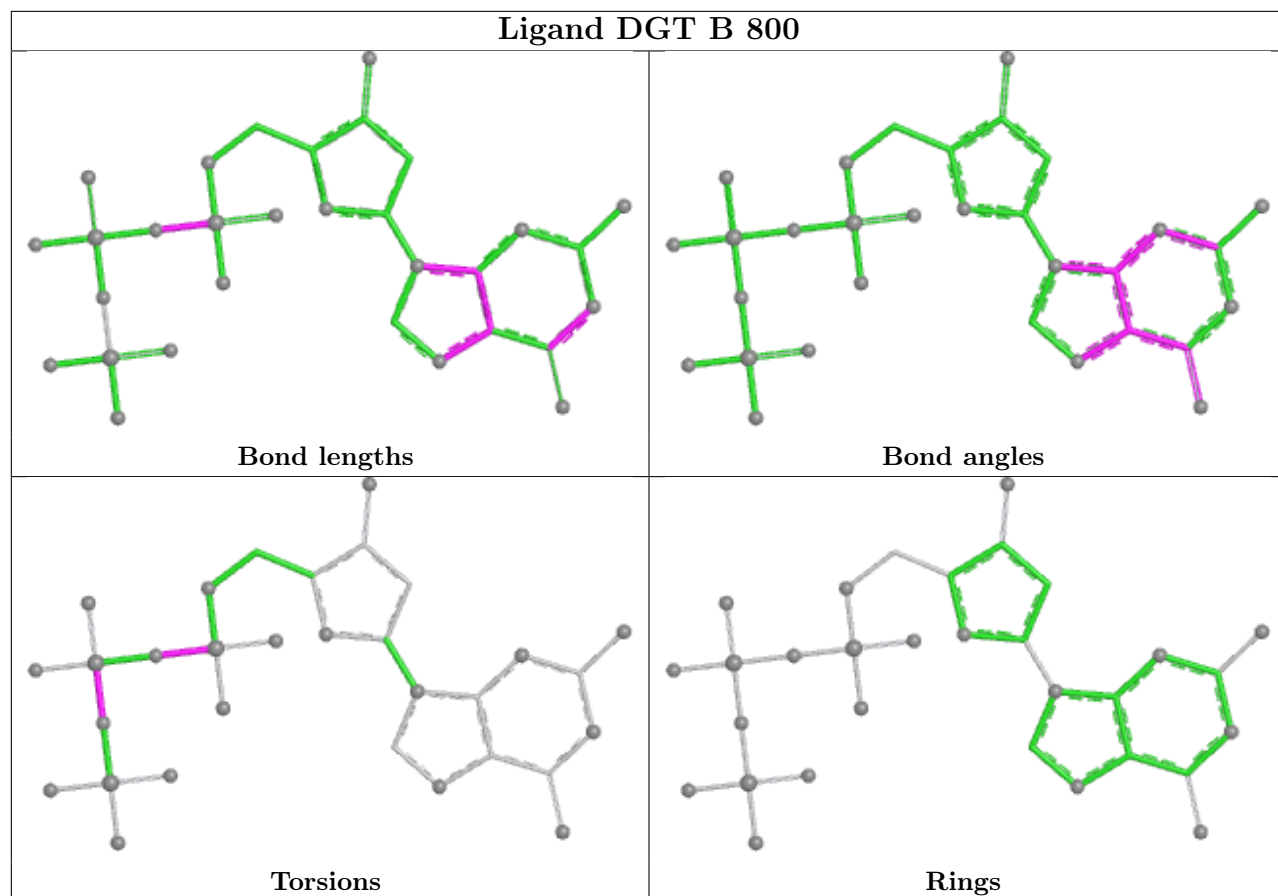
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

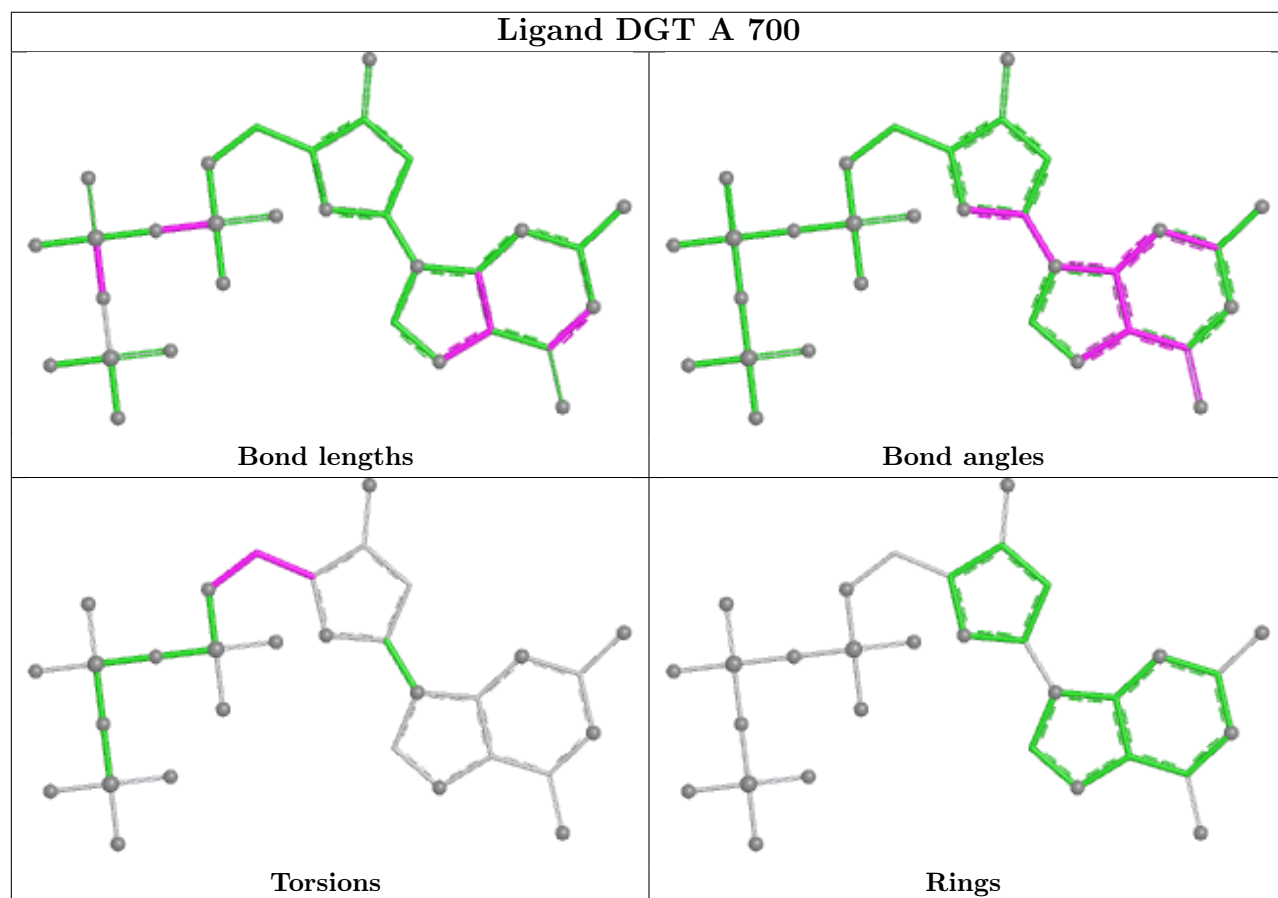
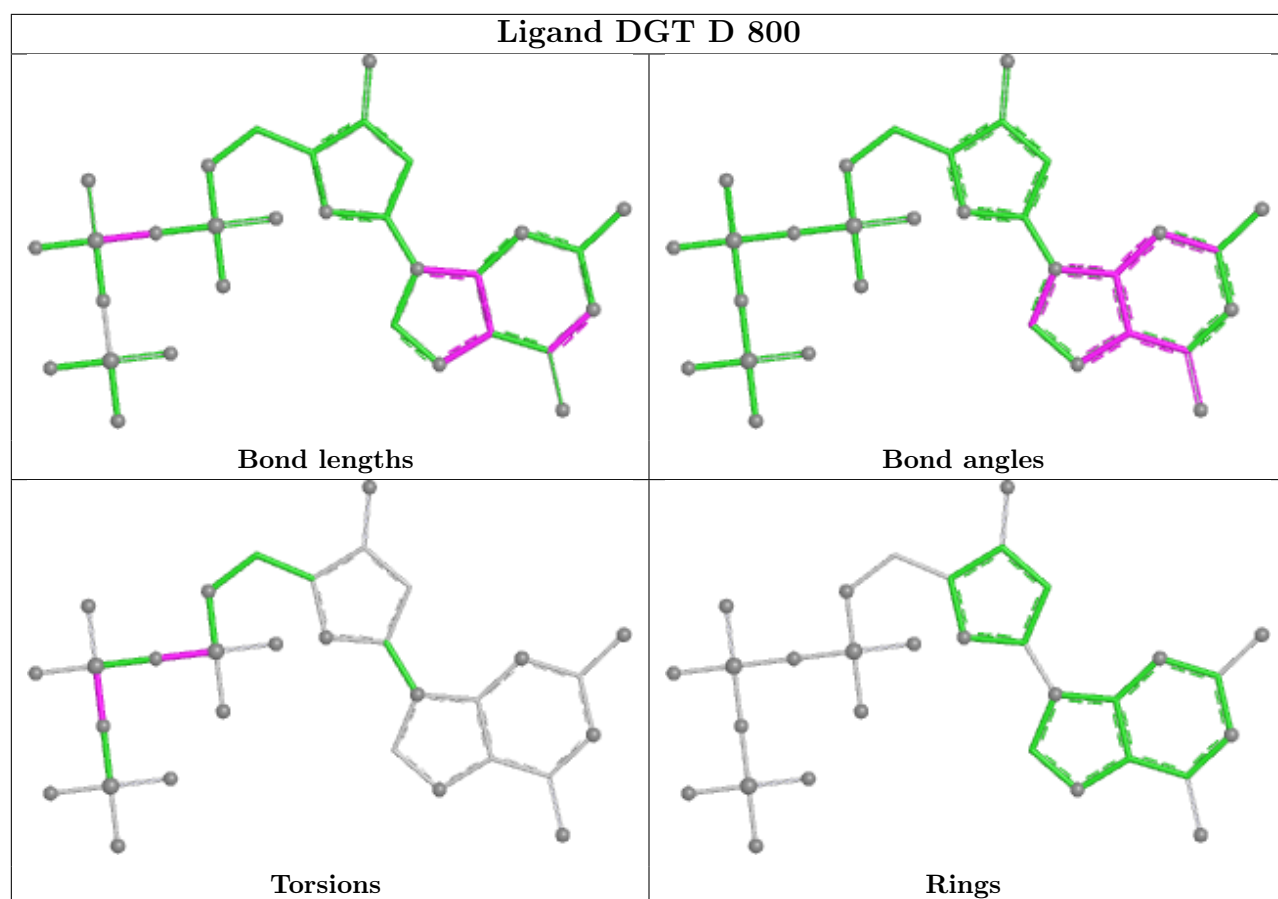


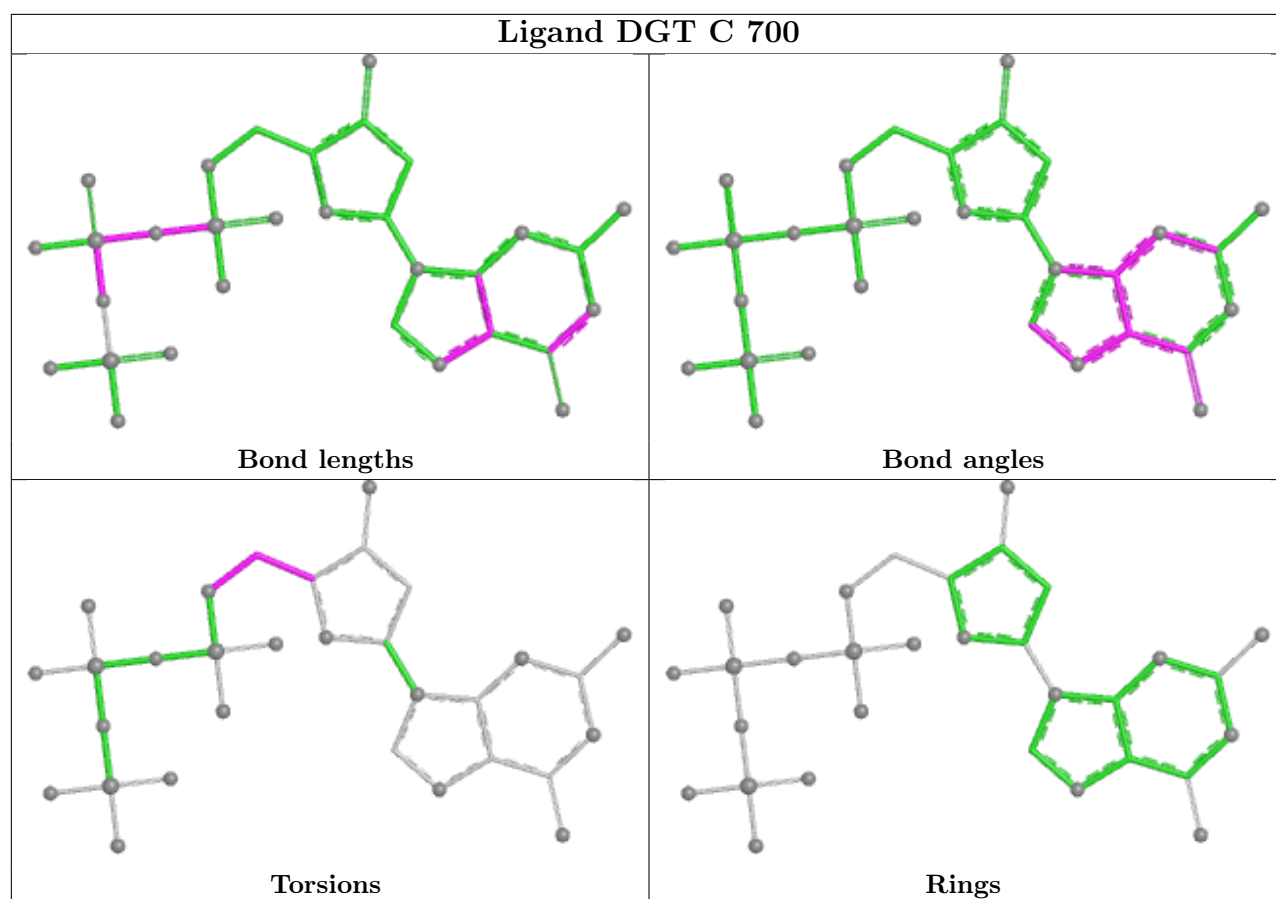












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	481/550 (87%)	0.48	27 (5%)	30 32	15, 41, 68, 89	7 (1%)
1	B	481/550 (87%)	0.23	21 (4%)	39 42	13, 34, 61, 78	4 (0%)
1	C	481/550 (87%)	0.49	24 (4%)	34 36	14, 42, 69, 94	5 (1%)
1	D	481/550 (87%)	0.22	19 (3%)	42 45	12, 34, 58, 75	7 (1%)
All	All	1924/2200 (87%)	0.35	91 (4%)	36 38	12, 38, 64, 94	23 (1%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	LEU	4.6
1	A	328	ASN	4.2
1	A	537	VAL	4.0
1	B	537	VAL	4.0
1	A	488	LEU	4.0
1	B	466	ILE	3.9
1	D	328	ASN	3.8
1	A	284	LEU	3.8
1	B	326	GLN	3.8
1	B	488	LEU	3.7
1	C	488	LEU	3.7
1	C	284	LEU	3.6
1	C	592	THR	3.5
1	A	466	ILE	3.5
1	C	326	GLN	3.3
1	B	284	LEU	3.3
1	D	465	GLN	3.3
1	D	404	GLY	3.2
1	D	396	TYR	3.1
1	A	115	MET	3.1
1	A	535	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	522[A]	CYS	3.1
1	D	466	ILE	3.1
1	A	598	TRP	3.1
1	C	591	ILE	3.0
1	D	276	LEU	3.0
1	B	535	ASN	3.0
1	A	276	LEU	2.9
1	A	468	ILE	2.9
1	D	535	ASN	2.8
1	A	487	VAL	2.8
1	C	487	VAL	2.8
1	C	537	VAL	2.8
1	D	491	VAL	2.8
1	D	490	ASP	2.8
1	A	465	GLN	2.8
1	C	493	LEU	2.8
1	C	215	HIS	2.7
1	B	405	LYS	2.7
1	A	463	THR	2.7
1	C	590	LEU	2.7
1	D	468	ILE	2.6
1	D	405	LYS	2.6
1	B	276	LEU	2.6
1	D	113	ASP	2.6
1	B	468	ILE	2.5
1	D	593	PRO	2.5
1	B	591	ILE	2.5
1	B	592	THR	2.5
1	B	215	HIS	2.4
1	C	492	LYS	2.4
1	B	465	GLN	2.4
1	D	599	ASN	2.4
1	D	344	ASP	2.4
1	A	326	GLN	2.4
1	C	562	LEU	2.3
1	A	293	ASN	2.3
1	D	464	GLY	2.3
1	A	347	LEU	2.3
1	A	327	ASN	2.3
1	D	215	HIS	2.3
1	A	343	VAL	2.3
1	C	491	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	534	LYS	2.2
1	A	590	LEU	2.2
1	A	325	ILE	2.2
1	B	469	LYS	2.2
1	C	577	ASN	2.2
1	A	404	GLY	2.2
1	C	403	GLY	2.2
1	C	404	GLY	2.2
1	C	468	ILE	2.1
1	A	599	ASN	2.1
1	B	464	GLY	2.1
1	A	489	LEU	2.1
1	B	325	ILE	2.1
1	B	115	MET	2.1
1	B	562	LEU	2.1
1	B	470	ARG	2.1
1	A	277	GLU	2.0
1	A	591	ILE	2.0
1	A	596	LYS	2.0
1	C	293	ASN	2.0
1	C	328	ASN	2.0
1	C	345	ASN	2.0
1	B	487	VAL	2.0
1	C	474	GLU	2.0
1	B	403	GLY	2.0
1	D	594	GLN	2.0
1	C	452	ASN	2.0
1	C	371[A]	ARG	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,

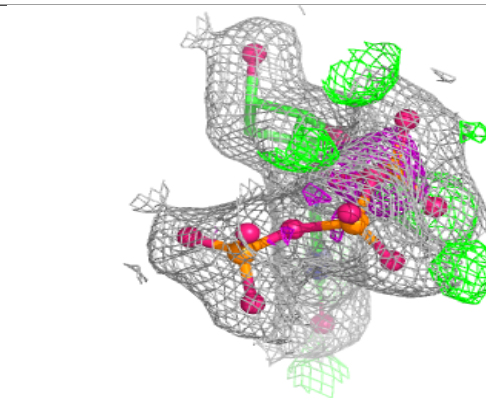
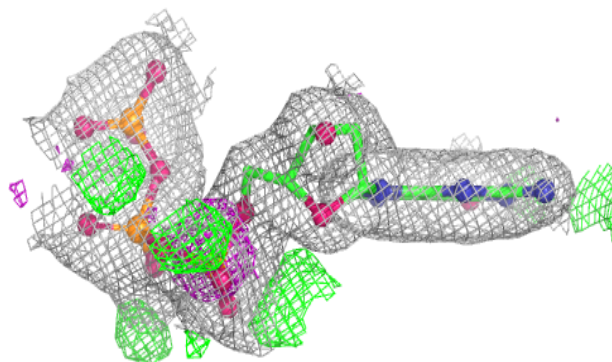
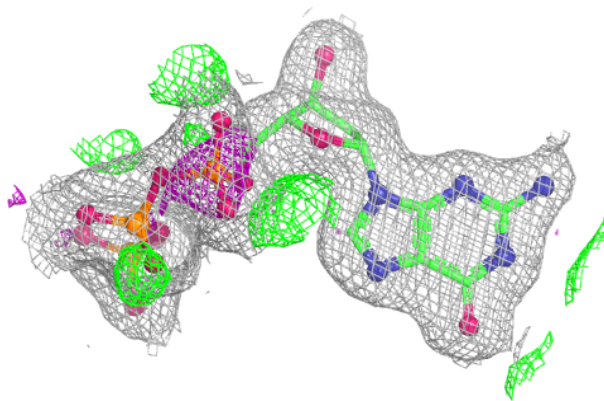
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DGT	A	700	31/31	0.94	0.08	29,35,43,44	0
2	DGT	C	700	31/31	0.94	0.07	30,36,43,45	0
2	DGT	D	700	31/31	0.95	0.07	25,28,35,36	0
2	DGT	C	900	31/31	0.97	0.05	28,29,36,38	0
2	DGT	B	700	31/31	0.97	0.06	23,28,33,34	0
2	DGT	B	900	31/31	0.98	0.05	24,25,29,31	0
2	DGT	A	900	31/31	0.98	0.05	26,27,33,35	0
2	DGT	C	800	31/31	0.98	0.05	25,28,31,31	0
2	DGT	A	800	31/31	0.98	0.05	24,27,29,30	0
2	DGT	B	800	31/31	0.98	0.04	21,22,26,27	0
2	DGT	D	800	31/31	0.98	0.05	22,22,24,24	0
2	DGT	D	900	31/31	0.98	0.04	23,24,29,30	0
3	MG	A	750	1/1	0.98	0.10	42,42,42,42	0
3	MG	B	850	1/1	0.98	0.07	24,24,24,24	0
3	MG	D	750	1/1	0.98	0.12	32,32,32,32	0
3	MG	A	850	1/1	0.99	0.04	28,28,28,28	0
3	MG	C	750	1/1	0.99	0.07	44,44,44,44	0
3	MG	C	850	1/1	0.99	0.05	27,27,27,27	0
3	MG	B	750	1/1	0.99	0.07	30,30,30,30	0
3	MG	D	850	1/1	0.99	0.06	24,24,24,24	0

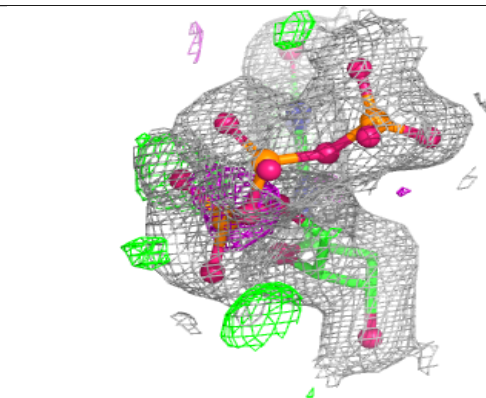
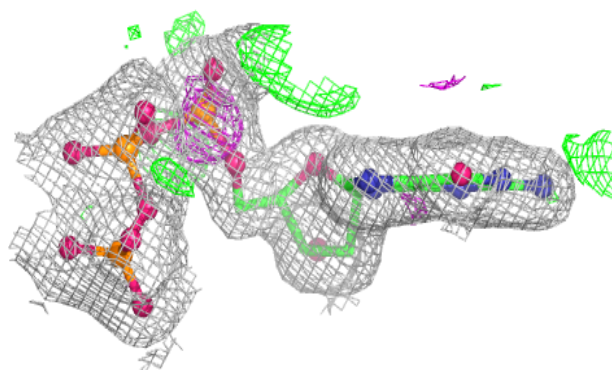
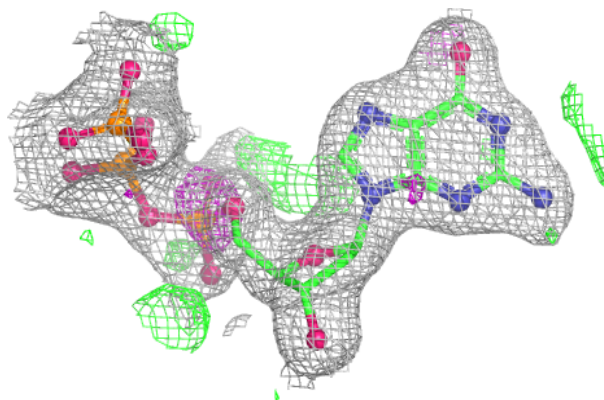
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT A 700:

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

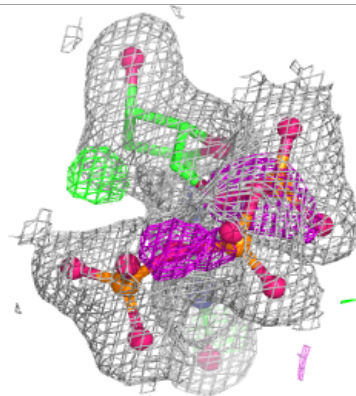
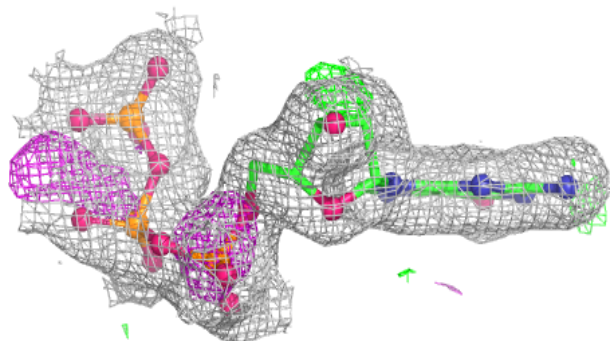
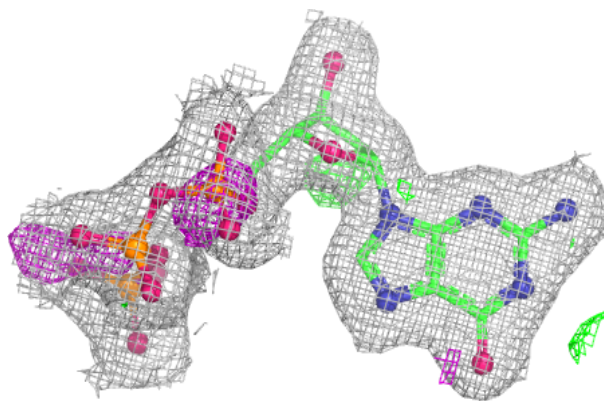
**Electron density around DGT C 700:**

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

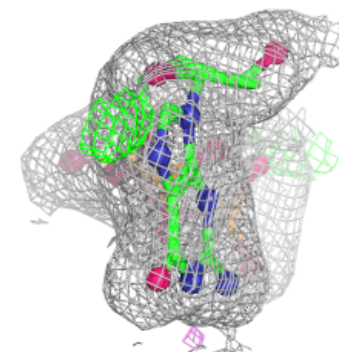
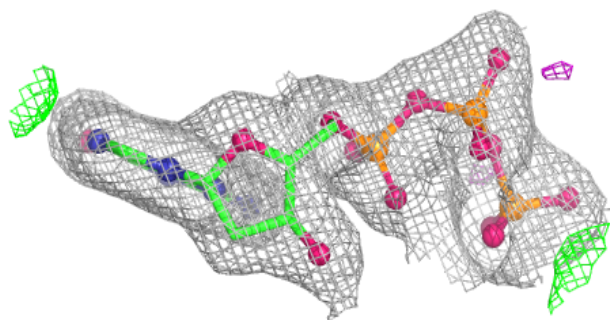
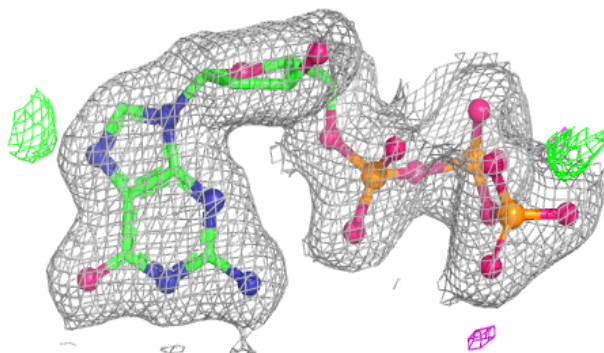


Electron density around DGT D 700:

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

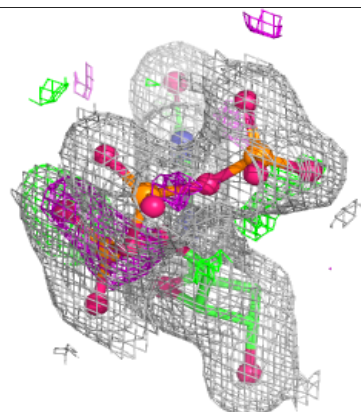
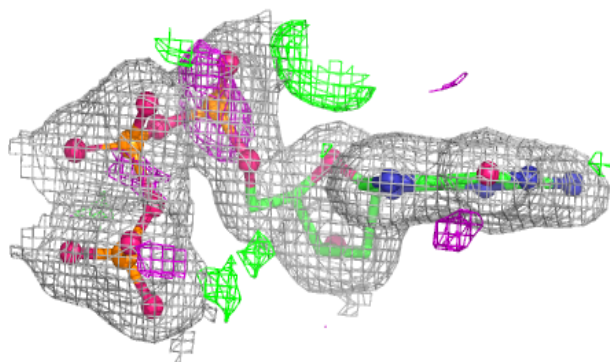
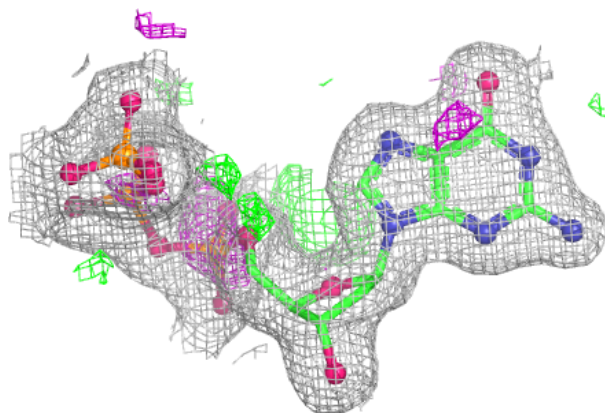
**Electron density around DGT C 900:**

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

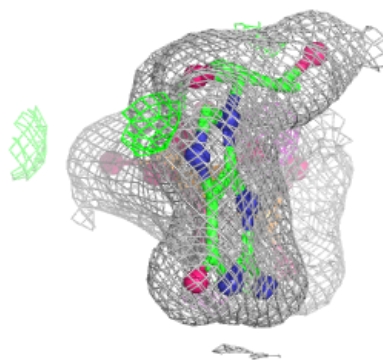
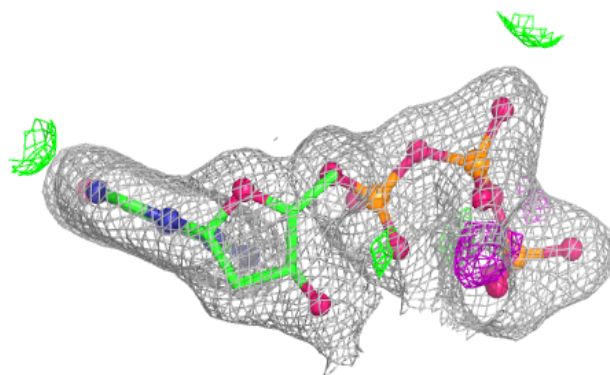
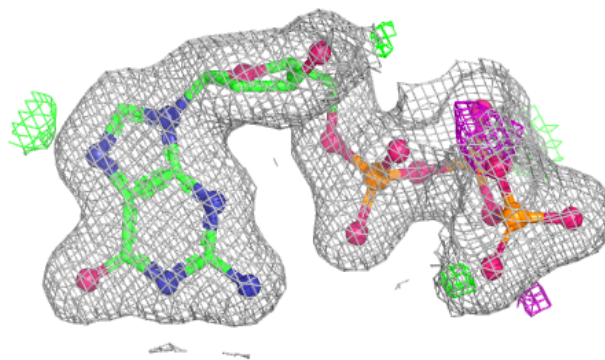


Electron density around DGT B 700:

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

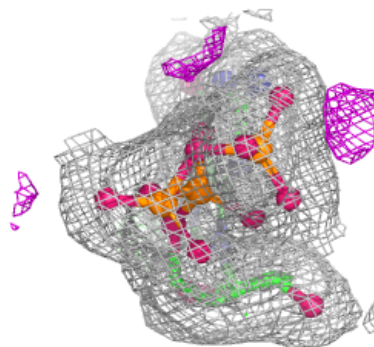
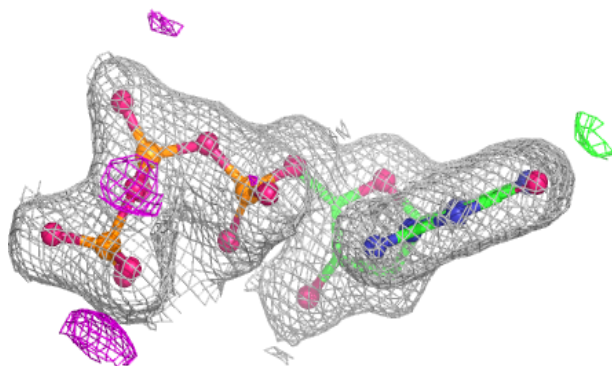
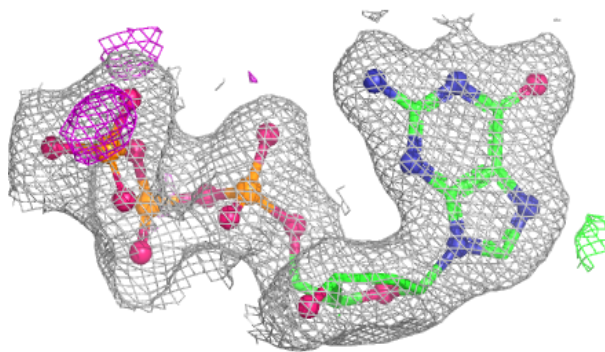
**Electron density around DGT B 900:**

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

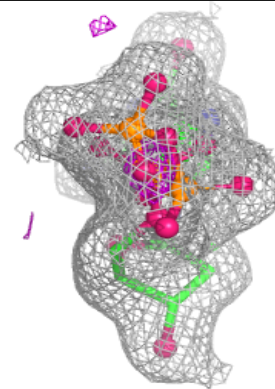
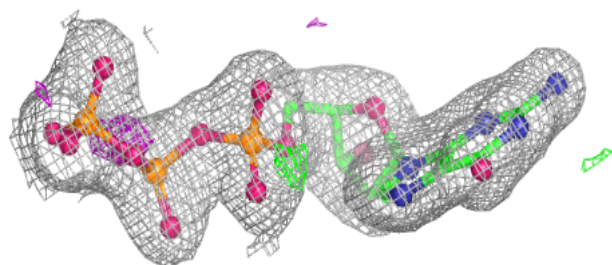
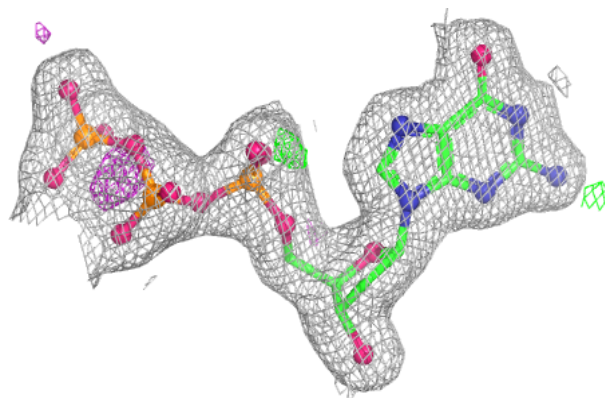


Electron density around DGT A 900:

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

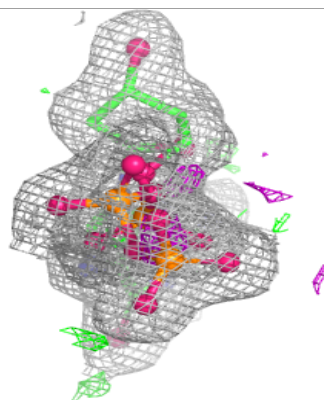
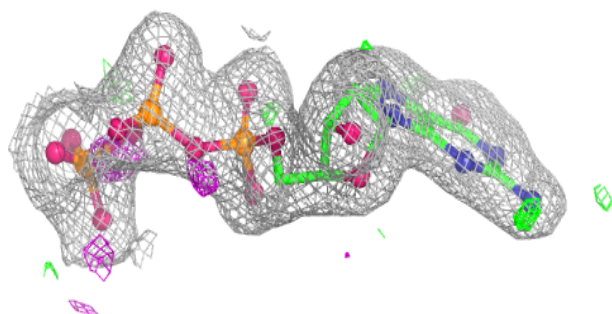
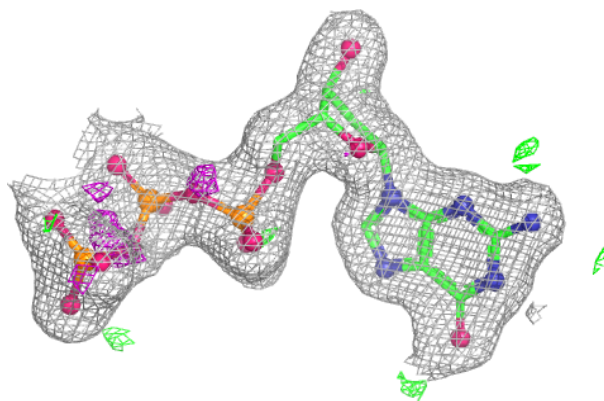
**Electron density around DGT C 800:**

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

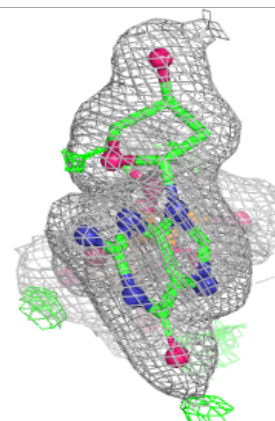
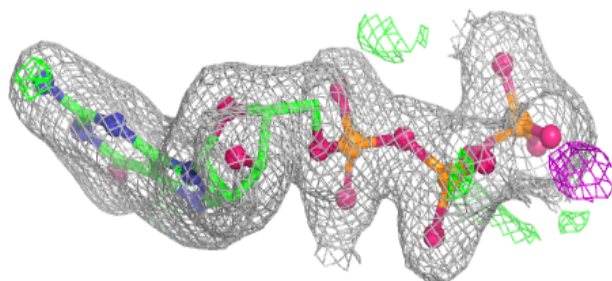
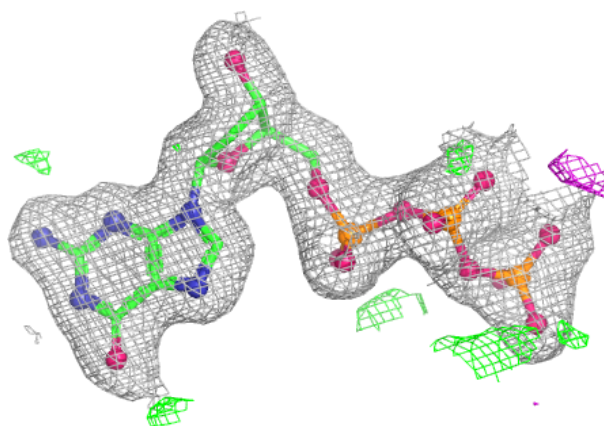


Electron density around DGT A 800:

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

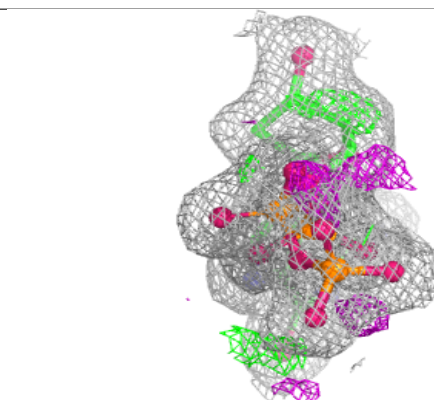
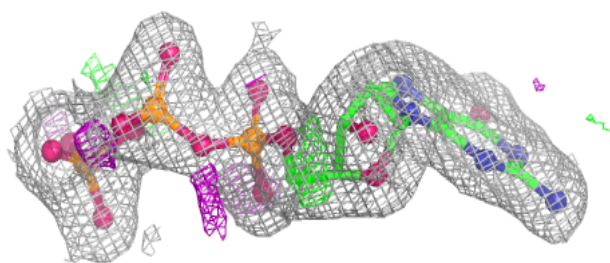
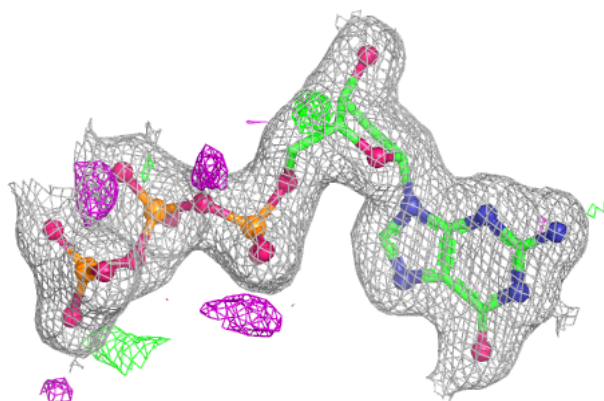
**Electron density around DGT B 800:**

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

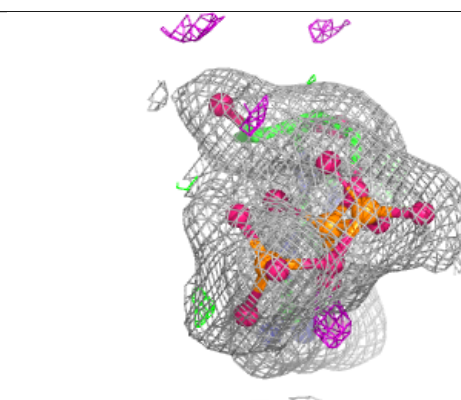
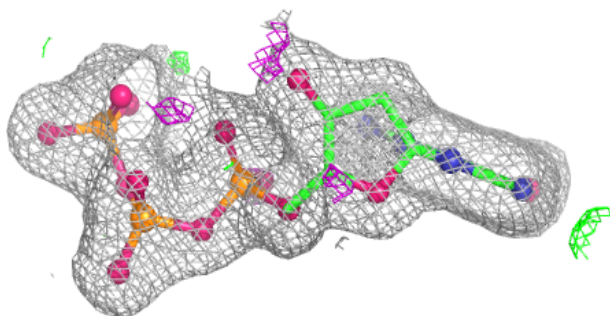
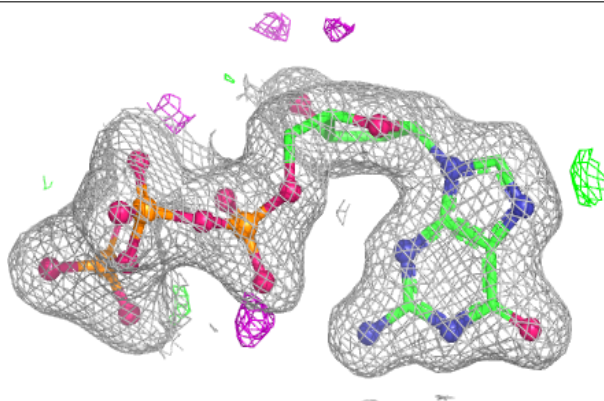


Electron density around DGT D 800:

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

**Electron density around DGT D 900:**

$2mF_o-DF_c$ (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.