



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:53 AM UTC

PDB ID : 7LU5 / pdb_00007lu5
Title : SAMHD1(113-626) H206R D207N R366H
Authors : Temple, J.T.; Bowen, N.E.
Deposited on : 2021-02-20
Resolution : 3.57 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

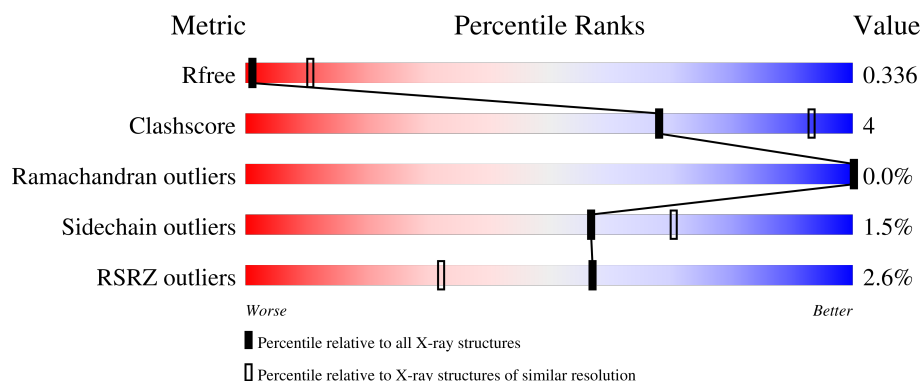
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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.



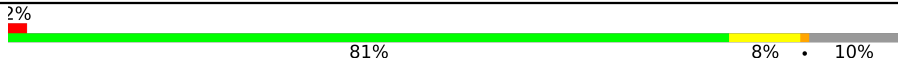
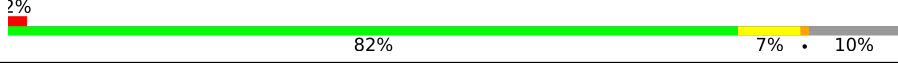
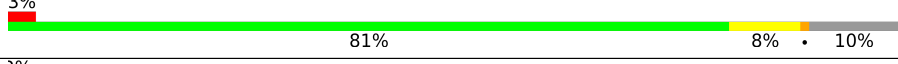
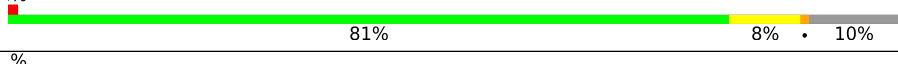
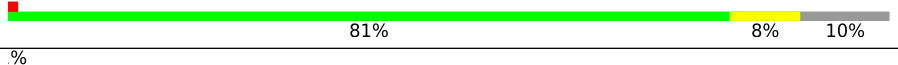
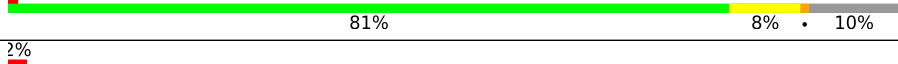
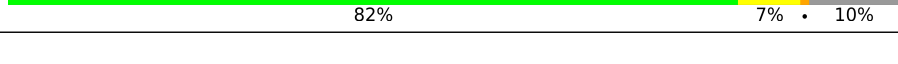
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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	3% 81% 9% 10%
1	B	535	4% 81% 9% 10%
1	C	535	3% 81% 8% 10%
1	D	535	2% 83% 7% 10%
1	E	535	2% 81% 9% 10%

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Mol	Chain	Length	Quality of chain
1	F	535	
1	G	535	
1	H	535	
1	I	535	
1	J	535	
1	K	535	
1	L	535	
1	M	535	
1	N	535	
1	O	535	
1	P	535	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 63936 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	0	0
			3932	2517	684	711	20			
1	B	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	C	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	D	481	Total	C	N	O	S	0	1	0
			3940	2521	686	713	20			
1	E	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	F	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	G	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	H	481	Total	C	N	O	S	0	1	0
			3940	2521	686	713	20			
1	I	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	J	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	K	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	L	481	Total	C	N	O	S	0	1	0
			3940	2521	686	713	20			
1	M	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	N	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	O	481	Total	C	N	O	S	0	0	0
			3932	2517	684	711	20			
1	P	481	Total	C	N	O	S	0	1	0
			3940	2521	686	713	20			

There are 384 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
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
A	366	HIS	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	HIS	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
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	HIS	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

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

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

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

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

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

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

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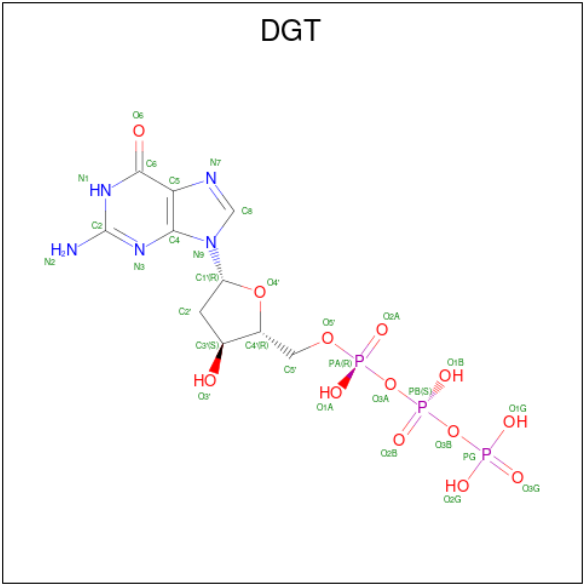
Chain	Residue	Modelled	Actual	Comment	Reference
O	92	MET	-	initiating methionine	UNP Q9Y3Z3
O	93	GLY	-	expression tag	UNP Q9Y3Z3
O	94	SER	-	expression tag	UNP Q9Y3Z3
O	95	SER	-	expression tag	UNP Q9Y3Z3
O	96	HIS	-	expression tag	UNP Q9Y3Z3
O	97	HIS	-	expression tag	UNP Q9Y3Z3
O	98	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
P	110	SER	-	expression tag	UNP Q9Y3Z3
P	111	HIS	-	expression tag	UNP Q9Y3Z3
P	112	MET	-	expression tag	UNP Q9Y3Z3
P	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
P	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
P	366	HIS	ARG	engineered mutation	UNP Q9Y3Z3

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	F	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	F	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	G	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	G	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	H	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	I	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	I	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	J	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	J	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	J	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	K	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	K	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	L	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	M	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	M	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	N	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	O	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	O	1	Total 31	C 10	N 5	O 13	P 3	0	0

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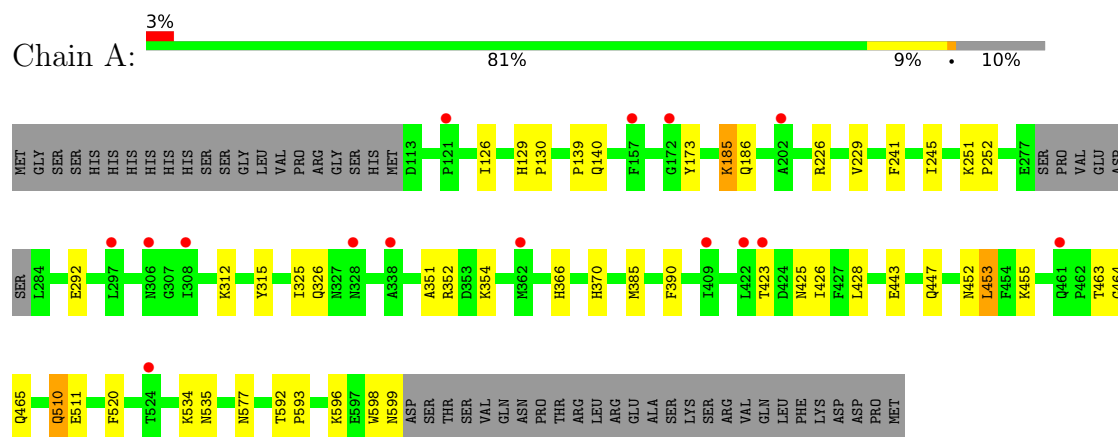
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

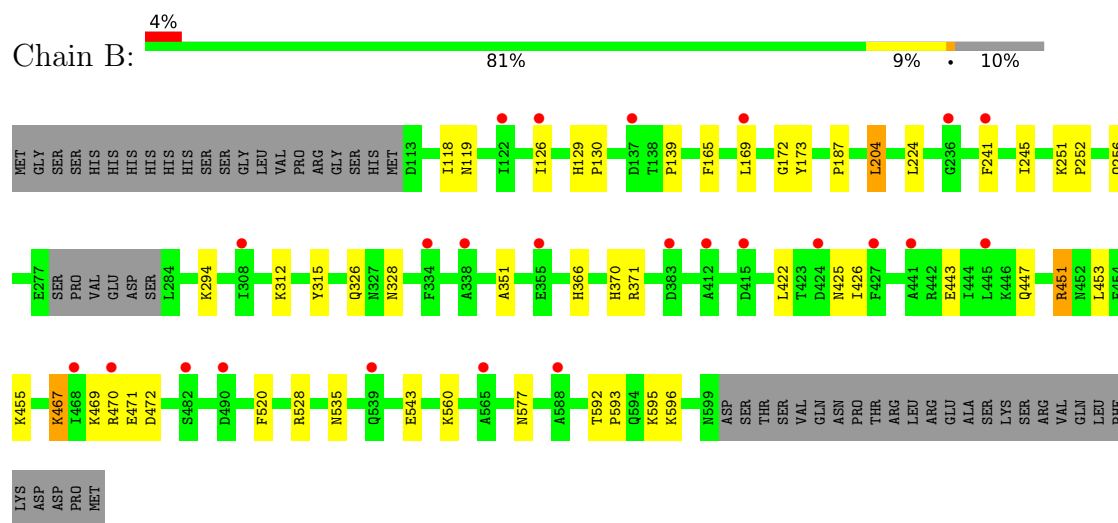
3 Residue-property plots [i](#)

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.

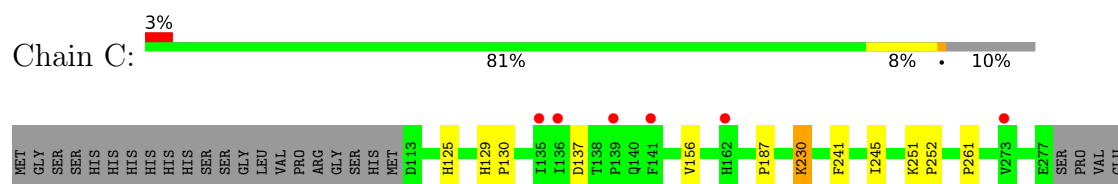
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

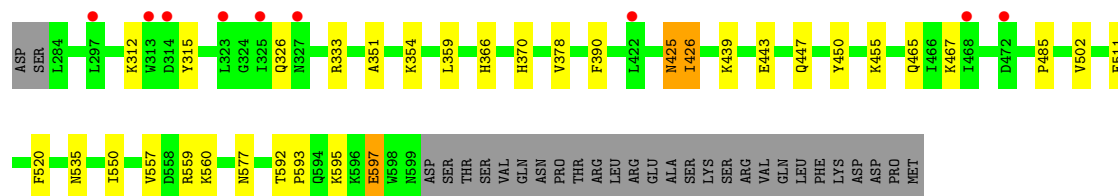


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

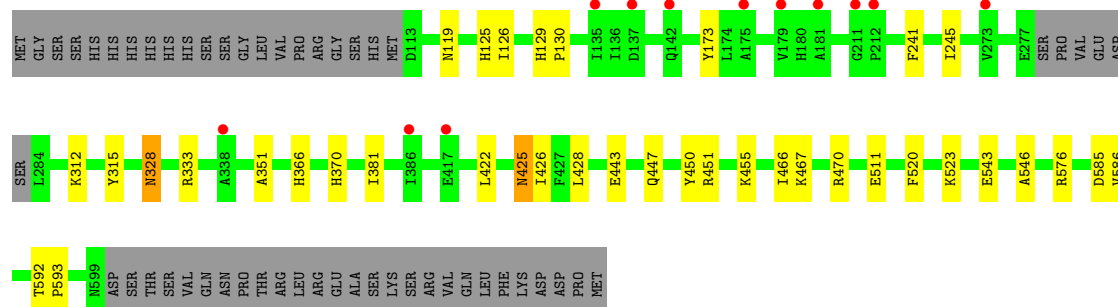
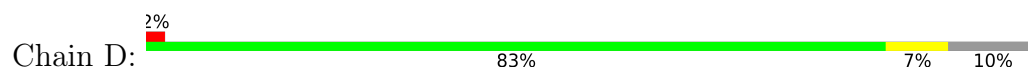


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

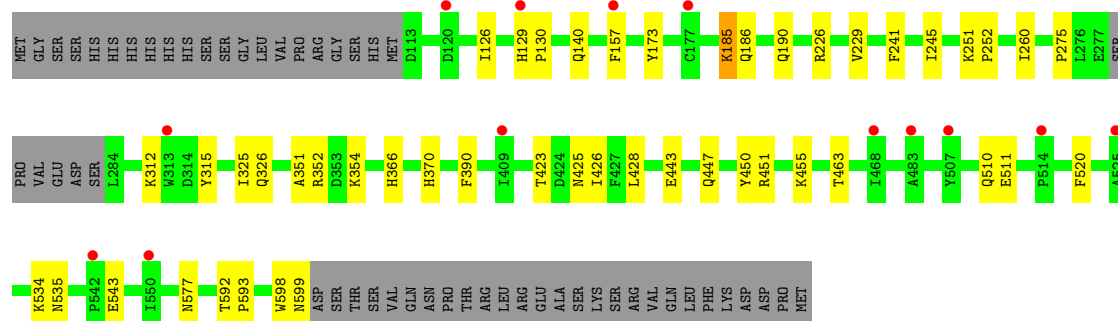
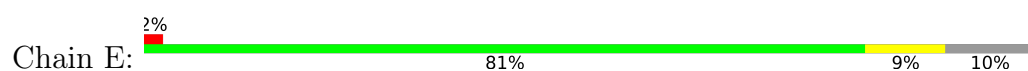




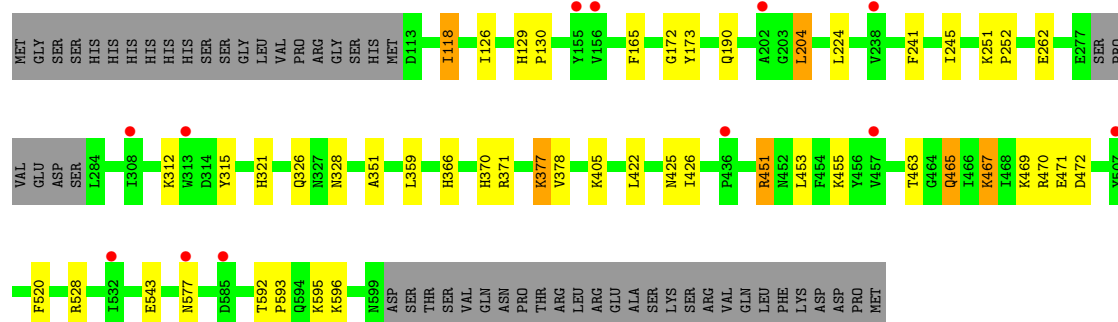
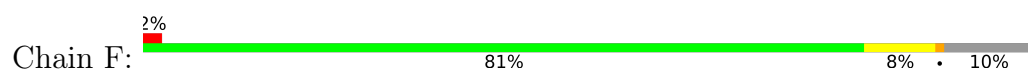
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

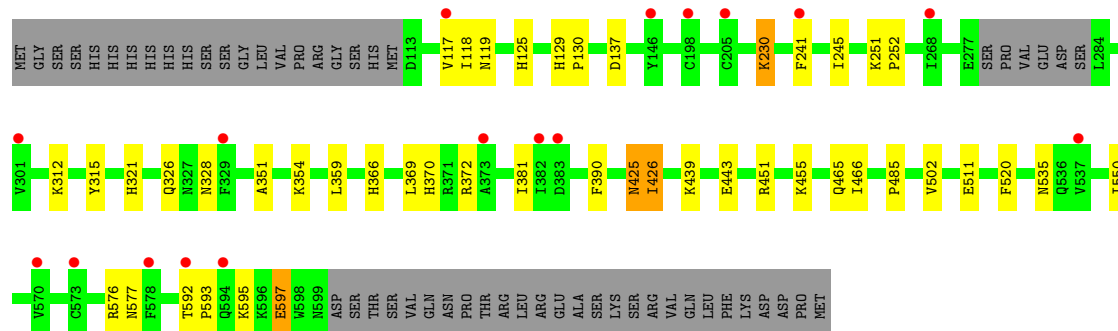


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



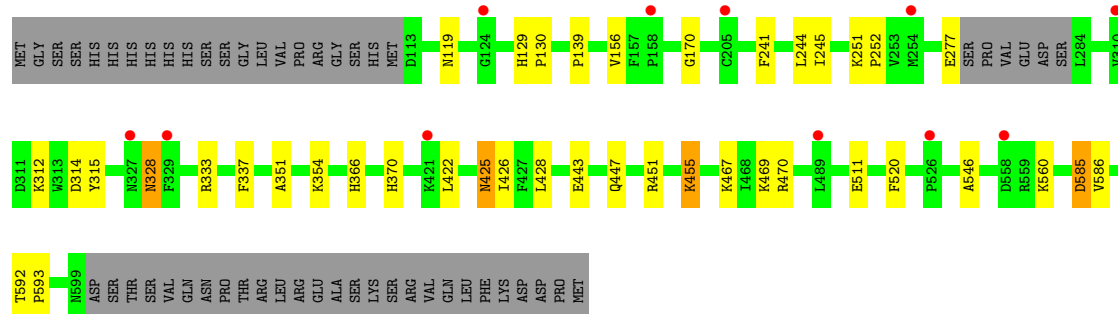
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain G: 



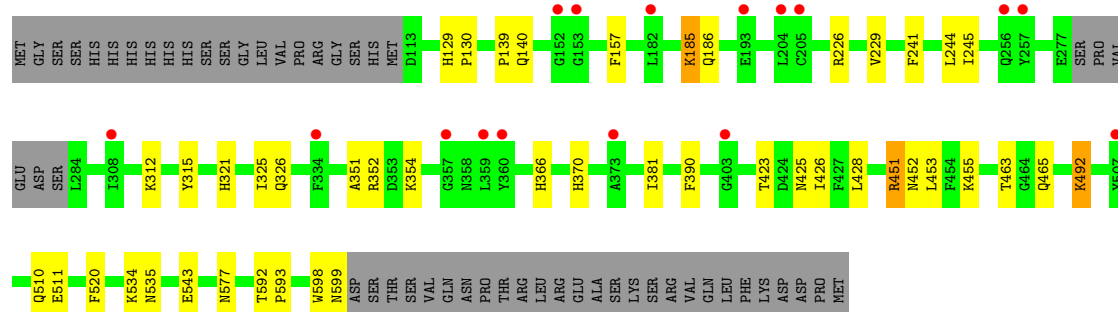
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain H: 



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

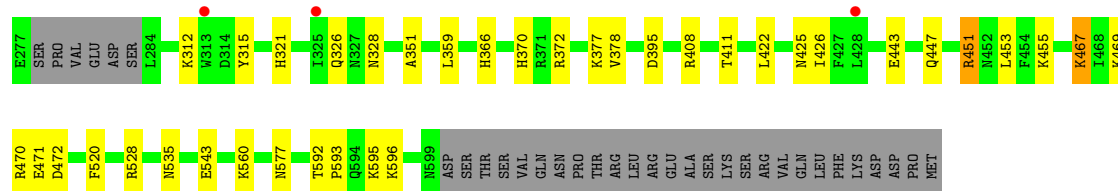
Chain I: 



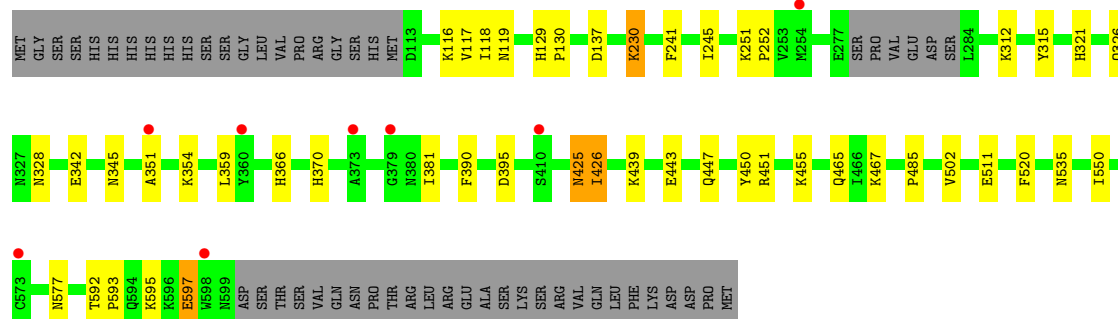
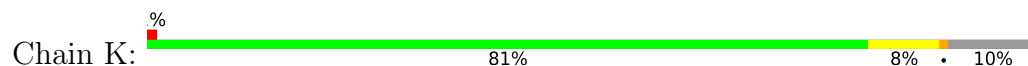
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain J: 

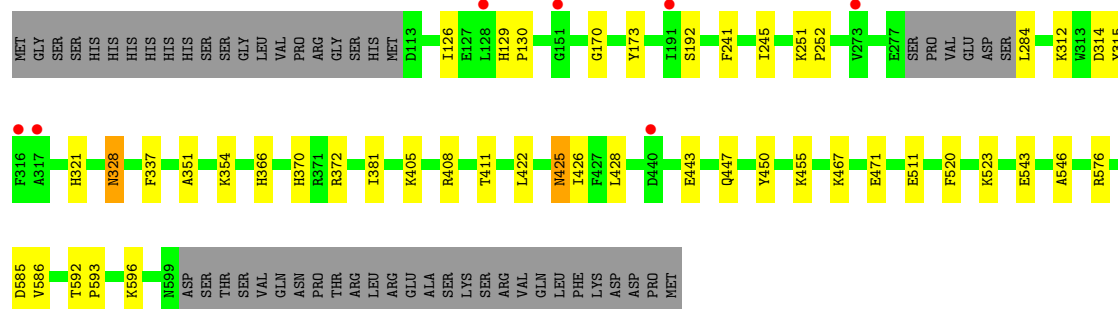
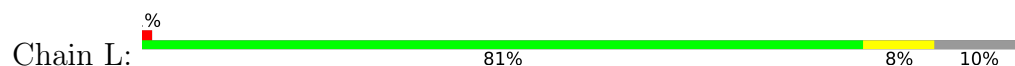




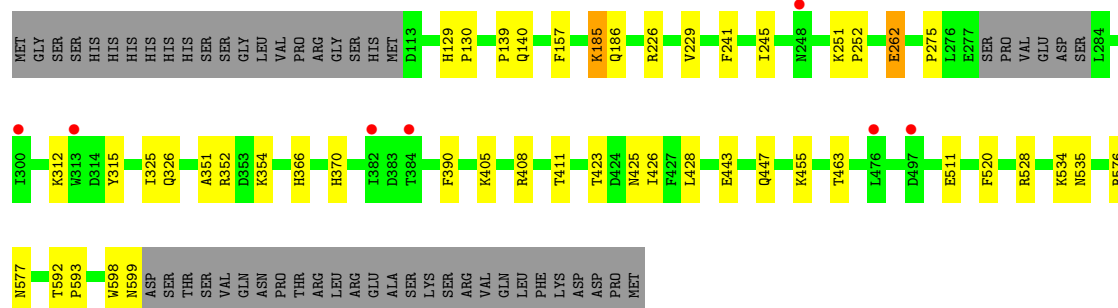
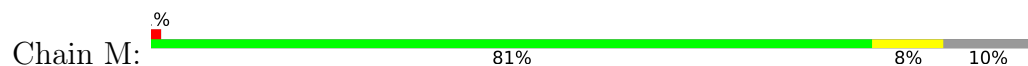
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



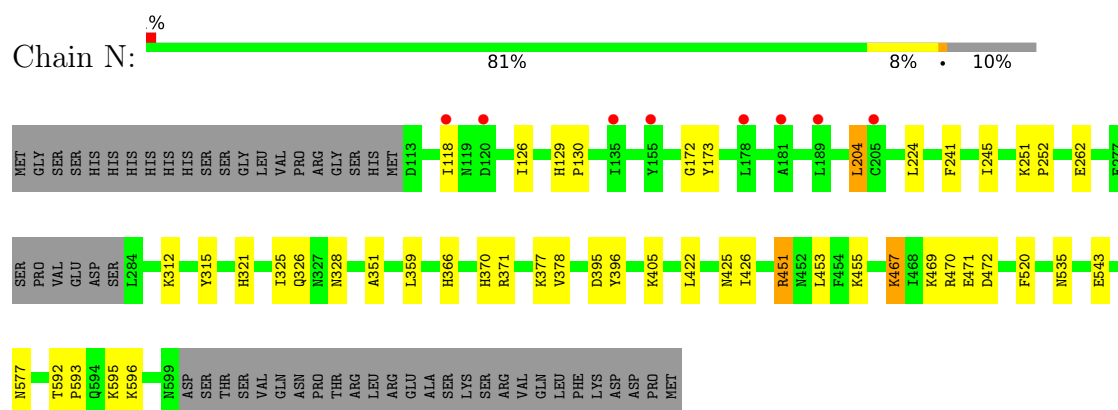
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



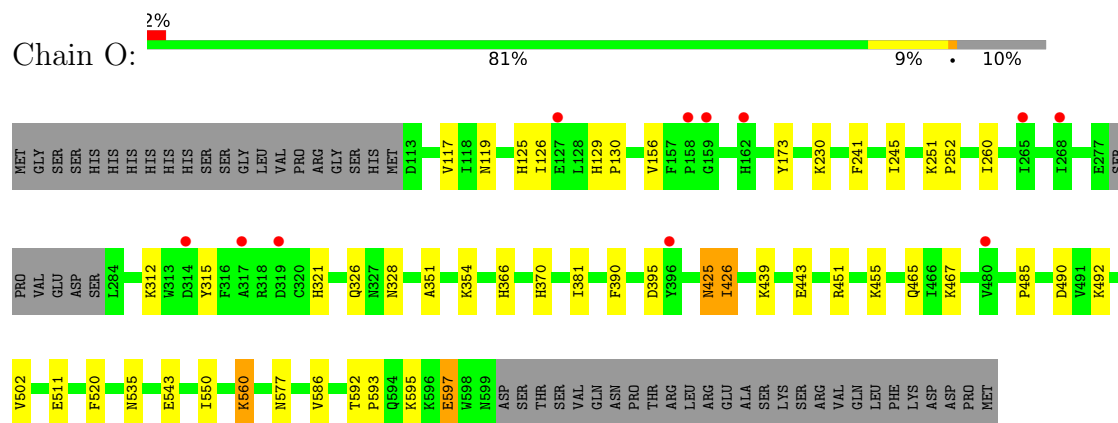
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



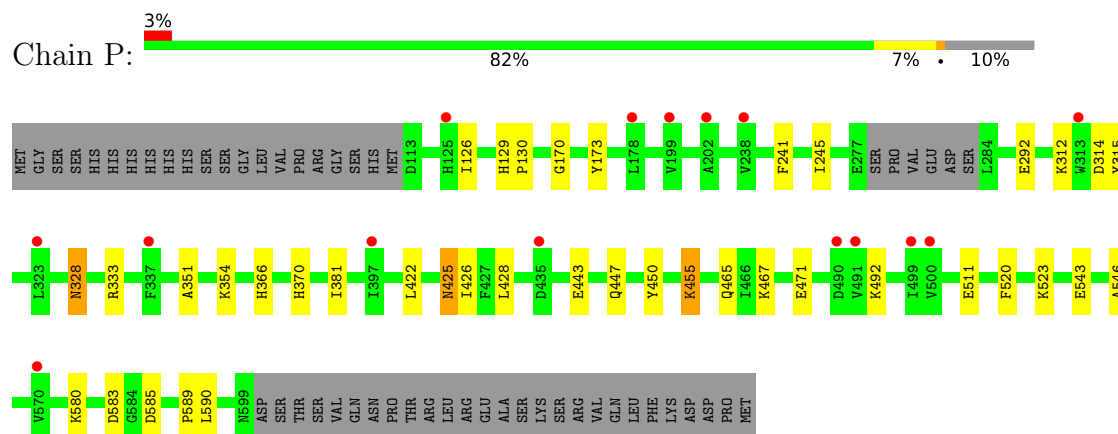
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



● 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	83.73Å 573.48Å 100.50Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	49.27 – 3.57 49.27 – 3.57	Depositor EDS
% Data completeness (in resolution range)	83.9 (49.27-3.57) 91.6 (49.27-3.57)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.236 , 0.274 0.298 , 0.336	Depositor DCC
R_{free} test set	4552 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	159.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 129.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.598 for H, K, L 0.402 for -H, -K, H+L	Depositor
Outliers	0 of 92616 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	63936	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	0/4025	1.25	8/5434 (0.1%)
1	B	0.89	2/4025 (0.0%)	1.24	6/5434 (0.1%)
1	C	0.88	1/4025 (0.0%)	1.24	4/5434 (0.1%)
1	D	0.87	0/4033	1.22	2/5445 (0.0%)
1	E	0.88	1/4025 (0.0%)	1.24	5/5434 (0.1%)
1	F	0.89	2/4025 (0.0%)	1.25	7/5434 (0.1%)
1	G	0.87	0/4025	1.23	4/5434 (0.1%)
1	H	0.87	0/4033	1.21	2/5445 (0.0%)
1	I	0.89	1/4025 (0.0%)	1.25	8/5434 (0.1%)
1	J	0.89	1/4025 (0.0%)	1.24	5/5434 (0.1%)
1	K	0.87	0/4025	1.23	4/5434 (0.1%)
1	L	0.87	0/4033	1.21	1/5445 (0.0%)
1	M	0.89	2/4025 (0.0%)	1.24	6/5434 (0.1%)
1	N	0.90	2/4025 (0.0%)	1.24	5/5434 (0.1%)
1	O	0.87	0/4025	1.23	4/5434 (0.1%)
1	P	0.88	0/4033	1.21	1/5445 (0.0%)
All	All	0.88	12/64432 (0.0%)	1.23	72/86988 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	261	PRO	N-CD	7.44	1.58	1.47
1	F	328	ASN	C-O	6.91	1.32	1.23
1	I	510	GLN	C-N	-6.51	1.23	1.33
1	N	328	ASN	C-O	6.33	1.32	1.23
1	J	328	ASN	C-O	6.21	1.31	1.23
1	M	275	PRO	C-O	-5.51	1.16	1.24
1	B	328	ASN	C-O	5.48	1.31	1.23
1	B	371	ARG	C-O	5.45	1.30	1.24
1	F	371	ARG	C-O	5.43	1.30	1.24
1	E	275	PRO	C-O	-5.37	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	371	ARG	C-O	5.24	1.30	1.24
1	M	262	GLU	CD-OE2	-5.06	1.15	1.25

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	485	PRO	N-CA-C	10.05	128.38	113.81
1	O	485	PRO	N-CA-C	9.95	128.23	113.81
1	G	485	PRO	N-CA-C	9.88	128.14	113.81
1	K	485	PRO	N-CA-C	9.86	128.11	113.81
1	C	559	ARG	N-CA-C	-8.51	102.08	111.36
1	E	140	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	A	140	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	C	557	VAL	N-CA-C	-7.58	105.33	112.83
1	M	140	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	I	140	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	I	452	ASN	CA-C-N	-7.42	109.50	122.64
1	I	452	ASN	C-N-CA	-7.42	109.50	122.64
1	I	534	LYS	CG-CD-CE	-7.24	94.65	111.30
1	E	534	LYS	CG-CD-CE	-7.23	94.68	111.30
1	M	534	LYS	CG-CD-CE	-7.19	94.76	111.30
1	E	186	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	D	328	ASN	CA-CB-CG	7.11	119.71	112.60
1	B	451	ARG	NE-CZ-NH1	-7.03	114.47	121.50
1	I	186	GLN	OE1-CD-NE2	-7.03	115.57	122.60
1	H	328	ASN	CA-CB-CG	6.94	119.54	112.60
1	A	534	LYS	CG-CD-CE	-6.93	95.37	111.30
1	M	186	GLN	OE1-CD-NE2	-6.89	115.71	122.60
1	A	186	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	L	328	ASN	CA-CB-CG	6.79	119.39	112.60
1	P	328	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	452	ASN	CA-C-N	-6.63	110.91	122.64
1	A	452	ASN	C-N-CA	-6.63	110.91	122.64
1	N	451	ARG	NE-CZ-NH1	-6.59	114.91	121.50
1	J	451	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	F	451	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	K	485	PRO	CA-C-O	-6.17	109.89	119.64
1	O	485	PRO	CA-C-O	-6.16	109.91	119.64
1	G	485	PRO	CA-C-O	-6.13	109.96	119.64
1	C	485	PRO	CA-C-O	-6.11	109.98	119.64
1	M	262	GLU	CB-CG-CD	6.03	122.85	112.60
1	I	185	LYS	CB-CG-CD	6.01	125.12	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LYS	CB-CG-CD	5.93	124.93	111.30
1	E	185	LYS	CB-CG-CD	5.88	124.83	111.30
1	M	185	LYS	CB-CG-CD	5.86	124.78	111.30
1	B	451	ARG	NE-CZ-NH2	5.84	124.45	119.20
1	I	492	LYS	CB-CG-CD	5.53	124.02	111.30
1	B	467	LYS	CB-CG-CD	5.49	123.92	111.30
1	F	467	LYS	CB-CG-CD	5.43	123.78	111.30
1	N	467	LYS	CB-CG-CD	5.38	123.68	111.30
1	N	451	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	G	328	ASN	CB-CA-C	5.36	118.97	109.65
1	E	455	LYS	CG-CD-CE	5.35	123.61	111.30
1	I	455	LYS	CG-CD-CE	5.35	123.60	111.30
1	O	328	ASN	CB-CA-C	5.31	118.88	109.65
1	K	328	ASN	CB-CA-C	5.30	118.88	109.65
1	J	467	LYS	CB-CG-CD	5.30	123.50	111.30
1	A	452	ASN	CA-C-O	-5.29	116.00	122.41
1	M	455	LYS	CG-CD-CE	5.25	123.39	111.30
1	F	262	GLU	CB-CG-CD	5.23	121.49	112.60
1	N	451	ARG	N-CA-C	-5.22	106.22	112.58
1	B	451	ARG	N-CA-C	-5.21	106.23	112.58
1	N	472	ASP	CB-CA-C	-5.20	102.65	111.02
1	J	262	GLU	CB-CG-CD	5.16	121.37	112.60
1	J	451	ARG	N-CA-C	-5.15	106.30	112.58
1	F	472	ASP	CB-CA-C	-5.15	102.73	111.02
1	D	451	ARG	N-CA-C	-5.12	106.34	112.58
1	G	451	ARG	N-CA-C	-5.11	106.34	112.58
1	J	472	ASP	CB-CA-C	-5.10	102.80	111.02
1	B	472	ASP	CB-CA-C	-5.09	102.82	111.02
1	F	451	ARG	N-CA-C	-5.09	106.37	112.58
1	K	451	ARG	N-CA-C	-5.08	106.38	112.58
1	A	455	LYS	CG-CD-CE	5.07	122.97	111.30
1	B	371	ARG	N-CA-CB	5.05	117.34	110.01
1	F	465	GLN	OE1-CD-NE2	5.05	127.65	122.60
1	F	451	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	H	451	ARG	N-CA-C	-5.04	106.43	112.58
1	O	451	ARG	N-CA-C	-5.04	106.44	112.58

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	3932	0	3915	30	2
1	B	3932	0	3915	43	0
1	C	3932	0	3915	35	0
1	D	3940	0	3920	26	2
1	E	3932	0	3915	31	0
1	F	3932	0	3915	36	14
1	G	3932	0	3915	37	14
1	H	3940	0	3920	31	0
1	I	3932	0	3915	30	6
1	J	3932	0	3915	34	6
1	K	3932	0	3915	40	2
1	L	3940	0	3920	32	3
1	M	3932	0	3915	29	5
1	N	3932	0	3915	31	3
1	O	3932	0	3915	38	5
1	P	3940	0	3920	26	6
2	A	93	0	36	5	0
2	B	62	0	24	2	0
2	C	62	0	24	8	0
2	D	31	0	12	1	0
2	E	93	0	36	3	0
2	F	62	0	24	6	0
2	G	62	0	24	4	0
2	H	31	0	12	7	0
2	I	62	0	24	0	0
2	J	93	0	36	12	0
2	K	62	0	24	4	0
2	L	31	0	12	2	0
2	M	62	0	24	1	0
2	N	31	0	12	0	0
2	O	93	0	36	4	0
2	P	62	0	24	6	0
All	All	63936	0	63044	455	34

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 (455) 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:J:543:GLU:HG3	1:L:543:GLU:HG3	1.72	0.70
1:N:543:GLU:HG3	1:P:543:GLU:HG3	1.73	0.70
1:N:377:LYS:NZ	2:P:701:DGT:O1G	2.25	0.69
2:D:701:DGT:H5'A	2:D:701:DGT:H8	1.74	0.69
1:J:118:ILE:HG12	2:K:701:DGT:H2'	1.75	0.68
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.74	0.68
1:D:511:GLU:HG2	1:D:546:ALA:HB3	1.75	0.68
1:H:511:GLU:HG2	1:H:546:ALA:HB3	1.76	0.68
2:J:701:DGT:O2A	1:K:117:VAL:HG23	1.94	0.67
1:N:118:ILE:HG12	2:O:702:DGT:H2'	1.75	0.67
1:F:172:GLY:HA3	1:F:204:LEU:HD13	1.77	0.67
1:B:118:ILE:HG12	2:C:701:DGT:H2'	1.78	0.66
1:F:165:PHE:HZ	2:F:702:DGT:O6	1.78	0.66
1:F:366:HIS:CE1	1:F:370:HIS:CD2	2.84	0.66
1:N:366:HIS:CE1	1:N:370:HIS:CD2	2.84	0.66
1:F:378:VAL:HG21	2:H:701:DGT:O3G	1.96	0.66
1:A:366:HIS:CE1	1:A:370:HIS:CD2	2.84	0.65
1:B:172:GLY:HA3	1:B:204:LEU:HD13	1.77	0.65
1:I:366:HIS:CE1	1:I:370:HIS:CD2	2.84	0.65
1:M:366:HIS:CE1	1:M:370:HIS:CD2	2.84	0.65
1:O:366:HIS:CE1	1:O:370:HIS:CD2	2.84	0.65
2:G:702:DGT:HN2A	1:H:119:ASN:ND2	1.93	0.65
1:D:366:HIS:CE1	1:D:370:HIS:CD2	2.84	0.65
1:J:172:GLY:HA3	1:J:204:LEU:HD13	1.77	0.65
1:G:366:HIS:CE1	1:G:370:HIS:CD2	2.84	0.65
1:L:366:HIS:CE1	1:L:370:HIS:CD2	2.84	0.65
1:J:366:HIS:CE1	1:J:370:HIS:CD2	2.84	0.65
1:C:366:HIS:CE1	1:C:370:HIS:CD2	2.84	0.65
1:H:366:HIS:CE1	1:H:370:HIS:CD2	2.85	0.65
1:K:345:ASN:CG	1:O:490:ASP:HB3	2.20	0.65
1:B:366:HIS:CE1	1:B:370:HIS:CD2	2.84	0.65
1:N:172:GLY:HA3	1:N:204:LEU:HD13	1.78	0.65
1:P:366:HIS:CE1	1:P:370:HIS:CD2	2.84	0.65
1:E:366:HIS:CE1	1:E:370:HIS:CD2	2.84	0.64
1:K:366:HIS:CE1	1:K:370:HIS:CD2	2.84	0.64
2:C:702:DGT:HN2A	1:D:119:ASN:ND2	1.96	0.64
1:L:511:GLU:HG2	1:L:546:ALA:HB3	1.78	0.64
1:F:118:ILE:HG12	2:F:702:DGT:H2'	1.79	0.64
1:M:511:GLU:O	1:M:511:GLU:HG3	2.00	0.62
1:E:511:GLU:O	1:E:511:GLU:HG3	2.00	0.62
1:J:165:PHE:HZ	2:K:701:DGT:O6	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:GLN:OE1	1:G:326:GLN:HB3	2.00	0.62
1:A:326:GLN:OE1	1:C:326:GLN:HB3	2.00	0.61
1:I:390:PHE:CE2	1:I:426:ILE:HD11	2.35	0.61
1:M:390:PHE:CE2	1:M:426:ILE:HD11	2.35	0.61
1:P:354:LYS:NZ	2:P:701:DGT:O1A	2.33	0.61
1:P:511:GLU:HG2	1:P:546:ALA:HB3	1.83	0.61
1:G:117:VAL:HG21	1:H:337:PHE:CZ	2.36	0.61
1:A:511:GLU:HG3	1:A:511:GLU:O	2.00	0.60
1:E:157:PHE:CE2	2:G:702:DGT:H1'	2.36	0.60
1:E:390:PHE:CE2	1:E:426:ILE:HD11	2.35	0.60
1:K:117:VAL:HG21	1:L:337:PHE:CZ	2.36	0.60
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.36	0.60
1:J:165:PHE:CZ	2:K:701:DGT:O6	2.55	0.60
1:I:511:GLU:HG3	1:I:511:GLU:O	2.01	0.60
1:H:354:LYS:NZ	2:H:701:DGT:O1A	2.35	0.60
1:F:165:PHE:CZ	2:F:702:DGT:O6	2.56	0.59
1:M:326:GLN:OE1	1:O:326:GLN:HB3	2.03	0.59
2:J:701:DGT:O2A	1:K:117:VAL:CG2	2.51	0.58
1:E:428:LEU:HD13	1:H:425:ASN:HB2	1.85	0.58
1:B:256:GLN:NE2	1:F:190:GLN:OE1	2.37	0.58
1:B:294:LYS:HE3	1:E:190:GLN:HE22	1.68	0.58
1:A:292:GLU:OE1	1:H:560:LYS:NZ	2.31	0.57
1:M:528:ARG:NH1	1:O:586:VAL:HG22	2.19	0.57
1:I:423:THR:O	1:I:426:ILE:HG12	2.05	0.57
1:M:428:LEU:HD13	1:P:425:ASN:HB2	1.86	0.57
1:N:425:ASN:ND2	1:O:425:ASN:OD1	2.38	0.57
1:G:117:VAL:HG23	2:H:701:DGT:O2A	2.04	0.56
1:E:423:THR:O	1:E:426:ILE:HG12	2.05	0.56
1:I:428:LEU:HD13	1:L:425:ASN:HB2	1.86	0.56
1:B:560:LYS:CE	1:P:292:GLU:OE1	2.53	0.56
1:A:423:THR:O	1:A:426:ILE:HG12	2.05	0.56
2:J:701:DGT:O1A	1:L:354:LYS:NZ	2.39	0.56
1:M:423:THR:O	1:M:426:ILE:HG12	2.05	0.56
1:A:366:HIS:CE1	1:A:370:HIS:NE2	2.75	0.55
1:J:378:VAL:HG21	2:J:701:DGT:O3G	2.05	0.55
1:I:366:HIS:CE1	1:I:370:HIS:NE2	2.75	0.55
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.88	0.55
1:E:366:HIS:CE1	1:E:370:HIS:NE2	2.74	0.55
1:L:366:HIS:CE1	1:L:370:HIS:NE2	2.75	0.55
1:P:366:HIS:CE1	1:P:370:HIS:NE2	2.75	0.55
1:F:366:HIS:CE1	1:F:370:HIS:NE2	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:428:LEU:CD1	1:P:425:ASN:HB2	2.36	0.55
1:D:366:HIS:CE1	1:D:370:HIS:NE2	2.75	0.55
1:I:326:GLN:OE1	1:K:326:GLN:HB3	2.07	0.55
1:M:366:HIS:CE1	1:M:370:HIS:NE2	2.75	0.55
1:N:378:VAL:HG21	2:P:701:DGT:O3G	2.06	0.55
1:G:366:HIS:CE1	1:G:370:HIS:NE2	2.75	0.55
1:E:428:LEU:CD1	1:H:425:ASN:HB2	2.36	0.55
1:B:366:HIS:CE1	1:B:370:HIS:NE2	2.75	0.55
1:C:187:PRO:CB	1:O:260:ILE:HD11	2.37	0.55
1:O:366:HIS:CE1	1:O:370:HIS:NE2	2.75	0.55
1:C:366:HIS:CE1	1:C:370:HIS:NE2	2.75	0.54
1:H:366:HIS:CE1	1:H:370:HIS:NE2	2.75	0.54
1:N:366:HIS:CE1	1:N:370:HIS:NE2	2.75	0.54
1:K:345:ASN:OD1	1:O:490:ASP:HB3	2.07	0.54
1:C:455:LYS:HA	1:C:455:LYS:HE2	1.90	0.54
1:J:366:HIS:CE1	1:J:370:HIS:NE2	2.75	0.54
1:K:366:HIS:CE1	1:K:370:HIS:NE2	2.75	0.54
1:B:560:LYS:NZ	1:P:292:GLU:OE1	2.39	0.54
1:I:428:LEU:CD1	1:L:425:ASN:HB2	2.37	0.54
1:K:455:LYS:HA	1:K:455:LYS:HE2	1.90	0.53
1:C:187:PRO:HB2	1:O:260:ILE:CD1	2.38	0.53
1:B:528:ARG:HH11	1:D:586:VAL:HG22	1.72	0.53
1:G:117:VAL:HG21	1:H:337:PHE:HZ	1.73	0.53
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.42	0.53
1:B:560:LYS:HE2	1:P:292:GLU:OE1	2.09	0.53
1:K:117:VAL:HG21	1:L:337:PHE:HZ	1.72	0.53
1:G:117:VAL:CG2	2:H:701:DGT:O2A	2.58	0.52
1:A:226:ARG:NH2	1:A:229:VAL:HG21	2.26	0.51
1:I:226:ARG:NH2	1:I:229:VAL:HG21	2.25	0.51
1:C:156:VAL:O	2:C:701:DGT:H1'	2.10	0.51
1:G:455:LYS:HE2	1:G:455:LYS:HA	1.92	0.51
1:I:451:ARG:HG3	2:L:701:DGT:N1	2.26	0.51
1:F:425:ASN:ND2	1:G:425:ASN:OD1	2.43	0.51
1:C:390:PHE:CZ	1:C:426:ILE:CG2	2.94	0.51
2:A:702:DGT:HN2A	1:B:119:ASN:HD21	1.59	0.51
1:D:351:ALA:O	1:D:520:PHE:HA	2.12	0.50
1:J:372:ARG:HG2	2:J:701:DGT:O6	2.10	0.50
1:K:390:PHE:CZ	1:K:426:ILE:CG2	2.95	0.50
1:P:351:ALA:O	1:P:520:PHE:HA	2.12	0.50
1:A:351:ALA:O	1:A:520:PHE:HA	2.12	0.50
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:ALA:O	1:F:520:PHE:HA	2.12	0.50
1:A:428:LEU:CD1	1:D:425:ASN:HB2	2.41	0.50
1:G:351:ALA:O	1:G:520:PHE:HA	2.12	0.50
1:M:351:ALA:O	1:M:520:PHE:HA	2.12	0.50
2:E:702:DGT:H3'	2:F:702:DGT:O3'	2.12	0.50
1:J:543:GLU:CG	1:L:543:GLU:HG3	2.41	0.50
1:L:351:ALA:O	1:L:520:PHE:HA	2.12	0.50
1:M:226:ARG:NH2	1:M:229:VAL:HG21	2.26	0.50
1:O:455:LYS:HE2	1:O:455:LYS:HA	1.94	0.50
1:G:390:PHE:CZ	1:G:426:ILE:CG2	2.94	0.50
1:I:351:ALA:O	1:I:520:PHE:HA	2.12	0.49
1:J:351:ALA:O	1:J:520:PHE:HA	2.12	0.49
1:K:351:ALA:O	1:K:520:PHE:HA	2.12	0.49
1:E:351:ALA:O	1:E:520:PHE:HA	2.12	0.49
1:I:425:ASN:HB2	1:L:428:LEU:HD13	1.95	0.49
1:N:351:ALA:O	1:N:520:PHE:HA	2.12	0.49
1:O:351:ALA:O	1:O:520:PHE:HA	2.12	0.49
1:B:351:ALA:O	1:B:520:PHE:HA	2.12	0.49
1:M:390:PHE:CE2	1:M:426:ILE:CD1	2.96	0.49
1:O:390:PHE:CZ	1:O:426:ILE:CG2	2.95	0.49
1:E:226:ARG:NH2	1:E:229:VAL:HG21	2.26	0.49
2:C:702:DGT:N2	1:D:119:ASN:ND2	2.61	0.49
1:H:351:ALA:O	1:H:520:PHE:HA	2.12	0.49
1:B:326:GLN:HB2	1:D:328:ASN:HA	1.95	0.49
2:A:703:DGT:H5'A	2:C:702:DGT:O1B	2.12	0.49
1:C:351:ALA:O	1:C:520:PHE:HA	2.12	0.49
1:M:425:ASN:HB2	1:P:428:LEU:HD13	1.94	0.49
1:I:592:THR:OG1	1:I:593:PRO:HD3	2.13	0.49
1:J:592:THR:OG1	1:J:593:PRO:HD3	2.13	0.49
1:F:451:ARG:HA	1:F:453:LEU:CD1	2.43	0.48
1:L:408:ARG:H	1:L:411:THR:HG1	1.60	0.48
1:M:408:ARG:H	1:M:411:THR:HG1	1.60	0.48
1:N:451:ARG:HA	1:N:453:LEU:CD1	2.43	0.48
1:K:592:THR:OG1	1:K:593:PRO:HD3	2.13	0.48
2:M:702:DGT:H3'	2:O:702:DGT:O3'	2.13	0.48
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.13	0.48
1:E:352:ARG:HG3	1:E:354:LYS:HG2	1.95	0.48
1:I:139:PRO:HD3	1:L:450:TYR:CE1	2.49	0.48
1:J:451:ARG:HA	1:J:453:LEU:CD1	2.43	0.48
1:J:425:ASN:ND2	1:K:425:ASN:OD1	2.46	0.48
1:A:390:PHE:CE2	1:A:426:ILE:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:GLU:CG	1:D:543:GLU:HG3	2.43	0.48
1:E:390:PHE:CE2	1:E:426:ILE:CD1	2.96	0.48
1:G:592:THR:OG1	1:G:593:PRO:HD3	2.13	0.48
1:A:352:ARG:HG3	1:A:354:LYS:HG2	1.96	0.48
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.13	0.48
1:E:592:THR:OG1	1:E:593:PRO:HD3	2.13	0.48
1:B:451:ARG:HA	1:B:453:LEU:CD1	2.43	0.48
1:M:592:THR:OG1	1:M:593:PRO:HD3	2.13	0.48
1:I:390:PHE:CE2	1:I:426:ILE:CD1	2.96	0.47
1:G:119:ASN:CB	2:H:701:DGT:H8	2.44	0.47
1:M:139:PRO:HD3	1:P:450:TYR:CE1	2.49	0.47
1:N:592:THR:OG1	1:N:593:PRO:HD3	2.14	0.47
1:F:592:THR:OG1	1:F:593:PRO:HD3	2.14	0.47
1:M:425:ASN:HB2	1:P:428:LEU:CD1	2.45	0.47
1:A:592:THR:OG1	1:A:593:PRO:HD3	2.13	0.47
2:A:702:DGT:O1B	1:C:378:VAL:HG21	2.15	0.47
1:F:469:LYS:HD3	1:F:471:GLU:OE2	2.15	0.47
1:G:119:ASN:HB2	2:H:701:DGT:H8	1.96	0.47
1:K:595:LYS:HE3	1:K:597:GLU:HG2	1.97	0.47
1:C:592:THR:N	1:C:593:PRO:CD	2.78	0.47
1:E:592:THR:N	1:E:593:PRO:CD	2.78	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:J:592:THR:N	1:J:593:PRO:CD	2.78	0.47
1:A:425:ASN:HB2	1:D:428:LEU:CD1	2.45	0.47
1:F:592:THR:N	1:F:593:PRO:CD	2.78	0.47
1:G:439:LYS:HE2	1:G:443:GLU:CG	2.45	0.47
1:N:592:THR:N	1:N:593:PRO:CD	2.78	0.47
1:B:294:LYS:HE3	1:E:190:GLN:NE2	2.31	0.46
1:B:451:ARG:HG3	2:B:701:DGT:N2	2.29	0.46
1:B:469:LYS:HD3	1:B:471:GLU:OE2	2.15	0.46
1:C:577:ASN:OD1	1:C:595:LYS:NZ	2.41	0.46
1:G:592:THR:N	1:G:593:PRO:CD	2.78	0.46
1:I:352:ARG:HG3	1:I:354:LYS:HG2	1.95	0.46
1:I:592:THR:N	1:I:593:PRO:CD	2.78	0.46
1:O:592:THR:OG1	1:O:593:PRO:HD3	2.13	0.46
1:A:598:TRP:O	1:A:599:ASN:HB2	2.16	0.46
2:A:702:DGT:H3'	2:C:701:DGT:O3'	2.15	0.46
1:I:598:TRP:O	1:I:599:ASN:HB2	2.15	0.46
1:K:592:THR:N	1:K:593:PRO:CD	2.78	0.46
1:N:469:LYS:HD3	1:N:471:GLU:OE2	2.15	0.46
1:O:119:ASN:CB	2:P:701:DGT:H8	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:PHE:CE2	2:K:702:DGT:H1'	2.50	0.46
1:J:359:LEU:HD23	1:J:359:LEU:HA	1.69	0.46
1:J:469:LYS:HD3	1:J:471:GLU:OE2	2.15	0.46
1:N:377:LYS:NZ	2:P:701:DGT:PG	2.87	0.46
1:H:592:THR:N	1:H:593:PRO:CD	2.79	0.46
1:K:439:LYS:HE2	1:K:443:GLU:CG	2.46	0.46
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.46
1:B:224:LEU:HD23	1:B:470:ARG:HH22	1.81	0.46
1:C:595:LYS:HG3	1:C:597:GLU:HG2	1.98	0.46
1:D:592:THR:N	1:D:593:PRO:CD	2.79	0.46
1:M:352:ARG:HG3	1:M:354:LYS:HG2	1.96	0.46
1:B:451:ARG:HD3	1:B:453:LEU:CD1	2.46	0.46
1:F:224:LEU:HD23	1:F:470:ARG:HH22	1.81	0.46
1:M:157:PHE:CE2	2:O:703:DGT:H1'	2.51	0.46
1:M:535:ASN:OD1	1:M:535:ASN:N	2.49	0.46
1:O:535:ASN:OD1	1:O:535:ASN:N	2.49	0.46
1:K:535:ASN:OD1	1:K:535:ASN:N	2.49	0.46
1:L:592:THR:N	1:L:593:PRO:CD	2.79	0.46
1:N:326:GLN:HB2	1:P:328:ASN:HA	1.98	0.46
1:A:510:GLN:HB3	1:A:511:GLU:H	1.67	0.46
1:L:192:SER:HB3	1:N:262:GLU:HB2	1.97	0.46
1:M:592:THR:N	1:M:593:PRO:CD	2.78	0.46
1:A:535:ASN:OD1	1:A:535:ASN:N	2.49	0.45
1:C:439:LYS:HE2	1:C:443:GLU:CG	2.46	0.45
1:I:451:ARG:HG3	2:L:701:DGT:C2	2.45	0.45
1:O:592:THR:N	1:O:593:PRO:CD	2.78	0.45
1:E:598:TRP:O	1:E:599:ASN:HB2	2.16	0.45
1:N:224:LEU:HD23	1:N:470:ARG:HH22	1.82	0.45
1:O:439:LYS:HE2	1:O:443:GLU:CG	2.45	0.45
1:G:381:ILE:HD12	1:G:381:ILE:HA	1.90	0.45
1:G:535:ASN:OD1	1:G:535:ASN:N	2.49	0.45
1:J:535:ASN:OD1	1:J:535:ASN:N	2.49	0.45
1:C:535:ASN:OD1	1:C:535:ASN:N	2.49	0.45
1:F:451:ARG:HD3	1:F:453:LEU:CD1	2.46	0.45
1:J:139:PRO:HD3	1:K:450:TYR:CE1	2.51	0.45
1:N:451:ARG:HD3	1:N:453:LEU:CD1	2.46	0.45
1:C:187:PRO:CB	1:O:260:ILE:CD1	2.94	0.45
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.91	0.45
1:E:535:ASN:OD1	1:E:535:ASN:N	2.49	0.45
1:K:595:LYS:HG3	1:K:597:GLU:HG2	1.99	0.45
2:A:702:DGT:HN2A	1:B:119:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:ARG:HD3	1:J:453:LEU:CD1	2.46	0.45
1:O:595:LYS:HG3	1:O:597:GLU:HG2	1.98	0.45
1:I:425:ASN:HB2	1:L:428:LEU:CD1	2.46	0.45
1:O:502:VAL:HG22	1:O:550:ILE:HD12	1.98	0.45
1:F:326:GLN:HB2	1:H:328:ASN:HA	1.99	0.45
1:J:224:LEU:HD23	1:J:470:ARG:HH22	1.81	0.45
1:B:535:ASN:OD1	1:B:535:ASN:N	2.49	0.44
1:G:502:VAL:HG22	1:G:550:ILE:HD12	1.98	0.44
1:G:577:ASN:OD1	1:G:595:LYS:NZ	2.41	0.44
1:I:535:ASN:OD1	1:I:535:ASN:N	2.49	0.44
1:J:326:GLN:HB2	1:L:328:ASN:HA	1.98	0.44
1:K:502:VAL:HG22	1:K:550:ILE:HD12	1.98	0.44
1:N:535:ASN:N	1:N:535:ASN:OD1	2.49	0.44
1:C:333:ARG:HB2	1:D:125:HIS:CE1	2.52	0.44
1:E:425:ASN:HB2	1:H:428:LEU:HD13	1.98	0.44
1:K:312:LYS:HA	1:K:315:TYR:CE2	2.53	0.44
1:A:139:PRO:HD3	1:D:450:TYR:CE1	2.52	0.44
1:D:312:LYS:HA	1:D:315:TYR:CE2	2.53	0.44
1:N:312:LYS:HA	1:N:315:TYR:CE2	2.53	0.44
1:O:312:LYS:HA	1:O:315:TYR:CE2	2.53	0.44
1:O:381:ILE:HD12	1:O:381:ILE:HA	1.90	0.44
1:F:405:LYS:HB3	1:F:405:LYS:HE2	1.77	0.44
1:G:312:LYS:HA	1:G:315:TYR:CE2	2.53	0.44
1:G:595:LYS:HG3	1:G:597:GLU:HG2	1.98	0.44
1:J:312:LYS:HA	1:J:315:TYR:CE2	2.53	0.44
1:M:598:TRP:O	1:M:599:ASN:HB2	2.17	0.44
1:N:405:LYS:HE2	1:N:405:LYS:HB3	1.77	0.44
1:L:192:SER:CB	1:N:262:GLU:HB2	2.48	0.44
1:O:595:LYS:HE3	1:O:597:GLU:HG2	1.99	0.44
1:P:422:LEU:HD12	1:P:426:ILE:HG13	2.00	0.44
1:M:312:LYS:HA	1:M:315:TYR:CE2	2.53	0.44
1:C:502:VAL:HG22	1:C:550:ILE:HD12	1.99	0.44
1:L:422:LEU:HD12	1:L:426:ILE:HG13	1.99	0.44
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.52	0.43
1:D:422:LEU:HD12	1:D:426:ILE:HG13	2.00	0.43
1:E:312:LYS:HA	1:E:315:TYR:CE2	2.53	0.43
1:F:377:LYS:HB2	1:F:377:LYS:HE2	1.33	0.43
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.53	0.43
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.53	0.43
1:F:129:HIS:CG	1:F:130:PRO:HD2	2.54	0.43
1:G:230:LYS:HB3	1:G:230:LYS:HE3	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:LYS:HE3	1:K:230:LYS:HB3	1.65	0.43
1:P:312:LYS:HA	1:P:315:TYR:CE2	2.53	0.43
1:B:451:ARG:HG3	1:C:137:ASP:OD2	2.18	0.43
1:C:230:LYS:HB3	1:C:230:LYS:HE3	1.64	0.43
1:C:595:LYS:HE3	1:C:597:GLU:HG2	1.99	0.43
1:F:312:LYS:HA	1:F:315:TYR:CE2	2.53	0.43
1:F:577:ASN:OD1	1:F:595:LYS:NZ	2.41	0.43
1:G:595:LYS:HE3	1:G:597:GLU:HG2	1.99	0.43
1:H:170:GLY:HA3	1:H:314:ASP:OD2	2.18	0.43
1:H:312:LYS:HA	1:H:315:TYR:CE2	2.53	0.43
1:K:359:LEU:HA	1:K:359:LEU:HD23	1.70	0.43
1:K:595:LYS:HE3	1:K:597:GLU:CG	2.48	0.43
1:P:170:GLY:HA3	1:P:314:ASP:OD2	2.18	0.43
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.54	0.43
1:F:528:ARG:HH12	1:H:585:ASP:HB3	1.84	0.43
1:K:129:HIS:CG	1:K:130:PRO:HD2	2.53	0.43
1:O:156:VAL:O	2:O:702:DGT:H1'	2.18	0.43
1:B:451:ARG:HG3	2:B:701:DGT:HN2	1.83	0.43
1:I:312:LYS:HA	1:I:315:TYR:CE2	2.53	0.43
1:J:451:ARG:HG3	1:K:137:ASP:OD2	2.18	0.43
1:L:170:GLY:HA3	1:L:314:ASP:OD1	2.19	0.43
1:C:187:PRO:HB3	1:O:260:ILE:HD11	1.99	0.43
1:J:577:ASN:OD1	1:J:595:LYS:NZ	2.41	0.43
1:E:129:HIS:CG	1:E:130:PRO:HD2	2.54	0.43
1:J:528:ARG:HH11	1:L:586:VAL:HG22	1.83	0.43
1:L:312:LYS:HA	1:L:315:TYR:CE2	2.53	0.43
1:O:560:LYS:H	1:O:560:LYS:HG2	1.51	0.43
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.53	0.43
1:C:125:HIS:NE2	1:D:333:ARG:HD2	2.34	0.43
1:G:118:ILE:HG12	2:G:701:DGT:H2'A	2.01	0.43
1:G:129:HIS:CG	1:G:130:PRO:HD2	2.54	0.43
1:H:129:HIS:CG	1:H:130:PRO:HD2	2.53	0.43
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.54	0.43
2:F:701:DGT:H8	2:F:701:DGT:H2'A	1.89	0.43
1:H:241:PHE:O	1:H:245:ILE:HG12	2.19	0.43
1:J:129:HIS:CG	1:J:130:PRO:HD2	2.54	0.43
2:J:702:DGT:H2'A	1:K:118:ILE:HG12	2.00	0.43
1:L:381:ILE:HD12	1:L:381:ILE:HA	1.91	0.43
1:N:543:GLU:CG	1:P:543:GLU:HG3	2.43	0.43
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.54	0.43
1:J:241:PHE:O	1:J:245:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:129:HIS:CG	1:L:130:PRO:HD2	2.53	0.43
1:N:129:HIS:CG	1:N:130:PRO:HD2	2.53	0.43
1:O:129:HIS:CG	1:O:130:PRO:HD2	2.53	0.43
1:A:241:PHE:O	1:A:245:ILE:HG12	2.19	0.42
1:B:422:LEU:HD12	1:B:426:ILE:HG13	2.01	0.42
1:M:129:HIS:CG	1:M:130:PRO:HD2	2.53	0.42
1:C:241:PHE:O	1:C:245:ILE:HG12	2.19	0.42
1:E:450:TYR:CE1	1:H:139:PRO:HD3	2.54	0.42
2:E:701:DGT:O1G	1:H:455:LYS:NZ	2.42	0.42
1:I:129:HIS:CG	1:I:130:PRO:HD2	2.54	0.42
1:J:422:LEU:HD12	1:J:426:ILE:HG13	2.01	0.42
1:N:241:PHE:O	1:N:245:ILE:HG12	2.19	0.42
1:N:422:LEU:HD12	1:N:426:ILE:HG13	2.01	0.42
1:F:321:HIS:CE1	1:G:321:HIS:CE1	3.06	0.42
1:J:251:LYS:HB2	1:J:252:PRO:HD3	2.02	0.42
1:P:129:HIS:CG	1:P:130:PRO:HD2	2.54	0.42
2:C:702:DGT:HN2A	1:D:119:ASN:HD21	1.63	0.42
2:J:702:DGT:O1G	1:K:116:LYS:NZ	2.52	0.42
2:J:703:DGT:O6	1:L:372:ARG:HG2	2.20	0.42
1:K:241:PHE:O	1:K:245:ILE:HG12	2.19	0.42
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.02	0.42
1:E:425:ASN:HB2	1:H:428:LEU:CD1	2.49	0.42
1:F:241:PHE:O	1:F:245:ILE:HG12	2.19	0.42
1:N:359:LEU:HD23	1:N:359:LEU:HA	1.69	0.42
1:P:241:PHE:O	1:P:245:ILE:HG12	2.19	0.42
1:E:598:TRP:O	1:E:599:ASN:CB	2.68	0.42
2:E:702:DGT:O6	1:G:372:ARG:HG2	2.19	0.42
1:F:377:LYS:H	1:F:377:LYS:HG3	1.67	0.42
2:G:702:DGT:N2	1:H:119:ASN:ND2	2.64	0.42
1:I:226:ARG:HH21	1:I:229:VAL:HG21	1.85	0.42
1:L:241:PHE:O	1:L:245:ILE:HG12	2.19	0.42
1:N:321:HIS:CE1	1:O:321:HIS:CE1	3.08	0.42
1:B:241:PHE:O	1:B:245:ILE:HG12	2.19	0.42
1:C:595:LYS:HE3	1:C:597:GLU:CG	2.49	0.42
1:F:451:ARG:HG3	1:G:137:ASP:OD2	2.20	0.42
1:H:422:LEU:HD12	1:H:426:ILE:HG13	2.00	0.42
1:M:241:PHE:O	1:M:245:ILE:HG12	2.19	0.42
1:N:577:ASN:OD1	1:N:595:LYS:NZ	2.41	0.42
1:A:226:ARG:HH21	1:A:229:VAL:HG21	1.85	0.42
1:E:241:PHE:O	1:E:245:ILE:HG12	2.19	0.42
1:F:359:LEU:HA	1:F:359:LEU:HD23	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:PHE:O	1:G:245:ILE:HG12	2.19	0.42
1:O:251:LYS:HB2	1:O:252:PRO:HD3	2.02	0.42
1:O:577:ASN:OD1	1:O:595:LYS:NZ	2.41	0.42
1:C:359:LEU:HA	1:C:359:LEU:HD23	1.70	0.42
1:D:241:PHE:O	1:D:245:ILE:HG12	2.19	0.42
1:E:425:ASN:ND2	1:H:425:ASN:OD1	2.53	0.42
1:F:251:LYS:HB2	1:F:252:PRO:HD3	2.02	0.42
1:F:422:LEU:HD12	1:F:426:ILE:HG13	2.01	0.42
1:I:241:PHE:O	1:I:245:ILE:HG12	2.19	0.42
1:O:119:ASN:ND2	2:P:701:DGT:H8	2.35	0.42
1:O:465:GLN:OE1	1:O:465:GLN:HA	2.20	0.42
1:A:598:TRP:O	1:A:599:ASN:CB	2.68	0.42
1:G:125:HIS:NE2	1:H:333:ARG:HD2	2.35	0.42
1:G:595:LYS:HE3	1:G:597:GLU:CG	2.49	0.42
1:K:465:GLN:OE1	1:K:465:GLN:HA	2.20	0.42
1:M:251:LYS:HB2	1:M:252:PRO:HD3	2.02	0.42
1:J:408:ARG:H	1:J:411:THR:HG1	1.65	0.41
1:O:595:LYS:HE3	1:O:597:GLU:CG	2.49	0.41
1:B:118:ILE:HG12	2:C:701:DGT:C2'	2.49	0.41
1:F:528:ARG:HH11	1:H:586:VAL:HG22	1.85	0.41
1:I:321:HIS:CE1	1:L:321:HIS:CE1	3.09	0.41
1:M:598:TRP:O	1:M:599:ASN:CB	2.67	0.41
1:O:241:PHE:O	1:O:245:ILE:HG12	2.19	0.41
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.02	0.41
1:B:256:GLN:NE2	1:F:190:GLN:HE22	2.18	0.41
1:B:577:ASN:OD1	1:B:595:LYS:NZ	2.41	0.41
2:J:701:DGT:H1'	1:K:119:ASN:HB2	2.02	0.41
1:L:251:LYS:HB2	1:L:252:PRO:HD3	2.03	0.41
1:L:284:LEU:HD23	1:L:284:LEU:HA	1.92	0.41
1:B:256:GLN:NE2	1:F:190:GLN:CD	2.78	0.41
1:H:251:LYS:HB2	1:H:252:PRO:HD3	2.02	0.41
1:J:321:HIS:CE1	1:K:321:HIS:CE1	3.08	0.41
1:K:381:ILE:HD12	1:K:381:ILE:HA	1.90	0.41
1:K:465:GLN:O	1:K:467:LYS:HG3	2.21	0.41
1:D:126:ILE:HG12	1:D:173:TYR:CD1	2.55	0.41
1:F:126:ILE:HG12	1:F:173:TYR:CD1	2.56	0.41
1:I:598:TRP:O	1:I:599:ASN:CB	2.68	0.41
1:O:465:GLN:O	1:O:467:LYS:HG3	2.21	0.41
1:A:385:MET:SD	1:A:453:LEU:HB3	2.61	0.41
1:B:256:GLN:NE2	1:F:190:GLN:NE2	2.68	0.41
1:K:577:ASN:OD1	1:K:595:LYS:NZ	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:465:GLN:OE1	1:G:465:GLN:HA	2.20	0.41
2:J:701:DGT:H8	1:K:119:ASN:HB2	2.03	0.41
1:A:251:LYS:HB2	1:A:252:PRO:HD3	2.03	0.41
1:E:443:GLU:O	1:E:447:GLN:HG2	2.21	0.41
1:F:465:GLN:O	1:F:465:GLN:HG3	2.19	0.41
1:K:443:GLU:O	1:K:447:GLN:HG2	2.21	0.41
1:N:126:ILE:HG12	1:N:173:TYR:CD1	2.56	0.41
1:P:126:ILE:HG12	1:P:173:TYR:CD1	2.56	0.41
1:B:139:PRO:HD3	1:C:450:TYR:CE1	2.56	0.41
1:C:465:GLN:O	1:C:467:LYS:HG3	2.21	0.41
1:E:126:ILE:HG12	1:E:173:TYR:CD1	2.56	0.41
1:G:251:LYS:HB2	1:G:252:PRO:HD3	2.02	0.41
1:O:125:HIS:NE2	1:P:333:ARG:HD2	2.36	0.41
1:P:443:GLU:O	1:P:447:GLN:HG2	2.21	0.41
1:E:251:LYS:HB2	1:E:252:PRO:HD3	2.03	0.41
1:G:119:ASN:HB2	2:H:701:DGT:H1'	2.03	0.41
1:G:359:LEU:HA	1:G:359:LEU:HD23	1.70	0.41
1:P:455:LYS:HE3	1:P:455:LYS:HA	2.03	0.41
1:B:187:PRO:CB	1:E:260:ILE:HD11	2.51	0.40
1:C:443:GLU:O	1:C:447:GLN:HG2	2.21	0.40
2:F:701:DGT:H2'	1:H:156:VAL:HG12	2.02	0.40
1:H:443:GLU:O	1:H:447:GLN:HG2	2.21	0.40
1:I:381:ILE:HD12	1:I:381:ILE:HA	1.91	0.40
2:J:701:DGT:H8	1:K:119:ASN:CB	2.51	0.40
1:L:126:ILE:HG12	1:L:173:TYR:CD1	2.56	0.40
1:L:443:GLU:O	1:L:447:GLN:HG2	2.21	0.40
1:M:443:GLU:O	1:M:447:GLN:HG2	2.21	0.40
1:B:126:ILE:HG12	1:B:173:TYR:CD1	2.56	0.40
1:O:492:LYS:HE3	1:O:492:LYS:HB3	1.94	0.40
1:P:381:ILE:HD12	1:P:381:ILE:HA	1.91	0.40
1:A:443:GLU:O	1:A:447:GLN:HG2	2.21	0.40
1:D:443:GLU:O	1:D:447:GLN:HG2	2.21	0.40
1:G:369:LEU:HD23	1:G:369:LEU:HA	1.96	0.40
1:H:244:LEU:C	1:H:244:LEU:HD23	2.47	0.40
1:J:451:ARG:HG3	2:J:702:DGT:N2	2.37	0.40
1:K:251:LYS:HB2	1:K:252:PRO:HD3	2.02	0.40
1:A:126:ILE:HG12	1:A:173:TYR:CD1	2.57	0.40
1:C:465:GLN:OE1	1:C:465:GLN:HA	2.20	0.40
1:I:244:LEU:C	1:I:244:LEU:HD23	2.47	0.40
1:J:443:GLU:O	1:J:447:GLN:HG2	2.22	0.40
1:M:226:ARG:HH21	1:M:229:VAL:HG21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:251:LYS:HB2	1:N:252:PRO:HD3	2.02	0.40
1:O:126:ILE:HG12	1:O:173:TYR:CD1	2.56	0.40
1:B:165:PHE:CZ	1:B:169:LEU:HD11	2.56	0.40
1:B:443:GLU:O	1:B:447:GLN:HG2	2.22	0.40

All (34) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:492:LYS:CE	1:J:395:ASP:OD1[1_454]	1.17	1.03
1:F:465:GLN:OE1	1:G:576:ARG:O[1_455]	1.19	1.01
1:F:465:GLN:OE1	1:G:576:ARG:C[1_455]	1.22	0.98
1:F:465:GLN:CD	1:G:576:ARG:C[1_455]	1.31	0.89
1:F:465:GLN:CD	1:G:576:ARG:O[1_455]	1.34	0.86
1:F:465:GLN:OE1	1:G:577:ASN:N[1_455]	1.41	0.79
1:M:405:LYS:NZ	1:N:396:TYR:OH[1_454]	1.43	0.77
1:I:492:LYS:CE	1:J:395:ASP:CG[1_454]	1.48	0.72
1:O:395:ASP:OD1	1:P:492:LYS:CE[1_556]	1.57	0.63
1:F:465:GLN:CG	1:G:576:ARG:O[1_455]	1.67	0.53
1:F:465:GLN:OE1	1:G:577:ASN:CA[1_455]	1.68	0.52
1:F:463:THR:O	1:G:466:ILE:CD1[1_455]	1.74	0.46
1:J:560:LYS:NZ	1:M:262:GLU:OE1[1_656]	1.77	0.43
1:F:465:GLN:CD	1:G:577:ASN:N[1_455]	1.78	0.42
1:I:492:LYS:NZ	1:J:395:ASP:OD1[1_454]	1.82	0.38
1:A:464:GLY:CA	1:D:466:ILE:CD1[1_455]	1.88	0.32
1:A:465:GLN:OE1	1:D:576:ARG:O[1_455]	1.88	0.32
1:I:492:LYS:CE	1:J:395:ASP:CB[1_454]	1.88	0.32
1:K:597:GLU:O	1:L:596:LYS:NZ[1_455]	1.89	0.31
1:O:395:ASP:OD1	1:P:492:LYS:NZ[1_556]	1.89	0.31
1:I:492:LYS:CD	1:J:395:ASP:CB[1_454]	1.90	0.30
1:O:395:ASP:CG	1:P:492:LYS:CE[1_556]	1.93	0.27
1:O:395:ASP:CG	1:P:492:LYS:CD[1_556]	1.98	0.22
1:F:465:GLN:NE2	1:G:577:ASN:N[1_455]	1.99	0.21
1:F:465:GLN:OE1	1:G:577:ASN:C[1_455]	2.01	0.19
1:M:405:LYS:CD	1:N:395:ASP:OD2[1_454]	2.01	0.19
1:M:576:ARG:NH1	1:P:465:GLN:OE1[1_455]	2.02	0.18
1:M:405:LYS:CE	1:N:395:ASP:OD2[1_454]	2.03	0.17
1:F:465:GLN:NE2	1:G:576:ARG:C[1_455]	2.05	0.15
1:K:395:ASP:OD2	1:L:405:LYS:NZ[1_556]	2.10	0.10
1:F:465:GLN:NE2	1:G:577:ASN:CG[1_455]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:THR:C	1:G:466:ILE:CD1[1_455]	2.14	0.06
1:I:465:GLN:OE1	1:L:576:ARG:CZ[1_455]	2.15	0.05
1:O:395:ASP:OD2	1:P:492:LYS:CE[1_556]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/535 (89%)	469 (98%)	8 (2%)	0	100	100
1	B	477/535 (89%)	469 (98%)	8 (2%)	0	100	100
1	C	477/535 (89%)	470 (98%)	7 (2%)	0	100	100
1	D	478/535 (89%)	471 (98%)	7 (2%)	0	100	100
1	E	477/535 (89%)	468 (98%)	9 (2%)	0	100	100
1	F	477/535 (89%)	469 (98%)	8 (2%)	0	100	100
1	G	477/535 (89%)	470 (98%)	7 (2%)	0	100	100
1	H	478/535 (89%)	470 (98%)	8 (2%)	0	100	100
1	I	477/535 (89%)	466 (98%)	11 (2%)	0	100	100
1	J	477/535 (89%)	469 (98%)	8 (2%)	0	100	100
1	K	477/535 (89%)	470 (98%)	7 (2%)	0	100	100
1	L	478/535 (89%)	471 (98%)	7 (2%)	0	100	100
1	M	477/535 (89%)	468 (98%)	9 (2%)	0	100	100
1	N	477/535 (89%)	468 (98%)	9 (2%)	0	100	100
1	O	477/535 (89%)	470 (98%)	7 (2%)	0	100	100
1	P	478/535 (89%)	470 (98%)	7 (2%)	1 (0%)	43	72
All	All	7636/8560 (89%)	7508 (98%)	127 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	589	PRO

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	427/477 (90%)	420 (98%)	7 (2%)	55	69
1	B	427/477 (90%)	423 (99%)	4 (1%)	70	76
1	C	427/477 (90%)	420 (98%)	7 (2%)	55	69
1	D	428/477 (90%)	422 (99%)	6 (1%)	59	71
1	E	427/477 (90%)	420 (98%)	7 (2%)	55	69
1	F	427/477 (90%)	420 (98%)	7 (2%)	55	69
1	G	427/477 (90%)	421 (99%)	6 (1%)	59	71
1	H	428/477 (90%)	421 (98%)	7 (2%)	55	69
1	I	427/477 (90%)	420 (98%)	7 (2%)	55	69
1	J	427/477 (90%)	422 (99%)	5 (1%)	63	73
1	K	427/477 (90%)	420 (98%)	7 (2%)	55	69
1	L	428/477 (90%)	422 (99%)	6 (1%)	59	71
1	M	427/477 (90%)	423 (99%)	4 (1%)	70	76
1	N	427/477 (90%)	422 (99%)	5 (1%)	63	73
1	O	427/477 (90%)	418 (98%)	9 (2%)	47	65
1	P	428/477 (90%)	419 (98%)	9 (2%)	47	65
All	All	6836/7632 (90%)	6733 (98%)	103 (2%)	57	70

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	325	ILE
1	A	453	LEU
1	A	463	THR

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Mol	Chain	Res	Type
1	A	510	GLN
1	A	577	ASN
1	A	596	LYS
1	B	204	LEU
1	B	455	LYS
1	B	467	LYS
1	B	596	LYS
1	C	230	LYS
1	C	354	LYS
1	C	425	ASN
1	C	426	ILE
1	C	511	GLU
1	C	560	LYS
1	C	597	GLU
1	D	425	ASN
1	D	455	LYS
1	D	467	LYS
1	D	470	ARG
1	D	523	LYS
1	D	585	ASP
1	E	185	LYS
1	E	325	ILE
1	E	451	ARG
1	E	463	THR
1	E	510	GLN
1	E	543	GLU
1	E	577	ASN
1	F	118	ILE
1	F	204	LEU
1	F	377	LYS
1	F	455	LYS
1	F	467	LYS
1	F	543	GLU
1	F	596	LYS
1	G	230	LYS
1	G	354	LYS
1	G	425	ASN
1	G	426	ILE
1	G	511	GLU
1	G	597	GLU
1	H	277	GLU
1	H	425	ASN

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Mol	Chain	Res	Type
1	H	455	LYS
1	H	467	LYS
1	H	469	LYS
1	H	470	ARG
1	H	585	ASP
1	I	185	LYS
1	I	325	ILE
1	I	451	ARG
1	I	453	LEU
1	I	463	THR
1	I	543	GLU
1	I	577	ASN
1	J	204	LEU
1	J	377	LYS
1	J	455	LYS
1	J	467	LYS
1	J	596	LYS
1	K	230	LYS
1	K	342	GLU
1	K	354	LYS
1	K	425	ASN
1	K	426	ILE
1	K	511	GLU
1	K	597	GLU
1	L	425	ASN
1	L	455	LYS
1	L	467	LYS
1	L	471	GLU
1	L	523	LYS
1	L	585	ASP
1	M	185	LYS
1	M	325	ILE
1	M	463	THR
1	M	577	ASN
1	N	204	LEU
1	N	325	ILE
1	N	455	LYS
1	N	467	LYS
1	N	596	LYS
1	O	117	VAL
1	O	230	LYS
1	O	354	LYS

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Mol	Chain	Res	Type
1	O	425	ASN
1	O	426	ILE
1	O	511	GLU
1	O	543	GLU
1	O	560	LYS
1	O	597	GLU
1	P	425	ASN
1	P	455	LYS
1	P	467	LYS
1	P	471	GLU
1	P	523	LYS
1	P	580	LYS
1	P	583	ASP
1	P	585	ASP
1	P	590	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (229) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	180	HIS
1	A	190	GLN
1	A	200	GLN
1	A	207	ASN
1	A	210	HIS
1	A	215	HIS
1	A	233	HIS
1	A	366	HIS
1	A	367	ASN
1	A	370	HIS
1	A	425	ASN
1	A	510	GLN
1	A	571	GLN
1	A	594	GLN
1	B	119	ASN
1	B	149	GLN
1	B	200	GLN
1	B	207	ASN
1	B	210	HIS
1	B	215	HIS
1	B	233	HIS
1	B	243	HIS

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Mol	Chain	Res	Type
1	B	256	GLN
1	B	322	HIS
1	B	366	HIS
1	B	367	ASN
1	B	425	ASN
1	B	571	GLN
1	C	149	GLN
1	C	200	GLN
1	C	207	ASN
1	C	210	HIS
1	C	233	HIS
1	C	235	GLN
1	C	322	HIS
1	C	366	HIS
1	C	447	GLN
1	C	452	ASN
1	C	571	GLN
1	C	594	GLN
1	D	119	ASN
1	D	149	GLN
1	D	200	GLN
1	D	207	ASN
1	D	210	HIS
1	D	233	HIS
1	D	235	GLN
1	D	243	HIS
1	D	248	ASN
1	D	322	HIS
1	D	326	GLN
1	D	366	HIS
1	D	447	GLN
1	D	539	GLN
1	D	571	GLN
1	D	594	GLN
1	E	149	GLN
1	E	180	HIS
1	E	190	GLN
1	E	200	GLN
1	E	207	ASN
1	E	210	HIS
1	E	215	HIS
1	E	233	HIS

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Mol	Chain	Res	Type
1	E	243	HIS
1	E	248	ASN
1	E	366	HIS
1	E	425	ASN
1	E	571	GLN
1	E	594	GLN
1	F	119	ASN
1	F	149	GLN
1	F	190	GLN
1	F	200	GLN
1	F	207	ASN
1	F	210	HIS
1	F	215	HIS
1	F	233	HIS
1	F	243	HIS
1	F	248	ASN
1	F	322	HIS
1	F	366	HIS
1	F	367	ASN
1	F	425	ASN
1	F	539	GLN
1	F	571	GLN
1	F	582	GLN
1	G	149	GLN
1	G	190	GLN
1	G	200	GLN
1	G	207	ASN
1	G	210	HIS
1	G	233	HIS
1	G	235	GLN
1	G	243	HIS
1	G	322	HIS
1	G	364	HIS
1	G	366	HIS
1	G	571	GLN
1	G	594	GLN
1	H	119	ASN
1	H	149	GLN
1	H	200	GLN
1	H	207	ASN
1	H	210	HIS
1	H	233	HIS

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Mol	Chain	Res	Type
1	H	235	GLN
1	H	322	HIS
1	H	326	GLN
1	H	364	HIS
1	H	366	HIS
1	H	539	GLN
1	H	571	GLN
1	H	594	GLN
1	I	149	GLN
1	I	180	HIS
1	I	190	GLN
1	I	200	GLN
1	I	207	ASN
1	I	210	HIS
1	I	215	HIS
1	I	233	HIS
1	I	243	HIS
1	I	248	ASN
1	I	366	HIS
1	I	367	ASN
1	I	425	ASN
1	I	571	GLN
1	I	594	GLN
1	J	119	ASN
1	J	149	GLN
1	J	200	GLN
1	J	207	ASN
1	J	210	HIS
1	J	215	HIS
1	J	233	HIS
1	J	243	HIS
1	J	248	ASN
1	J	322	HIS
1	J	366	HIS
1	J	367	ASN
1	J	425	ASN
1	J	539	GLN
1	J	571	GLN
1	K	149	GLN
1	K	190	GLN
1	K	200	GLN
1	K	207	ASN

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Mol	Chain	Res	Type
1	K	210	HIS
1	K	233	HIS
1	K	235	GLN
1	K	322	HIS
1	K	366	HIS
1	K	517	HIS
1	K	571	GLN
1	K	594	GLN
1	L	149	GLN
1	L	200	GLN
1	L	207	ASN
1	L	210	HIS
1	L	233	HIS
1	L	235	GLN
1	L	248	ASN
1	L	322	HIS
1	L	326	GLN
1	L	364	HIS
1	L	366	HIS
1	L	447	GLN
1	L	539	GLN
1	L	571	GLN
1	L	594	GLN
1	M	149	GLN
1	M	180	HIS
1	M	190	GLN
1	M	200	GLN
1	M	207	ASN
1	M	210	HIS
1	M	215	HIS
1	M	233	HIS
1	M	243	HIS
1	M	248	ASN
1	M	366	HIS
1	M	367	ASN
1	M	425	ASN
1	M	571	GLN
1	M	594	GLN
1	N	119	ASN
1	N	149	GLN
1	N	200	GLN
1	N	207	ASN

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Mol	Chain	Res	Type
1	N	210	HIS
1	N	215	HIS
1	N	233	HIS
1	N	243	HIS
1	N	248	ASN
1	N	322	HIS
1	N	366	HIS
1	N	367	ASN
1	N	425	ASN
1	N	571	GLN
1	O	149	GLN
1	O	190	GLN
1	O	200	GLN
1	O	207	ASN
1	O	210	HIS
1	O	233	HIS
1	O	235	GLN
1	O	243	HIS
1	O	322	HIS
1	O	366	HIS
1	O	571	GLN
1	O	594	GLN
1	P	149	GLN
1	P	200	GLN
1	P	207	ASN
1	P	210	HIS
1	P	233	HIS
1	P	235	GLN
1	P	248	ASN
1	P	322	HIS
1	P	326	GLN
1	P	364	HIS
1	P	366	HIS
1	P	447	GLN
1	P	539	GLN
1	P	571	GLN
1	P	594	GLN
1	P	599	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

32 ligands are modelled in this entry.

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	P	702	-	32,33,33	0.51	0	48,52,52	0.58	0
2	DGT	B	701	-	32,33,33	0.59	0	48,52,52	0.67	0
2	DGT	I	702	-	32,33,33	0.54	0	48,52,52	0.58	0
2	DGT	O	703	-	32,33,33	0.56	0	48,52,52	0.60	0
2	DGT	E	703	-	32,33,33	0.52	0	48,52,52	0.70	0
2	DGT	F	701	-	32,33,33	0.71	1 (3%)	48,52,52	0.58	0
2	DGT	J	703	-	32,33,33	0.74	1 (3%)	48,52,52	0.56	0
2	DGT	L	701	-	32,33,33	0.56	0	48,52,52	0.57	0
2	DGT	N	701	-	32,33,33	0.79	1 (3%)	48,52,52	0.54	0
2	DGT	H	701	-	32,33,33	0.62	0	48,52,52	0.68	0
2	DGT	K	701	-	32,33,33	0.51	0	48,52,52	0.59	0
2	DGT	G	702	-	32,33,33	0.59	0	48,52,52	0.69	0
2	DGT	E	701	-	32,33,33	0.50	0	48,52,52	0.69	0
2	DGT	D	701	-	32,33,33	0.60	0	48,52,52	0.55	0
2	DGT	C	701	-	32,33,33	0.50	0	48,52,52	0.60	0
2	DGT	J	702	-	32,33,33	0.57	0	48,52,52	0.69	0
2	DGT	A	703	-	32,33,33	0.52	0	48,52,52	0.80	2 (4%)
2	DGT	P	701	-	32,33,33	0.64	0	48,52,52	0.69	0
2	DGT	I	701	-	32,33,33	0.49	0	48,52,52	0.69	0
2	DGT	F	702	-	32,33,33	0.45	0	48,52,52	0.61	0
2	DGT	M	701	-	32,33,33	0.54	0	48,52,52	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DGT	A	701	-	32,33,33	0.55	0	48,52,52	0.70	0
2	DGT	K	702	-	32,33,33	0.53	0	48,52,52	0.59	0
2	DGT	E	702	-	32,33,33	0.53	0	48,52,52	0.59	0
2	DGT	A	702	-	32,33,33	0.55	0	48,52,52	0.56	0
2	DGT	C	702	-	32,33,33	0.52	0	48,52,52	0.55	0
2	DGT	B	702	-	32,33,33	0.73	0	48,52,52	0.57	0
2	DGT	M	702	-	32,33,33	0.57	0	48,52,52	0.58	0
2	DGT	O	701	-	32,33,33	0.59	0	48,52,52	0.67	0
2	DGT	G	701	-	32,33,33	0.56	0	48,52,52	0.67	0
2	DGT	J	701	-	32,33,33	0.59	0	48,52,52	0.68	0
2	DGT	O	702	-	32,33,33	0.46	0	48,52,52	0.61	0

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	P	702	-	-	5/22/34/34	0/3/3/3
2	DGT	B	701	-	-	8/22/34/34	0/3/3/3
2	DGT	I	702	-	-	6/22/34/34	0/3/3/3
2	DGT	O	703	-	-	4/22/34/34	0/3/3/3
2	DGT	E	703	-	-	7/22/34/34	0/3/3/3
2	DGT	F	701	-	-	5/22/34/34	0/3/3/3
2	DGT	J	703	-	-	5/22/34/34	0/3/3/3
2	DGT	L	701	-	-	7/22/34/34	0/3/3/3
2	DGT	N	701	-	-	5/22/34/34	0/3/3/3
2	DGT	H	701	-	-	7/22/34/34	0/3/3/3
2	DGT	K	701	-	-	2/22/34/34	0/3/3/3
2	DGT	G	702	-	-	3/22/34/34	0/3/3/3
2	DGT	E	701	-	-	6/22/34/34	0/3/3/3
2	DGT	D	701	-	-	6/22/34/34	0/3/3/3
2	DGT	C	701	-	-	2/22/34/34	0/3/3/3
2	DGT	J	702	-	-	8/22/34/34	0/3/3/3
2	DGT	A	703	-	-	6/22/34/34	0/3/3/3
2	DGT	P	701	-	-	7/22/34/34	0/3/3/3
2	DGT	I	701	-	-	6/22/34/34	0/3/3/3
2	DGT	F	702	-	-	2/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	M	701	-	-	6/22/34/34	0/3/3/3
2	DGT	A	701	-	-	6/22/34/34	0/3/3/3
2	DGT	K	702	-	-	4/22/34/34	0/3/3/3
2	DGT	E	702	-	-	5/22/34/34	0/3/3/3
2	DGT	A	702	-	-	4/22/34/34	0/3/3/3
2	DGT	C	702	-	-	5/22/34/34	0/3/3/3
2	DGT	B	702	-	-	6/22/34/34	0/3/3/3
2	DGT	M	702	-	-	5/22/34/34	0/3/3/3
2	DGT	O	701	-	-	8/22/34/34	0/3/3/3
2	DGT	G	701	-	-	8/22/34/34	0/3/3/3
2	DGT	J	701	-	-	7/22/34/34	0/3/3/3
2	DGT	O	702	-	-	2/22/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	703	DGT	PA-O3A	2.32	1.62	1.59
2	N	701	DGT	PA-O3A	2.28	1.62	1.59
2	F	701	DGT	PA-O3A	2.02	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	DGT	C1'-N9-C8	-2.55	122.20	127.91
2	A	703	DGT	C1'-N9-C4	2.43	132.06	125.50

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DGT	C5'-O5'-PA-O3A
2	A	701	DGT	C5'-O5'-PA-O2A
2	A	702	DGT	PB-O3B-PG-O1G
2	A	703	DGT	O4'-C1'-N9-C8
2	A	703	DGT	O4'-C1'-N9-C4
2	B	701	DGT	C5'-O5'-PA-O3A
2	B	701	DGT	C5'-O5'-PA-O1A
2	B	701	DGT	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	702	DGT	C5'-O5'-PA-O3A
2	B	702	DGT	C5'-O5'-PA-O1A
2	B	702	DGT	C5'-O5'-PA-O2A
2	B	702	DGT	O4'-C4'-C5'-O5'
2	C	702	DGT	O4'-C4'-C5'-O5'
2	D	701	DGT	C5'-O5'-PA-O3A
2	D	701	DGT	C5'-O5'-PA-O2A
2	D	701	DGT	C4'-C5'-O5'-PA
2	E	701	DGT	C5'-O5'-PA-O2A
2	E	702	DGT	PB-O3B-PG-O1G
2	F	701	DGT	C5'-O5'-PA-O3A
2	F	701	DGT	C5'-O5'-PA-O1A
2	F	701	DGT	C5'-O5'-PA-O2A
2	F	701	DGT	O4'-C4'-C5'-O5'
2	G	701	DGT	C5'-O5'-PA-O3A
2	G	701	DGT	C5'-O5'-PA-O1A
2	G	701	DGT	C5'-O5'-PA-O2A
2	G	702	DGT	O4'-C4'-C5'-O5'
2	H	701	DGT	C5'-O5'-PA-O3A
2	H	701	DGT	C5'-O5'-PA-O2A
2	H	701	DGT	C3'-C4'-C5'-O5'
2	I	701	DGT	C5'-O5'-PA-O3A
2	I	701	DGT	C5'-O5'-PA-O2A
2	I	702	DGT	PB-O3B-PG-O1G
2	J	701	DGT	PB-O3A-PA-O5'
2	J	701	DGT	C5'-O5'-PA-O3A
2	J	701	DGT	C5'-O5'-PA-O2A
2	J	701	DGT	C4'-C5'-O5'-PA
2	J	701	DGT	C3'-C4'-C5'-O5'
2	J	702	DGT	C5'-O5'-PA-O3A
2	J	702	DGT	C5'-O5'-PA-O1A
2	J	702	DGT	C5'-O5'-PA-O2A
2	J	703	DGT	C5'-O5'-PA-O3A
2	J	703	DGT	C5'-O5'-PA-O1A
2	J	703	DGT	C5'-O5'-PA-O2A
2	J	703	DGT	O4'-C4'-C5'-O5'
2	K	702	DGT	O4'-C4'-C5'-O5'
2	M	701	DGT	C5'-O5'-PA-O2A
2	M	702	DGT	PB-O3B-PG-O1G
2	N	701	DGT	C5'-O5'-PA-O3A
2	N	701	DGT	C5'-O5'-PA-O1A
2	N	701	DGT	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	N	701	DGT	O4'-C4'-C5'-O5'
2	O	701	DGT	C5'-O5'-PA-O3A
2	O	701	DGT	C5'-O5'-PA-O1A
2	O	701	DGT	C5'-O5'-PA-O2A
2	O	703	DGT	O4'-C4'-C5'-O5'
2	P	701	DGT	PB-O3A-PA-O5'
2	P	701	DGT	C5'-O5'-PA-O3A
2	P	701	DGT	C5'-O5'-PA-O2A
2	P	701	DGT	C4'-C5'-O5'-PA
2	P	701	DGT	C3'-C4'-C5'-O5'
2	C	701	DGT	C3'-C4'-C5'-O5'
2	D	701	DGT	C3'-C4'-C5'-O5'
2	F	702	DGT	C3'-C4'-C5'-O5'
2	K	701	DGT	C3'-C4'-C5'-O5'
2	O	702	DGT	C3'-C4'-C5'-O5'
2	H	701	DGT	C4'-C5'-O5'-PA
2	A	702	DGT	O4'-C4'-C5'-O5'
2	B	702	DGT	C3'-C4'-C5'-O5'
2	C	701	DGT	O4'-C4'-C5'-O5'
2	C	702	DGT	C3'-C4'-C5'-O5'
2	D	701	DGT	O4'-C4'-C5'-O5'
2	E	702	DGT	O4'-C4'-C5'-O5'
2	E	703	DGT	O4'-C4'-C5'-O5'
2	F	701	DGT	C3'-C4'-C5'-O5'
2	F	702	DGT	O4'-C4'-C5'-O5'
2	G	702	DGT	C3'-C4'-C5'-O5'
2	H	701	DGT	O4'-C4'-C5'-O5'
2	I	702	DGT	O4'-C4'-C5'-O5'
2	J	701	DGT	O4'-C4'-C5'-O5'
2	J	703	DGT	C3'-C4'-C5'-O5'
2	K	701	DGT	O4'-C4'-C5'-O5'
2	K	702	DGT	C3'-C4'-C5'-O5'
2	M	702	DGT	O4'-C4'-C5'-O5'
2	N	701	DGT	C3'-C4'-C5'-O5'
2	O	702	DGT	O4'-C4'-C5'-O5'
2	O	703	DGT	C3'-C4'-C5'-O5'
2	P	701	DGT	O4'-C4'-C5'-O5'
2	A	702	DGT	C3'-C4'-C5'-O5'
2	L	701	DGT	O4'-C4'-C5'-O5'
2	P	702	DGT	O4'-C4'-C5'-O5'
2	A	701	DGT	O4'-C4'-C5'-O5'
2	E	701	DGT	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	M	701	DGT	O4'-C4'-C5'-O5'
2	I	701	DGT	O4'-C4'-C5'-O5'
2	I	702	DGT	C3'-C4'-C5'-O5'
2	C	702	DGT	PB-O3B-PG-O3G
2	K	702	DGT	PB-O3B-PG-O3G
2	E	702	DGT	C3'-C4'-C5'-O5'
2	E	703	DGT	C3'-C4'-C5'-O5'
2	M	702	DGT	C3'-C4'-C5'-O5'
2	E	703	DGT	PG-O3B-PB-O2B
2	P	702	DGT	PG-O3B-PB-O2B
2	B	701	DGT	O4'-C1'-N9-C4
2	E	703	DGT	O4'-C1'-N9-C4
2	G	701	DGT	O4'-C1'-N9-C4
2	J	702	DGT	O4'-C1'-N9-C4
2	L	701	DGT	O4'-C1'-N9-C4
2	O	701	DGT	O4'-C1'-N9-C4
2	P	701	DGT	O4'-C1'-N9-C4
2	B	701	DGT	O4'-C1'-N9-C8
2	E	703	DGT	O4'-C1'-N9-C8
2	G	701	DGT	O4'-C1'-N9-C8
2	J	702	DGT	O4'-C1'-N9-C8
2	L	701	DGT	O4'-C1'-N9-C8
2	O	701	DGT	O4'-C1'-N9-C8
2	D	701	DGT	PB-O3A-PA-O5'
2	H	701	DGT	PB-O3A-PA-O5'
2	O	703	DGT	PB-O3B-PG-O3G
2	P	702	DGT	C3'-C4'-C5'-O5'
2	A	701	DGT	C5'-O5'-PA-O1A
2	A	703	DGT	C5'-O5'-PA-O2A
2	C	702	DGT	C5'-O5'-PA-O2A
2	E	701	DGT	C5'-O5'-PA-O3A
2	E	701	DGT	C5'-O5'-PA-O1A
2	E	702	DGT	C5'-O5'-PA-O2A
2	I	701	DGT	C5'-O5'-PA-O1A
2	I	702	DGT	C5'-O5'-PA-O2A
2	K	702	DGT	C5'-O5'-PA-O2A
2	M	701	DGT	C5'-O5'-PA-O3A
2	M	701	DGT	C5'-O5'-PA-O1A
2	M	702	DGT	C5'-O5'-PA-O2A
2	O	703	DGT	C5'-O5'-PA-O2A
2	B	701	DGT	PG-O3B-PB-O1B
2	G	701	DGT	PG-O3B-PB-O1B

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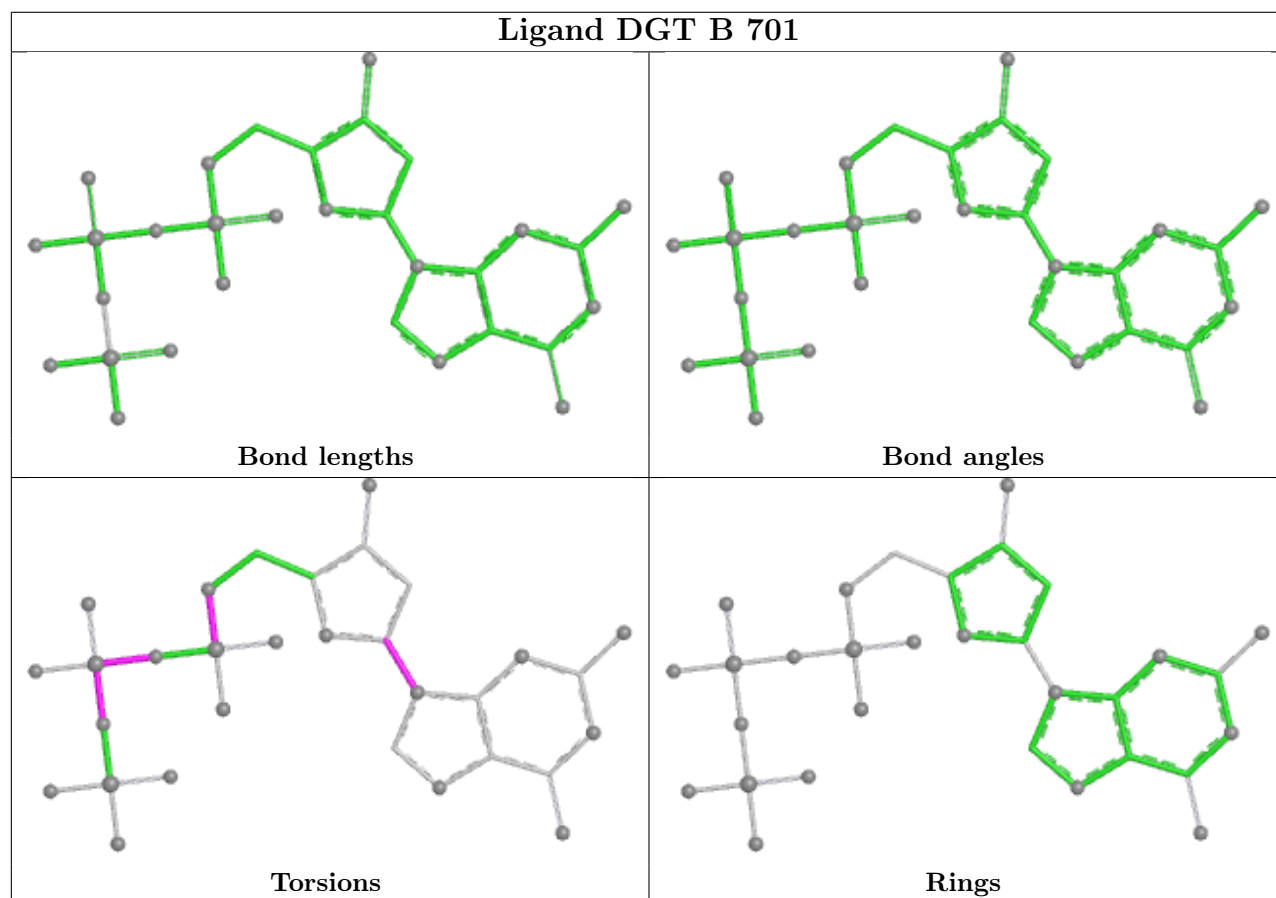
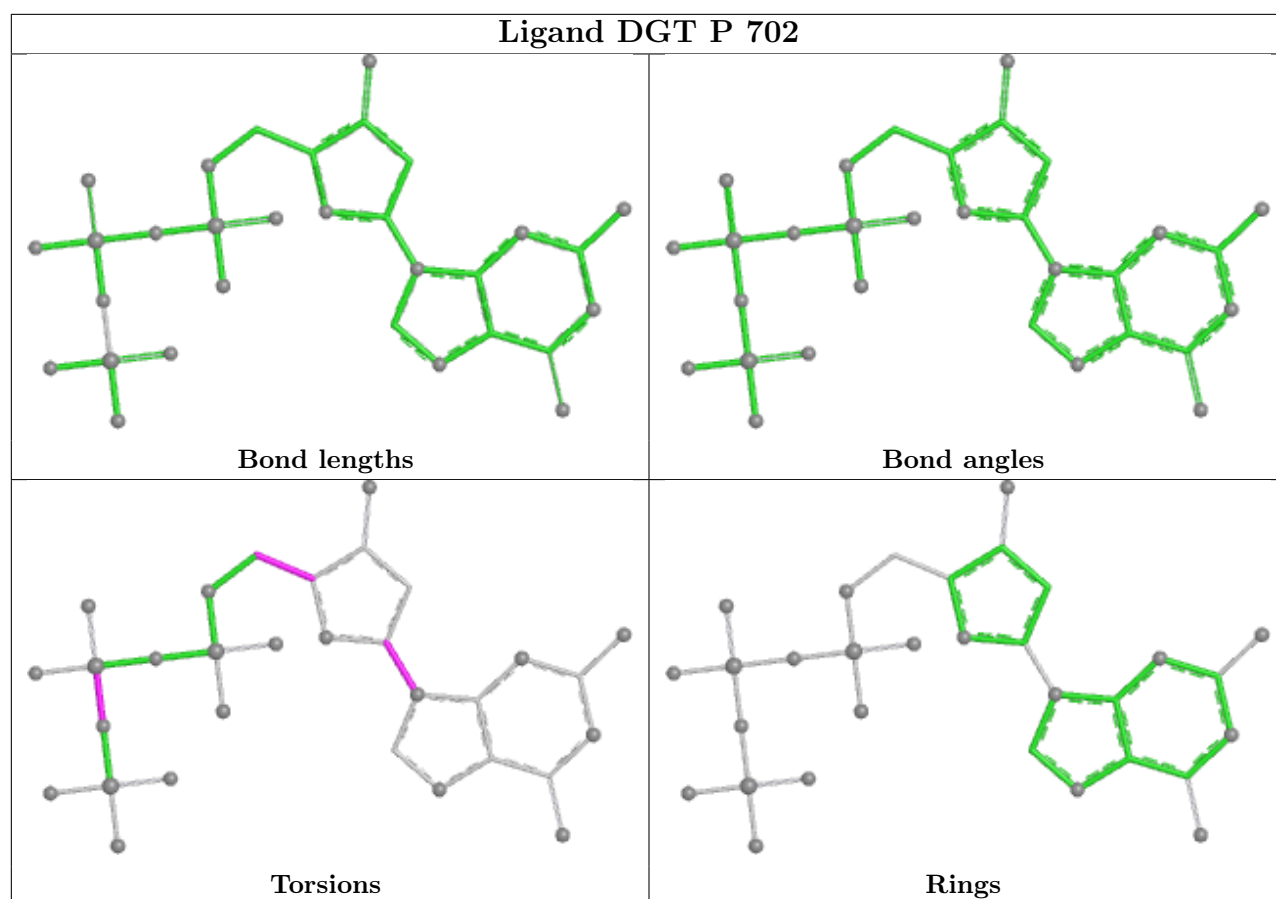
Mol	Chain	Res	Type	Atoms
2	J	702	DGT	PG-O3B-PB-O1B
2	L	701	DGT	PG-O3B-PB-O2B
2	O	701	DGT	PG-O3B-PB-O1B
2	P	702	DGT	PG-O3B-PB-O1B
2	L	701	DGT	C3'-C4'-C5'-O5'
2	G	702	DGT	PB-O3B-PG-O3G
2	E	703	DGT	PA-O3A-PB-O2B
2	L	701	DGT	PA-O3A-PB-O2B
2	H	701	DGT	O4'-C1'-N9-C4
2	J	701	DGT	O4'-C1'-N9-C4
2	A	702	DGT	PB-O3B-PG-O3G
2	E	702	DGT	PB-O3B-PG-O3G
2	I	702	DGT	PB-O3B-PG-O3G
2	M	702	DGT	PB-O3B-PG-O3G
2	J	702	DGT	PA-O3A-PB-O3B
2	O	701	DGT	PA-O3A-PB-O3B
2	A	703	DGT	PA-O3A-PB-O2B
2	B	701	DGT	PA-O3A-PB-O2B
2	E	703	DGT	PG-O3B-PB-O1B
2	G	701	DGT	PA-O3A-PB-O2B
2	J	702	DGT	PA-O3A-PB-O2B
2	L	701	DGT	PG-O3B-PB-O1B
2	O	701	DGT	PA-O3A-PB-O2B
2	B	701	DGT	PA-O3A-PB-O3B
2	G	701	DGT	PA-O3A-PB-O3B
2	P	702	DGT	O4'-C1'-N9-C4
2	A	701	DGT	C3'-C4'-C5'-O5'
2	A	703	DGT	C3'-C4'-C5'-O5'
2	E	701	DGT	C3'-C4'-C5'-O5'
2	I	701	DGT	C3'-C4'-C5'-O5'
2	M	701	DGT	C3'-C4'-C5'-O5'
2	A	703	DGT	O4'-C4'-C5'-O5'
2	A	701	DGT	PB-O3A-PA-O1A
2	B	702	DGT	PB-O3A-PA-O1A
2	C	702	DGT	PB-O3A-PA-O1A
2	E	701	DGT	PB-O3A-PA-O1A
2	I	701	DGT	PB-O3A-PA-O1A
2	I	702	DGT	PB-O3A-PA-O1A
2	M	701	DGT	PB-O3A-PA-O1A

There are no ring outliers.

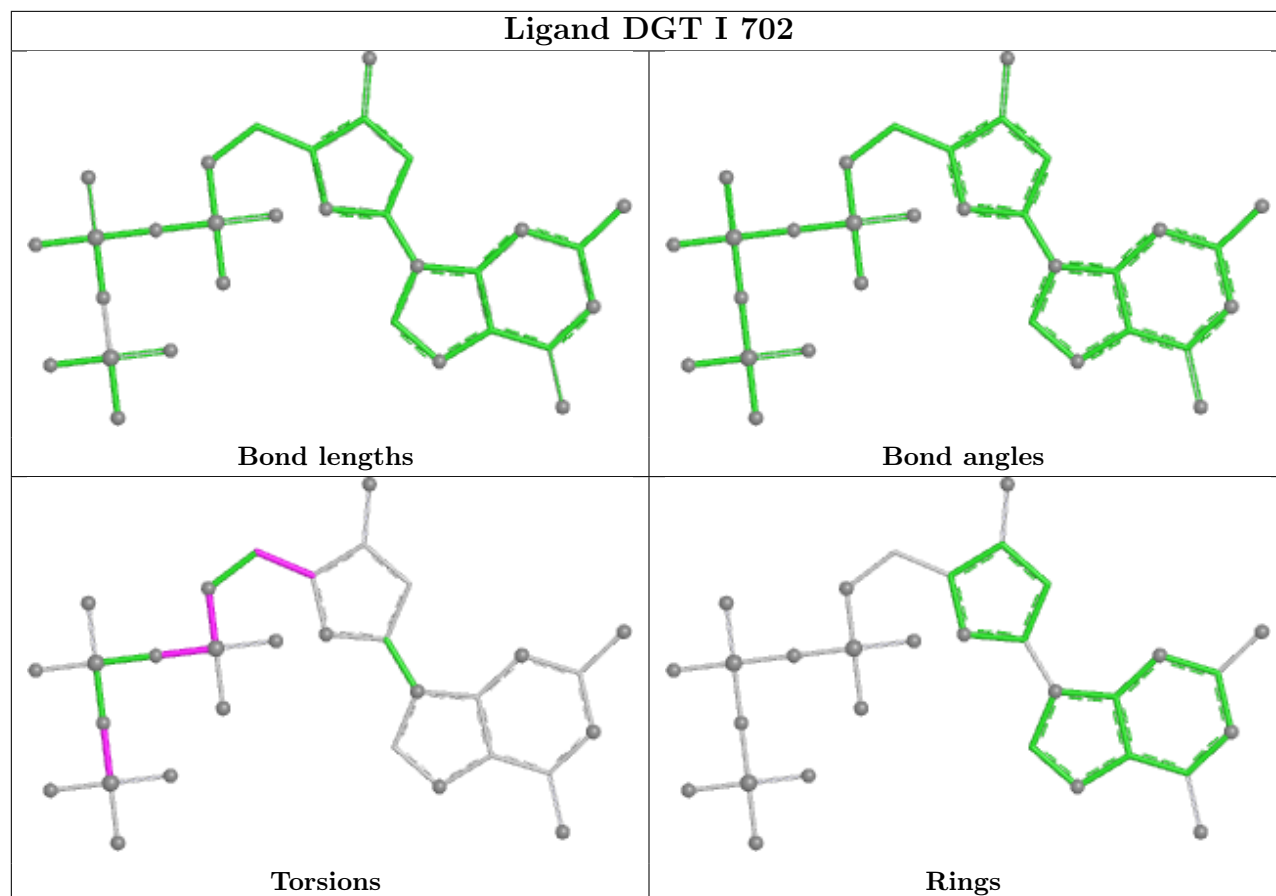
23 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	DGT	2	0
2	O	703	DGT	1	0
2	F	701	DGT	2	0
2	J	703	DGT	1	0
2	L	701	DGT	2	0
2	H	701	DGT	7	0
2	K	701	DGT	3	0
2	G	702	DGT	3	0
2	E	701	DGT	1	0
2	D	701	DGT	1	0
2	C	701	DGT	4	0
2	J	702	DGT	3	0
2	A	703	DGT	1	0
2	P	701	DGT	6	0
2	F	702	DGT	4	0
2	K	702	DGT	1	0
2	E	702	DGT	2	0
2	A	702	DGT	4	0
2	C	702	DGT	4	0
2	M	702	DGT	1	0
2	G	701	DGT	1	0
2	J	701	DGT	8	0
2	O	702	DGT	3	0

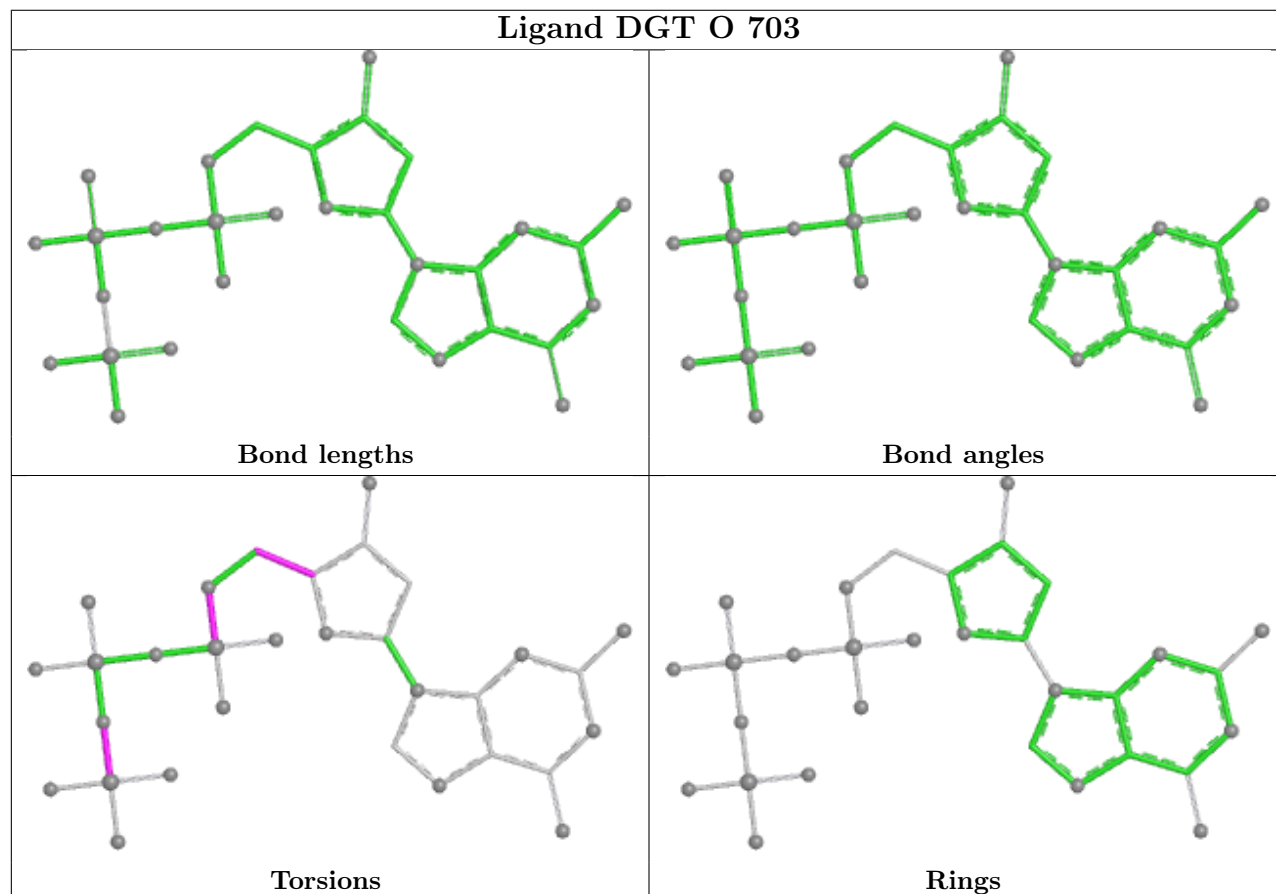
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



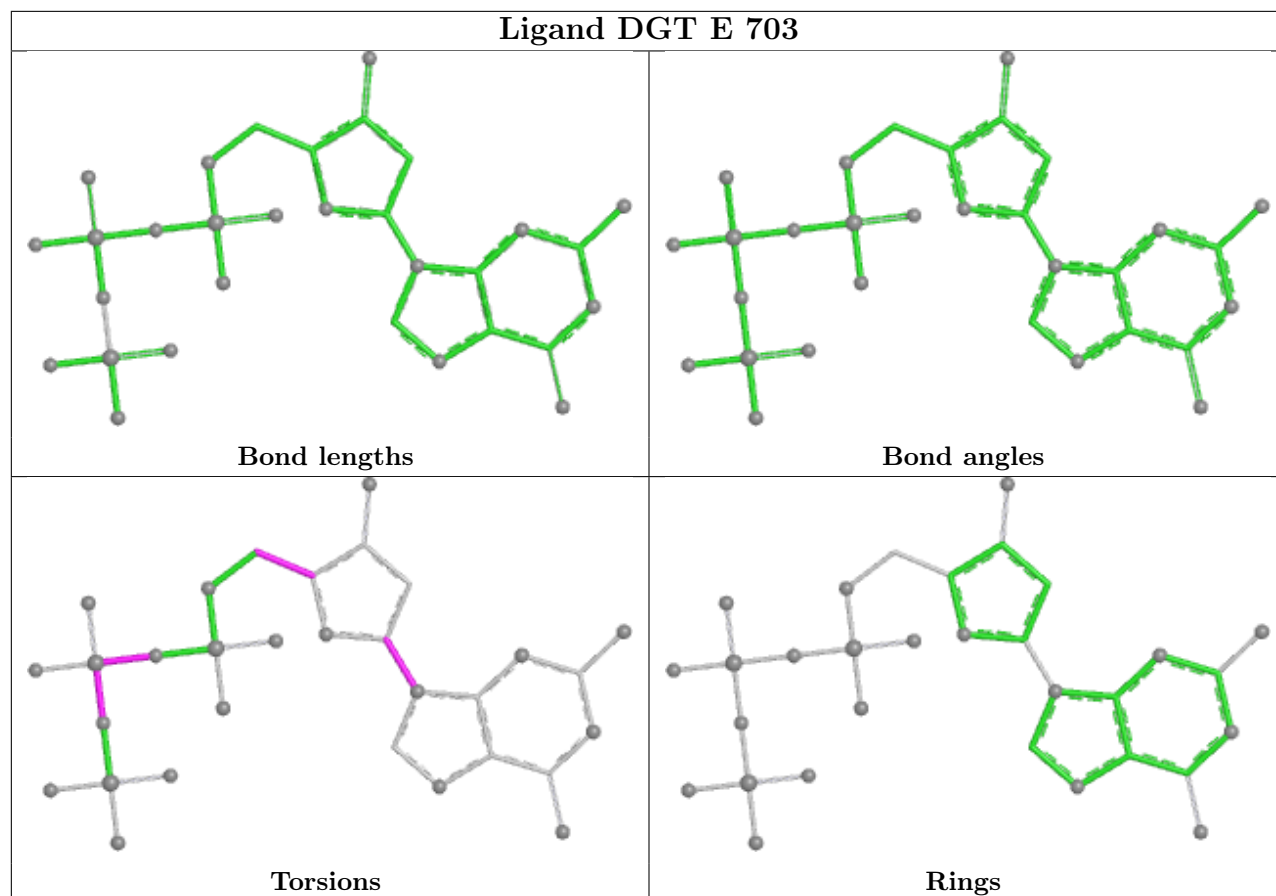
Ligand DGT I 702



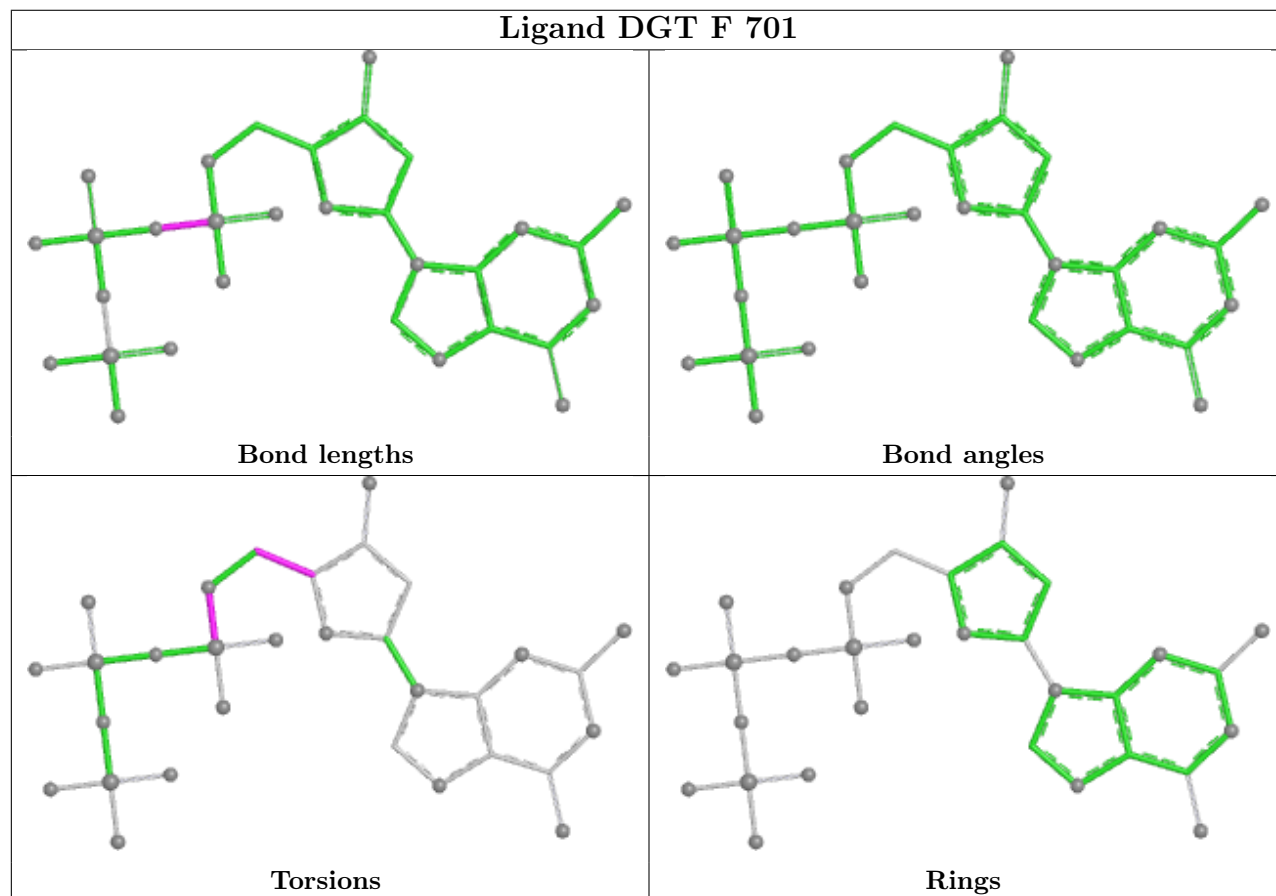
Ligand DGT O 703



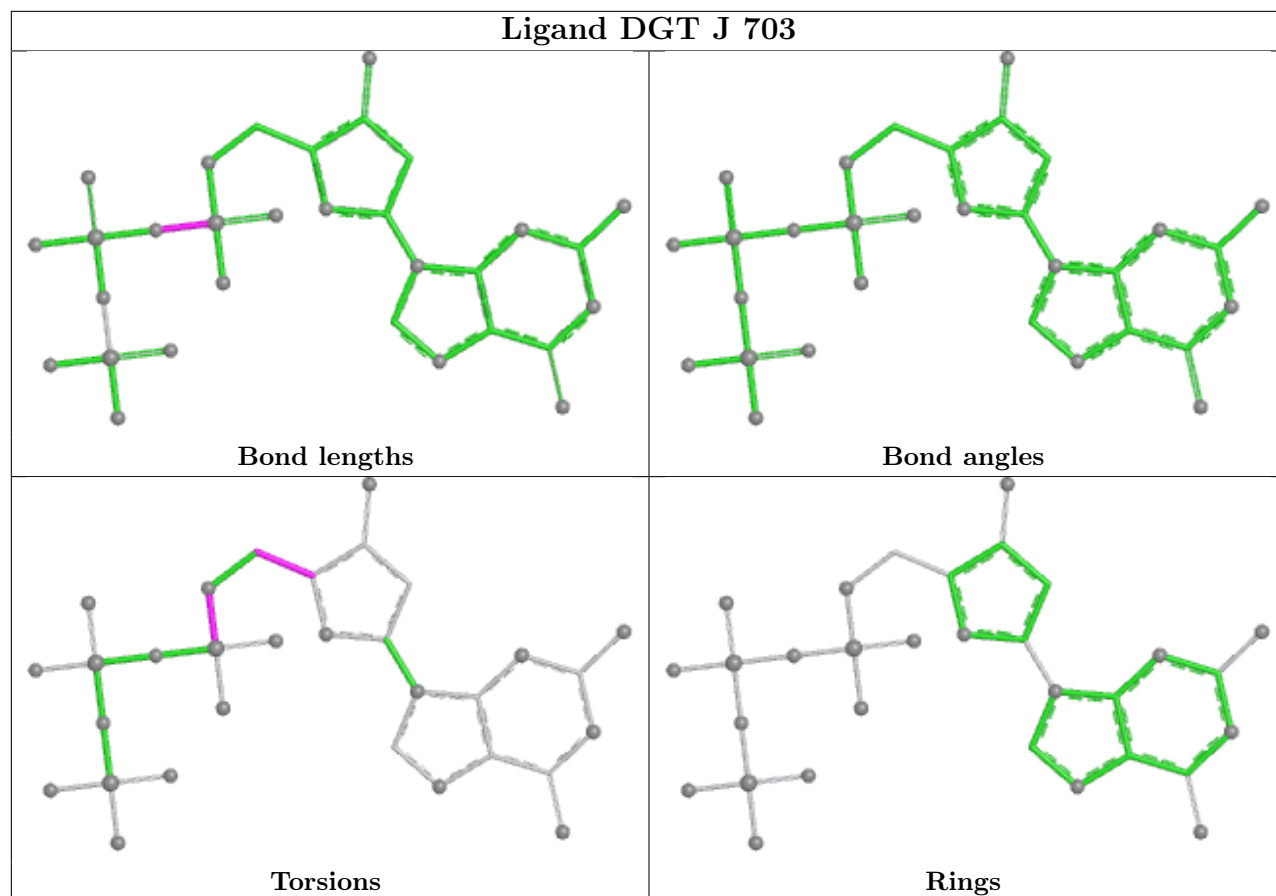
Ligand DGT E 703



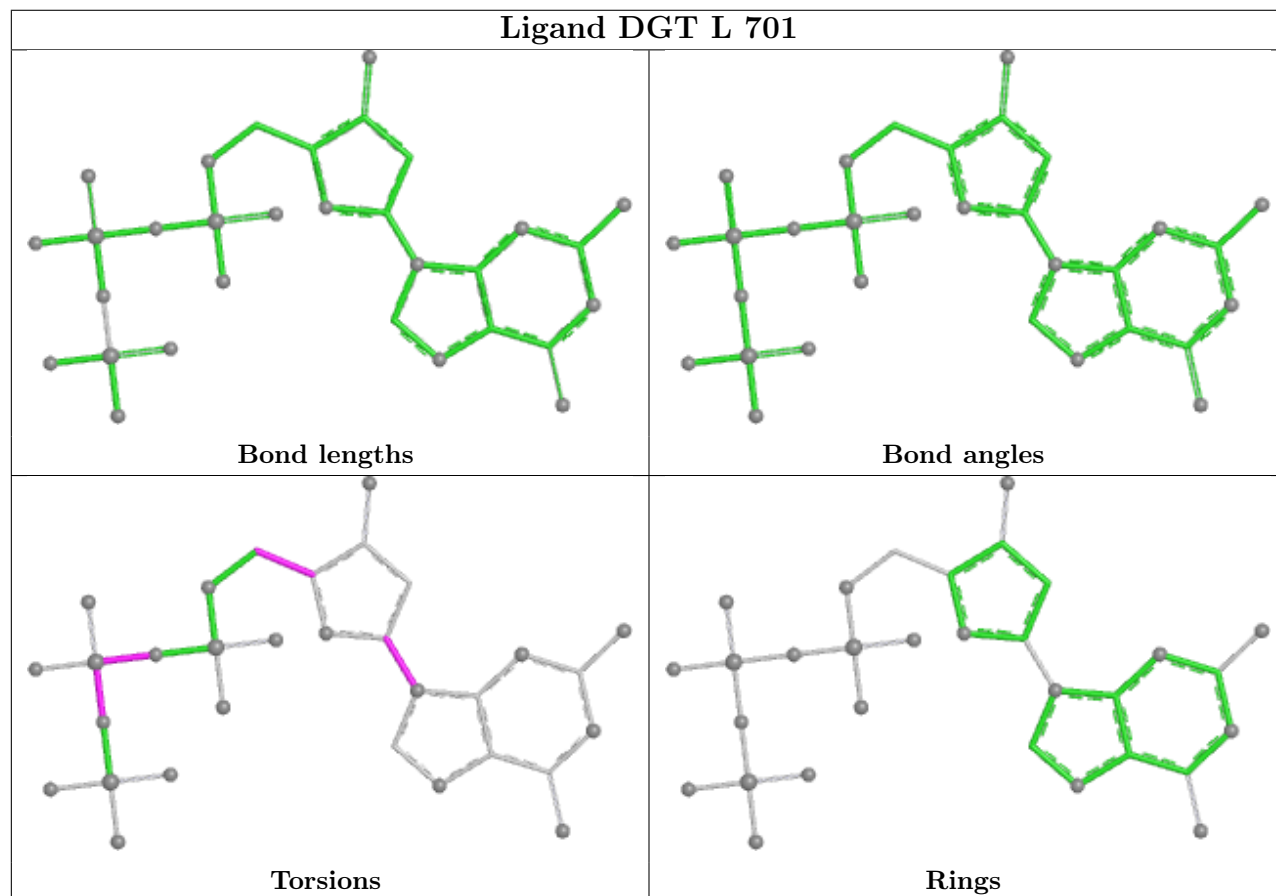
Ligand DGT F 701

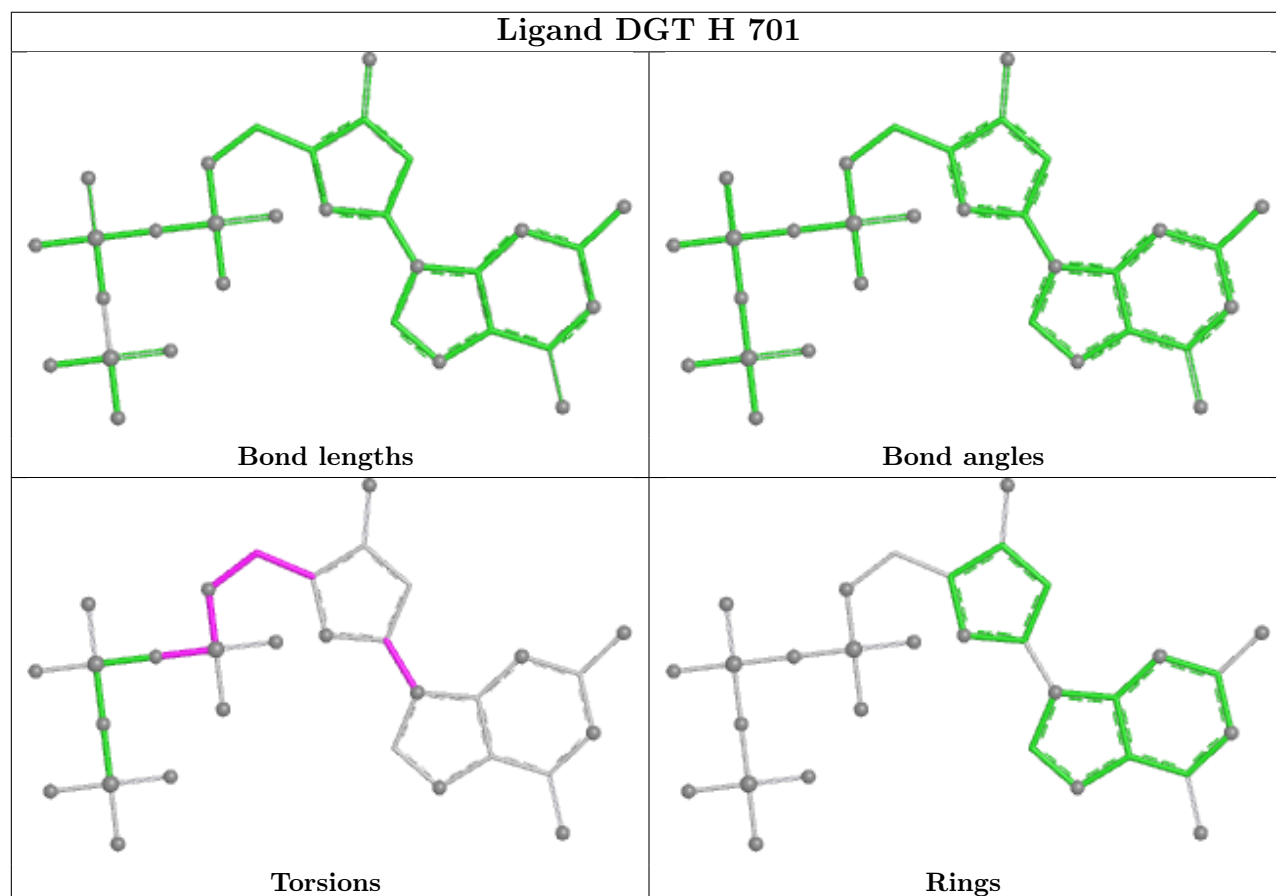
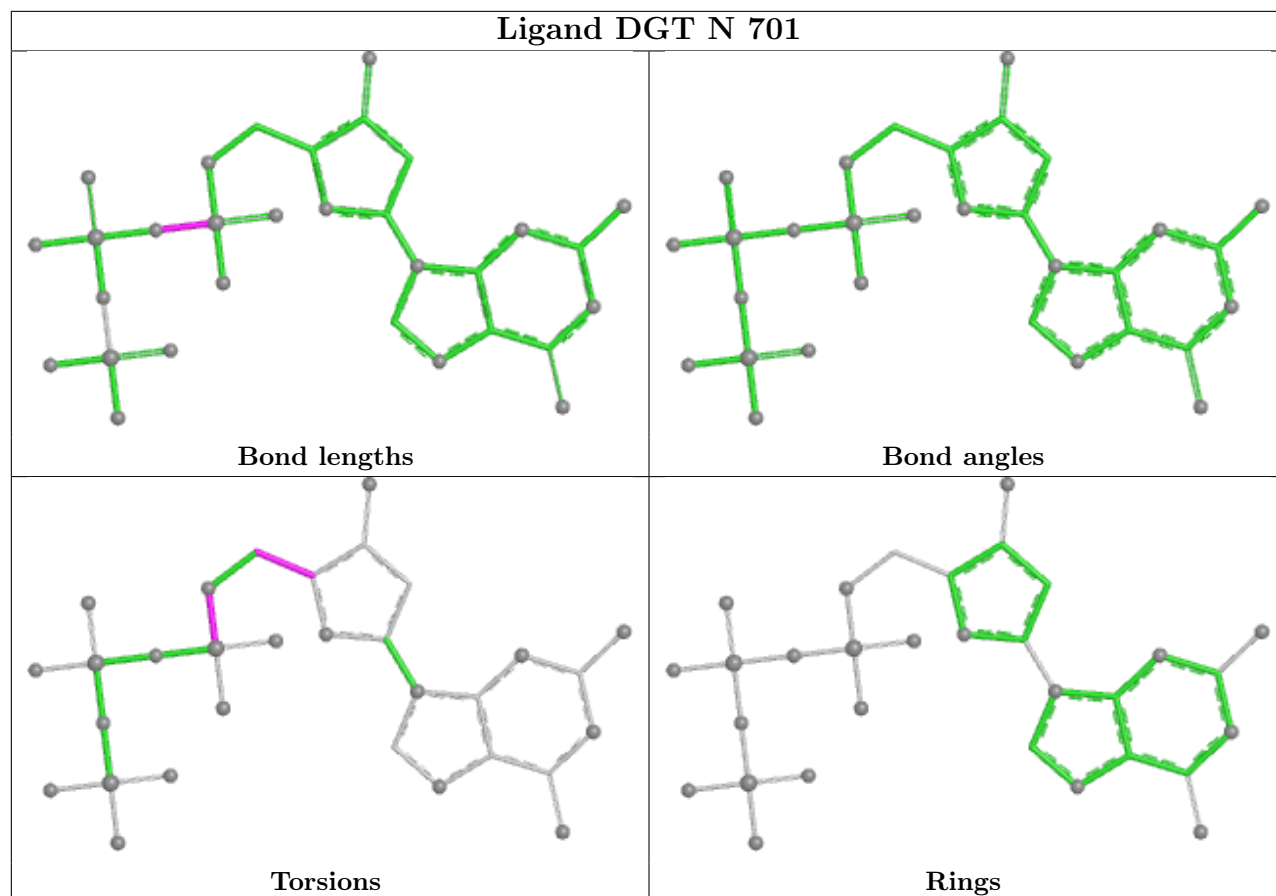


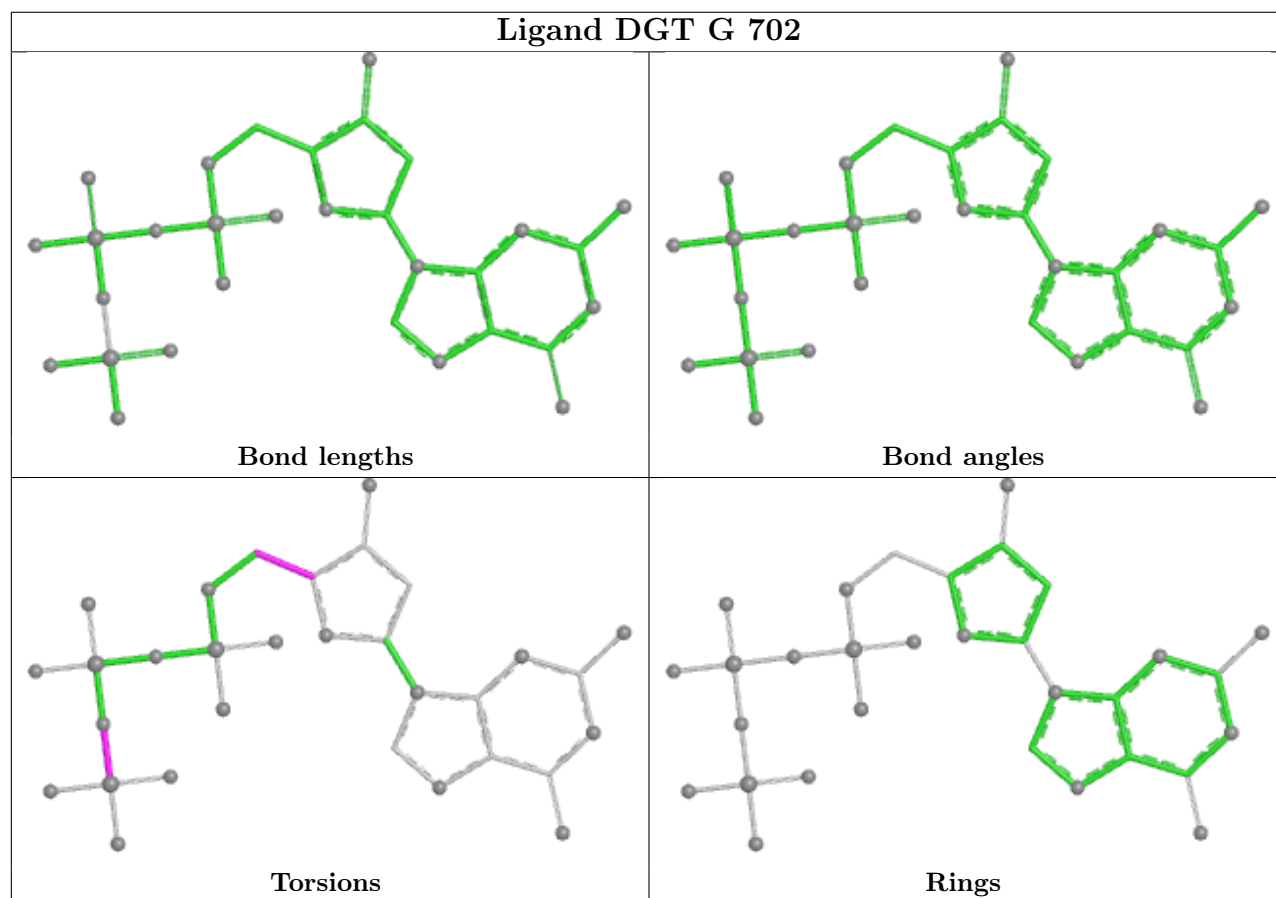
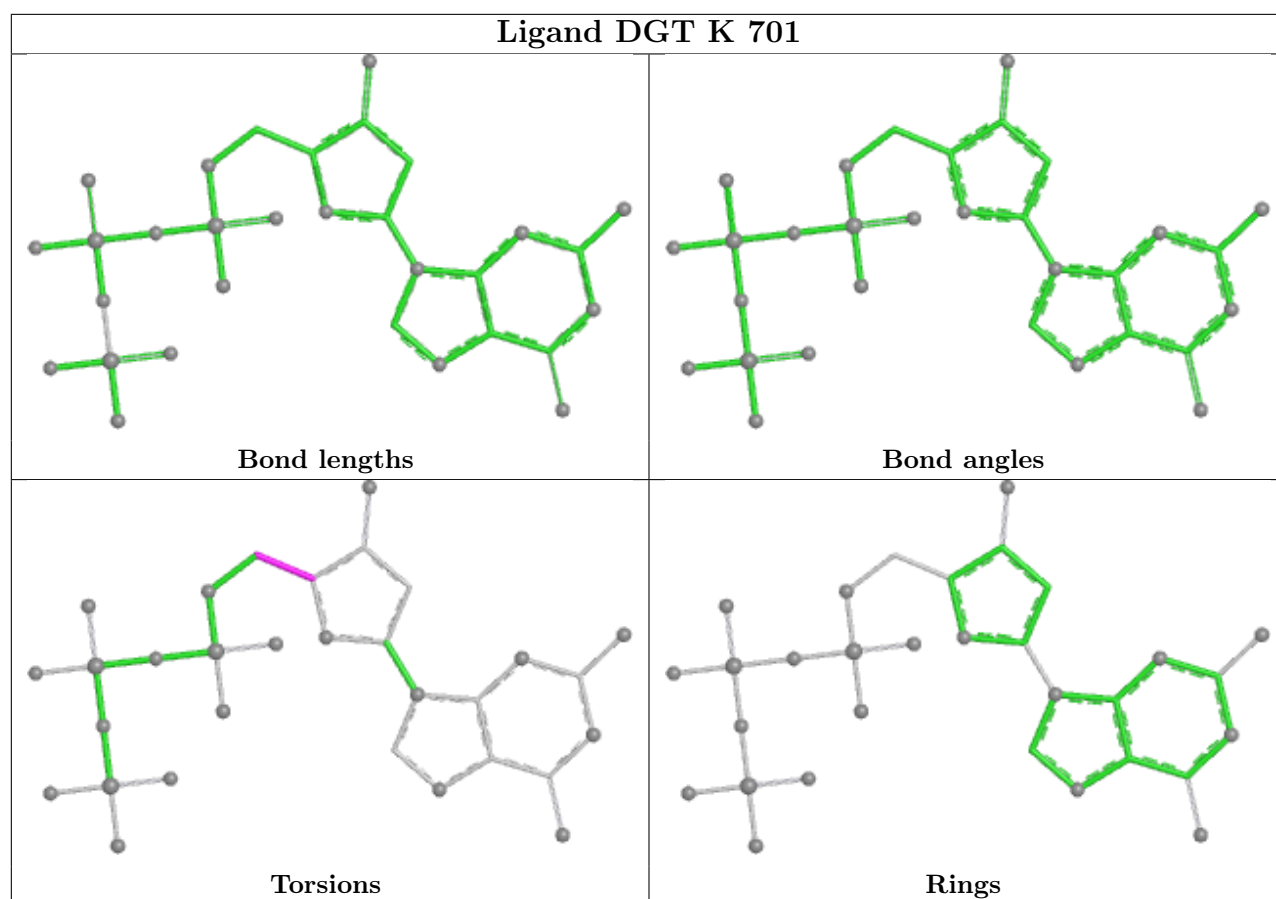
Ligand DGT J 703



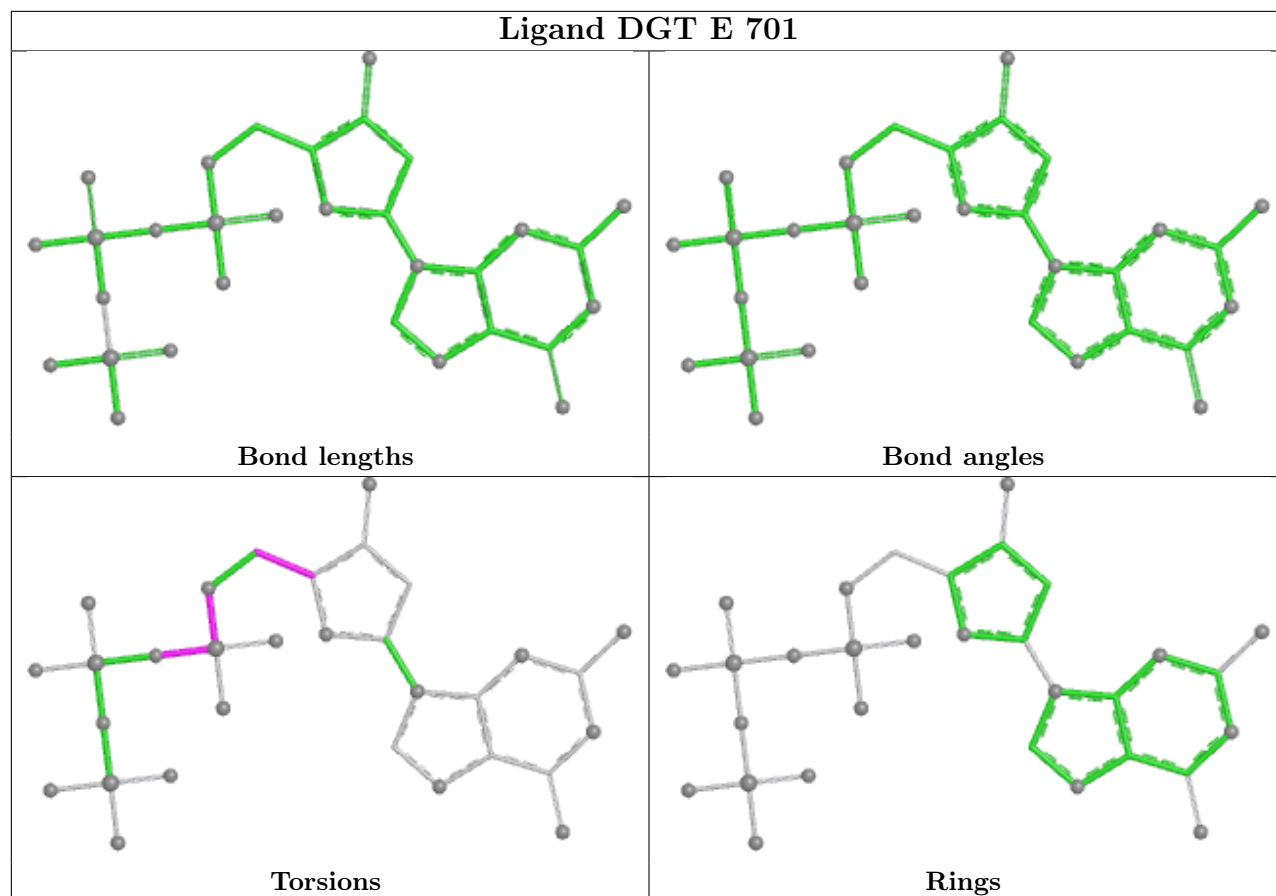
Ligand DGT L 701



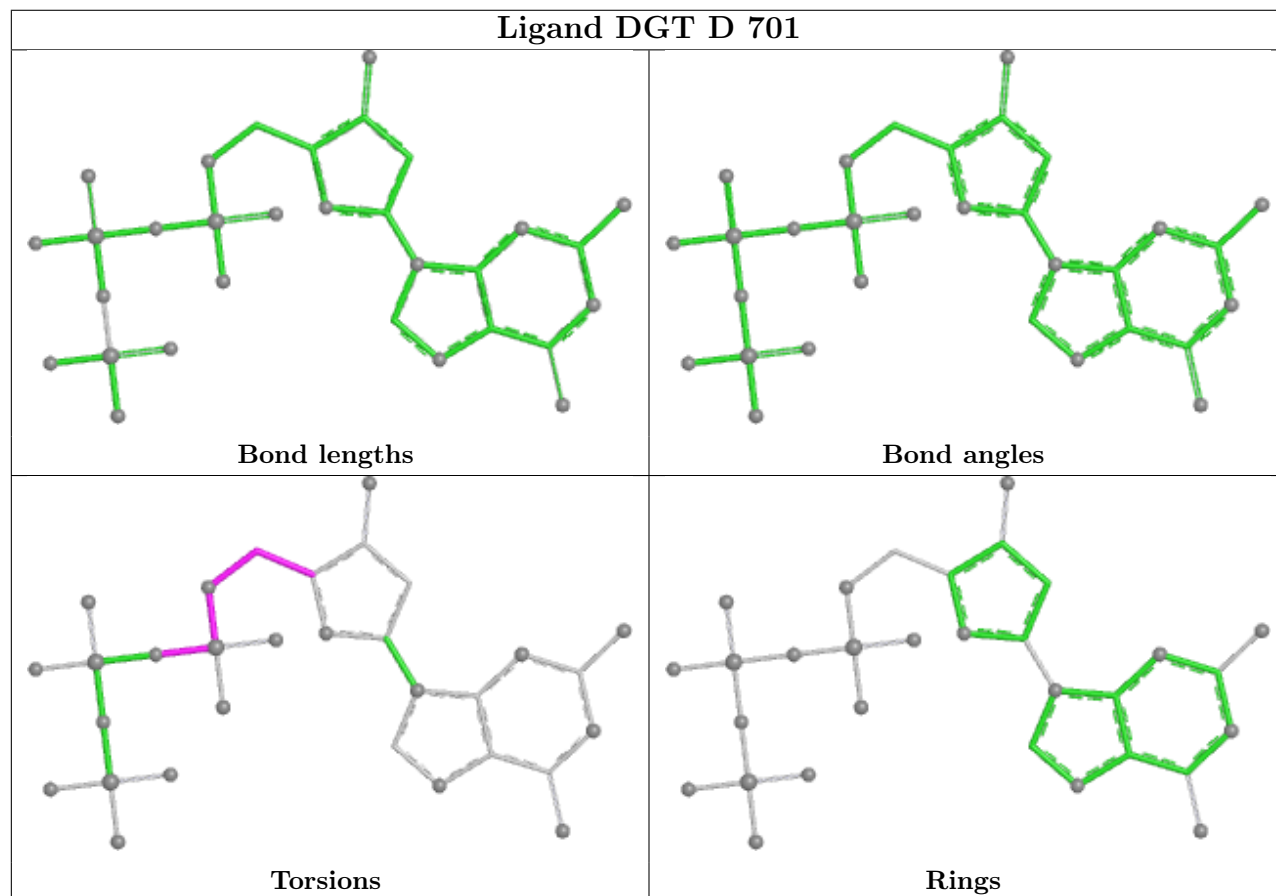


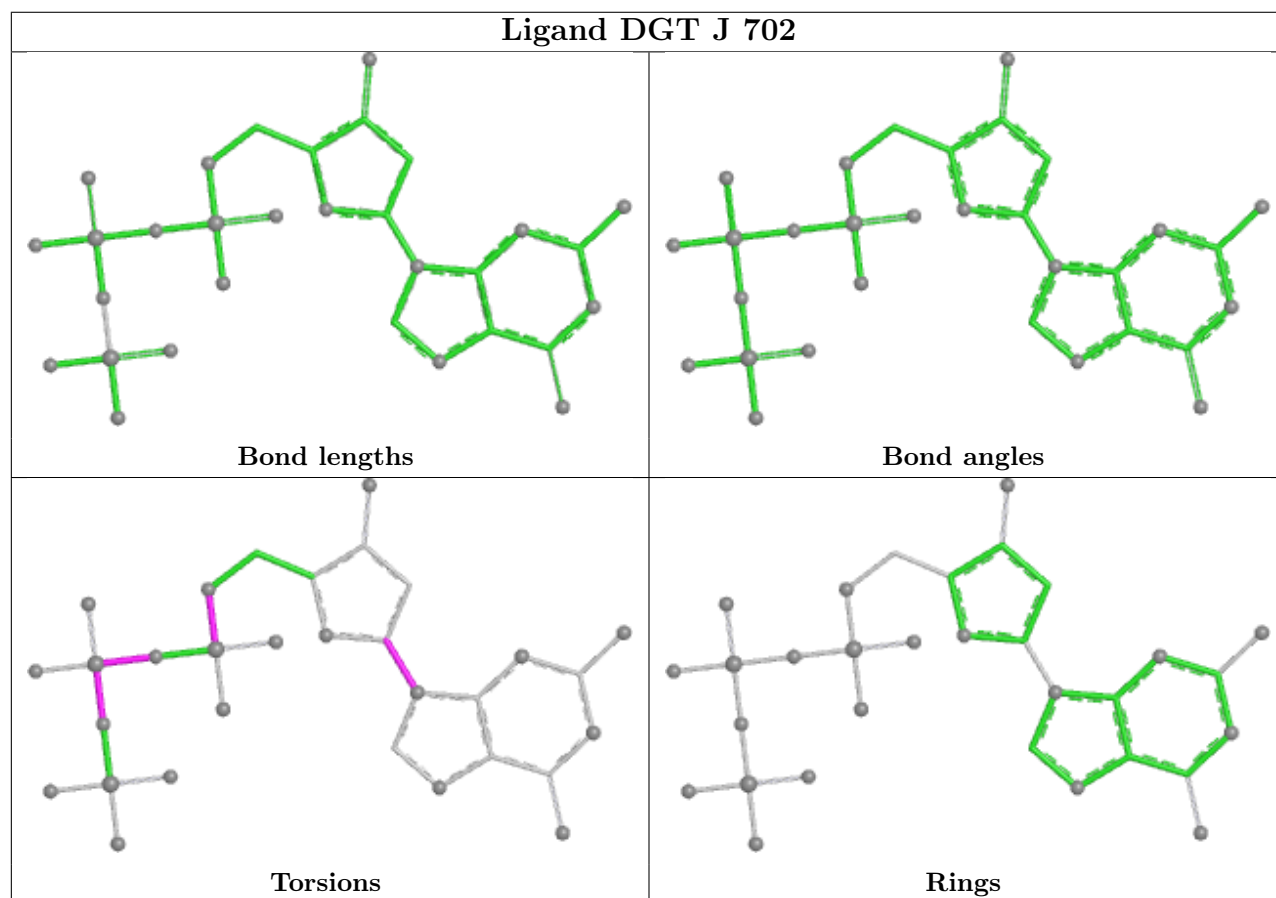
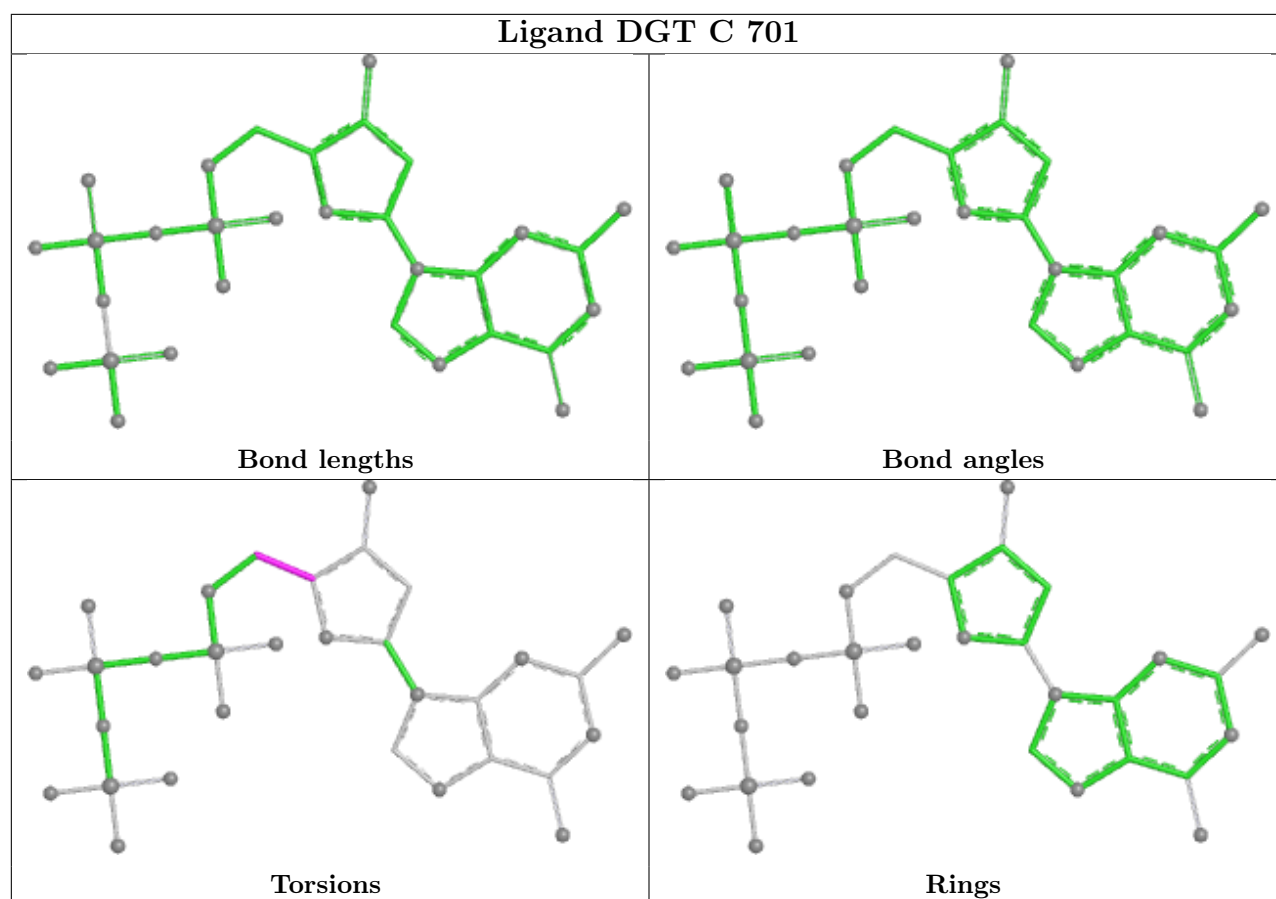


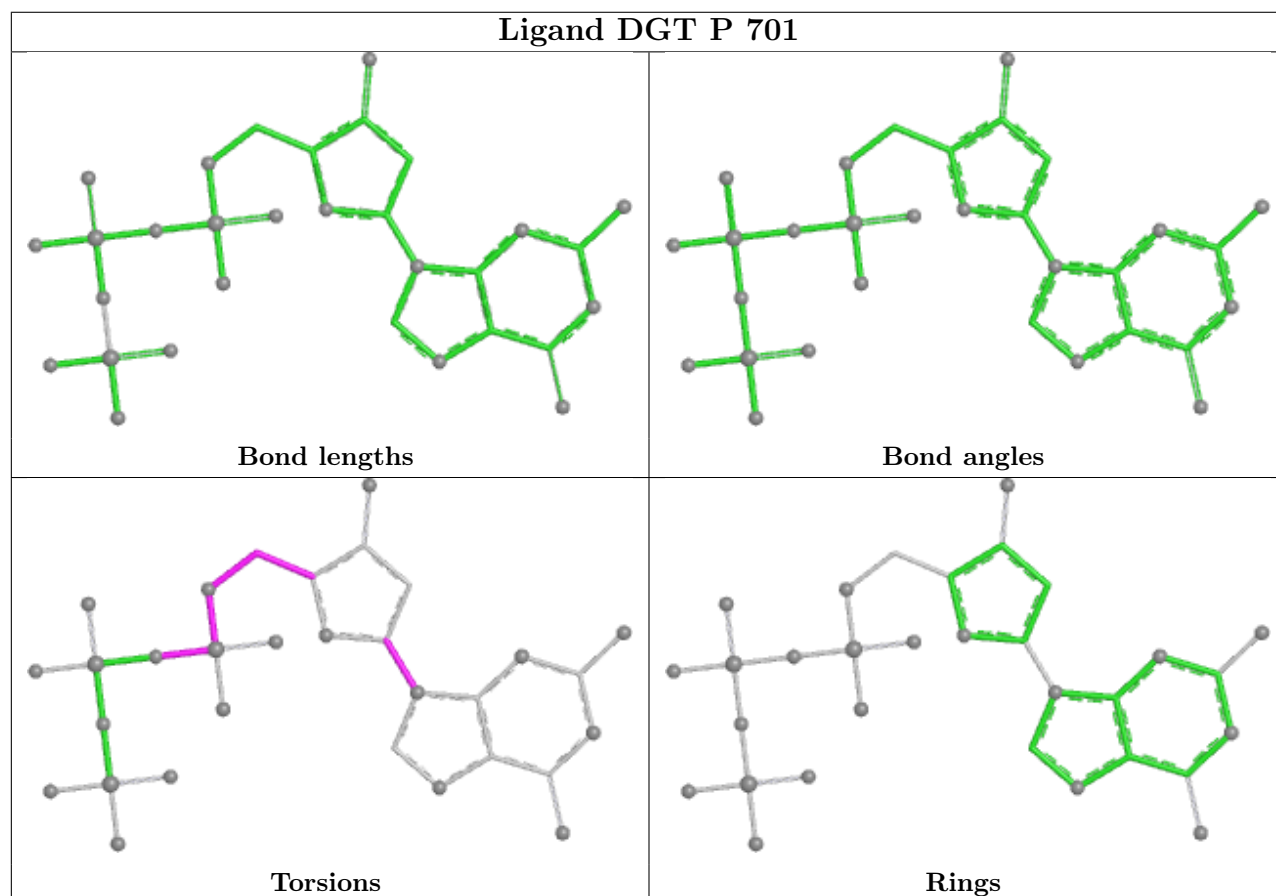
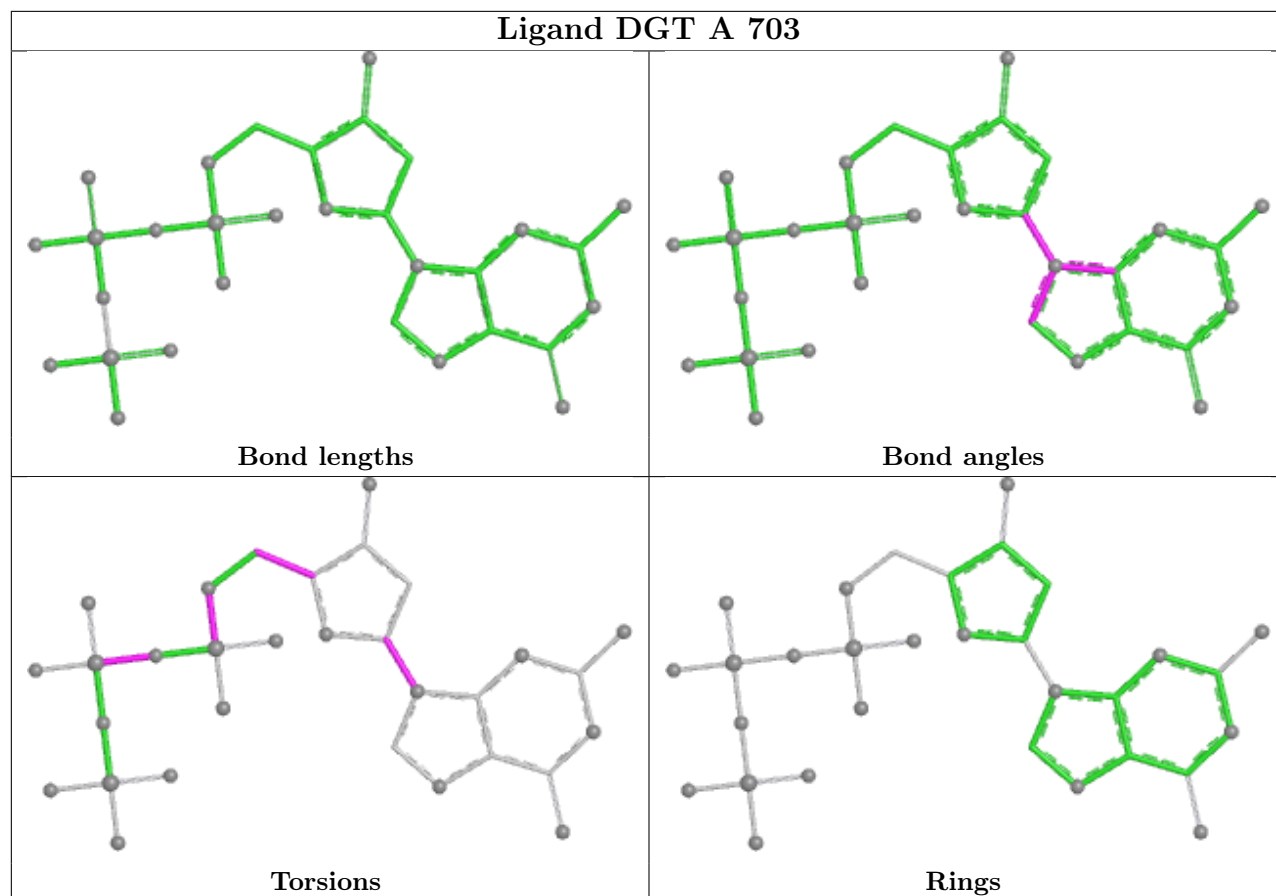
Ligand DGT E 701



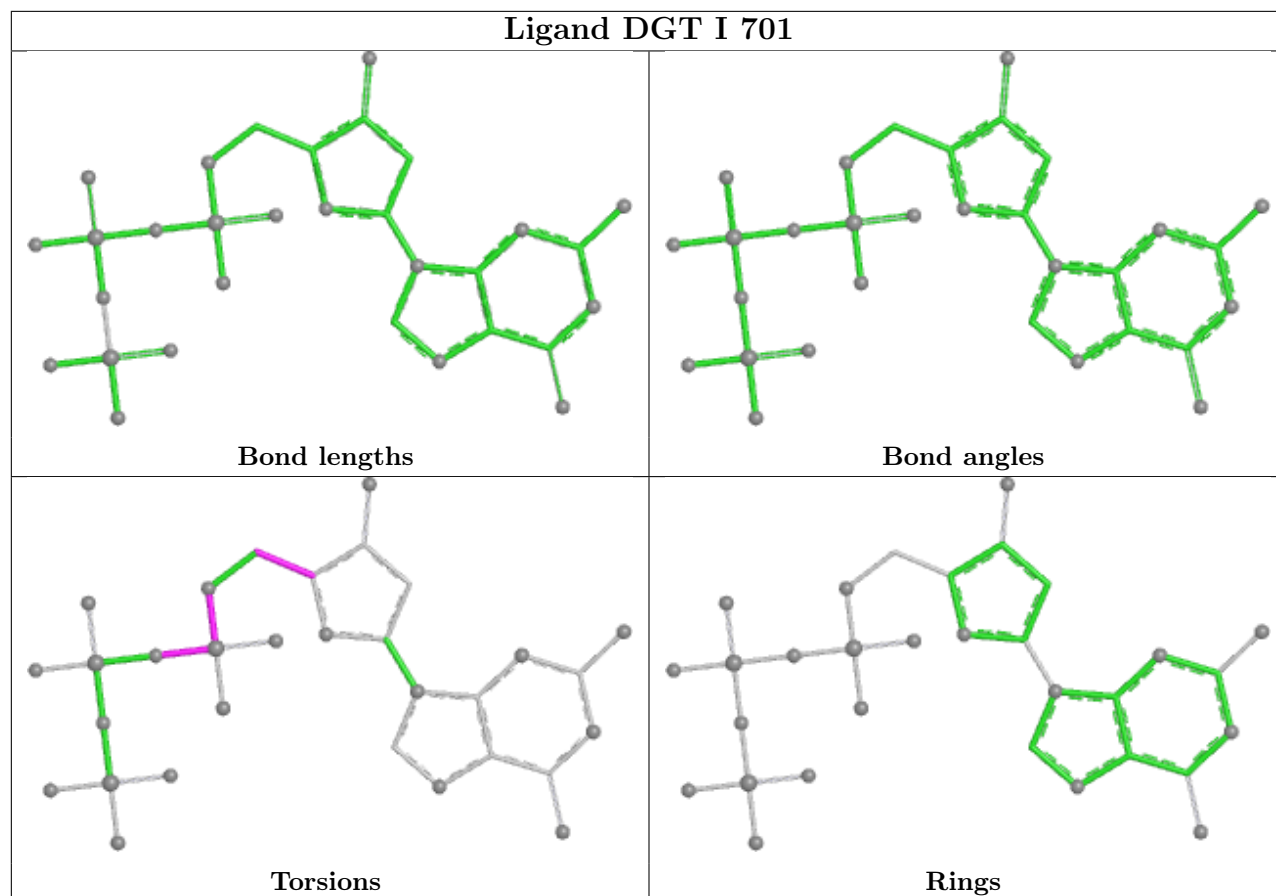
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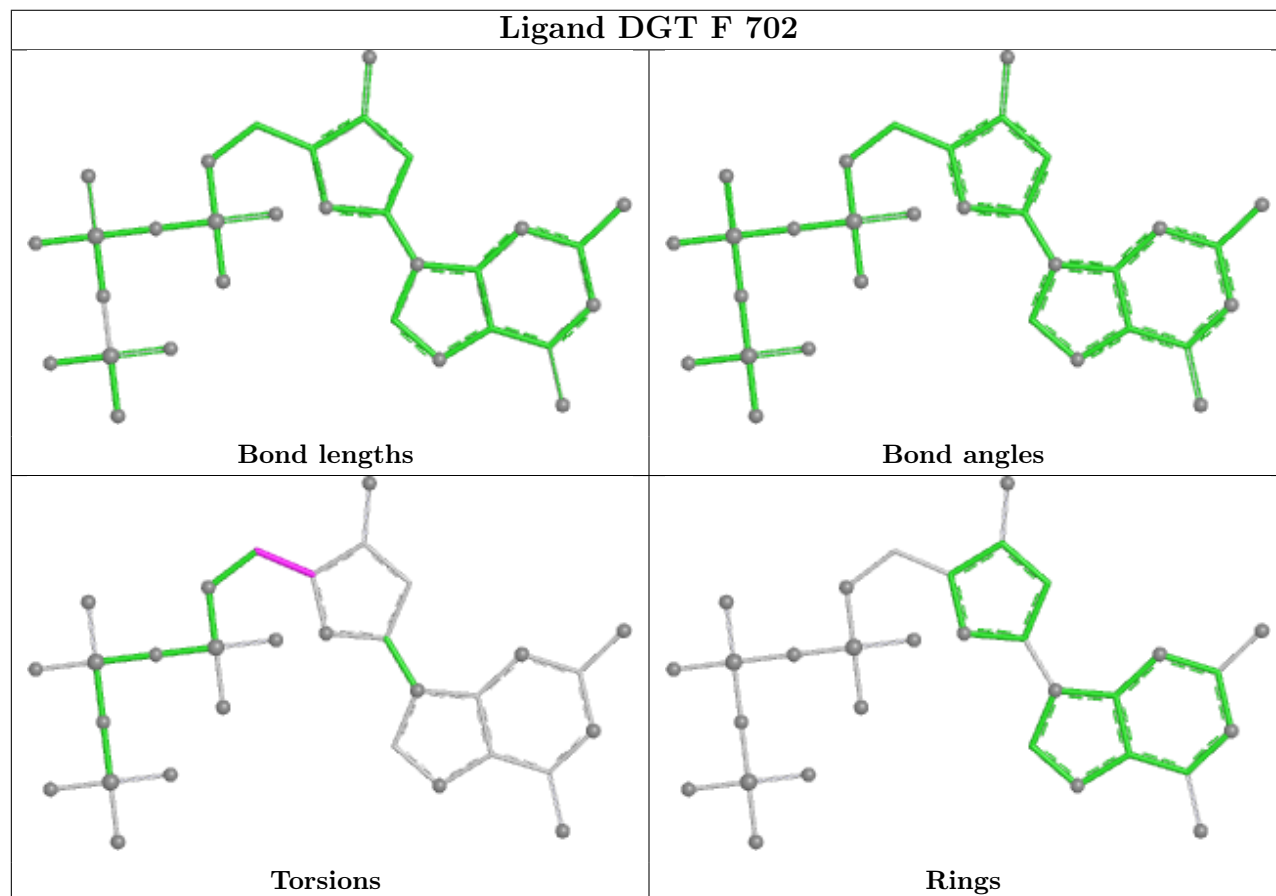


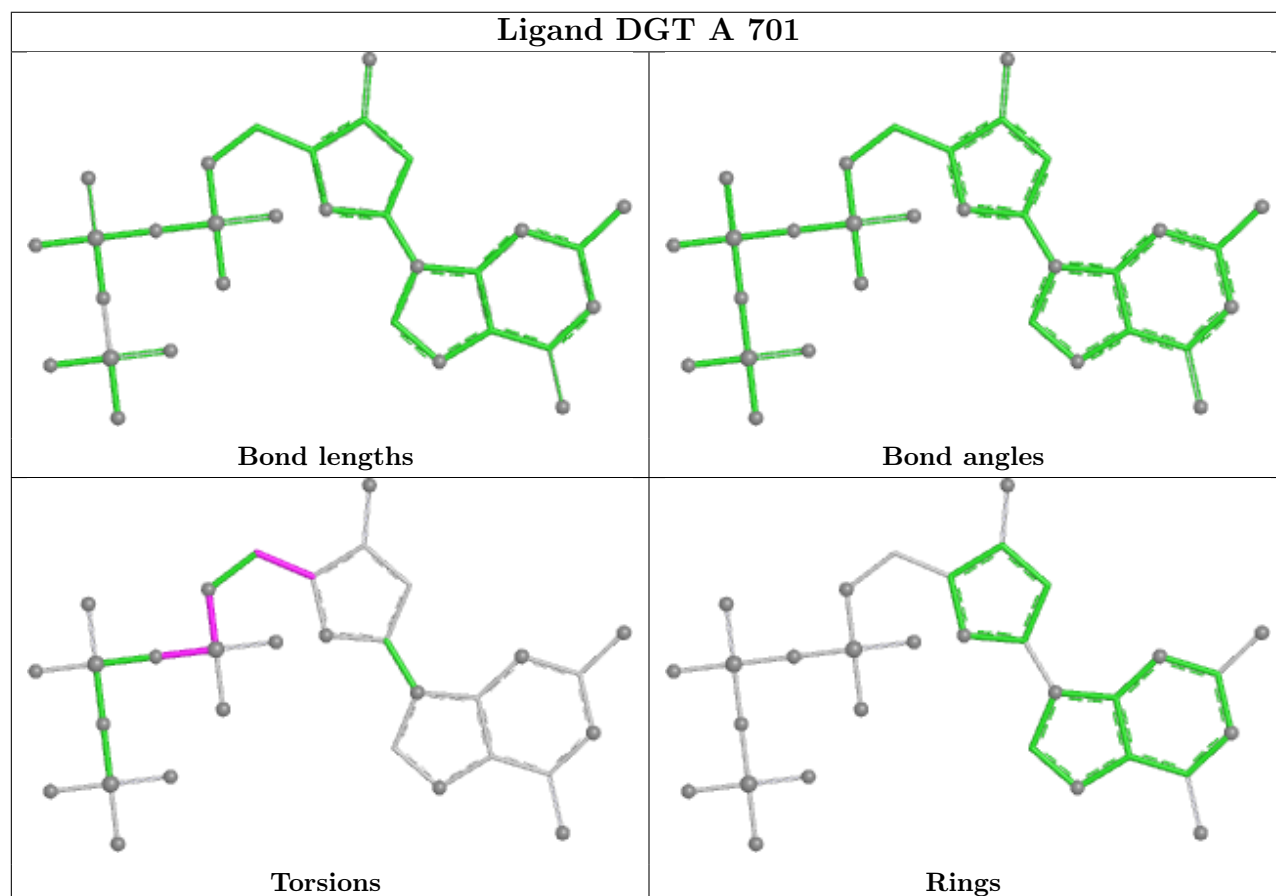
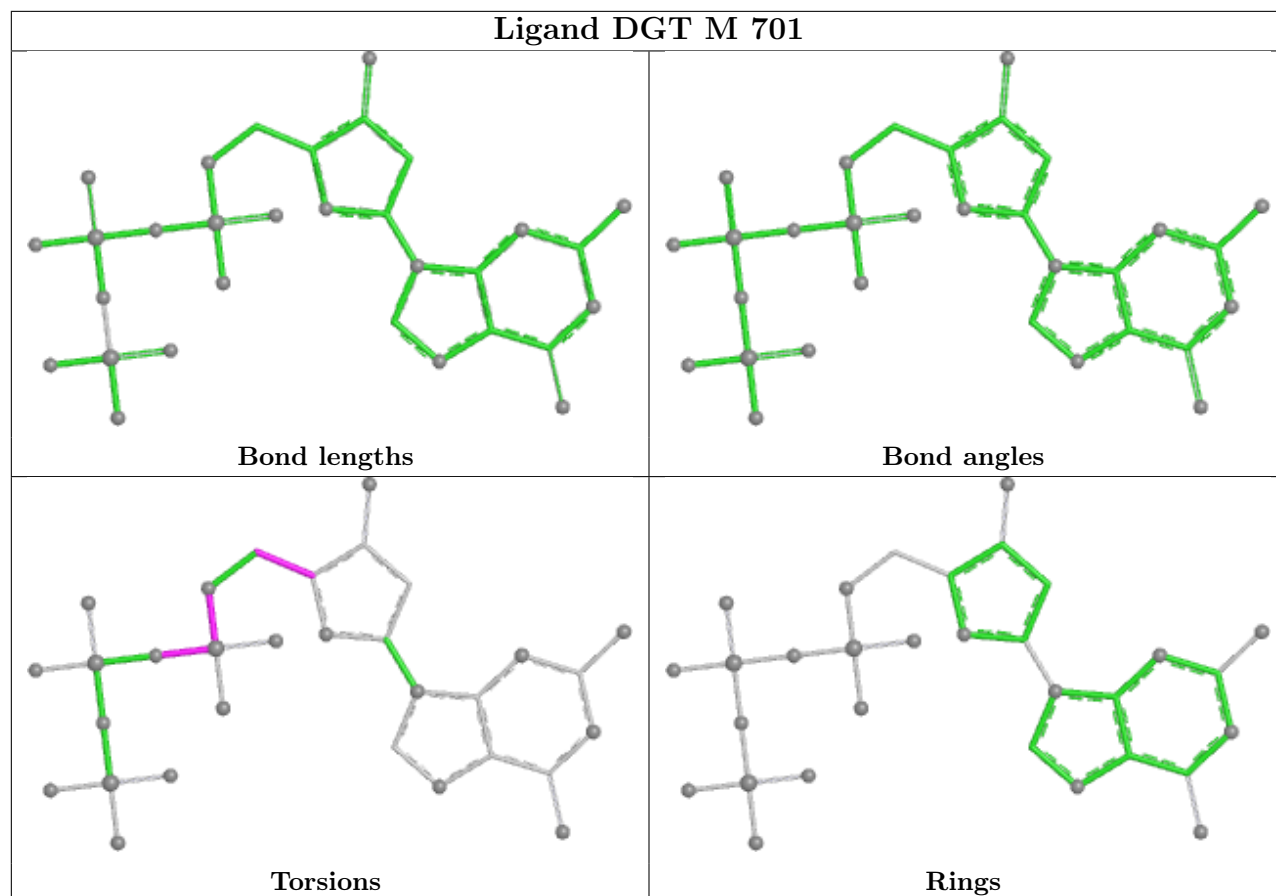


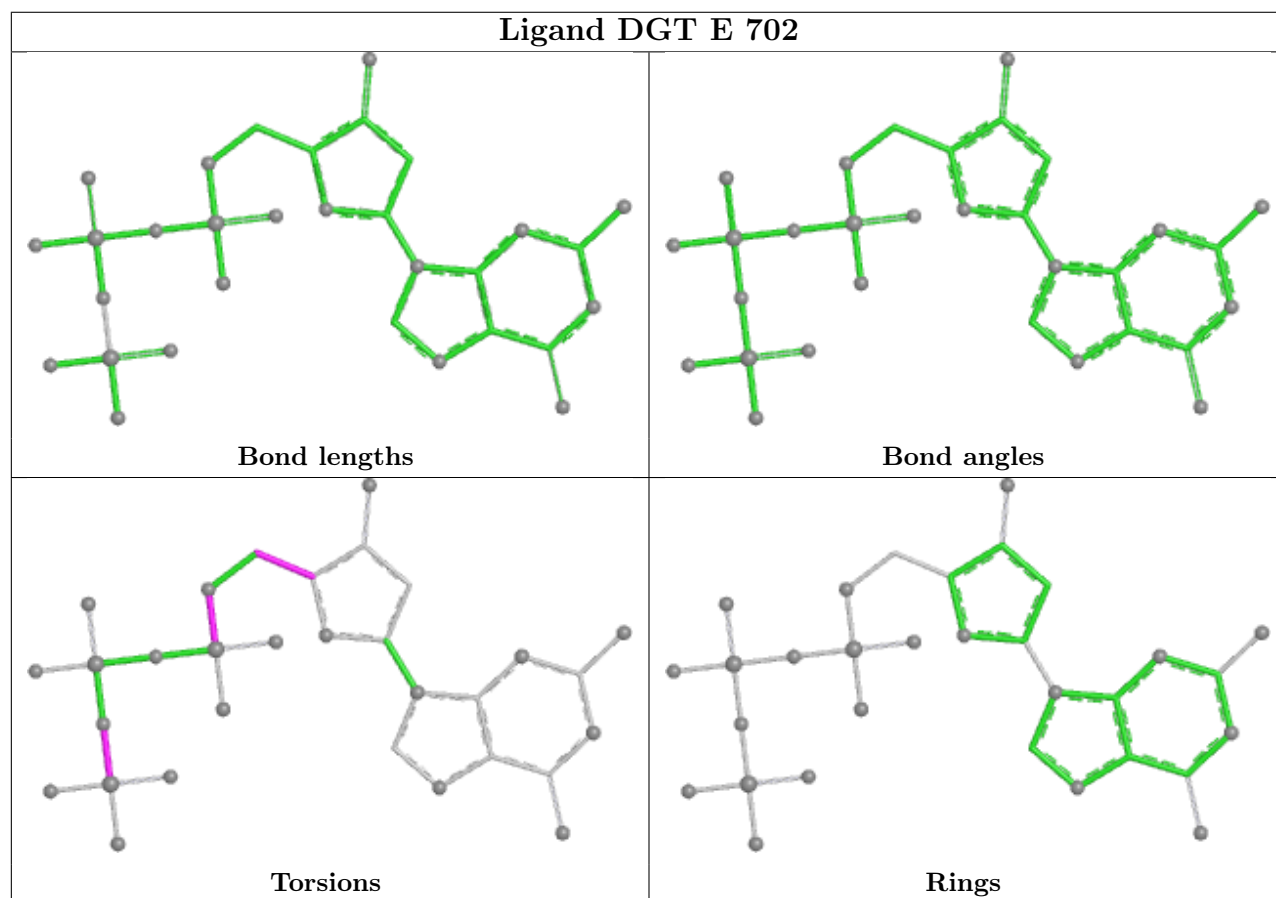
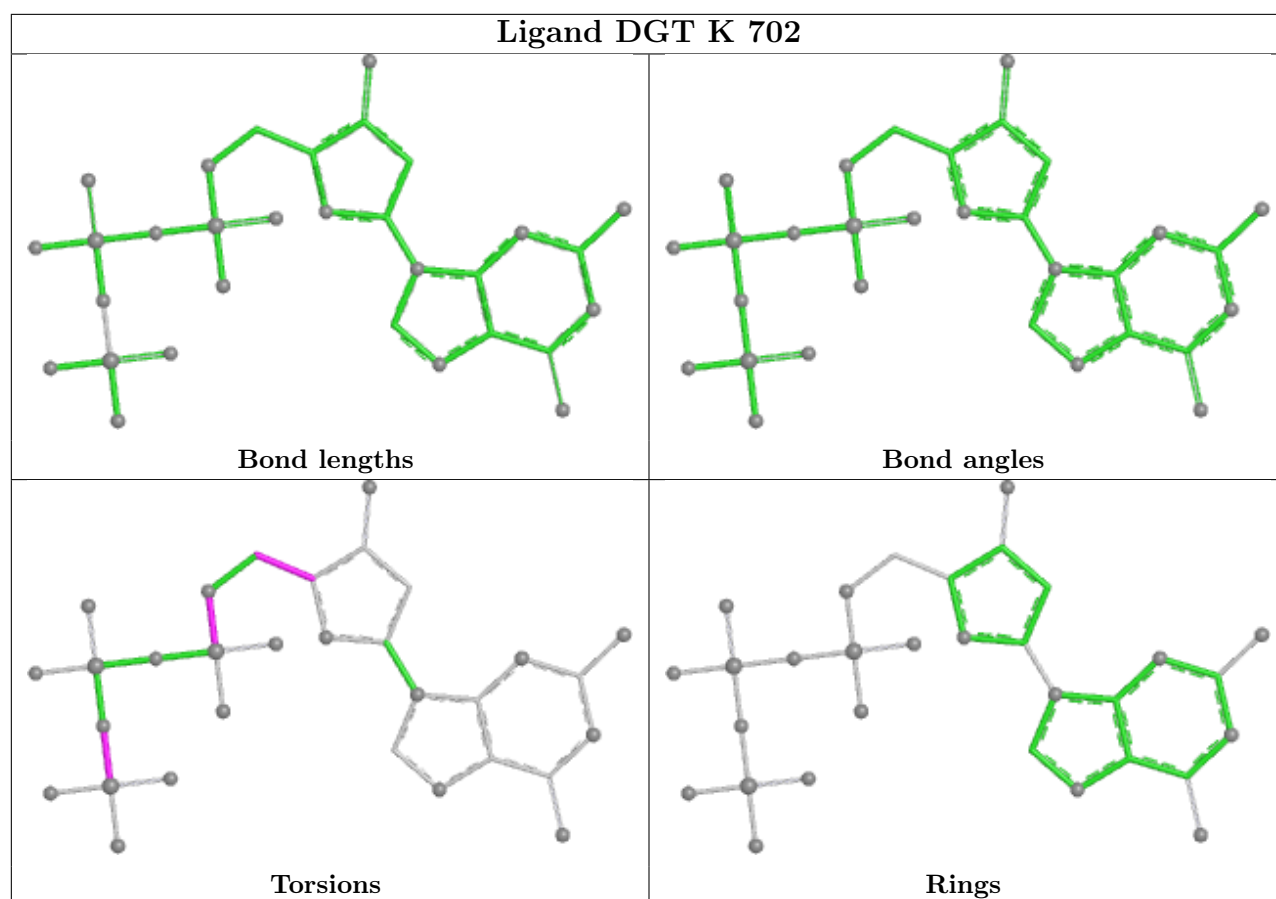
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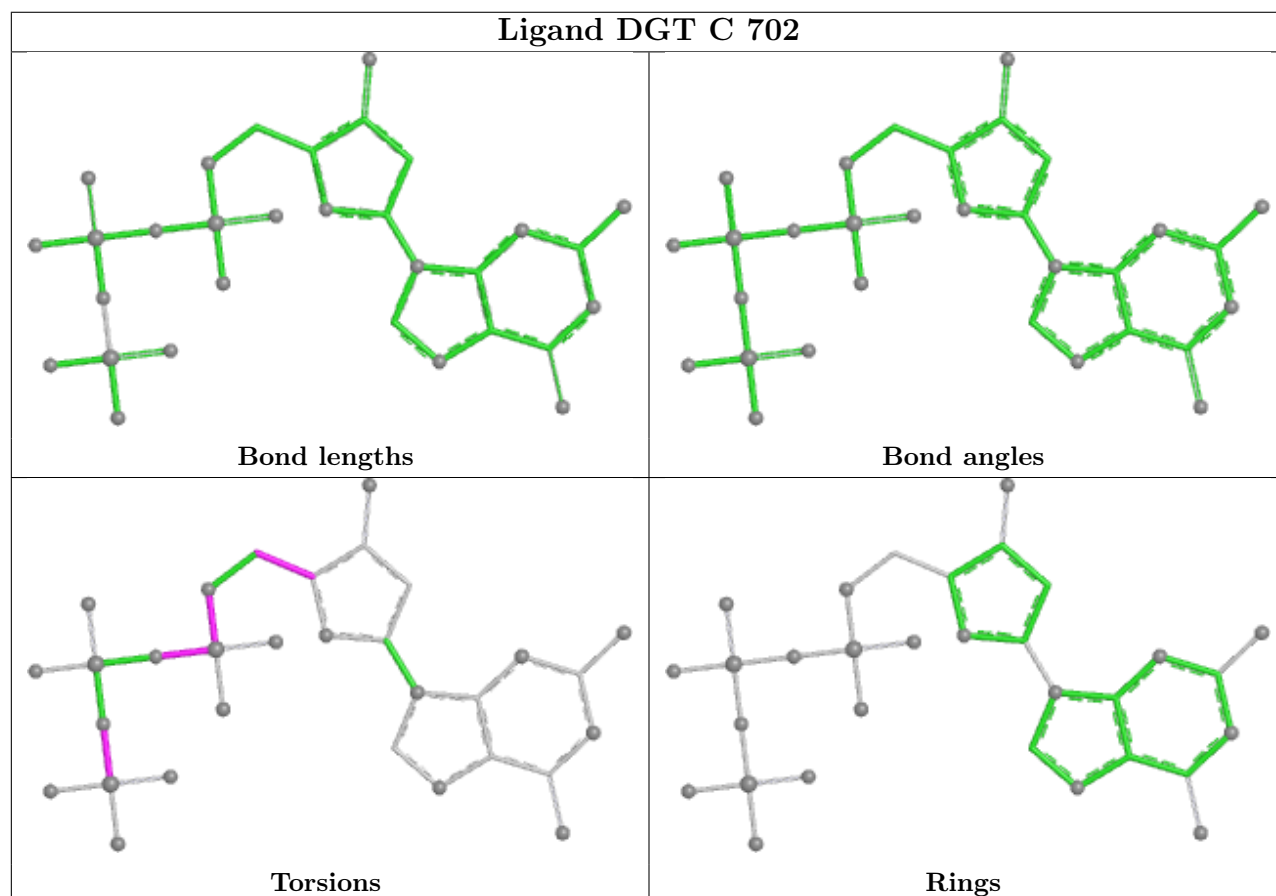
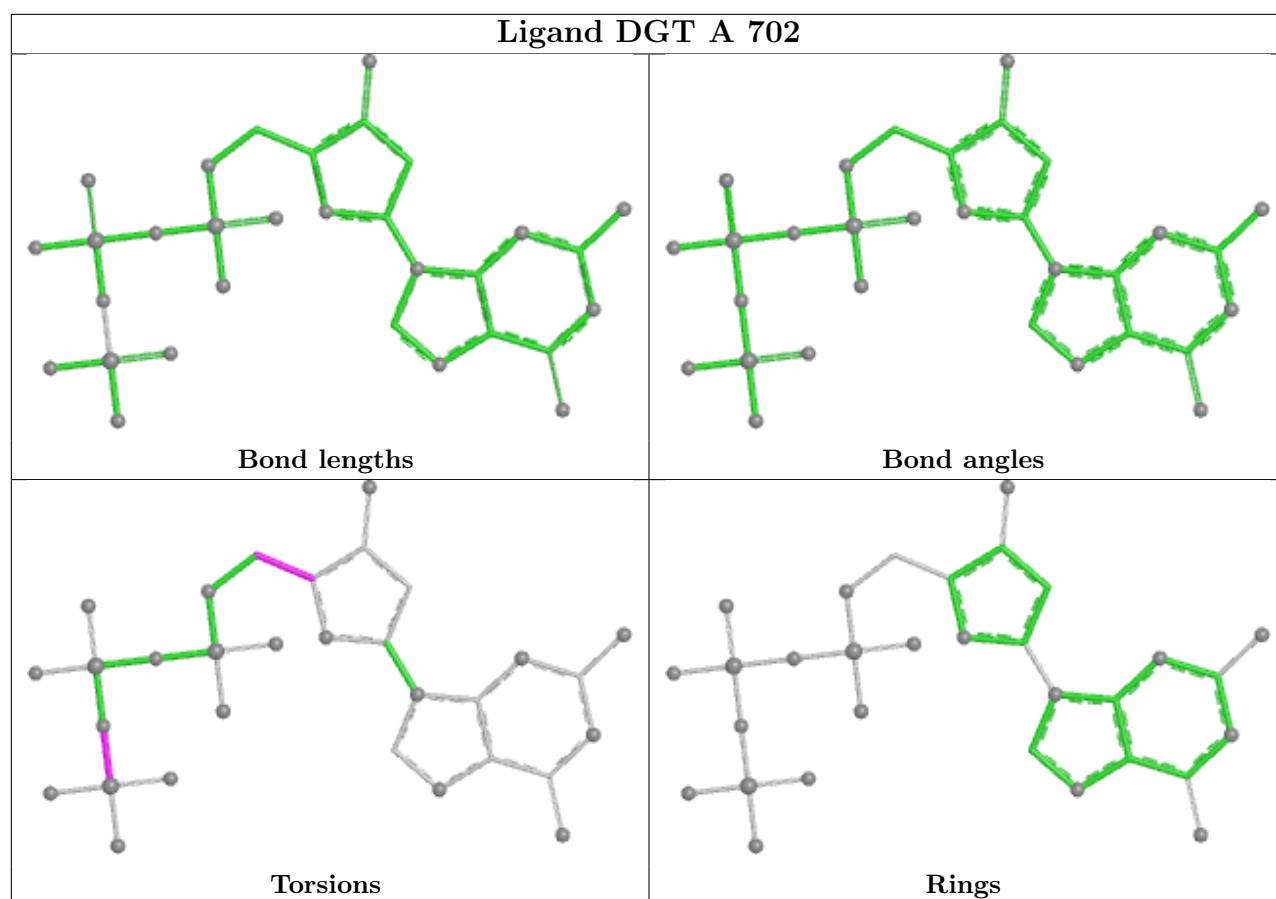


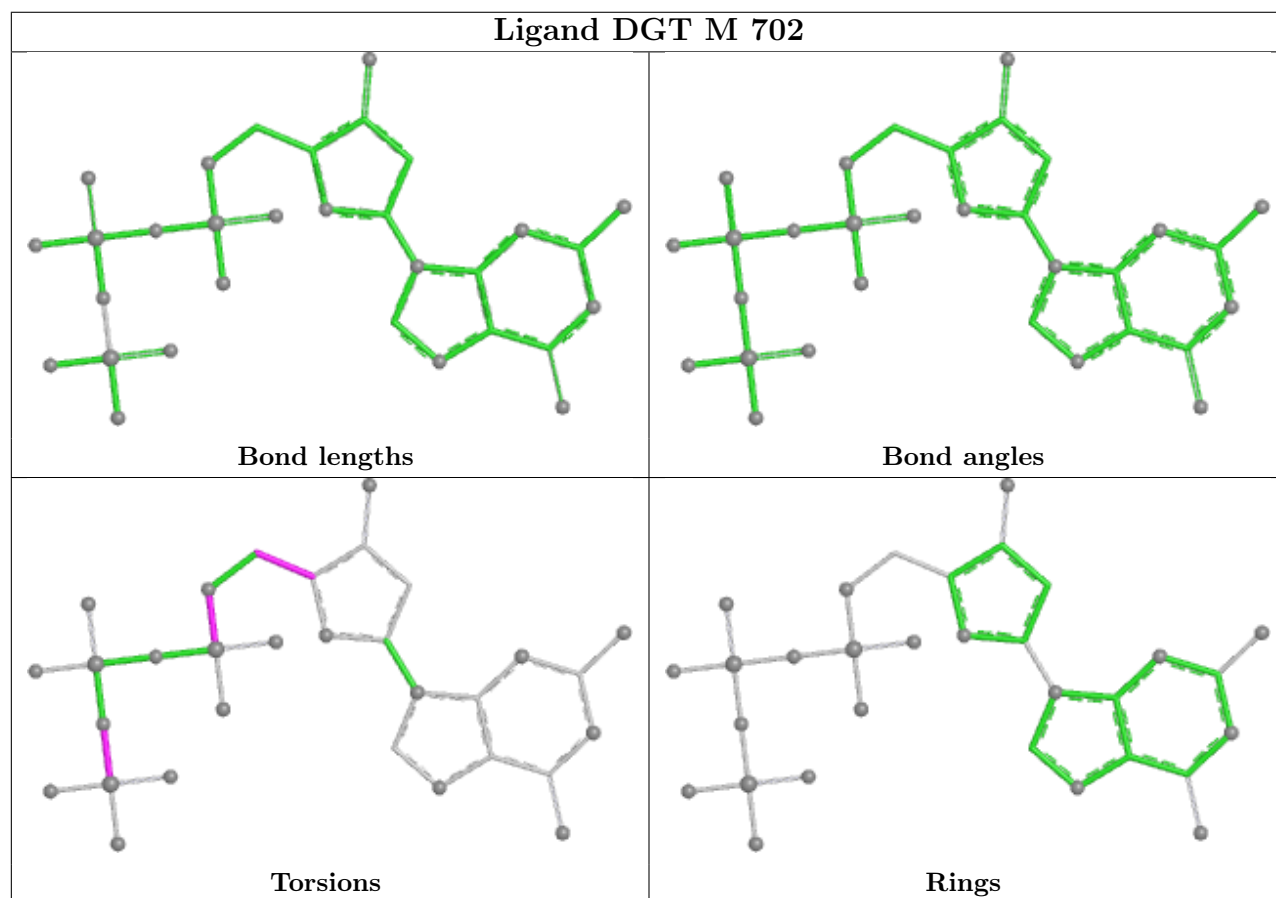
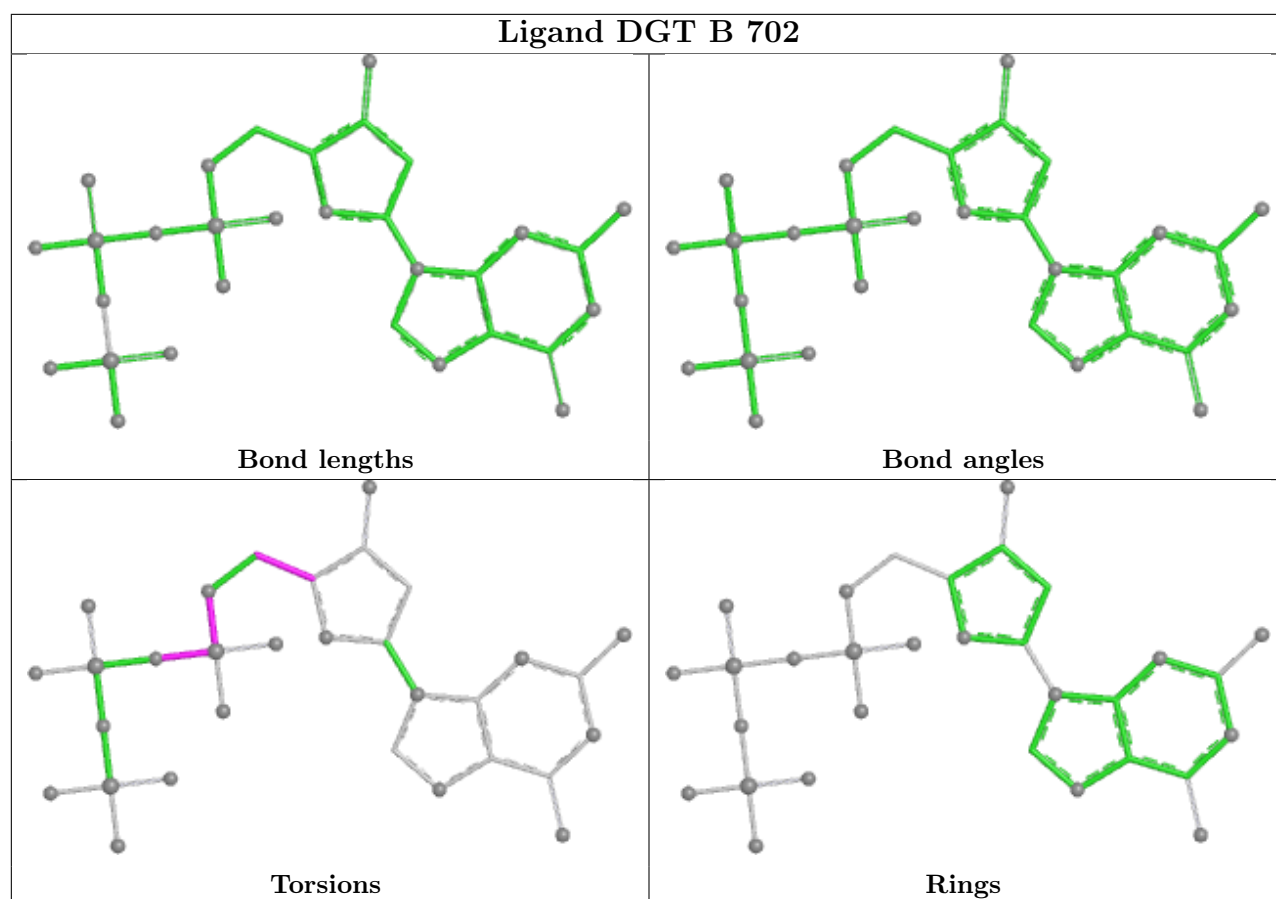
Ligand DGT F 702

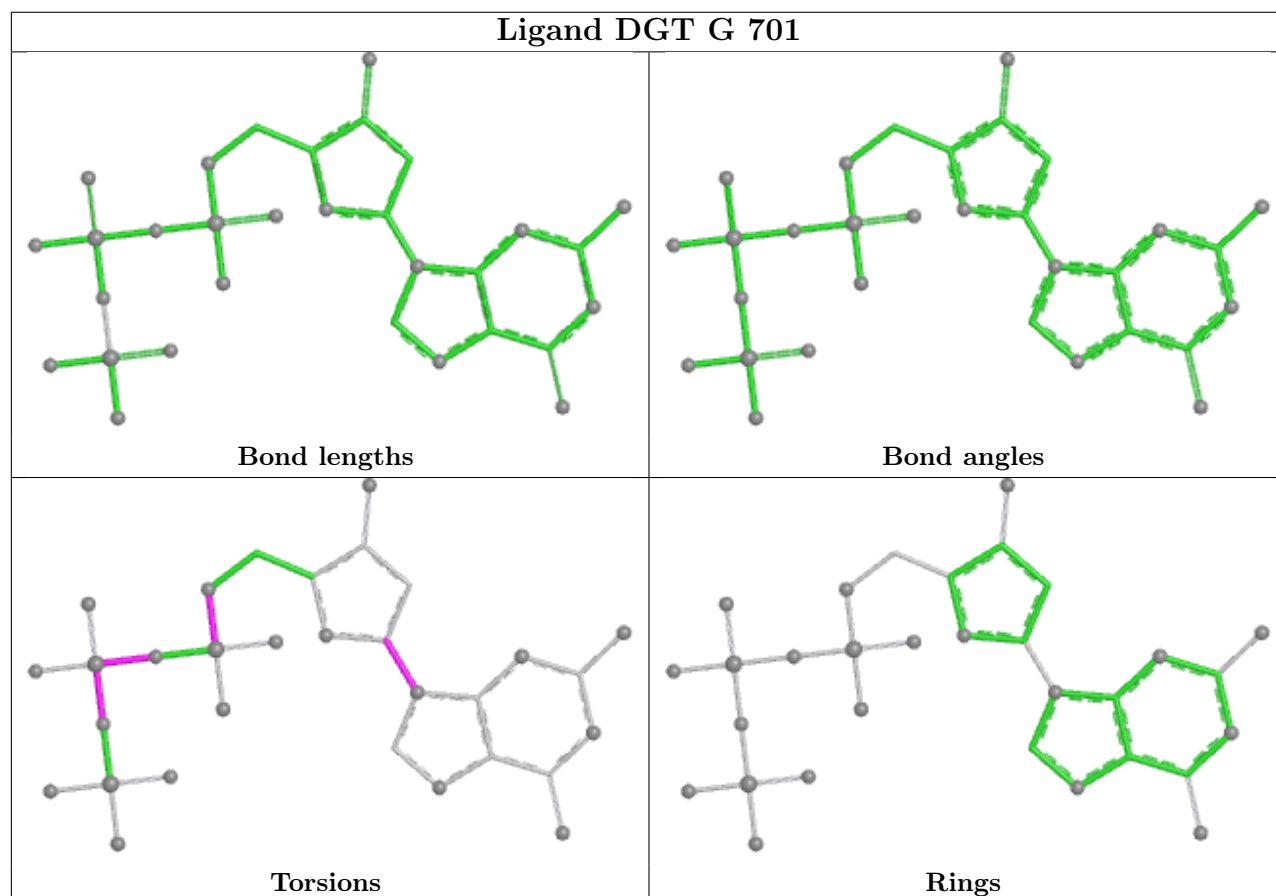
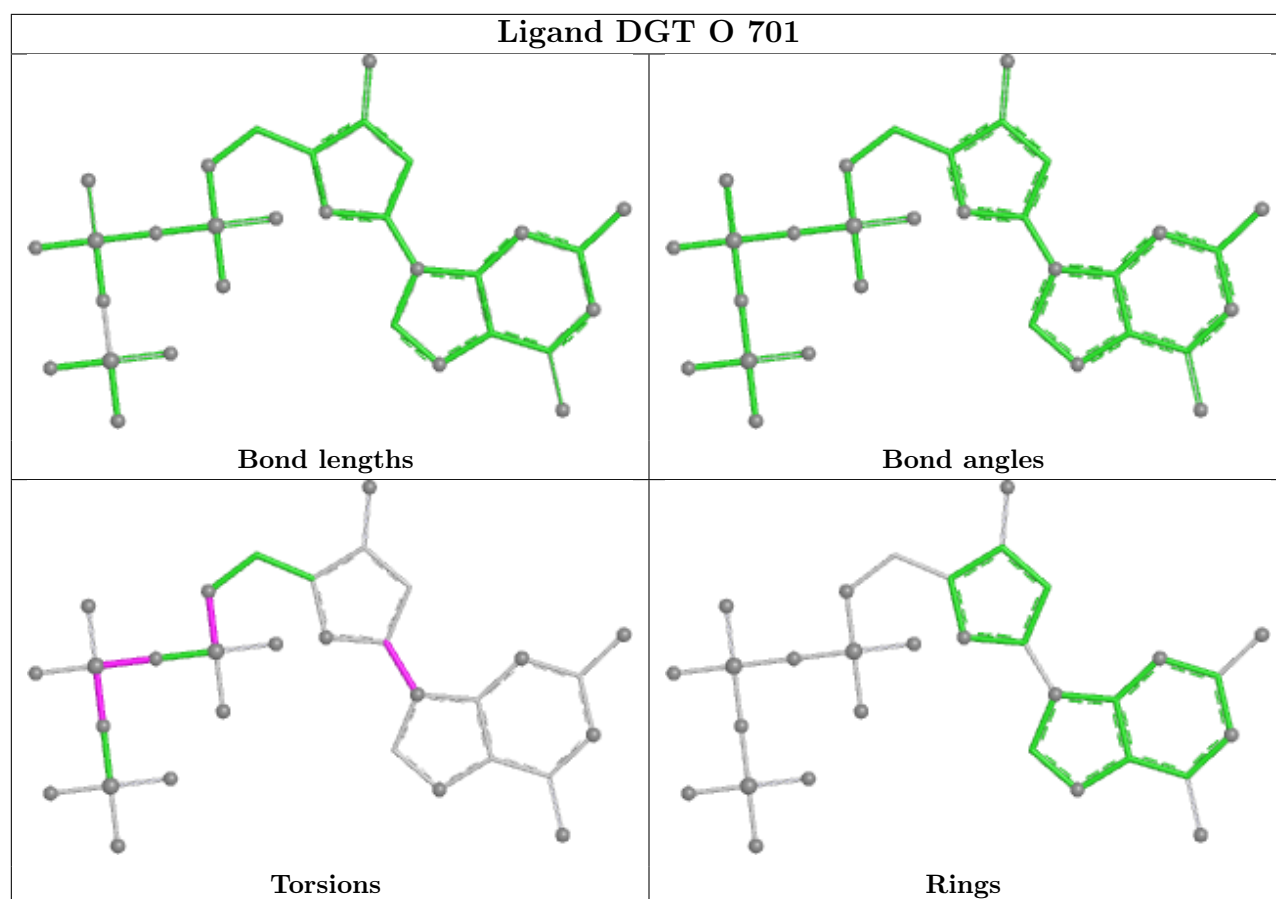




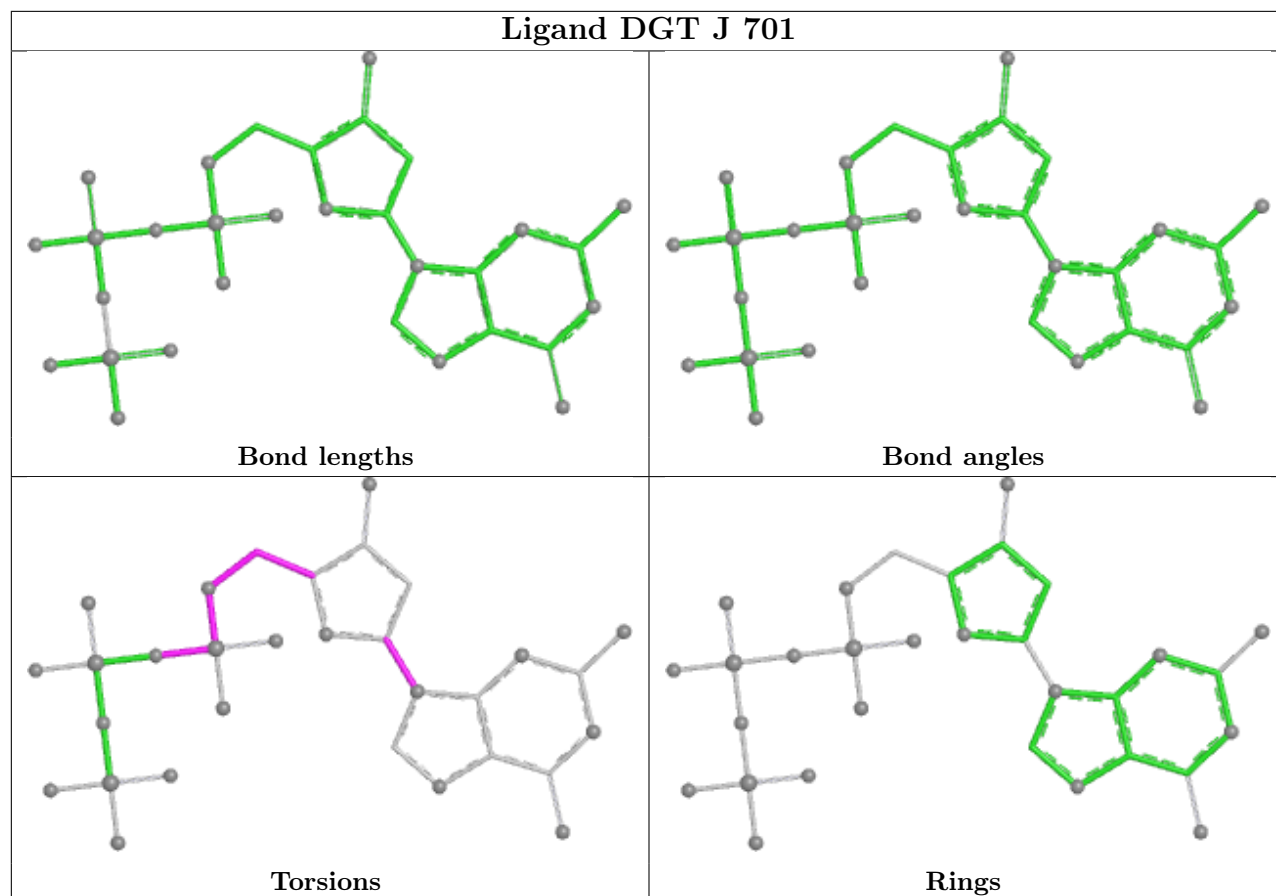




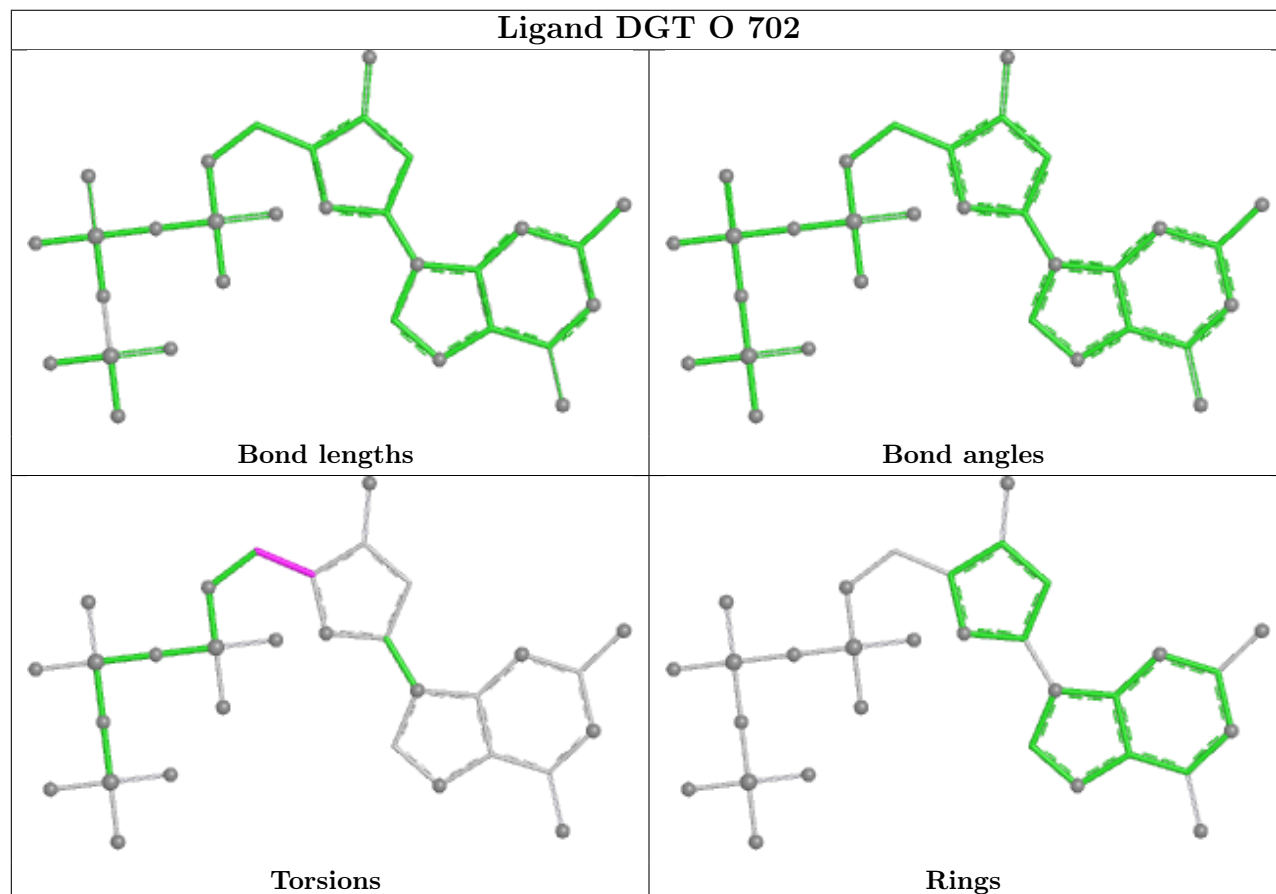




Ligand DGT J 701



Ligand DGT O 702



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	481/535 (89%)	0.10	15 (3%)	51	28	111, 176, 242, 304	0
1	B	481/535 (89%)	0.17	24 (4%)	34	19	101, 176, 237, 298	0
1	C	481/535 (89%)	0.19	15 (3%)	51	28	102, 179, 235, 265	0
1	D	481/535 (89%)	0.09	12 (2%)	58	33	82, 176, 239, 287	1 (0%)
1	E	481/535 (89%)	0.10	13 (2%)	56	31	87, 164, 223, 258	0
1	F	481/535 (89%)	0.08	12 (2%)	58	33	103, 182, 247, 317	0
1	G	481/535 (89%)	0.16	17 (3%)	47	26	108, 181, 254, 313	0
1	H	481/535 (89%)	0.06	11 (2%)	61	34	61, 178, 243, 303	1 (0%)
1	I	481/535 (89%)	0.16	16 (3%)	49	27	102, 187, 245, 283	0
1	J	481/535 (89%)	0.10	10 (2%)	63	36	120, 189, 262, 339	0
1	K	481/535 (89%)	0.07	8 (1%)	69	40	119, 193, 269, 307	0
1	L	481/535 (89%)	0.01	7 (1%)	72	44	75, 191, 275, 324	1 (0%)
1	M	481/535 (89%)	0.17	7 (1%)	72	44	128, 206, 278, 317	0
1	N	481/535 (89%)	0.01	8 (1%)	69	40	100, 185, 248, 270	0
1	O	481/535 (89%)	0.05	11 (2%)	61	34	116, 189, 270, 318	0
1	P	481/535 (89%)	0.10	15 (3%)	51	28	108, 193, 257, 341	1 (0%)
All	All	7696/8560 (89%)	0.10	201 (2%)	57	32	61, 184, 256, 341	4 (0%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	313	TRP	6.8
1	C	313	TRP	6.4
1	C	135	ILE	5.8
1	J	428	LEU	5.1
1	A	306	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	O	127	GLU	4.8
1	I	152	GLY	4.8
1	J	174	LEU	4.6
1	O	158	PRO	4.5
1	P	500	VAL	4.4
1	I	373	ALA	4.3
1	A	121	PRO	4.3
1	E	507	TYR	4.1
1	I	153	GLY	4.1
1	B	169	LEU	4.1
1	N	135	ILE	4.0
1	G	205	CYS	4.0
1	F	457	VAL	4.0
1	G	537	VAL	3.9
1	B	441	ALA	3.9
1	H	329	PHE	3.9
1	I	193	GLU	3.8
1	O	265	ILE	3.7
1	J	175	ALA	3.7
1	F	585	ASP	3.7
1	H	205	CYS	3.6
1	B	468	ILE	3.6
1	I	308	ILE	3.6
1	P	570	VAL	3.4
1	P	178	LEU	3.4
1	D	211	GLY	3.4
1	E	129	HIS	3.4
1	I	205	CYS	3.4
1	B	490	ASP	3.4
1	O	314	ASP	3.3
1	A	308	ILE	3.3
1	H	254	MET	3.3
1	I	204	LEU	3.3
1	K	598	TRP	3.3
1	L	191	ILE	3.2
1	G	117	VAL	3.2
1	B	122	ILE	3.2
1	G	573	CYS	3.2
1	G	146	TYR	3.1
1	A	524	THR	3.1
1	F	577	ASN	3.1
1	P	202	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	565	ALA	3.0
1	K	373	ALA	3.0
1	P	323	LEU	3.0
1	C	468	ILE	3.0
1	E	313	TRP	3.0
1	D	175	ALA	3.0
1	G	373	ALA	2.9
1	B	539	GLN	2.9
1	G	383	ASP	2.9
1	B	445	LEU	2.9
1	L	128	LEU	2.9
1	F	436	PRO	2.9
1	E	483	ALA	2.9
1	L	273	VAL	2.9
1	J	198	CYS	2.9
1	B	415	ASP	2.9
1	O	396	TYR	2.8
1	G	382	ILE	2.8
1	D	386	ILE	2.8
1	B	412	ALA	2.8
1	J	144	LEU	2.8
1	F	202	ALA	2.8
1	H	489	LEU	2.7
1	D	179	VAL	2.7
1	J	248	ASN	2.7
1	B	338	ALA	2.7
1	B	308	ILE	2.7
1	O	268	ILE	2.7
1	C	139	PRO	2.7
1	G	329	PHE	2.7
1	A	297	LEU	2.7
1	C	136	ILE	2.6
1	L	317	ALA	2.6
1	F	155	TYR	2.6
1	K	360	TYR	2.6
1	M	384	THR	2.6
1	A	172	GLY	2.6
1	B	424	ASP	2.6
1	E	120	ASP	2.6
1	F	507	TYR	2.6
1	B	126	ILE	2.6
1	B	137	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	327	ASN	2.6
1	G	268	ILE	2.6
1	G	198	CYS	2.6
1	M	382	ILE	2.6
1	A	422	LEU	2.6
1	D	338	ALA	2.6
1	L	316	PHE	2.6
1	A	409	ILE	2.5
1	N	118	ILE	2.5
1	N	120	ASP	2.5
1	E	468	ILE	2.5
1	C	273	VAL	2.5
1	H	327	ASN	2.5
1	P	397	ILE	2.5
1	A	328	ASN	2.5
1	J	325	ILE	2.5
1	P	499	ILE	2.5
1	K	254	MET	2.5
1	B	383	ASP	2.5
1	D	212	PRO	2.5
1	C	162	HIS	2.5
1	F	238	VAL	2.5
1	G	570	VAL	2.5
1	N	181	ALA	2.5
1	N	205	CYS	2.5
1	C	141	PHE	2.4
1	O	317	ALA	2.4
1	M	476	LEU	2.4
1	H	124	GLY	2.4
1	M	497	ASP	2.4
1	A	338	ALA	2.4
1	O	159	GLY	2.4
1	I	257	TYR	2.4
1	N	178	LEU	2.4
1	L	151	GLY	2.4
1	A	202	ALA	2.4
1	E	514	PRO	2.4
1	B	236	GLY	2.4
1	A	157	PHE	2.4
1	E	409	ILE	2.4
1	P	491	VAL	2.4
1	J	160	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	334	PHE	2.3
1	E	157	PHE	2.3
1	I	403	GLY	2.3
1	D	273	VAL	2.3
1	H	421	LYS	2.3
1	A	461	GLN	2.3
1	E	542	PRO	2.3
1	H	526	PRO	2.3
1	C	422	LEU	2.3
1	I	256	GLN	2.3
1	C	314	ASP	2.3
1	F	532	ILE	2.3
1	K	573	CYS	2.3
1	B	470	ARG	2.2
1	F	308	ILE	2.2
1	K	351	ALA	2.2
1	H	310	VAL	2.2
1	N	189	LEU	2.2
1	M	300	ILE	2.2
1	G	578	PHE	2.2
1	O	162	HIS	2.2
1	D	142	GLN	2.2
1	G	301	VAL	2.2
1	E	177	CYS	2.2
1	L	440	ASP	2.2
1	G	594	GLN	2.2
1	P	238	VAL	2.2
1	D	135	ILE	2.2
1	I	334	PHE	2.2
1	H	558	ASP	2.2
1	P	435	ASP	2.2
1	B	427	PHE	2.2
1	N	155	TYR	2.1
1	O	480	VAL	2.1
1	P	199	VAL	2.1
1	B	241	PHE	2.1
1	I	182	LEU	2.1
1	K	410	SER	2.1
1	D	137	ASP	2.1
1	O	319	ASP	2.1
1	P	125	HIS	2.1
1	F	156	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	337	PHE	2.1
1	C	323	LEU	2.1
1	B	588	ALA	2.1
1	F	313	TRP	2.1
1	P	313	TRP	2.1
1	B	355	GLU	2.1
1	I	359	LEU	2.1
1	E	525	ALA	2.1
1	M	248	ASN	2.1
1	G	241	PHE	2.1
1	A	423	THR	2.1
1	D	417	GLU	2.1
1	G	592	THR	2.1
1	J	135	ILE	2.1
1	I	507	TYR	2.1
1	J	313	TRP	2.1
1	E	550	ILE	2.1
1	A	362	MET	2.1
1	I	360	TYR	2.0
1	C	472	ASP	2.0
1	I	357	GLY	2.0
1	K	379	GLY	2.0
1	C	325	ILE	2.0
1	C	297	LEU	2.0
1	H	158	PRO	2.0
1	B	482	SER	2.0
1	D	181	ALA	2.0
1	P	490	ASP	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,

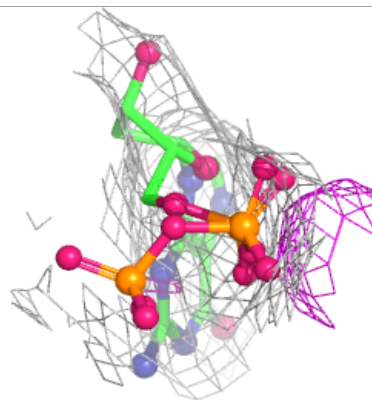
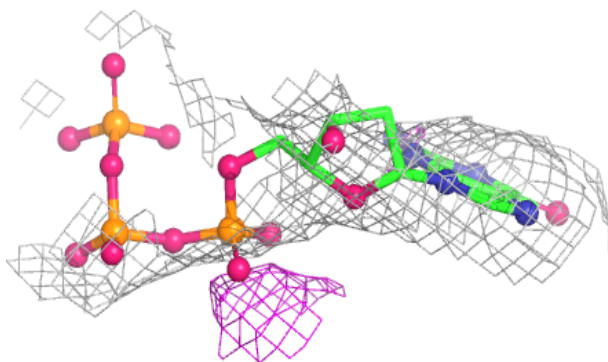
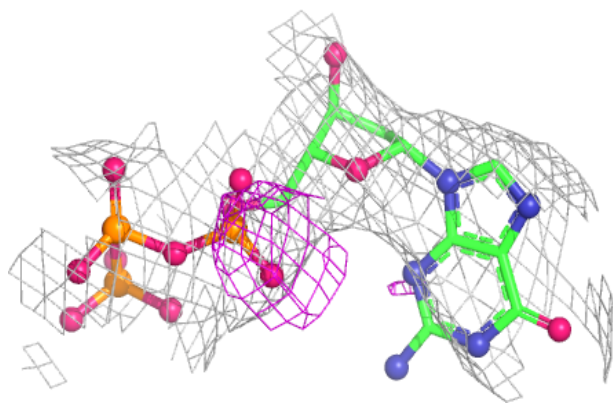
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DGT	P	701	31/31	0.70	0.12	108,163,260,277	0
2	DGT	F	701	31/31	0.71	0.12	115,163,258,286	0
2	DGT	J	701	31/31	0.72	0.11	158,196,236,251	0
2	DGT	J	703	31/31	0.77	0.10	148,179,222,224	0
2	DGT	B	702	31/31	0.79	0.12	123,161,221,241	0
2	DGT	I	701	31/31	0.80	0.10	119,176,216,232	0
2	DGT	K	701	31/31	0.80	0.11	146,190,210,214	0
2	DGT	G	701	31/31	0.80	0.10	114,167,193,203	0
2	DGT	E	702	31/31	0.81	0.09	104,152,183,186	0
2	DGT	M	702	31/31	0.81	0.09	111,145,210,237	0
2	DGT	A	703	31/31	0.81	0.16	118,158,255,262	0
2	DGT	C	702	31/31	0.82	0.10	105,162,186,208	0
2	DGT	F	702	31/31	0.84	0.10	120,163,193,201	0
2	DGT	M	701	31/31	0.84	0.08	77,162,195,234	0
2	DGT	N	701	31/31	0.85	0.08	121,182,200,207	0
2	DGT	A	701	31/31	0.85	0.10	79,136,185,195	0
2	DGT	D	701	31/31	0.86	0.08	111,173,229,241	0
2	DGT	O	703	31/31	0.86	0.09	101,149,199,203	0
2	DGT	J	702	31/31	0.86	0.10	109,172,198,208	0
2	DGT	L	701	31/31	0.87	0.12	139,192,250,256	0
2	DGT	C	701	31/31	0.87	0.09	84,132,159,171	0
2	DGT	K	702	31/31	0.87	0.08	106,157,197,225	0
2	DGT	A	702	31/31	0.88	0.09	78,102,159,161	0
2	DGT	O	701	31/31	0.88	0.08	104,155,198,238	0
2	DGT	O	702	31/31	0.90	0.09	103,170,202,219	0
2	DGT	H	701	31/31	0.90	0.09	106,142,204,224	0
2	DGT	G	702	31/31	0.90	0.08	92,119,161,175	0
2	DGT	E	701	31/31	0.91	0.10	155,194,231,249	0
2	DGT	P	702	31/31	0.91	0.11	122,171,232,248	0
2	DGT	I	702	31/31	0.92	0.07	123,168,202,210	0
2	DGT	E	703	31/31	0.93	0.09	97,159,257,259	0
2	DGT	B	701	31/31	0.94	0.07	101,133,155,171	0

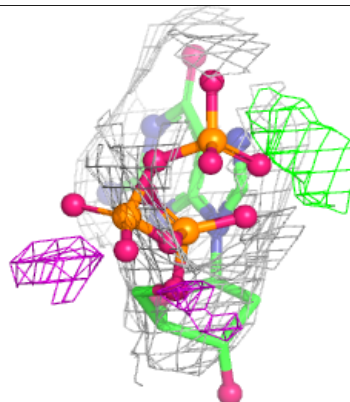
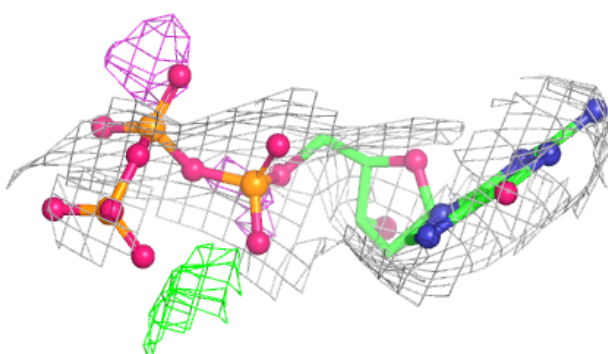
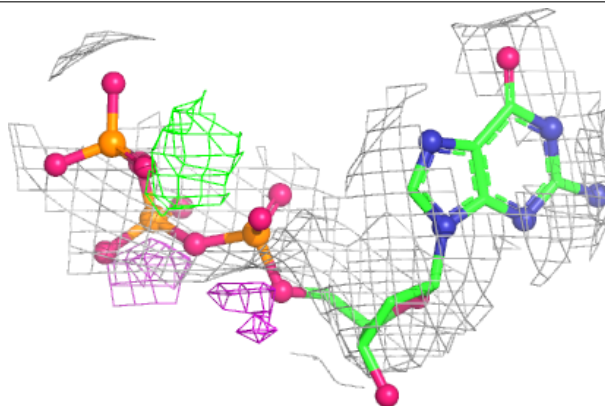
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT P 701:

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

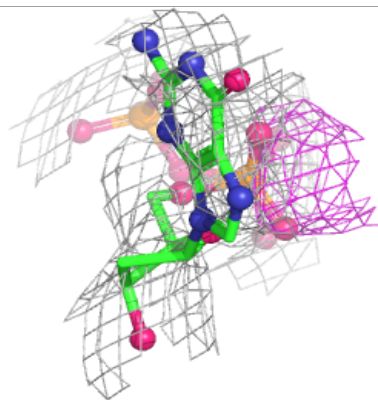
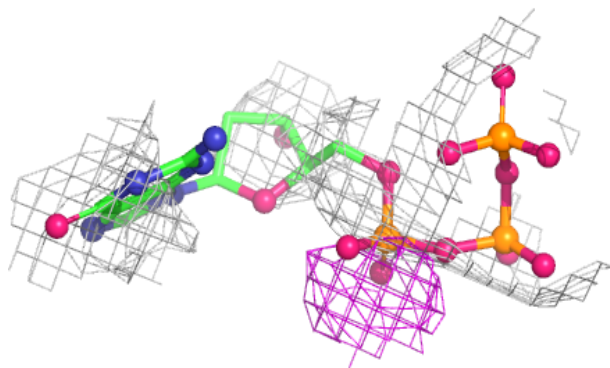
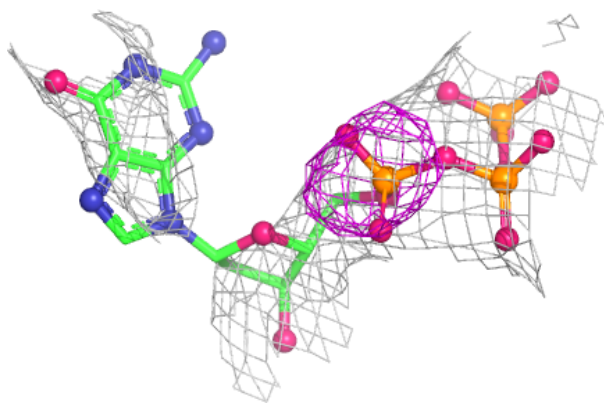
**Electron density around DGT F 701:**

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

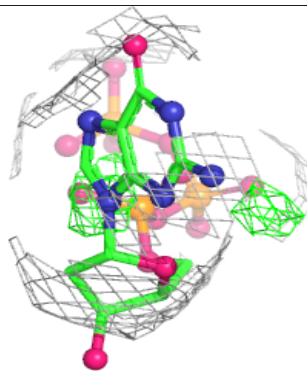
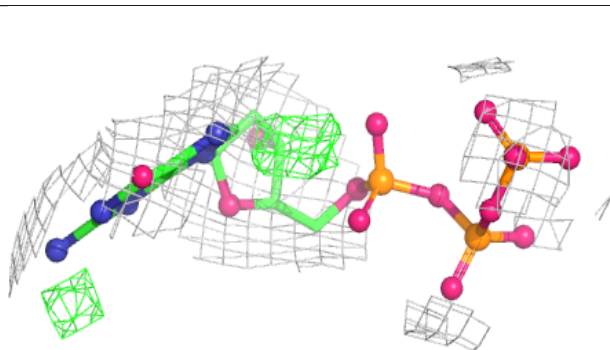
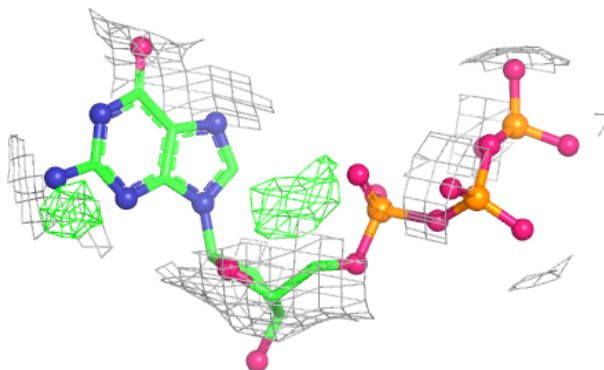


Electron density around DGT J 701:

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

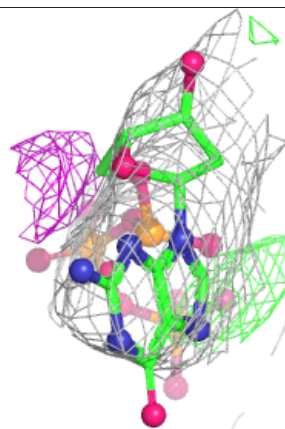
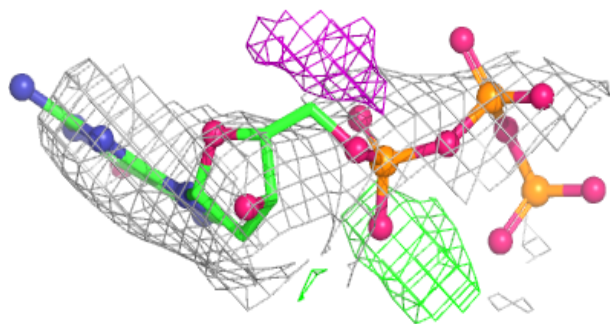
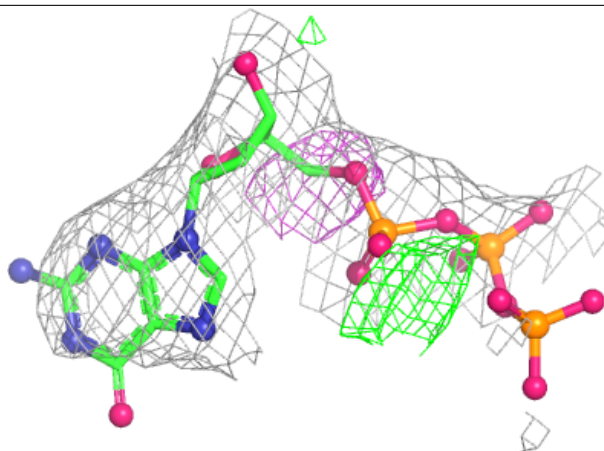
**Electron density around DGT J 703:**

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

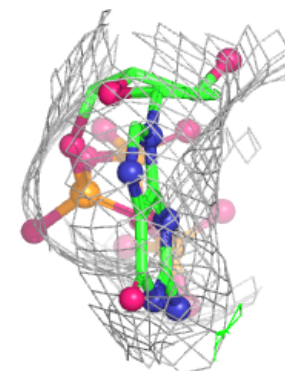
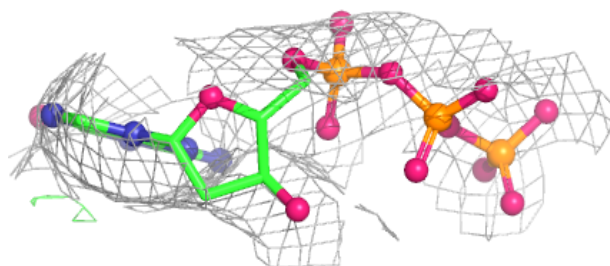
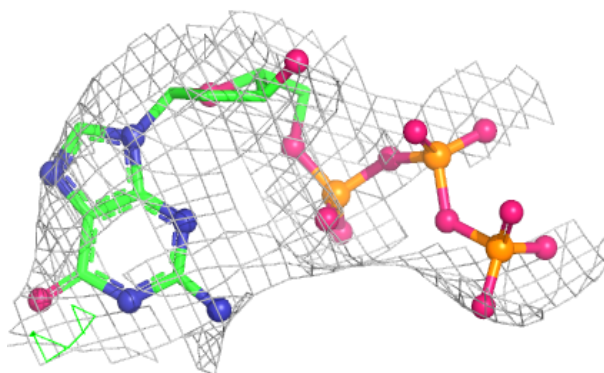


Electron density around DGT B 702:

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

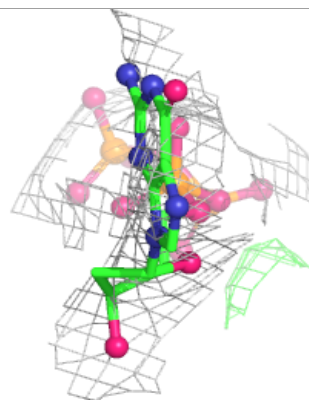
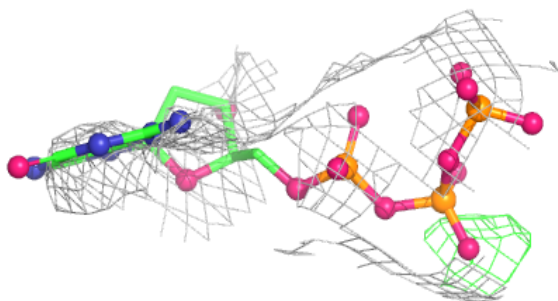
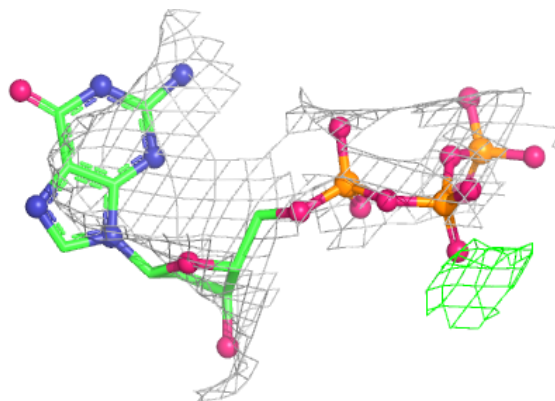
**Electron density around DGT I 701:**

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

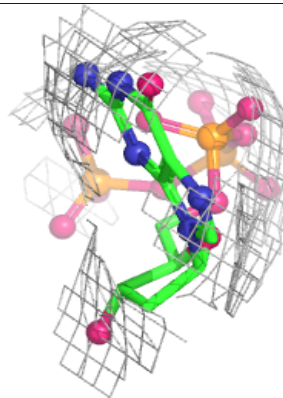
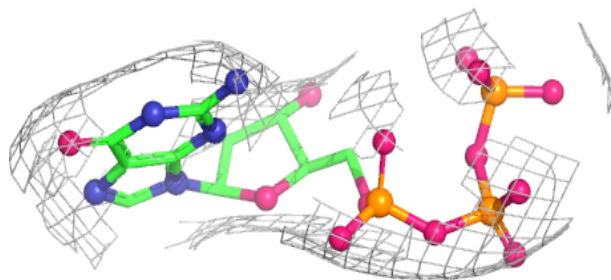
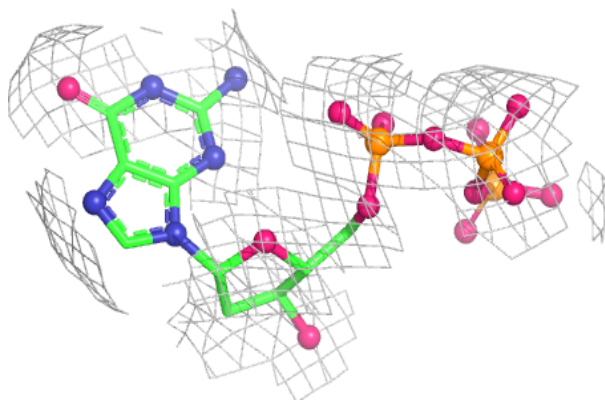


Electron density around DGT K 701:

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

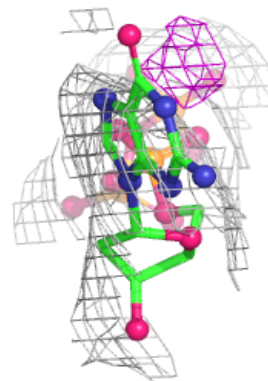
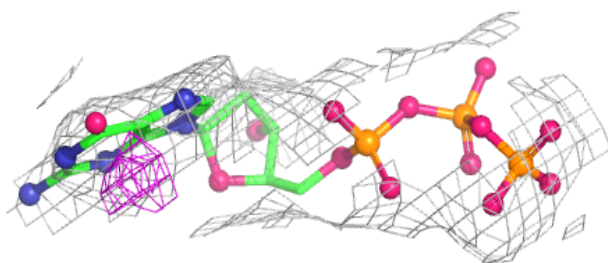
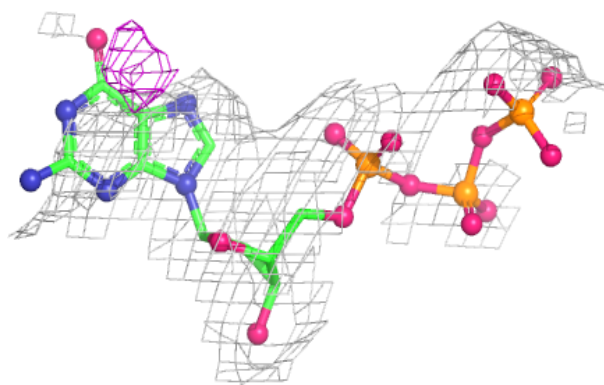
**Electron density around DGT G 701:**

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

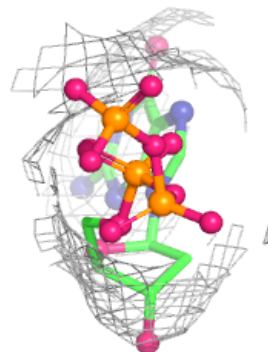
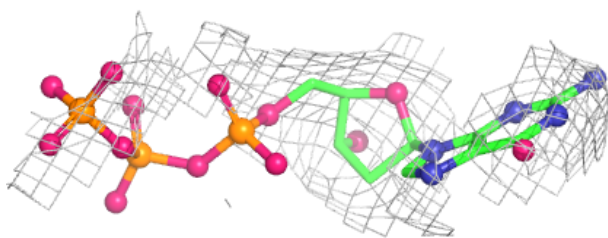
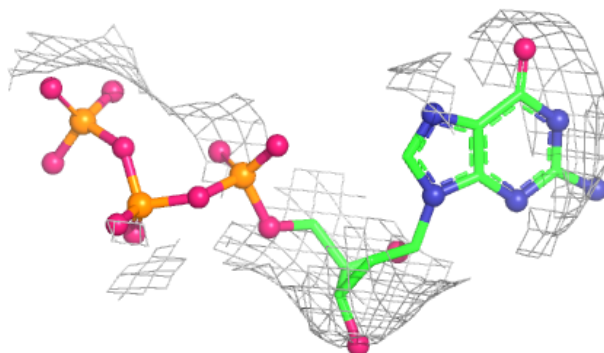


Electron density around DGT E 702:

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

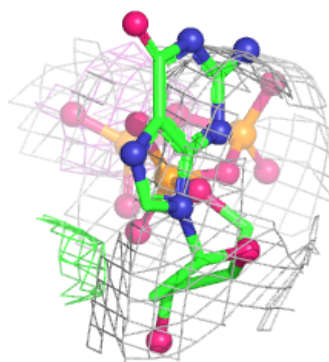
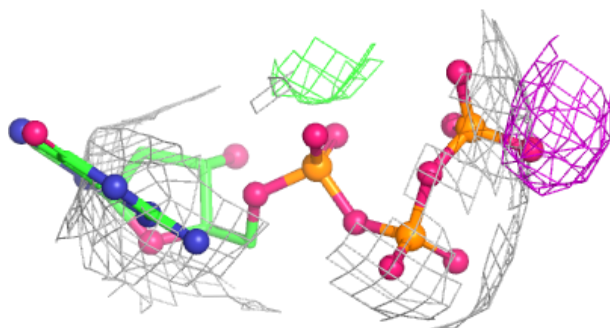
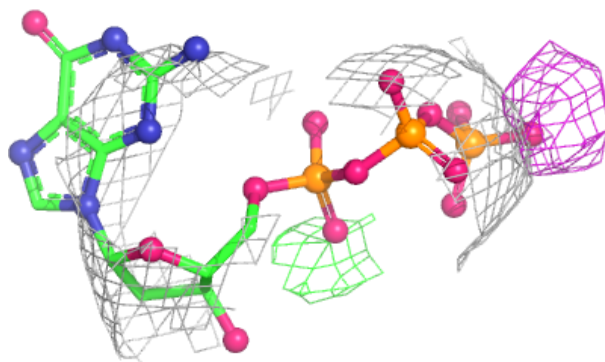
**Electron density around DGT M 702:**

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

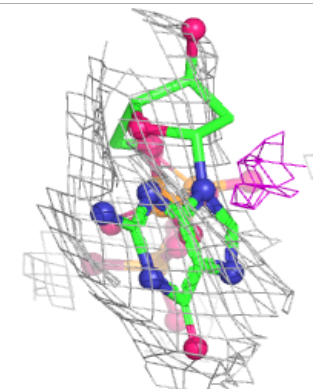
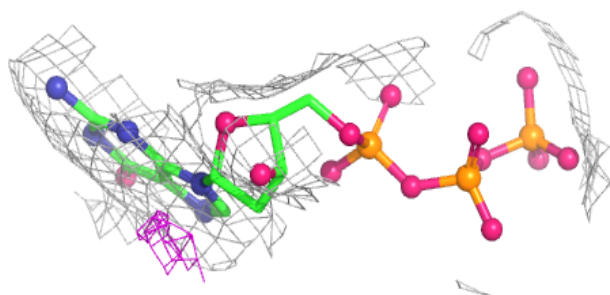
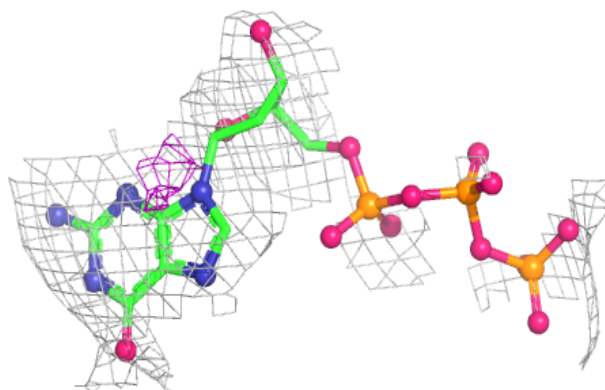


Electron density around DGT A 703:

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

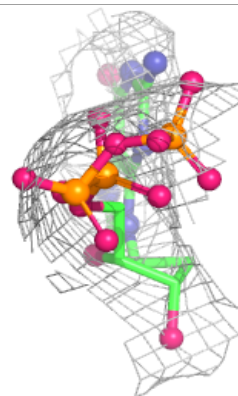
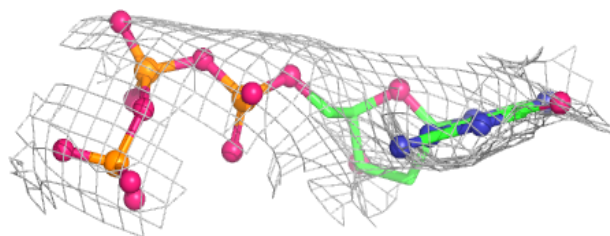
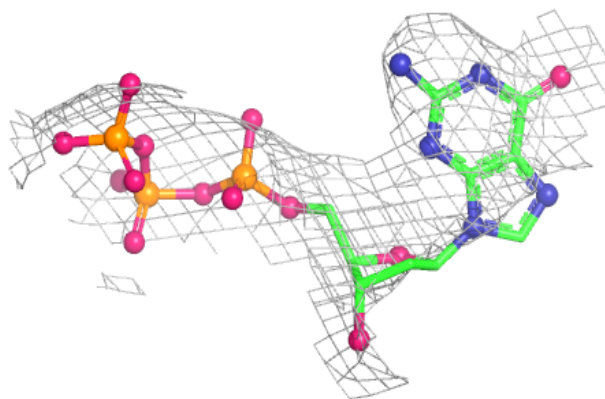
**Electron density around DGT C 702:**

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

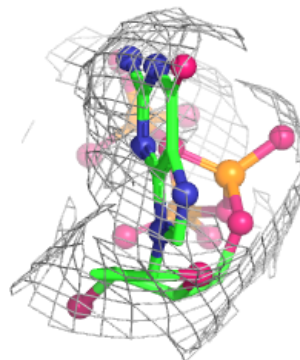
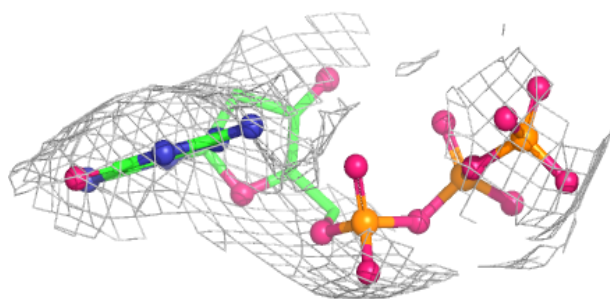
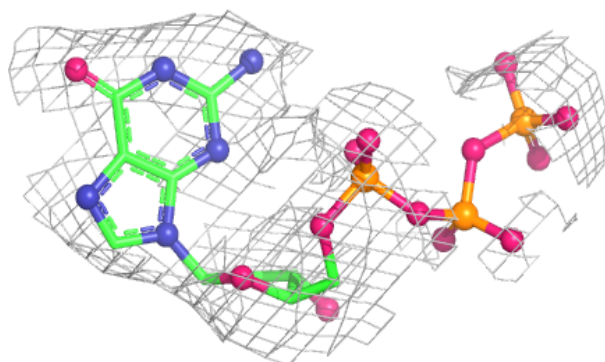


Electron density around DGT F 702:

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

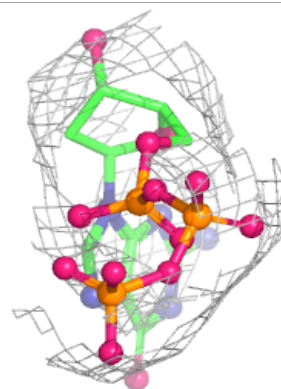
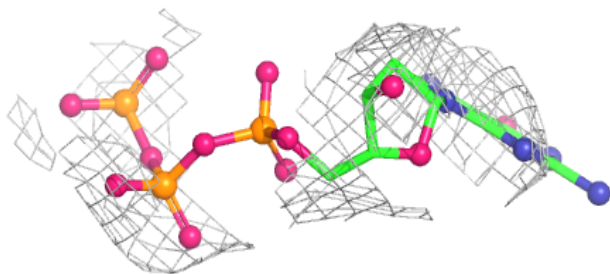
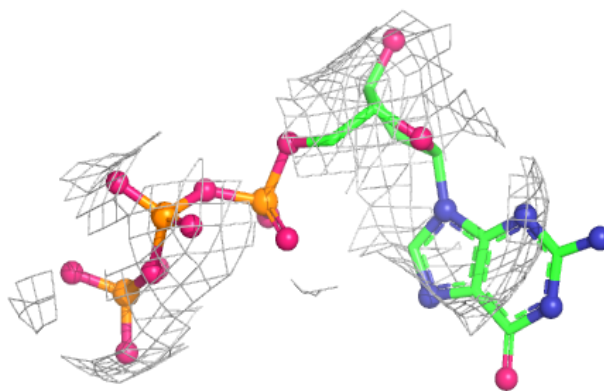
**Electron density around DGT M 701:**

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

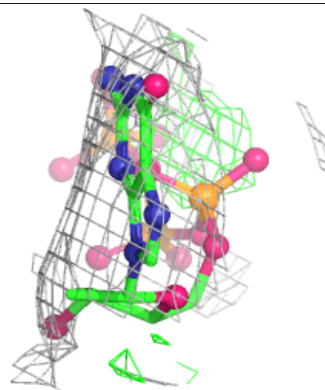
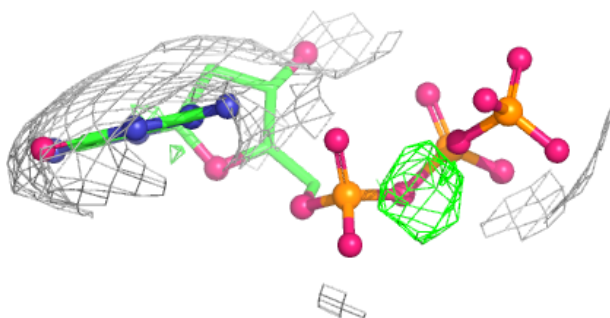
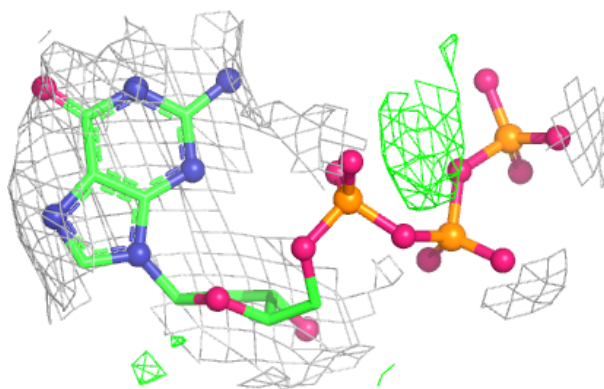


Electron density around DGT N 701:

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

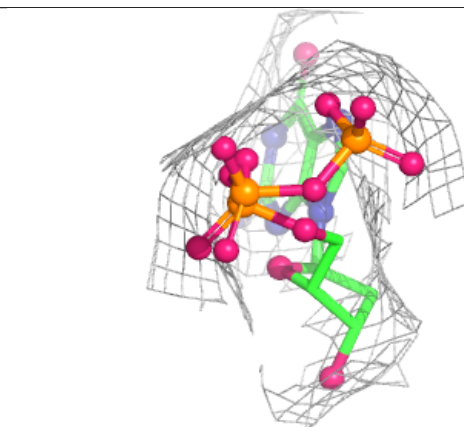
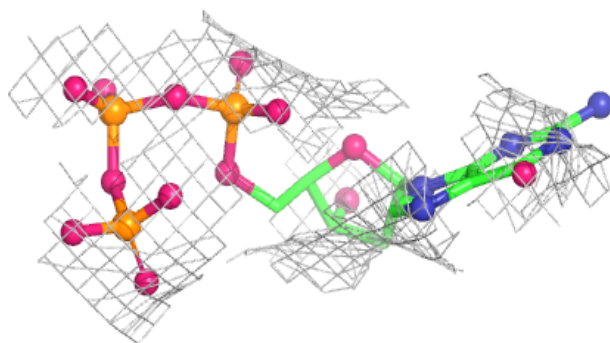
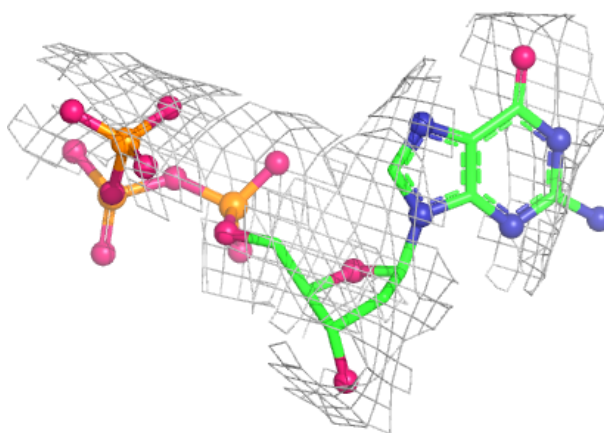
**Electron density around DGT A 701:**

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

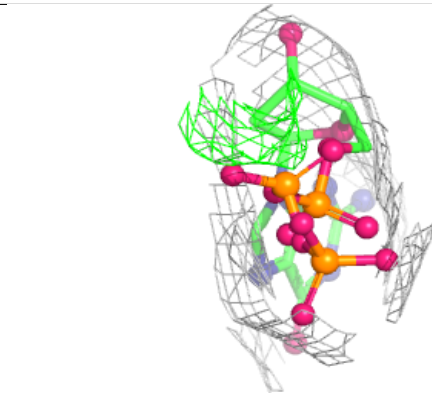
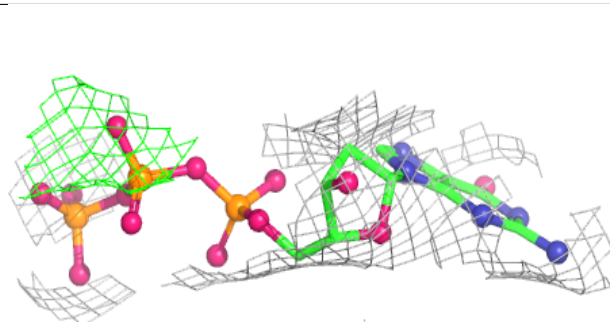
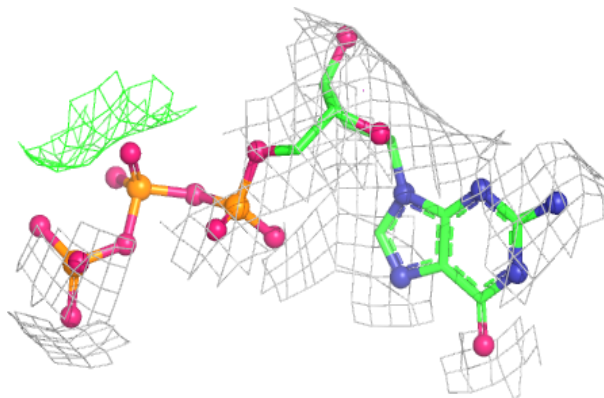


Electron density around DGT D 701:

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

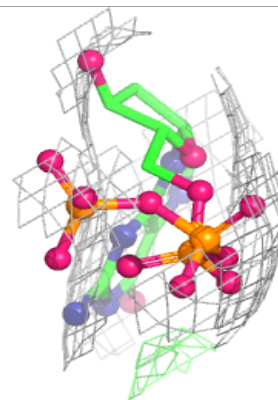
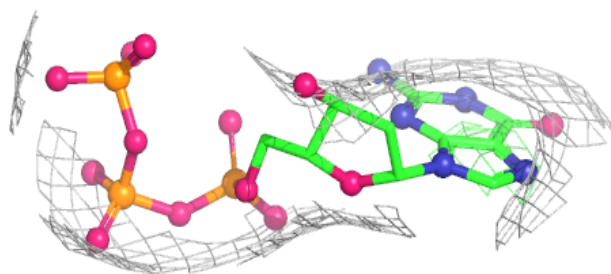
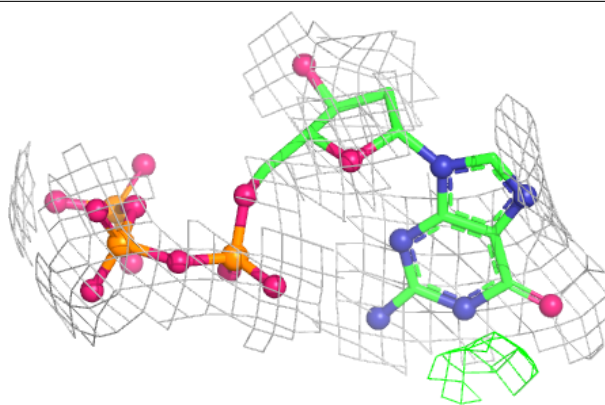
**Electron density around DGT O 703:**

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



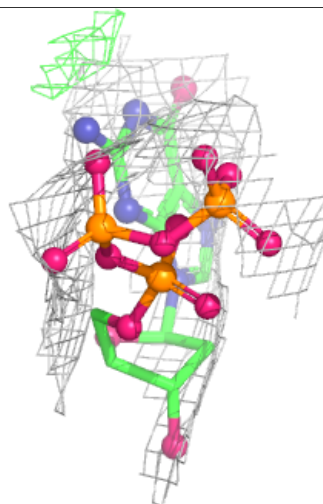
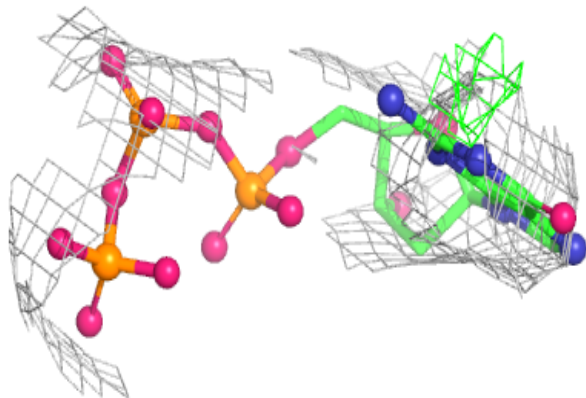
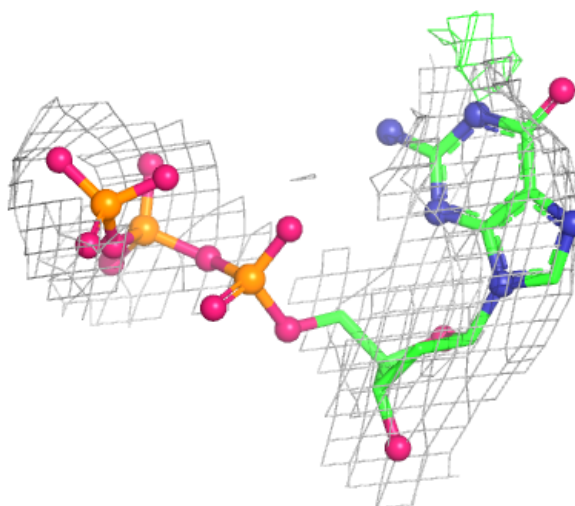
Electron density around DGT J 702:

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



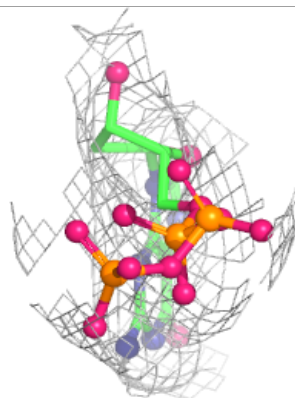
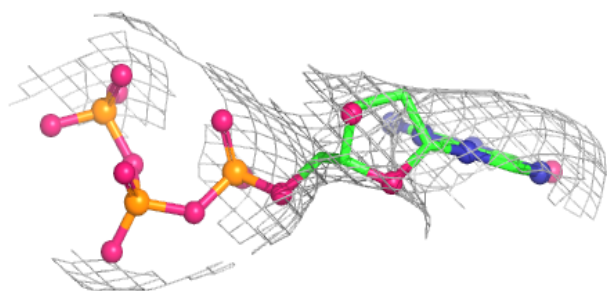
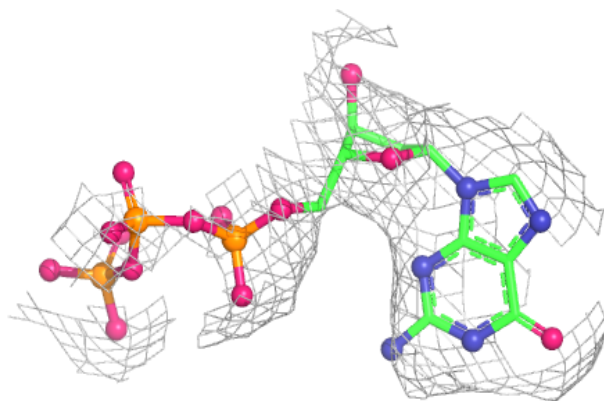
Electron density around DGT L 701:

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

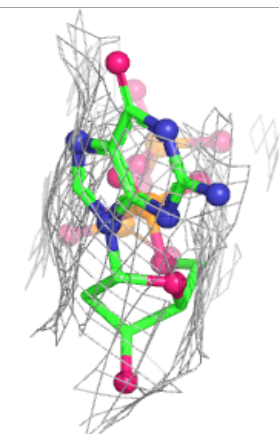
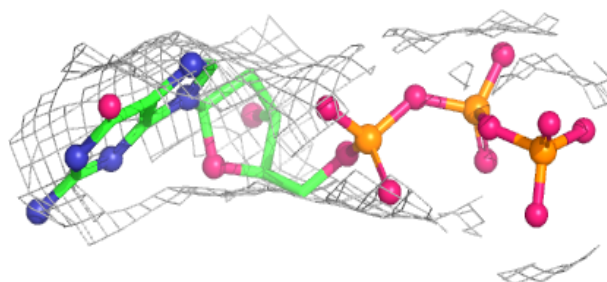
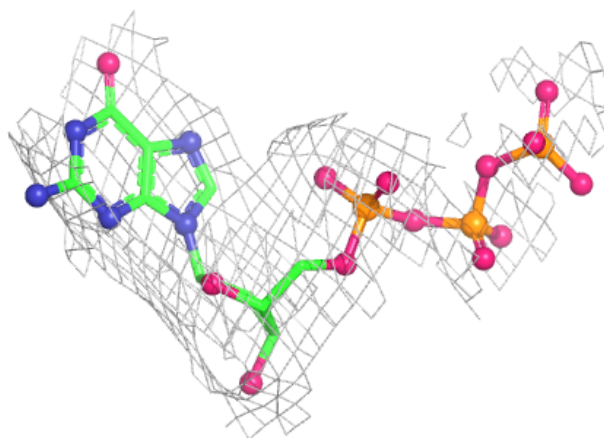


Electron density around DGT C 701:

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

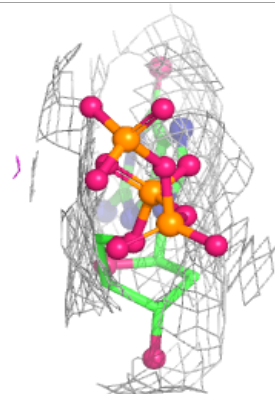
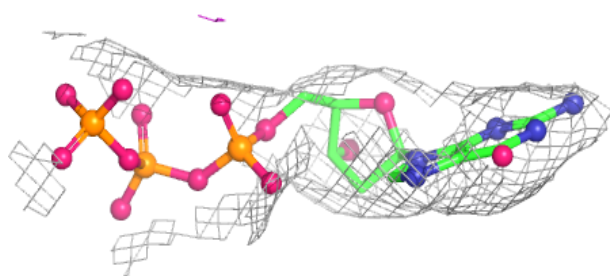
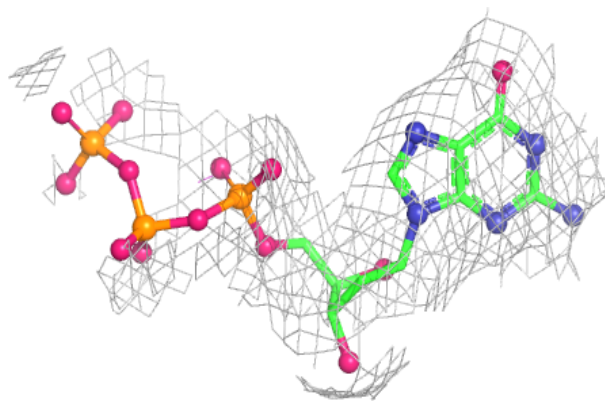
**Electron density around DGT K 702:**

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

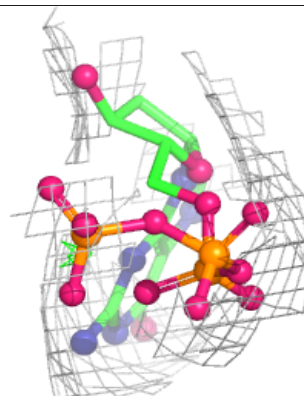
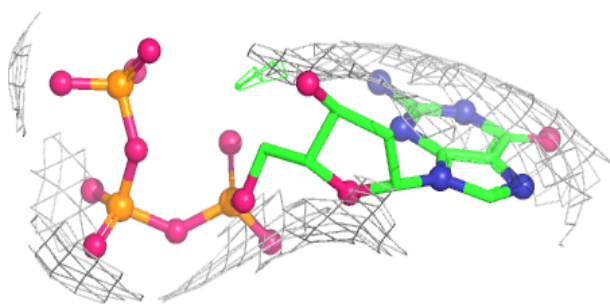
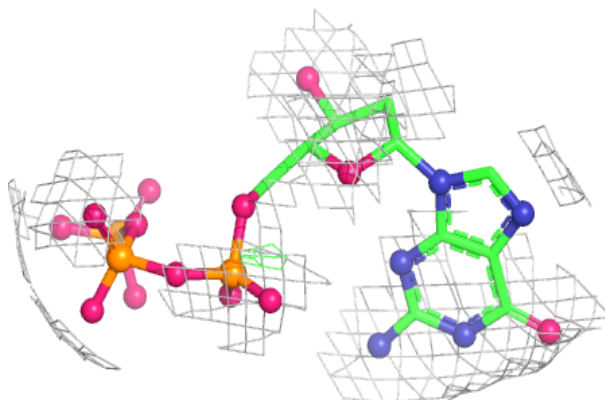


Electron density around DGT A 702:

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

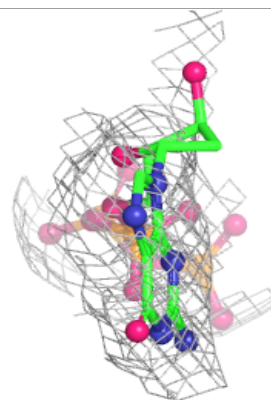
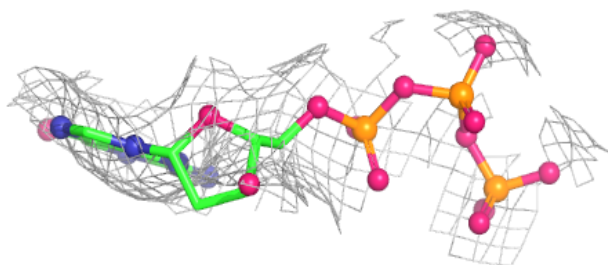
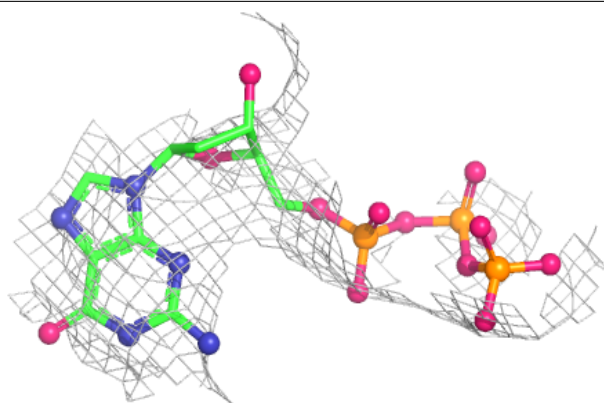
**Electron density around DGT O 701:**

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

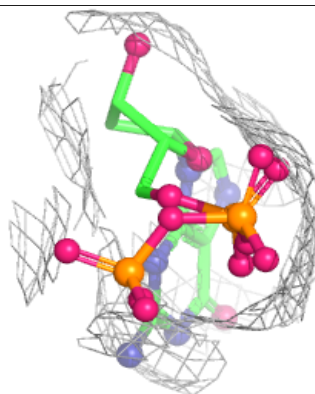
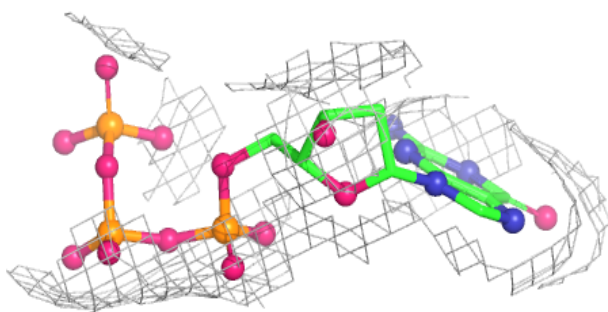
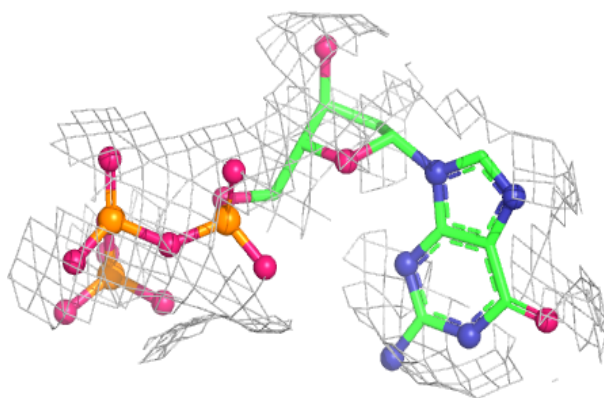


Electron density around DGT O 702:

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

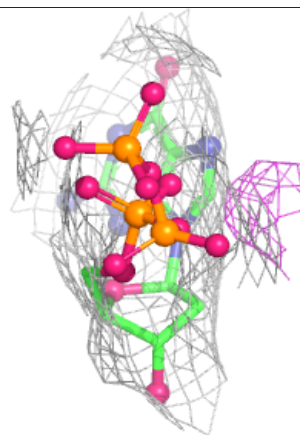
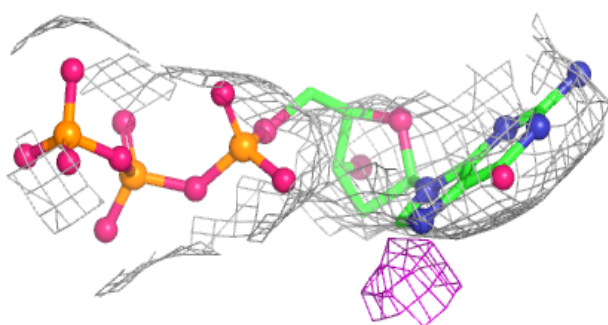
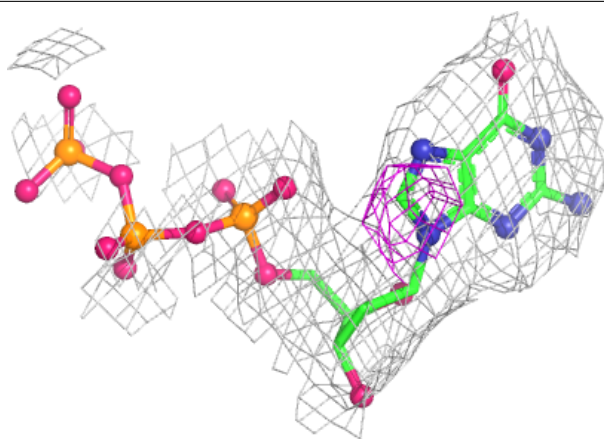
**Electron density around DGT H 701:**

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

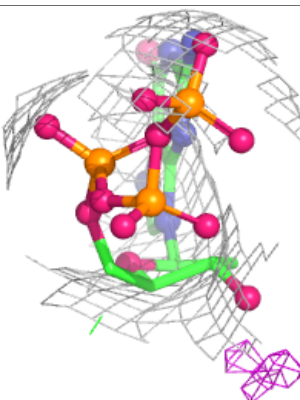
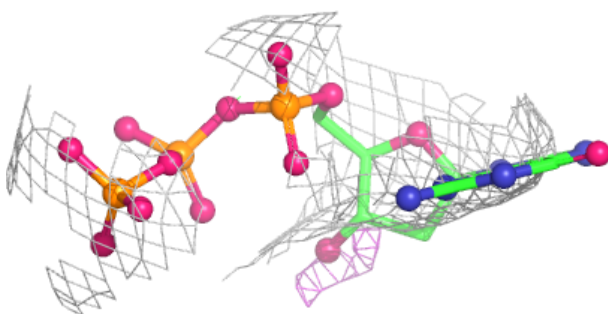
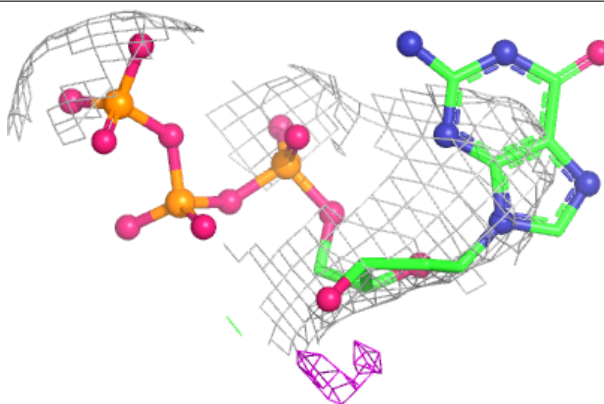


Electron density around DGT G 702:

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

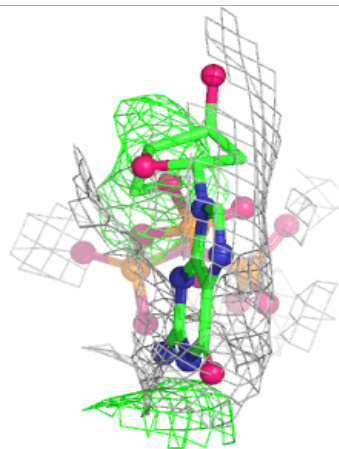
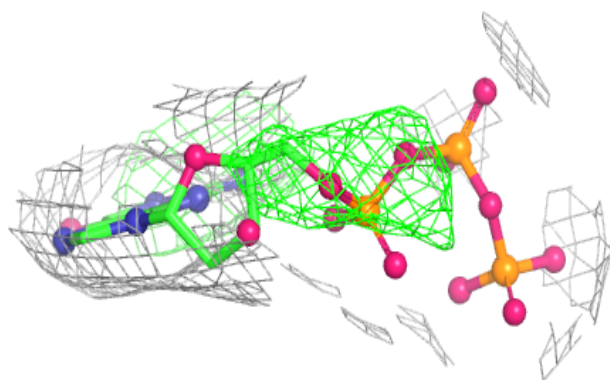
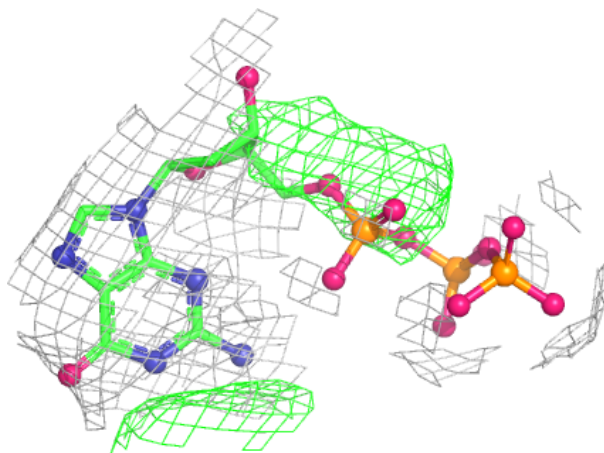
**Electron density around DGT E 701:**

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



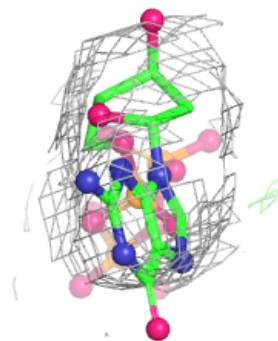
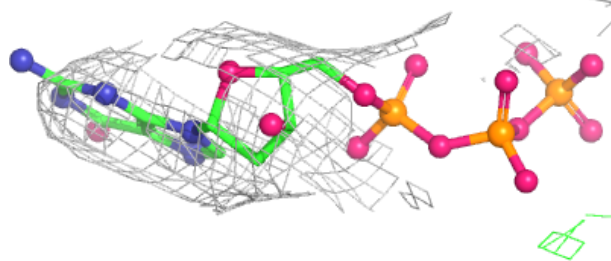
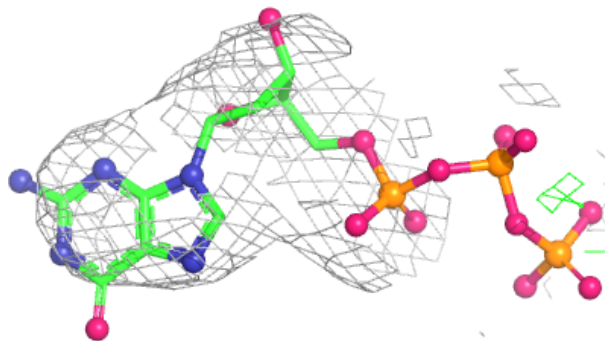
Electron density around DGT P 702:

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



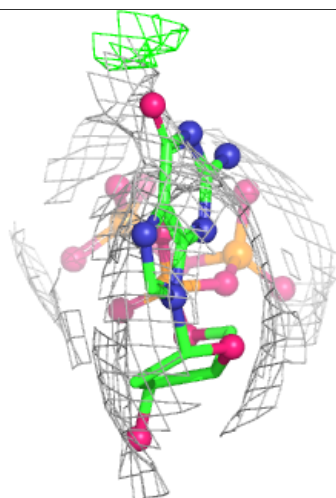
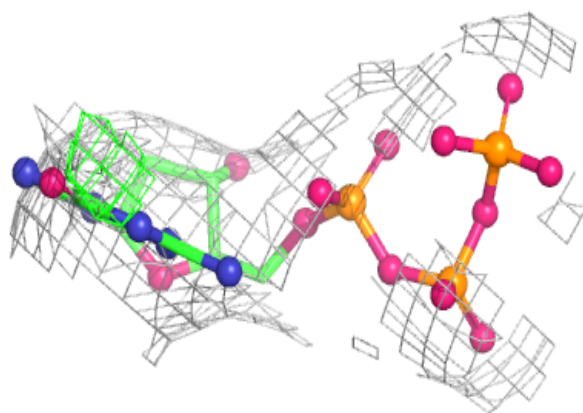
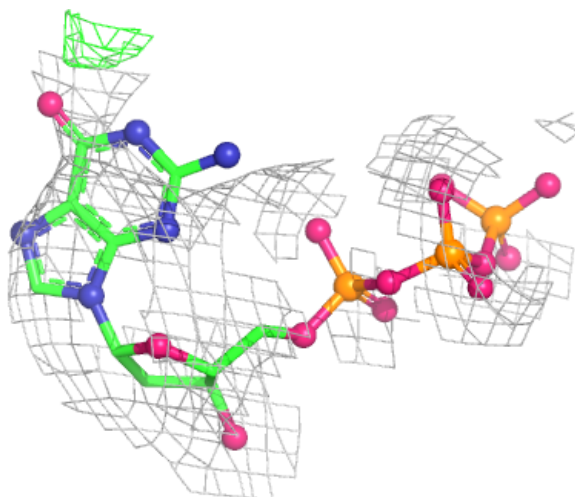
Electron density around DGT I 702:

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



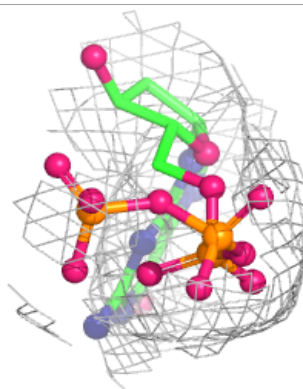
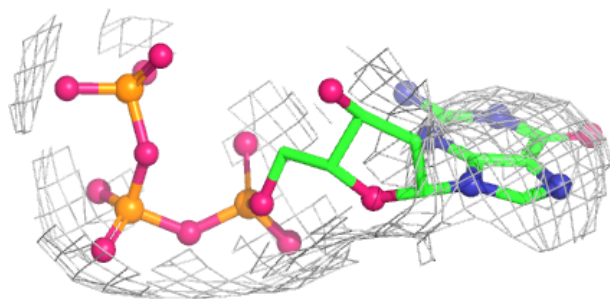
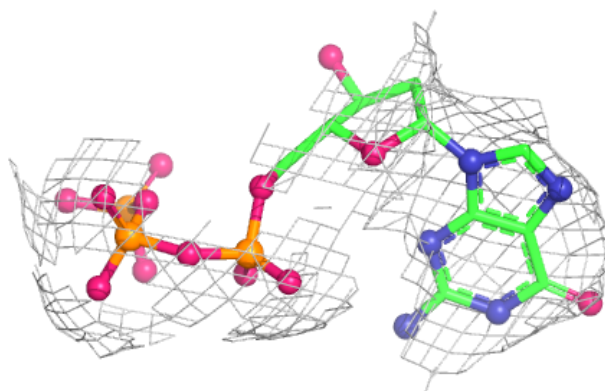
Electron density around DGT E 703:

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



Electron density around DGT B 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.