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wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:03 AM EDT

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

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

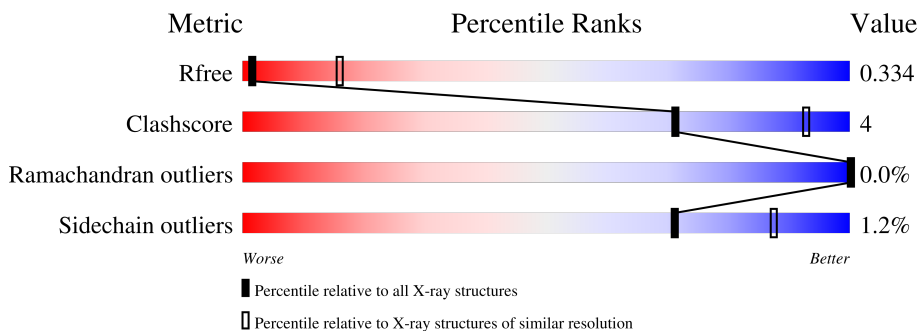|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.334
Clashscore		4
Ramachandran outliers		0.0%
Sidechain outliers		1.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	535	82% 8% · 10%
1	B	535	81% 8% 10%
1	C	535	82% 8% · 10%
1	D	535	83% 7% 10%
1	E	535	82% 7% 10%
1	F	535	82% 7% · 10%
1	G	535	82% 8% · 10%

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Mol	Chain	Length	Quality of chain
1	H	535	83% 7% · 10%
1	I	535	83% 7% 10%
1	J	535	81% 8% 10%
1	K	535	81% 8% · 10%
1	L	535	81% 8% 10%
1	M	535	82% 7% 10%
1	N	535	82% 8% 10%
1	O	535	81% 8% · 10%
1	P	535	82% 7% · 10%

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 3932	C 2517	N 684	O 711	S 20	0	0	0
1	B	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	C	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	D	481	Total 3940	C 2521	N 686	O 713	S 20	0	1	0
1	E	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	F	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	G	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	H	481	Total 3940	C 2521	N 686	O 713	S 20	0	1	0
1	I	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	J	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	K	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	L	481	Total 3940	C 2521	N 686	O 713	S 20	0	1	0
1	M	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	N	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	O	481	Total 3932	C 2517	N 684	O 711	S 20	0	0	0
1	P	481	Total 3940	C 2521	N 686	O 713	S 20	0	1	0

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

Continued from previous page...

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 (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

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

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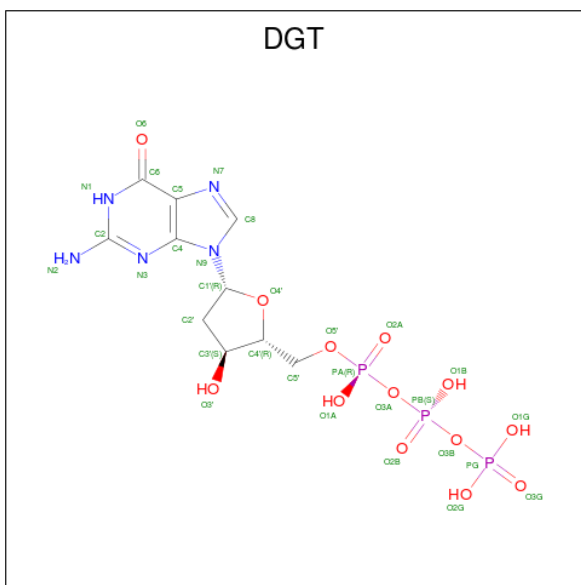
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	31	10	5	13	3	0	0
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G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

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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 ⓘ

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D: 83%   7%   10%

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain E: 82%   7%   10%

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain F: 82%   7%   •   10%

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain G: 82%   8%   •   10%

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain H:

83%   7%   ·   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** N119 H129 P130 P139 V156 G170 F241 I245 K251 P252 E277 SER PRO VAL GLU ASP SER L284 K312 W313 D314 Y315 N328 R333 F337

A351 K354 H366 H370 L422 **N425** I426 **F427** L428 E443 Q447 **K455** K469 R470 E511 F520 A546 K560 N577 **D585** V586 T592 P593 **N599** ASP SER THR SER VAL GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG

VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain I:

83%   7%   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** H129 P130 P139 F157 **K185** R226 V229 F241 I245 E277 SER PRO VAL GLU ASP SER L284 K312 Y315 H321 Q326 A351 R352 D353

K354 H366 H370 I381 F390 T423 **D424** **N425** I426 **F427** L428 **R451** **N452** L453 T463 **G464** Q465 K492 E511 F520 K534 N535 T592 P593 W598 **N599** ASP SER THR SER VAL GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU

PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain J:

81%   8%   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** I118 H129 P130 P139 F165 G172 **L204** L224 F241 I245 K251 P252 E262 E277 SER PRO VAL GLU ASP SER L284 K312 Y315

H321 Q326 A351 L359 H366 H370 **R371** R372 K377 V378 D395 L422 **N425** I426 E443 Q447 Y450 **R451** **N452** L453 K469 R470 E471 F520 R528 N535 E543 K560 N577 T592 P593 **Q594** **K595** **K596** **N599** ASP SER THR SER

VAL GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain K:

81%   8%   ·   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** V117 I118 N119 H129 P130 D137 **K230** F241 I245 K251 P252 E277 SER PRO VAL GLU ASP SER L284 K312 Y315 H321 Q326 E342

N345 A351 L359 H366 H370 I381 F390 D395 **N425** I426 K439 E443 Q447 Y450 K455 Q465 **I466** K467 R470 P485 V502 E511 F520 N535 I550 N577 T592 P593 **Q594** **K595** **K596** **E597** W598 **N599** ASP SER THR

SER VAL GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain L: 81%   8%   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER HIS MET **D113** I126 H129 P130 G170 Y173 S192 F241 I245 K251 P252 **E277** SER PRO VAL GLU ASP SER L284 K312 **W313** **D314** Y315 H321 **N328** F337

A351 K354 H366 H370 **R371** R372 I381 K405 L422 **M425** I426 **F427** **L428** E443 Q447 Y450 K455 E471 E511 F520 K523 E543 A546 R576 N577 D585 V586 T592 P593 K596 **N599** ASP SER THR SER VAL GLN

ASN PRO THR ARG LEU ARG GLU GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain M: 82%   7%   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** H129 P130 P139 F157 **K185** R226 V229 F241 I245 K251 P252 **E262** **E277** SER PRO VAL GLU ASP SER L284 K312 Y315 Q326

A351 R352 **D353** K354 H366 H370 F390 K405 T423 **D424** N425 I426 **F427** L428 E443 Q447 R451 T463 K486 E511 F520 R528 K534 N535 R576 T592 P593 **W598** N599 ASP SER THR SER VAL GLN ASN PRO THR ARG LEU ARG GLU ALA

SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain N: 82%   8%   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** I118 I126 H129 P130 G172 Y173 **L204** L224 F241 I245 K251 P252 E262 **E277** SER PRO VAL GLU ASP SER L284 K312 Y315 H321

I325 Q326 A351 L359 H366 H370 K377 V378 D395 Y396 K405 L422 N425 I426 Y450 **R451** N452 L453 K469 R470 E471 F520 N535 E543 N577 T592 P593 **Q594** K595 K596 **N599** ASP SER THR SER VAL GLN ASN PRO THR ARG LEU

ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain O: 81%   8%   ·   10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** V117 I118 N119 H125 I126 H129 P130 V156 Y173 K230 F241 I245 K251 P252 I260 **E277** SER PRO VAL GLU ASP SER L284 K312 Y315

H321 Q326 A351 H366 H370 I381 F390 D395 **M425** I426 K439 E443 K455 Q465 I466 K467 R470 P485 D490 **V491** K492 V502 E511 F520 N535 I550 **K560** N577 V586 T592 P593 **Q594** K595 K596 **E597** **W598** N599 ASP SER THR SER VAL GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain P:

82% 7% · 10%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET **D113** I126 H129 P130 G170 Y173 F241 I245 E277 SER PRO VAL GLU ASP SER L284 K288 E292 K312 W313 D314 Y315 N328 R333 A351

K354 H366 H370 I381 L422 M425 I426 F427 L428 E443 Q447 Y450 K455 Q465 E471 K492 E511 F520 K523 E543 A546 N577 K580 D583 G584 D585 P589 L590 N599 ASP SER THR SER VAL GLN ASN PRO THR

ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

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
$< I/\sigma(I) >$ [1]	2.20 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.236 , 0.274 0.297 , 0.334	Depositor DCC
R_{free} test set	4552 reflections (4.91%)	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)	0.31 , 122.4	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	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	0.85	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.62	0/4025	0.73	2/5434 (0.0%)
1	B	0.63	1/4025 (0.0%)	0.77	4/5434 (0.1%)
1	C	0.62	1/4025 (0.0%)	0.72	2/5434 (0.0%)
1	D	0.60	0/4033	0.70	0/5445
1	E	0.61	0/4025	0.72	2/5434 (0.0%)
1	F	0.63	1/4025 (0.0%)	0.76	4/5434 (0.1%)
1	G	0.60	0/4025	0.71	2/5434 (0.0%)
1	H	0.60	0/4033	0.69	0/5445
1	I	0.62	0/4025	0.73	2/5434 (0.0%)
1	J	0.63	1/4025 (0.0%)	0.76	4/5434 (0.1%)
1	K	0.59	0/4025	0.71	2/5434 (0.0%)
1	L	0.60	0/4033	0.69	0/5445
1	M	0.63	1/4025 (0.0%)	0.72	2/5434 (0.0%)
1	N	0.62	0/4025	0.76	4/5434 (0.1%)
1	O	0.60	0/4025	0.71	2/5434 (0.0%)
1	P	0.61	0/4033	0.70	0/5445
All	All	0.61	5/64432 (0.0%)	0.72	32/86988 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	262	GLU	CD-OE2	-9.01	1.15	1.25
1	C	261	PRO	N-CD	7.37	1.58	1.47
1	J	262	GLU	CD-OE2	-5.86	1.19	1.25
1	F	262	GLU	CD-OE2	-5.78	1.19	1.25
1	B	262	GLU	CD-OE2	-5.64	1.19	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	ARG	NE-CZ-NH1	-11.67	114.47	120.30

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	451	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	J	451	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	F	451	ARG	NE-CZ-NH1	-10.21	115.19	120.30
1	B	450	TYR	CB-CG-CD2	-9.76	115.14	121.00

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	42	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	35	14
1	G	3932	0	3915	37	14
1	H	3940	0	3920	30	0
1	I	3932	0	3915	29	6
1	J	3932	0	3915	33	6
1	K	3932	0	3915	39	2
1	L	3940	0	3920	31	3
1	M	3932	0	3915	28	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	93	0	36	11	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	448	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.

The worst 5 of 448 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

The worst 5 of 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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/535 (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%)	47	80
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%)	421 (99%)	6 (1%)	67	85
1	B	427/477 (90%)	426 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	427/477 (90%)	422 (99%)	5 (1%)	71	87
1	D	428/477 (90%)	421 (98%)	7 (2%)	62	83
1	E	427/477 (90%)	423 (99%)	4 (1%)	78	90
1	F	427/477 (90%)	423 (99%)	4 (1%)	78	90
1	G	427/477 (90%)	423 (99%)	4 (1%)	78	90
1	H	428/477 (90%)	422 (99%)	6 (1%)	67	85
1	I	427/477 (90%)	423 (99%)	4 (1%)	78	90
1	J	427/477 (90%)	424 (99%)	3 (1%)	84	93
1	K	427/477 (90%)	422 (99%)	5 (1%)	71	87
1	L	428/477 (90%)	421 (98%)	7 (2%)	62	83
1	M	427/477 (90%)	423 (99%)	4 (1%)	78	90
1	N	427/477 (90%)	424 (99%)	3 (1%)	84	93
1	O	427/477 (90%)	421 (99%)	6 (1%)	67	85
1	P	428/477 (90%)	416 (97%)	12 (3%)	43	73
All	All	6836/7632 (90%)	6755 (99%)	81 (1%)	71	87

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	451	ARG
1	P	425	ASN
1	M	486	LYS
1	O	425	ASN
1	P	523	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	539	GLN
1	P	539	GLN
1	J	599	ASN
1	P	366	HIS
1	O	207	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	F	701	-	26,33,33	0.95	1 (3%)	32,52,52	0.70	0
2	DGT	E	702	-	26,33,33	0.93	2 (7%)	32,52,52	0.74	1 (3%)
2	DGT	A	701	-	26,33,33	0.94	1 (3%)	32,52,52	0.90	1 (3%)
2	DGT	M	701	-	26,33,33	0.98	2 (7%)	32,52,52	0.86	1 (3%)
2	DGT	O	703	-	26,33,33	0.99	2 (7%)	32,52,52	0.80	0
2	DGT	E	703	-	26,33,33	0.95	2 (7%)	32,52,52	0.81	0
2	DGT	G	701	-	26,33,33	0.91	2 (7%)	32,52,52	0.76	1 (3%)
2	DGT	C	702	-	26,33,33	0.94	2 (7%)	32,52,52	0.82	0
2	DGT	N	701	-	26,33,33	1.01	2 (7%)	32,52,52	0.73	0
2	DGT	K	702	-	26,33,33	0.95	2 (7%)	32,52,52	0.82	1 (3%)
2	DGT	D	701	-	26,33,33	1.02	3 (11%)	32,52,52	0.69	0
2	DGT	C	701	-	26,33,33	0.92	2 (7%)	32,52,52	0.86	1 (3%)
2	DGT	O	702	-	26,33,33	0.92	1 (3%)	32,52,52	0.86	1 (3%)
2	DGT	A	703	-	26,33,33	0.97	2 (7%)	32,52,52	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	DGT	I	702	-	26,33,33	0.94	2 (7%)	32,52,52	0.72	0
2	DGT	J	702	-	26,33,33	0.92	2 (7%)	32,52,52	0.80	1 (3%)
2	DGT	J	703	-	26,33,33	0.96	1 (3%)	32,52,52	0.70	0
2	DGT	P	702	-	26,33,33	0.98	2 (7%)	32,52,52	0.72	0
2	DGT	B	701	-	26,33,33	0.97	2 (7%)	32,52,52	0.72	0
2	DGT	M	702	-	26,33,33	0.94	2 (7%)	32,52,52	0.73	0
2	DGT	B	702	-	26,33,33	0.96	2 (7%)	32,52,52	0.73	0
2	DGT	A	702	-	26,33,33	1.00	2 (7%)	32,52,52	0.70	0
2	DGT	H	701	-	26,33,33	0.97	2 (7%)	32,52,52	0.81	0
2	DGT	P	701	-	26,33,33	1.00	2 (7%)	32,52,52	0.82	0
2	DGT	I	701	-	26,33,33	0.92	2 (7%)	32,52,52	0.88	2 (6%)
2	DGT	J	701	-	26,33,33	0.95	2 (7%)	32,52,52	0.80	0
2	DGT	K	701	-	26,33,33	0.93	2 (7%)	32,52,52	0.80	1 (3%)
2	DGT	E	701	-	26,33,33	0.94	2 (7%)	32,52,52	0.88	1 (3%)
2	DGT	L	701	-	26,33,33	0.96	2 (7%)	32,52,52	0.75	0
2	DGT	O	701	-	26,33,33	0.92	2 (7%)	32,52,52	0.77	1 (3%)
2	DGT	G	702	-	26,33,33	0.97	1 (3%)	32,52,52	0.87	0
2	DGT	F	702	-	26,33,33	0.93	1 (3%)	32,52,52	0.85	1 (3%)

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	F	701	-	-	5/18/34/34	0/3/3/3
2	DGT	E	702	-	-	5/18/34/34	0/3/3/3
2	DGT	A	701	-	-	5/18/34/34	0/3/3/3
2	DGT	M	701	-	-	5/18/34/34	0/3/3/3
2	DGT	O	703	-	-	4/18/34/34	0/3/3/3
2	DGT	E	703	-	-	5/18/34/34	0/3/3/3
2	DGT	G	701	-	-	6/18/34/34	0/3/3/3
2	DGT	C	702	-	-	4/18/34/34	0/3/3/3
2	DGT	N	701	-	-	5/18/34/34	0/3/3/3
2	DGT	K	702	-	-	4/18/34/34	0/3/3/3
2	DGT	D	701	-	-	6/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	C	701	-	-	3/18/34/34	0/3/3/3
2	DGT	O	702	-	-	3/18/34/34	0/3/3/3
2	DGT	A	703	-	-	3/18/34/34	0/3/3/3
2	DGT	I	702	-	-	5/18/34/34	0/3/3/3
2	DGT	J	702	-	-	6/18/34/34	0/3/3/3
2	DGT	J	703	-	-	5/18/34/34	0/3/3/3
2	DGT	P	702	-	-	4/18/34/34	0/3/3/3
2	DGT	B	701	-	-	6/18/34/34	0/3/3/3
2	DGT	M	702	-	-	5/18/34/34	0/3/3/3
2	DGT	B	702	-	-	5/18/34/34	0/3/3/3
2	DGT	A	702	-	-	4/18/34/34	0/3/3/3
2	DGT	H	701	-	-	6/18/34/34	0/3/3/3
2	DGT	P	701	-	-	6/18/34/34	0/3/3/3
2	DGT	I	701	-	-	5/18/34/34	0/3/3/3
2	DGT	J	701	-	-	6/18/34/34	0/3/3/3
2	DGT	K	701	-	-	3/18/34/34	0/3/3/3
2	DGT	E	701	-	-	5/18/34/34	0/3/3/3
2	DGT	L	701	-	-	5/18/34/34	0/3/3/3
2	DGT	O	701	-	-	6/18/34/34	0/3/3/3
2	DGT	G	702	-	-	3/18/34/34	0/3/3/3
2	DGT	F	702	-	-	3/18/34/34	0/3/3/3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	701	DGT	C5-C6	-2.92	1.41	1.47
2	B	701	DGT	C5-C6	-2.87	1.41	1.47
2	D	701	DGT	C5-C6	-2.84	1.41	1.47
2	A	702	DGT	C5-C6	-2.83	1.41	1.47
2	H	701	DGT	C5-C6	-2.72	1.41	1.47

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	DGT	O6-C6-C5	2.58	129.41	124.37
2	E	701	DGT	O6-C6-C5	2.26	128.78	124.37
2	J	702	DGT	O6-C6-C5	2.20	128.67	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	702	DGT	O6-C6-C5	2.19	128.66	124.37
2	O	701	DGT	O6-C6-C5	2.12	128.52	124.37

There are no chirality outliers.

5 of 151 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	B	701	DGT	C5'-O5'-PA-O3A
2	B	701	DGT	C5'-O5'-PA-O1A

There are no ring outliers.

23 monomers are involved in 60 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT E 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT M 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT O 703

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT E 703

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT G 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT C 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT N 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT K 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT D 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT C 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT O 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT A 703

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT I 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT J 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT J 703

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT P 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT M 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT B 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT A 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT H 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT P 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT I 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT J 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT K 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT E 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT L 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT O 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT G 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT F 702

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
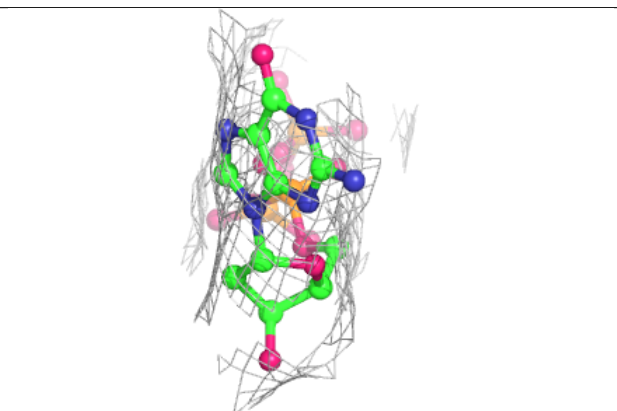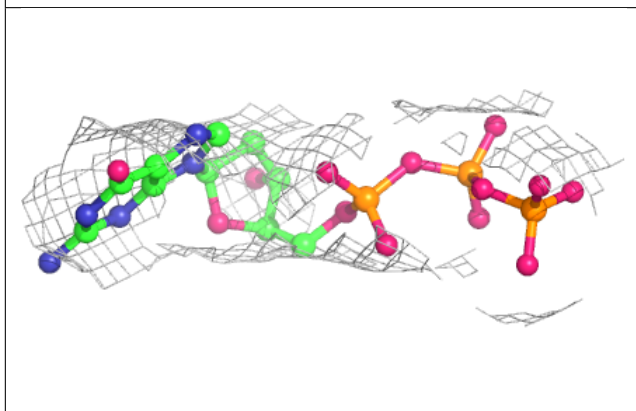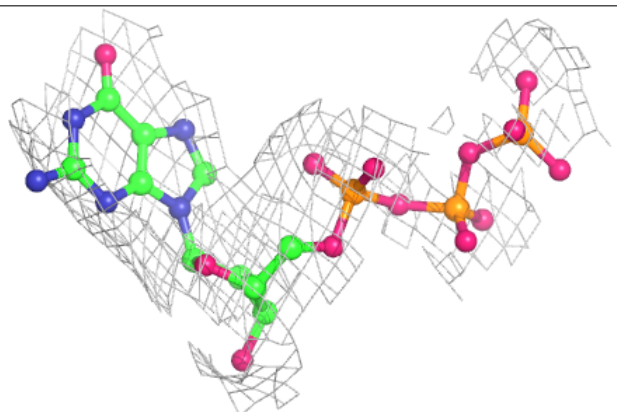
Electron density around DGT A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
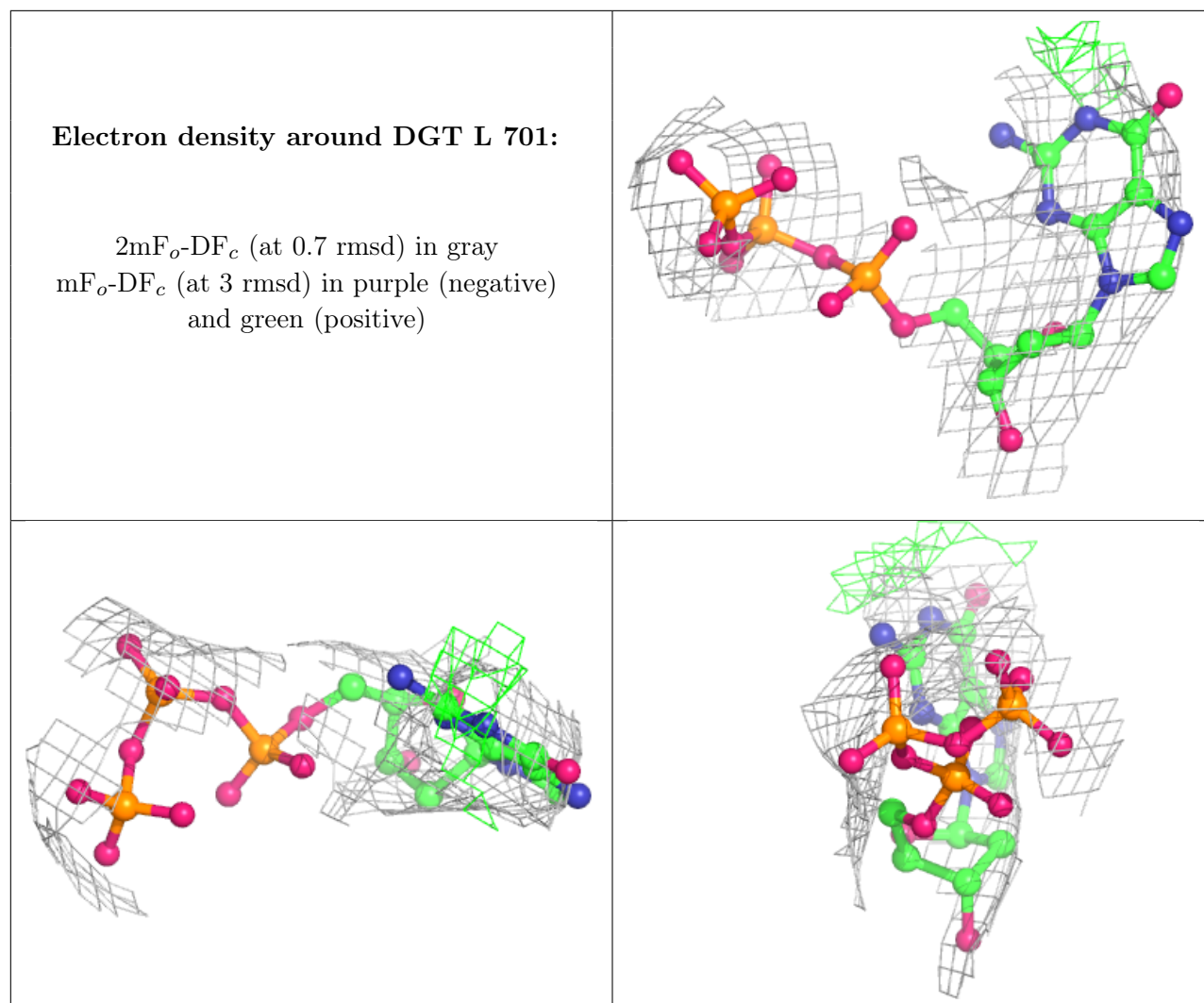mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
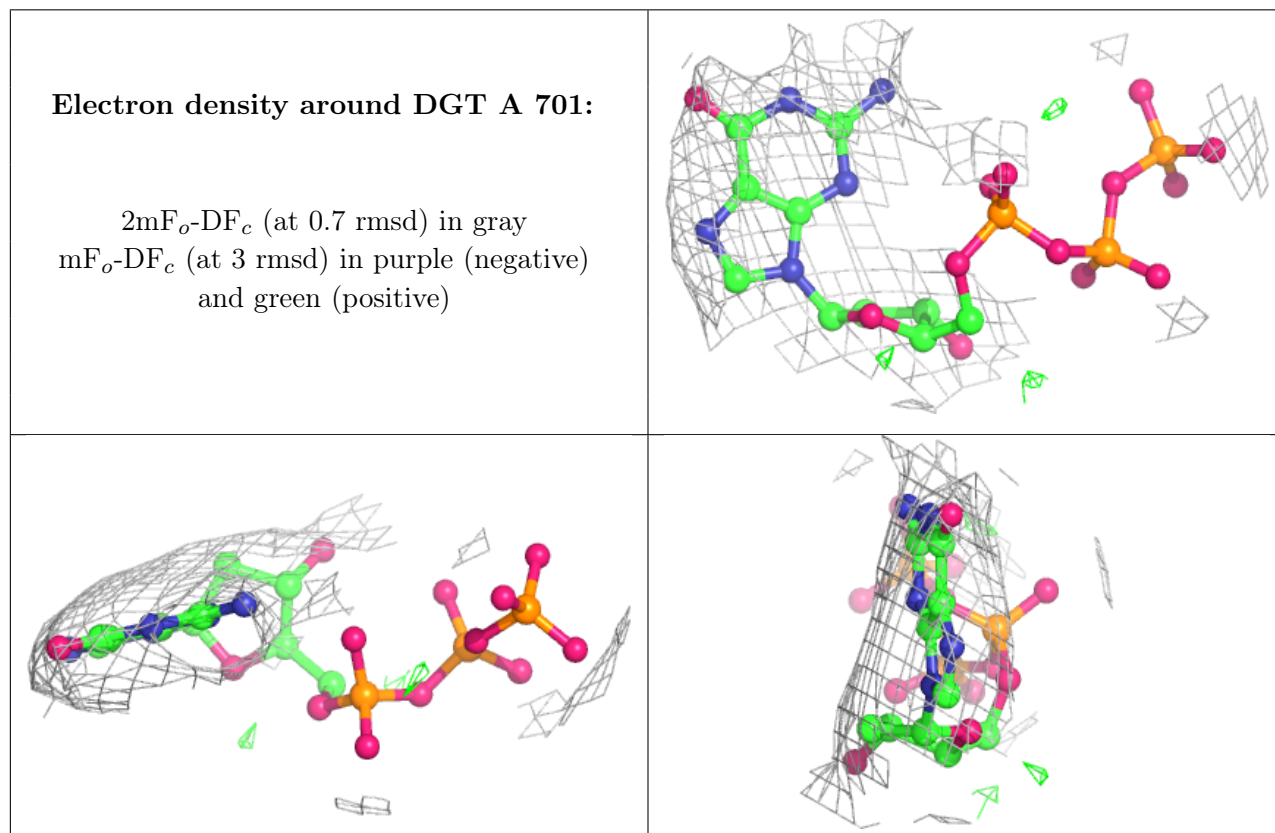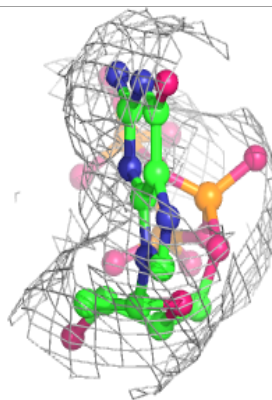
Electron density around DGT A 702:

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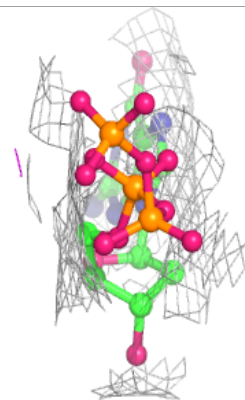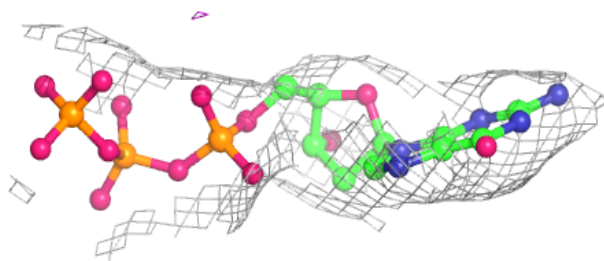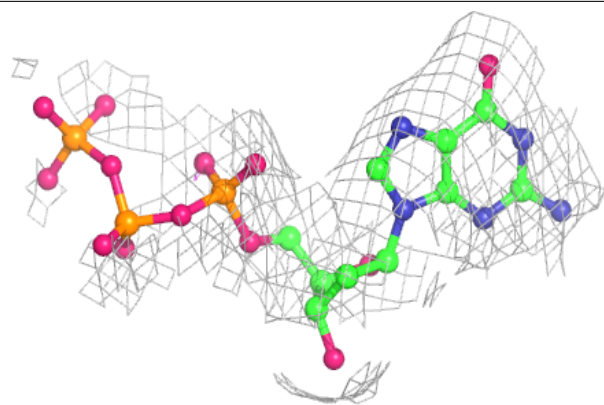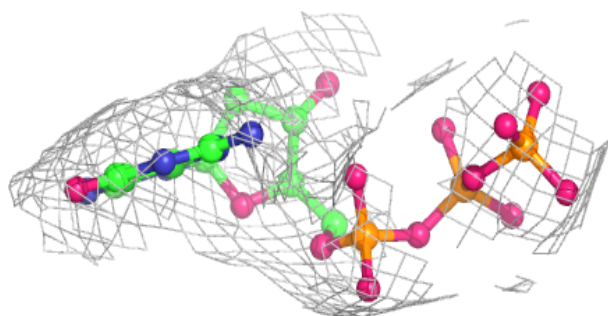

Electron density around DGT A 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
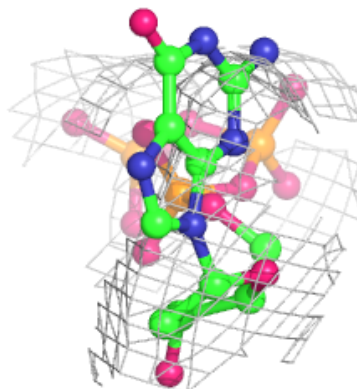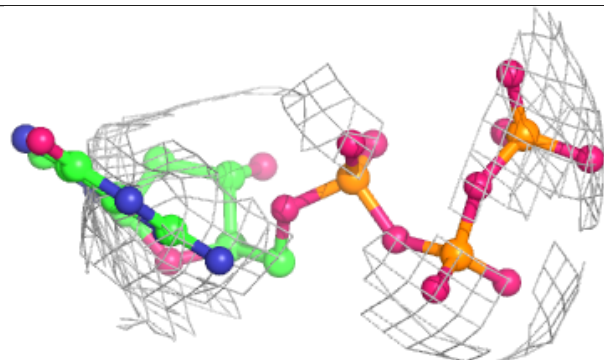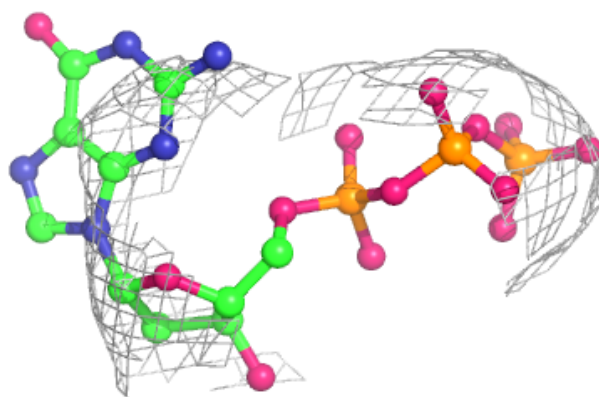
Electron density around DGT B 701:
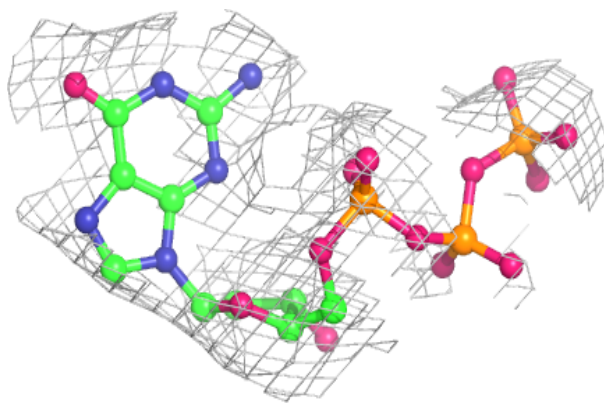
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
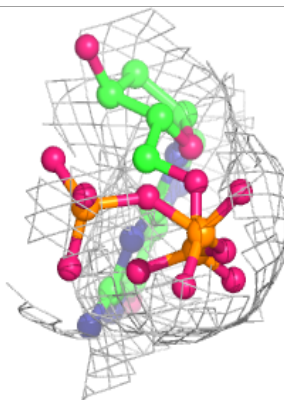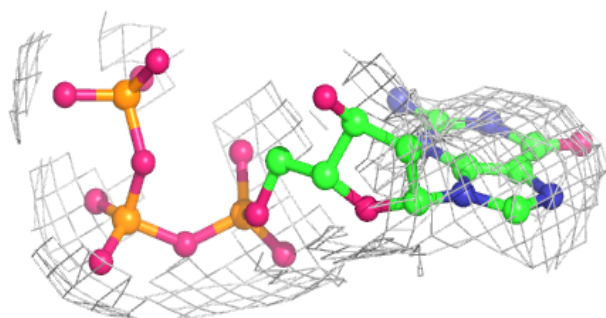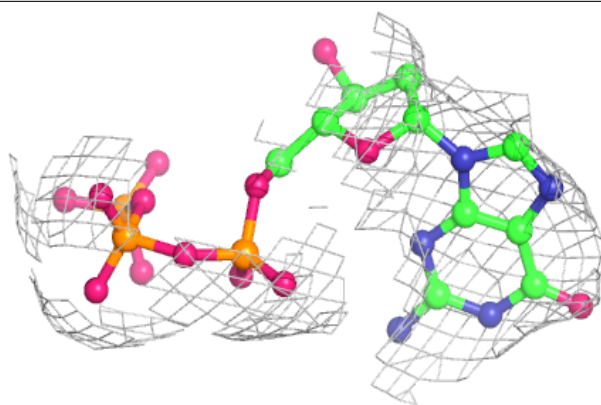
Electron density around DGT B 702:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
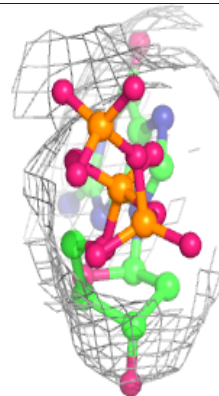and green (positive)
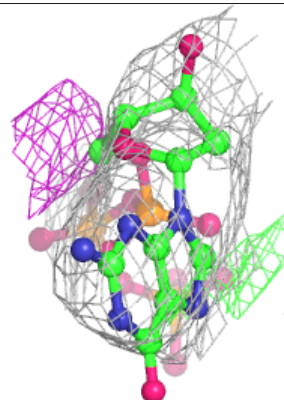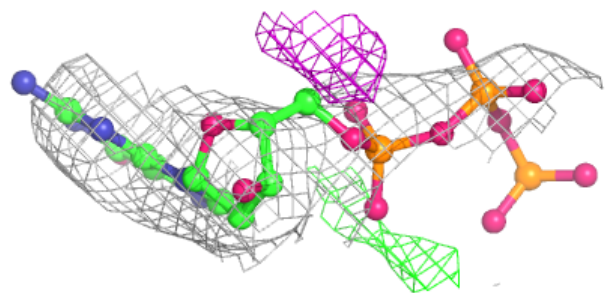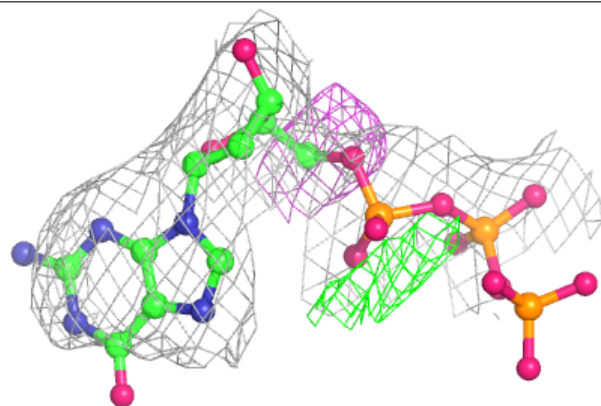
Electron density around DGT C 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
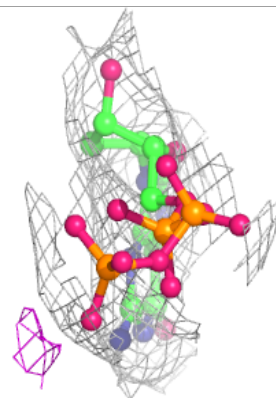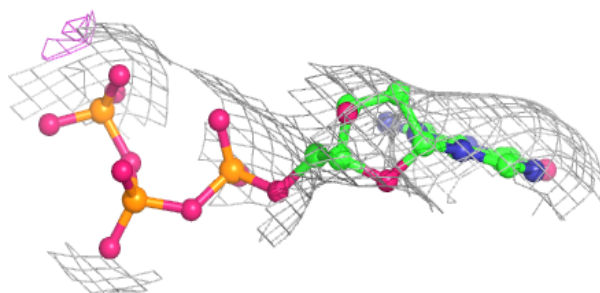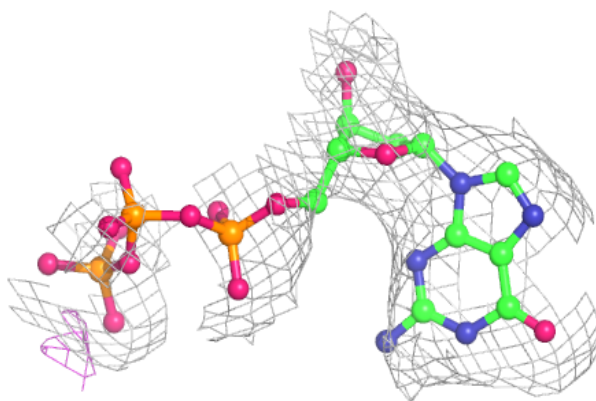
Electron density around DGT C 702:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
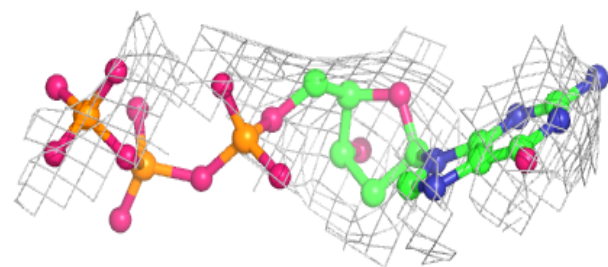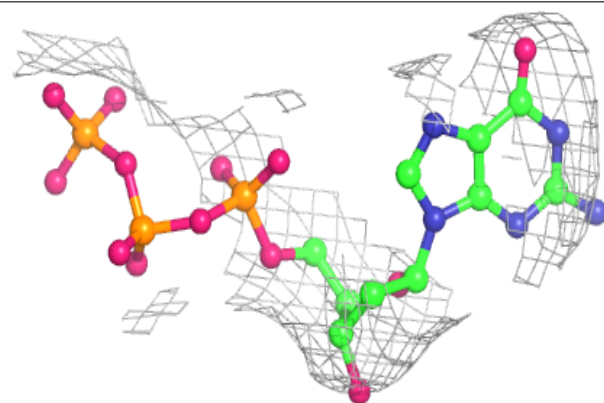and green (positive)
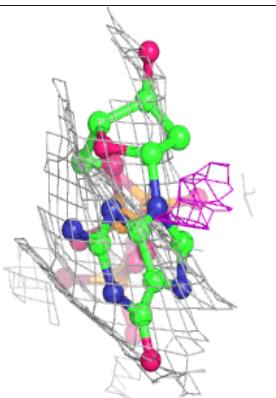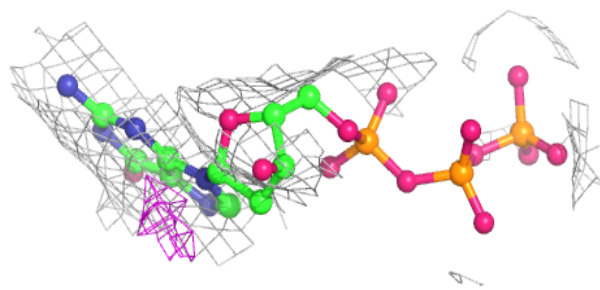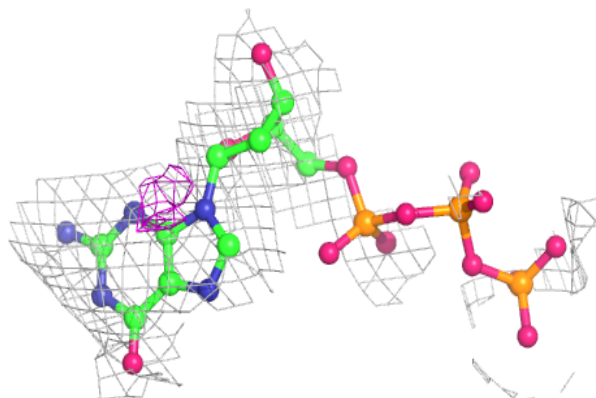
Electron density around DGT D 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
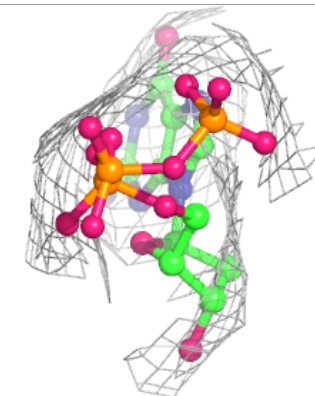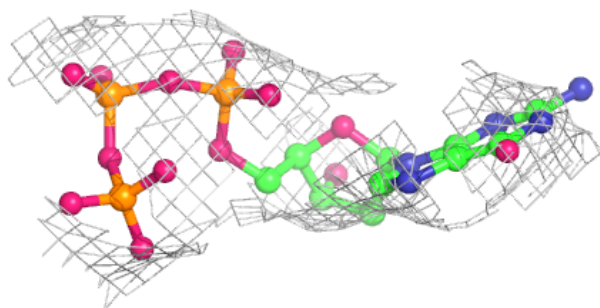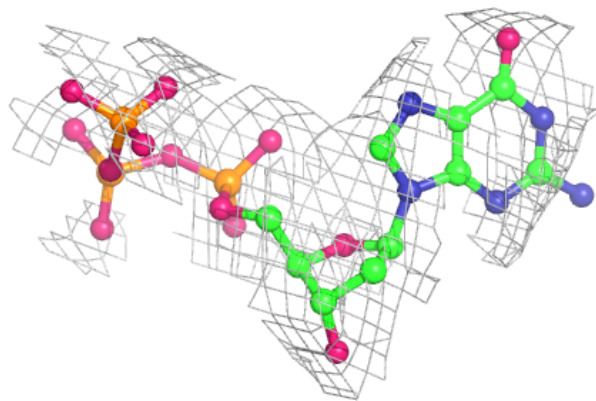
Electron density around DGT E 701:

$2mF_o$-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 E 702:

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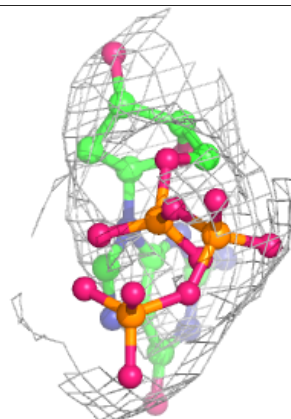and green (positive)

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)
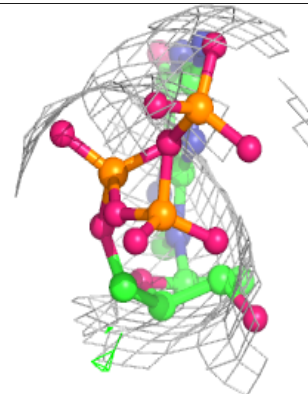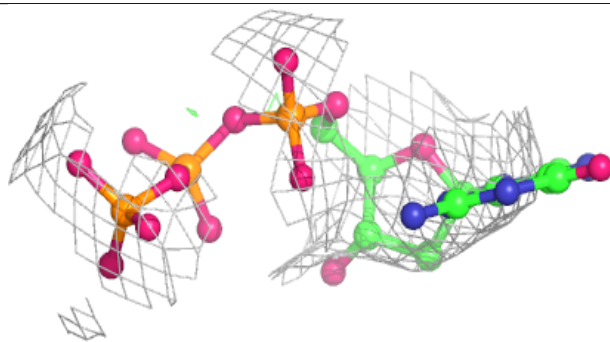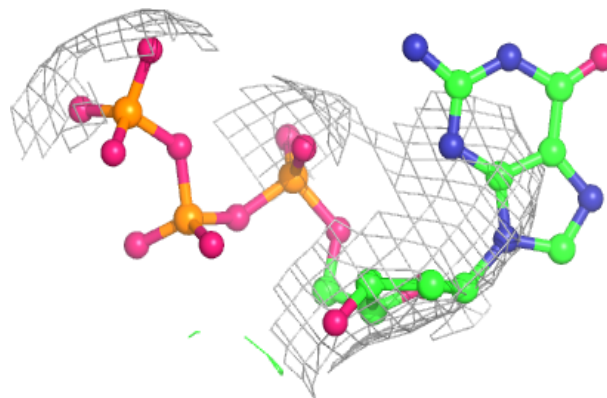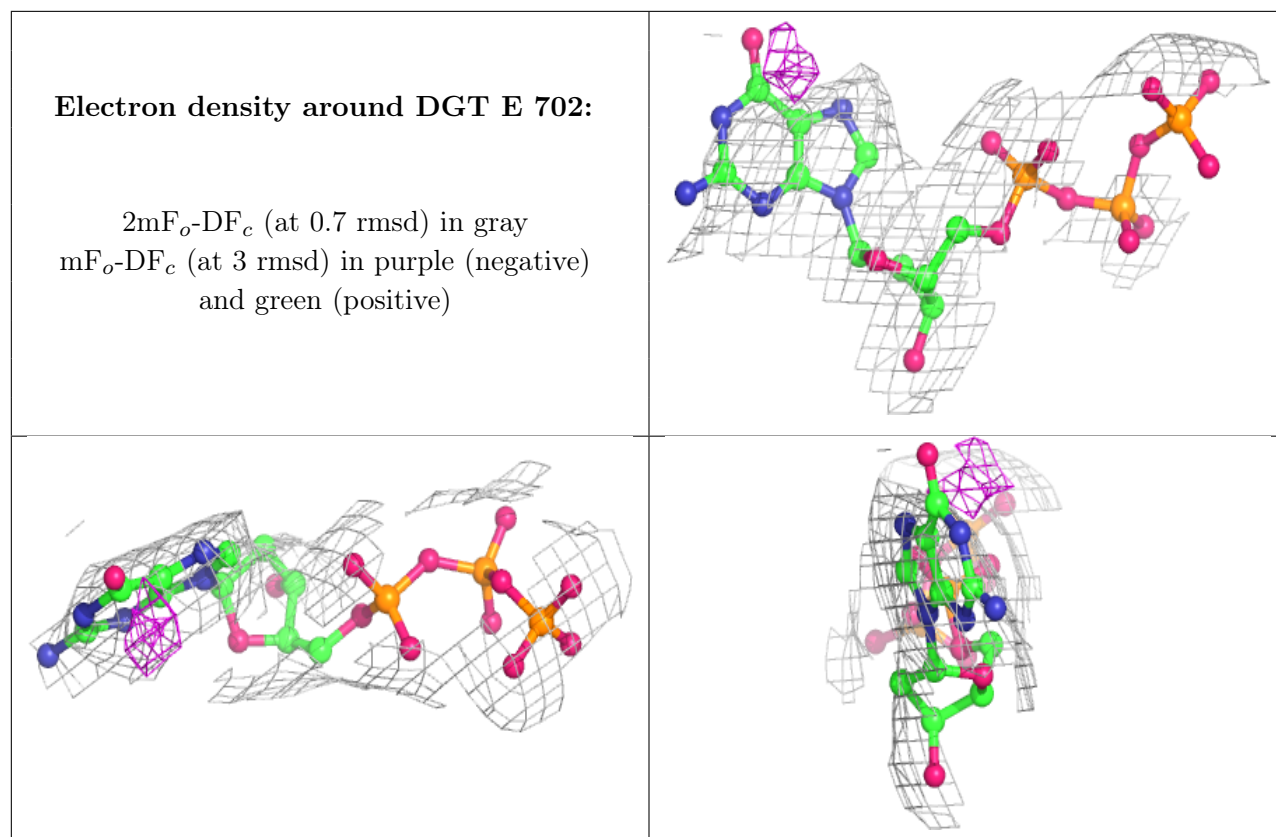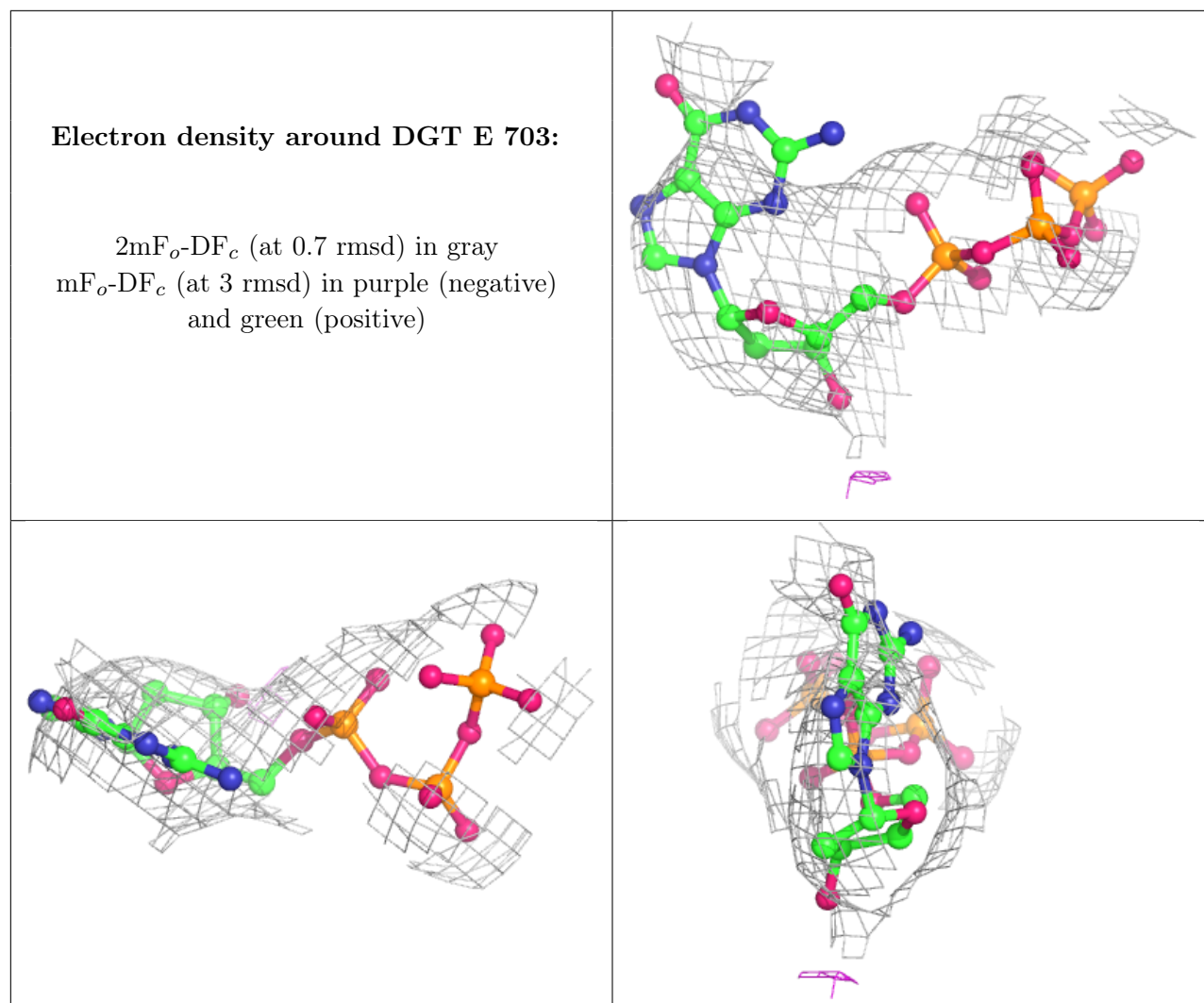
Electron density around DGT F 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
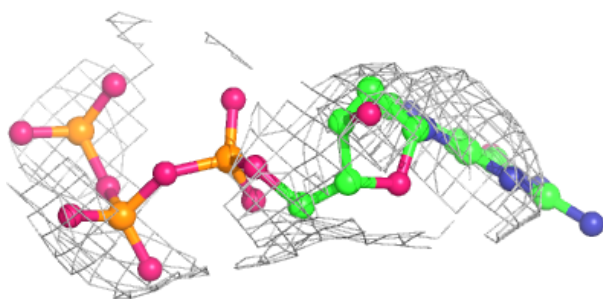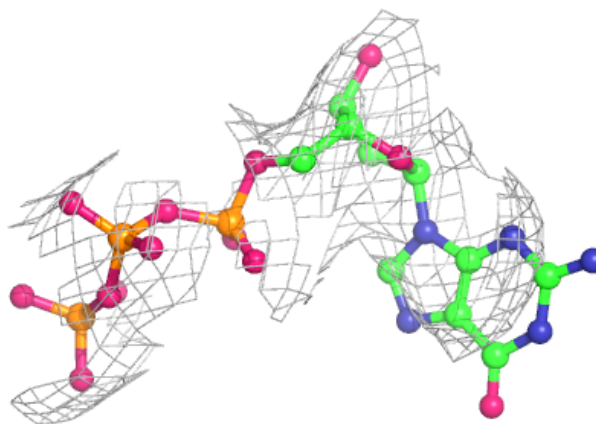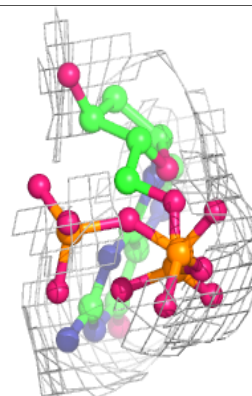and green (positive)
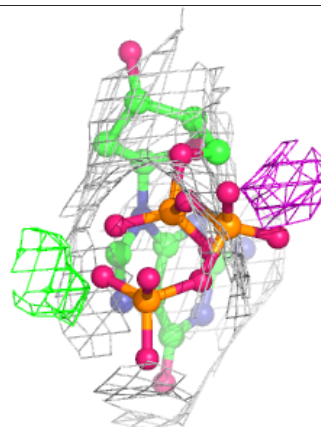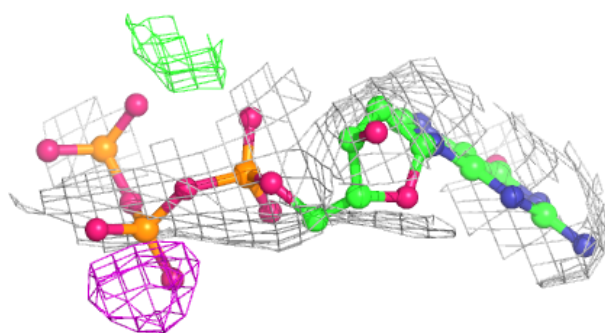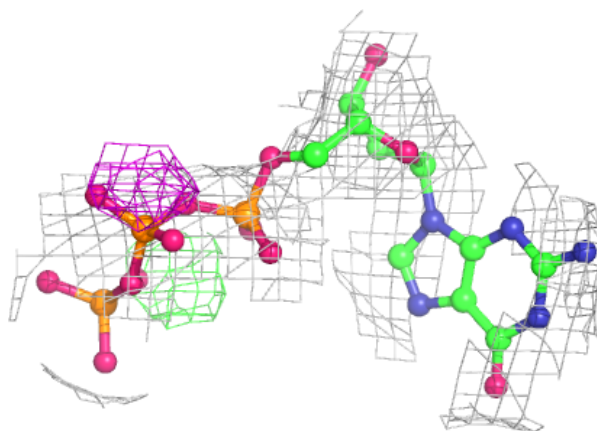
Electron density around DGT F 702:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
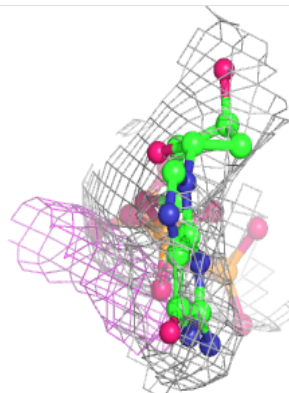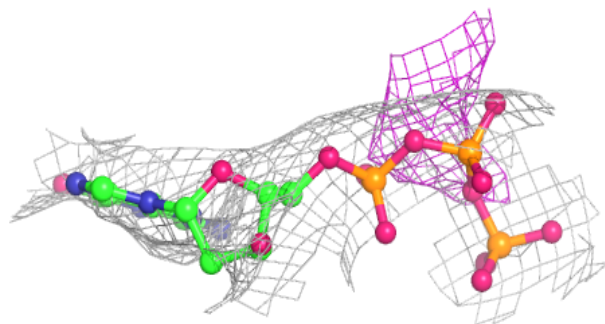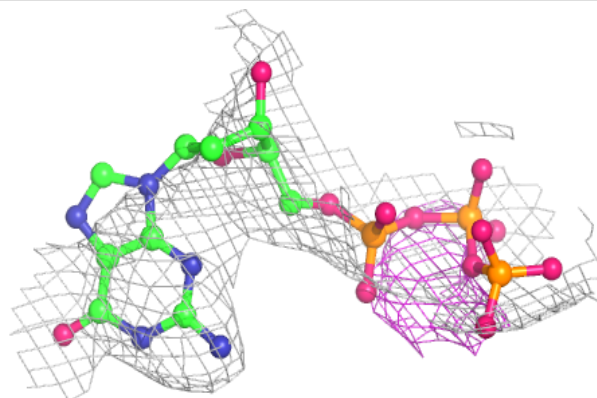
Electron density around DGT G 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
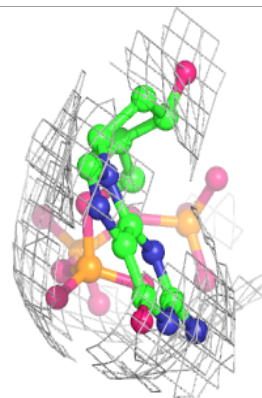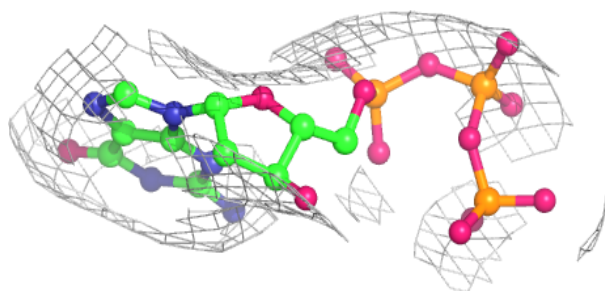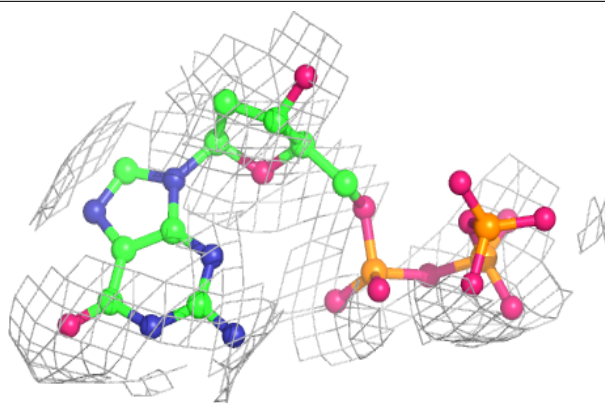
Electron density around DGT G 702:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
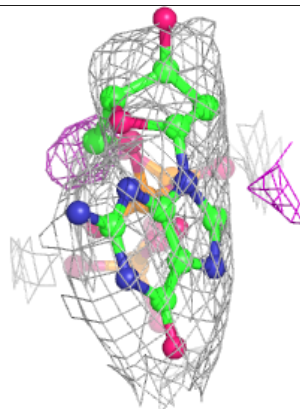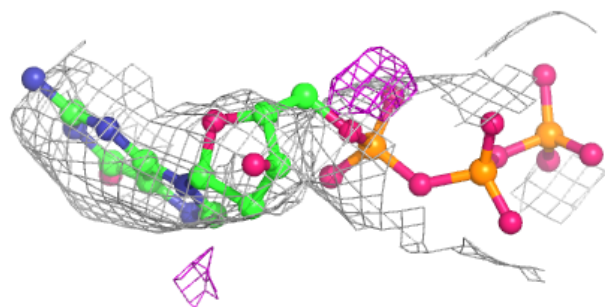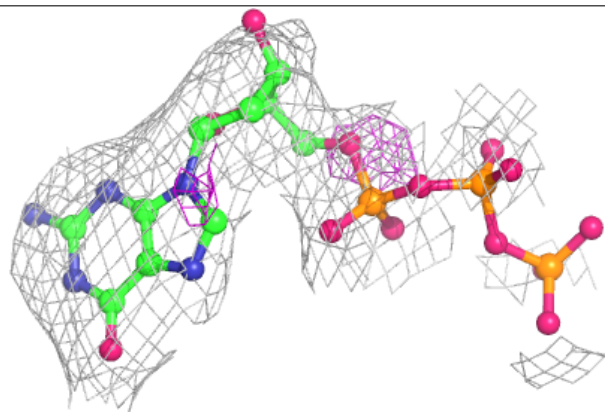
Electron density around DGT H 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
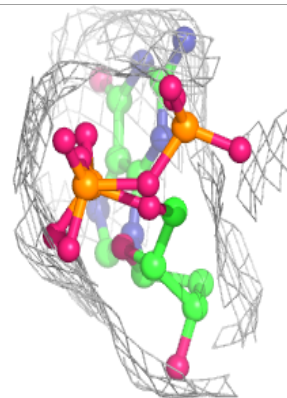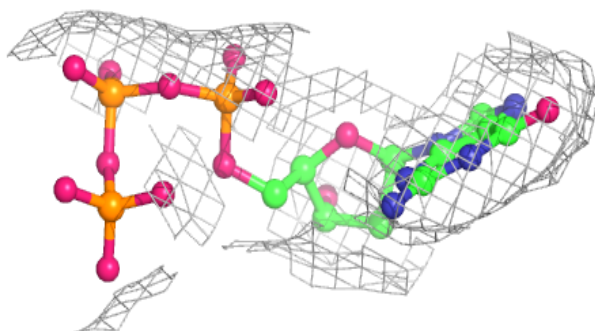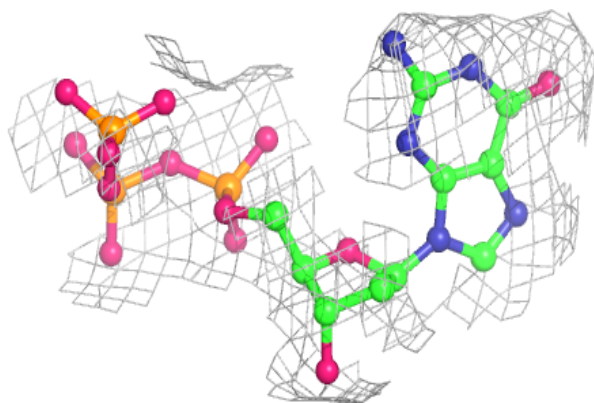
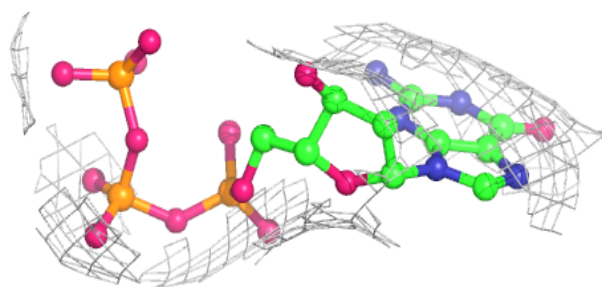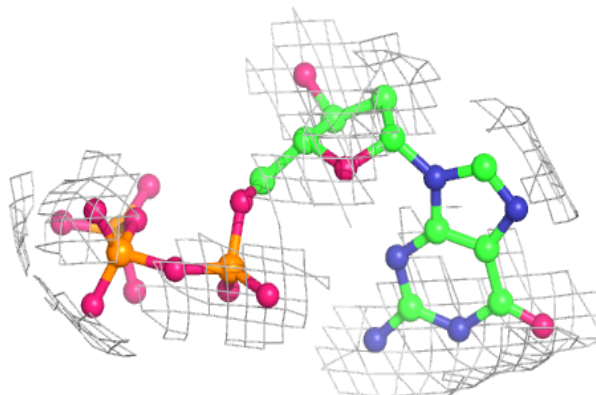**Electron density around DGT I 701:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
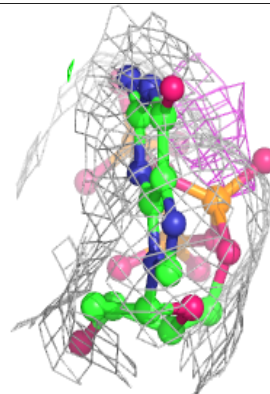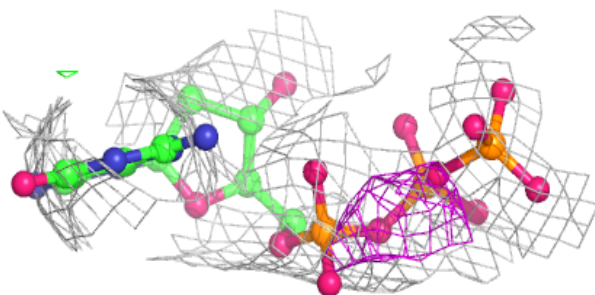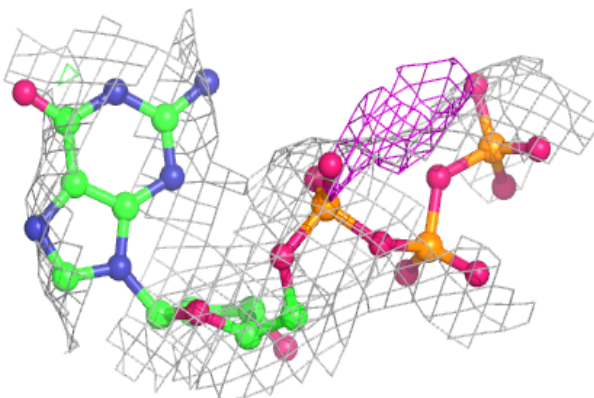
Electron density around DGT I 702:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
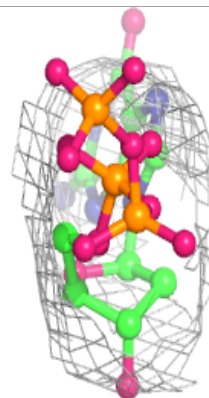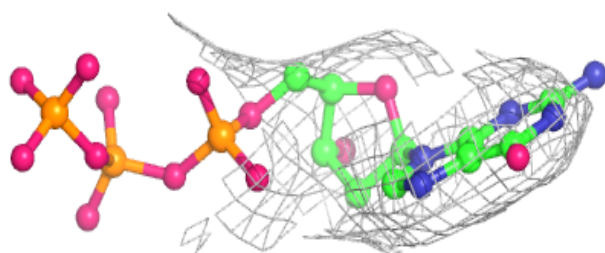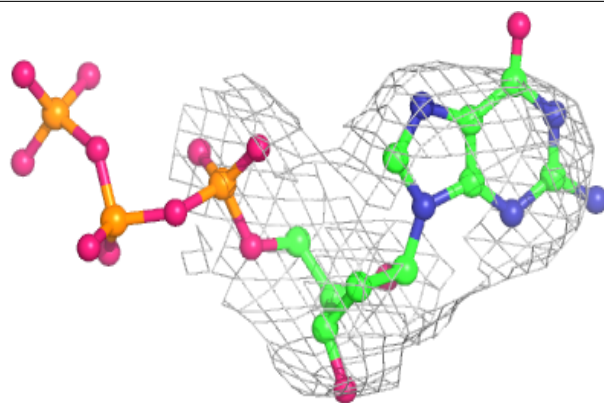
Electron density around DGT J 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
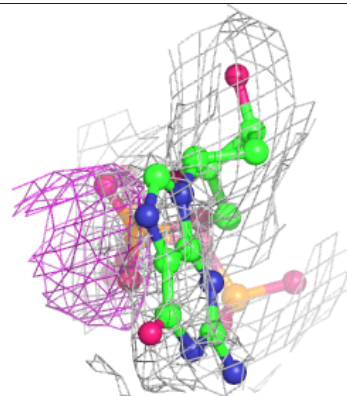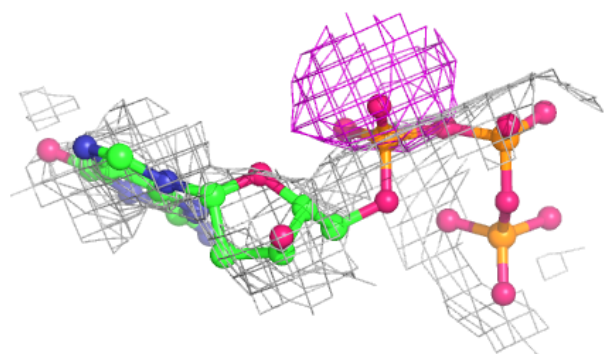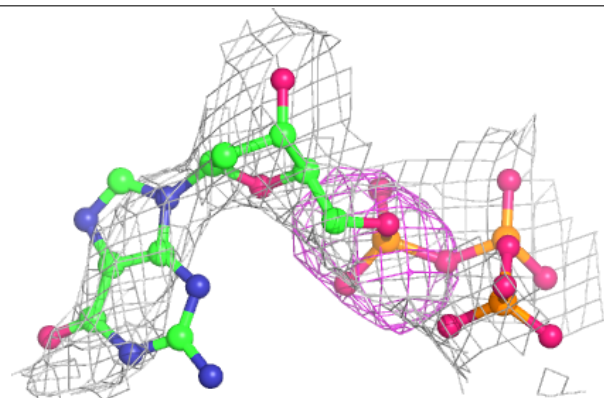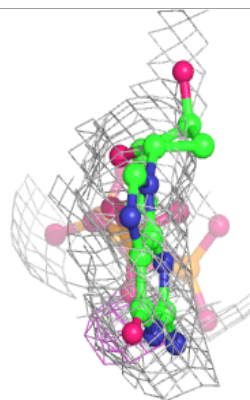
Electron density around DGT J 702:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
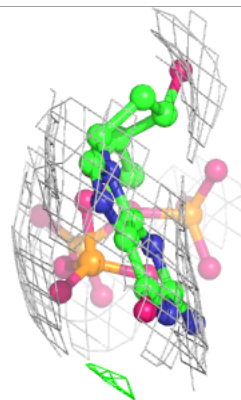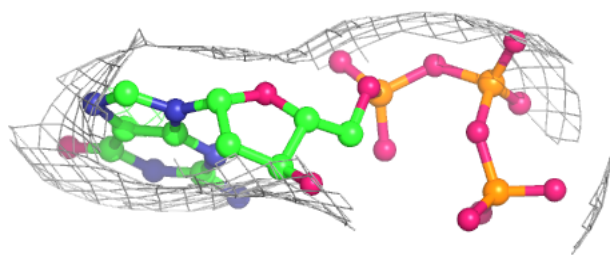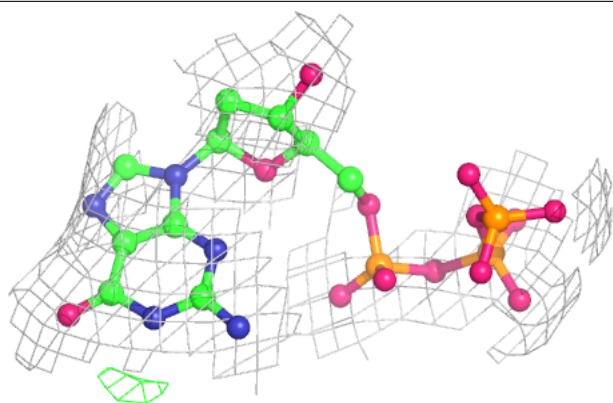
Electron density around DGT J 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
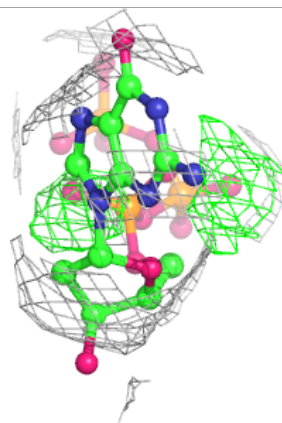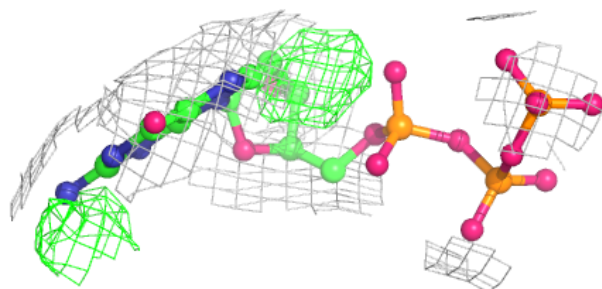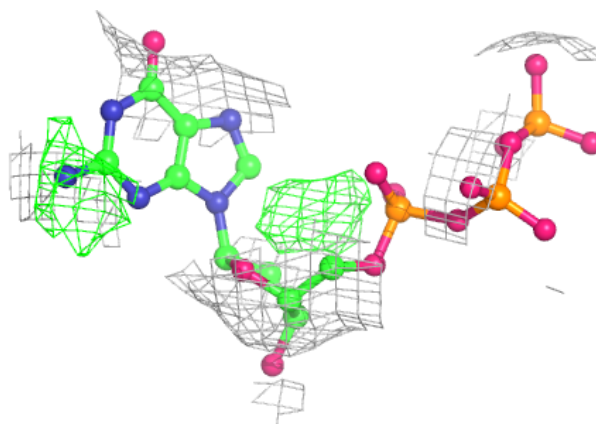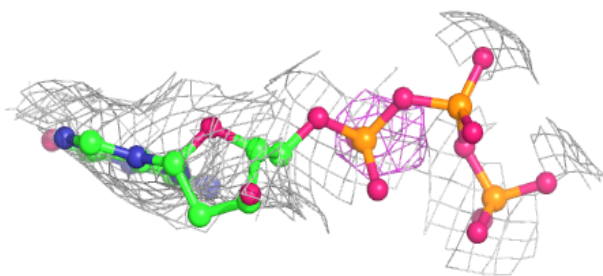
Electron density around DGT K 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
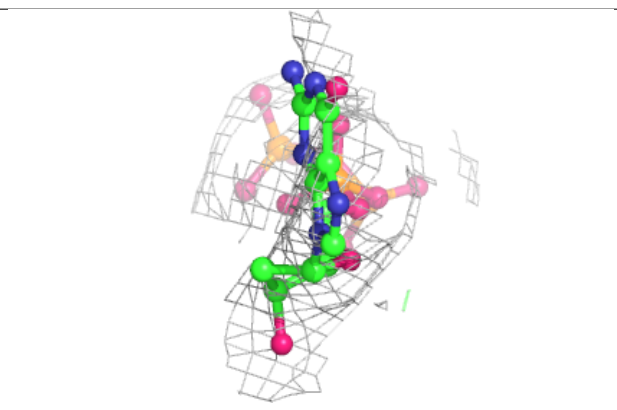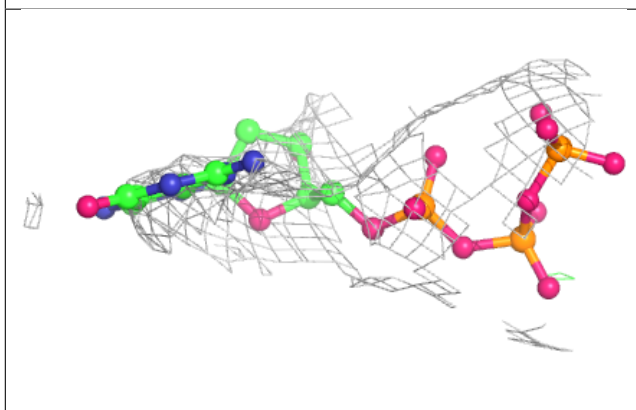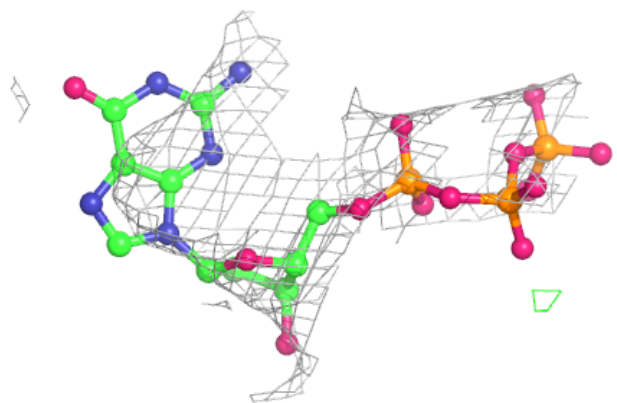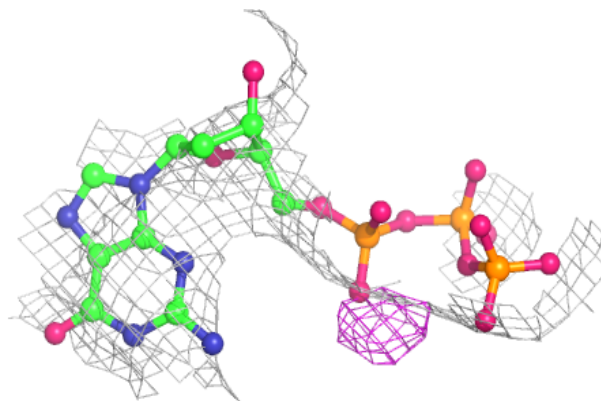

Electron density around DGT K 702:

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 L 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 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 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 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:

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

Electron density around DGT O 703:

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

Electron density around DGT P 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
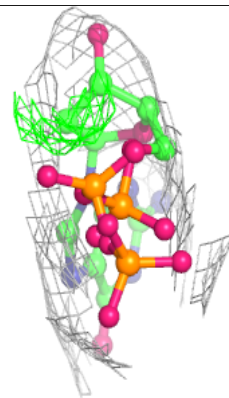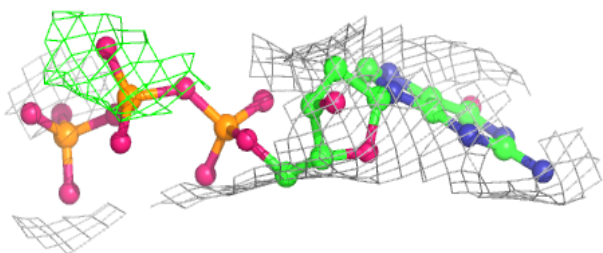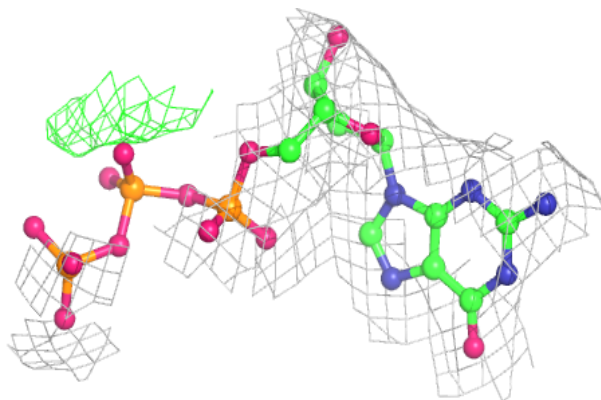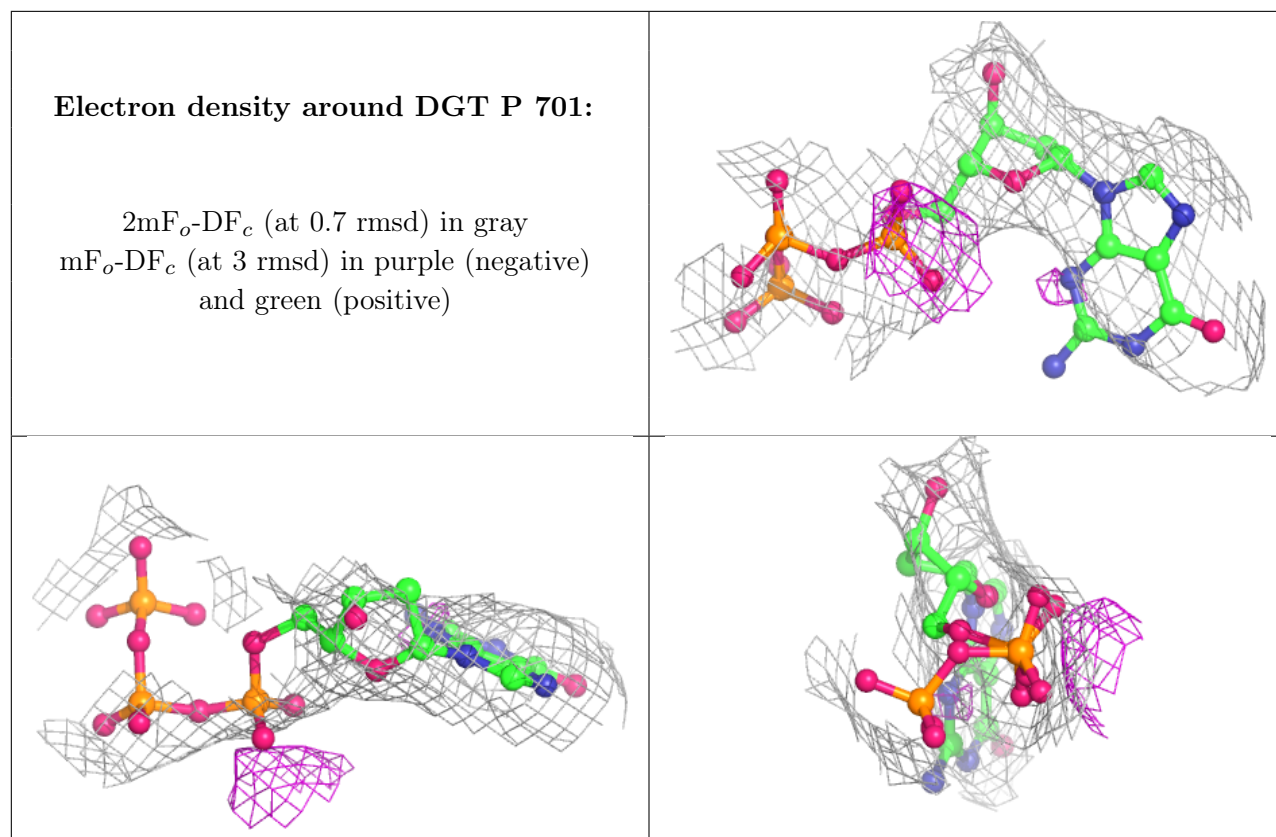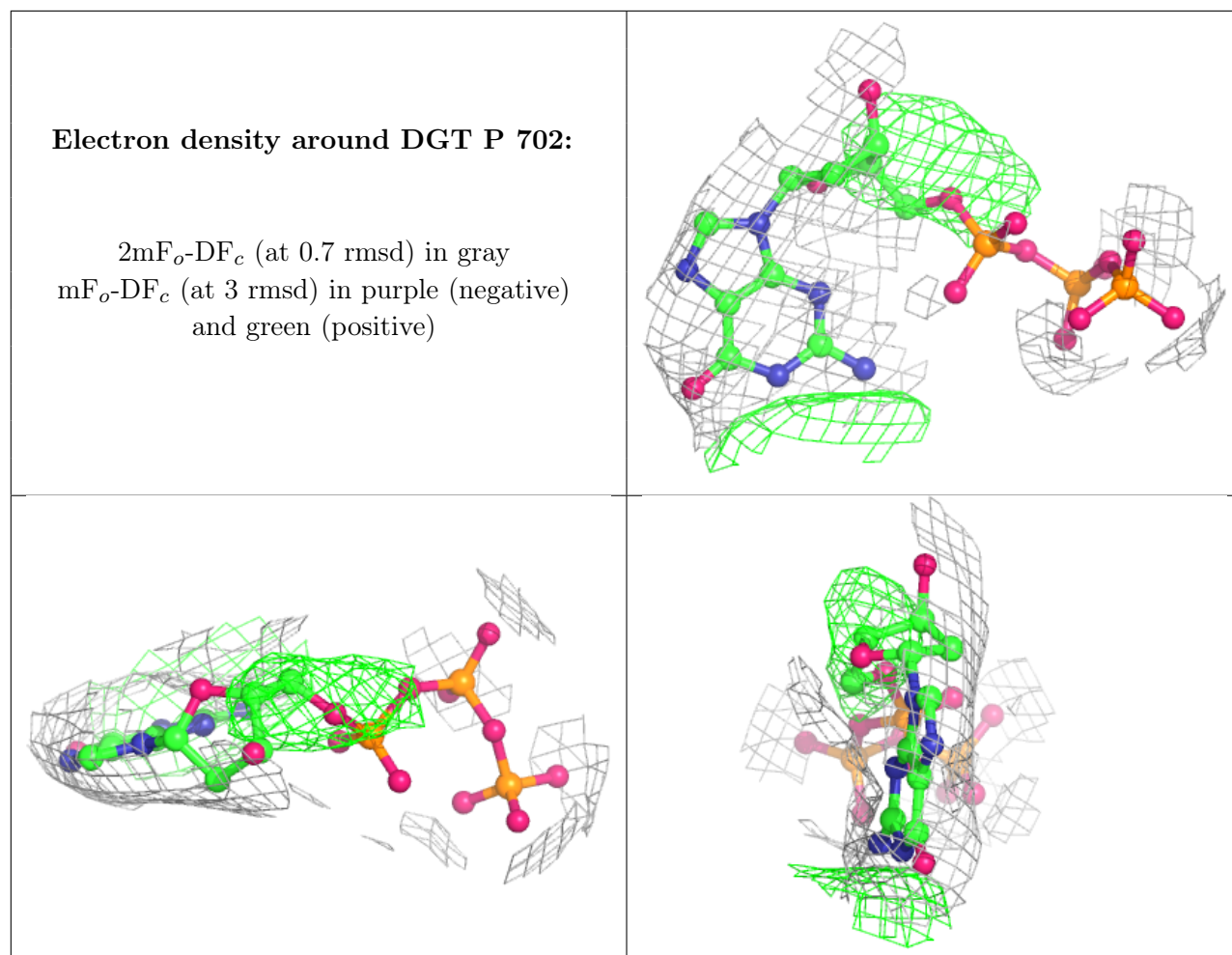
6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.