



Full wwPDB X-ray Structure Validation Report i

Mar 3, 2024 – 05:57 PM EST

PDB ID : 6DW5
Title : SAMHD1 Bound to Gemcitabine-TP in the Catalytic Pocket
Authors : Knecht, K.M.; Buzovetsky, O.; Schneider, C.; Thomas, D.; Srikanth, V.; Kaderali, L.; Tofoleanu, F.; Reiss, K.; Ferreiros, N.; Geisslinger, G.; Batista, V.S.; Ji, X.; Cinatl, J.; Keppler, O.T.; Xiong, Y.
Deposited on : 2018-06-26
Resolution : 1.93 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriaage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

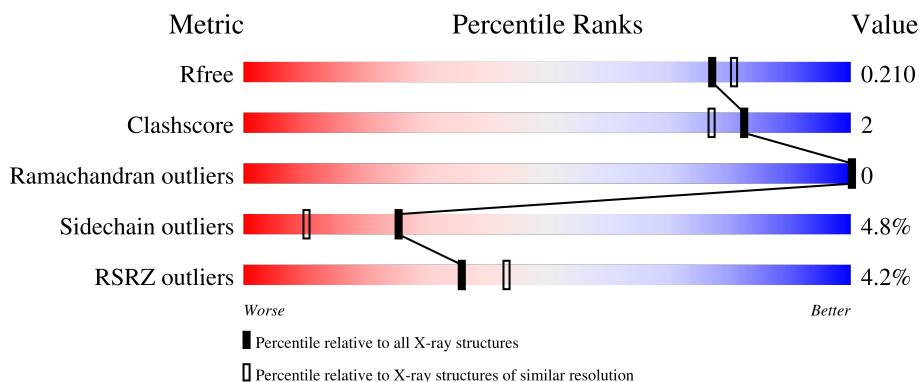
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

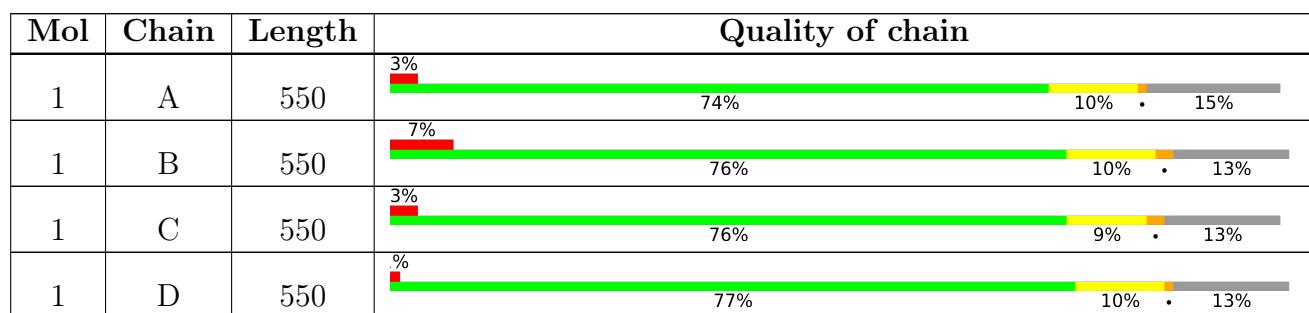
The reported resolution of this entry is 1.93 Å.

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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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.



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NI	C	701	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16603 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	468	Total	C 3825	N 2445	O 667	S 693	20	0	0
1	B	480	Total	C 3925	N 2513	O 684	S 708	20	0	0
1	C	481	Total	C 3933	N 2517	O 685	S 711	20	0	0
1	D	481	Total	C 3940	N 2522	O 687	S 711	20	0	1

There are 152 discrepancies between the modelled and reference sequences:

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

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

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

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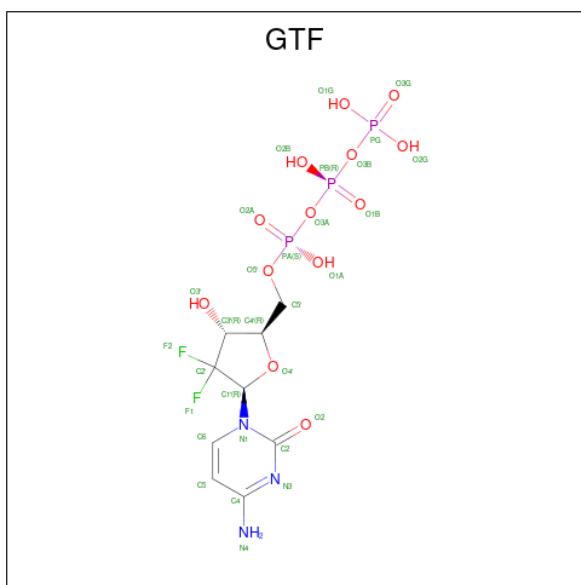
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag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

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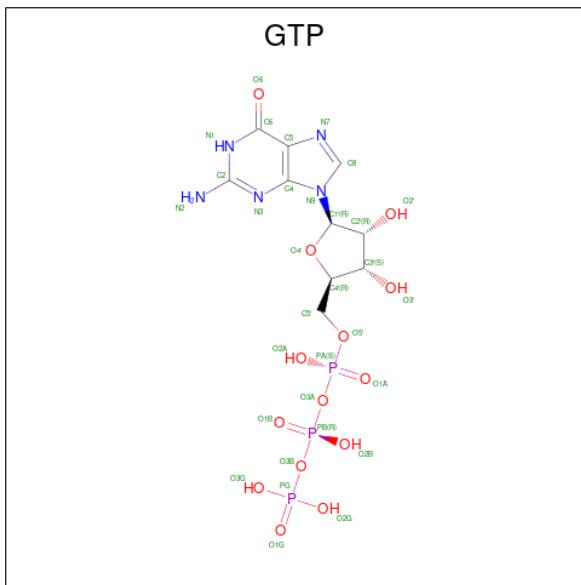
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-deoxy-2',2'-difluorocytidine 5'-(tetrahydrogen triphosphate) (three-letter code: GTF) (formula: C₉H₁₄F₂N₃O₁₃P₃).



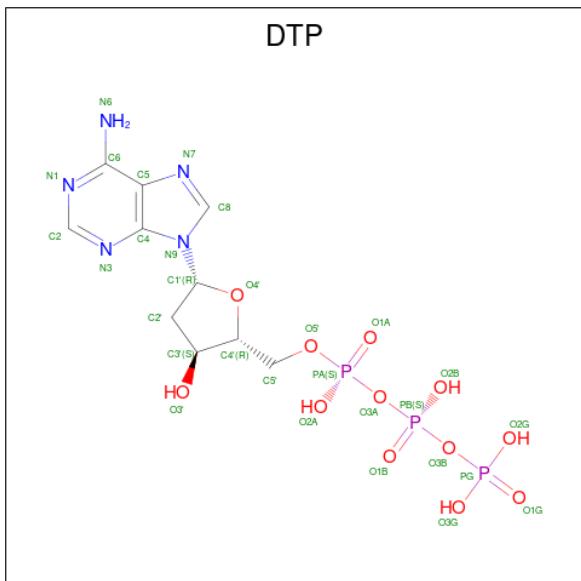
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		
2	B	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		
2	C	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		
2	D	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	32	10	5	14	3	0	0
3	B	1	32	10	5	14	3	0	0
3	B	1	32	10	5	14	3	0	0
3	D	1	32	10	5	14	3	0	0

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C 30	N 10	O 5	P 12	3	0
4	B	1	Total	C 30	N 10	O 5	P 12	3	0
4	C	1	Total	C 30	N 10	O 5	P 12	3	0
4	D	1	Total	C 30	N 10	O 5	P 12	3	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total Na 1 1		0	0
6	B	1	Total Na 1 1		0	0
6	C	2	Total Na 2 2		0	0

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total Ni 1 1		0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	164	Total O 164 164		0	0

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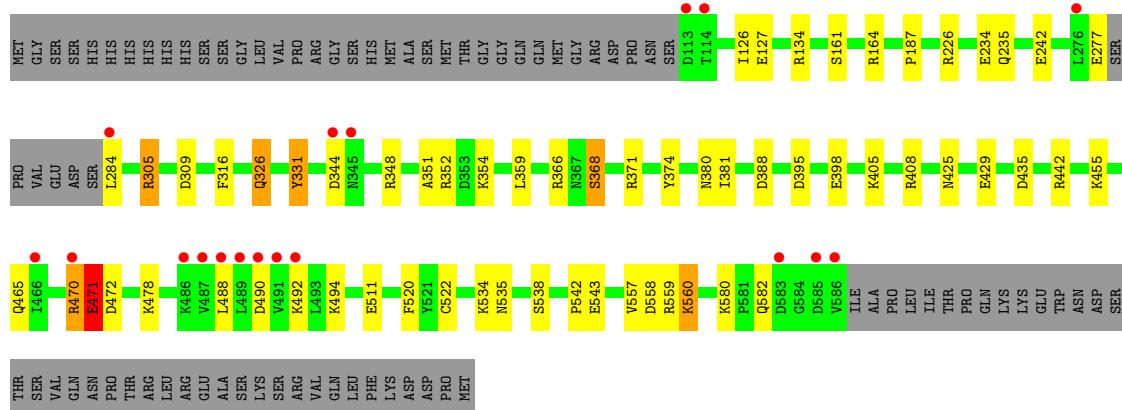
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	138	Total O 138 138	0	0
8	C	137	Total O 137 137	0	0
8	D	158	Total O 158 158	0	0

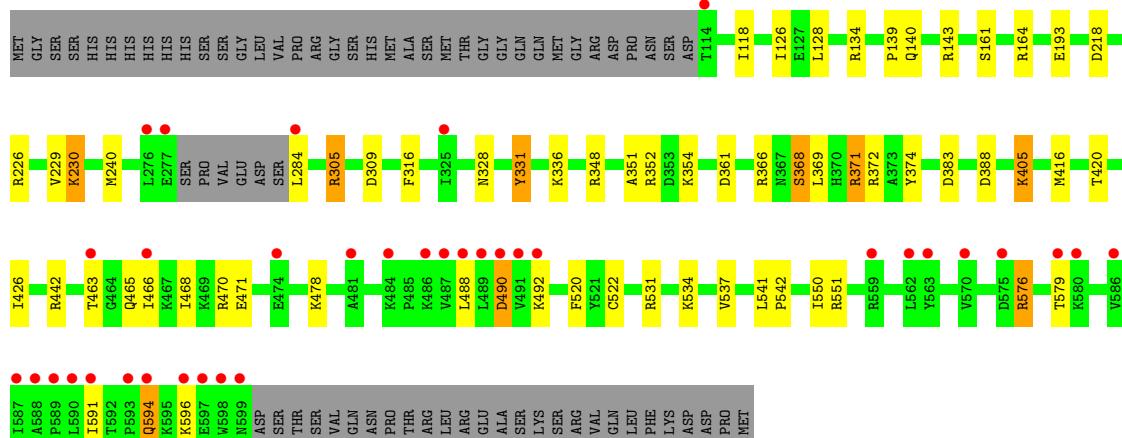
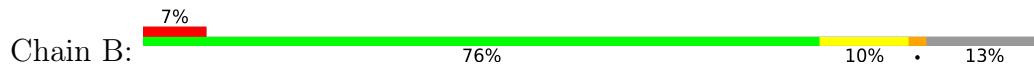
3 Residue-property plots

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

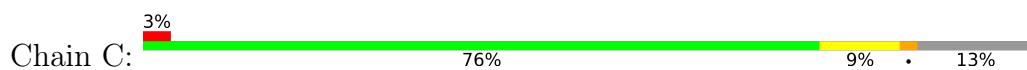
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

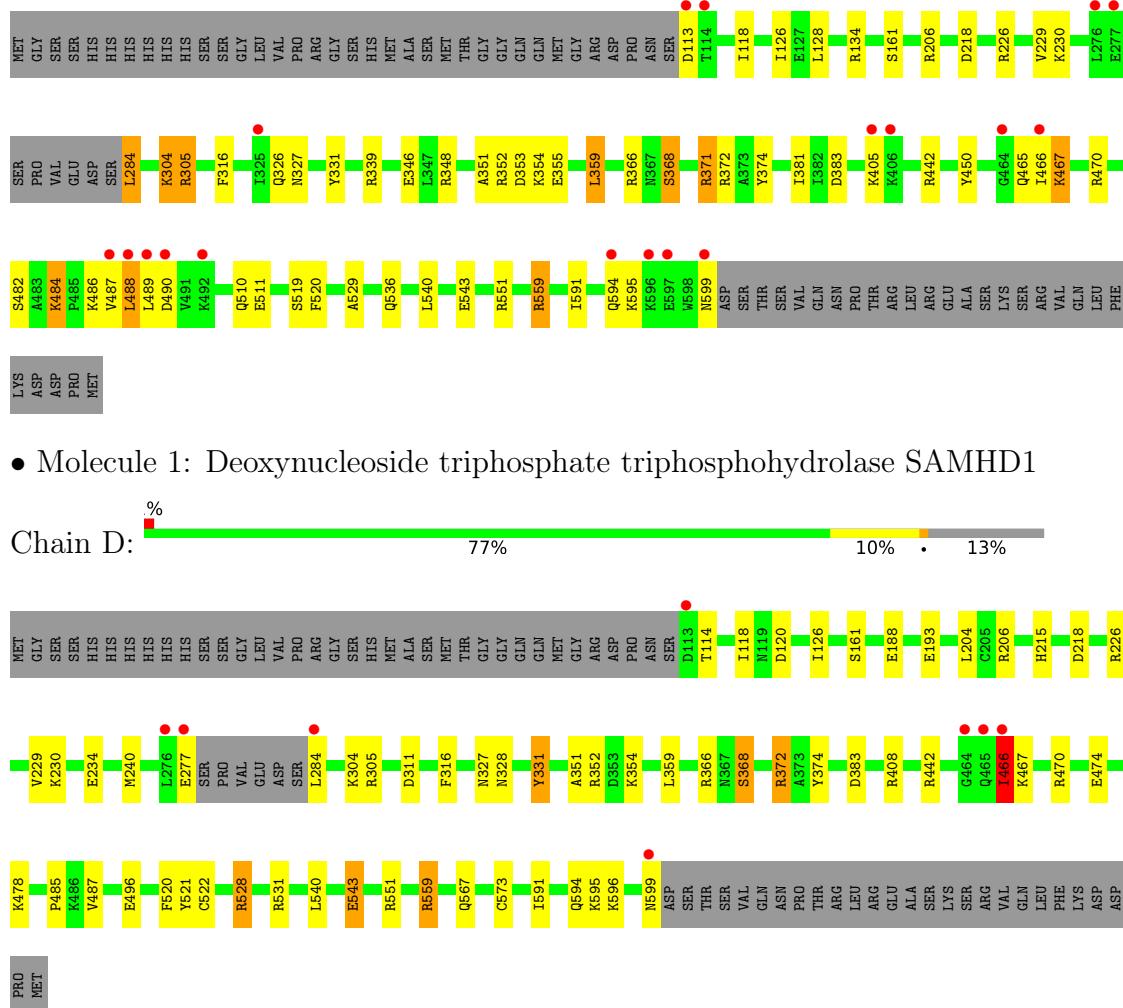


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.69 Å 142.90 Å 98.91 Å 90.00° 113.92° 90.00°	Depositor
Resolution (Å)	90.41 – 1.93 48.35 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.0 (90.41-1.93) 97.0 (48.35-1.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.95 (at 1.94 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R , R_{free}	0.173 , 0.205 0.181 , 0.210	Depositor DCC
R_{free} test set	7434 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16603	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, GTP, MG, NA, GTF, NI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.11	7/3913 (0.2%)	1.14	26/5279 (0.5%)
1	B	1.04	6/4017 (0.1%)	1.10	32/5422 (0.6%)
1	C	1.04	3/4025 (0.1%)	1.12	29/5433 (0.5%)
1	D	1.12	12/4036 (0.3%)	1.11	24/5448 (0.4%)
All	All	1.08	28/15991 (0.2%)	1.12	111/21582 (0.5%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	SER	CB-OG	12.57	1.58	1.42
1	C	161	SER	CB-OG	10.26	1.55	1.42
1	B	161	SER	CB-OG	9.29	1.54	1.42
1	C	368	SER	CB-OG	-8.60	1.31	1.42
1	B	368	SER	CB-OG	-8.13	1.31	1.42
1	B	371	ARG	CZ-NH2	7.87	1.43	1.33
1	D	521	TYR	CE1-CZ	-7.75	1.28	1.38
1	A	538	SER	CB-OG	7.58	1.52	1.42
1	D	188	GLU	CD-OE2	7.57	1.33	1.25
1	D	234	GLU	CD-OE1	7.48	1.33	1.25
1	D	368	SER	CB-OG	-7.25	1.32	1.42
1	A	368	SER	CB-OG	-7.18	1.32	1.42
1	D	327	ASN	C-O	-7.07	1.09	1.23
1	A	234	GLU	CD-OE1	6.64	1.32	1.25
1	D	193	GLU	CG-CD	6.32	1.61	1.51
1	A	429	GLU	CG-CD	6.02	1.60	1.51
1	D	496	GLU	CD-OE2	6.02	1.32	1.25
1	D	543	GLU	CD-OE1	5.94	1.32	1.25
1	A	511	GLU	CG-CD	5.91	1.60	1.51
1	D	408	ARG	CZ-NH1	5.76	1.40	1.33
1	B	193	GLU	CG-CD	5.74	1.60	1.51
1	A	398	GLU	CD-OE2	5.48	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	408	ARG	CD-NE	5.42	1.55	1.46
1	D	573	CYS	CB-SG	-5.34	1.73	1.81
1	B	161	SER	CA-CB	5.25	1.60	1.52
1	C	511	GLU	CG-CD	5.25	1.59	1.51
1	D	161	SER	CB-OG	5.17	1.49	1.42
1	B	193	GLU	CD-OE2	5.12	1.31	1.25

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	442	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	B	442	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	C	371	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	C	442	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	A	442	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	B	371	ARG	NE-CZ-NH1	-10.21	115.20	120.30
1	A	442	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	C	304	LYS	CD-CE-NZ	9.29	133.06	111.70
1	C	371	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	B	372	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	A	371	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	371	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	B	551	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	C	551	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	D	226	ARG	NE-CZ-NH2	7.97	124.29	120.30
1	D	366	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	C	352	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	B	531	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	372	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	D	531	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	366	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	408	ARG	CG-CD-NE	-7.28	96.52	111.80
1	D	442	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	218	ASP	CB-CG-OD1	7.15	124.73	118.30
1	C	134	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	388	ASP	CB-CG-OD1	7.03	124.63	118.30
1	C	226	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	C	488	LEU	CA-CB-CG	7.00	131.40	115.30
1	A	226	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	B	226	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	B	442	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	134	ARG	NE-CZ-NH2	6.62	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	366	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	535	ASN	CB-CA-C	-6.47	97.45	110.40
1	C	359	LEU	CB-CG-CD1	6.43	121.94	111.00
1	A	366	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	594	GLN	CB-CA-C	-6.30	97.79	110.40
1	C	442	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	366	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	348	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	353	ASP	CB-CG-OD1	6.15	123.84	118.30
1	C	359	LEU	CB-CG-CD2	6.13	121.42	111.00
1	C	206	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	522	CYS	CA-CB-SG	-6.10	103.02	114.00
1	A	316	PHE	CB-CG-CD1	6.07	125.05	120.80
1	A	305	ARG	CB-CG-CD	6.06	127.36	111.60
1	D	206	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	348	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	354	LYS	CB-CA-C	-6.04	98.33	110.40
1	C	352	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	B	388	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	371	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	D	559	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	466	ILE	N-CA-CB	5.99	124.58	110.80
1	D	372	ARG	CG-CD-NE	5.96	124.31	111.80
1	B	134	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	C	218	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	354	LYS	CB-CA-C	-5.89	98.61	110.40
1	D	551	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	B	551	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	B	383	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	206	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	371	ARG	CD-NE-CZ	5.77	131.68	123.60
1	D	528	ARG	CG-CD-NE	5.77	123.91	111.80
1	D	218	ASP	CB-CG-OD1	5.74	123.47	118.30
1	C	559	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	348	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	395	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	522	CYS	CA-CB-SG	-5.71	103.73	114.00
1	D	354	LYS	CB-CA-C	-5.69	99.02	110.40
1	D	528	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	206	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	383	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	316	PHE	CB-CG-CD1	5.66	124.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	LYS	CD-CE-NZ	5.65	124.70	111.70
1	D	218	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	C	366	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	120	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	366	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	352	ARG	CG-CD-NE	-5.42	100.41	111.80
1	D	311	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	371	ARG	CA-CB-CG	-5.42	101.48	113.40
1	C	371	ARG	CD-NE-CZ	5.42	131.18	123.60
1	D	316	PHE	CB-CG-CD1	5.39	124.57	120.80
1	B	134	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	471	GLU	CA-CB-CG	5.29	125.03	113.40
1	A	435	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	B	164	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	309	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	348	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	305	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	352	ARG	CG-CD-NE	-5.18	100.92	111.80
1	B	230	LYS	CA-CB-CG	5.18	124.79	113.40
1	C	467	LYS	N-CA-CB	5.18	119.92	110.60
1	B	594	GLN	CA-CB-CG	5.16	124.75	113.40
1	D	352	ARG	CG-CD-NE	-5.15	100.98	111.80
1	D	522	CYS	CA-CB-SG	-5.13	104.77	114.00
1	A	309	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	242	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	C	466	ILE	CB-CA-C	-5.12	101.37	111.60
1	B	576	ARG	CA-CB-CG	5.11	124.64	113.40
1	D	305	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	164	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	204	LEU	CA-CB-CG	5.09	127.02	115.30
1	C	316	PHE	CB-CG-CD2	-5.09	117.23	120.80
1	B	361	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	316	PHE	CB-CG-CD1	5.07	124.35	120.80
1	C	339	ARG	CG-CD-NE	5.07	122.45	111.80
1	B	388	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	284	LEU	CA-CB-CG	5.04	126.88	115.30
1	C	383	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	3825	0	3806	19	2
1	B	3925	0	3917	24	0
1	C	3933	0	3921	24	0
1	D	3940	0	3928	16	2
2	A	30	0	10	3	0
2	B	30	0	10	3	0
2	C	30	0	10	3	0
2	D	30	0	9	6	0
3	A	32	0	12	0	0
3	B	64	0	24	0	0
3	D	32	0	12	0	0
4	A	30	0	12	0	0
4	B	30	0	12	1	0
4	C	30	0	12	0	0
4	D	30	0	12	0	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
7	C	1	0	0	0	0
8	A	164	0	0	1	0
8	B	138	0	0	0	0
8	C	137	0	0	2	0
8	D	158	0	0	0	0
All	All	16603	0	15707	79	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (79) 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)
2:C:705:GTF:O4'	2:C:705:GTF:C1'	1.71	1.26
2:A:701:GTF:O4'	2:A:701:GTF:C1'	1.69	1.21
2:D:702:GTF:O4'	2:D:702:GTF:C1'	1.69	1.20
2:B:701:GTF:O4'	2:B:701:GTF:C1'	1.68	1.17
1:D:215:HIS:CE1	2:D:702:GTF:O1A	2.20	0.94
1:A:534:LYS:HE3	1:A:542:PRO:O	1.78	0.83
1:A:543:GLU:HG3	1:C:543:GLU:HG3	1.61	0.81
1:A:558:ASP:OD2	1:A:560:LYS:HG2	1.83	0.77
1:D:215:HIS:NE2	2:D:702:GTF:O1A	2.20	0.74
1:B:140:GLN:CG	1:B:240:MET:HE1	2.25	0.66
1:A:543:GLU:CG	1:C:543:GLU:HG3	2.28	0.64
1:D:591:ILE:O	1:D:594:GLN:HG2	1.97	0.64
1:C:591:ILE:O	1:C:594:GLN:HG2	1.98	0.63
1:B:591:ILE:O	1:B:594:GLN:HG2	2.00	0.61
1:B:140:GLN:HG3	1:B:240:MET:HE1	1.83	0.61
1:B:534:LYS:O	1:B:537:VAL:HG22	2.01	0.61
1:C:374:TYR:CE1	2:C:705:GTF:F1	2.45	0.60
1:A:470:ARG:C	1:A:470:ARG:HD3	2.24	0.58
1:A:326:GLN:HG2	1:C:327:ASN:O	2.03	0.58
1:C:326:GLN:NE2	8:C:801:HOH:O	2.21	0.58
1:D:374:TYR:CE1	2:D:702:GTF:F1	2.51	0.54
1:A:326:GLN:OE1	1:C:326:GLN:OE1	2.27	0.53
1:B:537:VAL:HG23	1:B:541:LEU:CD1	2.38	0.53
1:A:470:ARG:HD3	1:A:471:GLU:N	2.24	0.53
1:C:487:VAL:HG13	1:C:489:LEU:HG	1.89	0.53
1:A:380:ASN:OD1	8:A:801:HOH:O	2.19	0.52
1:D:215:HIS:HE1	2:D:702:GTF:O1A	1.82	0.52
1:D:595:LYS:O	1:D:599:ASN:ND2	2.43	0.51
1:A:374:TYR:CE1	2:A:701:GTF:F1	2.53	0.51
1:B:374:TYR:CE1	2:B:701:GTF:F1	2.53	0.51
1:C:595:LYS:O	1:C:599:ASN:ND2	2.43	0.51
1:C:305:ARG:HG2	1:C:348:ARG:NH1	2.26	0.51
1:B:328:ASN:HB3	1:D:328:ASN:HB3	1.92	0.50
1:D:487:VAL:HG21	1:D:567:GLN:HG3	1.93	0.50
1:C:374:TYR:CZ	2:C:705:GTF:F1	2.54	0.49
1:A:127:GLU:OE2	1:B:336:LYS:HE2	2.12	0.49
1:C:118:ILE:CD1	1:C:128:LEU:HD11	2.43	0.49
1:B:240:MET:HG2	1:B:416:MET:SD	2.53	0.48
2:A:701:GTF:F2	2:A:701:GTF:H5'	2.04	0.48
1:D:215:HIS:NE2	2:D:702:GTF:PA	2.88	0.47
1:C:354:LYS:HG3	1:C:355:GLU:OE2	2.16	0.46
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:PRO:HB2	1:D:487:VAL:HG22	1.98	0.45
1:C:371:ARG:NH2	8:C:811:HOH:O	2.49	0.45
1:B:537:VAL:HG23	1:B:541:LEU:HD12	1.99	0.45
1:B:537:VAL:CG2	1:B:541:LEU:CD1	2.95	0.45
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.45
1:B:490:ASP:OD2	1:B:490:ASP:N	2.50	0.44
1:C:118:ILE:HD11	1:C:128:LEU:CD1	2.47	0.44
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.91	0.44
1:C:482:SER:O	1:C:484:LYS:HE2	2.17	0.44
1:B:143:ARG:HD2	1:B:420:THR:HA	1.99	0.44
1:B:537:VAL:HG23	1:B:541:LEU:HD11	2.00	0.44
1:A:543:GLU:CG	1:C:543:GLU:CG	2.95	0.44
2:B:701:GTF:F2	2:B:701:GTF:C6	2.56	0.43
1:A:543:GLU:HG3	1:C:543:GLU:CG	2.40	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.18	0.43
1:B:468:ILE:HD12	1:B:550:ILE:HD11	2.00	0.43
1:D:118:ILE:HG23	1:D:126:ILE:HG12	2.01	0.43
1:A:126:ILE:HD13	1:A:126:ILE:HG21	1.65	0.43
1:B:139:PRO:HD3	1:C:450:TYR:CE1	2.54	0.43
1:D:240:MET:HB2	1:D:240:MET:HE2	1.96	0.43
4:B:704:DTP:N6	1:D:372:ARG:HG2	2.34	0.43
1:A:582:GLN:HG2	1:C:536:GLN:NE2	2.34	0.42
1:B:537:VAL:CG2	1:B:541:LEU:HD11	2.48	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.95	0.42
1:B:351:ALA:O	1:B:520:PHE:HA	2.20	0.42
1:A:331:TYR:C	1:A:331:TYR:CD1	2.92	0.42
1:B:331:TYR:CD1	1:B:331:TYR:C	2.92	0.42
1:B:463:THR:O	1:B:466:ILE:HD12	2.19	0.42
1:D:331:TYR:CD1	1:D:331:TYR:C	2.93	0.42
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.62	0.42
1:C:519:SER:HB3	1:C:529:ALA:HB1	2.03	0.41
1:B:118:ILE:CD1	1:B:128:LEU:HD11	2.51	0.41
1:B:541:LEU:HB3	1:B:542:PRO:HD2	2.02	0.41
1:D:126:ILE:HG21	1:D:126:ILE:HD13	1.74	0.41
1:B:126:ILE:HD13	1:B:126:ILE:HG21	1.66	0.40
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.93	0.40

All (2) 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:A:472:ASP:OD2	1:D:466:ILE:CD1[1_455]	1.73	0.47
1:A:472:ASP:OD2	1:D:466:ILE:CG1[1_455]	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	464/550 (84%)	456 (98%)	8 (2%)	0	100 100
1	B	476/550 (86%)	468 (98%)	8 (2%)	0	100 100
1	C	477/550 (87%)	466 (98%)	11 (2%)	0	100 100
1	D	478/550 (87%)	472 (99%)	6 (1%)	0	100 100
All	All	1895/2200 (86%)	1862 (98%)	33 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [\(i\)](#)

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	415/488 (85%)	392 (94%)	23 (6%)	21 8
1	B	426/488 (87%)	407 (96%)	19 (4%)	27 12
1	C	427/488 (88%)	406 (95%)	21 (5%)	25 10
1	D	428/488 (88%)	409 (96%)	19 (4%)	28 13
All	All	1696/1952 (87%)	1614 (95%)	82 (5%)	25 10

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	PRO
1	A	235	GLN
1	A	277	GLU
1	A	284	LEU
1	A	305	ARG
1	A	326	GLN
1	A	331	TYR
1	A	344	ASP
1	A	359	LEU
1	A	368	SER
1	A	405	LYS
1	A	425	ASN
1	A	465	GLN
1	A	470	ARG
1	A	471	GLU
1	A	478	LYS
1	A	488	LEU
1	A	490	ASP
1	A	492	LYS
1	A	494	LYS
1	A	559	ARG
1	A	560	LYS
1	A	580	LYS
1	B	229	VAL
1	B	230	LYS
1	B	284	LEU
1	B	305	ARG
1	B	331	TYR
1	B	368	SER
1	B	371	ARG
1	B	405	LYS
1	B	426	ILE
1	B	465	GLN
1	B	470	ARG
1	B	471	GLU
1	B	478	LYS
1	B	488	LEU
1	B	490	ASP
1	B	492	LYS
1	B	576	ARG
1	B	579	THR
1	B	596	LYS

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Mol	Chain	Res	Type
1	C	113	ASP
1	C	229	VAL
1	C	230	LYS
1	C	284	LEU
1	C	304	LYS
1	C	305	ARG
1	C	331	TYR
1	C	346	GLU
1	C	359	LEU
1	C	368	SER
1	C	405	LYS
1	C	465	GLN
1	C	467	LYS
1	C	470	ARG
1	C	484	LYS
1	C	486	LYS
1	C	488	LEU
1	C	490	ASP
1	C	510	GLN
1	C	540	LEU
1	C	559	ARG
1	D	114	THR
1	D	229	VAL
1	D	230	LYS
1	D	277	GLU
1	D	284	LEU
1	D	304	LYS
1	D	331	TYR
1	D	359	LEU
1	D	368	SER
1	D	466	ILE
1	D	467	LYS
1	D	470	ARG
1	D	474	GLU
1	D	478	LYS
1	D	528	ARG
1	D	540	LEU
1	D	543	GLU
1	D	559	ARG
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	A	364	HIS
1	A	465	GLN
1	A	539	GLN
1	B	465	GLN
1	B	527	ASN
1	C	465	GLN
1	C	535	ASN
1	C	599	ASN
1	D	571	GLN
1	D	599	ASN

5.3.3 RNA [\(i\)](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	D	703	5	26,34,34	1.52	5 (19%)	32,54,54	1.49	8 (25%)
4	DTP	C	702	5	26,32,32	1.37	5 (19%)	30,50,50	1.49	5 (16%)
2	GTF	B	701	5	25,31,31	4.58	14 (56%)	35,50,50	2.70	13 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DTP	A	703	5	26,32,32	1.47	5 (19%)	30,50,50	1.40	5 (16%)
2	GTF	A	701	5	25,31,31	5.07	15 (60%)	35,50,50	3.31	12 (34%)
3	GTP	B	702	5	26,34,34	1.71	6 (23%)	32,54,54	1.13	3 (9%)
2	GTF	D	702	5	25,31,31	4.90	13 (52%)	35,50,50	2.34	11 (31%)
4	DTP	B	704	5	26,32,32	1.21	2 (7%)	30,50,50	1.42	5 (16%)
3	GTP	A	702	5	26,34,34	1.62	4 (15%)	32,54,54	1.90	9 (28%)
4	DTP	D	701	5	26,32,32	1.17	1 (3%)	30,50,50	1.33	4 (13%)
2	GTF	C	705	-	25,31,31	4.93	16 (64%)	35,50,50	2.78	12 (34%)
3	GTP	B	703	5	26,34,34	1.63	7 (26%)	32,54,54	1.38	5 (15%)

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
3	GTP	D	703	5	-	1/18/38/38	0/3/3/3
4	DTP	C	702	5	-	2/18/34/34	0/3/3/3
2	GTF	B	701	5	-	5/22/42/42	0/2/2/2
4	DTP	A	703	5	-	1/18/34/34	0/3/3/3
2	GTF	A	701	5	-	3/22/42/42	0/2/2/2
3	GTP	B	702	5	-	6/18/38/38	0/3/3/3
2	GTF	D	702	5	-	5/22/42/42	0/2/2/2
4	DTP	B	704	5	-	3/18/34/34	0/3/3/3
3	GTP	A	702	5	-	2/18/38/38	0/3/3/3
4	DTP	D	701	5	-	1/18/34/34	0/3/3/3
2	GTF	C	705	-	-	4/22/42/42	0/2/2/2
3	GTP	B	703	5	-	7/18/38/38	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	GTF	O4'-C1'	17.40	1.71	1.42
2	A	701	GTF	O4'-C1'	16.18	1.69	1.42
2	D	702	GTF	O4'-C1'	15.84	1.69	1.42
2	B	701	GTF	O4'-C1'	15.07	1.68	1.42
2	D	702	GTF	C2-N3	8.34	1.53	1.36
2	A	701	GTF	C4-N3	8.02	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GTF	C2-N3	7.96	1.52	1.36
2	C	705	GTF	C2-N1	7.75	1.56	1.40
2	A	701	GTF	C2-N1	7.65	1.56	1.40
2	D	702	GTF	C2-N1	7.35	1.55	1.40
2	B	701	GTF	C6-N1	6.95	1.54	1.38
2	C	705	GTF	C2-N3	6.89	1.50	1.36
2	A	701	GTF	C6-N1	6.76	1.54	1.38
2	A	701	GTF	C6-C5	6.76	1.50	1.35
2	C	705	GTF	C6-C5	6.48	1.50	1.35
2	B	701	GTF	C2-N1	6.42	1.53	1.40
2	D	702	GTF	C6-C5	5.97	1.48	1.35
2	D	702	GTF	C6-N1	5.86	1.52	1.38
2	B	701	GTF	C6-C5	5.85	1.48	1.35
2	D	702	GTF	O3'-C3'	-5.85	1.31	1.42
2	B	701	GTF	C2-N3	5.72	1.48	1.36
2	B	701	GTF	O4'-C4'	-5.69	1.32	1.45
2	C	705	GTF	C6-N1	5.35	1.50	1.38
2	C	705	GTF	C4-N3	5.26	1.45	1.34
2	B	701	GTF	C4-N3	5.22	1.45	1.34
2	D	702	GTF	O4'-C4'	-5.18	1.33	1.45
2	C	705	GTF	O4'-C4'	-5.18	1.33	1.45
2	A	701	GTF	C4'-C3'	5.16	1.63	1.53
3	A	702	GTP	O4'-C1'	5.01	1.48	1.41
2	D	702	GTF	C4-N3	4.97	1.44	1.34
2	D	702	GTF	C4'-C3'	4.45	1.62	1.53
3	B	702	GTP	O4'-C1'	4.43	1.47	1.41
2	B	701	GTF	C4'-C3'	4.40	1.62	1.53
2	C	705	GTF	C4'-C3'	3.84	1.61	1.53
2	B	701	GTF	C4-N4	3.72	1.42	1.33
3	B	703	GTP	O4'-C1'	3.72	1.46	1.41
2	A	701	GTF	O4'-C4'	-3.69	1.36	1.45
3	B	702	GTP	C6-N1	-3.62	1.32	1.37
3	D	703	GTP	O4'-C1'	3.62	1.46	1.41
2	A	701	GTF	F2-C2'	3.56	1.45	1.37
2	D	702	GTF	C4-N4	3.52	1.42	1.33
4	A	703	DTP	C2-N3	3.49	1.37	1.32
2	A	701	GTF	C5-C4	3.27	1.50	1.42
2	B	701	GTF	C5-C4	3.21	1.50	1.42
3	B	703	GTP	C6-N1	-2.96	1.33	1.37
4	B	704	DTP	C2-N3	2.96	1.36	1.32
2	C	705	GTF	C1'-N1	2.91	1.55	1.47
3	B	703	GTP	PG-O3G	-2.90	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GTF	PA-O5'	2.84	1.70	1.59
2	C	705	GTF	F2-C2'	2.83	1.43	1.37
2	C	705	GTF	C5-C4	2.81	1.49	1.42
3	A	702	GTP	C4-N3	-2.81	1.30	1.37
2	A	701	GTF	O3'-C3'	-2.70	1.37	1.42
2	A	701	GTF	C5'-C4'	2.70	1.60	1.51
4	C	702	DTP	O4'-C1'	2.66	1.48	1.42
2	B	701	GTF	F2-C2'	2.65	1.43	1.37
2	B	701	GTF	PA-O5'	2.58	1.69	1.59
3	B	703	GTP	PB-O2B	-2.54	1.43	1.55
4	A	703	DTP	C4-N3	-2.50	1.32	1.35
3	B	702	GTP	O4'-C4'	-2.48	1.39	1.45
4	A	703	DTP	C5-C4	2.48	1.47	1.40
4	C	702	DTP	C5-N7	-2.48	1.30	1.39
3	A	702	GTP	O6-C6	2.47	1.28	1.23
2	A	701	GTF	C4-N4	2.46	1.39	1.33
2	C	705	GTF	F1-C2'	2.45	1.42	1.37
3	B	702	GTP	C2'-C1'	-2.43	1.50	1.53
4	C	702	DTP	C2-N1	-2.40	1.29	1.33
2	C	705	GTF	C5'-C4'	2.39	1.59	1.51
3	B	703	GTP	O2'-C2'	2.39	1.48	1.43
2	B	701	GTF	O3'-C3'	-2.36	1.38	1.42
2	D	702	GTF	C5-C4	2.36	1.48	1.42
2	D	702	GTF	C1'-N1	2.35	1.53	1.47
2	D	702	GTF	F2-C2'	2.34	1.42	1.37
2	A	701	GTF	C1'-N1	2.33	1.53	1.47
3	D	703	GTP	PG-O2G	-2.28	1.46	1.54
3	D	703	GTP	C2'-C1'	-2.27	1.50	1.53
4	A	703	DTP	O3'-C3'	2.25	1.48	1.43
3	B	703	GTP	O6-C6	2.24	1.27	1.23
4	B	704	DTP	O4'-C4'	-2.22	1.40	1.45
2	C	705	GTF	PA-O5'	2.21	1.68	1.59
4	C	702	DTP	PG-O2G	-2.20	1.46	1.54
4	C	702	DTP	C3'-C4'	-2.17	1.47	1.53
4	A	703	DTP	PA-O2A	-2.16	1.45	1.55
2	C	705	GTF	PG-O2G	-2.15	1.46	1.54
3	D	703	GTP	PB-O2B	-2.14	1.45	1.55
3	B	703	GTP	C4-N3	-2.13	1.32	1.37
3	B	702	GTP	PG-O3G	-2.13	1.46	1.54
4	D	701	DTP	PB-O2B	-2.10	1.45	1.55
3	D	703	GTP	PA-O2A	-2.10	1.45	1.55
2	B	701	GTF	C5'-C4'	2.07	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	GTF	C4-N4	2.04	1.38	1.33
3	A	702	GTP	O4'-C4'	-2.02	1.40	1.45
3	B	702	GTP	C2-N3	2.01	1.38	1.33

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GTF	F2-C2'-F1	11.36	118.17	105.20
2	B	701	GTF	O4'-C1'-N1	10.34	117.05	108.44
2	A	701	GTF	O4'-C1'-N1	9.25	116.14	108.44
2	C	705	GTF	O4'-C1'-N1	9.22	116.12	108.44
2	C	705	GTF	F2-C2'-F1	7.89	114.21	105.20
2	D	702	GTF	O4'-C1'-N1	6.51	113.86	108.44
2	A	701	GTF	F1-C2'-C1'	-6.25	97.36	110.97
2	D	702	GTF	F2-C2'-F1	5.42	111.39	105.20
2	A	701	GTF	O1A-PA-O5'	4.88	130.39	107.75
3	A	702	GTP	O6-C6-N1	4.53	126.00	120.65
2	D	702	GTF	C5'-C4'-C3'	-4.47	107.18	114.66
2	C	705	GTF	O2G-PG-O3B	4.43	119.50	104.64
2	A	701	GTF	O4'-C4'-C3'	-4.36	99.66	104.42
2	B	701	GTF	PB-O3A-PA	-4.19	118.46	132.83
2	B	701	GTF	N4-C4-N3	-4.14	110.71	117.97
2	B	701	GTF	O2-C2-N1	3.93	127.00	118.89
2	C	705	GTF	O5'-PA-O2A	3.84	124.06	109.07
4	C	702	DTP	N6-C6-N1	3.81	126.49	118.57
2	A	701	GTF	PB-O3A-PA	-3.80	119.80	132.83
3	A	702	GTP	O2G-PG-O3B	3.76	117.24	104.64
2	C	705	GTF	O2-C2-N3	-3.74	116.25	122.33
3	B	703	GTP	O6-C6-N1	3.71	125.03	120.65
2	B	701	GTF	F2-C2'-F1	3.67	109.40	105.20
2	D	702	GTF	O1G-PG-O3G	3.50	124.40	110.68
2	C	705	GTF	C5-C4-N3	3.47	127.23	121.33
2	B	701	GTF	F1-C2'-C1'	-3.47	103.41	110.97
4	D	701	DTP	C2'-C1'-N9	3.38	122.07	114.27
2	D	702	GTF	O2G-PG-O3B	-3.35	93.41	104.64
2	B	701	GTF	O5'-PA-O2A	3.32	122.06	109.07
2	D	702	GTF	PB-O3A-PA	-3.31	121.47	132.83
3	D	703	GTP	C3'-C2'-C1'	3.21	105.82	100.98
4	A	703	DTP	O3G-PG-O1G	3.12	122.89	110.68
2	A	701	GTF	O1G-PG-O3G	-3.06	98.71	110.68
2	D	702	GTF	O2-C2-N3	-3.05	117.37	122.33
4	C	702	DTP	C5-C6-N6	-2.99	115.80	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GTF	O1G-PG-O3B	2.99	114.65	104.64
4	B	704	DTP	N6-C6-N1	2.95	124.69	118.57
4	C	702	DTP	C2'-C1'-N9	2.91	120.98	114.27
2	B	701	GTF	O2G-PG-O1G	2.89	118.67	107.64
3	A	702	GTP	C3'-C2'-C1'	2.82	105.23	100.98
3	A	702	GTP	O6-C6-C5	-2.81	118.87	124.37
4	A	703	DTP	O2A-PA-O1A	2.75	125.83	112.24
3	B	703	GTP	PA-O3A-PB	-2.75	123.41	132.83
3	A	702	GTP	O3G-PG-O2G	2.74	118.12	107.64
2	A	701	GTF	O2G-PG-O1G	2.74	118.10	107.64
3	A	702	GTP	O2A-PA-O1A	2.73	125.75	112.24
4	B	704	DTP	C2-N1-C6	2.73	123.43	118.75
4	C	702	DTP	C2'-C3'-C4'	2.72	108.44	102.76
4	C	702	DTP	O2G-PG-O1G	2.67	121.13	110.68
2	B	701	GTF	C5-C4-N4	2.65	124.74	120.57
2	A	701	GTF	O1A-PA-O2A	-2.61	99.33	112.24
4	B	704	DTP	N3-C2-N1	-2.59	124.63	128.68
3	B	702	GTP	PA-O3A-PB	-2.59	123.95	132.83
3	D	703	GTP	O2'-C2'-C1'	-2.59	101.31	110.85
2	D	702	GTF	C5-C4-N3	2.57	125.71	121.33
2	C	705	GTF	O3'-C3'-C4'	2.57	118.48	112.40
4	D	701	DTP	O3G-PG-O1G	2.55	120.66	110.68
4	D	701	DTP	C4-C5-N7	-2.52	106.77	109.40
3	D	703	GTP	O3G-PG-O2G	2.49	117.15	107.64
3	B	703	GTP	O3G-PG-O2G	2.47	117.08	107.64
2	D	702	GTF	C4-N3-C2	-2.45	116.29	120.25
2	B	701	GTF	O2-C2-N3	-2.44	118.37	122.33
3	B	702	GTP	O3G-PG-O2G	2.43	116.91	107.64
4	A	703	DTP	N6-C6-N1	2.39	123.54	118.57
4	B	704	DTP	O3G-PG-O2G	2.38	116.73	107.64
3	D	703	GTP	O2A-PA-O5'	-2.37	96.73	107.75
2	D	702	GTF	N4-C4-N3	-2.37	113.81	117.97
3	A	702	GTP	O5'-C5'-C4'	2.37	117.14	108.99
3	B	703	GTP	O4'-C1'-C2'	2.36	110.37	106.93
2	A	701	GTF	O2-C2-N1	2.35	123.74	118.89
2	C	705	GTF	N4-C4-N3	-2.35	113.85	117.97
3	D	703	GTP	PA-O3A-PB	-2.33	124.83	132.83
2	D	702	GTF	F2-C2'-C1'	2.30	115.98	110.97
2	B	701	GTF	N1-C2-N3	-2.29	114.63	118.81
3	B	703	GTP	O3B-PG-O1G	-2.29	98.47	111.19
4	A	703	DTP	C2'-C1'-N9	2.29	119.55	114.27
2	C	705	GTF	C4-N3-C2	-2.27	116.59	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	705	GTF	PB-O3B-PG	-2.27	125.04	132.83
2	B	701	GTF	O4'-C4'-C3'	-2.23	101.99	104.42
3	D	703	GTP	O6-C6-C5	-2.22	120.04	124.37
3	A	702	GTP	O3'-C3'-C4'	-2.20	104.68	111.05
2	C	705	GTF	F2-C2'-C1'	2.19	115.74	110.97
3	A	702	GTP	O4'-C4'-C5'	-2.15	102.31	109.37
3	B	702	GTP	O2A-PA-O1A	2.09	122.55	112.24
4	A	703	DTP	O3G-PG-O3B	-2.08	97.67	104.64
3	D	703	GTP	C8-N7-C5	2.08	106.95	102.99
2	A	701	GTF	N1-C2-N3	-2.07	115.04	118.81
4	D	701	DTP	O3'-C3'-C2'	-2.04	103.60	110.90
2	C	705	GTF	O2-C2-N1	2.03	123.08	118.89
3	D	703	GTP	C5-C6-N1	2.02	117.51	113.95
4	B	704	DTP	O2A-PA-O1A	2.01	122.19	112.24
2	B	701	GTF	O1G-PG-O3G	-2.01	102.82	110.68

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	GTF	C5'-O5'-PA-O2A
2	C	705	GTF	PB-O3A-PA-O5'
2	C	705	GTF	C5'-O5'-PA-O1A
2	D	702	GTF	PB-O3B-PG-O1G
2	D	702	GTF	C3'-C4'-C5'-O5'
3	B	702	GTP	PB-O3B-PG-O2G
4	B	704	DTP	PB-O3B-PG-O2G
4	B	704	DTP	PB-O3B-PG-O3G
4	D	701	DTP	PB-O3B-PG-O3G
2	D	702	GTF	O4'-C4'-C5'-O5'
2	C	705	GTF	C4'-C5'-O5'-PA
4	C	702	DTP	PB-O3A-PA-O1A
2	B	701	GTF	C3'-C4'-C5'-O5'
2	D	702	GTF	C4'-C5'-O5'-PA
2	B	701	GTF	C4'-C5'-O5'-PA
3	A	702	GTP	C4'-C5'-O5'-PA
2	A	701	GTF	C4'-C5'-O5'-PA
3	B	702	GTP	C4'-C5'-O5'-PA
3	B	703	GTP	C4'-C5'-O5'-PA
4	A	703	DTP	PB-O3B-PG-O3G
2	B	701	GTF	C5'-O5'-PA-O3A
2	C	705	GTF	C5'-O5'-PA-O3A

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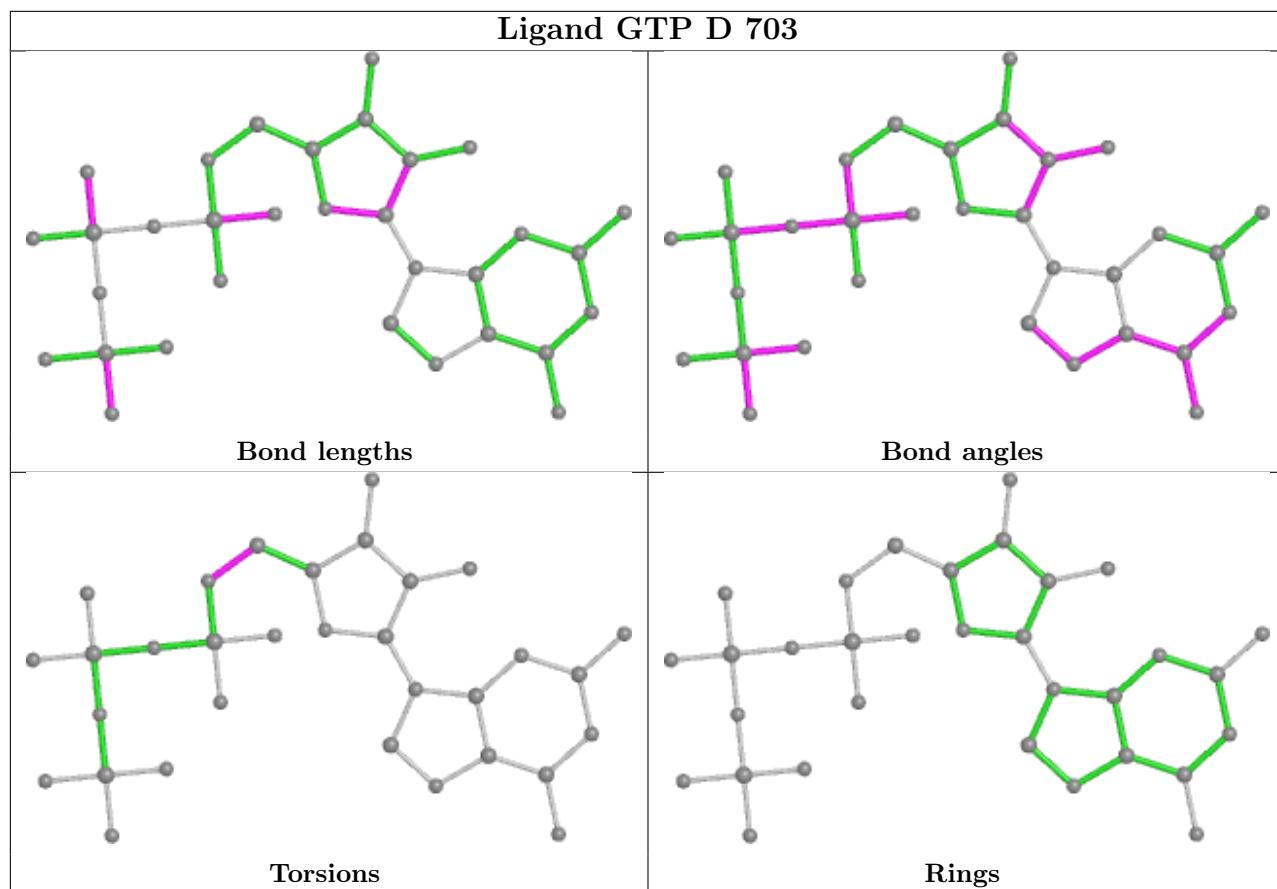
Mol	Chain	Res	Type	Atoms
3	B	703	GTP	C5'-O5'-PA-O3A
2	B	701	GTF	PB-O3A-PA-O2A
2	A	701	GTF	C5'-O5'-PA-O1A
2	D	702	GTF	PB-O3B-PG-O3G
3	B	702	GTP	PB-O3B-PG-O1G
3	B	702	GTP	PG-O3B-PB-O2B
3	B	703	GTP	PG-O3B-PB-O2B
3	B	703	GTP	PB-O3A-PA-O2A
4	C	702	DTP	PB-O3A-PA-O2A
3	A	702	GTP	PG-O3B-PB-O1B
3	B	702	GTP	PG-O3B-PB-O1B
3	B	703	GTP	PB-O3B-PG-O1G
4	B	704	DTP	PB-O3B-PG-O1G
3	D	703	GTP	C4'-C5'-O5'-PA
2	A	701	GTF	C5'-O5'-PA-O3A
3	B	702	GTP	PB-O3A-PA-O1A
3	B	703	GTP	PG-O3B-PB-O1B
3	B	703	GTP	C5'-O5'-PA-O1A

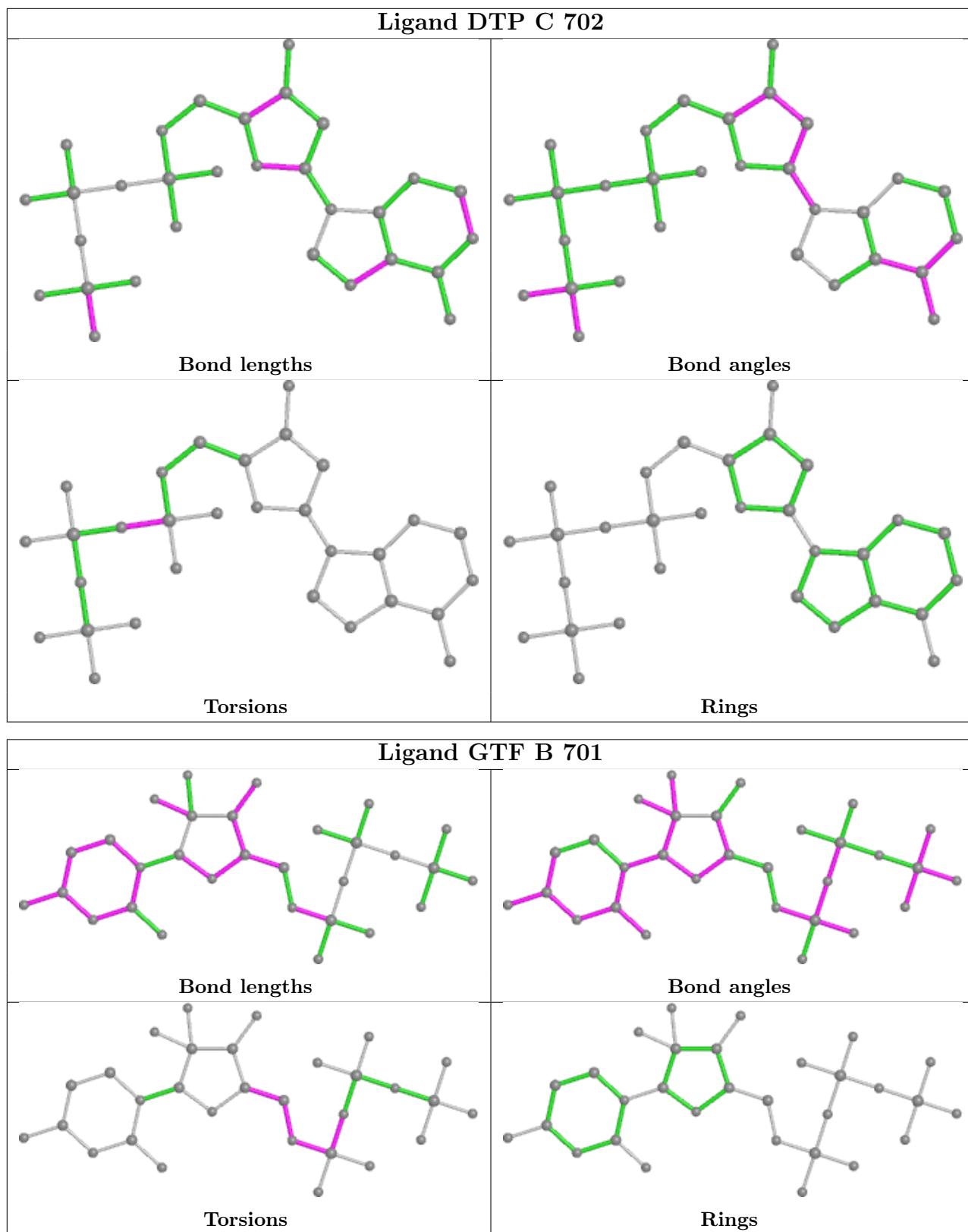
There are no ring outliers.

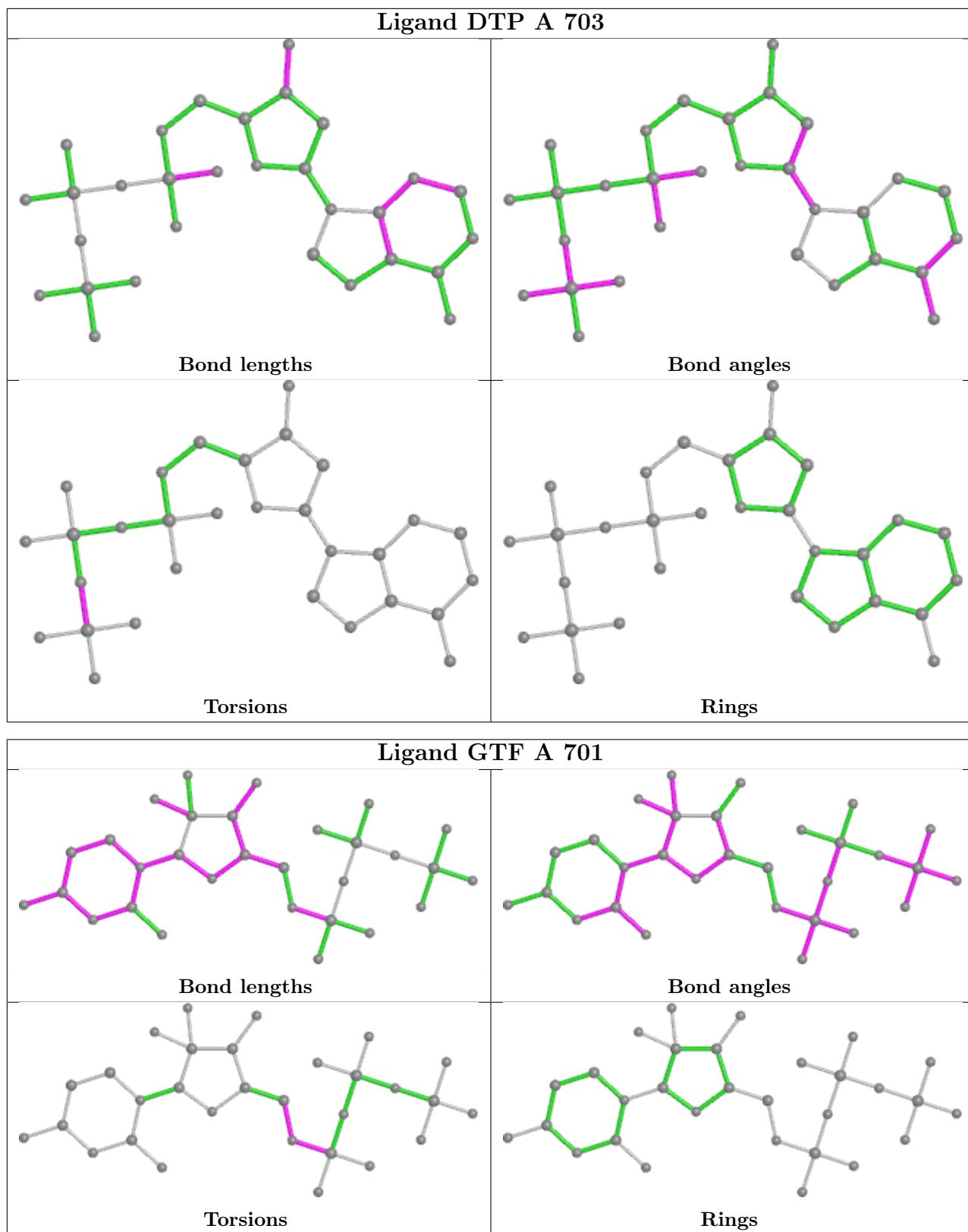
5 monomers are involved in 16 short contacts:

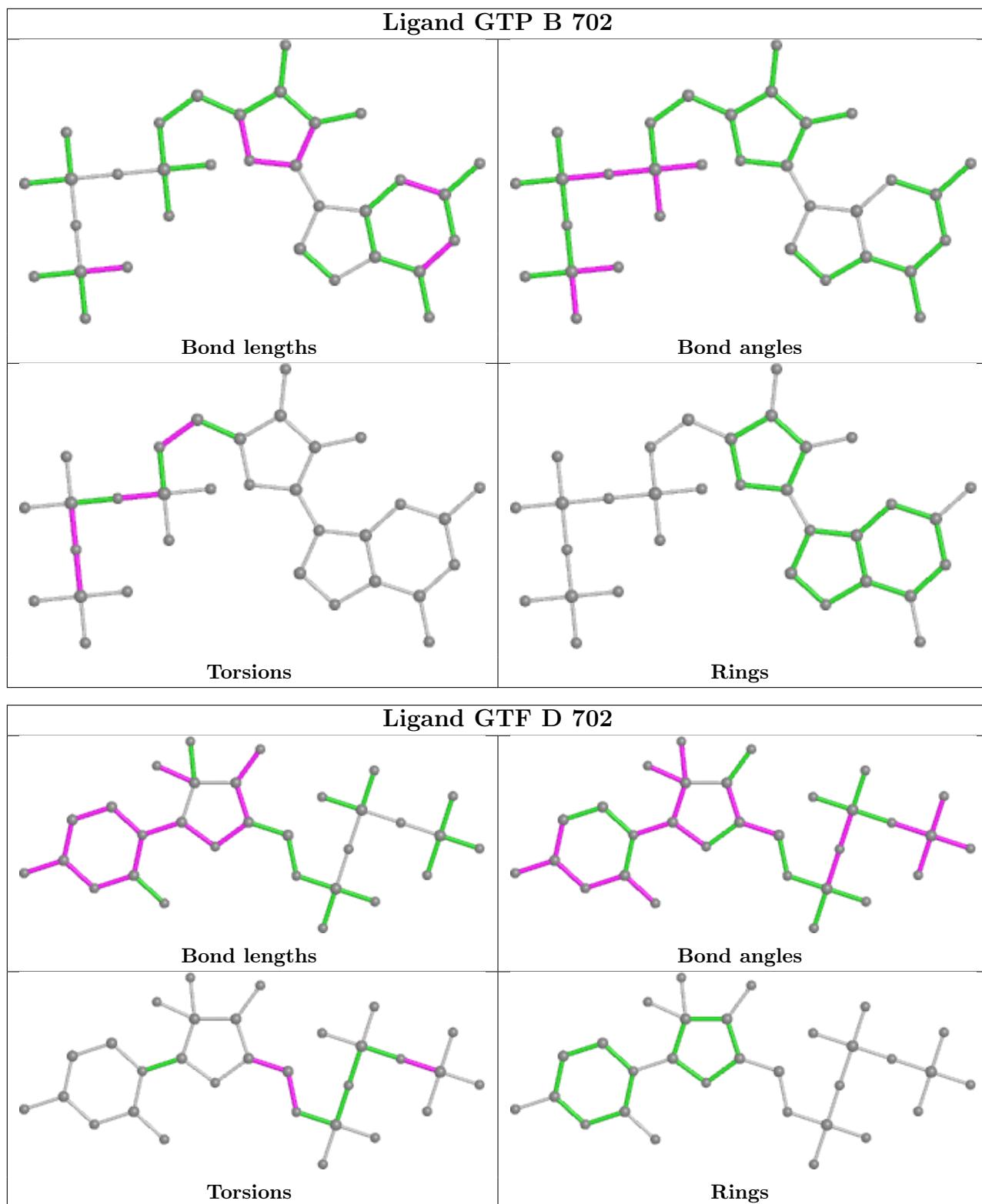
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	GTF	3	0
2	A	701	GTF	3	0
2	D	702	GTF	6	0
4	B	704	DTP	1	0
2	C	705	GTF	3	0

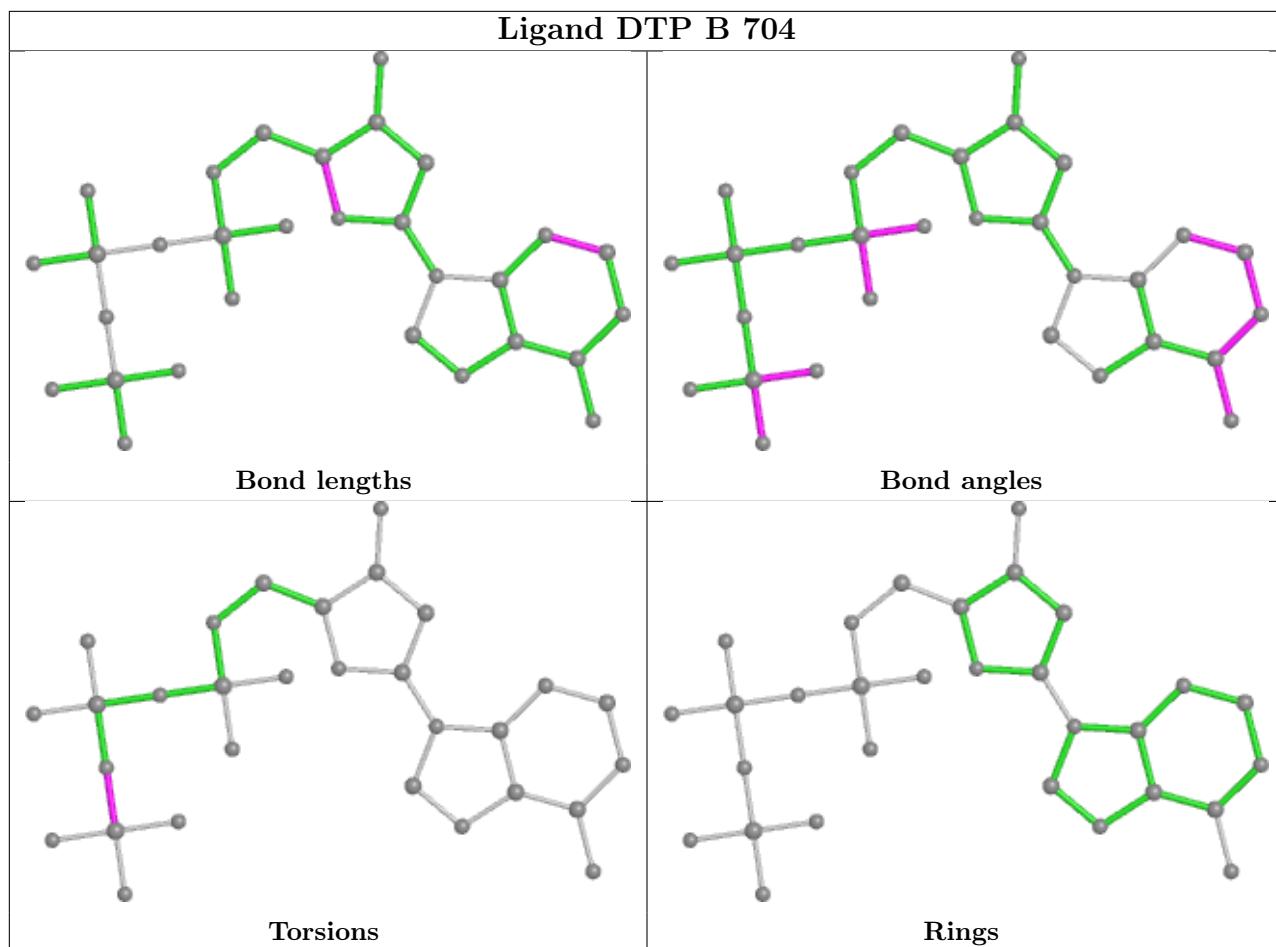
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

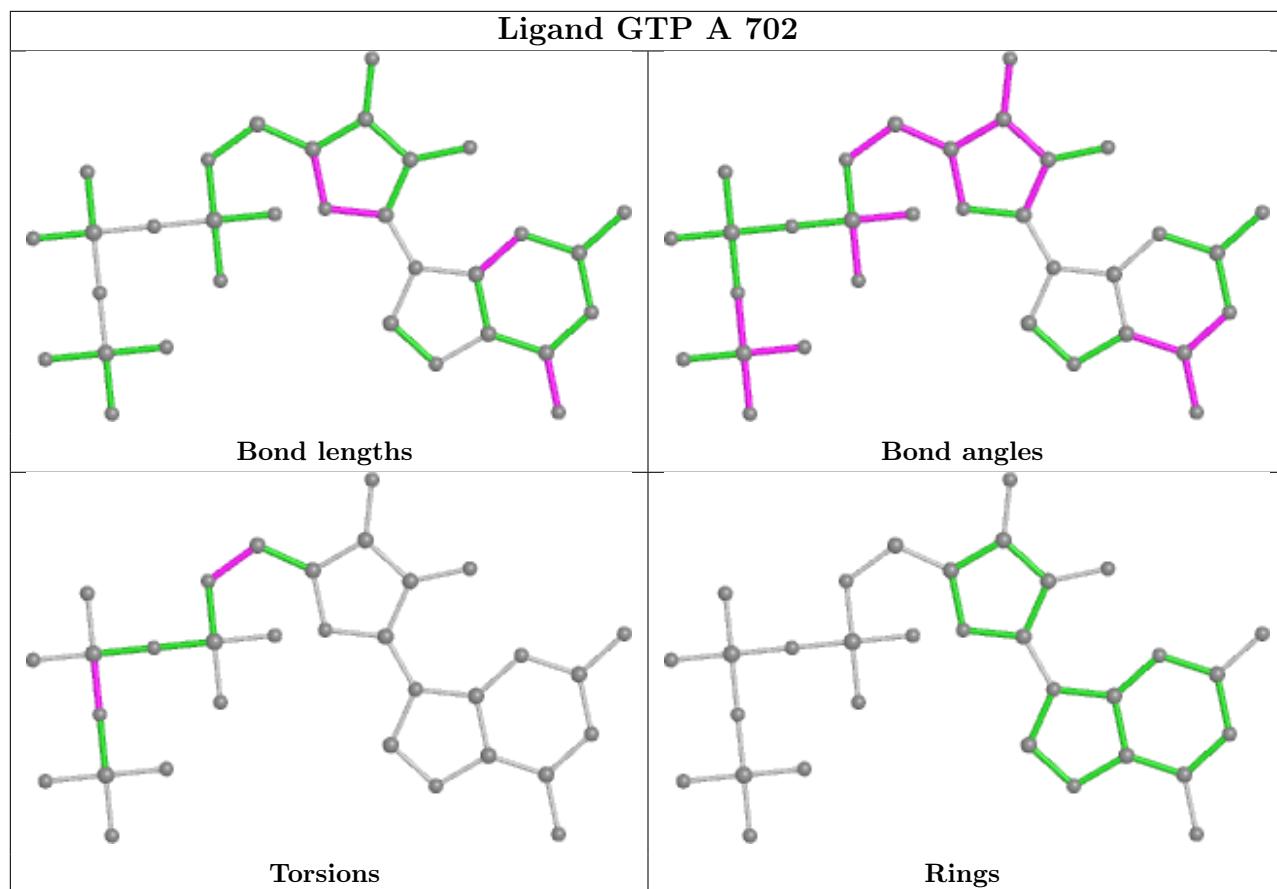


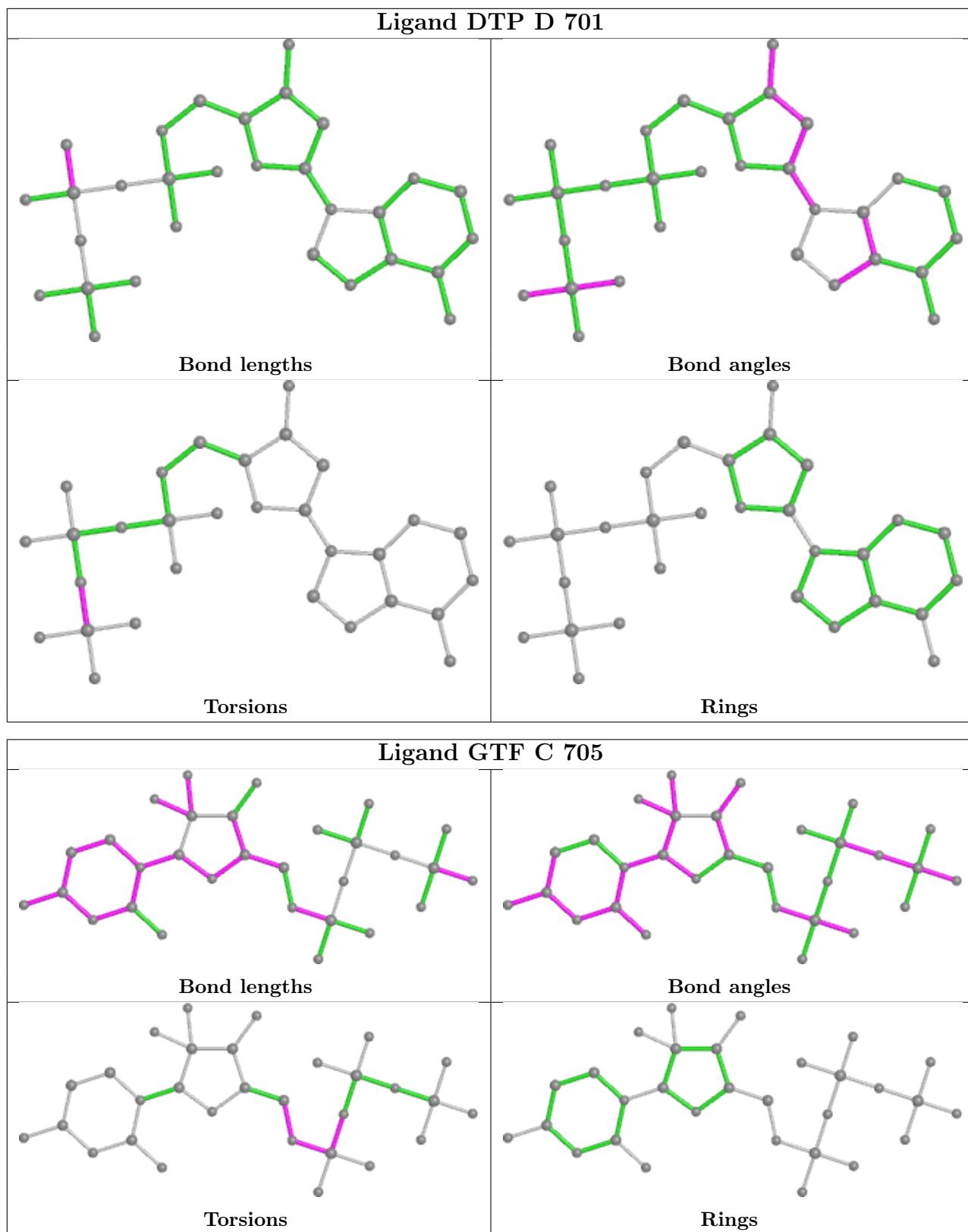


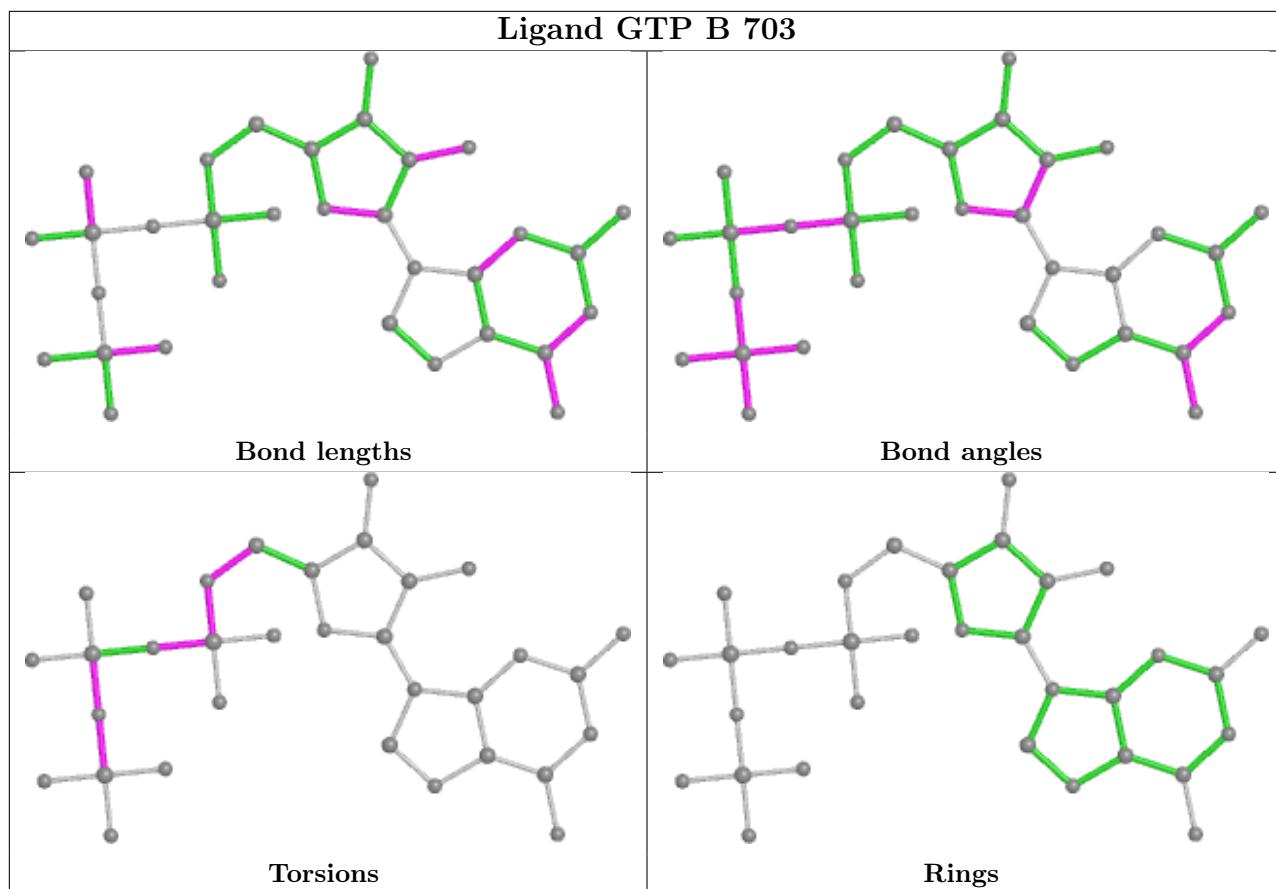












5.7 Other polymers [\(i\)](#)

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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/550 (85%)	-0.15	18 (3%) 40 48	14, 32, 67, 102	0
1	B	480/550 (87%)	0.12	36 (7%) 14 20	18, 37, 84, 118	0
1	C	481/550 (87%)	-0.12	18 (3%) 41 49	18, 35, 73, 105	0
1	D	481/550 (87%)	-0.28	8 (1%) 70 75	14, 31, 58, 108	0
All	All	1910/2200 (86%)	-0.11	80 (4%) 36 43	14, 33, 73, 118	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	9.1
1	B	490	ASP	7.2
1	C	466	ILE	7.0
1	A	488	LEU	7.0
1	C	488	LEU	6.9
1	C	277	GLU	6.8
1	D	276	LEU	6.4
1	A	486	LYS	6.2
1	B	591	ILE	6.2
1	B	590	LEU	6.2
1	D	113	ASP	5.6
1	A	276	LEU	5.5
1	C	487	VAL	5.5
1	A	490	ASP	5.3
1	C	276	LEU	5.3
1	B	276	LEU	5.1
1	B	599	ASN	5.0
1	C	489	LEU	4.6
1	C	596	LYS	4.5
1	A	491	VAL	4.4
1	C	113	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	487	VAL	4.1
1	D	465	GLN	4.1
1	B	489	LEU	4.0
1	D	466	ILE	4.0
1	B	594	GLN	4.0
1	B	466	ILE	3.9
1	B	597	GLU	3.9
1	B	570	VAL	3.8
1	A	489	LEU	3.7
1	B	596	LYS	3.7
1	B	487	VAL	3.6
1	A	492	LYS	3.6
1	A	284	LEU	3.5
1	A	586	VAL	3.5
1	C	490	ASP	3.5
1	D	464	GLY	3.5
1	D	277	GLU	3.4
1	B	563	TYR	3.4
1	B	277	GLU	3.3
1	A	470	ARG	3.2
1	B	114	THR	3.2
1	B	588	ALA	3.2
1	B	559	ARG	3.2
1	B	593	PRO	3.2
1	A	113	ASP	3.1
1	C	492	LYS	3.0
1	D	284	LEU	2.9
1	B	587	ILE	2.9
1	B	486	LYS	2.9
1	B	463	THR	2.8
1	C	599	ASN	2.8
1	A	466	ILE	2.8
1	D	599	ASN	2.7
1	B	589	PRO	2.7
1	B	284	LEU	2.7
1	A	344	ASP	2.6
1	C	114	THR	2.6
1	A	345	ASN	2.6
1	A	114	THR	2.6
1	A	583	ASP	2.6
1	B	579	THR	2.6
1	B	491	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	585	ASP	2.5
1	B	474	GLU	2.5
1	B	580	LYS	2.5
1	B	562	LEU	2.4
1	B	325	ILE	2.4
1	B	586	VAL	2.3
1	B	575	ASP	2.2
1	B	598	TRP	2.2
1	C	594	GLN	2.2
1	C	406	LYS	2.1
1	C	464	GLY	2.1
1	C	325	ILE	2.1
1	B	492	LYS	2.1
1	B	484	LYS	2.0
1	C	405	LYS	2.0
1	B	481	ALA	2.0
1	C	597	GLU	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 monosaccharides 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.

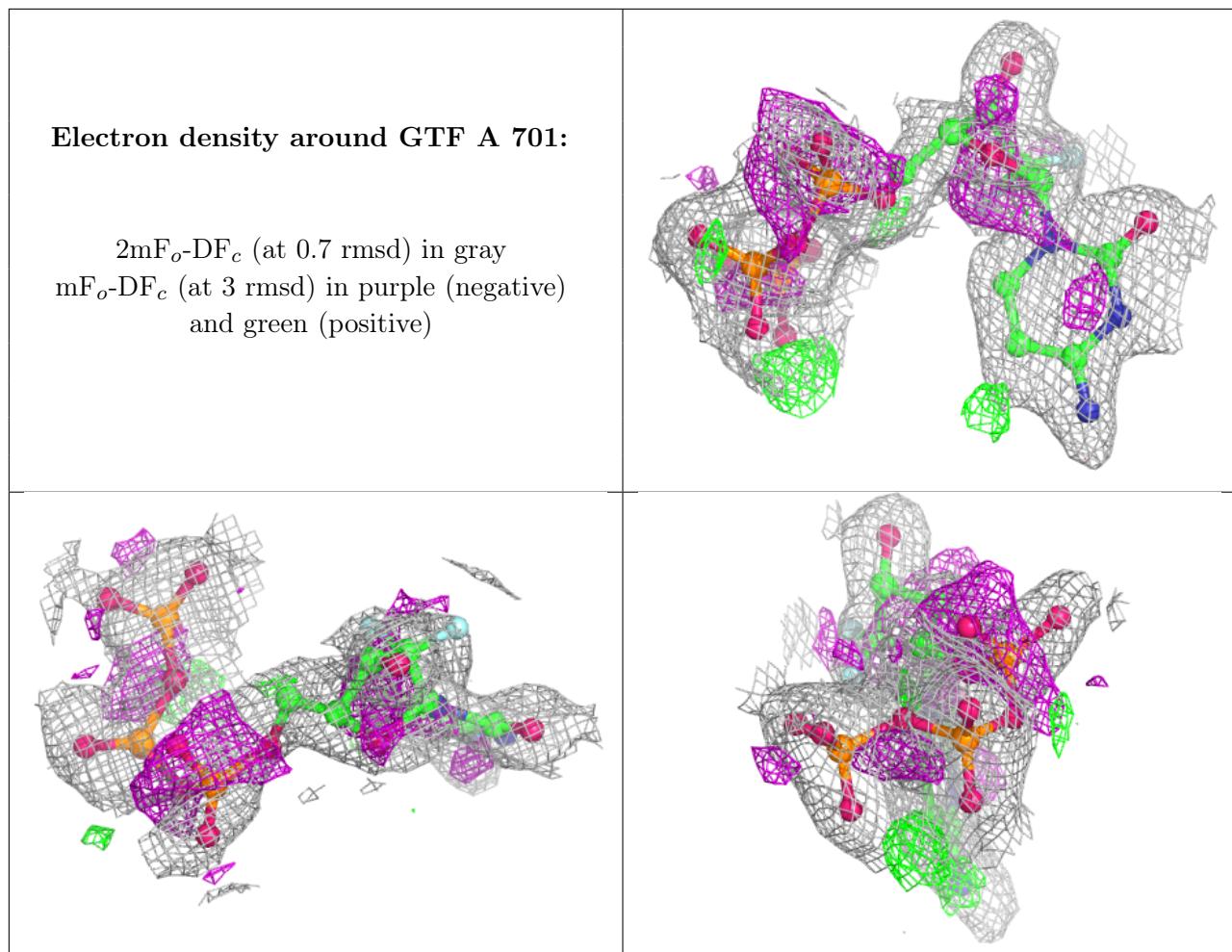
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NI	C	701	1/1	-0.10	0.50	239,239,239,239	0
5	MG	B	706	1/1	0.79	0.18	66,66,66,66	0
2	GTF	A	701	30/30	0.81	0.18	23,50,75,85	0
2	GTF	B	701	30/30	0.82	0.18	30,58,94,110	0
2	GTF	C	705	30/30	0.84	0.15	32,51,67,81	0
6	NA	B	705	1/1	0.86	0.19	40,40,40,40	0

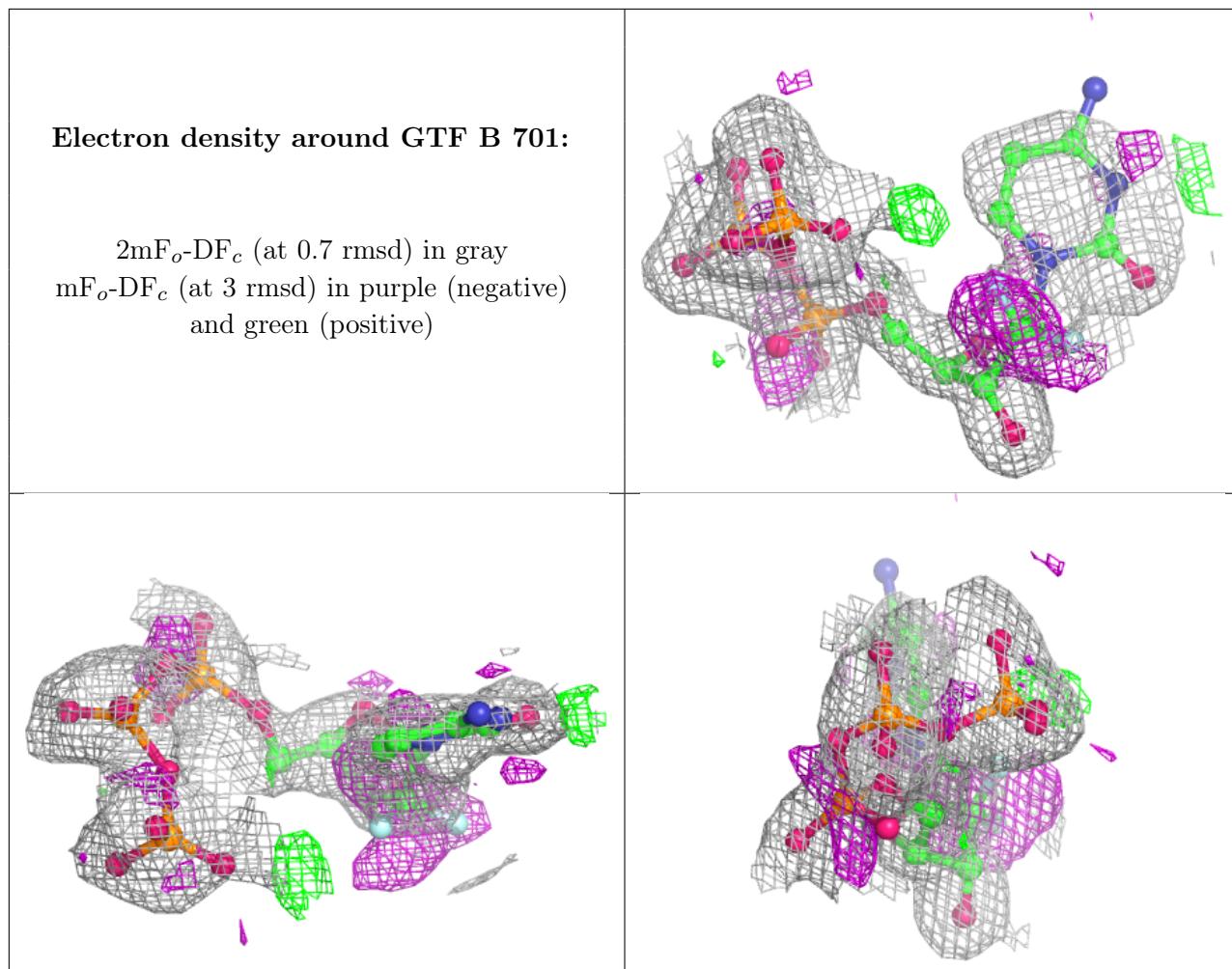
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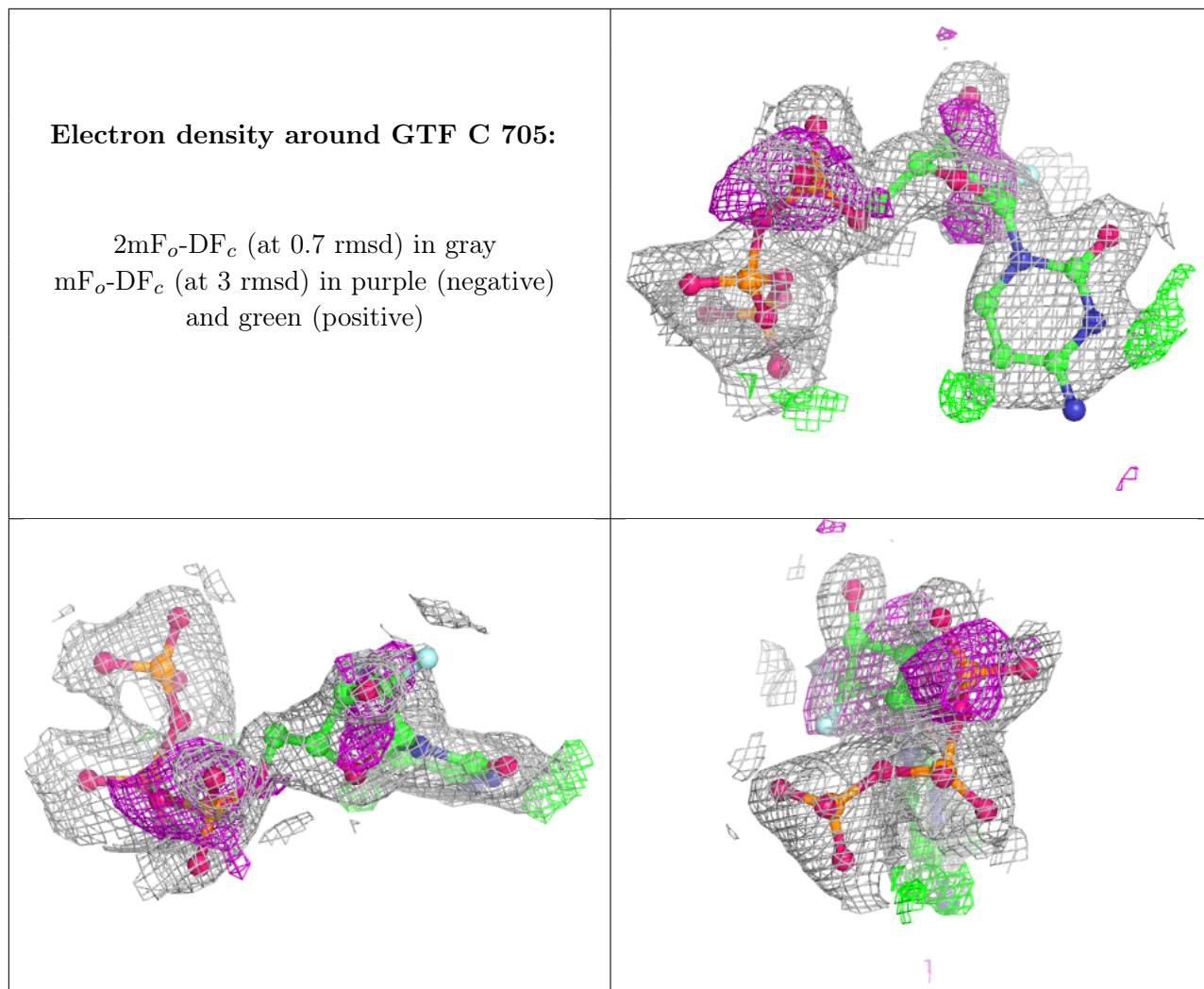
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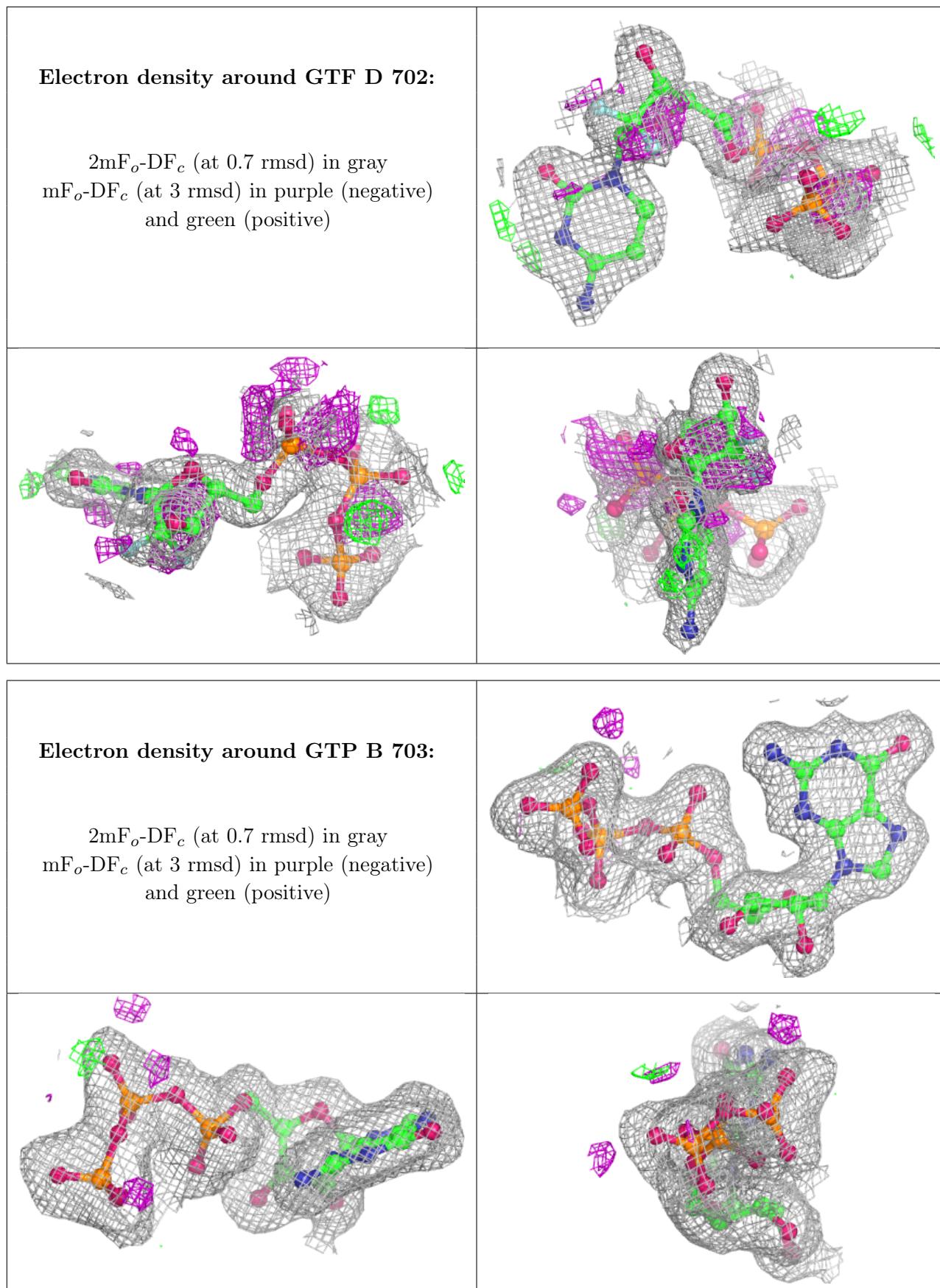
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GTF	D	702	30/30	0.88	0.14	25,45,67,70	0
5	MG	D	705	1/1	0.90	0.11	57,57,57,57	0
6	NA	A	706	1/1	0.93	0.07	37,37,37,37	0
5	MG	A	707	1/1	0.94	0.31	62,62,62,62	0
6	NA	C	707	1/1	0.94	0.15	39,39,39,39	0
5	MG	D	704	1/1	0.94	0.17	57,57,57,57	0
5	MG	A	708	1/1	0.95	0.23	53,53,53,53	0
5	MG	D	706	1/1	0.96	0.19	49,49,49,49	0
6	NA	C	706	1/1	0.97	0.09	56,56,56,56	0
3	GTP	B	703	32/32	0.99	0.06	21,23,30,30	0
5	MG	C	704	1/1	0.99	0.07	22,22,22,22	0
3	GTP	D	703	32/32	0.99	0.07	15,18,26,27	0
4	DTP	A	703	30/30	0.99	0.08	18,21,25,26	0
4	DTP	B	704	30/30	0.99	0.08	15,19,22,24	0
4	DTP	C	702	30/30	0.99	0.08	13,16,19,19	0
4	DTP	D	701	30/30	0.99	0.09	17,21,24,25	0
5	MG	A	704	1/1	0.99	0.05	24,24,24,24	0
3	GTP	A	702	32/32	0.99	0.07	14,16,21,21	0
3	GTP	B	702	32/32	0.99	0.07	18,21,29,29	0
5	MG	C	703	1/1	1.00	0.04	18,18,18,18	0
5	MG	A	705	1/1	1.00	0.04	20,20,20,20	0

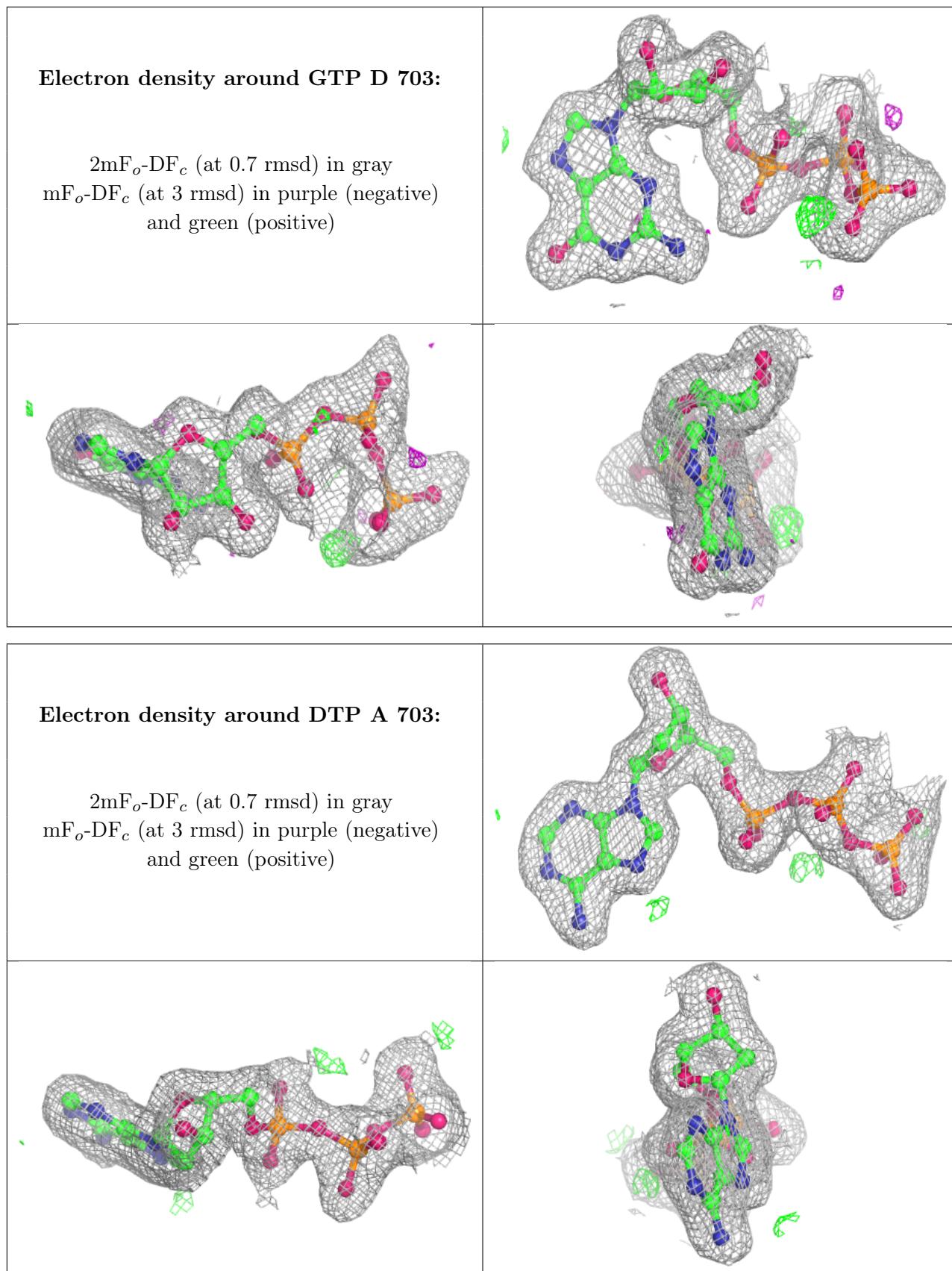
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

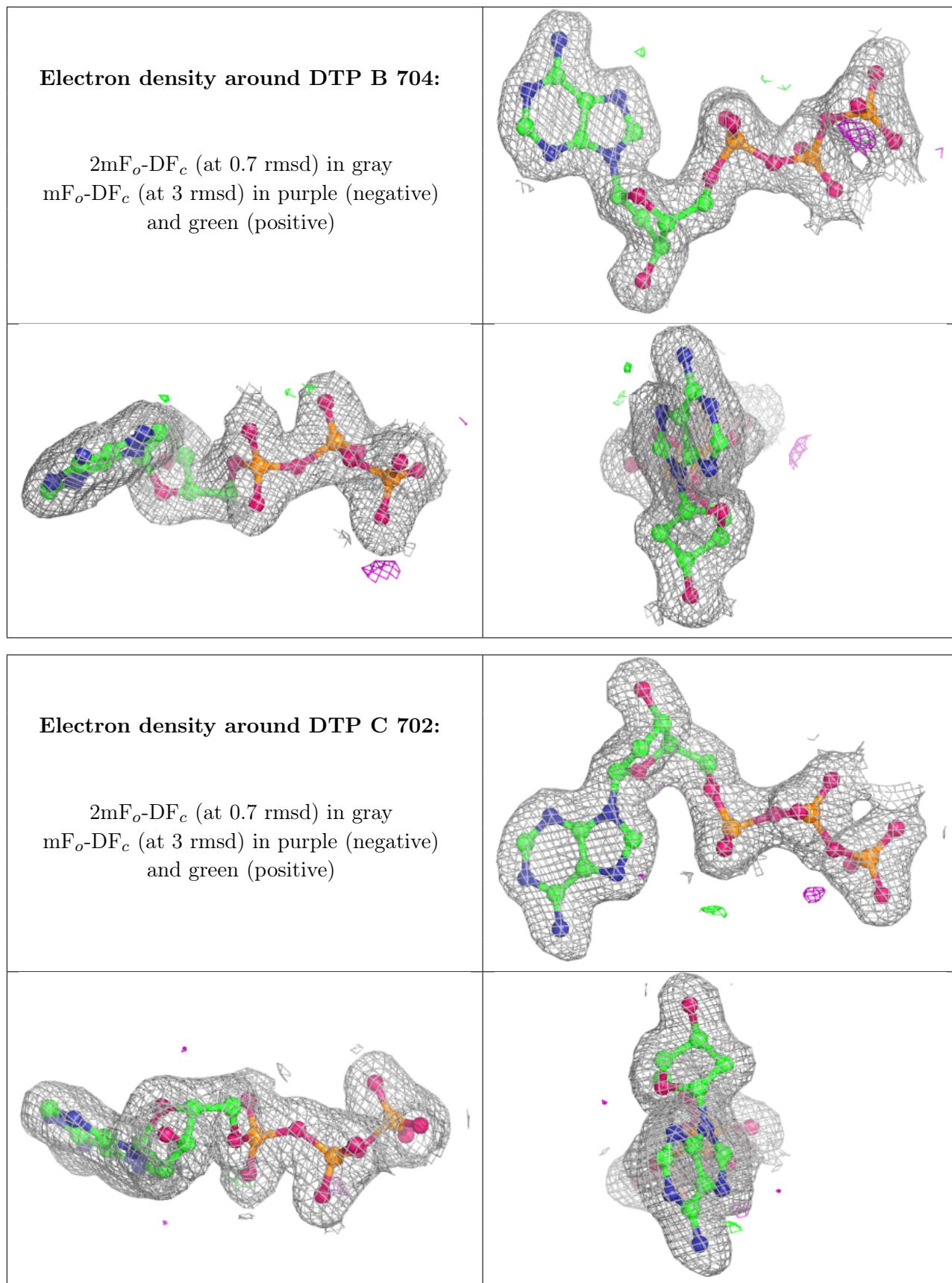


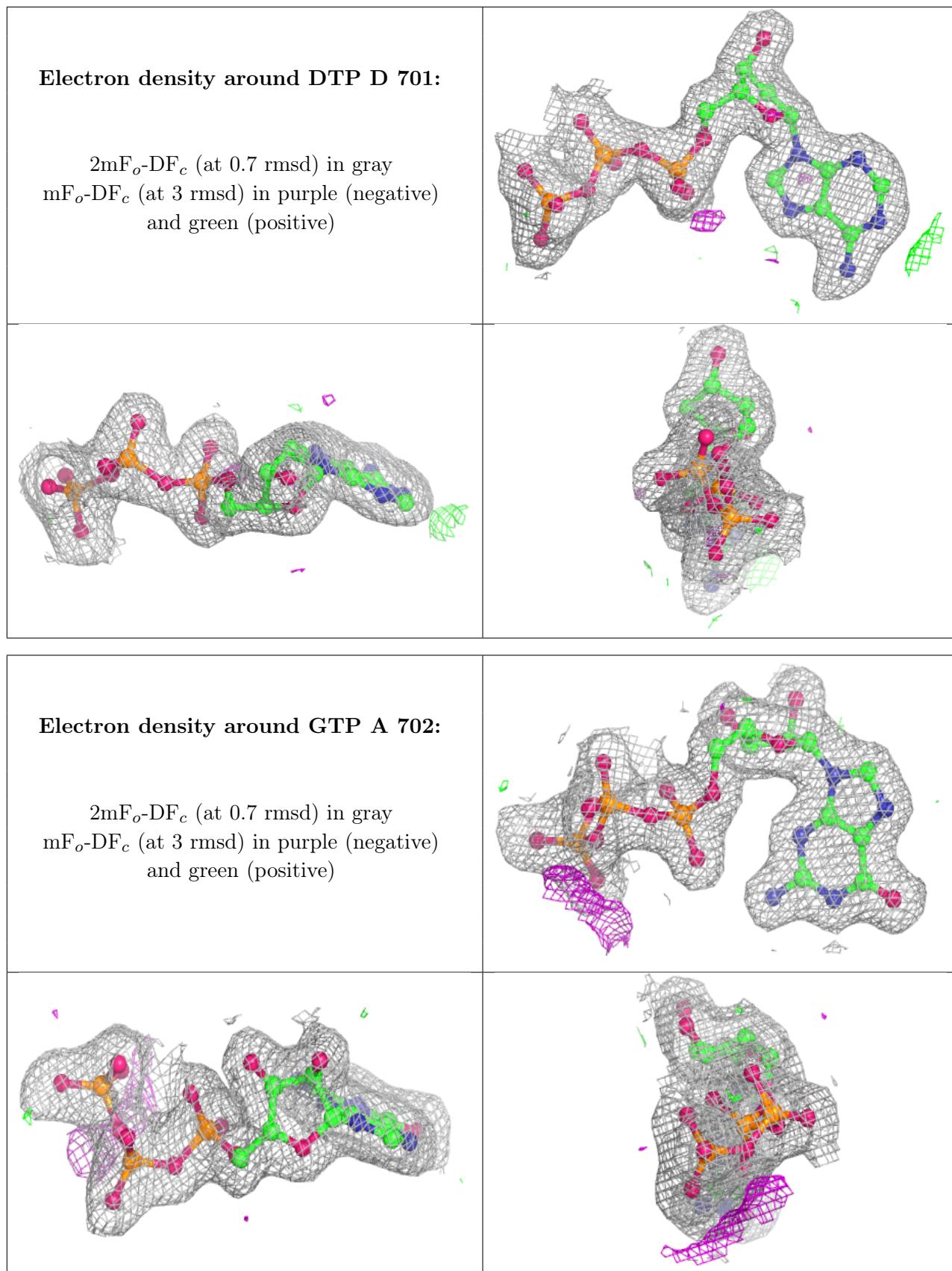


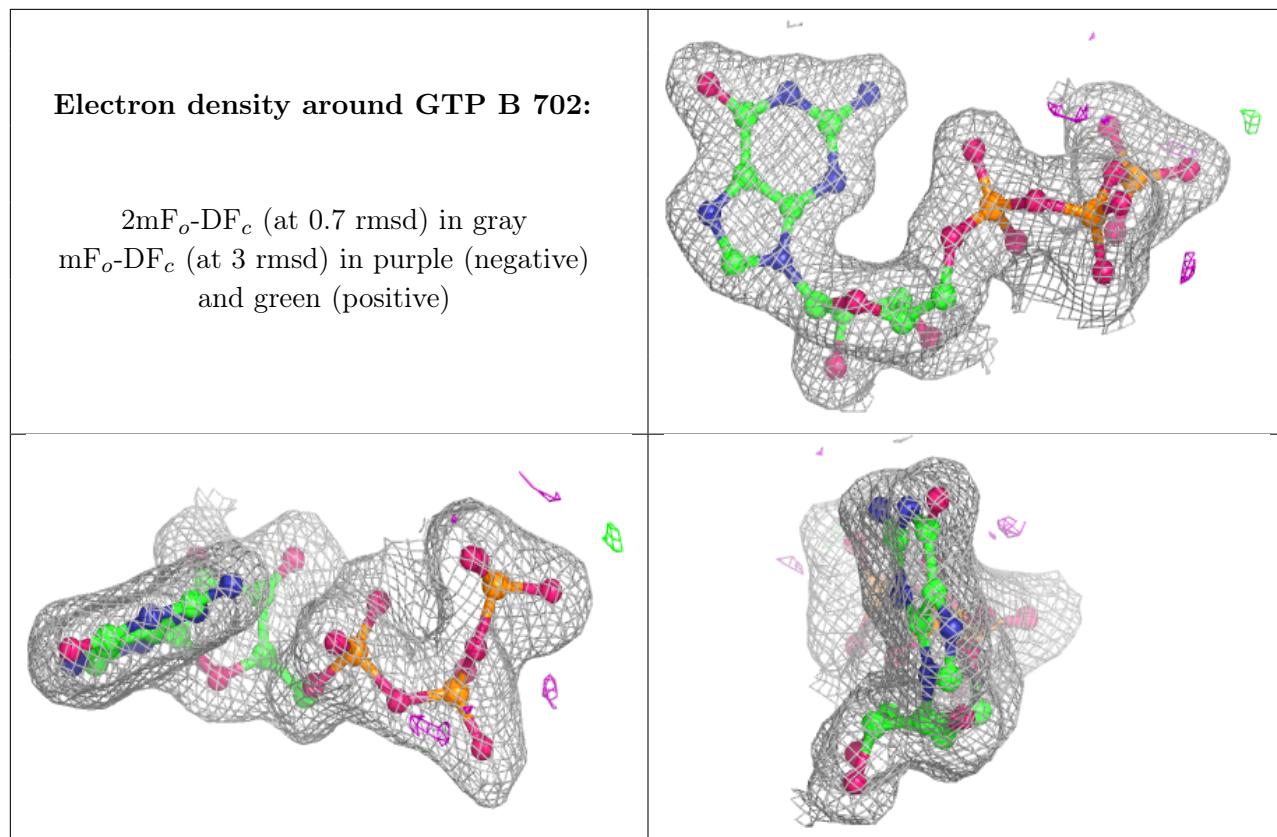












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.