



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:27 AM UTC

PDB ID : 4QG1 / pdb_00004qg1
Title : Crystal structure of the tetrameric GTP/dATP-bound SAMHD1 (RN206) mutant catalytic core
Authors : Koharudin, L.M.I.; Wu, Y.; DeLucia, M.; Mehrens, J.; Gronenborn, A.M.; Ahn, J.
Deposited on : 2014-05-22
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

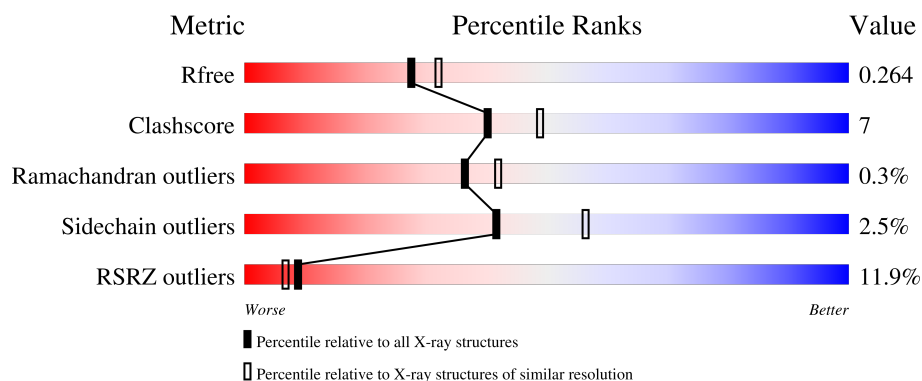
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	13% 73% 13% • 13%
1	B	550	8% 74% 13% • 13%
1	C	550	13% 74% 11% • 13%
1	D	550	8% 75% 11% • 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	B	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	C	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	D	481	Total	C	N	O	S	0	1	0
			3940	2522	687	711	20			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	expression tag	UNP Q9Y3Z3
A	78	GLY	-	expression tag	UNP Q9Y3Z3
A	79	SER	-	expression tag	UNP Q9Y3Z3
A	80	SER	-	expression tag	UNP Q9Y3Z3
A	81	HIS	-	expression tag	UNP Q9Y3Z3
A	82	HIS	-	expression tag	UNP Q9Y3Z3
A	83	HIS	-	expression tag	UNP Q9Y3Z3
A	84	HIS	-	expression tag	UNP Q9Y3Z3
A	85	HIS	-	expression tag	UNP Q9Y3Z3
A	86	HIS	-	expression tag	UNP Q9Y3Z3
A	87	SER	-	expression tag	UNP Q9Y3Z3
A	88	SER	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	LEU	-	expression tag	UNP Q9Y3Z3
A	91	VAL	-	expression tag	UNP Q9Y3Z3
A	92	PRO	-	expression tag	UNP Q9Y3Z3
A	93	ARG	-	expression tag	UNP Q9Y3Z3
A	94	GLY	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
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	-	expression tag	UNP Q9Y3Z3
B	78	GLY	-	expression tag	UNP Q9Y3Z3
B	79	SER	-	expression tag	UNP Q9Y3Z3
B	80	SER	-	expression tag	UNP Q9Y3Z3
B	81	HIS	-	expression tag	UNP Q9Y3Z3
B	82	HIS	-	expression tag	UNP Q9Y3Z3
B	83	HIS	-	expression tag	UNP Q9Y3Z3
B	84	HIS	-	expression tag	UNP Q9Y3Z3
B	85	HIS	-	expression tag	UNP Q9Y3Z3
B	86	HIS	-	expression tag	UNP Q9Y3Z3
B	87	SER	-	expression tag	UNP Q9Y3Z3
B	88	SER	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	LEU	-	expression tag	UNP Q9Y3Z3
B	91	VAL	-	expression tag	UNP Q9Y3Z3
B	92	PRO	-	expression tag	UNP Q9Y3Z3
B	93	ARG	-	expression tag	UNP Q9Y3Z3
B	94	GLY	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	MET	-	expression tag	UNP Q9Y3Z3
B	98	ALA	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	MET	-	expression tag	UNP Q9Y3Z3
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	-	expression tag	UNP Q9Y3Z3
C	78	GLY	-	expression tag	UNP Q9Y3Z3
C	79	SER	-	expression tag	UNP Q9Y3Z3
C	80	SER	-	expression tag	UNP Q9Y3Z3
C	81	HIS	-	expression tag	UNP Q9Y3Z3
C	82	HIS	-	expression tag	UNP Q9Y3Z3
C	83	HIS	-	expression tag	UNP Q9Y3Z3
C	84	HIS	-	expression tag	UNP Q9Y3Z3
C	85	HIS	-	expression tag	UNP Q9Y3Z3
C	86	HIS	-	expression tag	UNP Q9Y3Z3
C	87	SER	-	expression tag	UNP Q9Y3Z3
C	88	SER	-	expression tag	UNP Q9Y3Z3
C	89	GLY	-	expression tag	UNP Q9Y3Z3
C	90	LEU	-	expression tag	UNP Q9Y3Z3
C	91	VAL	-	expression tag	UNP Q9Y3Z3
C	92	PRO	-	expression tag	UNP Q9Y3Z3
C	93	ARG	-	expression tag	UNP Q9Y3Z3
C	94	GLY	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	MET	-	expression tag	UNP Q9Y3Z3
C	98	ALA	-	expression tag	UNP Q9Y3Z3
C	99	SER	-	expression tag	UNP Q9Y3Z3
C	100	MET	-	expression tag	UNP Q9Y3Z3
C	101	THR	-	expression tag	UNP Q9Y3Z3
C	102	GLY	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	GLN	-	expression tag	UNP Q9Y3Z3
C	105	GLN	-	expression tag	UNP Q9Y3Z3

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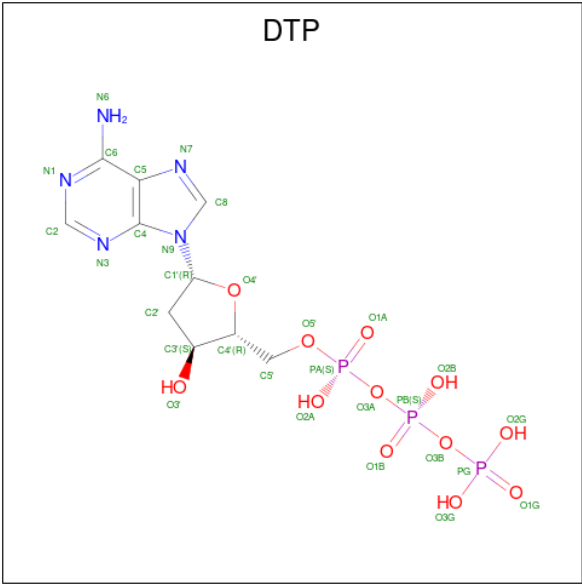
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C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	77	MET	-	expression tag	UNP Q9Y3Z3
D	78	GLY	-	expression tag	UNP Q9Y3Z3
D	79	SER	-	expression tag	UNP Q9Y3Z3
D	80	SER	-	expression tag	UNP Q9Y3Z3
D	81	HIS	-	expression tag	UNP Q9Y3Z3
D	82	HIS	-	expression tag	UNP Q9Y3Z3
D	83	HIS	-	expression tag	UNP Q9Y3Z3
D	84	HIS	-	expression tag	UNP Q9Y3Z3
D	85	HIS	-	expression tag	UNP Q9Y3Z3
D	86	HIS	-	expression tag	UNP Q9Y3Z3
D	87	SER	-	expression tag	UNP Q9Y3Z3
D	88	SER	-	expression tag	UNP Q9Y3Z3
D	89	GLY	-	expression tag	UNP Q9Y3Z3
D	90	LEU	-	expression tag	UNP Q9Y3Z3
D	91	VAL	-	expression tag	UNP Q9Y3Z3
D	92	PRO	-	expression tag	UNP Q9Y3Z3
D	93	ARG	-	expression tag	UNP Q9Y3Z3
D	94	GLY	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	MET	-	expression tag	UNP Q9Y3Z3
D	98	ALA	-	expression tag	UNP Q9Y3Z3
D	99	SER	-	expression tag	UNP Q9Y3Z3
D	100	MET	-	expression tag	UNP Q9Y3Z3
D	101	THR	-	expression tag	UNP Q9Y3Z3
D	102	GLY	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	GLN	-	expression tag	UNP Q9Y3Z3
D	105	GLN	-	expression tag	UNP Q9Y3Z3
D	106	MET	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	ARG	-	expression tag	UNP Q9Y3Z3
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'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)

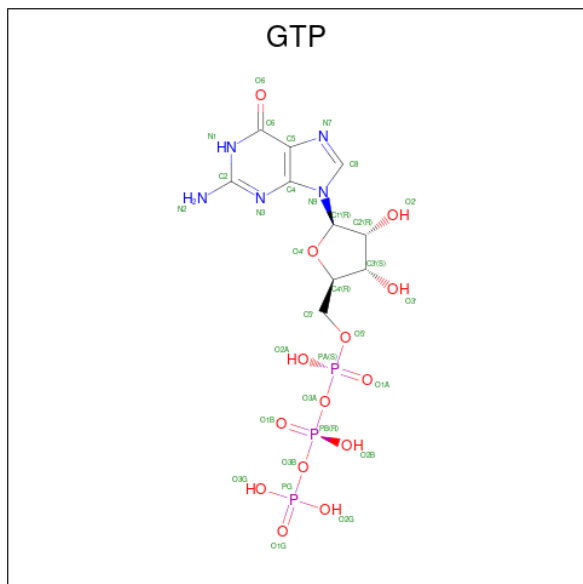


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	D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

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

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	37	Total O 37 37	0	0
5	B	56	Total O 56 56	0	0
5	C	38	Total O 38 38	0	0

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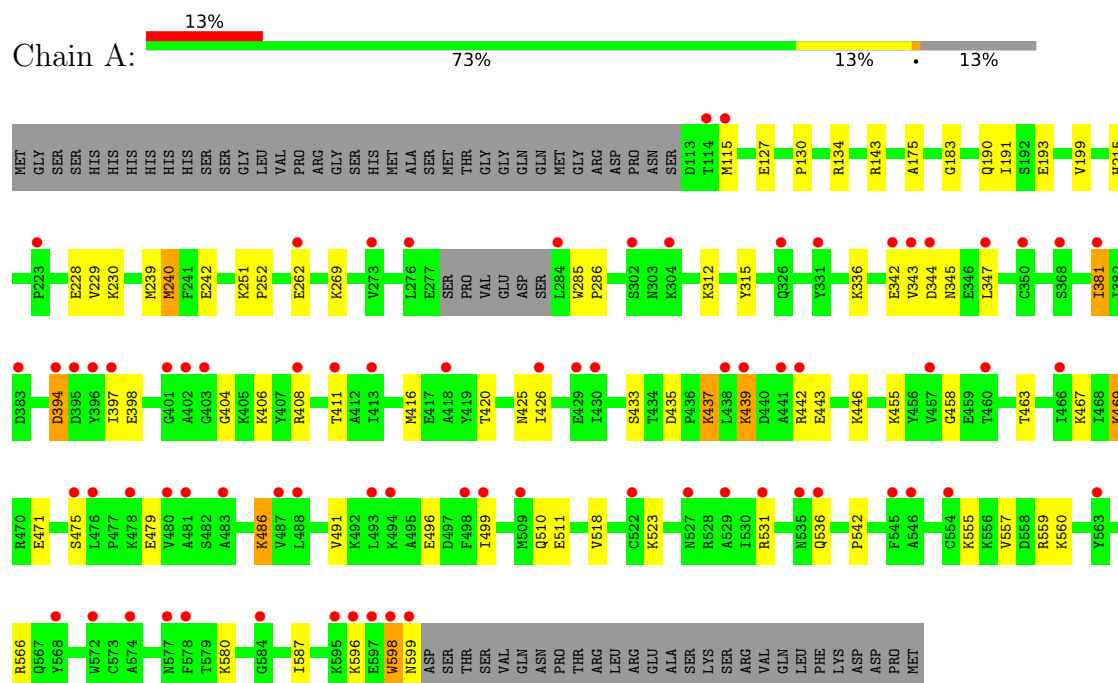
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	60	Total	O	0	0
			60	60		

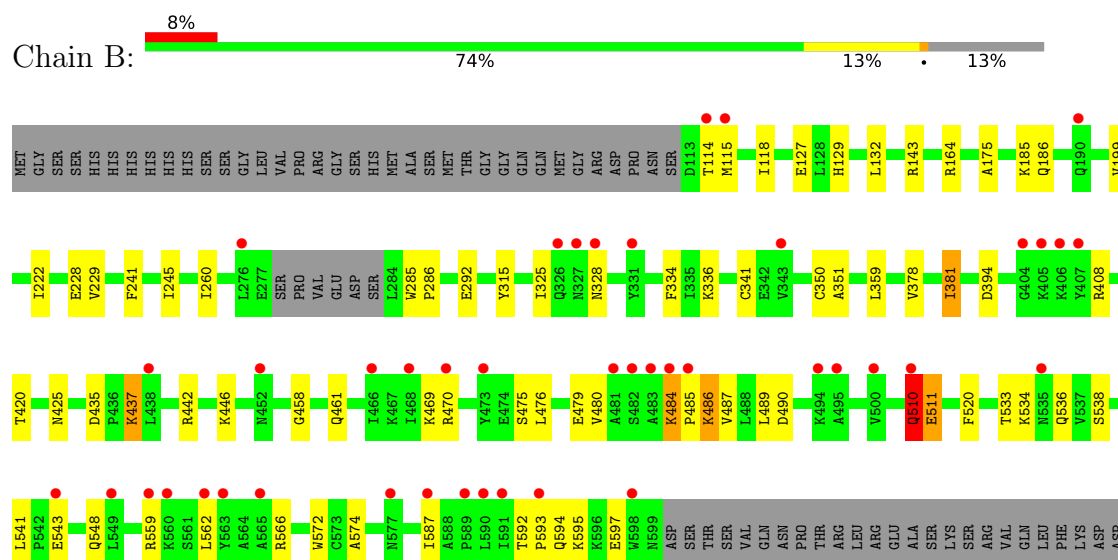
3 Residue-property plots [i](#)

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

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



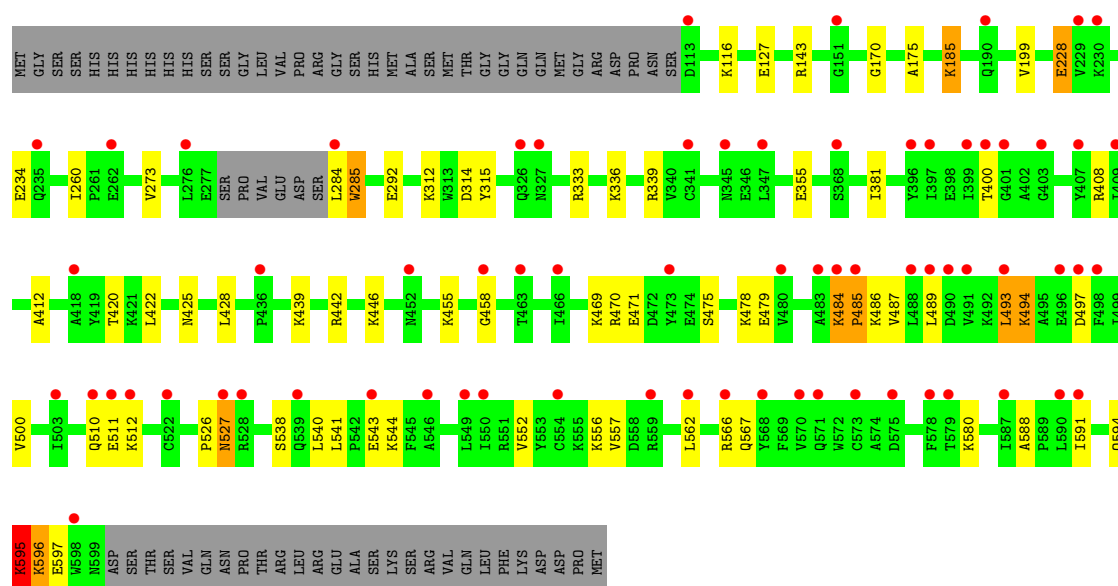
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



PRO
MET

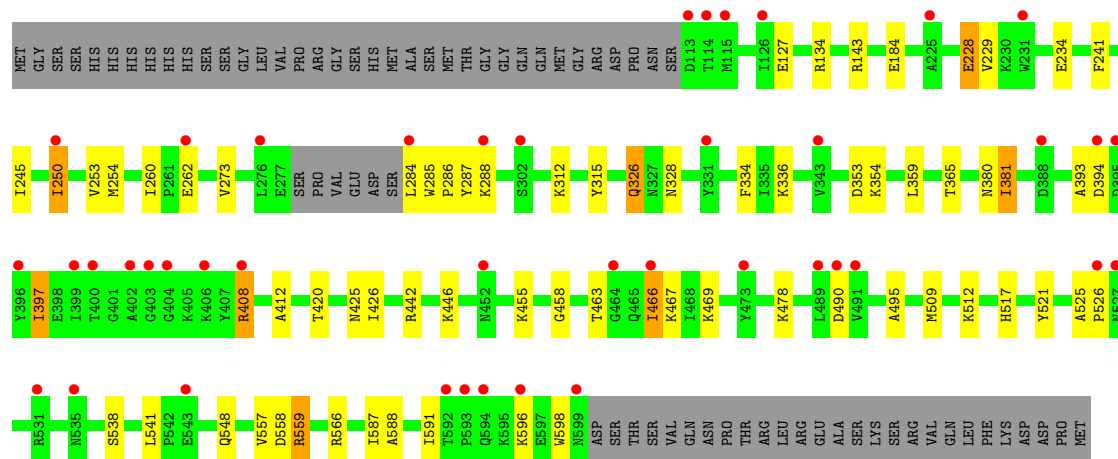
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C: 



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.69Å 146.72Å 99.26Å 90.00° 114.76° 90.00°	Depositor
Resolution (Å)	42.99 – 2.20 42.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.99-2.20) 93.9 (42.99-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496, REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.264 0.217 , 0.264	Depositor DCC
R_{free} test set	2002 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16302	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.41	0/4025	0.90	3/5433 (0.1%)
1	B	0.39	0/4025	0.91	11/5433 (0.2%)
1	C	0.40	0/4025	0.91	11/5433 (0.2%)
1	D	0.42	0/4036	0.90	13/5448 (0.2%)
All	All	0.41	0/16111	0.91	38/21747 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	LYS	CA-C-N	16.54	136.30	119.76
1	B	484	LYS	C-N-CA	16.54	136.30	119.76
1	C	596	LYS	N-CA-C	9.66	125.11	111.30
1	C	484	LYS	CA-C-N	9.07	131.18	119.84
1	C	484	LYS	C-N-CA	9.07	131.18	119.84
1	A	598	TRP	N-CA-C	-8.30	103.35	113.97
1	C	285	TRP	CA-C-N	7.17	127.78	120.04
1	C	285	TRP	C-N-CA	7.17	127.78	120.04
1	D	490	ASP	N-CA-C	-6.98	103.89	113.18
1	D	397	ILE	CA-C-N	-6.75	113.48	122.99
1	D	397	ILE	C-N-CA	-6.75	113.48	122.99
1	A	404	GLY	N-CA-C	-6.45	106.14	114.85
1	D	408	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	C	260	ILE	CA-C-N	6.29	126.50	119.32
1	C	260	ILE	C-N-CA	6.29	126.50	119.32
1	C	484	LYS	N-CA-C	6.12	118.29	109.48
1	D	525	ALA	CA-C-N	5.90	125.60	119.82
1	D	525	ALA	C-N-CA	5.90	125.60	119.82
1	D	229	VAL	N-CA-C	5.83	116.40	110.05
1	B	458	GLY	N-CA-C	5.70	118.91	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ILE	CA-C-N	5.53	125.62	119.32
1	B	260	ILE	C-N-CA	5.53	125.62	119.32
1	C	458	GLY	N-CA-C	5.50	118.61	110.42
1	B	325	ILE	CA-C-N	-5.50	114.02	122.87
1	B	325	ILE	C-N-CA	-5.50	114.02	122.87
1	D	260	ILE	CA-C-N	5.35	126.53	119.84
1	D	260	ILE	C-N-CA	5.35	126.53	119.84
1	B	592	THR	CA-C-N	-5.29	113.58	119.19
1	B	592	THR	C-N-CA	-5.29	113.58	119.19
1	A	458	GLY	N-CA-C	5.26	118.25	110.42
1	C	595	LYS	CA-C-N	-5.25	114.38	123.25
1	C	595	LYS	C-N-CA	-5.25	114.38	123.25
1	D	458	GLY	N-CA-C	5.23	118.22	110.42
1	D	408	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	222	ILE	CB-CA-C	-5.06	108.99	114.35
1	B	510	GLN	CB-CA-C	-5.06	110.35	117.23
1	D	598	TRP	CA-C-N	5.01	130.72	121.70
1	D	598	TRP	C-N-CA	5.01	130.72	121.70

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	3933	0	3919	67	0
1	B	3933	0	3921	42	0
1	C	3933	0	3919	52	0
1	D	3940	0	3926	56	0
2	A	60	0	24	3	0
2	B	60	0	24	2	0
2	C	60	0	24	1	0
2	D	60	0	24	2	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	11	2	0
4	C	32	0	11	2	0
4	D	64	0	22	1	0
5	A	37	0	0	0	0
5	B	56	0	0	0	0
5	C	38	0	0	0	0
5	D	60	0	0	1	0
All	All	16302	0	15825	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (210) 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:A:510:GLN:HG2	1:A:511:GLU:H	1.12	1.14
1:D:397:ILE:O	1:D:408:ARG:NH1	1.92	1.02
1:C:469:LYS:HD2	1:C:470:ARG:H	1.41	0.85
1:A:439:LYS:HE3	1:A:443:GLU:HG2	1.60	0.83
1:A:510:GLN:HG2	1:A:511:GLU:N	1.95	0.80
1:A:397:ILE:HG21	1:A:426:ILE:HD11	1.64	0.78
1:C:485:PRO:HB3	1:C:489:LEU:HD21	1.65	0.77
1:A:435:ASP:OD2	1:A:437:LYS:HG3	1.90	0.72
1:C:455:LYS:HG2	1:C:557:VAL:HG12	1.71	0.71
1:D:234:GLU:HB3	1:D:273:VAL:HG22	1.71	0.71
1:B:469:LYS:HD2	1:B:470:ARG:H	1.55	0.70
1:A:398:GLU:CD	1:A:406:LYS:HE3	2.18	0.69
1:A:559:ARG:HH21	1:A:560:LYS:HZ2	1.38	0.69
1:A:559:ARG:HH21	1:A:560:LYS:NZ	1.91	0.68
1:B:574:ALA:O	1:B:595:LYS:NZ	2.18	0.68
1:C:527:ASN:HD22	1:C:527:ASN:N	1.91	0.67
1:A:510:GLN:CG	1:A:511:GLU:H	1.94	0.66
1:D:328:ASN:OD1	1:D:365:THR:OG1	2.10	0.66
1:D:397:ILE:C	1:D:408:ARG:HH12	2.04	0.65
1:D:393:ALA:O	1:D:408:ARG:NH2	2.30	0.65
1:D:245:ILE:HD12	1:D:250:ILE:HD11	1.78	0.65
1:A:469:LYS:HB2	1:A:471:GLU:HG2	1.78	0.65
1:C:493:LEU:HD11	1:C:556:LYS:HD2	1.78	0.64
1:A:475:SER:O	1:A:479:GLU:HG3	1.99	0.62
1:A:408:ARG:HB3	1:A:408:ARG:CZ	2.29	0.62
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:LYS:O	1:B:486:LYS:HG3	2.00	0.62
1:C:339:ARG:HH21	1:C:527:ASN:ND2	1.99	0.60
1:B:425:ASN:OD1	1:C:425:ASN:ND2	2.33	0.60
1:D:285:TRP:O	1:D:288:LYS:NZ	2.32	0.60
1:A:394:ASP:C	1:A:408:ARG:HH12	2.08	0.60
1:B:574:ALA:HA	1:B:595:LYS:HE2	1.84	0.59
1:C:336:LYS:HE3	1:D:127:GLU:HG3	1.85	0.58
1:B:484:LYS:HD2	1:B:485:PRO:HD2	1.85	0.58
1:B:484:LYS:HD2	1:B:485:PRO:CD	2.34	0.58
1:C:442:ARG:O	1:C:446:LYS:HG3	2.03	0.57
1:A:394:ASP:O	1:A:408:ARG:NH1	2.26	0.57
1:C:493:LEU:HG	1:C:497:ASP:CB	2.35	0.57
1:D:467:LYS:HE3	1:D:548:GLN:HG3	1.86	0.57
1:A:394:ASP:C	1:A:408:ARG:HH22	2.13	0.57
1:C:475:SER:O	1:C:479:GLU:HG3	2.05	0.56
1:C:484:LYS:HB2	1:C:486:LYS:NZ	2.19	0.56
1:D:287:TYR:O	1:D:288:LYS:HD3	2.05	0.56
1:B:461:GLN:HG3	1:B:548:GLN:O	2.06	0.56
1:C:127:GLU:HG3	1:D:336:LYS:HE3	1.88	0.56
1:A:425:ASN:ND2	1:D:425:ASN:OD1	2.39	0.56
1:D:241:PHE:O	1:D:245:ILE:HG12	2.06	0.55
1:C:526:PRO:C	1:C:527:ASN:HD22	2.15	0.55
1:A:580:LYS:HG3	1:A:598:TRP:CE3	2.41	0.55
1:D:442:ARG:O	1:D:446:LYS:HG3	2.08	0.54
1:A:439:LYS:CE	1:A:443:GLU:HG2	2.34	0.53
1:A:518:VAL:O	1:A:531:ARG:NH1	2.41	0.53
1:B:538:SER:HB3	1:B:541:LEU:HG	1.90	0.53
1:D:397:ILE:HB	1:D:408:ARG:HH22	1.73	0.53
1:C:543:GLU:HG2	1:C:544:LYS:HG3	1.91	0.53
1:A:536:GLN:HE21	1:C:580:LYS:HB3	1.74	0.53
1:C:484:LYS:HB2	1:C:486:LYS:HE2	1.90	0.53
1:A:193:GLU:H	1:A:193:GLU:CD	2.16	0.53
1:C:442:ARG:HG2	1:C:446:LYS:HE2	1.90	0.52
1:C:484:LYS:HB2	1:C:486:LYS:CE	2.40	0.52
1:A:239:MET:HE2	1:A:416:MET:HE3	1.91	0.52
1:C:588:ALA:HB1	1:C:591:ILE:HD13	1.92	0.52
1:A:115:MET:HE3	1:A:127:GLU:HB3	1.92	0.52
1:D:397:ILE:CA	1:D:408:ARG:HH12	2.22	0.52
1:D:588:ALA:HB1	1:D:591:ILE:HD13	1.91	0.52
1:B:534:LYS:NZ	1:B:543:GLU:OE2	2.43	0.51
1:C:469:LYS:HD2	1:C:470:ARG:N	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:GLU:H	1:B:597:GLU:CD	2.18	0.51
1:B:442:ARG:O	1:B:446:LYS:HG3	2.11	0.51
1:C:469:LYS:HZ2	1:C:471:GLU:HG3	1.76	0.51
1:D:287:TYR:C	1:D:288:LYS:HD3	2.35	0.51
1:B:593:PRO:C	1:B:595:LYS:H	2.20	0.50
1:D:394:ASP:HA	1:D:408:ARG:HE	1.76	0.50
1:C:486:LYS:N	1:C:486:LYS:HD3	2.27	0.50
1:A:433:SER:OG	1:A:442:ARG:NH1	2.43	0.50
1:A:580:LYS:HD2	1:A:598:TRP:HB3	1.94	0.50
1:C:284:LEU:O	1:C:284:LEU:HD23	2.12	0.50
1:D:250:ILE:HD12	1:D:254:MET:HG3	1.94	0.50
1:A:342:GLU:HG2	1:A:347:LEU:CD2	2.42	0.49
1:C:339:ARG:NH2	1:C:527:ASN:ND2	2.60	0.49
1:A:397:ILE:H	1:A:408:ARG:HH21	1.60	0.49
1:B:435:ASP:OD2	1:B:437:LYS:HE2	2.12	0.49
1:A:439:LYS:HD3	1:A:442:ARG:NH2	2.28	0.49
1:C:185:LYS:HB3	1:C:185:LYS:HE2	1.66	0.48
1:D:538:SER:HB3	1:D:541:LEU:HG	1.96	0.48
1:A:408:ARG:H	1:A:411:THR:HG1	1.61	0.48
1:C:285:TRP:CD2	1:C:292:GLU:HG2	2.49	0.48
1:C:487:VAL:HG21	1:C:567:GLN:HG3	1.94	0.48
1:A:439:LYS:HD3	1:A:442:ARG:CZ	2.43	0.48
1:A:439:LYS:HD2	1:A:442:ARG:HB3	1.96	0.48
1:C:510:GLN:HG3	1:C:511:GLU:H	1.77	0.48
1:D:284:LEU:HG	1:D:285:TRP:H	1.78	0.48
1:D:354:LYS:NZ	2:D:702:DTP:O2A	2.41	0.48
1:B:378:VAL:O	1:B:381:ILE:HG22	2.14	0.48
1:A:486:LYS:HB3	1:A:486:LYS:HE2	1.46	0.48
1:B:479:GLU:HG2	1:B:572:TRP:HE1	1.79	0.48
1:A:343:VAL:O	1:A:345:ASN:N	2.47	0.47
1:A:336:LYS:HE3	1:B:127:GLU:HG3	1.96	0.47
1:C:594:GLN:O	1:C:595:LYS:O	2.30	0.47
1:A:215:HIS:NE2	2:A:701:DTP:O2A	2.43	0.47
1:C:333:ARG:NE	1:C:355:GLU:OE2	2.48	0.47
1:C:339:ARG:NH2	1:C:527:ASN:HD21	2.12	0.47
1:D:397:ILE:HG21	1:D:426:ILE:HD11	1.96	0.47
1:B:562:LEU:HD21	1:B:566:ARG:NH2	2.29	0.47
1:C:469:LYS:NZ	1:C:471:GLU:HG3	2.30	0.47
1:D:394:ASP:O	1:D:408:ARG:NE	2.48	0.47
1:D:455:LYS:HG2	1:D:557:VAL:HG12	1.97	0.47
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:701:GTP:O1G	1:C:116:LYS:NZ	2.41	0.47
1:A:531:ARG:HG2	1:A:531:ARG:HH11	1.80	0.46
1:B:566:ARG:HD3	1:B:587:ILE:HB	1.97	0.46
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.76	0.46
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.97	0.46
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.78	0.46
1:A:398:GLU:HB3	1:A:406:LYS:HD2	1.97	0.46
1:B:510:GLN:HB3	1:B:511:GLU:H	1.48	0.46
1:A:127:GLU:HG3	1:B:336:LYS:HE3	1.98	0.46
1:A:242:GLU:OE1	1:A:269:LYS:NZ	2.43	0.46
1:B:241:PHE:O	1:B:245:ILE:HG12	2.16	0.45
1:C:597:GLU:HG3	1:C:597:GLU:O	2.16	0.45
1:B:341:CYS:HB2	1:B:350:CYS:SG	2.56	0.45
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.51	0.45
1:A:439:LYS:HD3	1:A:442:ARG:NE	2.32	0.45
1:D:463:THR:O	1:D:466:ILE:HG22	2.16	0.45
1:D:509:MET:HE1	1:D:517:HIS:CD2	2.52	0.45
1:A:342:GLU:HG2	1:A:347:LEU:HD21	1.98	0.45
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.99	0.45
1:B:285:TRP:CG	1:B:292:GLU:HG2	2.52	0.45
1:D:241:PHE:CZ	1:D:245:ILE:HD11	2.52	0.45
1:D:285:TRP:HA	1:D:286:PRO:HD3	1.83	0.44
1:D:380:ASN:OD1	5:D:834:HOH:O	2.20	0.44
1:D:566:ARG:HD3	1:D:587:ILE:HB	1.99	0.44
1:B:328:ASN:CG	1:D:328:ASN:HD22	2.25	0.44
1:C:234:GLU:HB3	1:C:273:VAL:HG23	1.99	0.44
1:A:566:ARG:HD3	1:A:587:ILE:HB	2.00	0.44
1:B:484:LYS:NZ	1:B:487:VAL:O	2.44	0.44
1:B:394:ASP:O	1:B:408:ARG:HD2	2.18	0.44
1:A:215:HIS:HE2	2:A:701:DTP:PA	2.40	0.44
1:A:397:ILE:N	1:A:408:ARG:HH21	2.15	0.44
1:C:494:LYS:HE3	1:C:494:LYS:HB3	1.70	0.44
1:B:228:GLU:HG2	1:B:229:VAL:N	2.32	0.44
1:B:114:THR:OG1	1:B:115:MET:N	2.51	0.43
1:A:442:ARG:O	1:A:446:LYS:HG3	2.18	0.43
1:D:408:ARG:O	1:D:412:ALA:N	2.51	0.43
1:D:394:ASP:HA	1:D:408:ARG:HH21	1.83	0.43
1:C:500:VAL:HG22	1:C:552:VAL:HG22	1.99	0.43
1:D:284:LEU:HG	1:D:285:TRP:N	2.34	0.43
1:D:397:ILE:HB	1:D:408:ARG:HH12	1.84	0.43
1:B:129:HIS:HB3	1:B:132:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:701:DTP:O1B	4:D:701:GTP:H5''	2.19	0.43
1:D:467:LYS:HD2	1:D:467:LYS:HA	1.68	0.43
1:D:509:MET:HE2	1:D:512:LYS:HD2	2.01	0.43
1:A:439:LYS:HD2	1:A:439:LYS:HA	1.51	0.43
1:A:523:LYS:NZ	4:C:702:GTP:O2G	2.49	0.43
1:B:285:TRP:HA	1:B:286:PRO:HD3	1.86	0.42
1:B:594:GLN:O	1:B:594:GLN:HG3	2.19	0.42
1:D:394:ASP:C	1:D:408:ARG:NE	2.77	0.42
1:A:499:ILE:HD11	1:A:555:LYS:HE2	2.01	0.42
1:C:143:ARG:HD2	1:C:420:THR:HA	2.01	0.42
1:A:536:GLN:NE2	1:C:580:LYS:HD3	2.35	0.42
1:D:228:GLU:H	1:D:228:GLU:HG3	1.32	0.42
1:A:240:MET:HG2	1:A:416:MET:SD	2.59	0.42
1:B:484:LYS:HZ3	1:B:489:LEU:HD21	1.83	0.42
1:C:562:LEU:O	1:C:566:ARG:HG3	2.18	0.42
1:D:353:ASP:OD1	1:D:354:LYS:N	2.47	0.42
1:A:542:PRO:HB3	1:C:540:LEU:O	2.19	0.42
1:A:580:LYS:HA	1:A:598:TRP:CZ2	2.55	0.42
1:D:143:ARG:HD2	1:D:420:THR:HA	2.02	0.42
1:A:130:PRO:O	1:A:134:ARG:HG2	2.20	0.41
1:A:143:ARG:HD2	1:A:420:THR:HA	2.01	0.41
1:A:183:GLY:HA2	1:A:191:ILE:HD12	2.00	0.41
1:C:170:GLY:HA3	1:C:314:ASP:OD2	2.19	0.41
1:C:512:LYS:HA	1:C:512:LYS:HD3	1.75	0.41
1:B:476:LEU:O	1:B:480:VAL:HG23	2.20	0.41
1:C:484:LYS:HA	1:C:485:PRO:HD3	1.76	0.41
1:D:326:GLN:HE21	1:D:326:GLN:HB2	1.68	0.41
1:A:496:GLU:O	1:A:555:LYS:HD2	2.20	0.41
1:B:143:ARG:HD2	1:B:420:THR:HA	2.02	0.41
1:B:185:LYS:HG3	1:B:186:GLN:HG3	2.01	0.41
1:B:351:ALA:O	1:B:520:PHE:HA	2.19	0.41
4:B:701:GTP:H5''	2:D:702:DTP:O1B	2.20	0.41
1:C:412:ALA:HB3	1:C:422:LEU:HD22	2.02	0.41
1:D:467:LYS:HE3	1:D:548:GLN:CG	2.48	0.41
1:A:398:GLU:HB3	1:A:406:LYS:CD	2.51	0.41
1:D:312:LYS:HA	1:D:315:TYR:CE2	2.56	0.41
1:A:471:GLU:HG2	1:A:471:GLU:H	1.61	0.41
1:A:559:ARG:NH2	1:A:560:LYS:HZ2	2.12	0.41
1:B:334:PHE:CE1	1:B:359:LEU:HD21	2.56	0.41
1:A:285:TRP:HA	1:A:286:PRO:HD3	1.94	0.41
1:C:228:GLU:H	1:C:228:GLU:HG3	1.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:PHE:CE2	1:D:359:LEU:HD21	2.55	0.41
1:D:559:ARG:H	1:D:559:ARG:HG3	1.41	0.41
1:A:251:LYS:HB2	1:A:252:PRO:HD3	2.02	0.41
1:C:494:LYS:HG2	1:C:497:ASP:OD2	2.21	0.41
1:D:558:ASP:HB2	1:D:559:ARG:NH1	2.36	0.41
1:C:428:LEU:HD23	1:C:428:LEU:HA	1.90	0.41
1:B:315:TYR:CD2	2:B:702:DTP:H5'1	2.55	0.41
2:A:702:DTP:O1B	4:C:702:GTP:H5''	2.21	0.40
1:B:533:THR:OG1	1:B:536:GLN:HG3	2.20	0.40
1:C:538:SER:HB3	1:C:541:LEU:HG	2.02	0.40
1:A:228:GLU:HG2	1:A:229:VAL:N	2.36	0.40
1:B:164:ARG:HH22	2:B:702:DTP:H4'	1.85	0.40
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.56	0.40
1:D:134:ARG:NH2	1:D:253:VAL:HG22	2.36	0.40
1:D:408:ARG:HA	1:D:408:ARG:HD2	1.60	0.40
1:D:478:LYS:HG3	1:D:495:ALA:CB	2.52	0.40
1:D:241:PHE:CE1	1:D:245:ILE:HD11	2.56	0.40
1:A:467:LYS:N	1:A:467:LYS:HD2	2.35	0.40
1:D:521:TYR:CD1	1:D:526:PRO:HA	2.57	0.40
1:D:397:ILE:HB	1:D:408:ARG:NH2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/550 (87%)	460 (96%)	15 (3%)	2 (0%)	30	34
1	B	477/550 (87%)	461 (97%)	15 (3%)	1 (0%)	43	51
1	C	477/550 (87%)	457 (96%)	18 (4%)	2 (0%)	30	34
1	D	478/550 (87%)	461 (96%)	17 (4%)	0	100	100
All	All	1909/2200 (87%)	1839 (96%)	65 (3%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ASP
1	C	485	PRO
1	C	595	LYS
1	A	394	ASP
1	B	490	ASP

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	427/488 (88%)	414 (97%)	13 (3%)	36	49
1	B	427/488 (88%)	419 (98%)	8 (2%)	50	66
1	C	427/488 (88%)	416 (97%)	11 (3%)	40	55
1	D	428/488 (88%)	418 (98%)	10 (2%)	44	59
All	All	1709/1952 (88%)	1667 (98%)	42 (2%)	42	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	230	LYS
1	A	240	MET
1	A	262	GLU
1	A	381	ILE
1	A	437	LYS
1	A	439	LYS
1	A	463	THR
1	A	469	LYS
1	A	486	LYS
1	A	491	VAL
1	A	596	LYS
1	A	599	ASN
1	B	118	ILE
1	B	381	ILE

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Mol	Chain	Res	Type
1	B	437	LYS
1	B	475	SER
1	B	486	LYS
1	B	510	GLN
1	B	511	GLU
1	B	559	ARG
1	C	185	LYS
1	C	228	GLU
1	C	381	ILE
1	C	400	THR
1	C	408	ARG
1	C	439	LYS
1	C	478	LYS
1	C	493	LEU
1	C	494	LYS
1	C	527	ASN
1	C	596	LYS
1	D	184	GLU
1	D	228	GLU
1	D	250	ILE
1	D	262	GLU
1	D	326	GLN
1	D	381	ILE
1	D	466	ILE
1	D	469	LYS
1	D	559	ARG
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	235	GLN
1	A	326	GLN
1	A	370	HIS
1	A	375	GLN
1	A	380	ASN
1	A	425	ASN
1	A	567	GLN
1	B	149	GLN
1	B	235	GLN
1	B	248	ASN

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Mol	Chain	Res	Type
1	B	375	GLN
1	B	380	ASN
1	B	527	ASN
1	B	567	GLN
1	B	594	GLN
1	C	149	GLN
1	C	180	HIS
1	C	190	GLN
1	C	200	GLN
1	C	233	HIS
1	C	243	HIS
1	C	370	HIS
1	C	375	GLN
1	C	380	ASN
1	C	425	ASN
1	C	461	GLN
1	C	527	ASN
1	C	571	GLN
1	C	594	GLN
1	D	149	GLN
1	D	200	GLN
1	D	370	HIS
1	D	375	GLN
1	D	380	ASN
1	D	517	HIS
1	D	539	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTP	C	701	3	31,32,32	1.60	6 (19%)	46,50,50	1.79	9 (19%)
4	GTP	D	701	3	33,34,34	2.47	10 (30%)	50,54,54	1.60	9 (18%)
2	DTP	A	702	3	31,32,32	1.62	6 (19%)	46,50,50	1.78	8 (17%)
4	GTP	C	702	3	33,34,34	2.47	11 (33%)	50,54,54	1.62	8 (16%)
4	GTP	D	703	3	33,34,34	2.47	10 (30%)	50,54,54	1.62	7 (14%)
2	DTP	D	702	3	31,32,32	1.63	6 (19%)	46,50,50	1.77	9 (19%)
4	GTP	B	701	3	33,34,34	2.48	9 (27%)	50,54,54	1.60	9 (18%)
2	DTP	D	704	-	31,32,32	1.61	7 (22%)	46,50,50	1.76	9 (19%)
2	DTP	C	703	-	31,32,32	1.63	6 (19%)	46,50,50	1.81	9 (19%)
2	DTP	A	701	-	31,32,32	1.59	6 (19%)	46,50,50	1.77	9 (19%)
2	DTP	B	702	-	31,32,32	1.60	5 (16%)	46,50,50	1.80	10 (21%)
2	DTP	B	703	3	31,32,32	1.63	6 (19%)	46,50,50	1.84	9 (19%)

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	DTP	C	701	3	-	3/22/34/34	0/3/3/3
4	GTP	D	701	3	-	7/22/38/38	0/3/3/3
2	DTP	A	702	3	-	9/22/34/34	0/3/3/3
4	GTP	C	702	3	-	8/22/38/38	0/3/3/3
4	GTP	D	703	3	-	8/22/38/38	0/3/3/3
2	DTP	D	702	3	-	2/22/34/34	0/3/3/3
4	GTP	B	701	3	-	6/22/38/38	0/3/3/3
2	DTP	D	704	-	-	8/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	C	703	-	-	7/22/34/34	0/3/3/3
2	DTP	A	701	-	-	8/22/34/34	0/3/3/3
2	DTP	B	702	-	-	9/22/34/34	0/3/3/3
2	DTP	B	703	3	-	2/22/34/34	0/3/3/3

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	GTP	O6-C6	9.51	1.41	1.23
4	D	703	GTP	O6-C6	9.50	1.41	1.23
4	D	701	GTP	O6-C6	9.42	1.41	1.23
4	B	701	GTP	O6-C6	9.31	1.41	1.23
4	B	701	GTP	C2-N2	6.13	1.48	1.34
4	D	701	GTP	C2-N2	6.01	1.48	1.34
4	C	702	GTP	C2-N2	5.95	1.48	1.34
4	D	703	GTP	C2-N2	5.83	1.47	1.34
2	A	702	DTP	PB-O3B	4.57	1.64	1.59
2	C	703	DTP	PB-O3B	4.56	1.64	1.59
2	B	703	DTP	PB-O3B	4.38	1.64	1.59
2	B	702	DTP	PB-O3B	4.37	1.64	1.59
2	C	701	DTP	PB-O3B	4.27	1.64	1.59
2	A	701	DTP	PB-O3B	4.23	1.64	1.59
4	B	701	GTP	PB-O3A	-4.09	1.55	1.59
2	D	704	DTP	PB-O3B	3.99	1.63	1.59
4	D	703	GTP	PB-O3A	-3.91	1.55	1.59
2	B	702	DTP	C6-N6	3.90	1.44	1.34
2	B	703	DTP	C6-N6	3.88	1.44	1.34
2	A	702	DTP	C6-N6	3.83	1.44	1.34
2	D	702	DTP	PB-O3B	3.81	1.63	1.59
2	D	702	DTP	C6-N6	3.80	1.43	1.34
4	D	701	GTP	PB-O3A	-3.80	1.55	1.59
2	A	701	DTP	C6-N6	3.80	1.43	1.34
2	C	701	DTP	C6-N6	3.78	1.43	1.34
2	D	704	DTP	C6-N6	3.78	1.43	1.34
2	C	703	DTP	C6-N6	3.71	1.43	1.34
4	D	701	GTP	O2'-C2'	-3.13	1.35	1.43
4	B	701	GTP	O2'-C2'	-3.01	1.35	1.43
4	C	702	GTP	O2'-C2'	-2.99	1.35	1.43
4	C	702	GTP	PB-O3A	-2.93	1.56	1.59
2	D	702	DTP	O3'-C3'	-2.92	1.37	1.43
4	D	703	GTP	O2'-C2'	-2.91	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	DTP	O3'-C3'	-2.82	1.37	1.43
2	D	704	DTP	O3'-C3'	-2.80	1.37	1.43
2	D	702	DTP	PB-O3A	2.76	1.62	1.59
2	C	701	DTP	C5'-C4'	-2.75	1.43	1.51
2	B	702	DTP	O3'-C3'	-2.72	1.37	1.43
2	B	703	DTP	O3'-C3'	-2.70	1.37	1.43
2	B	703	DTP	C5'-C4'	-2.69	1.43	1.51
2	A	701	DTP	O3'-C3'	-2.69	1.37	1.43
2	C	703	DTP	O3'-C3'	-2.67	1.37	1.43
2	B	702	DTP	C5'-C4'	-2.67	1.43	1.51
2	D	704	DTP	PB-O3A	2.65	1.62	1.59
2	D	702	DTP	C5'-C4'	-2.64	1.43	1.51
2	A	701	DTP	C5'-C4'	-2.64	1.43	1.51
2	A	702	DTP	C5'-C4'	-2.64	1.43	1.51
2	A	702	DTP	O3'-C3'	-2.63	1.37	1.43
2	C	703	DTP	C5'-C4'	-2.59	1.43	1.51
2	D	704	DTP	C5'-C4'	-2.54	1.43	1.51
4	B	701	GTP	C5'-C4'	-2.52	1.44	1.51
4	D	701	GTP	C5'-C4'	-2.48	1.44	1.51
2	C	703	DTP	PB-O3A	2.39	1.62	1.59
2	D	704	DTP	C2'-C3'	-2.38	1.46	1.52
4	B	701	GTP	C6-N1	-2.35	1.34	1.38
4	C	702	GTP	C2'-C3'	-2.34	1.47	1.53
2	D	702	DTP	C2'-C3'	-2.34	1.46	1.52
2	C	703	DTP	C2'-C3'	-2.33	1.46	1.52
4	D	701	GTP	C2'-C3'	-2.31	1.47	1.53
4	C	702	GTP	C5'-C4'	-2.29	1.44	1.51
4	B	701	GTP	C3'-C4'	-2.29	1.47	1.53
2	B	702	DTP	PB-O3A	2.28	1.62	1.59
2	C	701	DTP	C2'-C3'	-2.27	1.47	1.52
4	C	702	GTP	PA-O3A	2.27	1.62	1.59
4	B	701	GTP	C2'-C3'	-2.27	1.47	1.53
2	A	702	DTP	PB-O3A	2.26	1.61	1.59
4	D	701	GTP	C3'-C4'	-2.26	1.47	1.53
4	C	702	GTP	C3'-C4'	-2.26	1.47	1.53
2	A	701	DTP	C2'-C3'	-2.26	1.47	1.52
4	D	703	GTP	C3'-C4'	-2.24	1.47	1.53
4	D	701	GTP	C5-N7	-2.22	1.34	1.39
4	D	703	GTP	C2'-C3'	-2.20	1.47	1.53
2	B	703	DTP	C2'-C3'	-2.19	1.47	1.52
2	A	702	DTP	C2'-C3'	-2.18	1.47	1.52
4	D	703	GTP	C5-N7	-2.17	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	GTP	C6-N1	-2.16	1.34	1.38
4	D	703	GTP	C6-N1	-2.15	1.34	1.38
2	C	701	DTP	PB-O3A	2.13	1.61	1.59
4	D	703	GTP	PG-O2G	-2.11	1.47	1.54
4	C	702	GTP	C5-N7	-2.11	1.34	1.39
4	D	703	GTP	C5'-C4'	-2.10	1.45	1.51
2	A	701	DTP	PB-O3A	2.10	1.61	1.59
4	D	701	GTP	C6-N1	-2.08	1.35	1.38
2	B	703	DTP	PB-O3A	2.07	1.61	1.59
4	B	701	GTP	PG-O2G	-2.07	1.47	1.54
4	C	702	GTP	PG-O2G	-2.06	1.47	1.54
4	D	701	GTP	PG-O2G	-2.01	1.47	1.54
2	D	704	DTP	PG-O3G	-2.00	1.47	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	GTP	C5-C4-N3	-5.68	119.35	128.39
4	D	701	GTP	C5-C4-N3	-5.67	119.36	128.39
4	D	703	GTP	C5-C4-N3	-5.52	119.61	128.39
4	B	701	GTP	C5-C4-N3	-5.41	119.78	128.39
2	A	702	DTP	C5-C4-N3	-5.27	119.47	126.72
2	A	701	DTP	C5-C4-N3	-5.13	119.66	126.72
2	B	703	DTP	N3-C2-N1	-5.10	120.87	128.58
2	C	701	DTP	C5-C4-N3	-5.06	119.75	126.72
2	C	703	DTP	C5-C4-N3	-5.05	119.76	126.72
2	D	702	DTP	N3-C2-N1	-5.04	120.96	128.58
2	B	702	DTP	N3-C2-N1	-4.98	121.04	128.58
2	B	702	DTP	C5-C4-N3	-4.91	119.96	126.72
2	D	704	DTP	N3-C2-N1	-4.90	121.17	128.58
2	C	703	DTP	N3-C2-N1	-4.82	121.29	128.58
2	A	701	DTP	N3-C2-N1	-4.76	121.37	128.58
2	A	702	DTP	N3-C2-N1	-4.72	121.44	128.58
2	C	701	DTP	N3-C2-N1	-4.67	121.51	128.58
2	D	704	DTP	C5-C4-N3	-4.66	120.30	126.72
2	D	702	DTP	C5-C4-N3	-4.52	120.49	126.72
2	B	703	DTP	C5-C4-N3	-4.48	120.54	126.72
4	D	701	GTP	C2-N3-C4	4.31	119.72	112.30
4	C	702	GTP	N9-C4-N3	4.27	134.48	125.95
4	D	703	GTP	C2-N3-C4	4.23	119.58	112.30
4	B	701	GTP	C2-N3-C4	4.12	119.39	112.30
4	C	702	GTP	C2-N3-C4	4.10	119.36	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	GTP	N9-C4-N3	4.05	134.04	125.95
2	B	703	DTP	N9-C8-N7	-4.00	108.27	113.94
2	A	702	DTP	C4-C5-N7	-3.70	106.35	110.58
4	B	701	GTP	N9-C4-N3	3.70	133.34	125.95
2	B	703	DTP	C4-C5-N7	-3.68	106.38	110.58
4	D	703	GTP	N9-C4-N3	3.68	133.31	125.95
2	D	702	DTP	N9-C8-N7	-3.65	108.76	113.94
2	C	701	DTP	C4-C5-N7	-3.59	106.48	110.58
2	A	702	DTP	C2-N3-C4	3.58	120.56	111.83
2	A	701	DTP	C2-N3-C4	3.51	120.40	111.83
2	C	703	DTP	C2-N3-C4	3.50	120.39	111.83
2	D	702	DTP	C4-C5-N7	-3.49	106.59	110.58
2	C	701	DTP	N9-C8-N7	-3.46	109.03	113.94
2	C	701	DTP	C2-N3-C4	3.45	120.25	111.83
2	A	701	DTP	N3-C4-N9	3.44	133.02	127.17
2	B	702	DTP	C2-N3-C4	3.44	120.22	111.83
2	B	703	DTP	C2-N3-C4	3.43	120.20	111.83
2	D	702	DTP	C2-N3-C4	3.42	120.19	111.83
2	C	703	DTP	N9-C8-N7	-3.42	109.08	113.94
2	D	704	DTP	N9-C8-N7	-3.42	109.09	113.94
2	A	701	DTP	N9-C8-N7	-3.41	109.10	113.94
2	C	703	DTP	N3-C4-N9	3.40	132.95	127.17
2	B	702	DTP	N3-C4-N9	3.38	132.92	127.17
2	B	703	DTP	C5-N7-C8	3.37	108.75	103.45
2	D	704	DTP	C2-N3-C4	3.30	119.89	111.83
2	C	701	DTP	C5-N7-C8	3.29	108.62	103.45
2	A	702	DTP	C5-N7-C8	3.28	108.61	103.45
2	D	704	DTP	O5'-C5'-C4'	3.27	120.12	108.99
2	A	702	DTP	N9-C8-N7	-3.27	109.30	113.94
2	B	702	DTP	N9-C8-N7	-3.25	109.32	113.94
2	A	701	DTP	C4-C5-N7	-3.23	106.89	110.58
2	D	704	DTP	N3-C4-N9	3.22	132.64	127.17
4	D	703	GTP	O5'-C5'-C4'	3.20	119.90	108.99
2	C	703	DTP	C4-C5-N7	-3.20	106.92	110.58
2	A	702	DTP	N3-C4-N9	3.18	132.57	127.17
2	C	701	DTP	N3-C4-N9	3.14	132.50	127.17
2	D	702	DTP	C5-N7-C8	3.13	108.37	103.45
2	A	701	DTP	C5-N7-C8	3.10	108.32	103.45
2	C	703	DTP	O5'-C5'-C4'	3.09	119.53	108.99
2	C	703	DTP	C5-N7-C8	3.07	108.27	103.45
2	B	702	DTP	O5'-C5'-C4'	3.06	119.42	108.99
2	B	703	DTP	C4-N9-C8	3.00	108.89	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	DTP	C4-C5-N7	-2.99	107.16	110.58
2	D	704	DTP	C4-C5-N7	-2.93	107.23	110.58
2	B	702	DTP	C5-N7-C8	2.91	108.03	103.45
2	D	704	DTP	C5-N7-C8	2.91	108.02	103.45
4	C	702	GTP	O3G-PG-O3B	2.91	114.39	104.64
4	D	703	GTP	O3G-PG-O3B	2.88	114.30	104.64
4	C	702	GTP	O5'-C5'-C4'	2.74	118.34	108.99
2	D	704	DTP	C4-N9-C8	2.71	108.59	105.74
4	B	701	GTP	O3G-PG-O3B	2.69	113.67	104.64
2	D	702	DTP	N3-C4-N9	2.69	131.74	127.17
2	B	703	DTP	N3-C4-N9	2.68	131.73	127.17
2	D	702	DTP	C4-N9-C8	2.65	108.52	105.74
2	A	701	DTP	O5'-C5'-C4'	2.61	117.88	108.99
2	C	703	DTP	C4-N9-C8	2.56	108.43	105.74
2	D	702	DTP	O2G-PG-O3B	2.55	113.18	104.64
2	B	702	DTP	C4-N9-C8	2.50	108.37	105.74
2	A	701	DTP	C4-N9-C8	2.50	108.36	105.74
2	C	701	DTP	O2G-PG-O3B	2.45	112.85	104.64
4	B	701	GTP	O5'-C5'-C4'	2.43	117.26	108.99
4	D	701	GTP	C2-N1-C6	-2.42	120.73	125.11
4	B	701	GTP	N9-C8-N7	-2.41	108.92	113.40
4	D	701	GTP	O5'-C5'-C4'	2.41	117.20	108.99
4	D	701	GTP	O3G-PG-O3B	2.40	112.69	104.64
4	B	701	GTP	C2-N1-C6	-2.37	120.82	125.11
4	C	702	GTP	C2-N1-C6	-2.34	120.87	125.11
2	C	701	DTP	C4-N9-C8	2.27	108.13	105.74
4	C	702	GTP	N9-C8-N7	-2.27	109.20	113.40
4	D	703	GTP	C2-N1-C6	-2.20	121.13	125.11
4	D	701	GTP	N9-C8-N7	-2.19	109.35	113.40
2	B	703	DTP	O5'-C5'-C4'	2.17	116.37	108.99
4	B	701	GTP	C8-N7-C5	2.16	108.10	104.26
4	D	701	GTP	C8-N7-C5	2.12	108.03	104.26
4	C	702	GTP	O6-C6-C5	-2.09	121.01	126.53
4	B	701	GTP	C4-C5-N7	-2.09	107.36	110.67
4	D	703	GTP	C4-C5-N7	-2.08	107.38	110.67
2	B	702	DTP	O3G-PG-O3B	2.03	111.44	104.64
4	D	701	GTP	C4-C5-N7	-2.02	107.47	110.67
2	A	702	DTP	O2G-PG-O3B	2.00	111.36	104.64

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DTP	C5'-O5'-PA-O1A
2	A	702	DTP	PB-O3B-PG-O2G
2	A	702	DTP	PB-O3B-PG-O3G
2	A	702	DTP	C5'-O5'-PA-O1A
2	A	702	DTP	C5'-O5'-PA-O2A
2	C	701	DTP	PB-O3B-PG-O2G
2	C	703	DTP	PB-O3A-PA-O5'
2	C	703	DTP	C5'-O5'-PA-O2A
2	D	704	DTP	C5'-O5'-PA-O1A
2	D	704	DTP	C5'-O5'-PA-O2A
2	D	704	DTP	C5'-O5'-PA-O3A
2	D	704	DTP	C4'-C5'-O5'-PA
4	B	701	GTP	PB-O3B-PG-O3G
4	C	702	GTP	PB-O3B-PG-O3G
4	C	702	GTP	C5'-O5'-PA-O3A
4	C	702	GTP	C5'-O5'-PA-O2A
4	D	701	GTP	PB-O3B-PG-O3G
4	D	703	GTP	PB-O3B-PG-O3G
2	A	702	DTP	O4'-C4'-C5'-O5'
2	C	703	DTP	C3'-C4'-C5'-O5'
2	C	703	DTP	O4'-C4'-C5'-O5'
2	A	701	DTP	C3'-C4'-C5'-O5'
2	B	702	DTP	C2'-C1'-N9-C4
2	A	701	DTP	C4'-C5'-O5'-PA
2	A	702	DTP	C3'-C4'-C5'-O5'
2	A	701	DTP	PB-O3A-PA-O5'
2	D	704	DTP	PB-O3A-PA-O5'
4	D	703	GTP	PB-O3B-PG-O2G
4	B	701	GTP	PB-O3A-PA-O2A
4	C	702	GTP	PB-O3A-PA-O2A
4	D	701	GTP	PB-O3A-PA-O2A
2	C	703	DTP	C4'-C5'-O5'-PA
2	A	701	DTP	O4'-C4'-C5'-O5'
2	A	701	DTP	C5'-O5'-PA-O2A
2	A	701	DTP	C5'-O5'-PA-O3A
2	A	702	DTP	C5'-O5'-PA-O3A
2	B	702	DTP	C5'-O5'-PA-O2A
2	B	702	DTP	C5'-O5'-PA-O3A
2	C	703	DTP	C5'-O5'-PA-O1A
2	C	703	DTP	C5'-O5'-PA-O3A
4	B	701	GTP	C5'-O5'-PA-O1A
4	C	702	GTP	C5'-O5'-PA-O1A
4	D	701	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	D	703	GTP	C5'-O5'-PA-O3A
4	D	703	GTP	C5'-O5'-PA-O1A
2	B	702	DTP	C4'-C5'-O5'-PA
2	A	702	DTP	PG-O3B-PB-O1B
2	B	702	DTP	PG-O3B-PB-O2B
4	D	703	GTP	PB-O3A-PA-O2A
2	B	703	DTP	PG-O3B-PB-O1B
2	C	701	DTP	PB-O3B-PG-O1G
4	B	701	GTP	PB-O3B-PG-O1G
4	D	703	GTP	PB-O3B-PG-O1G
2	C	701	DTP	PB-O3B-PG-O3G
4	B	701	GTP	PB-O3B-PG-O2G
4	D	701	GTP	PB-O3B-PG-O2G
2	B	702	DTP	PG-O3B-PB-O1B
2	D	702	DTP	PG-O3B-PB-O1B
2	D	704	DTP	PB-O3A-PA-O1A
4	D	701	GTP	PG-O3B-PB-O2B
4	D	703	GTP	PB-O3A-PA-O1A
2	A	701	DTP	C2'-C1'-N9-C4
4	C	702	GTP	C4'-C5'-O5'-PA
2	B	702	DTP	C2'-C1'-N9-C8
4	C	702	GTP	PB-O3B-PG-O1G
4	D	701	GTP	PB-O3B-PG-O1G
2	B	702	DTP	O4'-C1'-N9-C4
4	D	703	GTP	C4'-C5'-O5'-PA
2	B	702	DTP	O4'-C1'-N9-C8
4	D	701	GTP	C4'-C5'-O5'-PA
2	A	702	DTP	PG-O3B-PB-O2B
2	B	703	DTP	PG-O3B-PB-O2B
2	D	702	DTP	PG-O3B-PB-O2B
2	D	704	DTP	PB-O3A-PA-O2A
4	B	701	GTP	PG-O3B-PB-O2B
4	C	702	GTP	PG-O3B-PB-O2B
2	D	704	DTP	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 10 short contacts:

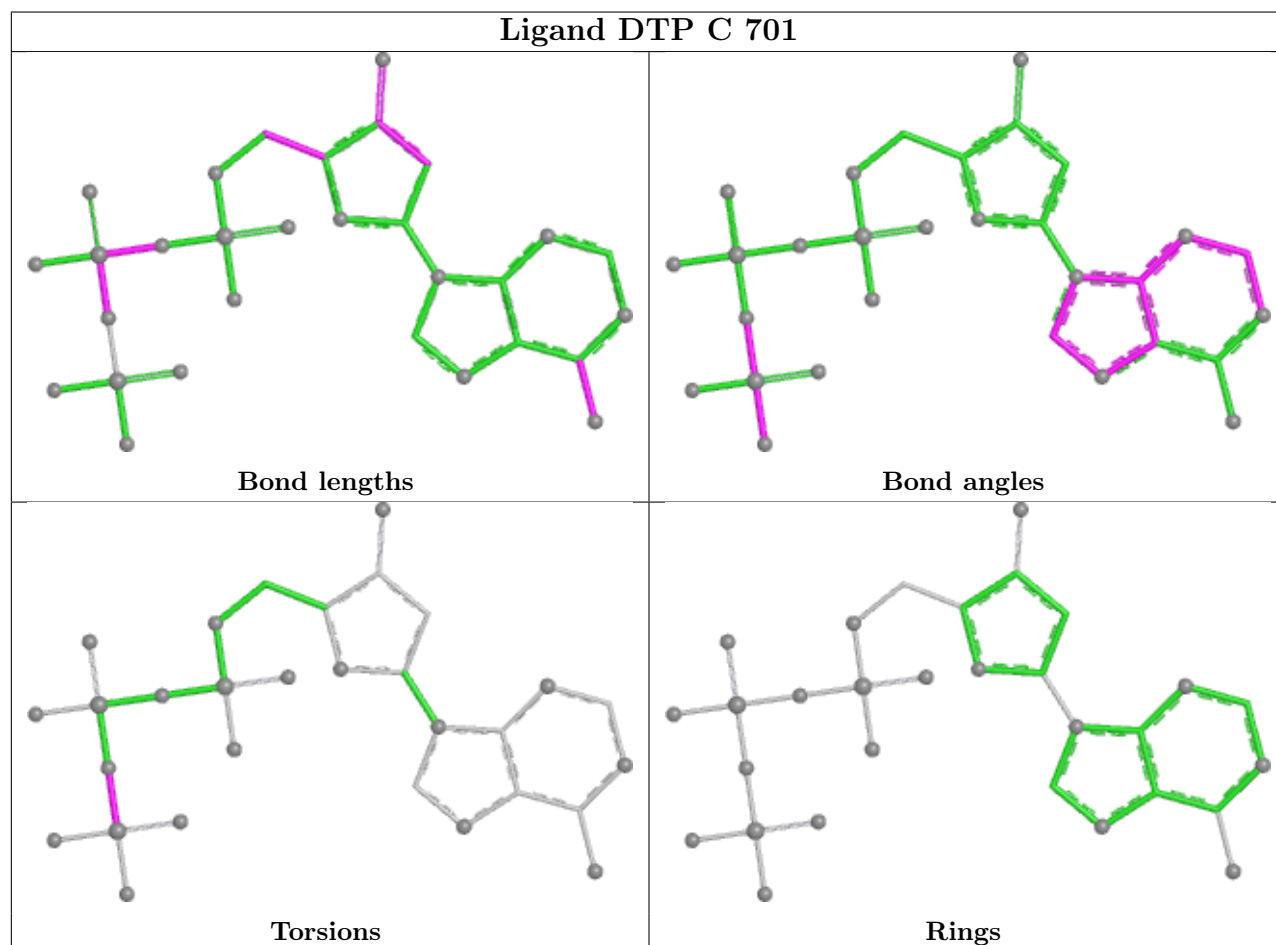
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	DTP	1	0
4	D	701	GTP	1	0
2	A	702	DTP	1	0

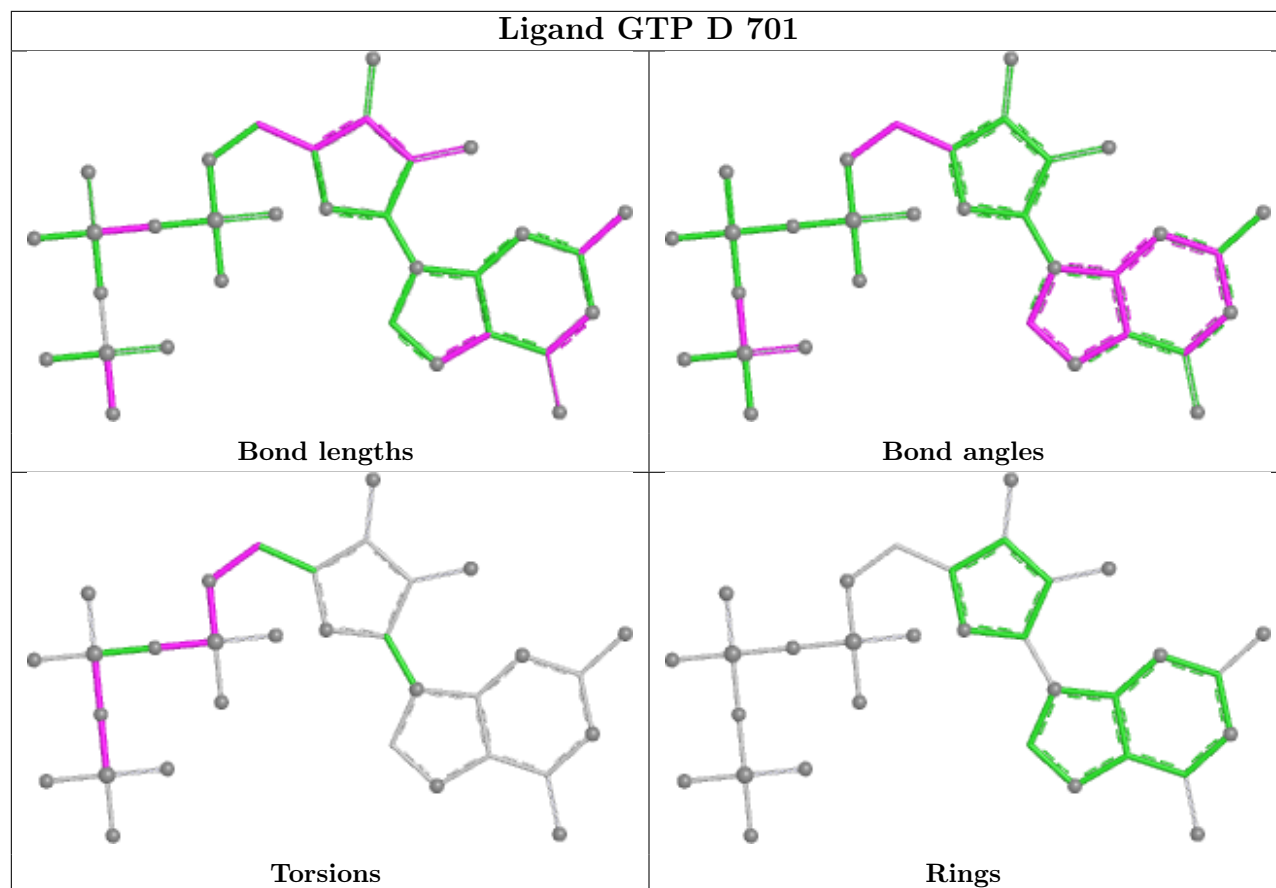
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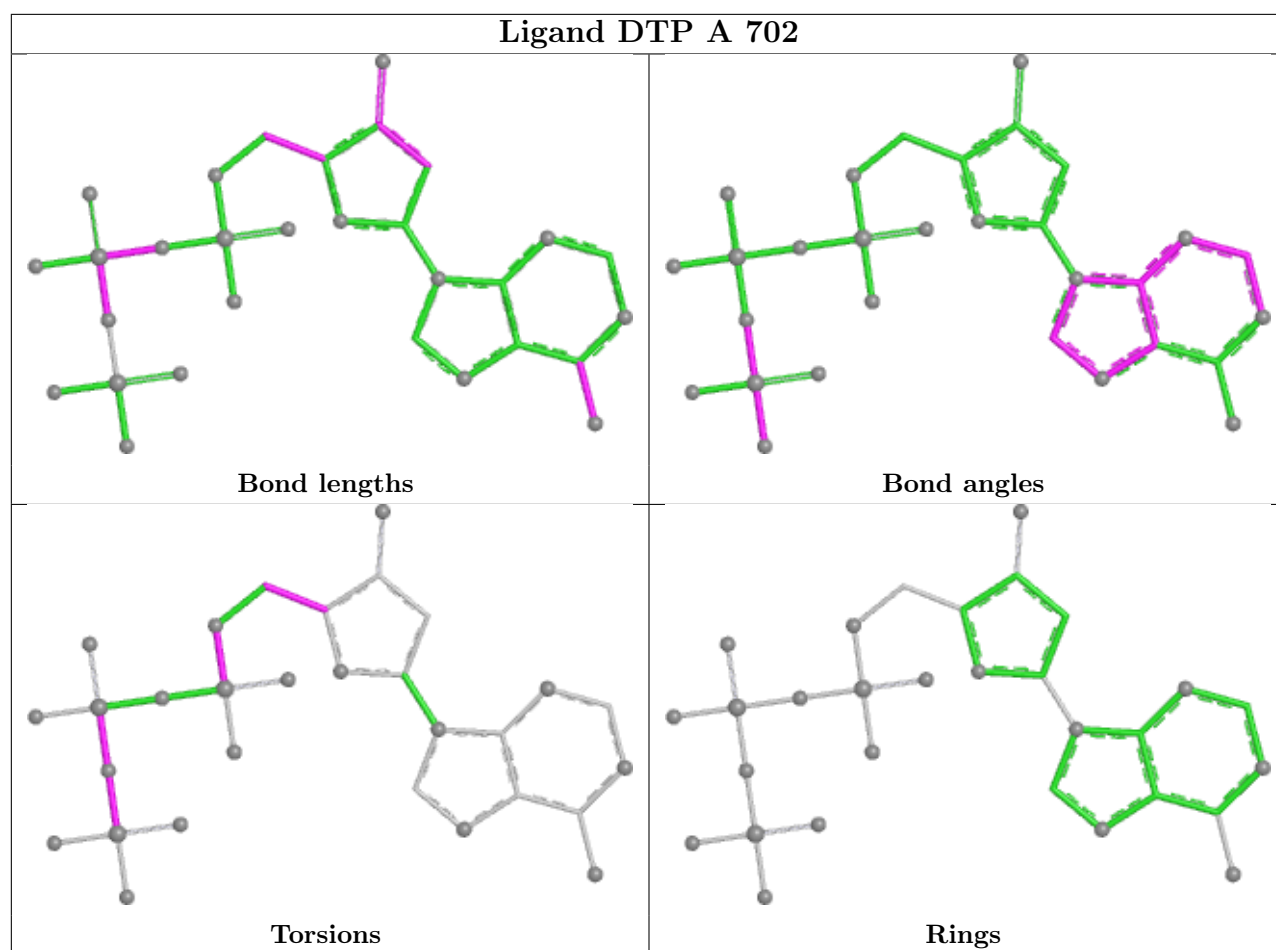
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	GTP	2	0
2	D	702	DTP	2	0
4	B	701	GTP	2	0
2	A	701	DTP	2	0
2	B	702	DTP	2	0

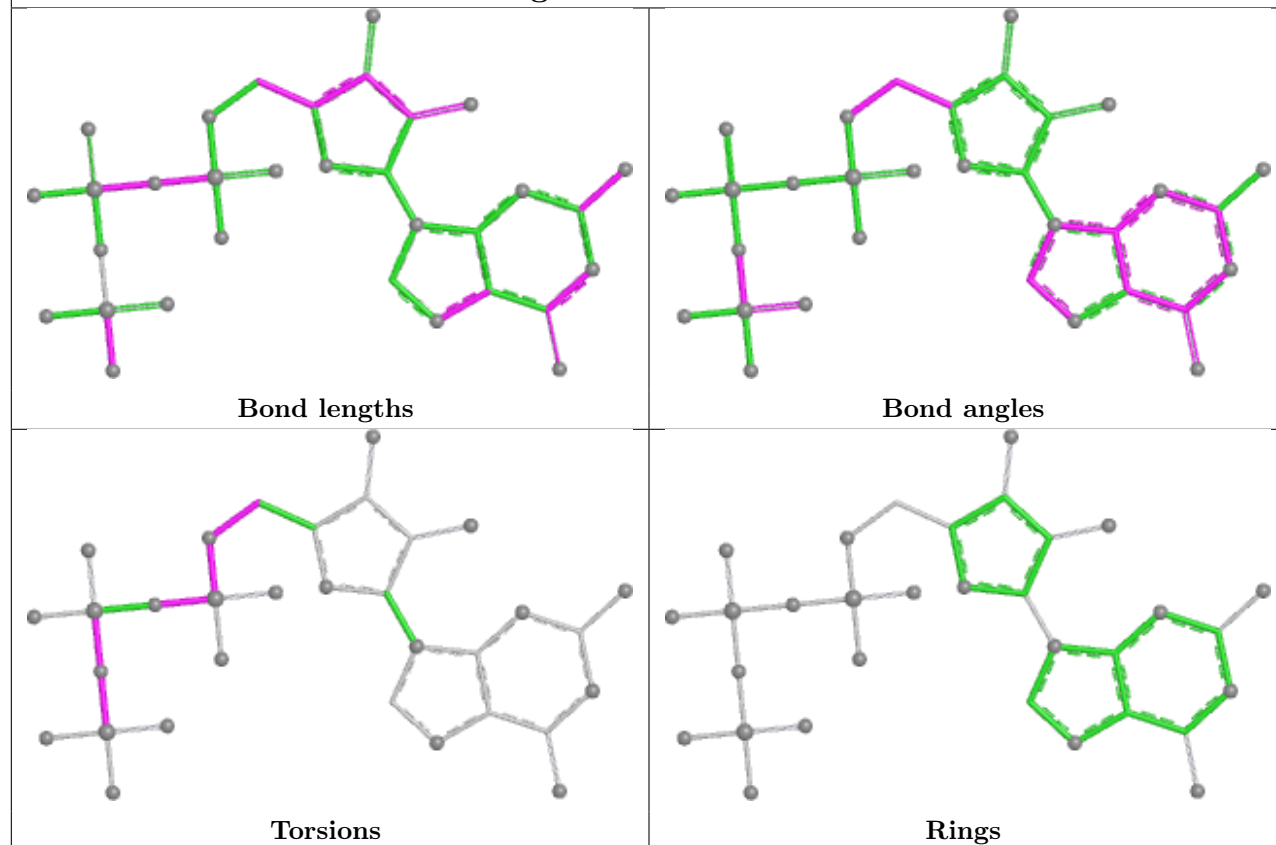
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



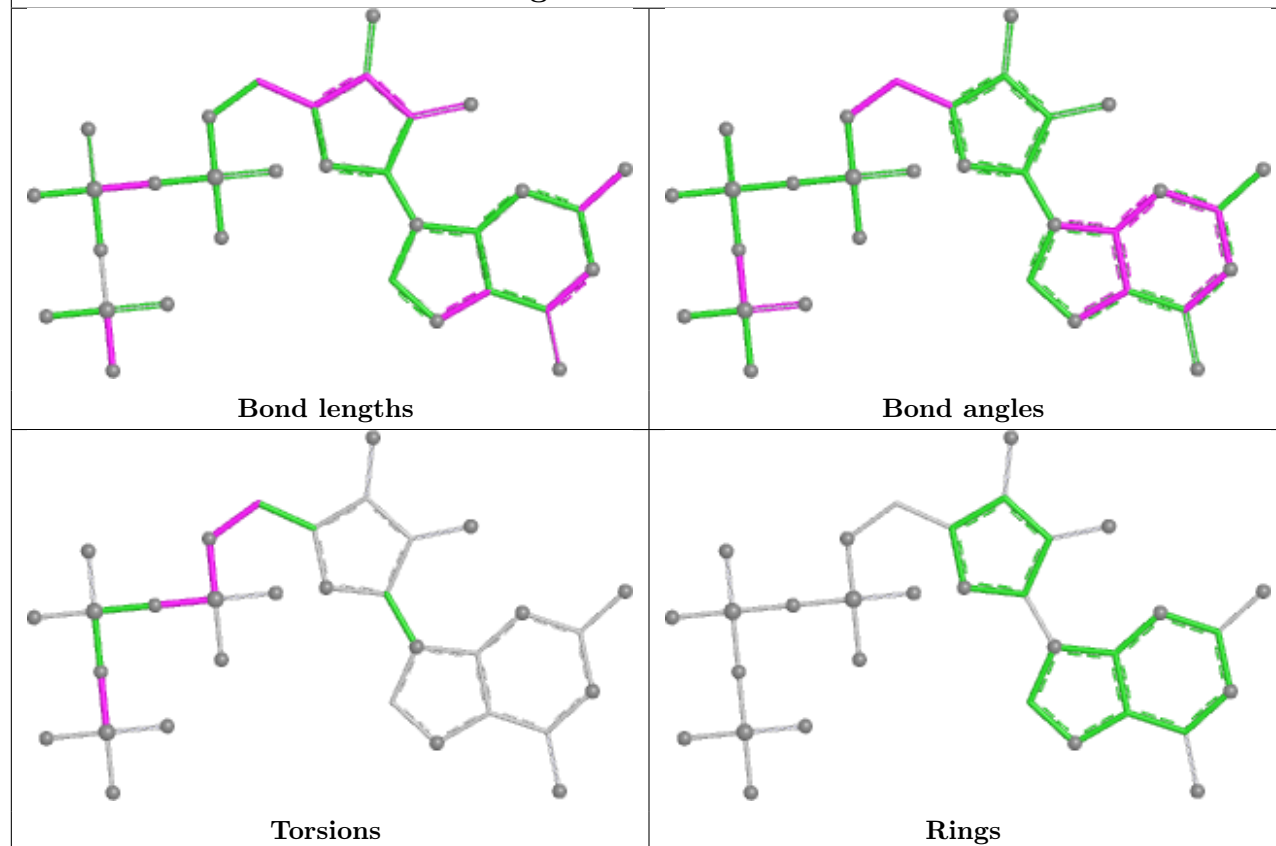


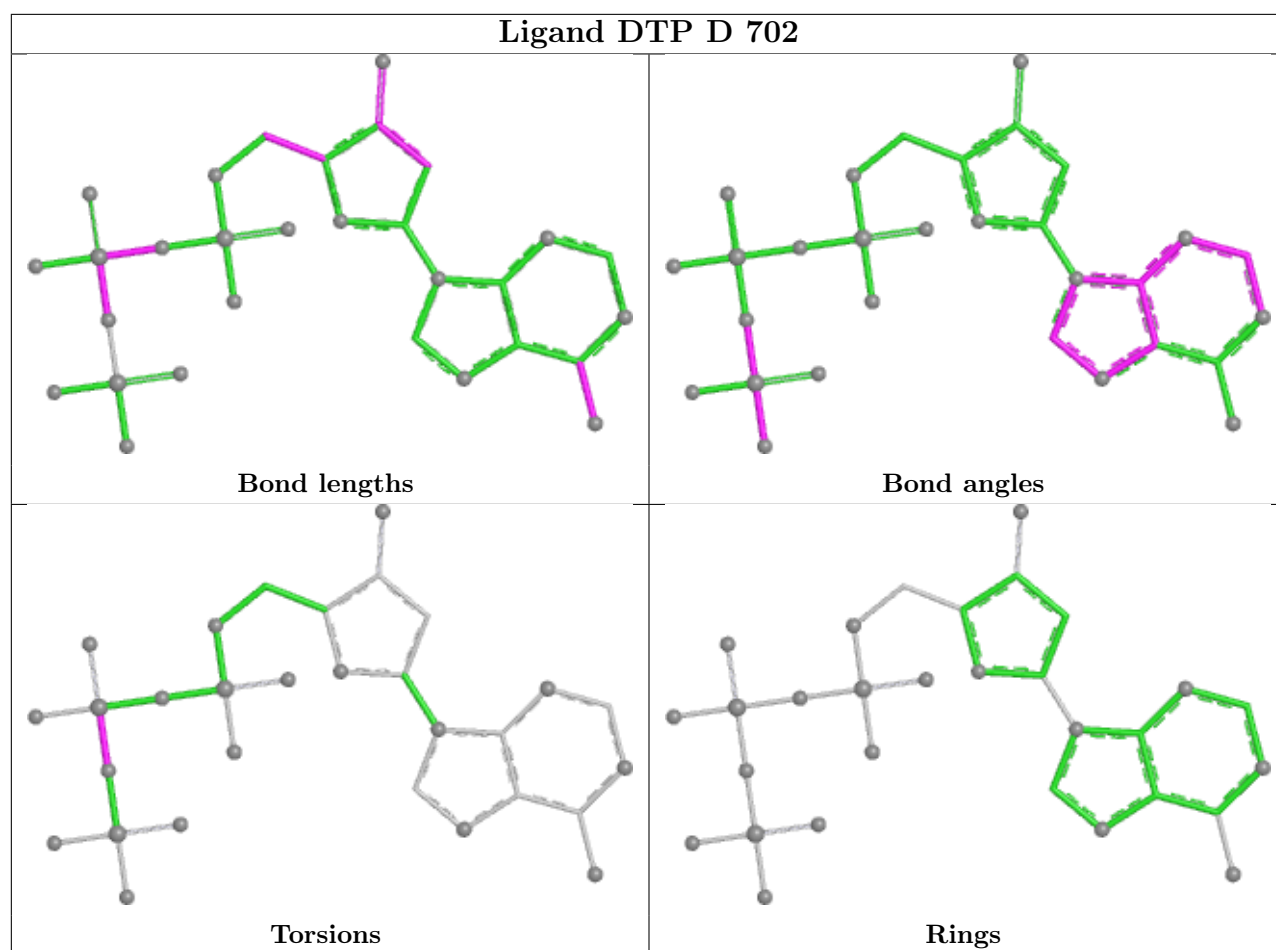


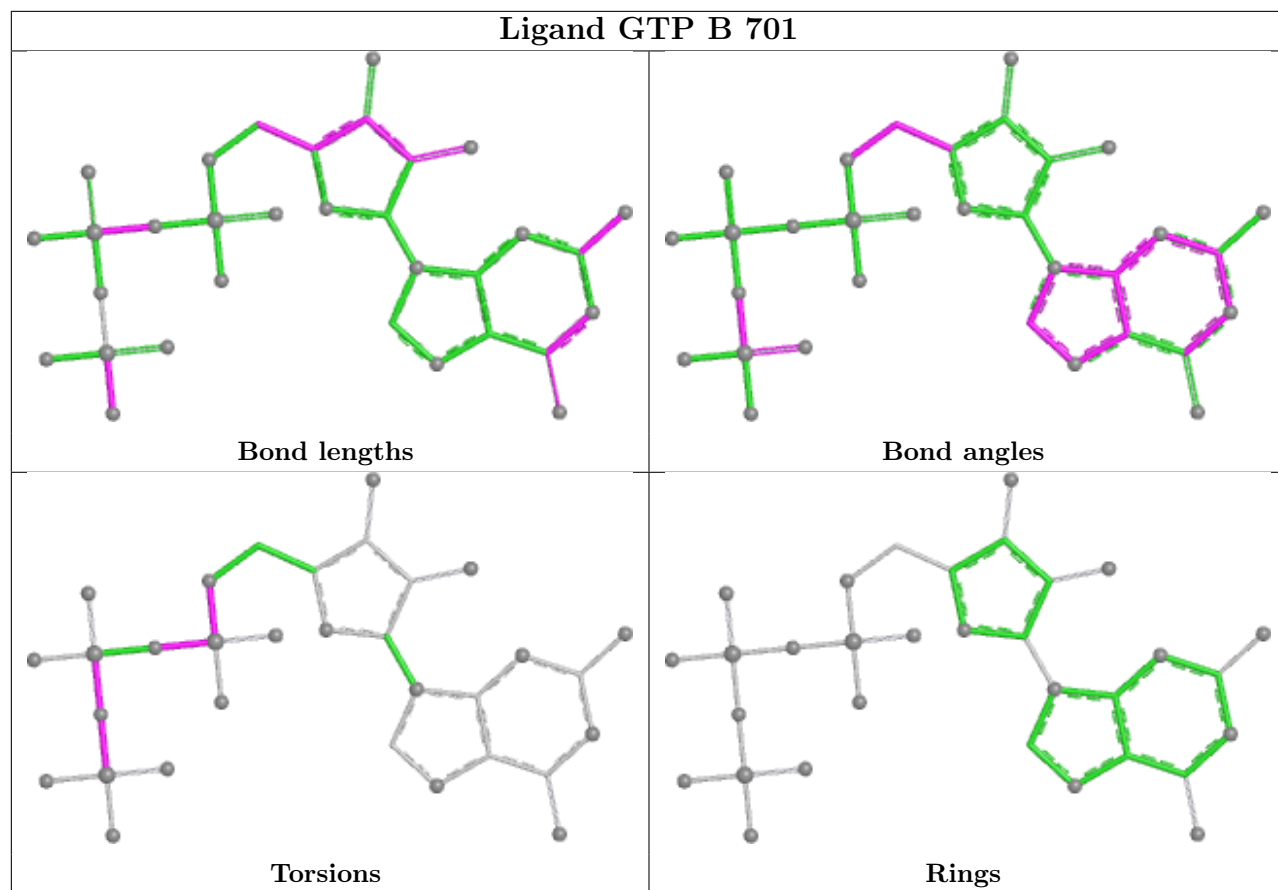
Ligand GTP C 702

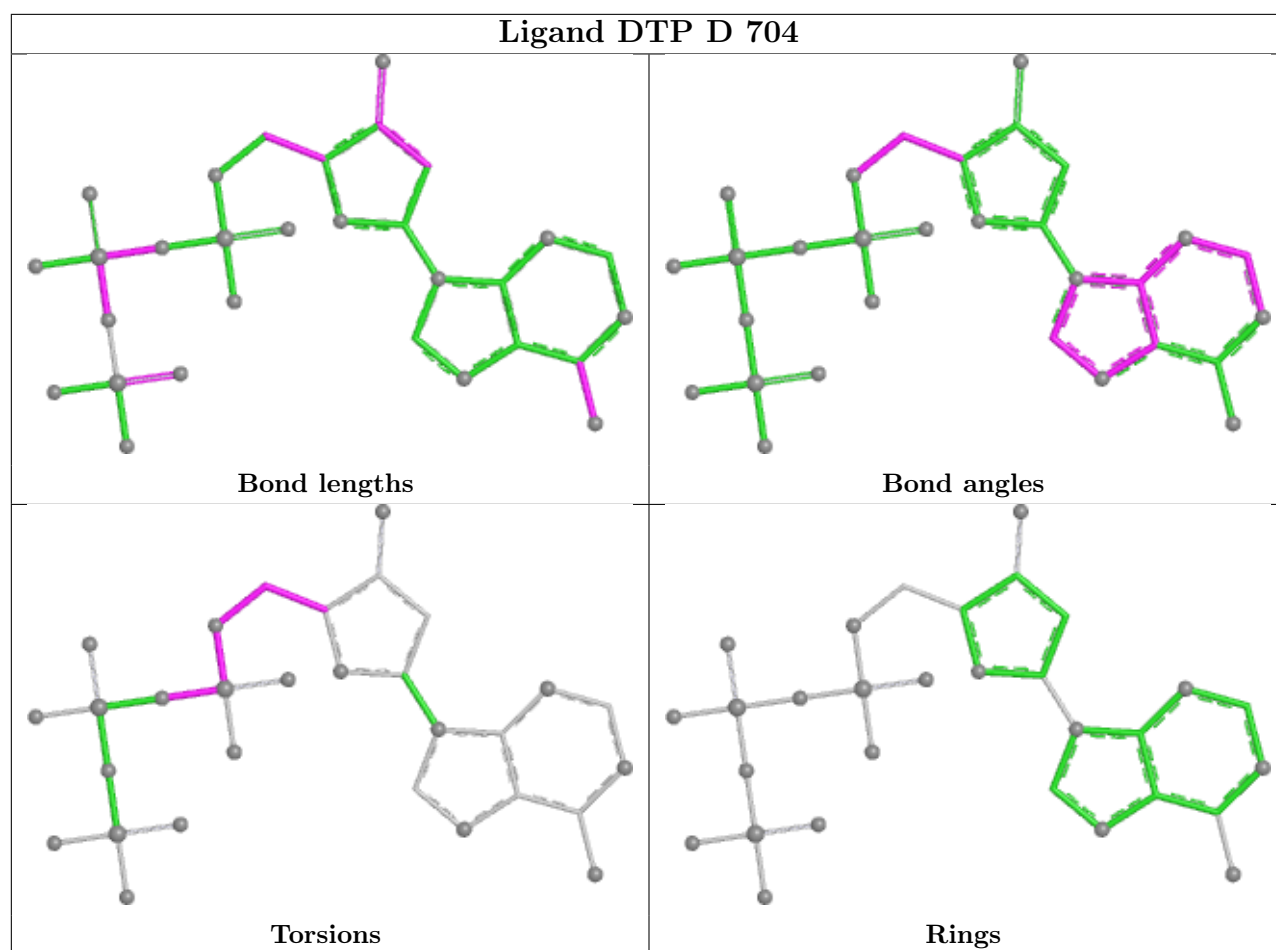


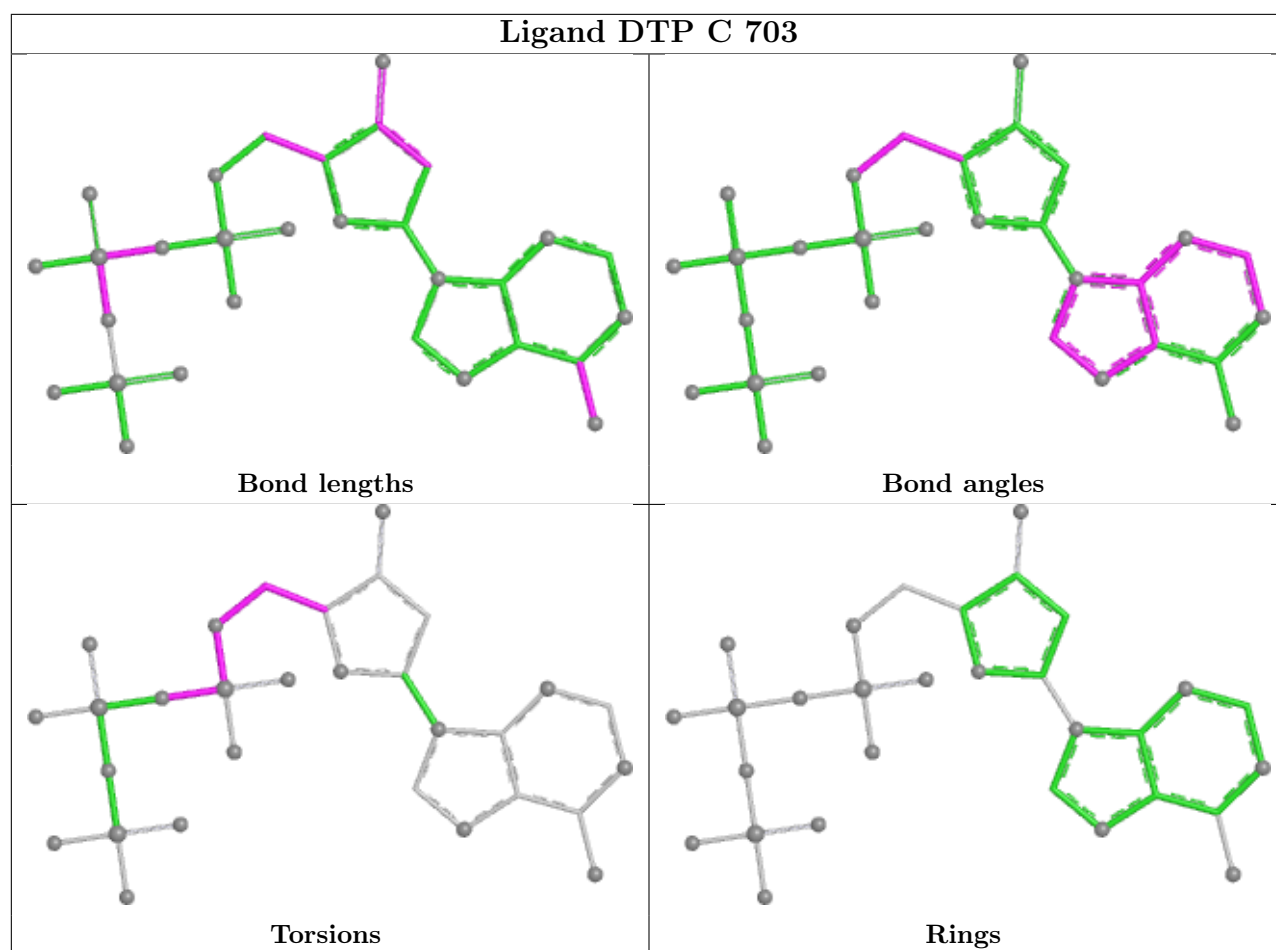
Ligand GTP D 703

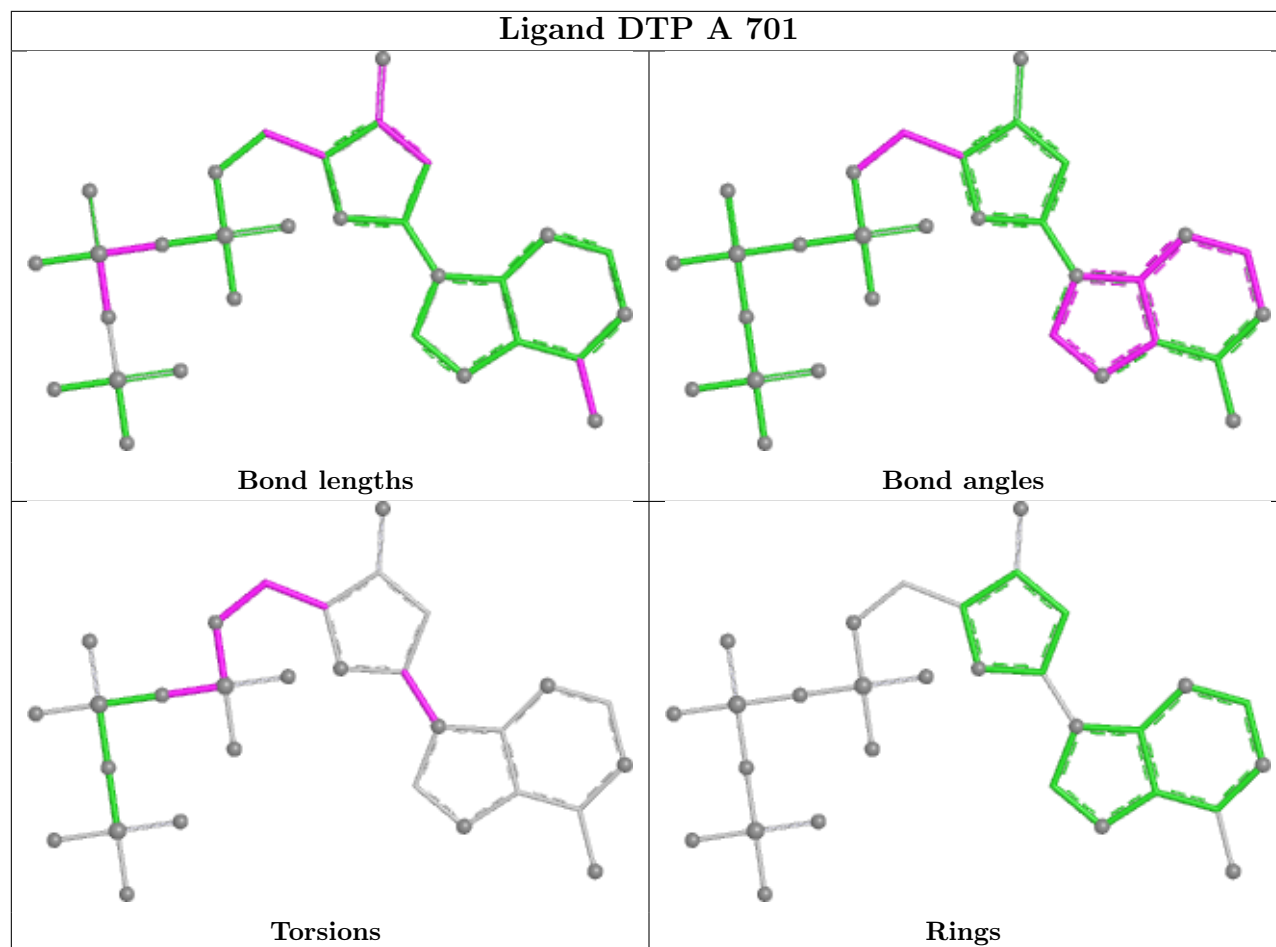


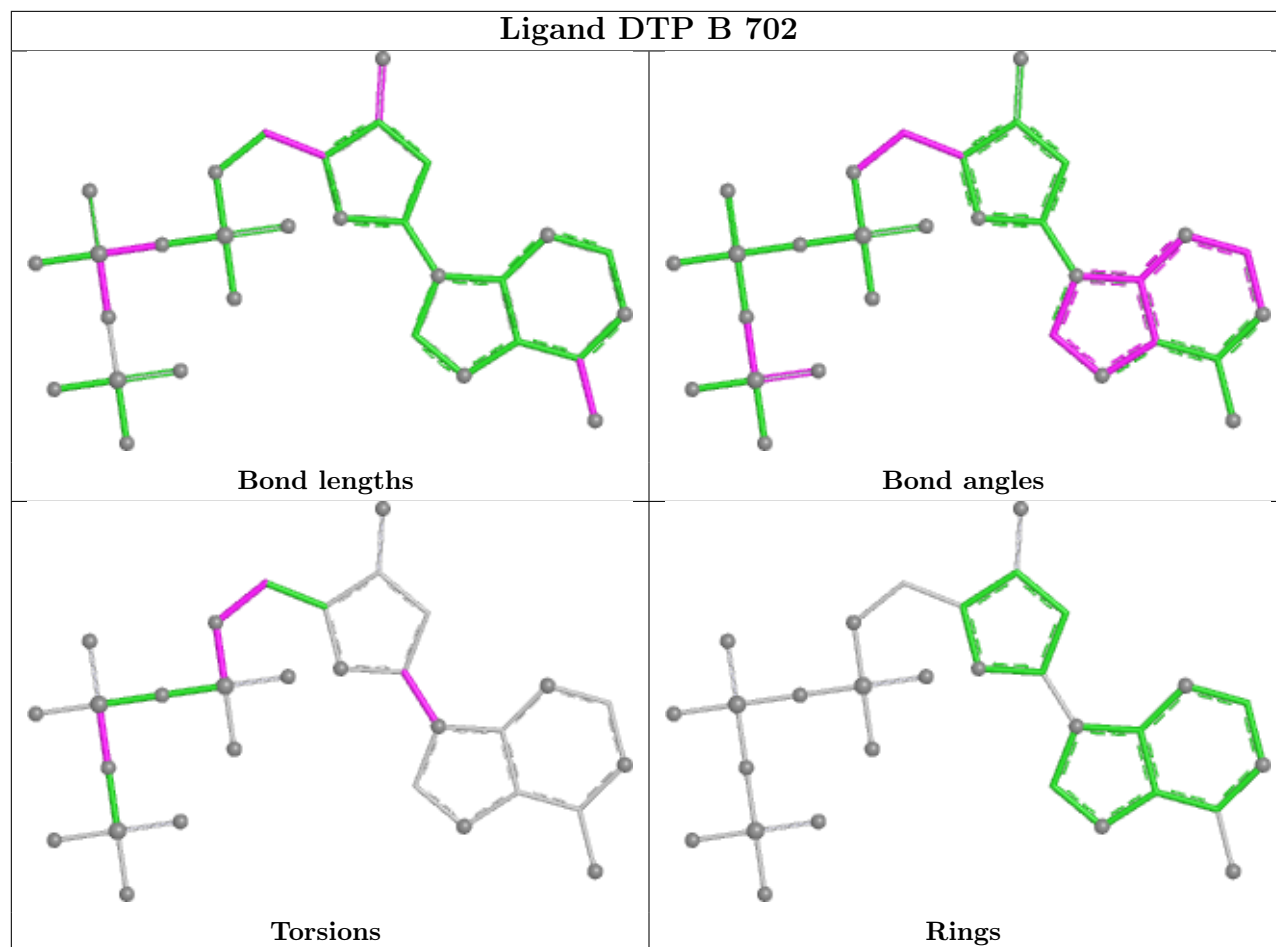


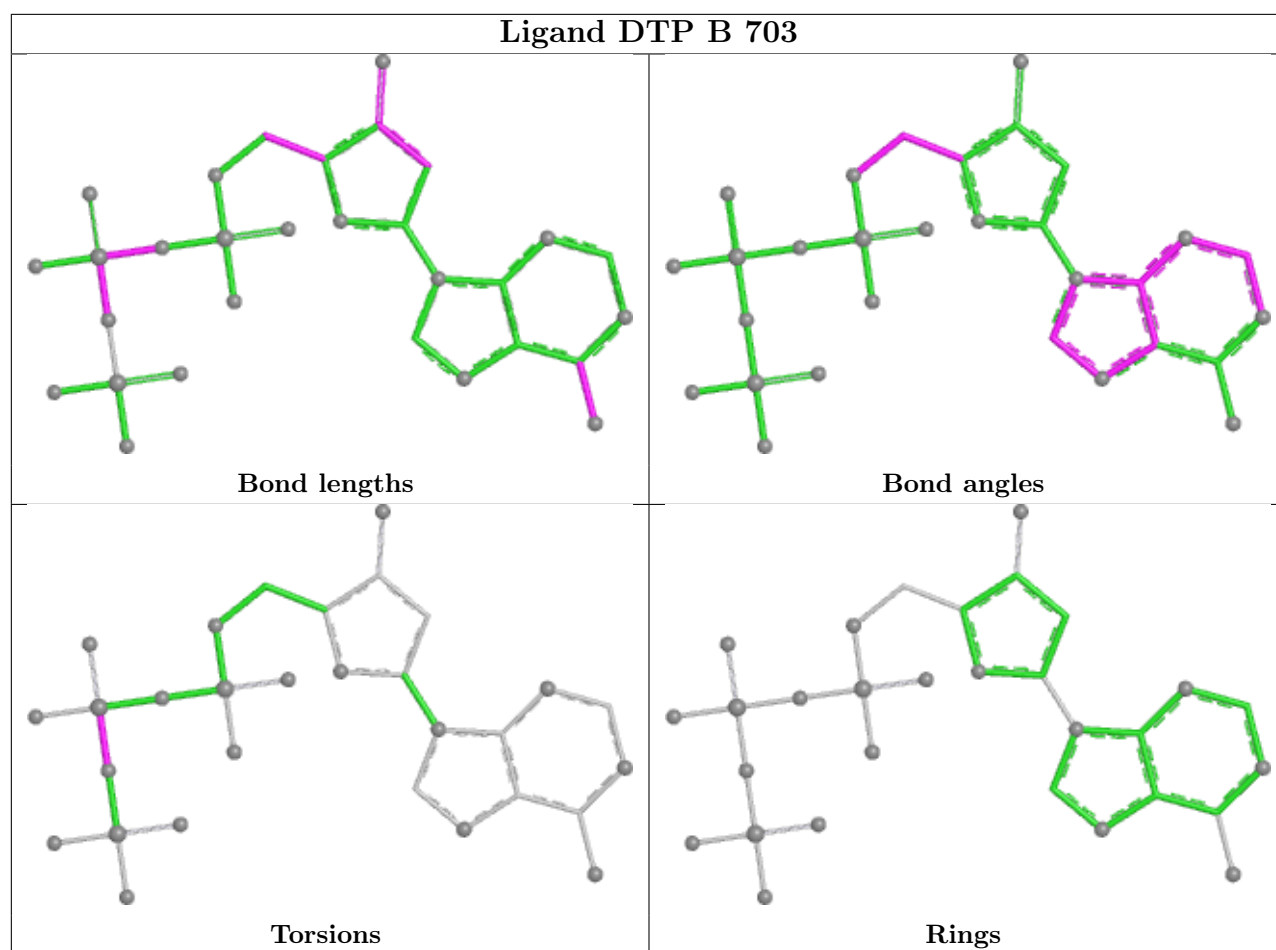












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/550 (87%)	1.12	74 (15%) 5 4	32, 52, 75, 107	460 (95%)
1	B	481/550 (87%)	0.82	43 (8%) 15 13	32, 49, 71, 94	444 (92%)
1	C	481/550 (87%)	1.05	69 (14%) 6 4	32, 49, 79, 122	457 (95%)
1	D	481/550 (87%)	0.80	42 (8%) 16 13	27, 44, 60, 73	466 (96%)
All	All	1924/2200 (87%)	0.95	228 (11%) 9 7	27, 49, 72, 122	1827 (94%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	595	LYS	6.6
1	A	598	TRP	6.1
1	D	490	ASP	5.2
1	A	439	LYS	4.8
1	D	526	PRO	4.7
1	D	115	MET	4.7
1	A	326	GLN	4.6
1	C	284	LEU	4.4
1	C	276	LEU	4.3
1	C	489	LEU	4.3
1	C	493	LEU	4.2
1	B	483	ALA	4.2
1	A	438	LEU	4.2
1	D	284	LEU	4.2
1	A	487	VAL	4.1
1	B	510	GLN	3.9
1	D	599	ASN	3.9
1	A	402	ALA	3.8
1	D	596	LYS	3.8
1	A	488	LEU	3.8
1	B	593	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	426	ILE	3.8
1	A	578	PHE	3.7
1	A	481	ALA	3.7
1	C	522	CYS	3.7
1	B	485	PRO	3.6
1	D	466	ILE	3.6
1	A	395	ASP	3.5
1	A	483	ALA	3.5
1	A	344	ASP	3.5
1	D	113	ASP	3.5
1	D	408	ARG	3.5
1	D	400	THR	3.4
1	D	114	THR	3.4
1	A	396	TYR	3.4
1	C	591	ILE	3.3
1	A	408	ARG	3.3
1	A	480	VAL	3.3
1	D	527	ASN	3.3
1	D	404	GLY	3.3
1	C	550	ILE	3.3
1	C	483	ALA	3.3
1	A	394	ASP	3.3
1	C	409	ILE	3.3
1	A	493	LEU	3.2
1	B	327	ASN	3.2
1	A	429	GLU	3.2
1	A	403	GLY	3.2
1	C	527	ASN	3.2
1	C	578	PHE	3.2
1	D	394	ASP	3.2
1	C	452	ASN	3.1
1	B	405	LYS	3.1
1	A	478	LYS	3.1
1	D	543	GLU	3.1
1	B	598	TRP	3.0
1	A	115	MET	3.0
1	A	343	VAL	3.0
1	A	466	ILE	3.0
1	A	529	ALA	3.0
1	C	488	LEU	3.0
1	D	452	ASN	3.0
1	C	598	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	590	LEU	2.9
1	B	326	GLN	2.9
1	C	510	GLN	2.9
1	D	396	TYR	2.9
1	C	151	GLY	2.9
1	C	327	ASN	2.9
1	C	403	GLY	2.9
1	C	485	PRO	2.9
1	D	343	VAL	2.9
1	C	568	TYR	2.9
1	D	225	ALA	2.9
1	B	190	GLN	2.9
1	C	399	ILE	2.9
1	A	599	ASN	2.9
1	C	326	GLN	2.8
1	C	466	ILE	2.8
1	A	442	ARG	2.8
1	D	276	LEU	2.8
1	B	407	TYR	2.8
1	A	418	ALA	2.8
1	A	441	ALA	2.8
1	A	494	LYS	2.8
1	B	484	LYS	2.8
1	A	499	ILE	2.8
1	C	400	THR	2.8
1	D	593	PRO	2.8
1	C	543	GLU	2.8
1	A	522	CYS	2.7
1	A	554	CYS	2.7
1	C	511	GLU	2.7
1	B	560	LYS	2.7
1	C	418	ALA	2.7
1	D	594	GLN	2.7
1	B	328	ASN	2.7
1	B	543	GLU	2.7
1	B	559	ARG	2.7
1	B	115	MET	2.7
1	A	568	TYR	2.6
1	C	473	TYR	2.6
1	D	406	LYS	2.6
1	C	490	ASP	2.6
1	A	223	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	397	ILE	2.6
1	D	250	ILE	2.6
1	B	562	LEU	2.6
1	A	584	GLY	2.6
1	B	482	SER	2.6
1	C	562	LEU	2.6
1	C	546	ALA	2.6
1	D	388	ASP	2.6
1	C	503	ILE	2.6
1	D	592	THR	2.5
1	B	495	ALA	2.5
1	D	535	ASN	2.5
1	C	262	GLU	2.5
1	B	331	TYR	2.5
1	D	395	ASP	2.5
1	A	457	VAL	2.4
1	B	468	ILE	2.4
1	C	491	VAL	2.4
1	B	438	LEU	2.4
1	A	401	GLY	2.4
1	B	589	PRO	2.4
1	C	566	ARG	2.4
1	A	397	ILE	2.4
1	A	545	PHE	2.4
1	D	399	ILE	2.4
1	A	331	TYR	2.4
1	A	563	TYR	2.4
1	A	574	ALA	2.4
1	C	463	THR	2.4
1	C	230	LYS	2.4
1	D	491	VAL	2.4
1	B	276	LEU	2.4
1	A	527	ASN	2.4
1	A	597	GLU	2.4
1	C	579	THR	2.4
1	A	381	ILE	2.4
1	A	531	ARG	2.4
1	C	528	ARG	2.4
1	A	546	ALA	2.3
1	A	498	PHE	2.3
1	C	229	VAL	2.3
1	D	126	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	470	ARG	2.3
1	C	401	GLY	2.3
1	A	536	GLN	2.3
1	A	276	LEU	2.3
1	B	590	LEU	2.3
1	C	549	LEU	2.3
1	A	535	ASN	2.3
1	C	345	ASN	2.3
1	C	436	PRO	2.3
1	B	466	ILE	2.3
1	C	573	CYS	2.3
1	B	481	ALA	2.3
1	D	531	ARG	2.3
1	B	114	THR	2.3
1	C	480	VAL	2.3
1	B	535	ASN	2.2
1	C	575	ASP	2.2
1	A	114	THR	2.2
1	A	262	GLU	2.2
1	A	475	SER	2.2
1	C	190	GLN	2.2
1	C	368	SER	2.2
1	B	406	LYS	2.2
1	A	476	LEU	2.2
1	D	464	GLY	2.2
1	C	571	GLN	2.2
1	B	565	ALA	2.2
1	A	302	SER	2.2
1	A	273	VAL	2.2
1	C	570	VAL	2.2
1	B	452	ASN	2.2
1	C	341	CYS	2.2
1	A	460	THR	2.2
1	B	473	TYR	2.2
1	C	396	TYR	2.2
1	A	347	LEU	2.2
1	B	549	LEU	2.2
1	D	489	LEU	2.2
1	B	343	VAL	2.2
1	C	458	GLY	2.2
1	C	539	GLN	2.2
1	D	403	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	368	SER	2.2
1	B	563	TYR	2.1
1	D	473	TYR	2.1
1	A	572	TRP	2.1
1	C	347	LEU	2.1
1	C	113	ASP	2.1
1	A	304	LYS	2.1
1	C	484	LYS	2.1
1	C	496	GLU	2.1
1	D	402	ALA	2.1
1	A	284	LEU	2.1
1	C	497	ASP	2.1
1	D	262	GLU	2.1
1	C	498	PHE	2.1
1	C	559	ARG	2.1
1	A	596	LYS	2.1
1	B	494	LYS	2.1
1	A	413	ILE	2.1
1	A	430	ILE	2.1
1	B	577	ASN	2.1
1	B	591	ILE	2.1
1	C	407	TYR	2.1
1	C	587	ILE	2.1
1	D	231	TRP	2.1
1	B	404	GLY	2.1
1	D	331	TYR	2.1
1	B	500	VAL	2.1
1	D	288	LYS	2.0
1	B	587	ILE	2.0
1	C	512	LYS	2.0
1	A	342	GLU	2.0
1	A	509	MET	2.0
1	A	411	THR	2.0
1	D	302	SER	2.0
1	A	350	CYS	2.0
1	C	235	GLN	2.0
1	C	554	CYS	2.0
1	A	383	ASP	2.0
1	A	577	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

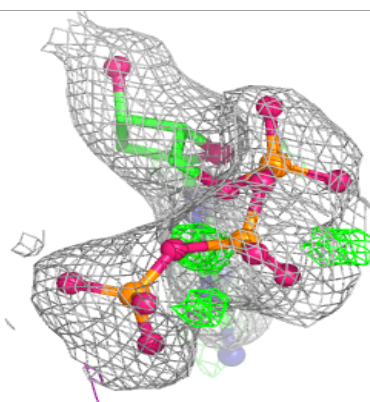
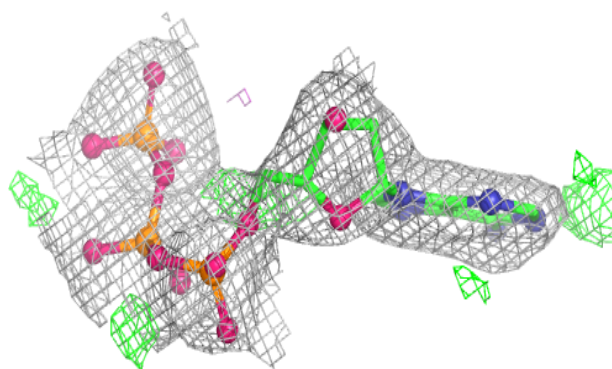
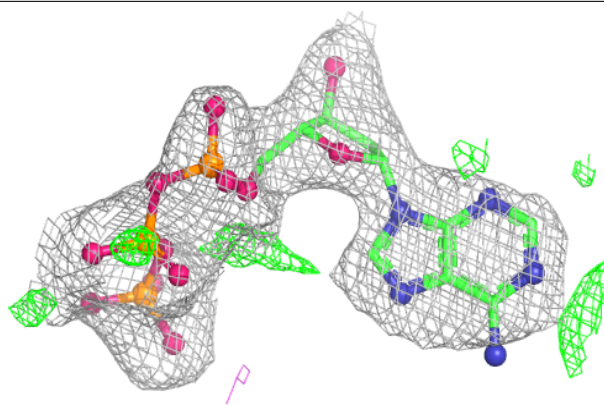
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	703	1/1	0.89	0.07	37,37,37,37	1
3	MG	D	705	1/1	0.89	0.08	60,60,60,60	0
2	DTP	A	701	30/30	0.90	0.13	55,60,71,73	28
3	MG	A	704	1/1	0.90	0.07	56,56,56,56	1
2	DTP	D	704	30/30	0.90	0.13	36,50,56,57	30
2	DTP	B	702	30/30	0.91	0.12	48,55,61,64	28
2	DTP	C	703	30/30	0.92	0.13	44,59,66,70	28
3	MG	C	704	1/1	0.94	0.06	62,62,62,62	0
4	GTP	D	701	32/32	0.95	0.07	48,53,61,69	32
4	GTP	C	702	32/32	0.96	0.08	42,53,62,68	32
4	GTP	B	701	32/32	0.96	0.07	43,50,58,63	32
2	DTP	B	703	30/30	0.97	0.07	32,44,57,60	20
2	DTP	C	701	30/30	0.97	0.07	48,52,58,60	18
2	DTP	A	702	30/30	0.97	0.07	47,53,57,60	21
2	DTP	D	702	30/30	0.97	0.06	43,48,56,56	19
4	GTP	D	703	32/32	0.97	0.07	37,46,52,59	32

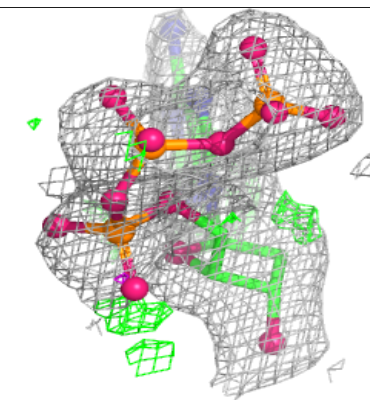
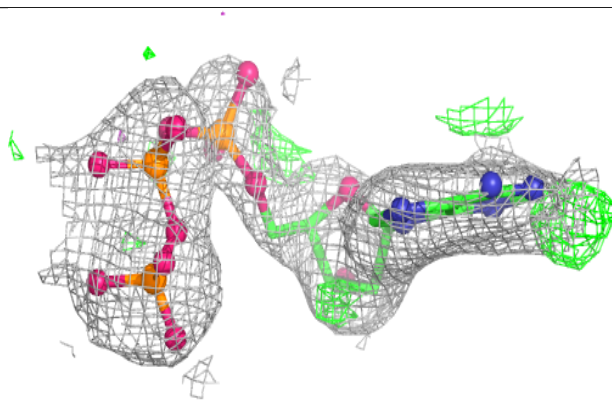
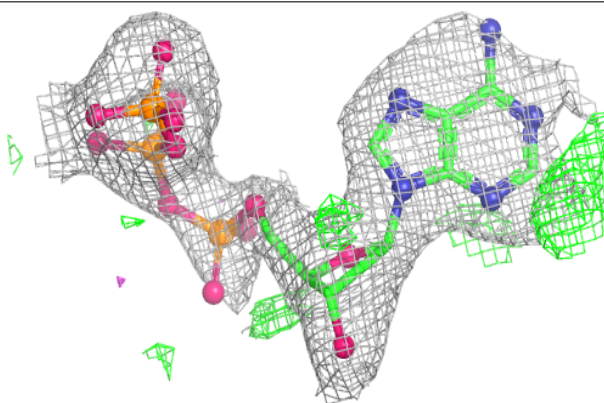
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP 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)

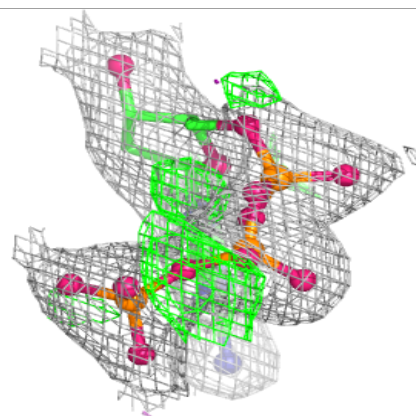
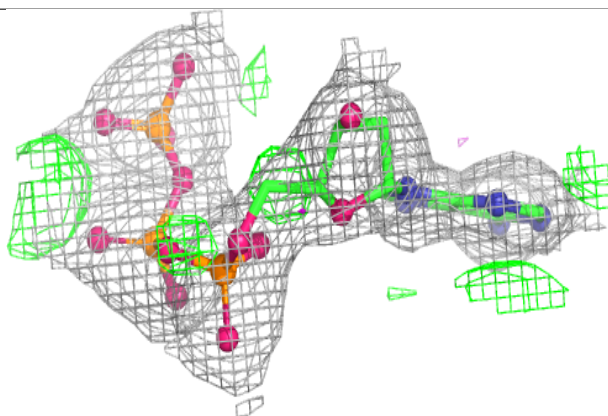
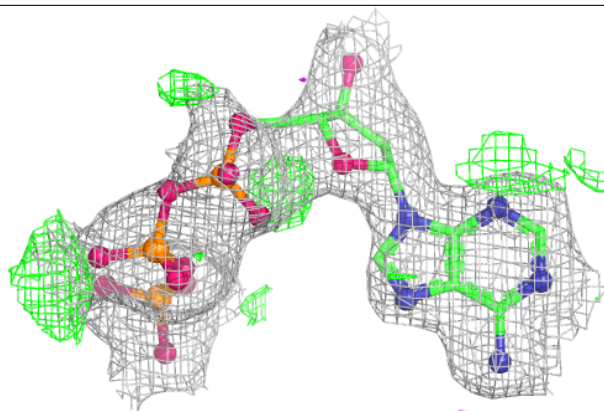
**Electron density around DTP D 704:**

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

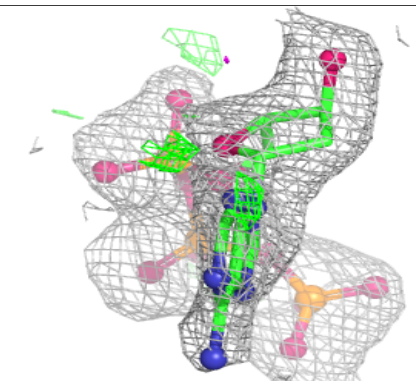
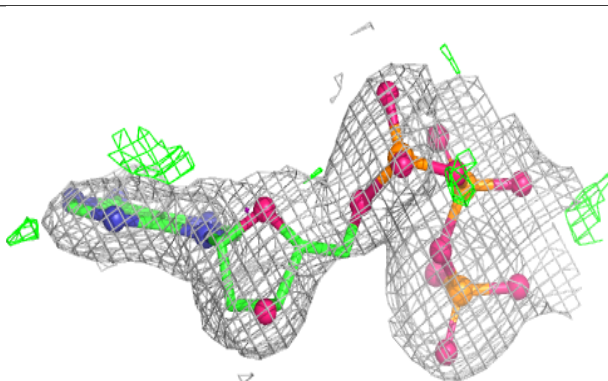
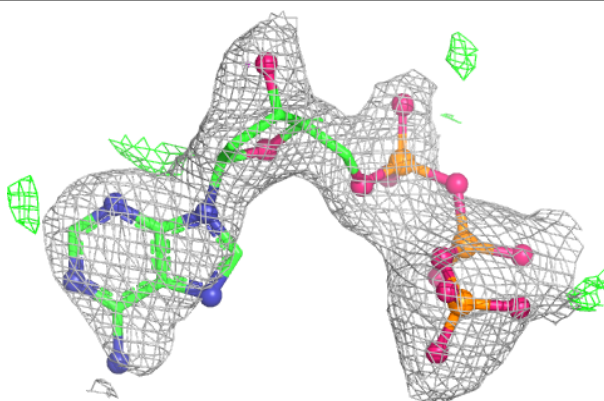


Electron density around DTP B 702:

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

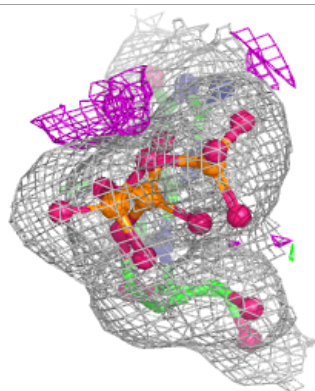
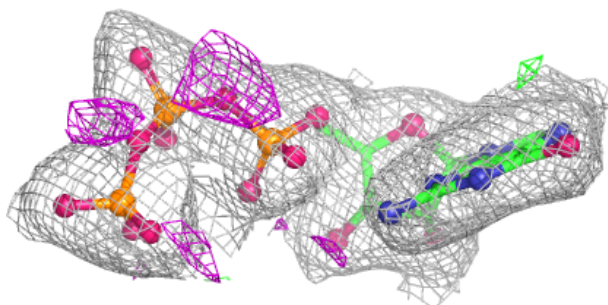
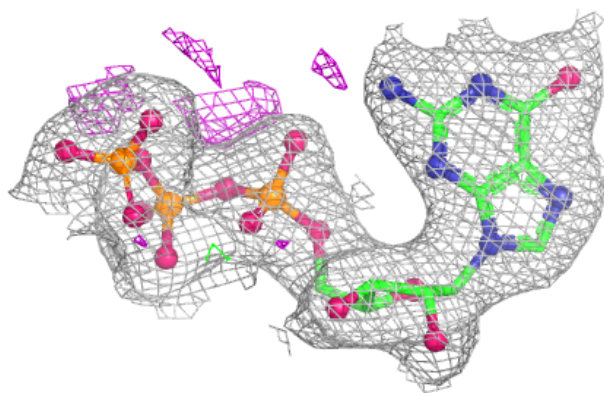
**Electron density around DTP C 703:**

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

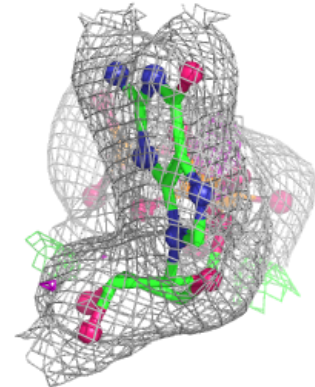
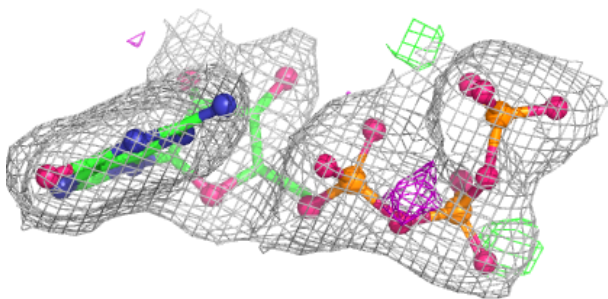
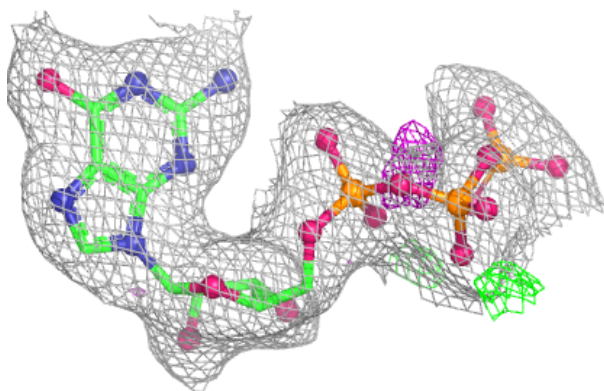


Electron density around GTP D 701:

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

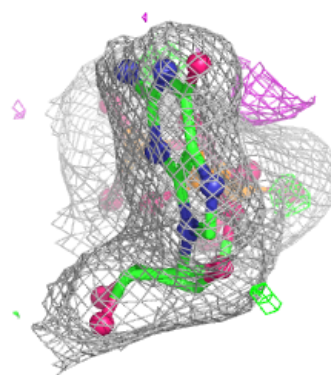
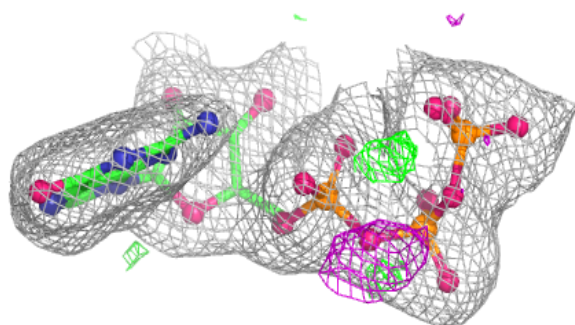
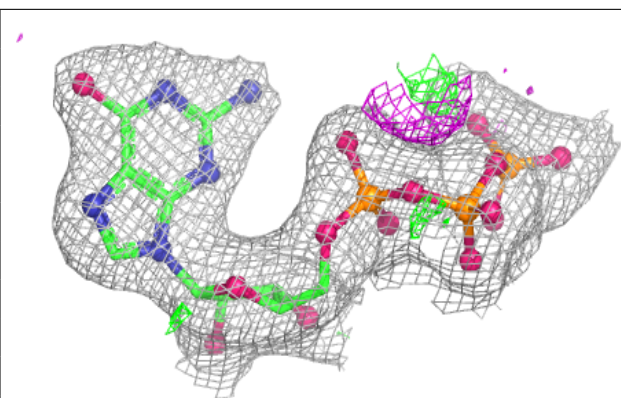
**Electron density around GTP C 702:**

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

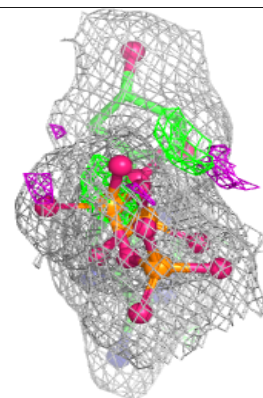
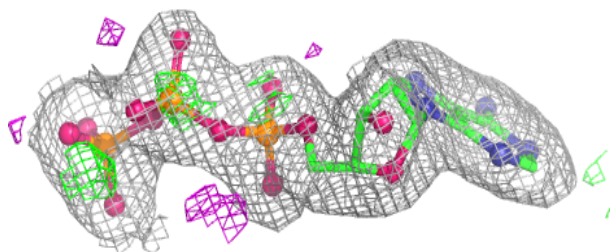
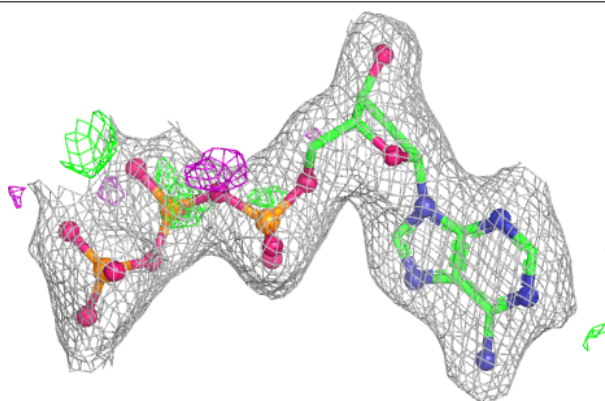


Electron density around GTP B 701:

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

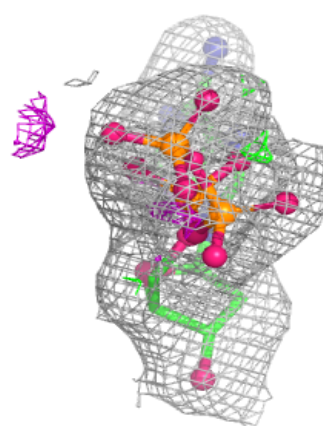
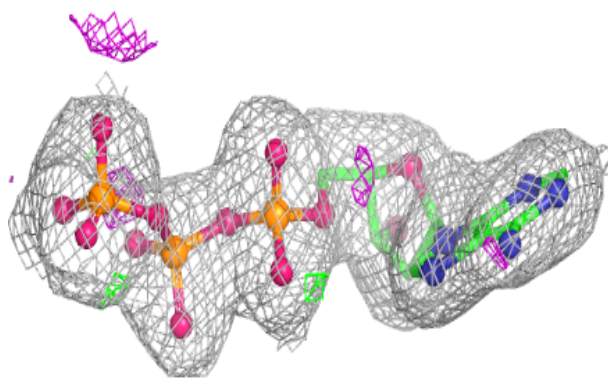
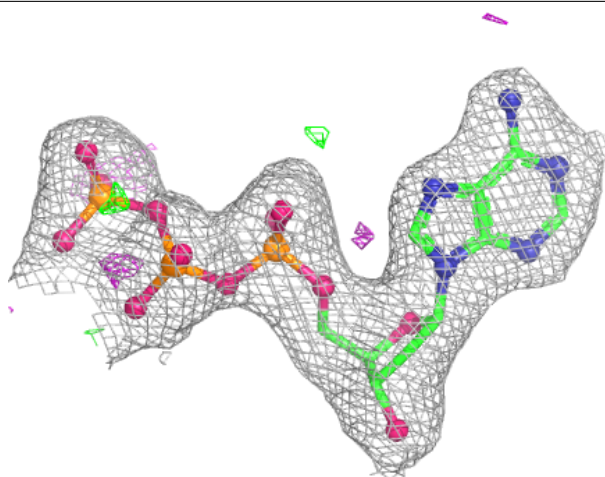
**Electron density around DTP B 703:**

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



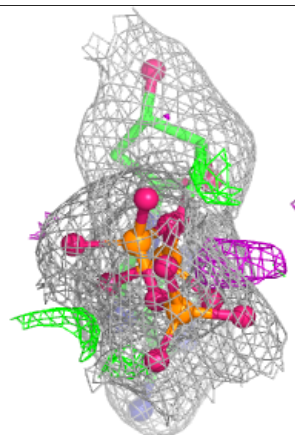
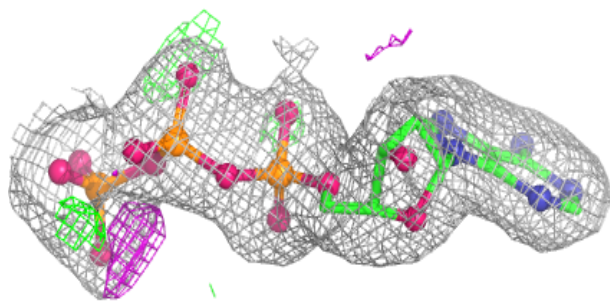
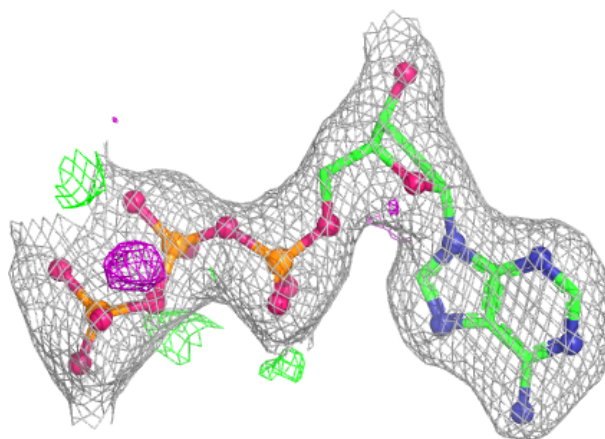
Electron density around DTP C 701:

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



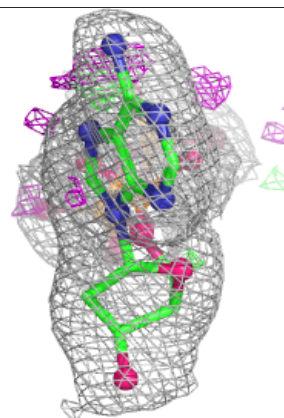
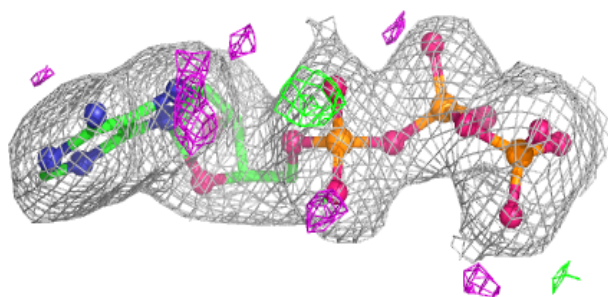
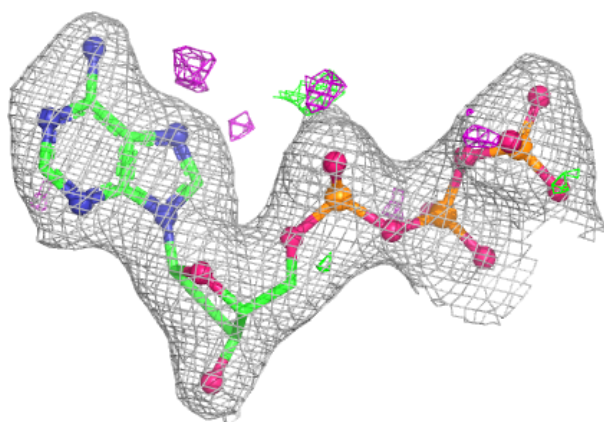
Electron density around DTP A 702:

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

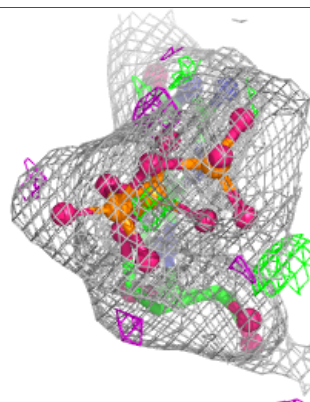
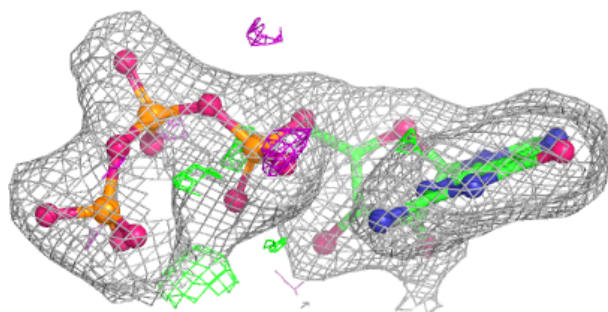
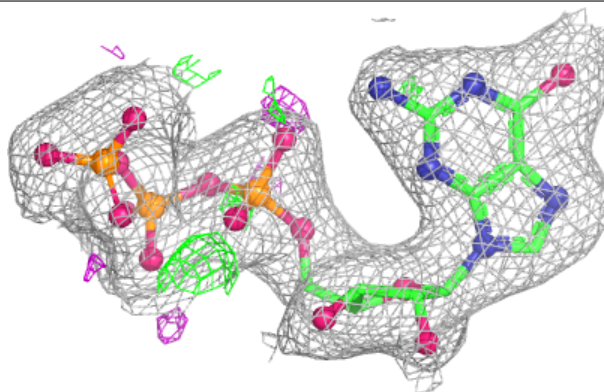


Electron density around DTP D 702:

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

**Electron density around GTP D 703:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.