



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:04 pm BST

PDB ID : 4QG2
Title : Crystal structure of the tetrameric GTP/dATP/ATP-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 : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

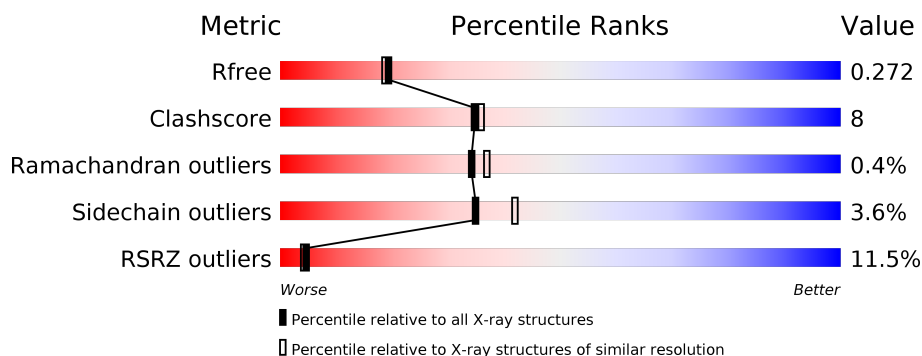
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	<div> <div>10%</div> <div>67% 19% • 13%</div> </div>
1	B	550	<div> <div>12%</div> <div>72% 14% • 13%</div> </div>
1	C	550	<div> <div>12%</div> <div>67% 19% • 13%</div> </div>
1	D	550	<div> <div>6%</div> <div>69% 17% • 13%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16094 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	1	0
			3939	2520	686	712	21			
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	1	0
			3939	2520	686	712	21			
1	D	481	Total	C	N	O	S	0	3	0
			3955	2528	689	717	21			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
A	78	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	79	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	80	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	81	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	82	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	83	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	84	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	85	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	86	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	87	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	88	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	90	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	91	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
A	92	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
A	93	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
A	94	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
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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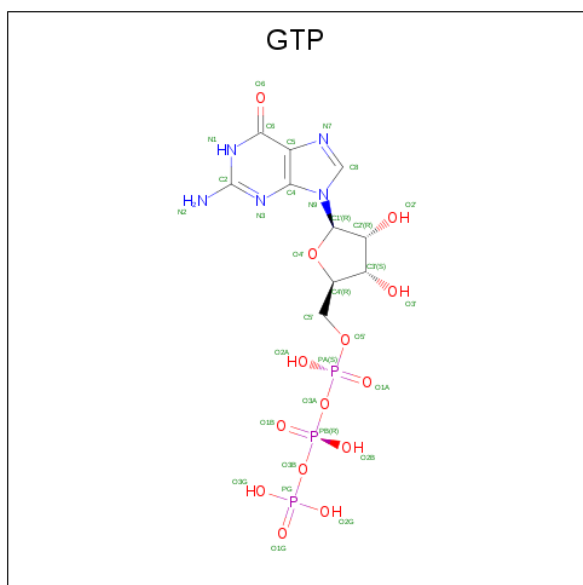
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C	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
C	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
C	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	112	SER	-	EXPRESSION 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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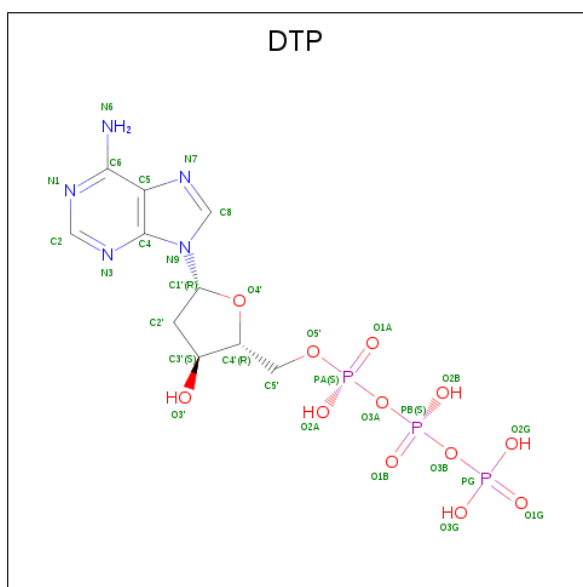
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
D	207	ASN	ASP	ENGINEERED MUTATION	UNP Q9Y3Z3

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

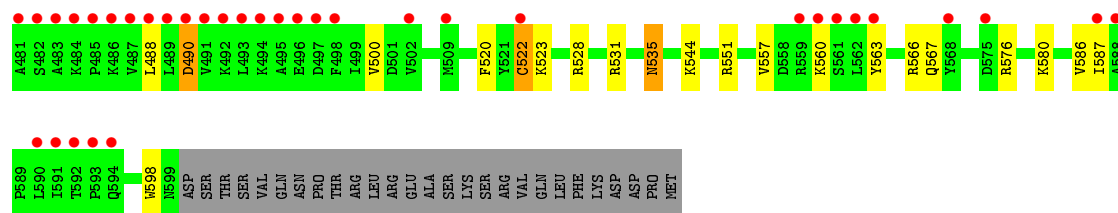
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	16	Total O 16 16	0	0

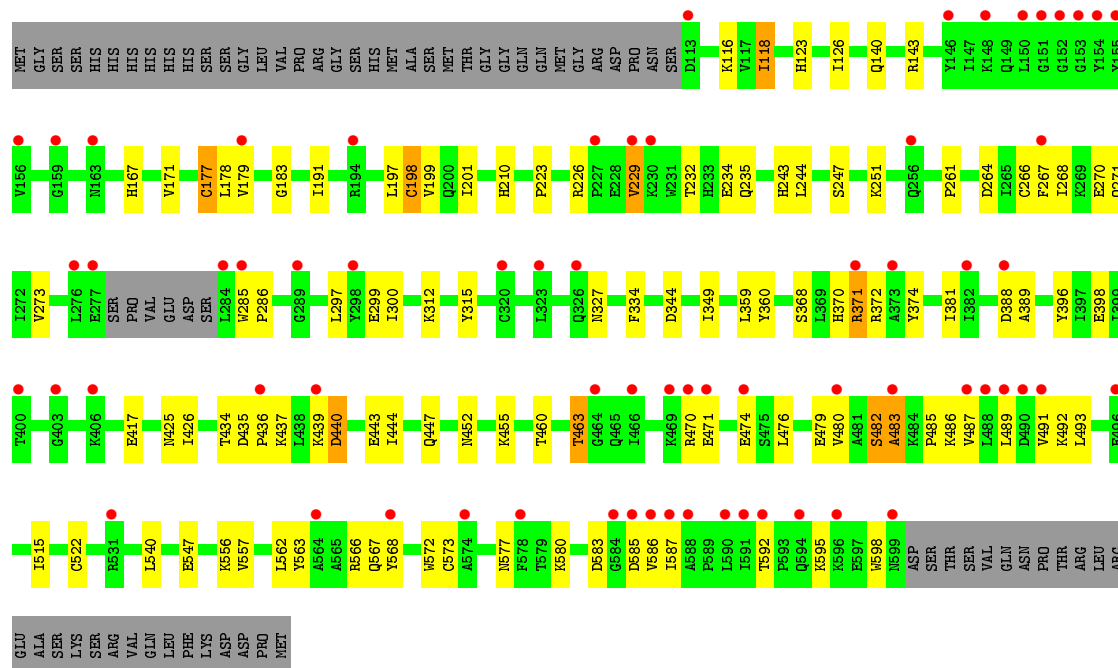
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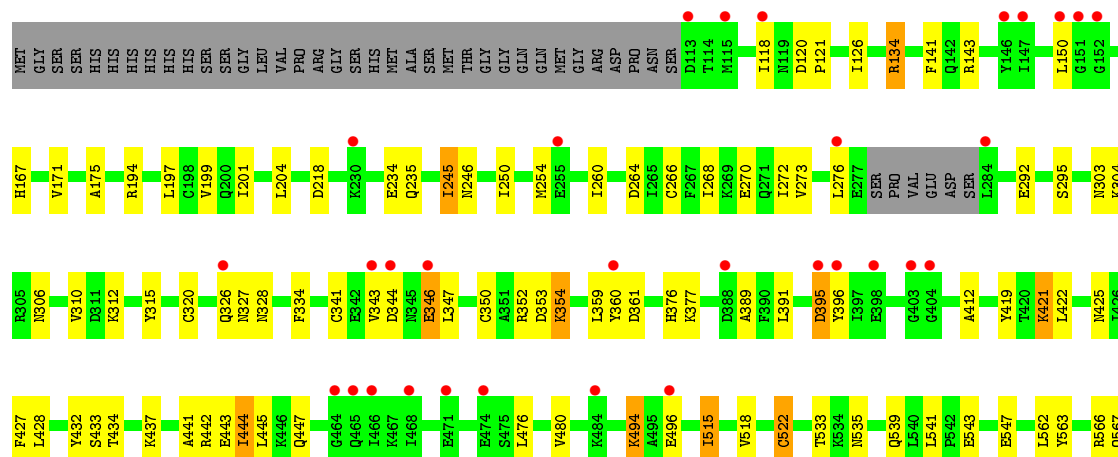
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	16	Total	O	0	0
			16	16		
5	D	26	Total	O	0	0
			26	26		

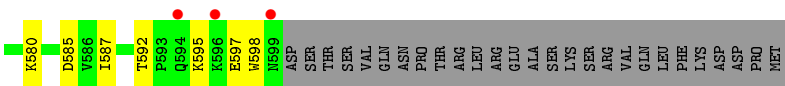


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.23Å 147.00Å 99.29Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	43.07 – 2.25 43.07 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.07-2.25) 91.7 (43.07-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.237 , 0.271 0.241 , 0.272	Depositor DCC
R_{free} test set	2008 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16094	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: 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	0.35	0/4031	0.57	1/5441 (0.0%)
1	B	0.28	0/4025	0.51	0/5433
1	C	0.32	0/4031	0.55	0/5441
1	D	0.31	0/4047	0.53	0/5463
All	All	0.32	0/16134	0.54	1/21778 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	MET	CA-CB-CG	5.60	122.83	113.30

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	3939	0	3923	85	0
1	B	3933	0	3921	52	0
1	C	3939	0	3923	82	0
1	D	3955	0	3933	69	0
2	A	32	0	11	0	0
2	B	64	0	22	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	32	0	11	0	0
3	A	30	0	12	0	0
3	B	30	0	12	3	0
3	C	30	0	12	0	0
3	D	30	0	12	0	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	18	0	0	2	0
5	B	16	0	0	2	0
5	C	16	0	0	1	0
5	D	26	0	0	4	0
All	All	16094	0	15792	263	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 8.

All (263) 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:D:389:ALA:HB2	1:D:444:ILE:HD11	1.42	0.99
1:C:566:ARG:HD3	1:C:587:ILE:HB	1.52	0.91
1:A:113:ASP:OD2	1:A:257:TYR:OH	1.90	0.87
1:A:425:ASN:ND2	1:D:425:ASN:OD1	2.11	0.83
1:C:299:GLU:N	1:C:299:GLU:OE1	2.12	0.82
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.14	0.81
1:D:328:ASN:ND2	5:D:819:HOH:O	2.12	0.80
1:A:591:ILE:O	1:A:594:GLN:NE2	2.14	0.80
1:C:198:CYS:SG	1:C:271:GLN:NE2	2.55	0.79
1:A:361:ASP:OD2	1:C:371:ARG:NH2	2.16	0.78
1:C:179:VAL:HG21	1:C:199:VAL:HG21	1.68	0.76
1:D:292:GLU:HB3	1:D:346:GLU:OE1	1.87	0.75
1:A:528:ARG:HH22	1:C:586:VAL:HG13	1.53	0.74
1:D:312:LYS:NZ	5:D:801:HOH:O	2.20	0.74
1:A:432:TYR:CG	1:D:421:LYS:HD3	2.22	0.73
1:C:243:HIS:CE1	1:C:417:GLU:HG3	2.24	0.72
1:B:400:THR:HG21	1:C:434:THR:HG21	1.71	0.71
1:A:385:MET:O	1:A:444:ILE:HD11	1.92	0.70
1:A:185:LYS:NZ	1:A:338:ALA:O	2.18	0.70
1:B:114:THR:HG22	1:B:115:MET:H	1.57	0.70
3:B:703:DTP:O1B	1:D:377:LYS:NZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:CYS:HB2	1:B:350:CYS:SG	2.33	0.69
1:A:129:HIS:HD2	1:A:131:LEU:H	1.40	0.69
1:A:417:GLU:O	5:A:811:HOH:O	2.11	0.69
1:A:525:ALA:HB3	1:A:528:ARG:CZ	2.23	0.68
1:B:243:HIS:NE2	1:B:417:GLU:OE1	2.21	0.67
1:C:243:HIS:HE1	1:C:417:GLU:HG3	1.59	0.67
1:B:476:LEU:HD22	1:B:500:VAL:HG11	1.77	0.67
1:C:123:HIS:ND1	5:C:805:HOH:O	2.30	0.65
1:D:433:SER:OG	1:D:442:ARG:NH1	2.29	0.65
1:A:232:THR:OG1	1:A:234:GLU:OE1	2.10	0.64
1:B:442:ARG:HG2	1:B:446:LYS:HE2	1.79	0.64
1:C:371:ARG:HH22	1:C:372:ARG:HH21	1.44	0.64
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.78	0.64
1:D:341:CYS:HB2	1:D:350:CYS:SG	2.38	0.64
1:C:223:PRO:HB3	1:C:470:ARG:NH2	2.12	0.64
1:C:251:LYS:HD3	1:C:261:PRO:HB3	1.80	0.62
1:D:533:THR:OG1	1:D:535:ASN:OD1	2.13	0.62
1:B:544:LYS:HE2	1:D:539:GLN:HB3	1.81	0.62
1:D:194:ARG:HH21	1:D:260:ILE:HB	1.63	0.62
1:A:129:HIS:CD2	1:A:131:LEU:H	2.18	0.62
1:A:115:MET:HE2	1:A:127:GLU:CB	2.30	0.61
1:B:371:ARG:NH2	1:D:361:ASP:OD2	2.22	0.61
1:A:428:LEU:HB3	1:A:432:TYR:CE2	2.35	0.61
1:C:232:THR:OG1	1:C:234:GLU:OE1	2.17	0.61
1:A:243:HIS:NE2	1:A:417:GLU:OE1	2.20	0.61
1:A:216:MET:SD	1:A:387:THR:OG1	2.56	0.61
1:B:531:ARG:NE	5:B:813:HOH:O	2.33	0.60
1:C:583:ASP:O	1:C:587:ILE:HG12	2.01	0.59
1:A:431:LEU:HD23	1:A:432:TYR:CE1	2.38	0.59
1:D:396:TYR:CD1	1:D:437:LYS:HB3	2.37	0.59
1:B:158:PRO:HG3	1:C:118:ILE:HD11	1.85	0.59
1:C:440:ASP:N	1:C:440:ASP:OD1	2.36	0.58
1:A:361:ASP:O	1:A:365:THR:HG23	2.03	0.58
1:A:433:SER:OG	1:A:442:ARG:NH1	2.36	0.58
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.42	0.58
1:C:566:ARG:HD3	1:C:587:ILE:CB	2.31	0.58
1:D:143:ARG:HD3	5:D:808:HOH:O	2.04	0.58
1:C:183:GLY:HA2	1:C:191:ILE:HD12	1.85	0.58
1:A:534:LYS:HE3	1:A:541:LEU:HB2	1.86	0.57
1:C:455:LYS:HG2	1:C:557:VAL:HG12	1.85	0.57
1:B:469:LYS:HD3	1:B:470:ARG:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LYS:NZ	3:B:703:DTP:O3G	2.38	0.57
1:D:234:GLU:HB3	1:D:273:VAL:HG22	1.87	0.57
1:A:172:GLY:HA3	1:A:204:LEU:HD12	1.87	0.57
1:B:580:LYS:HB2	1:B:598:TRP:CD2	2.40	0.56
1:A:432:TYR:CD1	1:D:421:LYS:HD3	2.41	0.56
1:A:528:ARG:HH22	1:C:586:VAL:CG1	2.16	0.56
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.87	0.55
1:D:334:PHE:CE2	1:D:359:LEU:HD21	2.41	0.55
1:A:525:ALA:HB3	1:A:528:ARG:NH2	2.22	0.55
1:C:388:ASP:OD1	1:C:389:ALA:N	2.39	0.55
1:A:130:PRO:O	1:A:134:ARG:HG2	2.07	0.55
1:C:266:CYS:O	1:C:270:GLU:HG3	2.06	0.55
1:D:150:LEU:O	5:D:815:HOH:O	2.18	0.55
1:C:371:ARG:NH2	1:C:372:ARG:HH21	2.05	0.54
1:D:566:ARG:HD3	1:D:587:ILE:HB	1.89	0.54
1:A:266:CYS:O	1:A:270:GLU:HG3	2.07	0.54
1:D:266:CYS:O	1:D:270:GLU:HG3	2.07	0.54
1:B:522:CYS:SG	1:B:523:LYS:N	2.80	0.54
1:D:441:ALA:O	1:D:444:ILE:HG13	2.08	0.54
1:B:479:GLU:OE1	1:B:576:ARG:NH1	2.41	0.53
1:A:462:PRO:HB2	1:A:466:ILE:HG23	1.89	0.53
1:C:474:GLU:N	1:C:474:GLU:OE1	2.42	0.53
1:D:250:ILE:HG22	1:D:254:MET:HG3	1.91	0.52
1:C:580:LYS:NZ	1:C:585:ASP:OD1	2.37	0.52
1:A:597:GLU:OE1	1:A:597:GLU:N	2.41	0.52
1:B:185:LYS:HG3	1:B:186:GLN:HG3	1.92	0.52
1:B:490:ASP:OD2	1:B:560:LYS:NZ	2.42	0.52
1:A:212:PRO:HD2	1:A:217:PHE:CD1	2.46	0.52
1:A:218:ASP:OD2	1:A:232:THR:HA	2.10	0.52
1:C:334:PHE:CE2	1:C:359:LEU:HD21	2.46	0.51
1:A:571:GLN:NE2	1:A:591:ILE:HD11	2.25	0.51
1:D:515:ILE:HA	1:D:518:VAL:HG12	1.92	0.51
1:B:143:ARG:NH2	1:B:210:HIS:O	2.31	0.51
1:D:395:ASP:OD1	1:D:395:ASP:N	2.43	0.51
1:A:522[A]:CYS:SG	1:A:523:LYS:N	2.83	0.51
1:D:592:THR:HG23	1:D:598:TRP:HE3	1.75	0.51
1:B:266:CYS:O	1:B:270:GLU:HG3	2.11	0.50
1:A:428:LEU:HD22	1:A:432:TYR:CZ	2.46	0.50
1:D:141:PHE:CZ	1:D:204:LEU:HD22	2.46	0.50
1:B:535:ASN:N	1:B:535:ASN:OD1	2.29	0.50
1:A:353:ASP:OD1	1:A:354:LYS:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:THR:HG21	1:C:573:CYS:SG	2.51	0.50
1:A:115:MET:HE2	1:A:127:GLU:HB3	1.92	0.50
1:C:264:ASP:O	1:C:268:ILE:HG13	2.12	0.50
1:A:528:ARG:HH12	1:C:586:VAL:HA	1.77	0.50
1:B:428:LEU:HD12	1:C:425:ASN:HB2	1.94	0.49
1:B:470:ARG:HD2	1:B:473:TYR:CE2	2.46	0.49
1:D:303:ASN:ND2	1:D:306:ASN:OD1	2.45	0.49
1:A:522[B]:CYS:SG	1:C:586:VAL:HG21	2.52	0.49
1:C:234:GLU:HB3	1:C:273:VAL:HG23	1.95	0.49
1:C:360:TYR:CZ	1:C:515:ILE:HG12	2.48	0.49
1:D:343:VAL:HG12	1:D:344:ASP:OD1	2.13	0.49
1:A:167:HIS:O	1:A:171:VAL:HG23	2.13	0.49
1:A:461:GLN:NE2	1:A:547:GLU:OE1	2.40	0.49
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.48	0.49
1:D:295:SER:OG	1:D:347:LEU:O	2.31	0.49
1:D:312:LYS:HA	1:D:315:TYR:CE2	2.48	0.48
1:A:580:LYS:HB2	1:A:598:TRP:CD2	2.48	0.48
1:B:197:LEU:O	1:B:201:ILE:HG13	2.13	0.48
1:B:563:TYR:O	1:B:567:GLN:HG2	2.12	0.48
1:A:320:CYS:SG	1:A:327:ASN:HB3	2.53	0.48
1:C:443:GLU:O	1:C:447:GLN:HG2	2.12	0.48
1:D:412:ALA:HB3	1:D:422:LEU:HD22	1.94	0.47
1:D:476:LEU:O	1:D:480:VAL:HG23	2.14	0.47
1:A:421:LYS:HE2	5:A:811:HOH:O	2.14	0.47
1:C:381:ILE:HA	1:C:381:ILE:HD12	1.81	0.47
1:D:419:TYR:CE1	1:D:422:LEU:HD23	2.49	0.47
1:D:264:ASP:O	1:D:268:ILE:HG13	2.15	0.47
1:C:232:THR:HG23	1:C:235:GLN:H	1.78	0.47
3:B:703:DTP:O2A	1:D:376:HIS:HE1	1.97	0.47
1:A:238:VAL:HG13	1:A:269:LYS:HD3	1.96	0.47
1:A:115:MET:HE2	1:A:127:GLU:CA	2.44	0.47
1:D:346:GLU:OE2	1:D:347:LEU:N	2.25	0.47
1:B:328:ASN:HA	1:D:326:GLN:HG3	1.97	0.47
1:C:388:ASP:OD1	1:C:444:ILE:HD13	2.15	0.46
1:C:493:LEU:HD23	1:C:556:LYS:HE2	1.96	0.46
1:D:346:GLU:CD	1:D:347:LEU:H	2.16	0.46
1:C:226:ARG:HH21	1:C:229:VAL:HG21	1.79	0.46
1:D:585:ASP:OD1	1:D:592:THR:HG21	2.15	0.46
1:A:591:ILE:HG13	1:A:594:GLN:HE22	1.79	0.46
1:C:177:CYS:SG	1:C:178:LEU:N	2.89	0.46
1:A:421:LYS:HD2	1:D:432:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:HG2	1:A:189:LEU:HD13	1.97	0.46
1:A:471:GLU:O	1:A:473:TYR:N	2.49	0.46
1:D:245:ILE:HG22	1:D:246:ASN:N	2.30	0.46
1:A:463:THR:O	1:A:466:ILE:HG22	2.15	0.46
1:B:352:ARG:NH2	1:B:354:LYS:HZ2	2.14	0.46
1:C:476:LEU:O	1:C:480:VAL:HG23	2.15	0.46
1:A:538:SER:OG	1:C:547:GLU:OE2	2.34	0.46
1:C:463:THR:OG1	1:C:577:ASN:O	2.33	0.46
1:A:563:TYR:O	1:A:567:GLN:HG2	2.15	0.45
1:C:482:SER:OG	1:C:483:ALA:N	2.47	0.45
1:A:332:LYS:O	1:A:336:LYS:HD3	2.17	0.45
1:B:459:GLU:OE2	1:B:551:ARG:NE	2.37	0.45
2:B:701:GTP:O1G	1:C:116:LYS:NZ	2.37	0.45
1:B:172:GLY:HA3	1:B:204:LEU:HD12	1.96	0.45
1:B:320:CYS:SG	1:B:327:ASN:HB3	2.56	0.45
1:A:334:PHE:CE1	1:A:359:LEU:HD11	2.52	0.45
1:B:353:ASP:OD1	1:B:354:LYS:N	2.50	0.45
1:C:179:VAL:HG23	1:C:300:ILE:HD13	1.98	0.45
1:C:223:PRO:HB3	1:C:470:ARG:HH21	1.82	0.45
1:C:368:SER:O	1:C:372:ARG:HG2	2.16	0.45
1:B:580:LYS:HD2	1:B:598:TRP:HB3	1.97	0.45
1:C:580:LYS:HB2	1:C:598:TRP:CD2	2.51	0.45
1:A:592:THR:HG23	1:A:598:TRP:HE3	1.82	0.45
1:B:377:LYS:NZ	1:D:354:LYS:HD2	2.32	0.45
1:A:234:GLU:OE1	1:A:234:GLU:N	2.42	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.45
1:C:583:ASP:O	1:C:586:VAL:HB	2.17	0.45
1:D:171:VAL:HG13	1:D:310:VAL:HG23	1.99	0.45
1:B:326:GLN:NE2	1:D:327:ASN:H	2.15	0.45
1:A:191:ILE:HD11	1:A:296:PHE:CE1	2.52	0.44
1:C:370:HIS:HA	1:C:374:TYR:HB2	1.99	0.44
1:A:580:LYS:HB2	1:A:598:TRP:CE2	2.52	0.44
1:D:580:LYS:HE3	1:D:585:ASP:OD1	2.17	0.44
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.87	0.44
1:C:563:TYR:O	1:C:567:GLN:HG2	2.17	0.44
1:C:285:TRP:HA	1:C:286:PRO:HD3	1.89	0.44
1:D:391:LEU:HA	1:D:391:LEU:HD23	1.79	0.44
1:D:427:PHE:CE2	1:D:445:LEU:HD22	2.53	0.44
1:C:183:GLY:CA	1:C:191:ILE:HD12	2.48	0.44
1:A:243:HIS:O	1:A:247:SER:OG	2.27	0.44
1:D:443:GLU:OE2	1:D:447:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:SER:OG	1:B:442:ARG:NH1	2.49	0.43
1:B:396:TYR:CD1	1:B:437:LYS:HD3	2.53	0.43
1:C:143:ARG:NH2	1:C:210:HIS:O	2.44	0.43
1:C:267:PHE:HZ	1:C:297:LEU:HB3	1.83	0.43
1:C:489:LEU:HB3	1:C:492:LYS:HE3	2.00	0.43
1:B:455:LYS:HG2	1:B:557:VAL:HG12	1.99	0.43
1:C:388:ASP:OD1	1:C:444:ILE:HG21	2.18	0.43
1:A:118:ILE:HG22	1:A:126:ILE:HB	2.00	0.43
1:A:264:ASP:O	1:A:268:ILE:HG13	2.18	0.43
1:D:421:LYS:O	1:D:421:LYS:HD2	2.19	0.43
1:A:250:ILE:HG22	1:A:254:MET:HG3	2.00	0.43
1:A:440:ASP:O	1:A:444:ILE:HG22	2.19	0.43
1:B:116:LYS:HE2	1:B:133:VAL:HG11	2.01	0.43
1:D:562:LEU:HD12	1:D:562:LEU:HA	1.80	0.43
1:A:471:GLU:C	1:A:473:TYR:H	2.22	0.43
1:D:320:CYS:SG	1:D:327:ASN:HB2	2.59	0.43
1:A:528:ARG:NH1	1:C:586:VAL:HA	2.33	0.43
1:D:352:ARG:HG3	1:D:354:LYS:H	1.84	0.43
1:A:541:LEU:HB3	1:A:542:PRO:HD2	2.00	0.42
1:B:333:ARG:O	1:B:337:PHE:HD2	2.02	0.42
1:B:378:VAL:HG11	2:B:701:GTP:H5'	2.01	0.42
1:B:488:LEU:O	1:B:488:LEU:HD12	2.19	0.42
1:C:493:LEU:HB2	1:C:568:TYR:HE2	1.83	0.42
1:D:134:ARG:HE	1:D:134:ARG:HB2	1.75	0.42
1:B:531:ARG:CZ	5:B:813:HOH:O	2.66	0.42
1:A:462:PRO:HG3	1:A:468:ILE:HD11	2.01	0.42
1:B:423:THR:O	1:B:426:ILE:HG22	2.20	0.42
1:A:197:LEU:O	1:A:201:ILE:HG13	2.19	0.42
1:C:243:HIS:CD2	1:C:247:SER:OG	2.72	0.42
1:C:439:LYS:O	1:C:443:GLU:HG2	2.19	0.42
1:B:586:VAL:HG21	1:D:522[B]:CYS:SG	2.60	0.42
1:A:359:LEU:HA	1:A:359:LEU:HD12	1.83	0.42
1:C:140:GLN:HB2	1:C:244:LEU:HD13	2.02	0.42
1:C:562:LEU:O	1:C:566:ARG:HG3	2.20	0.42
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.83	0.42
1:C:197:LEU:O	1:C:201:ILE:HG13	2.20	0.42
1:C:489:LEU:HB3	1:C:492:LYS:NZ	2.34	0.42
1:C:595:LYS:HG2	1:C:598:TRP:CE2	2.55	0.42
1:C:349:ILE:HG21	1:C:349:ILE:HD13	1.80	0.41
1:A:542:PRO:HB3	1:C:540:LEU:O	2.20	0.41
1:D:563:TYR:O	1:D:567:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:HIS:O	1:C:171:VAL:HG23	2.20	0.41
1:D:118:ILE:HG22	1:D:126:ILE:HG12	2.01	0.41
1:A:469:LYS:HB3	1:A:469:LYS:HE3	1.79	0.41
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.20	0.41
1:B:397:ILE:HD11	1:B:430:ILE:HG12	2.02	0.41
1:A:524:THR:OG1	1:C:586:VAL:HG11	2.21	0.41
2:B:701:GTP:C8	1:C:118:ILE:HD12	2.56	0.41
1:A:479:GLU:OE1	1:A:576:ARG:NH1	2.50	0.41
1:A:576:ARG:HE	1:A:576:ARG:HB3	1.56	0.41
1:B:116:LYS:HE3	2:B:702:GTP:HN22	1.85	0.41
1:D:360:TYR:CE2	1:D:541:LEU:HD13	2.56	0.41
1:A:441:ALA:O	1:A:444:ILE:HG23	2.21	0.41
1:B:409:ILE:CD1	1:B:426:ILE:HD11	2.51	0.41
1:C:493:LEU:HB2	1:C:568:TYR:CE2	2.55	0.41
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.03	0.41
1:D:595:LYS:HG2	1:D:598:TRP:CE2	2.56	0.41
1:A:485:PRO:HG2	1:A:489:LEU:HD11	2.02	0.41
1:B:351:ALA:O	1:B:520:PHE:HA	2.20	0.41
1:C:435:ASP:HA	1:C:436:PRO:HD2	1.96	0.41
1:C:479:GLU:HB3	1:C:572:TRP:HE1	1.85	0.41
1:A:538:SER:HB3	1:A:541:LEU:CD1	2.50	0.41
1:D:494:LYS:HB2	1:D:496:GLU:OE1	2.21	0.41
1:B:388:ASP:OD2	1:B:392:LYS:NZ	2.40	0.41
1:C:118:ILE:HG23	1:C:126:ILE:HG13	2.03	0.41
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.56	0.41
1:C:396:TYR:CD1	1:C:437:LYS:HD3	2.56	0.41
1:A:562:LEU:HD12	1:A:562:LEU:HA	1.88	0.40
1:D:197:LEU:O	1:D:201:ILE:HG13	2.22	0.40
1:C:492:LYS:HD3	1:C:492:LYS:HA	1.55	0.40
1:D:167:HIS:O	1:D:171:VAL:HG23	2.21	0.40
1:D:272:ILE:O	1:D:304:LYS:NZ	2.54	0.40
1:A:224:LEU:HB3	1:A:391:LEU:HD11	2.03	0.40
1:D:312:LYS:HA	1:D:315:TYR:CD2	2.57	0.40
1:D:352:ARG:HG3	1:D:353:ASP:N	2.35	0.40
1:B:566:ARG:HD3	1:B:587:ILE:HB	2.03	0.40
1:D:118:ILE:HG22	1:D:126:ILE:CG1	2.52	0.40
1:A:425:ASN:HB2	1:D:428:LEU:HD12	2.03	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	478/550 (87%)	464 (97%)	12 (2%)	2 (0%)	34	37
1	B	477/550 (87%)	466 (98%)	9 (2%)	2 (0%)	34	37
1	C	478/550 (87%)	464 (97%)	10 (2%)	4 (1%)	19	17
1	D	480/550 (87%)	471 (98%)	9 (2%)	0	100	100
All	All	1913/2200 (87%)	1865 (98%)	40 (2%)	8 (0%)	34	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	PRO
1	C	483	ALA
1	A	472	ASP
1	A	594	GLN
1	C	485	PRO
1	C	486	LYS
1	C	482	SER
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	428/488 (88%)	413 (96%)	15 (4%)	36	43
1	B	427/488 (88%)	414 (97%)	13 (3%)	41	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	428/488 (88%)	412 (96%)	16 (4%)	34	40
1	D	430/488 (88%)	412 (96%)	18 (4%)	30	34
All	All	1713/1952 (88%)	1651 (96%)	62 (4%)	35	42

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	189	LEU
1	A	229	VAL
1	A	348	ARG
1	A	359	LEU
1	A	439	LYS
1	A	444	ILE
1	A	446	LYS
1	A	463	THR
1	A	467	LYS
1	A	484	LYS
1	A	528	ARG
1	A	540	LEU
1	A	576	ARG
1	A	594	GLN
1	B	114	THR
1	B	118	ILE
1	B	230	LYS
1	B	234	GLU
1	B	326	GLN
1	B	345	ASN
1	B	400	THR
1	B	408	ARG
1	B	465	GLN
1	B	476	LEU
1	B	522	CYS
1	B	528	ARG
1	B	535	ASN
1	C	118	ILE
1	C	177	CYS
1	C	198	CYS
1	C	229	VAL
1	C	327	ASN
1	C	344	ASP

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Mol	Chain	Res	Type
1	C	371	ARG
1	C	398	GLU
1	C	426	ILE
1	C	440	ASP
1	C	452	ASN
1	C	463	THR
1	C	471	GLU
1	C	487	VAL
1	C	491	VAL
1	C	592	THR
1	D	134	ARG
1	D	218	ASP
1	D	235	GLN
1	D	245	ILE
1	D	276	LEU
1	D	346	GLU
1	D	354	LYS
1	D	395	ASP
1	D	421	LYS
1	D	434	THR
1	D	444	ILE
1	D	494	LYS
1	D	515	ILE
1	D	522[A]	CYS
1	D	522[B]	CYS
1	D	543	GLU
1	D	547	GLU
1	D	597	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	327	ASN
1	A	571	GLN
1	B	210	HIS
1	C	243	HIS
1	D	376	HIS
1	D	571	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	DTP	C	701	4	26,32,32	1.22	4 (15%)	30,50,50	1.54	5 (16%)
2	GTP	A	701	4	26,34,34	2.37	8 (30%)	33,54,54	1.69	8 (24%)
3	DTP	D	701	4	26,32,32	1.30	4 (15%)	30,50,50	1.51	5 (16%)
3	DTP	B	703	4	26,32,32	1.22	3 (11%)	30,50,50	1.54	4 (13%)
2	GTP	B	702	4	26,34,34	2.34	7 (26%)	33,54,54	1.70	9 (27%)
2	GTP	D	702	4	26,34,34	2.38	8 (30%)	33,54,54	1.75	9 (27%)
2	GTP	B	701	4	26,34,34	2.36	8 (30%)	33,54,54	1.73	9 (27%)
3	DTP	A	702	4	26,32,32	1.30	4 (15%)	30,50,50	1.43	5 (16%)

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	DTP	C	701	4	-	2/18/34/34	0/3/3/3
2	GTP	A	701	4	-	3/18/38/38	0/3/3/3
3	DTP	D	701	4	-	2/18/34/34	0/3/3/3
3	DTP	B	703	4	-	4/18/34/34	0/3/3/3
2	GTP	B	702	4	-	6/18/38/38	0/3/3/3
2	GTP	D	702	4	-	3/18/38/38	0/3/3/3
2	GTP	B	701	4	-	5/18/38/38	0/3/3/3
3	DTP	A	702	4	-	6/18/34/34	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GTP	C2-N2	7.23	1.48	1.33
2	D	702	GTP	C2-N2	7.19	1.48	1.33
2	A	701	GTP	C2-N2	7.17	1.48	1.33
2	B	702	GTP	C2-N2	7.15	1.48	1.33
2	D	702	GTP	O6-C6	6.81	1.41	1.24
2	B	701	GTP	O6-C6	6.74	1.41	1.24
2	A	701	GTP	O6-C6	6.71	1.41	1.24
2	B	702	GTP	O6-C6	6.71	1.41	1.24
2	D	702	GTP	O2'-C2'	-3.18	1.35	1.43
2	B	702	GTP	O2'-C2'	-3.14	1.35	1.43
2	B	701	GTP	O2'-C2'	-3.13	1.35	1.43
2	A	701	GTP	O2'-C2'	-3.12	1.35	1.43
2	A	701	GTP	C2'-C1'	-2.74	1.49	1.53
3	B	703	DTP	C6-N6	2.72	1.43	1.34
3	A	702	DTP	C6-N6	2.71	1.43	1.34
3	D	701	DTP	O3'-C3'	-2.71	1.37	1.43
3	C	701	DTP	O3'-C3'	-2.70	1.37	1.43
3	D	701	DTP	C6-N6	2.70	1.43	1.34
3	B	703	DTP	O3'-C3'	-2.68	1.37	1.43
3	A	702	DTP	O3'-C3'	-2.66	1.37	1.43
3	C	701	DTP	C6-N6	2.66	1.43	1.34
2	B	702	GTP	C2'-C1'	-2.64	1.49	1.53
2	B	701	GTP	C2'-C1'	-2.63	1.49	1.53
2	D	702	GTP	C2'-C1'	-2.62	1.49	1.53
3	B	703	DTP	C5'-C4'	-2.57	1.43	1.51
3	A	702	DTP	C5'-C4'	-2.49	1.43	1.51
2	B	701	GTP	C5'-C4'	-2.46	1.43	1.51
3	C	701	DTP	C5'-C4'	-2.41	1.44	1.51
3	D	701	DTP	C5'-C4'	-2.37	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	GTP	C5'-C4'	-2.34	1.44	1.51
2	A	701	GTP	C5'-C4'	-2.31	1.44	1.51
2	D	702	GTP	PG-O3G	-2.28	1.46	1.54
2	A	701	GTP	PG-O3G	-2.28	1.46	1.54
2	D	702	GTP	C5'-C4'	-2.25	1.44	1.51
2	A	701	GTP	C2'-C3'	-2.22	1.47	1.53
2	D	702	GTP	C3'-C4'	-2.22	1.47	1.53
2	B	701	GTP	C2'-C3'	-2.21	1.47	1.53
2	B	702	GTP	C3'-C4'	-2.18	1.47	1.53
2	B	702	GTP	C2'-C3'	-2.18	1.47	1.53
3	C	701	DTP	C2'-C3'	-2.15	1.47	1.52
2	B	701	GTP	C3'-C4'	-2.14	1.47	1.53
2	A	701	GTP	C3'-C4'	-2.09	1.47	1.53
2	D	702	GTP	C2'-C3'	-2.09	1.47	1.53
3	D	701	DTP	C2'-C3'	-2.06	1.47	1.52
3	A	702	DTP	C2'-C3'	-2.04	1.47	1.52
2	B	701	GTP	PG-O2G	-2.01	1.47	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	DTP	N3-C2-N1	-4.82	121.14	128.68
3	C	701	DTP	N3-C2-N1	-4.75	121.25	128.68
3	D	701	DTP	N3-C2-N1	-4.70	121.33	128.68
3	A	702	DTP	N3-C2-N1	-4.67	121.38	128.68
2	D	702	GTP	C5-C6-N1	-4.19	117.70	123.43
2	B	702	GTP	C5-C6-N1	-4.05	117.89	123.43
2	B	701	GTP	C5-C6-N1	-3.93	118.06	123.43
2	A	701	GTP	C5-C6-N1	-3.90	118.10	123.43
2	A	701	GTP	C2-N3-C4	3.69	119.57	115.36
2	B	701	GTP	C2-N3-C4	3.59	119.45	115.36
2	D	702	GTP	C2-N3-C4	3.56	119.42	115.36
2	A	701	GTP	N3-C2-N1	-3.45	122.62	127.22
2	B	702	GTP	C2-N3-C4	3.45	119.30	115.36
2	D	702	GTP	N3-C2-N1	-3.44	122.64	127.22
2	B	702	GTP	N3-C2-N1	-3.39	122.70	127.22
2	B	701	GTP	N3-C2-N1	-3.36	122.74	127.22
2	B	701	GTP	PA-O3A-PB	-3.27	121.59	132.83
3	B	703	DTP	PB-O3B-PG	-3.24	121.72	132.83
2	D	702	GTP	C6-N1-C2	3.23	121.06	115.93
3	D	701	DTP	PA-O3A-PB	-3.13	122.09	132.83
2	B	702	GTP	C6-N1-C2	3.12	120.89	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	DTP	PB-O3B-PG	-3.09	122.23	132.83
2	A	701	GTP	C6-N1-C2	3.01	120.71	115.93
2	B	701	GTP	C6-N1-C2	3.00	120.70	115.93
3	B	703	DTP	C4-C5-N7	-2.95	106.32	109.40
2	A	701	GTP	C3'-C2'-C1'	2.94	105.41	100.98
2	B	701	GTP	C3'-C2'-C1'	2.94	105.41	100.98
3	A	702	DTP	C4-C5-N7	-2.94	106.34	109.40
3	A	702	DTP	PA-O3A-PB	-2.92	122.80	132.83
2	D	702	GTP	C3'-C2'-C1'	2.91	105.36	100.98
2	D	702	GTP	O5'-C5'-C4'	2.84	118.76	108.99
3	C	701	DTP	C4-C5-N7	-2.83	106.45	109.40
3	D	701	DTP	C4-C5-N7	-2.80	106.48	109.40
2	B	702	GTP	PA-O3A-PB	-2.79	123.26	132.83
3	D	701	DTP	O5'-C5'-C4'	2.77	118.54	108.99
3	C	701	DTP	O5'-C5'-C4'	2.77	118.51	108.99
3	B	703	DTP	PA-O3A-PB	-2.74	123.42	132.83
3	C	701	DTP	PA-O3A-PB	-2.70	123.55	132.83
2	B	702	GTP	O5'-C5'-C4'	2.67	118.19	108.99
2	A	701	GTP	PA-O3A-PB	-2.65	123.74	132.83
2	D	702	GTP	PA-O3A-PB	-2.63	123.78	132.83
3	D	701	DTP	PB-O3B-PG	-2.58	123.97	132.83
2	B	701	GTP	O3G-PG-O3B	2.55	113.19	104.64
2	A	701	GTP	O5'-C5'-C4'	2.53	117.69	108.99
2	B	702	GTP	C3'-C2'-C1'	2.48	104.71	100.98
2	B	702	GTP	O3G-PG-O3B	2.48	112.94	104.64
3	A	702	DTP	O5'-C5'-C4'	2.30	116.92	108.99
2	B	701	GTP	PB-O3B-PG	-2.26	125.08	132.83
3	A	702	DTP	PB-O3B-PG	-2.22	125.21	132.83
2	B	702	GTP	PB-O3B-PG	-2.21	125.24	132.83
2	A	701	GTP	PB-O3B-PG	-2.20	125.28	132.83
2	D	702	GTP	PB-O3B-PG	-2.19	125.31	132.83
2	B	701	GTP	C5'-C4'-C3'	-2.12	107.25	115.18
2	D	702	GTP	C4-C5-N7	-2.02	107.30	109.40

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	DTP	PB-O3B-PG-O2G
3	B	703	DTP	PB-O3B-PG-O3G
2	B	702	GTP	PB-O3B-PG-O3G
2	B	701	GTP	PB-O3B-PG-O3G

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

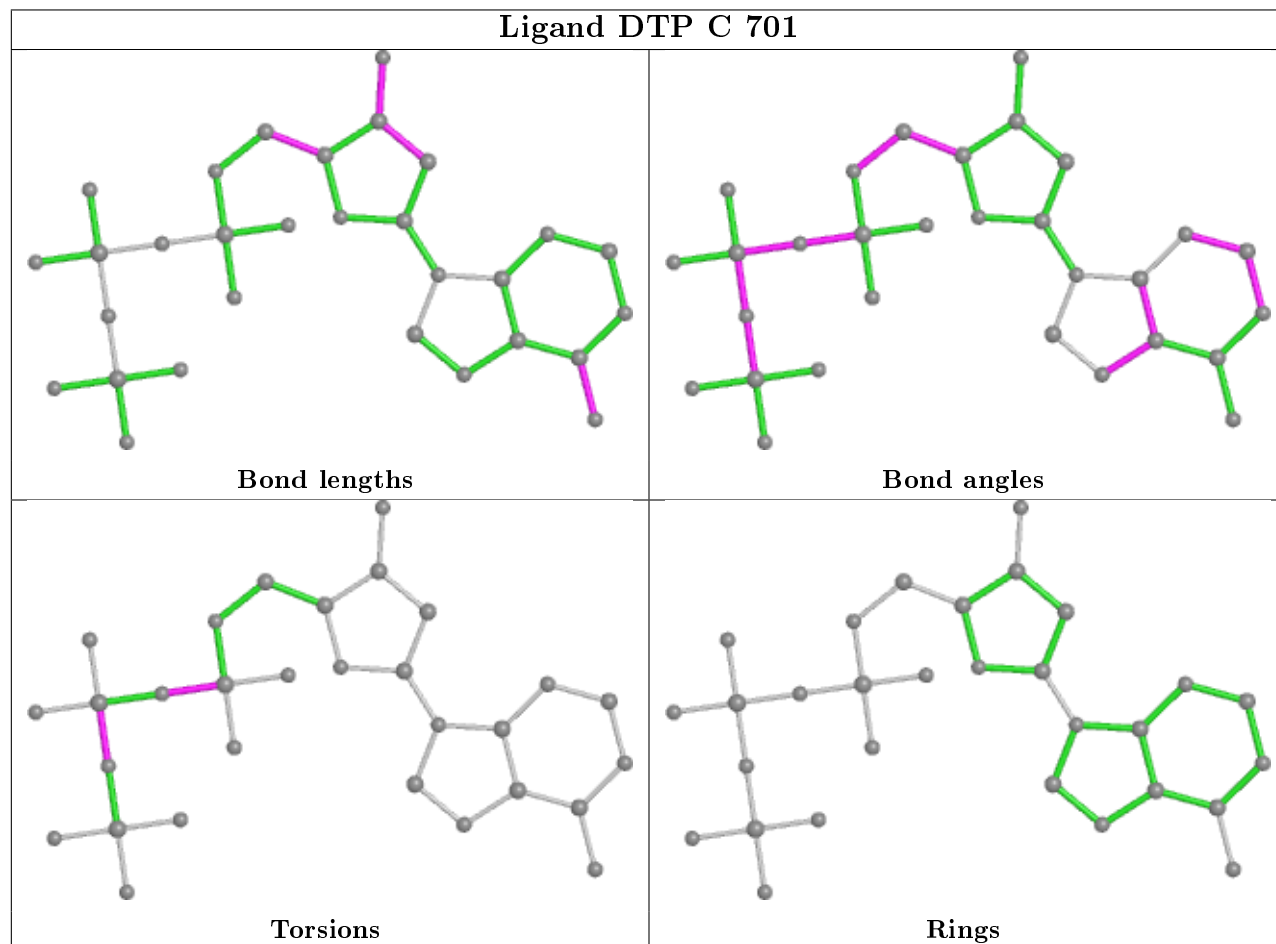
There are no ring outliers.

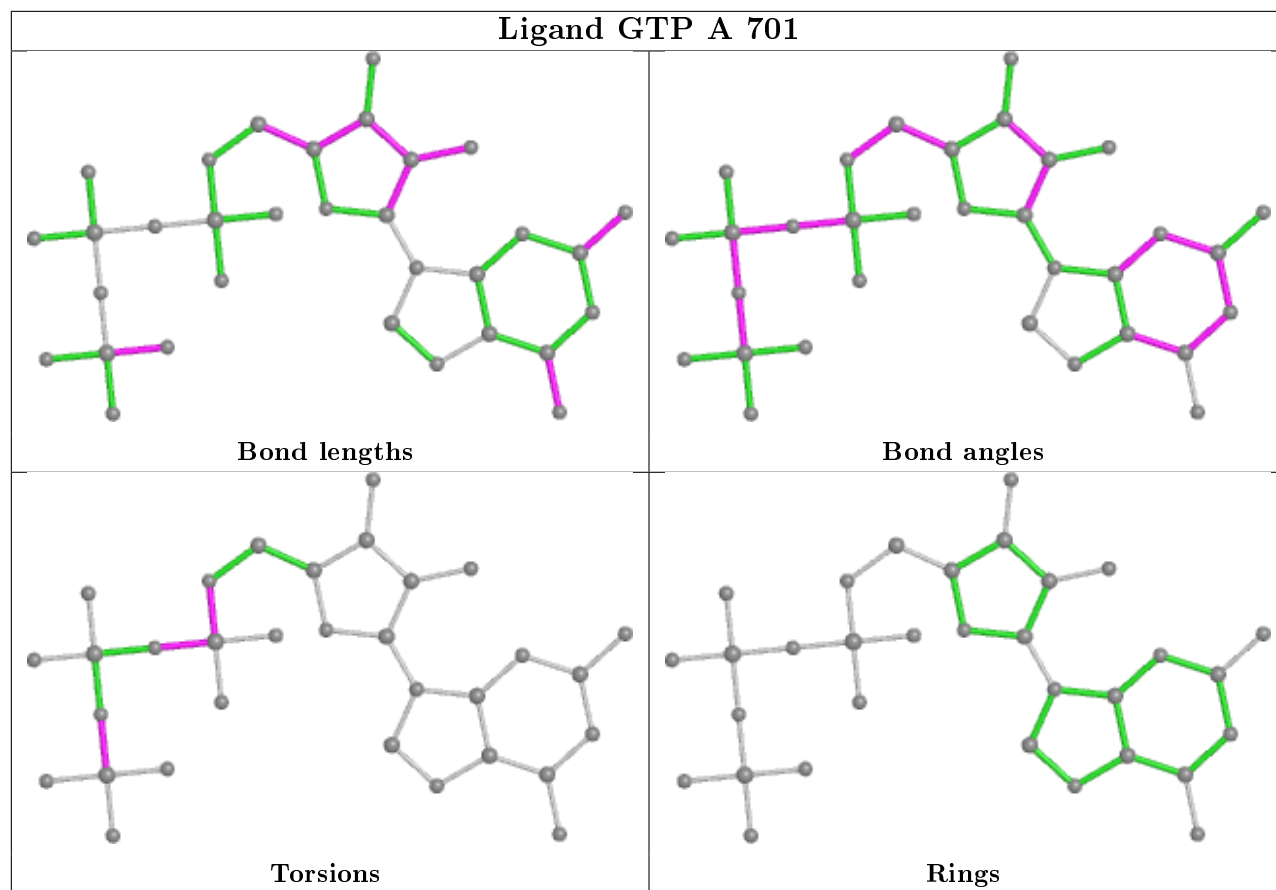
3 monomers are involved in 7 short contacts:

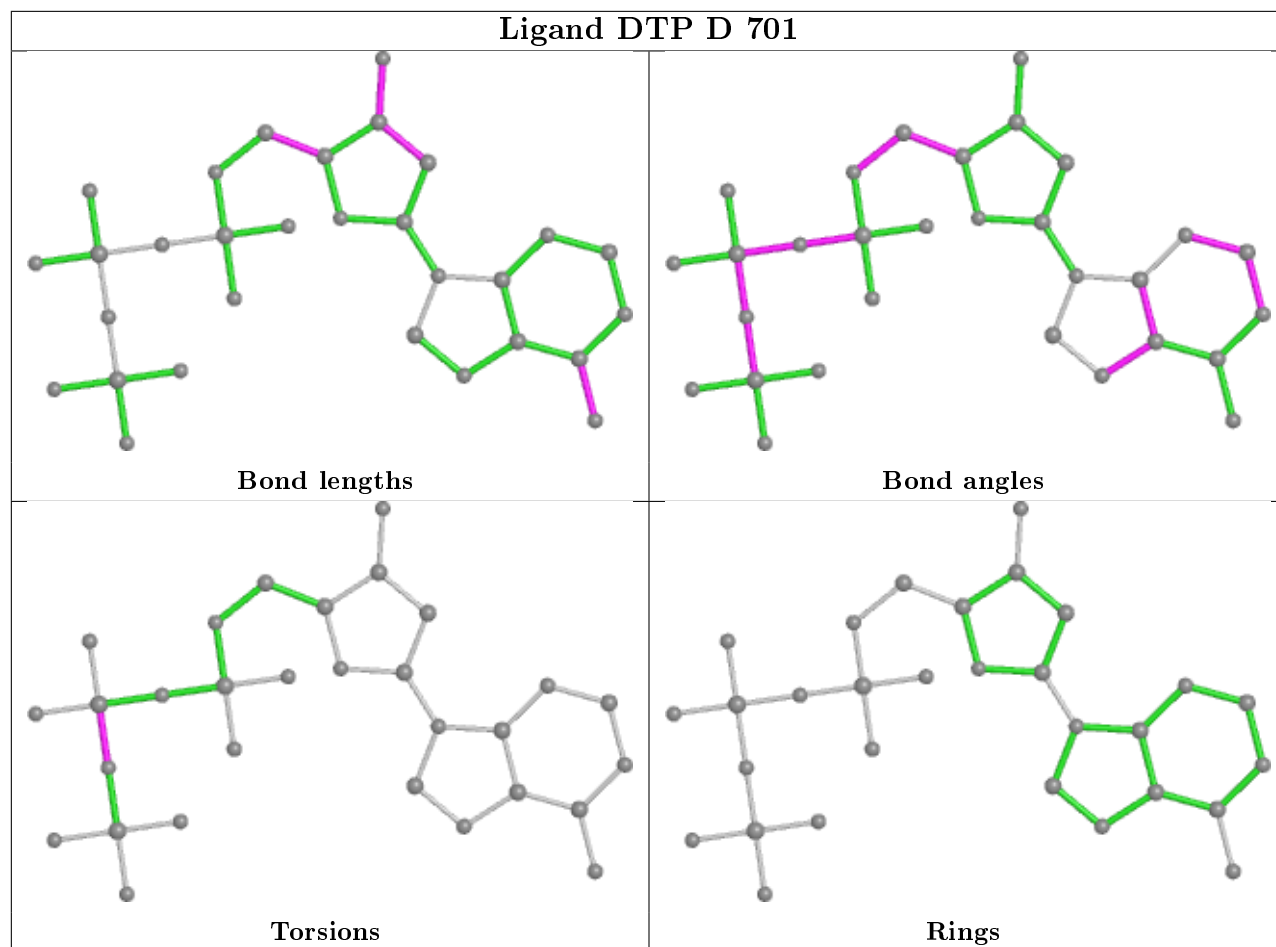
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	DTP	3	0
2	B	702	GTP	1	0
2	B	701	GTP	3	0

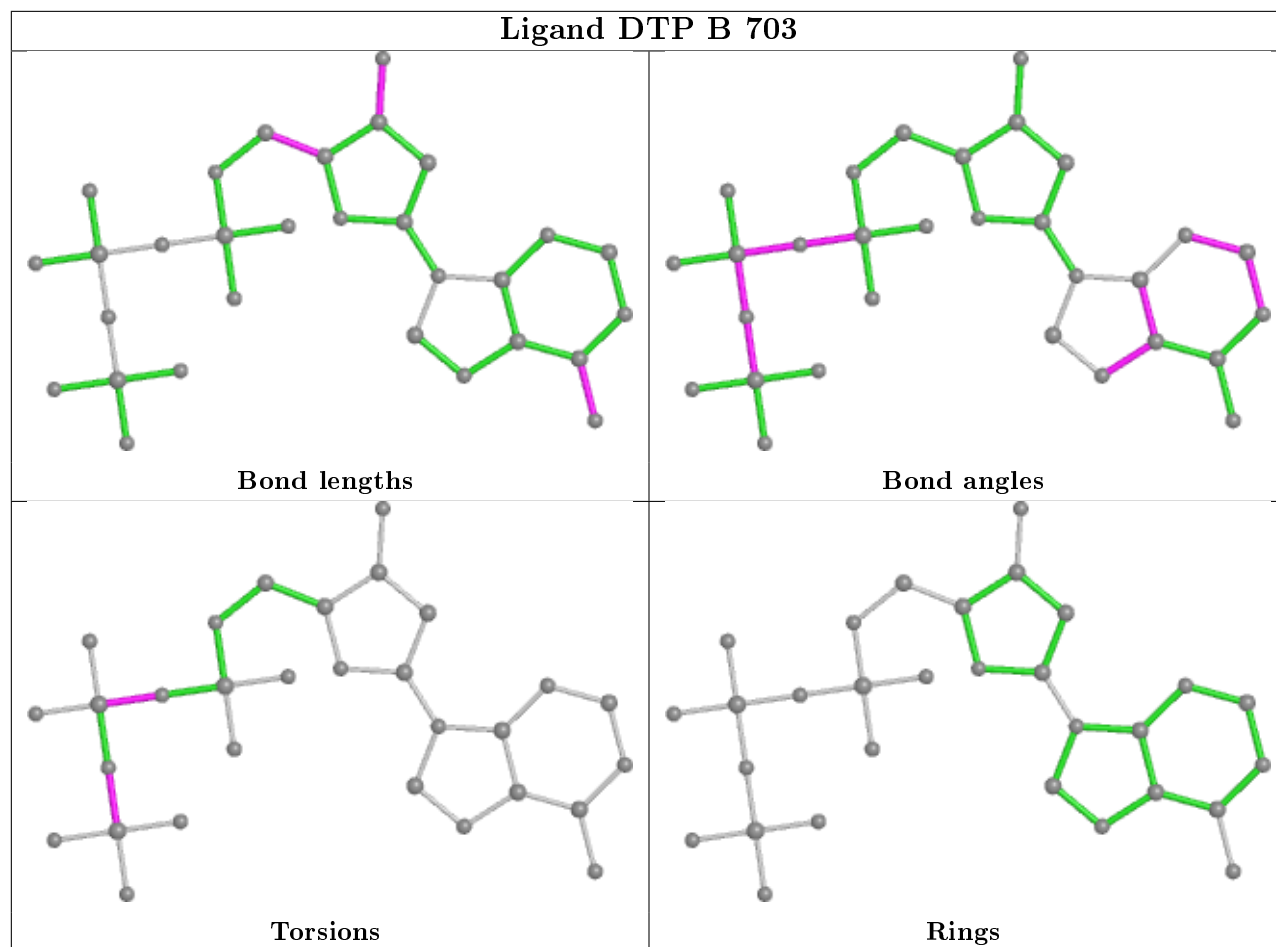
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

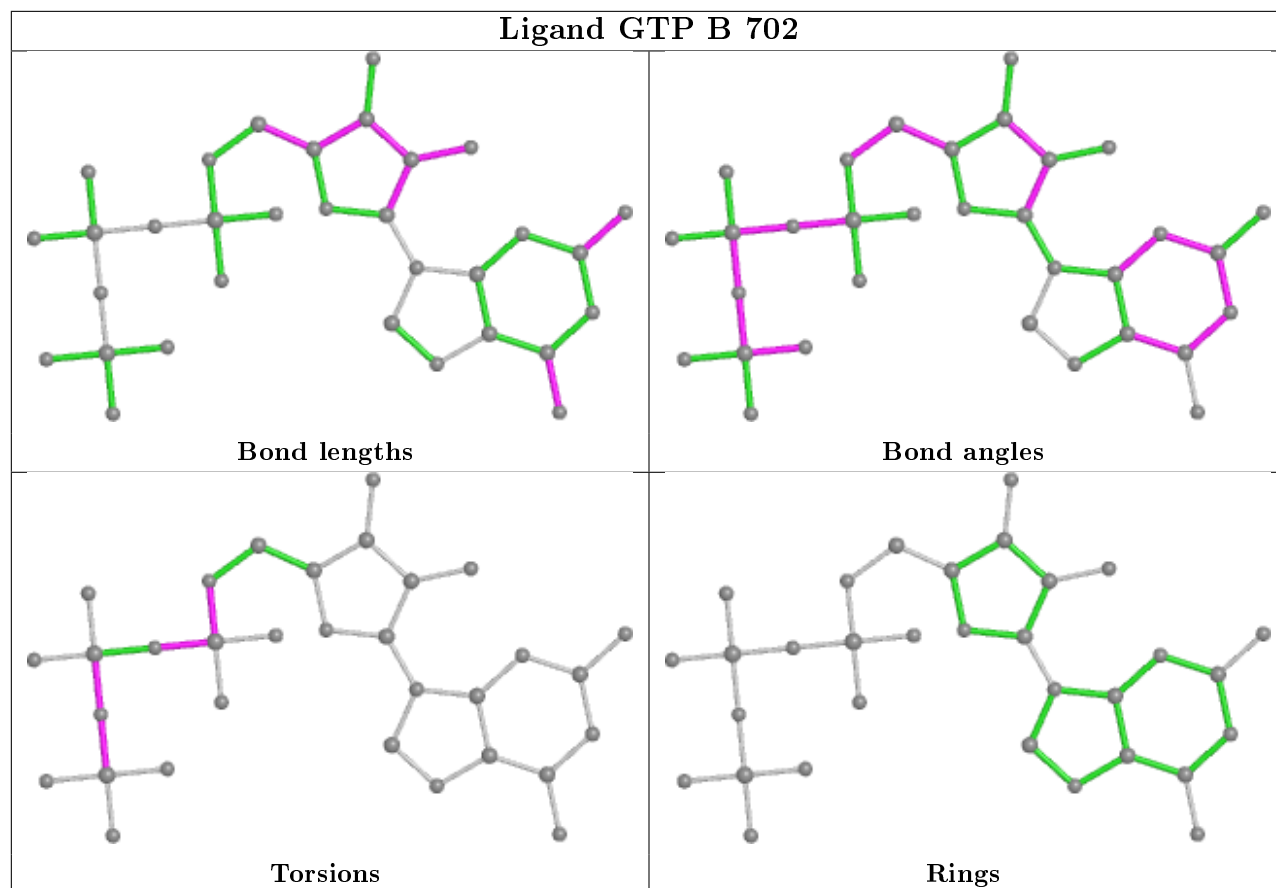




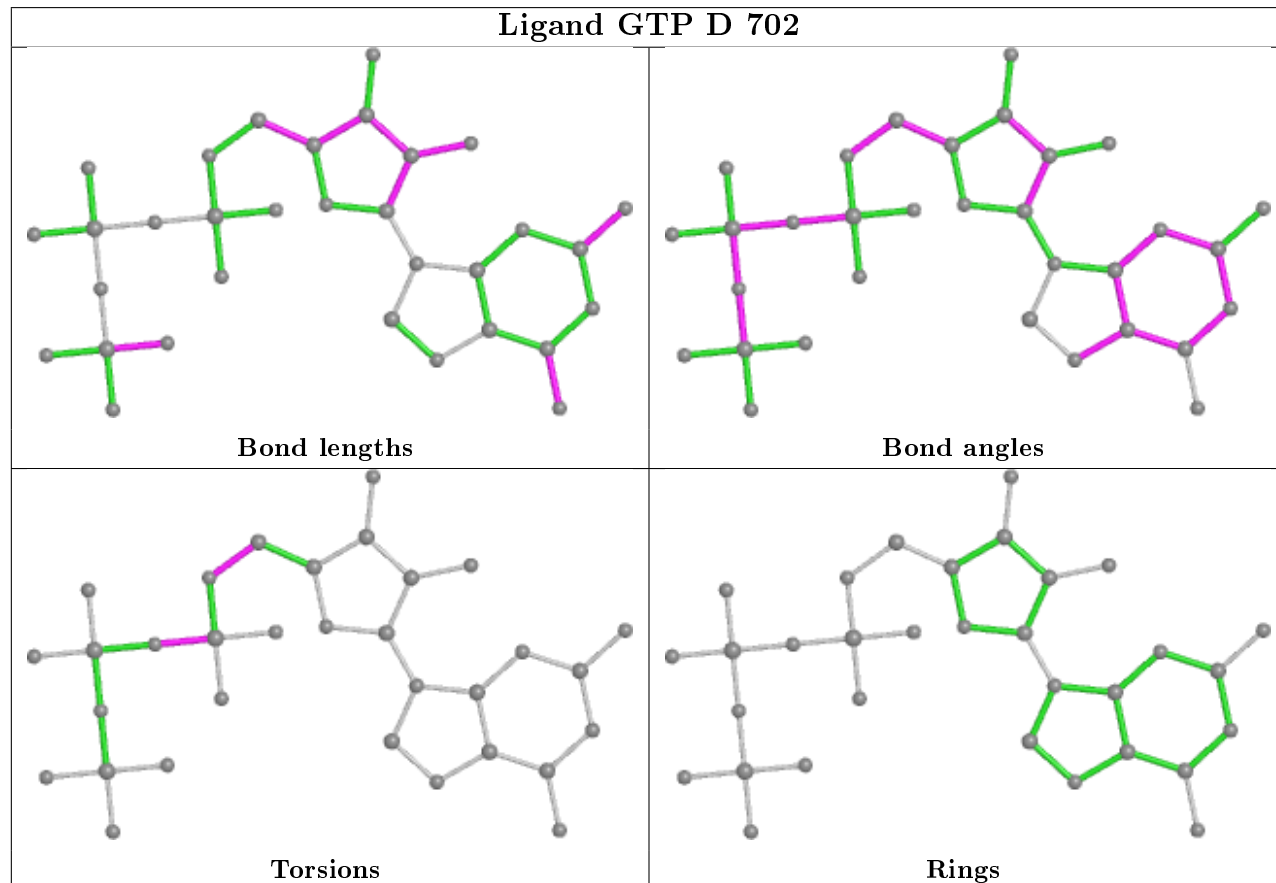


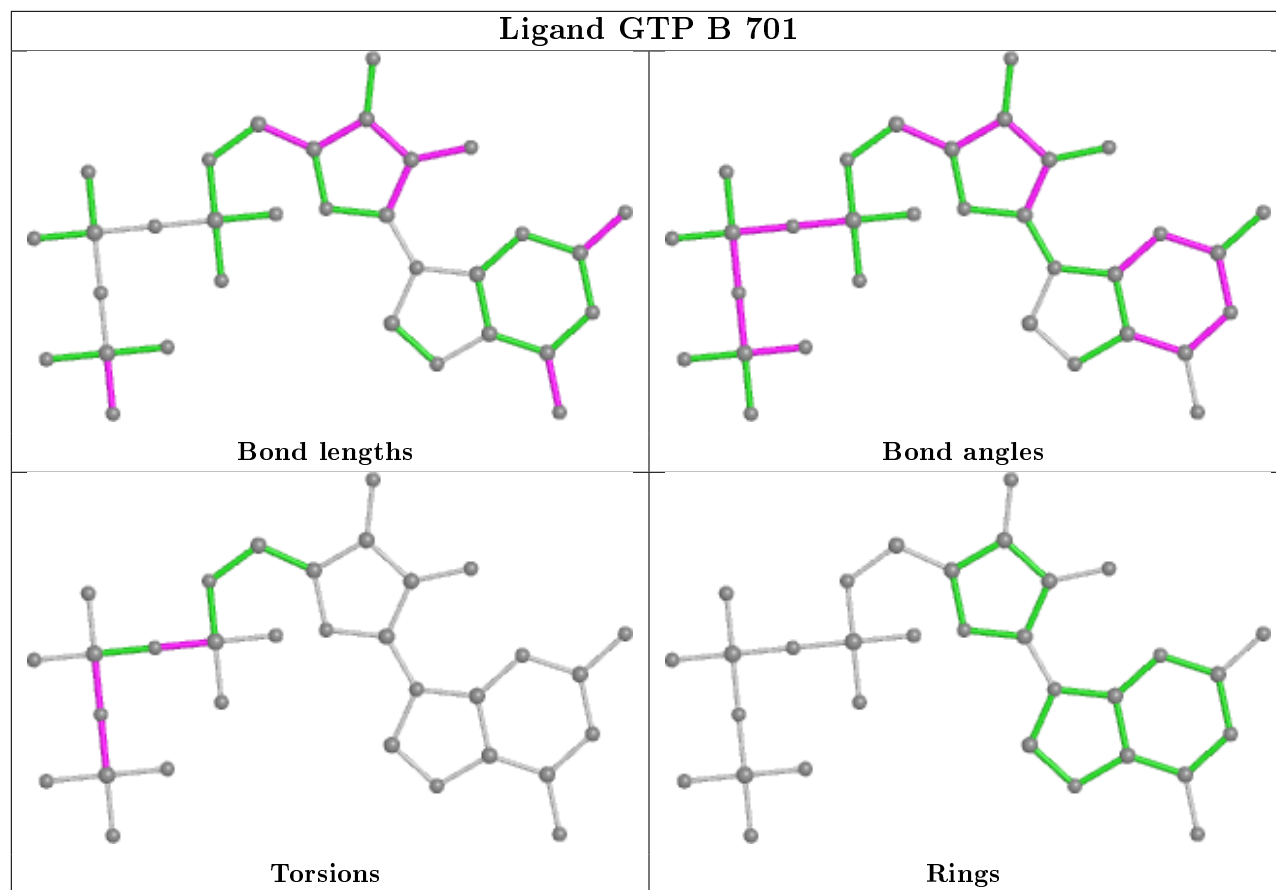


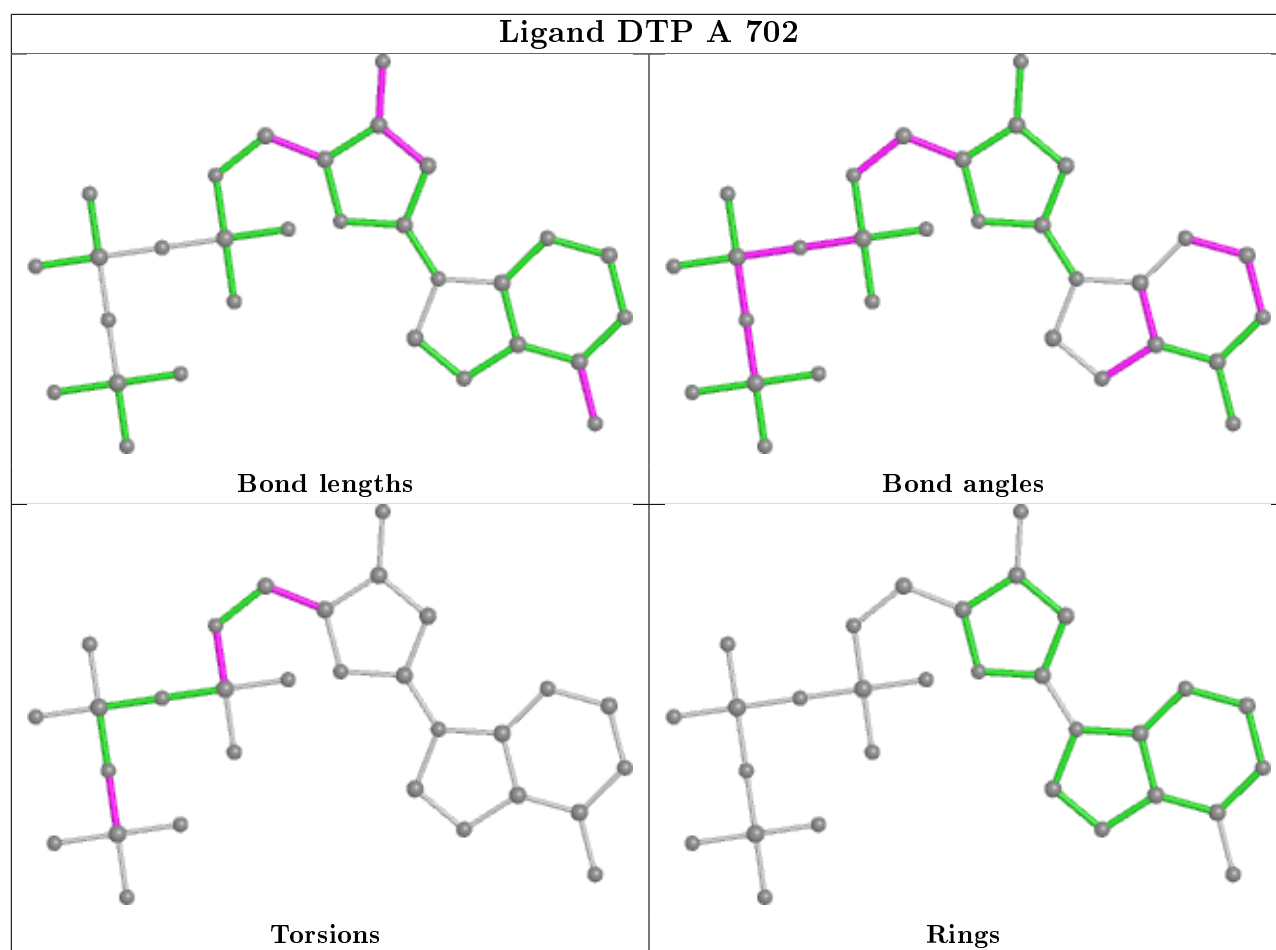
Ligand GTP B 702



Ligand GTP D 702







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/550 (87%)	0.85	57 (11%) 4 3	31, 73, 112, 127	183 (38%)
1	B	481/550 (87%)	0.75	64 (13%) 3 3	44, 68, 107, 123	171 (35%)
1	C	481/550 (87%)	0.94	67 (13%) 2 2	43, 71, 97, 123	206 (42%)
1	D	481/550 (87%)	0.55	34 (7%) 16 17	38, 61, 82, 96	202 (41%)
All	All	1924/2200 (87%)	0.77	222 (11%) 4 4	31, 68, 100, 127	762 (39%)

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	LEU	7.5
1	A	466	ILE	7.0
1	A	528	ARG	6.3
1	D	464	GLY	6.3
1	B	479	GLU	6.2
1	B	493	LEU	6.2
1	B	284	LEU	6.1
1	A	115	MET	6.0
1	A	481	ALA	5.9
1	D	113	ASP	5.9
1	C	488	LEU	5.8
1	C	489	LEU	5.4
1	B	492	LYS	5.3
1	C	590	LEU	5.0
1	B	562	LEU	4.7
1	B	568	TYR	4.6
1	A	489	LEU	4.6
1	D	599	ASN	4.6
1	C	113	ASP	4.6
1	A	487	VAL	4.6
1	C	229	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	490	ASP	4.5
1	C	586	VAL	4.5
1	D	465	GLN	4.4
1	A	230	LYS	4.4
1	C	151	GLY	4.4
1	A	483	ALA	4.4
1	D	326	GLN	4.3
1	C	276	LEU	4.3
1	B	594	GLN	4.2
1	C	596	LYS	4.2
1	D	466	ILE	4.2
1	B	563	TYR	4.1
1	A	465	GLN	4.1
1	B	489	LEU	4.1
1	C	568	TYR	4.1
1	B	114	THR	4.1
1	B	115	MET	3.9
1	B	560	LYS	3.9
1	C	487	VAL	3.9
1	C	591	ILE	3.8
1	B	113	ASP	3.8
1	C	592	THR	3.7
1	C	471	GLU	3.7
1	B	498	PHE	3.7
1	A	344	ASP	3.6
1	B	496	GLU	3.6
1	C	150	LEU	3.5
1	A	343	VAL	3.5
1	B	487	VAL	3.5
1	C	599	ASN	3.4
1	B	346	GLU	3.4
1	B	575	ASP	3.4
1	B	486	LYS	3.4
1	A	598	TRP	3.3
1	C	230	LYS	3.3
1	C	403	GLY	3.3
1	A	406	LYS	3.3
1	C	284	LEU	3.3
1	C	564	ALA	3.3
1	B	485	PRO	3.3
1	D	403	GLY	3.2
1	A	577	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	326	GLN	3.2
1	D	115	MET	3.2
1	D	596	LYS	3.2
1	A	469	LYS	3.2
1	D	496	GLU	3.1
1	D	360	TYR	3.1
1	C	285	TRP	3.1
1	B	483	ALA	3.1
1	A	327	ASN	3.1
1	B	590	LEU	3.1
1	D	468	ILE	3.1
1	A	486	LYS	3.1
1	C	227	PRO	3.1
1	B	588	ALA	3.1
1	C	490	ASP	3.1
1	C	400	THR	3.0
1	A	480	VAL	3.0
1	D	396	TYR	3.0
1	A	490	ASP	3.0
1	B	591	ILE	3.0
1	C	373	ALA	3.0
1	A	345	ASN	2.9
1	B	488	LEU	2.9
1	A	292	GLU	2.9
1	A	568	TYR	2.9
1	B	495	ALA	2.9
1	A	468	ILE	2.9
1	B	288	LYS	2.9
1	A	587	ILE	2.8
1	B	481	ALA	2.8
1	C	585	ASP	2.8
1	A	277	GLU	2.8
1	D	343	VAL	2.8
1	B	438	LEU	2.8
1	D	404	GLY	2.8
1	D	594	GLN	2.8
1	A	155	TYR	2.8
1	C	148	LYS	2.8
1	A	158	PRO	2.7
1	C	480	VAL	2.7
1	B	347	LEU	2.7
1	D	276	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	587	ILE	2.7
1	C	194	ARG	2.7
1	A	488	LEU	2.7
1	B	482	SER	2.7
1	A	558	ASP	2.6
1	C	298	TYR	2.6
1	C	474	GLU	2.6
1	B	491	VAL	2.6
1	B	559	ARG	2.6
1	A	148	LYS	2.6
1	C	464	GLY	2.6
1	D	388[A]	ASP	2.6
1	A	147	ILE	2.6
1	D	346	GLU	2.6
1	A	491	VAL	2.6
1	C	277	GLU	2.6
1	A	472	ASP	2.5
1	B	497	ASP	2.5
1	D	344	ASP	2.5
1	A	299	GLU	2.5
1	D	147	ILE	2.5
1	C	574	ALA	2.5
1	A	398	GLU	2.5
1	B	277	GLU	2.5
1	B	484	LYS	2.5
1	A	160	ALA	2.5
1	B	155	TYR	2.5
1	A	152	GLY	2.5
1	B	587	ILE	2.5
1	C	289	GLY	2.5
1	A	424	ASP	2.5
1	B	480	VAL	2.4
1	B	593	PRO	2.4
1	A	242	GLU	2.4
1	A	275	PRO	2.4
1	B	494	LYS	2.4
1	C	406	LYS	2.4
1	C	491	VAL	2.4
1	A	482	SER	2.4
1	B	327	ASN	2.4
1	A	276	LEU	2.3
1	A	434	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	439	LYS	2.3
1	A	293	ASN	2.3
1	A	522[A]	CYS	2.3
1	C	155	TYR	2.3
1	B	151	GLY	2.3
1	B	152	GLY	2.3
1	C	320	CYS	2.3
1	D	146	TYR	2.3
1	D	150	LEU	2.3
1	A	193	GLU	2.3
1	C	152	GLY	2.3
1	C	267	PHE	2.3
1	A	326	GLN	2.3
1	C	154	TYR	2.3
1	C	436	PRO	2.3
1	C	594	GLN	2.2
1	C	496	GLU	2.2
1	B	476	LEU	2.2
1	A	530	ILE	2.2
1	C	588	ALA	2.2
1	B	326	GLN	2.2
1	A	432	TYR	2.2
1	A	573	CYS	2.2
1	B	478	LYS	2.2
1	B	397	ILE	2.2
1	D	398	GLU	2.2
1	C	584	GLY	2.2
1	B	285	TRP	2.2
1	D	395	ASP	2.2
1	B	592	THR	2.2
1	D	118	ILE	2.2
1	B	436	PRO	2.2
1	D	484	LYS	2.1
1	A	213	PHE	2.1
1	B	399	ILE	2.1
1	C	531	ARG	2.1
1	D	255	GLU	2.1
1	B	161	SER	2.1
1	B	561	SER	2.1
1	C	371	ARG	2.1
1	D	152	GLY	2.1
1	B	440	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	470	ARG	2.1
1	A	347	LEU	2.1
1	C	153	GLY	2.1
1	D	471	GLU	2.1
1	B	370	HIS	2.1
1	C	388	ASP	2.1
1	B	429	GLU	2.1
1	C	163	ASN	2.1
1	B	502	VAL	2.1
1	A	146	TYR	2.1
1	A	478	LYS	2.1
1	C	146	TYR	2.1
1	C	159	GLY	2.1
1	A	222	ILE	2.1
1	C	382	ILE	2.1
1	B	522	CYS	2.1
1	C	156	VAL	2.1
1	C	578	PHE	2.1
1	B	150	LEU	2.0
1	B	509	MET	2.0
1	D	474	GLU	2.0
1	B	261	PRO	2.0
1	C	179	VAL	2.0
1	C	256	GLN	2.0
1	C	466	ILE	2.0
1	A	113	ASP	2.0
1	A	485	PRO	2.0
1	D	230	LYS	2.0
1	B	118	ILE	2.0
1	C	323	LEU	2.0
1	D	151	GLY	2.0
1	C	469	LYS	2.0
1	C	483	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

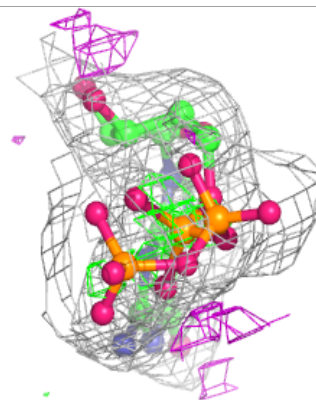
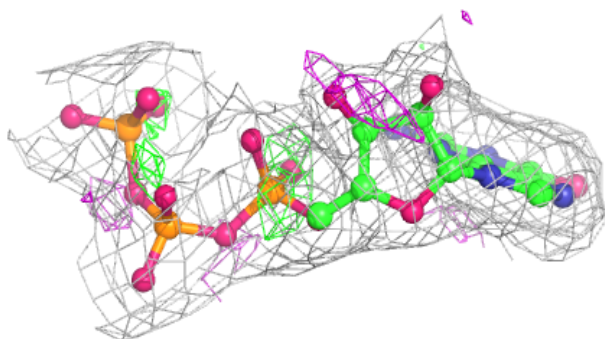
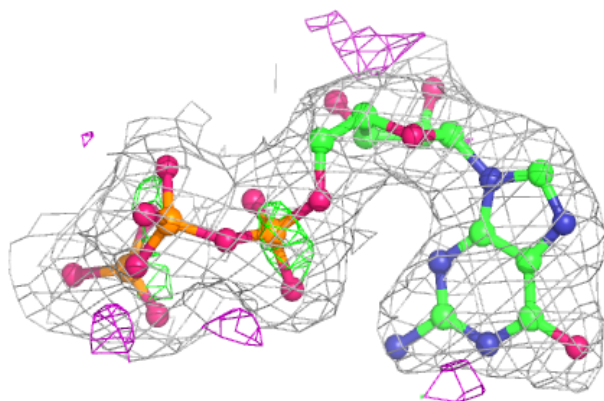
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	703	1/1	0.56	0.10	40,40,40,40	0
4	MG	D	703	1/1	0.80	0.05	56,56,56,56	0
4	MG	A	704	1/1	0.81	0.08	58,58,58,58	0
4	MG	C	702	1/1	0.85	0.10	56,56,56,56	0
2	GTP	A	701	32/32	0.94	0.18	47,57,63,67	0
3	DTP	C	701	30/30	0.95	0.16	44,48,57,60	14
3	DTP	B	703	30/30	0.95	0.16	32,41,57,72	11
2	GTP	B	702	32/32	0.95	0.14	40,54,62,68	0
2	GTP	D	702	32/32	0.96	0.14	31,50,61,80	0
3	DTP	A	702	30/30	0.96	0.18	32,48,60,62	11
3	DTP	D	701	30/30	0.97	0.15	40,47,54,55	14
2	GTP	B	701	32/32	0.97	0.12	40,55,63,66	0

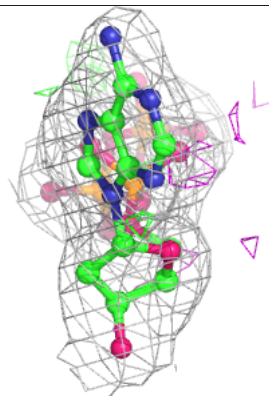
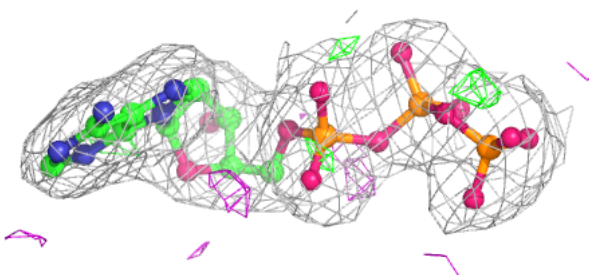
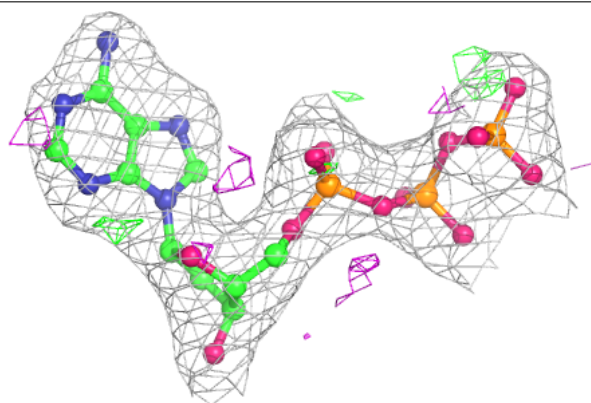
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

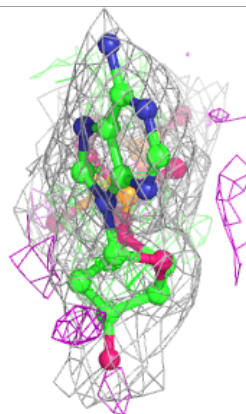
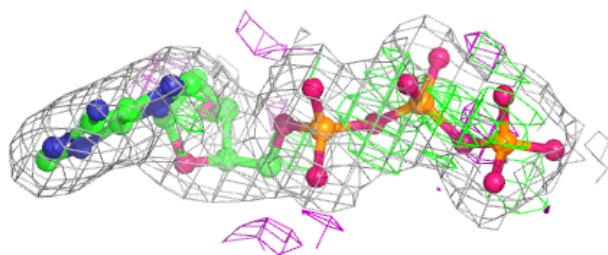
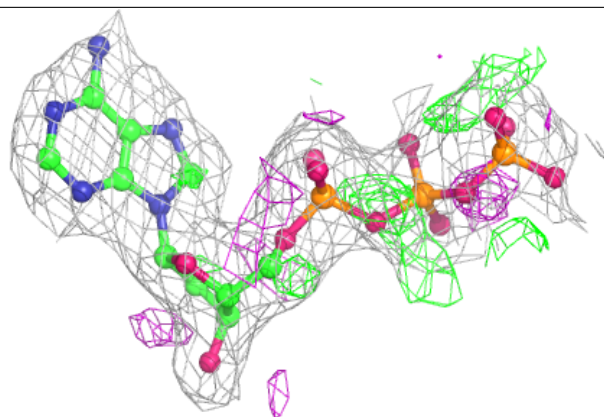
**Electron density around DTP C 701:**

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

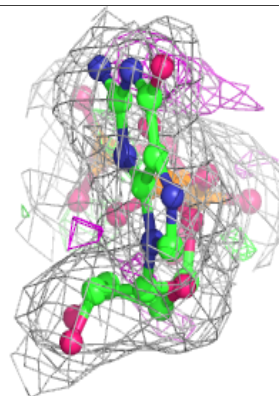
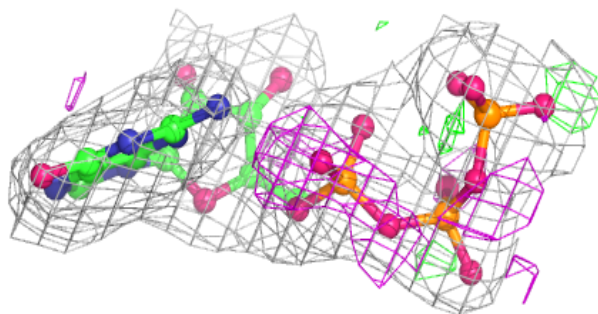
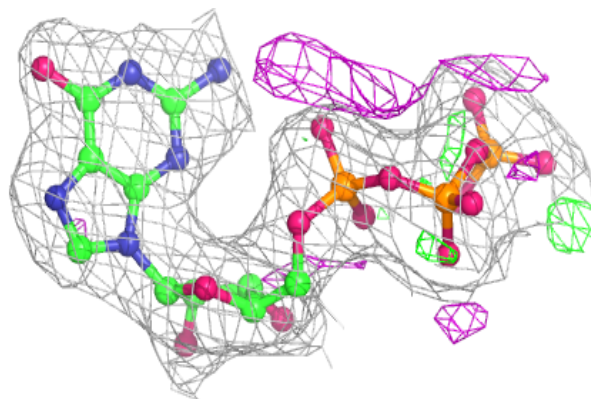


Electron density around DTP B 703:

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

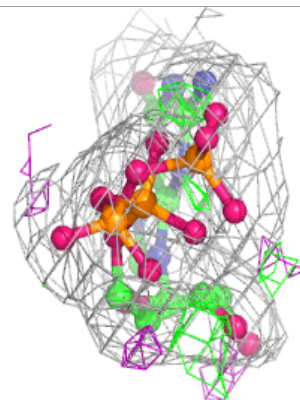
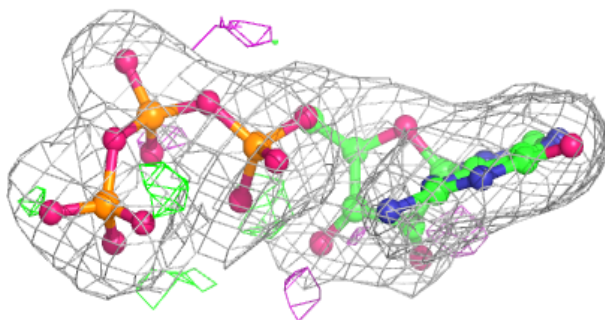
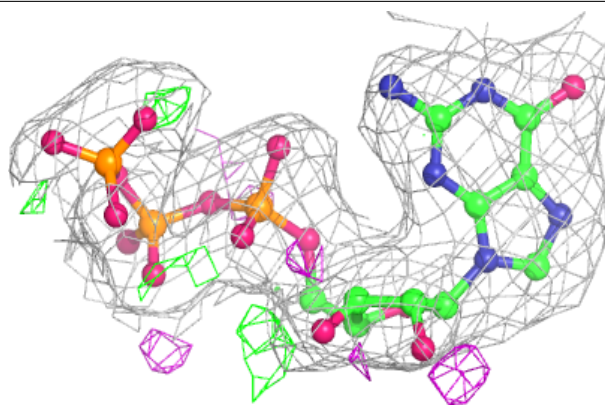
**Electron density around GTP B 702:**

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

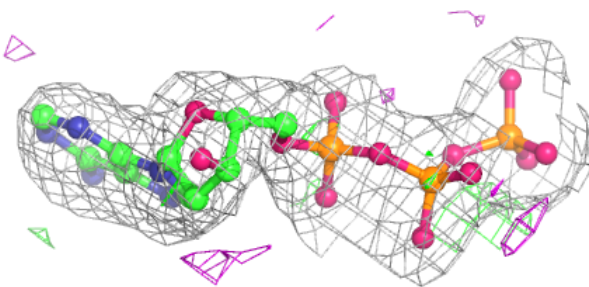
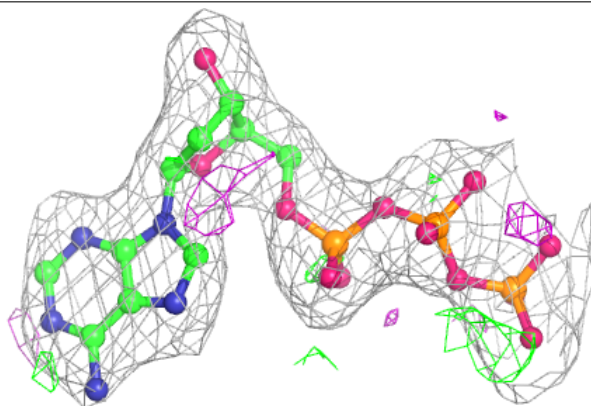


Electron density around GTP D 702:

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

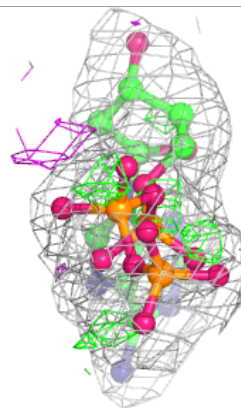
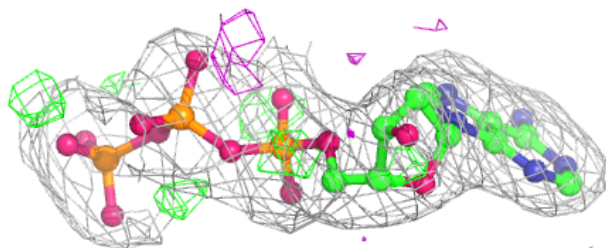
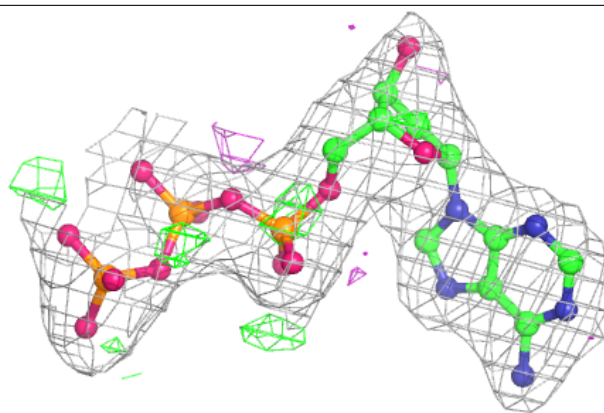
**Electron density around DTP A 702:**

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

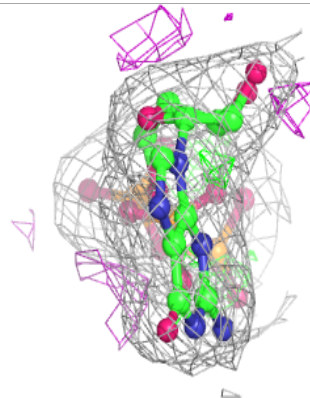
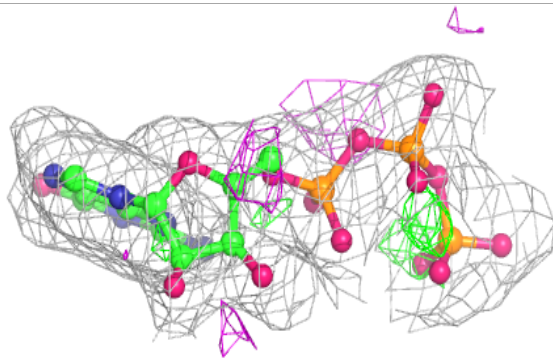
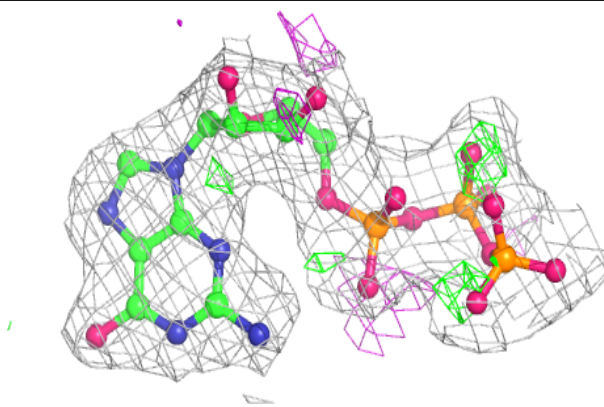


Electron density around DTP D 701:

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

**Electron density around GTP B 701:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.