



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:17 AM UTC

PDB ID : 4QG2 / pdb_00004qg2
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 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

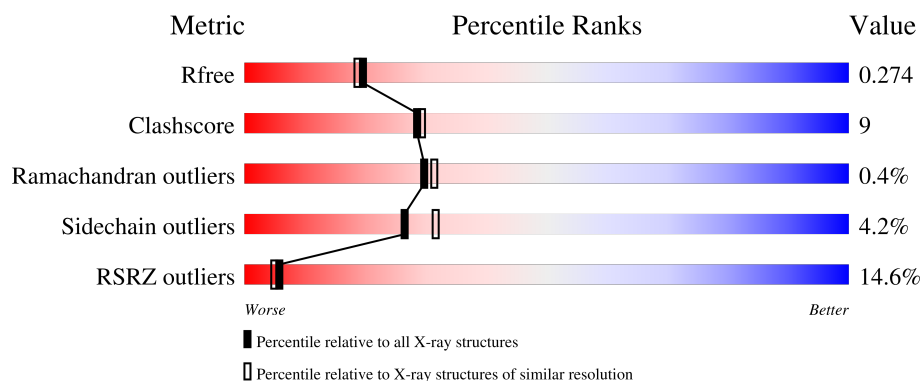
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	15% 65% 20% • 13%
1	B	550	11% 71% 15% • 13%
1	C	550	15% 66% 20% • 13%
1	D	550	10% 68% 18% • 13%

2 Entry composition

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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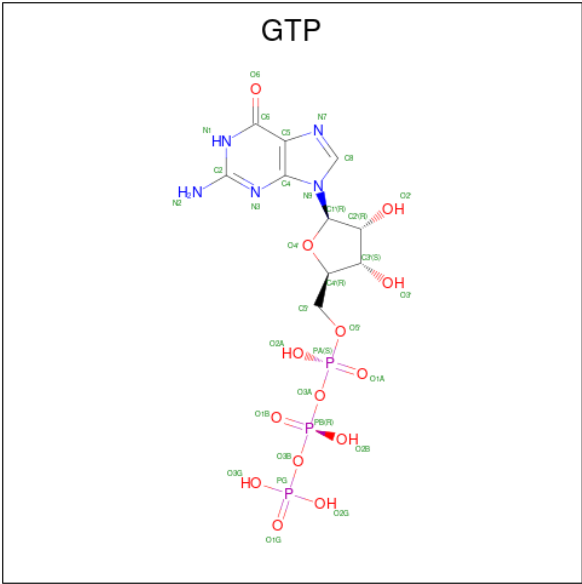
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C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression 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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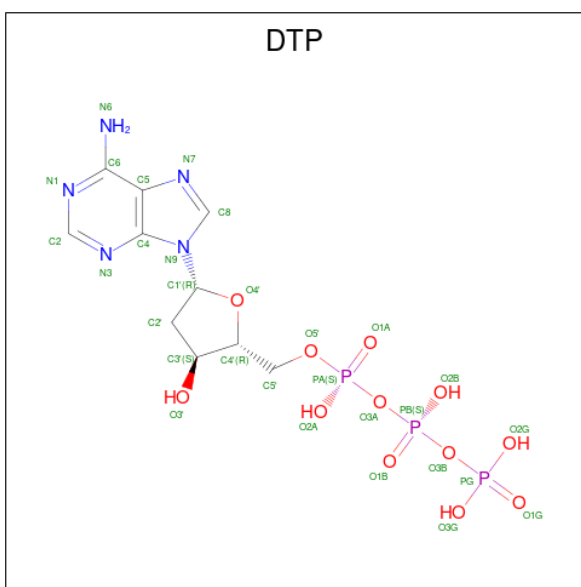
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

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

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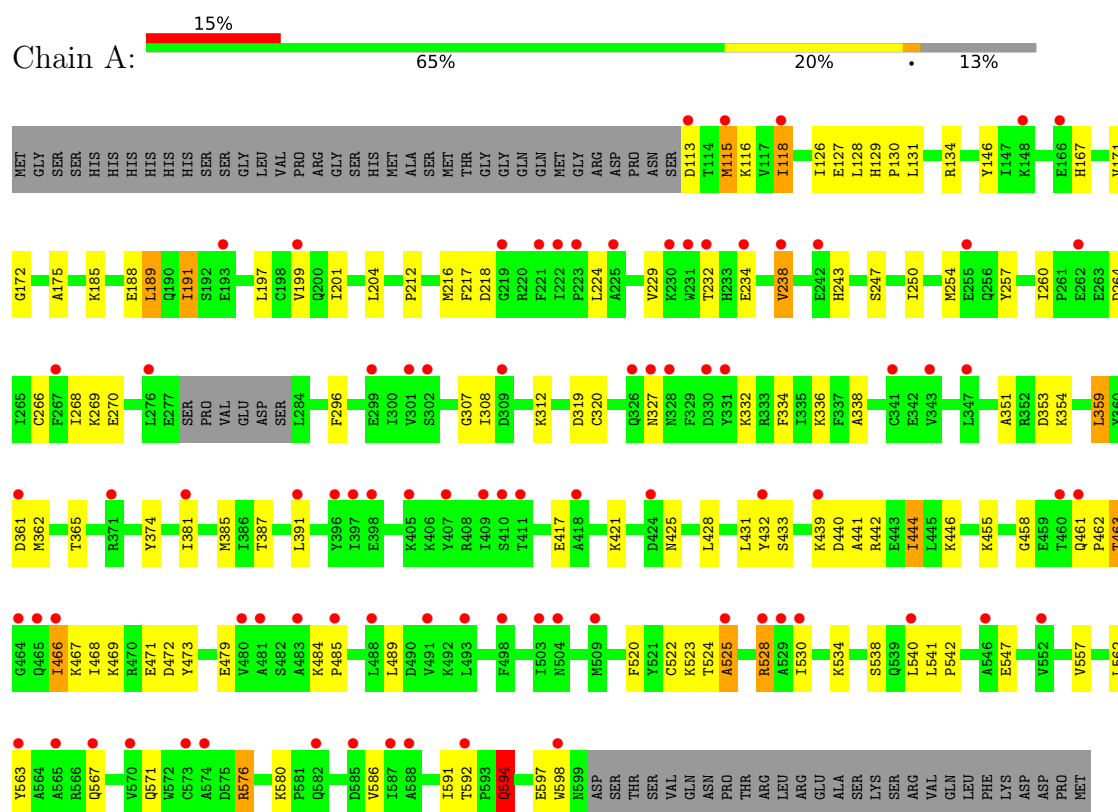
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	16	Total	O	0	0
			16	16		
5	D	26	Total	O	0	0
			26	26		

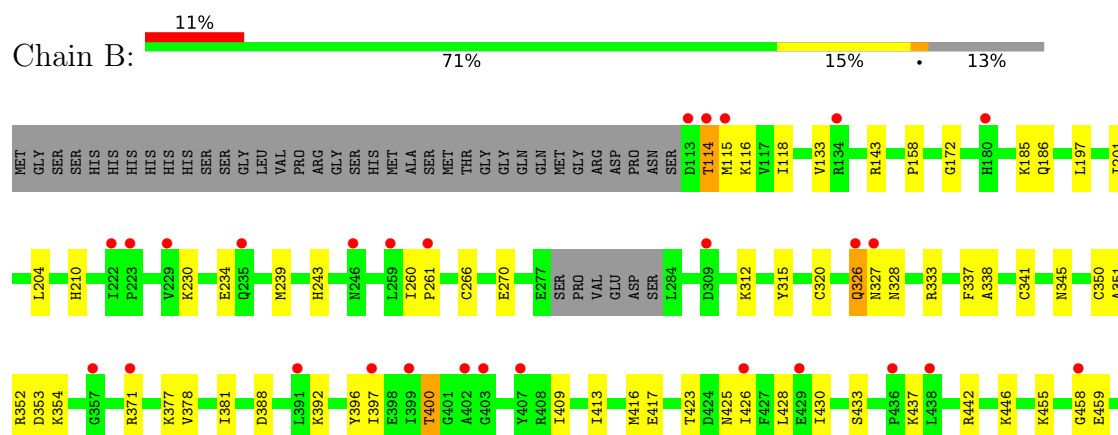
3 Residue-property plots

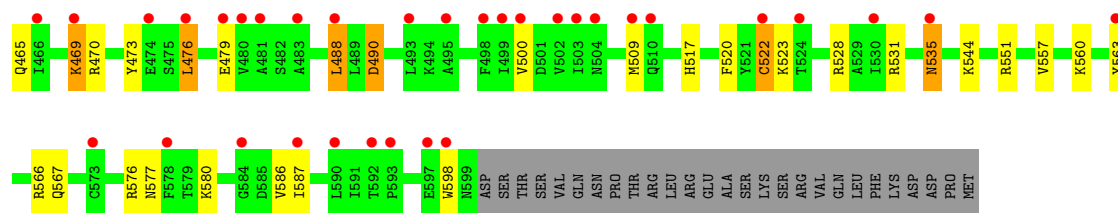
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

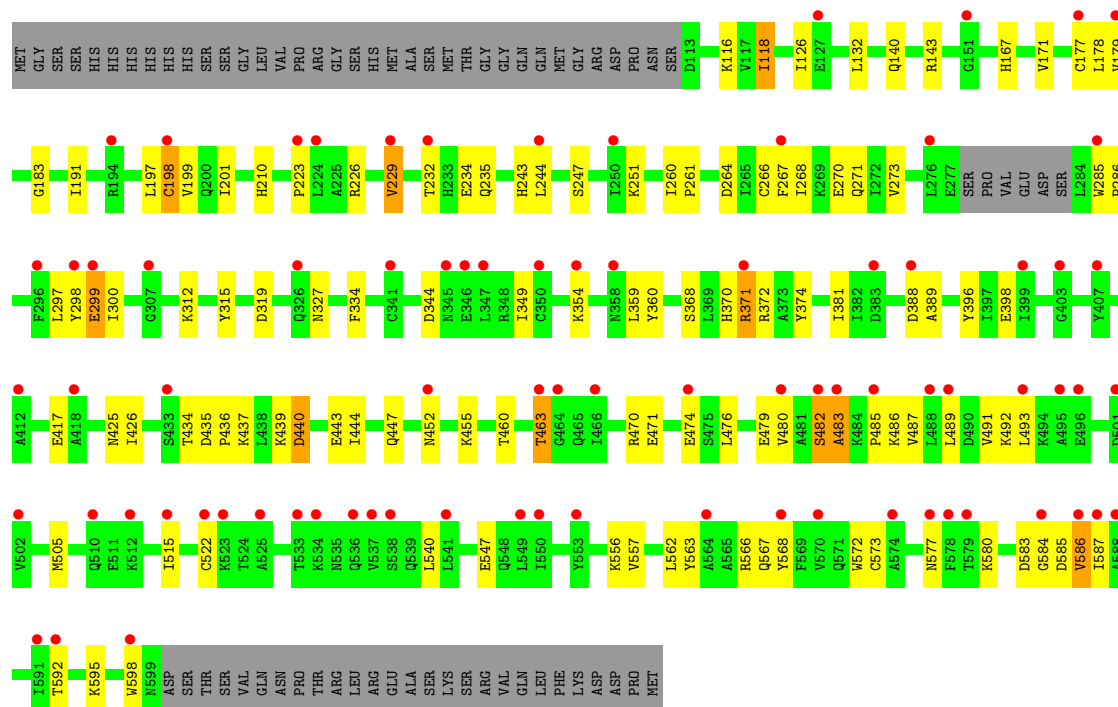


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

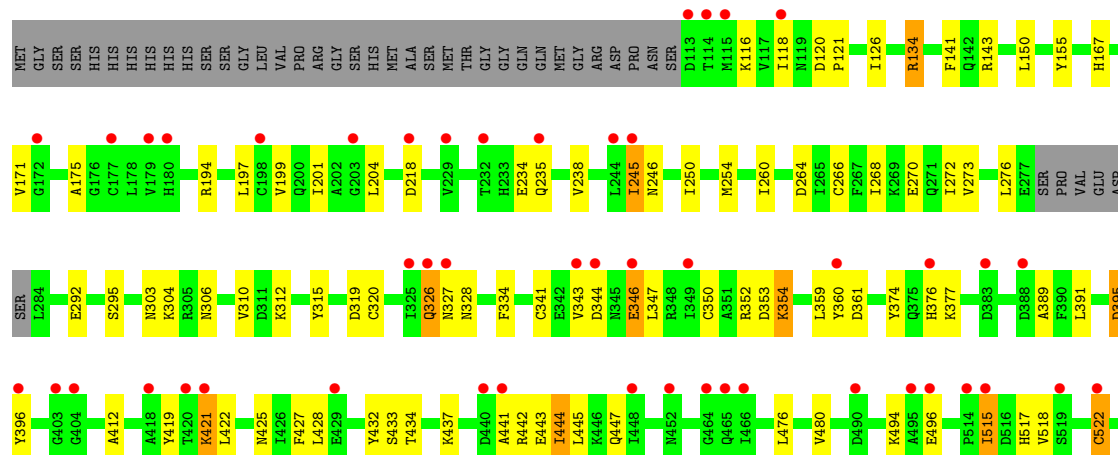


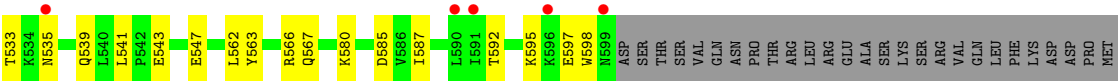


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• 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 , 0.274	Depositor DCC
R_{free} test set	2008 reflections (1.18%)	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 , 55.8	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

5.1 Standard geometry

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

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	0.42	0/4031	0.92	5/5441 (0.1%)
1	B	0.34	0/4025	0.84	3/5433 (0.1%)
1	C	0.38	0/4031	0.87	4/5441 (0.1%)
1	D	0.37	0/4047	0.83	0/5463
All	All	0.38	0/16134	0.87	12/21778 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	ALA	CA-C-N	9.41	130.56	120.12
1	A	525	ALA	C-N-CA	9.41	130.56	120.12
1	A	458	GLY	N-CA-C	7.88	122.17	110.42
1	A	260	ILE	CA-C-N	6.70	128.22	119.84
1	A	260	ILE	C-N-CA	6.70	128.22	119.84
1	B	260	ILE	CA-C-N	6.69	128.21	119.84
1	B	260	ILE	C-N-CA	6.69	128.21	119.84
1	C	260	ILE	CA-C-N	6.43	127.88	119.84
1	C	260	ILE	C-N-CA	6.43	127.88	119.84
1	B	458	GLY	N-CA-C	6.00	119.36	110.42
1	C	298	TYR	N-CA-C	5.87	120.57	113.17
1	C	586	VAL	CB-CA-C	-5.10	102.92	111.29

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	3939	0	3923	92	0
1	B	3933	0	3921	55	0
1	C	3939	0	3923	87	0
1	D	3955	0	3933	73	0
2	A	32	0	11	1	0
2	B	64	0	22	4	0
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	0	0
5	D	26	0	0	4	0
All	All	16094	0	15792	281	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 9.

All (281) 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:OE1	1:C:299:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:MET:HE1	1:A:128:LEU:N	2.04	0.73
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
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:A:115:MET:HE1	1:A:128:LEU:H	1.59	0.66
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:A:115:MET:HE3	1:A:116:LYS:N	2.13	0.63
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:308:ILE:HG12	1:A:362:MET:HE1	1.85	0.58
1:C:440:ASP:OD1	1:C:440:ASP:N	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
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:N	1:A:597:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:346:GLU:CD	1:D:347:LEU:H	2.16	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:N	1:D:395:ASP:OD1	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:OD1	1:B:535:ASN:N	2.29	0.50
1:A:353:ASP:OD1	1:A:354:LYS:N	2.44	0.50
1:C:460:THR:HG21	1:C:573:CYS:SG	2.51	0.50
1:A:115:MET:HE2	1:A:127:GLU:HG2	1.94	0.50
1:A:528:ARG:HH12	1:C:586:VAL:HA	1.77	0.50
1:C:264:ASP:O	1:C:268:ILE:HG13	2.12	0.50
1:B:388:ASP:OD2	1:B:392:LYS:NZ	2.40	0.49
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:B:185:LYS:NZ	1:B:338:ALA:O	2.24	0.48
1:A:471:GLU:C	1:A:473:TYR:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LYS:HE2	5:A:811:HOH:O	2.14	0.47
1:C:381:ILE:HD12	1:C:381:ILE:HA	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
3:B:703:DTP:O2A	1:D:376:HIS:HE1	1.97	0.47
1:C:232:THR:HG23	1:C:235:GLN:H	1.78	0.47
1:A:238:VAL:HG13	1:A:269:LYS:HD3	1.96	0.47
1:C:319:ASP:OD2	1:C:374:TYR:OH	2.30	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:C:226:ARG:HH21	1:C:229:VAL:HG21	1.79	0.46
2:A:701:GTP:O3G	1:D:116:LYS:NZ	2.42	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:A:421:LYS:HD2	1:D:432:TYR:CD1	2.50	0.46
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: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:177:CYS:SG	1:C:178:LEU:N	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:326:GLN:NE2	1:D:327:ASN:H	2.15	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:A:191:ILE:HD11	1:A:296:PHE:CE1	2.52	0.44
1:B:352:ARG:NH2	1:B:354:LYS:HZ2	2.15	0.44
1:B:509:MET:HE1	1:B:517:HIS:CD2	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:A:307:GLY:O	1:A:312:LYS:NZ	2.43	0.44
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.87	0.44
1:A:115:MET:HE3	1:A:115:MET:C	2.42	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:319:ASP:OD2	1:D:374:TYR:OH	2.31	0.44
1:D:391:LEU:HD23	1:D:391:LEU:HA	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:C:370:HIS:CB	1:C:505:MET:HE1	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
1:B:396:TYR:CD1	1:B:437:LYS:HD3	2.53	0.43
1:B:433:SER:OG	1:B:442:ARG:NH1	2.49	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:C:489:LEU:HB3	1:C:492:LYS:HZ1	1.82	0.43
1:C:370:HIS:HB3	1:C:505:MET:HE1	2.00	0.43
1:B:455:LYS:HG2	1:B:557:VAL:HG12	1.99	0.43
1:D:515:ILE:C	1:D:517:HIS:H	2.26	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:HD2	1:D:421:LYS:O	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:B:239:MET:HE2	1:B:416:MET:HE3	2.00	0.43
1:D:562:LEU:HD12	1:D:562:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:TYR:OH	1:D:155:TYR:OH	2.26	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:B:586:VAL:HG21	1:D:522[B]:CYS:SG	2.60	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:A:359:LEU:HD12	1:A:359:LEU:HA	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:C:584:GLY:C	1:C:586:VAL:H	2.28	0.42
1:A:381:ILE:HD12	1:A:381:ILE:HA	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:A:542:PRO:HB3	1:C:540:LEU:O	2.20	0.41
1:C:349:ILE:HG21	1:C:349:ILE:HD13	1.80	0.41
1:D:563:TYR:O	1:D:567:GLN:HG2	2.20	0.41
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:HE3	1:A:469:LYS:HB3	1.79	0.41
1:C:515:ILE:HD12	1:C:515:ILE:C	2.46	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:471:GLU:C	1:A:473:TYR:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:538:SER:HB3	1:A:541:LEU:CD1	2.50	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:D:494:LYS:HB2	1:D:496:GLU:OE1	2.21	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:A:319:ASP:OD2	1:A:374:TYR:OH	2.34	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:A:425:ASN:HB2	1:D:428:LEU:HD12	2.03	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/550 (87%)	464 (97%)	12 (2%)	2 (0%)	30	31
1	B	477/550 (87%)	466 (98%)	9 (2%)	2 (0%)	30	31
1	C	478/550 (87%)	464 (97%)	10 (2%)	4 (1%)	16	14
1	D	480/550 (87%)	471 (98%)	9 (2%)	0	100	100
All	All	1913/2200 (87%)	1865 (98%)	40 (2%)	8 (0%)	30	31

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%)	409 (96%)	19 (4%)	25	29
1	B	427/488 (88%)	411 (96%)	16 (4%)	30	37
1	C	428/488 (88%)	410 (96%)	18 (4%)	26	31
1	D	430/488 (88%)	411 (96%)	19 (4%)	25	29
All	All	1713/1952 (88%)	1641 (96%)	72 (4%)	26	31

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	118	ILE
1	A	189	LEU

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Mol	Chain	Res	Type
1	A	191	ILE
1	A	229	VAL
1	A	238	VAL
1	A	359	LEU
1	A	439	LYS
1	A	444	ILE
1	A	446	LYS
1	A	463	THR
1	A	466	ILE
1	A	467	LYS
1	A	484	LYS
1	A	528	ARG
1	A	530	ILE
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	413	ILE
1	B	465	GLN
1	B	469	LYS
1	B	476	LEU
1	B	488	LEU
1	B	522	CYS
1	B	528	ARG
1	B	535	ASN
1	B	577	ASN
1	C	118	ILE
1	C	132	LEU
1	C	198	CYS
1	C	229	VAL
1	C	299	GLU
1	C	327	ASN
1	C	344	ASP
1	C	354	LYS
1	C	371	ARG
1	C	398	GLU

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Mol	Chain	Res	Type
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	238	VAL
1	D	245	ILE
1	D	276	LEU
1	D	326	GLN
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	515	ILE
1	D	522[A]	CYS
1	D	522[B]	CYS
1	D	543	GLU
1	D	547	GLU
1	D	597	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	163	ASN
1	A	180	HIS
1	A	200	GLN
1	B	149	GLN
1	B	210	HIS
1	B	517	HIS
1	B	571	GLN
1	C	180	HIS
1	C	210	HIS
1	C	243	HIS

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Mol	Chain	Res	Type
1	D	180	HIS
1	D	210	HIS
1	D	376	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	702	4	31,32,32	1.65	6 (19%)	46,50,50	1.75	9 (19%)
2	GTP	D	702	4	33,34,34	2.51	11 (33%)	50,54,54	1.57	9 (18%)
3	DTP	D	701	4	31,32,32	1.64	6 (19%)	46,50,50	1.79	9 (19%)
2	GTP	B	702	4	33,34,34	2.48	10 (30%)	50,54,54	1.63	7 (14%)
3	DTP	C	701	4	31,32,32	1.57	6 (19%)	46,50,50	1.79	9 (19%)
3	DTP	B	703	4	31,32,32	1.52	7 (22%)	46,50,50	1.82	9 (19%)
2	GTP	B	701	4	33,34,34	2.50	10 (30%)	50,54,54	1.63	7 (14%)
2	GTP	A	701	4	33,34,34	2.50	11 (33%)	50,54,54	1.57	7 (14%)

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	A	702	4	-	7/22/34/34	0/3/3/3
2	GTP	D	702	4	-	3/22/38/38	0/3/3/3
3	DTP	D	701	4	-	3/22/34/34	0/3/3/3
2	GTP	B	702	4	-	5/22/38/38	0/3/3/3
3	DTP	C	701	4	-	2/22/34/34	0/3/3/3
3	DTP	B	703	4	-	5/22/34/34	0/3/3/3
2	GTP	B	701	4	-	5/22/38/38	0/3/3/3
2	GTP	A	701	4	-	3/22/38/38	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	702	GTP	O6-C6	9.54	1.41	1.23
2	B	701	GTP	O6-C6	9.46	1.41	1.23
2	A	701	GTP	O6-C6	9.42	1.41	1.23
2	B	702	GTP	O6-C6	9.41	1.41	1.23
2	B	701	GTP	C2-N2	6.06	1.48	1.34
2	D	702	GTP	C2-N2	6.02	1.48	1.34
2	A	701	GTP	C2-N2	6.01	1.48	1.34
2	B	702	GTP	C2-N2	5.99	1.48	1.34
3	A	702	DTP	PB-O3B	4.48	1.64	1.59
3	D	701	DTP	PB-O3B	4.37	1.64	1.59
3	C	701	DTP	PB-O3B	4.11	1.63	1.59
2	B	701	GTP	PB-O3A	-4.09	1.55	1.59
2	A	701	GTP	PB-O3A	-3.90	1.55	1.59
3	B	703	DTP	C6-N6	3.81	1.43	1.34
3	A	702	DTP	C6-N6	3.81	1.43	1.34
3	D	701	DTP	C6-N6	3.79	1.43	1.34
2	B	702	GTP	PB-O3A	-3.77	1.55	1.59
3	B	703	DTP	PB-O3B	3.74	1.63	1.59
3	C	701	DTP	C6-N6	3.73	1.43	1.34
2	D	702	GTP	PB-O3A	-3.69	1.55	1.59
2	D	702	GTP	O2'-C2'	-3.02	1.35	1.43
2	B	702	GTP	O2'-C2'	-2.98	1.35	1.43
2	B	701	GTP	O2'-C2'	-2.97	1.35	1.43
2	A	701	GTP	O2'-C2'	-2.96	1.35	1.43
3	D	701	DTP	O3'-C3'	-2.73	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	DTP	O3'-C3'	-2.72	1.37	1.43
3	B	703	DTP	O3'-C3'	-2.70	1.37	1.43
3	A	702	DTP	O3'-C3'	-2.69	1.37	1.43
3	B	703	DTP	C5'-C4'	-2.65	1.43	1.51
3	A	702	DTP	C5'-C4'	-2.57	1.43	1.51
3	C	701	DTP	PB-O3A	2.55	1.62	1.59
2	B	701	GTP	C5'-C4'	-2.54	1.43	1.51
2	B	701	GTP	C6-N1	-2.50	1.34	1.38
3	C	701	DTP	C5'-C4'	-2.48	1.44	1.51
2	B	702	GTP	C6-N1	-2.46	1.34	1.38
3	D	701	DTP	C5'-C4'	-2.45	1.44	1.51
2	B	702	GTP	C5'-C4'	-2.41	1.44	1.51
2	D	702	GTP	C6-N1	-2.41	1.34	1.38
3	A	702	DTP	PB-O3A	2.40	1.62	1.59
2	A	701	GTP	C5'-C4'	-2.39	1.44	1.51
3	D	701	DTP	PB-O3A	2.36	1.62	1.59
2	A	701	GTP	C6-N1	-2.35	1.34	1.38
2	D	702	GTP	PG-O3G	-2.35	1.46	1.54
2	A	701	GTP	PG-O3G	-2.35	1.46	1.54
2	D	702	GTP	C5'-C4'	-2.33	1.44	1.51
2	B	702	GTP	C5-N7	-2.26	1.34	1.39
2	A	701	GTP	C2'-C3'	-2.25	1.47	1.53
2	B	701	GTP	C5-N7	-2.25	1.34	1.39
2	B	701	GTP	C2'-C3'	-2.24	1.47	1.53
3	C	701	DTP	C2'-C3'	-2.24	1.47	1.52
2	D	702	GTP	C3'-C4'	-2.23	1.47	1.53
2	D	702	GTP	C5-N7	-2.21	1.34	1.39
2	B	702	GTP	C2'-C3'	-2.21	1.47	1.53
2	B	702	GTP	C3'-C4'	-2.20	1.47	1.53
2	A	701	GTP	C5-N7	-2.18	1.34	1.39
2	B	701	GTP	C3'-C4'	-2.15	1.47	1.53
3	D	701	DTP	C2'-C3'	-2.14	1.47	1.52
3	A	702	DTP	C2'-C3'	-2.12	1.47	1.52
2	D	702	GTP	C2'-C3'	-2.12	1.47	1.53
2	A	701	GTP	C3'-C4'	-2.11	1.47	1.53
2	B	701	GTP	PG-O2G	-2.07	1.47	1.54
3	B	703	DTP	C2'-C3'	-2.06	1.47	1.52
2	D	702	GTP	PG-O2G	-2.04	1.47	1.54
2	B	702	GTP	PG-O2G	-2.04	1.47	1.54
2	A	701	GTP	PG-O2G	-2.03	1.47	1.54
3	B	703	DTP	PG-O3G	-2.02	1.47	1.54
3	B	703	DTP	PB-O3A	2.00	1.61	1.59

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GTP	C5-C4-N3	-5.77	119.21	128.39
2	A	701	GTP	C5-C4-N3	-5.68	119.34	128.39
2	D	702	GTP	C5-C4-N3	-5.63	119.42	128.39
2	B	702	GTP	C5-C4-N3	-5.61	119.46	128.39
3	A	702	DTP	C5-C4-N3	-5.09	119.71	126.72
3	B	703	DTP	C5-C4-N3	-5.02	119.81	126.72
3	D	701	DTP	C5-C4-N3	-4.98	119.86	126.72
3	C	701	DTP	C5-C4-N3	-4.93	119.93	126.72
3	B	703	DTP	N3-C2-N1	-4.92	121.14	128.58
3	C	701	DTP	N3-C2-N1	-4.84	121.25	128.58
3	D	701	DTP	N3-C2-N1	-4.79	121.33	128.58
3	A	702	DTP	N3-C2-N1	-4.76	121.38	128.58
2	A	701	GTP	C2-N3-C4	4.22	119.57	112.30
2	B	701	GTP	C2-N3-C4	4.15	119.45	112.30
2	D	702	GTP	C2-N3-C4	4.13	119.42	112.30
2	B	702	GTP	C2-N3-C4	4.06	119.30	112.30
2	B	701	GTP	N9-C4-N3	3.99	133.93	125.95
2	B	702	GTP	N9-C4-N3	3.90	133.76	125.95
2	A	701	GTP	N9-C4-N3	3.90	133.74	125.95
2	D	702	GTP	N9-C4-N3	3.74	133.43	125.95
3	B	703	DTP	C4-C5-N7	-3.72	106.32	110.58
3	A	702	DTP	C4-C5-N7	-3.71	106.34	110.58
3	B	703	DTP	C2-N3-C4	3.63	120.70	111.83
3	C	701	DTP	C4-C5-N7	-3.61	106.45	110.58
3	D	701	DTP	C4-C5-N7	-3.59	106.48	110.58
3	B	703	DTP	N9-C8-N7	-3.56	108.88	113.94
3	A	702	DTP	C2-N3-C4	3.55	120.50	111.83
3	D	701	DTP	C2-N3-C4	3.54	120.47	111.83
3	C	701	DTP	C2-N3-C4	3.51	120.40	111.83
3	D	701	DTP	N9-C8-N7	-3.48	109.00	113.94
3	C	701	DTP	N9-C8-N7	-3.36	109.17	113.94
3	B	703	DTP	C5-N7-C8	3.34	108.71	103.45
3	A	702	DTP	N9-C8-N7	-3.26	109.31	113.94
3	D	701	DTP	C5-N7-C8	3.22	108.50	103.45
3	A	702	DTP	C5-N7-C8	3.17	108.44	103.45
3	C	701	DTP	C5-N7-C8	3.17	108.44	103.45
3	D	701	DTP	N3-C4-N9	2.93	132.15	127.17
3	B	703	DTP	N3-C4-N9	2.93	132.14	127.17
3	C	701	DTP	N3-C4-N9	2.91	132.11	127.17
3	A	702	DTP	N3-C4-N9	2.87	132.05	127.17
2	D	702	GTP	O5'-C5'-C4'	2.87	118.76	108.99
3	D	701	DTP	O5'-C5'-C4'	2.80	118.54	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	DTP	O5'-C5'-C4'	2.79	118.51	108.99
2	B	702	GTP	O5'-C5'-C4'	2.70	118.19	108.99
2	A	701	GTP	O5'-C5'-C4'	2.55	117.69	108.99
2	B	701	GTP	O3G-PG-O3B	2.55	113.19	104.64
2	B	702	GTP	O3G-PG-O3B	2.48	112.94	104.64
2	B	701	GTP	C2-N1-C6	-2.43	120.70	125.11
2	A	701	GTP	C2-N1-C6	-2.43	120.71	125.11
2	B	702	GTP	C2-N1-C6	-2.33	120.89	125.11
3	A	702	DTP	O5'-C5'-C4'	2.33	116.92	108.99
2	D	702	GTP	C2-N1-C6	-2.23	121.06	125.11
3	A	702	DTP	C5-C4-N9	2.23	108.24	105.81
2	B	701	GTP	C5'-C4'-C3'	-2.21	107.25	115.21
3	B	703	DTP	C4-N9-C8	2.19	108.03	105.74
3	D	701	DTP	C4-N9-C8	2.18	108.02	105.74
3	C	701	DTP	C4-N9-C8	2.14	107.98	105.74
2	D	702	GTP	C4-C5-N7	-2.13	107.30	110.67
2	A	701	GTP	C3'-C2'-C1'	2.09	105.41	101.46
2	B	701	GTP	C3'-C2'-C1'	2.09	105.41	101.46
2	A	701	GTP	N9-C8-N7	-2.08	109.55	113.40
2	D	702	GTP	N9-C8-N7	-2.07	109.57	113.40
2	D	702	GTP	C8-N7-C5	2.06	107.94	104.26
2	D	702	GTP	C3'-C2'-C1'	2.06	105.36	101.46
3	B	703	DTP	C5-C4-N9	2.05	108.05	105.81
2	B	702	GTP	N9-C8-N7	-2.05	109.61	113.40

There are no chirality outliers.

All (33) torsion outliers are listed below:

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

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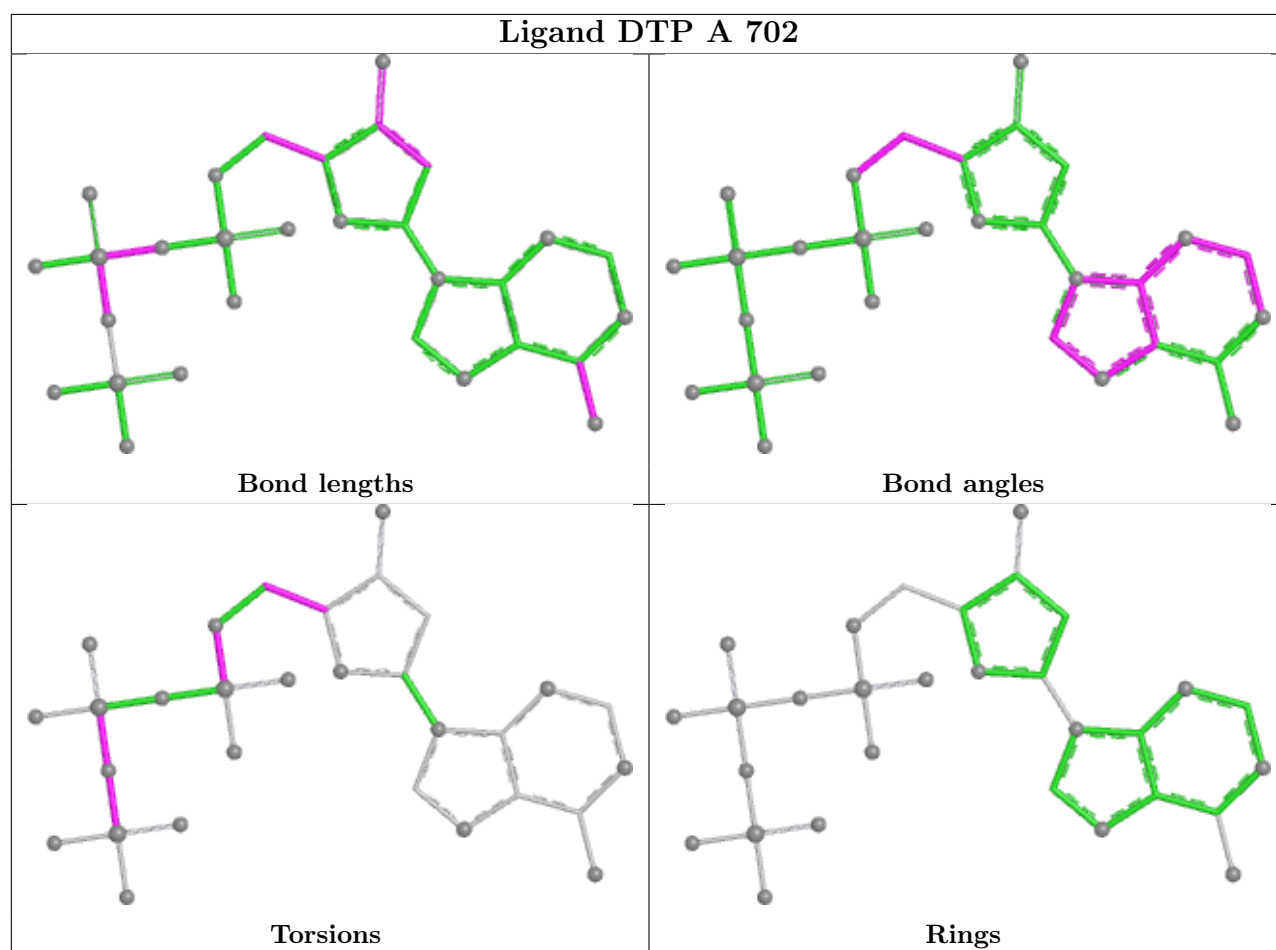
Mol	Chain	Res	Type	Atoms
3	C	701	DTP	PB-O3A-PA-O2A
2	B	702	GTP	C5'-O5'-PA-O1A
3	A	702	DTP	C5'-O5'-PA-O1A
3	A	702	DTP	C5'-O5'-PA-O3A
2	A	701	GTP	PB-O3A-PA-O1A
3	D	701	DTP	PG-O3B-PB-O2B
2	D	702	GTP	C4'-C5'-O5'-PA
3	B	703	DTP	PA-O3A-PB-O1B
3	C	701	DTP	PG-O3B-PB-O1B
2	B	701	GTP	PB-O3B-PG-O2G
2	B	701	GTP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

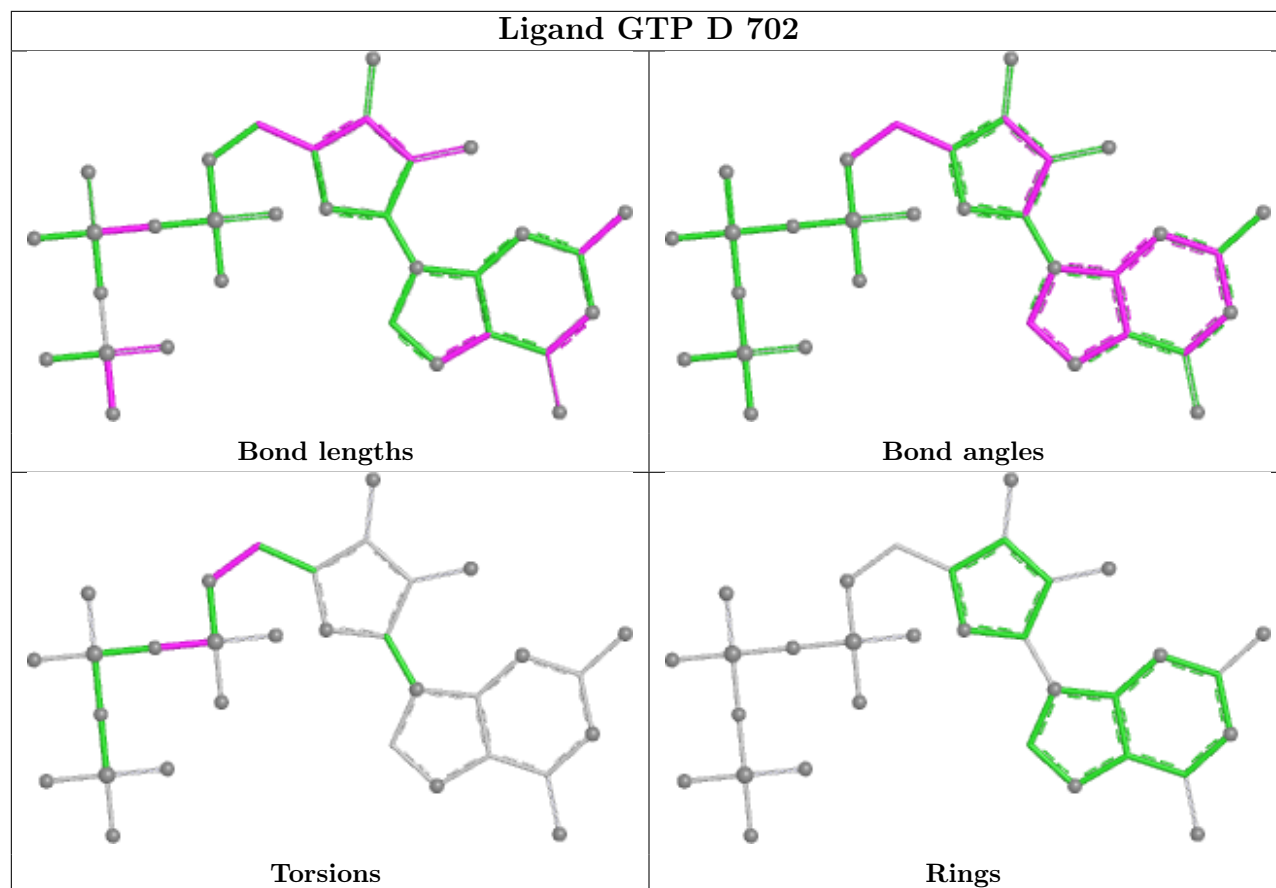
There are no ring outliers.

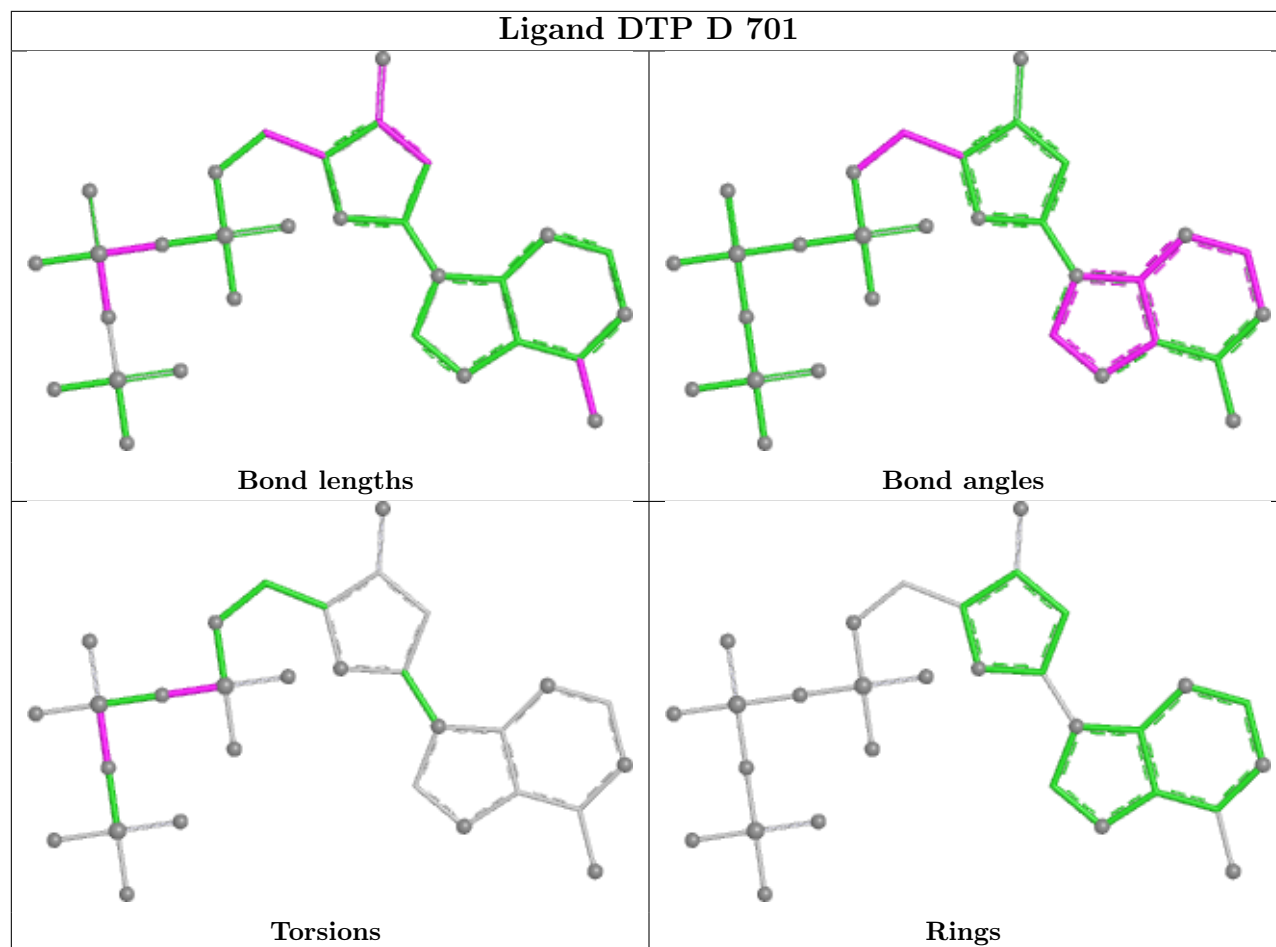
4 monomers are involved in 8 short contacts:

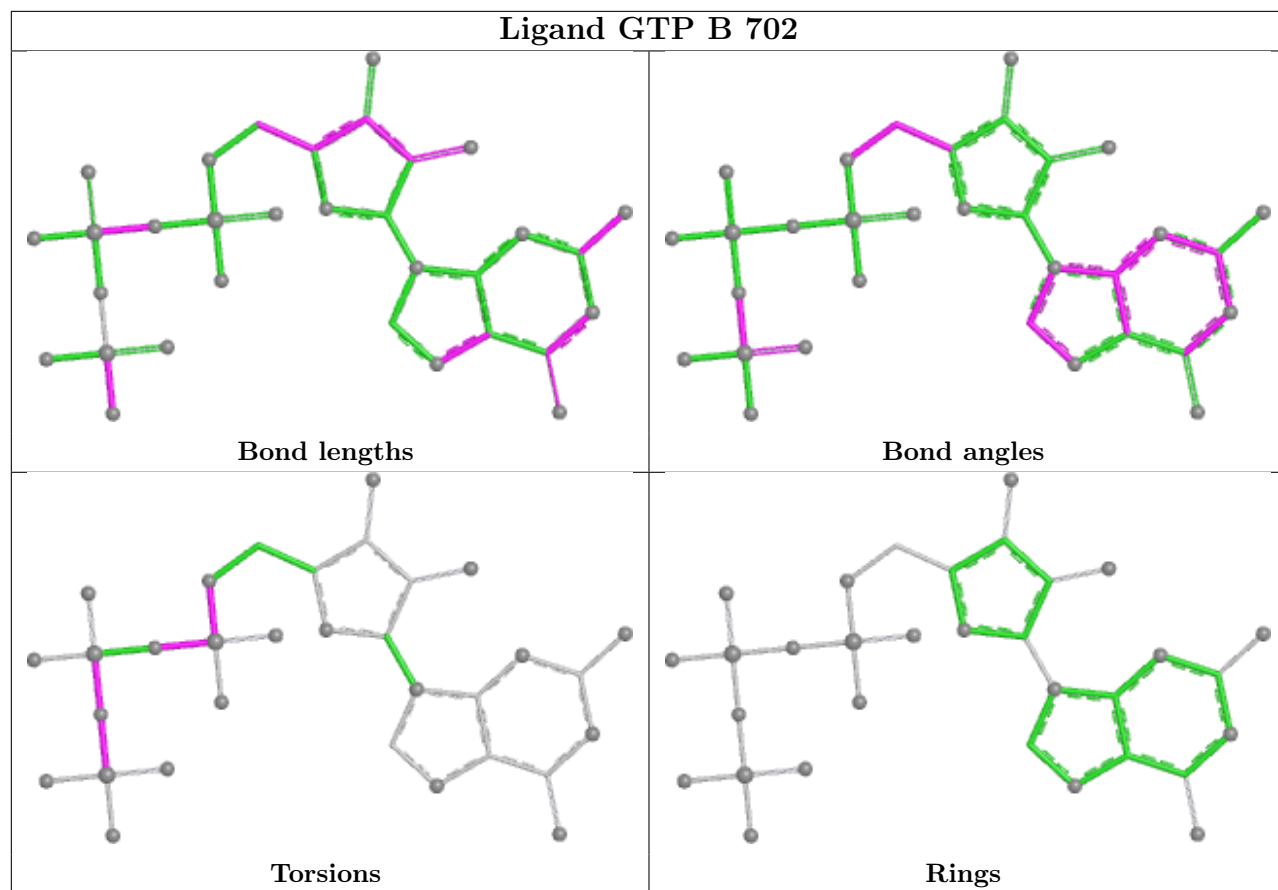
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	GTP	1	0
3	B	703	DTP	3	0
2	B	701	GTP	3	0
2	A	701	GTP	1	0

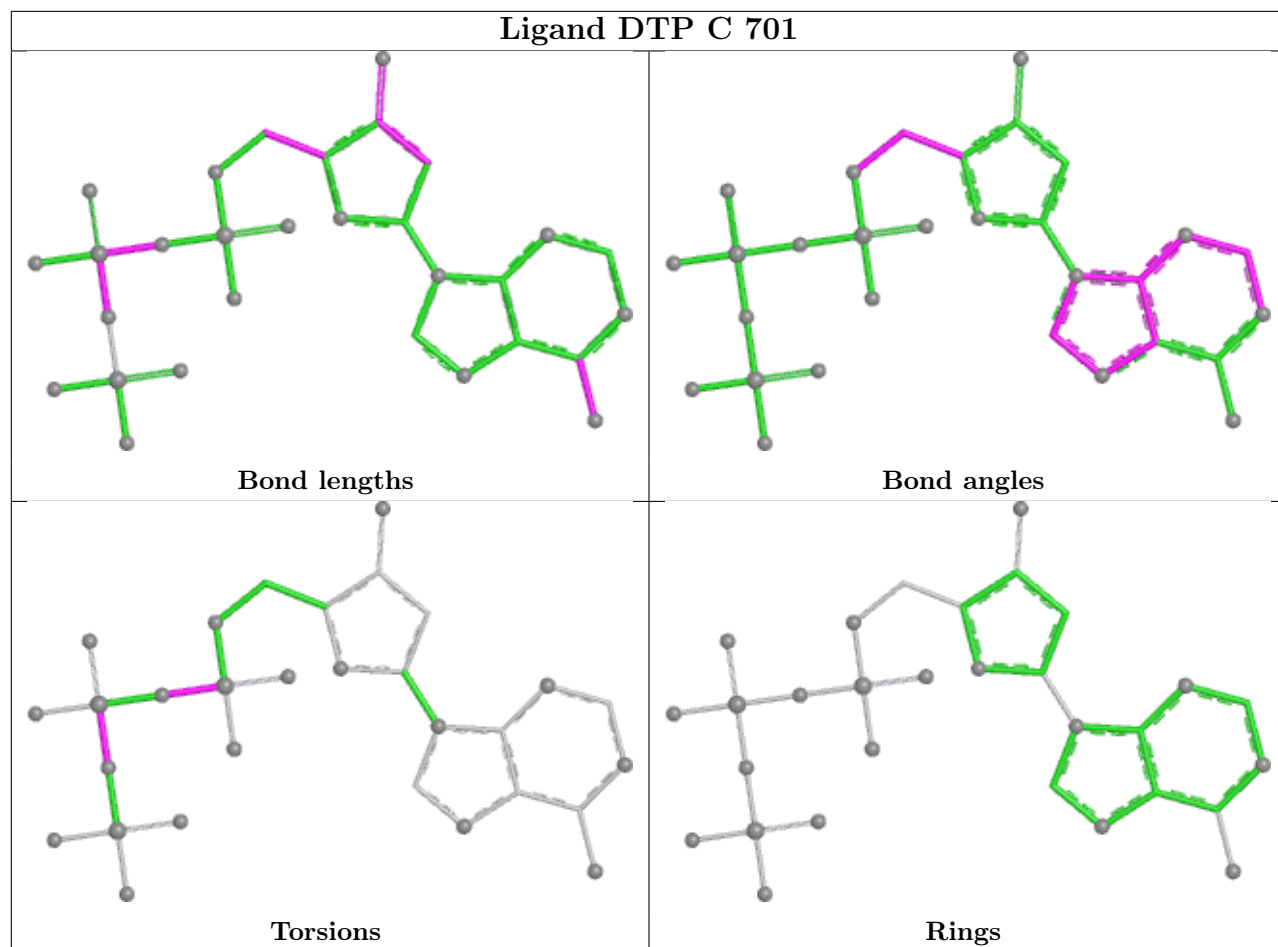
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



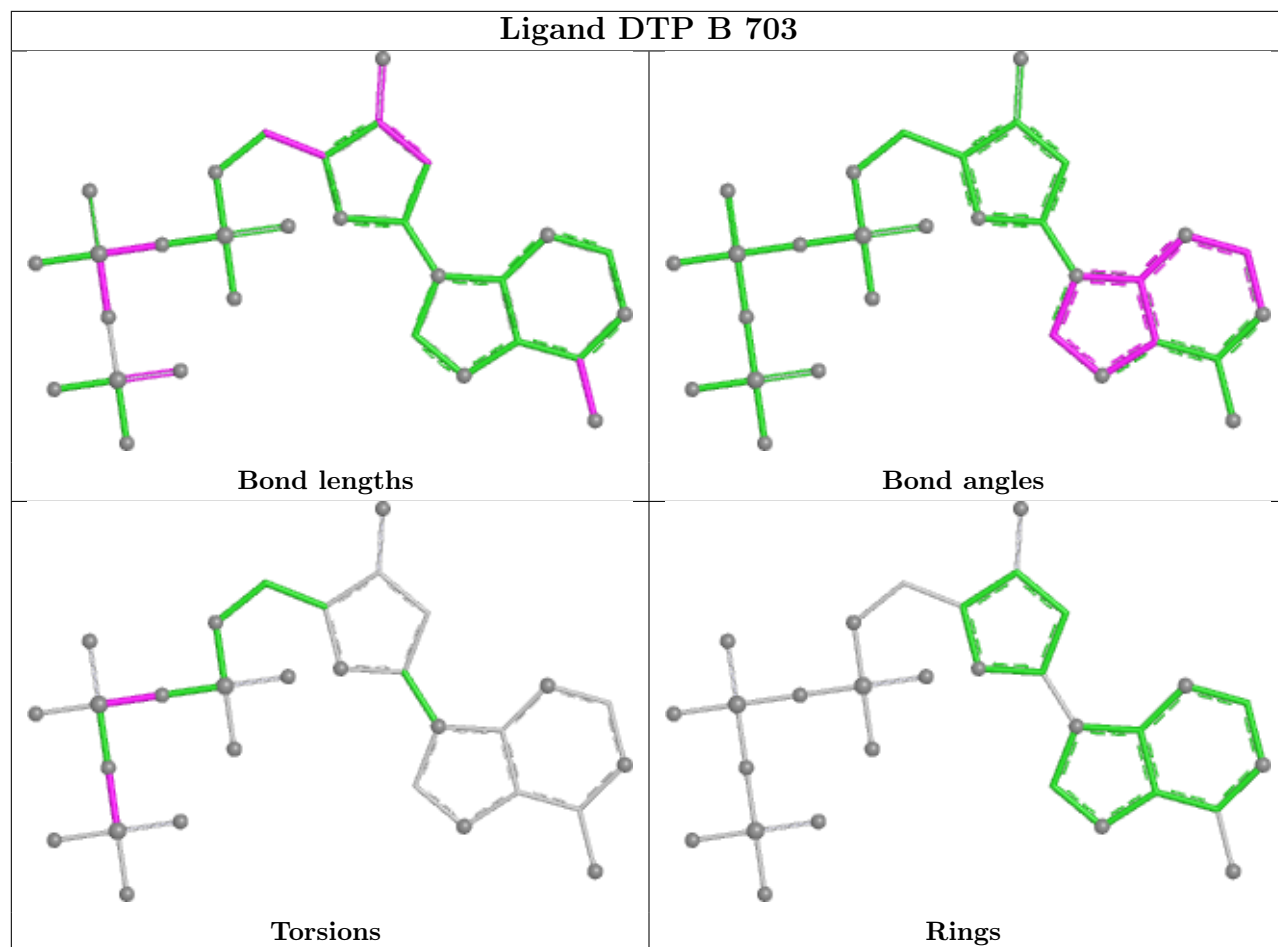




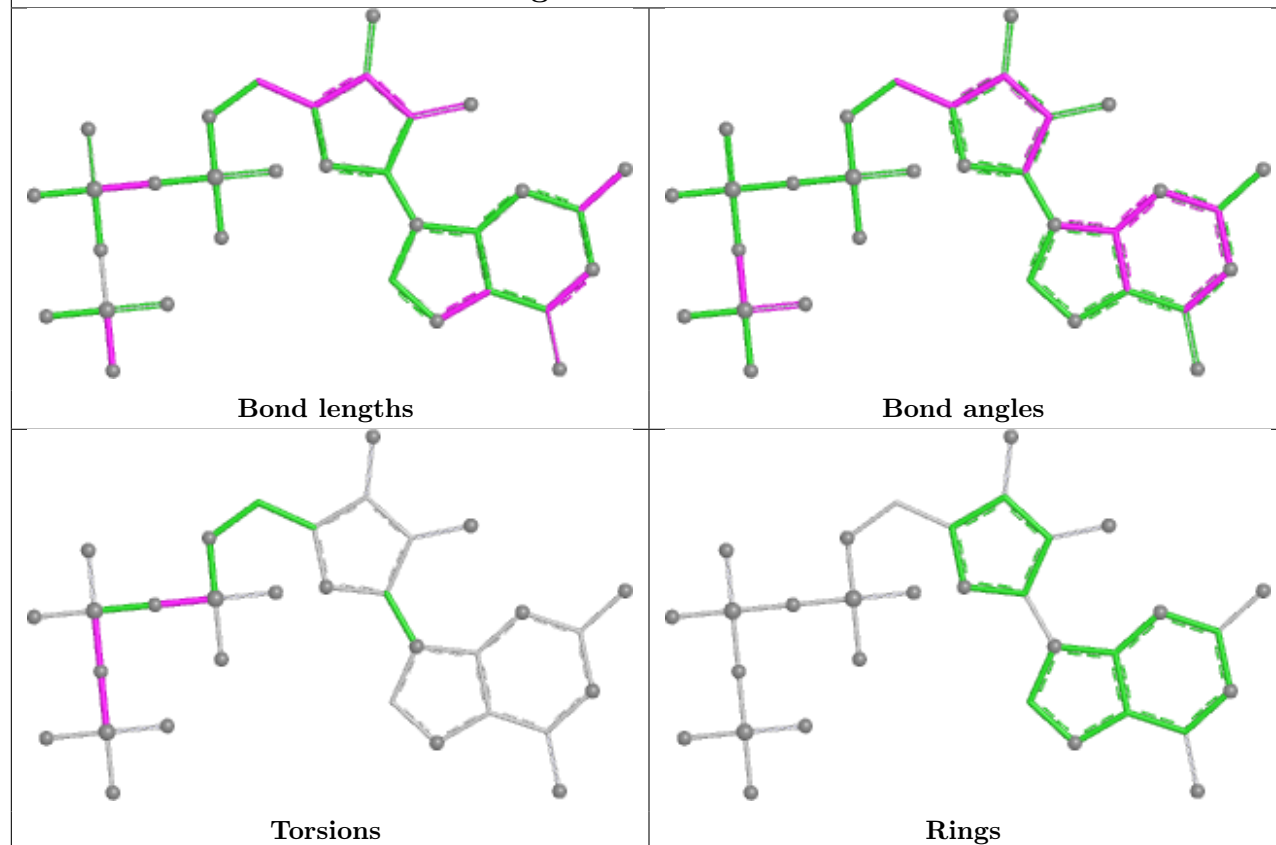




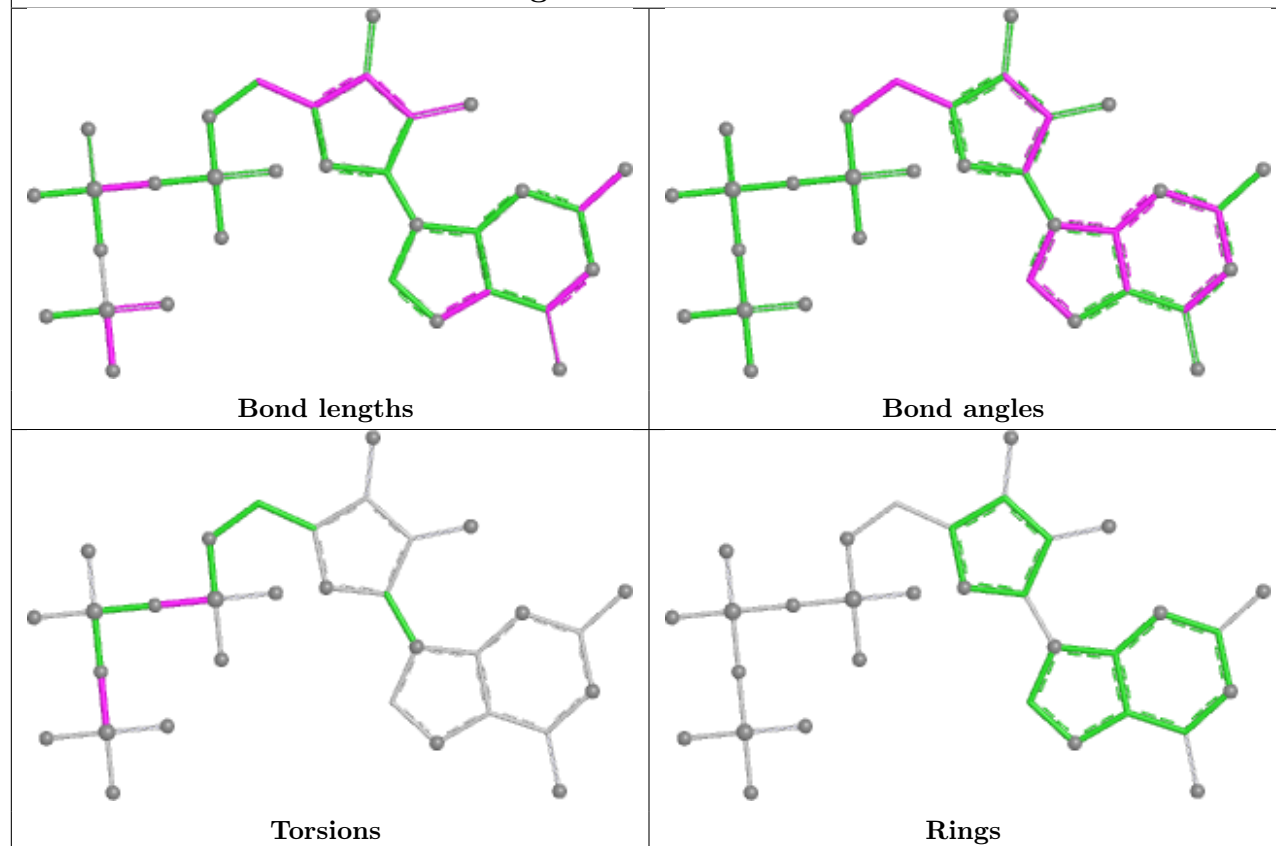
Ligand DTP B 703



Ligand GTP B 701



Ligand GTP A 701



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%)	1.32	85 (17%)	4 3	29, 65, 112, 127	184 (38%)
1	B	481/550 (87%)	1.15	61 (12%)	8 7	35, 62, 104, 123	171 (35%)
1	C	481/550 (87%)	1.30	81 (16%)	4 3	37, 62, 89, 123	207 (43%)
1	D	481/550 (87%)	1.05	53 (11%)	10 10	29, 56, 75, 91	205 (42%)
All	All	1924/2200 (87%)	1.21	280 (14%)	6 5	29, 61, 93, 127	767 (39%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	479	GLU	6.9
1	C	198	CYS	6.2
1	A	528	ARG	6.2
1	A	327	ASN	6.1
1	A	115	MET	5.6
1	D	326	GLN	5.1
1	D	496	GLU	4.8
1	D	403	GLY	4.6
1	D	360	TYR	4.4
1	B	114	THR	4.3
1	C	564	ALA	4.2
1	A	166	GLU	4.1
1	C	591	ILE	4.1
1	B	327	ASN	4.0
1	C	489	LEU	4.0
1	A	466	ILE	3.9
1	C	354	LYS	3.9
1	C	177	CYS	3.8
1	D	441	ALA	3.8
1	D	245	ILE	3.7
1	B	522	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	302	SER	3.6
1	C	388	ASP	3.6
1	B	480	VAL	3.6
1	C	483	ALA	3.4
1	D	172	GLY	3.4
1	A	432	TYR	3.4
1	A	326	GLN	3.4
1	C	224	LEU	3.3
1	C	232	THR	3.3
1	B	481	ALA	3.3
1	B	502	VAL	3.3
1	B	309	ASP	3.3
1	D	113	ASP	3.3
1	A	328	ASN	3.2
1	D	198	CYS	3.2
1	B	509	MET	3.2
1	C	574	ALA	3.2
1	C	307	GLY	3.2
1	C	346	GLU	3.2
1	C	533	THR	3.2
1	C	267	PHE	3.2
1	B	500	VAL	3.2
1	B	593	PRO	3.1
1	C	568	TYR	3.1
1	B	115	MET	3.1
1	A	225	ALA	3.1
1	B	488	LEU	3.1
1	A	465	GLN	3.1
1	D	404	GLY	3.1
1	D	421	LYS	3.1
1	B	407	TYR	3.0
1	A	409	ILE	3.0
1	A	530	ILE	3.0
1	B	397	ILE	3.0
1	C	525	ALA	3.0
1	A	242	GLU	3.0
1	A	598	TRP	3.0
1	A	574	ALA	3.0
1	B	590	LEU	3.0
1	B	466	ILE	3.0
1	A	234	GLU	3.0
1	C	488	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	480	VAL	2.9
1	C	586	VAL	2.9
1	D	343	VAL	2.9
1	C	464	GLY	2.9
1	C	577	ASN	2.9
1	A	481	ALA	2.9
1	B	598	TRP	2.9
1	C	480	VAL	2.9
1	A	341	CYS	2.9
1	B	246	ASN	2.9
1	D	344	ASP	2.9
1	C	298	TYR	2.8
1	C	598	TRP	2.8
1	D	599	ASN	2.8
1	A	563	TYR	2.8
1	C	537	VAL	2.8
1	A	223	PRO	2.8
1	B	510	GLN	2.8
1	D	235	GLN	2.8
1	A	331	TYR	2.8
1	C	296	PHE	2.8
1	D	591	ILE	2.8
1	A	148	LYS	2.8
1	C	495	ALA	2.8
1	C	578	PHE	2.8
1	A	113	ASP	2.7
1	A	118	ILE	2.7
1	B	326	GLN	2.7
1	C	223	PRO	2.7
1	A	262	GLU	2.7
1	D	346	GLU	2.7
1	A	418	ALA	2.7
1	A	424	ASP	2.7
1	C	474	GLU	2.7
1	A	347	LEU	2.7
1	B	259	LEU	2.7
1	B	578	PHE	2.7
1	A	570	VAL	2.7
1	D	490	ASP	2.7
1	C	403	GLY	2.7
1	D	515	ILE	2.7
1	B	573	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	418	ALA	2.7
1	C	536	GLN	2.7
1	C	553	TYR	2.7
1	D	596	LYS	2.7
1	A	503	ILE	2.7
1	D	519	SER	2.7
1	C	541	LEU	2.7
1	A	381	ILE	2.6
1	B	403	GLY	2.6
1	B	371	ARG	2.6
1	C	350	CYS	2.6
1	A	299	GLU	2.6
1	C	285	TRP	2.6
1	D	452[A]	ASN	2.6
1	A	238	VAL	2.6
1	C	371	ARG	2.6
1	C	522[A]	CYS	2.6
1	B	402	ALA	2.6
1	B	504	ASN	2.6
1	C	592	THR	2.6
1	D	464	GLY	2.6
1	C	229	VAL	2.6
1	B	399	ILE	2.6
1	D	396	TYR	2.6
1	A	565	ALA	2.5
1	B	535	ASN	2.5
1	A	410	SER	2.5
1	C	550	ILE	2.5
1	C	587	ILE	2.5
1	B	563	TYR	2.5
1	B	429	GLU	2.5
1	C	299	GLU	2.5
1	A	361	ASP	2.5
1	A	573	CYS	2.5
1	C	412	ALA	2.5
1	B	436	PRO	2.5
1	D	114	THR	2.5
1	C	179	VAL	2.5
1	A	407	TYR	2.5
1	C	452	ASN	2.5
1	A	219	GLY	2.5
1	A	464	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	261	PRO	2.5
1	A	221	PHE	2.5
1	C	515	ILE	2.5
1	D	229	VAL	2.5
1	D	325	ILE	2.5
1	B	476	LEU	2.5
1	C	326	GLN	2.5
1	C	463	THR	2.4
1	C	538	SER	2.4
1	A	587	ILE	2.4
1	C	250	ILE	2.4
1	A	493	LEU	2.4
1	D	244	LEU	2.4
1	A	483	ALA	2.4
1	A	529	ALA	2.4
1	C	579	THR	2.4
1	B	229	VAL	2.4
1	B	503	ILE	2.4
1	D	180	HIS	2.4
1	D	388[A]	ASP	2.4
1	A	343	VAL	2.4
1	B	530	ILE	2.4
1	D	115	MET	2.4
1	C	493	LEU	2.4
1	A	485	PRO	2.4
1	A	199	VAL	2.4
1	A	540	LEU	2.4
1	B	438	LEU	2.4
1	C	244	LEU	2.4
1	B	223	PRO	2.3
1	A	546	ALA	2.3
1	C	433	SER	2.3
1	D	118	ILE	2.3
1	D	376	HIS	2.3
1	A	567	GLN	2.3
1	D	514	PRO	2.3
1	B	357	GLY	2.3
1	A	592	THR	2.3
1	A	397	ILE	2.3
1	B	587	ILE	2.3
1	D	448	ILE	2.3
1	A	398	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	570	VAL	2.3
1	A	509	MET	2.3
1	A	232	THR	2.3
1	C	194	ARG	2.3
1	C	127	GLU	2.3
1	C	276	LEU	2.3
1	C	512	LYS	2.3
1	A	504	ASN	2.3
1	C	358	ASN	2.3
1	D	218	ASP	2.3
1	B	584	GLY	2.3
1	A	411	THR	2.3
1	A	439	LYS	2.3
1	A	267	PHE	2.2
1	C	502	VAL	2.3
1	A	309	ASP	2.2
1	A	330	ASP	2.2
1	A	525	ALA	2.2
1	A	460	THR	2.2
1	C	407	TYR	2.2
1	D	429	GLU	2.2
1	A	231	TRP	2.2
1	B	499	ILE	2.2
1	A	391	LEU	2.2
1	A	491	VAL	2.2
1	B	493	LEU	2.2
1	A	230	LYS	2.2
1	D	465	GLN	2.2
1	D	495	ALA	2.2
1	A	276	LEU	2.2
1	A	488	LEU	2.2
1	A	552	VAL	2.2
1	C	485	PRO	2.2
1	B	458	GLY	2.2
1	C	341	CYS	2.2
1	D	177	CYS	2.2
1	C	418	ALA	2.2
1	A	585	ASP	2.2
1	B	498	PHE	2.2
1	C	151	GLY	2.2
1	C	482	SER	2.2
1	D	232	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	420	THR	2.2
1	A	222	ILE	2.1
1	B	222	ILE	2.1
1	C	347	LEU	2.1
1	C	549	LEU	2.1
1	D	466	ILE	2.1
1	C	383	ASP	2.1
1	D	327	ASN	2.1
1	C	496	GLU	2.1
1	C	534	LYS	2.1
1	D	203	GLY	2.1
1	D	522[A]	CYS	2.1
1	B	391	LEU	2.1
1	B	426	ILE	2.1
1	C	466	ILE	2.1
1	D	349	ILE	2.1
1	A	193	GLU	2.1
1	B	474	GLU	2.1
1	C	345	ASN	2.1
1	D	383	ASP	2.1
1	D	535	ASN	2.1
1	D	179	VAL	2.1
1	A	498	PHE	2.1
1	B	524	THR	2.1
1	A	588	ALA	2.1
1	A	405	LYS	2.1
1	B	469	LYS	2.1
1	C	523	LYS	2.1
1	B	597	GLU	2.1
1	B	180	HIS	2.1
1	C	510	GLN	2.1
1	A	255	GLU	2.1
1	A	461	GLN	2.1
1	A	396	TYR	2.1
1	A	301	VAL	2.1
1	B	592	THR	2.0
1	B	483	ALA	2.0
1	C	588	ALA	2.0
1	B	235	GLN	2.0
1	B	113	ASP	2.0
1	C	501	ASP	2.0
1	D	440	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	399	ILE	2.0
1	C	584	GLY	2.0
1	B	495	ALA	2.0
1	A	582	GLN	2.0
1	D	590	LEU	2.0
1	A	371	ARG	2.0
1	B	134	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

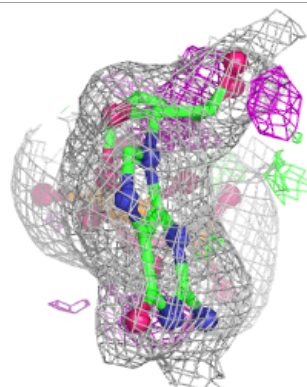
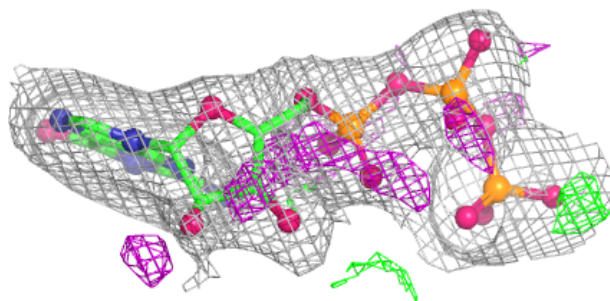
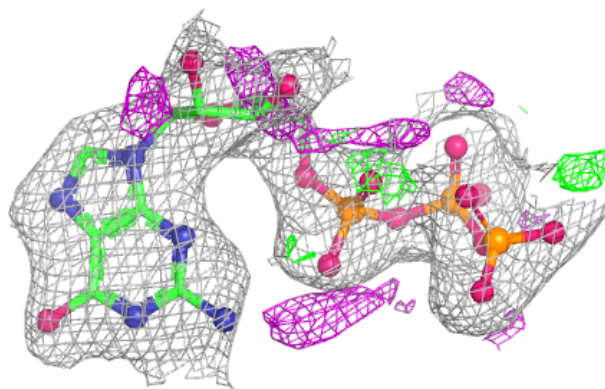
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	703	1/1	0.86	0.10	40,40,40,40	0
4	MG	D	703	1/1	0.89	0.09	56,56,56,56	0
4	MG	C	702	1/1	0.91	0.10	56,56,56,56	0
2	GTP	B	702	32/32	0.92	0.10	40,54,62,68	0
2	GTP	A	701	32/32	0.93	0.10	47,57,63,67	0
2	GTP	B	701	32/32	0.93	0.10	40,55,63,66	0
3	DTP	B	703	30/30	0.94	0.10	32,41,57,72	11
4	MG	A	704	1/1	0.95	0.11	58,58,58,58	0
3	DTP	C	701	30/30	0.95	0.09	44,48,57,60	14
2	GTP	D	702	32/32	0.95	0.09	31,50,61,80	0
3	DTP	A	702	30/30	0.96	0.08	32,48,60,62	11
3	DTP	D	701	30/30	0.96	0.08	40,47,54,55	14

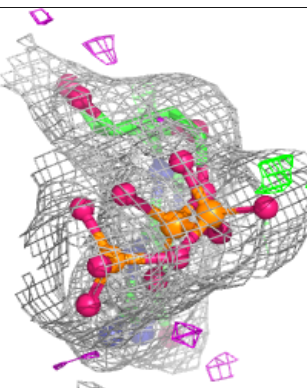
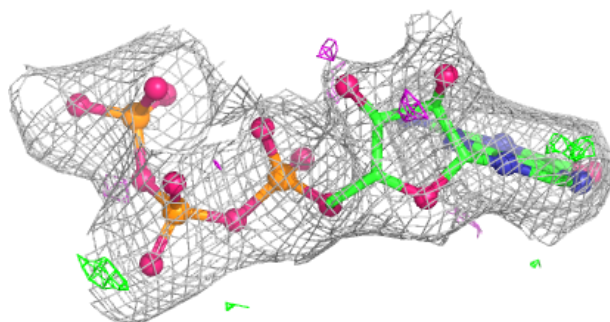
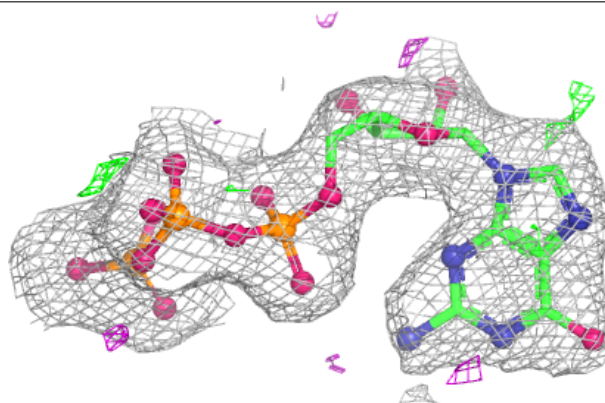
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

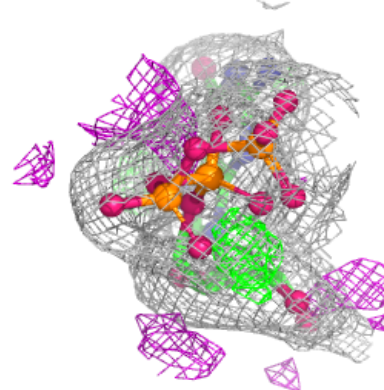
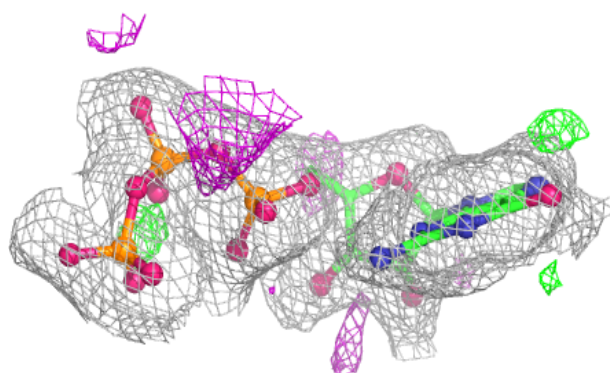
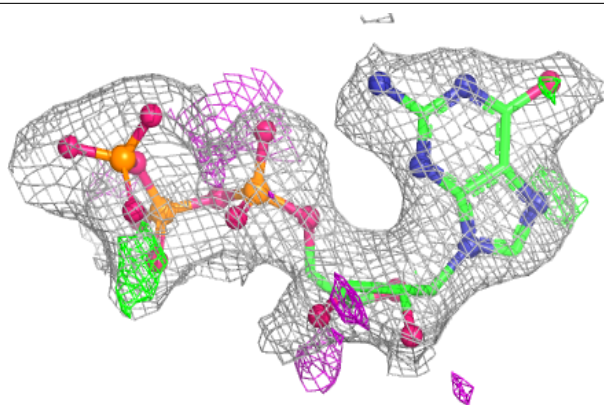
**Electron density around GTP A 701:**

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

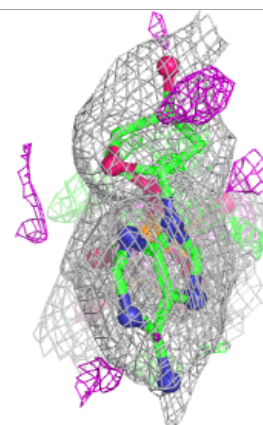
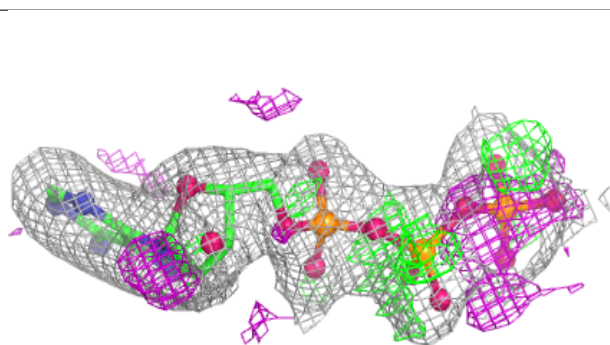
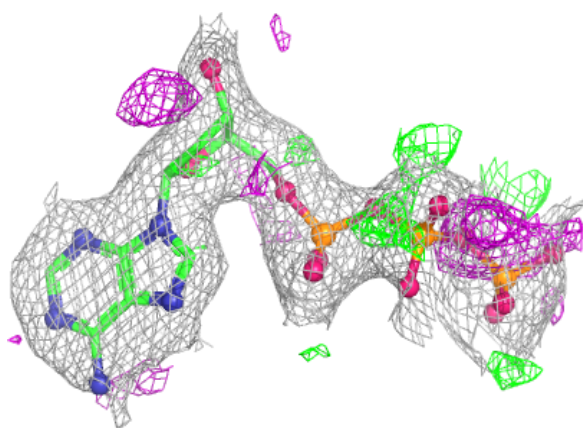


Electron density around GTP B 701:

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

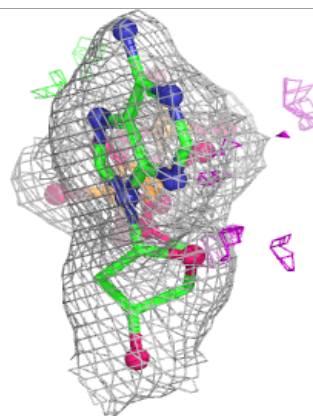
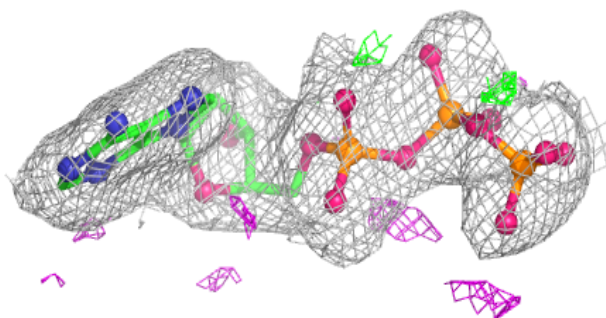
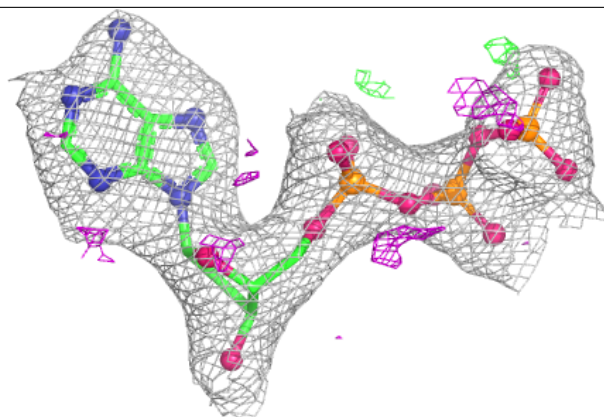
**Electron density around DTP B 703:**

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

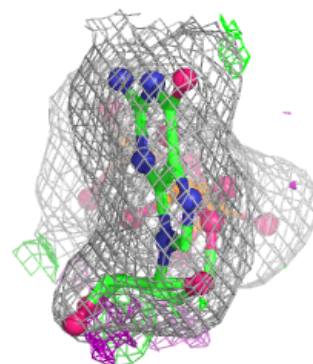
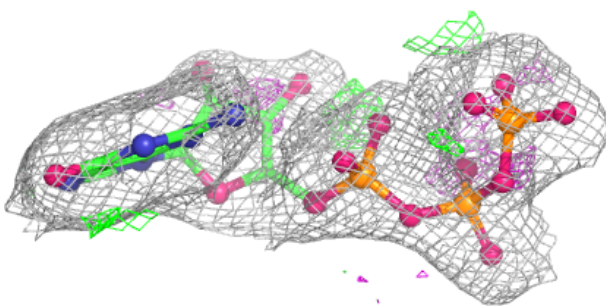
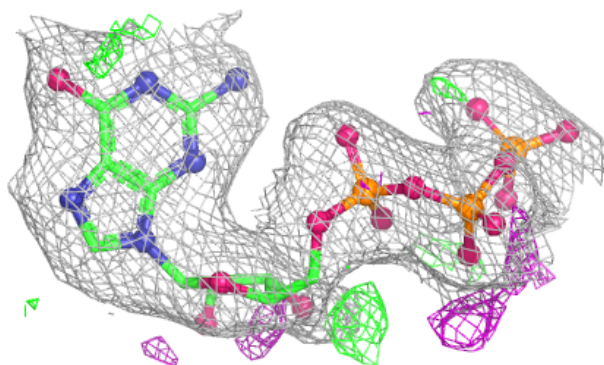


Electron density around DTP C 701:

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

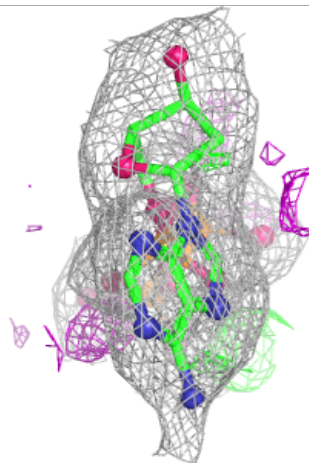
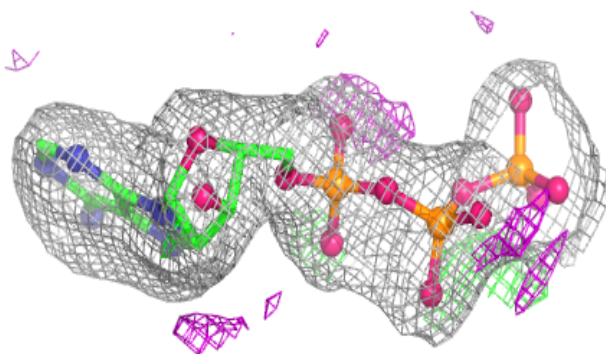
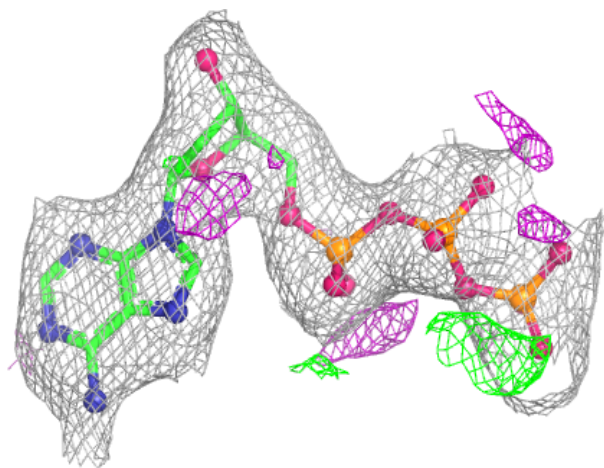
**Electron density around GTP D 702:**

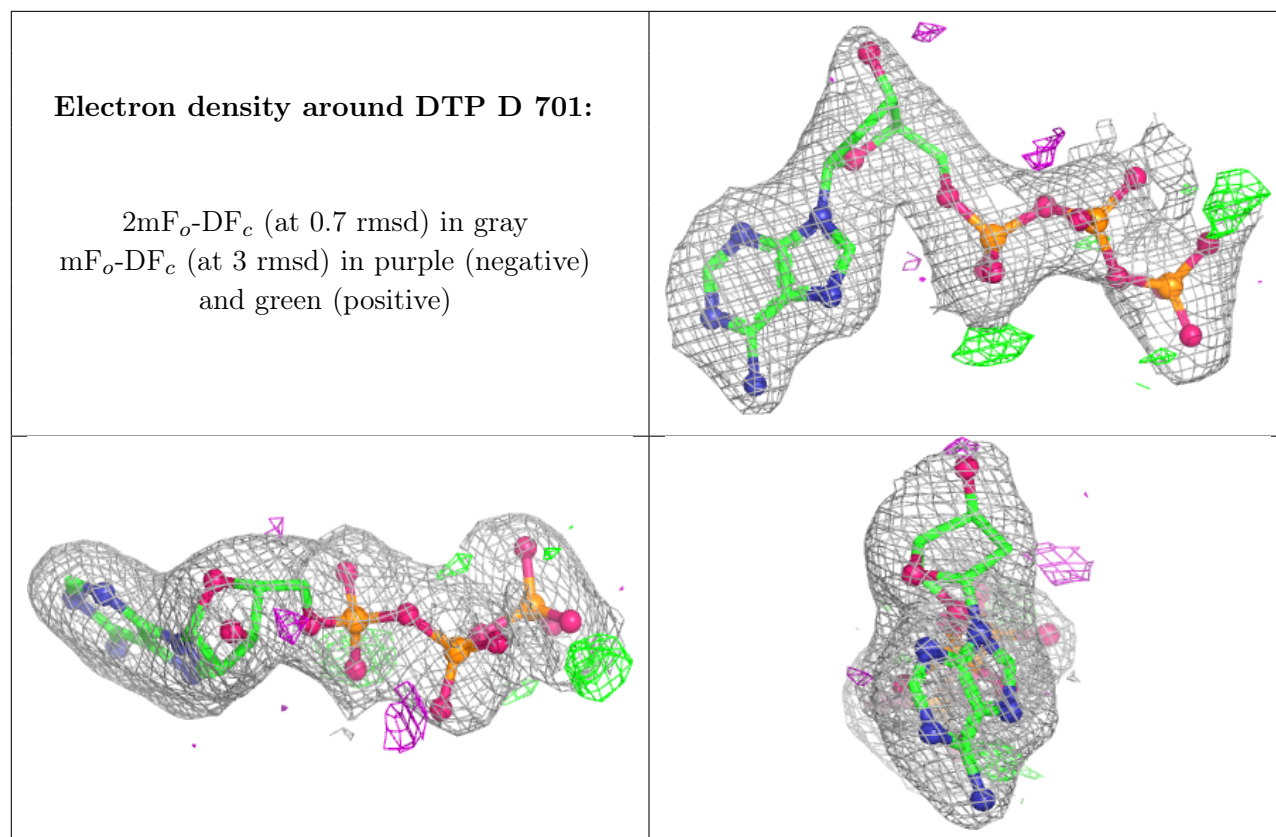
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.