Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 07:29 AM EDT

PDB ID	:	4RXS
Title	:	The structure of GTP-dTTP-bound SAMHD1
Authors	:	Zhu, C.F.; Wei, W.; Peng, X.; Dong, Y.H.; Gong, Y.; Yu, X.F.
Deposited on	:	2014-12-11
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

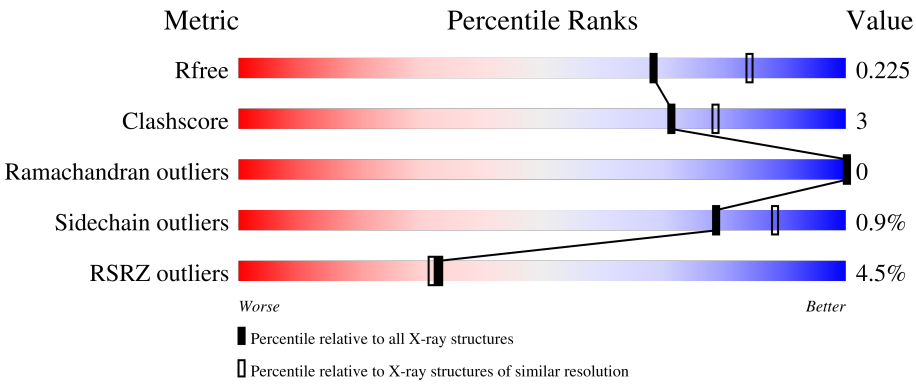
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	539	5%; 81%; 8%; • ; 11%
1	B	539	3%; 86%; 5%; 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8557 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
			Total	C	N	O	S			
1	A	481	3938	2523	683	713	19	0	0	0
1	B	492	4030	2583	699	729	19	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	SER	-	expression tag	UNP Q9Y3Z3
A	91	SER	-	expression tag	UNP Q9Y3Z3
A	92	HIS	-	expression tag	UNP Q9Y3Z3
A	93	HIS	-	expression tag	UNP Q9Y3Z3
A	94	HIS	-	expression tag	UNP Q9Y3Z3
A	95	HIS	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
A	97	HIS	-	expression tag	UNP Q9Y3Z3
A	98	SER	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	GLY	-	expression tag	UNP Q9Y3Z3
A	101	GLU	-	expression tag	UNP Q9Y3Z3
A	102	ASN	-	expression tag	UNP Q9Y3Z3
A	103	LEU	-	expression tag	UNP Q9Y3Z3
A	104	TYR	-	expression tag	UNP Q9Y3Z3
A	105	PHE	-	expression tag	UNP Q9Y3Z3
A	106	GLN	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	SER	-	expression tag	UNP Q9Y3Z3
A	266	TYR	CYS	conflict	UNP Q9Y3Z3
B	88	MET	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	SER	-	expression tag	UNP Q9Y3Z3

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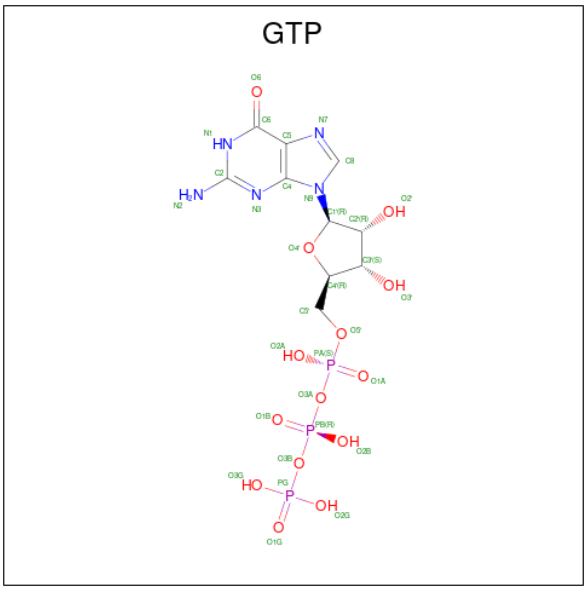
Chain	Residue	Modelled	Actual	Comment	Reference
B	91	SER	-	expression tag	UNP Q9Y3Z3
B	92	HIS	-	expression tag	UNP Q9Y3Z3
B	93	HIS	-	expression tag	UNP Q9Y3Z3
B	94	HIS	-	expression tag	UNP Q9Y3Z3
B	95	HIS	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	HIS	-	expression tag	UNP Q9Y3Z3
B	98	SER	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	GLY	-	expression tag	UNP Q9Y3Z3
B	101	GLU	-	expression tag	UNP Q9Y3Z3
B	102	ASN	-	expression tag	UNP Q9Y3Z3
B	103	LEU	-	expression tag	UNP Q9Y3Z3
B	104	TYR	-	expression tag	UNP Q9Y3Z3
B	105	PHE	-	expression tag	UNP Q9Y3Z3
B	106	GLN	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
B	266	TYR	CYS	conflict	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
			Total	C	N	O	P		
2	A	1	32	10	5	14	3	0	0

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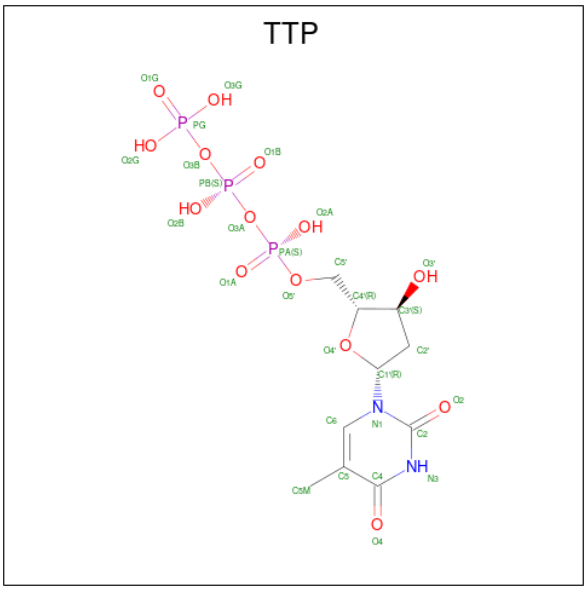
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	32	10	5	14	3	0	0

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	29	10	2	14	3	0	0
			Total	C	N	O	P		
3	A	1	29	10	2	14	3	0	0
			Total	C	N	O	P		
3	B	1	29	10	2	14	3	0	0
			Total	C	N	O	P		
3	B	1	29	10	2	14	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
			Total	Mg		
4	B	1	1	1	0	0

- Molecule 5 is water.

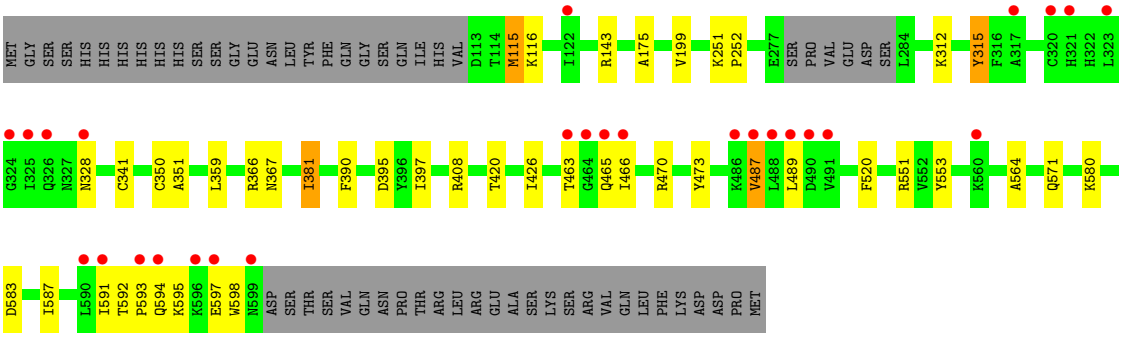
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	204	204	204	0	0
			Total	O		
5	B	203	203	203	0	0

3 Residue-property plots (i)

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

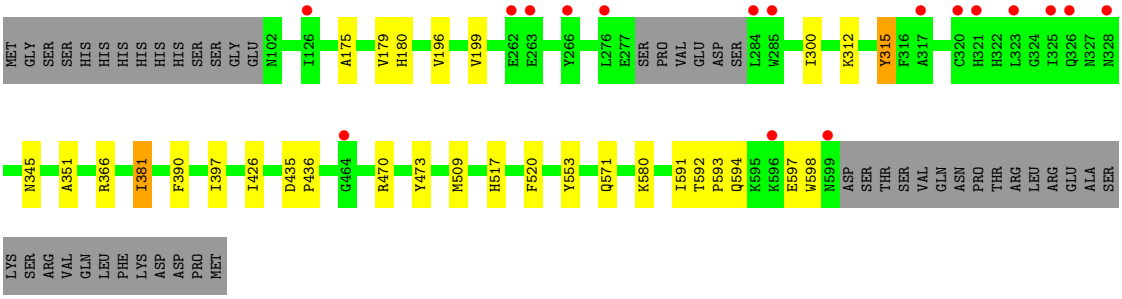
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.69Å 109.76Å 92.95Å 90.00° 122.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 48.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.20) 99.9 (48.96-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.194 , 0.222 0.199 , 0.225	Depositor DCC
R_{free} test set	3246 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8557	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TTP, 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	0.43	0/4032	0.62	0/5444
1	B	0.43	0/4127	0.61	0/5573
All	All	0.43	0/8159	0.61	0/11017

There are no bond length outliers.

There are no bond angle outliers.

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	3938	0	3917	34	0
1	B	4030	0	4003	22	0
2	A	64	0	24	0	0
3	A	58	0	26	2	0
3	B	58	0	26	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	204	0	0	2	0
5	B	203	0	0	0	0
All	All	8557	0	7996	56	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 3.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:LYS:HE3	1:A:597:GLU:HG3	1.74	0.70
1:B:179:VAL:CG1	1:B:196:VAL:HG22	2.24	0.68
1:B:179:VAL:HG23	1:B:300:ILE:CD1	2.25	0.67
1:B:591:ILE:O	1:B:594:GLN:HG2	1.98	0.63
1:B:381:ILE:HG12	1:B:553:TYR:CE2	2.34	0.62
1:B:179:VAL:HG23	1:B:300:ILE:HD13	1.81	0.61
1:A:381:ILE:HG12	1:A:553:TYR:CE2	2.37	0.59
1:A:328:ASN:OD1	1:A:328:ASN:N	2.39	0.56
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.88	0.56
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.87	0.56
1:A:315:TYR:CE2	3:A:802:TTP:H5'1	2.42	0.55
1:A:463:THR:O	1:A:466:ILE:HG12	2.07	0.54
1:B:312:LYS:HE3	1:B:366:ARG:HD2	1.90	0.54
1:A:312:LYS:HE3	1:A:366:ARG:HD2	1.90	0.53
1:A:397:ILE:HG21	1:A:426:ILE:HD11	1.92	0.51
1:B:179:VAL:HG11	1:B:196:VAL:HG22	1.93	0.51
1:A:470:ARG:HA	1:A:473:TYR:CE1	2.47	0.49
1:A:395:ASP:OD1	1:A:408:ARG:NH2	2.46	0.48
1:A:591:ILE:O	1:A:594:GLN:HB3	2.12	0.48
1:A:595:LYS:HE3	1:A:597:GLU:CG	2.43	0.48
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.95	0.48
1:A:591:ILE:O	1:A:594:GLN:OE1	2.32	0.47
1:A:367:ASN:HB2	5:A:1057:HOH:O	2.13	0.47
1:B:509:MET:HE1	1:B:517:HIS:CD2	2.49	0.47
1:A:115:MET:HG2	1:A:116:LYS:N	2.29	0.46
1:A:381:ILE:HD13	1:A:381:ILE:HA	1.85	0.46
1:B:315:TYR:CZ	3:B:702:TTP:H5'1	2.51	0.46
1:B:597:GLU:OE1	1:B:597:GLU:N	2.45	0.46
1:A:571:GLN:HE22	1:A:594:GLN:HE22	1.61	0.46
1:A:551:ARG:NH2	5:A:974:HOH:O	2.49	0.45
1:A:571:GLN:HE22	1:A:594:GLN:NE2	2.14	0.45
1:B:470:ARG:HA	1:B:473:TYR:CE1	2.52	0.45
1:B:580:LYS:HD3	1:B:598:TRP:HB3	1.99	0.45
1:B:381:ILE:CG1	1:B:553:TYR:CE2	3.00	0.45
1:A:315:TYR:CZ	3:A:802:TTP:H5'1	2.52	0.44
1:A:595:LYS:HG3	1:A:597:GLU:HG2	2.00	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:HB2	1:A:252:PRO:HD3	2.02	0.42
1:A:487:VAL:O	1:A:489:LEU:HD12	2.19	0.42
1:B:315:TYR:CE2	3:B:702:TTP:H5'1	2.54	0.42
1:A:143:ARG:HD2	1:A:420:THR:HA	2.01	0.42
1:B:179:VAL:HG12	1:B:180:HIS:N	2.34	0.42
1:B:592:THR:N	1:B:593:PRO:CD	2.83	0.41
1:B:390:PHE:CZ	1:B:426:ILE:HG23	2.55	0.41
1:A:390:PHE:CZ	1:A:426:ILE:HG23	2.55	0.41
1:A:489:LEU:HD23	1:A:564:ALA:HA	2.03	0.41
1:A:592:THR:N	1:A:593:PRO:CD	2.84	0.41
1:A:470:ARG:HA	1:A:473:TYR:CD1	2.55	0.41
1:A:580:LYS:HD3	1:A:598:TRP:HB3	2.02	0.41
1:A:381:ILE:CG1	1:A:553:TYR:CE2	3.03	0.41
1:A:341:CYS:HB2	1:A:350:CYS:SG	2.61	0.41
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.83	0.41
1:B:435:ASP:HA	1:B:436:PRO:HD2	1.97	0.40
1:B:571:GLN:HE22	1:B:594:GLN:HE22	1.69	0.40
1:A:583:ASP:O	1:A:587:ILE:HG12	2.22	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	477/539 (88%)	466 (98%)	11 (2%)	0	100	100
1	B	488/539 (90%)	480 (98%)	8 (2%)	0	100	100
All	All	965/1078 (90%)	946 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/481 (89%)	422 (99%)	5 (1%)	71	83
1	B	437/481 (91%)	434 (99%)	3 (1%)	84	91
All	All	864/962 (90%)	856 (99%)	8 (1%)	78	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	315	TYR
1	A	381	ILE
1	A	465	GLN
1	A	487	VAL
1	B	315	TYR
1	B	345	ASN
1	B	381	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	517	HIS
1	A	535	ASN
1	A	594	GLN
1	B	102	ASN
1	B	517	HIS
1	B	571	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	TTP	A	803	4	26,30,30	1.30	4 (15%)	39,47,47	1.71	9 (23%)
3	TTP	B	702	-	26,30,30	1.23	5 (19%)	39,47,47	2.00	8 (20%)
3	TTP	B	703	4	26,30,30	1.32	5 (19%)	39,47,47	1.98	10 (25%)
2	GTP	A	801	4	26,34,34	0.92	1 (3%)	32,54,54	1.30	4 (12%)
3	TTP	A	802	-	26,30,30	1.35	5 (19%)	39,47,47	1.96	8 (20%)
2	GTP	A	804	4	26,34,34	1.00	1 (3%)	32,54,54	1.41	4 (12%)

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	TTP	A	803	4	-	7/22/34/34	0/2/2/2
3	TTP	B	702	-	-	4/22/34/34	0/2/2/2
3	TTP	B	703	4	-	7/22/34/34	0/2/2/2
2	GTP	A	801	4	-	3/18/38/38	0/3/3/3
3	TTP	A	802	-	-	3/22/34/34	0/2/2/2
2	GTP	A	804	4	-	6/18/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TTP	C4-N3	-3.18	1.32	1.38
3	A	803	TTP	C6-C5	3.00	1.39	1.34
3	A	803	TTP	C4-N3	-2.84	1.33	1.38
3	B	703	TTP	C4-N3	-2.82	1.33	1.38
3	B	702	TTP	C2-N1	2.57	1.42	1.38
3	B	703	TTP	C6-N1	-2.57	1.33	1.38
3	B	703	TTP	C4-C5	2.55	1.49	1.44
3	B	703	TTP	C2-N3	-2.50	1.33	1.38
3	B	702	TTP	C4-N3	-2.49	1.34	1.38
2	A	804	GTP	C6-N1	-2.46	1.34	1.37
3	A	802	TTP	C6-C5	2.42	1.38	1.34
3	B	703	TTP	C6-C5	2.42	1.38	1.34
3	A	803	TTP	C2-N3	-2.40	1.33	1.38
3	A	802	TTP	C2-N1	2.40	1.42	1.38
3	A	802	TTP	C6-N1	-2.37	1.34	1.38
3	A	803	TTP	C4-C5	2.26	1.48	1.44
3	B	702	TTP	C2-N3	-2.19	1.34	1.38
2	A	801	GTP	C6-N1	-2.18	1.34	1.37
3	B	702	TTP	C6-C5	2.17	1.38	1.34
3	A	802	TTP	C2-N3	-2.10	1.34	1.38
3	B	702	TTP	C6-N1	-2.08	1.34	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	TTP	O4-C4-C5	-5.34	118.71	124.90
3	B	703	TTP	C4-N3-C2	-4.95	120.95	127.35
3	A	802	TTP	C5-C4-N3	4.74	119.36	115.31
3	A	802	TTP	C4-N3-C2	-4.72	121.24	127.35
3	B	703	TTP	N3-C2-N1	4.69	121.11	114.89
3	B	703	TTP	C5-C4-N3	4.69	119.31	115.31
3	B	702	TTP	C5-C4-N3	4.67	119.30	115.31
3	A	803	TTP	N3-C2-N1	4.53	120.90	114.89
3	A	802	TTP	N3-C2-N1	4.50	120.86	114.89
3	B	702	TTP	C4-N3-C2	-4.42	121.63	127.35
3	B	702	TTP	N3-C2-N1	4.14	120.39	114.89
3	A	803	TTP	C4-N3-C2	-3.86	122.35	127.35
3	B	702	TTP	PB-O3A-PA	-3.86	119.57	132.83
3	A	803	TTP	C5-C4-N3	3.86	118.60	115.31
3	A	802	TTP	PB-O3A-PA	-3.86	119.59	132.83
3	B	703	TTP	C5M-C5-C4	3.72	122.86	118.77
3	A	802	TTP	O4-C4-C5	-3.63	120.69	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	TTP	O4'-C1'-N1	3.52	114.15	107.86
2	A	804	GTP	C3'-C2'-C1'	3.38	106.06	100.98
3	B	703	TTP	O4'-C1'-N1	-3.29	101.99	107.86
2	A	801	GTP	PA-O3A-PB	-3.23	121.73	132.83
2	A	804	GTP	PA-O3A-PB	-3.22	121.78	132.83
3	B	703	TTP	C5-C6-N1	-3.08	120.17	123.34
3	B	703	TTP	C2'-C1'-N1	2.95	120.56	113.77
2	A	801	GTP	C3'-C2'-C1'	2.95	105.42	100.98
3	A	802	TTP	C5-C6-N1	-2.94	120.31	123.34
3	B	702	TTP	O4'-C1'-N1	2.88	113.01	107.86
3	A	803	TTP	C5-C6-N1	-2.69	120.57	123.34
2	A	804	GTP	O3G-PG-O2G	2.65	117.78	107.64
3	B	703	TTP	O2-C2-N1	-2.55	119.39	122.79
3	A	803	TTP	C2'-C1'-N1	2.55	119.65	113.77
3	A	802	TTP	C5M-C5-C4	2.48	121.50	118.77
3	B	703	TTP	O4-C4-C5	-2.37	122.16	124.90
2	A	804	GTP	O2G-PG-O3B	-2.37	96.70	104.64
2	A	801	GTP	C8-N7-C5	2.33	107.42	102.99
3	B	703	TTP	C5M-C5-C6	-2.31	119.76	122.85
3	A	803	TTP	O2G-PG-O1G	2.27	119.58	110.68
2	A	801	GTP	O3G-PG-O2G	2.25	116.23	107.64
3	A	803	TTP	O4-C4-C5	-2.24	122.31	124.90
3	A	803	TTP	O4'-C1'-N1	-2.22	103.89	107.86
3	A	803	TTP	O2G-PG-O3B	-2.11	97.57	104.64
3	B	702	TTP	C5-C6-N1	-2.07	121.21	123.34
3	B	702	TTP	C5M-C5-C4	2.07	121.04	118.77

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	TTP	C5'-O5'-PA-O1A
3	A	803	TTP	PB-O3B-PG-O2G
3	B	702	TTP	C5'-O5'-PA-O2A
3	B	702	TTP	C5'-O5'-PA-O3A
3	A	802	TTP	C5'-O5'-PA-O3A
2	A	804	GTP	PG-O3B-PB-O1B
3	A	802	TTP	PG-O3B-PB-O2B
3	B	703	TTP	PB-O3B-PG-O1G
2	A	804	GTP	C4'-C5'-O5'-PA
2	A	801	GTP	PB-O3A-PA-O2A
2	A	801	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	A	803	TTP	C2'-C1'-N1-C2
3	A	803	TTP	O4'-C1'-N1-C2
2	A	804	GTP	PB-O3A-PA-O2A
3	B	702	TTP	PG-O3B-PB-O1B
3	A	803	TTP	O4'-C1'-N1-C6
3	B	703	TTP	O4'-C1'-N1-C2
3	A	803	TTP	C2'-C1'-N1-C6
2	A	804	GTP	PB-O3B-PG-O2G
3	B	703	TTP	PB-O3B-PG-O2G
3	B	703	TTP	PB-O3B-PG-O3G
3	B	703	TTP	C2'-C1'-N1-C2
2	A	801	GTP	PG-O3B-PB-O1B
2	A	804	GTP	PG-O3B-PB-O2B
2	A	804	GTP	PB-O3A-PA-O1A
3	A	803	TTP	PB-O3A-PA-O1A
3	A	803	TTP	PG-O3B-PB-O2B
3	B	702	TTP	PG-O3B-PB-O2B
3	B	703	TTP	PB-O3A-PA-O1A
3	B	703	TTP	O4'-C1'-N1-C6

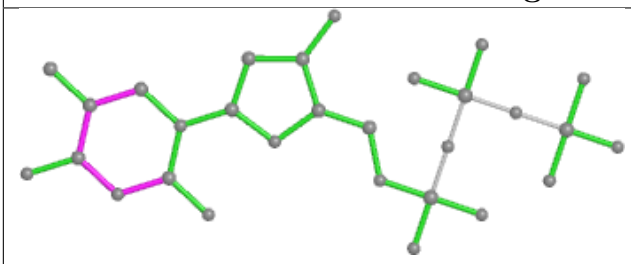
There are no ring outliers.

2 monomers are involved in 4 short contacts:

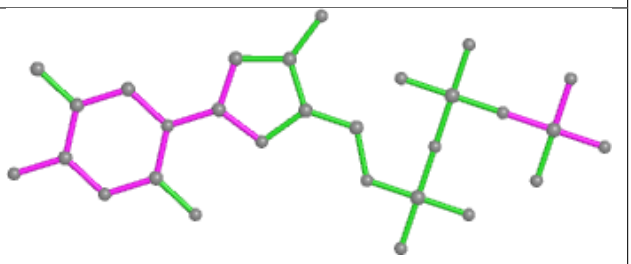
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	TTP	2	0
3	A	802	TTP	2	0

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

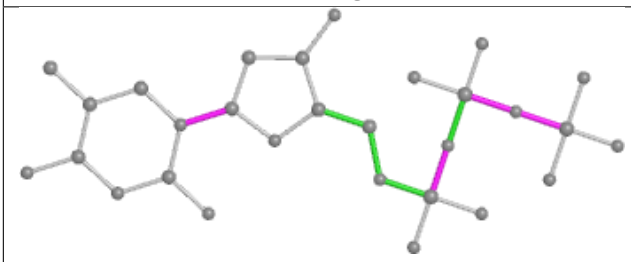
Ligand TTP A 803



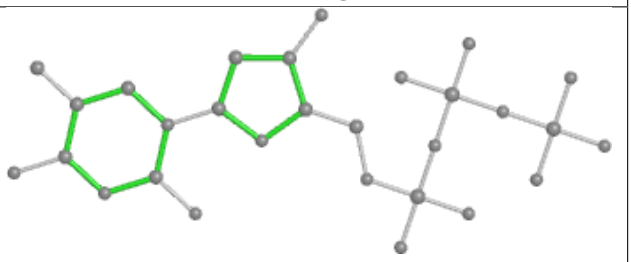
Bond lengths



Bond angles

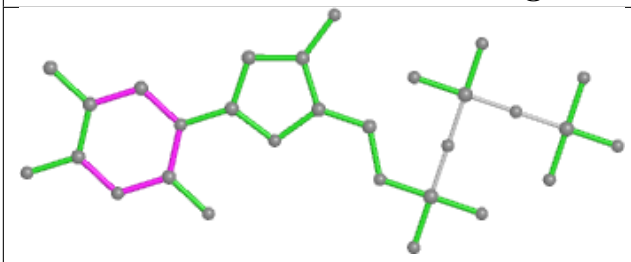


Torsions

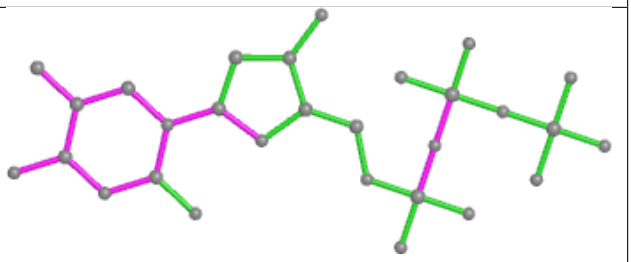


Rings

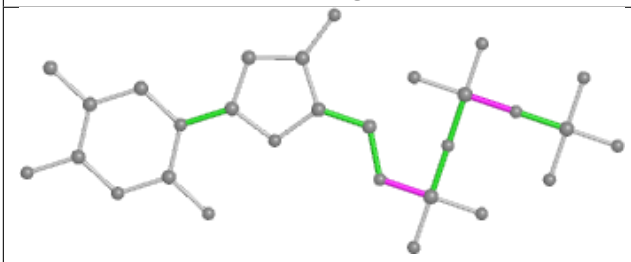
Ligand TTP B 702



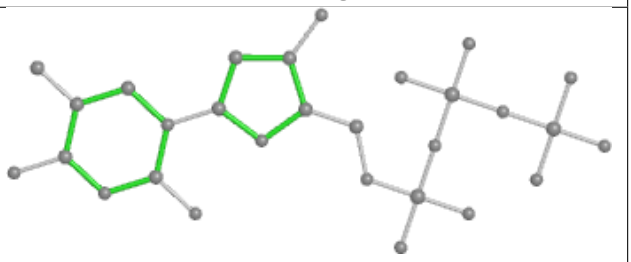
Bond lengths



Bond angles

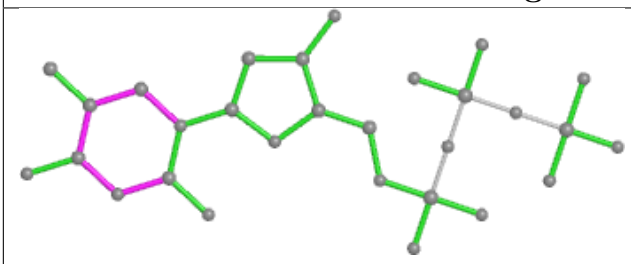


Torsions

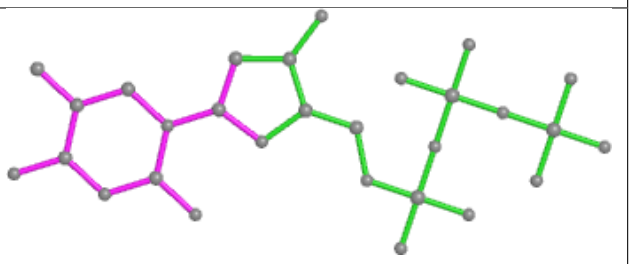


Rings

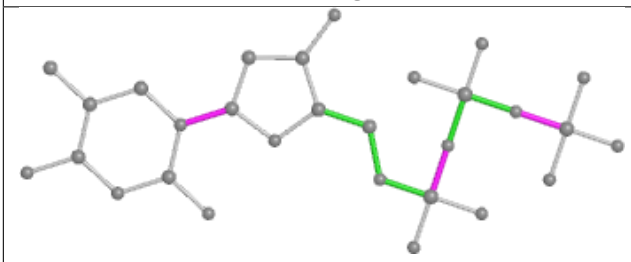
Ligand TTP B 703



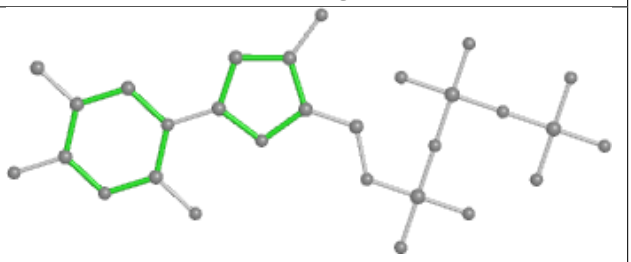
Bond lengths



Bond angles

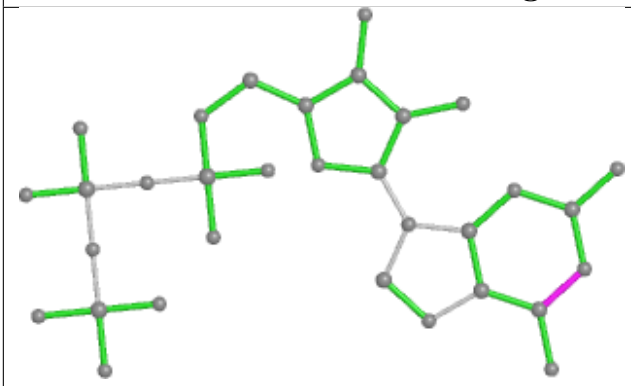


Torsions

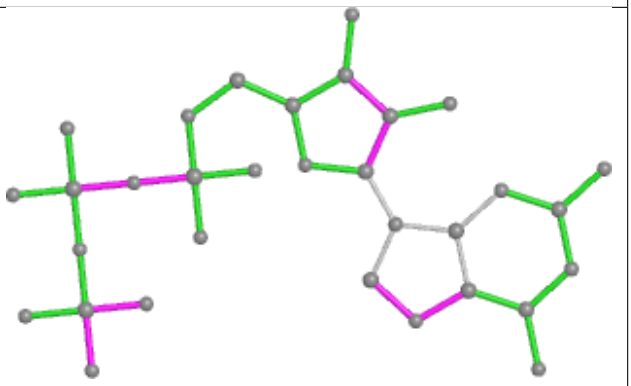


Rings

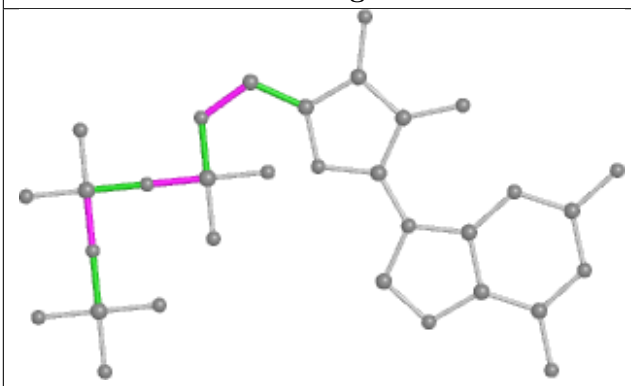
Ligand GTP A 801



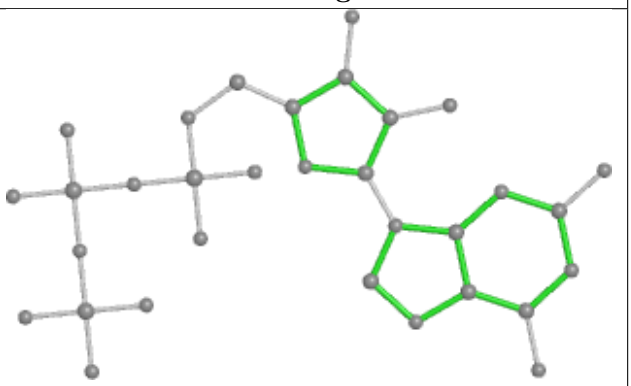
Bond lengths



Bond angles

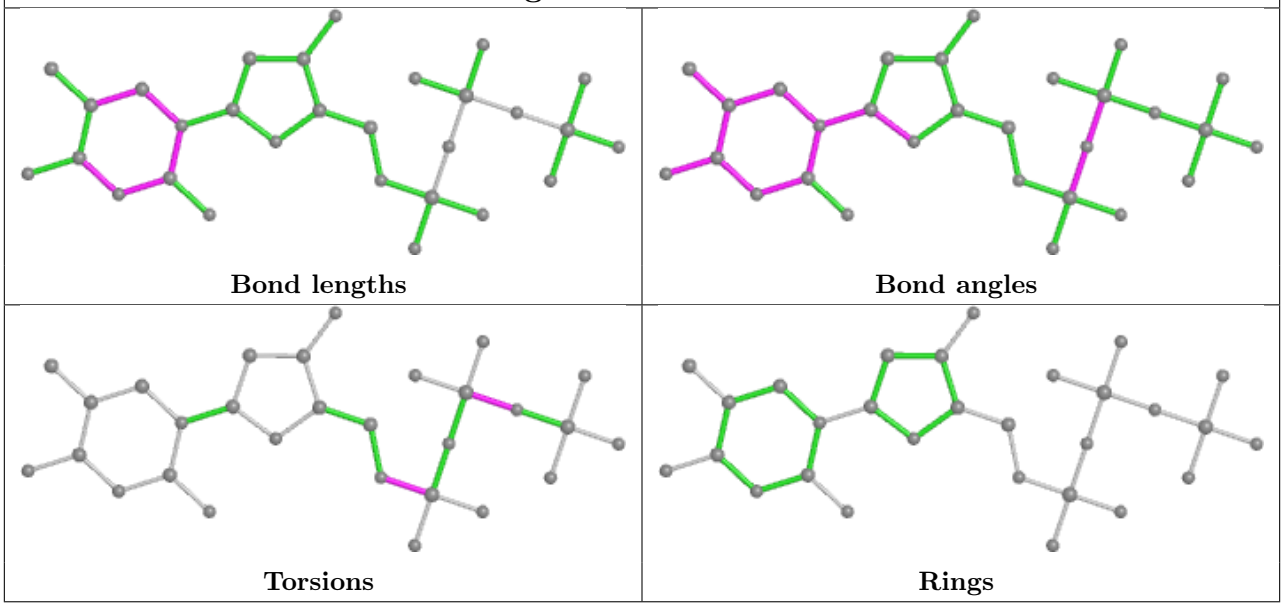


Torsions

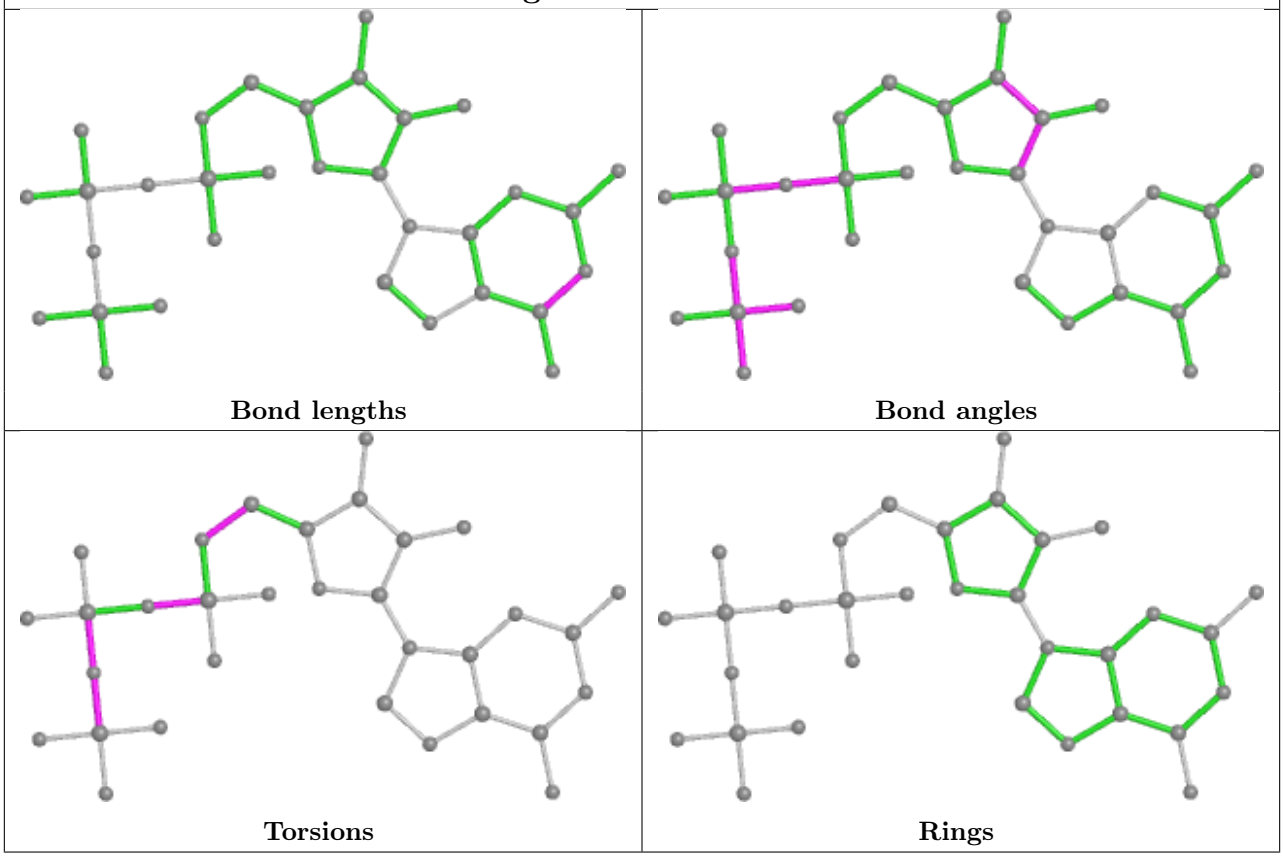


Rings

Ligand TTP A 802



Ligand GTP A 804



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	481/539 (89%)	0.06	27 (5%)	24	23	32, 49, 81, 106	0
1	B	492/539 (91%)	-0.07	17 (3%)	44	42	30, 46, 73, 105	0
All	All	973/1078 (90%)	-0.00	44 (4%)	33	32	30, 47, 75, 106	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	ASP	5.2
1	A	464	GLY	5.2
1	B	276	LEU	4.6
1	A	599	ASN	4.4
1	A	463	THR	4.2
1	A	488	LEU	3.9
1	A	590	LEU	3.8
1	A	326	GLN	3.6
1	B	328	ASN	3.6
1	B	266	TYR	3.6
1	B	326	GLN	3.5
1	B	464	GLY	3.4
1	A	320	CYS	3.2
1	A	325	ILE	3.1
1	A	491	VAL	3.1
1	B	325	ILE	3.0
1	A	597	GLU	2.9
1	A	489	LEU	2.9
1	B	596	LYS	2.9
1	B	317	ALA	2.8
1	A	596	LYS	2.8
1	A	591	ILE	2.8
1	A	465	GLN	2.7
1	A	487	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	599	ASN	2.6
1	B	262	GLU	2.6
1	B	320	CYS	2.5
1	A	122	ILE	2.5
1	A	466	ILE	2.5
1	A	328	ASN	2.5
1	B	263	GLU	2.5
1	A	486	LYS	2.4
1	A	323	LEU	2.4
1	A	593	PRO	2.3
1	A	321	HIS	2.3
1	A	594	GLN	2.2
1	B	284	LEU	2.2
1	B	323	LEU	2.2
1	A	560	LYS	2.1
1	A	324	GLY	2.1
1	A	317	ALA	2.1
1	B	126	ILE	2.1
1	B	285	TRP	2.1
1	B	321	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TTP	B	702	29/29	0.83	0.16	39,53,94,100	0
3	TTP	A	802	29/29	0.84	0.16	42,55,102,107	0
4	MG	A	805	1/1	0.94	0.10	37,37,37,37	0

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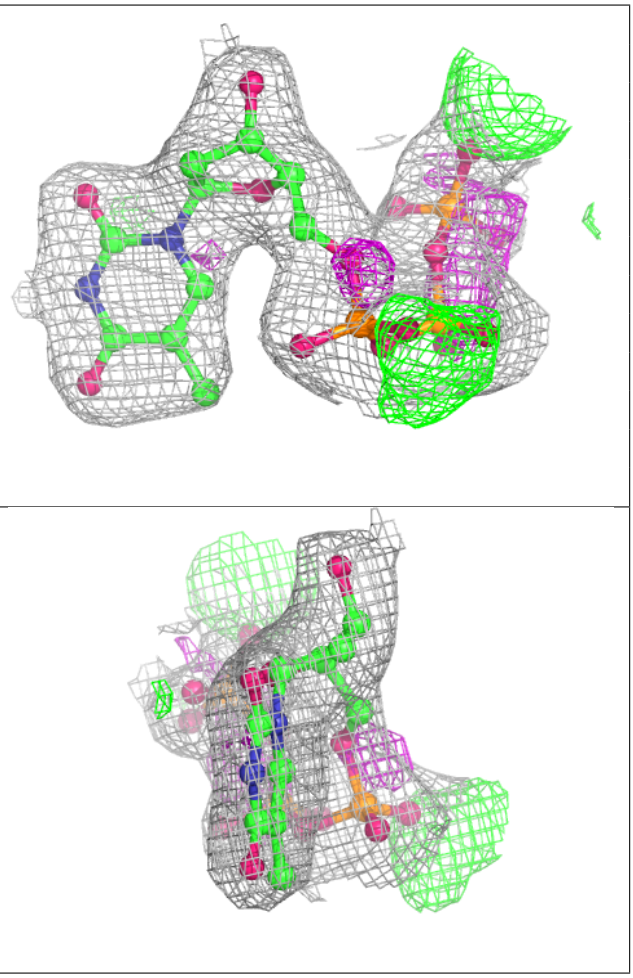
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TTP	B	703	29/29	0.98	0.17	30,34,36,38	0
2	GTP	A	804	32/32	0.98	0.14	32,35,39,39	0
4	MG	B	701	1/1	0.98	0.10	41,41,41,41	0
2	GTP	A	801	32/32	0.99	0.10	37,40,45,48	0
3	TTP	A	803	29/29	0.99	0.15	34,38,40,42	0

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.

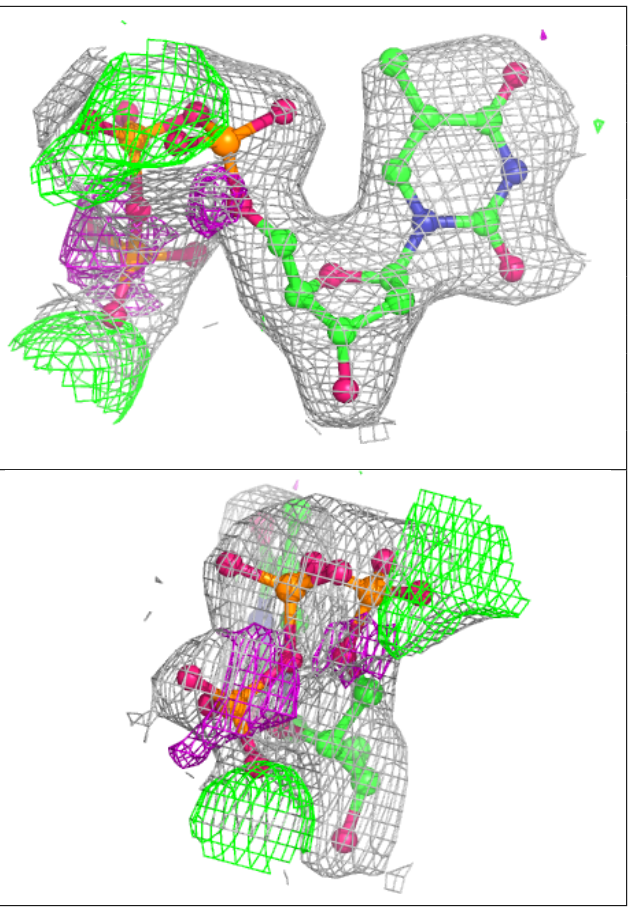
Electron density around TTP B 702:

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



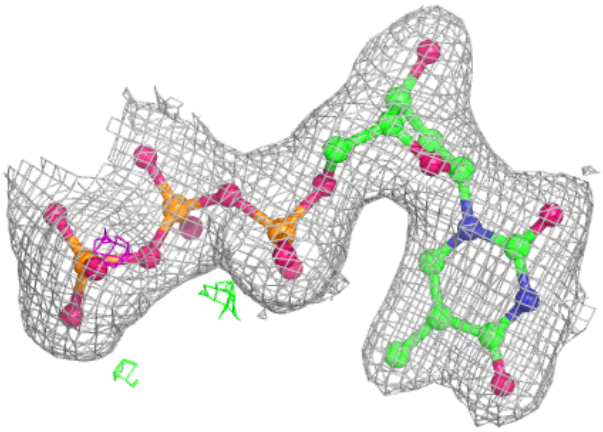
Electron density around TTP A 802:

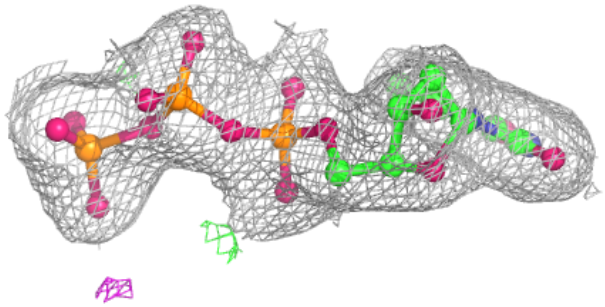
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

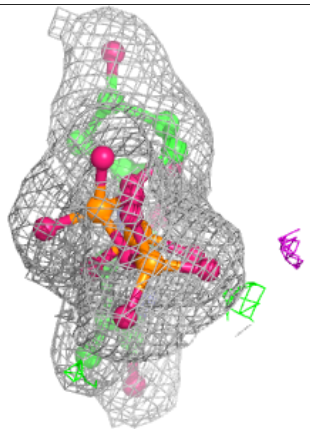


Electron density around TTP B 703:

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

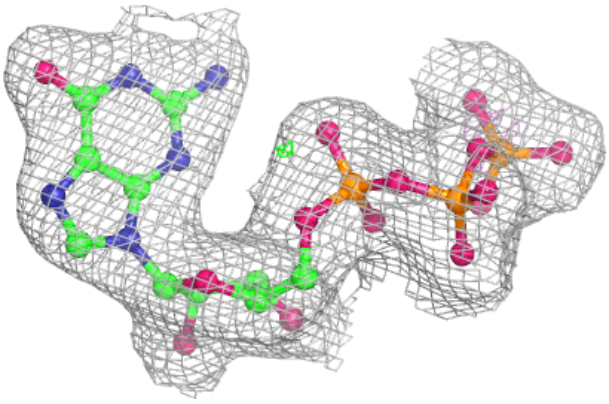


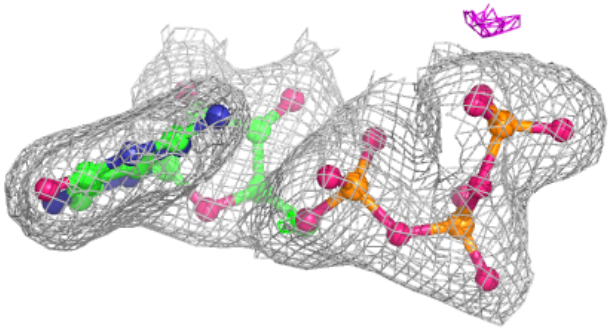


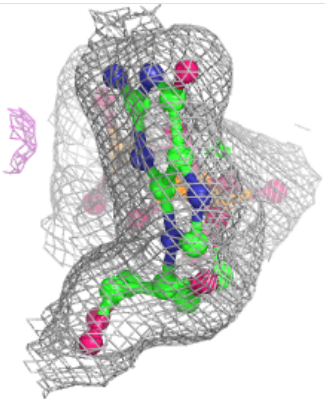


Electron density around GTP A 804:

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

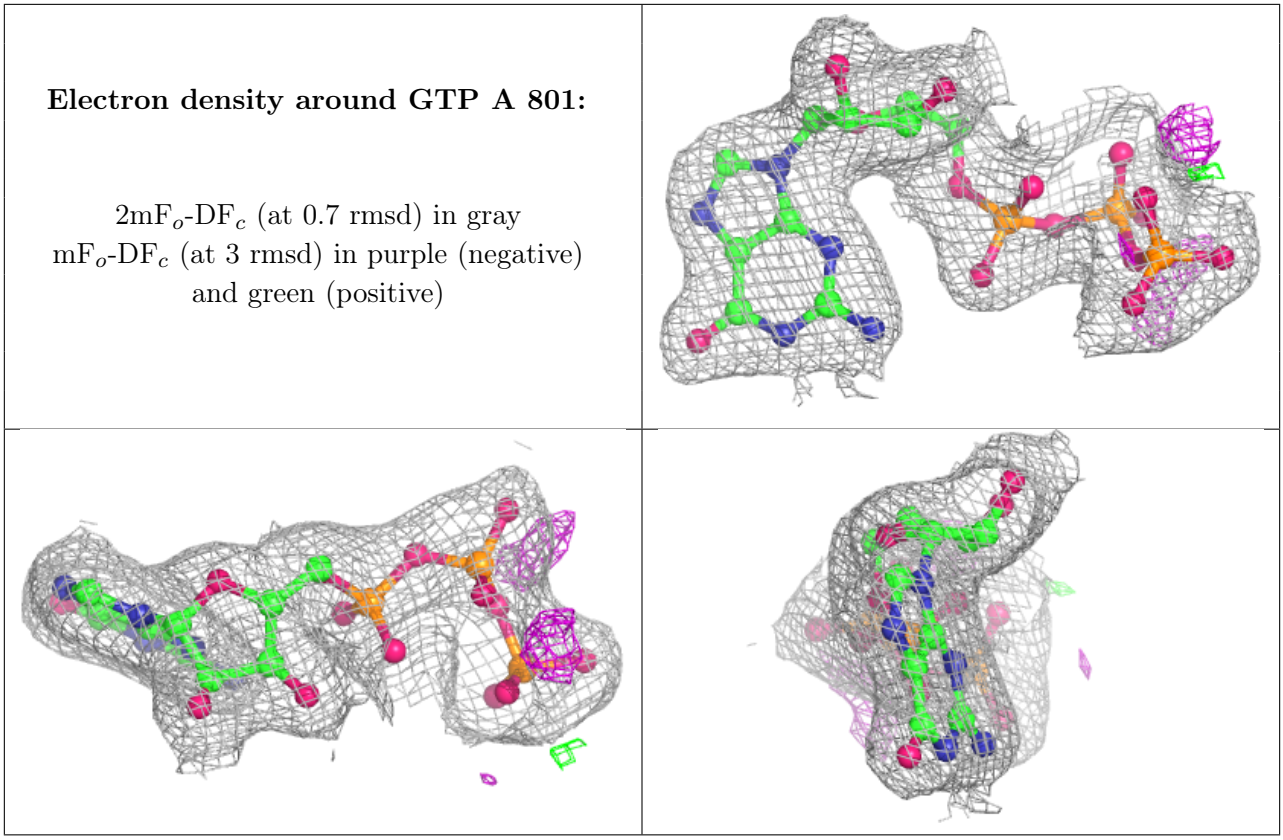






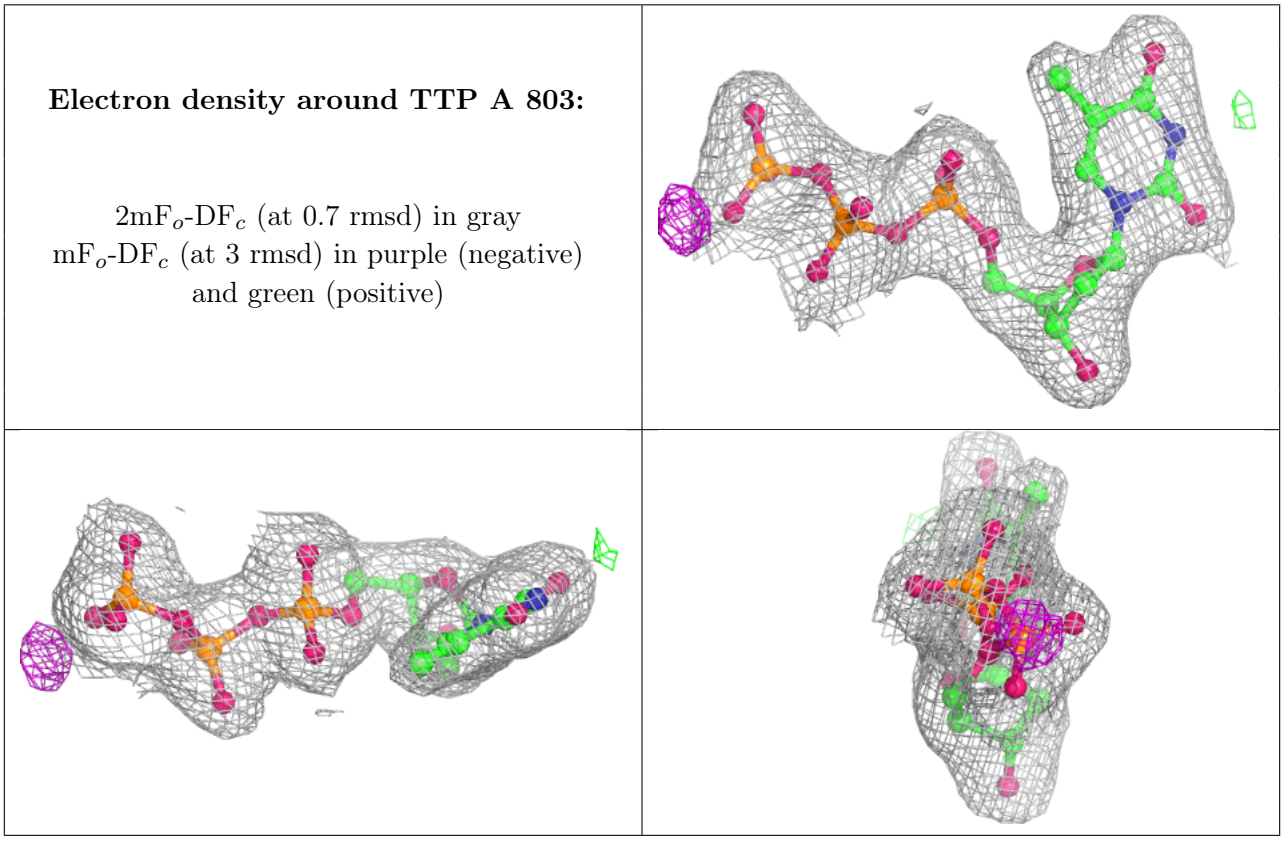
Electron density around GTP A 801:

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



Electron density around TTP A 803:

$2mF_o$-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.