Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 09:34 AM EDT

PDB ID	:	6PWY
Title	:	Structure of C. elegans ZK177.8, SAMHD1 ortholog
Authors	:	Lim, C.S.; Maehigashi, T.; Wade, L.R.; Bowen, N.; Knecht, K.; Xiong, Y.; Kim, B.
Deposited on	:	2019-07-24
Resolution	:	1.81 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:

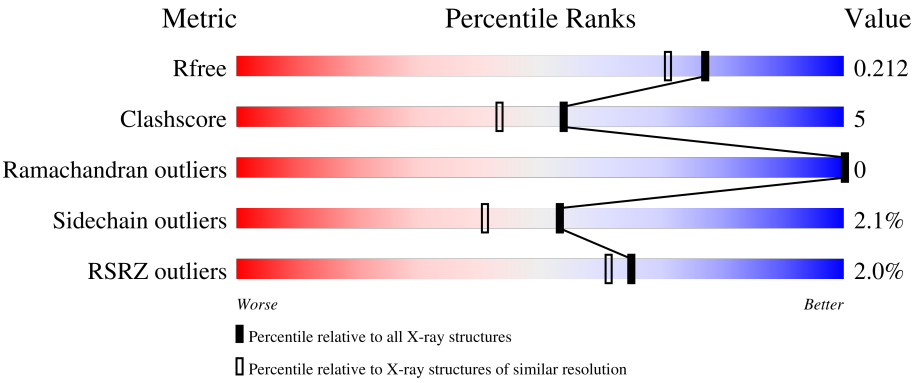
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	526	2% 85% 10%
1	B	526	2% 88% 8%
1	C	526	86% 10%
1	D	526	2% 85% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SIN	B	605	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18205 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.

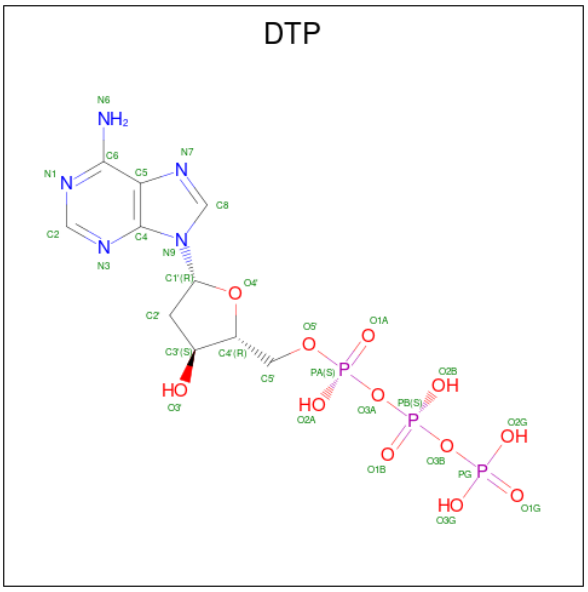
- Molecule 1 is a protein called ZK177.8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	4	0
			4040	2566	684	768	22			
1	B	513	Total	C	N	O	S	0	4	0
			4119	2615	703	779	22			
1	D	503	Total	C	N	O	S	0	4	0
			4033	2562	683	766	22			
1	C	513	Total	C	N	O	S	0	3	0
			4111	2609	702	778	22			

There are 12 discrepancies between the modelled and reference sequences:

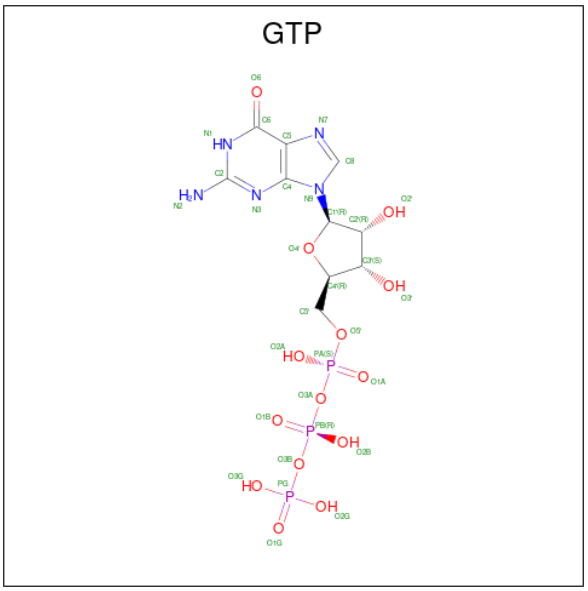
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP Q09374
A	134	ARG	HIS	engineered mutation	UNP Q09374
A	135	ASN	ASP	engineered mutation	UNP Q09374
B	40	MET	-	expression tag	UNP Q09374
B	134	ARG	HIS	engineered mutation	UNP Q09374
B	135	ASN	ASP	engineered mutation	UNP Q09374
D	40	MET	-	expression tag	UNP Q09374
D	134	ARG	HIS	engineered mutation	UNP Q09374
D	135	ASN	ASP	engineered mutation	UNP Q09374
C	40	MET	-	expression tag	UNP Q09374
C	134	ARG	HIS	engineered mutation	UNP Q09374
C	135	ASN	ASP	engineered mutation	UNP Q09374

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

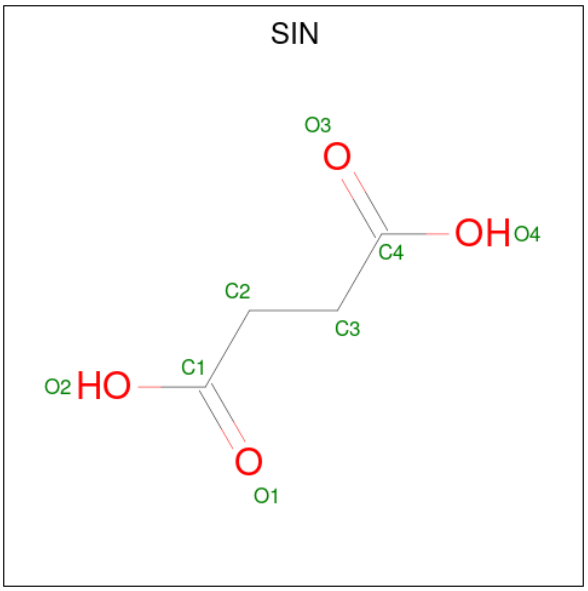


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

- Molecule 5 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 4 4	0	0
5	A	1	Total C O 8 4 4	0	0
5	B	1	Total C O 8 4 4	0	0
5	B	1	Total C O 8 4 4	0	0
5	C	1	Total C O 8 4 4	0	0
5	C	1	Total C O 8 4 4	0	0

- Molecule 6 is water.

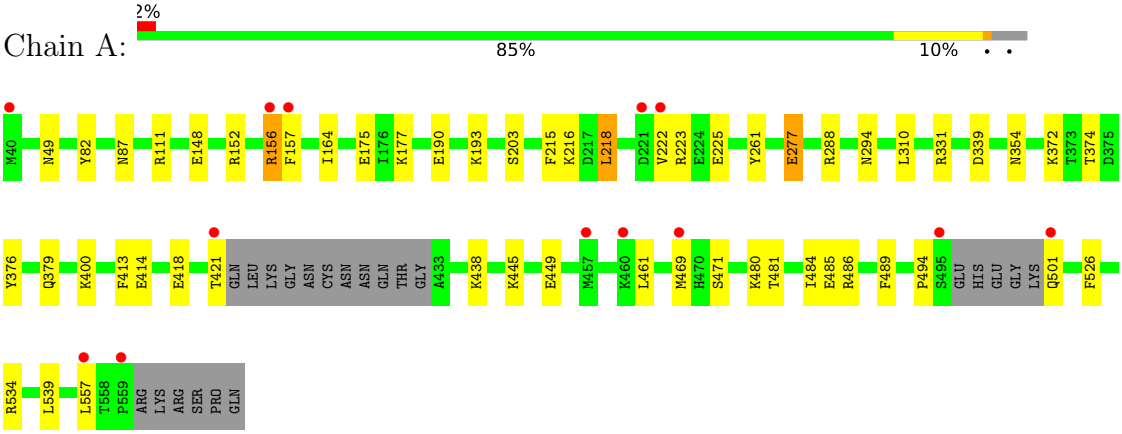
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	362	Total O 362 362	0	0
6	B	385	Total O 385 385	0	0
6	D	354	Total O 354 354	0	0
6	C	381	Total O 381 381	0	0

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.

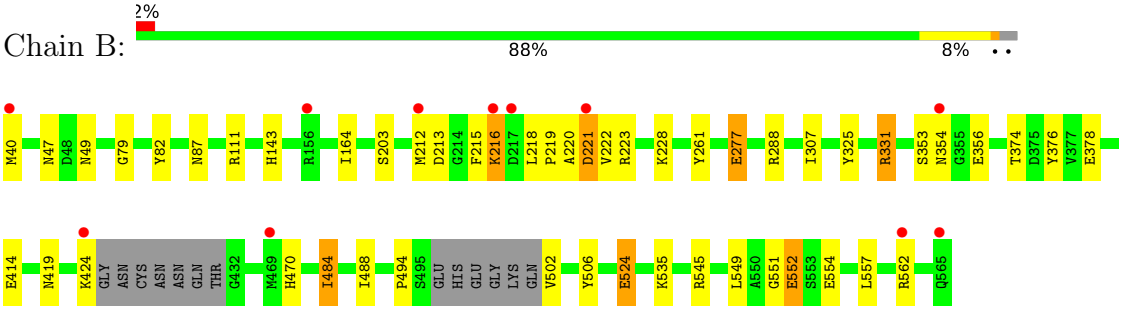
• Molecule 1: ZK177.8

Chain A:



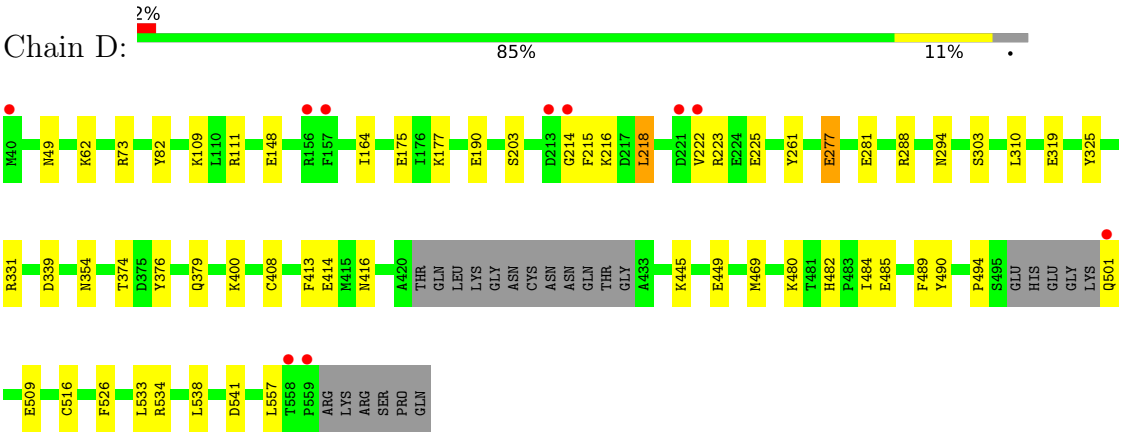
• Molecule 1: ZK177.8

Chain B:



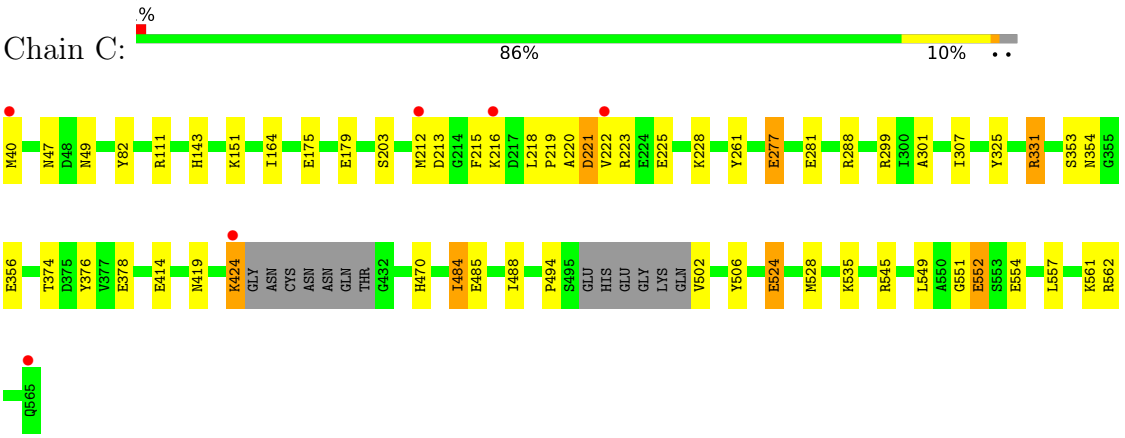
• Molecule 1: ZK177.8

Chain D:



• Molecule 1: ZK177.8

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.68Å 90.56Å 93.36Å 65.58° 65.49° 86.22°	Depositor
Resolution (Å)	46.03 – 1.81 46.03 – 1.81	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.03-1.81) 93.3 (46.03-1.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.182 , 0.209 0.188 , 0.212	Depositor DCC
R_{free} test set	10556 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.449 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18205	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: MG, DTP, GTP, SIN

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	0.90	7/4127 (0.2%)	0.85	0/5559
1	B	0.91	7/4204 (0.2%)	0.88	2/5660 (0.0%)
1	C	0.93	10/4196 (0.2%)	0.90	3/5649 (0.1%)
1	D	0.90	10/4120 (0.2%)	0.85	1/5549 (0.0%)
All	All	0.91	34/16647 (0.2%)	0.87	6/22417 (0.0%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	414	GLU	CD-OE1	9.22	1.35	1.25
1	A	190	GLU	CD-OE2	9.20	1.35	1.25
1	C	414	GLU	CD-OE1	8.74	1.35	1.25
1	D	277	GLU	CD-OE2	7.94	1.34	1.25
1	D	190	GLU	CD-OE2	7.64	1.34	1.25
1	D	277	GLU	CD-OE1	7.60	1.34	1.25
1	A	414	GLU	CD-OE1	7.39	1.33	1.25
1	A	277	GLU	CD-OE1	7.22	1.33	1.25
1	D	414	GLU	CD-OE1	7.21	1.33	1.25
1	B	277	GLU	CD-OE2	6.96	1.33	1.25
1	B	524	GLU	CD-OE1	6.89	1.33	1.25
1	A	485	GLU	CD-OE2	6.73	1.33	1.25
1	C	175	GLU	CD-OE2	6.41	1.32	1.25
1	D	485	GLU	CD-OE2	6.30	1.32	1.25
1	C	277	GLU	CD-OE2	6.14	1.32	1.25
1	D	148	GLU	CD-OE1	6.11	1.32	1.25
1	A	277	GLU	CD-OE2	5.98	1.32	1.25
1	C	378	GLU	CD-OE2	5.81	1.32	1.25
1	C	378	GLU	CD-OE1	5.73	1.31	1.25
1	C	485	GLU	CD-OE2	5.69	1.31	1.25
1	C	524	GLU	CD-OE1	5.68	1.31	1.25
1	D	319	GLU	CD-OE1	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	GLU	CD-OE2	5.57	1.31	1.25
1	D	281	GLU	CD-OE1	5.54	1.31	1.25
1	A	148	GLU	CD-OE1	5.43	1.31	1.25
1	B	552	GLU	CD-OE1	5.43	1.31	1.25
1	A	175	GLU	CD-OE2	5.30	1.31	1.25
1	B	378	GLU	CD-OE2	5.22	1.31	1.25
1	C	277	GLU	CD-OE1	5.21	1.31	1.25
1	B	552	GLU	CD-OE2	5.19	1.31	1.25
1	C	552	GLU	CD-OE1	5.19	1.31	1.25
1	C	179	GLU	CD-OE2	5.16	1.31	1.25
1	D	190	GLU	CD-OE1	5.07	1.31	1.25
1	B	277	GLU	CD-OE1	5.03	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	331	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	B	331	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	B	331	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	C	331	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	C	331	ARG	CG-CD-NE	-5.52	100.21	111.80
1	D	73	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	4040	0	4052	48	0
1	B	4119	0	4143	36	0
1	C	4111	0	4133	49	0
1	D	4033	0	4045	43	0
2	A	60	0	24	1	0
2	B	60	0	24	5	0
2	C	60	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	60	0	24	2	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	0	0
3	D	32	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	16	0	8	2	0
5	B	16	0	8	7	0
5	C	16	0	8	5	0
6	A	362	0	0	13	0
6	B	385	0	0	5	0
6	C	381	0	0	13	0
6	D	354	0	0	10	0
All	All	18205	0	16541	176	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 5.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:DTP:O2G	6:C:701:HOH:O	1.76	1.02
1:D:469:MET:HE3	1:D:469:MET:HA	1.40	1.02
1:A:469:MET:HE3	1:A:469:MET:HA	1.43	1.00
2:B:601:DTP:O2G	2:B:601:DTP:H5'1	1.63	0.99
1:A:376[B]:TYR:OH	1:D:376[B]:TYR:OH	1.55	0.95
1:B:143:HIS:HB2	5:B:605:SIN:H22	1.51	0.89
1:B:307:ILE:HG13	1:B:484:ILE:HD11	1.56	0.87
1:C:307:ILE:HG13	1:C:484:ILE:HD11	1.55	0.85
1:C:143:HIS:HB2	5:C:605:SIN:H22	1.55	0.85
1:C:299:ARG:HB2	1:C:488:ILE:CD1	2.11	0.80
1:A:469:MET:HA	1:A:469:MET:CE	2.14	0.76
1:D:469:MET:HA	1:D:469:MET:CE	2.17	0.73
1:C:281:GLU:OE2	6:C:702:HOH:O	2.08	0.71
1:C:164:ILE:HD11	1:C:203:SER:HB3	1.73	0.71
1:B:164:ILE:HD11	1:B:203:SER:HB3	1.72	0.70
1:B:277:GLU:HG2	6:B:825:HOH:O	1.91	0.70
1:D:400:LYS:NZ	6:D:702:HOH:O	2.25	0.68
1:A:534:ARG:NH1	6:A:701:HOH:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LYS:CE	6:D:958:HOH:O	2.43	0.67
1:D:215:PHE:HA	1:D:218:LEU:HD22	1.75	0.66
1:A:215:PHE:HA	1:A:218:LEU:HD22	1.76	0.66
1:A:164:ILE:HD11	1:A:203:SER:HB3	1.79	0.65
1:D:177:LYS:HE3	6:D:958:HOH:O	1.96	0.65
1:A:111:ARG:HD2	6:A:737:HOH:O	1.98	0.64
1:A:413:PHE:CD1	1:A:557:LEU:HD21	2.33	0.63
1:C:299:ARG:CB	1:C:488:ILE:CD1	2.76	0.62
1:D:164:ILE:HD11	1:D:203:SER:HB3	1.80	0.62
1:B:49:ASN:HA	5:C:604:SIN:H22	1.81	0.62
2:B:601:DTP:H5'1	2:B:601:DTP:PG	2.40	0.62
1:D:218:LEU:HG	1:D:222:VAL:HG11	1.82	0.61
1:A:218:LEU:HG	1:A:222:VAL:HG11	1.83	0.60
1:A:469:MET:HE3	1:A:469:MET:CA	2.28	0.60
1:B:221:ASP:OD2	1:B:221:ASP:N	2.34	0.60
1:C:552:GLU:HG3	1:C:557:LEU:HD11	1.83	0.60
1:B:552:GLU:HG3	1:B:557:LEU:HD11	1.84	0.59
2:D:602:DTP:O3B	2:D:602:DTP:H5'1	2.03	0.58
1:D:413:PHE:CD1	1:D:557:LEU:HD21	2.38	0.58
1:C:219:PRO:HB2	1:C:222:VAL:HG13	1.86	0.58
1:A:400:LYS:NZ	6:A:710:HOH:O	2.37	0.57
1:B:331:ARG:NH2	1:B:470:HIS:O	2.35	0.57
1:C:215:PHE:HA	1:C:218:LEU:HD22	1.87	0.57
2:B:601:DTP:C2	5:B:605:SIN:H21	2.34	0.57
1:A:216:LYS:O	1:A:223:ARG:NH2	2.35	0.56
1:C:554:GLU:OE1	6:C:703:HOH:O	2.17	0.56
1:D:277:GLU:HG2	6:D:747:HOH:O	2.05	0.56
1:C:331:ARG:NH2	1:C:470:HIS:O	2.35	0.56
1:A:469:MET:CE	1:A:469:MET:CA	2.81	0.56
1:B:554:GLU:OE1	6:B:701:HOH:O	2.17	0.55
1:C:277:GLU:HG2	6:C:815:HOH:O	2.05	0.55
1:A:177:LYS:CE	6:A:936:HOH:O	2.54	0.55
1:C:111:ARG:HD2	6:C:733:HOH:O	2.07	0.55
1:B:488[B]:ILE:CG1	1:B:506:TYR:CZ	2.90	0.54
1:D:484:ILE:HD11	1:D:489:PHE:HZ	1.72	0.54
1:C:535:LYS:HE2	6:C:931:HOH:O	2.06	0.54
1:B:535:LYS:HE2	6:B:960:HOH:O	2.07	0.54
1:A:49:ASN:HA	5:A:607:SIN:H32	1.90	0.54
2:C:601:DTP:C2	5:C:605:SIN:H21	2.38	0.53
1:A:177:LYS:HE3	6:A:936:HOH:O	2.08	0.53
1:D:216:LYS:O	1:D:223:ARG:NH2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ASP:OD2	1:C:221:ASP:N	2.40	0.53
1:D:177:LYS:HE2	6:D:958:HOH:O	2.06	0.53
1:C:424:LYS:CE	6:C:1005:HOH:O	2.57	0.53
1:D:111:ARG:HD2	6:D:738:HOH:O	2.08	0.53
1:C:419:ASN:ND2	6:C:705:HOH:O	2.29	0.53
1:B:488[B]:ILE:HG13	1:B:506:TYR:CE2	2.44	0.52
1:C:143:HIS:HB2	5:C:605:SIN:C2	2.35	0.52
1:A:374:THR:OG1	1:A:376[B]:TYR:HB3	2.10	0.52
1:C:220:ALA:HA	1:C:223:ARG:HG3	1.92	0.52
1:D:538:LEU:HD23	1:D:538:LEU:N	2.26	0.51
5:A:606:SIN:H32	1:D:49:ASN:HA	1.91	0.51
1:A:484:ILE:HD11	1:A:489:PHE:HZ	1.75	0.51
1:A:418:GLU:O	1:A:421:THR:HG22	2.12	0.50
1:B:488[B]:ILE:HD11	1:B:506:TYR:OH	2.11	0.50
1:D:469:MET:HE3	1:D:469:MET:CA	2.24	0.50
1:A:193:LYS:NZ	6:A:708:HOH:O	2.34	0.50
1:B:374:THR:OG1	1:B:376[A]:TYR:HB3	2.12	0.49
1:D:62:LYS:HE2	6:D:754:HOH:O	2.12	0.49
1:C:374:THR:OG1	1:C:376[B]:TYR:HB3	2.13	0.49
2:A:601:DTP:O2G	2:A:601:DTP:O2A	2.31	0.49
1:B:307:ILE:CG1	1:B:484:ILE:HD11	2.37	0.49
1:B:376[A]:TYR:CD1	1:C:376[A]:TYR:HB3	2.47	0.49
1:C:488:ILE:HG22	1:C:506:TYR:CZ	2.48	0.49
1:B:143:HIS:HB2	5:B:605:SIN:C2	2.35	0.49
1:D:408:CYS:HB3	1:D:534:ARG:HG3	1.94	0.49
1:A:331:ARG:HG2	1:A:526:PHE:HZ	1.78	0.48
5:B:606:SIN:C3	1:C:47:ASN:HB3	2.44	0.48
1:A:277:GLU:HG2	6:A:816:HOH:O	2.14	0.48
1:A:310:LEU:HB3	1:A:484:ILE:HD13	1.94	0.48
1:C:424:LYS:HE3	6:C:1005:HOH:O	2.14	0.48
1:C:299:ARG:HB2	1:C:488:ILE:HD12	1.95	0.48
1:D:374:THR:OG1	1:D:376[B]:TYR:HB3	2.14	0.47
1:A:177:LYS:HE2	6:A:936:HOH:O	2.14	0.47
1:C:299:ARG:CB	1:C:488:ILE:HD11	2.44	0.47
1:A:288:ARG:CD	1:A:494:PRO:HG2	2.44	0.47
1:D:288:ARG:CD	1:D:494:PRO:HG2	2.45	0.47
1:D:484:ILE:HD11	1:D:489:PHE:CZ	2.49	0.47
1:C:424:LYS:HE2	6:C:1005:HOH:O	2.15	0.47
1:B:47:ASN:HB3	5:C:604:SIN:H32	1.96	0.47
1:D:294:ASN:HB2	1:C:562:ARG:O	2.15	0.47
1:D:310:LEU:HB3	1:D:484:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:PRO:HB2	1:B:222:VAL:HG13	1.97	0.46
1:C:307:ILE:CG1	1:C:484:ILE:HD11	2.35	0.46
1:B:288:ARG:CD	1:B:494:PRO:HG2	2.45	0.46
1:B:376[B]:TYR:HB3	1:C:376[B]:TYR:CD1	2.51	0.46
1:C:288:ARG:CD	1:C:494:PRO:HG2	2.45	0.46
1:C:299:ARG:HB2	1:C:488:ILE:HD11	1.94	0.46
1:A:225:GLU:HA	1:A:225:GLU:OE2	2.16	0.46
1:B:325:TYR:CZ	2:B:601:DTP:H2'1	2.51	0.46
1:A:413:PHE:CG	1:A:557:LEU:HD11	2.50	0.46
1:B:545:ARG:NH2	1:B:549:LEU:HD21	2.31	0.46
1:C:301:ALA:HB2	1:C:488:ILE:HG13	1.98	0.46
1:D:225:GLU:OE2	1:D:225:GLU:HA	2.15	0.45
1:C:551:GLY:HA3	1:C:557:LEU:HD23	1.99	0.45
1:A:354:ASN:OD1	1:A:354:ASN:N	2.50	0.45
1:A:87:ASN:ND2	6:A:724:HOH:O	2.50	0.45
2:B:601:DTP:O2G	2:B:601:DTP:O3A	2.35	0.45
5:B:606:SIN:H22	1:C:49:ASN:HA	1.97	0.45
1:B:419:ASN:ND2	6:B:717:HOH:O	2.44	0.45
1:D:376[B]:TYR:OH	6:D:701:HOH:O	2.19	0.45
1:B:220:ALA:O	1:B:223:ARG:HB2	2.17	0.45
1:C:528:MET:SD	6:C:1054:HOH:O	2.61	0.44
1:C:151:LYS:HE3	6:C:1000:HOH:O	2.17	0.44
1:A:413:PHE:CD2	1:A:557:LEU:HD11	2.52	0.44
1:B:488[B]:ILE:HG13	1:B:506:TYR:CZ	2.51	0.44
1:C:545:ARG:NH2	1:C:549:LEU:HD21	2.32	0.44
1:A:376[A]:TYR:HD2	1:D:379:GLN:HG3	1.82	0.44
1:A:331:ARG:NH1	1:A:471:SER:OG	2.51	0.44
1:C:215:PHE:O	1:C:218:LEU:HB2	2.18	0.44
1:C:307:ILE:HG13	1:C:484:ILE:CD1	2.38	0.44
1:B:216:LYS:H	1:B:216:LYS:HG3	1.51	0.44
1:B:551:GLY:HA3	1:B:557:LEU:HD23	2.00	0.44
1:A:156:ARG:HG2	1:A:157:PHE:N	2.33	0.43
1:B:307:ILE:HG13	1:B:484:ILE:CD1	2.37	0.43
1:D:534:ARG:NE	6:D:728:HOH:O	2.52	0.43
1:A:288:ARG:HD2	1:A:494:PRO:HG2	2.00	0.43
1:A:294:ASN:HB2	1:B:562:ARG:O	2.19	0.43
1:A:331:ARG:HG2	1:A:526:PHE:CZ	2.54	0.43
1:A:331:ARG:HA	1:A:331:ARG:HD3	1.91	0.43
1:B:111:ARG:HD2	6:B:737:HOH:O	2.18	0.42
5:B:606:SIN:H32	1:C:47:ASN:HB3	2.01	0.42
1:A:461:LEU:CD1	1:A:539:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:GLU:HG3	1:C:561:LYS:HD2	2.01	0.42
1:B:228:LYS:HD2	1:B:228:LYS:HA	1.71	0.42
1:A:481:THR:HG21	1:A:486:ARG:HD2	2.01	0.42
1:D:354:ASN:OD1	1:D:354:ASN:N	2.50	0.42
1:D:445:LYS:O	1:D:449:GLU:HG3	2.19	0.42
1:A:152:ARG:NH2	6:A:728:HOH:O	2.52	0.42
1:A:379:GLN:HG3	1:D:376[A]:TYR:HD2	1.85	0.42
1:C:223:ARG:HG3	1:C:223:ARG:HH11	1.84	0.42
1:C:353:SER:O	1:C:354:ASN:HB2	2.20	0.42
1:A:372:LYS:HD2	6:A:941:HOH:O	2.19	0.41
1:A:445:LYS:O	1:A:449:GLU:HG3	2.19	0.41
1:D:331:ARG:HA	1:D:331:ARG:HD3	1.92	0.41
1:A:461:LEU:HD12	1:A:539:LEU:HD22	2.01	0.41
1:A:484:ILE:HD11	1:A:489:PHE:CZ	2.54	0.41
1:D:482:HIS:CE1	1:D:516:CYS:HB3	2.55	0.41
1:A:438:LYS:HG3	6:A:712:HOH:O	2.21	0.41
1:D:303[B]:SER:HG	1:D:490:TYR:HH	1.68	0.41
1:D:325:TYR:CZ	2:D:602:DTP:H2'1	2.56	0.41
1:A:501:GLN:NE2	6:A:739:HOH:O	2.54	0.41
1:B:470:HIS:HA	1:B:524:GLU:O	2.21	0.41
1:D:216:LYS:HA	1:D:223:ARG:NH2	2.36	0.41
1:D:331:ARG:HG2	1:D:526:PHE:HZ	1.86	0.41
1:D:501:GLN:NE2	6:D:735:HOH:O	2.53	0.41
1:B:79:GLY:HA3	5:B:605:SIN:C4	2.51	0.41
1:B:353:SER:O	1:B:354:ASN:HB2	2.20	0.41
1:C:223:ARG:HG3	1:C:223:ARG:NH1	2.36	0.41
1:C:470:HIS:HA	1:C:524:GLU:O	2.22	0.41
1:C:488:ILE:CG2	1:C:506:TYR:CZ	3.04	0.41
1:B:215:PHE:HA	1:B:218:LEU:HD22	2.03	0.40
1:D:416:ASN:HB2	6:C:900:HOH:O	2.21	0.40
1:D:214:GLY:O	1:D:218:LEU:HD13	2.22	0.40
1:C:228:LYS:HD2	1:C:228:LYS:HA	1.72	0.40
1:A:216:LYS:HA	1:A:223:ARG:NH2	2.36	0.40
1:D:288:ARG:HD2	1:D:494:PRO:HG2	2.03	0.40
1:C:325:TYR:CZ	2:C:601:DTP:H2'1	2.56	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	502/526 (95%)	494 (98%)	8 (2%)	0	100	100
1	B	511/526 (97%)	500 (98%)	11 (2%)	0	100	100
1	C	510/526 (97%)	499 (98%)	11 (2%)	0	100	100
1	D	501/526 (95%)	494 (99%)	7 (1%)	0	100	100
All	All	2024/2104 (96%)	1987 (98%)	37 (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	452/467 (97%)	446 (99%)	6 (1%)	69	61
1	B	460/467 (98%)	448 (97%)	12 (3%)	46	32
1	C	459/467 (98%)	447 (97%)	12 (3%)	46	32
1	D	451/467 (97%)	443 (98%)	8 (2%)	59	48
All	All	1822/1868 (98%)	1784 (98%)	38 (2%)	53	41

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	156	ARG

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Mol	Chain	Res	Type
1	A	218	LEU
1	A	261	TYR
1	A	339	ASP
1	A	480	LYS
1	B	40	MET
1	B	82	TYR
1	B	87	ASN
1	B	212	MET
1	B	213	ASP
1	B	216	LYS
1	B	221	ASP
1	B	261	TYR
1	B	356	GLU
1	B	424	LYS
1	B	484	ILE
1	B	502	VAL
1	D	82	TYR
1	D	109	LYS
1	D	218	LEU
1	D	261	TYR
1	D	339	ASP
1	D	480	LYS
1	D	533	LEU
1	D	541	ASP
1	C	40	MET
1	C	82	TYR
1	C	212	MET
1	C	213	ASP
1	C	216	LYS
1	C	221	ASP
1	C	225	GLU
1	C	261	TYR
1	C	356	GLU
1	C	424	LYS
1	C	484	ILE
1	C	502	VAL

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	87	ASN
1	B	210	GLN

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Mol	Chain	Res	Type
1	B	548	GLN
1	D	87	ASN
1	C	210	GLN
1	C	548	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 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DTP	D	602	-	26,32,32	0.87	1 (3%)	30,50,50	0.99	2 (6%)
3	GTP	D	603	4	26,34,34	1.06	3 (11%)	32,54,54	1.24	4 (12%)
3	GTP	C	602	4	26,34,34	1.22	3 (11%)	32,54,54	1.14	5 (15%)
2	DTP	C	601	-	26,32,32	0.92	1 (3%)	30,50,50	1.04	1 (3%)
3	GTP	A	602	4	26,34,34	1.06	3 (11%)	32,54,54	1.15	2 (6%)
2	DTP	C	603	4	26,32,32	1.03	2 (7%)	30,50,50	0.81	1 (3%)
5	SIN	A	607	-	7,7,7	1.44	1 (14%)	8,8,8	1.21	1 (12%)
5	SIN	B	605	-	7,7,7	0.81	0	8,8,8	1.32	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DTP	A	601	-	26,32,32	0.74	0	30,50,50	0.95	1 (3%)
3	GTP	B	602	4	26,34,34	1.23	3 (11%)	32,54,54	1.05	2 (6%)
5	SIN	B	606	-	7,7,7	1.07	0	8,8,8	1.16	0
5	SIN	A	606	-	7,7,7	1.23	0	8,8,8	2.09	3 (37%)
5	SIN	C	604	-	7,7,7	1.01	0	8,8,8	1.23	0
2	DTP	A	603	4	26,32,32	0.89	0	30,50,50	1.07	2 (6%)
2	DTP	B	601	-	26,32,32	0.86	1 (3%)	30,50,50	1.02	1 (3%)
2	DTP	D	604	4	26,32,32	0.94	0	30,50,50	1.01	1 (3%)
2	DTP	B	603	4	26,32,32	0.98	0	30,50,50	0.89	1 (3%)
5	SIN	C	605	-	7,7,7	1.61	2 (28%)	8,8,8	1.21	1 (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
2	DTP	D	602	-	-	1/18/34/34	0/3/3/3
3	GTP	D	603	4	-	3/18/38/38	0/3/3/3
3	GTP	C	602	4	-	3/18/38/38	0/3/3/3
2	DTP	C	601	-	-	1/18/34/34	0/3/3/3
3	GTP	A	602	4	-	2/18/38/38	0/3/3/3
2	DTP	C	603	4	-	4/18/34/34	0/3/3/3
5	SIN	A	607	-	-	2/5/5/5	-
5	SIN	B	605	-	-	2/5/5/5	-
2	DTP	A	601	-	-	3/18/34/34	0/3/3/3
3	GTP	B	602	4	-	3/18/38/38	0/3/3/3
5	SIN	B	606	-	-	1/5/5/5	-
5	SIN	A	606	-	-	3/5/5/5	-
5	SIN	C	604	-	-	1/5/5/5	-
2	DTP	A	603	4	-	4/18/34/34	0/3/3/3
2	DTP	B	601	-	-	1/18/34/34	0/3/3/3
2	DTP	D	604	4	-	4/18/34/34	0/3/3/3
2	DTP	B	603	4	-	2/18/34/34	0/3/3/3
5	SIN	C	605	-	-	3/5/5/5	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	GTP	C5-C6	-2.86	1.41	1.47
3	B	602	GTP	PG-O2G	-2.82	1.44	1.54
3	B	602	GTP	C5-C6	-2.81	1.41	1.47
5	C	605	SIN	O1-C1	2.73	1.31	1.22
3	A	602	GTP	C8-N7	-2.63	1.30	1.35
3	A	602	GTP	C5-C6	-2.61	1.42	1.47
2	C	601	DTP	PA-O5'	2.60	1.69	1.59
5	A	607	SIN	O3-C4	2.44	1.30	1.22
3	D	603	GTP	C5-C4	-2.41	1.36	1.43
2	C	603	DTP	C8-N7	-2.31	1.30	1.34
3	A	602	GTP	C5-C4	-2.21	1.37	1.43
2	C	603	DTP	PG-O3G	-2.21	1.46	1.54
3	B	602	GTP	C5-C4	-2.17	1.37	1.43
3	C	602	GTP	C5-C6	-2.17	1.43	1.47
2	D	602	DTP	C1'-N9	-2.16	1.43	1.49
3	D	603	GTP	C8-N7	-2.15	1.31	1.35
3	C	602	GTP	C5-C4	-2.15	1.37	1.43
5	C	605	SIN	O4-C4	-2.12	1.23	1.30
3	C	602	GTP	PG-O3G	-2.08	1.46	1.54
2	B	601	DTP	PA-O5'	2.01	1.67	1.59

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	606	SIN	C2-C3-C4	3.90	122.00	113.60
2	A	603	DTP	C5-C6-N6	3.74	126.03	120.35
3	D	603	GTP	C3'-C2'-C1'	3.34	106.01	100.98
2	C	601	DTP	C5-C6-N6	3.31	125.38	120.35
2	D	604	DTP	C5-C6-N6	3.13	125.10	120.35
2	B	601	DTP	C5-C6-N6	3.05	124.99	120.35
2	D	602	DTP	PA-O3A-PB	-2.93	122.77	132.83
2	A	601	DTP	C5-C6-N6	2.91	124.77	120.35
2	D	602	DTP	C5-C6-N6	2.78	124.58	120.35
3	D	603	GTP	O2G-PG-O3B	2.74	113.83	104.64
3	A	602	GTP	O2G-PG-O3B	2.72	113.77	104.64
3	A	602	GTP	C3'-C2'-C1'	2.70	105.05	100.98
2	B	603	DTP	C5-C6-N6	2.68	124.42	120.35
5	A	607	SIN	C2-C3-C4	2.61	119.23	113.60
5	A	606	SIN	O4-C4-C3	2.53	122.17	114.03
5	C	605	SIN	C3-C2-C1	2.50	118.97	113.60
3	C	602	GTP	O2'-C2'-C1'	-2.44	101.83	110.85
3	B	602	GTP	O3G-PG-O2G	2.41	116.83	107.64
5	A	606	SIN	O3-C4-C3	-2.37	115.47	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	603	DTP	O2A-PA-O1A	2.36	123.90	112.24
2	C	603	DTP	C5-C6-N6	2.27	123.81	120.35
3	C	602	GTP	C3'-C2'-C1'	2.25	104.36	100.98
3	B	602	GTP	C3'-C2'-C1'	2.21	104.31	100.98
3	D	603	GTP	O6-C6-C5	2.11	128.49	124.37
3	C	602	GTP	O3G-PG-O2G	2.10	115.64	107.64
3	C	602	GTP	O6-C6-C5	2.03	128.33	124.37
3	C	602	GTP	PA-O3A-PB	-2.03	125.87	132.83
3	D	603	GTP	O2'-C2'-C1'	-2.02	103.39	110.85
5	B	605	SIN	O1-C1-C2	-2.01	116.63	123.08

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	605	SIN	C1-C2-C3-C4
5	C	605	SIN	C1-C2-C3-C4
5	A	606	SIN	C1-C2-C3-C4
5	A	607	SIN	C1-C2-C3-C4
2	B	601	DTP	PG-O3B-PB-O3A
2	C	601	DTP	PB-O3B-PG-O1G
2	A	603	DTP	PA-O3A-PB-O2B
2	B	603	DTP	PA-O3A-PB-O1B
2	D	604	DTP	PA-O3A-PB-O2B
2	C	603	DTP	PA-O3A-PB-O1B
3	D	603	GTP	C4'-C5'-O5'-PA
2	A	601	DTP	PB-O3A-PA-O2A
3	B	602	GTP	C4'-C5'-O5'-PA
3	C	602	GTP	C4'-C5'-O5'-PA
2	A	601	DTP	PB-O3A-PA-O1A
2	A	603	DTP	PA-O3A-PB-O1B
2	A	603	DTP	PB-O3A-PA-O1A
2	D	602	DTP	PB-O3A-PA-O1A
2	D	604	DTP	PA-O3A-PB-O1B
2	D	604	DTP	PB-O3A-PA-O1A
2	C	603	DTP	PG-O3B-PB-O1B
2	C	603	DTP	PG-O3B-PB-O2B
3	A	602	GTP	C4'-C5'-O5'-PA
3	B	602	GTP	PB-O3A-PA-O1A
3	C	602	GTP	PB-O3A-PA-O2A
5	C	605	SIN	O1-C1-C2-C3
2	A	601	DTP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	A	603	DTP	PB-O3A-PA-O2A
2	B	603	DTP	PA-O3A-PB-O2B
2	D	604	DTP	PB-O3A-PA-O2A
2	C	603	DTP	PA-O3A-PB-O2B
3	A	602	GTP	PB-O3A-PA-O2A
3	B	602	GTP	PB-O3A-PA-O2A
3	D	603	GTP	PB-O3A-PA-O1A
3	D	603	GTP	PB-O3A-PA-O2A
3	C	602	GTP	PB-O3A-PA-O1A
5	C	605	SIN	O2-C1-C2-C3
5	A	606	SIN	C2-C3-C4-O4
5	A	607	SIN	O2-C1-C2-C3
5	C	604	SIN	C2-C3-C4-O4
5	B	605	SIN	C2-C3-C4-O3
5	B	606	SIN	C1-C2-C3-C4
5	A	606	SIN	C2-C3-C4-O3

There are no ring outliers.

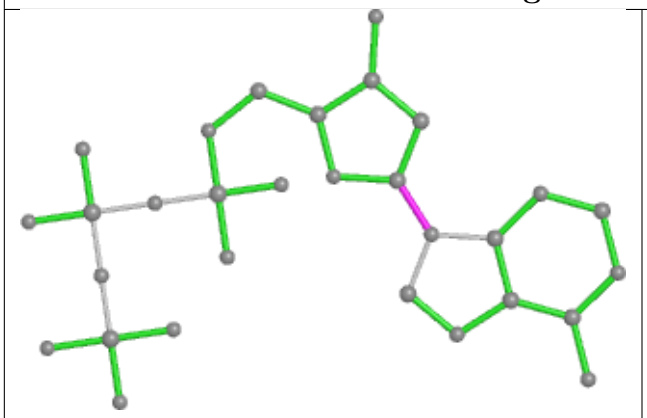
10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	DTP	2	0
2	C	601	DTP	3	0
5	A	607	SIN	1	0
5	B	605	SIN	4	0
2	A	601	DTP	1	0
5	B	606	SIN	3	0
5	A	606	SIN	1	0
5	C	604	SIN	2	0
2	B	601	DTP	5	0
5	C	605	SIN	3	0

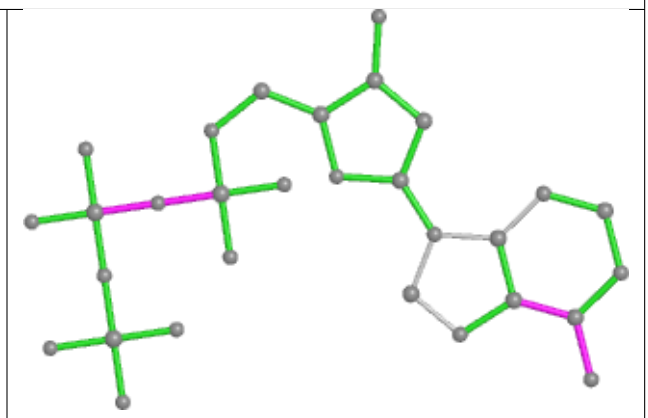
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

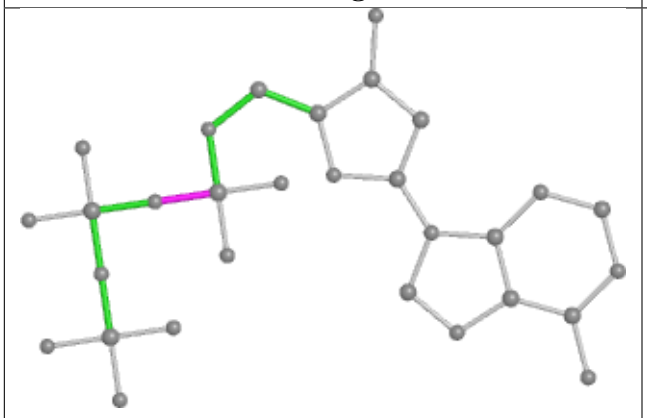
Ligand DTP D 602



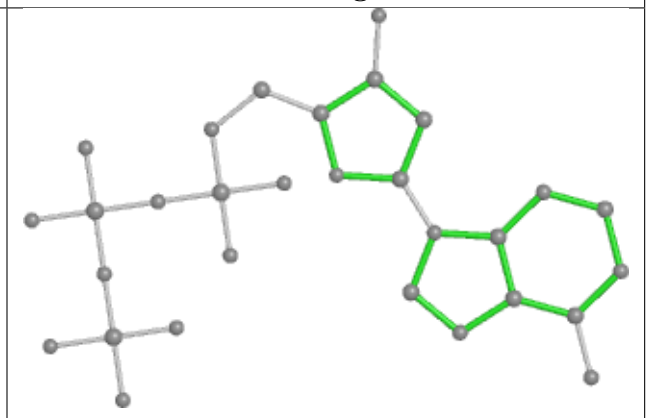
Bond lengths



Bond angles

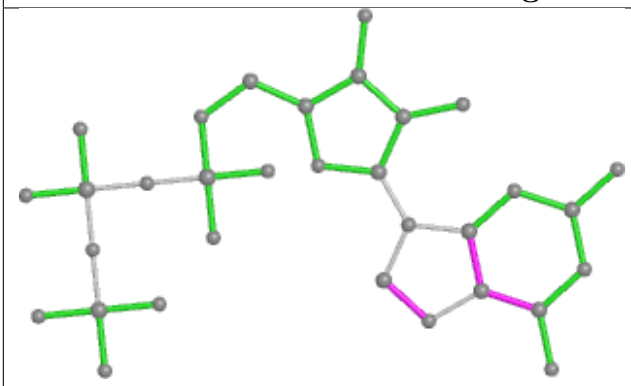


Torsions

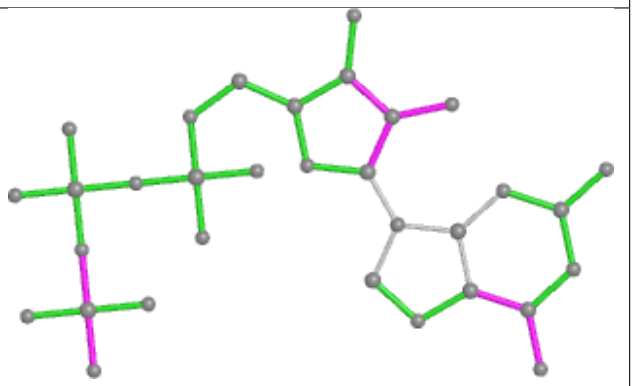


Rings

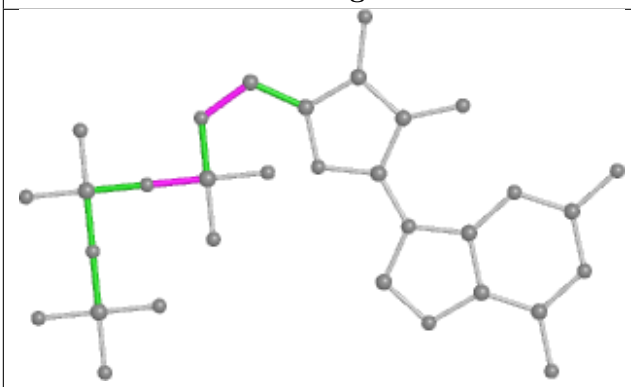
Ligand GTP D 603



Bond lengths



Bond angles



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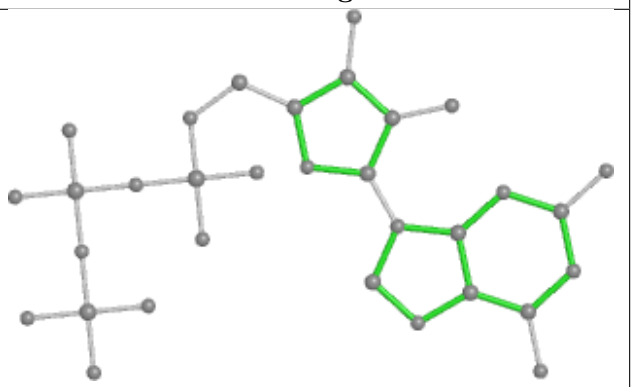
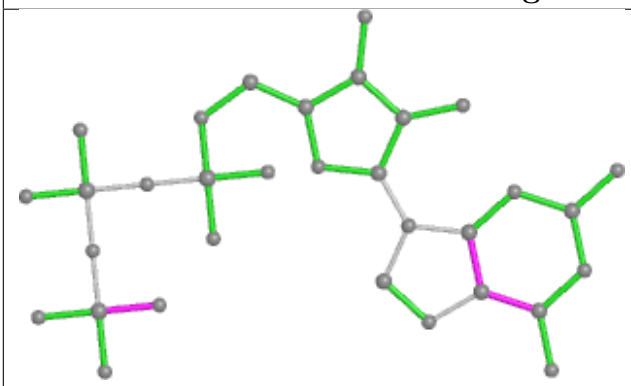


Rings

Ligand GTP C 602



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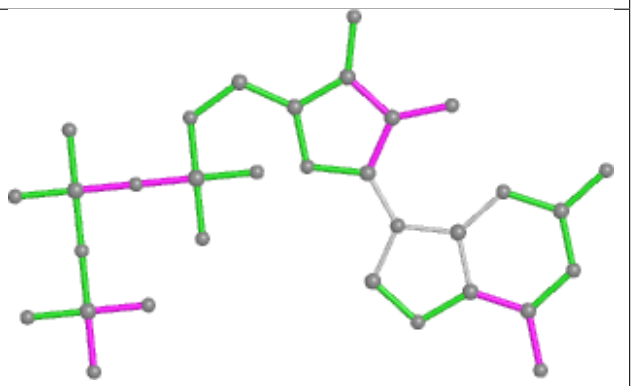
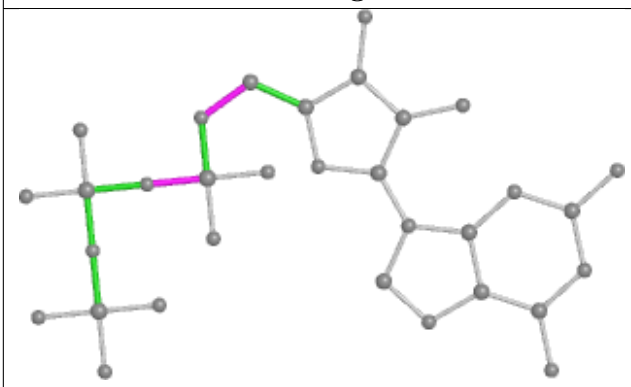


Bond angles



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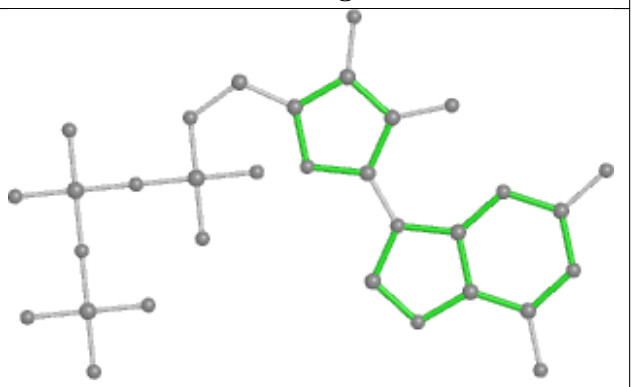
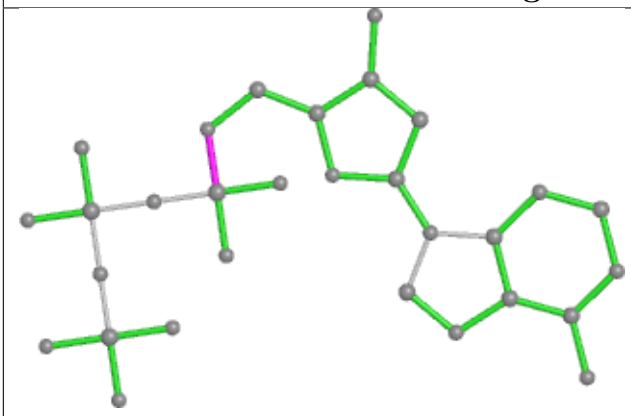


Rings

Ligand DTP C 601



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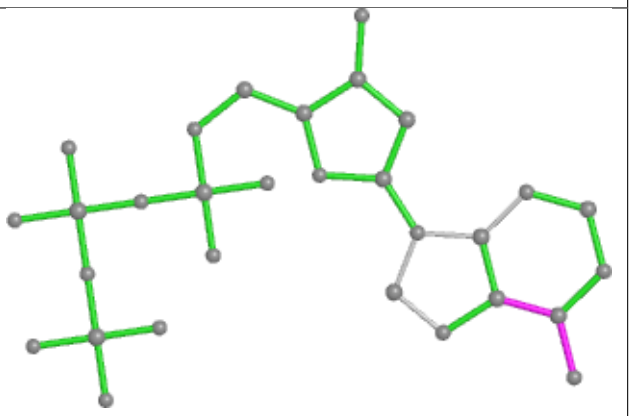

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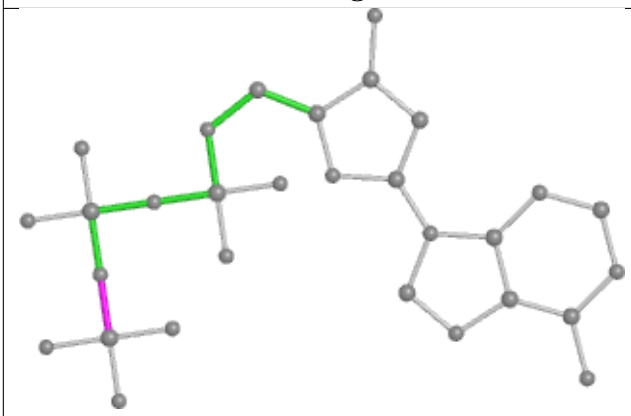

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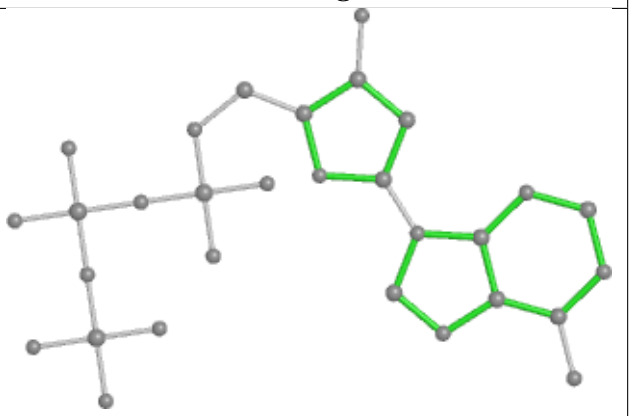
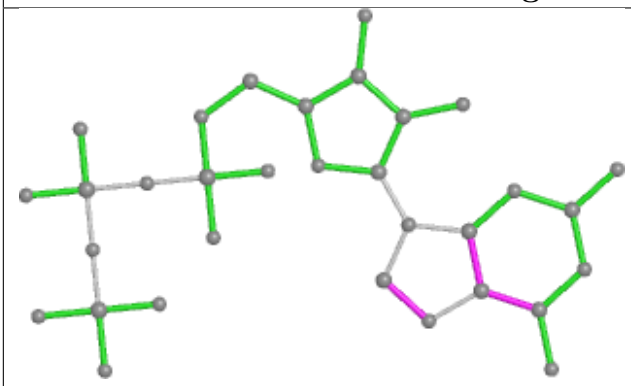


Rings

Ligand GTP A 602



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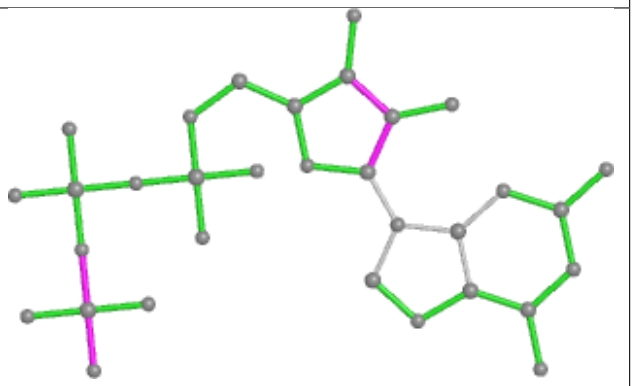

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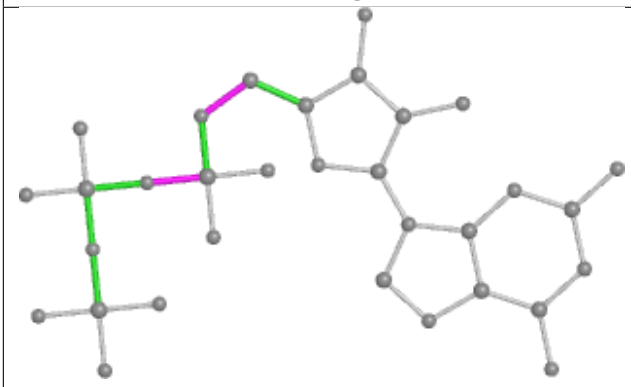

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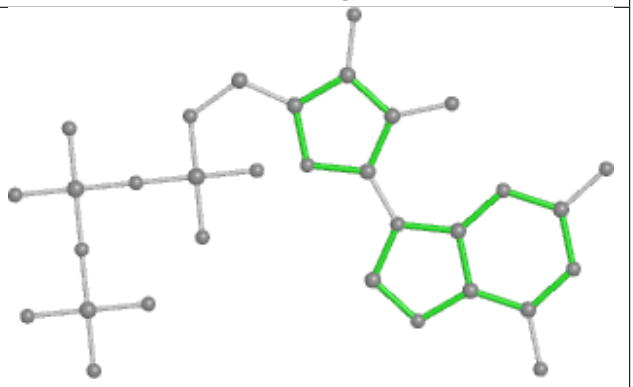
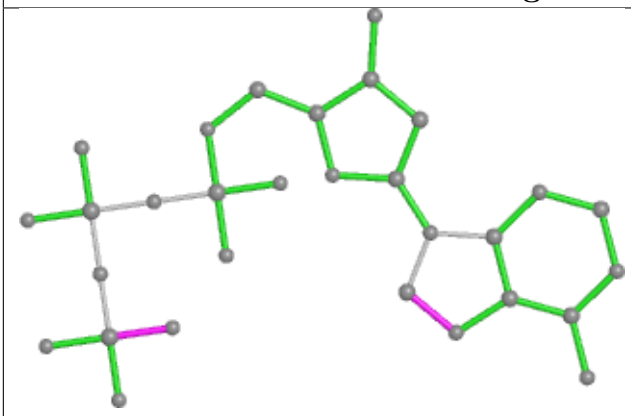


Rings

Ligand DTP C 603



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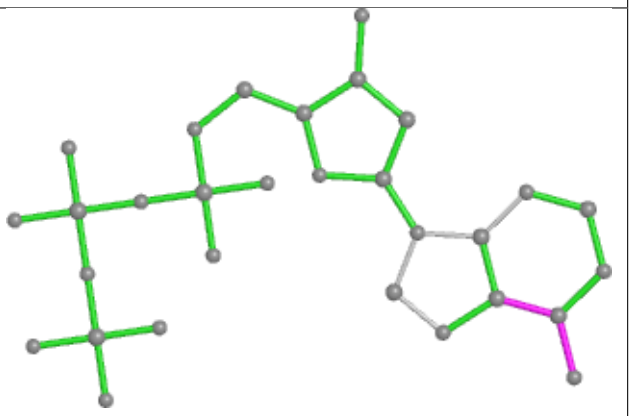

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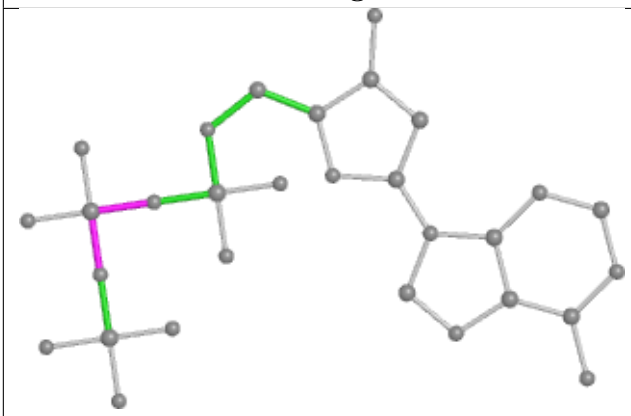

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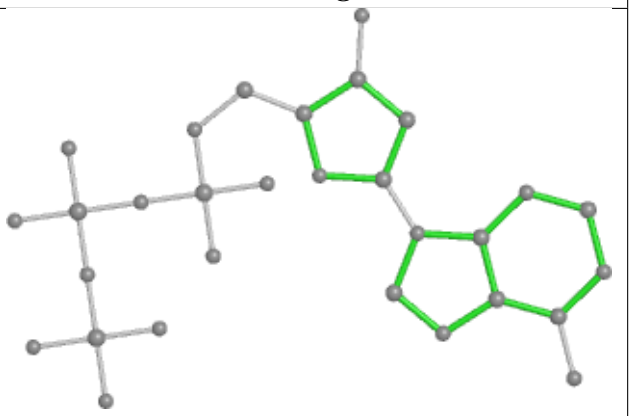
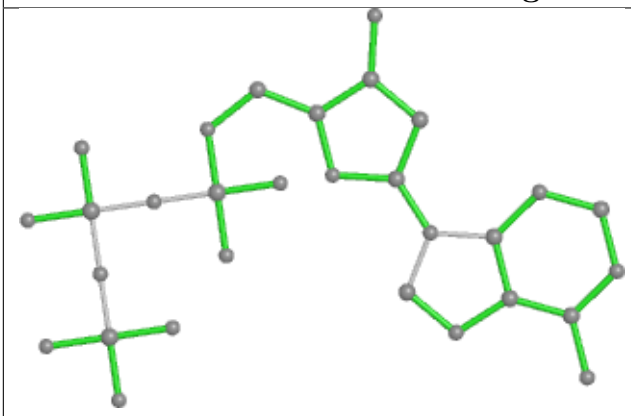


Rings

Ligand DTP A 601



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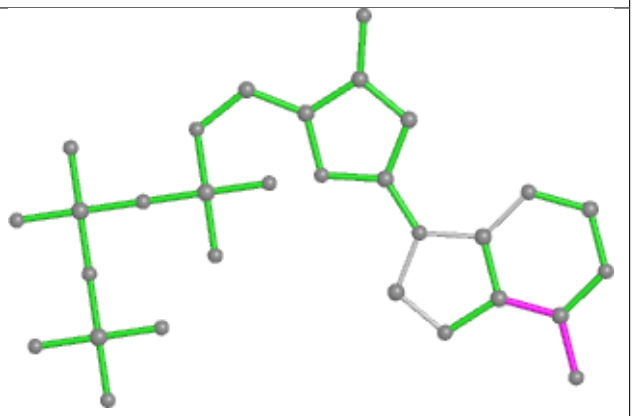

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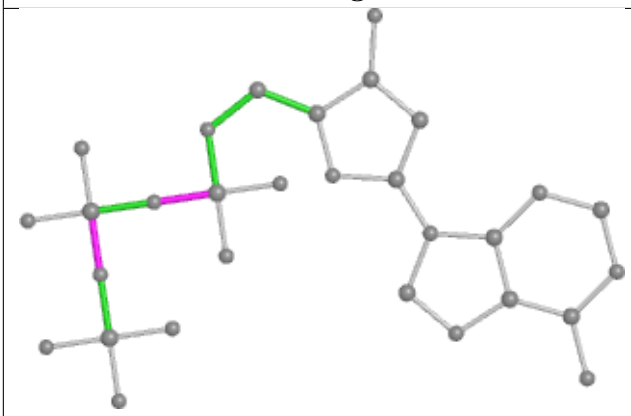

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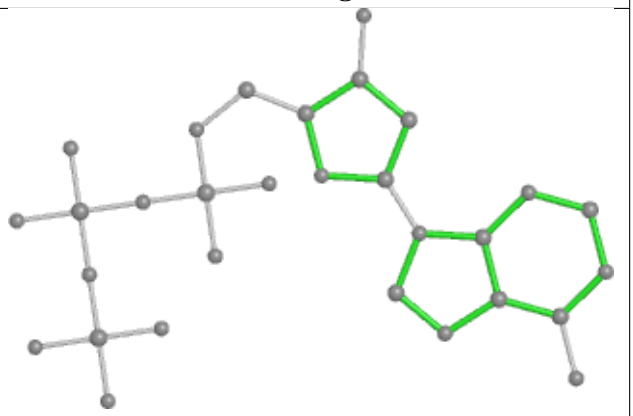
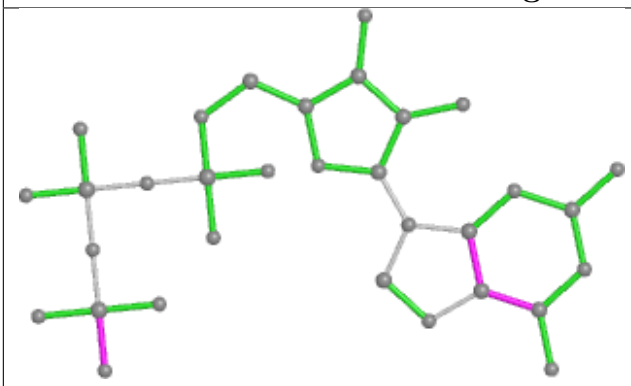


Rings

Ligand GTP B 602



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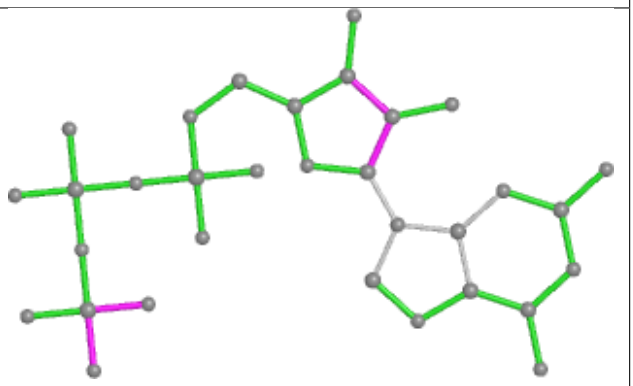

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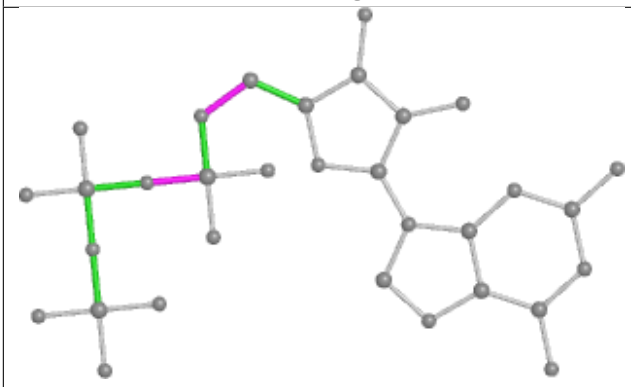

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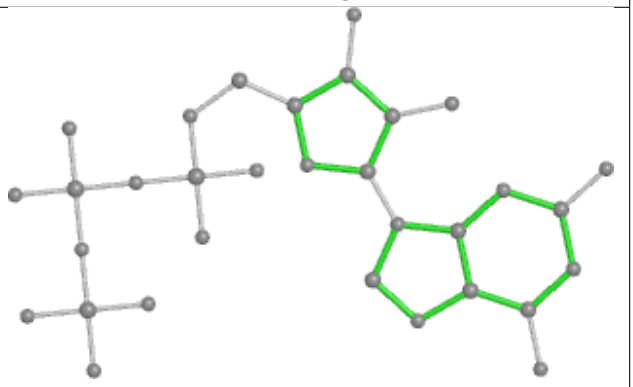
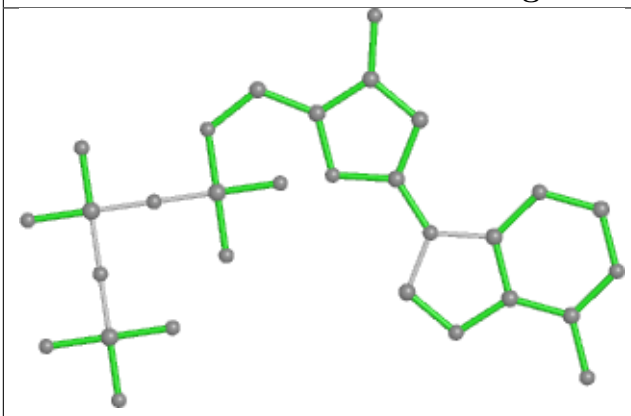


Rings

Ligand DTP A 603



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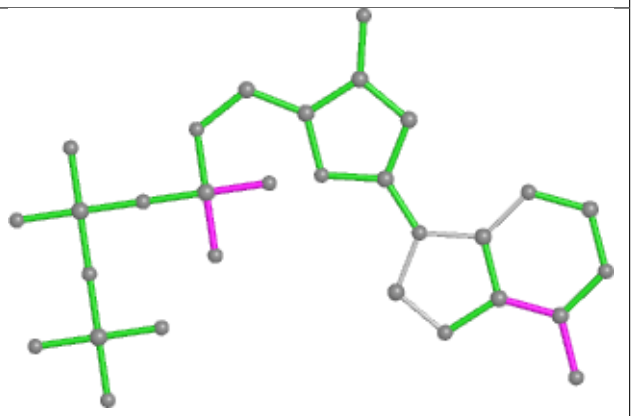

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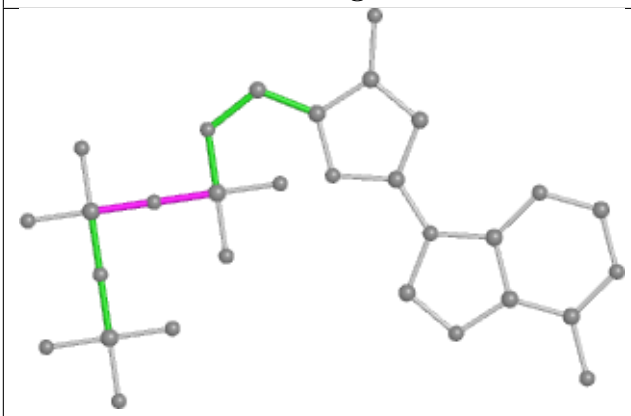

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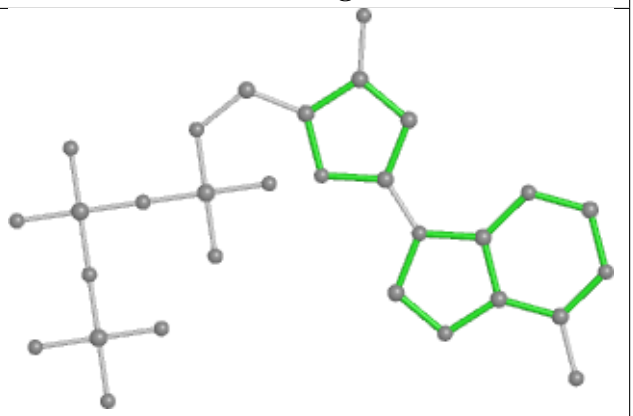
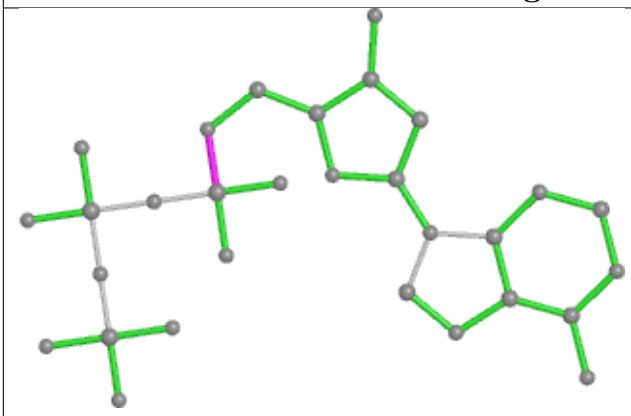


Rings

Ligand DTP B 601



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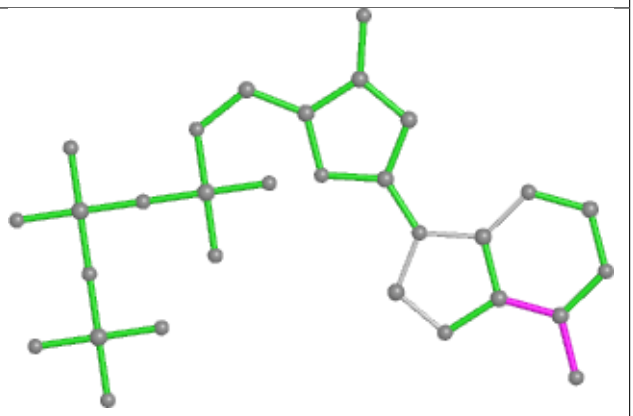

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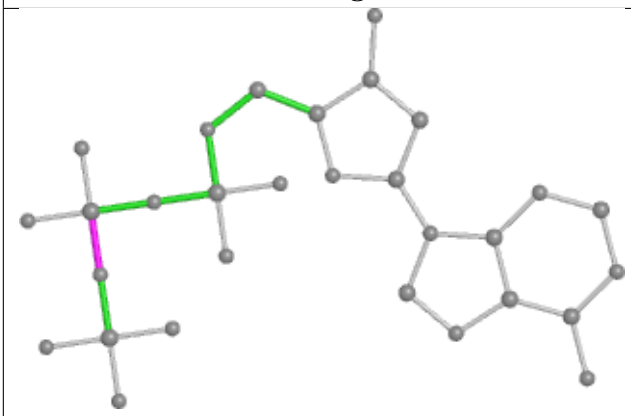

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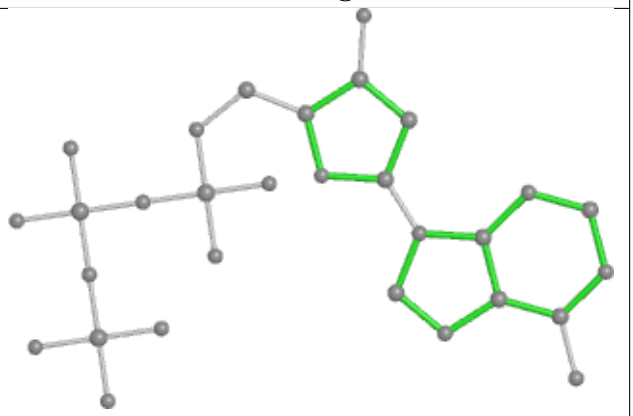
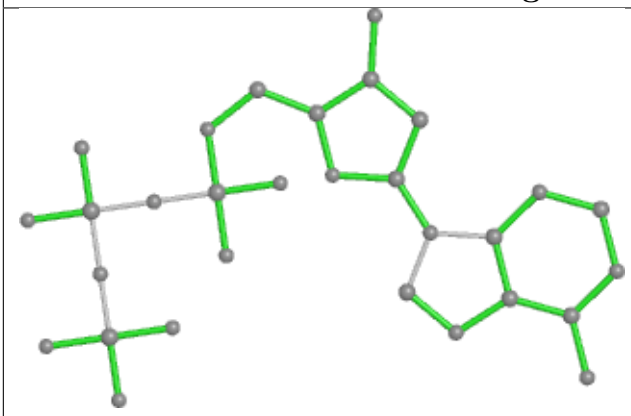


Rings

Ligand DTP D 604



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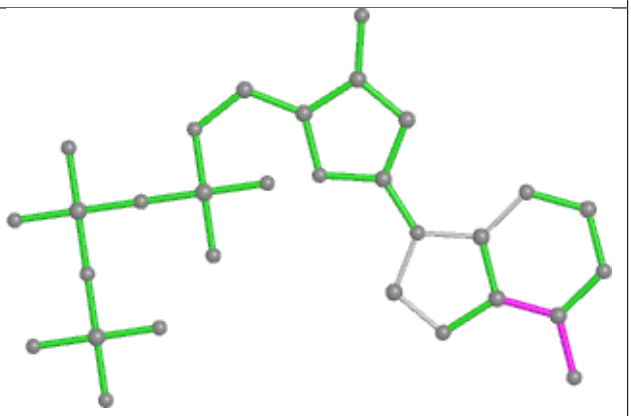

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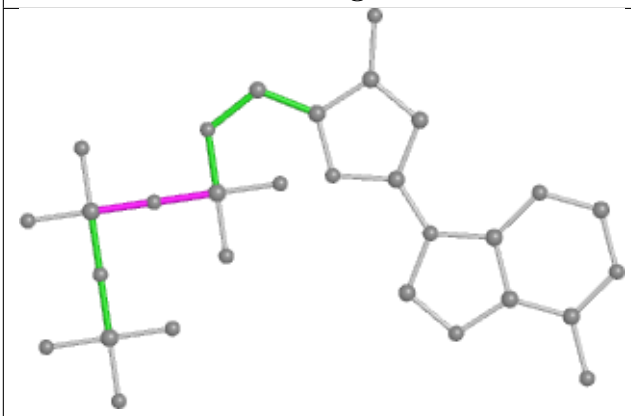

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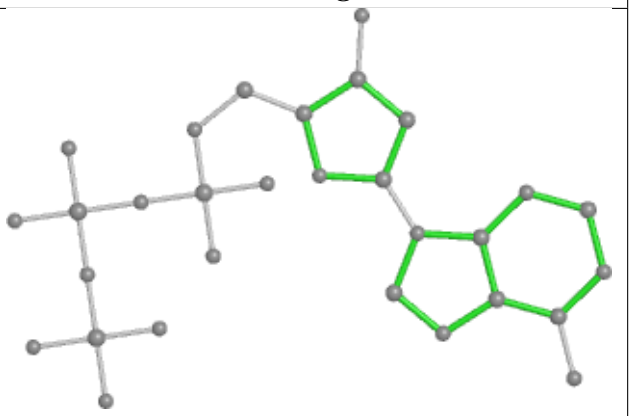
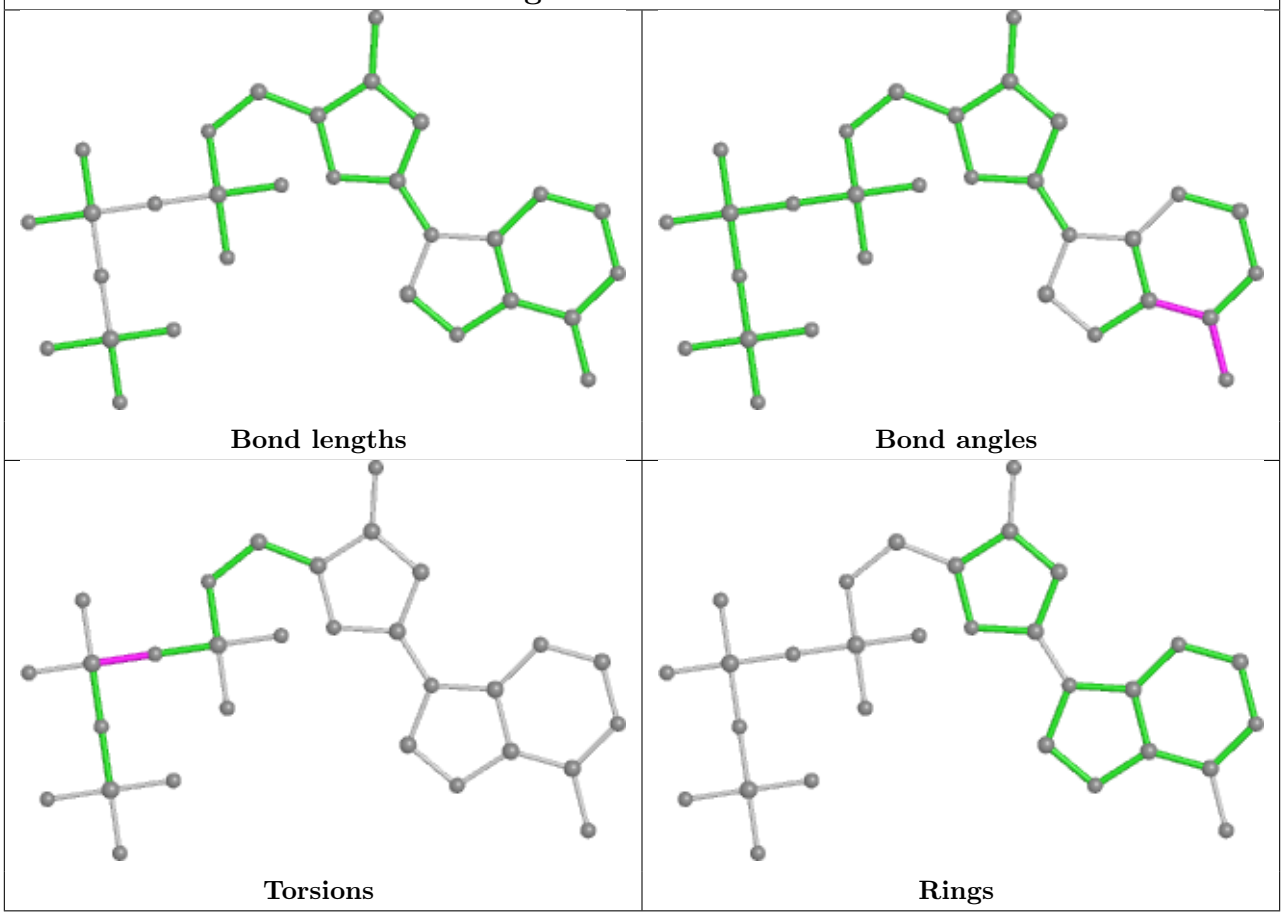


Rings

Ligand DTP B 603



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, 95^{th} 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	504/526 (95%)	-0.19	13 (2%)	56	51	11, 26, 66, 92	0
1	B	513/526 (97%)	-0.21	11 (2%)	63	59	9, 24, 66, 102	0
1	C	513/526 (97%)	-0.20	6 (1%)	79	76	10, 24, 67, 102	0
1	D	503/526 (95%)	-0.20	10 (1%)	65	61	10, 26, 64, 93	0
All	All	2033/2104 (96%)	-0.20	40 (1%)	65	61	9, 25, 67, 102	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	565	GLN	4.2
1	A	559	PRO	4.2
1	B	565	GLN	4.1
1	D	559	PRO	3.9
1	D	40	MET	3.7
1	A	157	PHE	3.7
1	D	213	ASP	3.6
1	D	156	ARG	3.5
1	C	40	MET	3.1
1	C	216	LYS	3.1
1	D	558	THR	2.9
1	D	222	VAL	2.9
1	D	214	GLY	2.7
1	A	156	ARG	2.7
1	A	222	VAL	2.7
1	A	501	GLN	2.7
1	A	557	LEU	2.6
1	B	212	MET	2.6
1	D	501	GLN	2.5
1	A	221	ASP	2.5
1	A	421	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	40	MET	2.5
1	B	424	LYS	2.5
1	D	157	PHE	2.5
1	A	457	MET	2.4
1	B	562	ARG	2.4
1	C	424	LYS	2.4
1	A	460	LYS	2.4
1	C	212	MET	2.3
1	B	221	ASP	2.3
1	C	222	VAL	2.3
1	B	216	LYS	2.3
1	A	40	MET	2.2
1	B	217	ASP	2.2
1	B	469	MET	2.2
1	B	354	ASN	2.1
1	B	156	ARG	2.0
1	A	495	SER	2.0
1	D	221	ASP	2.0
1	A	469	MET	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, 95^{th} 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
5	SIN	B	606	8/8	0.72	0.30	36,54,70,72	0
5	SIN	A	606	8/8	0.76	0.32	34,48,59,62	0
5	SIN	C	605	8/8	0.77	0.30	48,52,58,64	0
5	SIN	A	607	8/8	0.78	0.34	30,45,61,62	0

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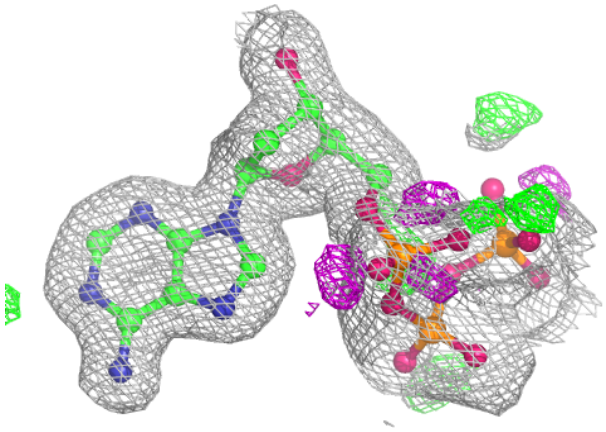
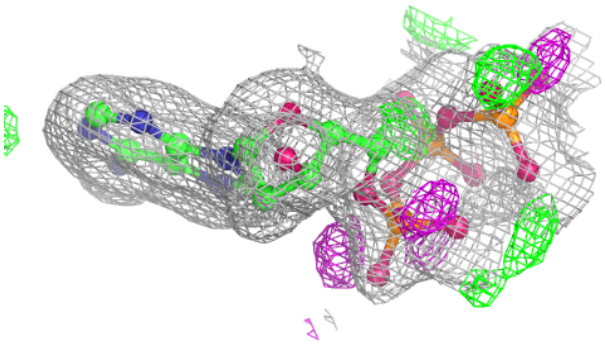
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SIN	B	605	8/8	0.79	0.38	50,52,55,66	0
5	SIN	C	604	8/8	0.82	0.29	37,45,57,72	0
2	DTP	A	601	30/30	0.94	0.09	19,22,125,128	0
2	DTP	B	601	30/30	0.94	0.10	14,20,90,103	0
2	DTP	C	601	30/30	0.95	0.09	16,20,93,102	0
2	DTP	D	602	30/30	0.96	0.09	17,25,120,129	0
3	GTP	B	602	32/32	0.98	0.10	10,11,18,20	0
3	GTP	D	603	32/32	0.98	0.09	12,15,22,23	0
3	GTP	C	602	32/32	0.98	0.09	9,11,17,19	0
4	MG	D	601	1/1	0.98	0.13	15,15,15,15	0
3	GTP	A	602	32/32	0.98	0.09	11,14,22,23	0
2	DTP	D	604	30/30	0.99	0.07	10,12,14,16	0
2	DTP	B	603	30/30	0.99	0.08	9,11,12,13	0
2	DTP	C	603	30/30	0.99	0.08	9,11,12,13	0
4	MG	A	605	1/1	0.99	0.12	18,18,18,18	0
4	MG	B	604	1/1	0.99	0.12	13,13,13,13	0
2	DTP	A	603	30/30	0.99	0.09	11,12,15,16	0
4	MG	A	604	1/1	1.00	0.13	12,12,12,12	0

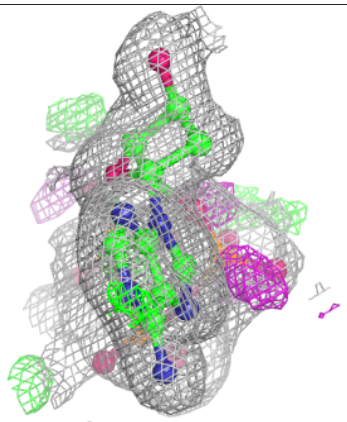
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP A 601:

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

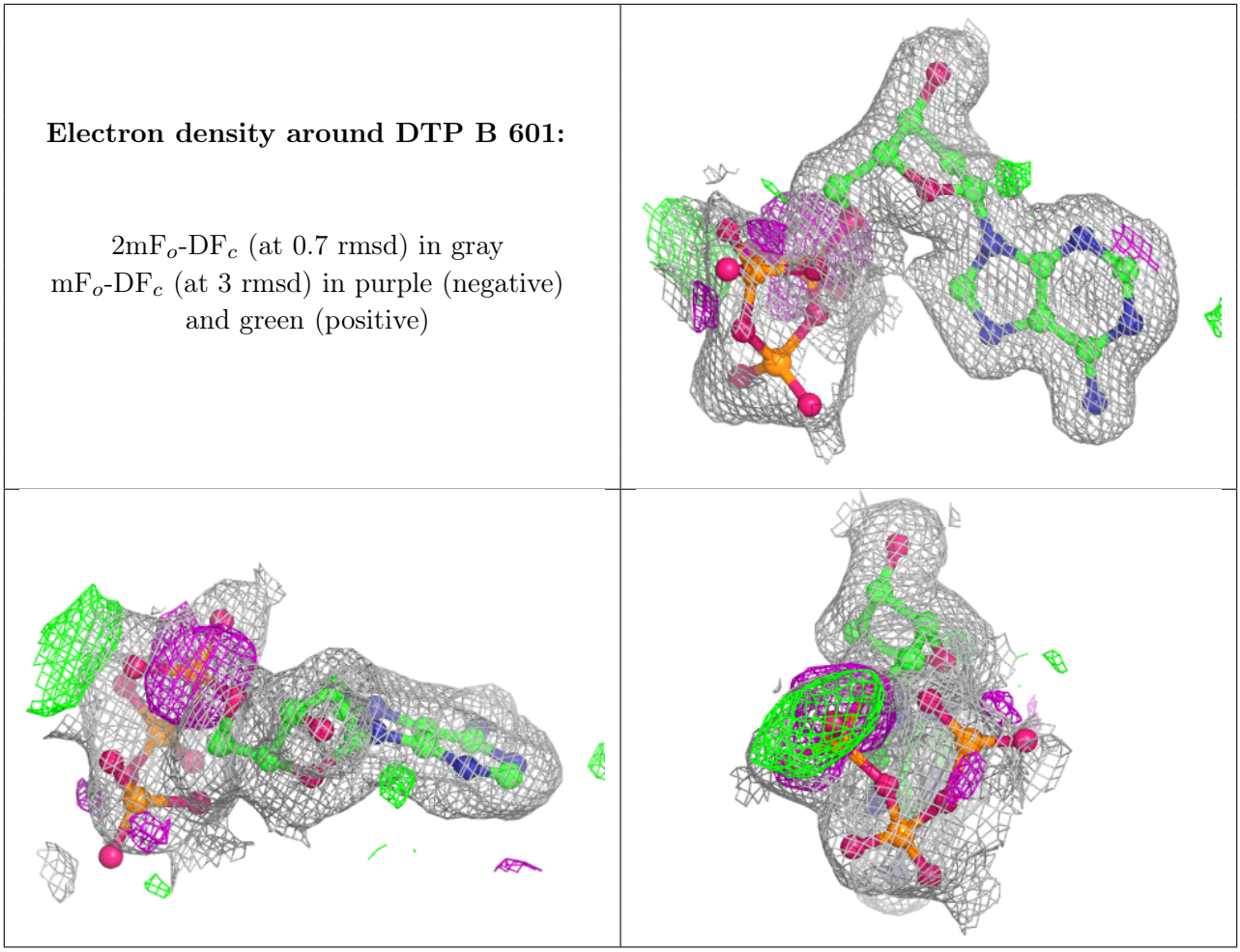






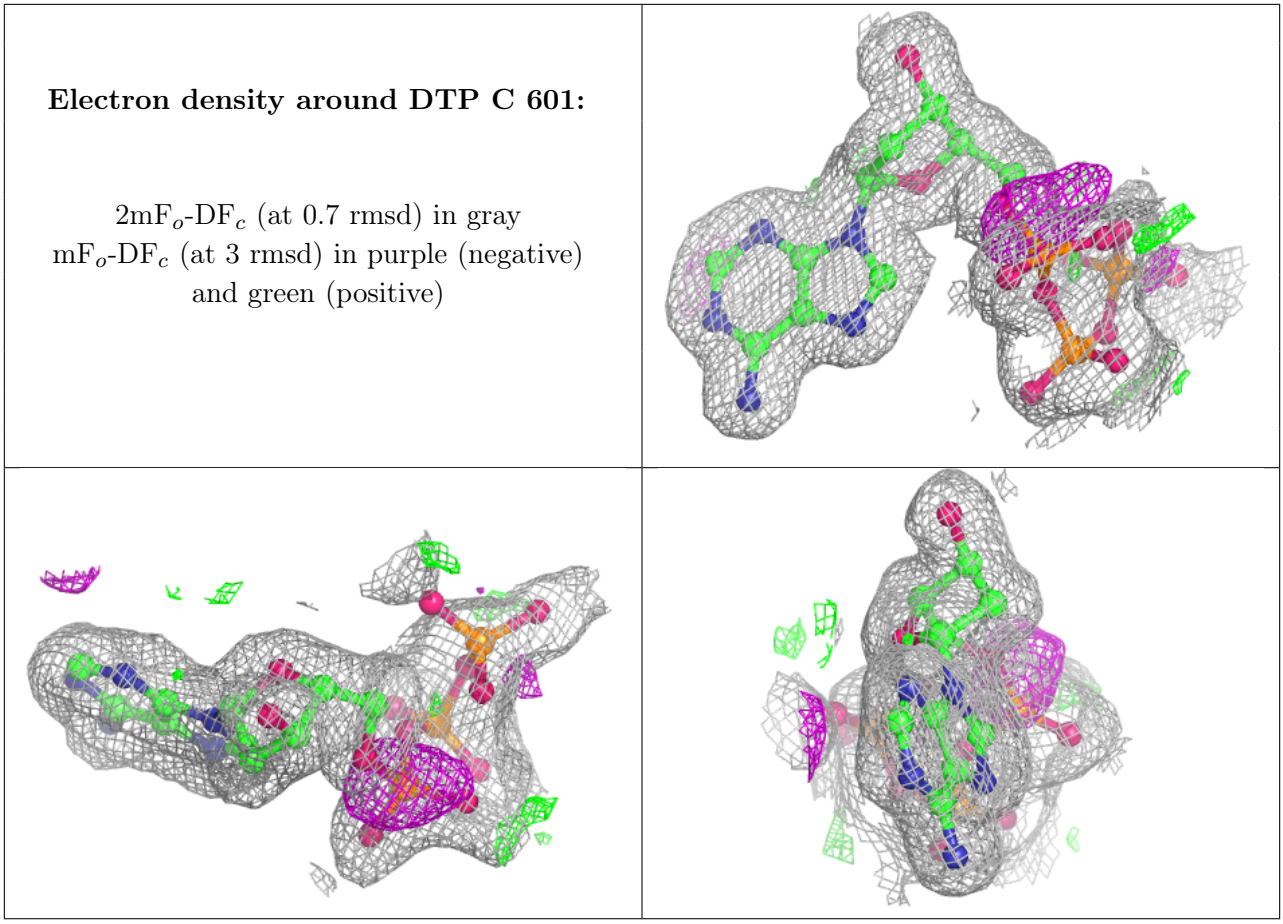
Electron density around DTP B 601:

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



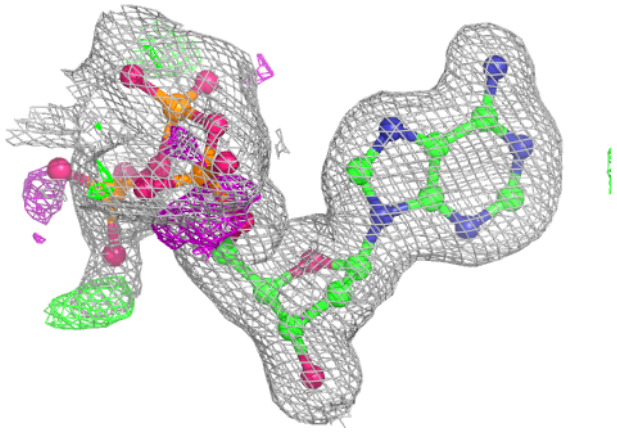
Electron density around DTP C 601:

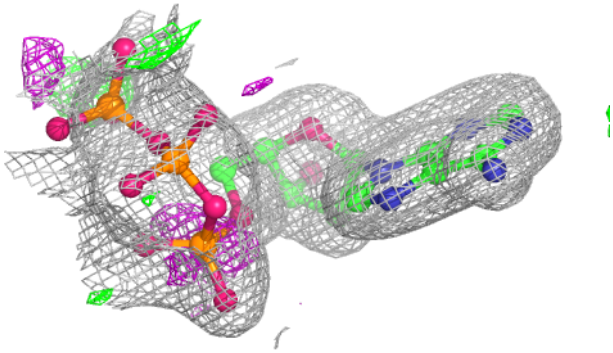
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

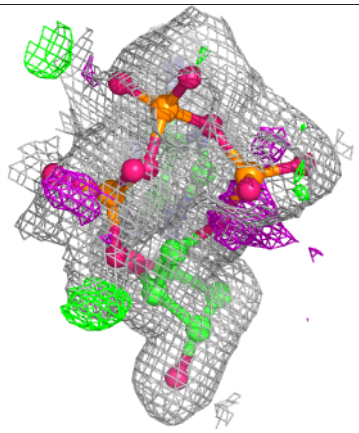


Electron density around DTP D 602:

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

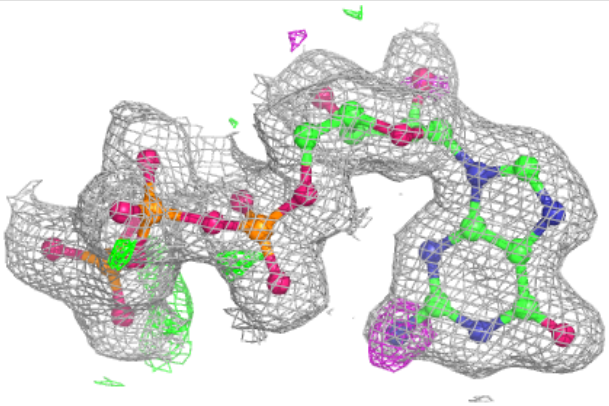


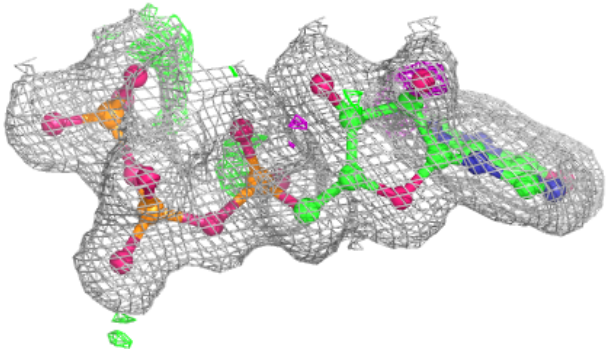


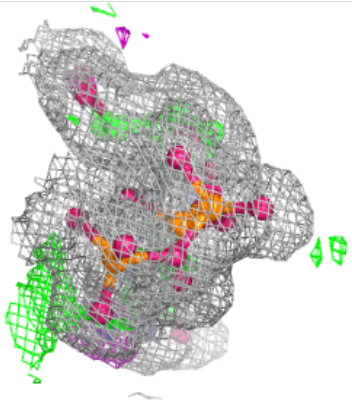


Electron density around GTP B 602:

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

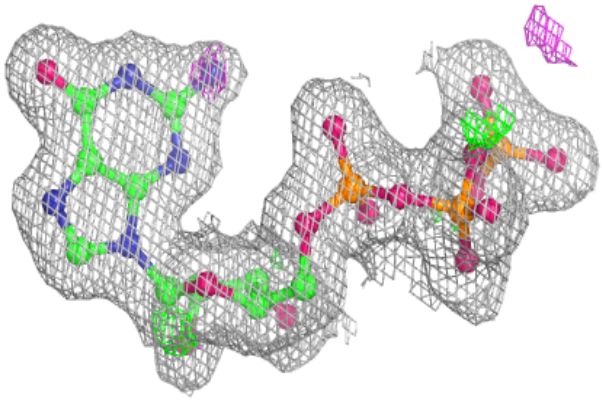


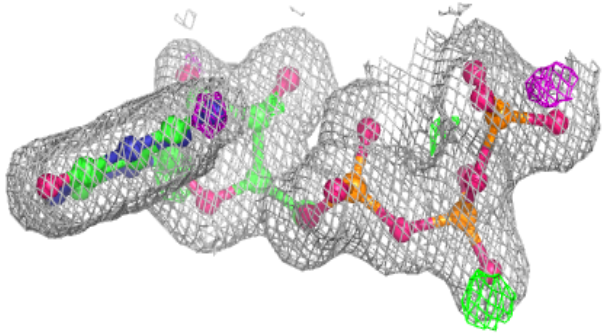


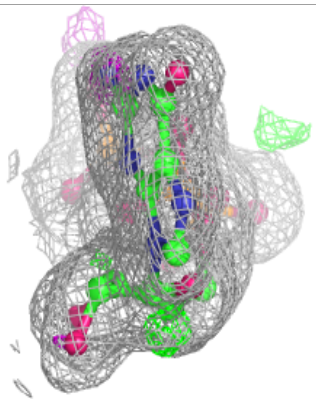


Electron density around GTP D 603:

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

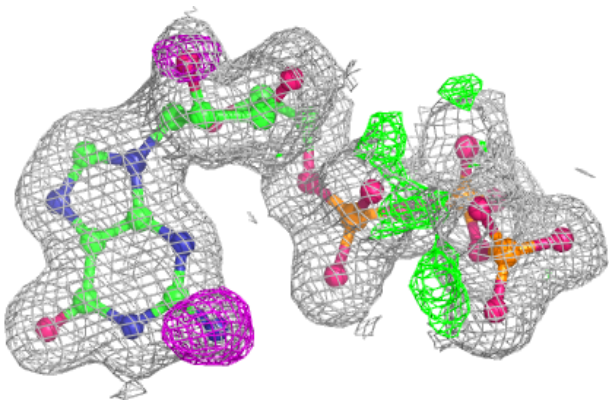


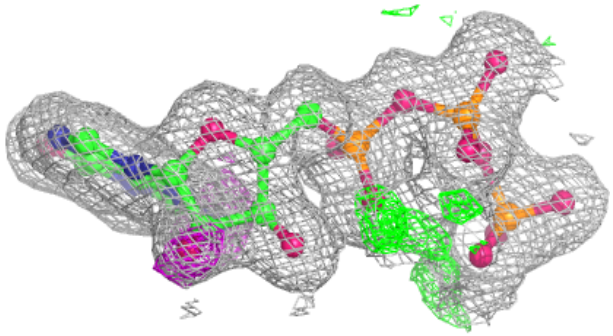


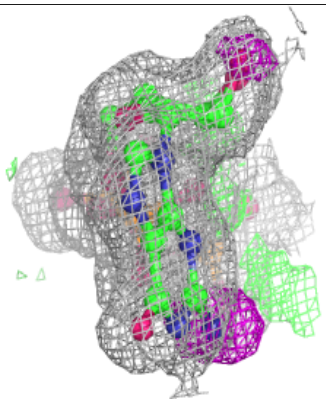


Electron density around GTP C 602:

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

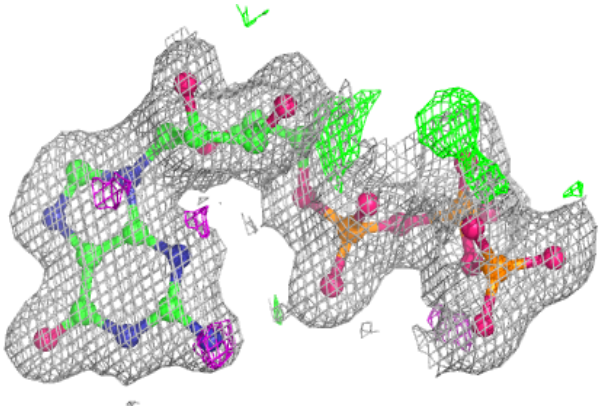


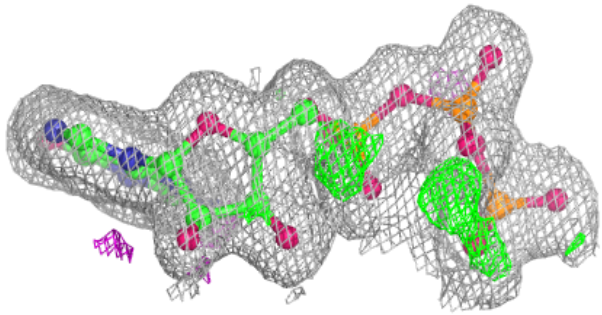


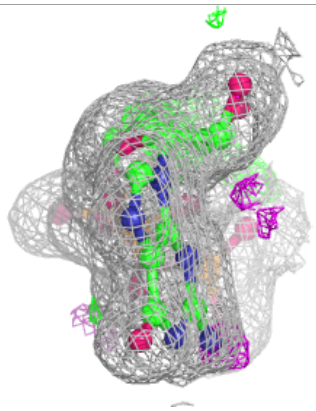


Electron density around GTP A 602:

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

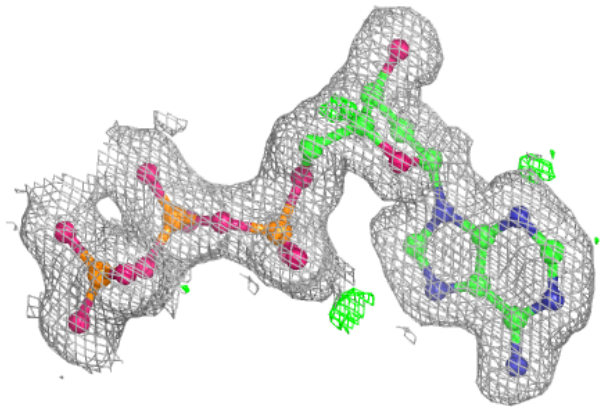


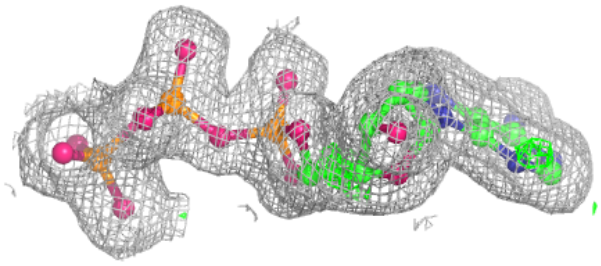


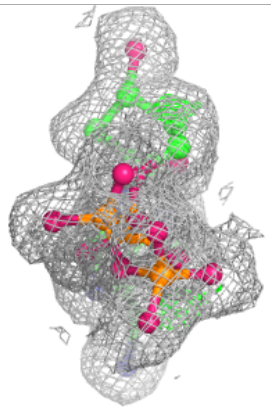


Electron density around DTP D 604:

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

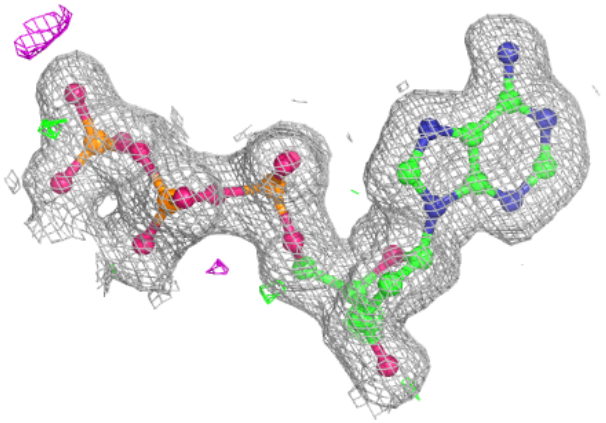


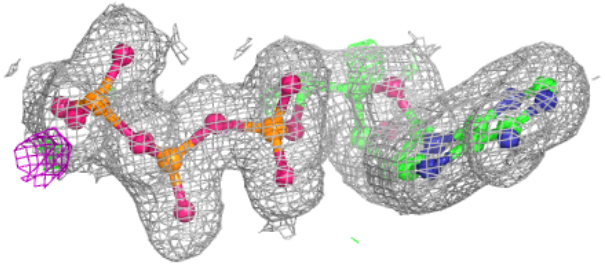


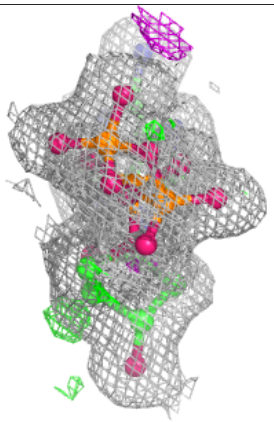


Electron density around DTP B 603:

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

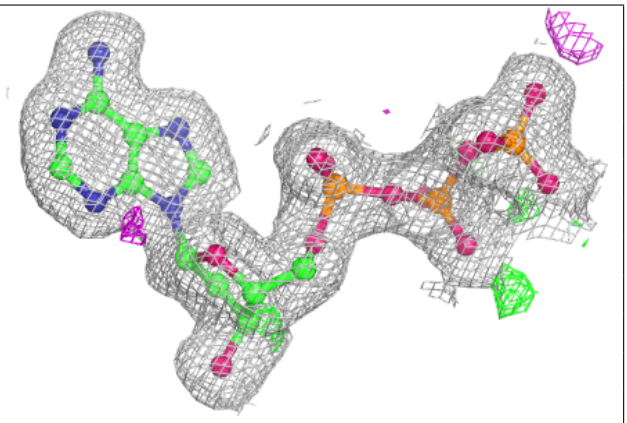


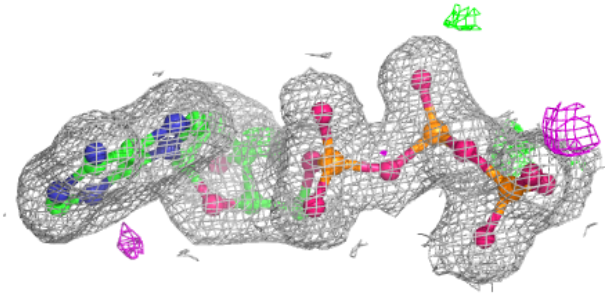


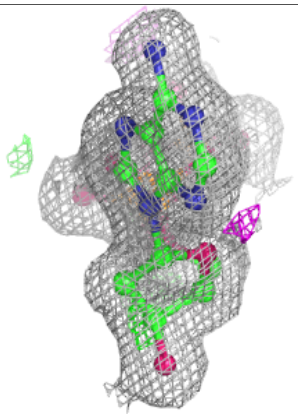


Electron density around DTP C 603:

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

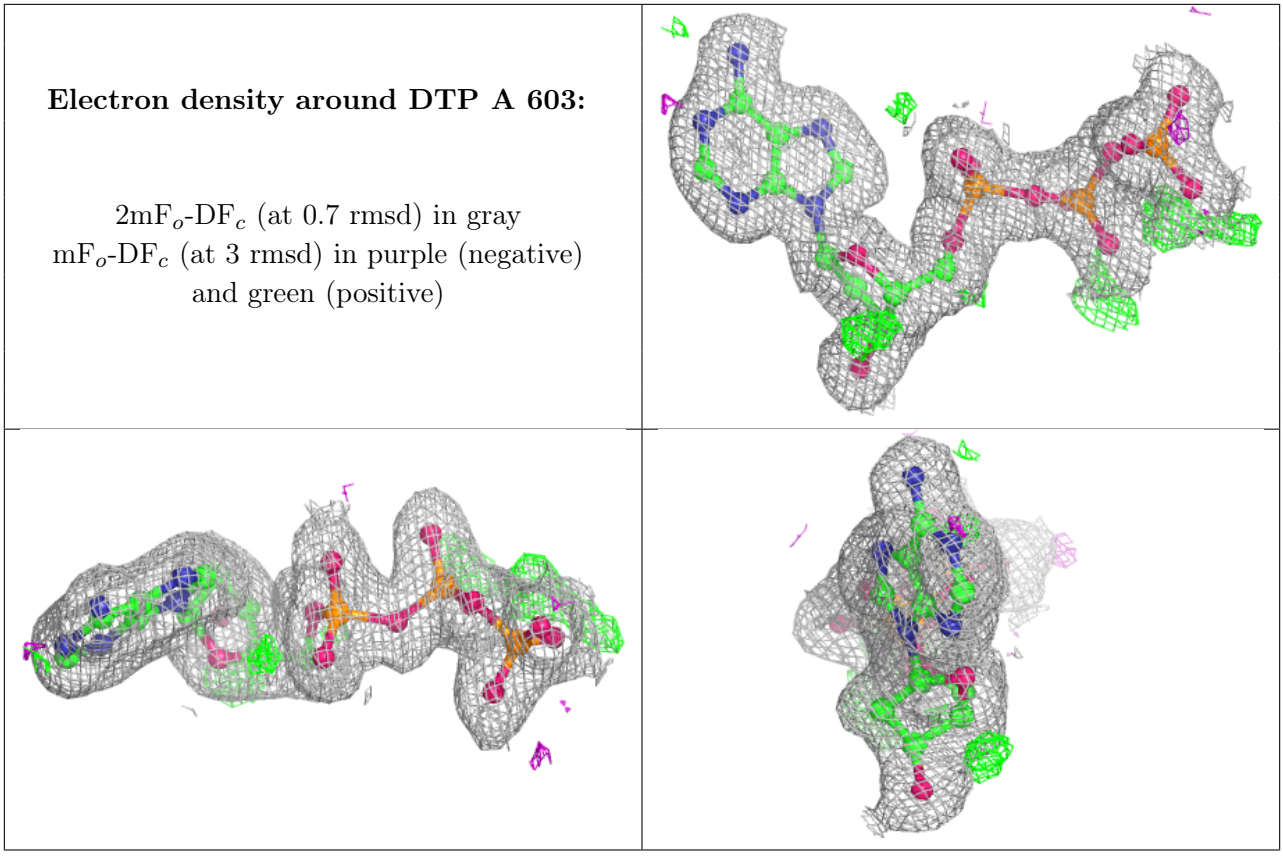






Electron density around DTP A 603:

$2mF_o$-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

There are no such residues in this entry.