Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 03:02 PM EDT

PDB ID	:	4ZWG
Title	:	Crystal structure of the GTP-dATP-bound catalytic core of SAMHD1 phosphomimetic T592E mutant
Authors	:	Tang, C.; Ji, X.; Xiong, Y.
Deposited on	:	2015-05-19
Resolution	:	2.30 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:

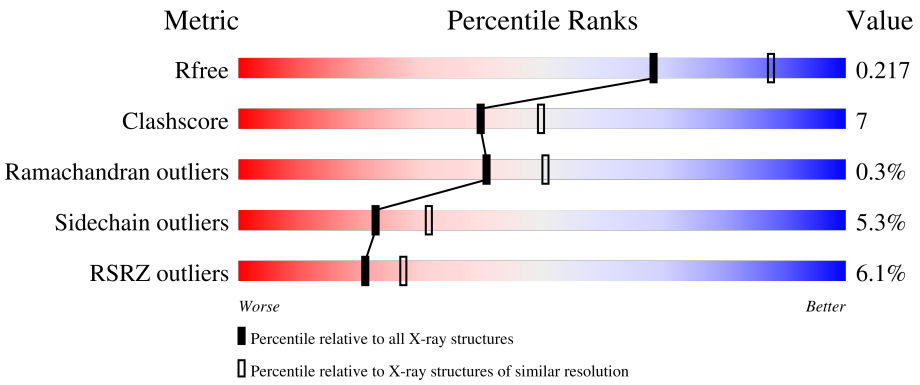
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	514	5% 75% 12% • 10%
1	B	514	5% 76% 12% • 11%
1	C	514	6% 80% 10% • 9%
1	D	514	5% 76% 10% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15653 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.

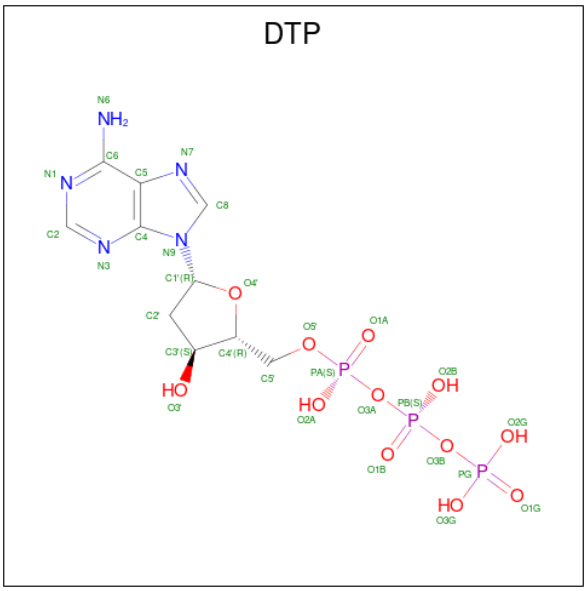
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	461	3779	2415	660	683	21	0	1	0
1	B	458	3751	2400	656	675	20	0	1	0
1	C	466	3810	2434	665	690	21	0	1	0
1	D	455	3735	2389	651	674	21	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

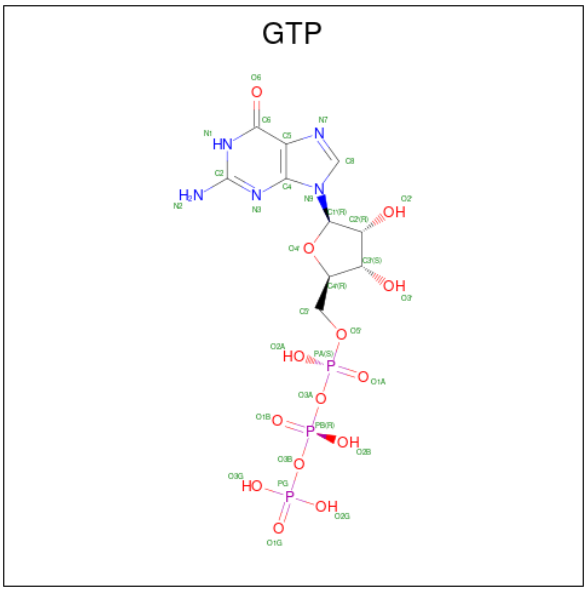
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	conflict	UNP Q9Y3Z3
A	207	ASN	ASP	conflict	UNP Q9Y3Z3
A	592	GLU	THR	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	conflict	UNP Q9Y3Z3
B	207	ASN	ASP	conflict	UNP Q9Y3Z3
B	592	GLU	THR	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	conflict	UNP Q9Y3Z3
C	207	ASN	ASP	conflict	UNP Q9Y3Z3
C	592	GLU	THR	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	conflict	UNP Q9Y3Z3
D	207	ASN	ASP	conflict	UNP Q9Y3Z3
D	592	GLU	THR	engineered mutation	UNP Q9Y3Z3

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



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

- Molecule 3 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		
3	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
3	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
3	B	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
3	C	1	32	10	5	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	2	2	2	0	0
			Total	Mg		
4	C	1	1	1	0	0
			Total	Mg		
4	D	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	86	86	86	0	0
			Total	O		
5	B	41	41	41	0	0

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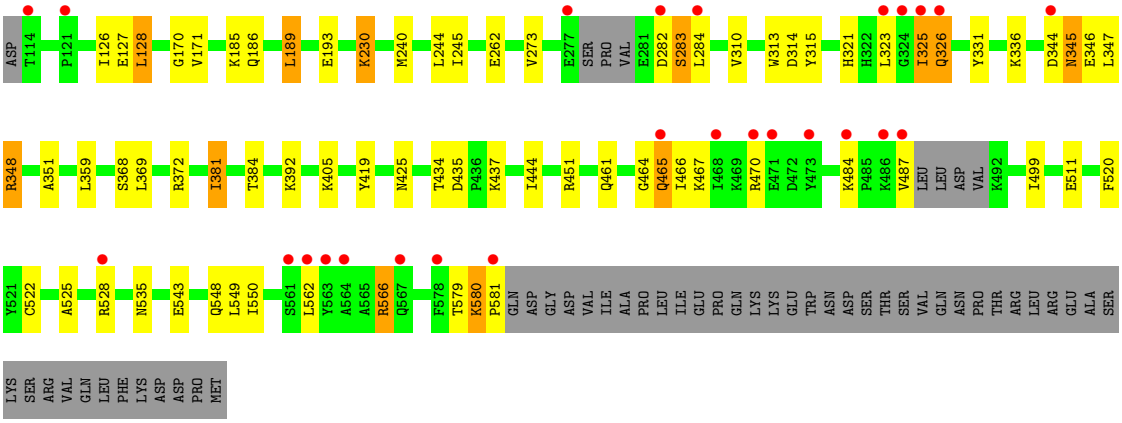
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	31	31	31	0	0
			Total	O		
5	D	48	48	48	0	0

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.

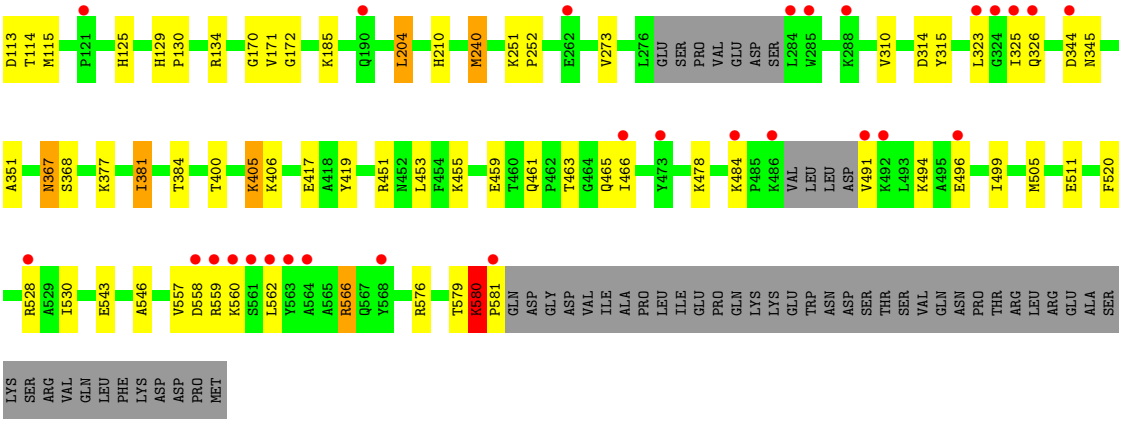
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



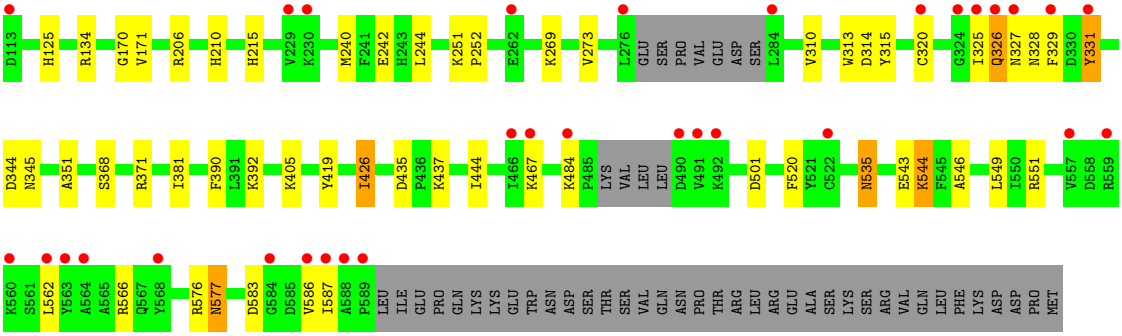
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:



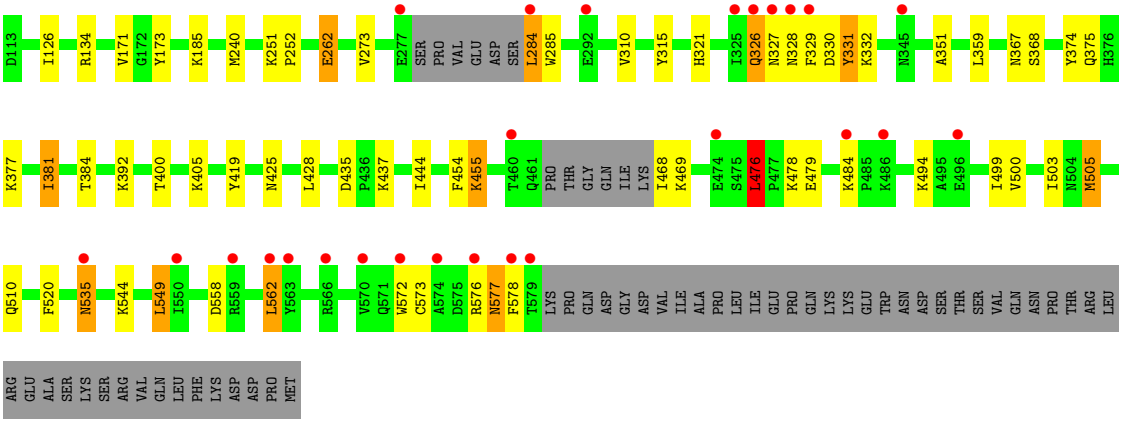
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.72Å 136.97Å 95.84Å 90.00° 113.96° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.30) 98.0 (49.71-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.205 , 0.246 0.212 , 0.217	Depositor DCC
R_{free} test set	4149 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15653	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: DTP, GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.60	1/3866 (0.0%)	0.75	0/5212
1	B	0.59	0/3841	0.75	1/5180 (0.0%)
1	C	0.59	0/3898	0.75	5/5259 (0.1%)
1	D	0.60	0/3820	0.76	2/5151 (0.0%)
All	All	0.59	1/15425 (0.0%)	0.75	8/20802 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	ARG	CZ-NH2	5.39	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	551	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	D	476	LEU	CB-CG-CD2	6.29	121.69	111.00
1	C	371	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	476	LEU	CB-CG-CD1	-5.98	100.83	111.00
1	C	551	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	501	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	549	LEU	CB-CG-CD1	5.24	119.91	111.00
1	B	478	LYS	CD-CE-NZ	5.01	123.22	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	465	GLN	Peptide

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	3779	0	3754	83	0
1	B	3751	0	3733	51	0
1	C	3810	0	3782	45	0
1	D	3735	0	3712	54	0
2	A	60	0	24	2	0
2	B	60	0	24	7	0
2	C	60	0	24	3	0
2	D	60	0	24	3	0
3	A	64	0	24	4	0
3	B	32	0	12	0	0
3	C	32	0	12	3	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	86	0	0	4	1
5	B	41	0	0	9	0
5	C	31	0	0	0	0
5	D	48	0	0	1	1
All	All	15653	0	15125	222	1

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

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:PHE:CE1	1:D:332:LYS:HB2	1.61	1.35
1:D:329:PHE:CE1	1:D:332:LYS:CB	2.16	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLU:OE2	1:C:269:LYS:NZ	1.72	1.21
1:D:329:PHE:HE1	1:D:332:LYS:CG	1.57	1.17
1:D:329:PHE:CE1	1:D:332:LYS:CG	2.29	1.16
1:D:329:PHE:HE1	1:D:332:LYS:HG3	0.98	1.14
1:D:329:PHE:CE1	1:D:332:LYS:HG3	1.82	1.13
1:A:465:GLN:HE21	1:A:466:ILE:N	1.45	1.12
1:A:451:ARG:HH21	3:A:702:GTP:H5'	1.16	1.08
1:B:367:ASN:ND2	1:B:505:MET:SD	2.27	1.07
1:A:465:GLN:NE2	1:A:466:ILE:H	1.53	1.05
1:D:329:PHE:CZ	1:D:332:LYS:CB	2.43	1.00
2:D:703:DTP:H8	2:D:703:DTP:H5'2	1.43	1.00
1:D:381:ILE:HD11	1:D:454:PHE:HB2	1.02	0.98
1:B:466:ILE:HG13	1:B:546:ALA:HB1	1.43	0.96
1:B:381:ILE:HD11	1:B:453:LEU:HB3	1.47	0.96
1:B:451:ARG:HH21	3:C:703:GTP:H5'	1.31	0.95
1:A:326:GLN:HG3	1:C:326:GLN:HB3	1.50	0.94
1:D:381:ILE:HD11	1:D:454:PHE:CB	1.97	0.94
1:D:381:ILE:CD1	1:D:454:PHE:HB2	1.96	0.92
1:A:465:GLN:HE21	1:A:466:ILE:H	0.95	0.91
1:B:461:GLN:HG3	1:B:580:LYS:HB3	1.54	0.90
1:C:125:HIS:H	1:D:329:PHE:HE2	1.20	0.90
1:D:329:PHE:CZ	1:D:332:LYS:HB2	2.06	0.88
1:A:344:ASP:O	1:A:345:ASN:ND2	2.08	0.87
1:D:375:GLN:NE2	1:D:505:MET:SD	2.48	0.86
1:A:461:GLN:HG3	1:A:580:LYS:HB2	1.56	0.86
1:A:326:GLN:CG	1:C:326:GLN:HB3	2.05	0.85
1:B:461:GLN:HG3	1:B:580:LYS:CB	2.07	0.84
1:D:503:ILE:HB	1:D:549:LEU:HD12	1.59	0.83
1:A:451:ARG:NH2	3:A:702:GTP:H5'	1.92	0.83
1:D:328:ASN:OD1	1:D:329:PHE:N	2.12	0.81
1:D:329:PHE:CD1	1:D:332:LYS:HB2	2.16	0.80
1:D:329:PHE:CZ	1:D:332:LYS:HB3	2.16	0.79
1:B:115:MET:HE2	1:B:129:HIS:HA	1.63	0.79
1:A:326:GLN:HB3	1:C:327:ASN:O	1.84	0.78
1:C:326:GLN:HE21	1:C:326:GLN:HA	1.49	0.77
1:B:466:ILE:CG1	1:B:546:ALA:HB1	2.16	0.75
1:A:465:GLN:NE2	1:A:466:ILE:N	2.22	0.73
1:B:405:LYS:CD	5:B:834:HOH:O	2.35	0.73
2:B:701:DTP:C2	5:B:827:HOH:O	2.36	0.72
1:D:326:GLN:H	1:D:326:GLN:HE21	1.37	0.72
1:A:326:GLN:CB	1:C:327:ASN:O	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASP:OD2	5:D:801:HOH:O	2.07	0.71
2:B:701:DTP:H2	5:B:827:HOH:O	1.90	0.70
1:A:461:GLN:CG	1:A:580:LYS:HB2	2.21	0.70
1:C:326:GLN:NE2	1:C:327:ASN:H	1.90	0.70
1:C:535:ASN:H	1:C:535:ASN:ND2	1.89	0.69
1:B:115:MET:CE	1:B:129:HIS:HA	2.21	0.69
1:C:320:CYS:HB3	1:C:325:ILE:O	1.93	0.69
1:C:313:TRP:HB3	1:C:331:TYR:HB3	1.75	0.69
1:A:325:ILE:HG13	1:A:326:GLN:N	2.08	0.68
1:B:326:GLN:HB3	1:D:328:ASN:HB2	1.75	0.67
1:A:451:ARG:HH21	3:A:702:GTP:C5'	1.99	0.67
1:A:525:ALA:HB3	1:C:586:VAL:HG11	1.77	0.67
2:D:703:DTP:H8	2:D:703:DTP:C5'	2.21	0.67
1:A:282:ASP:HA	1:A:283:SER:CB	2.25	0.67
2:A:701:DTP:H8	2:A:701:DTP:H5'2	1.77	0.67
1:B:417:GLU:HG3	5:B:829:HOH:O	1.94	0.67
1:A:525:ALA:O	5:A:801:HOH:O	2.14	0.66
1:B:377:LYS:O	1:B:381:ILE:HG23	1.95	0.66
3:A:706:GTP:H5"	2:B:703:DTP:O2B	1.96	0.65
1:B:451:ARG:NH2	3:C:703:GTP:H5'	2.08	0.65
1:D:384:THR:HG21	1:D:499:ILE:HD13	1.78	0.65
1:C:325:ILE:HG22	1:C:326:GLN:N	2.11	0.64
1:B:384:THR:HG21	1:B:499:ILE:HD13	1.77	0.64
1:C:327:ASN:ND2	1:C:329:PHE:O	2.29	0.64
1:A:384:THR:HG21	1:A:499:ILE:HD13	1.78	0.64
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.79	0.64
5:A:842:HOH:O	1:C:326:GLN:HB2	1.98	0.64
1:B:580:LYS:HD2	1:B:581:PRO:CD	2.28	0.63
1:D:479:GLU:OE1	1:D:576:ARG:HD3	1.98	0.63
1:A:535:ASN:OD1	1:A:535:ASN:N	2.31	0.63
1:B:113:ASP:OD1	1:B:114:THR:N	2.31	0.62
1:A:325:ILE:CD1	1:A:372:ARG:HH11	2.12	0.62
1:A:435:ASP:OD1	1:A:437:LYS:HG3	1.99	0.62
1:D:558:ASP:O	1:D:562:LEU:HD22	1.99	0.62
1:A:580:LYS:HG2	1:A:581:PRO:N	2.16	0.61
1:B:325:ILE:HG22	1:B:326:GLN:N	2.16	0.61
1:B:455:LYS:HE2	1:B:557:VAL:HB	1.82	0.60
1:D:535:ASN:H	1:D:535:ASN:HD22	1.46	0.60
1:A:435:ASP:OD2	1:A:437:LYS:HD2	2.02	0.59
1:A:282:ASP:HA	1:A:283:SER:HB2	1.83	0.59
1:A:522[A]:CYS:SG	1:C:586:VAL:HG11	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:NH2	2:C:704:DTP:O2B	2.35	0.59
1:A:230:LYS:HG2	1:A:230:LYS:O	2.02	0.59
1:D:535:ASN:H	1:D:535:ASN:ND2	2.01	0.59
1:A:230:LYS:HD3	5:A:853:HOH:O	2.03	0.59
1:B:558:ASP:O	1:B:560:LYS:N	2.38	0.57
1:C:215:HIS:CD2	2:C:704:DTP:C8	2.88	0.57
1:C:326:GLN:HA	1:C:326:GLN:NE2	2.18	0.57
1:B:172:GLY:HA3	1:B:204:LEU:HD13	1.86	0.56
1:B:113:ASP:HB3	1:B:130:PRO:HG3	1.87	0.56
1:D:126:ILE:HD12	1:D:173:TYR:CE1	2.41	0.56
1:B:461:GLN:HG3	1:B:580:LYS:HB2	1.85	0.56
1:A:325:ILE:HD12	1:A:372:ARG:NH1	2.21	0.55
1:C:544:LYS:HE2	1:C:546:ALA:O	2.07	0.55
1:B:451:ARG:HH21	3:C:703:GTP:C5'	2.11	0.55
1:B:580:LYS:HD2	1:B:581:PRO:N	2.22	0.55
1:D:240:MET:HE2	1:D:419:TYR:HD2	1.72	0.55
1:B:405:LYS:HD3	5:B:834:HOH:O	2.04	0.55
1:B:466:ILE:HG13	1:B:546:ALA:CB	2.29	0.54
1:A:321:HIS:CE1	1:D:321:HIS:CE1	2.95	0.54
1:A:313:TRP:HB3	1:A:331:TYR:HB3	1.88	0.54
1:A:323:LEU:CB	1:A:325:ILE:HG23	2.38	0.54
1:A:580:LYS:CG	1:A:581:PRO:HD2	2.38	0.54
1:D:326:GLN:H	1:D:326:GLN:NE2	2.05	0.54
1:C:210:HIS:NE2	2:C:704:DTP:O1A	2.39	0.54
1:D:576:ARG:O	1:D:577:ASN:HB2	2.08	0.54
1:A:325:ILE:HD12	1:A:372:ARG:HH11	1.72	0.53
1:D:262:GLU:OE1	1:D:262:GLU:HA	2.08	0.53
1:A:522[B]:CYS:SG	1:C:583:ASP:HB3	2.48	0.53
1:B:466:ILE:O	1:B:466:ILE:HG22	2.07	0.53
1:A:186:GLN:CB	1:A:189:LEU:HD22	2.39	0.53
1:A:525:ALA:HB3	1:C:586:VAL:CG1	2.39	0.53
1:D:476:LEU:HD12	1:D:500:VAL:HG11	1.90	0.53
1:A:466:ILE:HG22	1:A:466:ILE:O	2.09	0.52
1:A:326:GLN:O	1:C:328:ASN:ND2	2.43	0.52
1:D:384:THR:CG2	1:D:499:ILE:HD13	2.39	0.52
1:D:476:LEU:CD1	1:D:572:TRP:CZ2	2.93	0.51
1:A:464:GLY:O	1:A:467:LYS:HE3	2.10	0.51
1:A:522[B]:CYS:SG	1:C:583:ASP:CB	2.99	0.51
1:A:579:THR:HG22	1:A:580:LYS:N	2.26	0.51
1:B:384:THR:CG2	1:B:499:ILE:HD13	2.41	0.51
2:B:701:DTP:N7	5:B:803:HOH:O	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:THR:O	1:A:580:LYS:HB3	2.12	0.50
1:A:336:LYS:HE3	1:B:125:HIS:O	2.12	0.50
1:A:345:ASN:ND2	1:A:345:ASN:C	2.65	0.49
1:B:579:THR:O	1:B:580:LYS:HB3	2.10	0.49
1:A:326:GLN:HG2	1:C:326:GLN:CD	2.33	0.49
1:C:325:ILE:CG2	1:C:326:GLN:N	2.74	0.49
1:B:461:GLN:CG	1:B:580:LYS:HB2	2.43	0.49
1:B:325:ILE:CG2	1:B:326:GLN:N	2.75	0.48
1:A:425:ASN:ND2	1:D:425:ASN:OD1	2.46	0.48
1:A:325:ILE:HD13	1:A:372:ARG:HH11	1.79	0.48
2:A:701:DTP:H8	2:A:701:DTP:C5'	2.44	0.48
1:B:461:GLN:CG	1:B:580:LYS:CB	2.86	0.48
1:D:351:ALA:O	1:D:520:PHE:HA	2.13	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:B:461:GLN:HB2	1:B:579:THR:HG23	1.96	0.47
1:A:580:LYS:HG2	1:A:581:PRO:CD	2.45	0.47
1:A:580:LYS:HG3	1:A:581:PRO:HD2	1.96	0.47
1:D:435:ASP:OD2	1:D:437:LYS:HE3	2.14	0.47
1:D:375:GLN:NE2	1:D:505:MET:CE	2.78	0.47
1:A:528:ARG:HD3	1:C:586:VAL:HG22	1.96	0.47
1:C:326:GLN:NE2	1:C:327:ASN:N	2.60	0.47
1:D:251:LYS:HB2	1:D:252:PRO:HD3	1.97	0.46
1:C:576:ARG:O	1:C:577:ASN:HB2	2.16	0.46
1:A:323:LEU:HB2	1:A:325:ILE:HG23	1.96	0.46
1:A:580:LYS:CG	1:A:581:PRO:CD	2.94	0.46
1:C:390:PHE:CZ	1:C:426:ILE:CG2	2.99	0.46
1:B:461:GLN:HE21	1:B:580:LYS:HB2	1.81	0.46
1:C:566:ARG:HG2	1:C:587:ILE:HD12	1.98	0.46
1:A:465:GLN:HE21	1:A:465:GLN:CA	2.29	0.46
1:A:466:ILE:HG23	1:A:548:GLN:NE2	2.31	0.46
1:A:323:LEU:HB3	1:A:325:ILE:HG23	1.99	0.45
1:A:240:MET:HE2	1:A:419:TYR:HD2	1.80	0.45
1:D:381:ILE:HD13	1:D:381:ILE:O	2.16	0.45
1:D:284:LEU:HD13	1:D:285:TRP:N	2.32	0.45
1:D:374:TYR:CE1	2:D:703:DTP:H2'1	2.51	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.17	0.45
1:A:323:LEU:HB3	1:A:325:ILE:CG2	2.46	0.45
1:A:325:ILE:CG1	1:A:326:GLN:N	2.78	0.45
2:B:701:DTP:C2	5:B:804:HOH:O	2.66	0.45
1:D:573:CYS:O	1:D:577:ASN:O	2.35	0.45
1:A:313:TRP:HB3	1:A:331:TYR:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HG13	1:C:310:VAL:HG23	1.99	0.44
1:C:577:ASN:N	1:C:577:ASN:HD22	2.15	0.44
1:D:330:ASP:OD1	1:D:331:TYR:CE1	2.70	0.44
1:A:549:LEU:C	1:A:550:ILE:HD12	2.38	0.44
1:A:580:LYS:HG2	1:A:581:PRO:HD2	1.99	0.44
1:C:351:ALA:O	1:C:520:PHE:HA	2.18	0.44
1:A:425:ASN:HB2	1:D:428:LEU:HD13	2.00	0.44
1:A:434:THR:HG21	1:D:400:THR:CB	2.47	0.44
1:B:240:MET:CE	1:B:419:TYR:HB3	2.48	0.44
1:A:282:ASP:CA	1:A:283:SER:CB	2.96	0.44
1:A:346:GLU:OE1	1:A:348:ARG:NH1	2.50	0.43
1:C:344:ASP:O	1:C:345:ASN:HB2	2.18	0.43
1:D:468:ILE:HG23	1:D:469:LYS:CD	2.49	0.43
1:D:577:ASN:O	1:D:578:PHE:CG	2.71	0.43
1:B:580:LYS:CD	1:B:581:PRO:HD2	2.48	0.43
1:A:326:GLN:CD	1:C:326:GLN:HB3	2.38	0.43
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.91	0.43
1:B:566:ARG:HD2	1:B:566:ARG:HA	1.70	0.43
1:C:326:GLN:NE2	1:C:326:GLN:CA	2.81	0.43
1:D:392:LYS:HD2	1:D:444:ILE:CD1	2.49	0.43
1:B:405:LYS:HD2	5:B:834:HOH:O	2.10	0.43
1:C:435:ASP:OD2	1:C:437:LYS:HE3	2.19	0.43
1:D:171:VAL:HG13	1:D:310:VAL:HG23	2.00	0.43
1:B:210:HIS:NE2	2:B:701:DTP:O1A	2.43	0.42
1:B:528:ARG:HE	1:B:530:ILE:HG22	1.84	0.42
1:A:244:LEU:C	1:A:244:LEU:HD23	2.39	0.42
1:A:392:LYS:HD2	1:A:444:ILE:CD1	2.48	0.42
1:C:170:GLY:HA3	1:C:314:ASP:OD1	2.20	0.42
2:B:701:DTP:N3	5:B:804:HOH:O	2.37	0.42
1:A:384:THR:CG2	1:A:499:ILE:HD13	2.45	0.42
1:B:400:THR:OG1	1:B:406:LYS:HE2	2.20	0.42
1:A:566:ARG:HH22	1:A:581:PRO:HB2	1.85	0.42
1:B:171:VAL:HG13	1:B:310:VAL:HG23	2.01	0.42
1:B:323:LEU:HD13	1:B:325:ILE:HD12	2.01	0.42
1:A:262:GLU:H	1:A:262:GLU:CD	2.23	0.41
1:A:326:GLN:CG	1:C:326:GLN:CB	2.90	0.41
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.02	0.41
1:B:580:LYS:HD2	1:B:581:PRO:CG	2.50	0.41
1:A:171:VAL:HG13	1:A:310:VAL:HG23	2.00	0.41
1:B:344:ASP:O	1:B:345:ASN:HB2	2.20	0.41
1:D:330:ASP:OD1	1:D:330:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:LYS:HG3	1:D:562:LEU:HD11	2.01	0.41
1:C:240:MET:HE2	1:C:419:TYR:HD2	1.84	0.41
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.02	0.41
1:D:329:PHE:CZ	1:D:332:LYS:CG	2.95	0.41
1:B:170:GLY:HA3	1:B:314:ASP:OD1	2.21	0.41
1:C:244:LEU:C	1:C:244:LEU:HD23	2.41	0.41
1:A:170:GLY:HA3	1:A:314:ASP:OD1	2.21	0.41
1:C:392:LYS:HD2	1:C:444:ILE:CD1	2.50	0.41
1:B:459:GLU:O	1:B:580:LYS:HG3	2.21	0.41
1:A:325:ILE:HG12	1:A:369:LEU:HD21	2.03	0.40
1:A:345:ASN:ND2	5:A:812:HOH:O	2.55	0.40
1:D:558:ASP:C	1:D:562:LEU:HD22	2.42	0.40
1:A:126:ILE:HD13	1:A:126:ILE:HG21	1.88	0.40
1:A:127:GLU:O	1:A:128:LEU:HD13	2.22	0.40
1:A:325:ILE:CD1	1:A:372:ARG:NH1	2.81	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:880:HOH:O	5:D:836:HOH:O[2_848]	2.14	0.06

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	456/514 (89%)	444 (97%)	9 (2%)	3 (1%)	22 26
1	B	453/514 (88%)	443 (98%)	8 (2%)	2 (0%)	34 42
1	C	461/514 (90%)	452 (98%)	9 (2%)	0	100 100
1	D	450/514 (88%)	442 (98%)	7 (2%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1820/2056 (88%)	1781 (98%)	33 (2%)	6 (0%)	41 50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	B	559	ARG
1	A	284	LEU
1	B	580	LYS
1	D	577	ASN
1	A	580	LYS

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	410/459 (89%)	386 (94%)	24 (6%)	19 27
1	B	406/459 (88%)	385 (95%)	21 (5%)	23 32
1	C	413/459 (90%)	397 (96%)	16 (4%)	32 46
1	D	405/459 (88%)	379 (94%)	26 (6%)	17 23
All	All	1634/1836 (89%)	1547 (95%)	87 (5%)	22 31

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	185	LYS
1	A	189	LEU
1	A	193	GLU
1	A	230	LYS
1	A	245	ILE
1	A	273	VAL
1	A	315	TYR
1	A	325	ILE

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	345	ASN
1	A	347	LEU
1	A	359	LEU
1	A	368	SER
1	A	381	ILE
1	A	405	LYS
1	A	465	GLN
1	A	470	ARG
1	A	484	LYS
1	A	487	VAL
1	A	511	GLU
1	A	543	GLU
1	A	562	LEU
1	A	566	ARG
1	B	134	ARG
1	B	185	LYS
1	B	204	LEU
1	B	240	MET
1	B	273	VAL
1	B	315	TYR
1	B	367	ASN
1	B	368	SER
1	B	381	ILE
1	B	405	LYS
1	B	463	THR
1	B	484	LYS
1	B	491	VAL
1	B	494	LYS
1	B	496	GLU
1	B	511	GLU
1	B	543	GLU
1	B	562	LEU
1	B	566	ARG
1	B	576	ARG
1	B	580	LYS
1	C	134	ARG
1	C	273	VAL
1	C	315	TYR
1	C	326	GLN
1	C	331	TYR
1	C	368	SER

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Mol	Chain	Res	Type
1	C	381	ILE
1	C	405	LYS
1	C	426	ILE
1	C	467	LYS
1	C	484	LYS
1	C	535	ASN
1	C	543	GLU
1	C	544	LYS
1	C	562	LEU
1	C	577	ASN
1	D	134	ARG
1	D	185	LYS
1	D	262	GLU
1	D	273	VAL
1	D	284	LEU
1	D	315	TYR
1	D	326	GLN
1	D	327	ASN
1	D	331	TYR
1	D	359	LEU
1	D	367	ASN
1	D	368	SER
1	D	377	LYS
1	D	381	ILE
1	D	405	LYS
1	D	455	LYS
1	D	476	LEU
1	D	478	LYS
1	D	484	LYS
1	D	494	LYS
1	D	505	MET
1	D	510	GLN
1	D	535	ASN
1	D	544	LYS
1	D	549	LEU
1	D	562	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	322	HIS

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	328	ASN
1	A	370	HIS
1	A	425	ASN
1	A	461	GLN
1	A	465	GLN
1	B	215	HIS
1	B	322	HIS
1	B	328	ASN
1	B	370	HIS
1	B	375	GLN
1	B	425	ASN
1	B	461	GLN
1	C	322	HIS
1	C	326	GLN
1	C	328	ASN
1	C	370	HIS
1	C	535	ASN
1	C	577	ASN
1	D	243	HIS
1	D	322	HIS
1	D	326	GLN
1	D	327	ASN
1	D	370	HIS
1	D	375	GLN
1	D	535	ASN
1	D	567	GLN
1	D	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DTP	A	703	4	26,32,32	1.01	0	30,50,50	1.75	5 (16%)
2	DTP	D	702	4	26,32,32	1.01	2 (7%)	30,50,50	1.36	5 (16%)
2	DTP	D	703	-	26,32,32	1.00	2 (7%)	30,50,50	1.53	7 (23%)
2	DTP	A	701	-	26,32,32	1.01	2 (7%)	30,50,50	1.43	6 (20%)
3	GTP	A	702	4	26,34,34	1.14	1 (3%)	32,54,54	1.93	11 (34%)
3	GTP	A	706	4	26,34,34	1.02	1 (3%)	32,54,54	1.53	6 (18%)
2	DTP	C	701	4	26,32,32	0.95	1 (3%)	30,50,50	1.48	6 (20%)
2	DTP	B	703	4	26,32,32	1.17	1 (3%)	30,50,50	1.73	7 (23%)
2	DTP	C	704	-	26,32,32	1.21	3 (11%)	30,50,50	1.52	5 (16%)
2	DTP	B	701	-	26,32,32	1.14	3 (11%)	30,50,50	1.41	4 (13%)
3	GTP	C	703	4	26,34,34	1.25	3 (11%)	32,54,54	1.78	10 (31%)
3	GTP	B	702	4	26,34,34	0.99	1 (3%)	32,54,54	1.61	10 (31%)

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	A	703	4	-	1/18/34/34	0/3/3/3
2	DTP	D	702	4	-	2/18/34/34	0/3/3/3
2	DTP	D	703	-	-	1/18/34/34	0/3/3/3
2	DTP	A	701	-	-	7/18/34/34	0/3/3/3
3	GTP	A	702	4	-	6/18/38/38	0/3/3/3
3	GTP	A	706	4	-	3/18/38/38	0/3/3/3
2	DTP	C	701	4	-	6/18/34/34	0/3/3/3
2	DTP	B	703	4	-	1/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	C	704	-	-	7/18/34/34	0/3/3/3
2	DTP	B	701	-	-	8/18/34/34	0/3/3/3
3	GTP	C	703	4	-	7/18/38/38	0/3/3/3
3	GTP	B	702	4	-	11/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	GTP	C6-N1	-3.23	1.33	1.37
2	C	704	DTP	C5-C4	3.21	1.49	1.40
2	B	701	DTP	C5-C4	3.17	1.49	1.40
2	D	703	DTP	C5-C4	2.91	1.48	1.40
2	A	701	DTP	C5-C4	2.88	1.48	1.40
3	A	702	GTP	C6-N1	-2.61	1.34	1.37
2	D	702	DTP	C2-N3	2.45	1.36	1.32
2	D	703	DTP	C2-N3	2.39	1.35	1.32
2	B	703	DTP	C5-C4	2.34	1.47	1.40
2	A	701	DTP	C2-N3	2.25	1.35	1.32
2	C	704	DTP	C2-N3	2.23	1.35	1.32
2	C	701	DTP	C5-C4	2.23	1.46	1.40
2	C	704	DTP	C6-C5	2.20	1.51	1.43
2	D	702	DTP	C5-C4	2.19	1.46	1.40
2	B	701	DTP	C2-N3	2.15	1.35	1.32
3	A	706	GTP	O4'-C1'	2.13	1.44	1.41
3	C	703	GTP	PG-O2G	-2.06	1.46	1.54
2	B	701	DTP	C6-C5	2.04	1.50	1.43
3	B	702	GTP	C5-C4	2.02	1.48	1.43
3	C	703	GTP	C5-C4	2.01	1.48	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	703	DTP	N3-C2-N1	-4.36	121.86	128.68
2	C	701	DTP	N3-C2-N1	-4.31	121.94	128.68
3	C	703	GTP	C3'-C2'-C1'	4.01	107.01	100.98
2	C	704	DTP	N3-C2-N1	-3.92	122.54	128.68
2	D	703	DTP	N3-C2-N1	-3.92	122.55	128.68
2	B	703	DTP	N3-C2-N1	-3.90	122.58	128.68
3	A	702	GTP	C3'-C2'-C1'	3.85	106.78	100.98
2	A	701	DTP	N3-C2-N1	-3.68	122.92	128.68
2	A	703	DTP	C4-C5-N7	-3.68	105.56	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	GTP	O4'-C4'-C5'	-3.67	97.31	109.37
2	B	703	DTP	PB-O3B-PG	-3.58	120.55	132.83
3	C	703	GTP	PA-O3A-PB	-3.57	120.57	132.83
2	D	702	DTP	N3-C2-N1	-3.57	123.10	128.68
3	A	706	GTP	C8-N7-C5	3.57	109.79	102.99
2	B	701	DTP	C4-C5-N7	-3.35	105.91	109.40
3	A	706	GTP	PB-O3B-PG	-3.33	121.39	132.83
2	A	701	DTP	PA-O3A-PB	-3.27	121.61	132.83
2	C	704	DTP	C4-C5-N7	-3.23	106.03	109.40
3	A	702	GTP	PB-O3B-PG	-3.20	121.83	132.83
2	B	703	DTP	PA-O3A-PB	-3.14	122.06	132.83
2	B	701	DTP	N3-C2-N1	-3.06	123.90	128.68
2	B	703	DTP	C4-C5-N7	-3.04	106.23	109.40
2	B	703	DTP	C2'-C1'-N9	3.04	121.29	114.27
3	A	702	GTP	PA-O3A-PB	-3.04	122.39	132.83
3	A	706	GTP	O3G-PG-O2G	3.01	119.14	107.64
3	A	702	GTP	O2A-PA-O5'	2.99	121.61	107.75
3	A	702	GTP	O6-C6-N1	2.97	124.16	120.65
2	D	703	DTP	PB-O3B-PG	-2.93	122.76	132.83
3	C	703	GTP	PB-O3B-PG	-2.80	123.20	132.83
2	C	701	DTP	C2-N1-C6	2.76	123.47	118.75
2	A	703	DTP	O5'-PA-O1A	-2.71	98.49	109.07
3	A	702	GTP	N2-C2-N3	-2.70	114.49	119.74
2	B	703	DTP	C2-N1-C6	2.69	123.36	118.75
3	A	706	GTP	O3G-PG-O3B	-2.65	95.75	104.64
2	A	701	DTP	PB-O3B-PG	-2.60	123.92	132.83
3	C	703	GTP	O4'-C4'-C5'	-2.59	100.84	109.37
2	B	701	DTP	PB-O3B-PG	-2.56	124.03	132.83
2	D	703	DTP	O3G-PG-O2G	2.52	117.26	107.64
2	D	702	DTP	C5-C6-N6	-2.49	116.56	120.35
3	B	702	GTP	O2A-PA-O1A	2.48	124.50	112.24
3	C	703	GTP	O2A-PA-O5'	-2.47	96.26	107.75
3	A	706	GTP	O2A-PA-O1A	2.46	124.41	112.24
3	B	702	GTP	O2B-PB-O1B	2.46	124.40	112.24
2	D	703	DTP	PA-O3A-PB	-2.41	124.54	132.83
3	A	702	GTP	C8-N7-C5	2.41	107.58	102.99
2	A	703	DTP	C2'-C3'-C4'	2.41	107.78	102.76
3	B	702	GTP	C8-N7-C5	2.41	107.58	102.99
3	C	703	GTP	O3B-PG-O1G	-2.40	97.86	111.19
3	B	702	GTP	O3G-PG-O3B	2.38	112.62	104.64
2	C	704	DTP	C5-C6-N6	2.38	123.97	120.35
3	B	702	GTP	O3B-PG-O1G	-2.37	98.03	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	DTP	PA-O3A-PB	-2.37	124.69	132.83
2	C	701	DTP	C2'-C3'-C4'	2.36	107.68	102.76
3	A	702	GTP	O5'-C5'-C4'	2.35	117.08	108.99
2	C	704	DTP	PB-O3B-PG	-2.34	124.79	132.83
2	A	701	DTP	O3G-PG-O2G	2.31	116.47	107.64
2	C	701	DTP	PB-O3B-PG	-2.28	125.00	132.83
2	C	704	DTP	C2-N1-C6	2.28	122.65	118.75
3	B	702	GTP	O5'-C5'-C4'	2.26	116.78	108.99
3	C	703	GTP	O2A-PA-O1A	2.25	123.34	112.24
3	B	702	GTP	PA-O3A-PB	-2.24	125.15	132.83
3	C	703	GTP	O2G-PG-O1G	2.23	119.40	110.68
2	C	701	DTP	O2G-PG-O3B	2.22	112.07	104.64
2	D	702	DTP	C2'-C1'-N9	2.21	119.36	114.27
2	D	702	DTP	N6-C6-N1	2.21	123.16	118.57
3	B	702	GTP	O2G-PG-O1G	2.20	119.31	110.68
3	C	703	GTP	O2B-PB-O1B	2.20	123.13	112.24
3	C	703	GTP	O3G-PG-O3B	2.20	112.02	104.64
2	D	702	DTP	O2G-PG-O3B	-2.19	97.28	104.64
2	D	703	DTP	O2A-PA-O1A	2.17	122.98	112.24
2	D	703	DTP	C2-N1-C6	2.17	122.46	118.75
2	D	703	DTP	N6-C6-N1	2.16	123.06	118.57
3	B	702	GTP	C3'-C2'-C1'	2.15	104.21	100.98
3	A	702	GTP	O6-C6-C5	-2.14	120.19	124.37
2	A	701	DTP	C4-C5-N7	-2.13	107.17	109.40
2	A	703	DTP	C2'-C1'-N9	2.06	119.03	114.27
2	A	701	DTP	C2-N1-C6	2.06	122.28	118.75
3	A	706	GTP	PA-O3A-PB	-2.05	125.80	132.83
3	B	702	GTP	O5'-PA-O1A	-2.04	101.10	109.07
3	A	702	GTP	O3G-PG-O2G	2.03	115.39	107.64
2	B	703	DTP	C5-C6-N6	2.01	123.41	120.35
2	C	701	DTP	O3G-PG-O1G	2.01	118.53	110.68

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DTP	C5'-O5'-PA-O1A
2	A	701	DTP	C5'-O5'-PA-O2A
2	B	701	DTP	C5'-O5'-PA-O3A
2	B	701	DTP	C3'-C4'-C5'-O5'
2	C	701	DTP	PB-O3B-PG-O3G
2	C	704	DTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	C	704	DTP	C5'-O5'-PA-O1A
2	C	704	DTP	C5'-O5'-PA-O3A
2	C	704	DTP	C3'-C4'-C5'-O5'
2	D	703	DTP	PB-O3A-PA-O5'
3	A	702	GTP	C5'-O5'-PA-O1A
3	B	702	GTP	PB-O3B-PG-O2G
3	B	702	GTP	PB-O3B-PG-O3G
3	B	702	GTP	C5'-O5'-PA-O2A
3	C	703	GTP	C5'-O5'-PA-O1A
2	A	701	DTP	O4'-C4'-C5'-O5'
2	A	701	DTP	C3'-C4'-C5'-O5'
2	C	704	DTP	O4'-C4'-C5'-O5'
2	B	701	DTP	O4'-C4'-C5'-O5'
2	A	701	DTP	PB-O3B-PG-O1G
2	C	701	DTP	PB-O3A-PA-O1A
2	D	702	DTP	PG-O3B-PB-O1B
3	A	706	GTP	C4'-C5'-O5'-PA
3	A	702	GTP	C4'-C5'-O5'-PA
3	B	702	GTP	C4'-C5'-O5'-PA
2	C	701	DTP	PB-O3B-PG-O2G
3	A	702	GTP	C5'-O5'-PA-O3A
3	B	702	GTP	C5'-O5'-PA-O3A
3	C	703	GTP	C5'-O5'-PA-O3A
2	A	701	DTP	PB-O3A-PA-O1A
2	C	701	DTP	PG-O3B-PB-O2B
2	C	701	DTP	PB-O3A-PA-O2A
3	A	702	GTP	PB-O3A-PA-O1A
3	B	702	GTP	PG-O3B-PB-O1B
3	B	702	GTP	PB-O3A-PA-O2A
3	C	703	GTP	PB-O3A-PA-O1A
2	B	701	DTP	C5'-O5'-PA-O1A
2	B	701	DTP	C5'-O5'-PA-O2A
3	C	703	GTP	C5'-O5'-PA-O2A
2	B	701	DTP	PA-O3A-PB-O2B
2	C	701	DTP	PG-O3B-PB-O1B
2	D	702	DTP	PG-O3B-PB-O2B
3	B	702	GTP	PG-O3B-PB-O2B
3	C	703	GTP	PB-O3A-PA-O2A
3	C	703	GTP	O4'-C4'-C5'-O5'
3	A	702	GTP	O4'-C4'-C5'-O5'
2	A	703	DTP	PG-O3B-PB-O1B
3	B	702	GTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	701	DTP	PB-O3B-PG-O2G
2	C	704	DTP	PB-O3B-PG-O2G
2	A	701	DTP	C5'-O5'-PA-O3A
2	B	703	DTP	C5'-O5'-PA-O3A
3	A	706	GTP	C5'-O5'-PA-O3A
3	A	702	GTP	PB-O3A-PA-O2A
3	A	706	GTP	PG-O3B-PB-O1B
3	C	703	GTP	PG-O3B-PB-O2B
2	B	701	DTP	C4'-C5'-O5'-PA
2	C	704	DTP	C5'-O5'-PA-O2A
3	B	702	GTP	C5'-O5'-PA-O1A
3	B	702	GTP	PB-O3B-PG-O1G

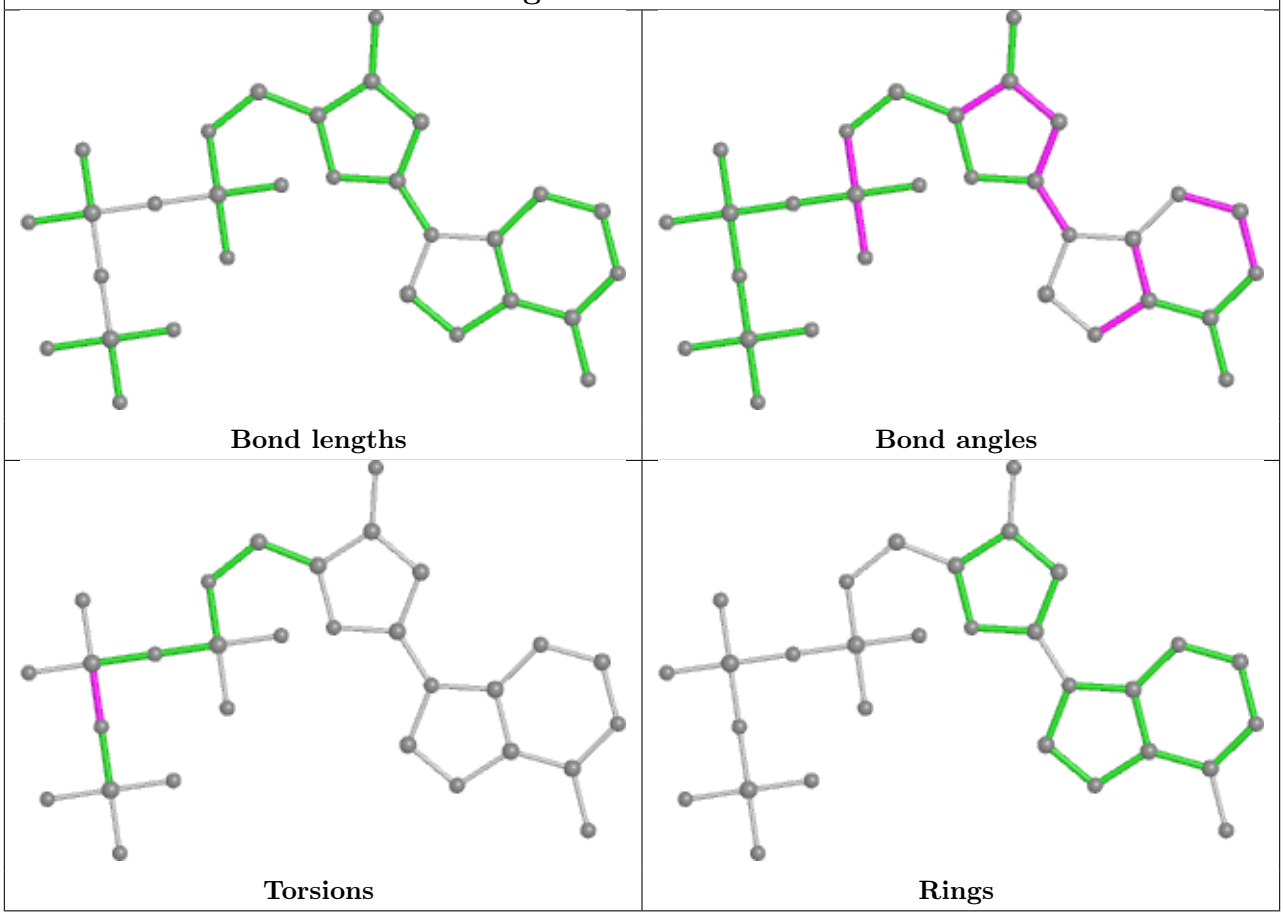
There are no ring outliers.

8 monomers are involved in 21 short contacts:

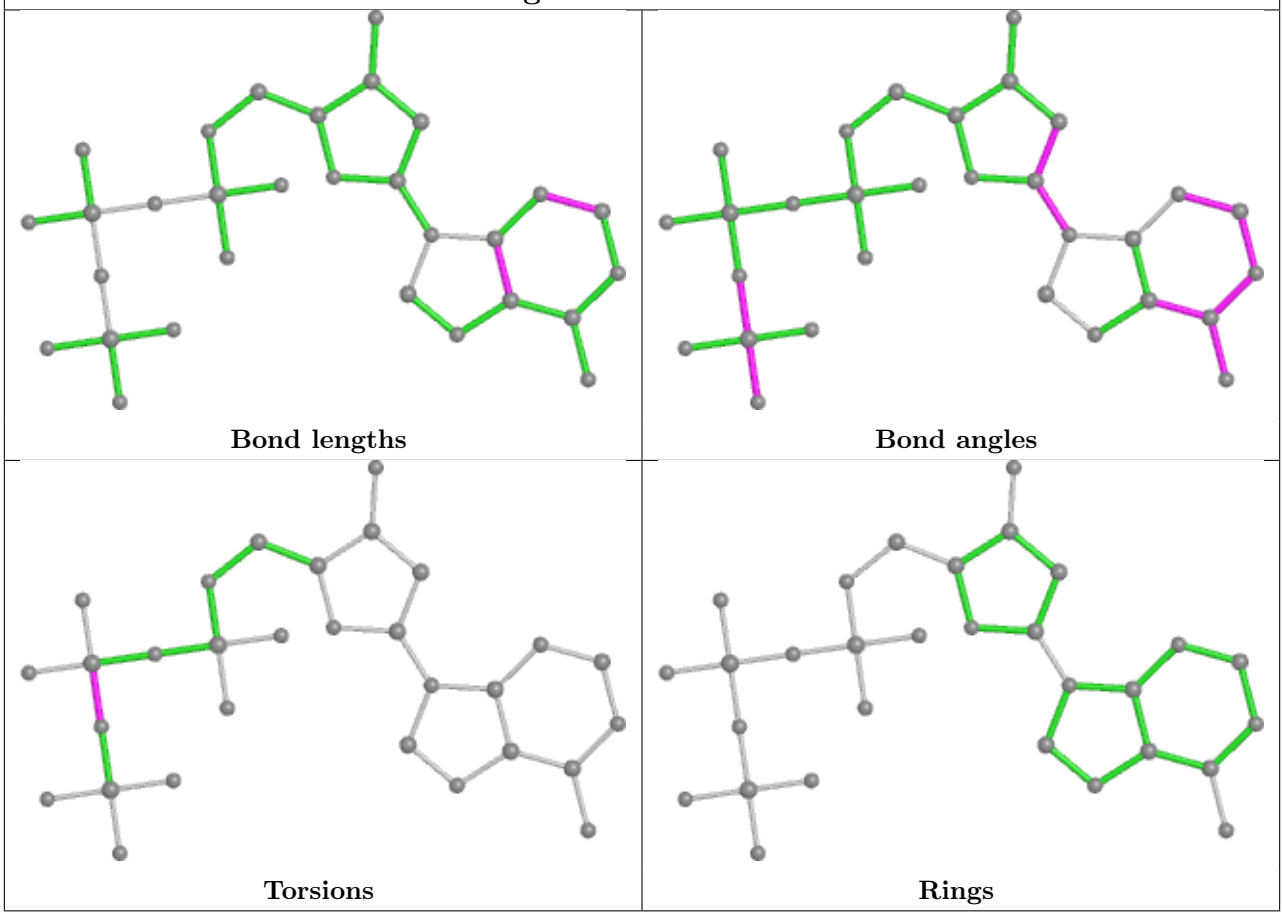
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	703	DTP	3	0
2	A	701	DTP	2	0
3	A	702	GTP	3	0
3	A	706	GTP	1	0
2	B	703	DTP	1	0
2	C	704	DTP	3	0
2	B	701	DTP	6	0
3	C	703	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A 703



Ligand DTP D 702



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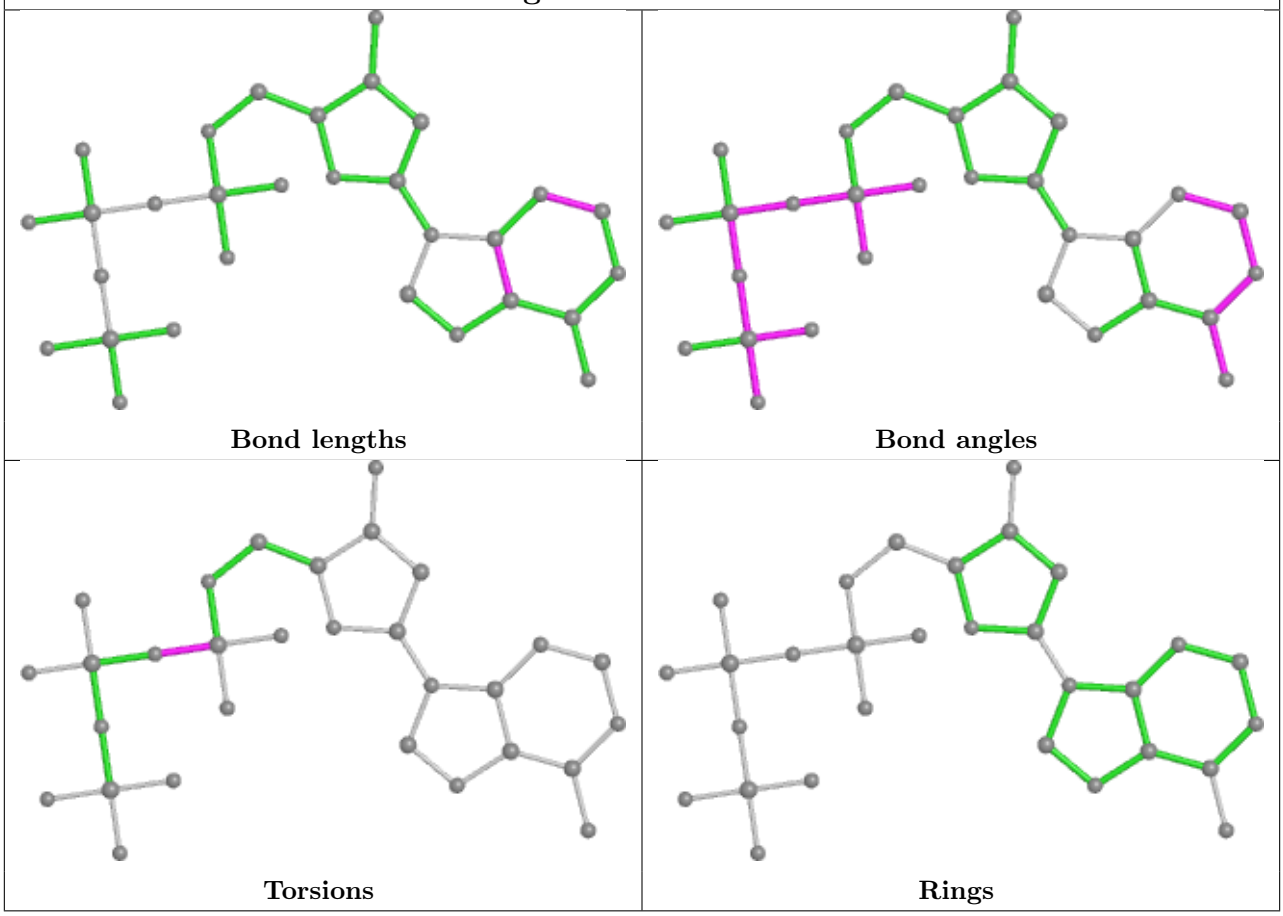

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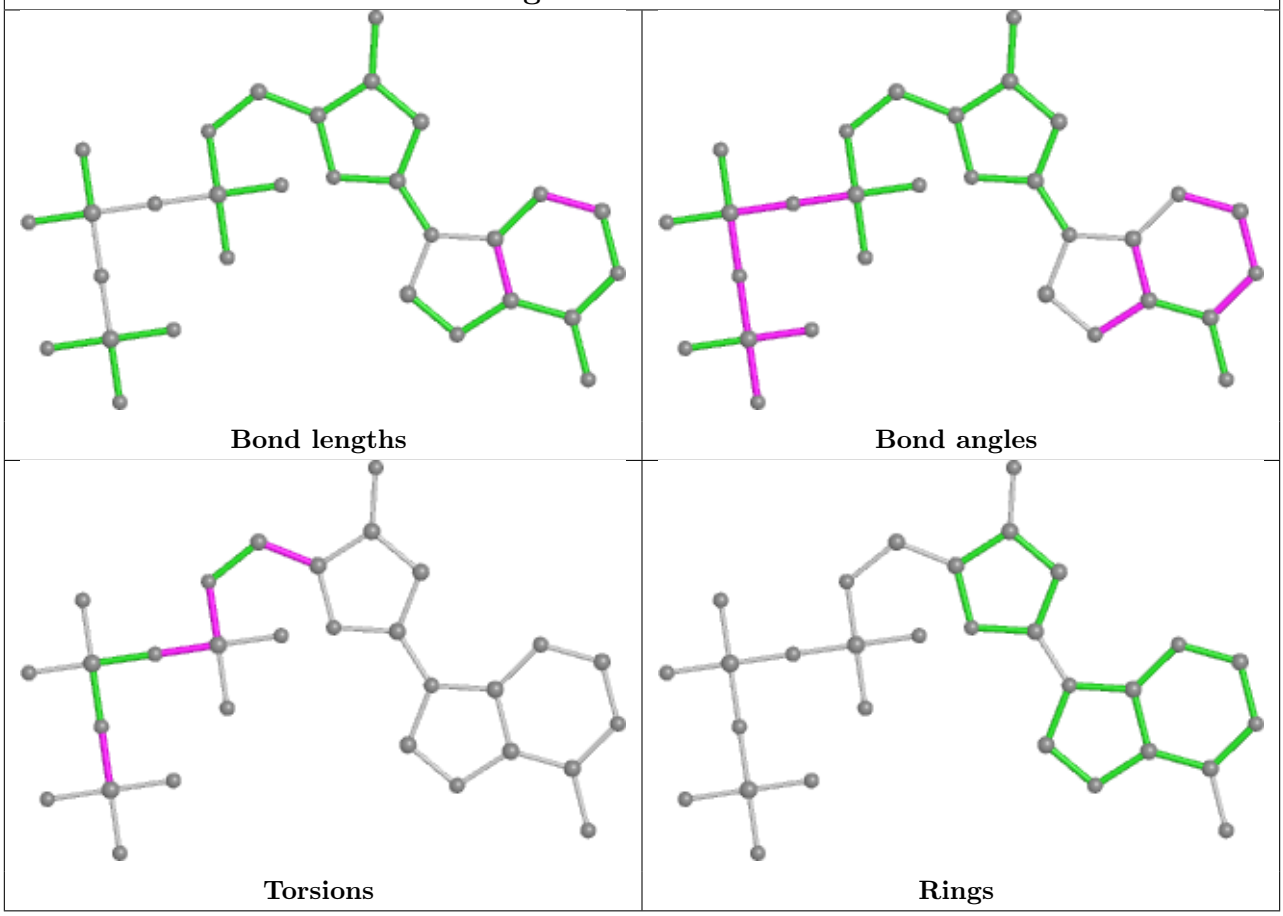

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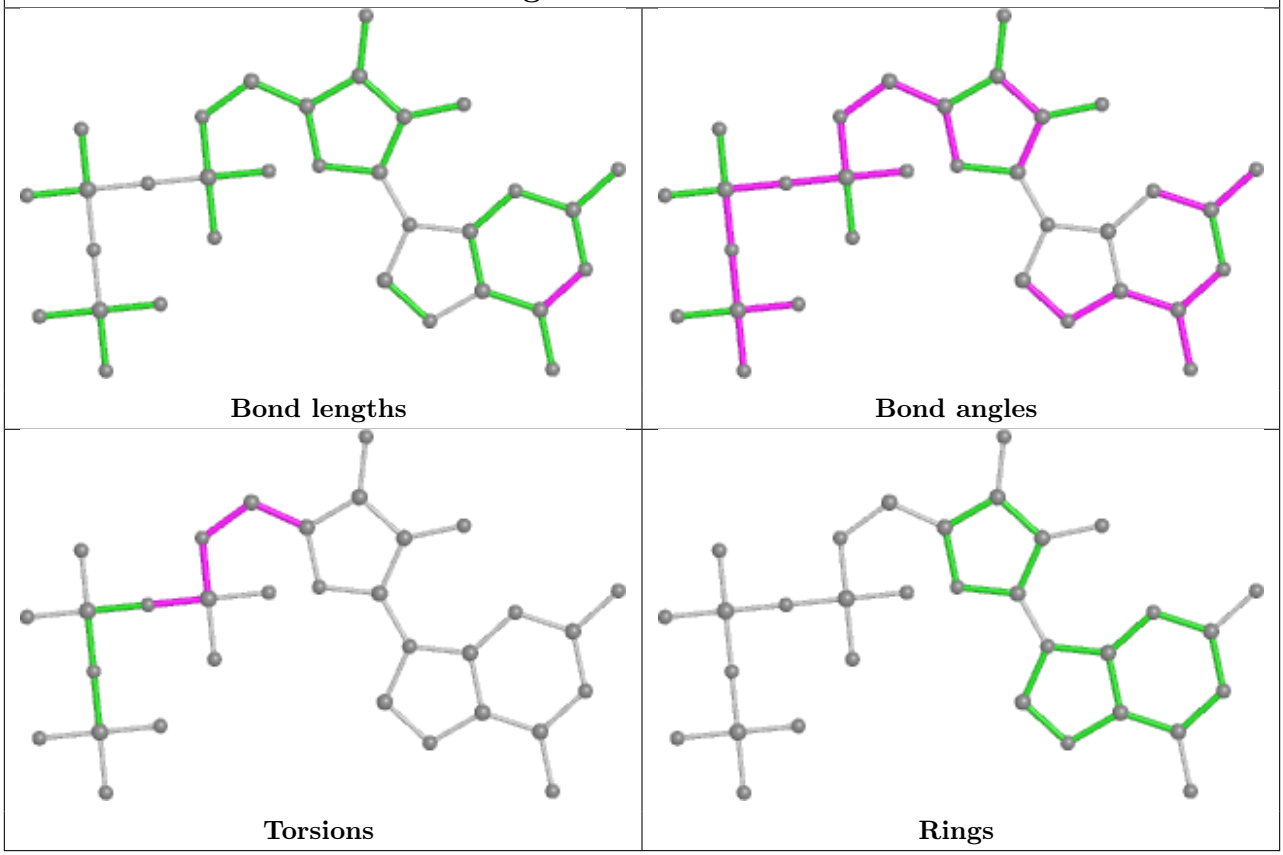

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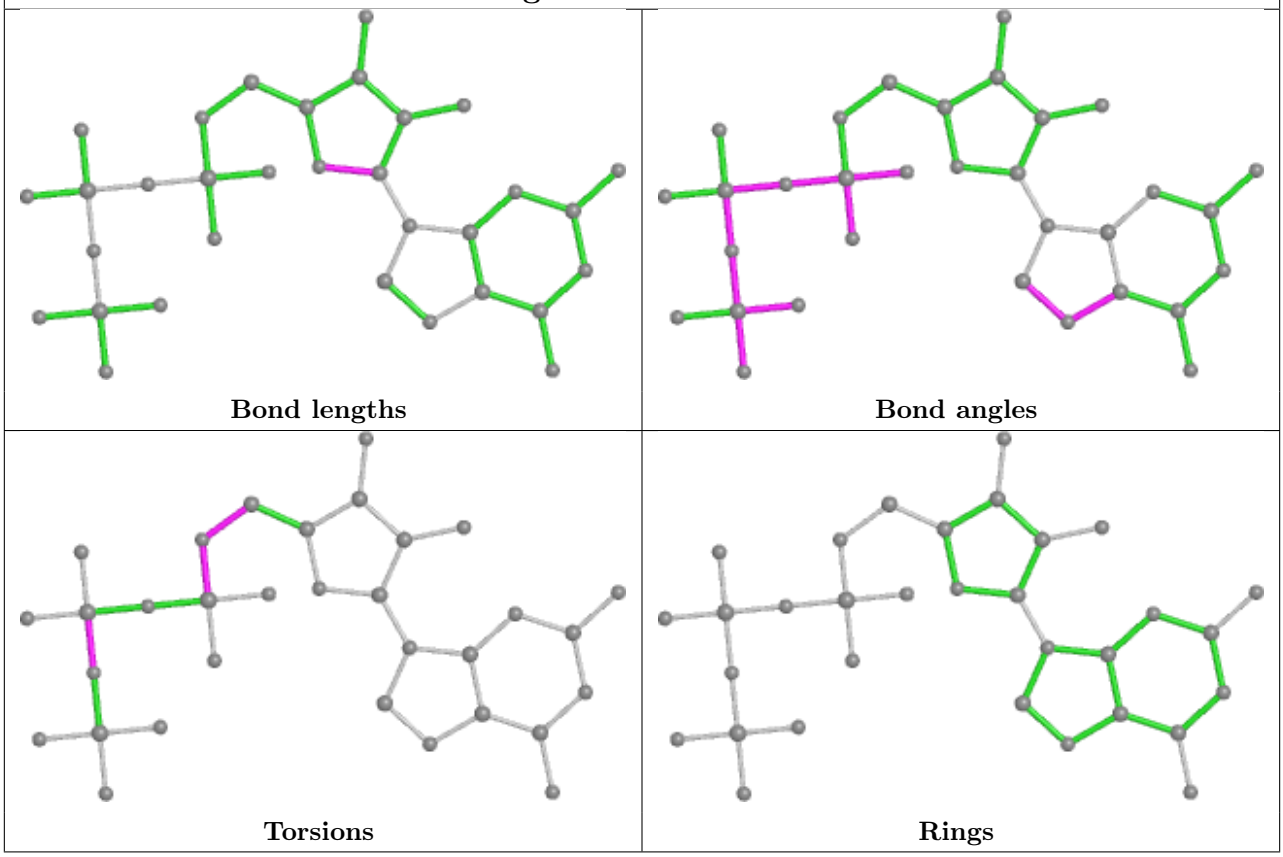

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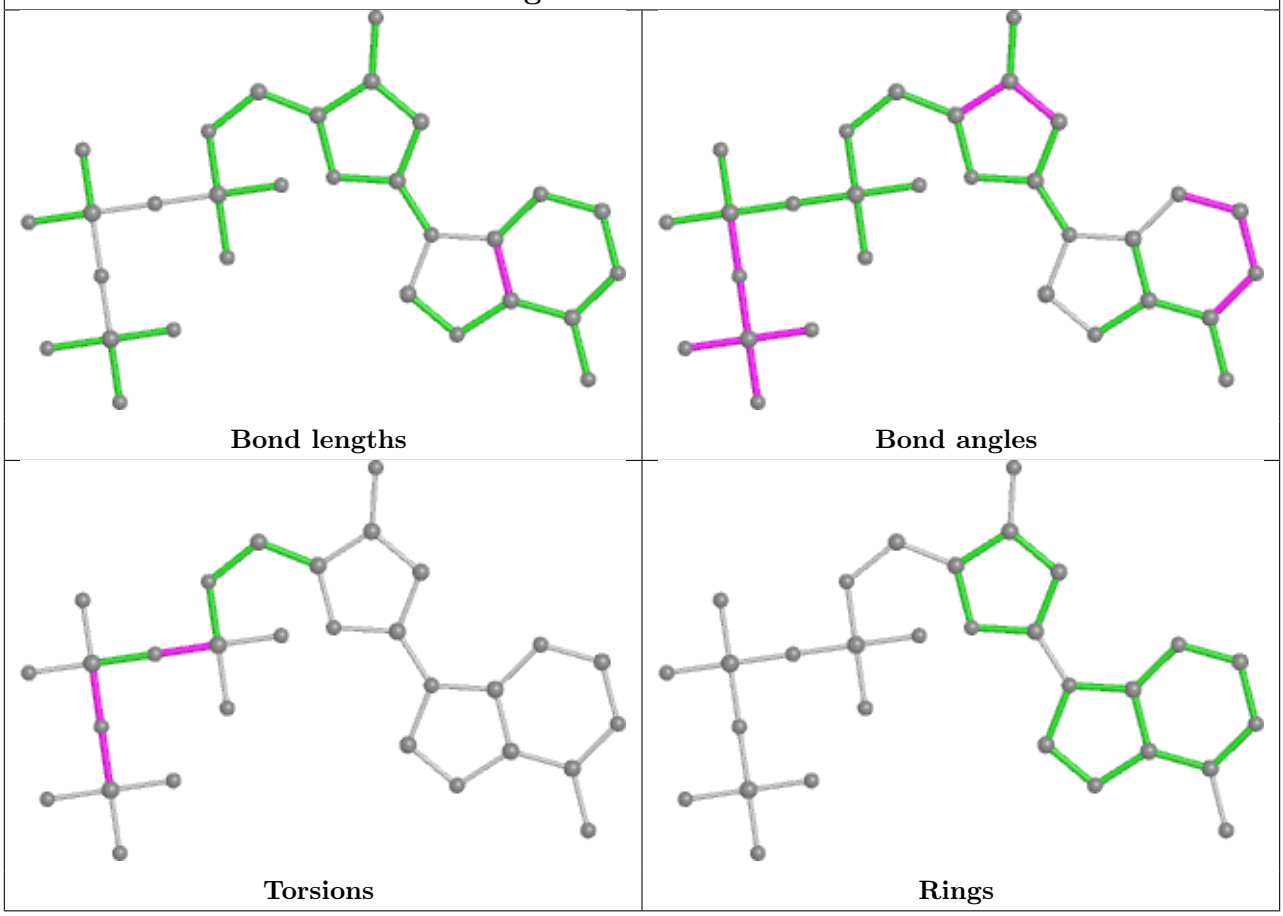

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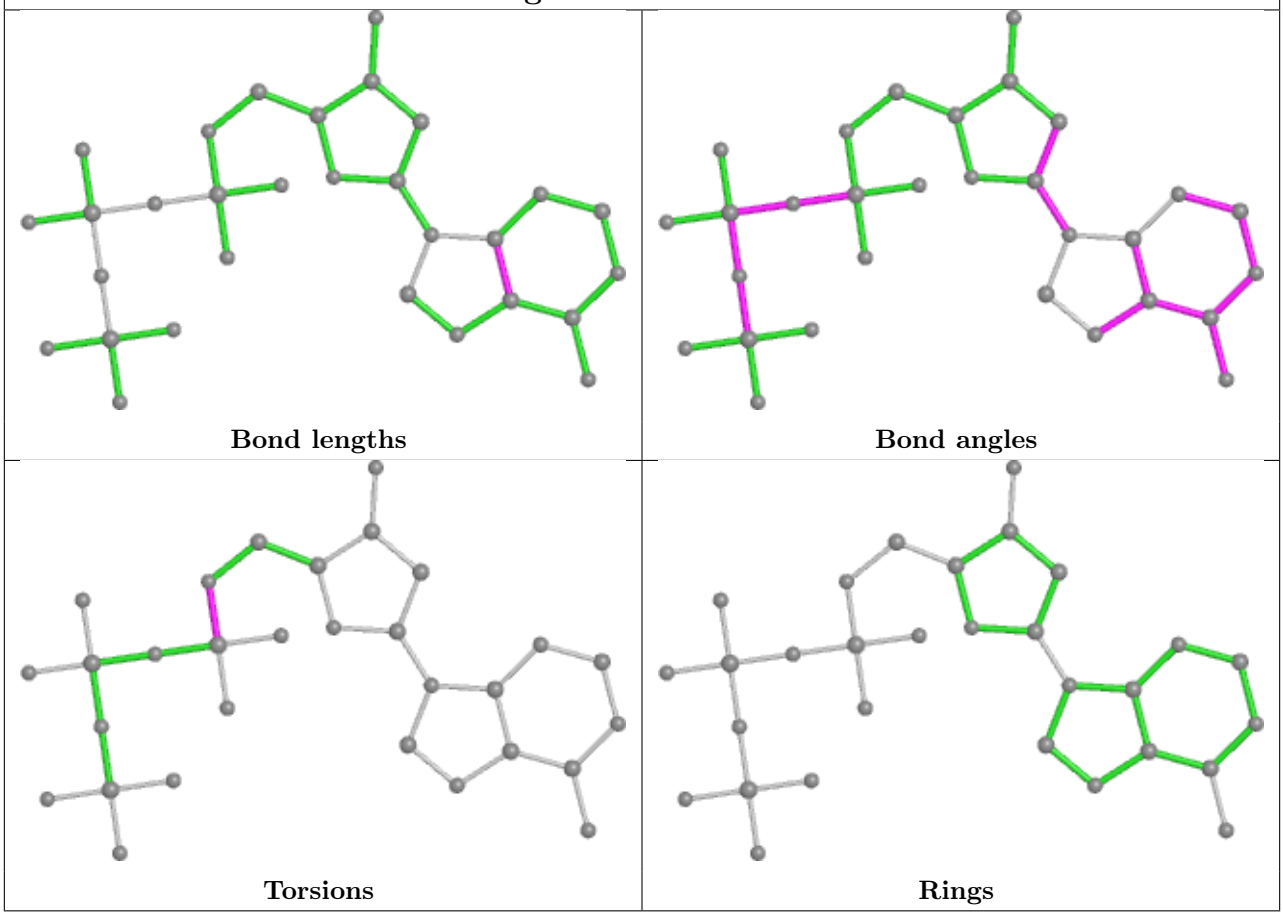

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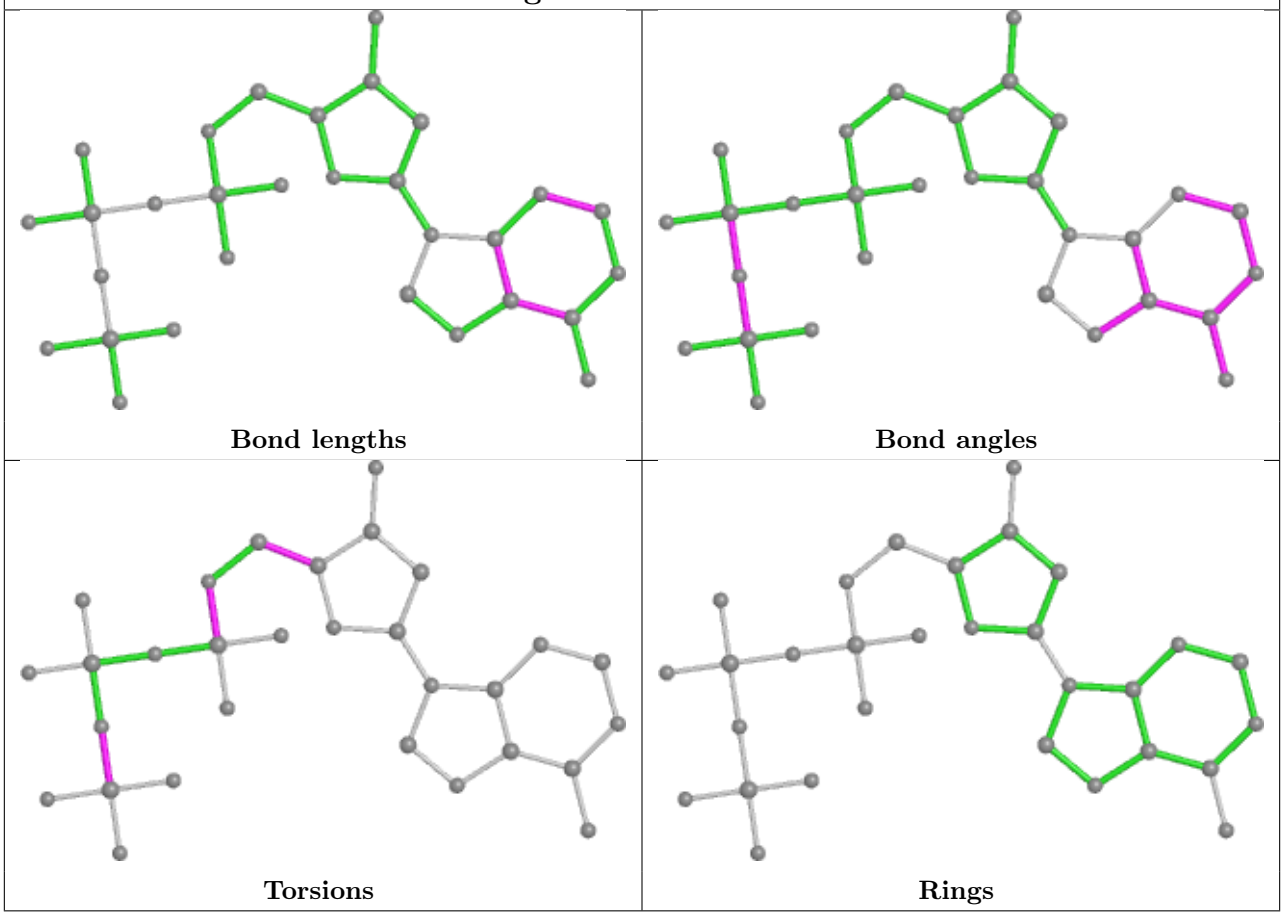

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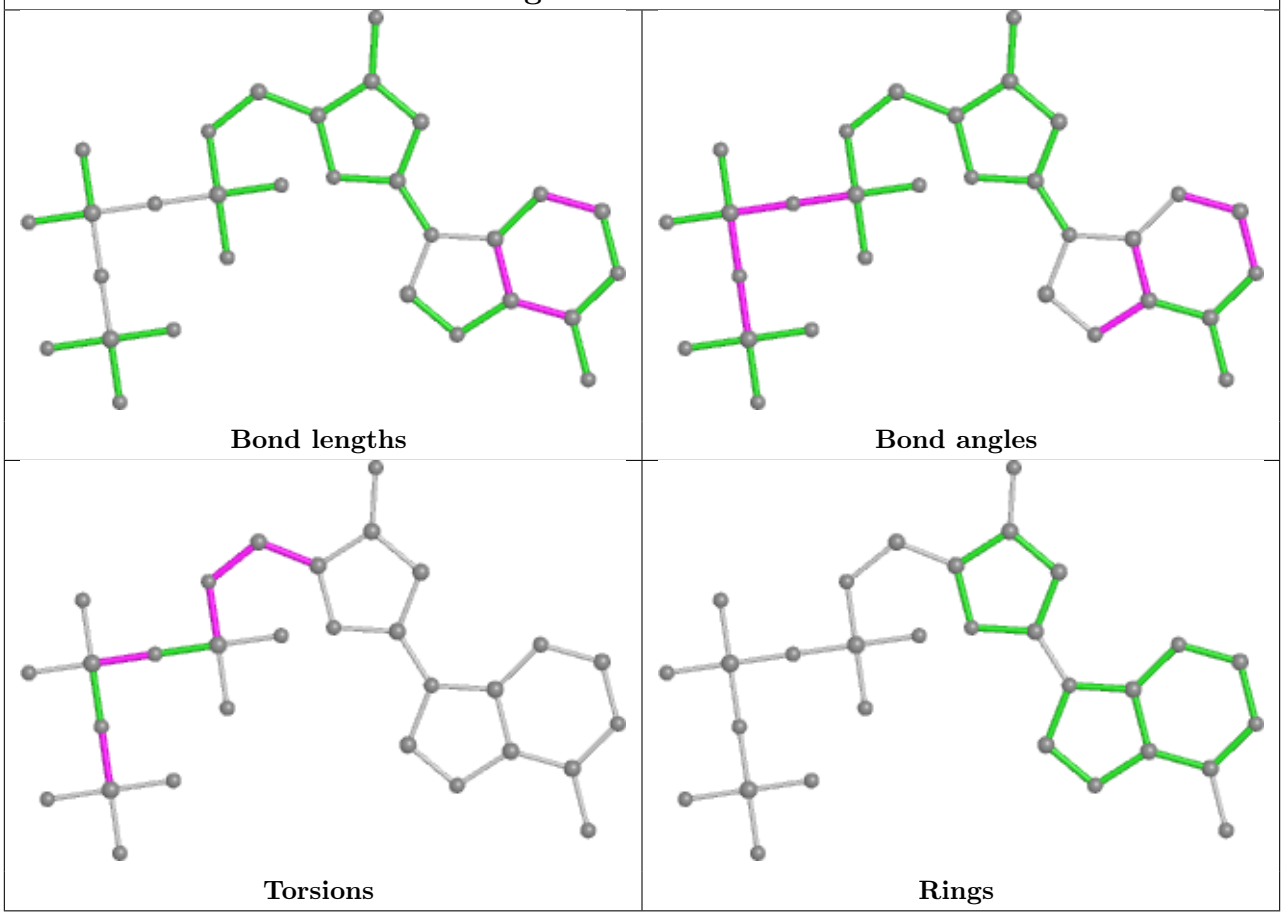

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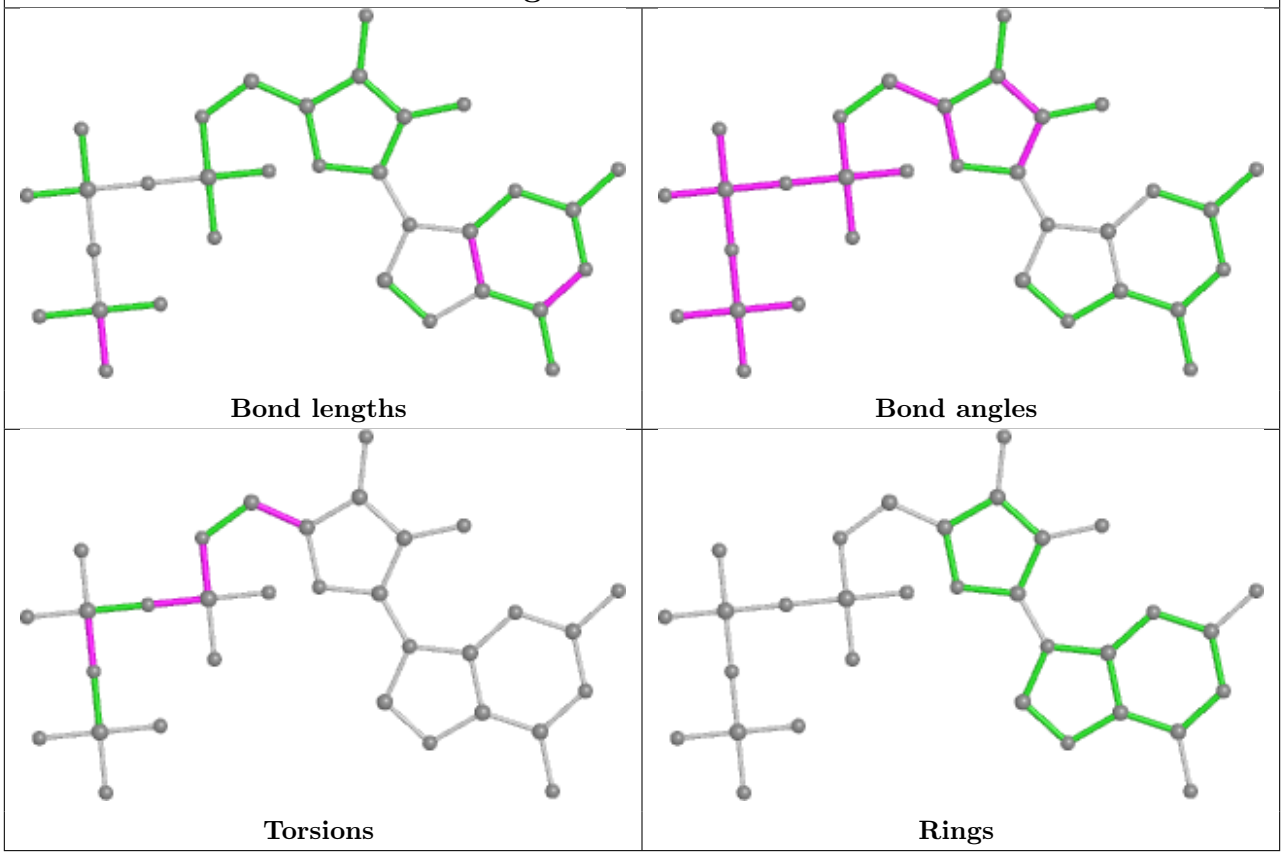

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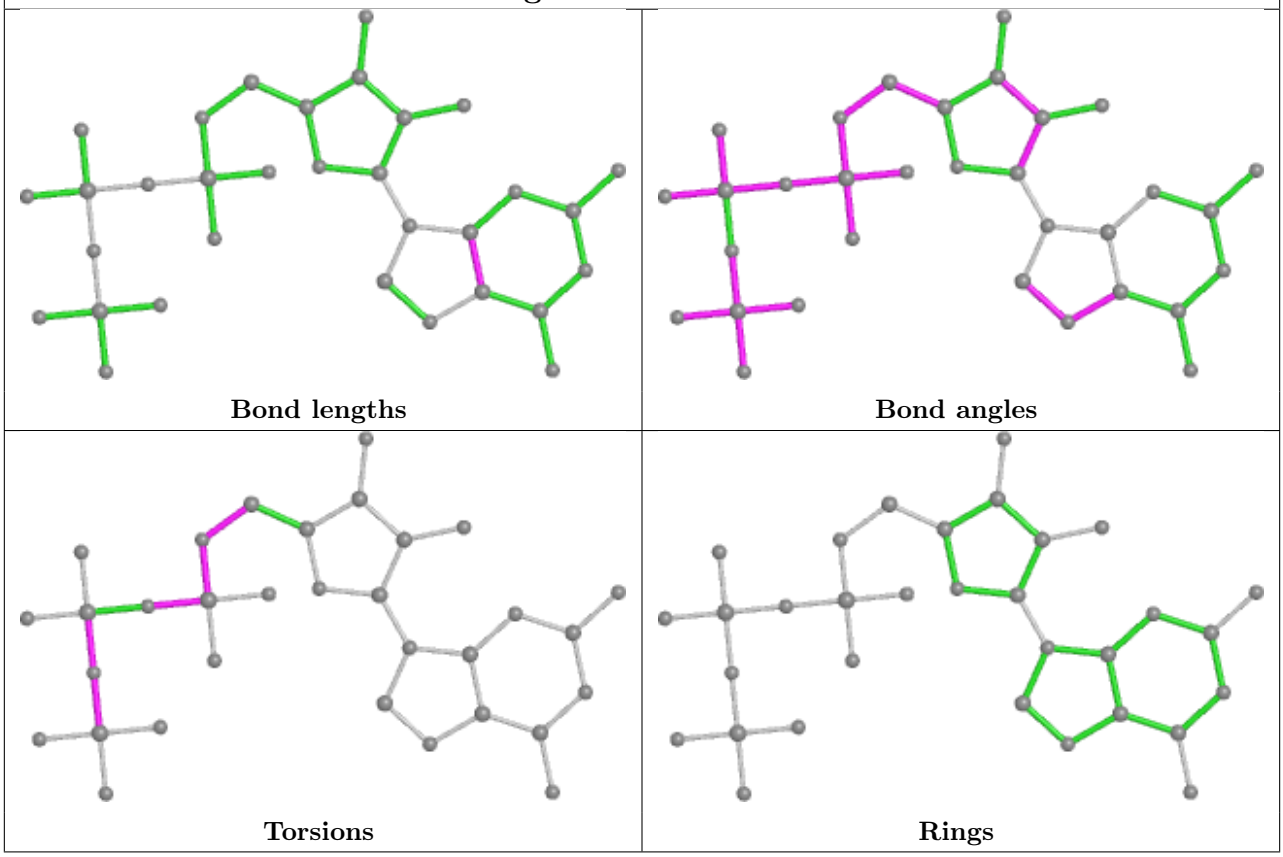

5.7 Other polymers (i)

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	461/514 (89%)	0.16	26 (5%)	24	30	19, 35, 66, 95	0
1	B	458/514 (89%)	0.26	28 (6%)	21	27	18, 37, 71, 97	0
1	C	466/514 (90%)	0.24	32 (6%)	16	22	18, 35, 67, 99	0
1	D	455/514 (88%)	0.21	26 (5%)	23	30	19, 36, 69, 93	0
All	All	1840/2056 (89%)	0.22	112 (6%)	21	27	18, 36, 69, 99	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	LEU	6.9
1	C	490	ASP	6.4
1	B	492	LYS	6.1
1	C	325	ILE	6.1
1	C	491	VAL	5.9
1	B	563	TYR	5.9
1	A	465	GLN	5.7
1	C	466	ILE	5.5
1	D	579	THR	5.3
1	A	563	TYR	5.2
1	A	277	GLU	4.9
1	B	466	ILE	4.9
1	C	326	GLN	4.8
1	D	326	GLN	4.3
1	A	468	ILE	4.3
1	D	284	LEU	4.3
1	D	277	GLU	4.2
1	D	562	LEU	4.2
1	B	486	LYS	4.0
1	B	562	LEU	4.0
1	B	560	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	578	PHE	3.9
1	A	562	LEU	3.8
1	C	329	PHE	3.7
1	C	588	ALA	3.7
1	C	492	LYS	3.7
1	C	262	GLU	3.7
1	D	325	ILE	3.7
1	B	326	GLN	3.7
1	C	587	ILE	3.7
1	B	491	VAL	3.6
1	A	581	PRO	3.6
1	D	329	PHE	3.5
1	D	563	TYR	3.5
1	B	528	ARG	3.4
1	A	486	LYS	3.4
1	A	528	ARG	3.4
1	B	564	ALA	3.4
1	D	559	ARG	3.4
1	A	325	ILE	3.4
1	B	325	ILE	3.4
1	C	568	TYR	3.3
1	A	473	TYR	3.3
1	B	561	SER	3.3
1	A	484	LYS	3.3
1	D	460	THR	3.3
1	D	574	ALA	3.2
1	C	284	LEU	3.2
1	B	559	ARG	3.1
1	C	113	ASP	3.0
1	C	484	LYS	3.0
1	C	327	ASN	3.0
1	C	584	GLY	3.0
1	C	562	LEU	2.9
1	B	581	PRO	2.8
1	B	190	GLN	2.8
1	B	496	GLU	2.8
1	A	487	VAL	2.8
1	B	484	LYS	2.8
1	D	570	VAL	2.7
1	D	345	ASN	2.7
1	D	566	ARG	2.7
1	A	561	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	568	TYR	2.7
1	C	560	LYS	2.7
1	A	114	THR	2.7
1	C	563	TYR	2.6
1	C	589	PRO	2.6
1	D	327	ASN	2.6
1	B	324	GLY	2.6
1	C	557	VAL	2.6
1	B	285	TRP	2.6
1	D	572	TRP	2.6
1	C	230	LYS	2.6
1	C	320	CYS	2.5
1	B	344	ASP	2.5
1	B	473	TYR	2.5
1	A	284	LEU	2.5
1	B	323	LEU	2.4
1	D	328	ASN	2.4
1	B	121	PRO	2.4
1	A	564	ALA	2.4
1	C	564	ALA	2.4
1	C	324	GLY	2.3
1	A	471	GLU	2.3
1	A	323	LEU	2.3
1	A	578	PHE	2.3
1	D	576	ARG	2.3
1	B	262	GLU	2.3
1	C	586	VAL	2.2
1	D	484	LYS	2.2
1	C	522[A]	CYS	2.2
1	A	282	ASP	2.2
1	A	470	ARG	2.2
1	C	331	TYR	2.2
1	D	474	GLU	2.2
1	A	567	GLN	2.2
1	D	496	GLU	2.2
1	A	326	GLN	2.2
1	D	550	ILE	2.1
1	A	344	ASP	2.1
1	C	276	LEU	2.1
1	C	467	LYS	2.1
1	A	324	GLY	2.1
1	D	535	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	288	LYS	2.1
1	D	486	LYS	2.1
1	D	292	GLU	2.0
1	A	121	PRO	2.0
1	B	558	ASP	2.0
1	C	229	VAL	2.0
1	C	559	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

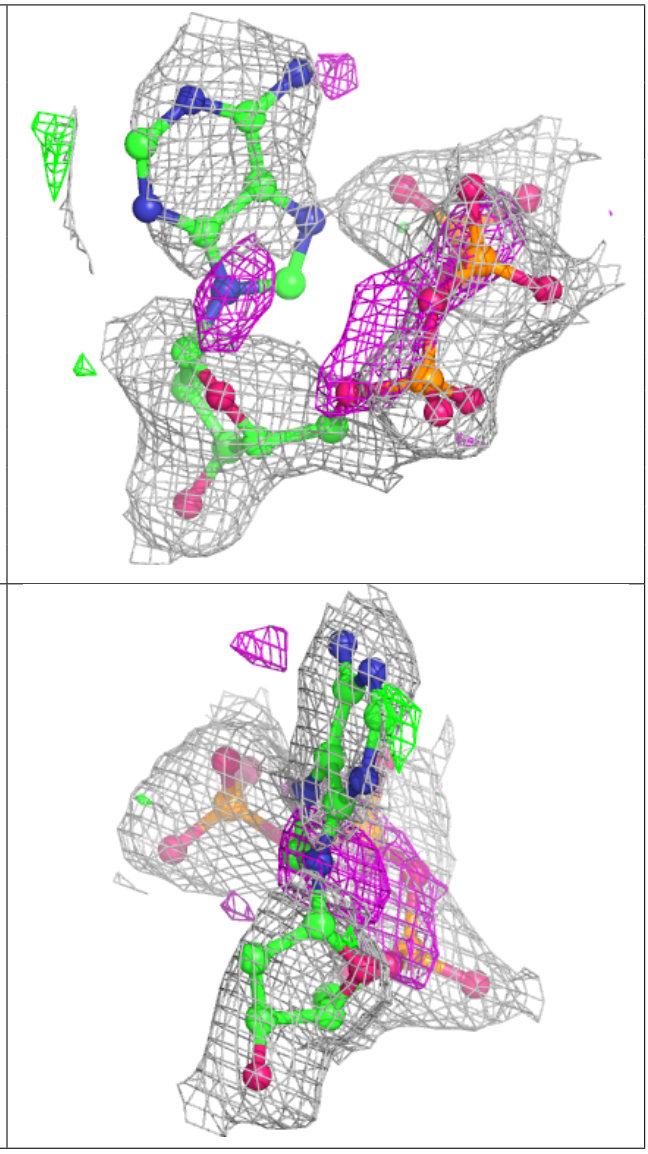
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DTP	A	701	30/30	0.74	0.24	44,75,85,87	0
2	DTP	B	701	30/30	0.77	0.25	48,76,92,96	0
2	DTP	C	704	30/30	0.77	0.30	44,75,97,108	0
2	DTP	D	703	30/30	0.81	0.23	46,73,85,94	0
2	DTP	D	702	30/30	0.97	0.11	19,24,29,31	0
4	MG	A	704	1/1	0.97	0.08	26,26,26,26	0
4	MG	A	705	1/1	0.97	0.08	29,29,29,29	0
4	MG	C	702	1/1	0.97	0.08	31,31,31,31	0
3	GTP	A	706	32/32	0.98	0.11	22,26,33,35	0
3	GTP	C	703	32/32	0.98	0.10	20,23,28,30	0
2	DTP	B	703	30/30	0.98	0.11	23,26,30,35	0
2	DTP	A	703	30/30	0.98	0.11	21,22,24,25	0
3	GTP	A	702	32/32	0.98	0.09	19,23,29,30	0
4	MG	D	701	1/1	0.98	0.05	27,27,27,27	0
3	GTP	B	702	32/32	0.99	0.10	23,24,27,27	0
2	DTP	C	701	30/30	0.99	0.09	21,23,27,29	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.

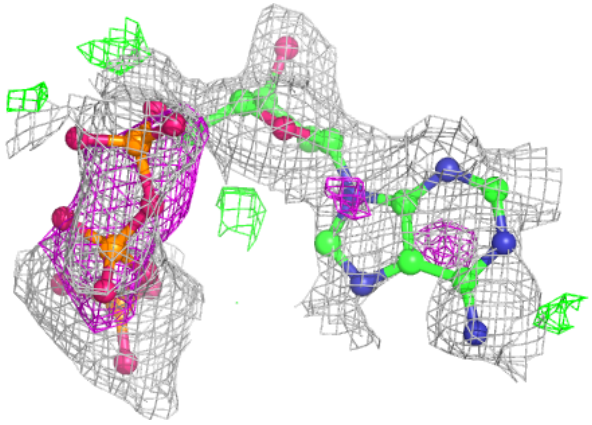
Electron density around DTP A 701:

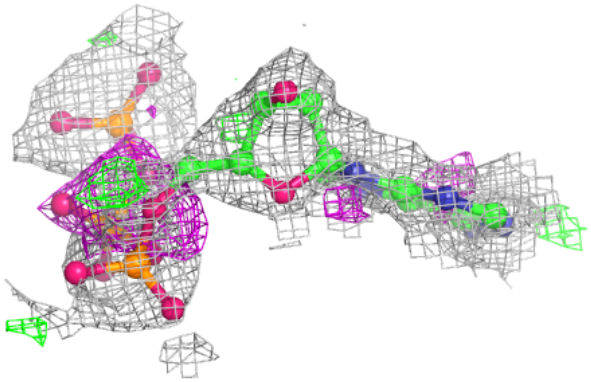
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

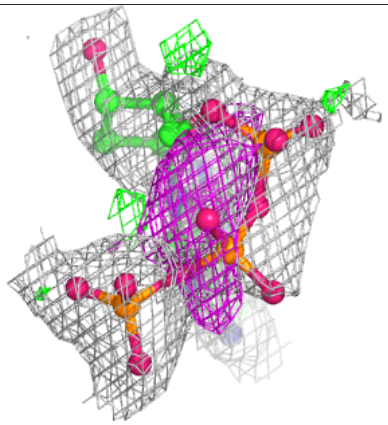


Electron density around DTP B 701:

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

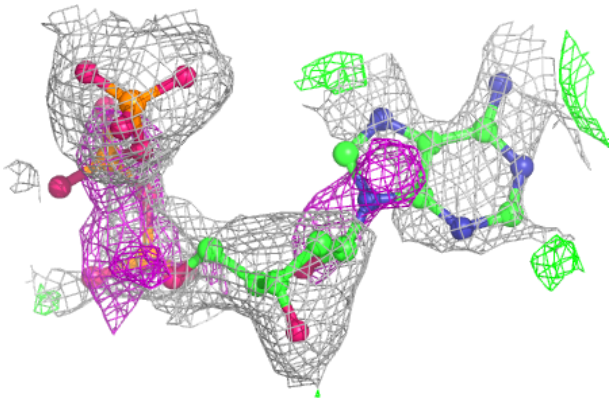


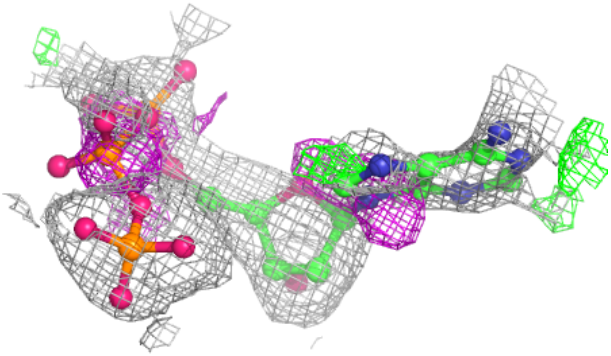


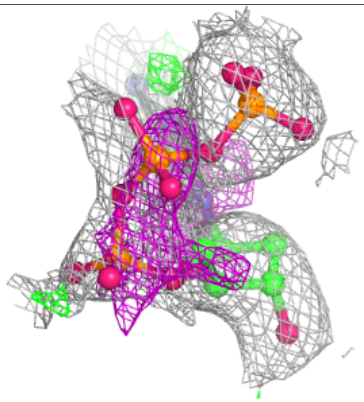


Electron density around DTP C 704:

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







Electron density around DTP D 703:

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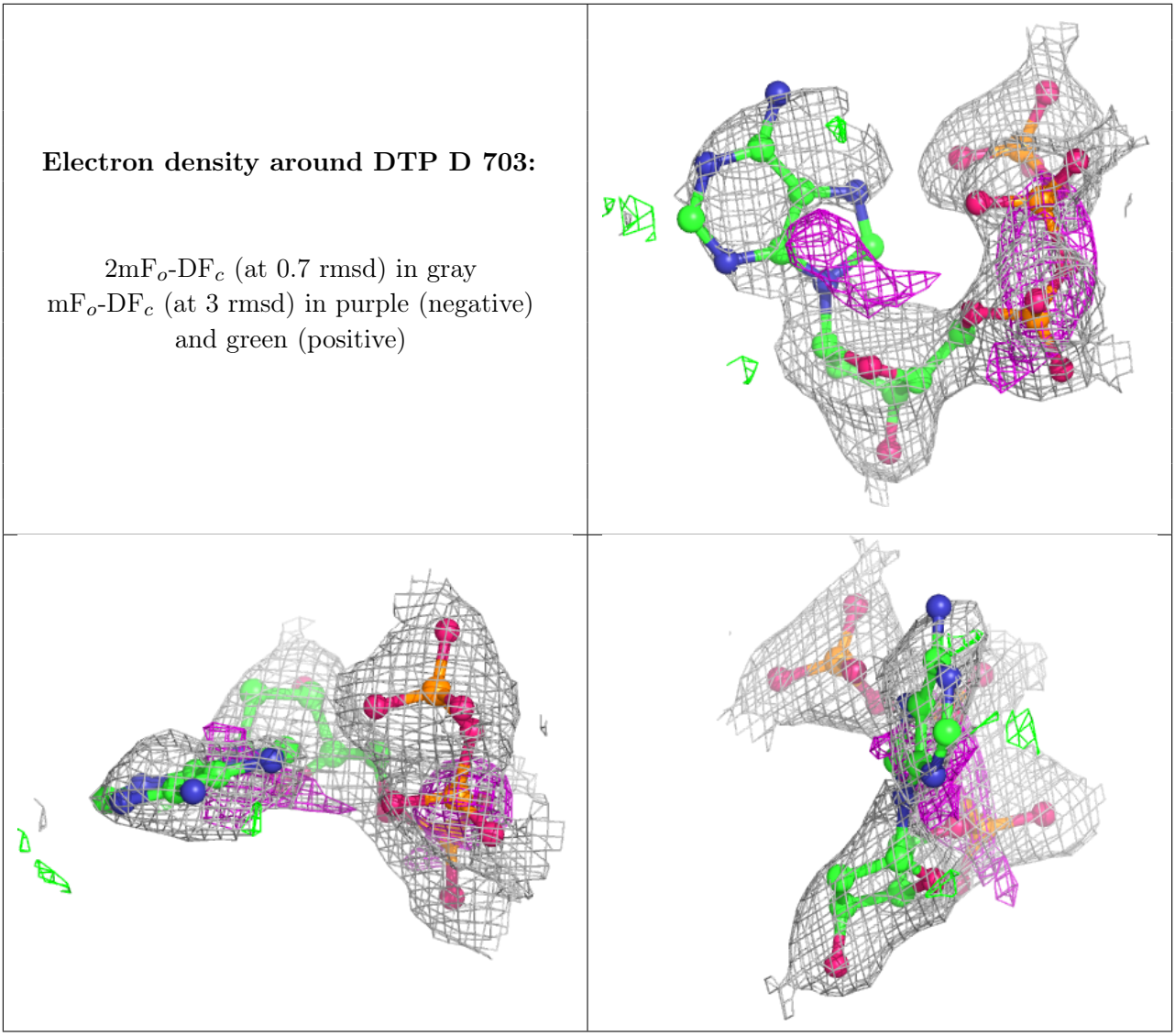
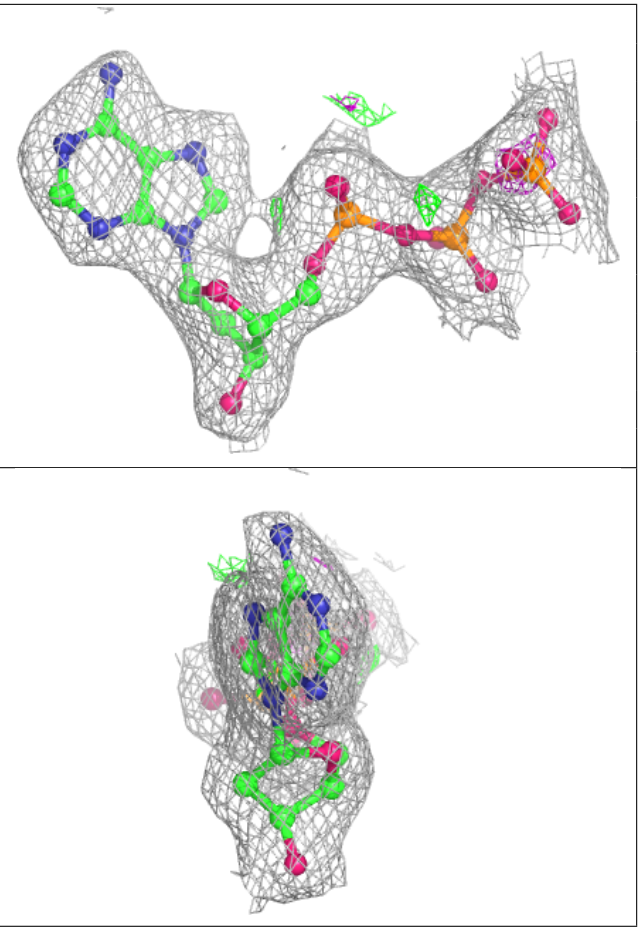
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



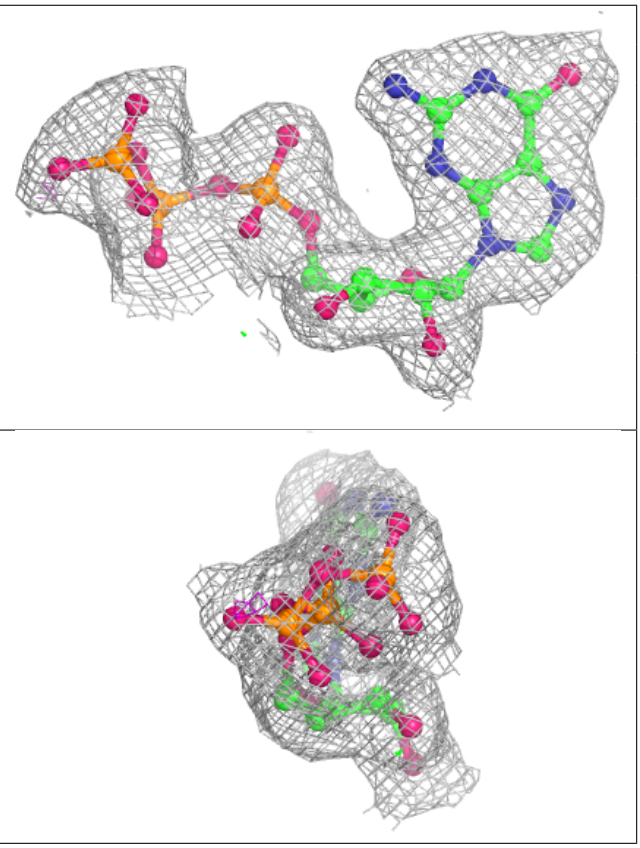
Electron density around DTP D 702:

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



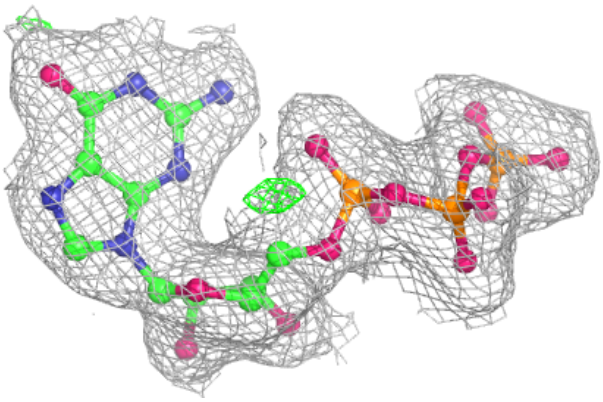
Electron density around GTP A 706:

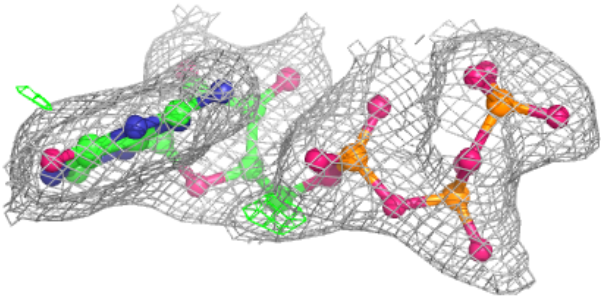
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

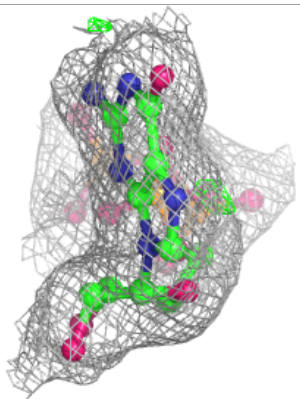


Electron density around GTP C 703:

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

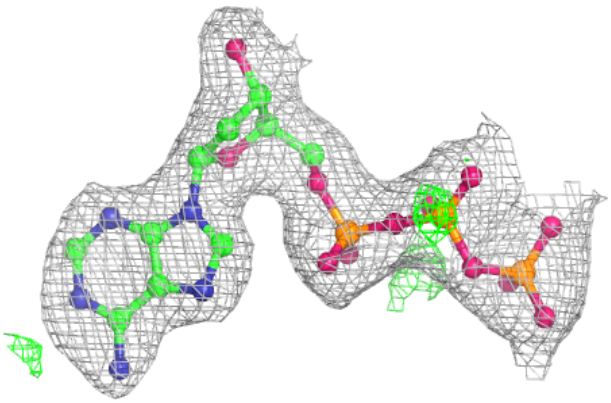


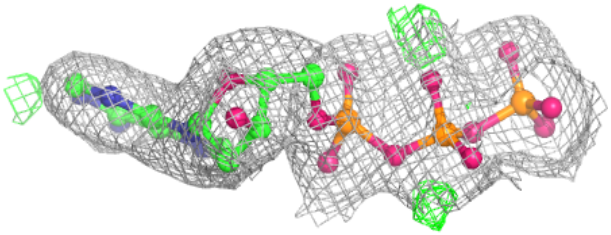


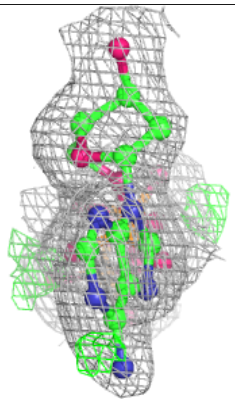


Electron density around DTP B 703:

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

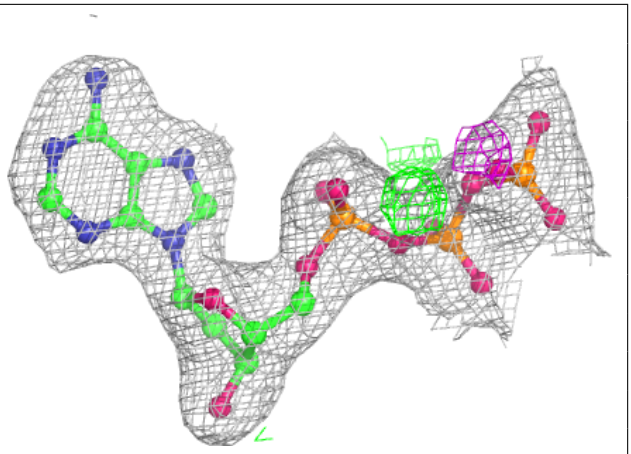


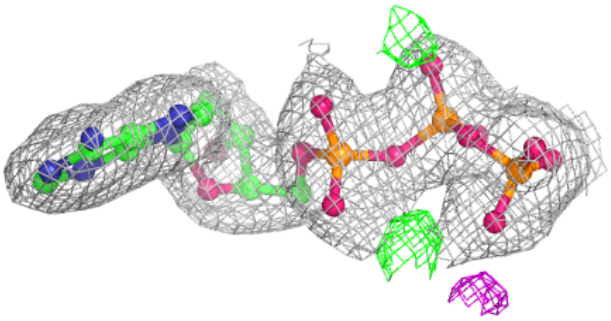


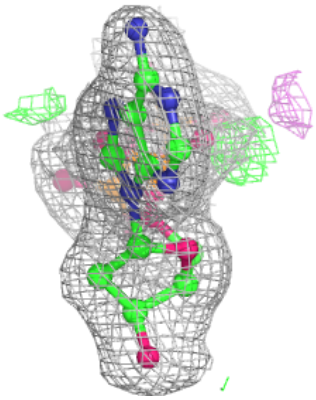


Electron density around DTP A 703:

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

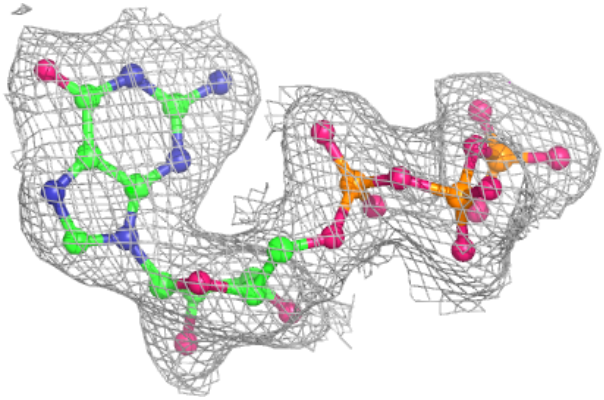


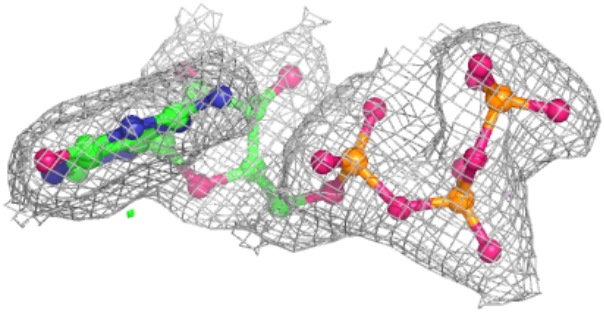


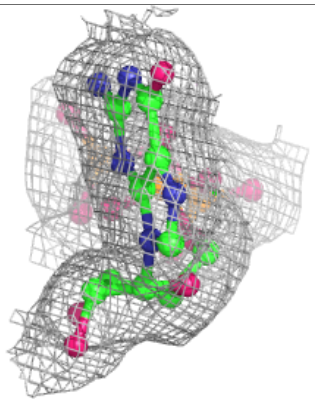


Electron density around GTP A 702:

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

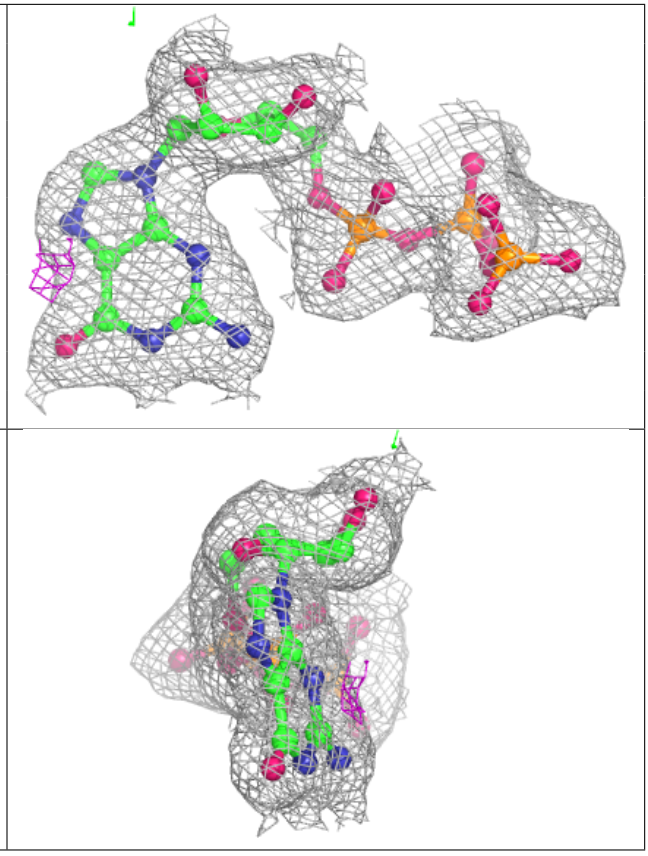


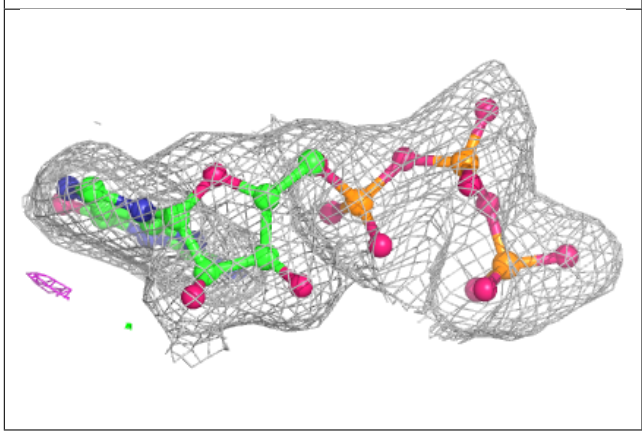




Electron density around GTP B 702:

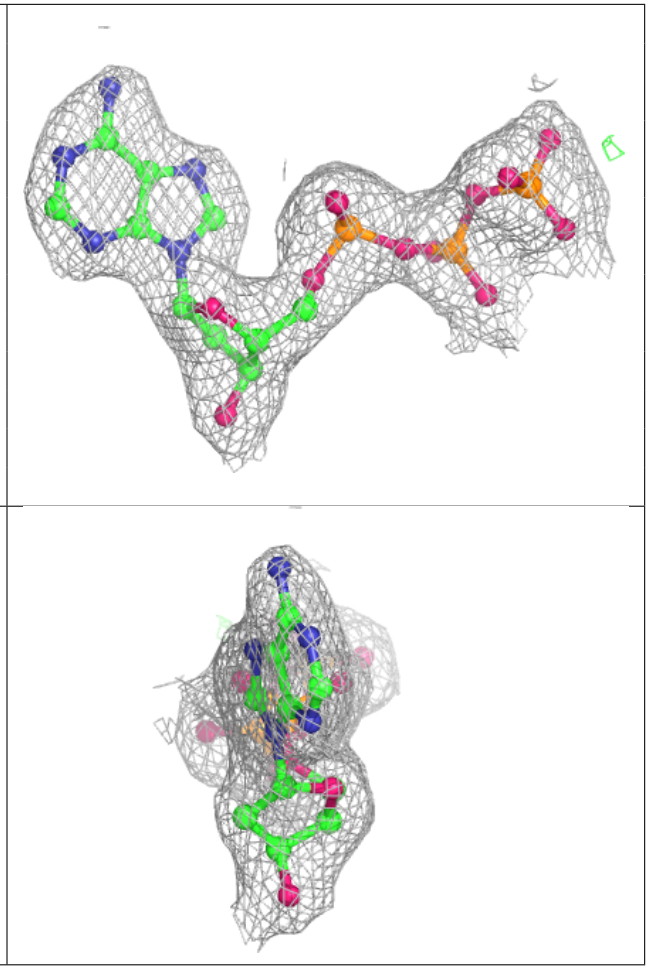
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around DTP C 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.