Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 08:52 pm GMT

PDB ID	:	1UVK
Title	:	The structural basis for RNA specificity and Ca2 inhibition of an RNA-dependent RNA polymerase phi6p2 dead-end complex
Authors	:	Salgado, P.S.; Makeyev, E.V.; Butcher, S.; Bamford, D.; Stuart, D.I.; Grimes, J.M.
Deposited on	:	2004-01-21
Resolution	:	2.45 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:

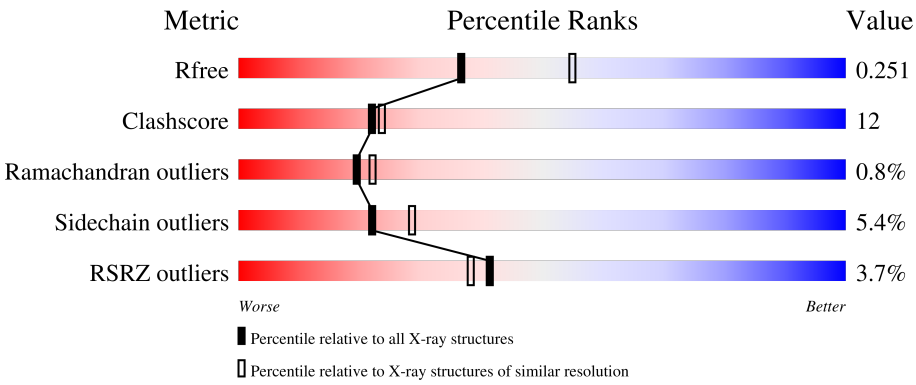
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	664	3% 77% 20% •
1	C	664	2% 76% 21% •
1	E	664	6% 77% 21% •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16257 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	664	5265	3342	914	977	32	0	0	0
1	C	664	5265	3342	914	977	32	0	0	0
1	E	664	5265	3342	914	977	32	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
C	456	MET	ILE	conflict	UNP P11124
E	456	MET	ILE	conflict	UNP P11124

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	1	1	1	0	0
2	C	1	1	1	0	0
2	E	1	1	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	C	2	2	2	0	0

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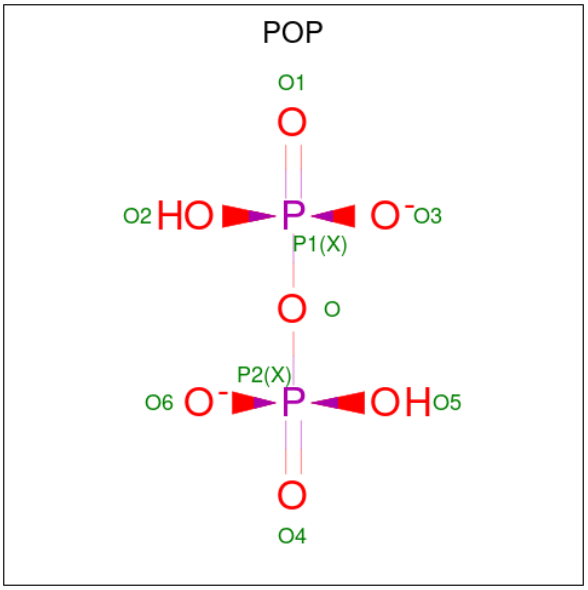
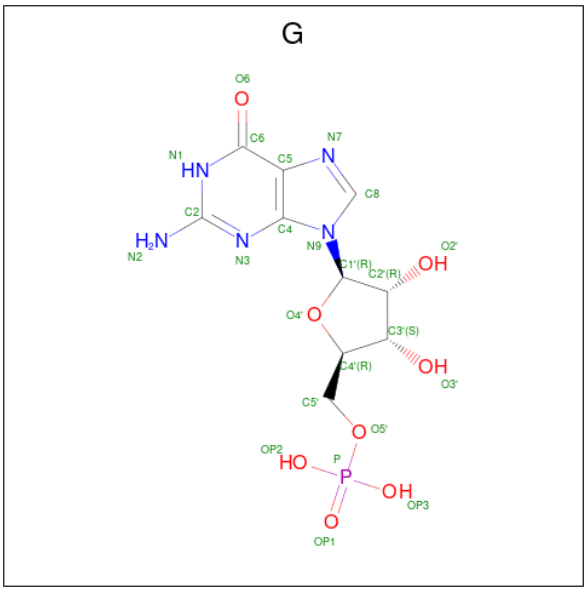
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	E	2	2	2	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



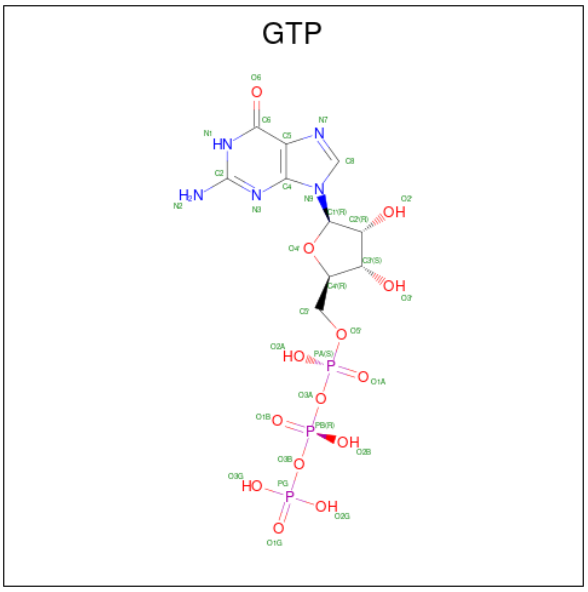
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	9	7	2	0	0
4	C	1	9	7	2	0	0
4	E	1	9	7	2	0	0

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
5	C	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
5	E	1	23	10	5	7	1	0	0

- Molecule 6 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		
6	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
6	C	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
6	E	1	32	10	5	14	3	0	0

- Molecule 7 is water.

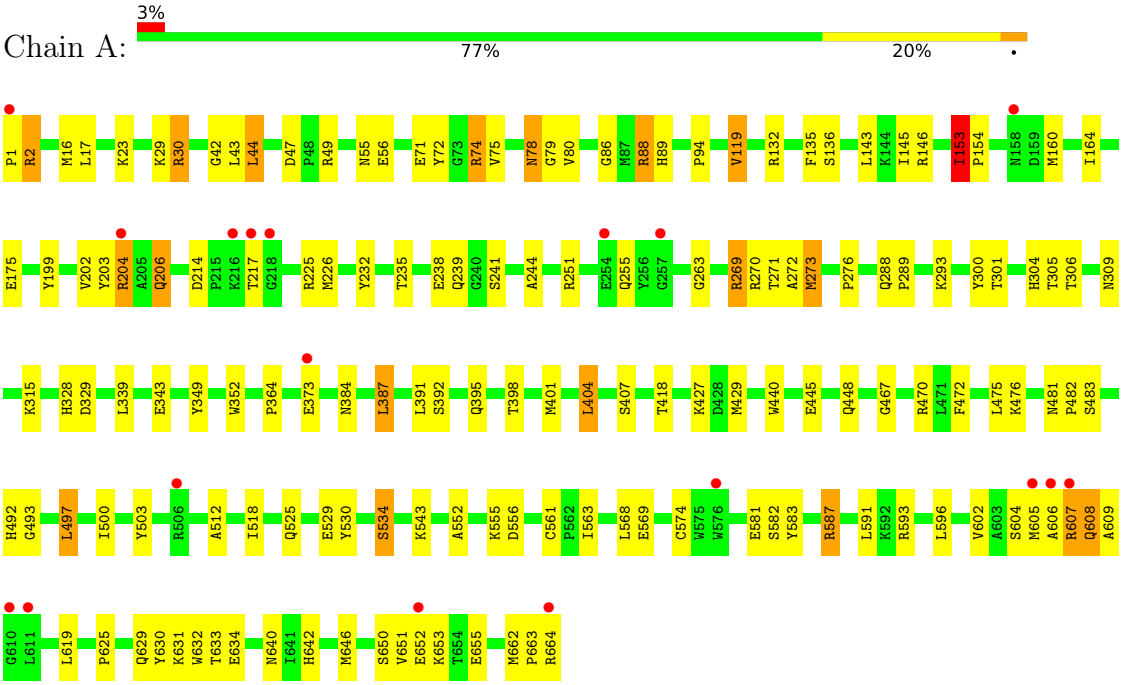
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	84	84	84	0	0
			Total	O		
7	C	87	87	87	0	0
			Total	O		
7	E	90	90	90	0	0

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.

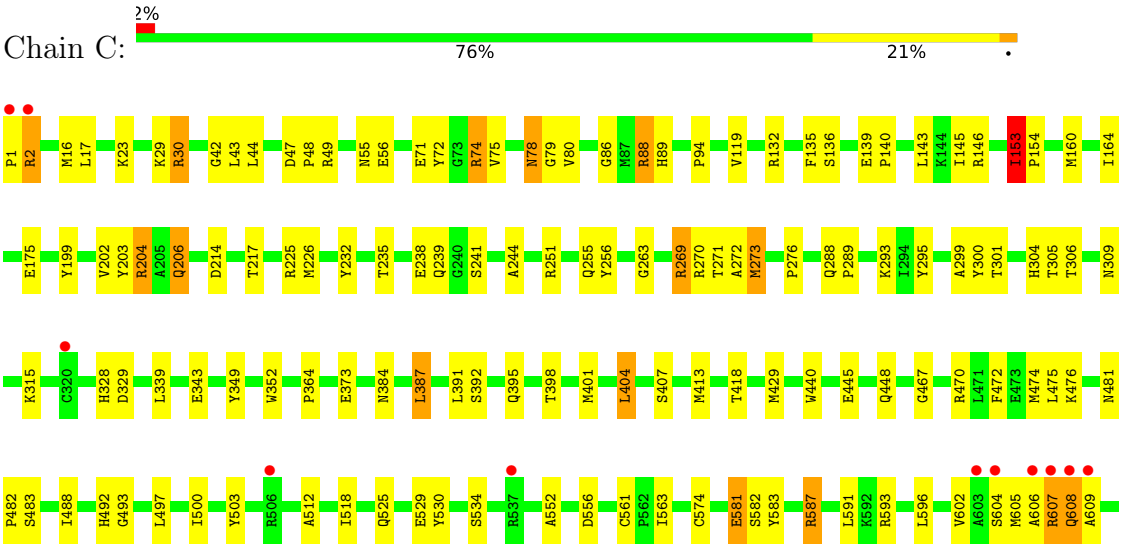
• Molecule 1: RNA-directed RNA polymerase

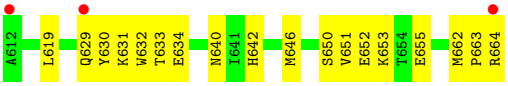
Chain A:



• Molecule 1: RNA-directed RNA polymerase

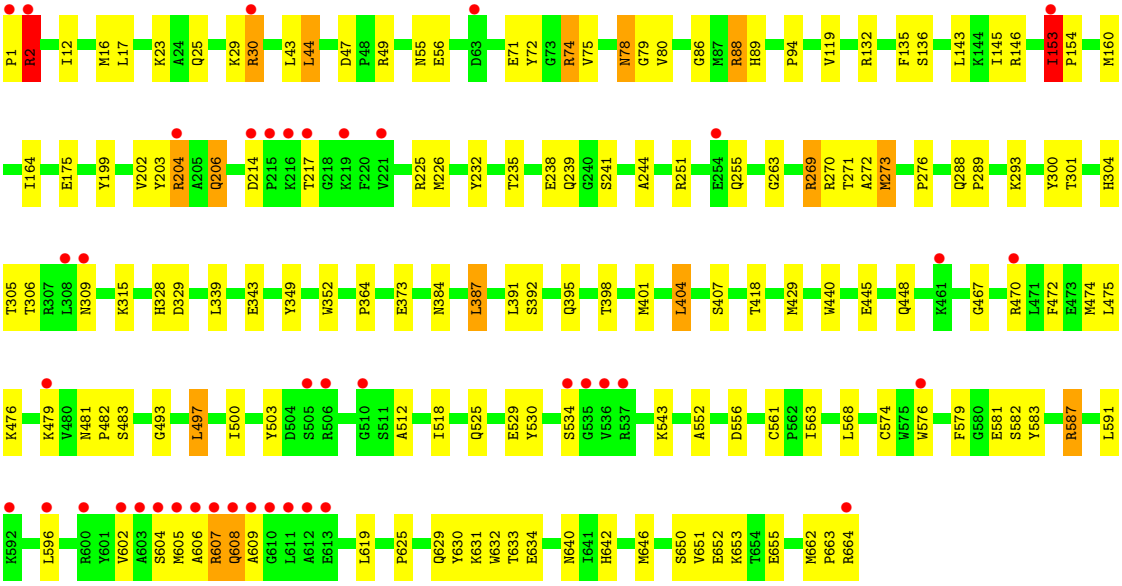
Chain C:





• Molecule 1: RNA-directed RNA polymerase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.29Å 93.80Å 140.77Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	19.98 – 2.45 20.02 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.98-2.45) 97.5 (20.02-2.45)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.68 (at 2.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.265 0.228 , 0.251	Depositor DCC
R_{free} test set	4874 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16257	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: POP, MG, MN, GTP

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	0.77	1/5396 (0.0%)	0.90	9/7297 (0.1%)
1	C	0.77	1/5396 (0.0%)	0.90	9/7297 (0.1%)
1	E	0.77	1/5396 (0.0%)	0.90	9/7297 (0.1%)
All	All	0.77	3/16188 (0.0%)	0.90	27/21891 (0.1%)

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	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	153	ILE	CA-CB	-9.66	1.32	1.54
1	C	153	ILE	CA-CB	-9.65	1.32	1.54
1	A	153	ILE	CA-CB	-9.64	1.32	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	153	ILE	C-N-CD	11.76	153.09	128.40
1	A	153	ILE	C-N-CD	11.75	153.08	128.40
1	C	153	ILE	C-N-CD	11.75	153.07	128.40
1	E	153	ILE	CG1-CB-CG2	9.46	132.22	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ILE	CG1-CB-CG2	9.46	132.21	111.40
1	C	153	ILE	CG1-CB-CG2	9.46	132.21	111.40
1	A	153	ILE	C-N-CA	-8.51	86.24	122.00
1	E	153	ILE	C-N-CA	-8.51	86.24	122.00
1	C	153	ILE	C-N-CA	-8.50	86.29	122.00
1	A	153	ILE	N-CA-C	8.45	133.80	111.00
1	C	153	ILE	N-CA-C	8.44	133.79	111.00
1	E	153	ILE	N-CA-C	8.44	133.78	111.00
1	A	153	ILE	CB-CA-C	-6.86	97.89	111.60
1	E	153	ILE	CB-CA-C	-6.86	97.89	111.60
1	C	153	ILE	CB-CA-C	-6.84	97.91	111.60
1	C	88	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	206	GLN	N-CA-C	-6.72	92.84	111.00
1	E	88	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	206	GLN	N-CA-C	-6.72	92.86	111.00
1	A	88	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	E	206	GLN	N-CA-C	-6.71	92.87	111.00
1	C	153	ILE	CA-CB-CG1	-5.94	99.71	111.00
1	A	153	ILE	CA-CB-CG1	-5.94	99.72	111.00
1	E	153	ILE	CA-CB-CG1	-5.94	99.72	111.00
1	A	404	LEU	CA-CB-CG	5.43	127.79	115.30
1	C	404	LEU	CA-CB-CG	5.43	127.78	115.30
1	E	404	LEU	CA-CB-CG	5.42	127.77	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
1	C	199	TYR	Sidechain
1	E	199	TYR	Sidechain

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	5265	0	5165	124	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5265	0	5165	128	1
1	E	5265	0	5165	124	7
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
4	A	9	0	0	0	0
4	C	9	0	0	0	0
4	E	9	0	0	0	0
5	A	23	0	12	2	0
5	C	23	0	12	2	0
5	E	23	0	12	2	0
6	A	32	0	11	4	0
6	C	32	0	11	4	0
6	E	32	0	11	4	0
7	A	84	0	0	4	1
7	C	87	0	0	6	2
7	E	90	0	0	11	1
All	All	16257	0	15564	373	9

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 12.

All (373) 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:C:153:ILE:HG23	1:C:154:PRO:CD	1.50	1.41
1:A:153:ILE:HG23	1:A:154:PRO:CD	1.50	1.39
1:E:153:ILE:HG23	1:E:154:PRO:CD	1.50	1.38
1:A:153:ILE:HG23	1:A:154:PRO:N	1.61	1.14
1:A:608:GLN:HE22	1:C:593:ARG:CZ	1.58	1.14
1:A:206:GLN:NE2	1:A:270:ARG:HE	1.51	1.09
1:C:206:GLN:NE2	1:C:270:ARG:HE	1.51	1.09
1:A:153:ILE:HG23	1:A:154:PRO:HD2	1.35	1.08
1:E:576:TRP:CE3	7:E:874:HOH:O	2.03	1.08
1:E:206:GLN:NE2	1:E:270:ARG:HE	1.51	1.07
1:E:153:ILE:HG23	1:E:154:PRO:N	1.61	1.06
1:C:153:ILE:HG23	1:C:154:PRO:HD2	1.34	1.05
1:E:153:ILE:HG23	1:E:154:PRO:HD2	1.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HG23	1:C:154:PRO:N	1.61	1.03
1:E:153:ILE:CG2	1:E:154:PRO:CD	2.37	1.03
1:C:153:ILE:CG2	1:C:154:PRO:CD	2.37	1.03
1:A:153:ILE:CG2	1:A:154:PRO:CD	2.37	1.02
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.12	0.95
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.12	0.95
1:C:581:GLU:OE1	7:C:801:HOH:O	1.89	0.90
1:E:576:TRP:HB3	7:E:874:HOH:O	1.71	0.90
1:A:561:CYS:HB3	7:A:851:HOH:O	1.73	0.89
1:C:561:CYS:HB3	7:C:851:HOH:O	1.73	0.89
1:E:251:ARG:HH11	1:E:255:GLN:HE22	1.12	0.89
1:E:561:CYS:HB3	7:E:853:HOH:O	1.73	0.89
1:C:153:ILE:CG2	1:C:154:PRO:N	2.37	0.88
1:A:153:ILE:CG2	1:A:154:PRO:N	2.37	0.87
1:E:576:TRP:HE3	7:E:874:HOH:O	1.45	0.86
1:E:206:GLN:HE21	1:E:270:ARG:HE	1.23	0.85
1:E:364:PRO:HA	1:E:387:LEU:HD22	1.59	0.84
1:C:206:GLN:HE21	1:C:270:ARG:HE	1.23	0.84
1:A:206:GLN:HE21	1:A:270:ARG:HE	1.23	0.84
1:C:364:PRO:HA	1:C:387:LEU:HD22	1.59	0.83
1:A:364:PRO:HA	1:A:387:LEU:HD22	1.59	0.83
1:A:608:GLN:NE2	1:C:593:ARG:CZ	2.40	0.83
6:E:706:GTP:O1G	6:E:706:GTP:N7	2.12	0.82
6:A:706:GTP:N7	6:A:706:GTP:O1G	2.12	0.82
6:C:706:GTP:N7	6:C:706:GTP:O1G	2.12	0.82
1:A:555:LYS:NZ	7:A:801:HOH:O	2.01	0.81
1:E:49:ARG:NH1	7:E:801:HOH:O	2.14	0.79
1:E:153:ILE:CG2	1:E:154:PRO:N	2.37	0.79
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.19	0.77
1:E:74:ARG:HB3	1:E:503:TYR:CD2	2.19	0.77
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.19	0.77
1:C:301:THR:HG23	1:C:440:TRP:O	1.85	0.76
1:C:226:MET:HE1	1:C:244:ALA:HB2	1.66	0.76
1:A:301:THR:HG23	1:A:440:TRP:O	1.85	0.76
1:E:301:THR:HG23	1:E:440:TRP:O	1.85	0.75
1:C:55:ASN:OD1	1:C:88:ARG:NH2	2.19	0.75
1:A:55:ASN:OD1	1:A:88:ARG:NH2	2.19	0.75
1:E:55:ASN:OD1	1:E:88:ARG:NH2	2.19	0.75
1:C:629:GLN:O	1:C:629:GLN:HG2	1.87	0.74
1:A:629:GLN:O	1:A:629:GLN:HG2	1.87	0.74
1:E:629:GLN:O	1:E:629:GLN:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:GLU:OE2	6:C:706:GTP:O2G	2.08	0.71
1:A:529:GLU:OE2	6:A:706:GTP:O2G	2.08	0.71
1:E:529:GLU:OE2	6:E:706:GTP:O2G	2.08	0.70
1:A:206:GLN:NE2	1:A:270:ARG:NE	2.35	0.69
1:E:153:ILE:CG2	1:E:154:PRO:HD2	2.17	0.69
1:A:226:MET:HE1	1:A:244:ALA:HB2	1.74	0.68
1:C:153:ILE:CG2	1:C:154:PRO:HD2	2.17	0.68
1:C:206:GLN:NE2	1:C:270:ARG:NE	2.35	0.68
1:A:206:GLN:HE21	1:A:270:ARG:NE	1.92	0.68
1:C:206:GLN:HE21	1:C:270:ARG:NE	1.92	0.68
1:E:226:MET:HE1	1:E:244:ALA:HB2	1.74	0.67
5:E:704:G:O6	6:E:706:GTP:O2G	2.14	0.66
5:C:704:G:O6	6:C:706:GTP:O2G	2.14	0.66
5:A:704:G:O6	6:A:706:GTP:O2G	2.14	0.65
1:E:206:GLN:HE21	1:E:270:ARG:NE	1.92	0.65
1:E:206:GLN:HE22	1:E:270:ARG:HE	1.41	0.65
1:E:78:ASN:ND2	1:E:80:VAL:H	1.94	0.65
1:C:206:GLN:HE22	1:C:270:ARG:HE	1.41	0.64
1:C:78:ASN:ND2	1:C:80:VAL:H	1.94	0.64
1:E:206:GLN:NE2	1:E:270:ARG:NE	2.35	0.64
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.80	0.64
1:A:78:ASN:ND2	1:A:80:VAL:H	1.94	0.64
1:A:206:GLN:HE22	1:A:270:ARG:HE	1.41	0.63
1:A:153:ILE:CG2	1:A:154:PRO:HD2	2.17	0.62
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.80	0.62
1:E:288:GLN:HB3	1:E:289:PRO:HD3	1.80	0.62
1:C:581:GLU:CG	7:C:801:HOH:O	2.47	0.62
1:E:78:ASN:HD22	1:E:79:GLY:N	1.98	0.61
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.36	0.61
1:C:78:ASN:HD22	1:C:79:GLY:N	1.98	0.60
1:E:203:TYR:CE1	1:E:271:THR:HG22	2.36	0.60
1:A:78:ASN:HD22	1:A:79:GLY:N	1.98	0.60
1:A:153:ILE:CG2	1:A:154:PRO:HD3	2.32	0.60
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.36	0.60
1:C:75:VAL:HG12	1:C:493:GLY:HA2	1.84	0.60
1:A:427:LYS:HE3	1:E:12:ILE:HG21	1.84	0.59
1:A:608:GLN:HE22	1:C:593:ARG:NE	1.98	0.59
1:A:75:VAL:HG12	1:A:493:GLY:HA2	1.84	0.59
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.38	0.59
1:E:75:VAL:HG12	1:E:493:GLY:HA2	1.84	0.59
1:A:71:GLU:CD	1:A:71:GLU:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.38	0.59
1:A:226:MET:HE2	1:A:244:ALA:HA	1.83	0.59
1:E:642:HIS:CE1	1:E:646:MET:HG3	2.38	0.59
1:C:71:GLU:CD	1:C:71:GLU:H	2.06	0.59
1:A:608:GLN:HE22	1:C:593:ARG:NH1	1.99	0.58
1:E:579:PHE:HE2	7:E:801:HOH:O	1.86	0.58
1:A:608:GLN:NE2	1:C:593:ARG:NH1	2.50	0.58
1:E:226:MET:HE2	1:E:244:ALA:HA	1.84	0.58
1:E:71:GLU:CD	1:E:71:GLU:H	2.06	0.58
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.69	0.58
1:A:119:VAL:O	1:E:25:GLN:HG3	2.04	0.57
1:E:576:TRP:CD2	7:E:874:HOH:O	2.43	0.57
1:E:203:TYR:HE1	1:E:271:THR:HG22	1.69	0.57
1:A:301:THR:HB	1:A:448:GLN:O	2.06	0.56
1:A:304:HIS:HA	1:A:309:ASN:HD21	1.71	0.56
1:A:418:THR:HG22	1:A:467:GLY:C	2.26	0.56
1:E:304:HIS:HA	1:E:309:ASN:HD21	1.71	0.56
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.69	0.56
1:C:304:HIS:HA	1:C:309:ASN:HD21	1.70	0.56
1:E:418:THR:HG22	1:E:467:GLY:C	2.26	0.56
1:A:606:ALA:C	1:A:608:GLN:H	2.09	0.56
1:C:301:THR:HB	1:C:448:GLN:O	2.06	0.56
1:C:418:THR:HG22	1:C:467:GLY:C	2.26	0.56
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.88	0.55
1:C:606:ALA:C	1:C:608:GLN:H	2.09	0.55
1:E:153:ILE:CG2	1:E:154:PRO:HD3	2.32	0.55
1:E:606:ALA:C	1:E:608:GLN:H	2.09	0.55
1:A:606:ALA:HB3	1:A:609:ALA:HB2	1.88	0.55
1:C:153:ILE:CG2	1:C:154:PRO:HD3	2.32	0.55
1:E:301:THR:HB	1:E:448:GLN:O	2.06	0.55
1:C:300:TYR:HD1	1:C:301:THR:HG22	1.71	0.54
1:E:606:ALA:HB3	1:E:609:ALA:HB2	1.88	0.54
1:E:300:TYR:HD1	1:E:301:THR:HG22	1.71	0.54
1:A:300:TYR:HD1	1:A:301:THR:HG22	1.71	0.54
1:A:17:LEU:O	1:A:153:ILE:O	2.26	0.54
1:E:576:TRP:CG	7:E:874:HOH:O	2.61	0.53
1:C:17:LEU:O	1:C:153:ILE:O	2.26	0.53
1:A:407:SER:HA	1:A:448:GLN:HE22	1.74	0.53
1:E:132:ARG:HH11	1:E:429:MET:HE2	1.74	0.53
1:C:475:LEU:HD21	1:C:482:PRO:HG3	1.91	0.53
1:C:251:ARG:NH1	1:C:255:GLN:HE22	1.95	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.45	0.52
1:E:17:LEU:O	1:E:153:ILE:O	2.26	0.52
1:A:136:SER:OG	1:A:293:LYS:NZ	2.43	0.52
1:C:136:SER:OG	1:C:293:LYS:NZ	2.43	0.52
1:E:587:ARG:NH1	7:E:804:HOH:O	2.43	0.52
1:A:475:LEU:HD21	1:A:482:PRO:HG3	1.91	0.52
1:E:136:SER:OG	1:E:293:LYS:NZ	2.43	0.52
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.45	0.52
1:E:175:GLU:HA	1:E:352:TRP:CE3	2.45	0.52
1:A:88:ARG:HD3	1:A:263:GLY:O	2.10	0.52
1:C:88:ARG:HD3	1:C:263:GLY:O	2.10	0.52
1:E:364:PRO:HA	1:E:387:LEU:CD2	2.37	0.52
1:E:475:LEU:HD21	1:E:482:PRO:HG3	1.91	0.52
1:E:407:SER:HA	1:E:448:GLN:HE22	1.74	0.52
1:E:88:ARG:HD3	1:E:263:GLY:O	2.10	0.51
1:A:2:ARG:HD2	1:A:2:ARG:O	2.11	0.51
1:C:407:SER:HA	1:C:448:GLN:HE22	1.74	0.51
1:A:587:ARG:NH1	7:A:803:HOH:O	2.43	0.51
1:C:481:ASN:ND2	1:C:483:SER:O	2.44	0.51
1:C:587:ARG:NH1	7:C:803:HOH:O	2.43	0.51
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.46	0.51
1:E:481:ASN:ND2	1:E:483:SER:O	2.44	0.51
1:A:481:ASN:ND2	1:A:483:SER:O	2.44	0.51
1:C:2:ARG:HD2	1:C:2:ARG:O	2.11	0.51
1:E:576:TRP:CB	7:E:874:HOH:O	2.41	0.51
1:C:602:VAL:HG11	1:C:605:MET:HG3	1.93	0.50
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.46	0.50
1:E:2:ARG:HD2	1:E:2:ARG:O	2.11	0.50
1:C:78:ASN:HD22	1:C:78:ASN:C	2.14	0.50
1:C:581:GLU:HG3	7:C:801:HOH:O	2.11	0.50
1:A:401:MET:HE2	1:A:401:MET:HA	1.94	0.50
1:E:78:ASN:HD22	1:E:78:ASN:C	2.14	0.50
1:E:175:GLU:HA	1:E:352:TRP:CD2	2.46	0.49
1:C:72:TYR:CZ	1:C:476:LYS:HD3	2.47	0.49
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.12	0.49
1:E:72:TYR:CZ	1:E:476:LYS:HD3	2.47	0.49
1:A:593:ARG:CG	1:C:42:GLY:HA2	2.43	0.49
1:C:1:PRO:HD2	1:C:238:GLU:OE2	2.13	0.49
1:A:534:SER:O	1:C:48:PRO:HG2	2.13	0.49
6:C:706:GTP:N7	6:C:706:GTP:PG	2.85	0.49
1:E:47:ASP:OD1	1:E:49:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:HD22	1:A:78:ASN:C	2.14	0.49
1:C:339:LEU:C	1:C:339:LEU:HD23	2.33	0.49
1:E:251:ARG:NH1	1:E:255:GLN:HE22	1.95	0.49
1:E:602:VAL:HG11	1:E:605:MET:HG3	1.93	0.49
1:A:72:TYR:CZ	1:A:476:LYS:HD3	2.47	0.49
1:A:339:LEU:C	1:A:339:LEU:HD23	2.33	0.49
1:A:1:PRO:HD2	1:A:238:GLU:OE2	2.13	0.49
1:E:1:PRO:HD2	1:E:238:GLU:OE2	2.13	0.49
6:A:706:GTP:N7	6:A:706:GTP:PG	2.85	0.48
1:A:602:VAL:HG11	1:A:605:MET:HG3	1.94	0.48
1:E:339:LEU:C	1:E:339:LEU:HD23	2.33	0.48
6:E:706:GTP:N7	6:E:706:GTP:PG	2.85	0.48
1:E:401:MET:CE	1:E:401:MET:HA	2.43	0.48
1:A:72:TYR:CE1	1:A:476:LYS:HD3	2.48	0.48
1:C:401:MET:CE	1:C:401:MET:HA	2.43	0.48
1:E:72:TYR:CE1	1:E:476:LYS:HD3	2.48	0.48
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.12	0.48
1:E:56:GLU:HG2	1:E:574:CYS:SG	2.54	0.48
1:C:56:GLU:HG2	1:C:574:CYS:SG	2.54	0.48
1:A:401:MET:HA	1:A:401:MET:CE	2.43	0.48
1:A:56:GLU:HG2	1:A:574:CYS:SG	2.54	0.48
1:A:364:PRO:HA	1:A:387:LEU:CD2	2.37	0.47
1:C:72:TYR:CE1	1:C:476:LYS:HD3	2.48	0.47
1:A:305:THR:OG1	1:A:306:THR:N	2.47	0.47
1:E:602:VAL:CG1	1:E:605:MET:HG3	2.45	0.47
1:A:602:VAL:CG1	1:A:605:MET:HG3	2.45	0.47
1:C:602:VAL:CG1	1:C:605:MET:HG3	2.45	0.47
1:A:153:ILE:HA	1:A:153:ILE:HD12	1.41	0.47
1:C:86:GLY:O	1:C:89:HIS:HD2	1.98	0.47
1:A:427:LYS:HE3	1:E:12:ILE:CG2	2.45	0.47
1:C:235:THR:O	1:C:238:GLU:HG3	2.15	0.47
1:C:132:ARG:HH11	1:C:429:MET:HE2	1.80	0.47
1:E:305:THR:OG1	1:E:306:THR:N	2.47	0.47
1:C:606:ALA:O	1:C:608:GLN:N	2.45	0.47
1:A:235:THR:O	1:A:238:GLU:HG3	2.15	0.46
1:E:235:THR:O	1:E:238:GLU:HG3	2.14	0.46
1:E:145:ILE:HD12	1:E:164:ILE:HD13	1.98	0.46
1:E:606:ALA:O	1:E:608:GLN:N	2.45	0.46
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.98	0.46
1:E:204:ARG:HD2	1:E:530:TYR:OH	2.15	0.46
1:C:304:HIS:HA	1:C:309:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLY:O	1:E:89:HIS:HD2	1.98	0.46
1:E:304:HIS:HA	1:E:309:ASN:ND2	2.30	0.46
1:C:401:MET:HA	1:C:401:MET:HE2	1.97	0.46
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.77	0.46
1:A:86:GLY:O	1:A:89:HIS:HD2	1.98	0.46
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.98	0.46
1:E:232:TYR:HA	1:E:239:GLN:O	2.15	0.46
1:A:232:TYR:HA	1:A:239:GLN:O	2.15	0.45
1:A:304:HIS:HA	1:A:309:ASN:ND2	2.30	0.45
1:C:226:MET:HE2	1:C:244:ALA:HA	1.97	0.45
1:A:132:ARG:HH12	1:A:429:MET:HG3	1.82	0.45
1:C:2:ARG:O	1:C:2:ARG:CD	2.65	0.45
1:C:204:ARG:HD2	1:C:530:TYR:OH	2.15	0.45
1:C:305:THR:OG1	1:C:306:THR:N	2.47	0.45
1:C:395:GLN:HB3	1:C:398:THR:HG22	1.98	0.45
1:E:640:ASN:OD1	1:E:640:ASN:N	2.48	0.45
1:C:662:MET:HB3	1:C:663:PRO:CD	2.47	0.45
1:E:395:GLN:HB3	1:E:398:THR:HG22	1.98	0.45
1:C:232:TYR:HA	1:C:239:GLN:O	2.15	0.45
1:A:204:ARG:HD2	1:A:530:TYR:OH	2.15	0.45
1:A:315:LYS:HE3	1:A:512:ALA:O	2.17	0.45
1:A:395:GLN:HB3	1:A:398:THR:HG22	1.98	0.45
1:A:607:ARG:O	1:A:608:GLN:HG3	2.16	0.45
1:C:132:ARG:HH12	1:C:429:MET:HG3	1.82	0.45
1:E:132:ARG:HH12	1:E:429:MET:HG3	1.82	0.45
1:E:607:ARG:O	1:E:608:GLN:HG3	2.16	0.45
1:E:315:LYS:HE3	1:E:512:ALA:O	2.17	0.45
1:C:135:PHE:HB3	1:C:349:TYR:OH	2.16	0.44
1:C:226:MET:HE1	1:C:244:ALA:CB	2.44	0.44
1:E:135:PHE:HB3	1:E:349:TYR:OH	2.16	0.44
1:A:135:PHE:HB3	1:A:349:TYR:OH	2.16	0.44
1:A:662:MET:HB3	1:A:663:PRO:CD	2.47	0.44
1:C:587:ARG:HA	1:C:587:ARG:HD2	1.77	0.44
1:E:2:ARG:O	1:E:2:ARG:CD	2.64	0.44
1:E:662:MET:HB3	1:E:663:PRO:CD	2.47	0.44
1:A:270:ARG:NH2	5:A:704:G:O2'	2.50	0.44
1:E:270:ARG:NH2	5:E:704:G:O2'	2.50	0.44
1:C:474:MET:HB2	1:C:474:MET:HE2	1.83	0.44
1:C:607:ARG:O	1:C:608:GLN:HG3	2.16	0.44
1:A:2:ARG:O	1:A:2:ARG:CD	2.65	0.44
1:A:160:MET:O	1:A:164:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:650:SER:OG	1:E:653:LYS:CG	2.66	0.44
1:A:525:GLN:NE2	1:A:583:TYR:OH	2.51	0.44
1:C:270:ARG:NH2	5:C:704:G:O2'	2.50	0.44
1:C:315:LYS:HE3	1:C:512:ALA:O	2.17	0.44
1:C:364:PRO:HA	1:C:387:LEU:CD2	2.37	0.44
1:C:640:ASN:OD1	1:C:640:ASN:N	2.48	0.44
1:E:328:HIS:HD2	1:E:329:ASP:OD1	2.01	0.44
1:E:652:GLU:H	1:E:652:GLU:CD	2.21	0.44
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.01	0.43
1:A:407:SER:OG	1:A:448:GLN:NE2	2.51	0.43
1:C:204:ARG:HE	1:C:204:ARG:HB3	1.56	0.43
1:C:650:SER:OG	1:C:653:LYS:CG	2.66	0.43
1:E:160:MET:O	1:E:164:ILE:HG12	2.18	0.43
1:A:273:MET:HE2	1:A:392:SER:HA	2.00	0.43
1:C:407:SER:OG	1:C:448:GLN:NE2	2.51	0.43
1:C:652:GLU:H	1:C:652:GLU:CD	2.21	0.43
1:E:202:VAL:CG2	1:E:272:ALA:HB3	2.48	0.43
1:A:29:LYS:O	1:A:30:ARG:C	2.57	0.43
1:A:640:ASN:OD1	1:A:640:ASN:N	2.48	0.43
1:C:328:HIS:HD2	1:C:329:ASP:OD1	2.01	0.43
1:C:413:MET:HE1	1:C:488:ILE:HG13	2.01	0.43
1:A:75:VAL:HG21	1:A:500:ILE:HG21	2.01	0.43
1:A:251:ARG:NH1	1:A:255:GLN:HE22	1.95	0.43
1:C:251:ARG:HB2	1:C:255:GLN:NE2	2.33	0.43
1:C:525:GLN:NE2	1:C:583:TYR:OH	2.51	0.43
1:E:387:LEU:HD12	1:E:387:LEU:HA	1.75	0.43
1:A:214:ASP:HB3	1:A:217:THR:OG1	2.18	0.43
1:E:525:GLN:NE2	1:E:583:TYR:OH	2.51	0.43
1:E:587:ARG:HA	1:E:587:ARG:HD2	1.77	0.43
1:A:650:SER:OG	1:A:653:LYS:HG3	2.18	0.43
1:C:160:MET:O	1:C:164:ILE:HG12	2.18	0.43
1:C:251:ARG:HB2	1:C:255:GLN:HE21	1.84	0.43
1:E:75:VAL:HG21	1:E:500:ILE:HG21	2.01	0.43
1:E:214:ASP:HB3	1:E:217:THR:OG1	2.18	0.43
1:E:407:SER:OG	1:E:448:GLN:NE2	2.51	0.43
1:E:650:SER:OG	1:E:653:LYS:HG3	2.19	0.43
1:E:251:ARG:HB2	1:E:255:GLN:NE2	2.34	0.43
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.77	0.43
1:A:251:ARG:HB2	1:A:255:GLN:NE2	2.34	0.43
1:A:305:THR:H	1:A:309:ASN:ND2	2.17	0.43
1:C:214:ASP:HB3	1:C:217:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASN:HD22	1:E:80:VAL:H	1.64	0.43
1:A:651:VAL:O	1:A:655:GLU:HB2	2.19	0.43
1:C:202:VAL:CG2	1:C:272:ALA:HB3	2.48	0.43
1:C:663:PRO:HD2	1:C:664:ARG:H	1.83	0.43
1:E:663:PRO:HD2	1:E:664:ARG:H	1.83	0.43
1:A:251:ARG:HB2	1:A:255:GLN:HE21	1.84	0.43
1:A:650:SER:OG	1:A:653:LYS:CG	2.66	0.43
1:E:305:THR:H	1:E:309:ASN:ND2	2.17	0.43
1:A:78:ASN:HD22	1:A:80:VAL:H	1.64	0.42
1:E:251:ARG:HB2	1:E:255:GLN:HE21	1.84	0.42
1:A:663:PRO:HD2	1:A:664:ARG:H	1.83	0.42
1:E:132:ARG:CZ	1:E:343:GLU:OE2	2.67	0.42
1:A:132:ARG:CZ	1:A:343:GLU:OE2	2.68	0.42
1:A:652:GLU:CD	1:A:652:GLU:H	2.21	0.42
1:C:29:LYS:O	1:C:30:ARG:C	2.57	0.42
1:C:633:THR:O	1:C:634:GLU:C	2.58	0.42
1:E:273:MET:HE2	1:E:392:SER:HA	2.00	0.42
1:A:42:GLY:O	1:C:256:TYR:HB3	2.20	0.42
1:E:518:ILE:HG21	1:E:563:ILE:HD11	2.01	0.42
1:E:568:LEU:HA	1:E:568:LEU:HD23	1.82	0.42
1:A:202:VAL:CG2	1:A:272:ALA:HB3	2.48	0.42
1:C:651:VAL:O	1:C:655:GLU:HB2	2.19	0.42
1:E:633:THR:O	1:E:634:GLU:C	2.58	0.42
1:A:86:GLY:O	1:A:89:HIS:CD2	2.73	0.42
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.55	0.42
1:A:633:THR:O	1:A:634:GLU:C	2.58	0.42
1:E:474:MET:HB2	1:E:474:MET:HE2	1.84	0.42
1:E:651:VAL:O	1:E:655:GLU:HB2	2.19	0.42
1:A:593:ARG:HG2	1:C:42:GLY:HA2	2.02	0.42
1:A:606:ALA:O	1:A:608:GLN:N	2.45	0.42
1:C:153:ILE:HB	1:C:276:PRO:HB3	2.02	0.42
1:C:273:MET:HE2	1:C:392:SER:HA	2.00	0.42
1:C:305:THR:H	1:C:309:ASN:ND2	2.17	0.42
1:E:153:ILE:HD12	1:E:153:ILE:HA	1.41	0.42
1:A:153:ILE:HB	1:A:276:PRO:HB3	2.02	0.42
1:C:132:ARG:CZ	1:C:343:GLU:OE2	2.67	0.42
1:C:650:SER:OG	1:C:653:LYS:HG3	2.19	0.42
1:E:29:LYS:O	1:E:30:ARG:C	2.57	0.42
1:E:225:ARG:HD3	1:E:225:ARG:HA	1.87	0.42
1:C:86:GLY:O	1:C:89:HIS:CD2	2.73	0.41
1:C:225:ARG:HA	1:C:225:ARG:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:MET:HA	1:E:401:MET:HE2	2.02	0.41
1:E:631:LYS:HE3	1:E:632:TRP:CZ2	2.55	0.41
1:C:518:ILE:HG21	1:C:563:ILE:HD11	2.01	0.41
1:C:631:LYS:HE3	1:C:632:TRP:CZ2	2.55	0.41
1:C:75:VAL:HG21	1:C:500:ILE:HG21	2.01	0.41
1:E:94:PRO:CB	1:E:269:ARG:HG3	2.51	0.41
1:E:49:ARG:CZ	7:E:801:HOH:O	2.59	0.41
1:A:225:ARG:HA	1:A:225:ARG:HD3	1.87	0.41
1:A:552:ALA:HB3	1:A:619:LEU:HD13	2.03	0.41
1:C:552:ALA:HB3	1:C:619:LEU:HD13	2.03	0.41
1:C:596:LEU:CD2	1:C:608:GLN:HG2	2.51	0.41
1:E:153:ILE:HB	1:E:276:PRO:HB3	2.02	0.41
1:A:492:HIS:HB2	7:A:876:HOH:O	2.21	0.41
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.51	0.41
1:A:518:ILE:HG21	1:A:563:ILE:HD11	2.01	0.41
1:C:202:VAL:O	1:C:202:VAL:HG23	2.21	0.41
1:C:295:TYR:O	1:C:299:ALA:HB2	2.21	0.41
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.92	0.41
1:A:596:LEU:CD2	1:A:608:GLN:HG2	2.51	0.41
1:C:392:SER:O	1:C:398:THR:HG21	2.21	0.41
1:C:492:HIS:HB2	7:C:877:HOH:O	2.21	0.41
1:A:392:SER:O	1:A:398:THR:HG21	2.21	0.40
1:A:543:LYS:O	1:A:625:PRO:HD2	2.21	0.40
1:E:202:VAL:O	1:E:202:VAL:HG23	2.21	0.40
1:A:568:LEU:HA	1:A:568:LEU:HD23	1.81	0.40
1:C:78:ASN:HD22	1:C:80:VAL:H	1.64	0.40
1:C:153:ILE:HD12	1:C:153:ILE:HA	1.41	0.40
1:E:552:ALA:HB3	1:E:619:LEU:HD13	2.03	0.40
1:E:596:LEU:CD2	1:E:608:GLN:HG2	2.51	0.40
1:C:94:PRO:CB	1:C:269:ARG:HG3	2.51	0.40
1:C:139:GLU:HA	1:C:140:PRO:HD3	1.96	0.40
1:E:543:LYS:O	1:E:625:PRO:HD2	2.21	0.40

All (9) 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)
7:A:861:HOH:O	7:C:804:HOH:O[2_646]	0.65	1.55
7:C:862:HOH:O	7:E:805:HOH:O[2_555]	1.48	0.72
1:E:479:LYS:NZ	1:E:607:ARG:C[2_445]	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:LYS:NZ	1:E:608:GLN:N[2_445]	1.93	0.27
1:A:569:GLU:OE2	1:E:1:PRO:CB[2_555]	2.08	0.12
1:C:607:ARG:CD	1:E:44:LEU:CD1[1_655]	2.12	0.08
1:E:479:LYS:CD	1:E:608:GLN:CB[2_445]	2.12	0.08
1:A:652:GLU:OE2	1:E:664:ARG:NH2[2_545]	2.15	0.05
1:E:479:LYS:NZ	1:E:607:ARG:O[2_445]	2.19	0.01

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	662/664 (100%)	629 (95%)	28 (4%)	5 (1%)	19	22
1	C	662/664 (100%)	630 (95%)	27 (4%)	5 (1%)	19	22
1	E	662/664 (100%)	629 (95%)	27 (4%)	6 (1%)	17	19
All	All	1986/1992 (100%)	1888 (95%)	82 (4%)	16 (1%)	19	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ILE
1	A	608	GLN
1	C	153	ILE
1	C	608	GLN
1	E	153	ILE
1	E	608	GLN
1	A	607	ARG
1	A	630	TYR
1	C	607	ARG
1	C	630	TYR
1	E	607	ARG
1	E	630	TYR
1	A	604	SER

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Mol	Chain	Res	Type
1	C	604	SER
1	E	604	SER
1	E	2	ARG

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	557/557 (100%)	527 (95%)	30 (5%)	22	28
1	C	557/557 (100%)	527 (95%)	30 (5%)	22	28
1	E	557/557 (100%)	527 (95%)	30 (5%)	22	28
All	All	1671/1671 (100%)	1581 (95%)	90 (5%)	22	28

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	16	MET
1	A	23	LYS
1	A	30	ARG
1	A	43	LEU
1	A	44	LEU
1	A	74	ARG
1	A	78	ASN
1	A	119	VAL
1	A	143	LEU
1	A	146	ARG
1	A	204	ARG
1	A	241	SER
1	A	269	ARG
1	A	273	MET
1	A	373	GLU
1	A	384	ASN
1	A	387	LEU
1	A	391	LEU

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	445	GLU
1	A	470	ARG
1	A	472	PHE
1	A	497	LEU
1	A	534	SER
1	A	556	ASP
1	A	581	GLU
1	A	582	SER
1	A	587	ARG
1	A	591	LEU
1	C	2	ARG
1	C	16	MET
1	C	23	LYS
1	C	30	ARG
1	C	43	LEU
1	C	44	LEU
1	C	74	ARG
1	C	78	ASN
1	C	119	VAL
1	C	143	LEU
1	C	146	ARG
1	C	204	ARG
1	C	241	SER
1	C	269	ARG
1	C	273	MET
1	C	373	GLU
1	C	384	ASN
1	C	387	LEU
1	C	391	LEU
1	C	404	LEU
1	C	445	GLU
1	C	470	ARG
1	C	472	PHE
1	C	497	LEU
1	C	534	SER
1	C	556	ASP
1	C	581	GLU
1	C	582	SER
1	C	587	ARG
1	C	591	LEU
1	E	2	ARG

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Mol	Chain	Res	Type
1	E	16	MET
1	E	23	LYS
1	E	30	ARG
1	E	43	LEU
1	E	44	LEU
1	E	74	ARG
1	E	78	ASN
1	E	119	VAL
1	E	143	LEU
1	E	146	ARG
1	E	204	ARG
1	E	241	SER
1	E	269	ARG
1	E	273	MET
1	E	373	GLU
1	E	384	ASN
1	E	387	LEU
1	E	391	LEU
1	E	404	LEU
1	E	445	GLU
1	E	470	ARG
1	E	472	PHE
1	E	497	LEU
1	E	534	SER
1	E	556	ASP
1	E	581	GLU
1	E	582	SER
1	E	587	ARG
1	E	591	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	191	GLN
1	A	206	GLN
1	A	255	GLN
1	A	309	ASN

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Mol	Chain	Res	Type
1	A	328	HIS
1	A	448	GLN
1	A	525	GLN
1	A	608	GLN
1	C	15	GLN
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	191	GLN
1	C	206	GLN
1	C	255	GLN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
1	C	525	GLN
1	E	26	GLN
1	E	78	ASN
1	E	89	HIS
1	E	91	ASN
1	E	191	GLN
1	E	206	GLN
1	E	255	GLN
1	E	309	ASN
1	E	328	HIS
1	E	448	GLN
1	E	525	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
6	GTP	C	706	5,3	26,34,34	0.98	1 (3%)	32,54,54	0.81	1 (3%)
6	GTP	A	706	5,3	26,34,34	0.98	1 (3%)	32,54,54	0.81	1 (3%)
6	GTP	E	706	5,3	26,34,34	0.97	1 (3%)	32,54,54	0.82	1 (3%)

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
6	GTP	C	706	5,3	-	3/18/38/38	0/3/3/3
6	GTP	A	706	5,3	-	3/18/38/38	0/3/3/3
6	GTP	E	706	5,3	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	706	GTP	C8-N7	-2.73	1.30	1.35
6	A	706	GTP	C8-N7	-2.70	1.30	1.35
6	E	706	GTP	C8-N7	-2.67	1.30	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	706	GTP	O6-C6-C5	2.19	128.64	124.37
6	E	706	GTP	O6-C6-C5	2.18	128.64	124.37
6	C	706	GTP	O6-C6-C5	2.17	128.61	124.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	706	GTP	C5'-O5'-PA-O1A
6	A	706	GTP	C5'-O5'-PA-O2A
6	C	706	GTP	C5'-O5'-PA-O1A
6	C	706	GTP	C5'-O5'-PA-O2A
6	E	706	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
6	E	706	GTP	C5'-O5'-PA-O2A
6	A	706	GTP	C5'-O5'-PA-O3A
6	C	706	GTP	C5'-O5'-PA-O3A
6	E	706	GTP	C5'-O5'-PA-O3A

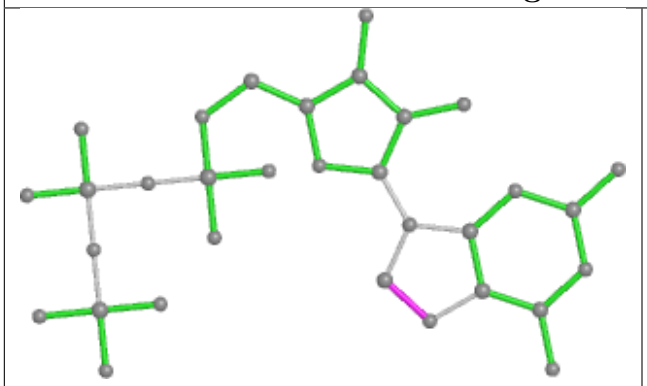
There are no ring outliers.

3 monomers are involved in 12 short contacts:

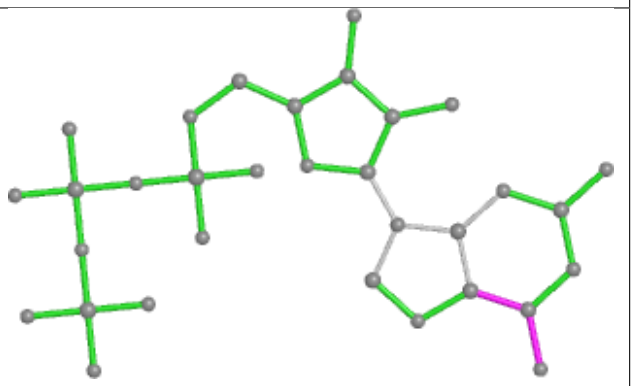
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	706	GTP	4	0
6	A	706	GTP	4	0
6	E	706	GTP	4	0

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.

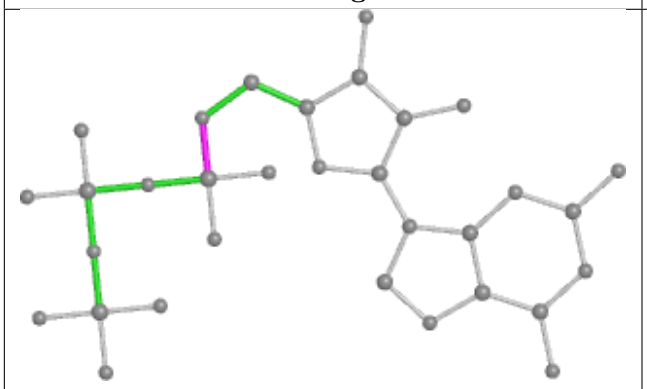
Ligand GTP C 706



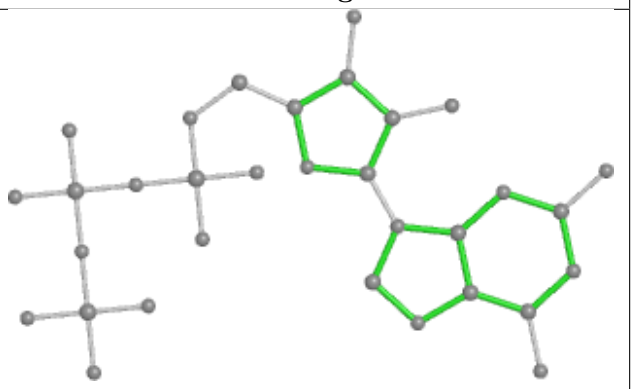
Bond lengths



Bond angles

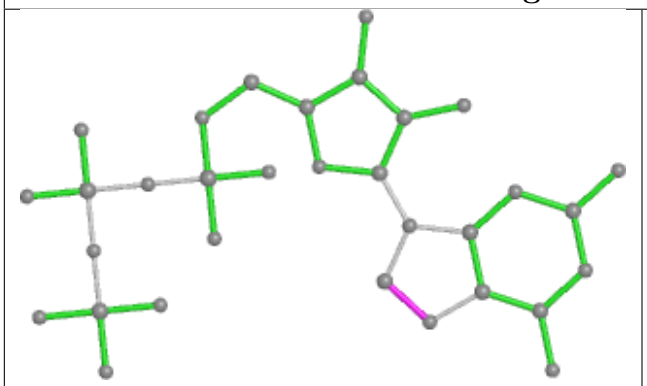


Torsions

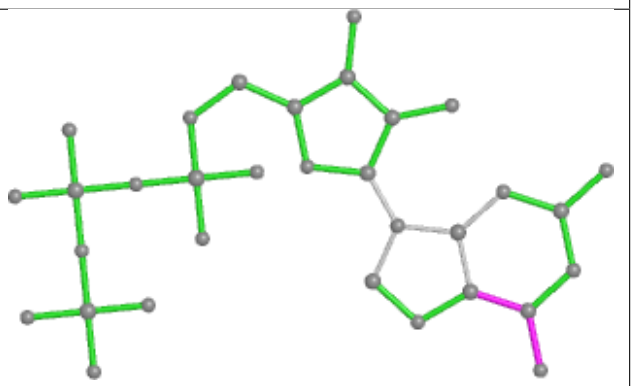


Rings

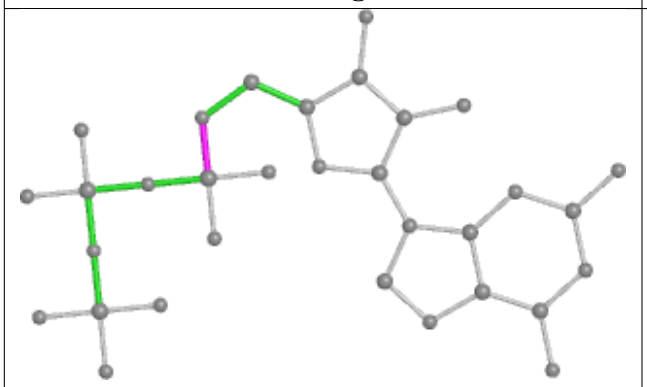
Ligand GTP A 706



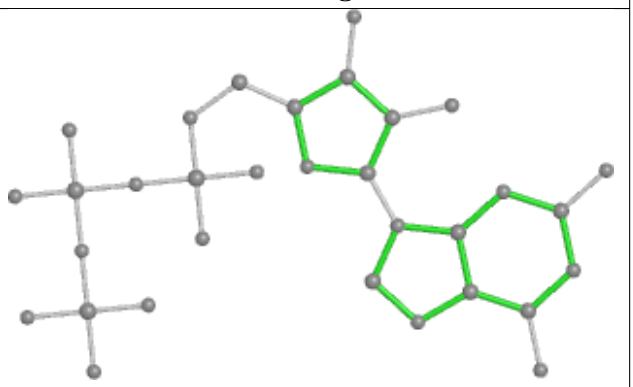
Bond lengths



Bond angles

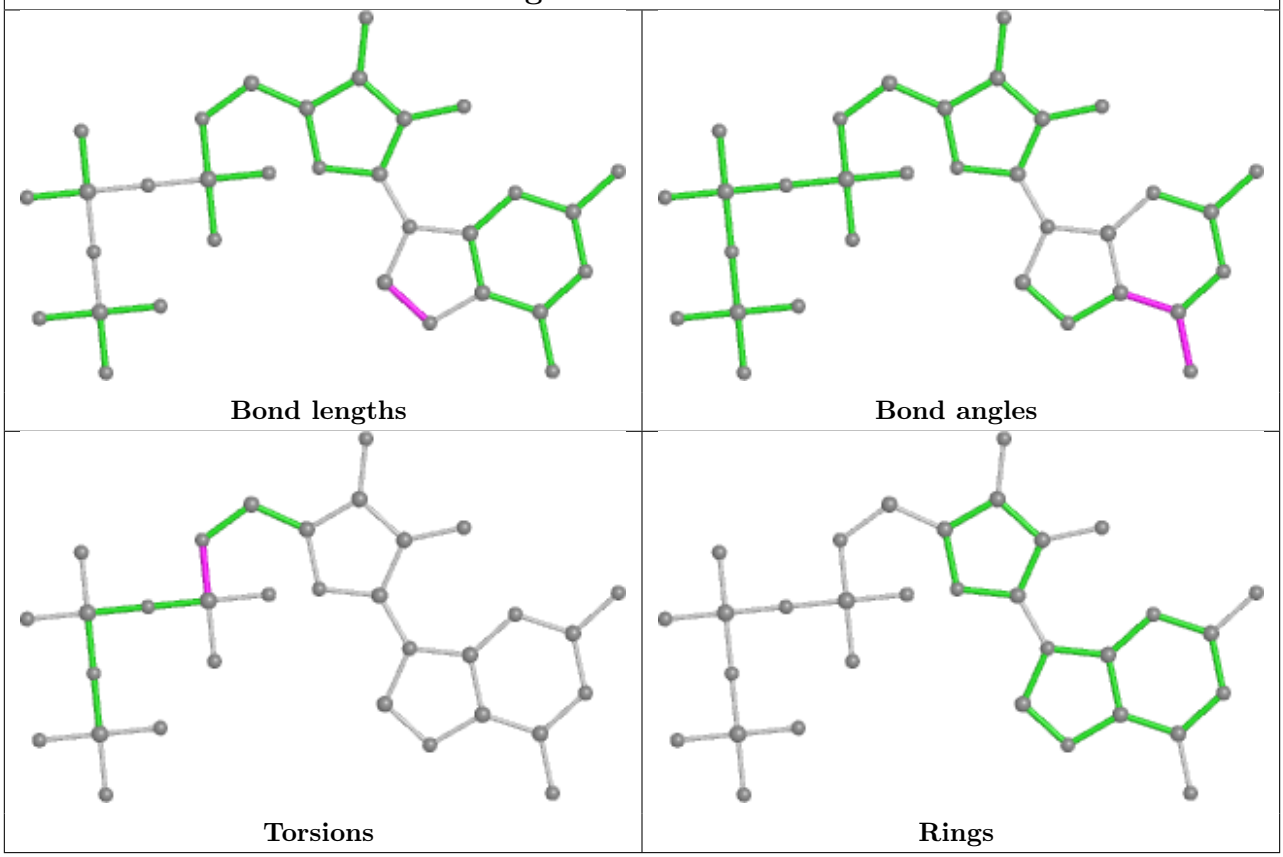


Torsions



Rings

Ligand GTP E 706



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
6	GTP	A	706	5,3	26,34,34	0.98	1 (3%)	32,54,54	0.81	1 (3%)
4	POP	C	701	3	6,8,8	1.26	0	13,13,13	0.91	0
5	G	C	704	6	18,25,26	1.10	2 (11%)	19,37,40	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	G	E	704	6	18,25,26	1.10	2 (11%)	19,37,40	0.78	0
4	POP	E	701	3	6,8,8	1.26	0	13,13,13	0.91	0
6	GTP	C	706	5,3	26,34,34	0.98	1 (3%)	32,54,54	0.81	1 (3%)
5	G	A	704	6	18,25,26	1.10	2 (11%)	19,37,40	0.78	0
4	POP	A	703	3	6,8,8	1.26	0	13,13,13	0.91	0
6	GTP	E	706	5,3	26,34,34	0.97	1 (3%)	32,54,54	0.82	1 (3%)

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
6	GTP	A	706	5,3	-	3/18/38/38	0/3/3/3
4	POP	C	701	3	-	0/6/6/6	-
5	G	C	704	6	-	0/3/25/26	0/3/3/3
5	G	E	704	6	-	0/3/25/26	0/3/3/3
4	POP	E	701	3	-	0/6/6/6	-
6	GTP	C	706	5,3	-	3/18/38/38	0/3/3/3
5	G	A	704	6	-	0/3/25/26	0/3/3/3
4	POP	A	703	3	-	0/6/6/6	-
6	GTP	E	706	5,3	-	3/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	704	G	C5-C6	-2.78	1.41	1.47
5	C	704	G	C5-C6	-2.76	1.41	1.47
5	A	704	G	C5-C6	-2.75	1.41	1.47
6	C	706	GTP	C8-N7	-2.73	1.30	1.35
6	A	706	GTP	C8-N7	-2.70	1.30	1.35
6	E	706	GTP	C8-N7	-2.67	1.30	1.35
5	C	704	G	C8-N7	-2.42	1.30	1.35
5	A	704	G	C8-N7	-2.42	1.30	1.35
5	E	704	G	C8-N7	-2.37	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	706	GTP	O6-C6-C5	2.19	128.64	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	706	GTP	O6-C6-C5	2.18	128.64	124.37
6	C	706	GTP	O6-C6-C5	2.17	128.61	124.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	706	GTP	C5'-O5'-PA-O1A
6	A	706	GTP	C5'-O5'-PA-O2A
6	C	706	GTP	C5'-O5'-PA-O1A
6	C	706	GTP	C5'-O5'-PA-O2A
6	E	706	GTP	C5'-O5'-PA-O1A
6	E	706	GTP	C5'-O5'-PA-O2A
6	A	706	GTP	C5'-O5'-PA-O3A
6	C	706	GTP	C5'-O5'-PA-O3A
6	E	706	GTP	C5'-O5'-PA-O3A

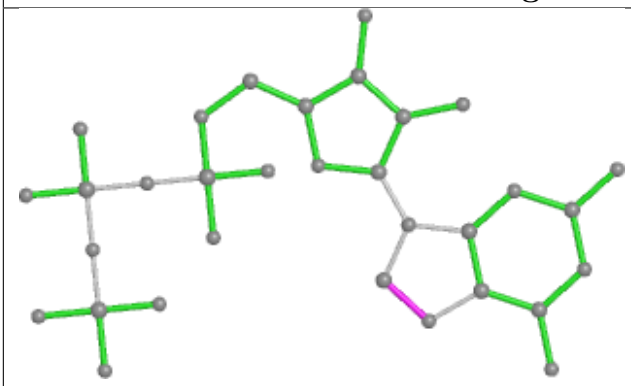
There are no ring outliers.

6 monomers are involved in 15 short contacts:

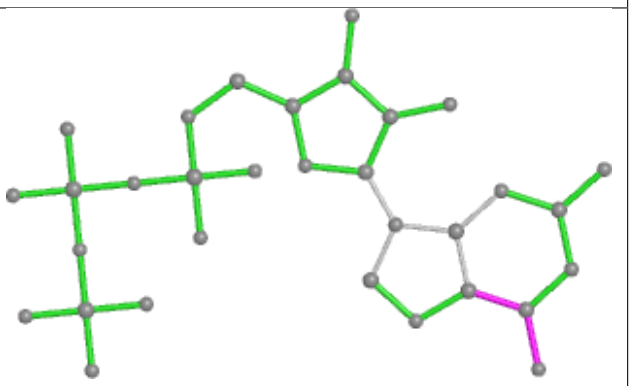
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	706	GTP	4	0
5	C	704	G	2	0
5	E	704	G	2	0
6	C	706	GTP	4	0
5	A	704	G	2	0
6	E	706	GTP	4	0

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.

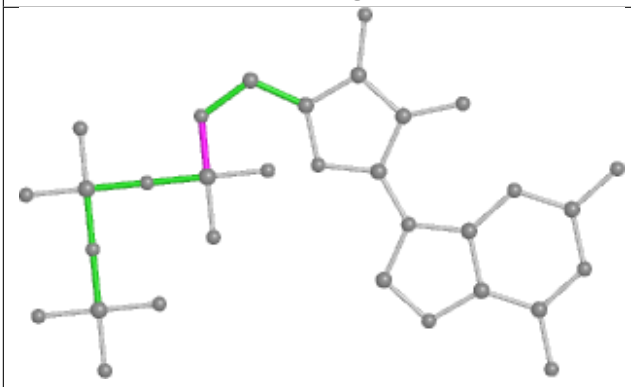
Ligand GTP A 706



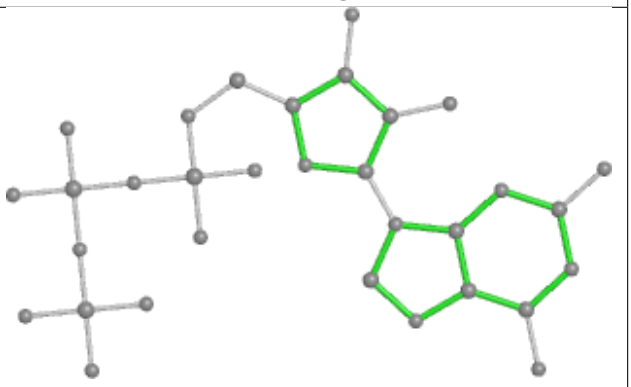
Bond lengths



Bond angles

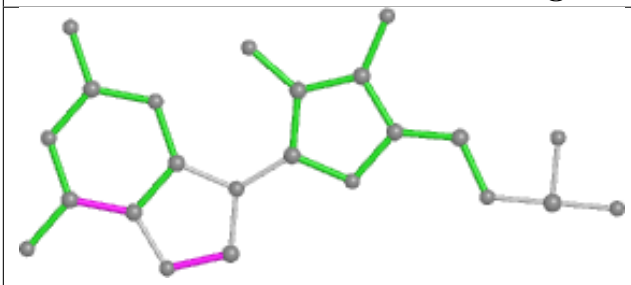


Torsions

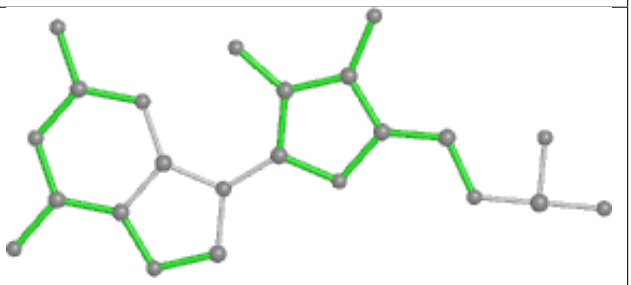


Rings

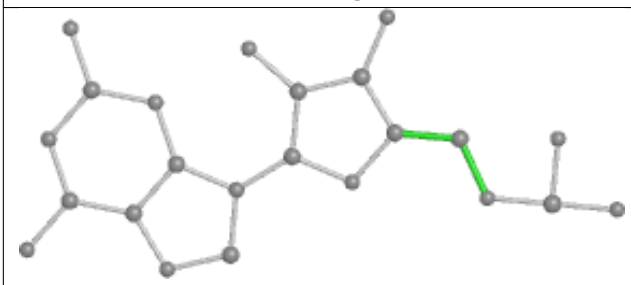
Ligand G C 704



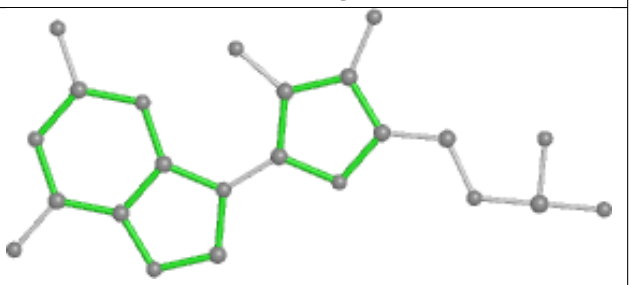
Bond lengths



Bond angles

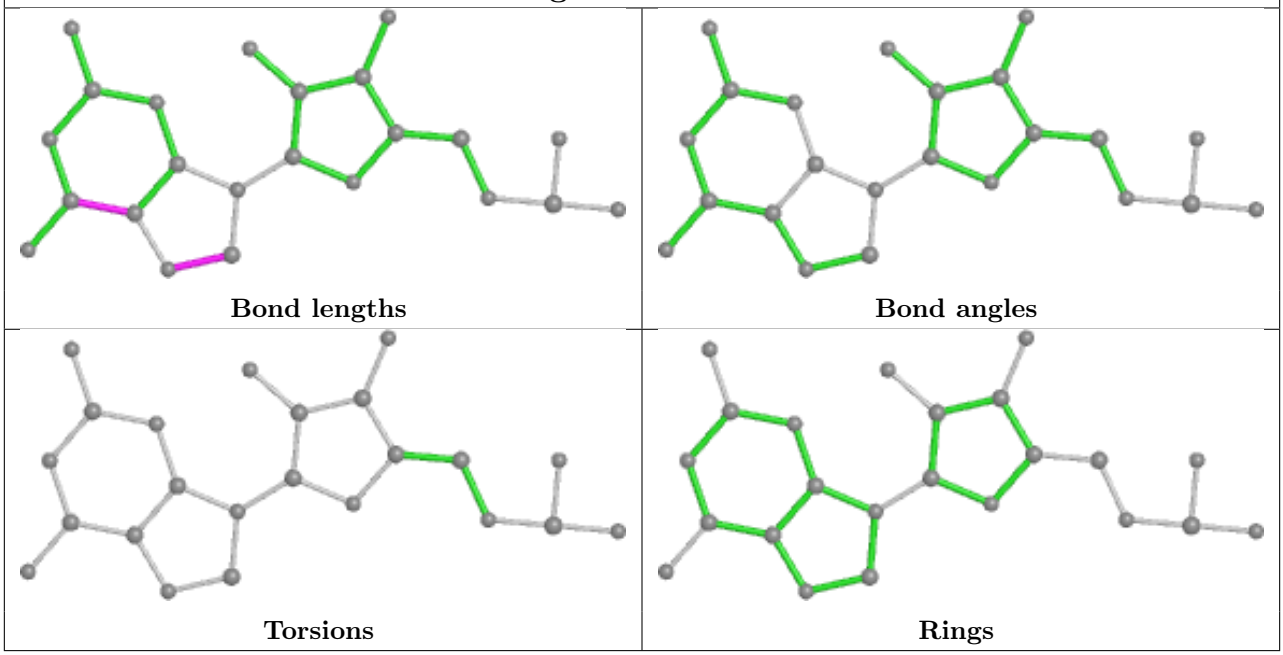


Torsions

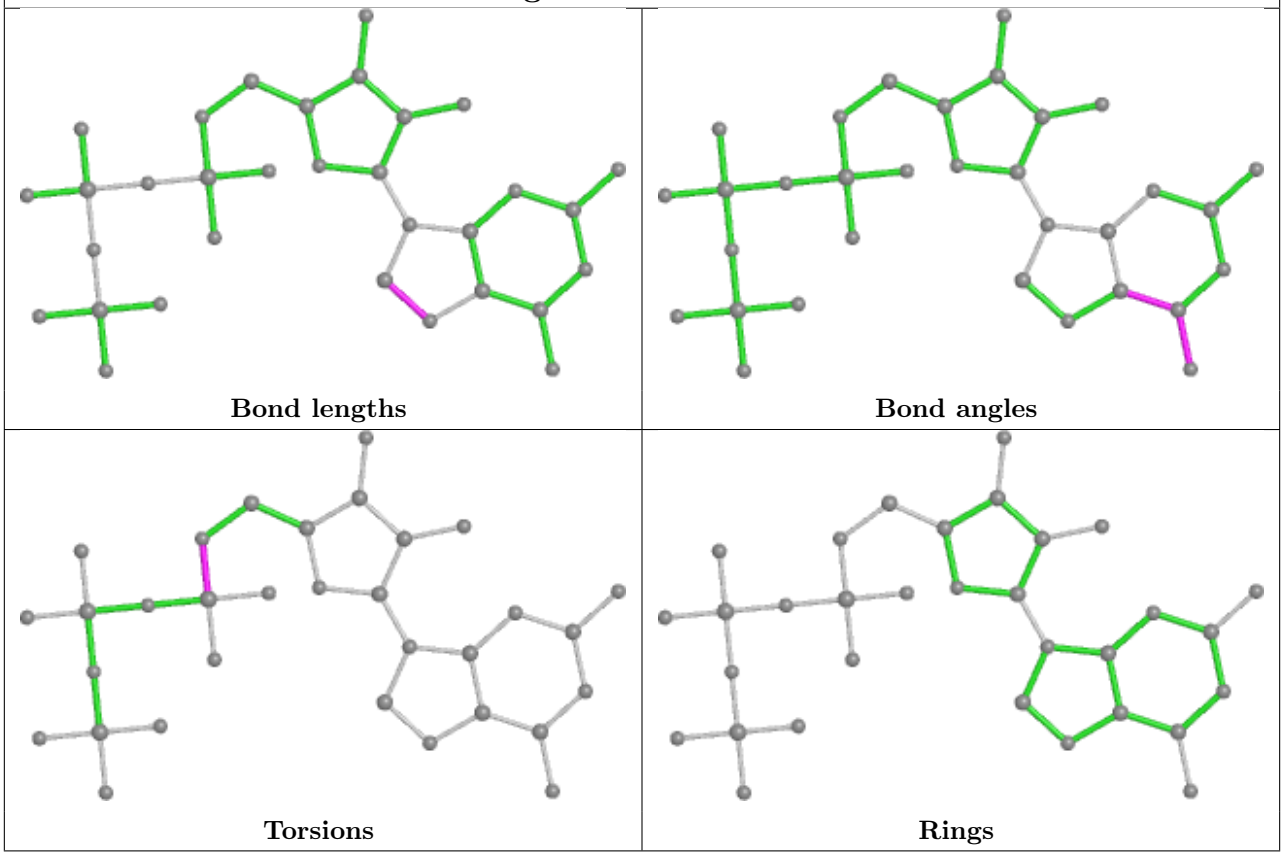


Rings

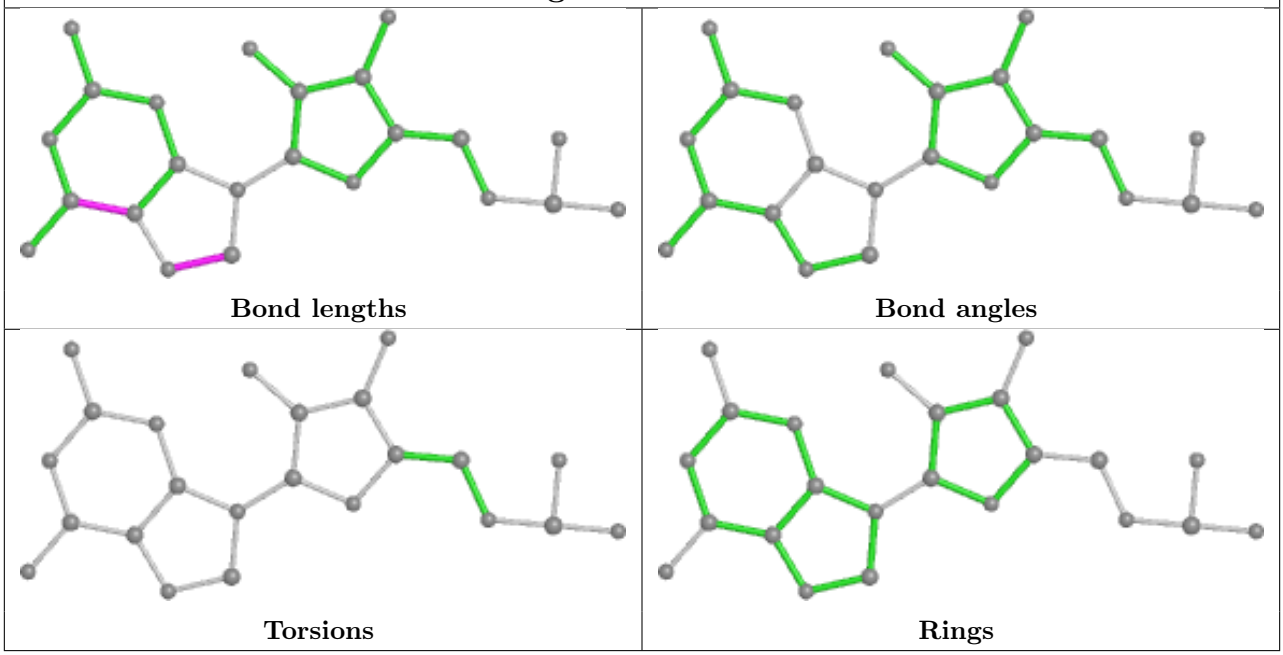
Ligand G E 704



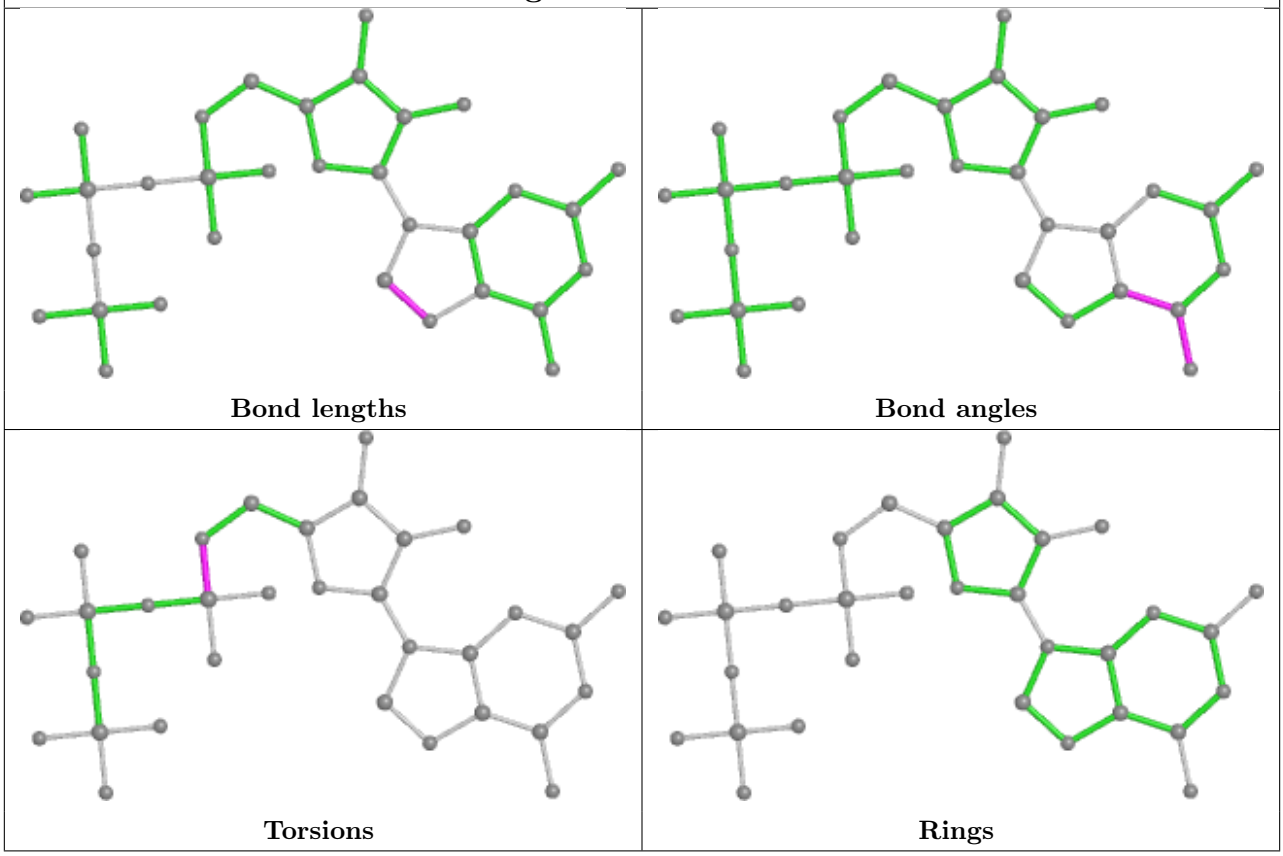
Ligand GTP C 706



Ligand G A 704



Ligand GTP E 706



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	664/664 (100%)	-0.01	18 (2%)	54	50	22, 38, 66, 119	0
1	C	664/664 (100%)	0.07	14 (2%)	63	60	22, 38, 66, 119	0
1	E	664/664 (100%)	0.23	42 (6%)	20	16	22, 38, 66, 119	0
All	All	1992/1992 (100%)	0.10	74 (3%)	41	38	22, 38, 66, 119	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	607	ARG	11.7
1	E	608	GLN	10.9
1	C	608	GLN	9.3
1	C	607	ARG	8.7
1	E	1	PRO	7.6
1	E	609	ALA	7.6
1	E	664	ARG	7.5
1	C	664	ARG	6.8
1	E	604	SER	6.6
1	A	664	ARG	6.5
1	E	610	GLY	6.3
1	E	603	ALA	6.3
1	A	1	PRO	6.2
1	E	606	ALA	6.0
1	C	603	ALA	5.5
1	E	537	ARG	5.4
1	C	609	ALA	4.9
1	A	606	ALA	4.5
1	C	604	SER	4.2
1	A	257	GLY	4.1
1	A	607	ARG	4.0
1	C	606	ALA	4.0
1	E	215	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	536	VAL	3.9
1	E	535	GLY	3.9
1	E	612	ALA	3.8
1	C	537	ARG	3.7
1	E	506	ARG	3.6
1	C	1	PRO	3.5
1	A	216	LYS	3.5
1	E	510	GLY	3.4
1	E	576	TRP	3.3
1	E	308	LEU	3.3
1	E	596	LEU	3.3
1	E	605	MET	3.2
1	E	505	SER	3.2
1	C	2	ARG	3.1
1	A	610	GLY	3.1
1	E	611	LEU	3.0
1	A	576	TRP	3.0
1	A	506	ARG	3.0
1	E	254	GLU	2.9
1	E	600	ARG	2.9
1	E	216	LYS	2.9
1	C	629	GLN	2.8
1	E	602	VAL	2.8
1	E	613	GLU	2.8
1	C	612	ALA	2.8
1	E	2	ARG	2.8
1	E	219	LYS	2.7
1	A	217	THR	2.7
1	C	506	ARG	2.7
1	E	214	ASP	2.7
1	E	461	LYS	2.7
1	E	204	ARG	2.7
1	A	254	GLU	2.5
1	A	652	GLU	2.5
1	E	479	LYS	2.4
1	A	611	LEU	2.4
1	C	320	CYS	2.4
1	A	204	ARG	2.3
1	E	470	ARG	2.3
1	E	30	ARG	2.3
1	E	217	THR	2.3
1	A	218	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	63	ASP	2.2
1	E	534	SER	2.2
1	E	221	VAL	2.2
1	A	605	MET	2.1
1	E	592	LYS	2.1
1	E	309	ASN	2.1
1	E	153	ILE	2.0
1	A	158	ASN	2.0
1	A	373	GLU	2.0

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

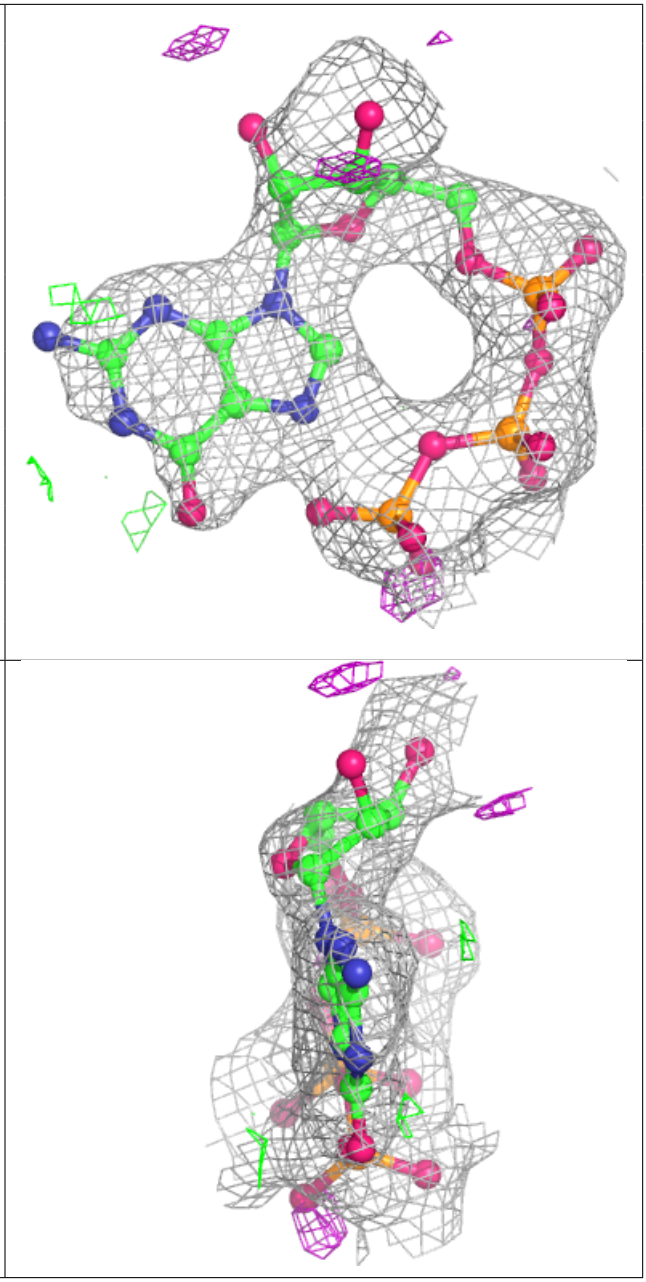
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GTP	A	706	32/32	0.88	0.20	53,63,70,74	0
6	GTP	C	706	32/32	0.91	0.18	53,63,70,74	0
6	GTP	E	706	32/32	0.91	0.17	53,63,70,74	0

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

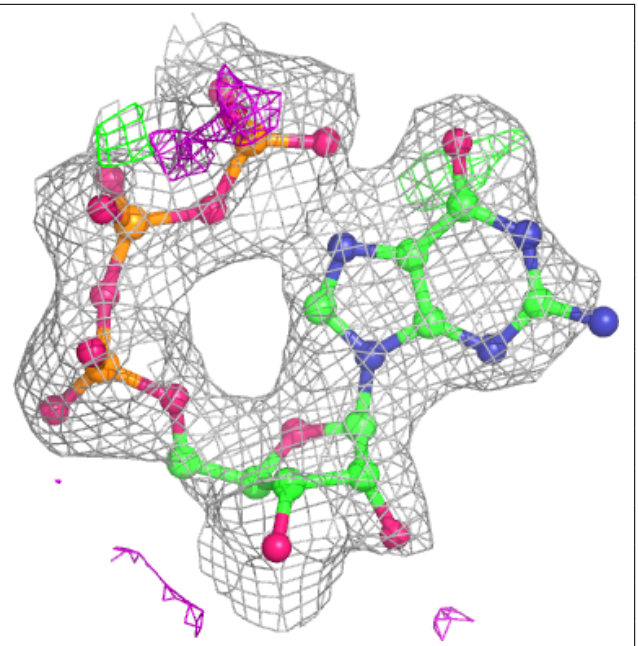
Electron density around GTP A 706:

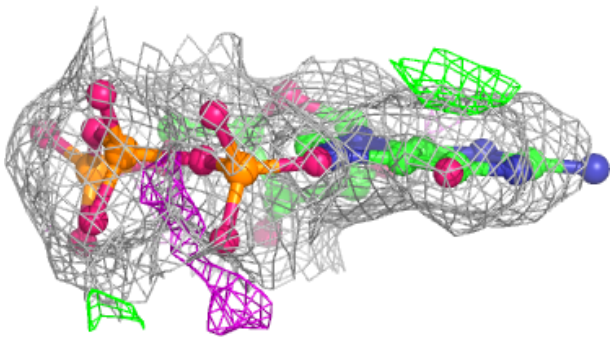
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

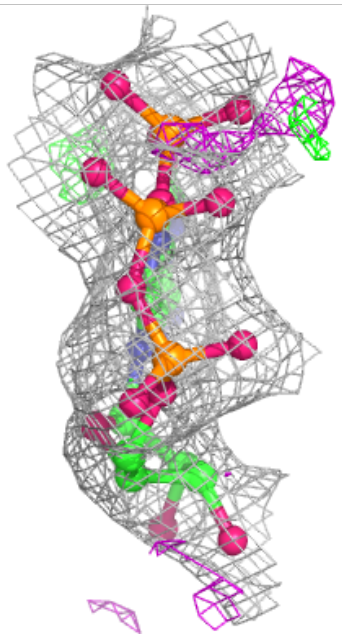


Electron density around GTP C 706:

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

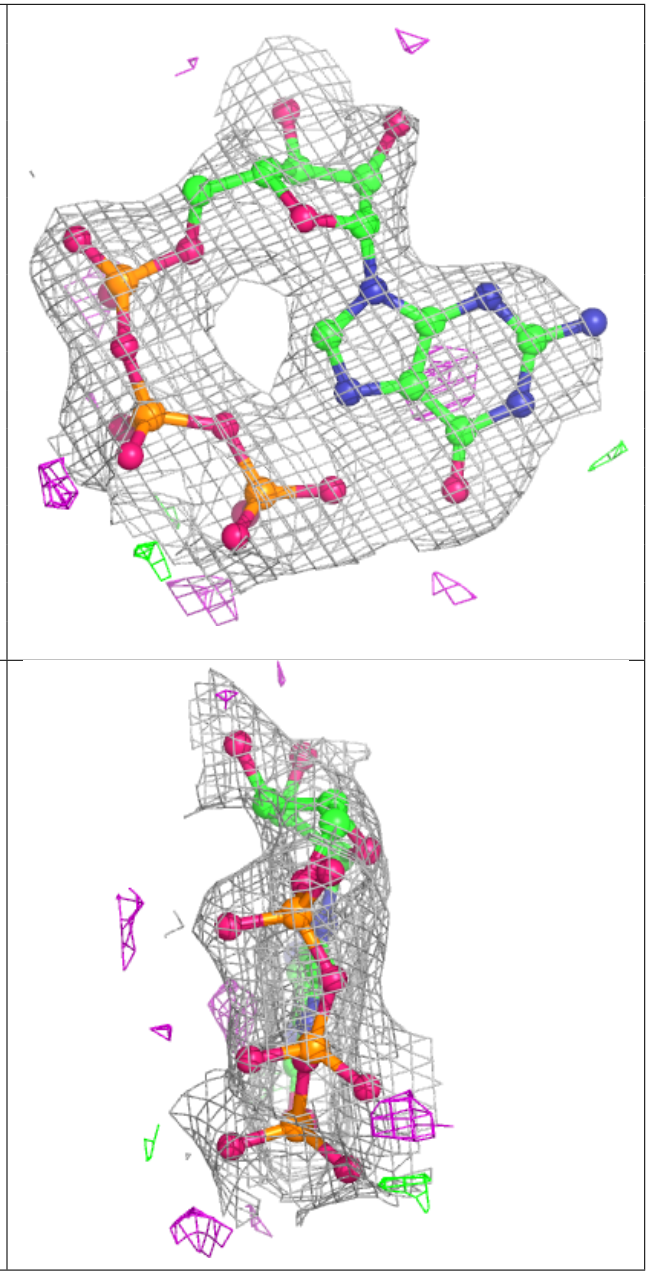






Electron density around GTP E 706:

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



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

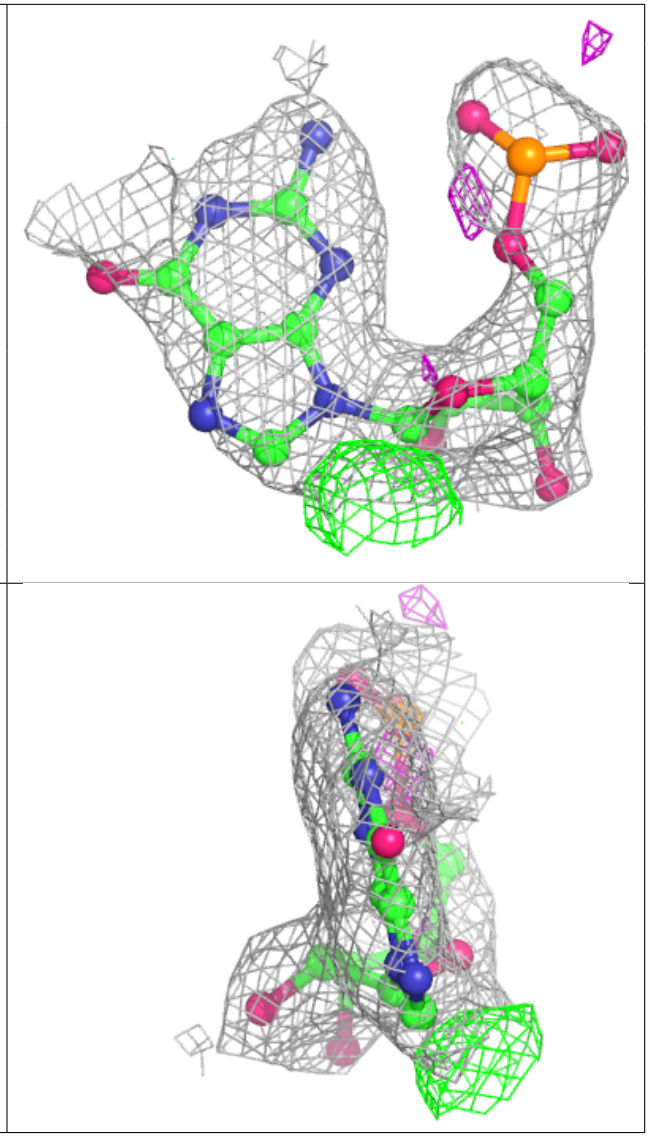
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	E	702	1/1	0.74	0.14	58,58,58,58	0
4	POP	A	703	9/9	0.77	0.31	108,111,113,113	0
3	MG	C	702	1/1	0.79	0.16	58,58,58,58	0
3	MG	C	705	1/1	0.81	0.12	35,35,35,35	0
5	G	A	704	23/24	0.81	0.30	53,73,80,81	0
3	MG	A	705	1/1	0.82	0.10	35,35,35,35	0
5	G	C	704	23/24	0.82	0.28	53,73,80,81	0
3	MG	A	702	1/1	0.83	0.11	58,58,58,58	0
3	MG	E	705	1/1	0.84	0.10	35,35,35,35	0
4	POP	E	701	9/9	0.85	0.22	108,111,113,113	0
6	GTP	A	706	32/32	0.88	0.20	53,63,70,74	0
5	G	E	704	23/24	0.89	0.24	53,73,80,81	0
4	POP	C	701	9/9	0.90	0.19	108,111,113,113	0
6	GTP	C	706	32/32	0.91	0.18	53,63,70,74	0
6	GTP	E	706	32/32	0.91	0.17	53,63,70,74	0
2	MN	E	703	1/1	0.93	0.05	50,50,50,50	0
2	MN	A	701	1/1	0.97	0.06	50,50,50,50	0
2	MN	C	703	1/1	0.97	0.10	50,50,50,50	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.

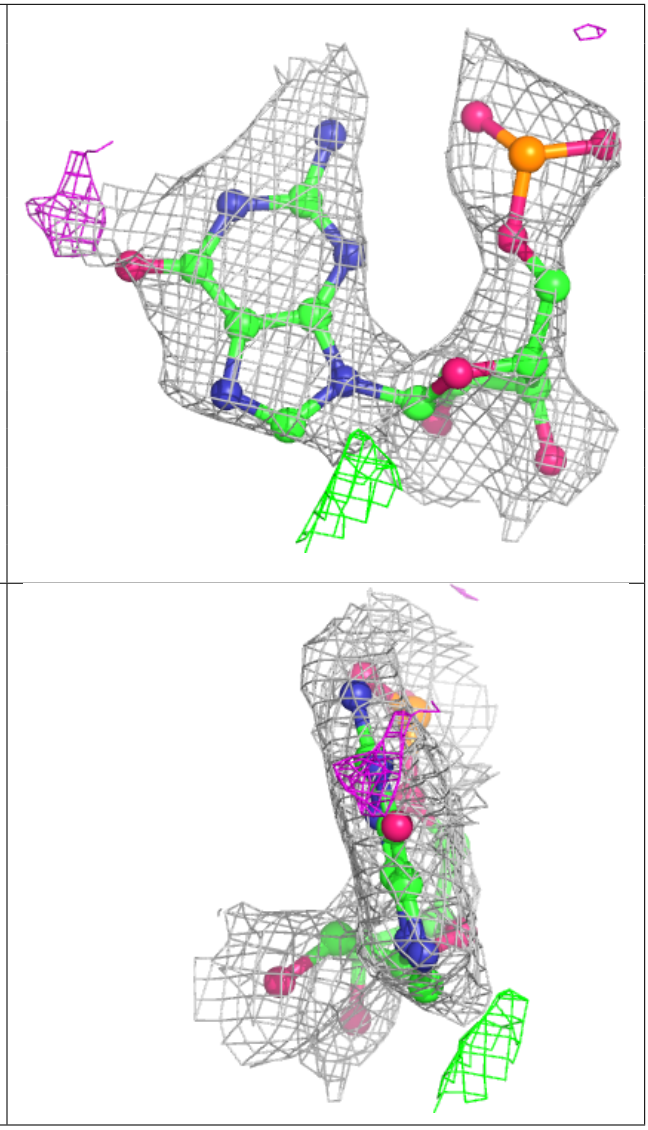
Electron density around G A 704:

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



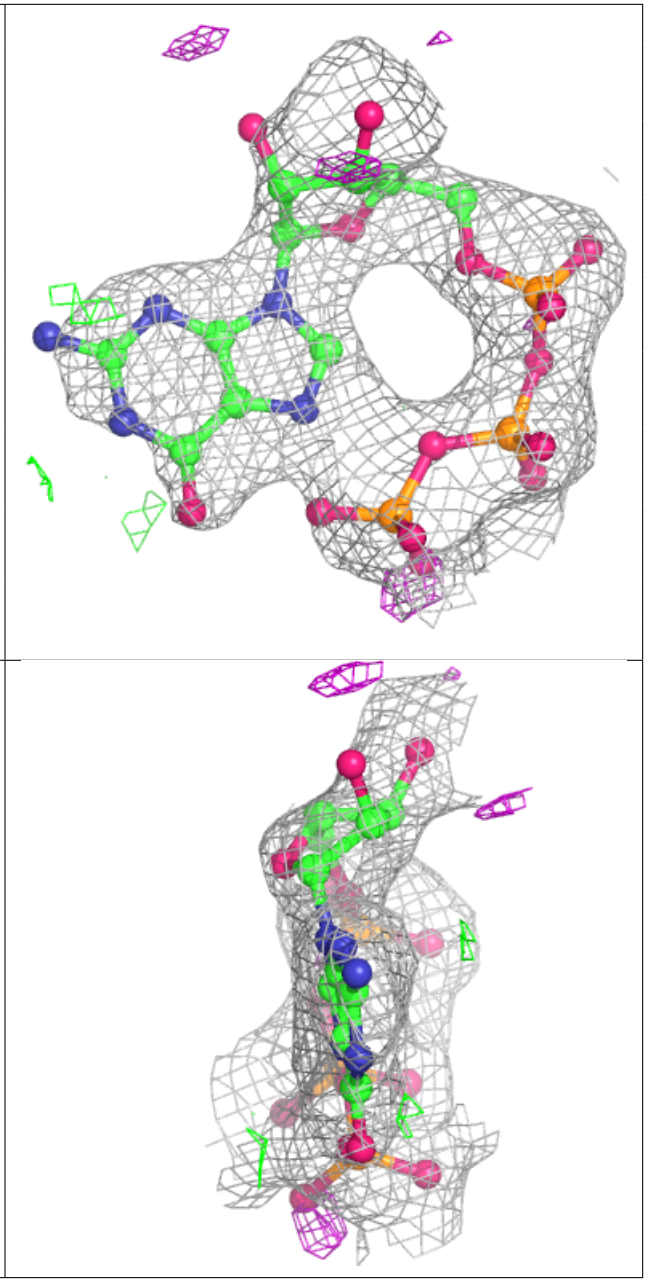
Electron density around G C 704:

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



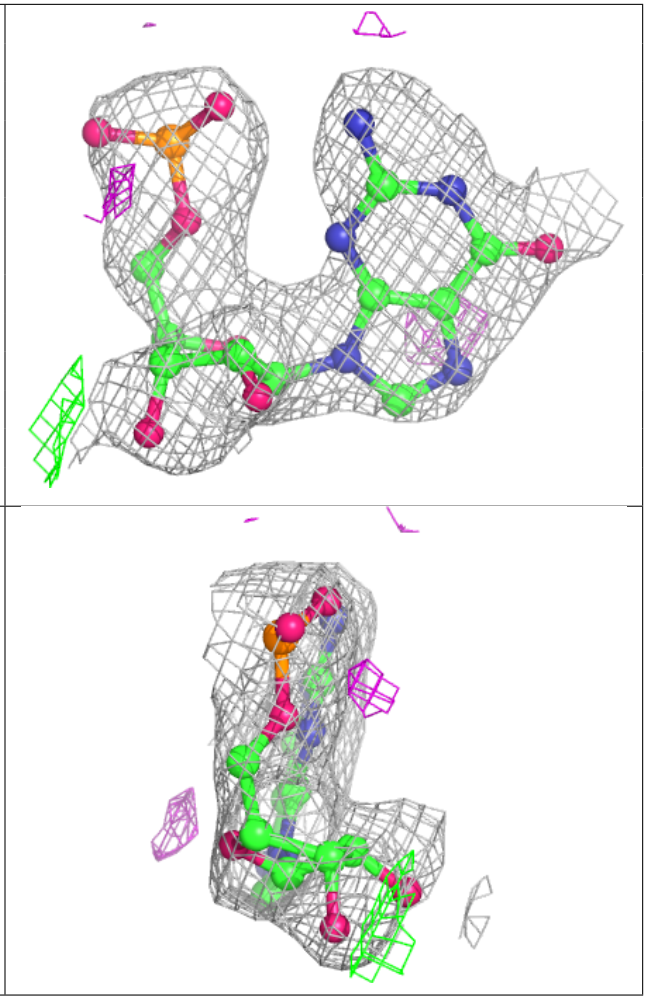
Electron density around GTP A 706:

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



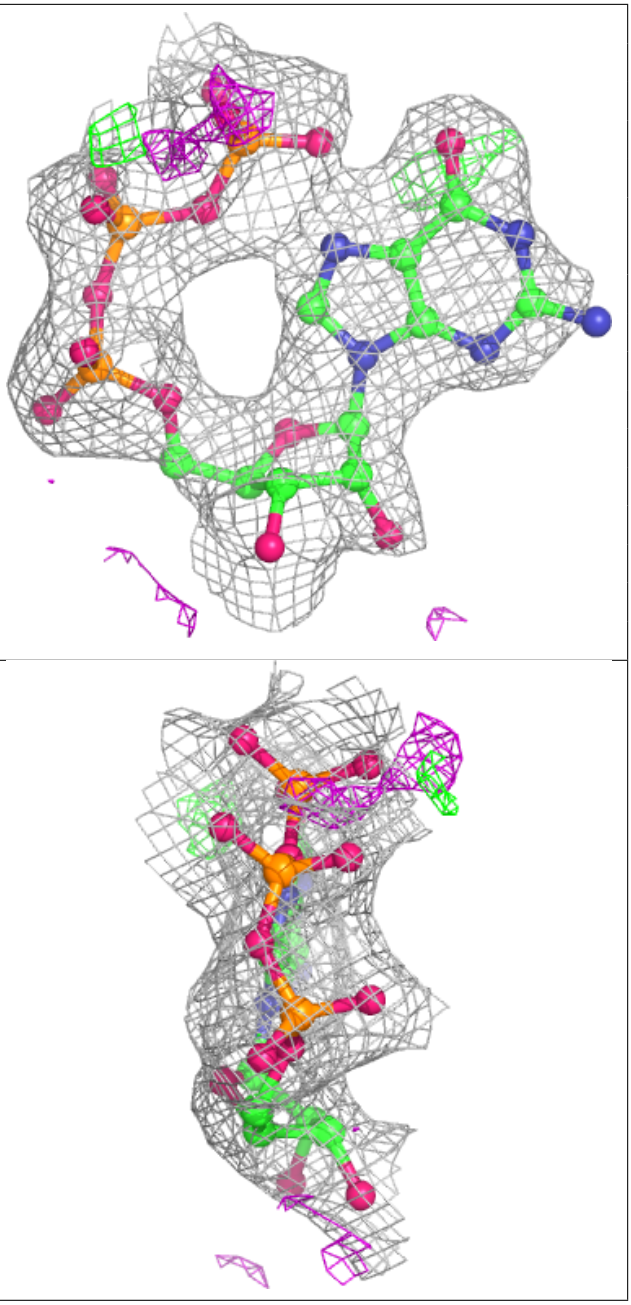
Electron density around G E 704:

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



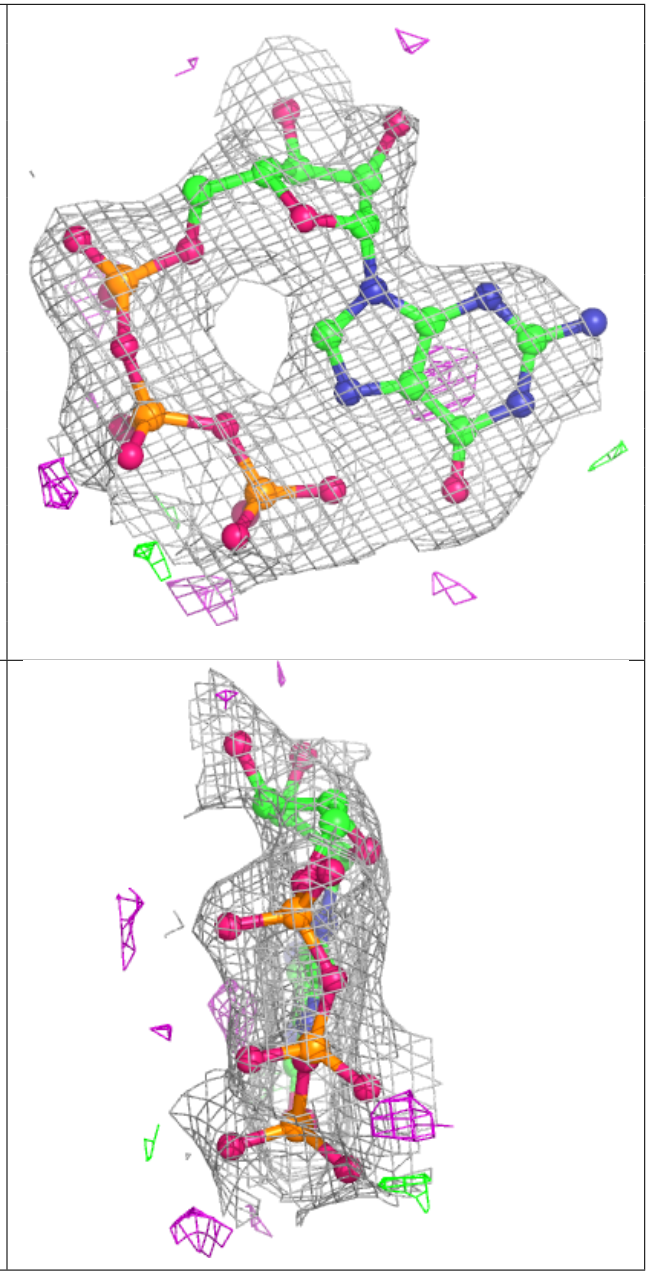
Electron density around GTP C 706:

$2mF_o$-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 E 706:

$2mF_o$-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.