Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:45 pm BST

PDB ID	:	6OIX
Title	:	Structure of Escherichia coli dGTPase bound to GTP
Authors	:	Barnes, C.O.; Wu, Y.; Calero, G.
Deposited on	:	2019-04-09
Resolution	:	3.15 Å(reported)

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

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

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

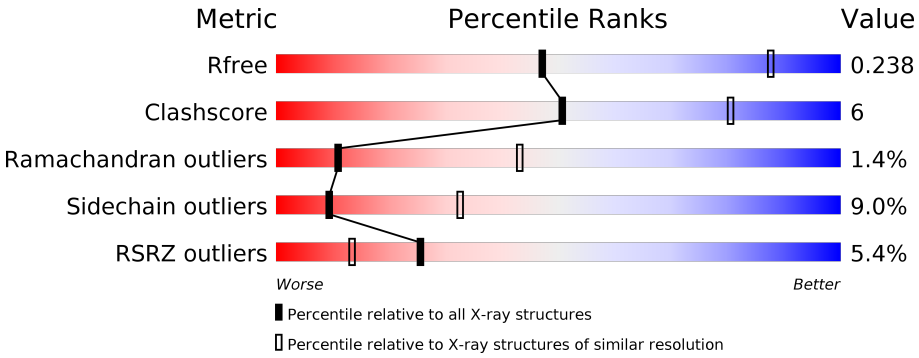
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 on 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	505	3% 75% 18% • 6%
1	B	505	10% 74% 16% • 7%
1	C	505	4% 74% 18% • 5%
1	D	505	9% 75% 16% • 7%
1	E	505	2% 76% 16% • 5%
1	F	505	3% 76% 15% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GTP	B	601	-	-	-	X

2 Entry composition (i)

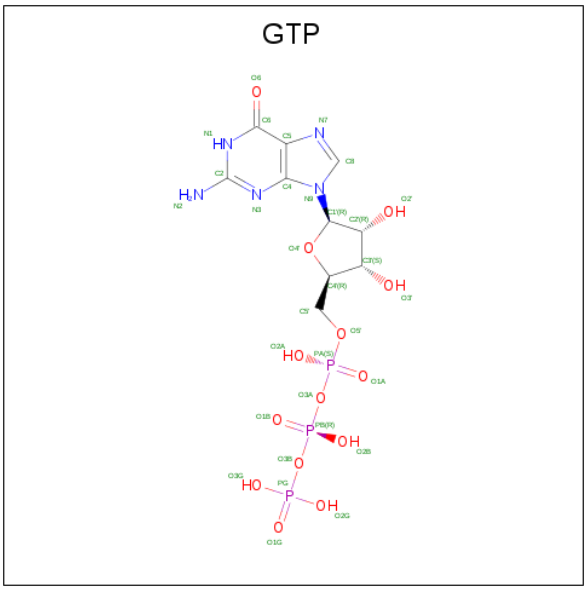
There are 4 unique types of molecules in this entry. The entry contains 24160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Deoxyguanosinetriphosphate triphosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3980	2549	708	708	15			
1	B	471	Total	C	N	O	S	0	0	0
			3921	2515	694	697	15			
1	C	478	Total	C	N	O	S	0	0	0
			3982	2552	708	706	16			
1	D	472	Total	C	N	O	S	0	0	0
			3927	2514	699	698	16			
1	E	478	Total	C	N	O	S	0	0	0
			3982	2549	708	709	16			
1	F	475	Total	C	N	O	S	0	0	0
			3954	2536	702	700	16			

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is water.

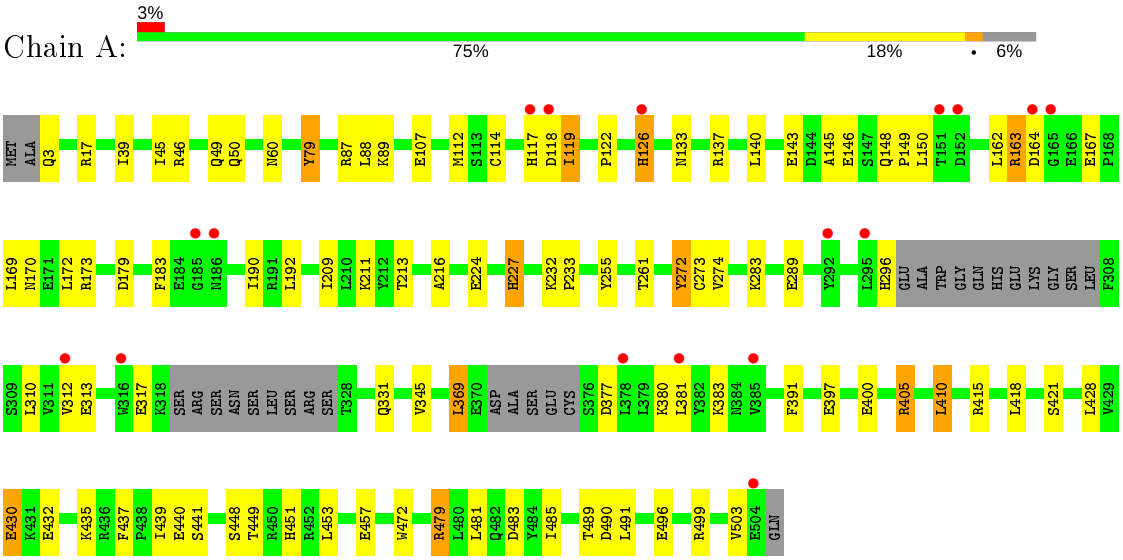
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	22	Total	O	0	0
			22	22		
4	C	38	Total	O	0	0
			38	38		
4	D	21	Total	O	0	0
			21	21		
4	E	49	Total	O	0	0
			49	49		
4	F	46	Total	O	0	0
			46	46		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

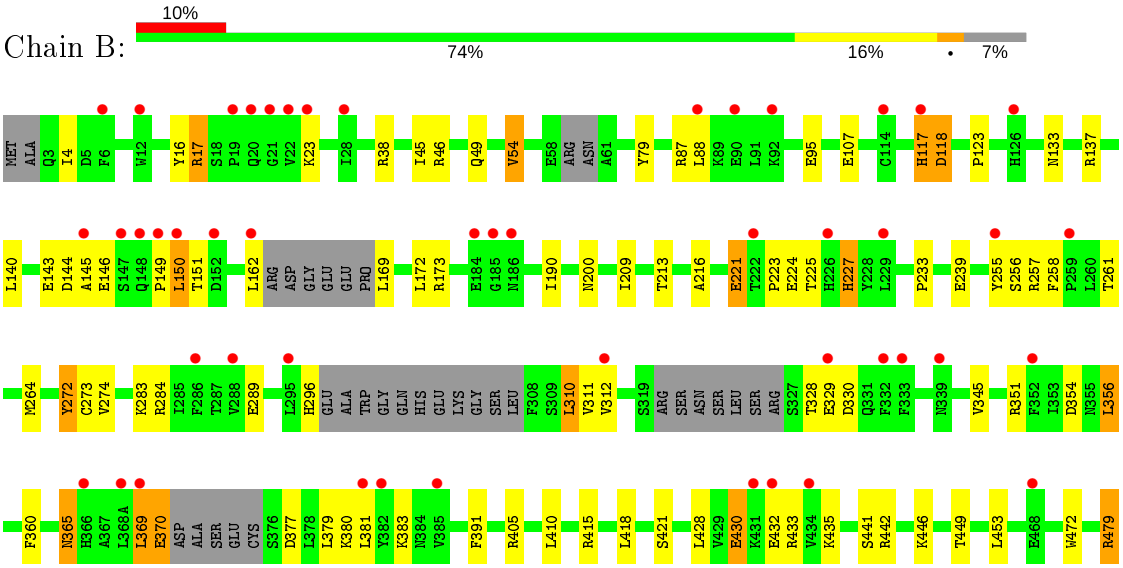
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

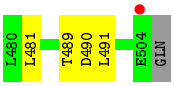
Chain A:



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

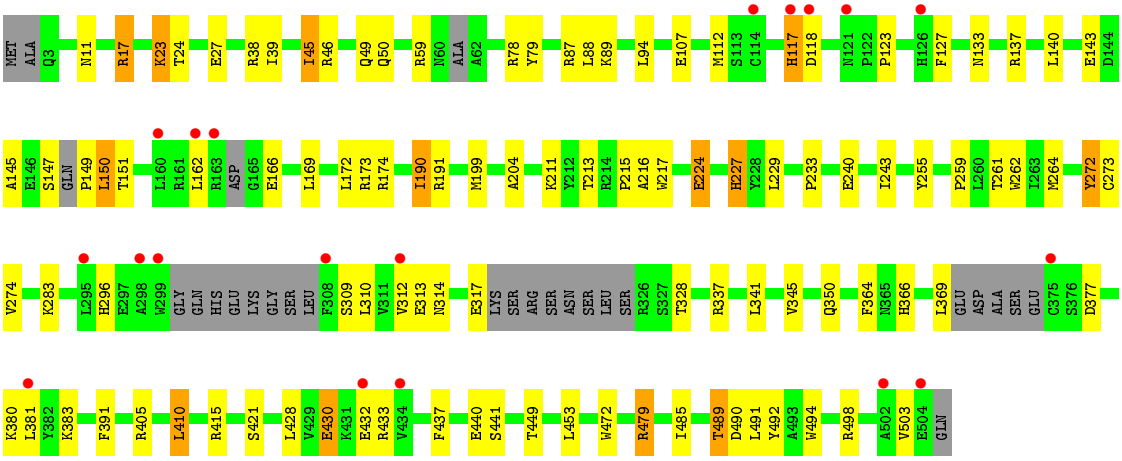
Chain B:





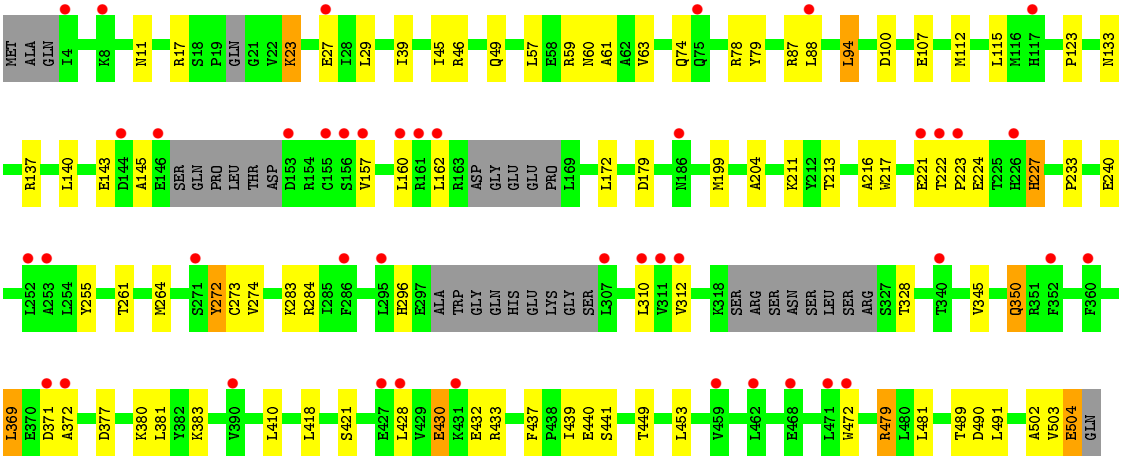
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain C:



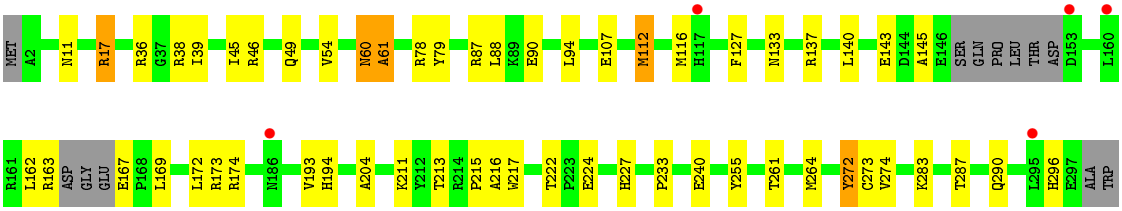
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

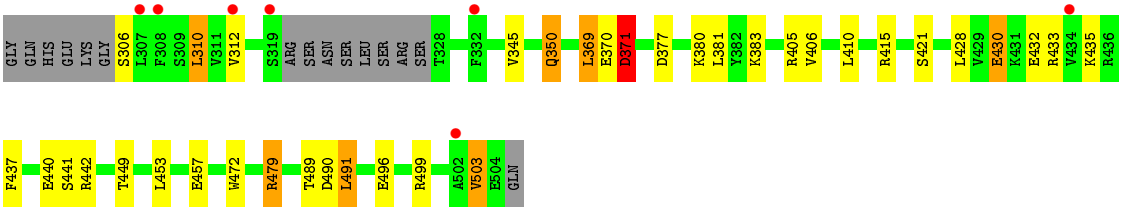
Chain D:



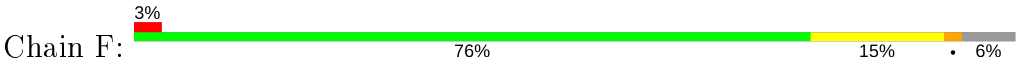
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

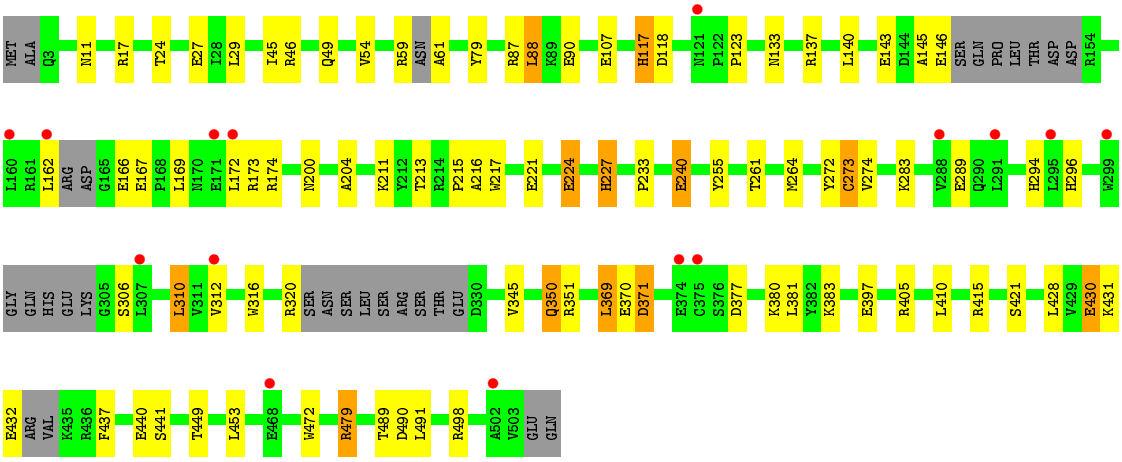
Chain E:





- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	191.59Å 191.59Å 292.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.75 – 3.15 39.36 – 3.11	Depositor EDS
% Data completeness (in resolution range)	91.6 (31.75-3.15) 88.8 (39.36-3.11)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.190 , 0.208 0.218 , 0.238	Depositor DCC
R_{free} test set	2647 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	97.5	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 99.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24160	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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

5.1 Standard geometry

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

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	0.56	0/4077	0.72	1/5511 (0.0%)
1	B	0.49	0/4015	0.70	3/5426 (0.1%)
1	C	0.56	0/4078	0.74	3/5508 (0.1%)
1	D	0.48	0/4018	0.71	2/5424 (0.0%)
1	E	0.54	1/4077 (0.0%)	0.73	1/5508 (0.0%)
1	F	0.53	0/4049	0.71	2/5467 (0.0%)
All	All	0.53	1/24314 (0.0%)	0.72	12/32844 (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	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	112	MET	SD-CE	-6.64	1.40	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	60	ASN	C-N-CA	8.20	142.19	121.70
1	C	117	HIS	N-CA-C	-5.74	95.52	111.00
1	F	117	HIS	N-CA-C	-5.74	95.52	111.00
1	A	163	ARG	C-N-CA	5.73	136.02	121.70
1	B	365	ASN	CA-CB-CG	-5.73	100.80	113.40
1	C	123	PRO	C-N-CA	-5.68	107.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	123	PRO	C-N-CA	-5.63	107.62	121.70
1	D	59	ARG	C-N-CA	5.56	135.61	121.70
1	C	199	MET	N-CA-C	-5.51	96.11	111.00
1	D	123	PRO	C-N-CA	-5.47	108.04	121.70
1	B	123	PRO	C-N-CA	-5.42	108.16	121.70
1	B	117	HIS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	60	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3980	0	3954	55	0
1	B	3921	0	3893	46	0
1	C	3982	0	3944	54	0
1	D	3927	0	3906	40	0
1	E	3982	0	3955	46	0
1	F	3954	0	3924	40	0
2	A	32	0	12	4	0
2	B	32	0	12	2	0
2	C	32	0	12	1	0
2	D	32	0	12	0	0
2	E	32	0	12	0	0
2	F	32	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	40	0	0	2	0
4	B	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	38	0	0	0	0
4	D	21	0	0	0	0
4	E	49	0	0	1	0
4	F	46	0	0	2	0
All	All	24160	0	23648	270	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (270) 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:150:LEU:HB3	1:C:151:THR:HA	1.16	1.13
1:B:17:ARG:HH22	1:B:38:ARG:HH22	1.05	1.02
1:E:272:TYR:HD2	1:E:273:CYS:HG	1.04	0.96
1:C:150:LEU:HB3	1:C:151:THR:CA	1.92	0.96
1:C:17:ARG:HH22	1:C:38:ARG:HH22	1.10	0.96
1:A:400:GLU:OE2	1:B:442:ARG:NE	2.00	0.94
1:B:4:ILE:HD13	1:B:356:LEU:HD12	1.55	0.88
1:A:126:HIS:H	1:A:126:HIS:CD2	1.92	0.85
1:C:262:TRP:HZ3	1:C:366:HIS:O	1.57	0.85
1:A:122:PRO:HG3	1:A:183:PHE:CE1	2.12	0.83
2:A:601:GTP:O2G	4:A:701:HOH:O	1.97	0.82
1:C:262:TRP:HH2	1:C:364:PHE:O	1.65	0.79
1:B:310:LEU:HD12	1:B:311:VAL:HG23	1.64	0.77
1:F:79:TYR:HD2	1:F:345:VAL:HG11	1.50	0.77
1:C:17:ARG:NH2	1:C:38:ARG:HH22	1.81	0.77
1:B:17:ARG:NH2	1:B:38:ARG:HH22	1.82	0.77
1:E:79:TYR:HD2	1:E:345:VAL:HG11	1.51	0.76
1:C:79:TYR:HD2	1:C:345:VAL:HG11	1.51	0.75
1:C:50:GLN:HG3	1:E:61:ALA:HB1	1.68	0.75
1:F:351:ARG:HH12	1:F:370:GLU:HG3	1.52	0.75
1:A:119:ILE:HG23	1:A:192:LEU:HD23	1.69	0.74
1:B:351:ARG:HH12	1:B:370:GLU:HG3	1.52	0.74
1:B:144:ASP:HB3	1:B:150:LEU:HD21	1.71	0.72
1:B:79:TYR:HD2	1:B:345:VAL:HG11	1.53	0.72
1:D:272:TYR:HD2	1:D:273:CYS:HG	1.37	0.72
1:B:227:HIS:HB2	4:B:704:HOH:O	1.92	0.70
1:C:262:TRP:CZ3	1:C:366:HIS:O	2.45	0.67
1:B:150:LEU:H	1:B:150:LEU:HD22	1.59	0.67
1:D:79:TYR:HD2	1:D:345:VAL:HG11	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:GLU:HG3	1:F:316:TRP:HH2	1.60	0.66
1:A:122:PRO:HG3	1:A:183:PHE:HE1	1.60	0.65
1:C:262:TRP:CH2	1:C:364:PHE:O	2.48	0.64
1:C:479:ARG:HG3	1:C:479:ARG:HH11	1.63	0.63
1:C:79:TYR:CD2	1:C:345:VAL:HG11	2.33	0.62
1:B:272:TYR:HD2	1:B:273:CYS:HG	1.47	0.62
1:C:224:GLU:HA	1:C:227:HIS:ND1	2.15	0.62
1:D:79:TYR:CD2	1:D:345:VAL:HG11	2.35	0.62
1:F:79:TYR:CD2	1:F:345:VAL:HG11	2.34	0.62
1:A:79:TYR:CD2	1:A:345:VAL:HG11	2.35	0.61
1:A:272:TYR:HD2	1:A:273:CYS:HG	1.49	0.61
1:D:224:GLU:HA	1:D:227:HIS:HD2	1.66	0.61
1:C:272:TYR:HD2	1:C:273:CYS:HG	1.48	0.60
1:D:479:ARG:HG3	1:D:479:ARG:HH11	1.66	0.60
1:A:79:TYR:HD2	1:A:345:VAL:HG11	1.65	0.60
1:C:494:TRP:CD1	1:C:498:ARG:HD3	2.36	0.60
1:B:272:TYR:HD2	1:B:273:CYS:SG	2.24	0.60
1:F:273:CYS:SG	1:F:383:LYS:HD2	2.43	0.59
1:E:39:ILE:HB	1:E:112:MET:CE	2.33	0.59
1:B:479:ARG:HG3	1:B:479:ARG:HH11	1.68	0.59
1:A:272:TYR:HD2	1:A:273:CYS:SG	2.25	0.59
1:B:79:TYR:CD2	1:B:345:VAL:HG11	2.35	0.58
1:F:224:GLU:HA	1:F:227:HIS:HD2	1.68	0.58
1:E:79:TYR:CD2	1:E:345:VAL:HG11	2.36	0.58
1:E:479:ARG:HG3	1:E:479:ARG:HH11	1.67	0.58
1:E:287:THR:HG23	1:E:290:GLN:H	1.69	0.57
1:A:122:PRO:HG3	1:A:183:PHE:CZ	2.40	0.57
1:C:272:TYR:HD2	1:C:273:CYS:SG	2.27	0.57
1:F:479:ARG:HG3	1:F:479:ARG:HH11	1.68	0.57
1:B:145:ALA:HA	1:B:162:LEU:HD11	1.85	0.57
1:F:294:HIS:HD2	4:F:736:HOH:O	1.86	0.57
1:F:217:TRP:CH2	1:F:240:GLU:HG2	2.40	0.57
1:B:257:ARG:HG2	1:B:261:THR:OG1	2.05	0.56
1:C:145:ALA:HA	1:C:162:LEU:HD11	1.86	0.56
1:A:391:PHE:CD1	2:A:601:GTP:C5	2.93	0.56
1:D:46:ARG:O	1:D:49:GLN:HG2	2.06	0.56
1:E:145:ALA:HA	1:E:162:LEU:HD11	1.88	0.56
1:A:46:ARG:O	1:A:49:GLN:HG2	2.06	0.55
1:D:94:LEU:HD23	1:D:100:ASP:HA	1.88	0.55
1:D:224:GLU:HA	1:D:227:HIS:CD2	2.40	0.55
1:A:224:GLU:HA	1:A:227:HIS:ND1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:TRP:HH2	1:C:240:GLU:HG3	1.71	0.55
1:F:46:ARG:O	1:F:49:GLN:HG2	2.06	0.55
1:A:479:ARG:HH11	1:A:479:ARG:HG2	1.71	0.55
1:C:313:GLU:O	1:C:317:GLU:OE1	2.24	0.55
1:E:46:ARG:O	1:E:49:GLN:HG2	2.07	0.55
1:A:119:ILE:HG23	1:A:192:LEU:CD2	2.38	0.54
1:B:4:ILE:CD1	1:B:356:LEU:HD12	2.35	0.54
1:A:122:PRO:CG	1:A:183:PHE:CE1	2.87	0.54
1:C:410:LEU:HD12	1:C:485:ILE:HD12	1.89	0.54
1:D:272:TYR:HD2	1:D:273:CYS:SG	2.30	0.54
1:B:54:VAL:HG11	1:B:391:PHE:HE1	1.73	0.54
1:A:122:PRO:CG	1:A:183:PHE:HE1	2.20	0.54
1:B:46:ARG:O	1:B:49:GLN:HG2	2.07	0.54
1:A:145:ALA:HA	1:A:162:LEU:HD11	1.89	0.54
1:A:397:GLU:HB3	1:B:442:ARG:HG2	1.89	0.54
1:D:145:ALA:HA	1:D:162:LEU:HD11	1.88	0.54
1:A:410:LEU:HD12	1:A:485:ILE:HD12	1.90	0.54
1:C:217:TRP:CH2	1:C:240:GLU:HG3	2.43	0.54
1:F:216:ALA:HA	1:F:233:PRO:HB3	1.89	0.53
1:A:216:ALA:HA	1:A:233:PRO:HB3	1.90	0.53
1:F:145:ALA:HA	1:F:162:LEU:HD11	1.90	0.53
1:B:356:LEU:HD13	1:B:360:PHE:HB2	1.90	0.53
1:C:46:ARG:O	1:C:49:GLN:HG2	2.09	0.53
1:E:216:ALA:HA	1:E:233:PRO:HB3	1.91	0.53
1:D:350:GLN:NE2	1:D:350:GLN:HA	2.24	0.53
1:C:216:ALA:HA	1:C:233:PRO:HB3	1.91	0.52
1:B:216:ALA:HA	1:B:233:PRO:HB3	1.90	0.52
1:F:224:GLU:HA	1:F:227:HIS:CD2	2.45	0.52
1:A:172:LEU:HD11	1:A:472:TRP:CZ2	2.45	0.52
1:C:479:ARG:NH1	1:C:479:ARG:HG3	2.23	0.52
1:E:217:TRP:HH2	1:E:240:GLU:HG3	1.75	0.51
1:A:126:HIS:CD2	1:A:126:HIS:N	2.72	0.51
1:F:172:LEU:HD11	1:F:472:TRP:CZ2	2.45	0.51
1:C:259:PRO:O	1:C:262:TRP:HD1	1.93	0.51
1:E:172:LEU:HD11	1:E:472:TRP:CZ2	2.46	0.51
1:C:229:LEU:HD21	1:C:262:TRP:CH2	2.46	0.51
1:C:337:ARG:O	1:C:341:LEU:HD23	2.11	0.50
1:D:222:THR:OG1	1:D:223:PRO:HA	2.12	0.50
1:A:126:HIS:NE2	4:A:703:HOH:O	2.35	0.50
1:D:216:ALA:HA	1:D:233:PRO:HB3	1.93	0.50
1:A:400:GLU:OE2	1:B:442:ARG:CZ	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:SER:HB2	1:A:451:HIS:ND1	2.27	0.50
2:A:601:GTP:C8	2:A:601:GTP:H5'	2.47	0.50
1:D:479:ARG:HG3	1:D:479:ARG:NH1	2.27	0.50
1:C:172:LEU:HD11	1:C:472:TRP:CZ2	2.47	0.49
1:D:172:LEU:HD11	1:D:472:TRP:CZ2	2.46	0.49
1:C:494:TRP:HD1	1:C:498:ARG:HD3	1.78	0.49
1:E:479:ARG:HG3	1:E:479:ARG:NH1	2.26	0.49
1:F:17:ARG:NH2	1:F:200:ASN:HD22	2.09	0.49
1:D:94:LEU:CD2	1:D:100:ASP:HA	2.41	0.49
1:A:50:GLN:HG3	1:F:61:ALA:HB1	1.94	0.49
1:A:418:LEU:HD11	1:A:481:LEU:HD23	1.95	0.49
1:D:179:ASP:OD1	1:D:216:ALA:HB3	2.12	0.49
1:D:369:LEU:HD22	1:D:369:LEU:N	2.27	0.49
1:B:377:ASP:HA	1:B:380:LYS:HD2	1.94	0.49
1:E:350:GLN:NE2	1:E:350:GLN:HA	2.28	0.48
1:F:350:GLN:HA	1:F:350:GLN:NE2	2.28	0.48
1:E:377:ASP:HA	1:E:380:LYS:HD2	1.95	0.48
1:A:313:GLU:O	1:A:317:GLU:OE1	2.32	0.48
1:A:369:LEU:N	1:A:369:LEU:HD22	2.28	0.48
1:A:211:LYS:HA	1:A:261:THR:HG21	1.96	0.48
1:B:133:ASN:O	1:B:137:ARG:HB2	2.14	0.48
1:E:371:ASP:HA	1:E:380:LYS:NZ	2.29	0.48
1:E:217:TRP:CH2	1:E:240:GLU:HG3	2.48	0.48
1:A:133:ASN:O	1:A:137:ARG:HB2	2.13	0.48
1:F:371:ASP:HA	1:F:380:LYS:NZ	2.29	0.48
1:A:114:CYS:O	1:A:117:HIS:ND1	2.36	0.47
1:C:147:SER:C	1:C:149:PRO:HG2	2.35	0.47
1:F:29:LEU:HD12	4:F:730:HOH:O	2.14	0.47
1:F:479:ARG:HG3	1:F:479:ARG:NH1	2.29	0.47
1:C:17:ARG:HH22	1:C:38:ARG:NH2	1.93	0.47
1:E:17:ARG:HH22	1:E:38:ARG:HH22	1.61	0.47
1:B:117:HIS:O	1:B:118:ASP:HB2	2.14	0.47
1:B:479:ARG:NH1	1:B:479:ARG:HG3	2.29	0.47
1:C:428:LEU:HD11	1:C:441:SER:HA	1.97	0.47
1:C:59:ARG:HH11	1:E:491:LEU:HD23	1.79	0.47
1:A:232:LYS:HD2	2:A:601:GTP:O1G	2.14	0.47
1:E:36:ARG:HA	1:E:112:MET:HE1	1.96	0.47
1:A:391:PHE:CD2	1:A:391:PHE:N	2.80	0.47
1:A:377:ASP:HA	1:A:380:LYS:HD2	1.95	0.47
1:B:54:VAL:HG11	1:B:391:PHE:CE1	2.49	0.47
1:F:306:SER:C	1:F:310:LEU:HD12	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:ASP:HA	1:D:380:LYS:HD2	1.95	0.47
1:B:172:LEU:HD11	1:B:472:TRP:CZ2	2.50	0.46
1:C:377:ASP:HA	1:C:380:LYS:HD2	1.97	0.46
1:F:377:ASP:HA	1:F:380:LYS:HD2	1.96	0.46
1:A:479:ARG:NH1	1:A:479:ARG:HG2	2.31	0.46
1:C:117:HIS:O	1:C:118:ASP:HB2	2.16	0.46
1:E:496:GLU:HG2	1:E:499:ARG:HH21	1.81	0.46
1:F:169:LEU:HD23	1:F:173:ARG:NH1	2.30	0.46
1:B:405:ARG:HG3	1:B:405:ARG:HH11	1.81	0.46
1:E:211:LYS:HA	1:E:261:THR:HG21	1.97	0.46
1:A:369:LEU:H	1:A:369:LEU:HD22	1.81	0.45
1:B:16:TYR:H	1:B:200:ASN:ND2	2.14	0.45
1:D:418:LEU:HD11	1:D:481:LEU:HD23	1.98	0.45
1:B:221:GLU:O	1:B:223:PRO:HD3	2.15	0.45
1:E:369:LEU:HD22	1:E:369:LEU:N	2.32	0.45
1:A:169:LEU:HD23	1:A:173:ARG:NH1	2.30	0.45
1:F:213:THR:HB	1:F:255:TYR:HA	1.98	0.45
1:C:273:CYS:SG	1:C:383:LYS:HA	2.56	0.45
1:C:211:LYS:HA	1:C:261:THR:HG21	1.99	0.45
1:D:504:GLU:OE2	1:D:504:GLU:HA	2.16	0.45
1:E:169:LEU:HD23	1:E:173:ARG:NH1	2.31	0.45
1:E:405:ARG:HG3	1:E:405:ARG:HH11	1.82	0.45
1:A:163:ARG:HB2	1:A:167:GLU:OE1	2.16	0.45
1:B:428:LEU:HD11	1:B:441:SER:HA	1.99	0.45
1:D:133:ASN:O	1:D:137:ARG:HB2	2.17	0.45
1:F:133:ASN:O	1:F:137:ARG:HB2	2.17	0.45
1:D:369:LEU:HD22	1:D:369:LEU:H	1.81	0.45
1:D:428:LEU:HD11	1:D:441:SER:HA	1.98	0.45
1:E:369:LEU:HD22	1:E:369:LEU:H	1.82	0.45
1:F:369:LEU:HD22	1:F:369:LEU:N	2.32	0.45
1:C:11:ASN:H	1:C:204:ALA:HB2	1.81	0.44
1:D:39:ILE:HG13	1:D:199:MET:HE1	1.99	0.44
1:E:133:ASN:O	1:E:137:ARG:HB2	2.17	0.44
1:E:428:LEU:HD11	1:E:441:SER:HA	1.99	0.44
1:E:503:VAL:HG12	1:F:498:ARG:HG2	1.99	0.44
1:A:410:LEU:HA	1:A:410:LEU:HD22	1.84	0.44
1:A:451:HIS:CD2	1:A:483:ASP:HB3	2.52	0.44
1:D:211:LYS:HA	1:D:261:THR:HG21	1.99	0.44
1:D:437:PHE:HB3	1:D:440:GLU:HB2	1.99	0.44
1:F:428:LEU:HD11	1:F:441:SER:HA	1.99	0.44
1:C:133:ASN:O	1:C:137:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD11	1:B:481:LEU:HD23	1.99	0.44
1:F:59:ARG:C	1:F:61:ALA:HB2	2.38	0.44
1:A:437:PHE:HB3	1:A:440:GLU:HB2	2.00	0.44
1:B:356:LEU:O	1:B:356:LEU:HD13	2.18	0.44
1:A:428:LEU:HD11	1:A:441:SER:HA	2.00	0.44
1:F:369:LEU:HD22	1:F:369:LEU:H	1.83	0.44
1:A:179:ASP:OD1	1:A:216:ALA:HB3	2.18	0.43
1:C:391:PHE:HB3	2:C:601:GTP:C6	2.53	0.43
1:B:329:GLU:HG3	1:B:330:ASP:H	1.84	0.43
1:E:273:CYS:SG	1:E:383:LYS:HA	2.58	0.43
1:A:213:THR:HB	1:A:255:TYR:HA	2.00	0.43
1:B:169:LEU:HD23	1:B:173:ARG:NH1	2.33	0.43
1:B:391:PHE:HB3	2:B:601:GTP:O6	2.18	0.43
1:D:11:ASN:H	1:D:204:ALA:HB2	1.84	0.43
1:D:439:ILE:HD13	1:E:127:PHE:HE2	1.81	0.43
1:B:258:PHE:HB3	1:B:261:THR:HG23	2.01	0.43
1:C:23:LYS:HA	1:C:27:GLU:OE1	2.19	0.43
1:F:211:LYS:HA	1:F:261:THR:HG21	2.00	0.43
1:B:369:LEU:HD13	1:B:379:LEU:HD11	2.00	0.43
1:D:213:THR:HB	1:D:255:TYR:HA	2.00	0.43
1:D:74:GLN:OE1	1:D:115:LEU:HD13	2.19	0.42
1:C:489:THR:HG23	1:C:492:TYR:HB3	2.01	0.42
1:C:213:THR:HB	1:C:255:TYR:HA	2.00	0.42
1:E:116:MET:CE	1:E:193:VAL:HG11	2.49	0.42
1:E:437:PHE:HB3	1:E:440:GLU:HB2	2.00	0.42
1:E:11:ASN:H	1:E:204:ALA:HB2	1.83	0.42
1:A:273:CYS:SG	1:A:383:LYS:HA	2.60	0.42
1:C:437:PHE:HB3	1:C:440:GLU:HB2	2.01	0.42
1:C:489:THR:HG23	1:C:492:TYR:CB	2.49	0.42
1:D:57:LEU:HD12	1:D:57:LEU:H	1.83	0.42
1:F:11:ASN:H	1:F:204:ALA:HB2	1.84	0.42
1:D:350:GLN:HE21	1:D:350:GLN:HA	1.83	0.42
1:B:273:CYS:SG	1:B:383:LYS:HA	2.60	0.42
1:B:272:TYR:CE1	2:B:601:GTP:H5"	2.55	0.42
1:E:442:ARG:HG2	1:F:397:GLU:HB3	2.01	0.42
1:A:405:ARG:HE	1:A:405:ARG:HB2	1.56	0.42
1:D:273:CYS:SG	1:D:383:LYS:HA	2.59	0.42
1:F:437:PHE:HB3	1:F:440:GLU:HB2	2.02	0.42
1:F:117:HIS:O	1:F:118:ASP:HB2	2.19	0.41
1:F:24:THR:HB	1:F:27:GLU:H	1.85	0.41
1:C:190:ILE:HG21	1:C:243:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:HD13	1:D:112:MET:HB3	2.00	0.41
1:D:61:ALA:HB1	1:D:63:VAL:HG12	2.01	0.41
1:A:400:GLU:OE2	1:B:442:ARG:NH2	2.53	0.41
1:F:306:SER:O	1:F:310:LEU:HD12	2.20	0.41
1:C:24:THR:HB	1:C:27:GLU:H	1.84	0.41
1:E:163:ARG:HB2	1:E:167:GLU:OE1	2.20	0.41
1:A:39:ILE:HD13	1:A:112:MET:HB3	2.02	0.41
1:C:39:ILE:HD13	1:C:112:MET:HB3	2.01	0.41
1:C:215:PRO:HB3	1:C:217:TRP:CH2	2.55	0.41
1:C:39:ILE:O	1:C:45:ILE:HG12	2.20	0.41
1:D:23:LYS:HA	1:D:27:GLU:OE1	2.19	0.41
1:E:213:THR:HB	1:E:255:TYR:HA	2.02	0.41
1:A:496:GLU:HG2	1:A:499:ARG:HH21	1.85	0.41
1:B:213:THR:HB	1:B:255:TYR:HA	2.02	0.41
1:F:145:ALA:HB1	1:F:174:ARG:HG2	2.01	0.41
1:A:170:ASN:HA	1:A:173:ARG:HD2	2.03	0.41
1:C:169:LEU:HD23	1:C:173:ARG:NH1	2.36	0.41
1:B:190:ILE:HG13	1:B:209:ILE:HD12	2.03	0.41
1:A:397:GLU:OE1	1:B:442:ARG:HG2	2.21	0.41
1:D:217:TRP:HH2	1:D:240:GLU:HG2	1.86	0.41
1:F:215:PRO:HB3	1:F:217:TRP:CH2	2.55	0.41
1:A:439:ILE:HD13	1:C:127:PHE:HE2	1.86	0.40
1:D:502:ALA:HB1	1:E:406:VAL:HG23	2.03	0.40
1:E:194:HIS:HD2	4:E:728:HOH:O	2.04	0.40
1:E:39:ILE:HB	1:E:112:MET:HE2	2.03	0.40
1:E:479:ARG:HH11	1:E:479:ARG:CG	2.34	0.40
1:F:88:LEU:HD12	1:F:88:LEU:HA	1.96	0.40
1:C:94:LEU:HA	1:C:94:LEU:HD12	1.85	0.40
1:D:157:VAL:HG11	1:D:160:LEU:HD23	2.03	0.40
1:E:39:ILE:HD13	1:E:112:MET:HB3	2.03	0.40
1:A:190:ILE:HG13	1:A:209:ILE:HD12	2.03	0.40
1:E:306:SER:C	1:E:310:LEU:HD12	2.42	0.40
1:E:94:LEU:HD12	1:E:94:LEU:HA	1.86	0.40
1:C:145:ALA:HB1	1:C:174:ARG:HG2	2.03	0.40
1:E:145:ALA:HB1	1:E:174:ARG:HG2	2.03	0.40
1:E:215:PRO:HB3	1:E:217:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/505 (93%)	445 (95%)	19 (4%)	5 (1%)	14	48
1	B	459/505 (91%)	430 (94%)	20 (4%)	9 (2%)	7	34
1	C	464/505 (92%)	437 (94%)	20 (4%)	7 (2%)	10	41
1	D	460/505 (91%)	429 (93%)	24 (5%)	7 (2%)	10	41
1	E	468/505 (93%)	442 (94%)	19 (4%)	7 (2%)	10	41
1	F	461/505 (91%)	438 (95%)	18 (4%)	5 (1%)	14	48
All	All	2781/3030 (92%)	2621 (94%)	120 (4%)	40 (1%)	11	43

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	GLU
1	D	60	ASN
1	E	61	ALA
1	E	222	THR
1	E	371	ASP
1	F	167	GLU
1	A	164	ASP
1	B	54	VAL
1	C	328	THR
1	E	54	VAL
1	F	54	VAL
1	F	371	ASP
1	A	432	GLU
1	B	225	THR
1	B	328	THR
1	B	432	GLU
1	C	150	LEU
1	C	432	GLU
1	D	328	THR
1	D	432	GLU

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Mol	Chain	Res	Type
1	E	432	GLU
1	A	430	GLU
1	B	118	ASP
1	B	430	GLU
1	C	23	LYS
1	C	430	GLU
1	D	272	TYR
1	D	372	ALA
1	D	430	GLU
1	E	430	GLU
1	F	272	TYR
1	F	430	GLU
1	A	272	TYR
1	B	23	LYS
1	B	272	TYR
1	C	272	TYR
1	E	272	TYR
1	A	149	PRO
1	B	149	PRO
1	D	23	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	427/450 (95%)	386 (90%)	41 (10%)	8 29
1	B	421/450 (94%)	378 (90%)	43 (10%)	7 27
1	C	426/450 (95%)	389 (91%)	37 (9%)	10 34
1	D	421/450 (94%)	386 (92%)	35 (8%)	11 37
1	E	427/450 (95%)	391 (92%)	36 (8%)	11 37
1	F	422/450 (94%)	385 (91%)	37 (9%)	10 34
All	All	2544/2700 (94%)	2315 (91%)	229 (9%)	9 32

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	17	ARG
1	A	45	ILE
1	A	60	ASN
1	A	79	TYR
1	A	87	ARG
1	A	88	LEU
1	A	89	LYS
1	A	107	GLU
1	A	118	ASP
1	A	119	ILE
1	A	126	HIS
1	A	140	LEU
1	A	143	GLU
1	A	146	GLU
1	A	148	GLN
1	A	150	LEU
1	A	227	HIS
1	A	274	VAL
1	A	283	LYS
1	A	289	GLU
1	A	296	HIS
1	A	310	LEU
1	A	312	VAL
1	A	331	GLN
1	A	369	LEU
1	A	381	LEU
1	A	405	ARG
1	A	410	LEU
1	A	415	ARG
1	A	421	SER
1	A	430	GLU
1	A	435	LYS
1	A	449	THR
1	A	453	LEU
1	A	457	GLU
1	A	479	ARG
1	A	489	THR
1	A	490	ASP
1	A	491	LEU
1	A	503	VAL
1	B	17	ARG
1	B	45	ILE

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Mol	Chain	Res	Type
1	B	87	ARG
1	B	88	LEU
1	B	95	GLU
1	B	107	GLU
1	B	140	LEU
1	B	143	GLU
1	B	146	GLU
1	B	150	LEU
1	B	151	THR
1	B	221	GLU
1	B	224	GLU
1	B	227	HIS
1	B	239	GLU
1	B	256	SER
1	B	264	MET
1	B	274	VAL
1	B	283	LYS
1	B	284	ARG
1	B	289	GLU
1	B	296	HIS
1	B	310	LEU
1	B	312	VAL
1	B	354	ASP
1	B	356	LEU
1	B	365	ASN
1	B	369	LEU
1	B	370	GLU
1	B	381	LEU
1	B	410	LEU
1	B	415	ARG
1	B	421	SER
1	B	430	GLU
1	B	433	ARG
1	B	435	LYS
1	B	446	LYS
1	B	449	THR
1	B	453	LEU
1	B	479	ARG
1	B	489	THR
1	B	490	ASP
1	B	491	LEU
1	C	17	ARG

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Mol	Chain	Res	Type
1	C	45	ILE
1	C	78	ARG
1	C	87	ARG
1	C	88	LEU
1	C	89	LYS
1	C	107	GLU
1	C	140	LEU
1	C	143	GLU
1	C	190	ILE
1	C	191	ARG
1	C	224	GLU
1	C	227	HIS
1	C	264	MET
1	C	274	VAL
1	C	283	LYS
1	C	296	HIS
1	C	309	SER
1	C	310	LEU
1	C	312	VAL
1	C	314	ASN
1	C	350	GLN
1	C	369	LEU
1	C	381	LEU
1	C	405	ARG
1	C	410	LEU
1	C	415	ARG
1	C	421	SER
1	C	430	GLU
1	C	433	ARG
1	C	449	THR
1	C	453	LEU
1	C	479	ARG
1	C	489	THR
1	C	490	ASP
1	C	491	LEU
1	C	503	VAL
1	D	17	ARG
1	D	29	LEU
1	D	45	ILE
1	D	78	ARG
1	D	87	ARG
1	D	88	LEU

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Mol	Chain	Res	Type
1	D	94	LEU
1	D	107	GLU
1	D	140	LEU
1	D	143	GLU
1	D	221	GLU
1	D	227	HIS
1	D	264	MET
1	D	274	VAL
1	D	283	LYS
1	D	284	ARG
1	D	296	HIS
1	D	310	LEU
1	D	312	VAL
1	D	350	GLN
1	D	369	LEU
1	D	371	ASP
1	D	381	LEU
1	D	410	LEU
1	D	421	SER
1	D	430	GLU
1	D	433	ARG
1	D	449	THR
1	D	453	LEU
1	D	479	ARG
1	D	489	THR
1	D	490	ASP
1	D	491	LEU
1	D	503	VAL
1	D	504	GLU
1	E	17	ARG
1	E	45	ILE
1	E	78	ARG
1	E	87	ARG
1	E	88	LEU
1	E	90	GLU
1	E	107	GLU
1	E	140	LEU
1	E	143	GLU
1	E	224	GLU
1	E	227	HIS
1	E	264	MET
1	E	274	VAL

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Mol	Chain	Res	Type
1	E	283	LYS
1	E	296	HIS
1	E	310	LEU
1	E	312	VAL
1	E	350	GLN
1	E	369	LEU
1	E	370	GLU
1	E	371	ASP
1	E	381	LEU
1	E	410	LEU
1	E	415	ARG
1	E	421	SER
1	E	430	GLU
1	E	433	ARG
1	E	435	LYS
1	E	449	THR
1	E	453	LEU
1	E	457	GLU
1	E	479	ARG
1	E	489	THR
1	E	490	ASP
1	E	491	LEU
1	E	503	VAL
1	F	45	ILE
1	F	87	ARG
1	F	88	LEU
1	F	90	GLU
1	F	107	GLU
1	F	140	LEU
1	F	143	GLU
1	F	146	GLU
1	F	166	GLU
1	F	221	GLU
1	F	224	GLU
1	F	227	HIS
1	F	240	GLU
1	F	264	MET
1	F	273	CYS
1	F	274	VAL
1	F	283	LYS
1	F	296	HIS
1	F	310	LEU

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Mol	Chain	Res	Type
1	F	312	VAL
1	F	320	ARG
1	F	350	GLN
1	F	369	LEU
1	F	381	LEU
1	F	405	ARG
1	F	410	LEU
1	F	415	ARG
1	F	421	SER
1	F	430	GLU
1	F	431	LYS
1	F	432	GLU
1	F	449	THR
1	F	453	LEU
1	F	479	ARG
1	F	489	THR
1	F	490	ASP
1	F	491	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	126	HIS
1	A	226	HIS
1	B	200	ASN
1	B	226	HIS
1	B	339	ASN
1	B	350	GLN
1	C	226	HIS
1	C	294	HIS
1	C	331	GLN
1	C	350	GLN
1	C	366	HIS
1	C	389	HIS
1	D	226	HIS
1	D	227	HIS
1	E	226	HIS
1	F	226	HIS
1	F	227	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GTP	F	601	-	26,34,34	1.06	2 (7%)	33,54,54	2.01	4 (12%)
2	GTP	D	601	-	26,34,34	1.09	2 (7%)	33,54,54	2.04	4 (12%)
2	GTP	C	601	-	26,34,34	1.36	2 (7%)	33,54,54	2.11	4 (12%)
2	GTP	A	601	-	26,34,34	1.30	2 (7%)	33,54,54	2.23	11 (33%)
2	GTP	E	601	-	26,34,34	1.16	2 (7%)	33,54,54	2.06	4 (12%)
2	GTP	B	601	-	26,34,34	1.13	2 (7%)	33,54,54	2.03	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	F	601	-	-	4/18/38/38	0/3/3/3
2	GTP	D	601	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	C	601	-	-	2/18/38/38	0/3/3/3
2	GTP	A	601	-	-	3/18/38/38	0/3/3/3
2	GTP	E	601	-	-	5/18/38/38	0/3/3/3
2	GTP	B	601	-	-	1/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	GTP	C6-C5	4.79	1.49	1.41
2	A	601	GTP	C6-C5	4.05	1.48	1.41
2	E	601	GTP	C6-N1	3.69	1.39	1.33
2	C	601	GTP	C6-N1	3.65	1.39	1.33
2	B	601	GTP	C6-N1	3.64	1.39	1.33
2	F	601	GTP	C6-N1	3.50	1.39	1.33
2	E	601	GTP	C6-C5	3.45	1.47	1.41
2	D	601	GTP	C6-N1	3.39	1.38	1.33
2	B	601	GTP	C6-C5	3.31	1.47	1.41
2	D	601	GTP	C6-C5	3.30	1.47	1.41
2	F	601	GTP	C6-C5	2.69	1.46	1.41
2	A	601	GTP	C2'-C1'	-2.06	1.50	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	GTP	C5-C6-N1	-8.43	111.91	123.43
2	C	601	GTP	C5-C6-N1	-8.42	111.92	123.43
2	D	601	GTP	C5-C6-N1	-8.26	112.13	123.43
2	B	601	GTP	C5-C6-N1	-8.19	112.23	123.43
2	F	601	GTP	C5-C6-N1	-8.18	112.24	123.43
2	E	601	GTP	C6-N1-C2	5.95	125.39	115.93
2	B	601	GTP	C6-N1-C2	5.94	125.37	115.93
2	D	601	GTP	C6-N1-C2	5.94	125.37	115.93
2	C	601	GTP	C6-N1-C2	5.93	125.36	115.93
2	F	601	GTP	C6-N1-C2	5.82	125.17	115.93
2	A	601	GTP	C2-N3-C4	4.84	120.88	115.36
2	A	601	GTP	PB-O3B-PG	-4.54	117.24	132.83
2	A	601	GTP	PA-O3A-PB	-4.39	117.77	132.83
2	A	601	GTP	C6-C5-C4	-4.31	116.68	120.80
2	A	601	GTP	C5-C6-N1	-4.03	117.91	123.43
2	C	601	GTP	C6-C5-C4	-3.64	117.32	120.80
2	A	601	GTP	C6-N1-C2	3.56	121.58	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	GTP	C4-C5-N7	-3.40	105.86	109.40
2	B	601	GTP	C6-C5-C4	-3.33	117.62	120.80
2	D	601	GTP	C6-C5-C4	-3.24	117.70	120.80
2	F	601	GTP	C6-C5-C4	-3.19	117.75	120.80
2	E	601	GTP	C6-C5-C4	-3.08	117.85	120.80
2	A	601	GTP	C3'-C2'-C1'	2.91	105.36	100.98
2	B	601	GTP	N3-C2-N1	-2.86	123.41	127.22
2	F	601	GTP	N3-C2-N1	-2.81	123.47	127.22
2	C	601	GTP	N3-C2-N1	-2.80	123.49	127.22
2	D	601	GTP	N3-C2-N1	-2.72	123.59	127.22
2	E	601	GTP	N3-C2-N1	-2.68	123.65	127.22
2	A	601	GTP	N3-C2-N1	-2.41	124.00	127.22
2	A	601	GTP	C1'-N9-C4	-2.36	122.50	126.64
2	A	601	GTP	O3G-PG-O2G	2.24	116.21	107.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	GTP	C5'-O5'-PA-O3A
2	D	601	GTP	PB-O3B-PG-O2G
2	D	601	GTP	C5'-O5'-PA-O1A
2	C	601	GTP	PB-O3B-PG-O3G
2	E	601	GTP	C5'-O5'-PA-O3A
2	E	601	GTP	C5'-O5'-PA-O2A
2	B	601	GTP	PB-O3B-PG-O2G
2	D	601	GTP	O4'-C4'-C5'-O5'
2	D	601	GTP	C3'-C4'-C5'-O5'
2	C	601	GTP	O4'-C4'-C5'-O5'
2	D	601	GTP	C5'-O5'-PA-O3A
2	F	601	GTP	C5'-O5'-PA-O1A
2	F	601	GTP	C5'-O5'-PA-O2A
2	F	601	GTP	PA-O3A-PB-O2B
2	E	601	GTP	PB-O3A-PA-O2A
2	D	601	GTP	PB-O3B-PG-O3G
2	A	601	GTP	O4'-C4'-C5'-O5'
2	A	601	GTP	PB-O3A-PA-O1A
2	A	601	GTP	PB-O3A-PA-O2A
2	E	601	GTP	PB-O3A-PA-O1A
2	E	601	GTP	C5'-O5'-PA-O1A
2	D	601	GTP	PB-O3B-PG-O1G

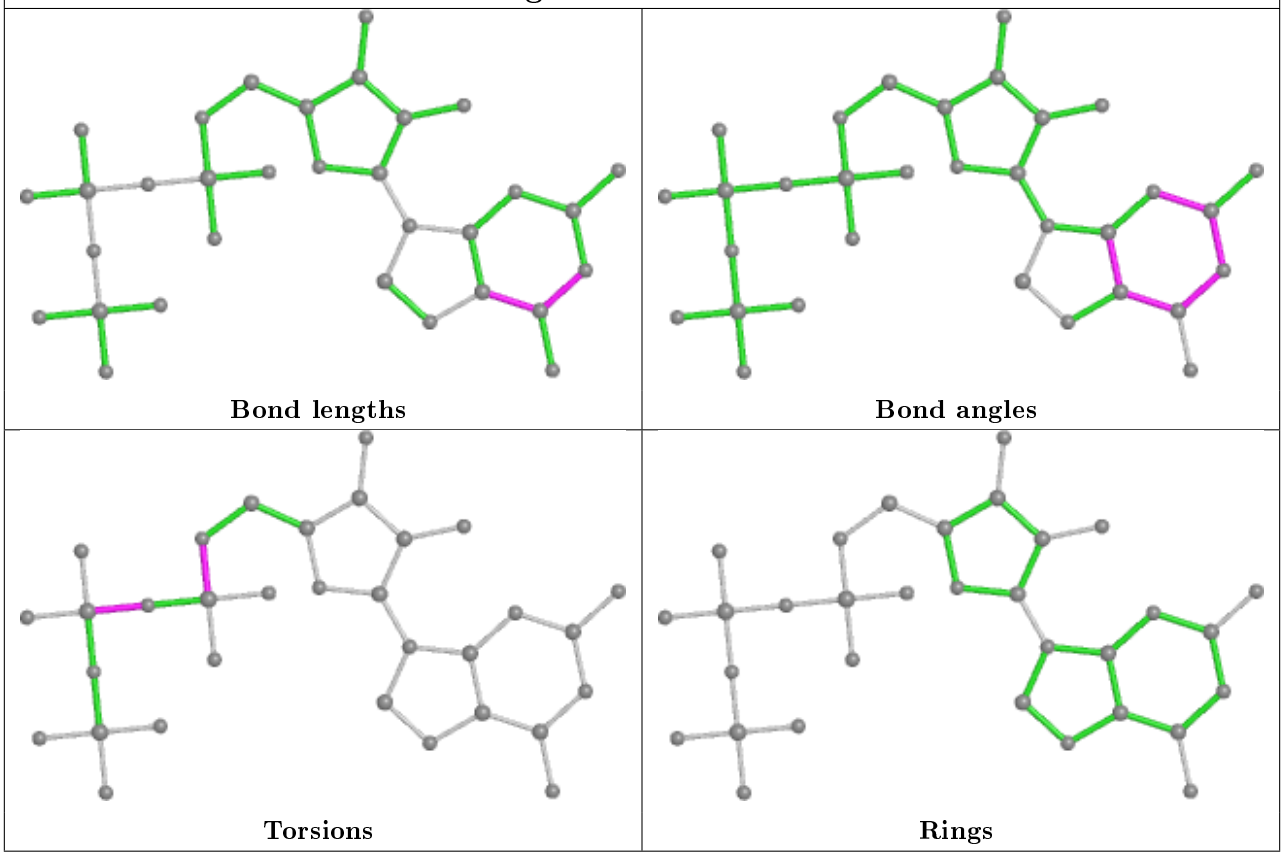
There are no ring outliers.

3 monomers are involved in 7 short contacts:

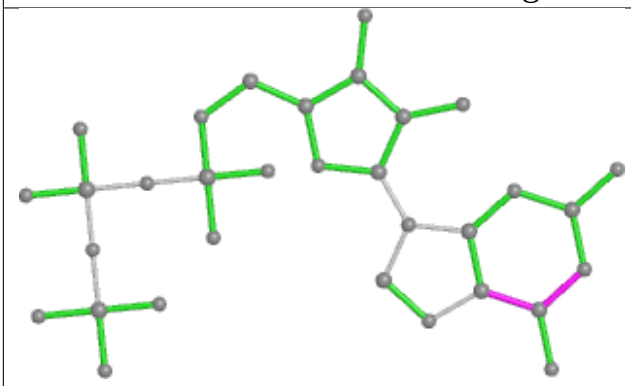
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	GTP	1	0
2	A	601	GTP	4	0
2	B	601	GTP	2	0

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

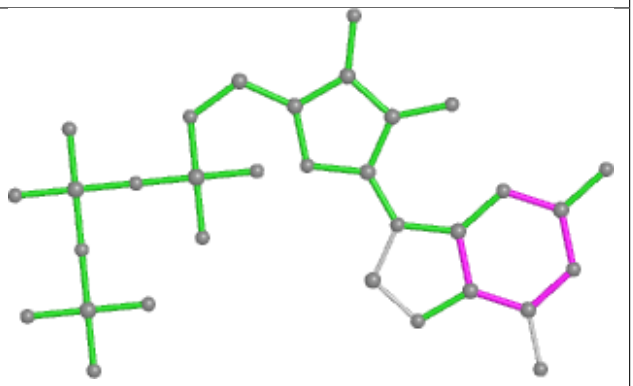
Ligand GTP F 601



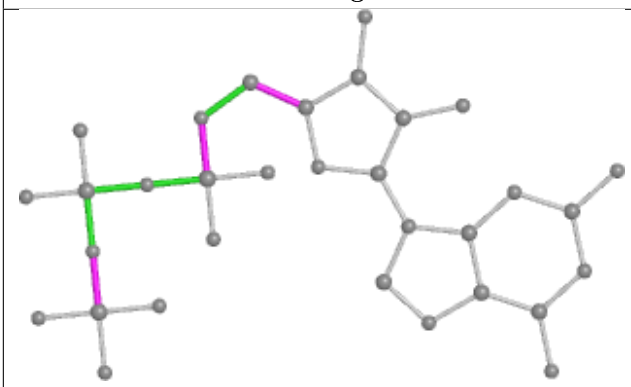
Ligand GTP D 601



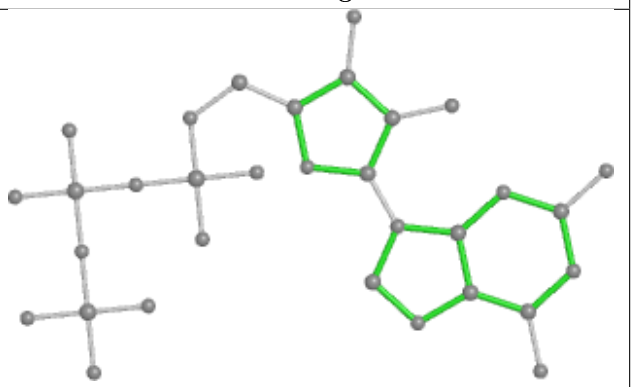
Bond lengths



Bond angles

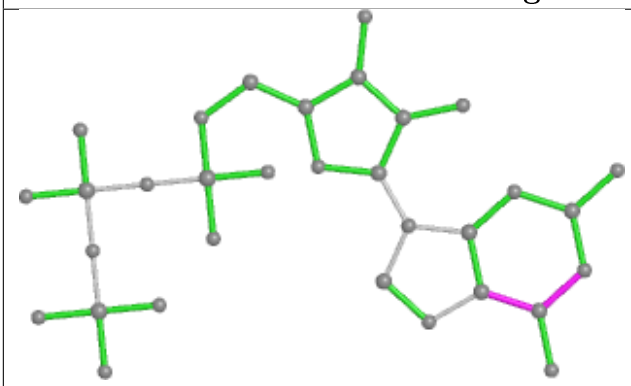


Torsions

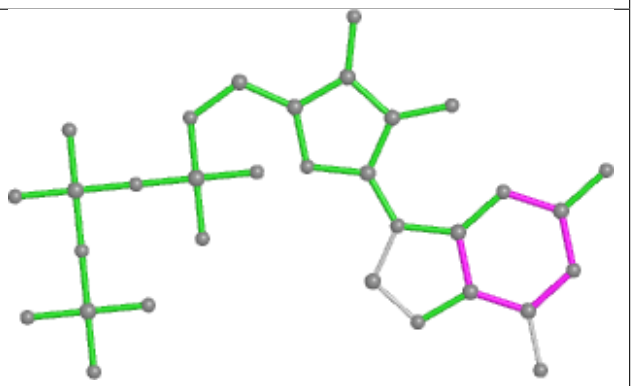


Rings

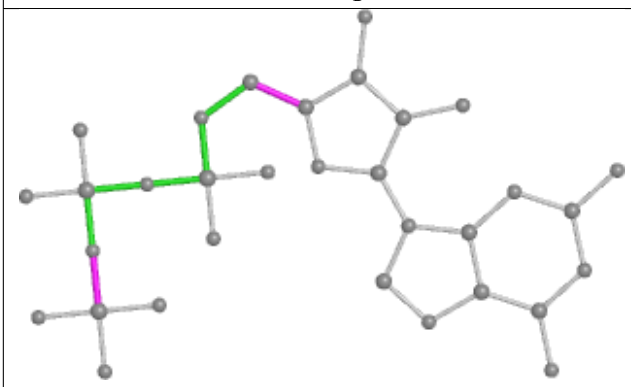
Ligand GTP C 601



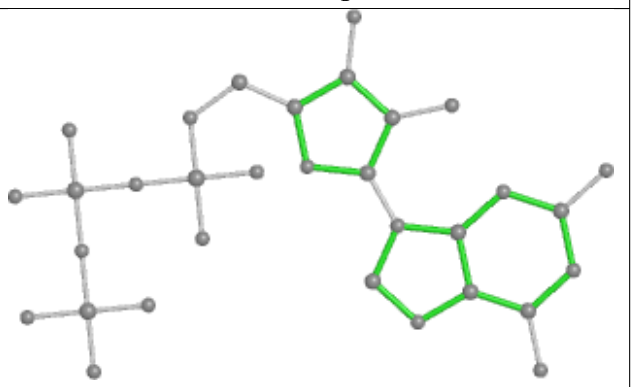
Bond lengths



Bond angles

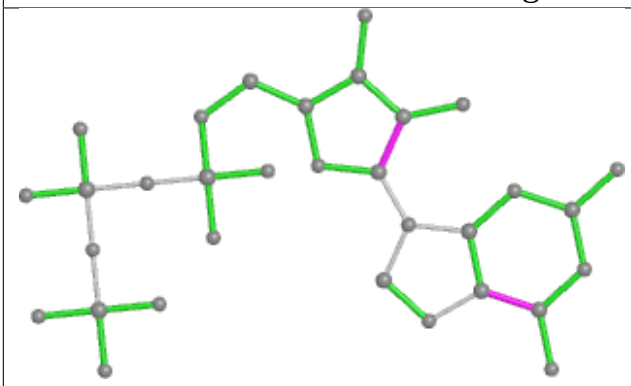


Torsions

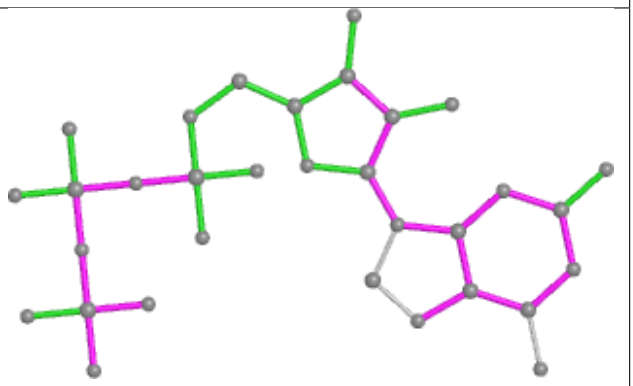


Rings

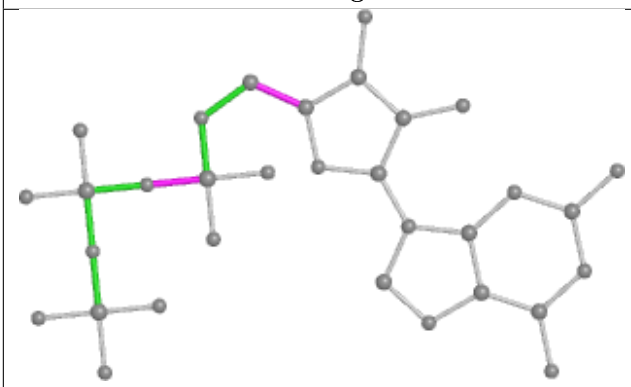
Ligand GTP A 601



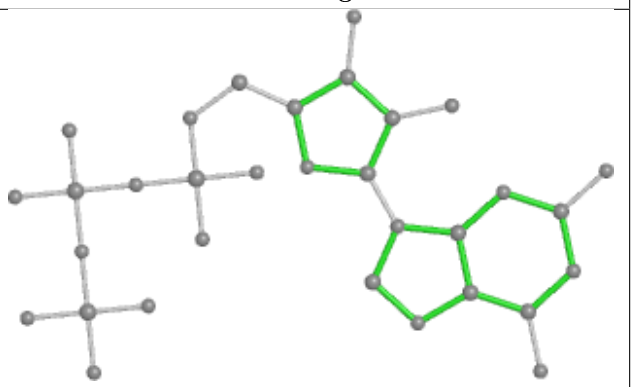
Bond lengths



Bond angles

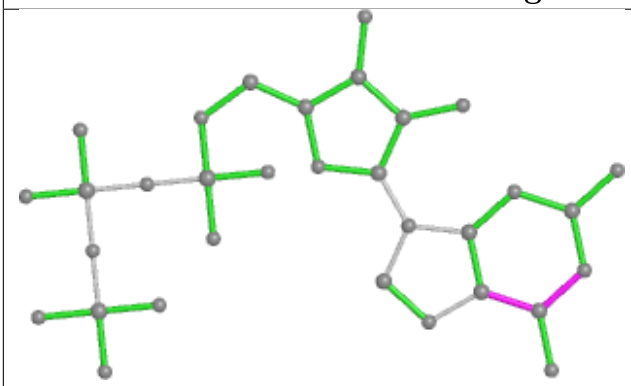


Torsions

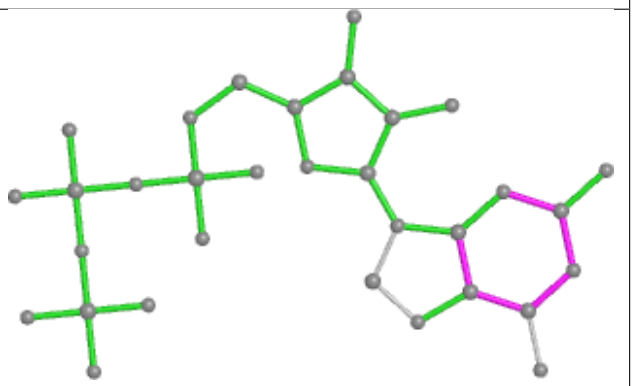


Rings

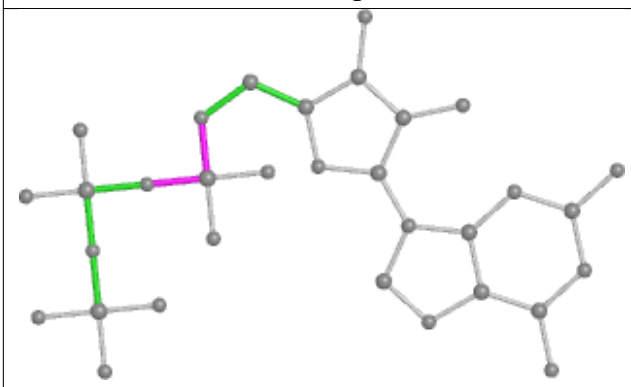
Ligand GTP E 601



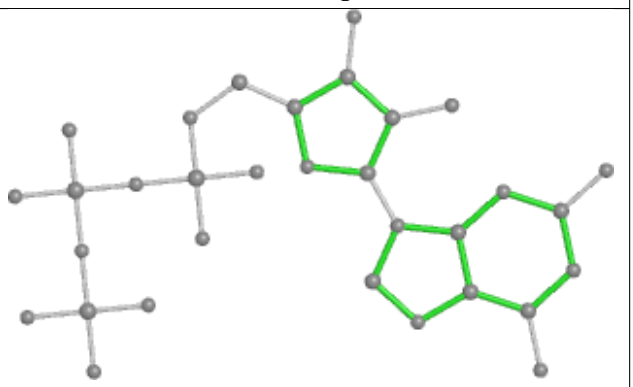
Bond lengths



Bond angles

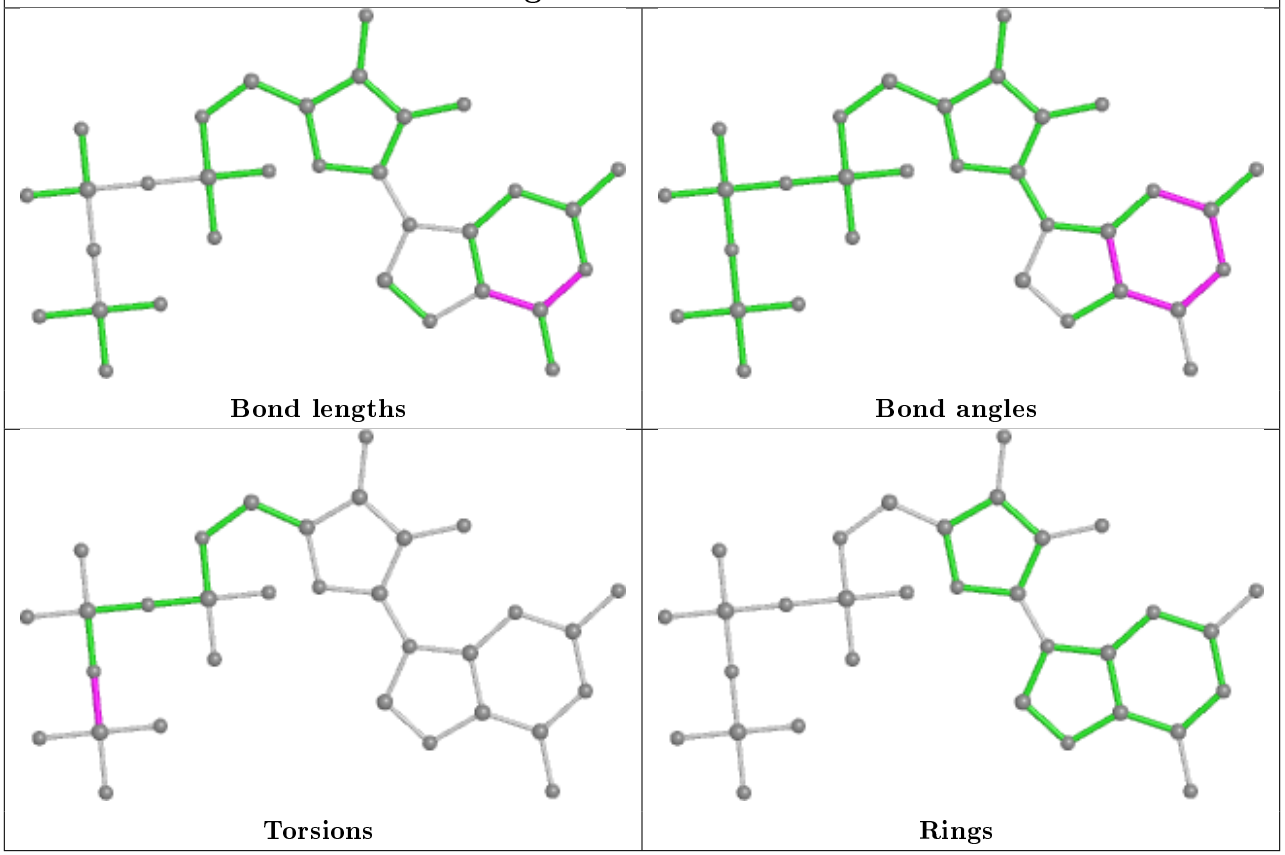


Torsions



Rings

Ligand GTP B 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	477/505 (94%)	0.19	17 (3%) 42 26	47, 99, 160, 189	1 (0%)
1	B	471/505 (93%)	0.55	49 (10%) 6 3	56, 145, 198, 211	2 (0%)
1	C	478/505 (94%)	0.18	19 (3%) 38 23	51, 102, 161, 186	2 (0%)
1	D	472/505 (93%)	0.53	43 (9%) 9 5	58, 146, 185, 200	0
1	E	478/505 (94%)	0.16	12 (2%) 57 42	57, 108, 162, 190	0
1	F	475/505 (94%)	0.20	15 (3%) 47 30	52, 111, 160, 194	2 (0%)
All	All	2851/3030 (94%)	0.30	155 (5%) 25 13	47, 119, 177, 211	7 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	TRP	5.4
1	B	20	GLN	4.8
1	D	311	VAL	4.7
1	D	155	CYS	4.3
1	B	21	GLY	4.2
1	B	19	PRO	4.0
1	B	117	HIS	3.9
1	A	117	HIS	3.8
1	D	372	ALA	3.7
1	B	504	GLU	3.7
1	D	431	LYS	3.7
1	D	312	VAL	3.7
1	A	165	GLY	3.7
1	A	295	LEU	3.6
1	D	186	ASN	3.6
1	D	427	GLU	3.5
1	D	295	LEU	3.5
1	A	292	TYR	3.4
1	B	22	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	329	GLU	3.3
1	E	295	LEU	3.3
1	C	504	GLU	3.2
1	C	502	ALA	3.2
1	A	126	HIS	3.2
1	B	295	LEU	3.1
1	B	255	TYR	3.1
1	D	156	SER	3.0
1	F	295	LEU	3.0
1	C	434	VAL	3.0
1	B	382	TYR	3.0
1	B	88	LEU	2.9
1	B	126	HIS	2.9
1	F	299	TRP	2.9
1	B	186	ASN	2.9
1	C	118	ASP	2.9
1	B	369	LEU	2.9
1	B	226	HIS	2.8
1	C	299	TRP	2.8
1	D	471	LEU	2.8
1	B	286	PHE	2.8
1	D	4	ILE	2.8
1	D	253	ALA	2.8
1	E	502	ALA	2.8
1	B	222	THR	2.8
1	C	160	LEU	2.8
1	B	312	VAL	2.8
1	B	431	LYS	2.8
1	C	375	CYS	2.8
1	F	307	LEU	2.7
1	F	160	LEU	2.7
1	C	295	LEU	2.7
1	D	428	LEU	2.7
1	B	468	GLU	2.7
1	B	23	LYS	2.7
1	E	117	HIS	2.7
1	B	152	ASP	2.7
1	B	148	GLN	2.7
1	A	151	THR	2.7
1	D	160	LEU	2.7
1	C	308	PHE	2.7
1	D	468	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	121	ASN	2.7
1	F	172	LEU	2.6
1	F	468	GLU	2.6
1	E	160	LEU	2.6
1	F	288	VAL	2.6
1	E	153	ASP	2.6
1	D	310	LEU	2.6
1	F	291	LEU	2.6
1	A	118	ASP	2.6
1	A	385	VAL	2.6
1	A	504	GLU	2.6
1	D	271	SER	2.6
1	D	222	THR	2.5
1	D	462	LEU	2.5
1	F	162	LEU	2.5
1	E	308	PHE	2.5
1	B	90	GLU	2.5
1	B	162	LEU	2.5
1	D	144	ASP	2.5
1	C	163	ARG	2.5
1	B	259	PRO	2.5
1	D	226	HIS	2.5
1	A	186	ASN	2.5
1	B	368(A)	LEU	2.5
1	B	332	PHE	2.5
1	C	298	ALA	2.5
1	B	6	PHE	2.4
1	B	147	SER	2.4
1	D	223	PRO	2.4
1	C	126	HIS	2.4
1	D	221	GLU	2.4
1	D	286	PHE	2.4
1	D	307	LEU	2.4
1	D	459	VAL	2.4
1	B	145	ALA	2.4
1	A	378	LEU	2.4
1	B	114	CYS	2.4
1	B	28	ILE	2.4
1	B	352	PHE	2.4
1	F	502	ALA	2.4
1	C	121	ASN	2.3
1	D	27	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	117	HIS	2.3
1	E	319	SER	2.3
1	C	432	GLU	2.3
1	D	157	VAL	2.3
1	D	8	LYS	2.3
1	D	88	LEU	2.3
1	D	371	ASP	2.3
1	F	312	VAL	2.3
1	D	146	GLU	2.3
1	B	92	LYS	2.3
1	D	117	HIS	2.3
1	C	312	VAL	2.3
1	A	316	TRP	2.2
1	D	472	TRP	2.2
1	E	307	LEU	2.2
1	A	152	ASP	2.2
1	A	164	ASP	2.2
1	F	375	CYS	2.2
1	D	340	THR	2.2
1	D	360	PHE	2.2
1	B	434	VAL	2.2
1	D	153	ASP	2.2
1	C	381	LEU	2.2
1	D	161	ARG	2.2
1	B	366	HIS	2.2
1	C	114	CYS	2.2
1	E	332	PHE	2.2
1	B	385	VAL	2.2
1	D	252	LEU	2.2
1	B	381	LEU	2.1
1	E	312	VAL	2.1
1	B	333	PHE	2.1
1	F	171	GLU	2.1
1	B	288	VAL	2.1
1	B	149	PRO	2.1
1	A	185	GLY	2.1
1	B	150	LEU	2.1
1	B	339	ASN	2.1
1	B	184	GLU	2.1
1	B	432	GLU	2.1
1	A	312	VAL	2.1
1	D	75	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	2.0
1	E	434	VAL	2.0
1	F	374	GLU	2.0
1	B	185	GLY	2.0
1	E	186	ASN	2.0
1	D	390	VAL	2.0
1	B	229	LEU	2.0
1	C	162	LEU	2.0
1	D	162	LEU	2.0
1	D	352	PHE	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 carbohydrates in this entry.

6.4 Ligands (i)

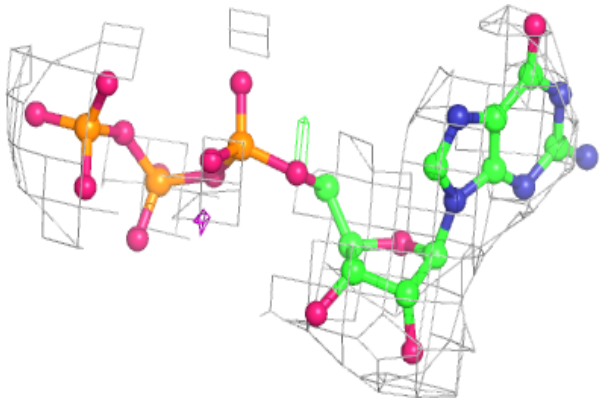
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

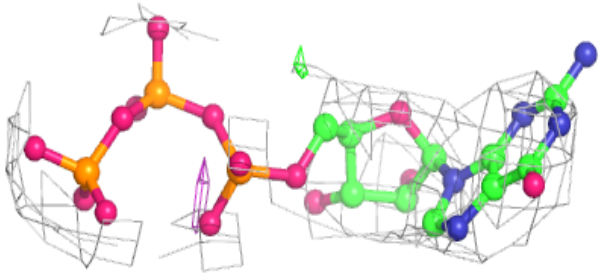
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GTP	D	601	32/32	0.71	0.37	153,164,208,208	0
2	GTP	B	601	32/32	0.71	0.41	174,179,230,231	0
2	GTP	F	601	32/32	0.77	0.33	111,127,169,170	0
2	GTP	C	601	32/32	0.78	0.40	95,113,159,162	0
3	MN	E	602	1/1	0.78	0.38	212,212,212,212	0
3	MN	A	602	1/1	0.81	0.42	170,170,170,170	0
2	GTP	E	601	32/32	0.82	0.33	108,122,166,168	32
3	MN	B	602	1/1	0.82	0.20	174,174,174,174	0
3	MN	C	602	1/1	0.85	0.71	189,189,189,189	0
2	GTP	A	601	32/32	0.85	0.29	106,131,164,165	0
3	MN	D	602	1/1	0.90	0.32	179,179,179,179	0
3	MN	F	602	1/1	0.95	0.34	167,167,167,167	0

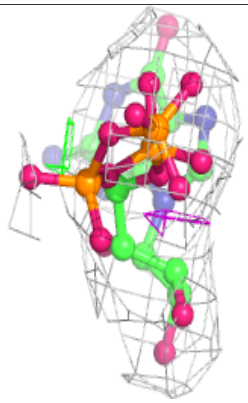
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP D 601:

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

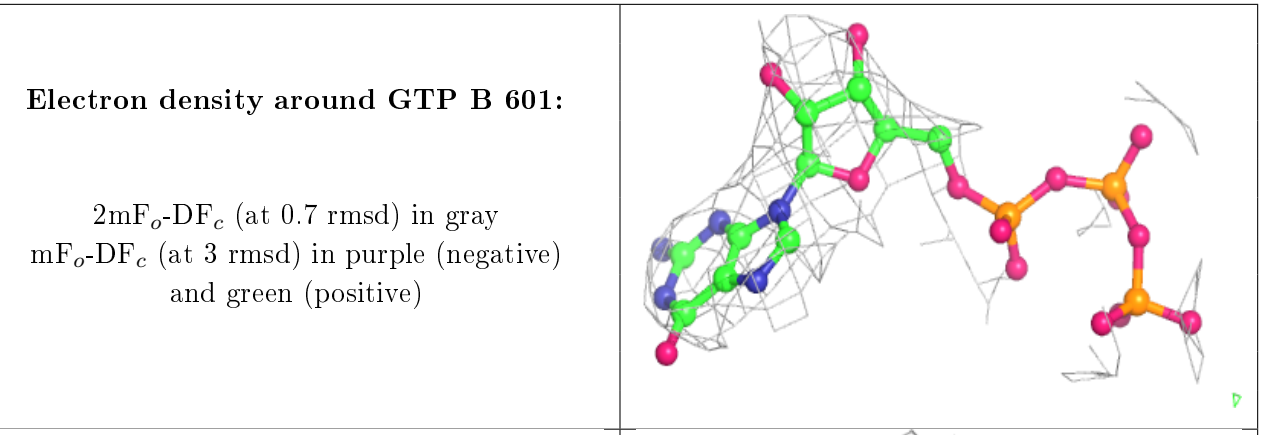


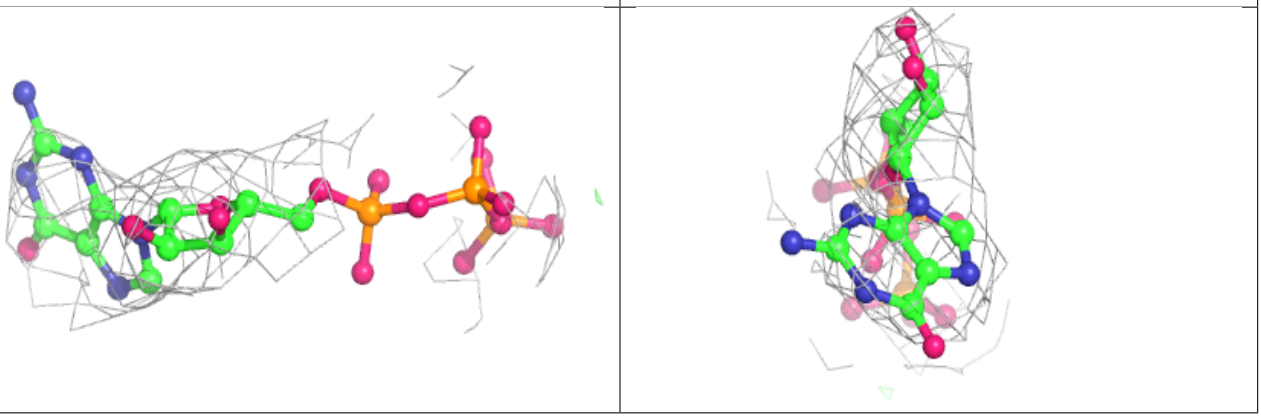




Electron density around GTP B 601:

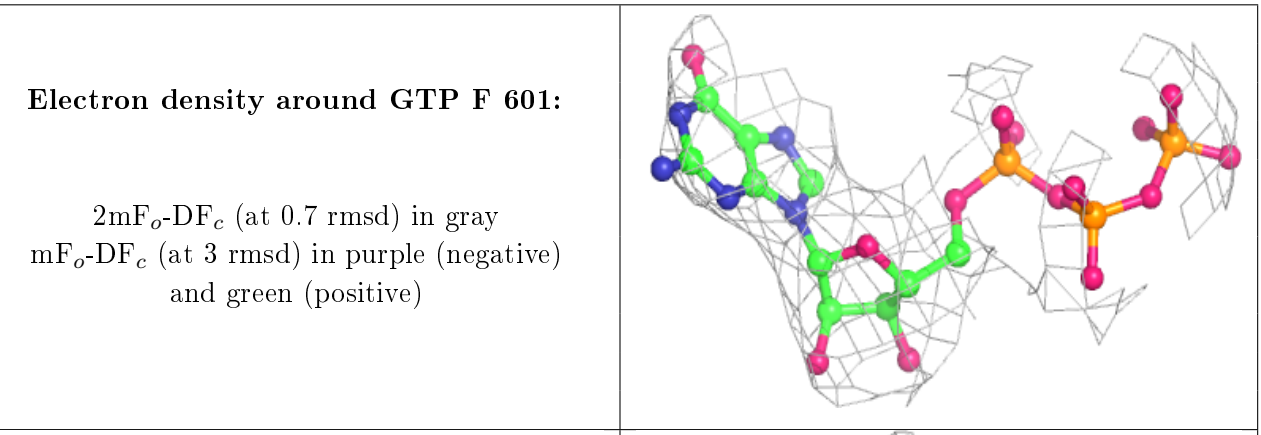
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

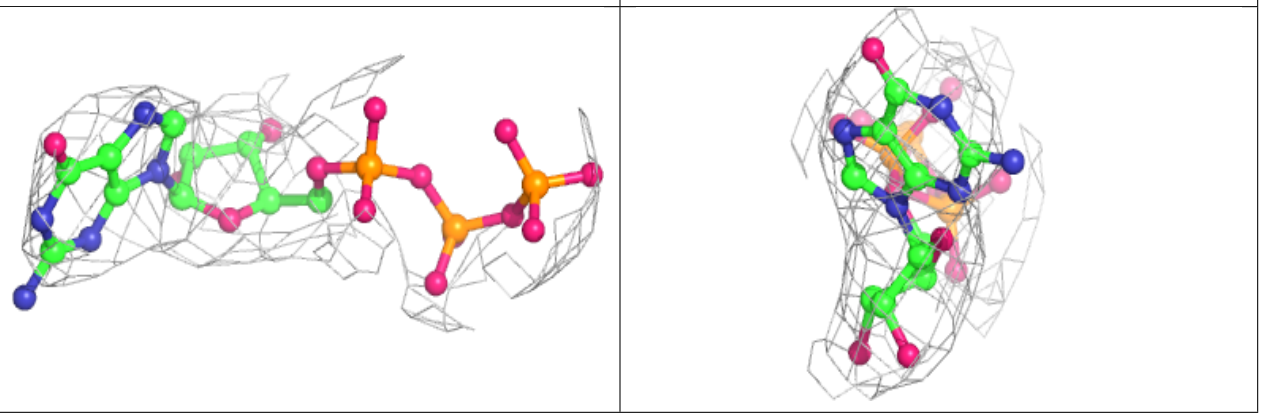




Electron density around GTP F 601:

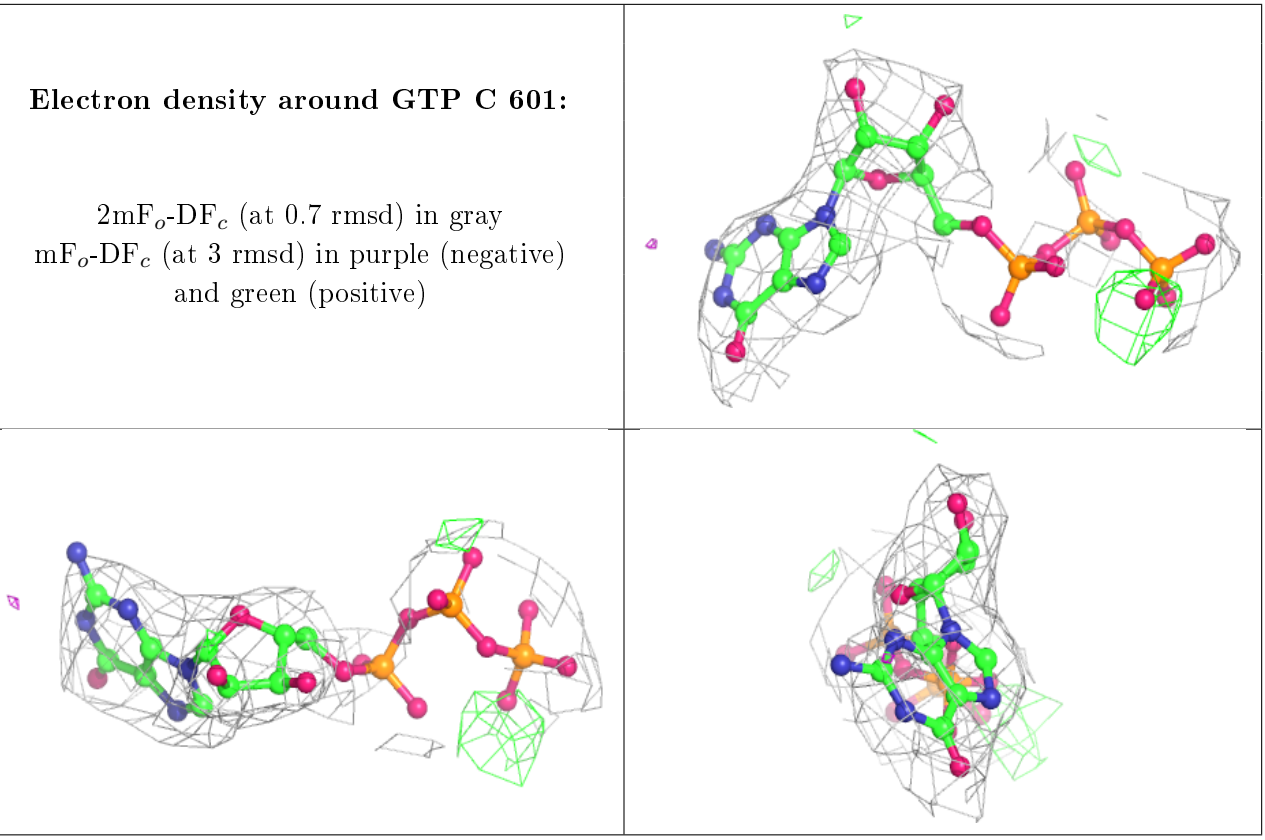
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





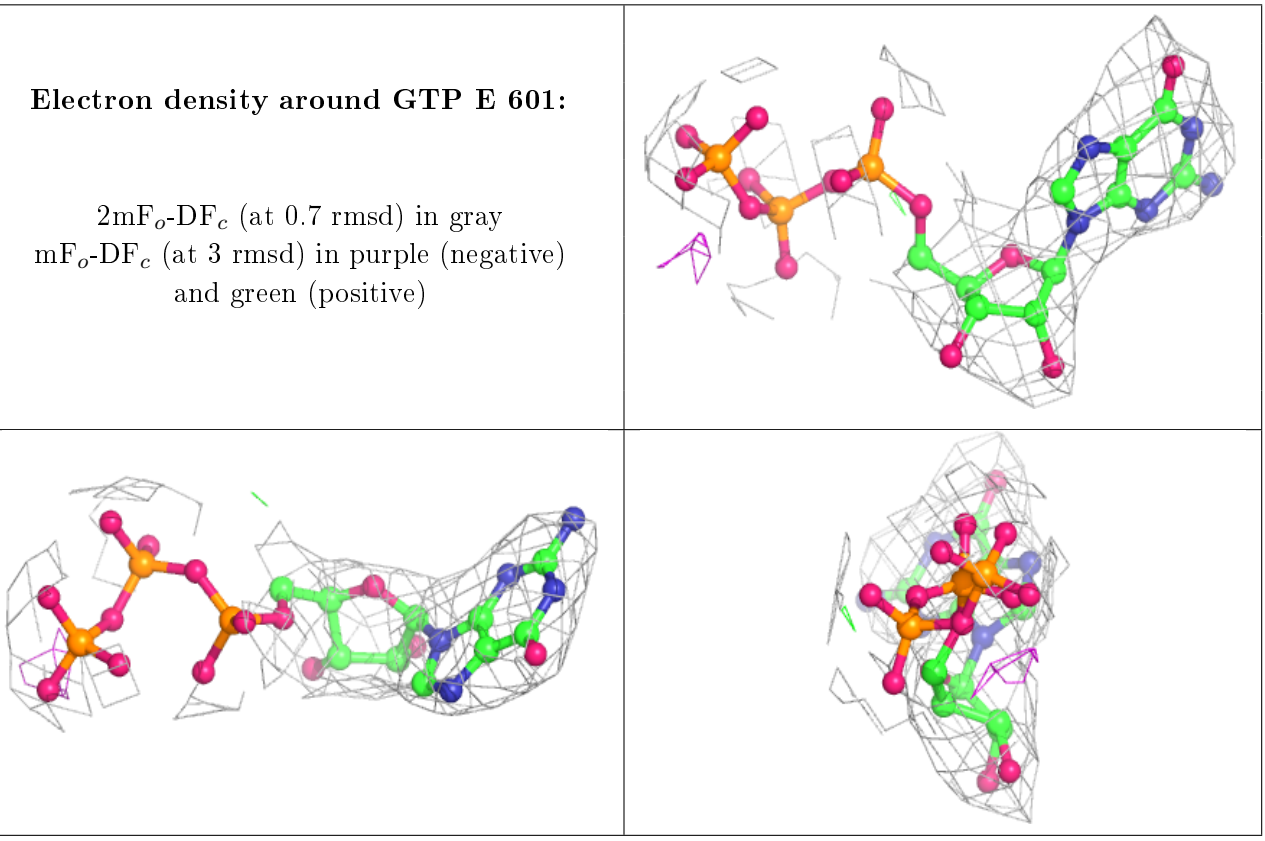
Electron density around GTP C 601:

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



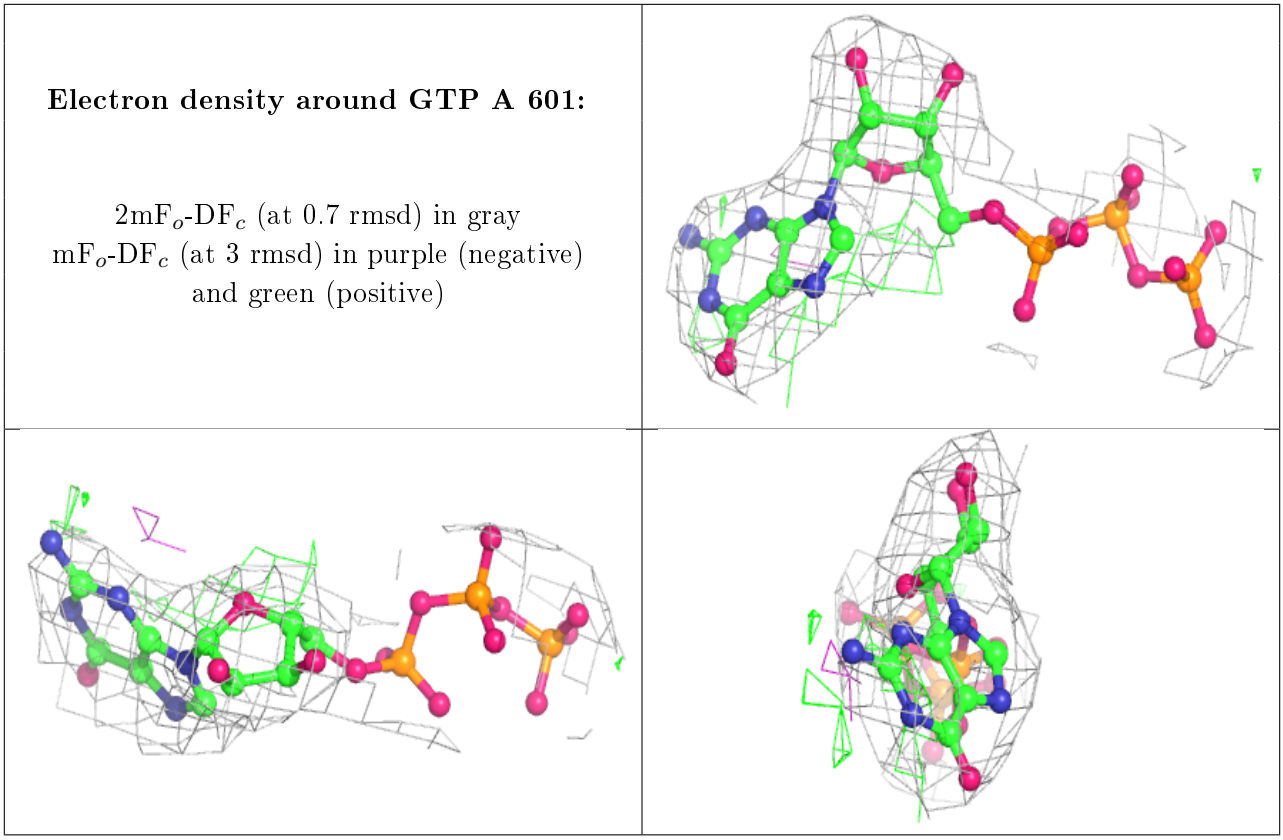
Electron density around GTP E 601:

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



Electron density around GTP A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.