



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:02 PM UTC

PDB ID : 9MG6 / pdb_00009mg6
Title : Structure of *Saccharomyces cerevisiae* mRNA cap (guanine-N7) methyltransferase variant, Abd1-K163R-K311R-F387Y-Y416F, in complex with sinefungin and GTP
Authors : Nilson, D.J.; Ghosh, A.
Deposited on : 2024-12-10
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

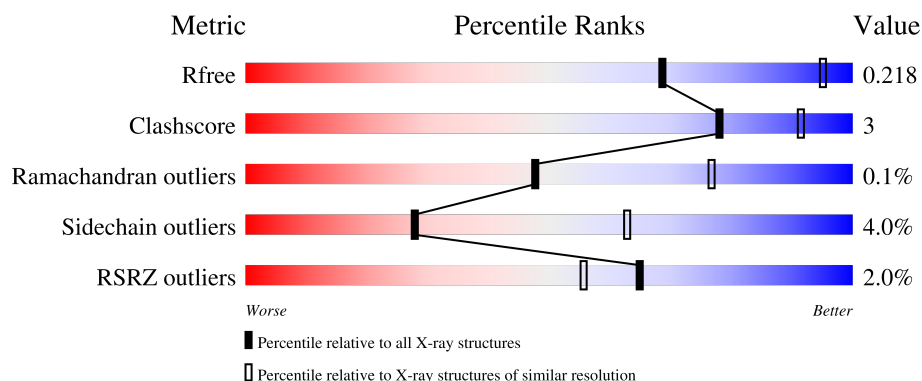
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	296	4% 91% 8%
1	B	296	% 90% 9%
1	C	296	% 91% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7661 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.

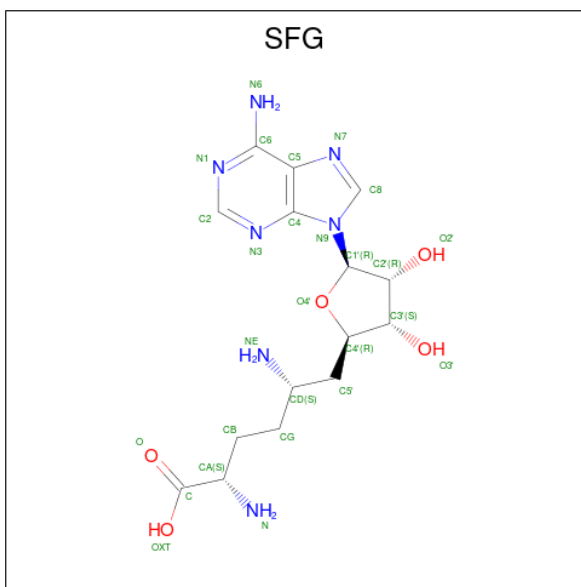
- Molecule 1 is a protein called mRNA cap guanine-N7 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2378	1539	388	440	11			
1	B	295	Total	C	N	O	S	0	0	0
			2391	1544	392	444	11			
1	C	295	Total	C	N	O	S	0	0	0
			2394	1547	395	441	11			

There are 12 discrepancies between the modelled and reference sequences:

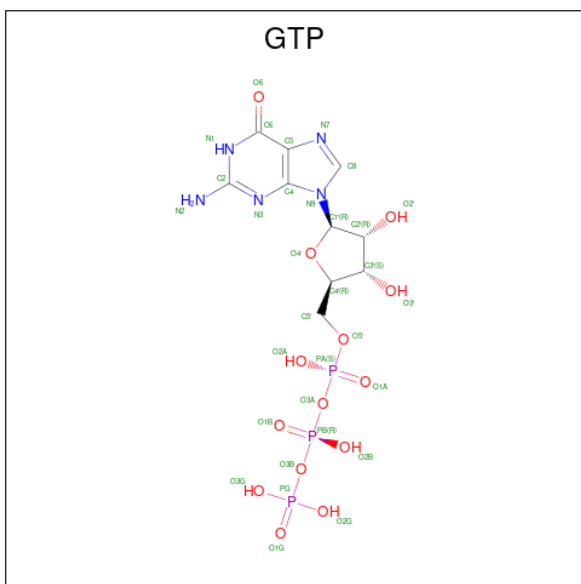
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	ARG	LYS	engineered mutation	UNP A6ZLH5
A	311	ARG	LYS	engineered mutation	UNP A6ZLH5
A	387	TYR	PHE	engineered mutation	UNP A6ZLH5
A	416	PHE	TYR	engineered mutation	UNP A6ZLH5
B	163	ARG	LYS	engineered mutation	UNP A6ZLH5
B	311	ARG	LYS	engineered mutation	UNP A6ZLH5
B	387	TYR	PHE	engineered mutation	UNP A6ZLH5
B	416	PHE	TYR	engineered mutation	UNP A6ZLH5
C	163	ARG	LYS	engineered mutation	UNP A6ZLH5
C	311	ARG	LYS	engineered mutation	UNP A6ZLH5
C	387	TYR	PHE	engineered mutation	UNP A6ZLH5
C	416	PHE	TYR	engineered mutation	UNP A6ZLH5

- Molecule 2 is SINEFUNGIN (CCD ID: SFG) (formula: $C_{15}H_{23}N_7O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		
2	B	1	Total	C	N	O	0	0
			27	15	7	5		
2	C	1	Total	C	N	O	0	0
			27	15	7	5		

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



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

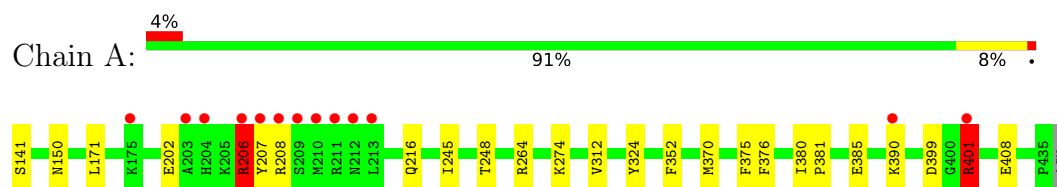
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total 78	O 78	0	0
6	B	81	Total 81	O 81	0	0
6	C	81	Total 81	O 81	0	0

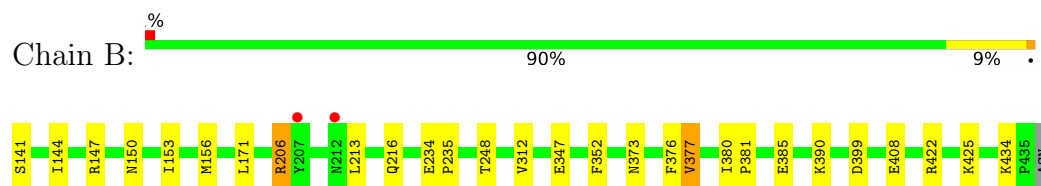
3 Residue-property plots [i](#)

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.

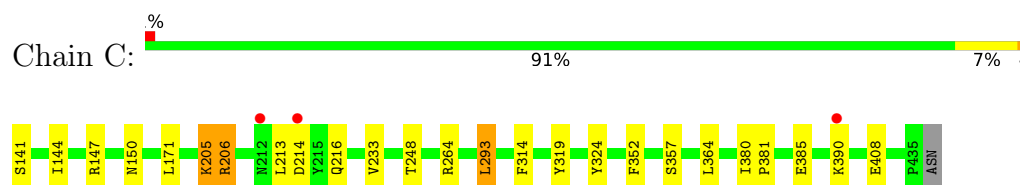
- Molecule 1: mRNA cap guanine-N7 methyltransferase



- Molecule 1: mRNA cap guanine-N7 methyltransferase



- Molecule 1: mRNA cap guanine-N7 methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.78Å 201.17Å 160.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.98 – 2.80 17.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (17.98-2.80) 99.4 (17.98-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.74Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.178 , 0.215 0.185 , 0.218	Depositor DCC
R_{free} test set	2445 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.068 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.084 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7661	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SFG, SO4, GTP, EDO

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	0/2442	0.98	4/3301 (0.1%)
1	B	0.55	0/2455	1.00	2/3317 (0.1%)
1	C	0.56	0/2458	0.99	5/3319 (0.2%)
All	All	0.55	0/7355	0.99	11/9937 (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	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	352	PHE	CA-CB-CG	-6.12	107.68	113.80
1	B	352	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	352	PHE	CA-CB-CG	-5.97	107.83	113.80
1	C	205	LYS	CB-CA-C	-5.96	101.53	110.88
1	C	214	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	324	TYR	N-CA-CB	-5.39	103.99	112.13
1	A	207	TYR	N-CA-C	-5.39	105.48	111.36
1	A	324	TYR	N-CA-CB	-5.12	104.41	112.13
1	C	314	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	399	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	399	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ARG	Sidechain
1	A	264	ARG	Sidechain
1	A	401	ARG	Sidechain
1	C	264	ARG	Sidechain

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	2378	0	2289	10	0
1	B	2391	0	2309	16	0
1	C	2394	0	2327	9	0
2	A	27	0	22	1	0
2	B	27	0	22	1	0
2	C	27	0	22	1	0
3	A	32	0	12	3	0
3	B	32	0	12	5	0
3	C	32	0	12	4	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	C	4	0	6	0	0
5	A	20	0	0	0	0
5	B	20	0	0	0	0
5	C	25	0	0	0	0
6	A	78	0	0	2	0
6	B	81	0	0	3	0
6	C	81	0	0	2	0
All	All	7661	0	7051	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (41) 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:B:153:ILE:HA	1:B:156:MET:HE2	1.73	0.70
2:A:501:SFG:NE	3:A:502:GTP:N7	2.41	0.69
2:C:501:SFG:NE	3:C:502:GTP:N7	2.44	0.66
1:B:425:LYS:HE2	6:B:654:HOH:O	1.98	0.63
2:B:501:SFG:NE	3:B:502:GTP:N7	2.48	0.62
1:A:141:SER:N	6:A:603:HOH:O	2.42	0.52
1:C:206:ARG:HH11	1:C:206:ARG:HG3	1.75	0.51
1:A:202:GLU:O	1:A:206:ARG:HB3	2.10	0.51
1:C:206:ARG:HH11	1:C:206:ARG:CG	2.24	0.50
1:C:141:SER:N	6:C:601:HOH:O	2.43	0.50
1:B:422:ARG:HD2	6:B:667:HOH:O	2.11	0.50
3:A:502:GTP:H3'	6:A:644:HOH:O	2.11	0.50
1:B:147:ARG:HG2	3:B:502:GTP:H5''	1.94	0.50
1:B:347:GLU:OE2	3:B:502:GTP:N1	2.44	0.49
1:B:206:ARG:CG	1:B:206:ARG:HH11	2.27	0.48
1:B:206:ARG:HH11	1:B:206:ARG:HB2	1.79	0.47
1:C:293:LEU:HB3	1:C:319:TYR:CE2	2.50	0.47
1:B:150:ASN:ND2	3:B:502:GTP:O2'	2.49	0.46
1:A:370:MET:HE3	1:A:375:PHE:HD1	1.80	0.46
1:C:150:ASN:ND2	3:C:502:GTP:O2'	2.50	0.45
1:A:380:ILE:N	1:A:381:PRO:CD	2.80	0.45
1:A:150:ASN:ND2	3:A:502:GTP:O2'	2.50	0.44
1:C:380:ILE:N	1:C:381:PRO:CD	2.80	0.44
1:A:171:LEU:HB2	1:A:248:THR:HG22	1.99	0.44
1:B:171:LEU:HB2	1:B:248:THR:HG22	2.00	0.44
1:B:373:ASN:O	1:B:377:VAL:HG13	2.18	0.43
1:C:380:ILE:CG2	1:C:381:PRO:HD3	2.49	0.43
1:B:234:GLU:N	1:B:235:PRO:CD	2.81	0.43
1:B:380:ILE:CG2	1:B:381:PRO:HD3	2.48	0.43
1:B:380:ILE:N	1:B:381:PRO:CD	2.81	0.43
3:B:502:GTP:H3'	6:B:641:HOH:O	2.19	0.43
1:C:171:LEU:HB2	1:C:248:THR:HG22	2.00	0.43
1:A:380:ILE:CG2	1:A:381:PRO:HD3	2.48	0.43
1:A:401:ARG:HA	1:A:401:ARG:HD3	1.66	0.43
1:C:147:ARG:HG2	3:C:502:GTP:H5''	2.02	0.42
1:B:153:ILE:HD13	1:B:156:MET:CE	2.49	0.42
1:A:208:ARG:H	1:A:208:ARG:HG2	1.34	0.41
3:C:502:GTP:H3'	6:C:651:HOH:O	2.20	0.41
1:B:141:SER:HB3	1:B:144:ILE:HD12	2.02	0.41
1:B:376:PHE:CZ	1:B:380:ILE:HD13	2.56	0.40
1:A:376:PHE:CZ	1:A:380:ILE:HD13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	293/296 (99%)	284 (97%)	8 (3%)	1 (0%)	36	66
1	B	293/296 (99%)	287 (98%)	6 (2%)	0	100	100
1	C	293/296 (99%)	286 (98%)	7 (2%)	0	100	100
All	All	879/888 (99%)	857 (98%)	21 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ARG

5.3.2 Protein sidechains

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	250/260 (96%)	241 (96%)	9 (4%)	31	66
1	B	254/260 (98%)	245 (96%)	9 (4%)	32	67
1	C	255/260 (98%)	243 (95%)	12 (5%)	23	57
All	All	759/780 (97%)	729 (96%)	30 (4%)	28	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	A	216	GLN

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Mol	Chain	Res	Type
1	A	245	ILE
1	A	274	LYS
1	A	312	VAL
1	A	385	GLU
1	A	390	LYS
1	A	401	ARG
1	A	408	GLU
1	B	206	ARG
1	B	213	LEU
1	B	216	GLN
1	B	312	VAL
1	B	377	VAL
1	B	385	GLU
1	B	390	LYS
1	B	408	GLU
1	B	434	LYS
1	C	144	ILE
1	C	205	LYS
1	C	206	ARG
1	C	213	LEU
1	C	216	GLN
1	C	233	VAL
1	C	293	LEU
1	C	357	SER
1	C	364	LEU
1	C	385	GLU
1	C	390	LYS
1	C	408	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	151	ASN
1	B	150	ASN
1	C	150	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands 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	$\# Z > 2$
5	SO4	A	507	-	4,4,4	0.31	0	6,6,6	0.13	0
3	GTP	B	502	-	33,34,34	1.06	2 (6%)	50,54,54	0.72	0
5	SO4	B	505	-	4,4,4	0.29	0	6,6,6	0.10	0
3	GTP	C	502	-	33,34,34	1.20	2 (6%)	50,54,54	0.74	1 (2%)
5	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SFG	A	501	-	28,29,29	0.52	0	34,42,42	0.58	0
5	SO4	B	508	-	4,4,4	0.33	0	6,6,6	0.08	0
5	SO4	C	506	-	4,4,4	0.27	0	6,6,6	0.16	0
4	EDO	A	503	-	3,3,3	0.30	0	2,2,2	0.44	0
5	SO4	A	505	-	4,4,4	0.29	0	6,6,6	0.13	0
5	SO4	B	507	-	4,4,4	0.43	0	6,6,6	0.08	0
5	SO4	C	504	-	4,4,4	0.25	0	6,6,6	0.21	0
5	SO4	C	507	-	4,4,4	0.31	0	6,6,6	0.19	0
4	EDO	B	503	-	3,3,3	0.35	0	2,2,2	0.44	0
2	SFG	C	501	-	28,29,29	0.54	0	34,42,42	0.59	0
2	SFG	B	501	-	28,29,29	0.51	0	34,42,42	0.49	0
4	EDO	C	503	-	3,3,3	0.30	0	2,2,2	0.34	0
5	SO4	C	508	-	4,4,4	0.31	0	6,6,6	0.15	0
4	EDO	B	504	-	3,3,3	0.21	0	2,2,2	0.19	0
5	SO4	B	506	-	4,4,4	0.30	0	6,6,6	0.12	0
5	SO4	A	506	-	4,4,4	0.30	0	6,6,6	0.24	0
3	GTP	A	502	-	33,34,34	0.93	2 (6%)	50,54,54	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	C	505	-	4,4,4	0.35	0	6,6,6	0.19	0

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
4	EDO	B	504	-	-	0/1/1/1	-
3	GTP	B	502	-	-	1/22/38/38	0/3/3/3
4	EDO	B	503	-	-	0/1/1/1	-
2	SFG	C	501	-	-	4/17/33/33	0/3/3/3
3	GTP	C	502	-	-	0/22/38/38	0/3/3/3
3	GTP	A	502	-	-	3/22/38/38	0/3/3/3
2	SFG	B	501	-	-	5/17/33/33	0/3/3/3
4	EDO	C	503	-	-	1/1/1/1	-
2	SFG	A	501	-	-	4/17/33/33	0/3/3/3
4	EDO	A	503	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	GTP	PA-O3A	5.19	1.65	1.59
3	B	502	GTP	PA-O3A	4.30	1.64	1.59
3	A	502	GTP	PA-O3A	3.58	1.63	1.59
3	C	502	GTP	PB-O3A	2.95	1.62	1.59
3	B	502	GTP	PB-O3A	2.61	1.62	1.59
3	A	502	GTP	PB-O3A	2.24	1.61	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	GTP	O2A-PA-O3A	2.04	112.80	107.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	SFG	NE-CD-CG-CB
2	A	501	SFG	C5'-CD-CG-CB

Continued on next page...

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Mol	Chain	Res	Type	Atoms
2	B	501	SFG	NE-CD-CG-CB
2	B	501	SFG	C5'-CD-CG-CB
2	C	501	SFG	O-C-CA-N
2	C	501	SFG	N-CA-CB-CG
2	C	501	SFG	C-CA-CB-CG
2	C	501	SFG	OXT-C-CA-N
3	B	502	GTP	PA-O3A-PB-O1B
2	B	501	SFG	OXT-C-CA-N
2	A	501	SFG	OXT-C-CA-CB
3	A	502	GTP	O4'-C4'-C5'-O5'
3	A	502	GTP	PG-O3B-PB-O2B
2	A	501	SFG	O-C-CA-CB
4	C	503	EDO	O1-C1-C2-O2
2	B	501	SFG	O-C-CA-CB
2	B	501	SFG	OXT-C-CA-CB
3	A	502	GTP	PG-O3B-PB-O1B

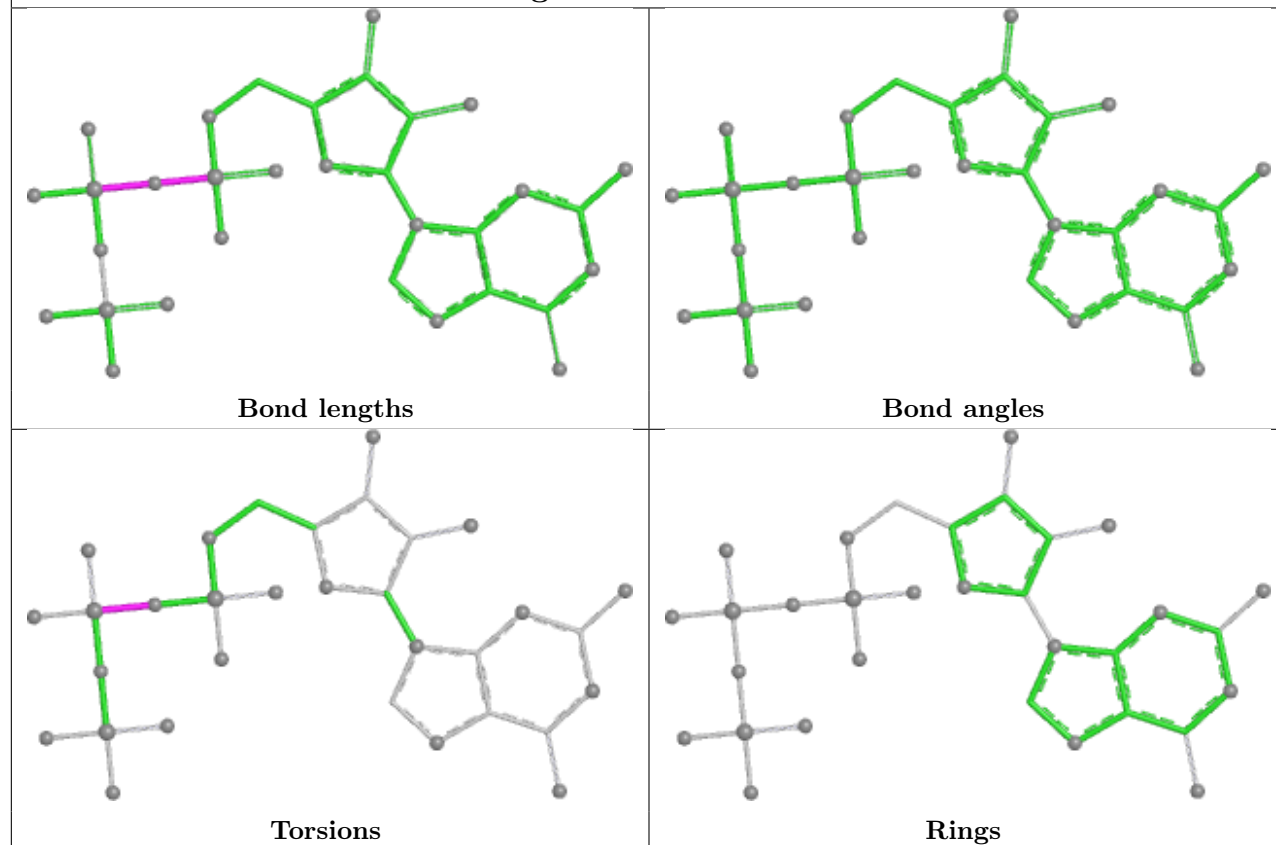
There are no ring outliers.

6 monomers are involved in 12 short contacts:

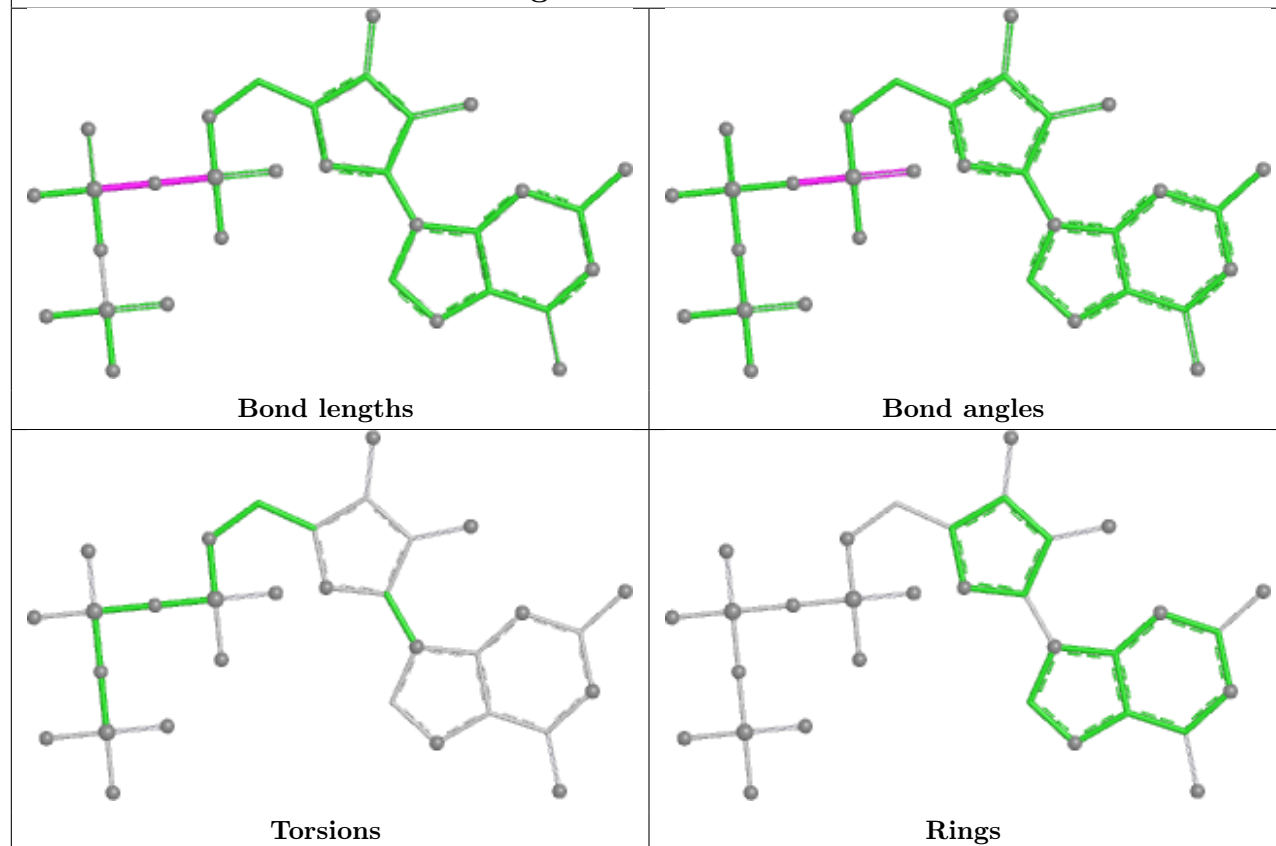
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	GTP	5	0
3	C	502	GTP	4	0
2	A	501	SFG	1	0
2	C	501	SFG	1	0
2	B	501	SFG	1	0
3	A	502	GTP	3	0

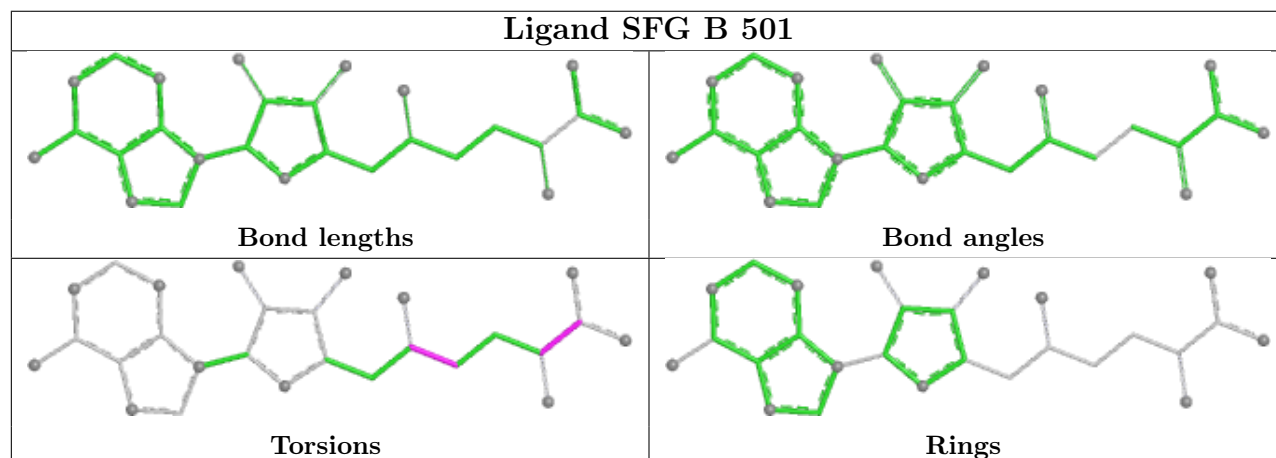
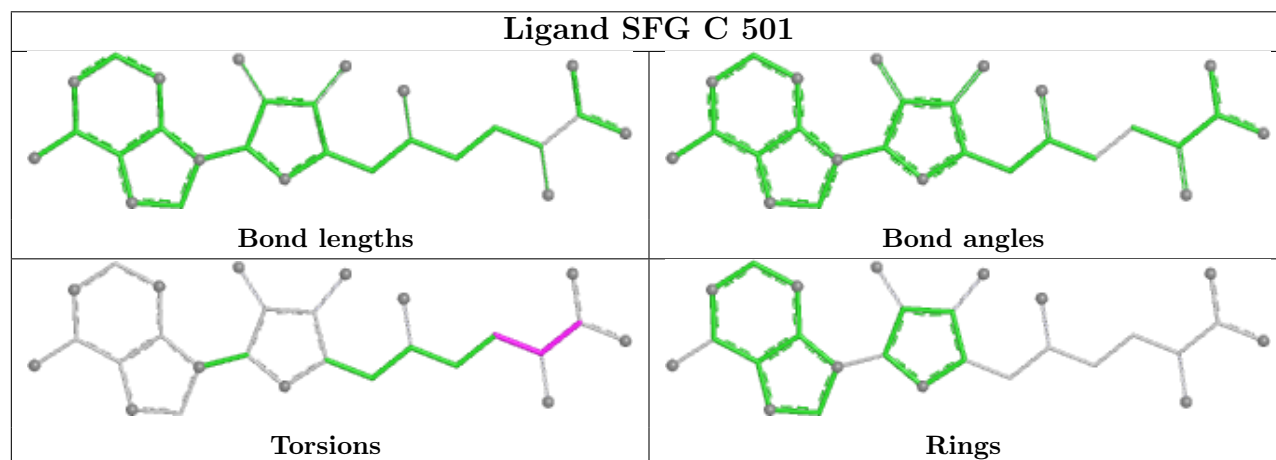
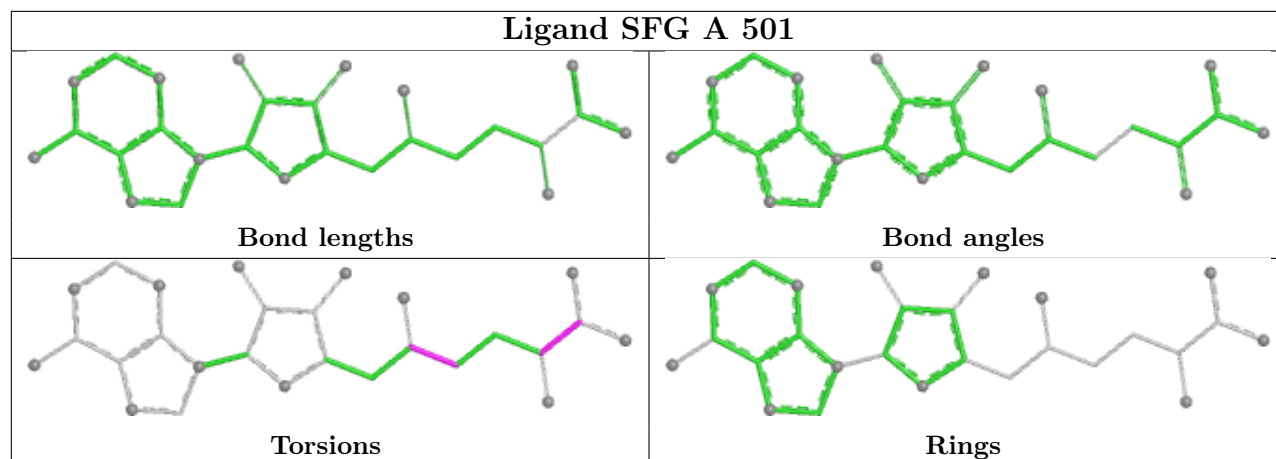
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

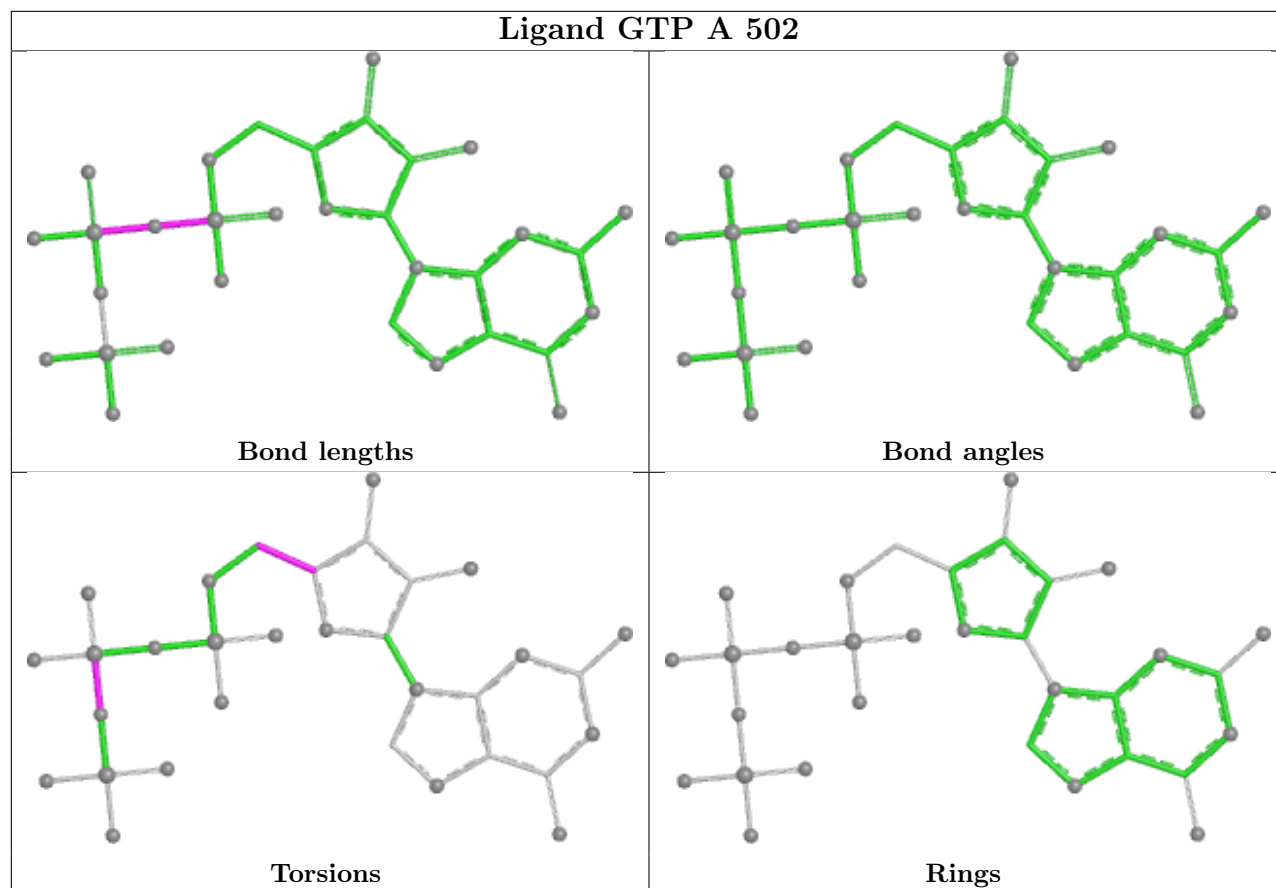
Ligand GTP B 502



Ligand GTP C 502







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	295/296 (99%)	-0.27	13 (4%) 39 31	16, 31, 65, 119	0
1	B	295/296 (99%)	-0.41	2 (0%) 84 77	18, 30, 59, 79	0
1	C	295/296 (99%)	-0.39	3 (1%) 79 72	17, 29, 58, 73	0
All	All	885/888 (99%)	-0.36	18 (2%) 65 56	16, 30, 62, 119	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	SER	5.2
1	A	206	ARG	4.7
1	A	213	LEU	4.6
1	A	211	ARG	4.6
1	A	207	TYR	4.5
1	A	208	ARG	3.6
1	A	212	ASN	3.5
1	A	204	HIS	2.8
1	B	212	ASN	2.6
1	A	203	ALA	2.4
1	A	210	MET	2.3
1	B	207	TYR	2.3
1	C	390	LYS	2.2
1	A	401	ARG	2.2
1	C	214	ASP	2.1
1	A	175	LYS	2.1
1	A	390	LYS	2.1
1	C	212	ASN	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

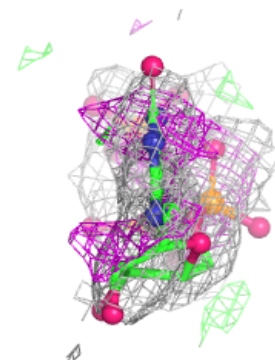
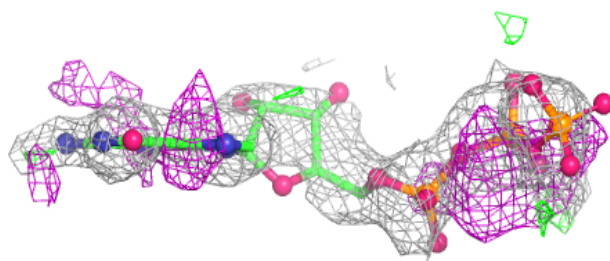
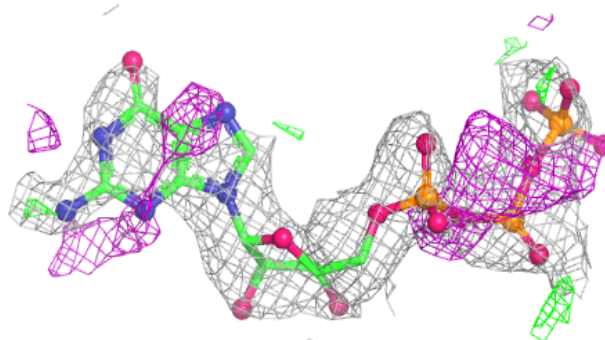
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GTP	C	502	32/32	0.74	0.20	87,108,125,133	0
4	EDO	B	503	4/4	0.80	0.21	46,47,52,53	0
4	EDO	C	503	4/4	0.80	0.20	45,54,56,59	0
5	SO4	A	506	5/5	0.80	0.13	89,92,100,100	0
4	EDO	A	503	4/4	0.81	0.21	55,56,62,64	0
3	GTP	B	502	32/32	0.82	0.17	82,102,117,124	0
3	GTP	A	502	32/32	0.82	0.16	81,105,137,141	0
4	EDO	B	504	4/4	0.88	0.15	33,36,36,36	0
5	SO4	B	506	5/5	0.89	0.16	67,71,88,90	0
5	SO4	C	507	5/5	0.91	0.12	61,71,74,75	0
5	SO4	B	507	5/5	0.92	0.13	59,72,81,82	0
5	SO4	C	508	5/5	0.94	0.18	59,68,70,74	0
5	SO4	B	508	5/5	0.95	0.13	67,72,77,79	0
5	SO4	C	506	5/5	0.95	0.11	48,52,55,55	0
2	SFG	A	501	27/27	0.95	0.09	30,36,59,63	0
2	SFG	C	501	27/27	0.95	0.09	30,34,53,66	0
2	SFG	B	501	27/27	0.96	0.07	30,38,57,59	0
5	SO4	A	507	5/5	0.97	0.11	63,66,69,74	0
5	SO4	B	505	5/5	0.97	0.08	42,44,50,52	0
5	SO4	C	505	5/5	0.99	0.08	26,27,27,28	0
5	SO4	A	504	5/5	0.99	0.07	34,35,36,37	0
5	SO4	A	505	5/5	0.99	0.07	43,44,47,48	0
5	SO4	C	504	5/5	0.99	0.08	24,26,29,31	0

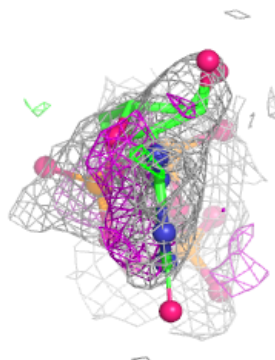
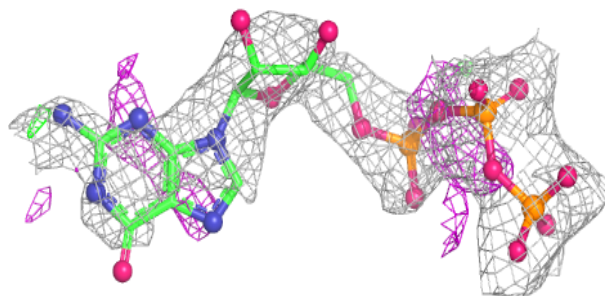
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP C 502:

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

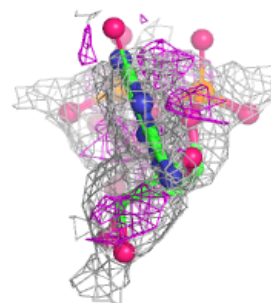
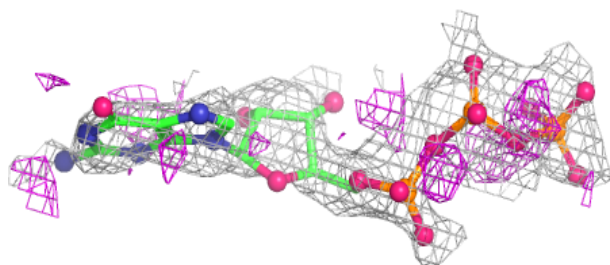
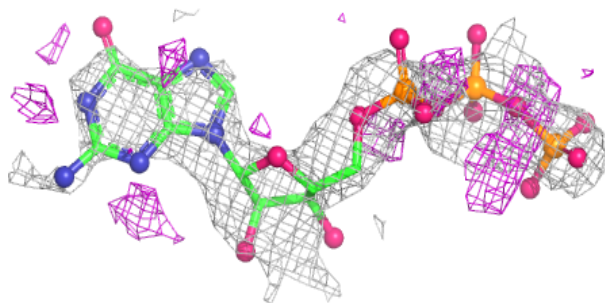
**Electron density around GTP B 502:**

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

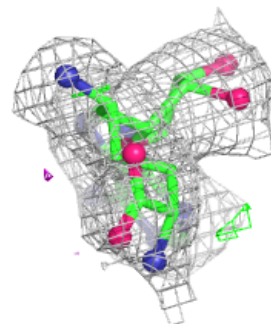
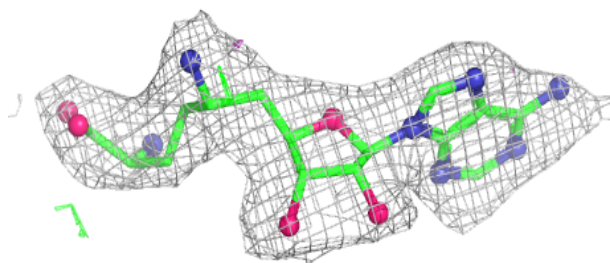
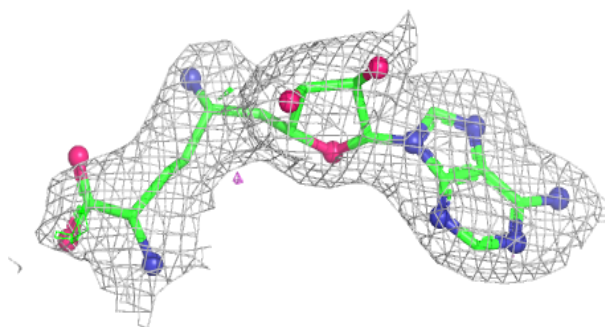


Electron density around GTP A 502:

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

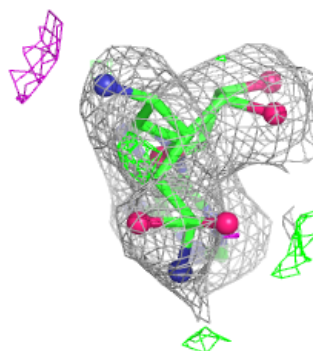
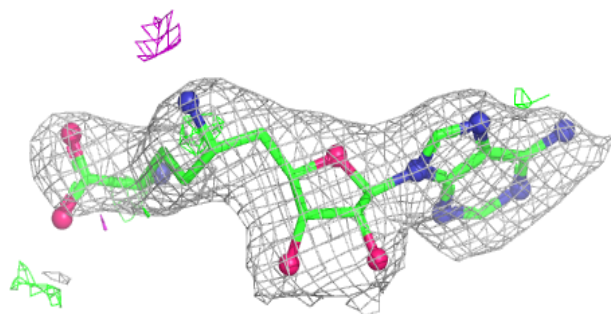
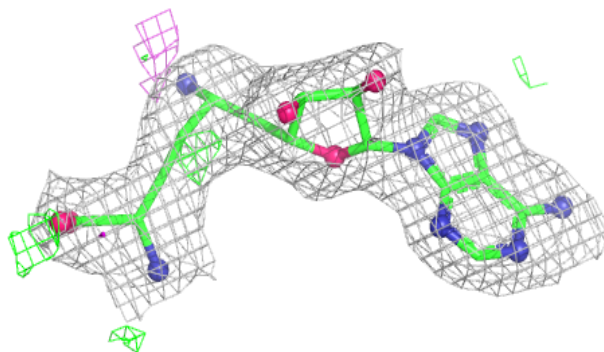
**Electron density around SFG A 501:**

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

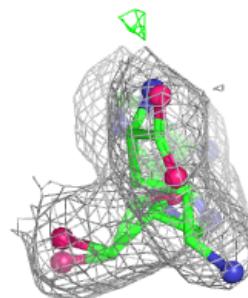
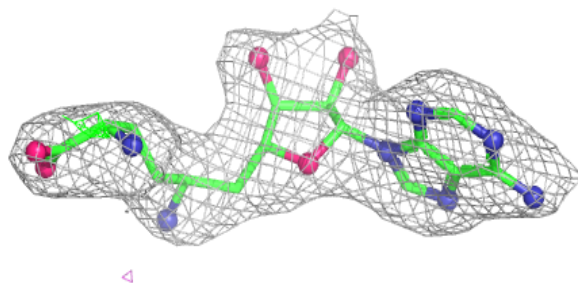
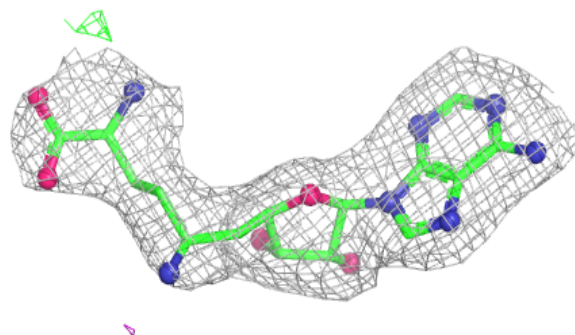


Electron density around SFG C 501:

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

**Electron density around SFG B 501:**

$2mF_o-DF_c$ (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.