



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:57 am BST

PDB ID : 5CK3
Title : Signal recognition particle receptor SRb-GTP/SRX complex from
Chaetomium thermophilum
Authors : Jadhav, B.R.; Wild, K.; Sinning, I.
Deposited on : 2015-07-15
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

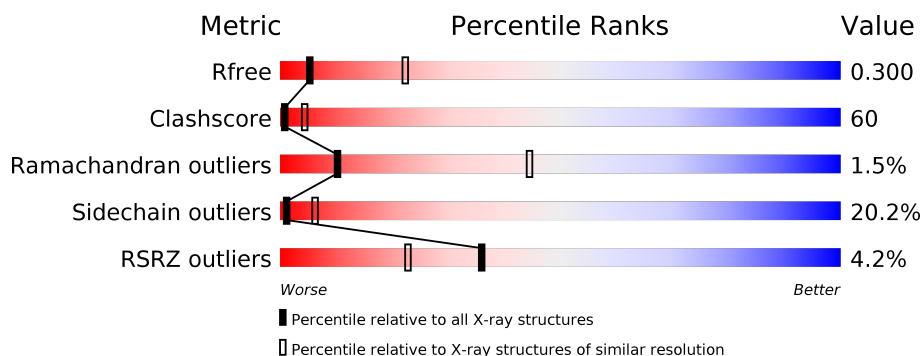
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	181	
1	C	181	
1	E	181	
2	B	307	
2	D	307	
2	F	307	

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
4	GTP	B	402	-	-	X	-
4	GTP	F	401	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7908 atoms, of which 8 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 SRX domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1090	707	178	203	2			
1	C	105	Total	C	N	O	S	0	0	0
			873	576	136	160	1			
1	E	104	Total	C	N	O	S	0	0	0
			843	555	131	155	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP G0S1R8
A	-6	LYS	-	expression tag	UNP G0S1R8
A	-5	HIS	-	expression tag	UNP G0S1R8
A	-4	HIS	-	expression tag	UNP G0S1R8
A	-3	HIS	-	expression tag	UNP G0S1R8
A	-2	HIS	-	expression tag	UNP G0S1R8
A	-1	HIS	-	expression tag	UNP G0S1R8
A	0	HIS	-	expression tag	UNP G0S1R8
A	1	MET	-	expression tag	UNP G0S1R8
A	2	SER	-	expression tag	UNP G0S1R8
C	-7	MET	-	initiating methionine	UNP G0S1R8
C	-6	LYS	-	expression tag	UNP G0S1R8
C	-5	HIS	-	expression tag	UNP G0S1R8
C	-4	HIS	-	expression tag	UNP G0S1R8
C	-3	HIS	-	expression tag	UNP G0S1R8
C	-2	HIS	-	expression tag	UNP G0S1R8
C	-1	HIS	-	expression tag	UNP G0S1R8
C	0	HIS	-	expression tag	UNP G0S1R8
C	1	MET	-	expression tag	UNP G0S1R8
C	2	SER	-	expression tag	UNP G0S1R8
E	-7	MET	-	initiating methionine	UNP G0S1R8
E	-6	LYS	-	expression tag	UNP G0S1R8
E	-5	HIS	-	expression tag	UNP G0S1R8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP G0S1R8
E	-3	HIS	-	expression tag	UNP G0S1R8
E	-2	HIS	-	expression tag	UNP G0S1R8
E	-1	HIS	-	expression tag	UNP G0S1R8
E	0	HIS	-	expression tag	UNP G0S1R8
E	1	MET	-	expression tag	UNP G0S1R8
E	2	SER	-	expression tag	UNP G0S1R8

- Molecule 2 is a protein called Putative signal recognition particle protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	270	Total	C	N	O	S	0	0	0
			2067	1313	362	388	4			
2	D	230	Total	C	N	O	S	0	0	0
			1789	1148	307	330	4			
2	F	147	Total	C	N	O	S	0	0	0
			1128	725	200	202	1			

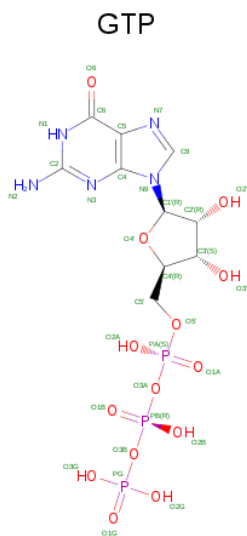
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	MET	-	initiating methionine	UNP G0S401
B	42	GLY	-	expression tag	UNP G0S401
D	41	MET	-	initiating methionine	UNP G0S401
D	42	GLY	-	expression tag	UNP G0S401
F	41	MET	-	initiating methionine	UNP G0S401
F	42	GLY	-	expression tag	UNP G0S401

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

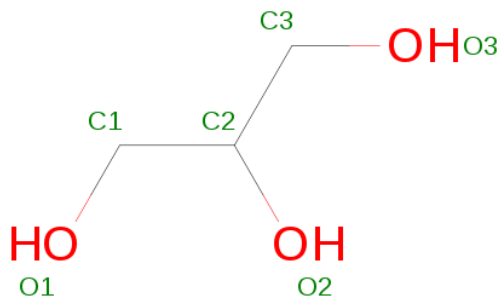
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



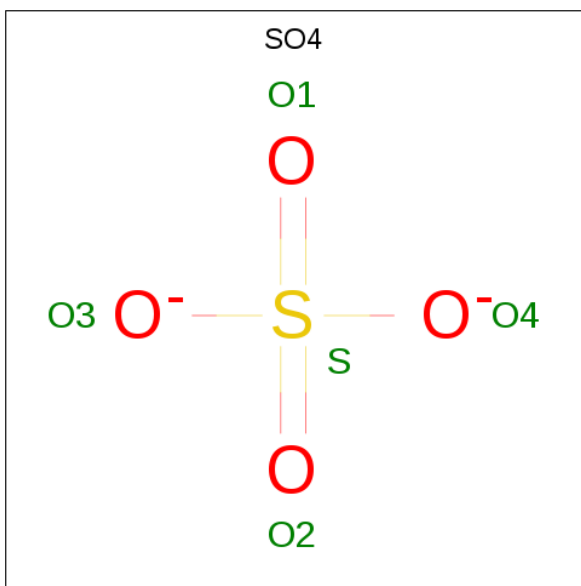
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	F	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

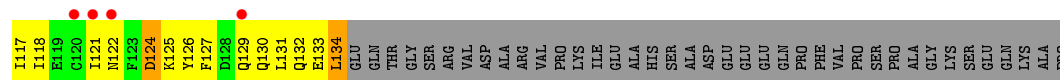


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

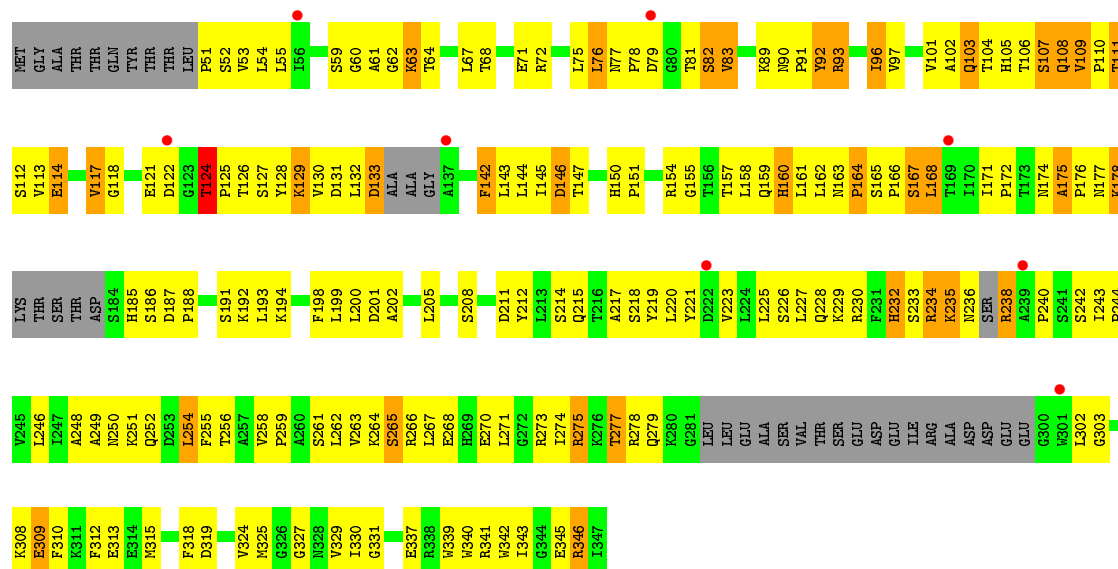
- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



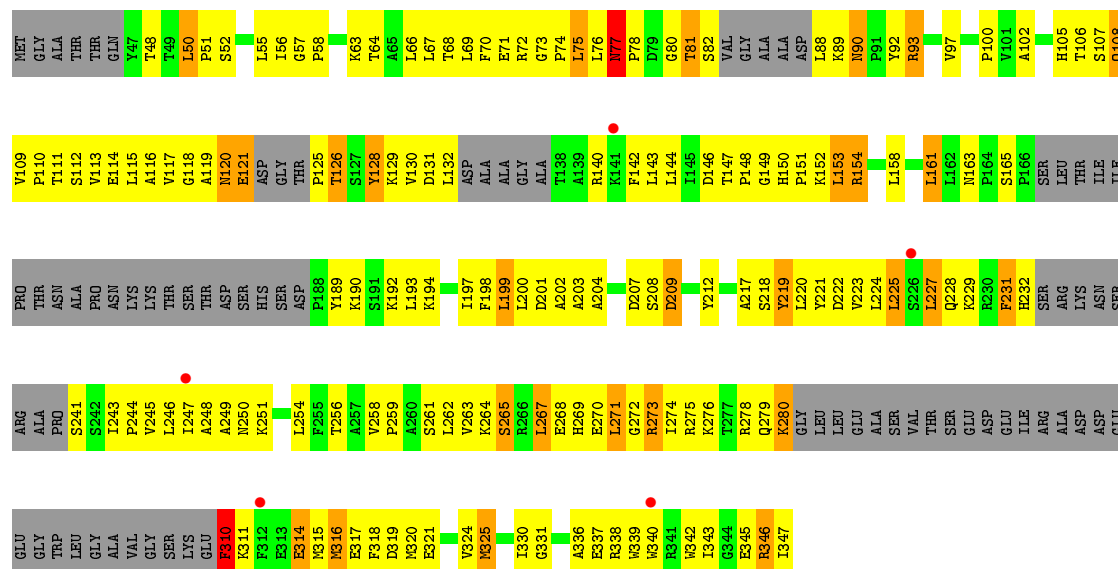
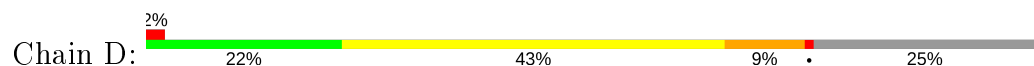
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		



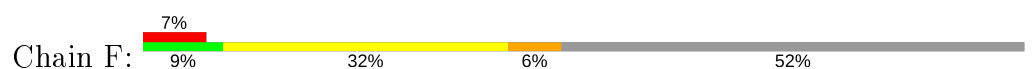
• Molecule 2: Putative signal recognition particle protein



• Molecule 2: Putative signal recognition particle protein



• Molecule 2: Putative signal recognition particle protein



E345 R346 I347	GLU	ALA	VAL	SER	VAL	THR	SER	GLU	ASP	GLU	ILE	ILE	ARG	ALA	ASP	ASP	GLU	GLU	GLY	TRP	LEU	GLY	GLY	ALA	VAL	VAL	PHE	LYS	PHE	GLU	GLU	MET	MET	GLU	PHE	ASP	MET	GLU	VAL	GLU	THR	ASP	GLY	ASN	PRO	ASP	GLY	THR	SER	VAL	GLY	ALA	ALA	ASP	LEU	LYS	ASN	PRO	TYR	ARG	K94	P95	I96	F97	T98	S99	P100
	V223	L224	L225	S226	L227	Q228	K229	R230	F231	HIS	SER	ARG	LYS	ASN	ALA	SER	THR	ILE	ILE	PRO	THR	ASN	ALA	PRO	ASN	LYS	THR	SER	THR	ALA	ASN	GLU	GLY	ASP	THR	PRO	THR	SER	TYR	LYS	VAL	ASP	LEU	ASP	ALA	ALA	GLY	LEU	THR	ALA	ASP	LEU	LYS	ASN	PRO	TYR	ARG	K94	P95	I96	F97	T98	S99	P100			
	V258	P259	A260	S261	L262	V263	K264	S265	R266	L267	E268	H269	E270	L271	G272	R273	I274	R275	K276	THR	ARG	GLN	LYS	GLY	LEU	D222																																									
	V322	E323	V324	G326	G326	G327	N328	V329	ILE	GLY	D332	G336	A336	E337	R338	W339	N340	R341	N342	I343	G344																																														
	LEU	ASN	PRO	SER	PRO	SER	THR	ILE	ILE	PRO	THR	ASN	ALA	PRO	ASN	LYS	THR	SER	THR	ALA	ASN	GLU	GLY	ASP	THR	PRO	THR	SER	TYR	LYS	VAL	ASP	LEU	ASP	ALA	ALA	GLY	LEU	THR	ALA	ASP	LEU	LYS	ASN	PRO	TYR	ARG	K94	P95	I96	F97	T98	S99	P100													
	V101	A102	Q103	T104	H105	T106	S107	Q108	V109	P110	T111	S112	V113	GLU	LEU	ALA	PRO	ASN	LYS	THR	SER	THR	ALA	ASN	GLU	GLY	ASP	THR	PRO	THR	SER	TYR	LYS	VAL	ASP	LEU	ASP	ALA	ALA	GLY	LEU	THR	ALA	ASP	LEU	LYS	ASN	PRO	TYR	ARG	K94	P95	I96	F97	T98	S99	P100										
	LEU	ASN	PRO	SER	PRO	SER	THR	ILE	ILE	PRO	THR	ASN	ALA	PRO	ASN	LYS	THR	SER	THR	ALA	ASN	GLU	GLY	ASP	THR	PRO	THR	SER	TYR	LYS	VAL	ASP	LEU	ASP	ALA	ALA	GLY	LEU	THR	ALA	ASP	LEU	LYS	ASN	PRO	TYR	ARG	K94	P95	I96	F97	T98	S99	P100													
	V223	L224	L225	S226	L227	Q228	K229	R230	F231	HIS	SER	ARG	LYS	ASN	ALA	SER	THR	ILE	ILE	PRO	THR	ASN	ALA	PRO	ASN	LYS	THR	SER	THR	ALA	ASN	GLU	GLY	ASP	THR	PRO	THR	SER	TYR	LYS	VAL	ASP	LEU	ASP	ALA	ALA	GLY	LEU	THR	ALA	ASP	LEU	LYS	ASN	PRO	TYR	ARG	K94	P95	I96	F97	T98	S99	P100			
	V258	P259	A260	S261	L262	V263	K264	S265	R266	L267	E268	H269	E270	L271	G272	R273	I274	R275	K276	THR	ARG	GLN	LYS	GLY	LEU	D222																																									
	V322	E323	V324	G326	G326	G327	N328	V329	ILE	GLY	D332	G336	A336	E337	R338	W339	N340	R341	N342	I343	G344																																														
LEU	ASN	PRO	SER	PRO	SER	THR	ILE	ILE	PRO	THR	ASN	ALA	PRO	ASN	LYS	THR	SER	THR	ALA	ASN	GLU	GLY	ASP	THR	PRO	THR	SER	TYR	LYS	VAL	ASP	LEU	ASP	ALA	ALA	GLY	LEU	THR	ALA	ASP	LEU	LYS	ASN	PRO	TYR	ARG	K94	P95	I96	F97	T98	S99	P100														

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.28 Å 83.61 Å 90.21 Å 90.00° 105.23° 90.00°	Depositor
Resolution (Å)	45.47 – 3.20 45.47 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.47-3.20) 99.2 (45.47-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.19 Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, R_{free}	0.276 , 0.300 0.276 , 0.300	Depositor DCC
R_{free} test set	1077 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7908	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GOL, MG, SO4

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	0.38	0/1118	0.73	4/1522 (0.3%)
1	C	0.35	0/894	0.63	1/1218 (0.1%)
1	E	0.25	0/858	0.47	0/1160
2	B	0.36	0/2110	0.55	1/2859 (0.0%)
2	D	0.40	2/1825 (0.1%)	0.60	2/2469 (0.1%)
2	F	0.35	1/1146 (0.1%)	0.56	1/1549 (0.1%)
All	All	0.36	3/7951 (0.0%)	0.59	9/10777 (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	2
1	C	0	2
2	D	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	310	PHE	CD2-CE2	5.28	1.49	1.39
2	F	110	PRO	N-CD	5.23	1.55	1.47
2	D	110	PRO	N-CD	5.04	1.54	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASP	CB-CG-OD2	-6.60	112.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	VAL	C-N-CD	6.09	141.19	128.40
1	C	66	LEU	CA-CB-CG	6.07	129.27	115.30
2	F	109	VAL	C-N-CD	5.87	140.73	128.40
2	D	109	VAL	C-N-CD	5.59	140.15	128.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	HIS	Peptide
1	A	64	HIS	Peptide
1	C	63	GLN	Peptide
1	C	65	SER	Peptide
2	D	88	LEU	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	1090	0	1076	152	0
1	C	873	0	859	90	0
1	E	843	0	839	123	0
2	B	2067	0	2093	201	0
2	D	1789	0	1821	224	0
2	F	1128	0	1166	226	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	B	32	0	12	14	0
4	D	32	0	12	1	0
4	F	32	0	12	14	0
5	B	6	8	8	1	0
6	B	5	0	0	1	0
All	All	7900	8	7898	948	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 60.

The worst 5 of 948 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:197:ILE:HG22	2:F:246:LEU:HB3	1.29	1.15
2:F:111:THR:O	2:F:145:ILE:HG23	1.46	1.14
2:D:55:LEU:HD21	2:D:146:ASP:HA	1.24	1.13
2:D:246:LEU:HB2	2:D:342:TRP:HZ3	1.03	1.11
2:F:259:PRO:HG2	2:F:262:LEU:HB2	1.24	1.08

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	133/181 (74%)	111 (84%)	18 (14%)	4 (3%)	4	28
1	C	99/181 (55%)	90 (91%)	7 (7%)	2 (2%)	7	38
1	E	92/181 (51%)	88 (96%)	4 (4%)	0	100	100
2	B	260/307 (85%)	237 (91%)	18 (7%)	5 (2%)	8	39
2	D	216/307 (70%)	204 (94%)	10 (5%)	2 (1%)	17	56
2	F	131/307 (43%)	116 (88%)	14 (11%)	1 (1%)	19	58
All	All	931/1464 (64%)	846 (91%)	71 (8%)	14 (2%)	10	44

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	164	PRO
1	A	84	SER
2	B	124	THR
1	C	121	ILE
1	A	62	ASP

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	122/161 (76%)	96 (79%)	26 (21%)	1	5
1	C	99/161 (62%)	73 (74%)	26 (26%)	0	2
1	E	96/161 (60%)	72 (75%)	24 (25%)	0	2
2	B	225/255 (88%)	186 (83%)	39 (17%)	2	10
2	D	196/255 (77%)	157 (80%)	39 (20%)	1	6
2	F	122/255 (48%)	102 (84%)	20 (16%)	2	11
All	All	860/1248 (69%)	686 (80%)	174 (20%)	1	6

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	90	TRP
2	D	108	GLN
2	F	144	LEU
1	C	109	GLN
1	C	130	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	GLN
2	D	77	ASN
2	D	250	ASN
1	C	130	GLN
2	D	108	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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$
4	GTP	F	401	3	26,34,34	0.96	1 (3%)	33,54,54	1.87	7 (21%)
5	GOL	B	403	-	5,5,5	0.41	0	5,5,5	0.29	0
6	SO4	B	404	-	4,4,4	0.15	0	6,6,6	0.06	0
4	GTP	B	402	3	26,34,34	0.98	1 (3%)	33,54,54	1.89	7 (21%)
4	GTP	D	401	3	26,34,34	1.05	1 (3%)	33,54,54	1.99	10 (30%)

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	GTP	F	401	3	-	3/18/38/38	0/3/3/3
5	GOL	B	403	-	-	4/4/4/4	-
4	GTP	B	402	3	-	1/18/38/38	0/3/3/3
4	GTP	D	401	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)
4	D	401	GTP	C6-N1	3.24	1.38	1.33
4	B	402	GTP	C6-N1	3.22	1.38	1.33
4	F	401	GTP	C6-N1	2.93	1.38	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	GTP	N3-C2-N1	-5.73	119.58	127.22
4	B	402	GTP	N3-C2-N1	-5.41	120.01	127.22
4	F	401	GTP	N3-C2-N1	-5.21	120.27	127.22
4	B	402	GTP	C2-N3-C4	4.56	120.56	115.36
4	F	401	GTP	C2-N3-C4	4.41	120.40	115.36

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	403	GOL	O1-C1-C2-C3
5	B	403	GOL	C1-C2-C3-O3
4	D	401	GTP	C5'-O5'-PA-O1A
4	F	401	GTP	O4'-C4'-C5'-O5'
4	F	401	GTP	C3'-C4'-C5'-O5'

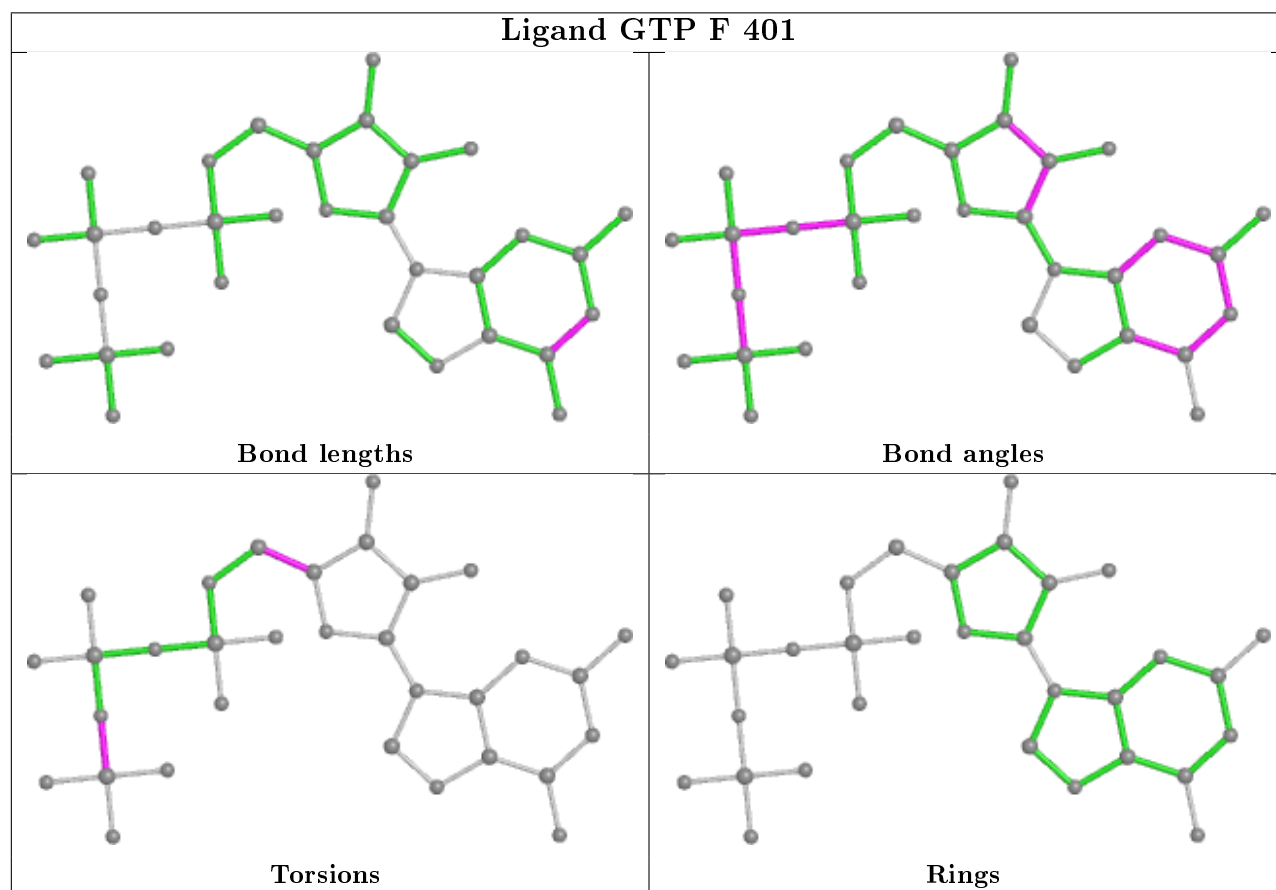
There are no ring outliers.

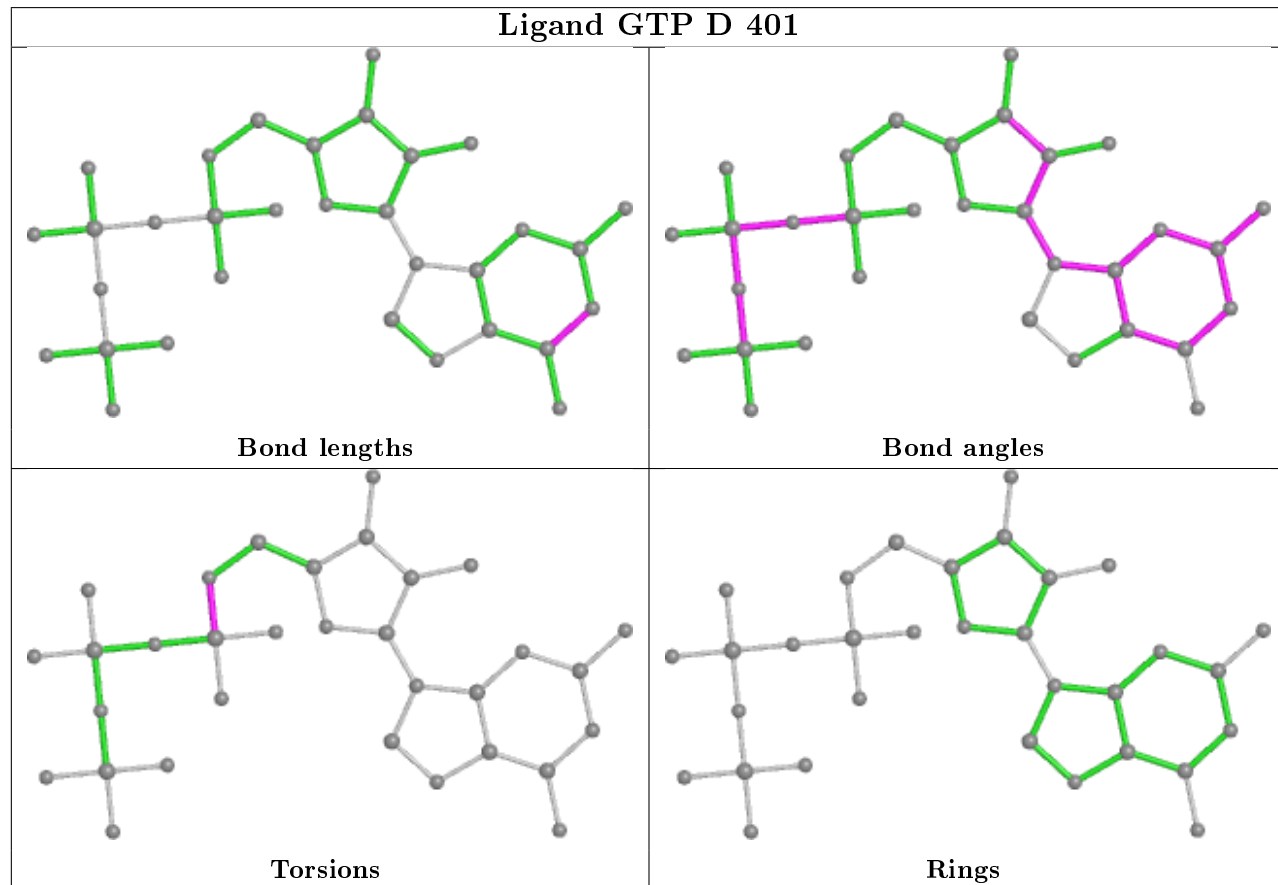
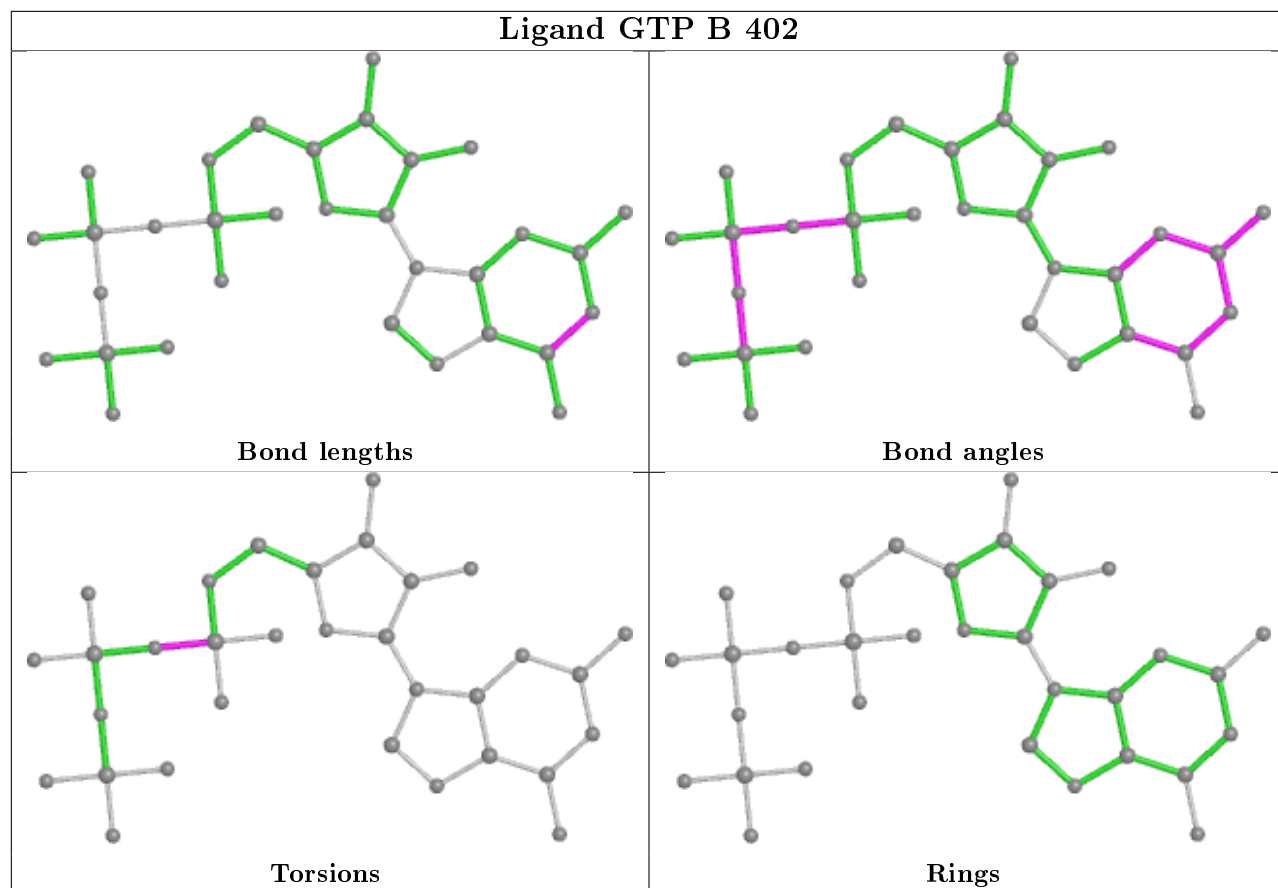
5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	401	GTP	14	0
5	B	403	GOL	1	0
6	B	404	SO4	1	0
4	B	402	GTP	14	0
4	D	401	GTP	1	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	135/181 (74%)	0.10	4 (2%) 50 34	36, 74, 119, 132	0
1	C	105/181 (58%)	-0.07	0 100 100	40, 68, 96, 105	0
1	E	104/181 (57%)	0.29	5 (4%) 30 18	72, 94, 112, 117	0
2	B	270/307 (87%)	0.07	8 (2%) 50 34	37, 66, 113, 131	0
2	D	230/307 (74%)	0.18	5 (2%) 62 48	47, 81, 121, 135	0
2	F	147/307 (47%)	0.81	20 (13%) 3 2	84, 121, 153, 160	0
All	All	991/1464 (67%)	0.22	42 (4%) 36 23	36, 83, 129, 160	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	197	ILE	4.5
1	A	53	ALA	4.5
1	A	60	LYS	4.4
1	E	38	ILE	4.4
1	E	120	CYS	3.9

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

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

6.3 Carbohydrates ⓘ

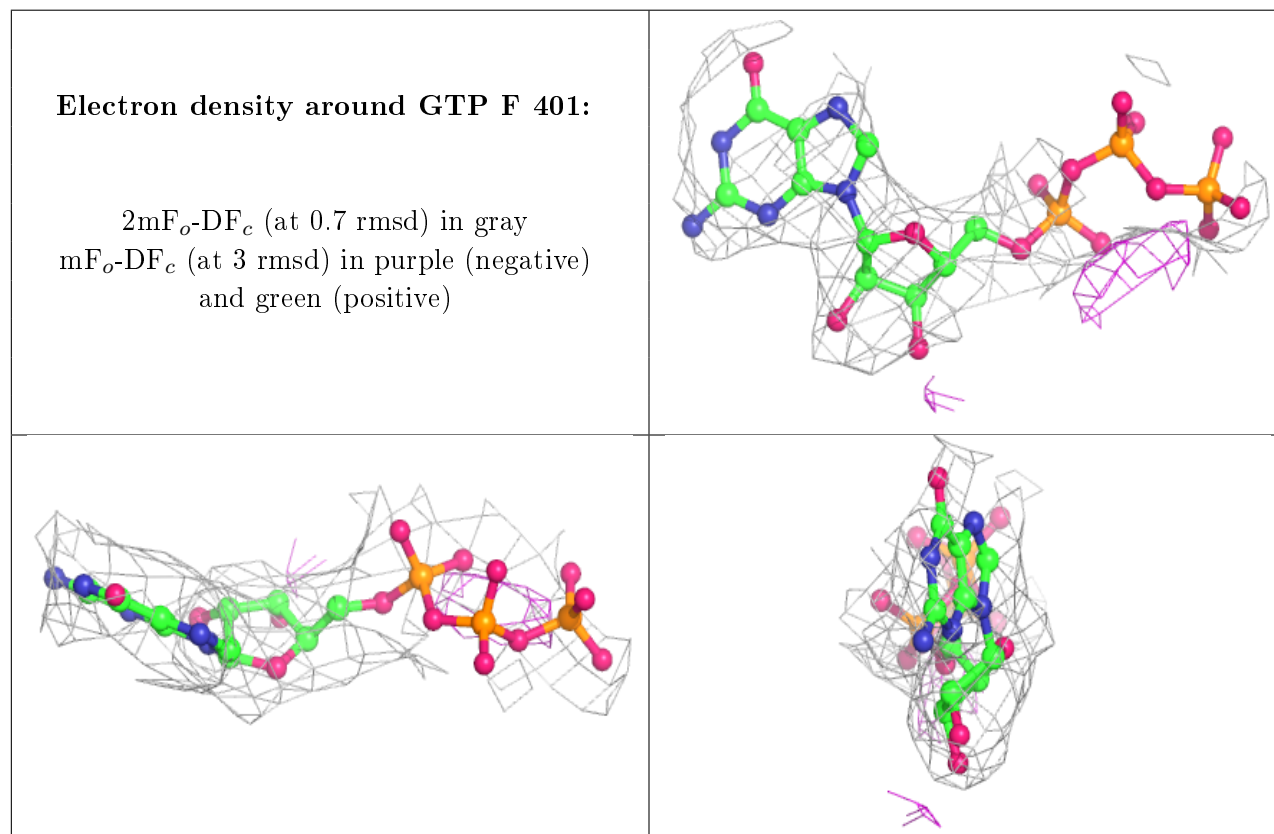
There are no carbohydrates in this entry.

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.

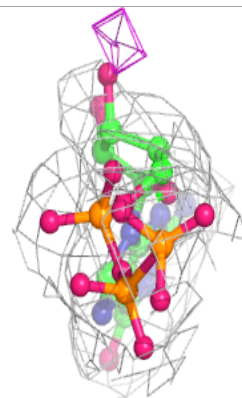
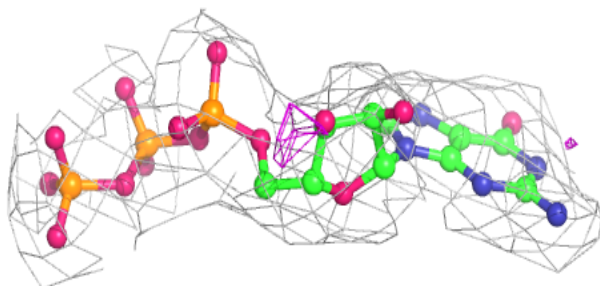
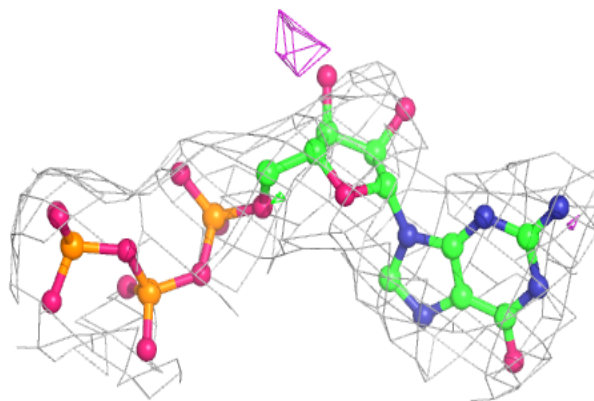
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	B	404	5/5	0.84	0.31	111,113,123,128	0
5	GOL	B	403	6/6	0.88	0.22	50,68,78,81	0
4	GTP	F	401	32/32	0.90	0.17	86,108,117,121	0
3	MG	F	400	1/1	0.94	0.09	104,104,104,104	0
3	MG	D	400	1/1	0.94	0.10	53,53,53,53	0
4	GTP	D	401	32/32	0.95	0.19	49,58,67,78	0
4	GTP	B	402	32/32	0.96	0.17	26,42,51,59	0
3	MG	B	401	1/1	0.96	0.14	42,42,42,42	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.

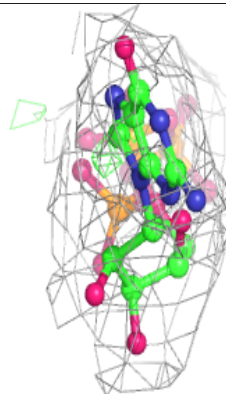
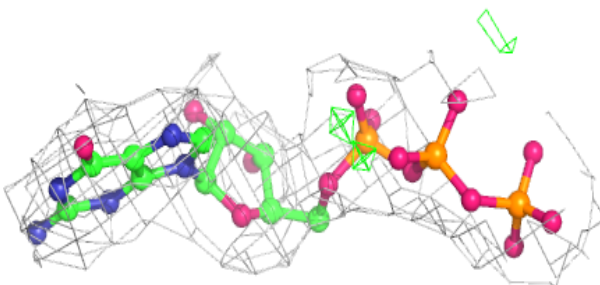
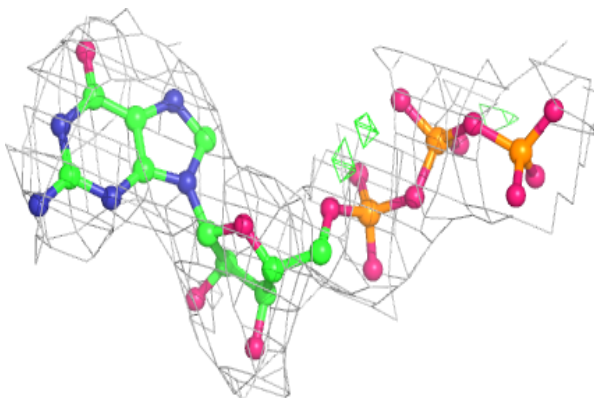


Electron density around GTP D 401:

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

**Electron density around GTP B 402:**

$2mF_o-DF_c$ (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.