wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 02:33 AM EDT

PDB ID	:	3WYF
Title	:	Crystal structure of Xpo1p-Yrb2p-Gsp1p-GTP complex
Authors	:	Koyama, M.; Shirai, N.; Matsuura, Y.
Deposited on	:	2014-08-26
Resolution	:	2.22 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

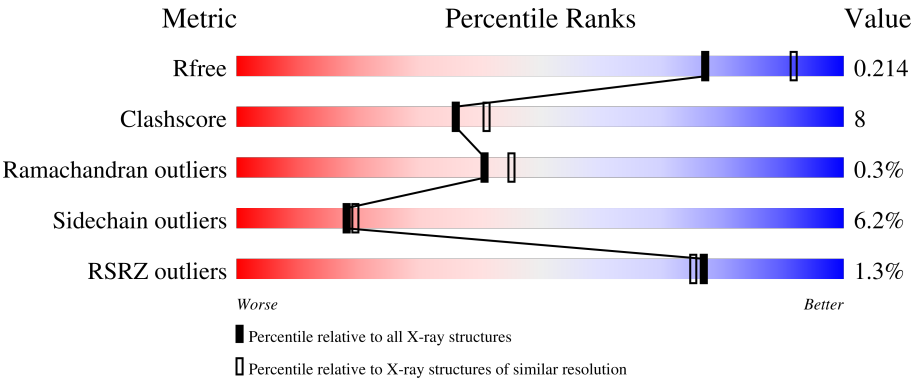
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	2% 68% 16% 14%
1	D	219	65% 18% 16%
2	B	238	4% 43% 14% 39%
2	E	238	3% 35% 19% 40%
3	C	1049	% 81% 17%

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Mol	Chain	Length	Quality of chain
3	F	1049	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22420 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 Gsp1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1492	973	252	262	5			
1	D	185	Total	C	N	O	S	0	0	0
			1459	953	245	257	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LEU	GLN	engineered mutation	UNP E7KFU1
D	71	LEU	GLN	engineered mutation	UNP E7KFU1

- Molecule 2 is a protein called Ran-specific GTPase-activating protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1073	691	180	200	2			
2	E	142	Total	C	N	O	S	0	0	0
			1074	690	181	201	2			

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1040	Total	C	N	O	S	0	0	0
			8322	5348	1361	1573	40			
3	F	1005	Total	C	N	O	S	0	0	0
			8046	5179	1316	1512	39			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P30822
C	0	ALA	-	expression tag	UNP P30822

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	ASN	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	TYR	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	LYS	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	PHE	deletion	UNP P30822
F	-1	GLY	-	expression tag	UNP P30822
F	0	ALA	-	expression tag	UNP P30822
F	?	-	VAL	deletion	UNP P30822
F	?	-	GLN	deletion	UNP P30822
F	?	-	ARG	deletion	UNP P30822

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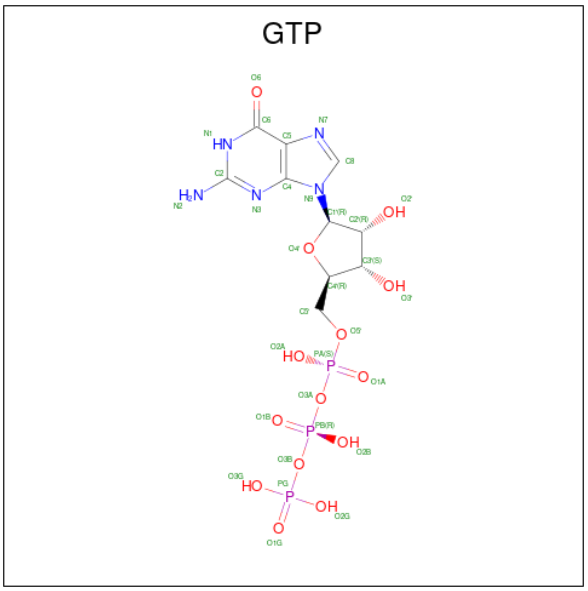
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	LEU	deletion	UNP P30822
F	?	-	PRO	deletion	UNP P30822
F	?	-	ALA	deletion	UNP P30822
F	?	-	THR	deletion	UNP P30822
F	?	-	GLU	deletion	UNP P30822
F	?	-	MET	deletion	UNP P30822
F	?	-	SER	deletion	UNP P30822
F	?	-	PRO	deletion	UNP P30822
F	?	-	LEU	deletion	UNP P30822
F	?	-	ILE	deletion	UNP P30822
F	?	-	GLN	deletion	UNP P30822
F	?	-	LEU	deletion	UNP P30822
F	?	-	SER	deletion	UNP P30822
F	?	-	VAL	deletion	UNP P30822
F	?	-	GLY	deletion	UNP P30822
F	?	-	SER	deletion	UNP P30822
F	?	-	GLN	deletion	UNP P30822
F	?	-	ALA	deletion	UNP P30822
F	?	-	ILE	deletion	UNP P30822
F	?	-	SER	deletion	UNP P30822
F	?	-	THR	deletion	UNP P30822
F	?	-	GLY	deletion	UNP P30822
F	?	-	SER	deletion	UNP P30822
F	?	-	GLY	deletion	UNP P30822
F	?	-	ALA	deletion	UNP P30822
F	?	-	LEU	deletion	UNP P30822
F	?	-	ASN	deletion	UNP P30822
F	?	-	PRO	deletion	UNP P30822
F	?	-	GLU	deletion	UNP P30822
F	?	-	TYR	deletion	UNP P30822
F	?	-	MET	deletion	UNP P30822
F	?	-	LYS	deletion	UNP P30822
F	?	-	ARG	deletion	UNP P30822
F	?	-	PHE	deletion	UNP P30822

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	84	Total O 84 84	0	0
6	B	11	Total O 11 11	0	0
6	C	351	Total O 351 351	0	0
6	D	86	Total O 86 86	0	0
6	E	10	Total O 10 10	0	0

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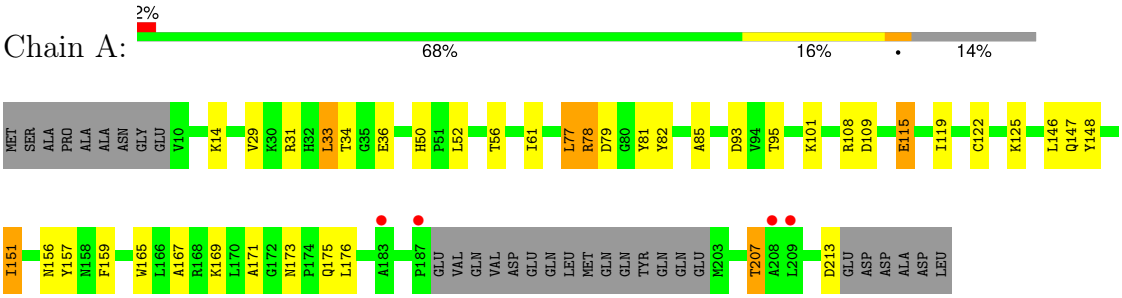
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	346	Total 346	O 346	0	0

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.

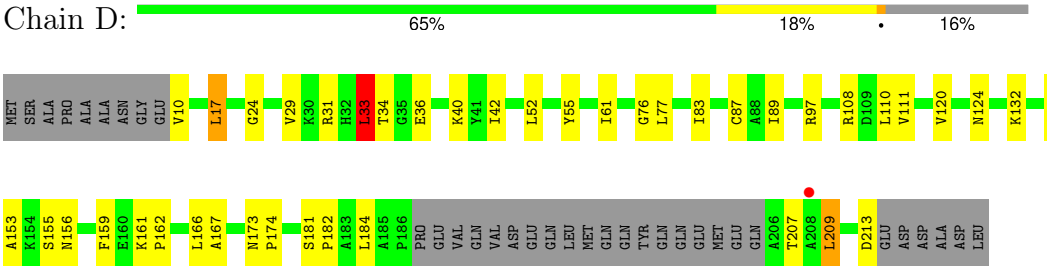
• Molecule 1: Gsp1p

Chain A:



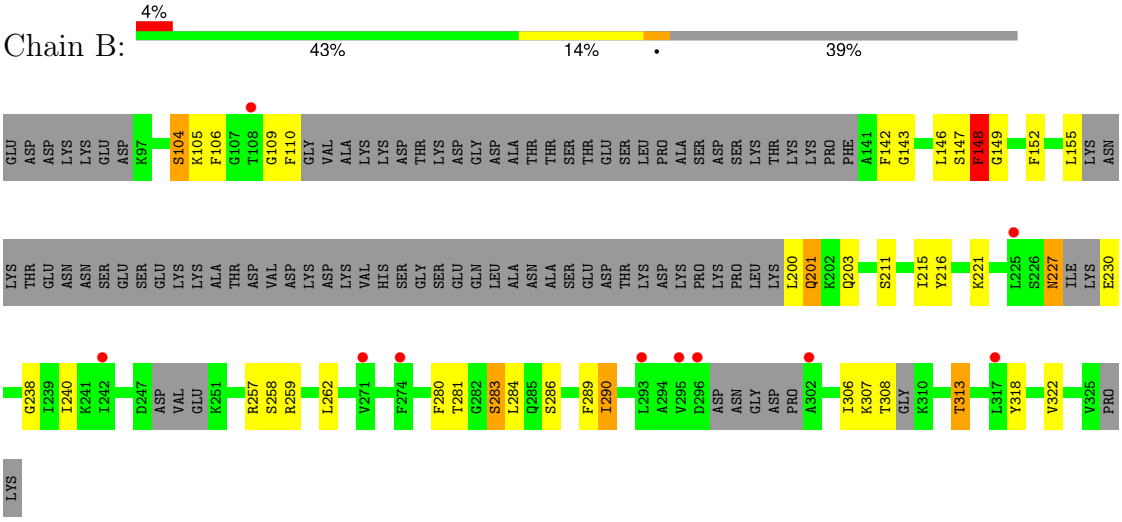
• Molecule 1: Gsp1p

Chain D:



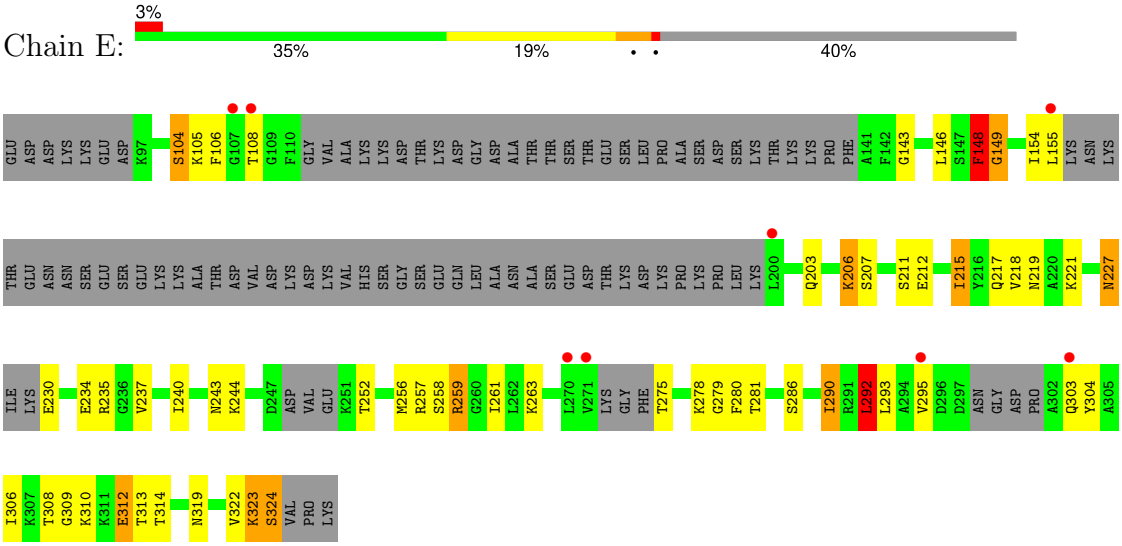
• Molecule 2: Ran-specific GTPase-activating protein 2

Chain B:



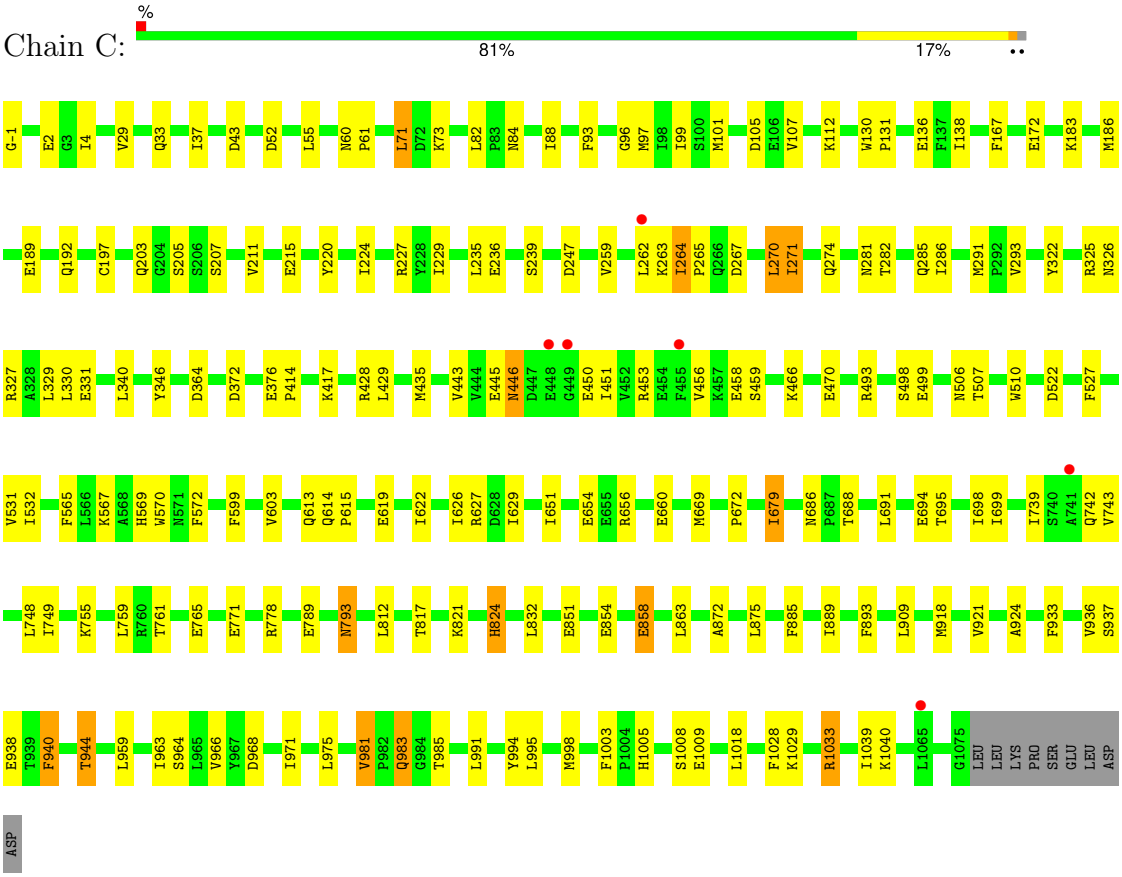
• Molecule 2: Ran-specific GTPase-activating protein 2

Chain E:



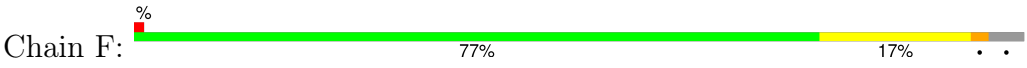
• Molecule 3: Exportin-1

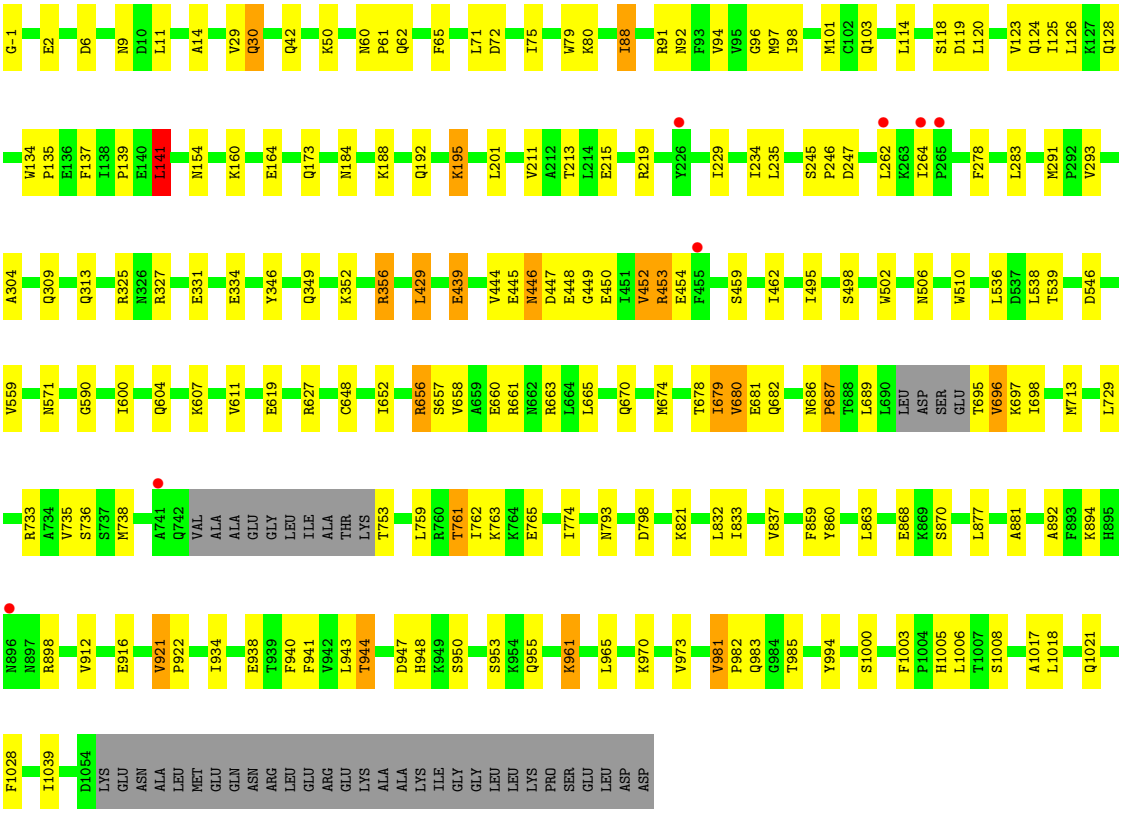
Chain C:



• Molecule 3: Exportin-1

Chain F:




G-1 E2 D6 N9 D10 L11 A14 V29 Q30 Q42 K50 N60 P61 Q62 F65 L71 D72 I75 W79 K80 I88 R91 N92 F93 V94 V95 G96 M97 I98 M101 C102 Q103 L114 S118 D119 L120 V123 Q124 I125 L126 K127 Q128
W134 P135 E136 F137 I138 P139 E140 L141 N154 K160 E164 Q173 N184 K188 Q192 K195 L201 V211 A212 T213 L214 E215 R219 Y226 I229 I234 L235 S245 P246 D247 L262 K263 I264 P265 F278 L283 M291 P292 V293
A304 Q309 Q313 R325 N326 R327 E331 E334 Y346 Q349 K352 R356 L429 E439 V444 E445 N446 D447 E448 G449 E450 I451 V452 R453 E454 P455 S459 I462 I495 S498 W502 N506 W510 L536 D537 L538 T539 D546
V559 N571 G590 I600 Q604 K607 V611 E619 R627 C648 I652 R656 S657 V658 A659 E660 R661 N662 R663 L664 L665 Q670 M674 T678 I679 V680 E681 Q682 N686 P687 T688 L689 L690 LEU ASP SER GLU T695 V696 K697 I698 M713 L729
R733 A734 V735 S736 S737 M738 A741 Q742 VAL ALA ALA GLU GLY LEU ILE ALA THR LYS T753 L759 R760 T761 I762 K763 K764 E765 I774 N793 D798 K821 L832 I833 V837 F859 Y860 L863 E868 K869 S870 L877 A881 A892 F893 K894 H895
N896 N897 R898 V912 E916 V921 P922 I934 E938 T939 F940 F941 V942 L943 T944 D947 H948 K949 S950 S953 K964 Q955 K961 L965 K970 V973 V981 P982 Q983 G984 T985 Y994 S1000 F1003 P1004 H1005 L1006 T1007 S1008 A1017 L1018 Q1021
F1028 I1039 D1054 LYS GLU ASN ALA LEU MET GLU GLN ASN ARG LEU GLU ARG GLU LYS ALA ALA LYS ILE GLY GLY LEU LEU LYS PRO SER GLU LEU ASP ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.49Å 155.95Å 149.82Å 90.00° 106.91° 90.00°	Depositor
Resolution (Å)	33.69 – 2.22 33.69 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.69-2.22) 98.7 (33.69-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.175 , 0.214 0.175 , 0.214	Depositor DCC
R_{free} test set	9411 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 21.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.226 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.776 for H, K, L 0.224 for H, -K, -H-L	Depositor
Outliers	0 of 187295 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22420	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: MG, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.73	0/1531	0.87	1/2079 (0.0%)
1	D	0.72	0/1497	0.88	5/2033 (0.2%)
2	B	0.48	0/1082	0.75	0/1449
2	E	0.52	0/1082	0.85	3/1444 (0.2%)
3	C	0.68	0/8480	0.82	6/11503 (0.1%)
3	F	0.64	0/8202	0.78	1/11129 (0.0%)
All	All	0.66	0/21874	0.81	16/29637 (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
2	B	0	1
2	E	0	2
3	C	0	1
3	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	149	GLY	N-CA-C	-6.59	96.63	113.10
2	E	279	GLY	N-CA-C	-6.58	96.64	113.10
3	F	141	LEU	CA-CB-CG	6.50	130.26	115.30
1	D	142	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	E	292	LEU	CA-CB-CG	5.98	129.05	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	148	PHE	Peptide
3	C	376	GLU	Mainchain
2	E	148	PHE	Peptide
2	E	278	LYS	Peptide
3	F	687	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1492	0	1486	33	0
1	D	1459	0	1453	29	0
2	B	1073	0	1044	28	0
2	E	1074	0	1064	47	0
3	C	8322	0	8330	115	0
3	F	8046	0	8052	122	0
4	A	32	0	12	1	0
4	D	32	0	12	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	84	0	0	2	0
6	B	11	0	0	0	0
6	C	351	0	0	8	1
6	D	86	0	0	1	0
6	E	10	0	0	2	0
6	F	346	0	0	5	1
All	All	22420	0	21453	342	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 342 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:B:280:PHE:O	2:B:286:SER:HB2	1.19	1.28
2:E:308:THR:HG21	2:E:313:THR:OG1	1.48	1.12
2:B:280:PHE:O	2:B:286:SER:CB	2.05	1.02
1:A:34:THR:OG1	1:A:36:GLU:HG2	1.65	0.97
3:C:1033:ARG:HG3	3:C:1033:ARG:HH11	1.30	0.96

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1274:HOH:O	6:F:1158:HOH:O[1_656]	2.17	0.03

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	185/219 (84%)	179 (97%)	6 (3%)	0	100	100
1	D	181/219 (83%)	171 (94%)	9 (5%)	1 (1%)	25	25
2	B	130/238 (55%)	115 (88%)	13 (10%)	2 (2%)	10	7
2	E	128/238 (54%)	112 (88%)	13 (10%)	3 (2%)	6	3
3	C	1038/1049 (99%)	1008 (97%)	29 (3%)	1 (0%)	51	60
3	F	999/1049 (95%)	958 (96%)	40 (4%)	1 (0%)	51	60
All	All	2661/3012 (88%)	2543 (96%)	110 (4%)	8 (0%)	41	45

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	312	GLU
2	E	323	LYS
3	F	681	GLU
2	B	105	LYS

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Mol	Chain	Res	Type
2	E	105	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	157/188 (84%)	150 (96%)	7 (4%)	27 33
1	D	153/188 (81%)	144 (94%)	9 (6%)	19 22
2	B	107/205 (52%)	92 (86%)	15 (14%)	3 2
2	E	109/205 (53%)	90 (83%)	19 (17%)	2 1
3	C	927/955 (97%)	882 (95%)	45 (5%)	25 29
3	F	900/955 (94%)	850 (94%)	50 (6%)	21 23
All	All	2353/2696 (87%)	2208 (94%)	145 (6%)	18 19

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	452	VAL
3	F	1000	SER
3	F	571	ASN
3	F	761	THR
3	C	656	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	227	ASN
3	F	49	GLN
3	F	1005	HIS
2	E	269	GLN
3	F	18	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	A	301	5	29,34,34	1.59	5 (17%)	35,54,54	1.68	7 (20%)
4	GTP	D	301	5	29,34,34	1.44	4 (13%)	35,54,54	1.62	9 (25%)

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	A	301	5	-	5/18/38/38	0/3/3/3
4	GTP	D	301	5	-	7/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GTP	PB-O3A	5.23	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	GTP	PA-O3A	4.28	1.64	1.59
4	D	301	GTP	O4'-C1'	3.23	1.45	1.40
4	A	301	GTP	O4'-C1'	2.58	1.44	1.40
4	A	301	GTP	PB-O3B	-2.53	1.56	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	301	GTP	C8-N7-C5	3.97	109.30	102.55
4	A	301	GTP	O3A-PA-O1A	3.92	122.49	110.70
4	D	301	GTP	C2-N1-C6	-3.35	118.97	125.11
4	A	301	GTP	O2B-PB-O3B	3.30	116.18	107.27
4	D	301	GTP	C8-N7-C5	3.09	107.81	102.55

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GTP	C5'-O5'-PA-O2A
4	D	301	GTP	C5'-O5'-PA-O3A
4	D	301	GTP	C5'-O5'-PA-O2A
4	D	301	GTP	O4'-C4'-C5'-O5'
4	D	301	GTP	C3'-C4'-C5'-O5'

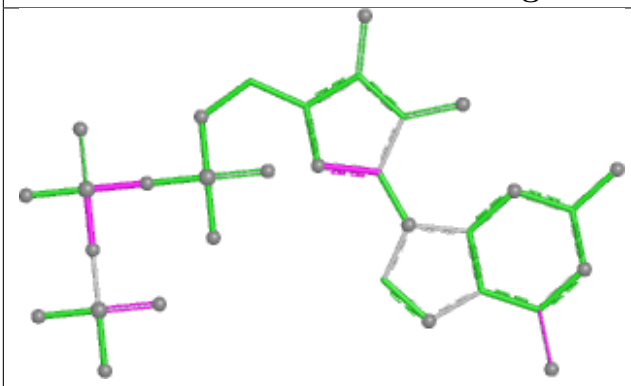
There are no ring outliers.

1 monomer is involved in 1 short contact:

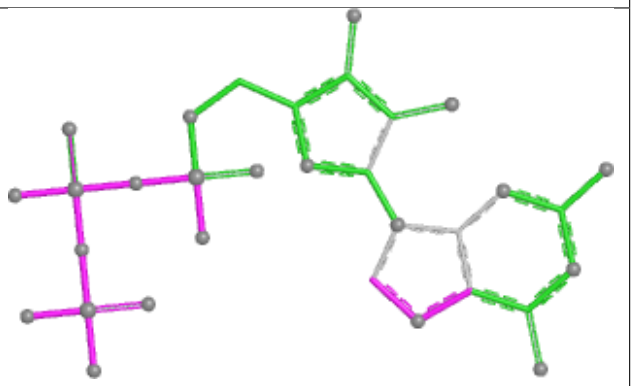
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GTP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

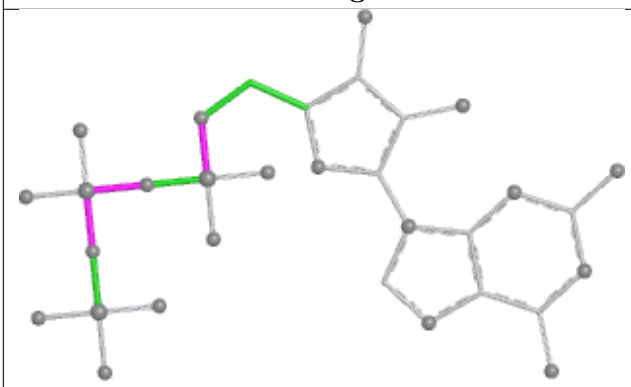
Ligand GTP A 301



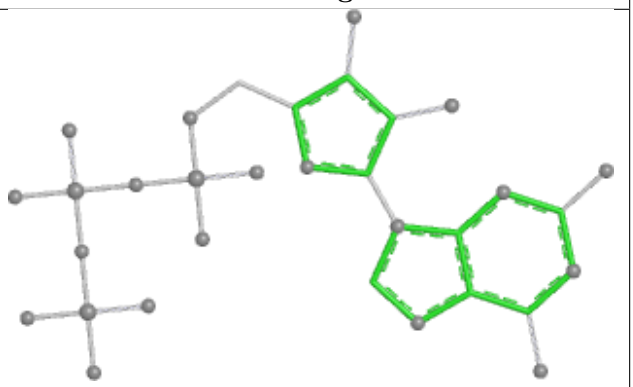
Bond lengths



Bond angles

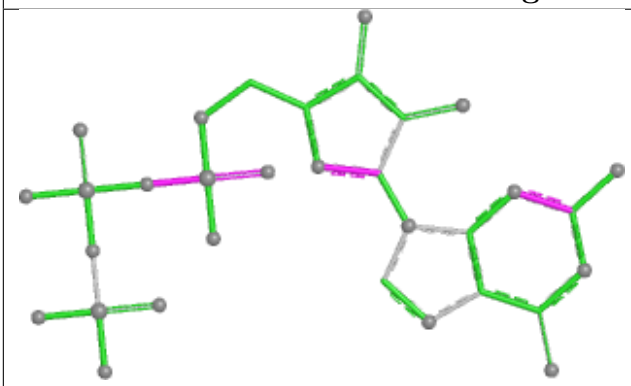


Torsions

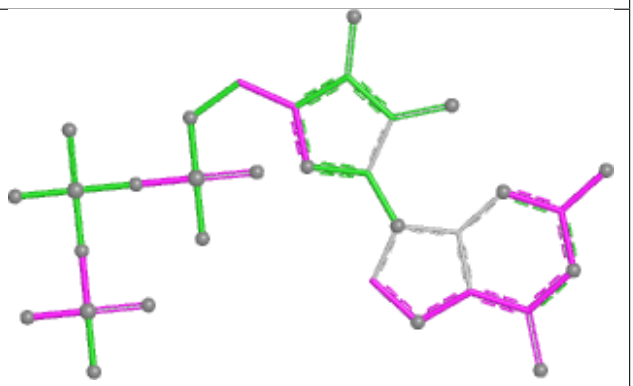


Rings

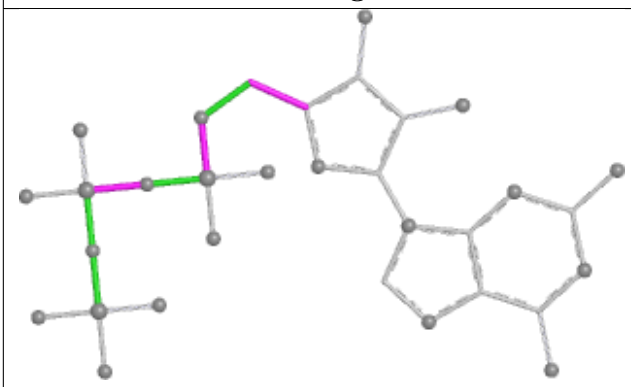
Ligand GTP D 301



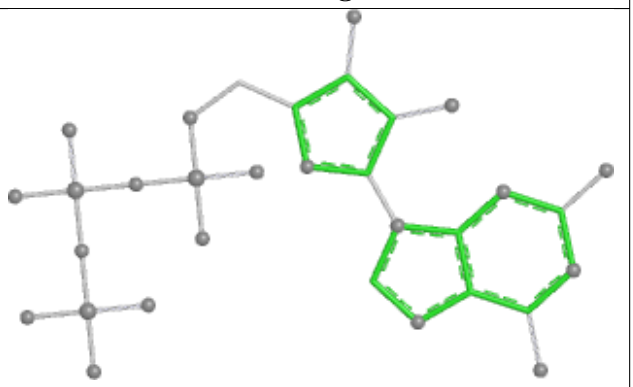
Bond lengths



Bond angles



Torsions



Rings

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, 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	189/219 (86%)	-0.11	4 (2%)	63	61	19, 32, 80, 108	0
1	D	185/219 (84%)	-0.25	1 (0%)	91	90	22, 34, 61, 76	0
2	B	144/238 (60%)	0.47	10 (6%)	16	15	41, 69, 90, 104	0
2	E	142/238 (59%)	0.33	8 (5%)	24	23	34, 62, 91, 105	0
3	C	1040/1049 (99%)	-0.14	6 (0%)	89	88	17, 36, 60, 98	0
3	F	1005/1049 (95%)	-0.11	7 (0%)	87	86	18, 39, 65, 101	0
All	All	2705/3012 (89%)	-0.08	36 (1%)	77	75	17, 39, 73, 108	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	295	VAL	5.2
3	F	264	ILE	4.8
2	B	295	VAL	4.3
3	C	448	GLU	4.2
2	B	302	ALA	3.8

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 monosaccharides in this entry.

6.4 Ligands (i)

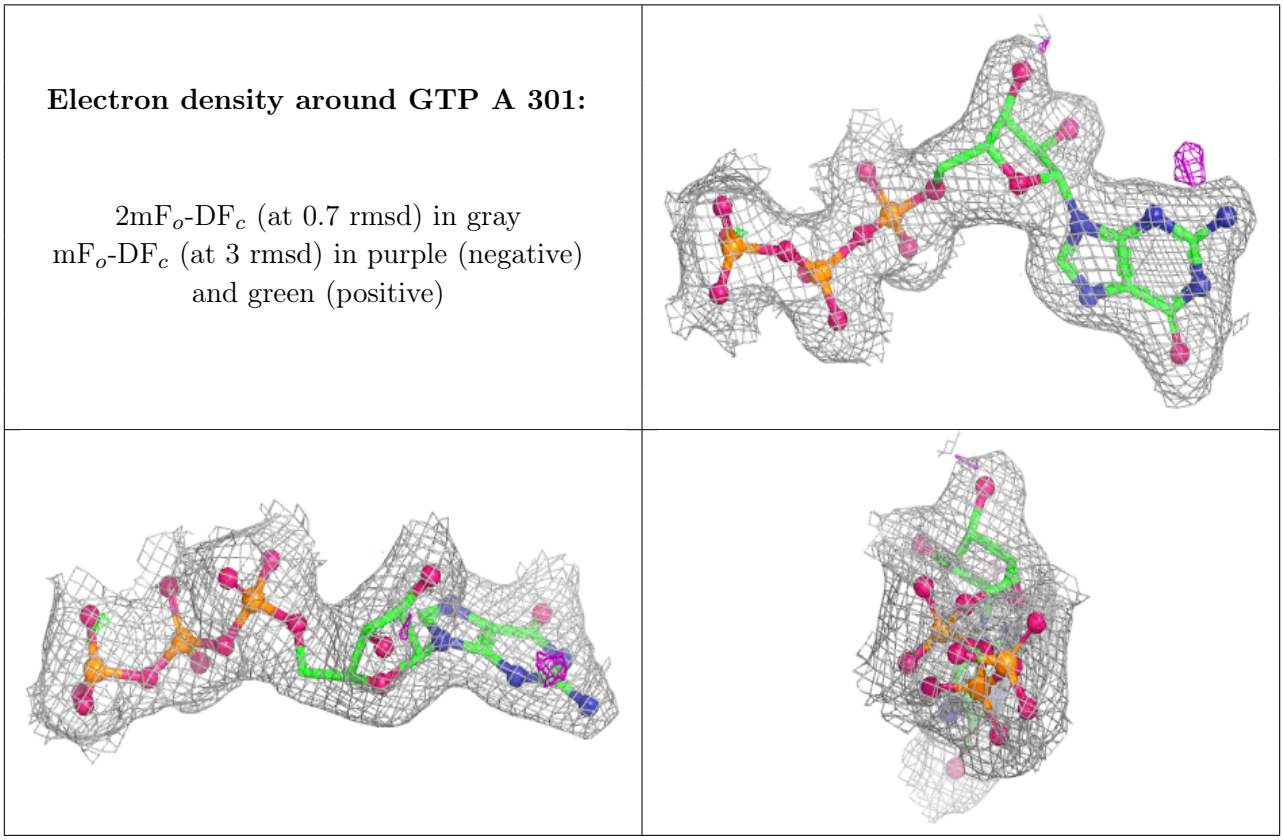
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GTP	A	301	32/32	0.98	0.13	21,27,30,31	0
5	MG	A	302	1/1	0.98	0.10	24,24,24,24	0
4	GTP	D	301	32/32	0.99	0.12	23,28,34,38	0
5	MG	D	302	1/1	0.99	0.08	27,27,27,27	0

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

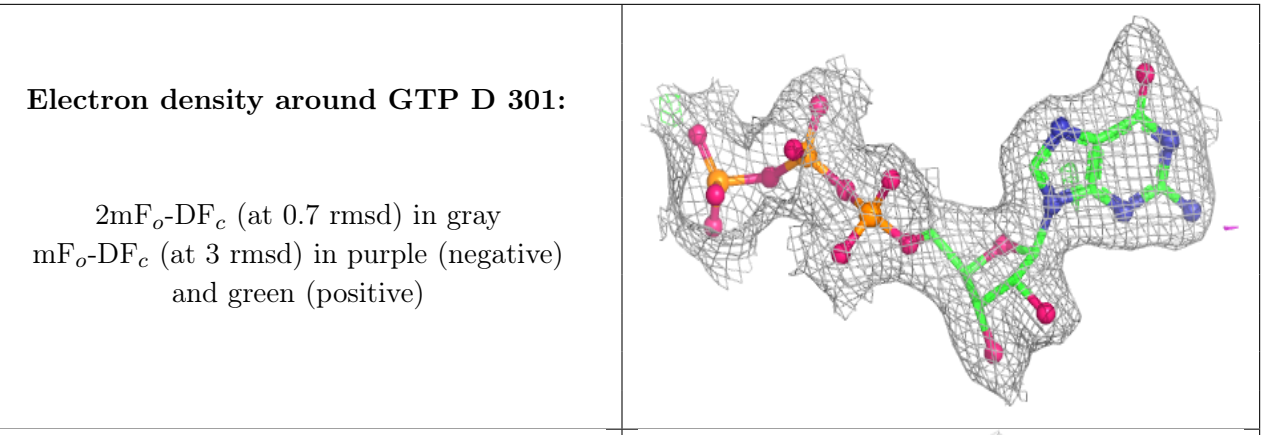
Electron density around GTP A 301:

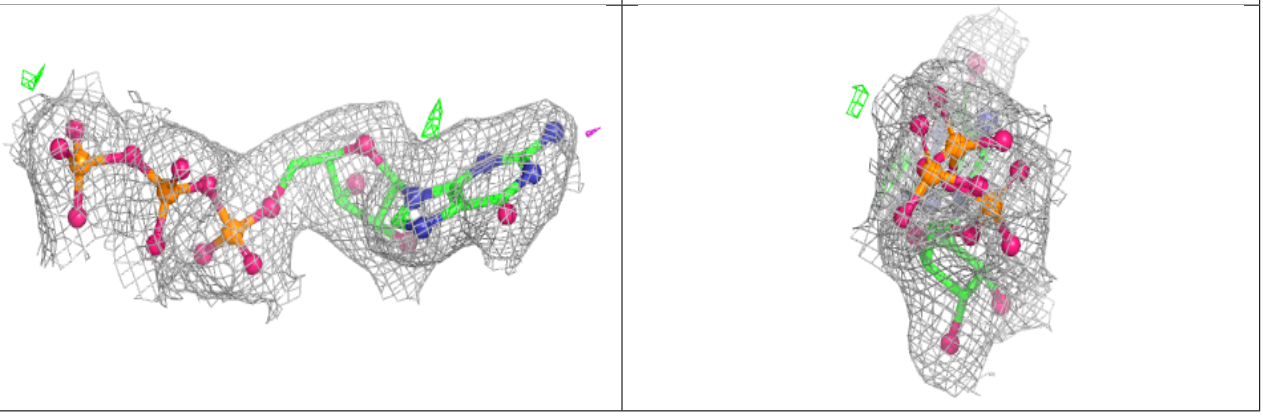
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP D 301:

$2mF_o$-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.