wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 02:57 AM EDT

PDB ID	:	3NBZ
Title	:	Crystal structure of the HIV-1 Rev NES-CRM1-RanGTP nuclear export complex (crystal I)
Authors	:	Guttler, T.; Madl, T.; Neumann, P.; Deichsel, D.; Corsini, L.; Monecke, T.; Ficner, R.; Sattler, M.; Gorlich, D.
Deposited on	:	2010-06-04
Resolution	:	2.80 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:

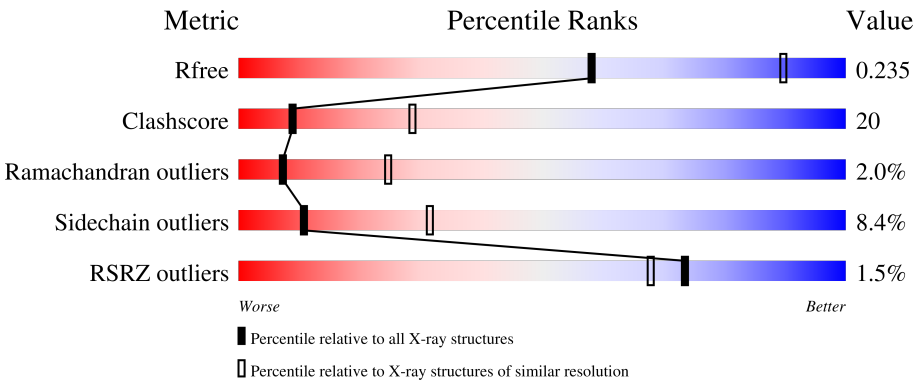
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	1073	% 58% 34% • •
1	D	1073	% 57% 35% • •
2	B	362	2% 42% 33% 6% 20%
2	E	362	2% 45% 32% • 19%

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Mol	Chain	Length	Quality of chain
3	C	176	% 61% 31% 6%
3	F	176	% 56% 37% 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25144 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 Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1038	8394	5387	1411	1543	53	0	0	0
1	D	1038	8394	5387	1411	1543	53	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 2 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	291	2339	1491	403	430	15	0	0	0
2	E	293	2354	1500	405	434	15	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
B	1	PRO	-	expression tag	UNP O95149
B	2	VAL	-	expression tag	UNP O95149
B	3	PRO	-	expression tag	UNP O95149
B	4	LEU	-	expression tag	UNP O95149
B	5	GLN	-	expression tag	UNP O95149
B	6	LEU	-	expression tag	UNP O95149

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	PRO	-	expression tag	UNP O95149
B	8	PRO	-	expression tag	UNP O95149
B	9	LEU	-	expression tag	UNP O95149
B	10	GLU	-	expression tag	UNP O95149
B	11	ARG	-	expression tag	UNP O95149
B	12	LEU	-	expression tag	UNP O95149
B	13	THR	-	expression tag	UNP O95149
B	14	LEU	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149
E	1	PRO	-	expression tag	UNP O95149
E	2	VAL	-	expression tag	UNP O95149
E	3	PRO	-	expression tag	UNP O95149
E	4	LEU	-	expression tag	UNP O95149
E	5	GLN	-	expression tag	UNP O95149
E	6	LEU	-	expression tag	UNP O95149
E	7	PRO	-	expression tag	UNP O95149
E	8	PRO	-	expression tag	UNP O95149
E	9	LEU	-	expression tag	UNP O95149
E	10	GLU	-	expression tag	UNP O95149
E	11	ARG	-	expression tag	UNP O95149
E	12	LEU	-	expression tag	UNP O95149
E	13	THR	-	expression tag	UNP O95149
E	14	LEU	-	expression tag	UNP O95149

- Molecule 3 is a protein called GTP-binding nuclear protein Ran.

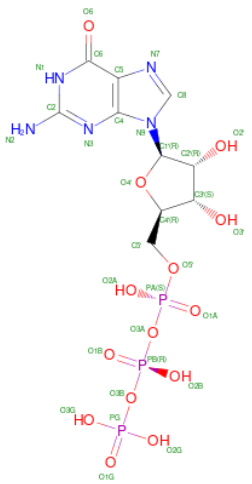
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	173	1405	914	246	240	5	0	0	0
			Total	C	N	O	S			
3	F	173	1405	914	246	240	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	engineered mutation	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826

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

GTP



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	C	1	1	1	0	0
5	F	1	1	1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	C	1	1	1	0	0
6	D	1	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	237	237	237	0	0

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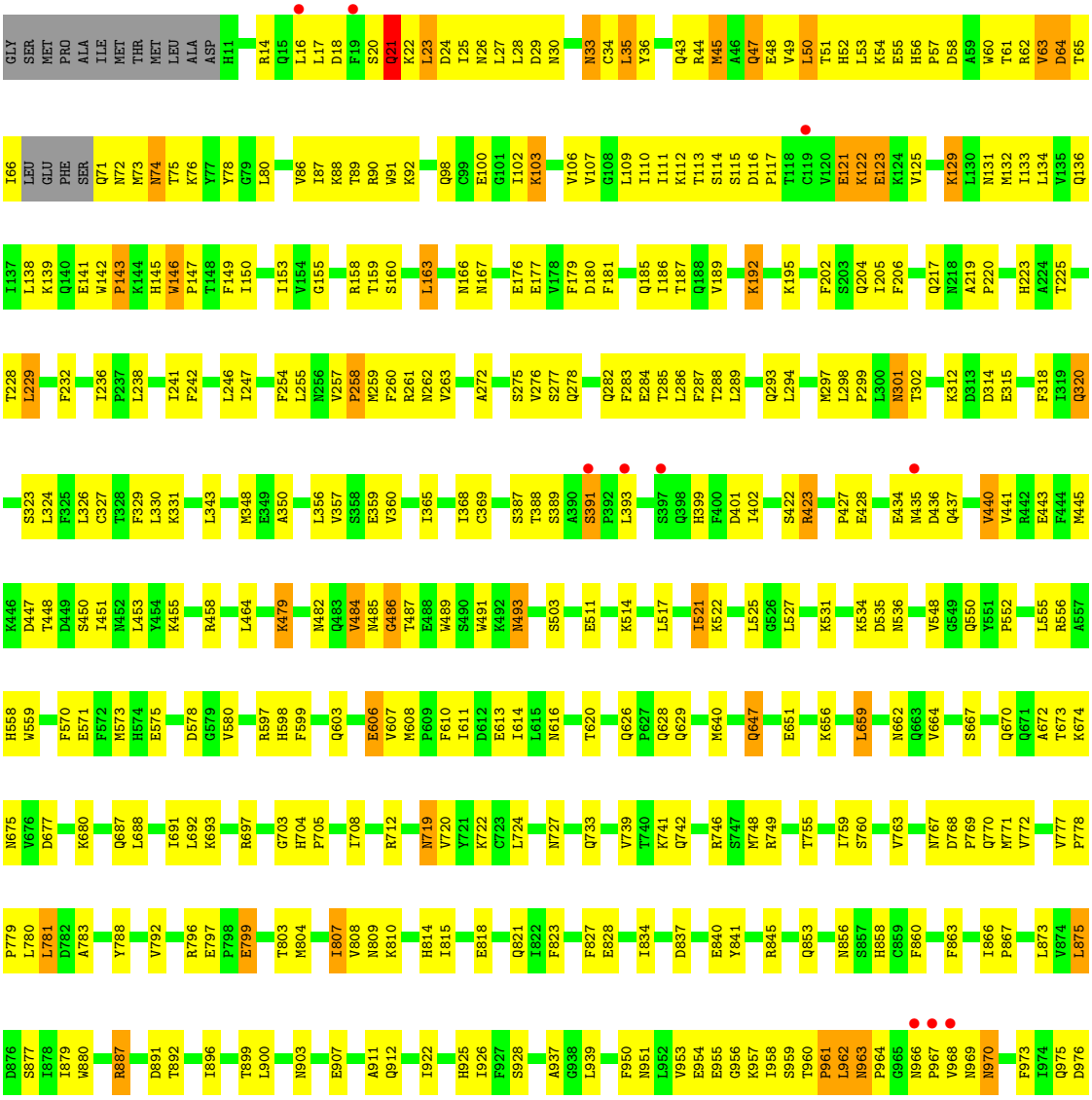
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	94	Total O 94 94	0	0
7	C	53	Total O 53 53	0	0
7	D	279	Total O 279 279	0	0
7	E	71	Total O 71 71	0	0
7	F	51	Total O 51 51	0	0

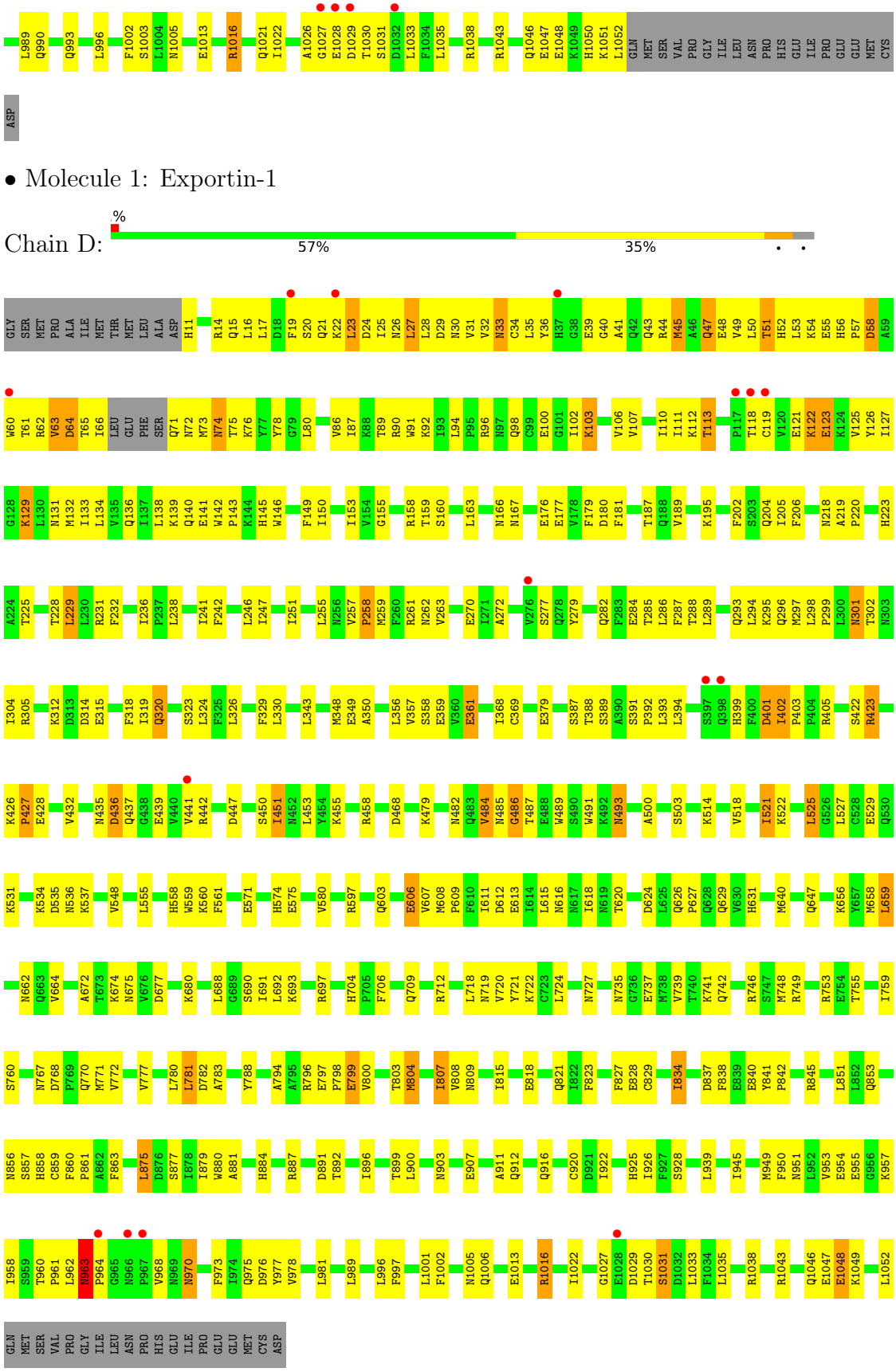
3 Residue-property plots (i)

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: Exportin-1

Chain A:





• Molecule 1: Exportin-1

Chain D: % 57% 35%

• Molecule 2: Snurportin-1

Chain B: 2% 42% 33% 6% 20%

GLY SER PRO VAL P3 L4 Q5 L6 P7 P8 L9 E10 R11 L12 T13 L14 S15 Q16 D17 L18 N19 H25 P26 R27 Y31 K32 S33 K34 Y35 L38 E39 Q40 S41 E42 R43 R44 R45 E49 K52 S53 K54 R55 H61 L65 D69 W70 T71 G72 M73 GLU SER GLU

GLU GLU ASN LYS LYS ASP ASP GLU GLU MET ASP ILE ASP THR VAL K92 P95 K96 N100 Q101 L104 S105 E106 I109 D110 V111 P112 L115 I120 V121 V122 V123 G127 K128 R129 A130 S135 S138 Y142 N150 R151 F152 S153 S154 L155 G158 G159 N160

R161 R162 N163 S164 Y169 T170 I171 Y176 Q181 T182 Y183 Y184 V188 M189 C190 W191 R192 D198 S210 K211 L212 P213 E214 E215 E216 G217 K223 L224 N225 N234 F235 E240 S241 L242 C243 D244 V245 L246 S247 M248 F252 L257 L258 F259 Y260 H261 K262 Q263 T264

H265 S270 T271 P272 L273 V274 L277 Y280 M281 V282 S283 D284 V285 L286 G287 V288 A289 V290 P291 A292 G293 P294 L295 T296 T297 LYS PRO ASP TYR ALA GLY HIS GLN LEU GLN GLN ILE MET GLU HIS LYS LYS SER GLN LYS GLU GLY MET LYS GLU LYS LEU THR HIS LYS ALA SER

GLU ASN GLY HIS TYR GLU LEU GLU HIS LEU SER THR PRO LYS LEU LYS GLY S347 S350 P351 D352 H353 C356 L357 M358 E359 N360

- Molecule 2: Snurportin-1

Chain E: 2% 45% 32% 19%

GLY SER PRO VAL P3 L4 Q5 L6 P7 P8 L9 E10 R11 L12 T13 L14 S15 Q16 D17 L18 N19 H25 P26 S29 Q30 Y31 K32 S33 K34 L38 E39 Q40 S41 E42 R43 R44 R45 L48 E49 L50 Q51 K52 S53 K54 R55 V59 N60 H61 R64 L65 W70 T71 G72

M73 GLU SER GLU GLU GLU ASN LYS LYS ASP ASP GLU GLU MET ASP ILE ASP T90 V91 K92 K93 L94 P95 K96 N100 Q101 S105 E106 I109 D110 V111 P112 L115 E118 W119 I120 V121 V122 V123 K128 R129 A130 S135 S138 Y142 N150 L155 R161

R162 N163 S164 T165 A166 K167 D168 Y169 T170 I171 Y176 Q181 T182 Y183 Y184 D187 V188 M189 C190 W191 R192 P195 M208 H209 S210 K211 L212 P213 E216 N225 N234 F235 E240 D244 V245 L246 S247 M248 D249 F250 P251 F252 L258 F259 Y260 H261 K262 Q263 T264

H265 S270 T271 P272 L273 V274 L277 R278 P279 Y280 M281 V282 L286 V290 P291 A292 G293 P294 T297 LYS PRO ASP TYR ALA GLY HIS GLN LEU GLN GLN ILE MET GLU HIS LYS LYS SER GLN LYS GLU GLY MET LYS GLU LYS LEU THR HIS LYS ALA SER GLU ASN GLY HIS

TYR GLU LEU GLU HIS LEU SER THR PRO LYS LEU LYS GLY S347 S348 H349 S350 P351 D352 H353 P354 L357 M358 E359 N360

- Molecule 3: GTP-binding nuclear protein Ran

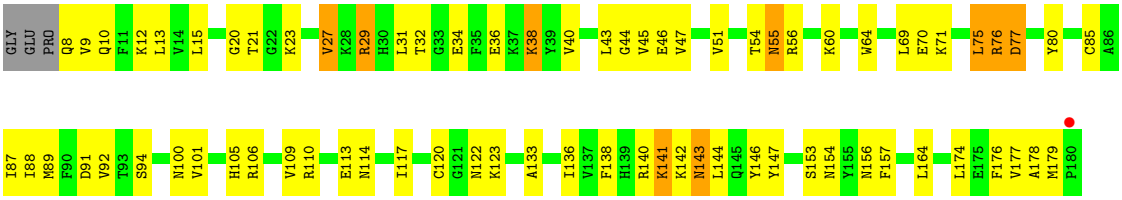
Chain C: % 61% 31% 6%

GLY GLU PRO Q8 V9 Q10 F11 K12 L13 V14 L15 T21 G22 K23 V27 K28 R29 H30 L31 T32 G33 E34 F35 E36 K37 K38 Y39 V40 A41 T42 L43 G44 V45 E46 V51 T54 N55 R56 K60 W64 A67 E70 L75 R76 D77 Y80 C85 A86 I87

I88 M89 V101 P102 H105 R106 V109 R110 I117 N122 K123 F138 H139 R140 K141 K142 N143 L144 D148 S153 N154 Y155 N156 F157 E158 K159 P160 L164 L174 E175 F176 V177 A178 M179 P180

• Molecule 3: GTP-binding nuclear protein Ran

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.66Å 224.62Å 164.02Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	38.90 – 2.80 38.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.1 (38.90-2.80) 81.4 (38.90-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.226 , 0.285 0.226 , 0.235	Depositor DCC
R_{free} test set	5702 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.119 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25144	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.31	0/8566	0.47	0/11604
1	D	0.31	0/8566	0.48	0/11604
2	B	0.34	0/2404	0.53	0/3263
2	E	0.34	0/2419	0.53	0/3283
3	C	0.32	0/1440	0.48	0/1945
3	F	0.32	0/1440	0.49	0/1945
All	All	0.32	0/24835	0.49	0/33644

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8394	0	8460	325	0
1	D	8394	0	8460	347	0
2	B	2339	0	2295	114	0
2	E	2354	0	2311	110	0
3	C	1405	0	1434	52	0
3	F	1405	0	1434	62	0
4	C	32	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	32	0	12	2	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	237	0	0	17	0
7	B	94	0	0	7	0
7	C	53	0	0	6	0
7	D	279	0	0	22	0
7	E	71	0	0	3	0
7	F	51	0	0	6	0
All	All	25144	0	24418	992	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 20.

The worst 5 of 992 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:E:290:VAL:H	2:E:291:PRO:HD3	1.09	1.10
2:B:52:LYS:HZ3	2:B:264:THR:HA	1.17	1.08
2:E:52:LYS:HZ3	2:E:264:THR:HA	1.18	1.02
1:D:45:MET:HE3	3:F:44:GLY:HA3	1.46	0.98
1:A:131:ASN:HD21	1:A:166:ASN:HD21	1.12	0.95

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	1034/1073 (96%)	931 (90%)	85 (8%)	18 (2%)	9 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1034/1073 (96%)	933 (90%)	83 (8%)	18 (2%)	9	29
2	B	285/362 (79%)	251 (88%)	23 (8%)	11 (4%)	3	10
2	E	287/362 (79%)	249 (87%)	28 (10%)	10 (4%)	3	12
3	C	171/176 (97%)	157 (92%)	13 (8%)	1 (1%)	25	56
3	F	171/176 (97%)	154 (90%)	16 (9%)	1 (1%)	25	56
All	All	2982/3222 (93%)	2675 (90%)	248 (8%)	59 (2%)	7	24

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	963	ASN
2	B	216	GLU
1	D	123	GLU
1	D	963	ASN

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	942/973 (97%)	869 (92%)	73 (8%)	13	35
1	D	942/973 (97%)	870 (92%)	72 (8%)	13	36
2	B	263/327 (80%)	236 (90%)	27 (10%)	7	21
2	E	265/327 (81%)	244 (92%)	21 (8%)	12	34
3	C	152/154 (99%)	136 (90%)	16 (10%)	7	20
3	F	152/154 (99%)	133 (88%)	19 (12%)	4	14
All	All	2716/2908 (93%)	2488 (92%)	228 (8%)	11	31

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	156	ASN

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Mol	Chain	Res	Type
3	F	76	ARG
1	D	320	GLN
3	F	71	LYS
2	E	189	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	55	ASN
2	E	61	HIS
1	D	166	ASN
2	E	51	GLN
3	F	30	HIS

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 6 ligands modelled in this entry, 4 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	F	217	5	26,34,34	1.12	1 (3%)	32,54,54	1.53	5 (15%)
4	GTP	C	217	5	26,34,34	1.16	2 (7%)	32,54,54	1.57	6 (18%)

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	217	5	-	7/18/38/38	0/3/3/3
4	GTP	C	217	5	-	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	C	217	GTP	C5-C6	-3.73	1.39	1.47
4	F	217	GTP	C5-C6	-3.70	1.39	1.47
4	C	217	GTP	O4'-C4'	-2.03	1.40	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	217	GTP	PB-O3B-PG	-4.55	117.22	132.83
4	F	217	GTP	PA-O3A-PB	-4.08	118.84	132.83
4	F	217	GTP	PB-O3B-PG	-3.20	121.83	132.83
4	C	217	GTP	C8-N7-C5	3.16	109.02	102.99
4	C	217	GTP	C5-C6-N1	3.07	119.37	113.95

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	217	GTP	PB-O3B-PG-O3G
4	F	217	GTP	PB-O3B-PG-O2G
4	F	217	GTP	C5'-O5'-PA-O3A
4	F	217	GTP	O4'-C4'-C5'-O5'
4	F	217	GTP	C3'-C4'-C5'-O5'

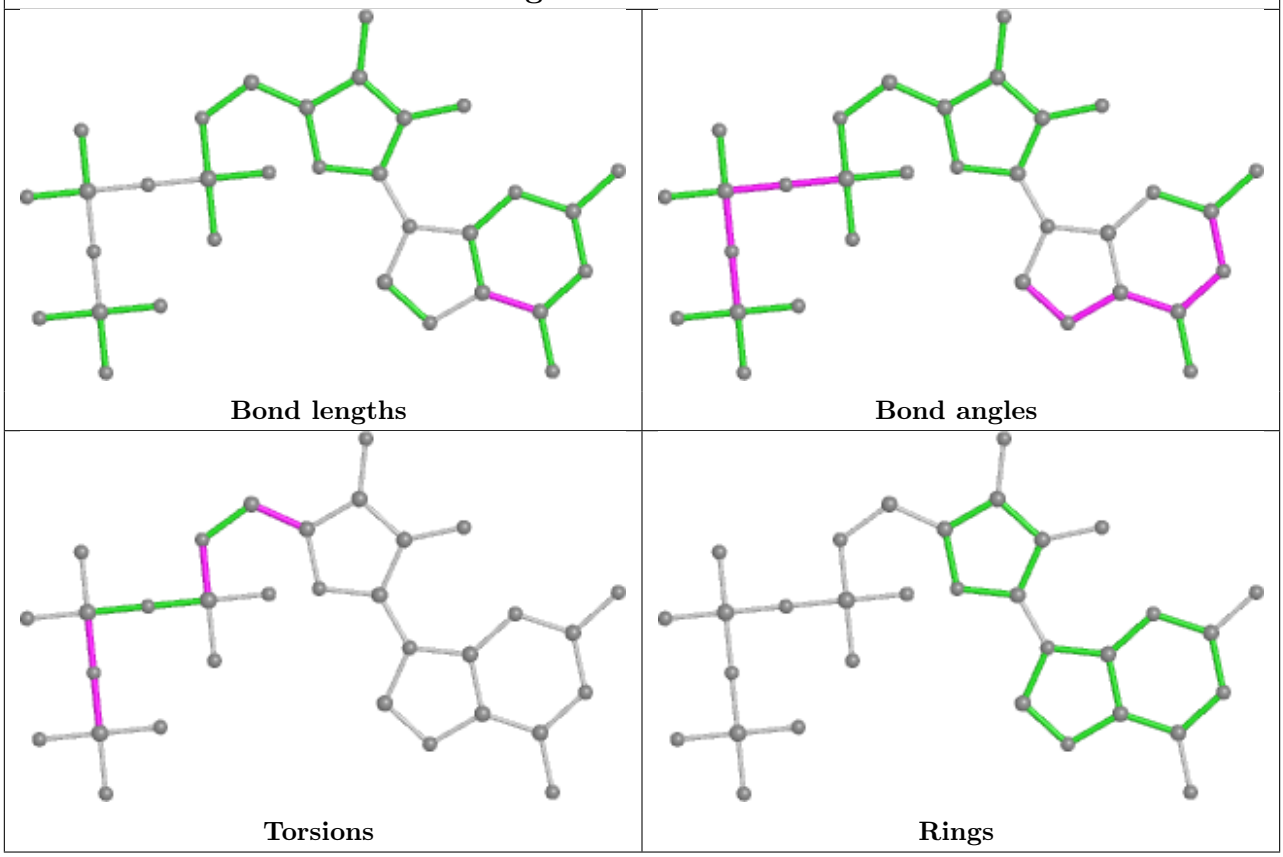
There are no ring outliers.

2 monomers are involved in 6 short contacts:

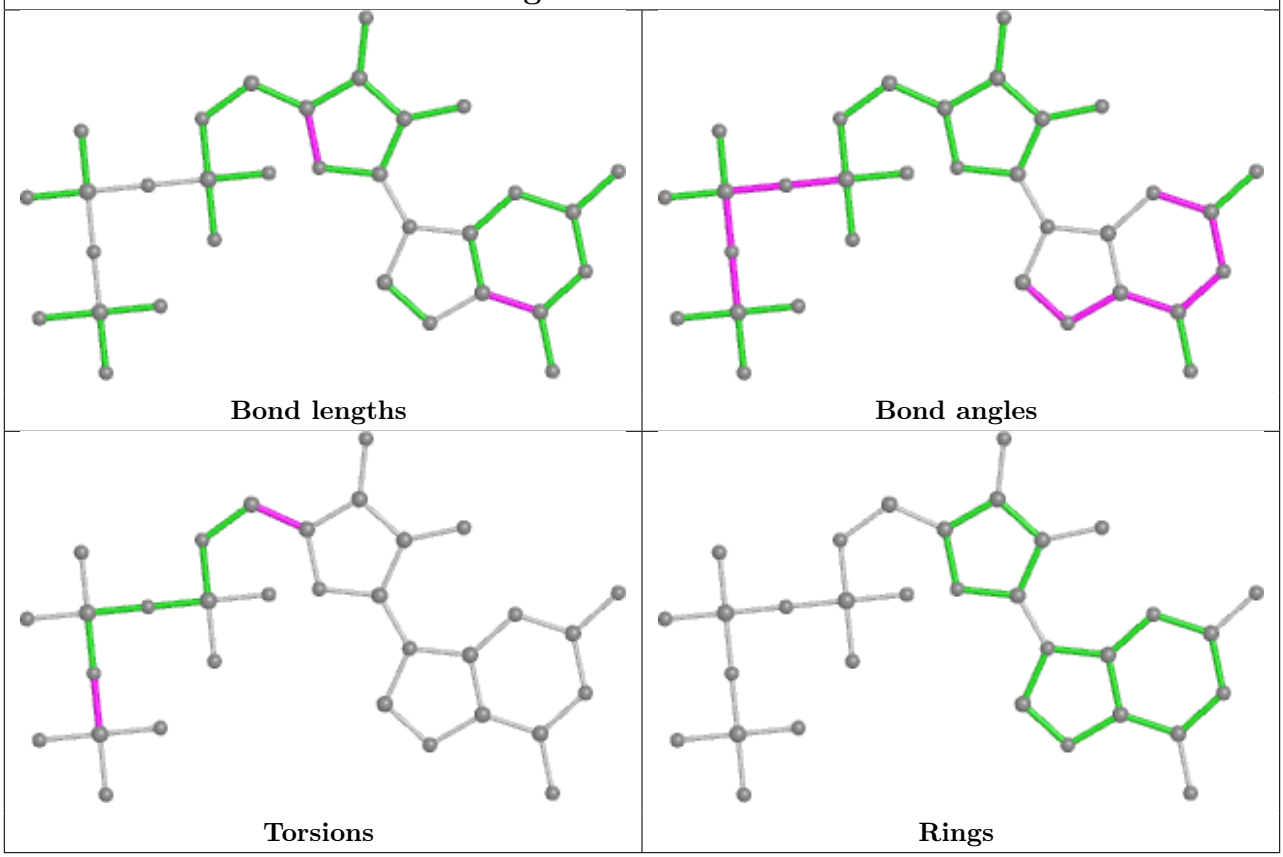
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	217	GTP	2	0
4	C	217	GTP	4	0

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

Ligand GTP F 217



Ligand GTP C 217



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	1038/1073 (96%)	-0.21	14 (1%)	77	72	14, 47, 107, 152	0
1	D	1038/1073 (96%)	-0.17	15 (1%)	75	70	14, 47, 103, 176	0
2	B	291/362 (80%)	-0.12	8 (2%)	54	44	15, 44, 116, 167	0
2	E	293/362 (80%)	-0.13	7 (2%)	59	49	15, 45, 123, 167	0
3	C	173/176 (98%)	-0.32	1 (0%)	89	86	21, 39, 79, 132	0
3	F	173/176 (98%)	-0.29	1 (0%)	89	86	20, 39, 79, 106	0
All	All	3006/3222 (93%)	-0.19	46 (1%)	73	68	14, 45, 106, 176	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	966	ASN	6.6
1	A	967	PRO	5.9
2	B	32	LYS	5.8
1	D	1028	GLU	4.8
2	E	360	ASN	4.7

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 monosaccharides in this entry.

6.4 Ligands (i)

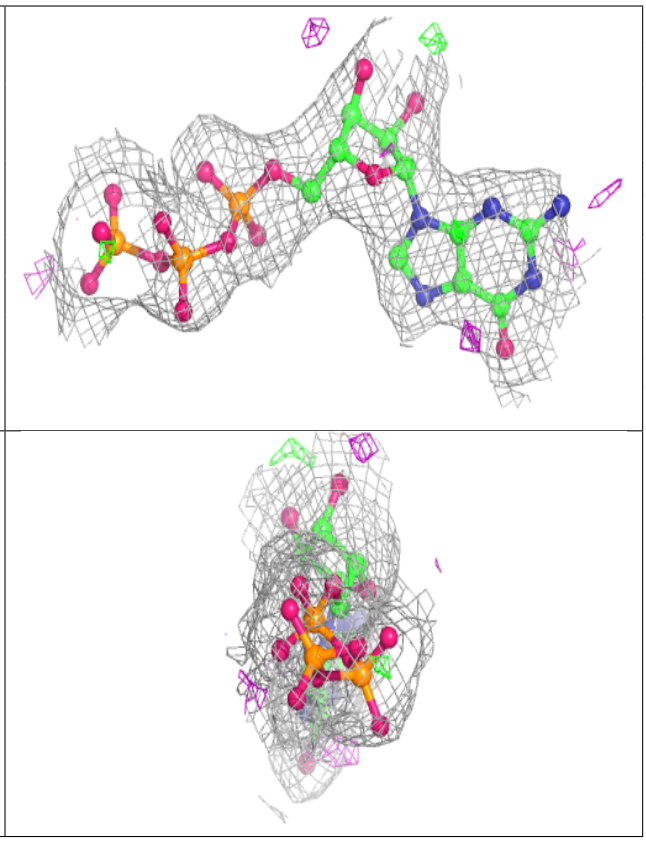
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	D	1072	1/1	0.85	0.19	52,52,52,52	0
6	NA	C	1	1/1	0.93	0.20	42,42,42,42	0
5	MG	F	218	1/1	0.95	0.17	26,26,26,26	0
4	GTP	C	217	32/32	0.97	0.15	12,29,37,71	0
4	GTP	F	217	32/32	0.97	0.16	16,34,50,56	0
5	MG	C	218	1/1	0.97	0.13	14,14,14,14	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.

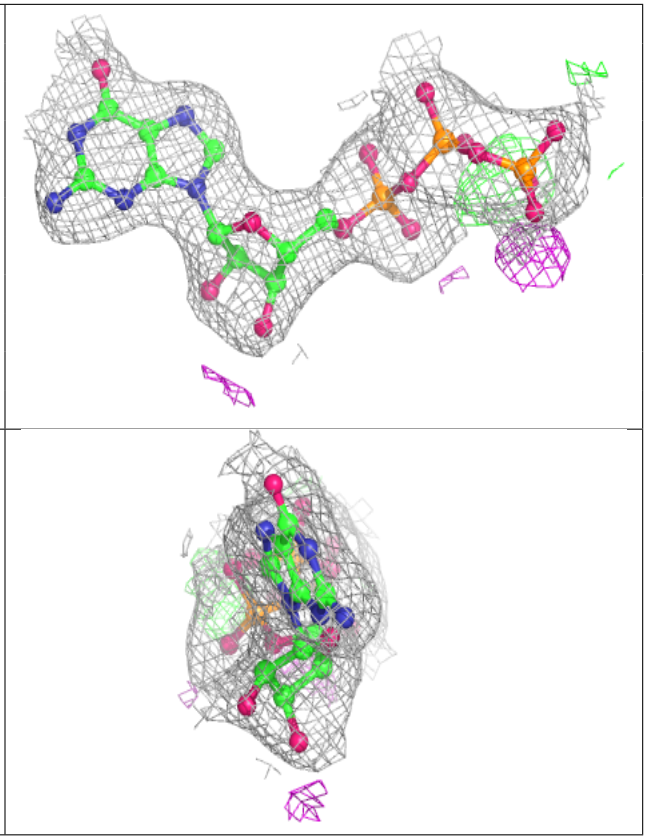
Electron density around GTP C 217:

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 217:

$2mF_o$-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.