wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 03:10 PM JST

PDB ID	:	7D74
EMDB ID	:	EMD-30601
Title	:	Cryo-EM structure of GMPPA/GMPPB complex bound to GTP (state II)
Authors	:	Zheng, L.; Liu, Z.; Wang, Y.; Yang, F.; Wang, J.; Qing, J.; cai, X.; Mo, X.; Gao, N.; Jia, D.
Deposited on	:	2020-10-02
Resolution	:	3.10 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

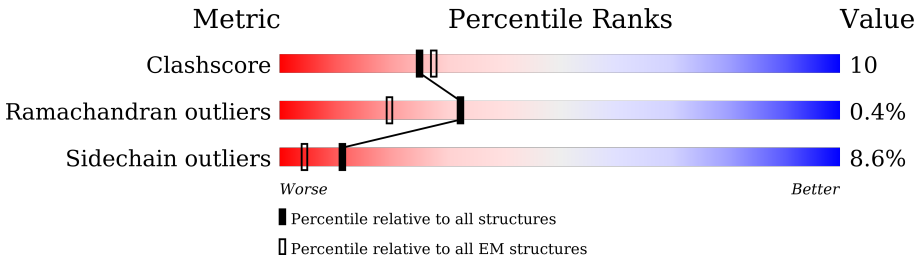
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	86% 9%
1	B	420	86% 10%
1	C	420	5% 83% 12%
1	D	420	85% 10%
2	E	360	82% 69% 28%
2	F	360	61% 72% 24%
2	G	360	81% 72% 24%
2	H	360	58% 77% 21%

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Mol	Chain	Length	Quality of chain
2	I	360	65% 75% 23%
2	J	360	85% 67% 28% 5%
2	K	360	57% 78% 20%
2	L	360	82% 70% 25%

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
3	GTP	E	401	-	-	X	-
3	GTP	F	401	-	-	X	-
3	GTP	G	401	-	-	X	-
3	GTP	H	401	-	-	X	-
3	GTP	J	401	-	-	X	-
3	GTP	K	401	-	-	X	-
3	GTP	L	401	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35353 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

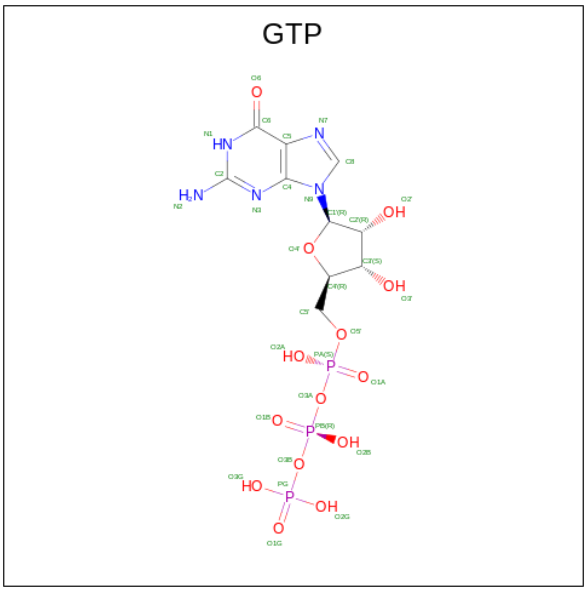
- Molecule 1 is a protein called Mannose-1-phosphate guanyltransferase alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	406	Total 3167	C 2028	N 560	O 568	S 11	0	0
1	D	406	Total 3167	C 2028	N 560	O 568	S 11	0	0
1	B	406	Total 3167	C 2028	N 560	O 568	S 11	0	0
1	C	406	Total 3167	C 2028	N 560	O 568	S 11	0	0

- Molecule 2 is a protein called Mannose-1-phosphate guanyltransferase beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	360	Total 2785	C 1769	N 487	O 507	S 22	0	0
2	F	360	Total 2789	C 1772	N 488	O 507	S 22	0	0
2	G	359	Total 2782	C 1767	N 487	O 506	S 22	0	0
2	H	360	Total 2789	C 1772	N 488	O 507	S 22	0	0
2	I	360	Total 2789	C 1772	N 488	O 507	S 22	0	0
2	J	360	Total 2789	C 1772	N 488	O 507	S 22	0	0
2	K	360	Total 2789	C 1772	N 488	O 507	S 22	0	0
2	L	360	Total 2789	C 1772	N 488	O 507	S 22	0	0

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



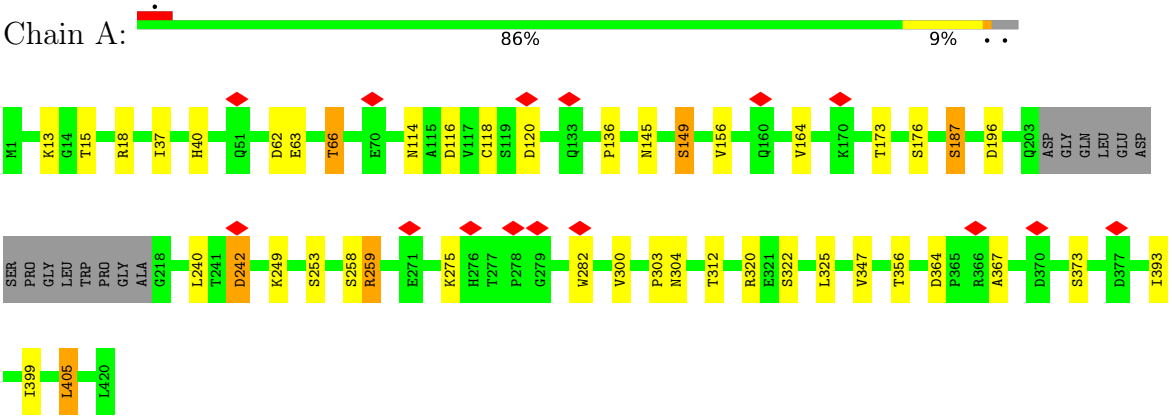
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	L	1	Total	C	N	O	P	0
			32	10	5	14	3	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

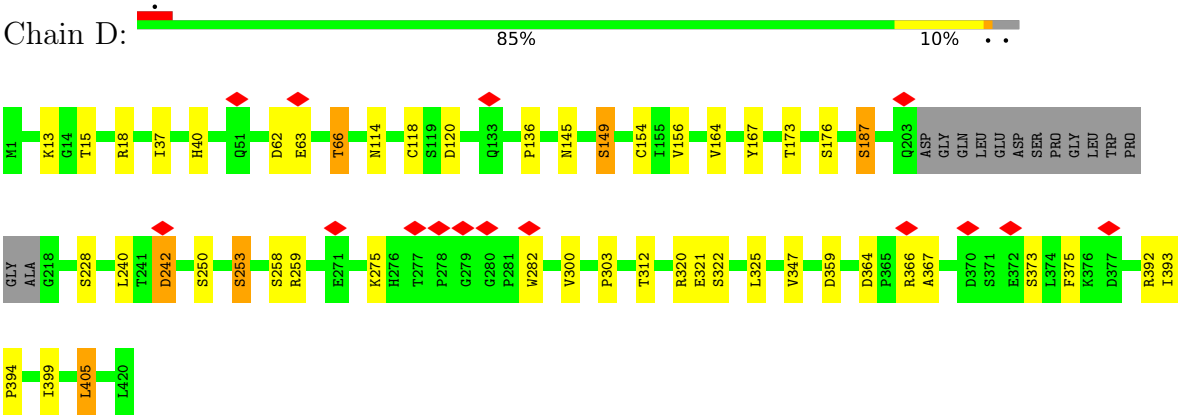
• Molecule 1: Mannose-1-phosphate guanyltransferase alpha

Chain A:



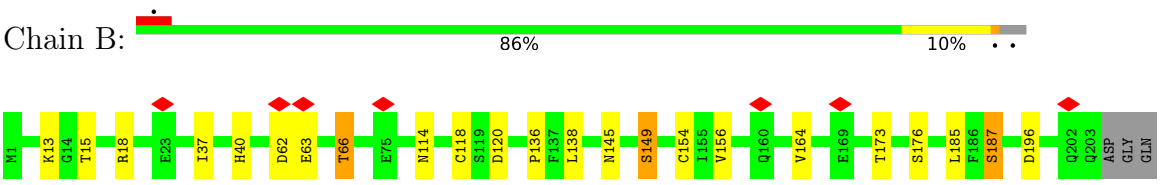
• Molecule 1: Mannose-1-phosphate guanyltransferase alpha

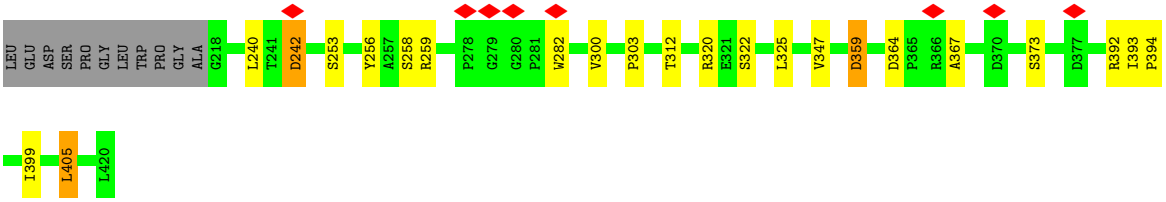
Chain D:



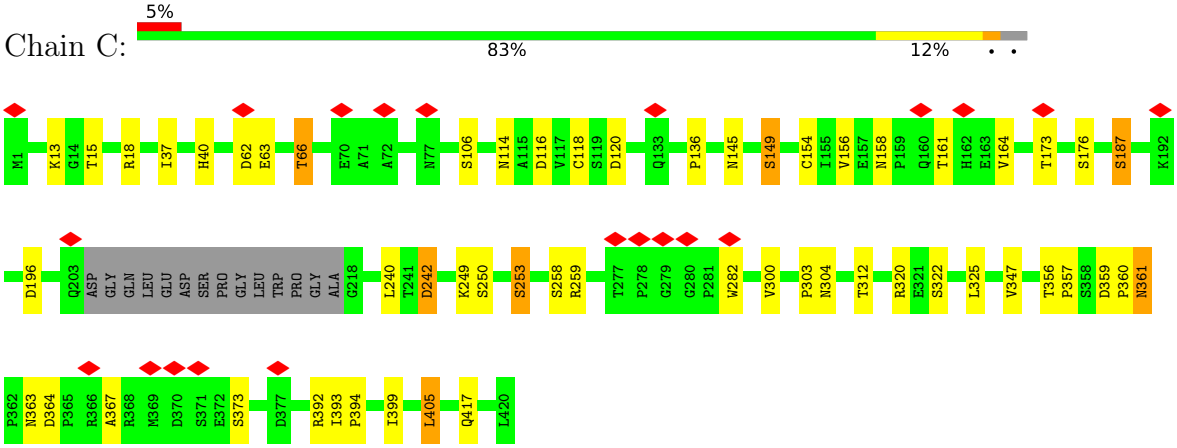
• Molecule 1: Mannose-1-phosphate guanyltransferase alpha

Chain B:

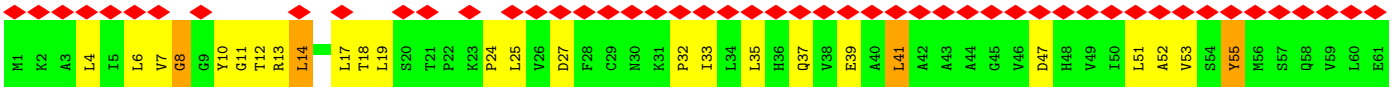


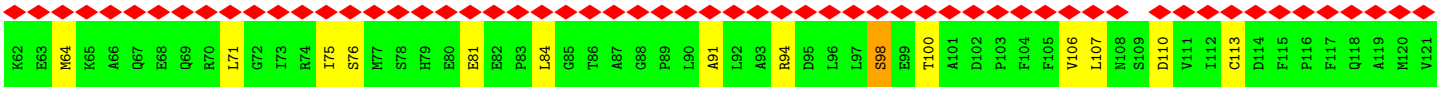


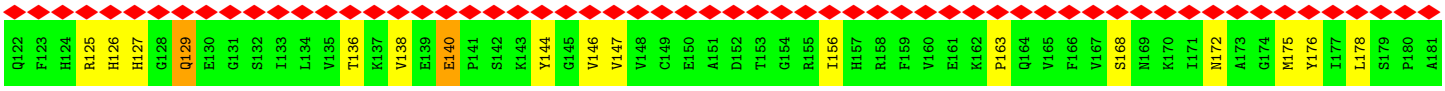
• Molecule 1: Mannose-1-phosphate guanyltransferase alpha

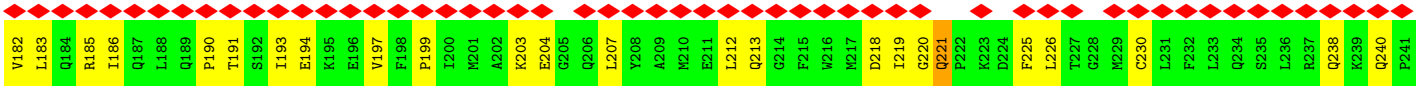


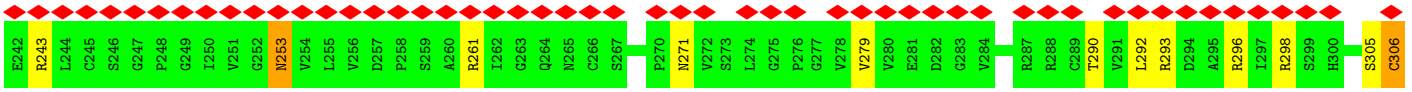
• Molecule 2: Mannose-1-phosphate guanyltransferase beta

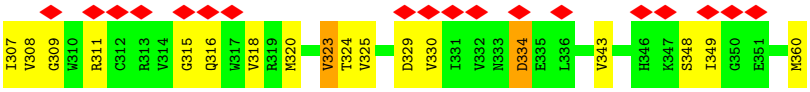




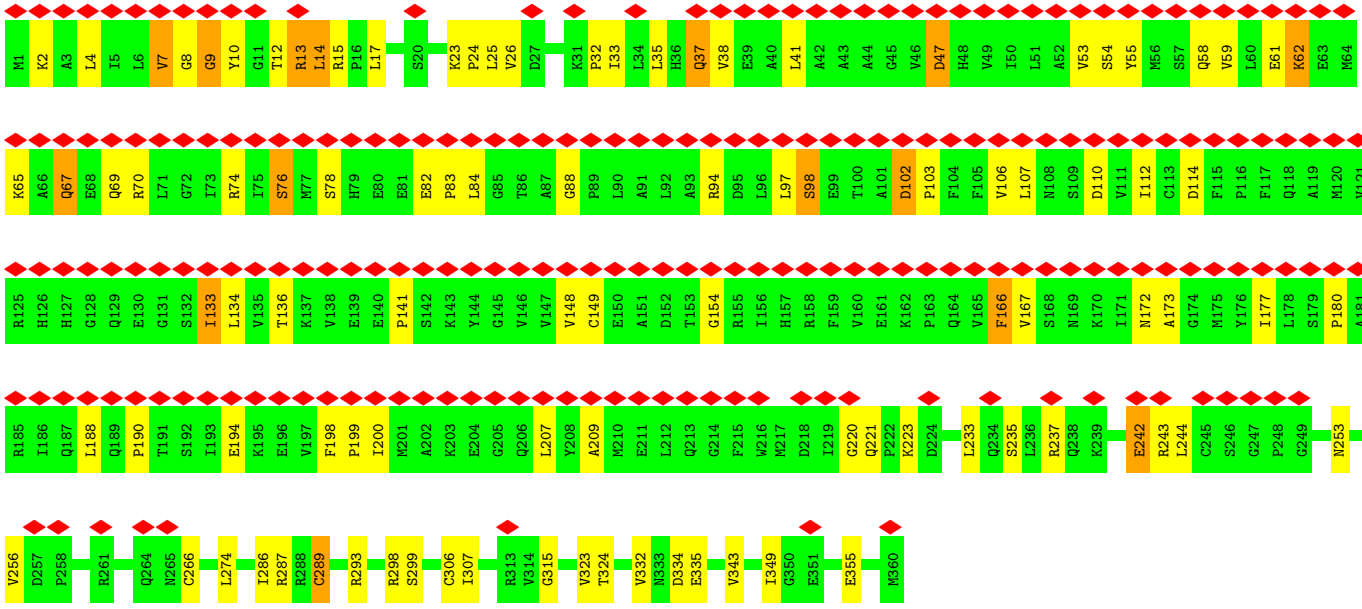






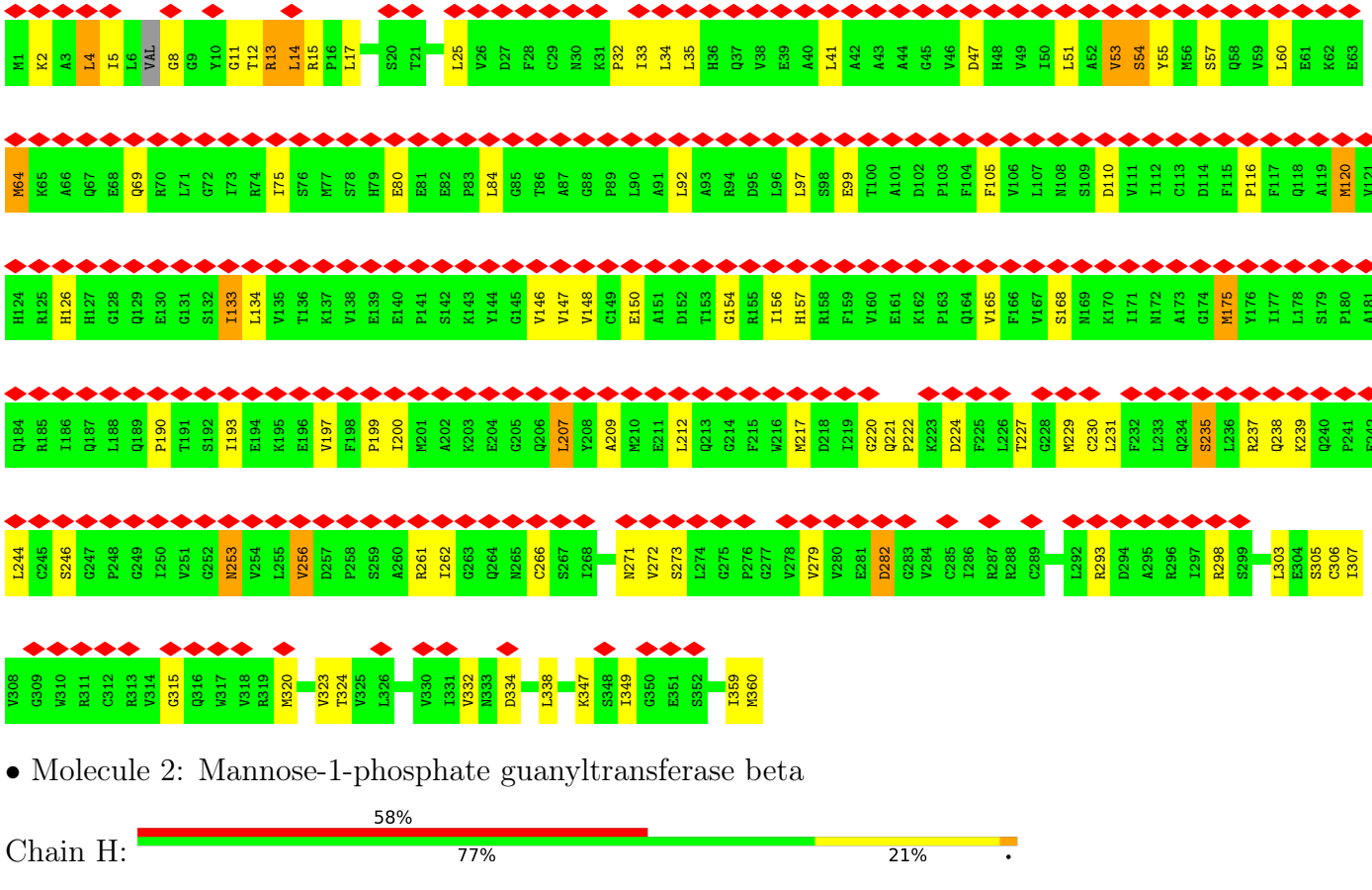


• Molecule 2: Mannose-1-phosphate guanyltransferase beta



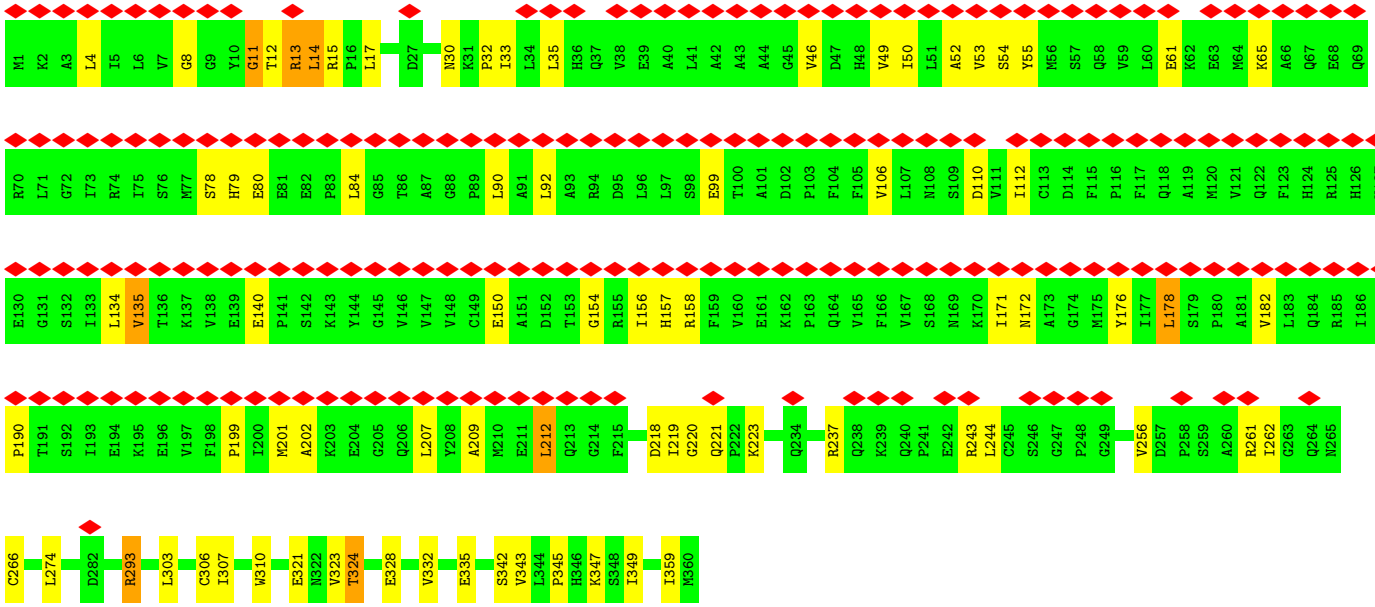
• Molecule 2: Mannose-1-phosphate guanyltransferase beta

Chain G:



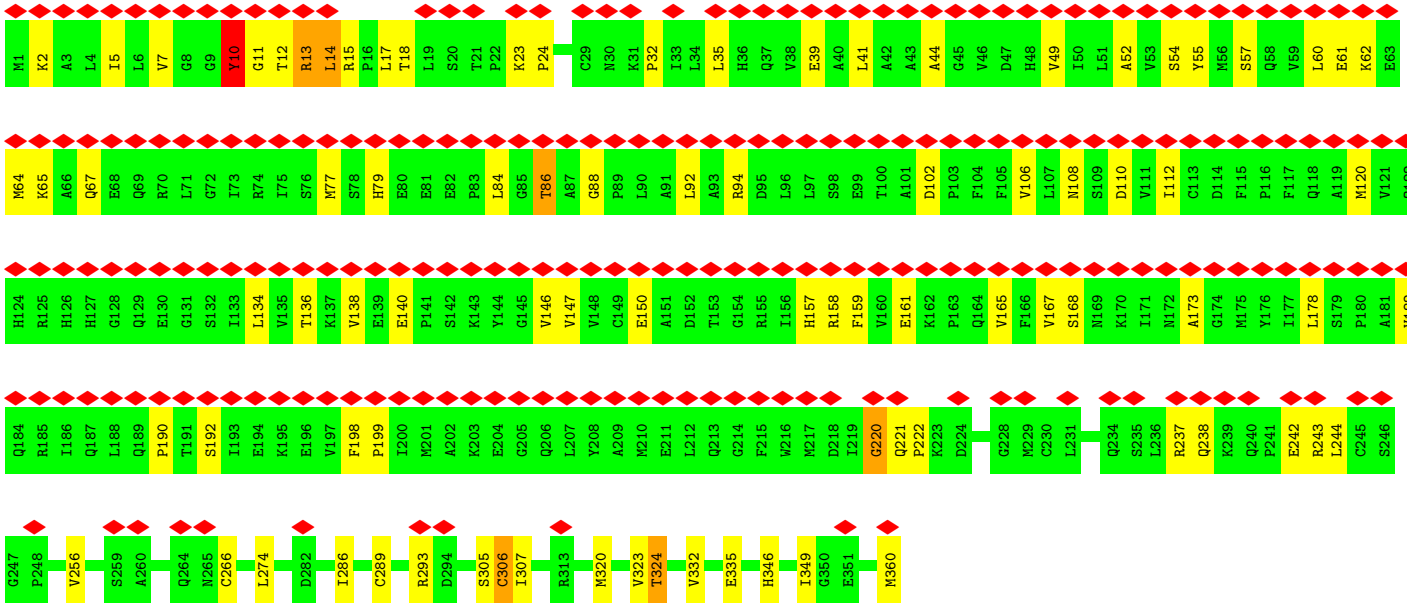
• Molecule 2: Mannose-1-phosphate guanyltransferase beta

Chain H:



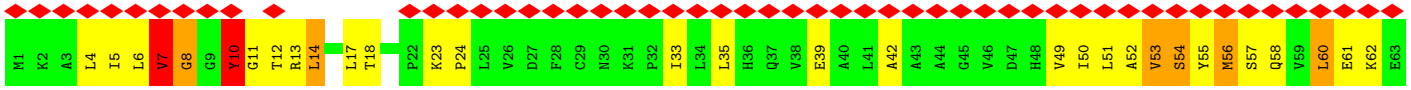
• Molecule 2: Mannose-1-phosphate guanyltransferase beta

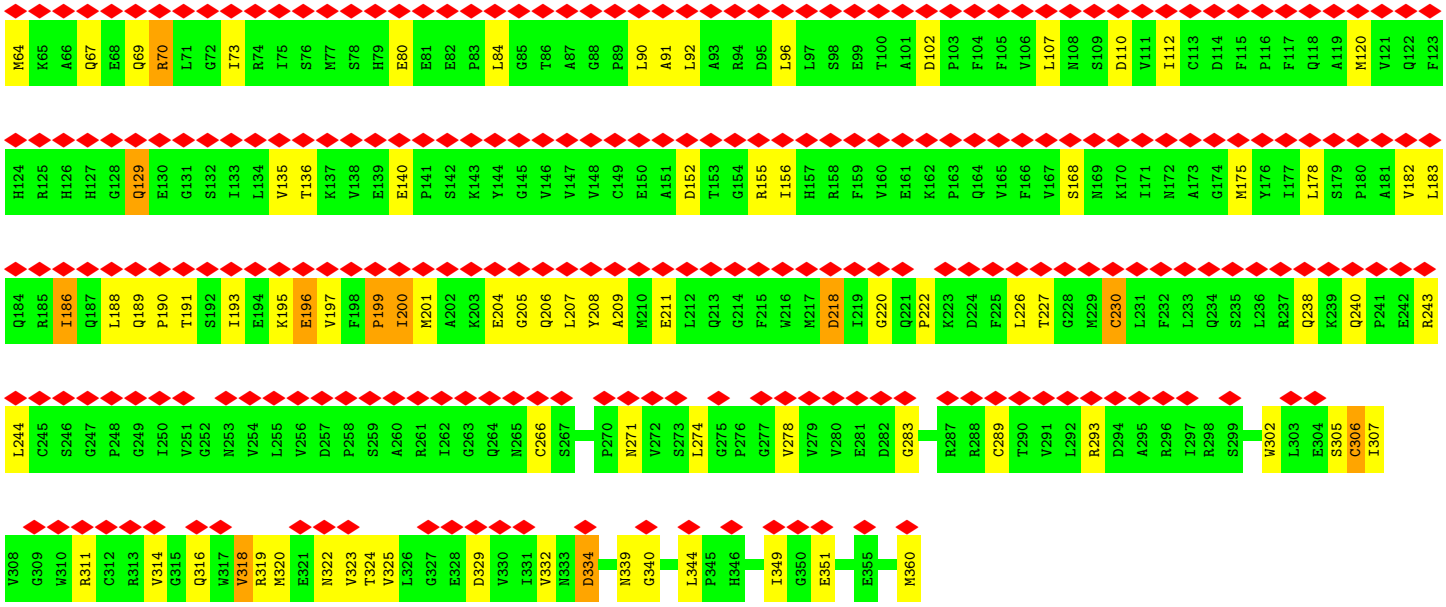
Chain I:



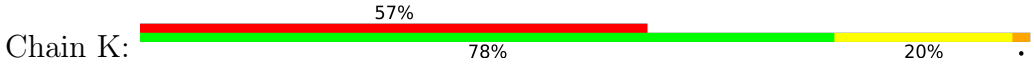
• Molecule 2: Mannose-1-phosphate guanyltransferase beta

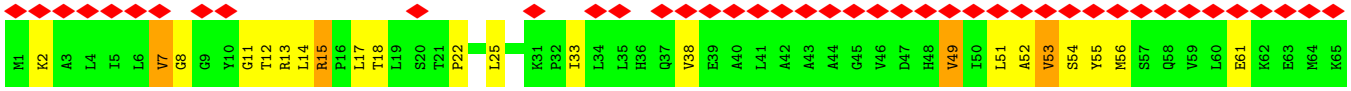
Chain J:

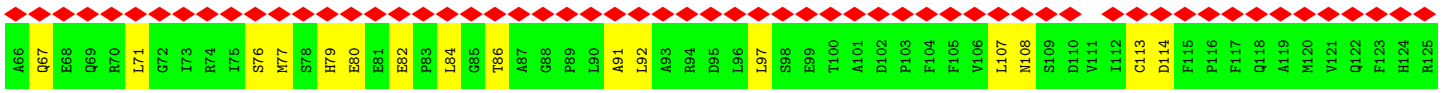


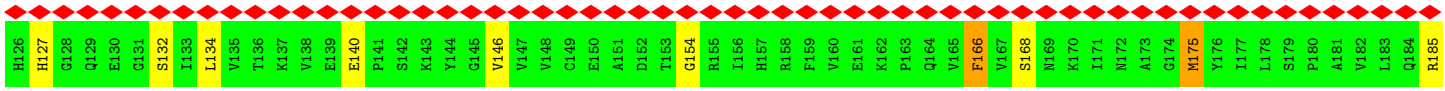


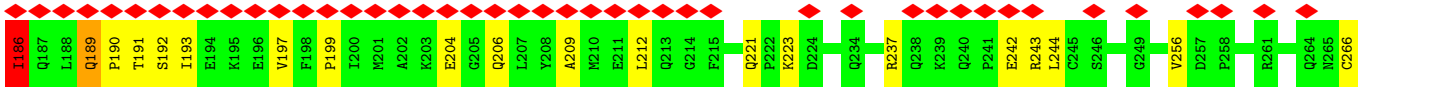
• Molecule 2: Mannose-1-phosphate guanyltransferase beta



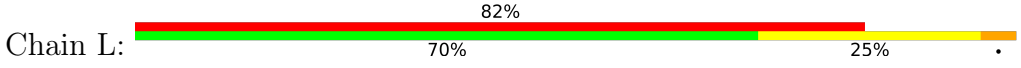


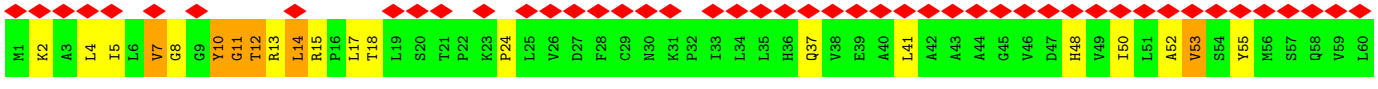


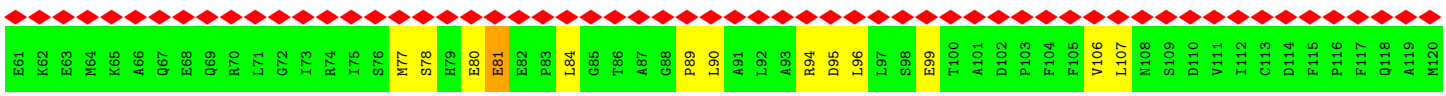


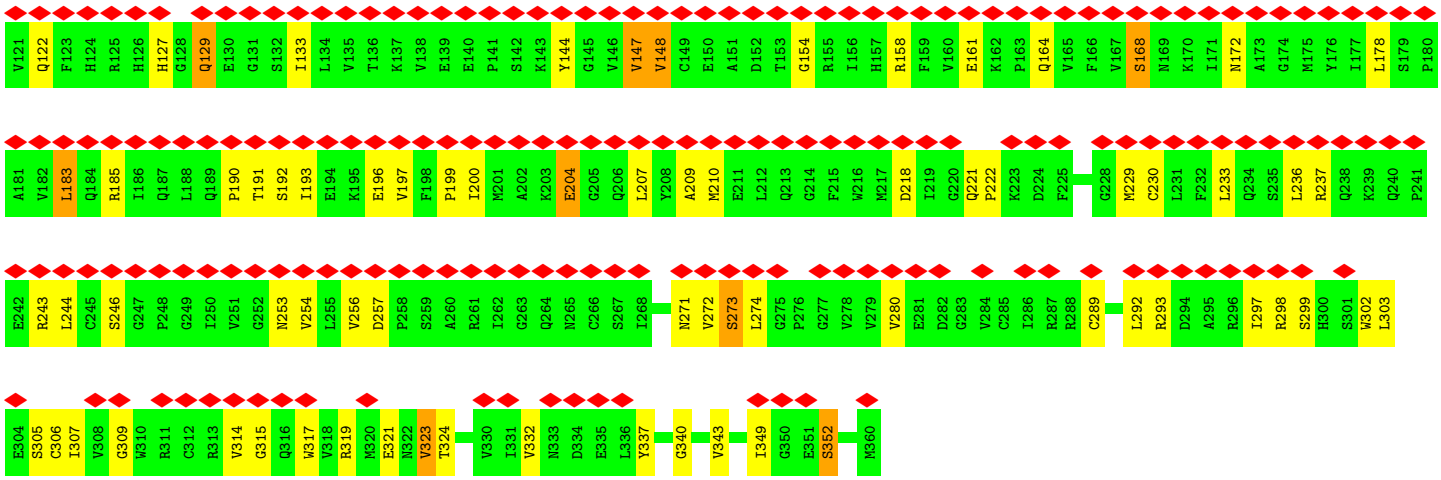


• Molecule 2: Mannose-1-phosphate guanyltransferase beta








V121 Q122 F123 H124 R125 H126 H127 G128 Q129 E130 G131 S132 I133 L134 V135 T136 K137 V138 E139 E140 P141 S142 K143 Y144 G145 V146 V147 V148 C149 E150 A151 D152 T153 G154 R155 I156 H157 R158 F159 V160 E161 K162 P163 Q164 V165 F166 V167 S168 N169 K170 I171 N172 A173 G174 M175 Y176 I177 L178 S179 P180
A181 V182 L183 Q184 R185 I186 Q187 L188 Q189 P190 T191 S192 I193 E194 K195 E196 V197 F198 P199 I200 M201 A202 K203 E204 G205 Q206 L207 Y208 A209 M210 E211 L212 Q213 G214 F215 W216 M217 D218 I219 G220 Q221 P222 K223 D224 F225 G228 M229 C230 L231 F232 L233 Q234 S235 L236 R237 Q238 K239 Q240 P241
E242 R243 L244 C245 S246 G247 P248 G249 I250 V251 G252 N253 V254 L255 V256 D257 P258 S259 A260 R261 I262 G263 Q264 N265 C266 S267 I268 N271 V272 S273 L274 G275 P276 G277 V278 V279 V280 E281 D282 G283 V284 C285 I286 R287 R288 C289 L292 R293 D294 A295 R296 I297 R298 S299 H300 S301 W302 L303
E304 S305 C306 I307 V308 G309 W310 R311 C312 R313 V314 G315 Q316 W317 V318 R319 M320 E321 N322 V323 T324 V330 I331 V332 N333 D334 E335 L336 Y337 G340 V343 I349 G350 E351 S352 M360

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.170	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0365	Depositor
Map size (Å)	252.48001, 252.48001, 252.48001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/3248	0.58	2/4420 (0.0%)
1	B	0.38	0/3248	0.57	2/4420 (0.0%)
1	C	0.38	0/3248	0.58	2/4420 (0.0%)
1	D	0.38	0/3248	0.57	1/4420 (0.0%)
2	E	0.44	0/2840	0.75	3/3850 (0.1%)
2	F	0.45	0/2844	0.77	2/3854 (0.1%)
2	G	0.44	0/2836	0.82	3/3841 (0.1%)
2	H	0.40	0/2844	0.71	3/3854 (0.1%)
2	I	0.46	0/2844	0.77	2/3854 (0.1%)
2	J	0.40	0/2844	0.78	6/3854 (0.2%)
2	K	0.41	0/2844	0.71	4/3854 (0.1%)
2	L	0.42	0/2844	0.80	2/3854 (0.1%)
All	All	0.41	0/35732	0.70	32/48495 (0.1%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	220	GLY	C-N-CA	5.78	136.15	121.70
2	F	9	GLY	N-CA-C	5.75	127.47	113.10
2	E	240	GLN	CA-CB-CG	5.72	125.99	113.40
1	D	405	LEU	CA-CB-CG	-5.71	102.16	115.30
1	B	405	LEU	CA-CB-CG	-5.71	102.16	115.30

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	3167	0	3184	22	0
1	B	3167	0	3184	22	0
1	C	3167	0	3184	30	0
1	D	3167	0	3184	25	0
2	E	2785	0	2829	91	0
2	F	2789	0	2840	102	0
2	G	2782	0	2830	74	0
2	H	2789	0	2838	59	0
2	I	2789	0	2840	72	0
2	J	2789	0	2840	125	0
2	K	2789	0	2838	47	0
2	L	2789	0	2840	80	0
3	A	32	0	12	1	0
3	B	32	0	12	1	0
3	C	32	0	12	1	0
3	D	32	0	12	1	0
3	E	32	0	12	16	0
3	F	32	0	12	30	0
3	G	32	0	12	13	0
3	H	32	0	12	15	0
3	I	32	0	12	8	0
3	J	32	0	12	14	0
3	K	32	0	12	13	0
3	L	32	0	12	13	0
All	All	35353	0	35575	727	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 10.

The worst 5 of 727 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:7:VAL:CG1	2:E:24:PRO:HG2	1.35	1.55
2:E:8:GLY:HA3	3:E:401:GTP:N3	1.22	1.51
2:F:7:VAL:CG2	2:F:24:PRO:HG3	1.43	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:GLY:HA3	3:F:401:GTP:N3	1.12	1.43
2:I:346:HIS:CG	2:J:10:TYR:CE1	2.13	1.35

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 PDB entries followed by that with respect to all EM entries.

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	402/420 (96%)	391 (97%)	11 (3%)	0	100	100
1	B	402/420 (96%)	392 (98%)	10 (2%)	0	100	100
1	C	402/420 (96%)	392 (98%)	10 (2%)	0	100	100
1	D	402/420 (96%)	392 (98%)	10 (2%)	0	100	100
2	E	358/360 (99%)	334 (93%)	21 (6%)	3 (1%)	16	48
2	F	358/360 (99%)	332 (93%)	23 (6%)	3 (1%)	16	48
2	G	355/360 (99%)	331 (93%)	24 (7%)	0	100	100
2	H	358/360 (99%)	336 (94%)	21 (6%)	1 (0%)	37	68
2	I	358/360 (99%)	336 (94%)	20 (6%)	2 (1%)	22	53
2	J	358/360 (99%)	333 (93%)	22 (6%)	3 (1%)	16	48
2	K	358/360 (99%)	335 (94%)	22 (6%)	1 (0%)	37	68
2	L	358/360 (99%)	333 (93%)	22 (6%)	3 (1%)	16	48
All	All	4469/4560 (98%)	4237 (95%)	216 (5%)	16 (0%)	32	63

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	8	GLY
2	F	10	TYR
2	I	10	TYR

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Mol	Chain	Res	Type
2	J	8	GLY
2	L	10	TYR

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 PDB entries followed by that with respect to all EM entries.

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	344/354 (97%)	324 (94%)	20 (6%)	17 45
1	B	344/354 (97%)	325 (94%)	19 (6%)	18 47
1	C	344/354 (97%)	325 (94%)	19 (6%)	18 47
1	D	344/354 (97%)	326 (95%)	18 (5%)	19 48
2	E	310/311 (100%)	274 (88%)	36 (12%)	4 18
2	F	311/311 (100%)	277 (89%)	34 (11%)	5 21
2	G	310/311 (100%)	273 (88%)	37 (12%)	4 17
2	H	311/311 (100%)	289 (93%)	22 (7%)	12 39
2	I	311/311 (100%)	281 (90%)	30 (10%)	7 26
2	J	311/311 (100%)	274 (88%)	37 (12%)	4 17
2	K	311/311 (100%)	286 (92%)	25 (8%)	10 34
2	L	311/311 (100%)	276 (89%)	35 (11%)	4 20
All	All	3862/3904 (99%)	3530 (91%)	332 (9%)	11 31

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	293	ARG
2	K	166	PHE
2	J	49	VAL
2	J	230	CYS
2	L	53	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	316	GLN
2	I	122	GLN
2	L	127	HIS
2	H	127	HIS
2	H	316	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
3	GTP	G	401	-	26,34,34	1.05	1 (3%)	32,54,54	3.23	9 (28%)
3	GTP	H	401	-	26,34,34	1.04	1 (3%)	32,54,54	3.23	9 (28%)
3	GTP	L	401	-	26,34,34	1.04	1 (3%)	32,54,54	3.23	9 (28%)
3	GTP	A	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.51	5 (15%)
3	GTP	C	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.51	4 (12%)
3	GTP	B	501	-	26,34,34	1.16	2 (7%)	32,54,54	1.50	4 (12%)
3	GTP	K	401	-	26,34,34	1.05	1 (3%)	32,54,54	3.23	9 (28%)
3	GTP	E	401	-	26,34,34	1.05	1 (3%)	32,54,54	3.23	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GTP	D	501	-	26,34,34	1.17	2 (7%)	32,54,54	1.51	5 (15%)
3	GTP	J	401	-	26,34,34	1.05	1 (3%)	32,54,54	3.23	9 (28%)
3	GTP	I	401	-	26,34,34	1.04	1 (3%)	32,54,54	3.23	9 (28%)
3	GTP	F	401	-	26,34,34	1.04	1 (3%)	32,54,54	3.23	9 (28%)

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
3	GTP	G	401	-	-	2/18/38/38	0/3/3/3
3	GTP	H	401	-	-	2/18/38/38	0/3/3/3
3	GTP	L	401	-	-	2/18/38/38	0/3/3/3
3	GTP	A	501	-	-	5/18/38/38	0/3/3/3
3	GTP	C	501	-	-	5/18/38/38	0/3/3/3
3	GTP	B	501	-	-	5/18/38/38	0/3/3/3
3	GTP	K	401	-	-	2/18/38/38	0/3/3/3
3	GTP	E	401	-	-	2/18/38/38	0/3/3/3
3	GTP	D	501	-	-	5/18/38/38	0/3/3/3
3	GTP	J	401	-	-	2/18/38/38	0/3/3/3
3	GTP	I	401	-	-	2/18/38/38	0/3/3/3
3	GTP	F	401	-	-	2/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	GTP	C5-C6	-3.27	1.40	1.47
3	A	501	GTP	C5-C6	-3.25	1.40	1.47
3	C	501	GTP	C5-C6	-3.25	1.40	1.47
3	B	501	GTP	C5-C6	-3.23	1.40	1.47
3	A	501	GTP	C6-N1	-3.21	1.33	1.37

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	401	GTP	N2-C2-N3	-12.03	96.32	119.74
3	E	401	GTP	N2-C2-N3	-12.02	96.35	119.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	401	GTP	N2-C2-N3	-12.01	96.36	119.74
3	J	401	GTP	N2-C2-N3	-12.00	96.37	119.74
3	G	401	GTP	N2-C2-N3	-12.00	96.38	119.74

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GTP	C5'-O5'-PA-O3A
3	A	501	GTP	C5'-O5'-PA-O2A
3	D	501	GTP	C5'-O5'-PA-O3A
3	D	501	GTP	C5'-O5'-PA-O2A
3	B	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

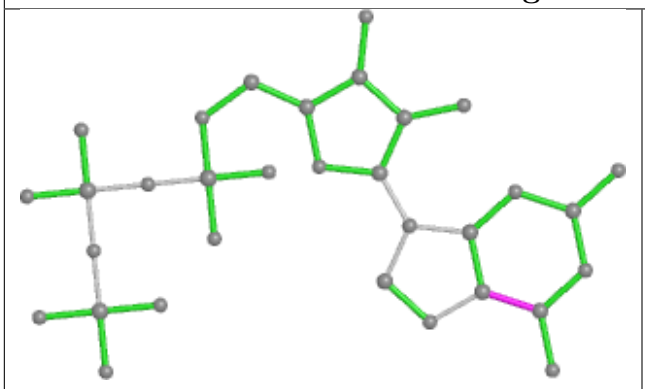
12 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	GTP	13	0
3	H	401	GTP	15	0
3	L	401	GTP	13	0
3	A	501	GTP	1	0
3	C	501	GTP	1	0
3	B	501	GTP	1	0
3	K	401	GTP	13	0
3	E	401	GTP	16	0
3	D	501	GTP	1	0
3	J	401	GTP	14	0
3	I	401	GTP	8	0
3	F	401	GTP	30	0

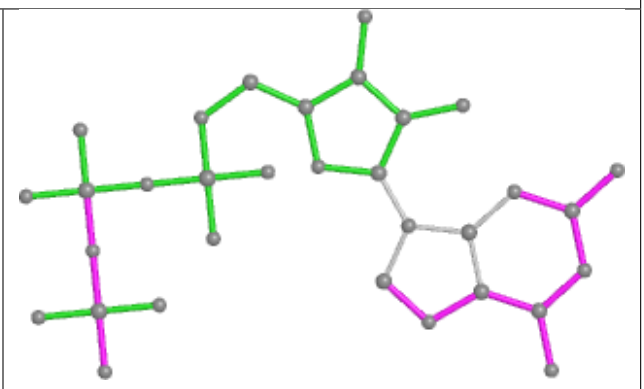
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

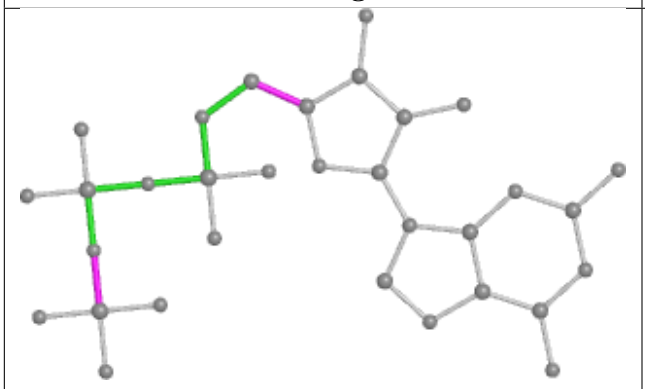
Ligand GTP G 401



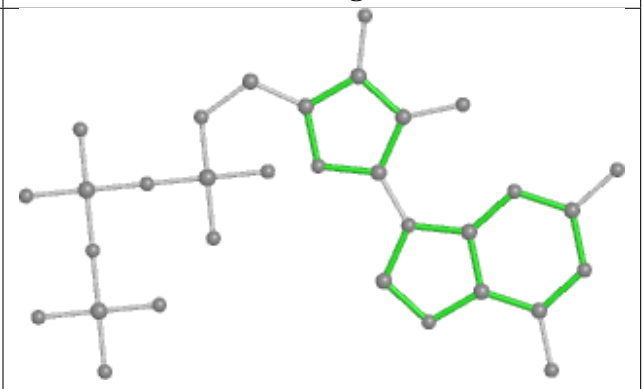
Bond lengths



Bond angles

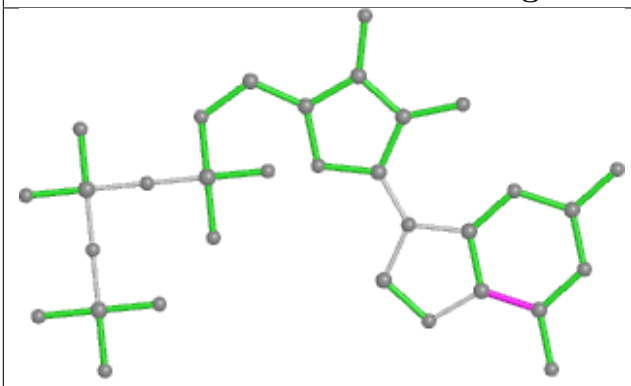


Torsions



Rings

Ligand GTP H 401



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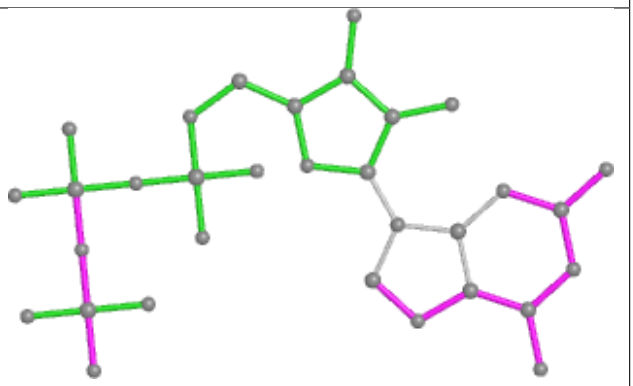

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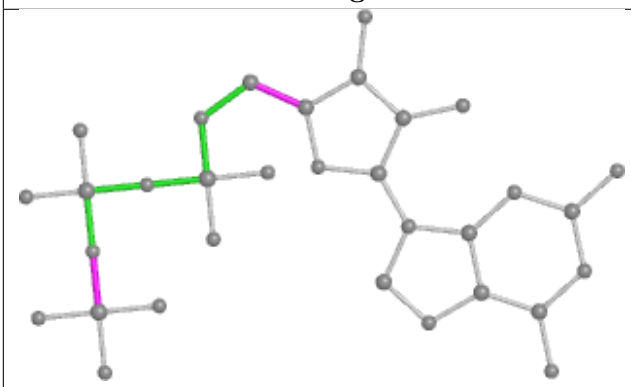

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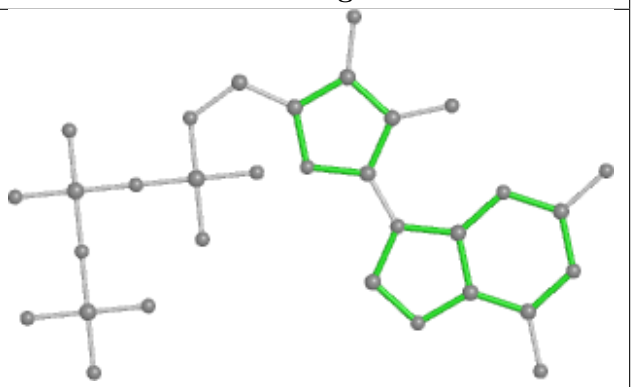
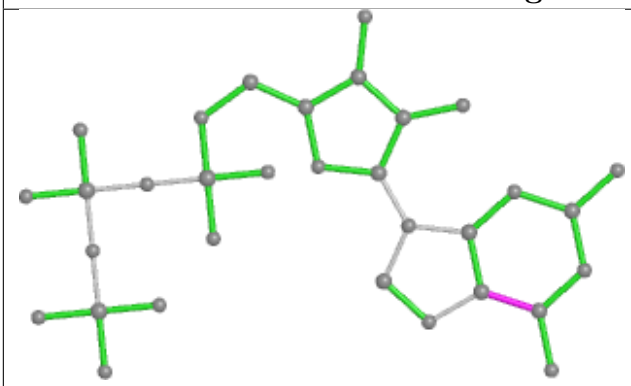


Rings

Ligand GTP L 401



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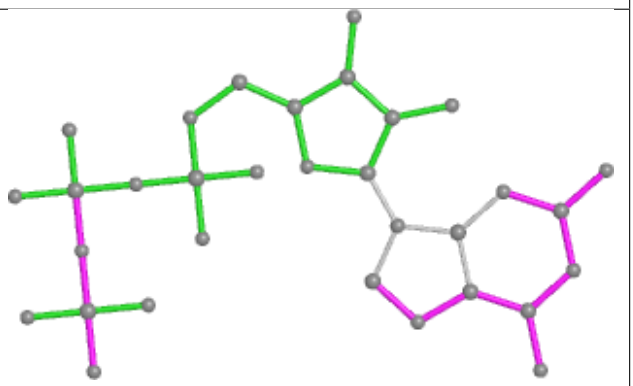

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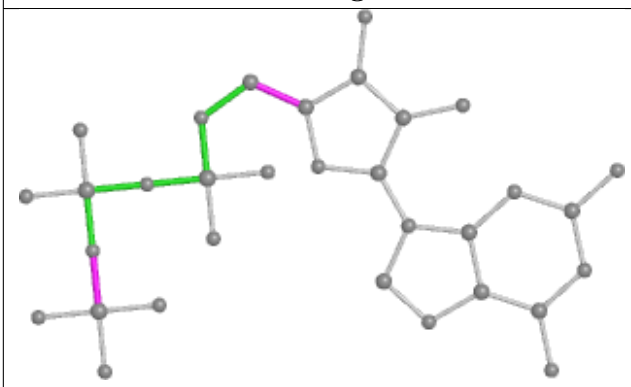

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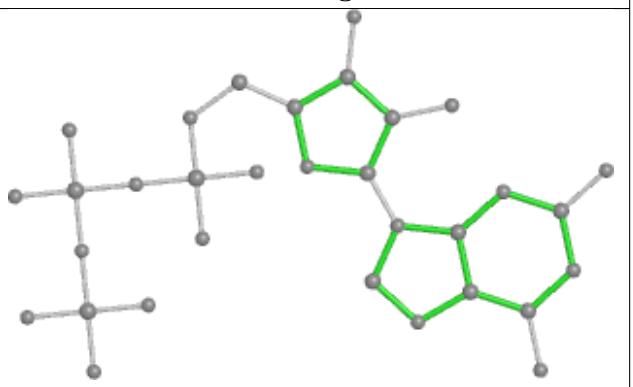
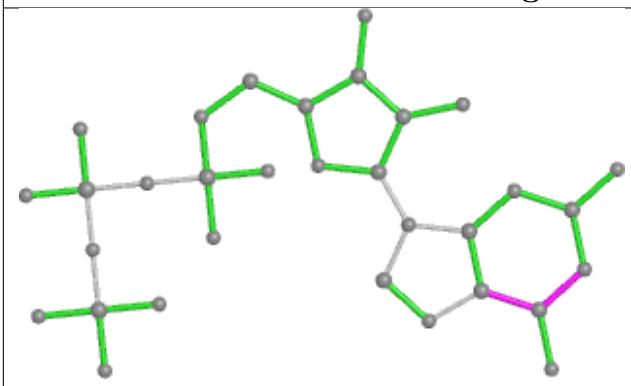


Rings

Ligand GTP A 501



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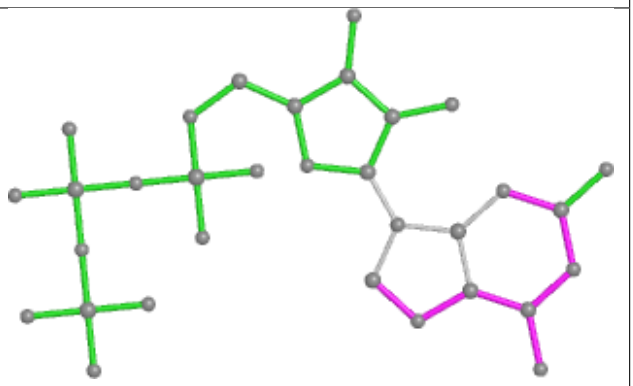

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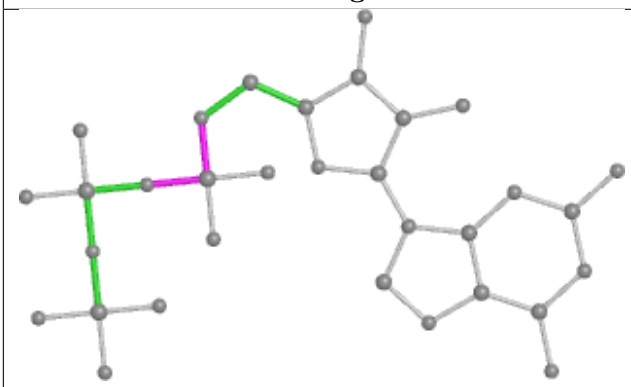

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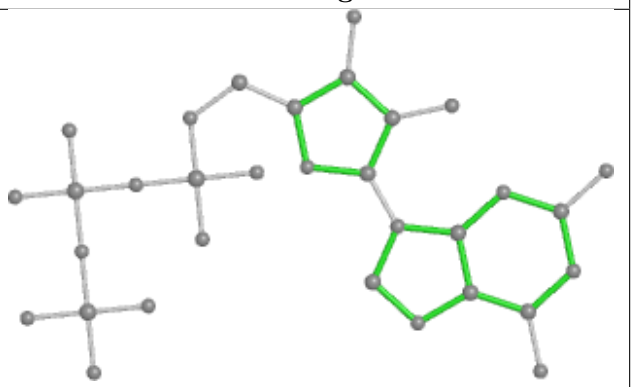
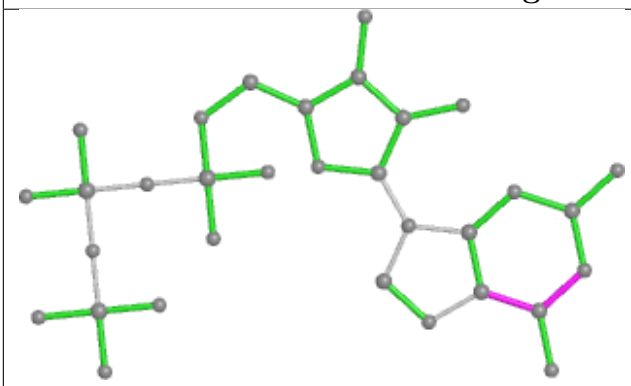


Rings

Ligand GTP C 501



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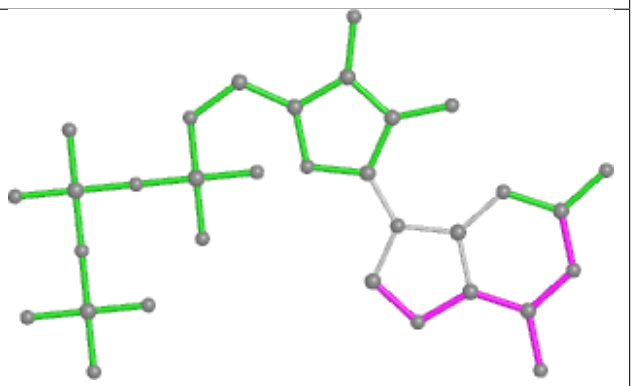

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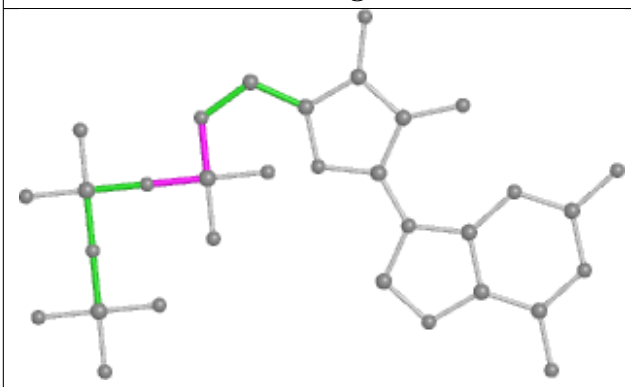

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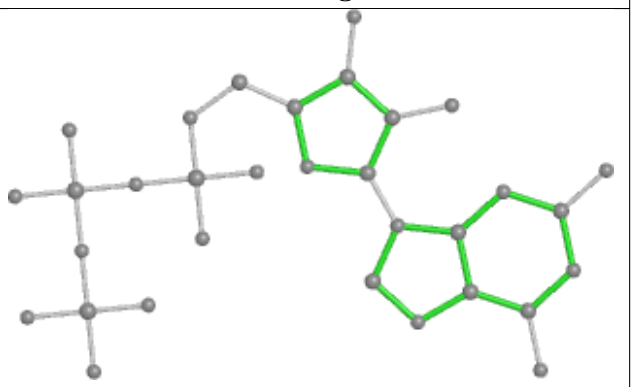
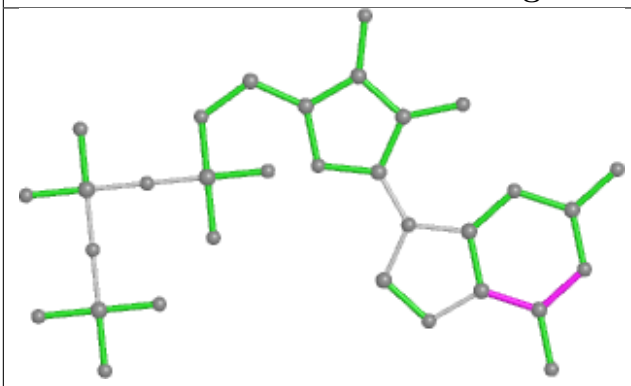


Rings

Ligand GTP B 501



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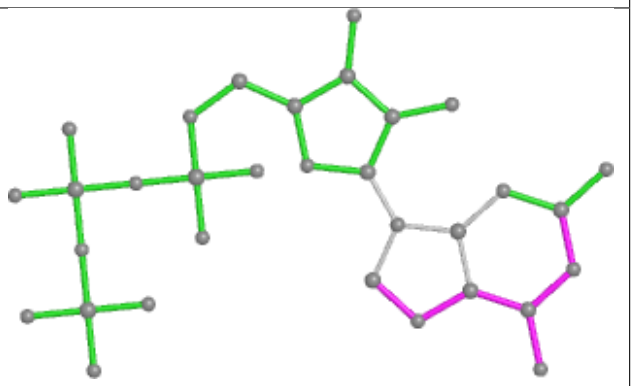
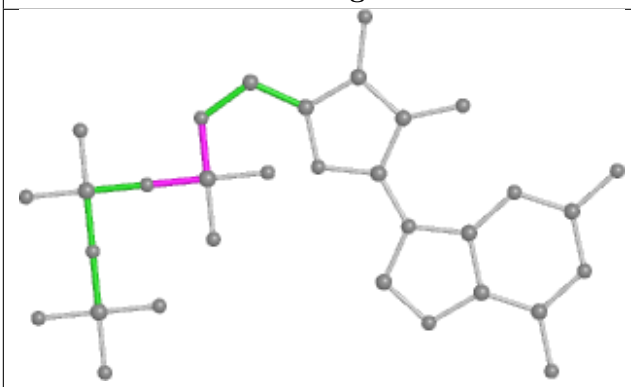


Bond angles



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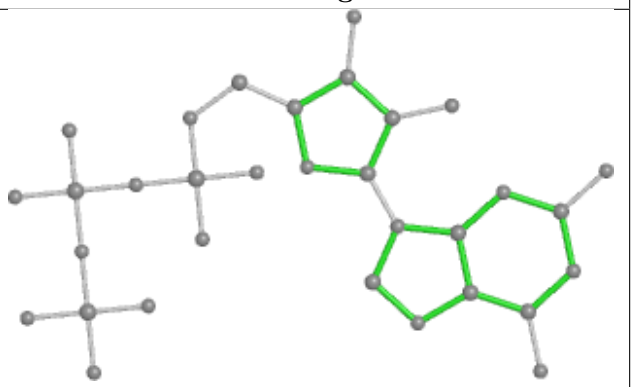
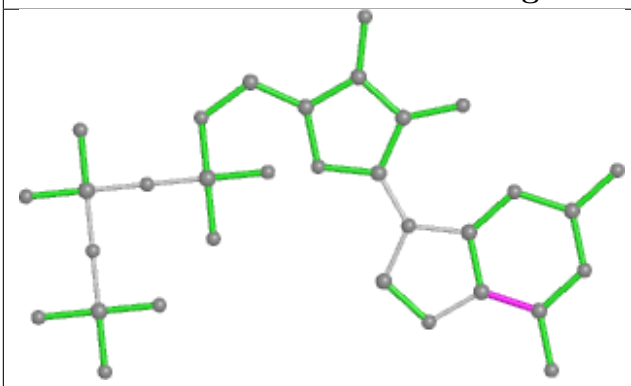
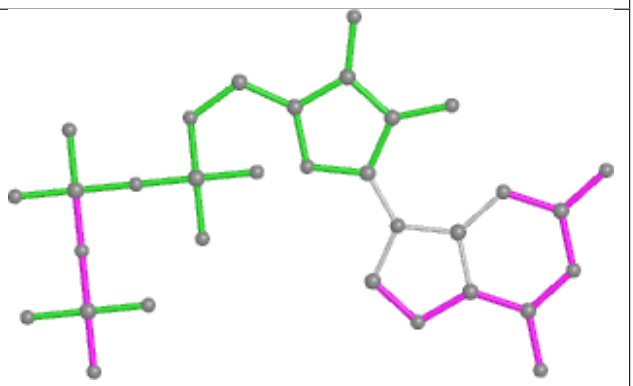


Rings

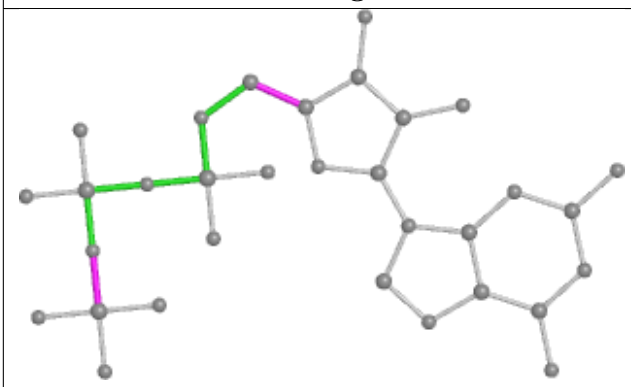
Ligand GTP K 401



Bond lengths



Bond angles



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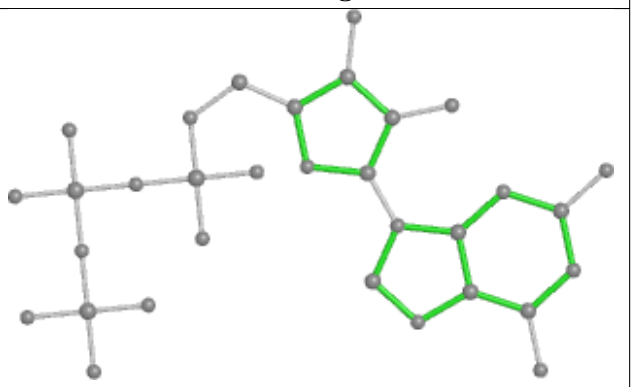
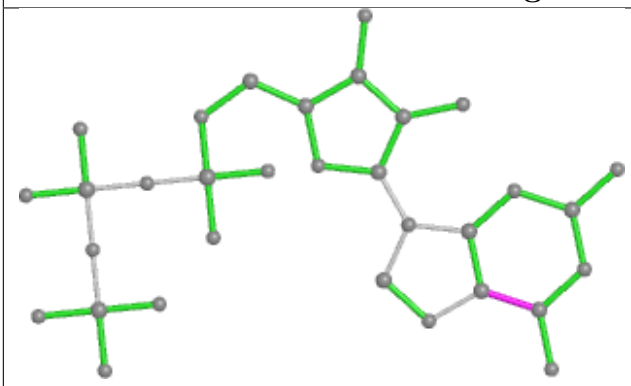
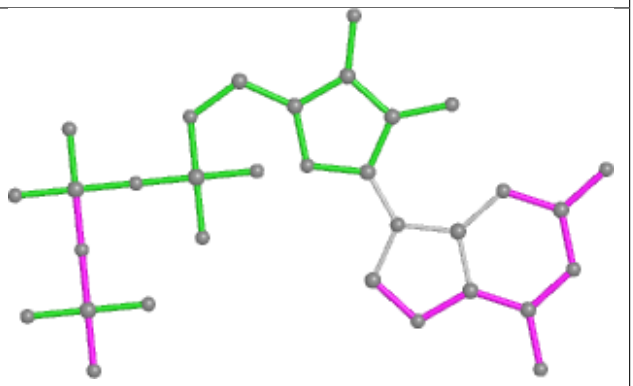


Rings

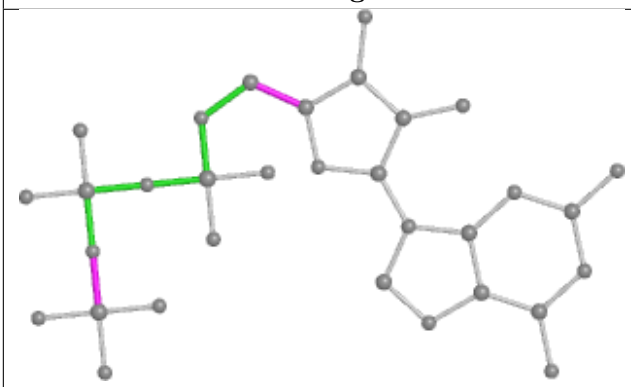
Ligand GTP E 401



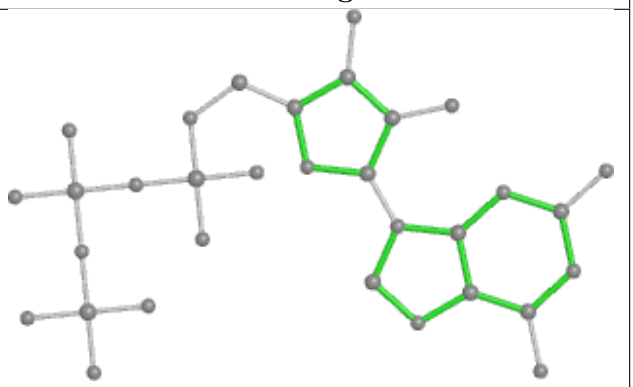
Bond lengths



Bond angles

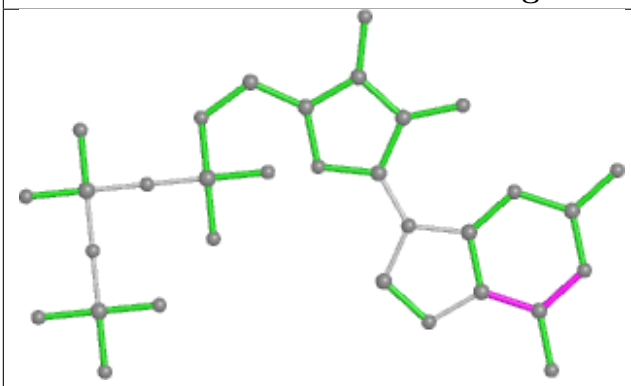


Torsions

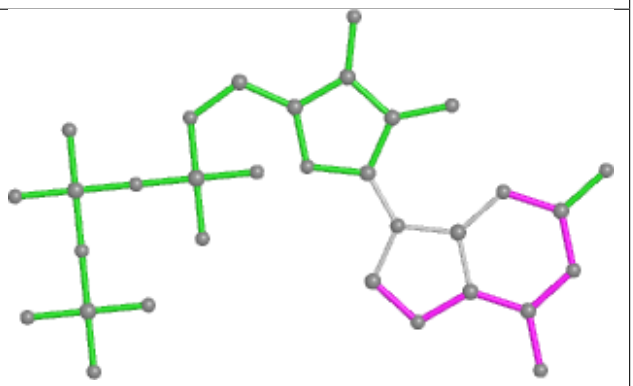


Rings

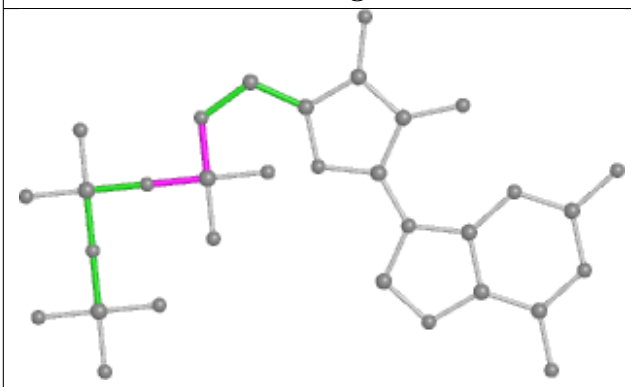
Ligand GTP D 501



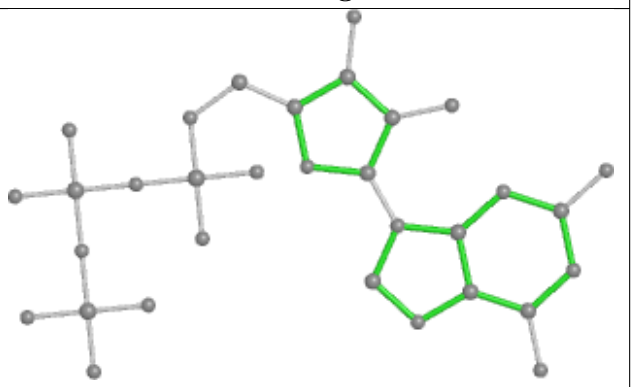
Bond lengths



Bond angles

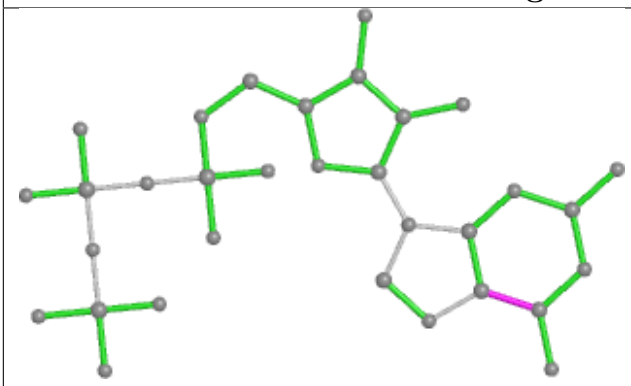


Torsions

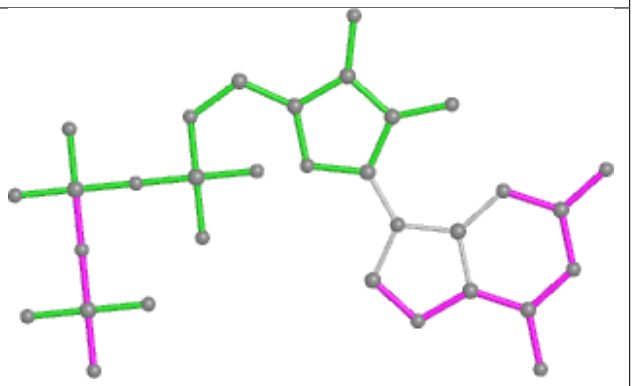


Rings

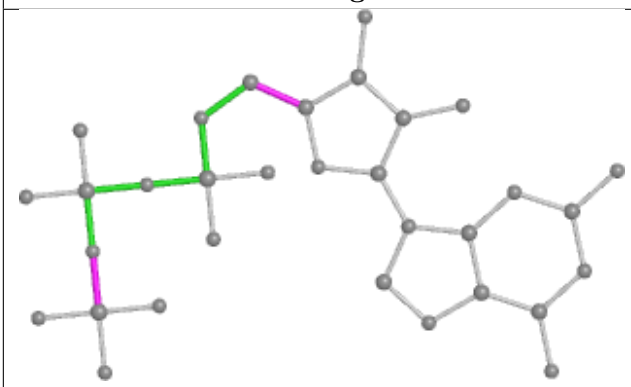
Ligand GTP J 401



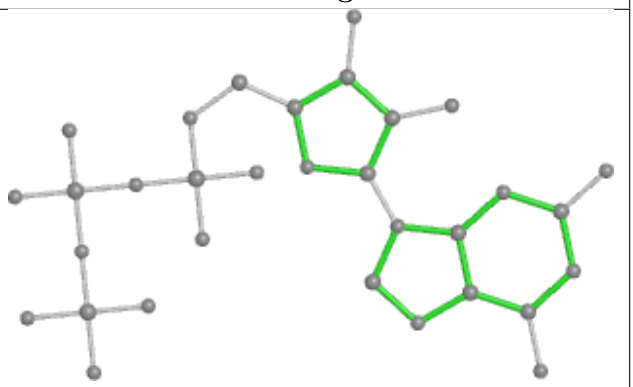
Bond lengths



Bond angles

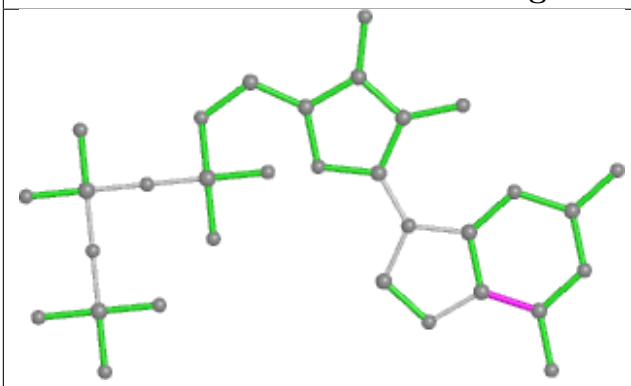


Torsions

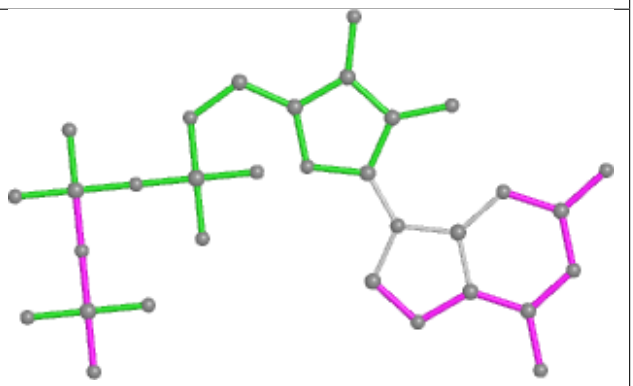


Rings

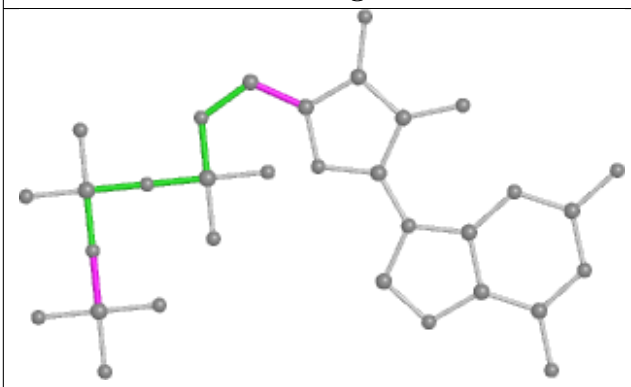
Ligand GTP I 401



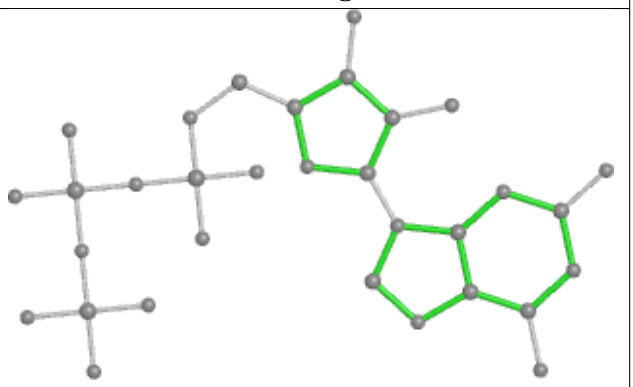
Bond lengths



Bond angles

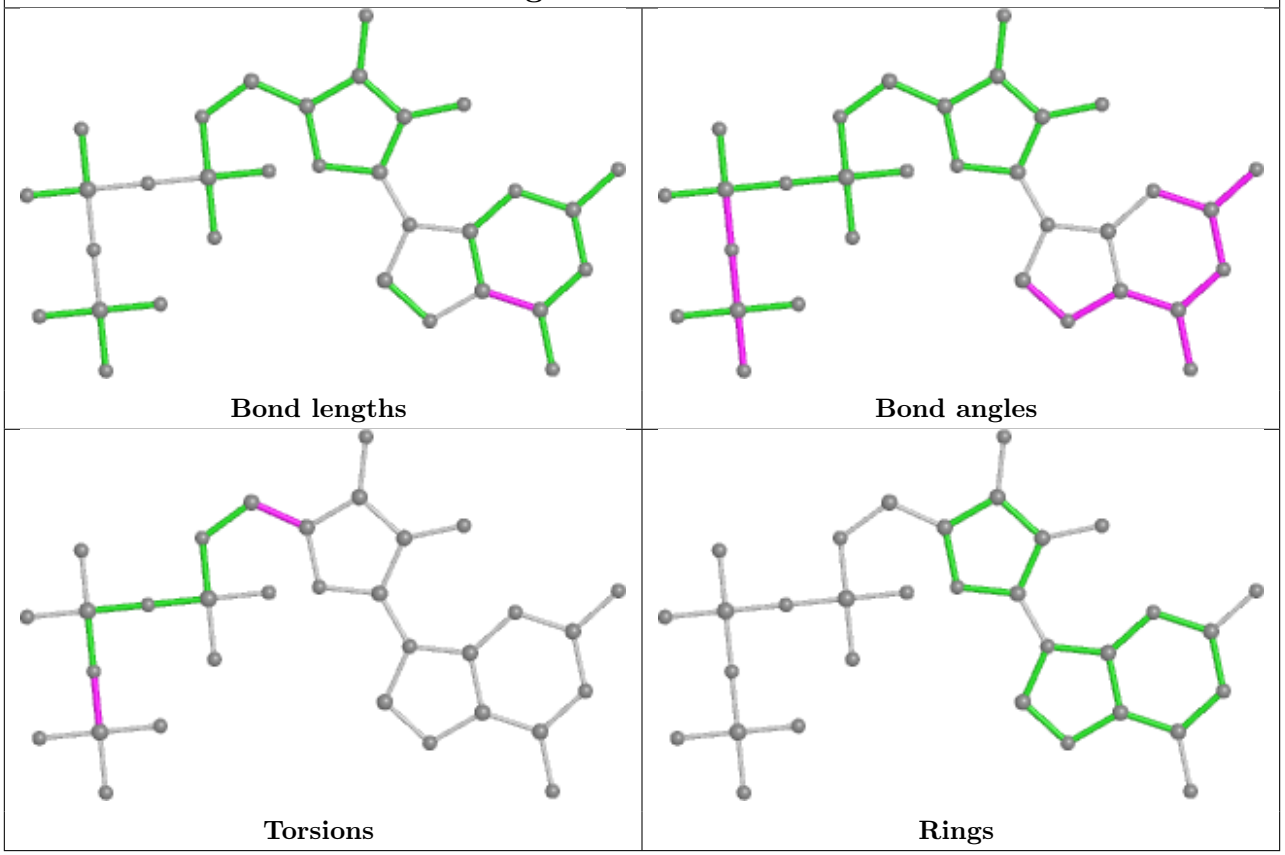


Torsions



Rings

Ligand GTP F 401



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.

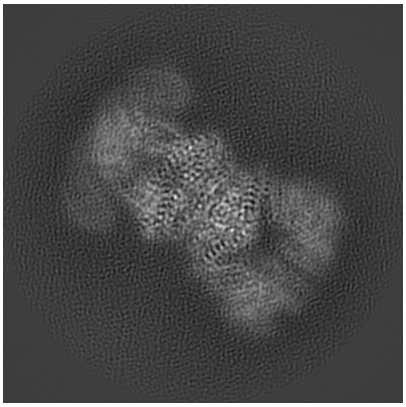
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30601. These allow visual inspection of the internal detail of the map and identification of artifacts.

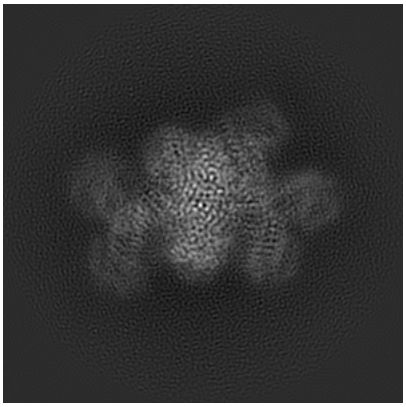
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

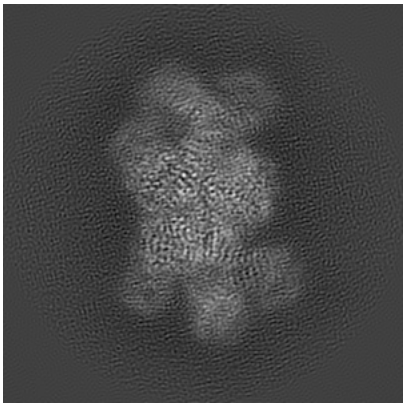
6.1.1 Primary map



X



Y

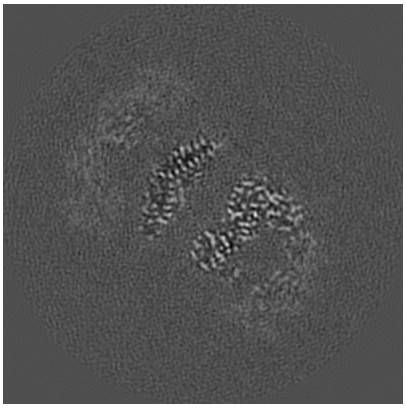


Z

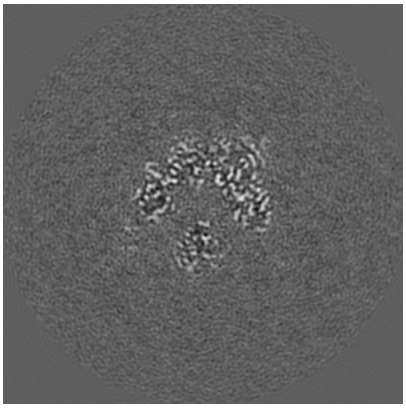
The images above show the map projected in three orthogonal directions.

6.2 Central slices

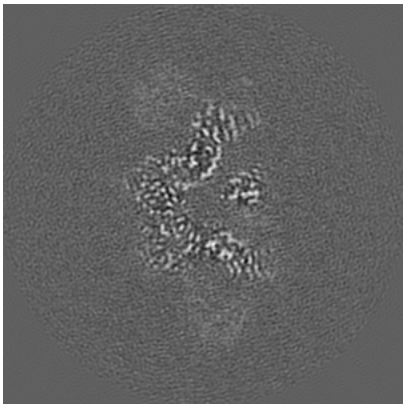
6.2.1 Primary map



X Index: 120



Y Index: 120

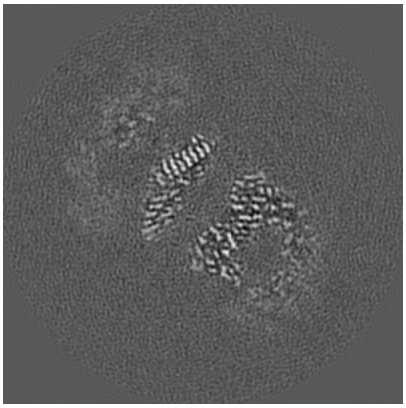


Z Index: 120

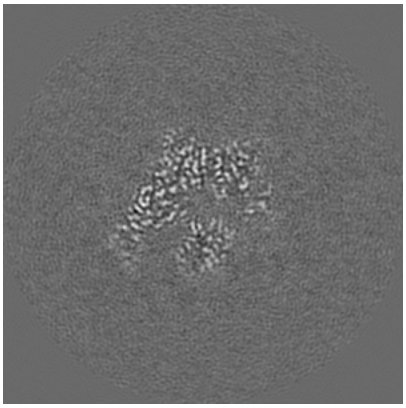
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

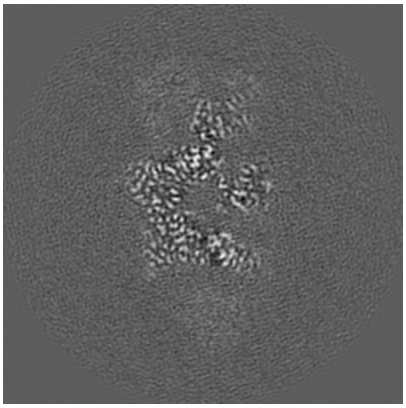
6.3.1 Primary map



X Index: 118



Y Index: 126

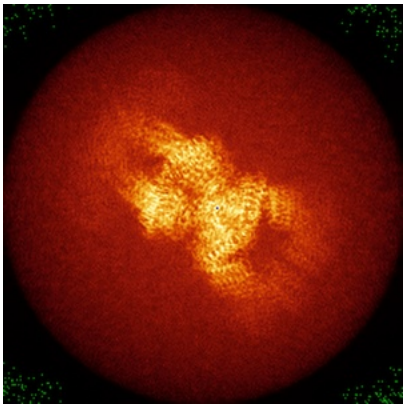


Z Index: 115

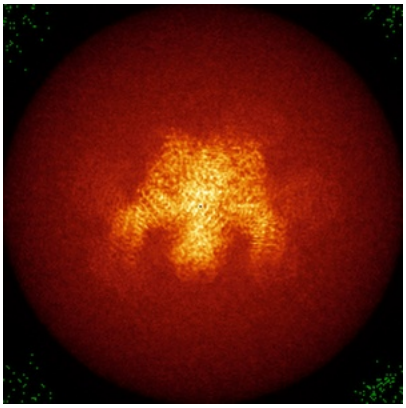
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

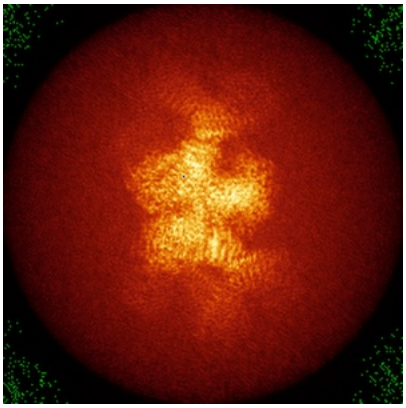
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0365. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

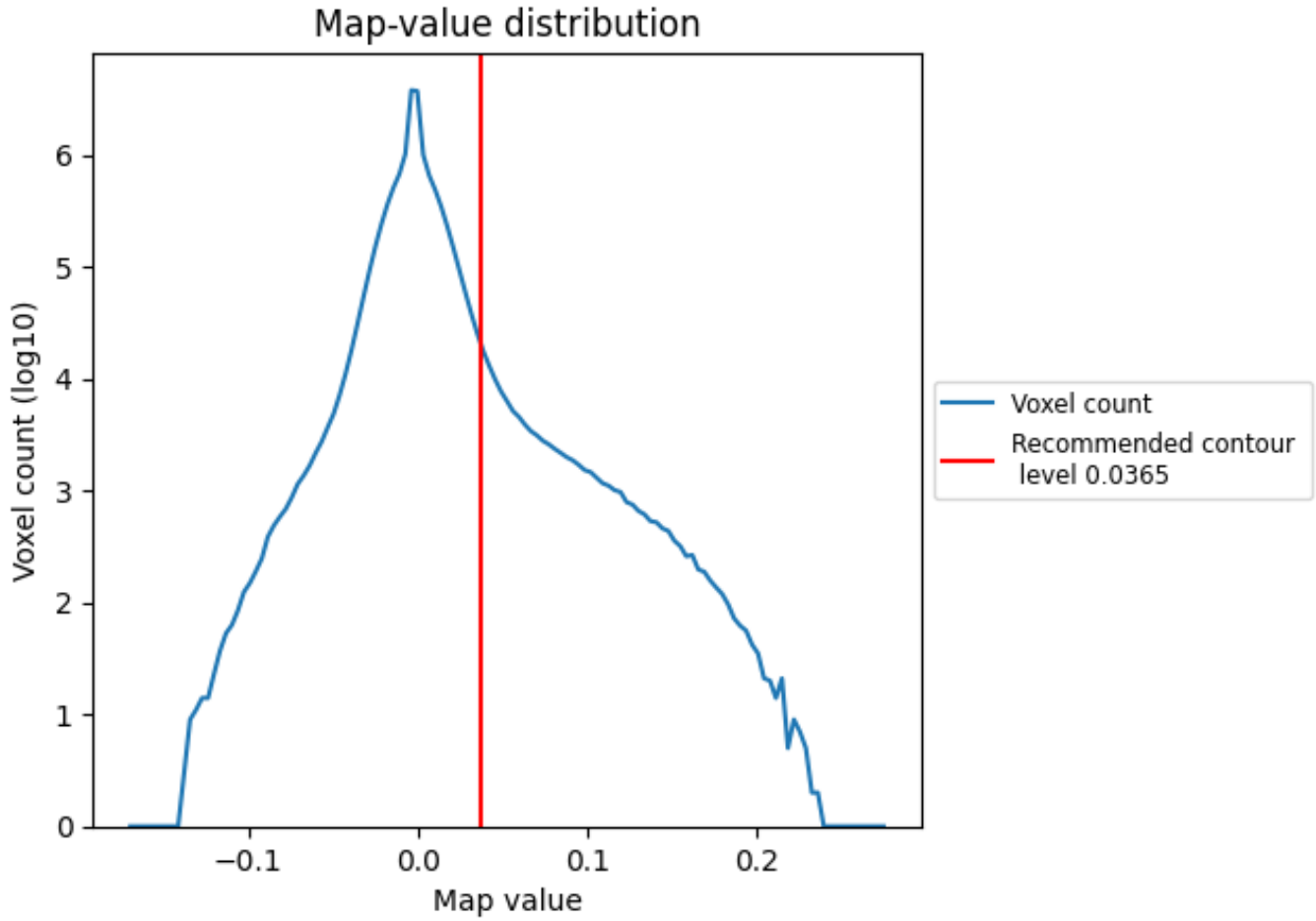
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

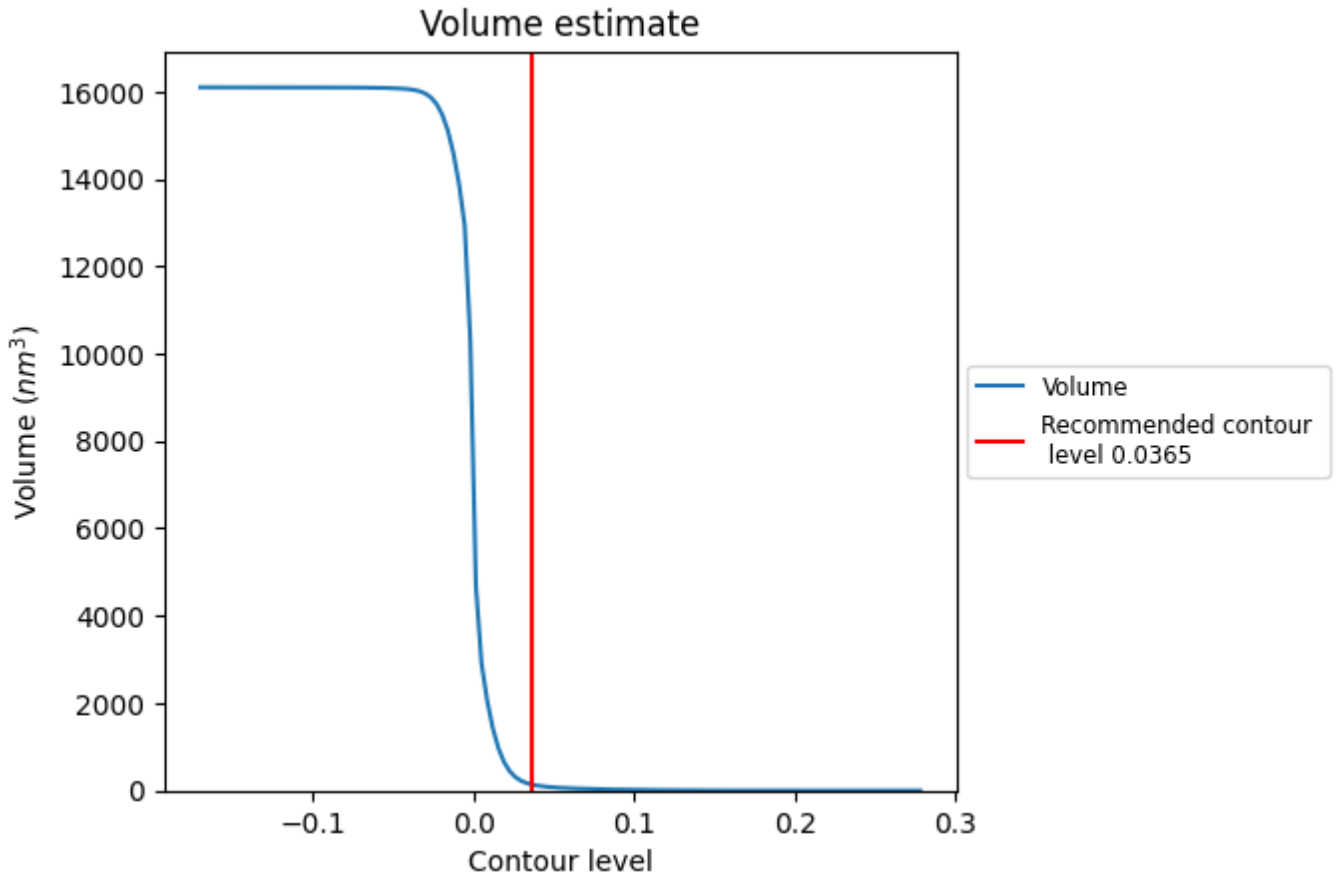
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

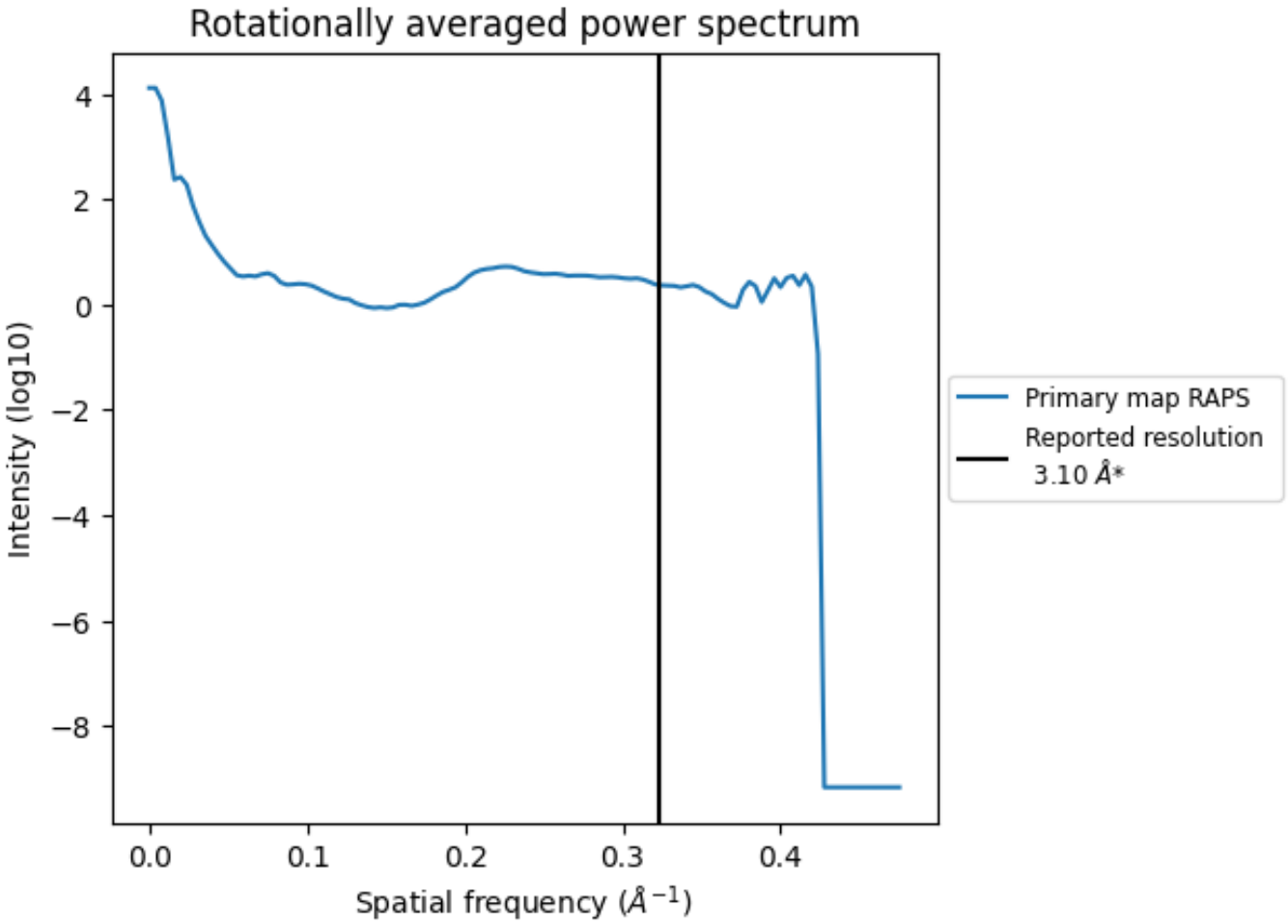
7.2 Volume estimate (i)



The volume at the recommended contour level is 138 nm^3; this corresponds to an approximate mass of 125 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

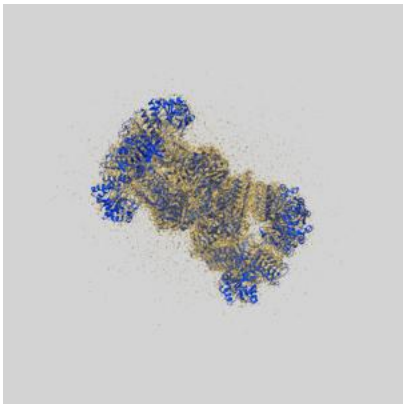
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

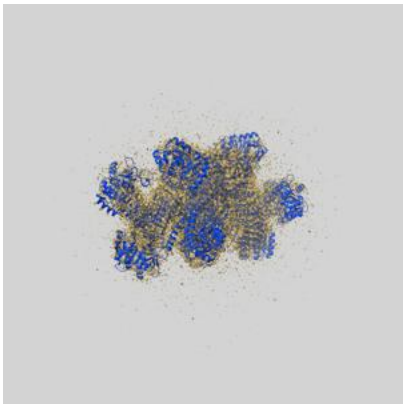
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30601 and PDB model 7D74. Per-residue inclusion information can be found in section 3 on page 6.

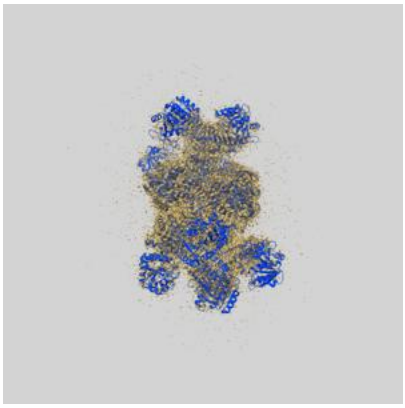
9.1 Map-model overlay



X



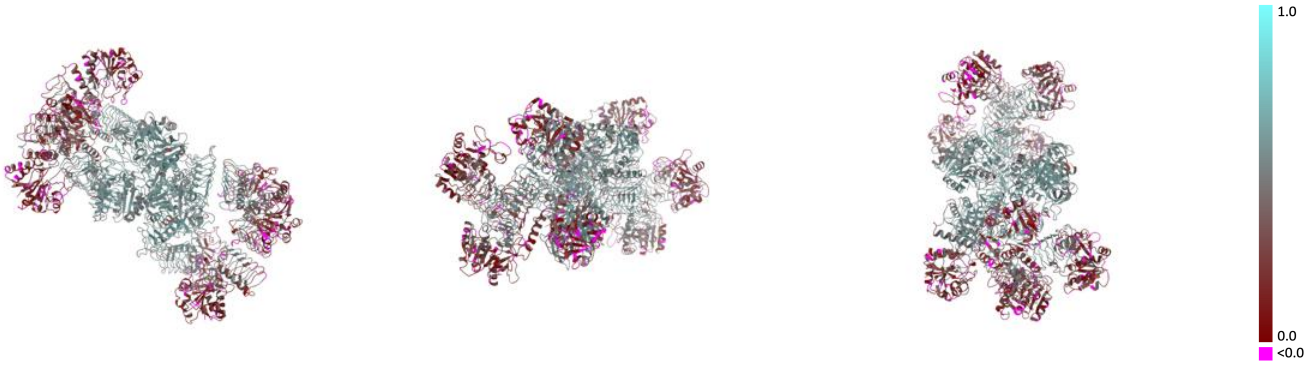
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0365 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

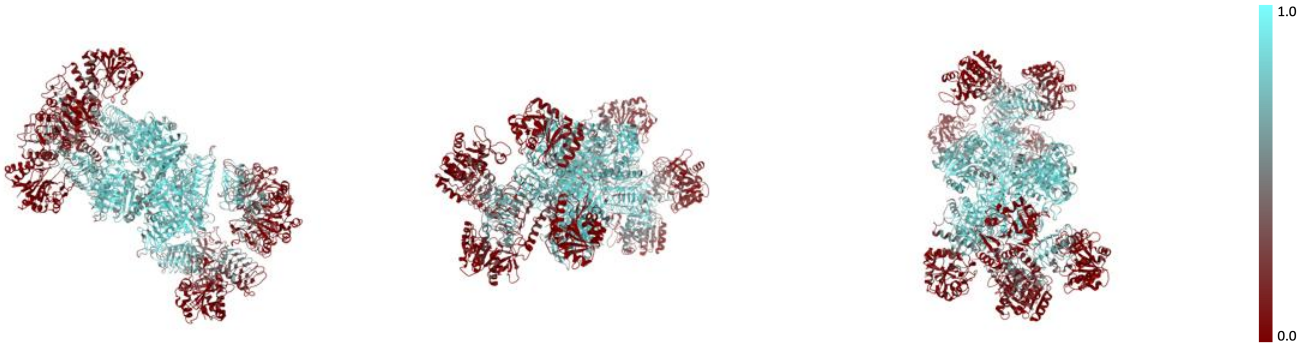
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

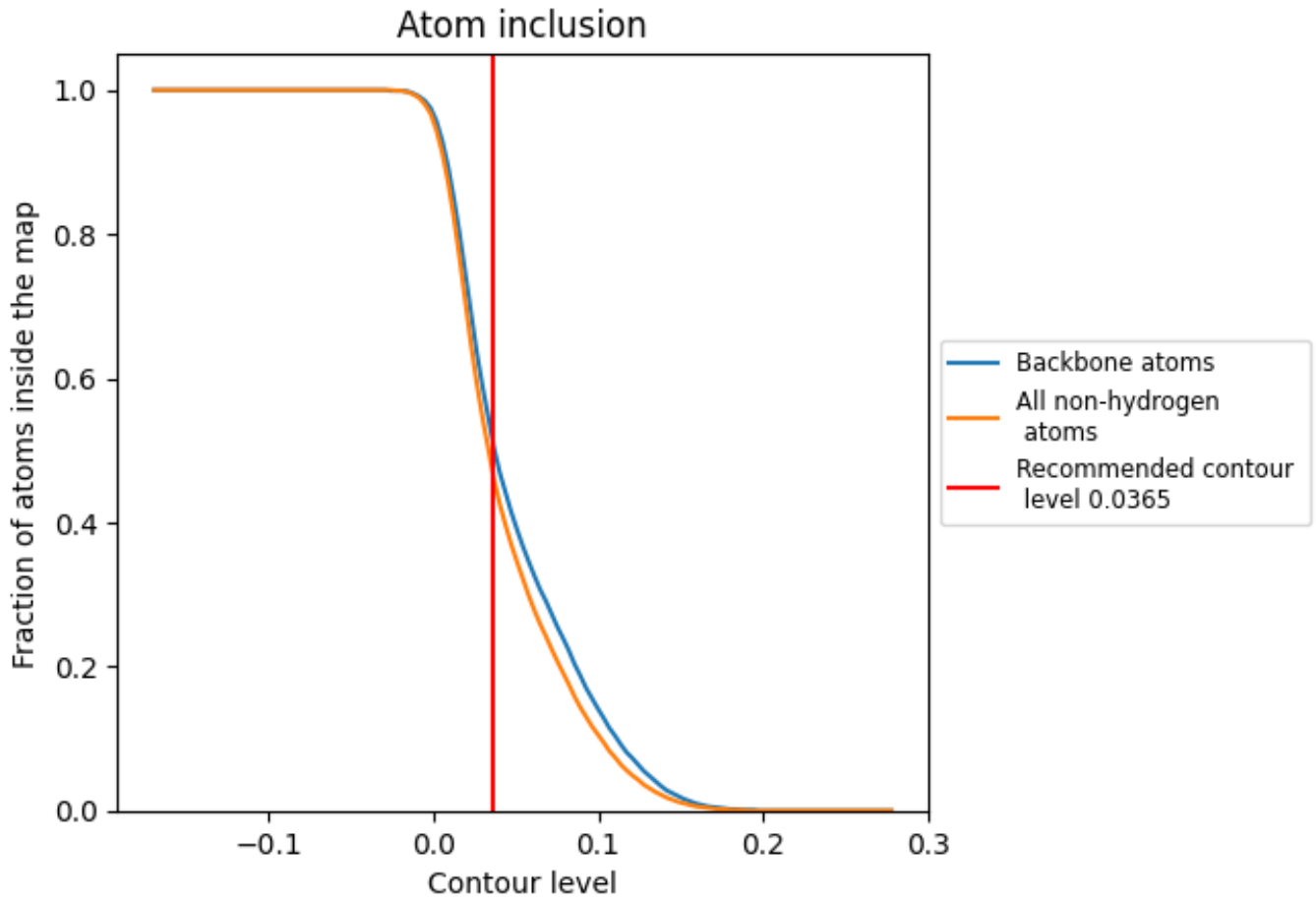
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0365).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0365) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.3940
A	0.8190	0.5710
B	0.8130	0.5660
C	0.8020	0.5640
D	0.8120	0.5620
E	0.1640	0.2230
F	0.3460	0.3490
G	0.1850	0.2680
H	0.3850	0.3680
I	0.3060	0.3230
J	0.1560	0.2210
K	0.3760	0.3540
L	0.1870	0.2730