wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 12:03 PM EST

PDB ID	:	7RMC
EMDB ID	:	EMD-24560
Title	:	Yeast CTP Synthase (Ura7) filament bound to CTP at low pH
Authors	:	Hansen, J.M.; Lynch, E.M.; Farrell, D.P.; DiMaio, F.; Quispe, J.; Kollman, J.M.
Deposited on	:	2021-07-27
Resolution	:	3.50 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:

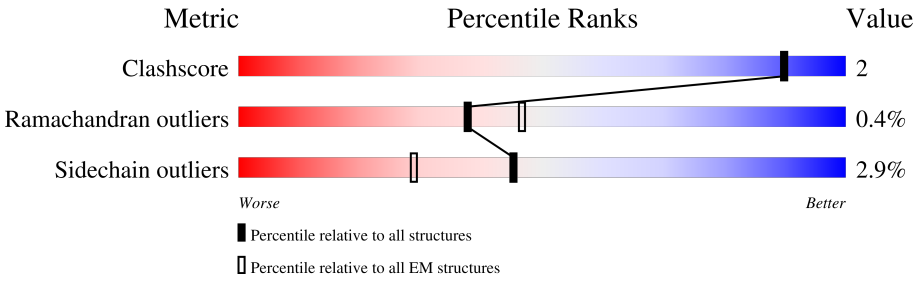
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	D	561	100% 93% 6% •
1	E	561	82% 93% 6% •
1	F	561	82% 93% 6% •
1	Q	561	84% 94% 5% •
1	R	561	15% 93% 6% •
1	S	561	100% 93% 6% •
1	T	561	15% 93% 6% •
1	U	561	100% 93% 6% •

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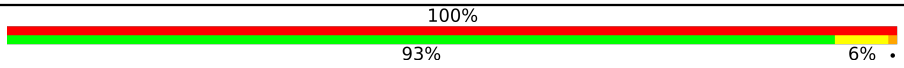
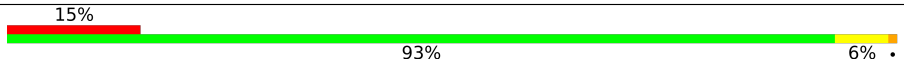
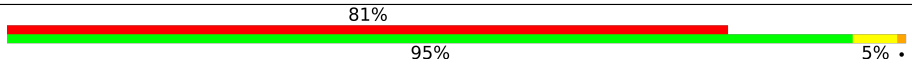
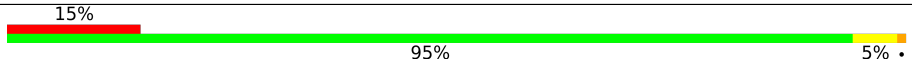
Mol	Chain	Length	Quality of chain
1	V	561	
1	W	561	
1	g	561	
1	h	561	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 106824 atoms, of which 53244 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 CTP synthase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	V	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	D	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	E	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	F	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	g	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	Q	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	S	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	U	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	h	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	R	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	T	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		
1	W	561	Total	C	H	N	O	S	0	0
			8844	2804	4437	746	833	24		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	?	-	PRO	deletion	UNP P28274
V	?	-	GLU	deletion	UNP P28274
V	?	-	ILE	deletion	UNP P28274
V	?	-	ASP	deletion	UNP P28274
V	?	-	LYS	deletion	UNP P28274
V	?	-	GLU	deletion	UNP P28274

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Chain	Residue	Modelled	Actual	Comment	Reference
V	?	-	THR	deletion	UNP P28274
V	?	-	MET	deletion	UNP P28274
V	?	-	GLY	deletion	UNP P28274
V	?	-	GLY	deletion	UNP P28274
V	?	-	SER	deletion	UNP P28274
D	?	-	PRO	deletion	UNP P28274
D	?	-	GLU	deletion	UNP P28274
D	?	-	ILE	deletion	UNP P28274
D	?	-	ASP	deletion	UNP P28274
D	?	-	LYS	deletion	UNP P28274
D	?	-	GLU	deletion	UNP P28274
D	?	-	THR	deletion	UNP P28274
D	?	-	MET	deletion	UNP P28274
D	?	-	GLY	deletion	UNP P28274
D	?	-	GLY	deletion	UNP P28274
D	?	-	SER	deletion	UNP P28274
E	?	-	PRO	deletion	UNP P28274
E	?	-	GLU	deletion	UNP P28274
E	?	-	ILE	deletion	UNP P28274
E	?	-	ASP	deletion	UNP P28274
E	?	-	LYS	deletion	UNP P28274
E	?	-	GLU	deletion	UNP P28274
E	?	-	THR	deletion	UNP P28274
E	?	-	MET	deletion	UNP P28274
E	?	-	GLY	deletion	UNP P28274
E	?	-	GLY	deletion	UNP P28274
E	?	-	SER	deletion	UNP P28274
F	?	-	PRO	deletion	UNP P28274
F	?	-	GLU	deletion	UNP P28274
F	?	-	ILE	deletion	UNP P28274
F	?	-	ASP	deletion	UNP P28274
F	?	-	LYS	deletion	UNP P28274
F	?	-	GLU	deletion	UNP P28274
F	?	-	THR	deletion	UNP P28274
F	?	-	MET	deletion	UNP P28274
F	?	-	GLY	deletion	UNP P28274
F	?	-	GLY	deletion	UNP P28274
F	?	-	SER	deletion	UNP P28274
g	?	-	PRO	deletion	UNP P28274
g	?	-	GLU	deletion	UNP P28274
g	?	-	ILE	deletion	UNP P28274
g	?	-	ASP	deletion	UNP P28274

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Chain	Residue	Modelled	Actual	Comment	Reference
g	?	-	LYS	deletion	UNP P28274
g	?	-	GLU	deletion	UNP P28274
g	?	-	THR	deletion	UNP P28274
g	?	-	MET	deletion	UNP P28274
g	?	-	GLY	deletion	UNP P28274
g	?	-	GLY	deletion	UNP P28274
g	?	-	SER	deletion	UNP P28274
Q	?	-	PRO	deletion	UNP P28274
Q	?	-	GLU	deletion	UNP P28274
Q	?	-	ILE	deletion	UNP P28274
Q	?	-	ASP	deletion	UNP P28274
Q	?	-	LYS	deletion	UNP P28274
Q	?	-	GLU	deletion	UNP P28274
Q	?	-	THR	deletion	UNP P28274
Q	?	-	MET	deletion	UNP P28274
Q	?	-	GLY	deletion	UNP P28274
Q	?	-	GLY	deletion	UNP P28274
Q	?	-	SER	deletion	UNP P28274
S	?	-	PRO	deletion	UNP P28274
S	?	-	GLU	deletion	UNP P28274
S	?	-	ILE	deletion	UNP P28274
S	?	-	ASP	deletion	UNP P28274
S	?	-	LYS	deletion	UNP P28274
S	?	-	GLU	deletion	UNP P28274
S	?	-	THR	deletion	UNP P28274
S	?	-	MET	deletion	UNP P28274
S	?	-	GLY	deletion	UNP P28274
S	?	-	GLY	deletion	UNP P28274
S	?	-	SER	deletion	UNP P28274
U	?	-	PRO	deletion	UNP P28274
U	?	-	GLU	deletion	UNP P28274
U	?	-	ILE	deletion	UNP P28274
U	?	-	ASP	deletion	UNP P28274
U	?	-	LYS	deletion	UNP P28274
U	?	-	GLU	deletion	UNP P28274
U	?	-	THR	deletion	UNP P28274
U	?	-	MET	deletion	UNP P28274
U	?	-	GLY	deletion	UNP P28274
U	?	-	GLY	deletion	UNP P28274
U	?	-	SER	deletion	UNP P28274
h	?	-	PRO	deletion	UNP P28274
h	?	-	GLU	deletion	UNP P28274

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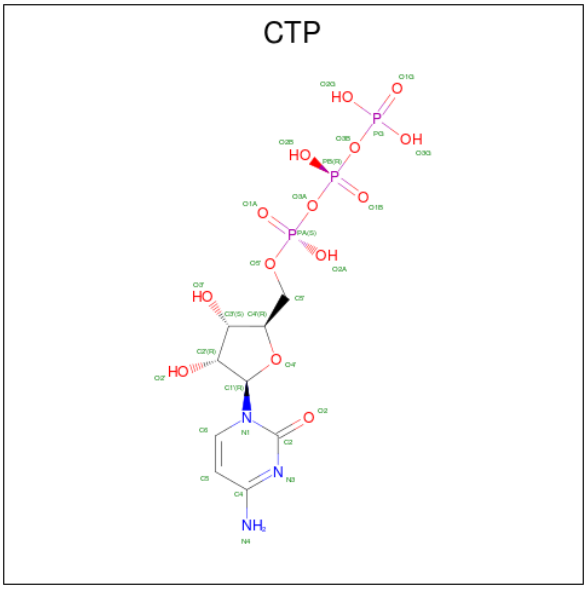
Chain	Residue	Modelled	Actual	Comment	Reference
h	?	-	ILE	deletion	UNP P28274
h	?	-	ASP	deletion	UNP P28274
h	?	-	LYS	deletion	UNP P28274
h	?	-	GLU	deletion	UNP P28274
h	?	-	THR	deletion	UNP P28274
h	?	-	MET	deletion	UNP P28274
h	?	-	GLY	deletion	UNP P28274
h	?	-	GLY	deletion	UNP P28274
h	?	-	SER	deletion	UNP P28274
R	?	-	PRO	deletion	UNP P28274
R	?	-	GLU	deletion	UNP P28274
R	?	-	ILE	deletion	UNP P28274
R	?	-	ASP	deletion	UNP P28274
R	?	-	LYS	deletion	UNP P28274
R	?	-	GLU	deletion	UNP P28274
R	?	-	THR	deletion	UNP P28274
R	?	-	MET	deletion	UNP P28274
R	?	-	GLY	deletion	UNP P28274
R	?	-	GLY	deletion	UNP P28274
R	?	-	SER	deletion	UNP P28274
T	?	-	PRO	deletion	UNP P28274
T	?	-	GLU	deletion	UNP P28274
T	?	-	ILE	deletion	UNP P28274
T	?	-	ASP	deletion	UNP P28274
T	?	-	LYS	deletion	UNP P28274
T	?	-	GLU	deletion	UNP P28274
T	?	-	THR	deletion	UNP P28274
T	?	-	MET	deletion	UNP P28274
T	?	-	GLY	deletion	UNP P28274
T	?	-	GLY	deletion	UNP P28274
T	?	-	SER	deletion	UNP P28274
W	?	-	PRO	deletion	UNP P28274
W	?	-	GLU	deletion	UNP P28274
W	?	-	ILE	deletion	UNP P28274
W	?	-	ASP	deletion	UNP P28274
W	?	-	LYS	deletion	UNP P28274
W	?	-	GLU	deletion	UNP P28274
W	?	-	THR	deletion	UNP P28274
W	?	-	MET	deletion	UNP P28274
W	?	-	GLY	deletion	UNP P28274
W	?	-	GLY	deletion	UNP P28274
W	?	-	SER	deletion	UNP P28274

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	V	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	V	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	D	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	D	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	E	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	E	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	F	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	F	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	g	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	g	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	Q	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	Q	1	Total	C	N	O	P	0
			58	18	6	28	6	

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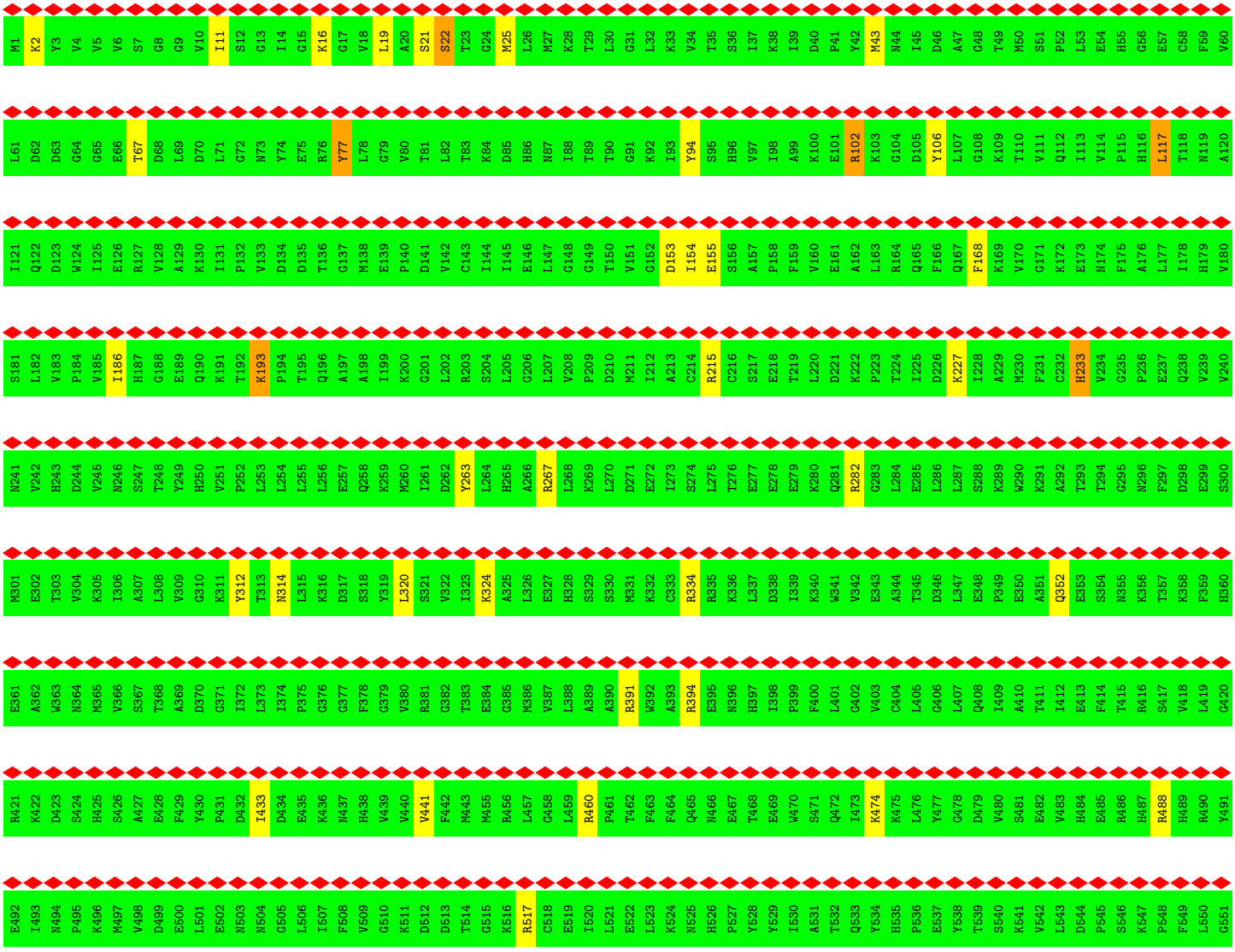
Mol	Chain	Residues	Atoms					AltConf
2	S	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	S	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	U	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	U	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	h	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	h	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	R	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	R	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	T	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	T	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	W	1	Total	C	N	O	P	0
			58	18	6	28	6	
2	W	1	Total	C	N	O	P	0
			58	18	6	28	6	

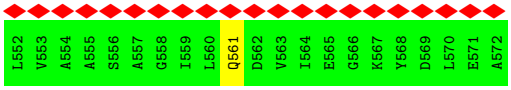
3 Residue-property plots (i)

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.

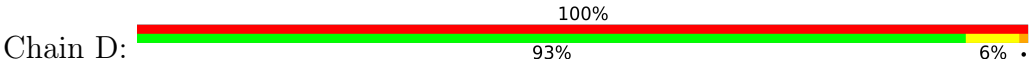
- Molecule 1: CTP synthase 1

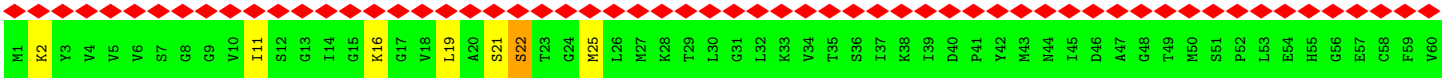
Chain V:

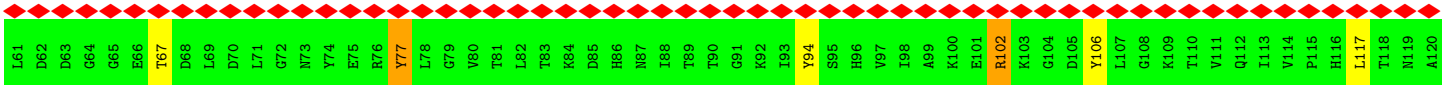


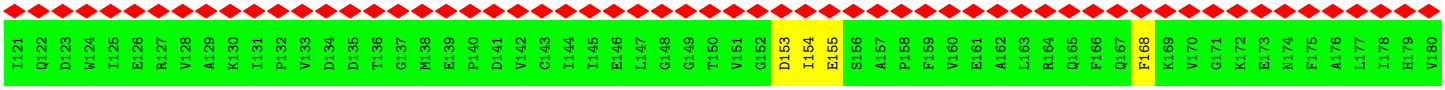


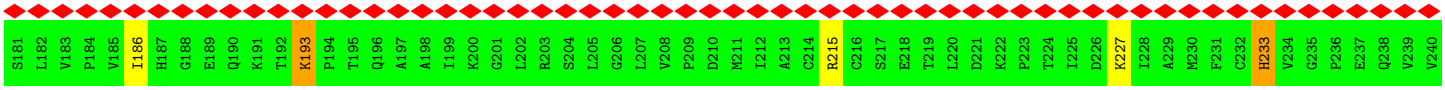
• Molecule 1: CTP synthase 1

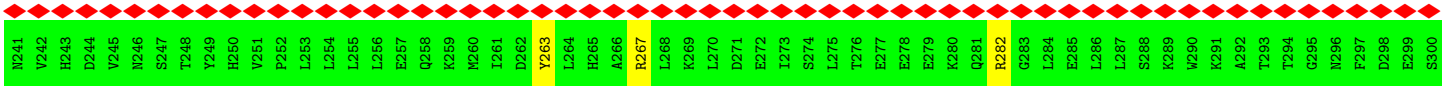


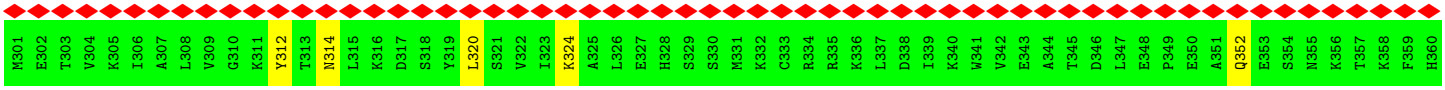


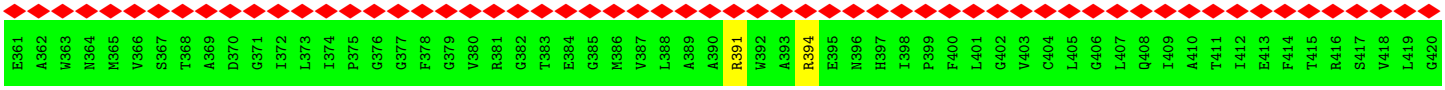


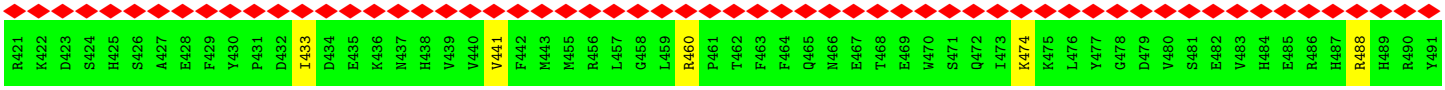


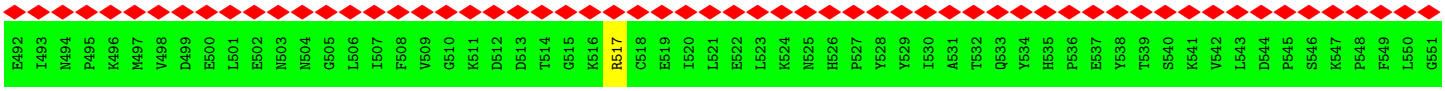


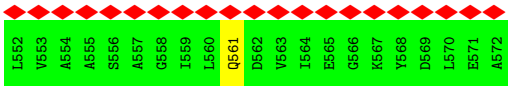




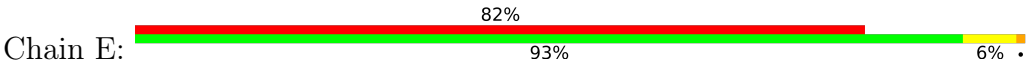


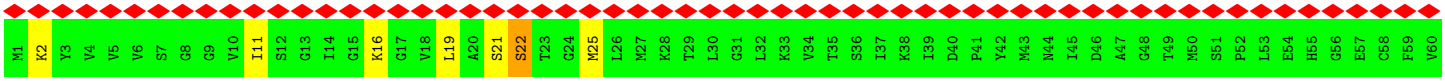


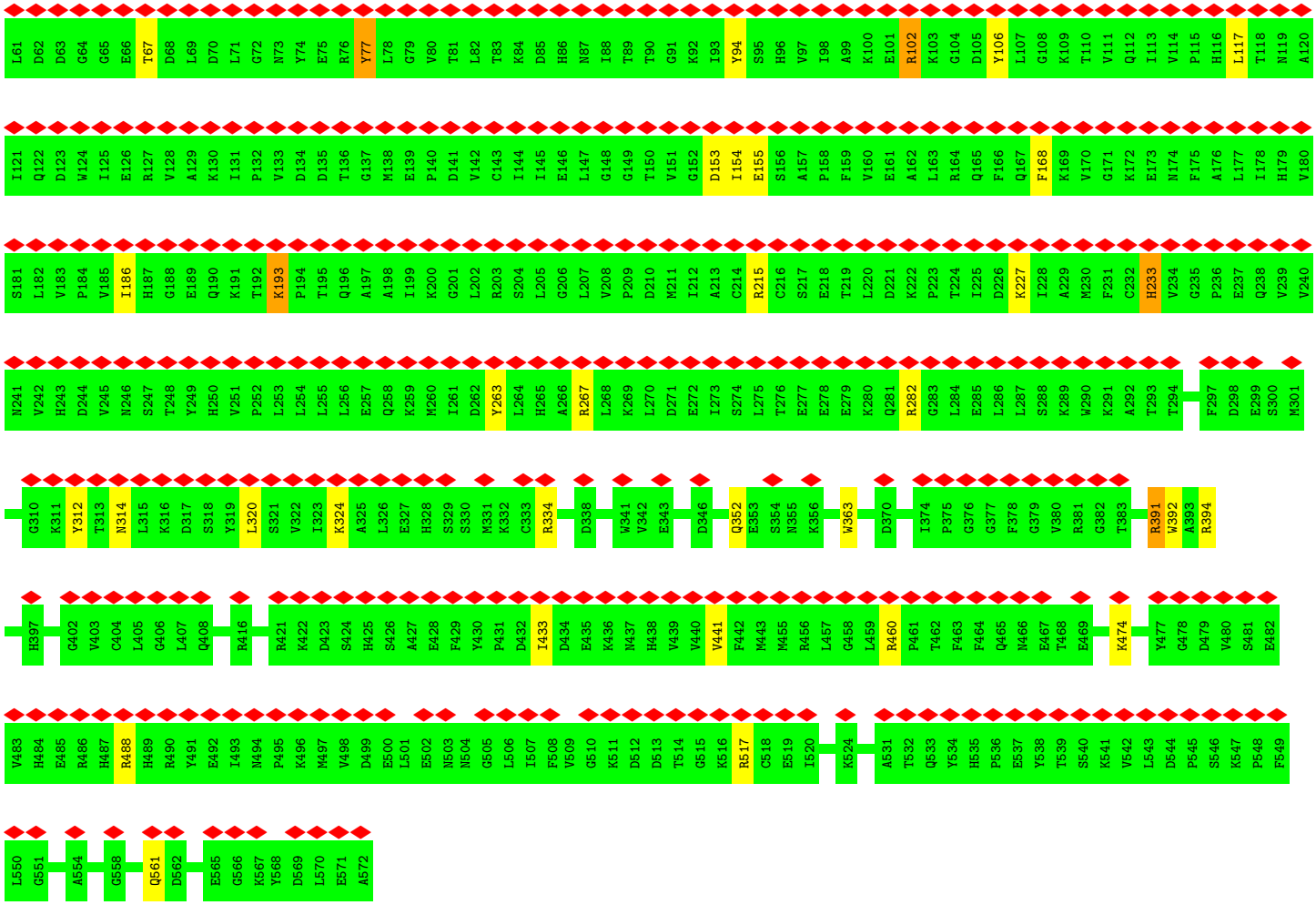




• Molecule 1: CTP synthase 1

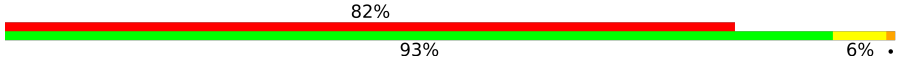


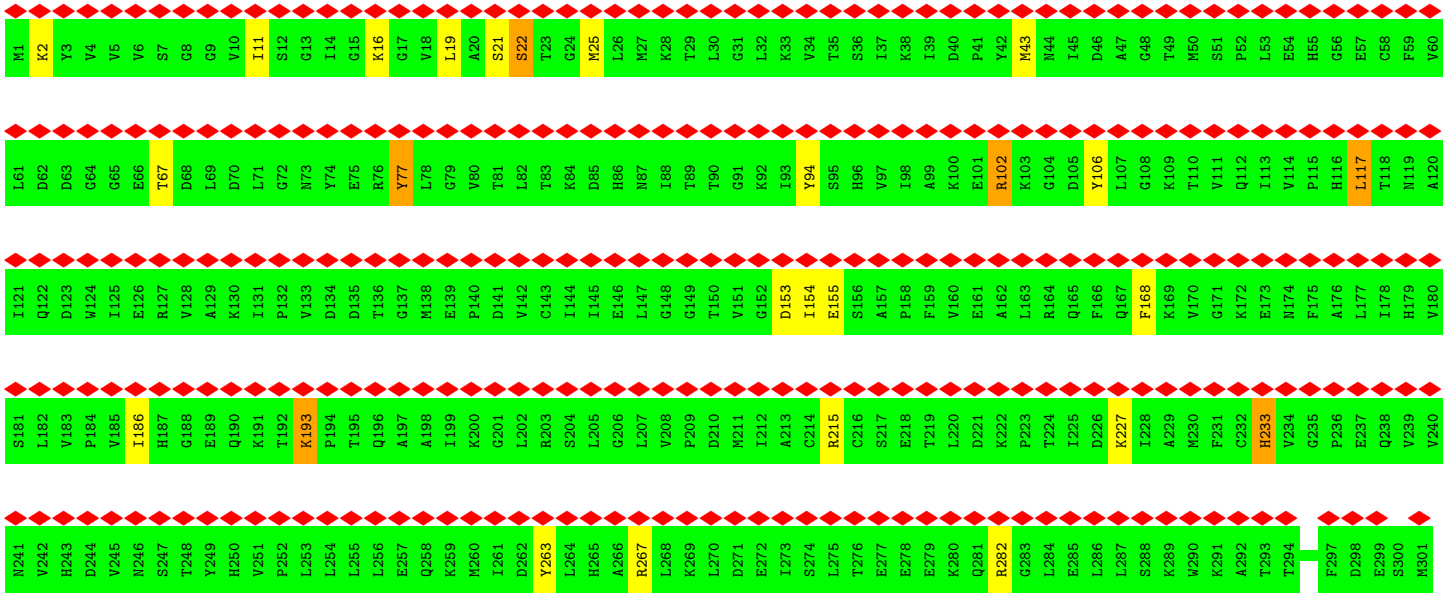


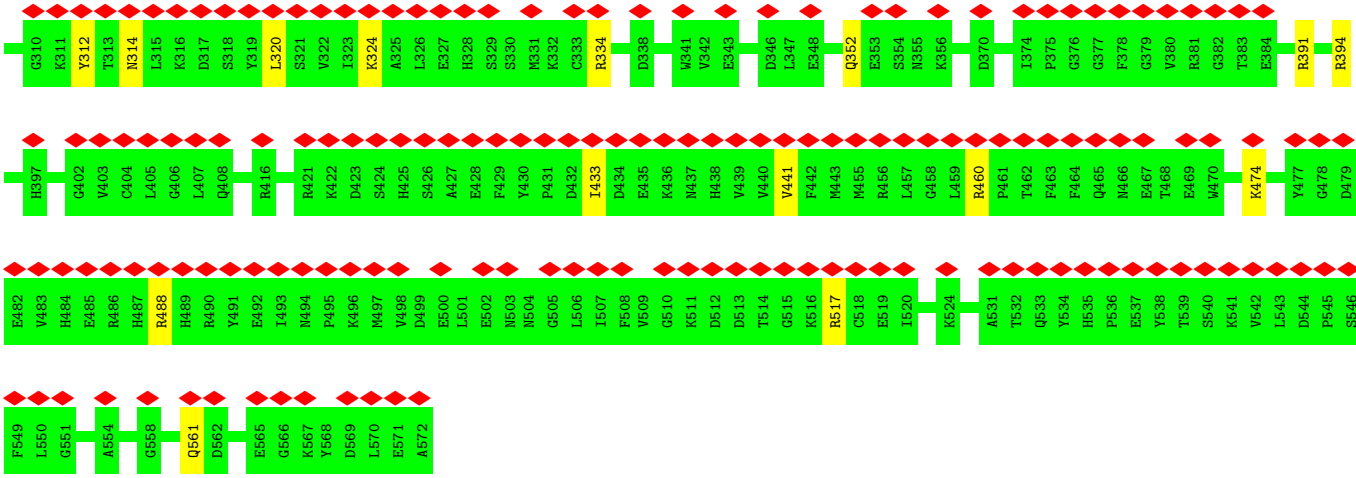


• Molecule 1: CTP synthase 1

Chain F:

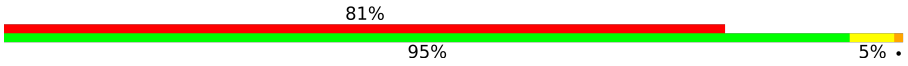


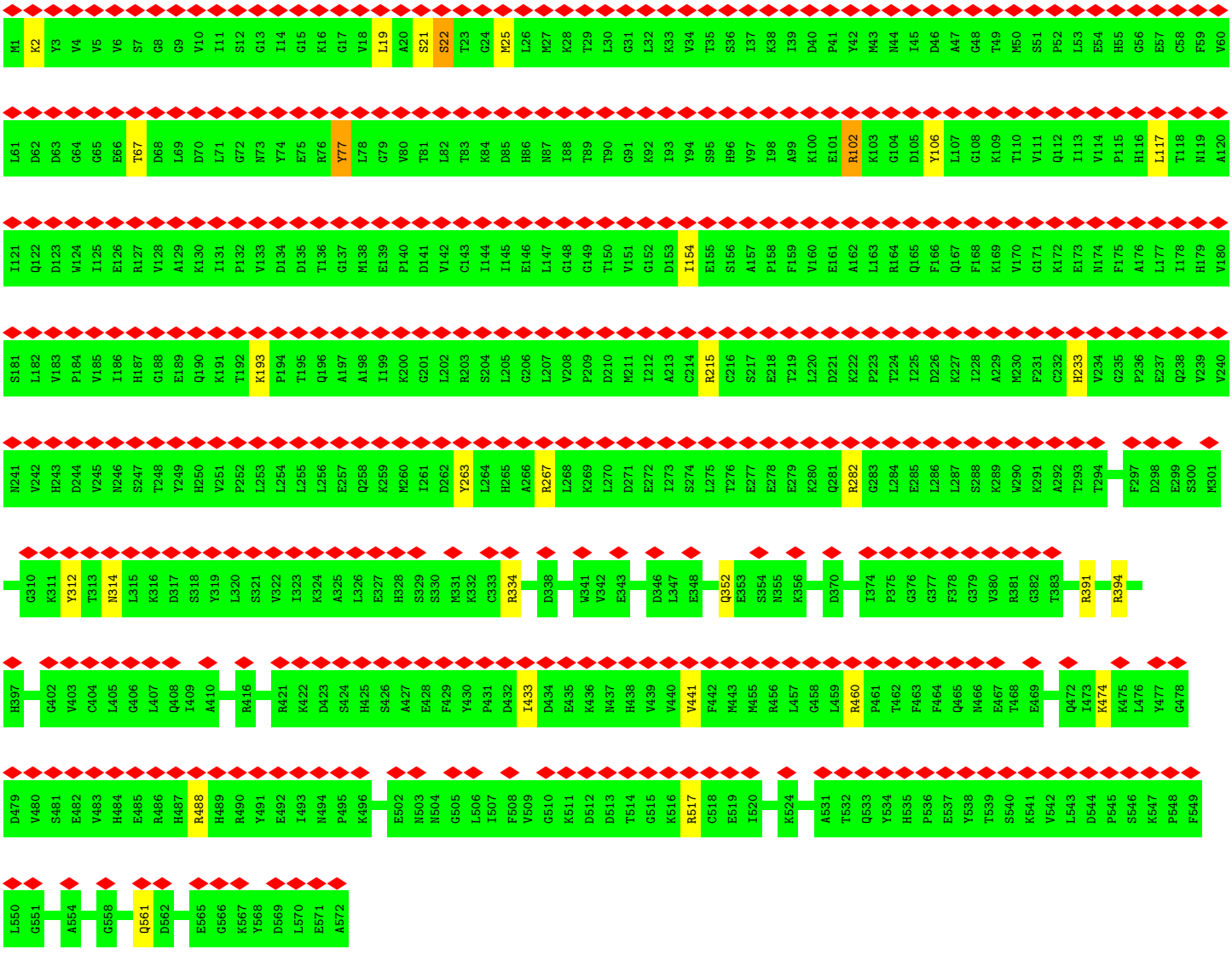




• Molecule 1: CTP synthase 1

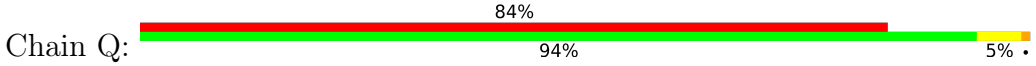
Chain g:

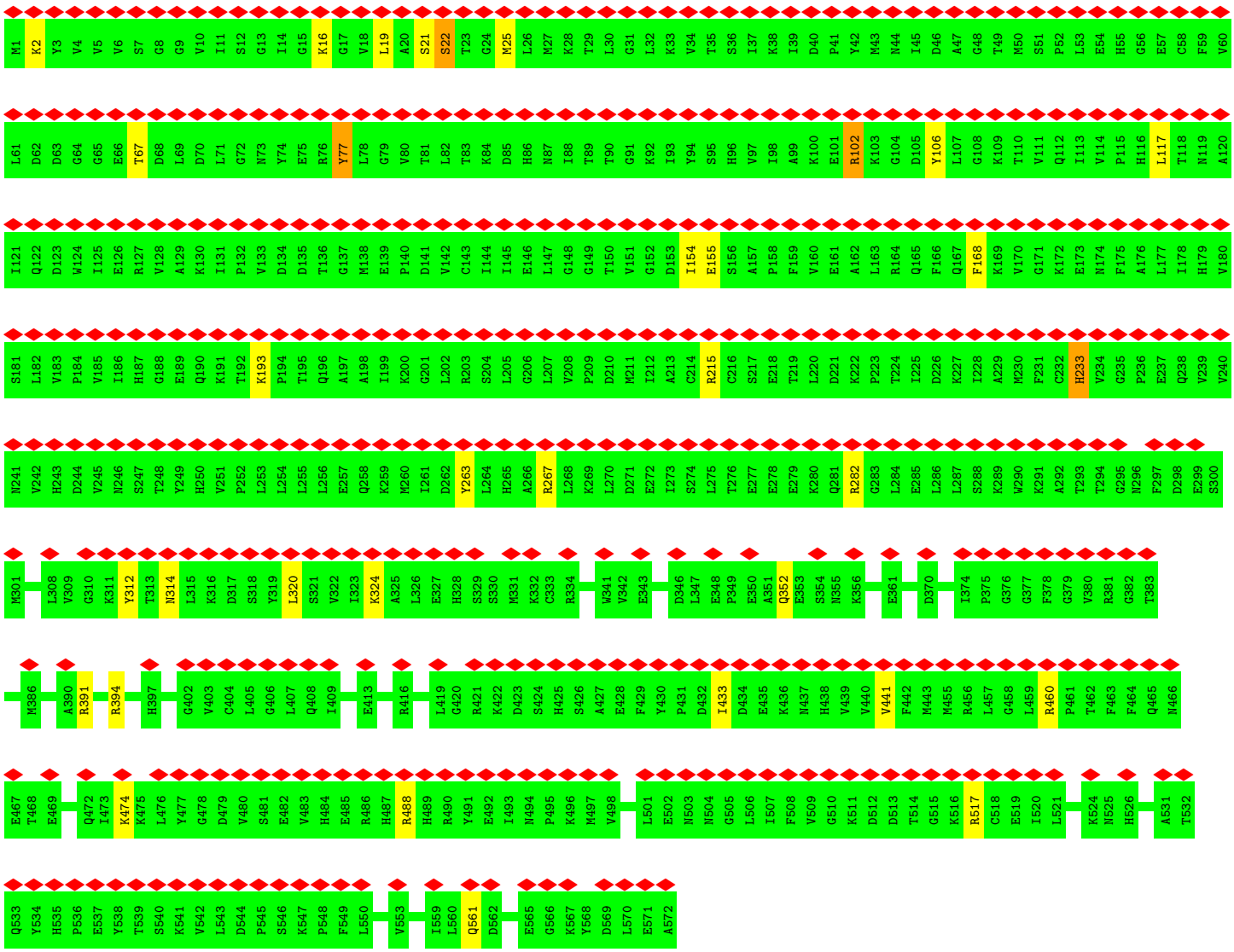




• Molecule 1: CTP synthase 1

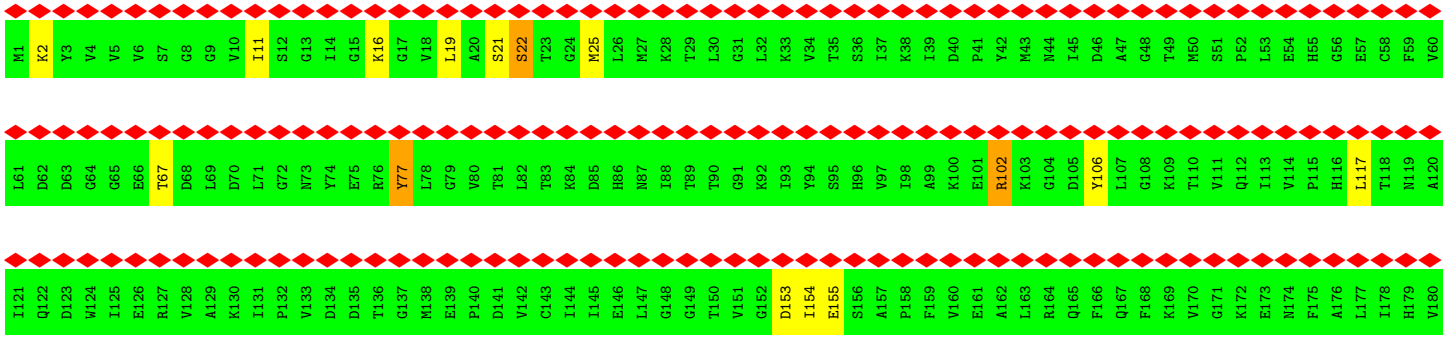
Chain Q:





• Molecule 1: CTP synthase 1

Chain S:



S181 L182 V183 P184 V185 I186 H187 G188 E189 Q190 K191 T192 K193 P194 T195 Q196 A197 A198 I199 K200 G201 L202 R203 S204 L205 G206 L207 V208 P209 D210 M211 I212 A213 C214 R215 C216 S217 E218 T219 L220 D221 K222 P223 T224 I225 D226 K227 I228 A229 M230 F231 C232 H233 V234 G235 P236 E237 Q238 V239 V240

N241 V242 H243 D244 V245 N246 S247 T248 Y249 H250 V251 P252 L253 L254 L255 L256 E257 Q258 K259 M260 I261 D262 Y263 L264 H265 A266 R267 L268 K269 L270 D271 E272 I273 S274 L275 T276 E277 E278 E279 K280 Q281 R282 G283 L284 E285 L286 L287 S288 K289 W290 K291 A292 T293 T294 G295 N296 F297 D298 E299 S300

M301 E302 T303 V304 K305 I306 A307 L308 V309 G310 K311 Y312 T313 N314 L315 K316 D317 S318 Y319 L320 S321 V322 I323 K324 A325 L326 E327 H328 S329 S330 M331 K332 C333 R334 R335 K336 L337 D338 I339 K340 W341 V342 E343 A344 T345 D346 L347 E348 P349 E350 A351 Q352 E353 S354 N355 K356 T357 K358 F359 H360

E361 A362 W363 N364 M365 V366 S367 T368 A369 D370 G371 I372 L373 I374 P375 G376 G377 F378 G379 V380 R381 G382 T383 E384 G385 M386 V387 L388 A389 A390 R391 W392 A393 R394 E395 N396 H397 I398 P399 F400 L401 G402 V403 C404 L405 G406 L407 Q408 I409 A410 T411 I412 E413 F414 T415 R416 S417 V418 L419 G420

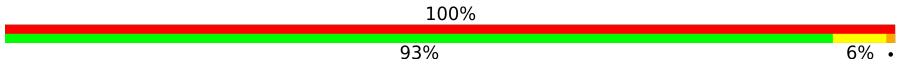
R421 K422 D423 S424 H425 S426 A427 E428 F429 Y430 P431 D432 I433 D434 E435 K436 N437 H438 V439 V440 V441 F442 M443 M455 R456 L457 G458 L459 R460 P461 T462 F463 F464 Q465 N466 E467 T468 E469 W470 S471 Q472 I473 K474 K475 L476 Y477 G478 D479 V480 S481 E482 V483 H484 E485 R486 H487 R488 H489 R490 Y491

E492 I493 N494 P495 K496 M497 V498 D499 E500 L501 E502 N503 N504 G505 L506 I507 F508 V509 G510 K511 D512 D513 T514 G515 K516 R517 C518 E519 I520 L521 E522 L523 K524 N525 H526 P527 Y528 Y529 I530 A531 T532 Q533 Y534 H535 P536 E537 Y538 T539 S540 K541 V542 L543 D544 P545 S546 K547 P548 F549 L550 G551

L552 V553 A554 A555 S556 A557 G558 I559 L560 Q561 D562 V563 I564 E565 G566 K567 Y568 D569 L570 E571 A572

• Molecule 1: CTP synthase 1

Chain U:



M1 K2 Y3 V4 V5 V6 S7 G8 G9 V10 I11 S12 G13 I14 G15 K16 G17 V18 L19 A20 S21 S22 T23 G24 M25 L26 M27 K28 T29 L30 G31 L32 K33 V34 T35 S36 I37 K38 I39 D40 P41 Y42 M43 N44 I45 D46 A47 G48 T49 M50 S51 P52 L53 E54 H55 G56 E57 C58 F59 V60

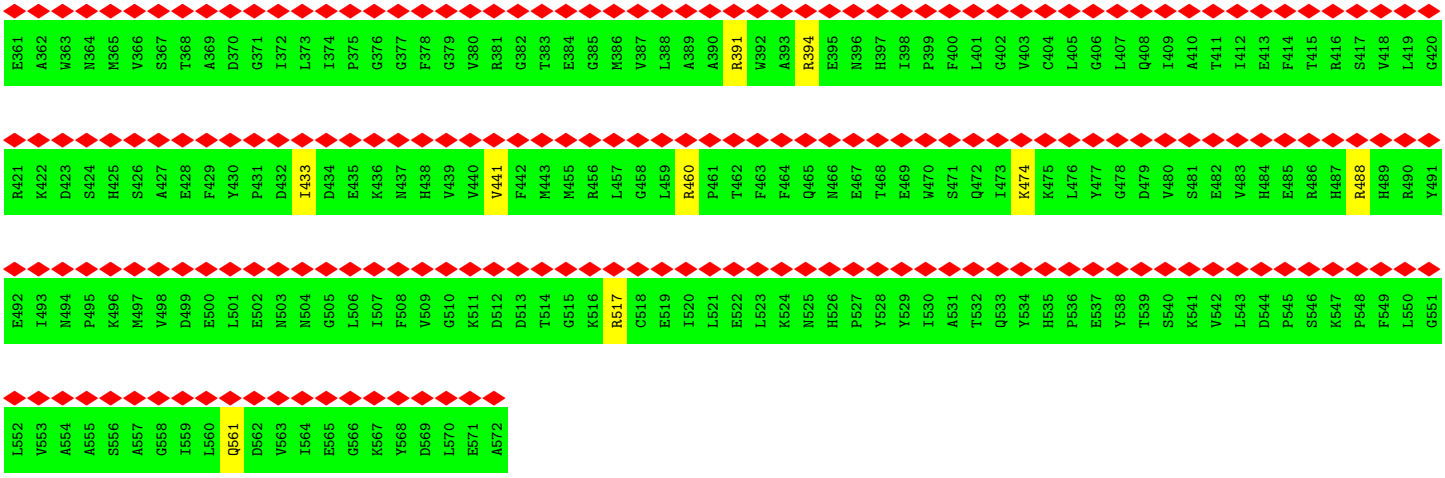
L61 D62 D63 G64 G65 E66 T67 D68 L69 D70 L71 G72 N73 Y74 E75 R76 Y77 L78 G79 V80 T81 L82 T83 K84 D85 H86 N87 I88 T89 T90 G91 K92 I93 Y94 S95 H96 V97 I98 A99 K100 E101 R102 K103 G104 D105 Y106 L107 G108 K109 T110 V111 Q112 I113 V114 P115 H116 L117 T118 N119 A120

I121 Q122 D123 W124 I125 E126 R127 V128 A129 K130 I131 P132 V133 D134 D135 T136 G137 M138 E139 P140 D141 V142 C143 I144 I145 E146 L147 G148 G149 T150 V151 G152 D153 I154 E155 S156 A157 P158 F159 V160 E161 A162 L163 R164 Q165 F166 Q167 F168 K169 V170 G171 K172 E173 N174 F175 A176 L177 I178 H179 V180

S181 L182 V183 P184 V185 I186 H187 G188 E189 Q190 K191 T192 K193 P194 T195 Q196 A197 A198 I199 K200 G201 L202 R203 S204 L205 G206 L207 V208 P209 D210 M211 I212 A213 C214 R215 C216 S217 E218 T219 L220 D221 K222 P223 T224 I225 D226 K227 I228 A229 M230 F231 C232 H233 V234 G235 P236 E237 Q238 V239 V240

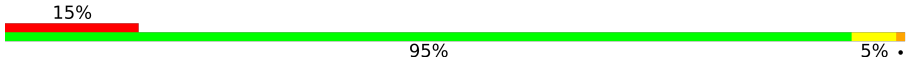
N241 V242 H243 D244 V245 N246 S247 T248 Y249 H250 V251 P252 L253 L254 L255 L256 E257 Q258 K259 M260 I261 D262 Y263 L264 H265 A266 R267 L268 K269 L270 D271 E272 I273 S274 L275 T276 E277 E278 E279 K280 Q281 R282 G283 L284 E285 L286 L287 S288 K289 W290 K291 A292 T293 T294 G295 N296 F297 D298 E299 S300

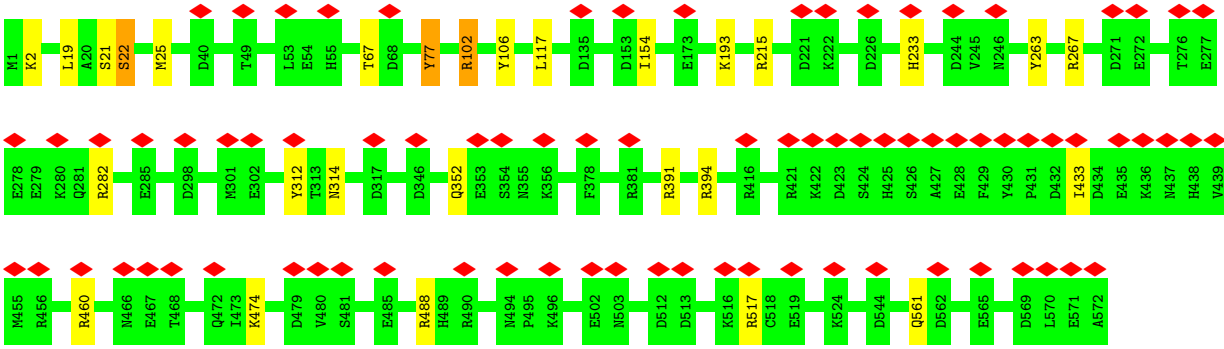
M301 E302 T303 V304 K305 I306 A307 L308 V309 G310 K311 Y312 T313 N314 L315 K316 D317 S318 Y319 L320 S321 V322 I323 K324 A325 L326 E327 H328 S329 S330 M331 K332 C333 R334 R335 K336 L337 D338 I339 K340 W341 V342 E343 A344 T345 D346 L347 E348 P349 E350 A351 Q352 E353 S354 N355 K356 T357 K358 F359 H360



• Molecule 1: CTP synthase 1

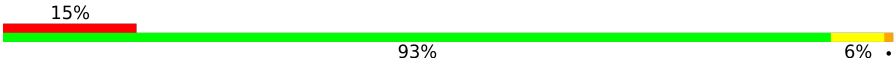
Chain h:

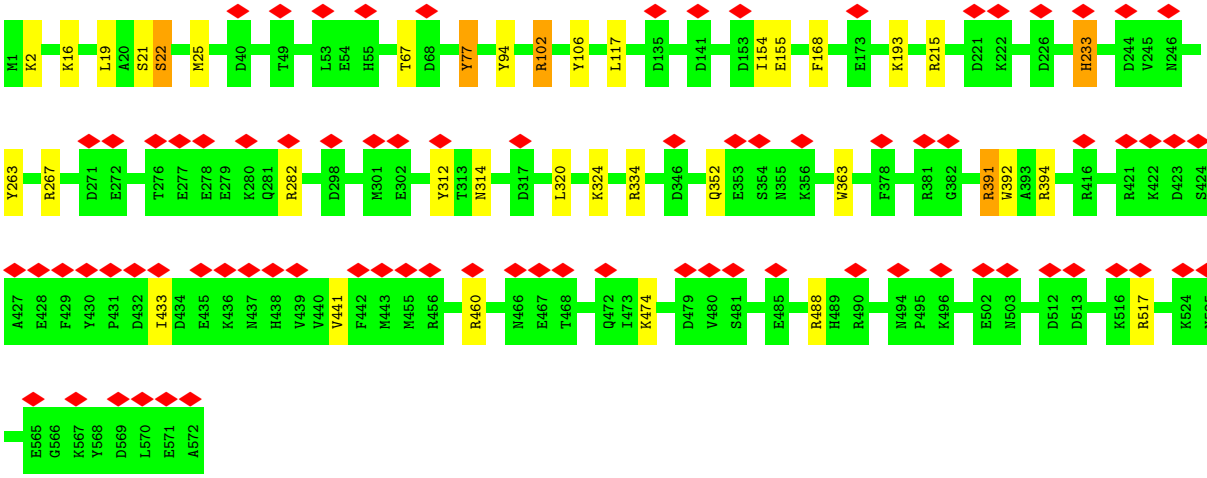




• Molecule 1: CTP synthase 1

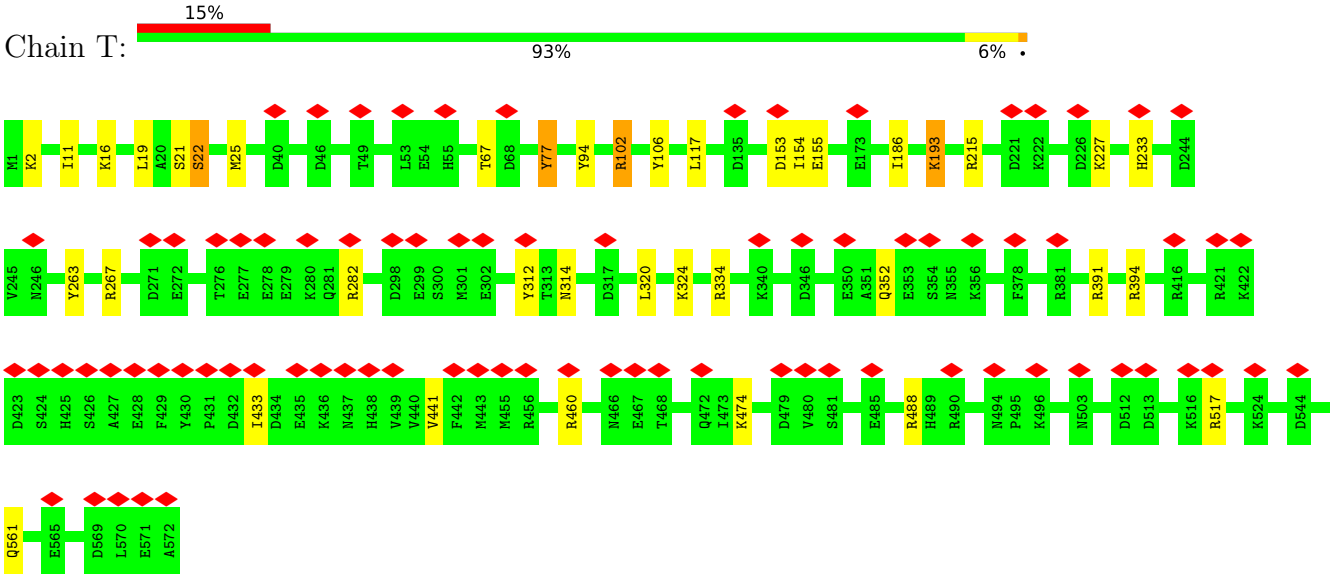
Chain R:





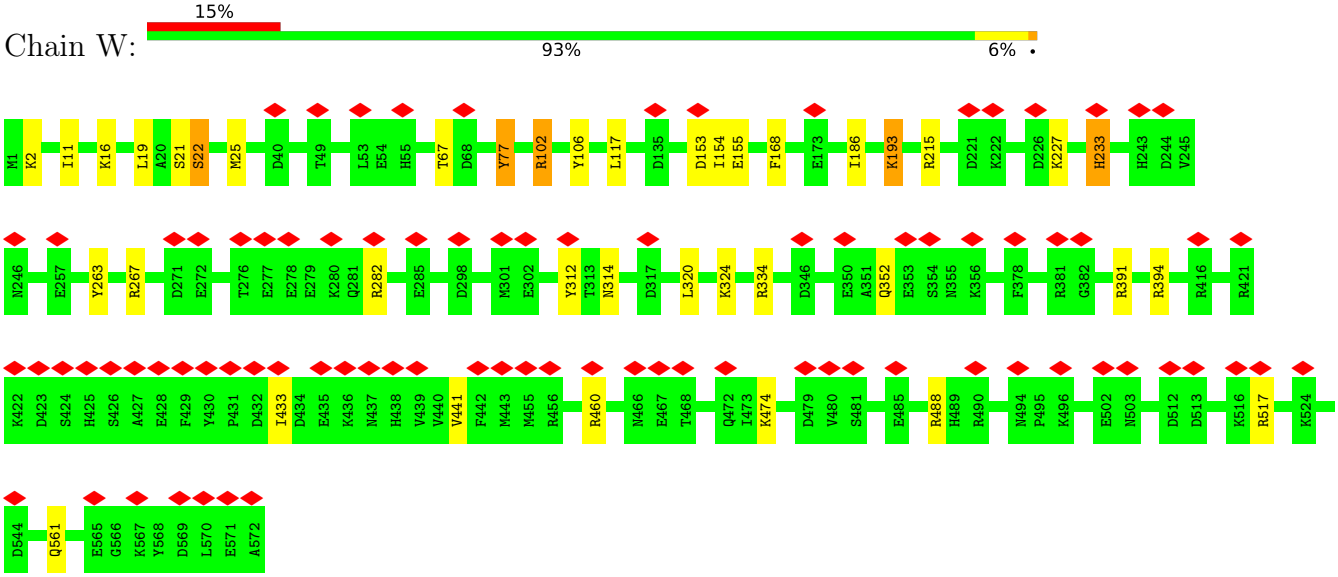
• Molecule 1: CTP synthase 1

Chain T:



• Molecule 1: CTP synthase 1

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	64010	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	90	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	10.548	Depositor
Minimum map value	-5.796	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.226	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTP

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	D	0.62	0/4494	1.03	14/6076 (0.2%)
1	E	0.63	0/4494	1.03	15/6076 (0.2%)
1	F	0.62	0/4494	1.03	16/6076 (0.3%)
1	Q	0.63	0/4494	1.03	15/6076 (0.2%)
1	R	0.62	0/4494	1.03	15/6076 (0.2%)
1	S	0.62	0/4494	1.03	15/6076 (0.2%)
1	T	0.62	0/4494	1.03	15/6076 (0.2%)
1	U	0.62	0/4494	1.03	15/6076 (0.2%)
1	V	0.62	0/4494	1.03	15/6076 (0.2%)
1	W	0.62	0/4494	1.03	15/6076 (0.2%)
1	g	0.63	0/4494	1.03	15/6076 (0.2%)
1	h	0.62	0/4494	1.03	14/6076 (0.2%)
All	All	0.62	0/53928	1.03	179/72912 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	2	4
1	E	2	4
1	F	2	4
1	Q	2	4
1	R	2	4
1	S	2	4
1	T	2	4
1	U	2	4
1	V	2	4
1	W	2	4
1	g	2	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	h	2	4
All	All	24	48

There are no bond length outliers.

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	67	THR	CA-CB-OG1	9.34	128.61	109.00
1	V	67	THR	CA-CB-OG1	9.32	128.58	109.00
1	U	67	THR	CA-CB-OG1	9.32	128.58	109.00
1	E	67	THR	CA-CB-OG1	9.32	128.56	109.00
1	R	67	THR	CA-CB-OG1	9.32	128.57	109.00

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	V	22	SER	CA
1	V	77	TYR	CA
1	D	22	SER	CA
1	D	77	TYR	CA
1	E	22	SER	CA

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	102	ARG	Sidechain
1	V	102	ARG	Sidechain
1	V	106	TYR	Sidechain
1	V	263	TYR	Sidechain
1	V	391	ARG	Sidechain

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	D	4407	4437	4436	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4407	4437	4436	26	0
1	F	4407	4437	4436	19	0
1	Q	4407	4437	4436	8	0
1	R	4407	4437	4436	20	0
1	S	4407	4437	4436	13	0
1	T	4407	4437	4436	16	0
1	U	4407	4437	4436	15	0
1	V	4407	4437	4436	19	0
1	W	4407	4437	4436	15	0
1	g	4407	4437	4436	0	0
1	h	4407	4437	4436	0	0
2	D	58	0	24	7	0
2	E	58	0	24	7	0
2	F	58	0	24	7	0
2	Q	58	0	24	6	0
2	R	58	0	24	6	0
2	S	58	0	24	7	0
2	T	58	0	24	8	0
2	U	58	0	24	7	0
2	V	58	0	24	7	0
2	W	58	0	24	7	0
2	g	58	0	24	0	0
2	h	58	0	24	0	0
All	All	53580	53244	53520	118	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 2.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:LYS:HE3	2:F:602:CTP:O2	1.64	0.98
1:V:324:LYS:HE3	2:V:602:CTP:O2	1.64	0.98
1:Q:324:LYS:HE3	2:Q:602:CTP:O2	1.64	0.98
1:S:324:LYS:HE3	2:S:602:CTP:O2	1.64	0.97
1:D:324:LYS:HE3	2:D:602:CTP:O2	1.64	0.96

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	D	557/561 (99%)	530 (95%)	25 (4%)	2 (0%)	34	72
1	E	557/561 (99%)	530 (95%)	25 (4%)	2 (0%)	34	72
1	F	557/561 (99%)	529 (95%)	26 (5%)	2 (0%)	34	72
1	Q	557/561 (99%)	530 (95%)	25 (4%)	2 (0%)	34	72
1	R	557/561 (99%)	529 (95%)	26 (5%)	2 (0%)	34	72
1	S	557/561 (99%)	530 (95%)	25 (4%)	2 (0%)	34	72
1	T	557/561 (99%)	530 (95%)	25 (4%)	2 (0%)	34	72
1	U	557/561 (99%)	530 (95%)	25 (4%)	2 (0%)	34	72
1	V	557/561 (99%)	529 (95%)	26 (5%)	2 (0%)	34	72
1	W	557/561 (99%)	529 (95%)	26 (5%)	2 (0%)	34	72
1	g	557/561 (99%)	530 (95%)	25 (4%)	2 (0%)	34	72
1	h	557/561 (99%)	529 (95%)	26 (5%)	2 (0%)	34	72
All	All	6684/6732 (99%)	6355 (95%)	305 (5%)	24 (0%)	38	72

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	433	ILE
1	D	433	ILE
1	E	433	ILE
1	F	433	ILE
1	g	433	ILE

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	D	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	E	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	F	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	Q	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	R	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	S	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	T	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	U	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	V	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	W	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	g	486/486 (100%)	472 (97%)	14 (3%)	42	71
1	h	486/486 (100%)	472 (97%)	14 (3%)	42	71
All	All	5832/5832 (100%)	5664 (97%)	168 (3%)	45	71

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	h	22	SER
1	T	22	SER
1	h	154	ILE
1	R	25	MET
1	T	314	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	352	GLN
1	h	352	GLN
1	W	352	GLN
1	R	352	GLN
1	g	352	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
2	CTP	g	601	-	26,30,30	1.45	4 (15%)	39,47,47	1.81	6 (15%)
2	CTP	Q	601	-	26,30,30	1.45	3 (11%)	39,47,47	1.82	7 (17%)
2	CTP	W	601	-	26,30,30	1.46	4 (15%)	39,47,47	1.80	6 (15%)
2	CTP	F	601	-	26,30,30	1.46	4 (15%)	39,47,47	1.80	6 (15%)
2	CTP	h	602	-	26,30,30	1.35	4 (15%)	39,47,47	1.41	6 (15%)
2	CTP	W	602	-	26,30,30	1.35	5 (19%)	39,47,47	1.40	6 (15%)
2	CTP	S	602	-	26,30,30	1.33	3 (11%)	39,47,47	1.42	6 (15%)
2	CTP	Q	602	-	26,30,30	1.33	4 (15%)	39,47,47	1.42	6 (15%)
2	CTP	g	602	-	26,30,30	1.35	4 (15%)	39,47,47	1.40	6 (15%)
2	CTP	h	601	-	26,30,30	1.46	4 (15%)	39,47,47	1.81	6 (15%)
2	CTP	D	601	-	26,30,30	1.44	3 (11%)	39,47,47	1.81	7 (17%)
2	CTP	E	601	-	26,30,30	1.45	3 (11%)	39,47,47	1.82	7 (17%)
2	CTP	S	601	-	26,30,30	1.45	3 (11%)	39,47,47	1.81	7 (17%)
2	CTP	T	602	-	26,30,30	1.33	3 (11%)	39,47,47	1.42	6 (15%)
2	CTP	T	601	-	26,30,30	1.45	3 (11%)	39,47,47	1.83	7 (17%)
2	CTP	E	602	-	26,30,30	1.33	4 (15%)	39,47,47	1.42	6 (15%)
2	CTP	R	601	-	26,30,30	1.45	3 (11%)	39,47,47	1.82	7 (17%)
2	CTP	V	602	-	26,30,30	1.35	4 (15%)	39,47,47	1.41	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CTP	R	602	-	26,30,30	1.32	3 (11%)	39,47,47	1.43	6 (15%)
2	CTP	D	602	-	26,30,30	1.33	3 (11%)	39,47,47	1.42	6 (15%)
2	CTP	U	601	-	26,30,30	1.46	4 (15%)	39,47,47	1.80	6 (15%)
2	CTP	V	601	-	26,30,30	1.45	4 (15%)	39,47,47	1.80	6 (15%)
2	CTP	U	602	-	26,30,30	1.35	4 (15%)	39,47,47	1.41	6 (15%)
2	CTP	F	602	-	26,30,30	1.36	4 (15%)	39,47,47	1.41	6 (15%)

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
2	CTP	g	601	-	-	9/22/38/38	0/2/2/2
2	CTP	Q	601	-	-	8/22/38/38	0/2/2/2
2	CTP	W	601	-	-	8/22/38/38	0/2/2/2
2	CTP	F	601	-	-	9/22/38/38	0/2/2/2
2	CTP	h	602	-	-	9/22/38/38	0/2/2/2
2	CTP	W	602	-	-	9/22/38/38	0/2/2/2
2	CTP	S	602	-	-	7/22/38/38	0/2/2/2
2	CTP	Q	602	-	-	7/22/38/38	0/2/2/2
2	CTP	g	602	-	-	9/22/38/38	0/2/2/2
2	CTP	h	601	-	-	8/22/38/38	0/2/2/2
2	CTP	D	601	-	-	8/22/38/38	0/2/2/2
2	CTP	E	601	-	-	8/22/38/38	0/2/2/2
2	CTP	S	601	-	-	8/22/38/38	0/2/2/2
2	CTP	T	602	-	-	7/22/38/38	0/2/2/2
2	CTP	T	601	-	-	8/22/38/38	0/2/2/2
2	CTP	E	602	-	-	7/22/38/38	0/2/2/2
2	CTP	R	601	-	-	8/22/38/38	0/2/2/2
2	CTP	V	602	-	-	8/22/38/38	0/2/2/2
2	CTP	R	602	-	-	7/22/38/38	0/2/2/2
2	CTP	D	602	-	-	7/22/38/38	0/2/2/2
2	CTP	U	601	-	-	8/22/38/38	0/2/2/2
2	CTP	V	601	-	-	8/22/38/38	0/2/2/2
2	CTP	U	602	-	-	9/22/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTP	F	602	-	-	9/22/38/38	0/2/2/2

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	CTP	C6-N1	-3.13	1.30	1.38
2	S	601	CTP	C6-N1	-3.12	1.30	1.38
2	T	601	CTP	C6-N1	-3.11	1.30	1.38
2	V	601	CTP	C6-N1	-3.11	1.30	1.38
2	Q	601	CTP	C6-N1	-3.10	1.30	1.38

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	601	CTP	PB-O3B-PG	-6.81	109.47	132.83
2	g	601	CTP	PB-O3B-PG	-6.80	109.49	132.83
2	Q	601	CTP	PB-O3B-PG	-6.80	109.49	132.83
2	T	601	CTP	PB-O3B-PG	-6.80	109.49	132.83
2	U	601	CTP	PB-O3B-PG	-6.80	109.49	132.83

There are no chirality outliers.

5 of 193 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	601	CTP	C2'-C1'-N1-C6
2	V	601	CTP	C5'-O5'-PA-O1A
2	V	601	CTP	C5'-O5'-PA-O2A
2	V	602	CTP	C3'-C4'-C5'-O5'
2	V	602	CTP	C5'-O5'-PA-O1A

There are no ring outliers.

20 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	601	CTP	2	0
2	W	601	CTP	3	0
2	F	601	CTP	3	0
2	W	602	CTP	4	0
2	S	602	CTP	4	0
2	Q	602	CTP	4	0
2	D	601	CTP	3	0

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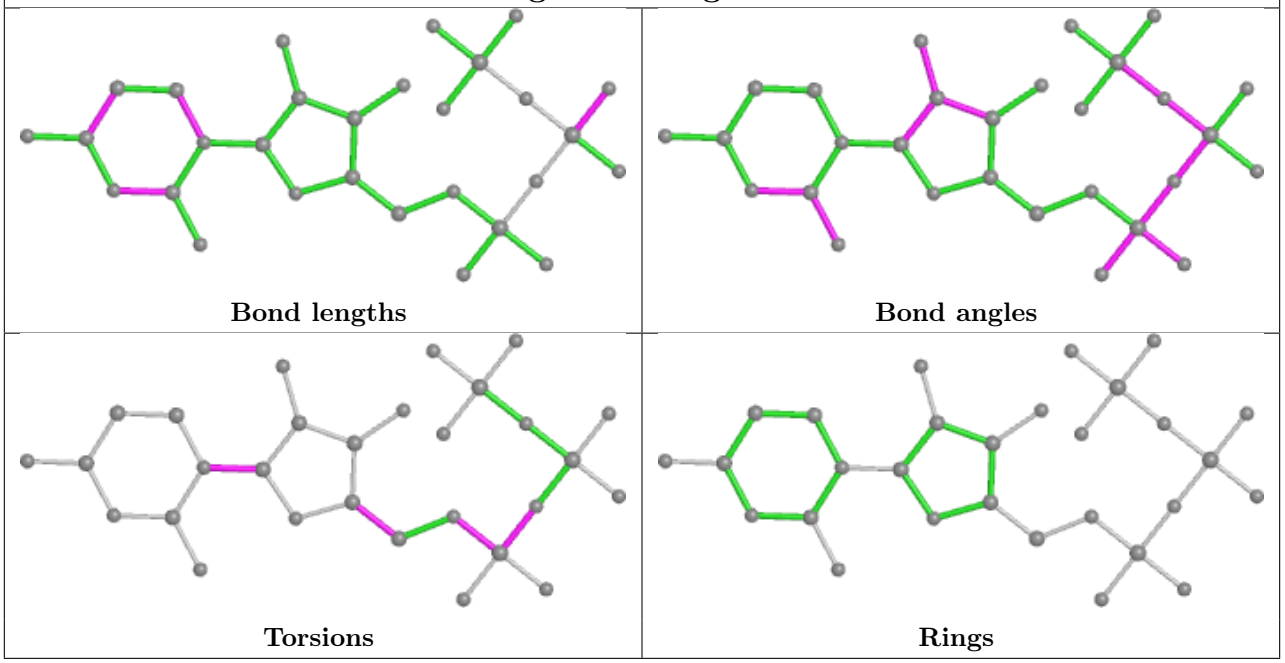
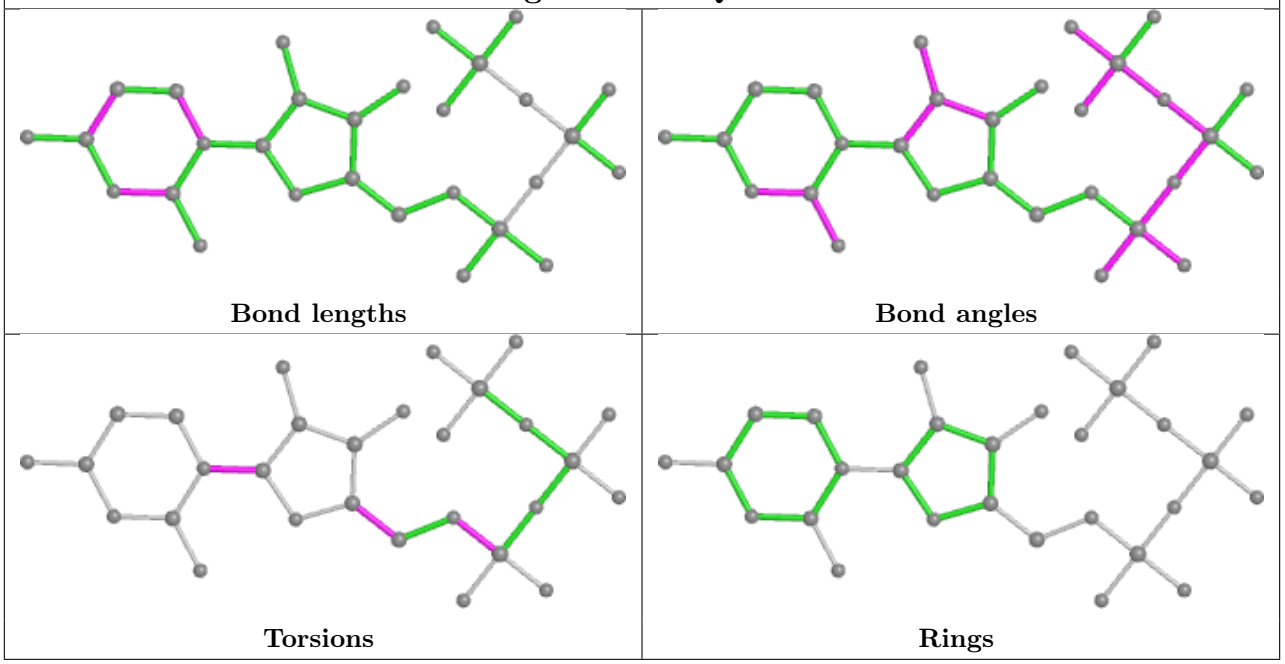
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	CTP	3	0
2	S	601	CTP	3	0
2	T	602	CTP	5	0
2	T	601	CTP	3	0
2	E	602	CTP	4	0
2	R	601	CTP	2	0
2	V	602	CTP	4	0
2	R	602	CTP	4	0
2	D	602	CTP	4	0
2	U	601	CTP	3	0
2	V	601	CTP	3	0
2	U	602	CTP	4	0
2	F	602	CTP	4	0

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.

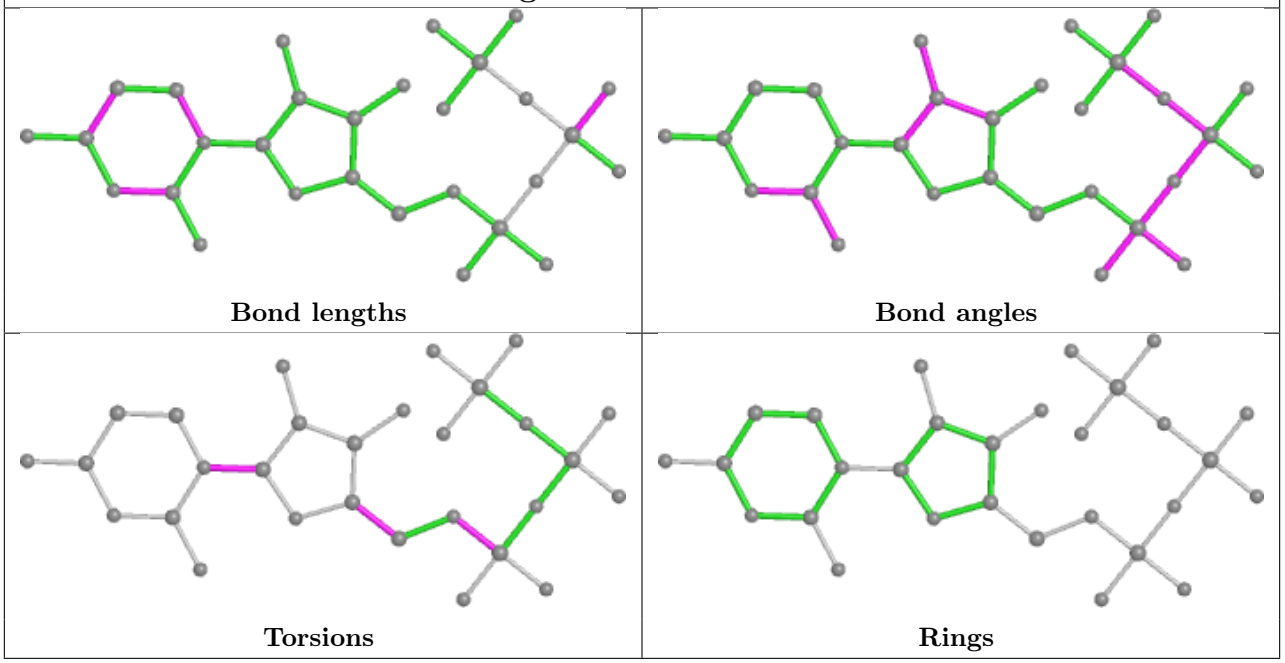
Ligand CTP g 601



Ligand CTP Q 601



Ligand CTP W 601



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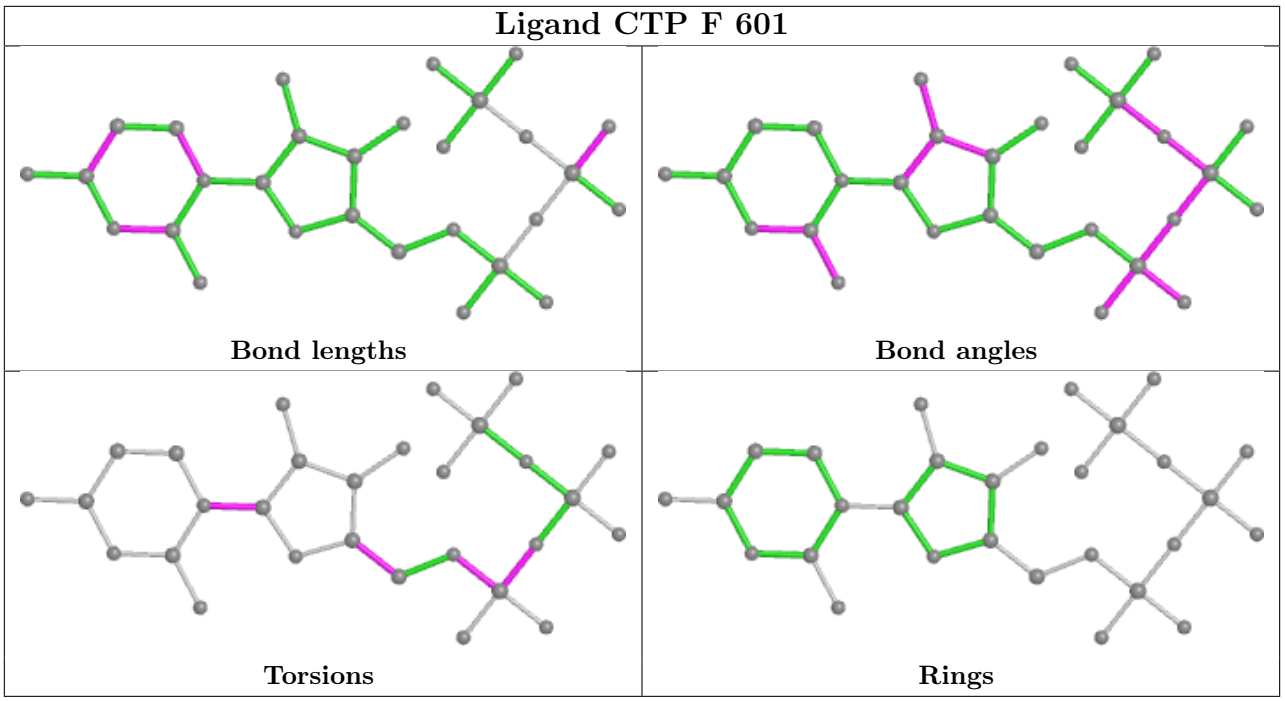
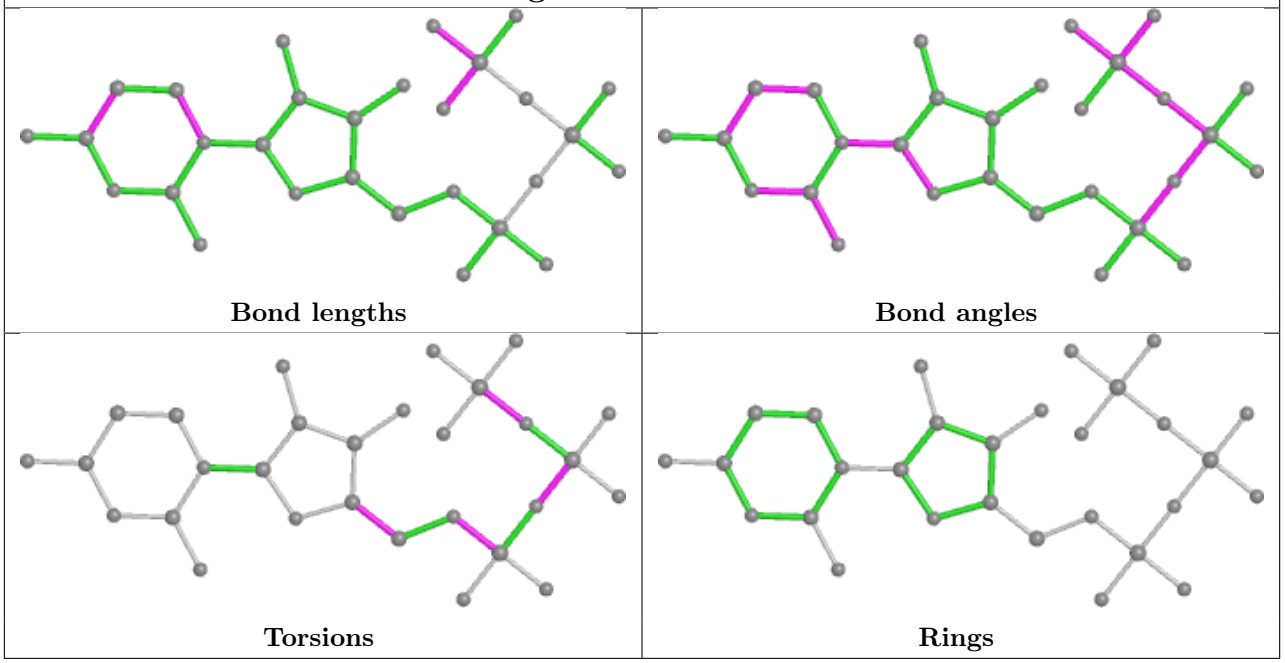


Ligand CTP h 602



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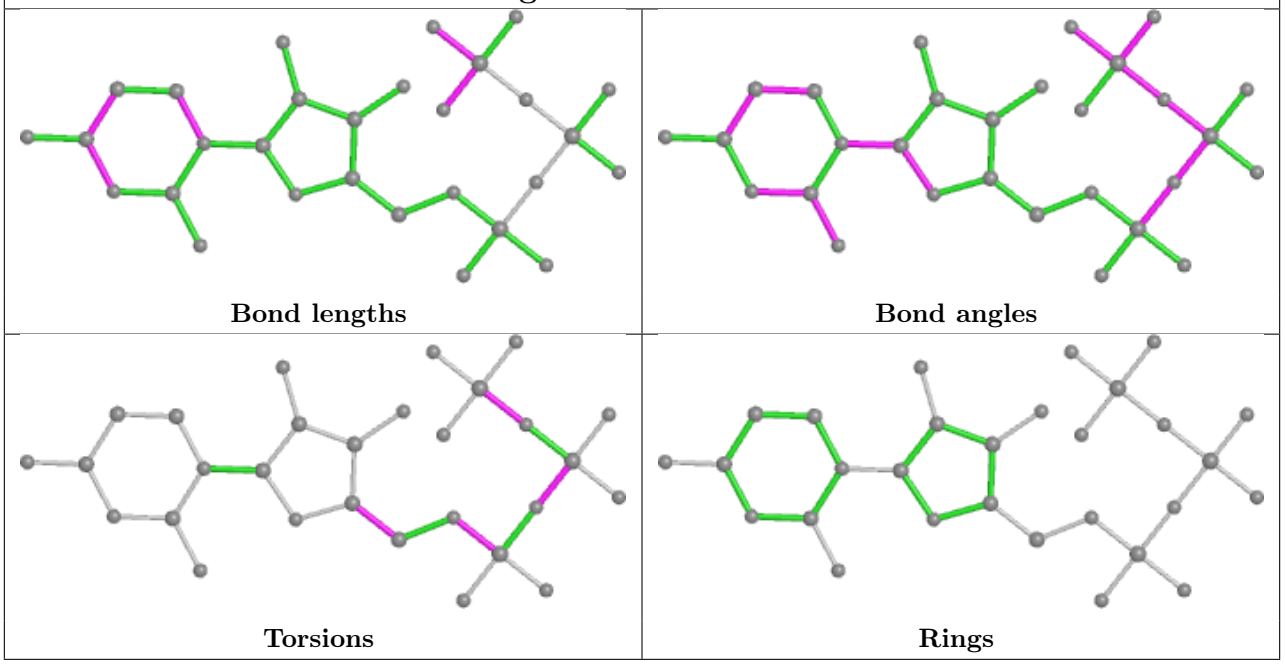

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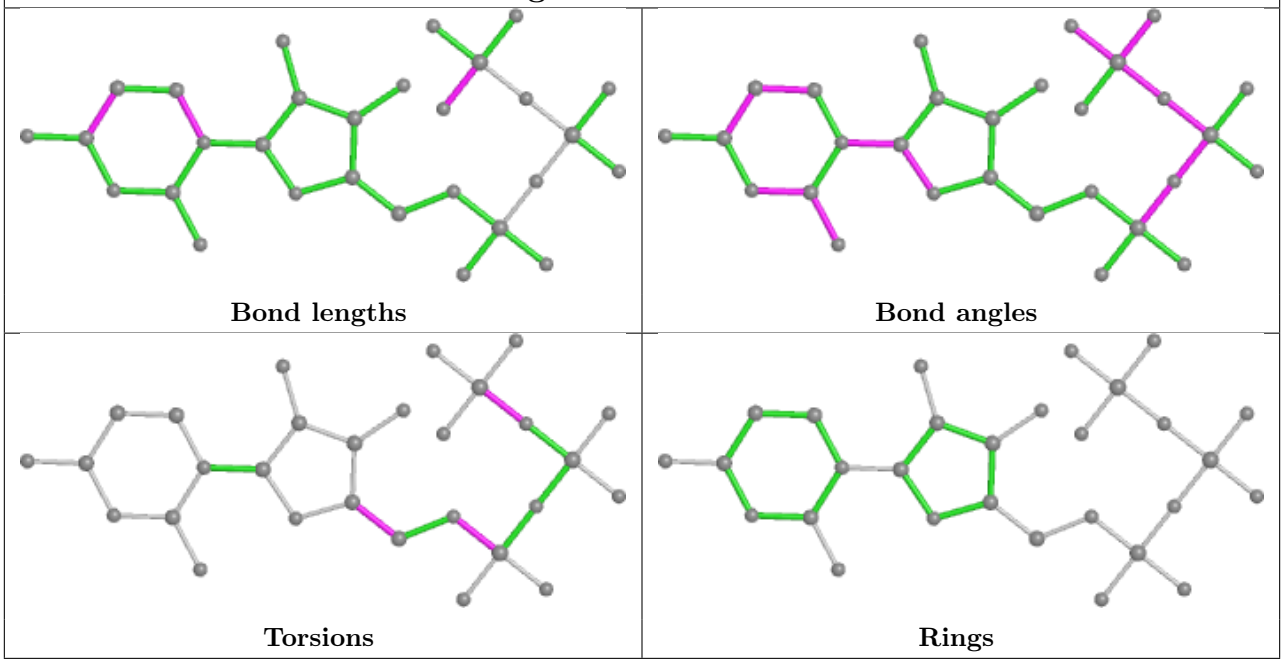

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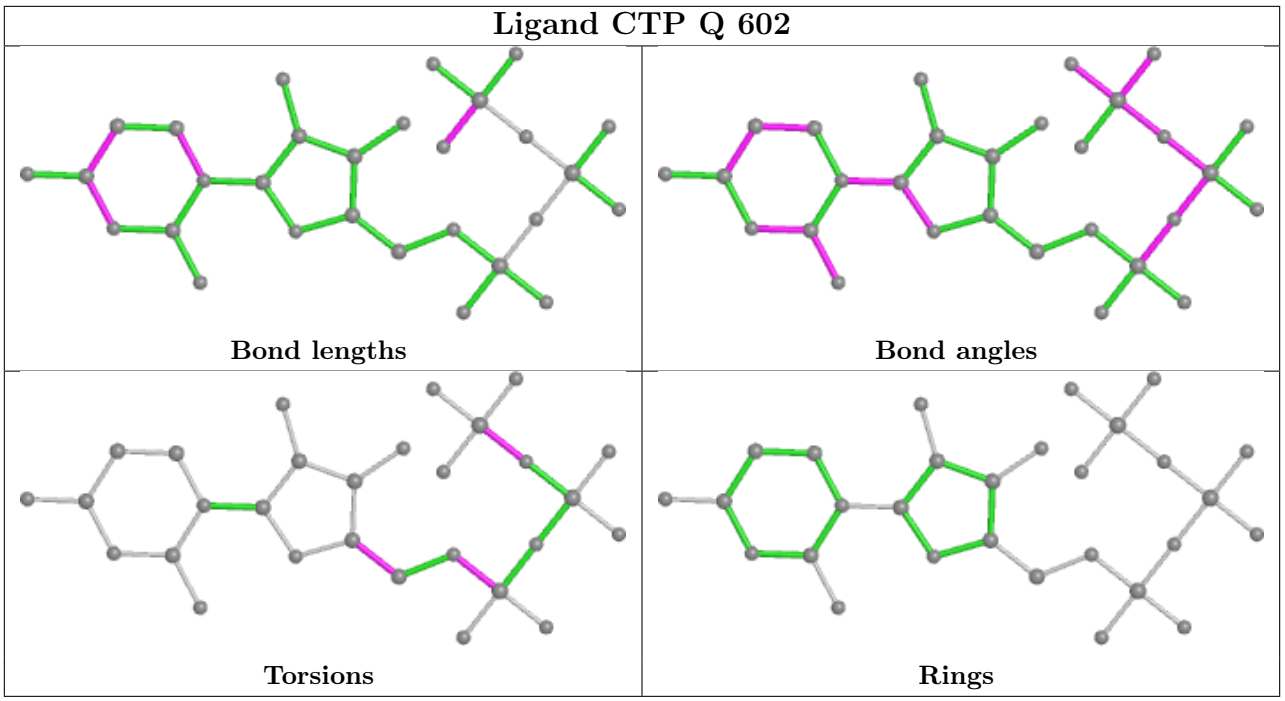

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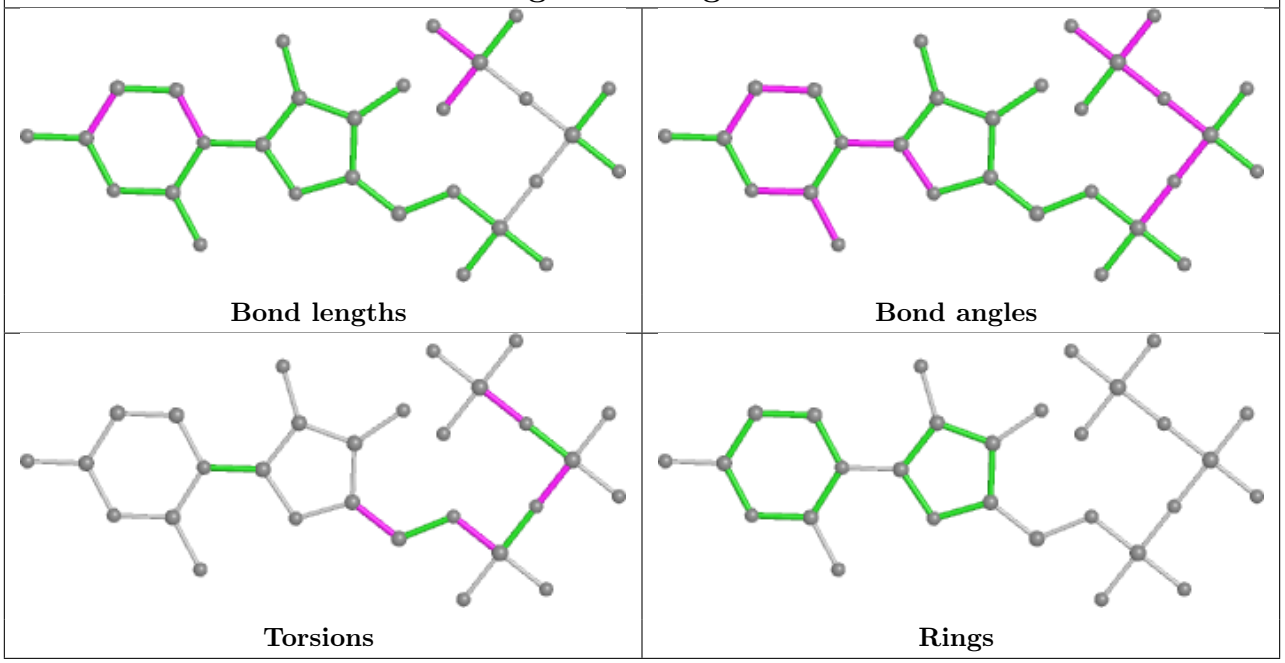

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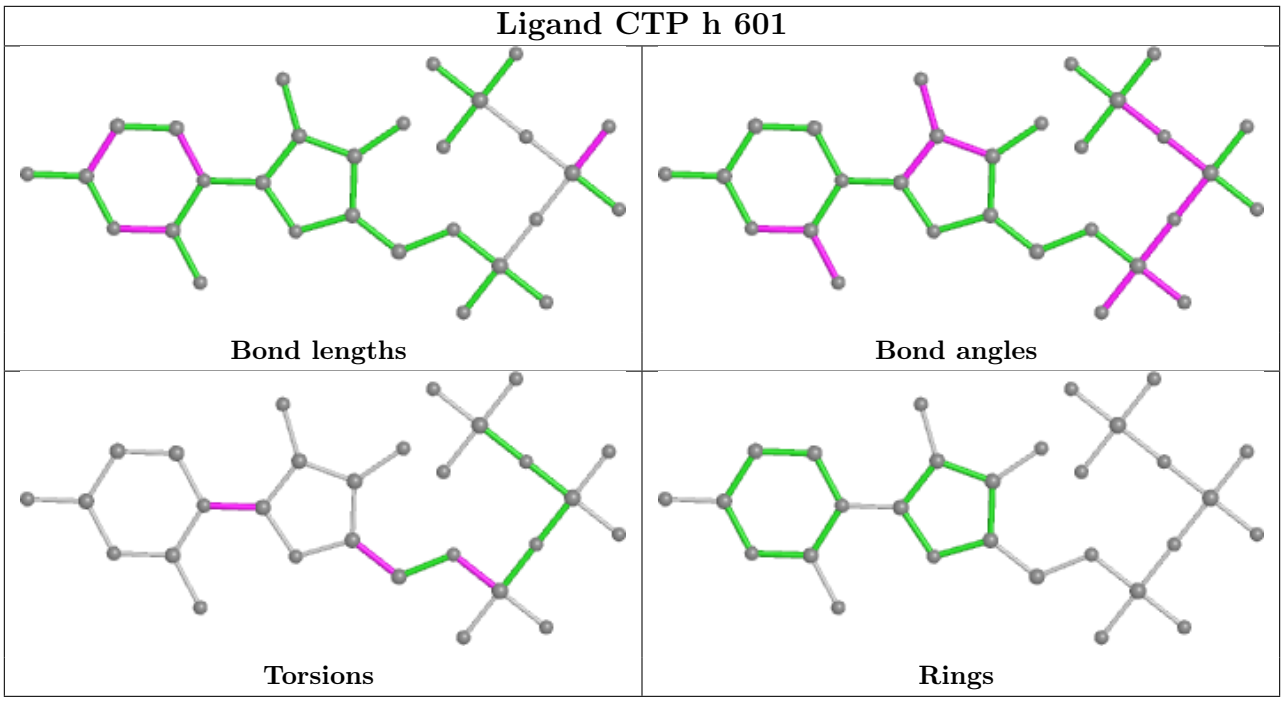
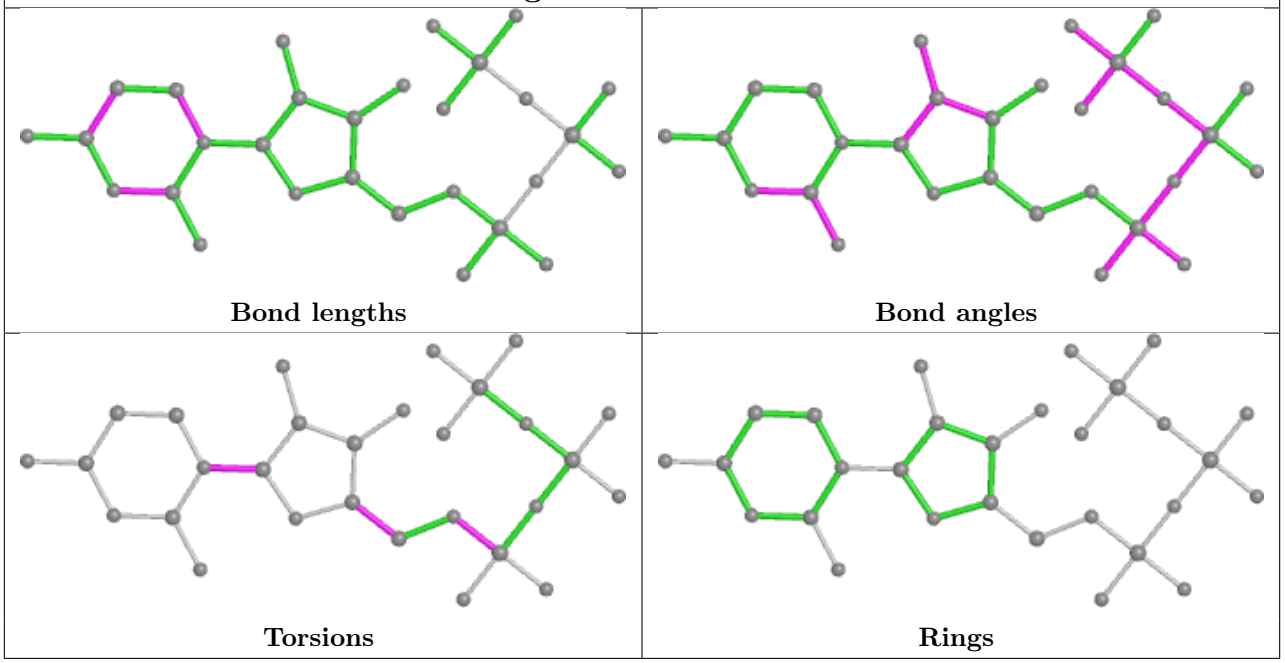


Ligand CTP D 601



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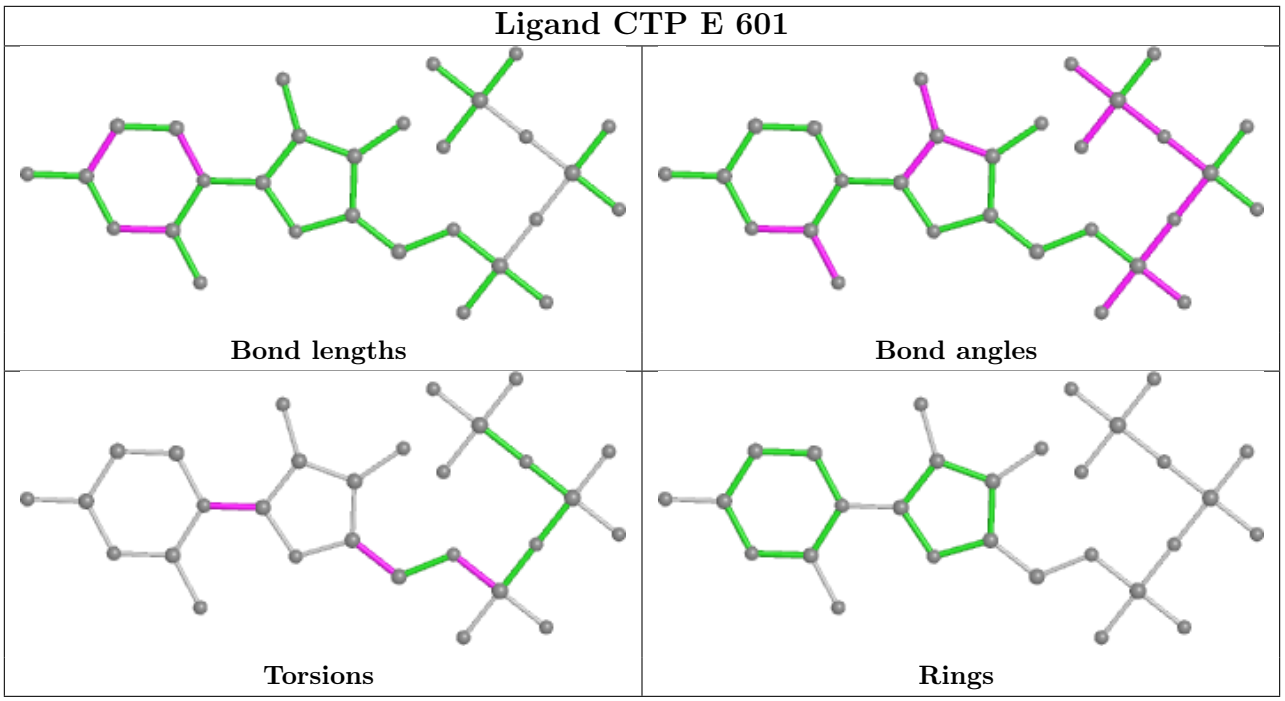

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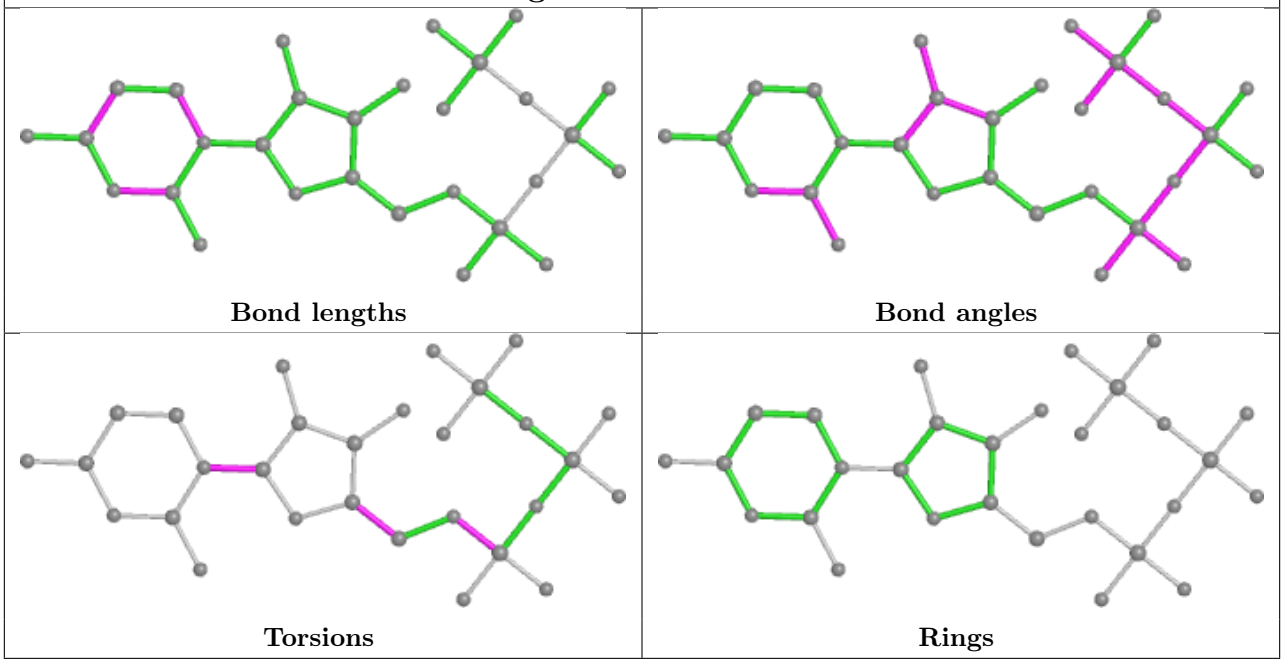

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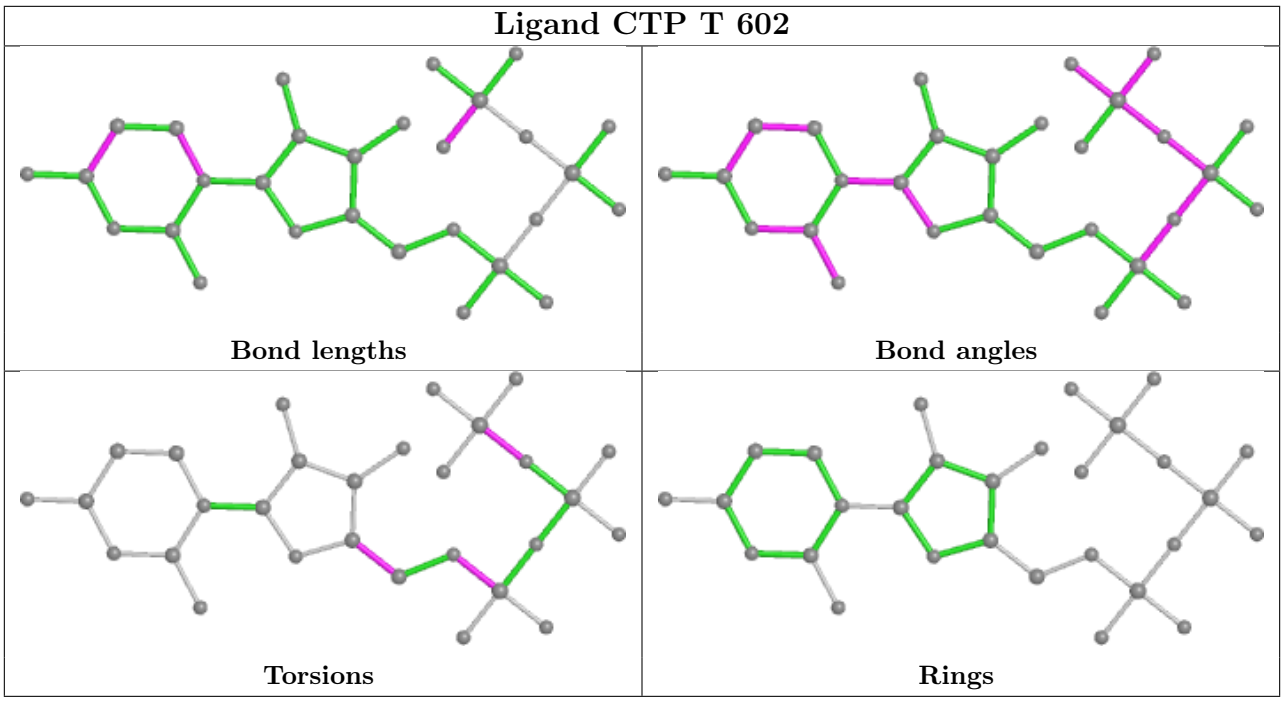

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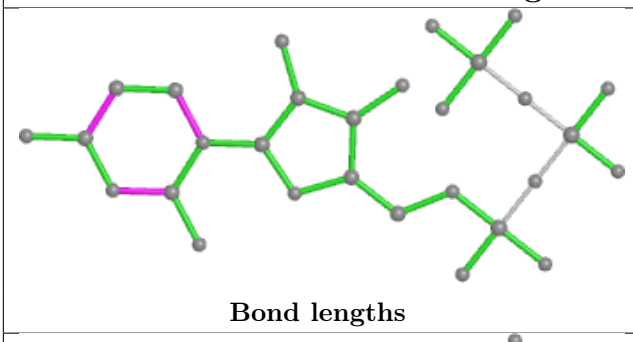
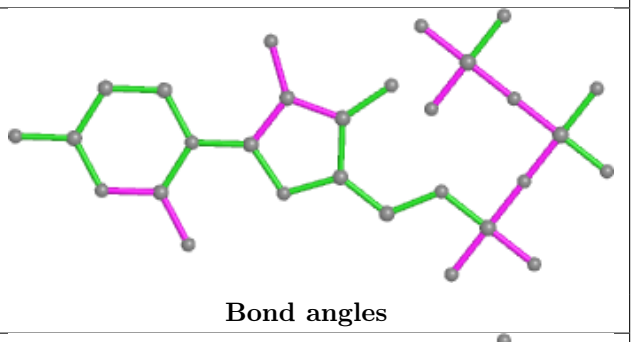
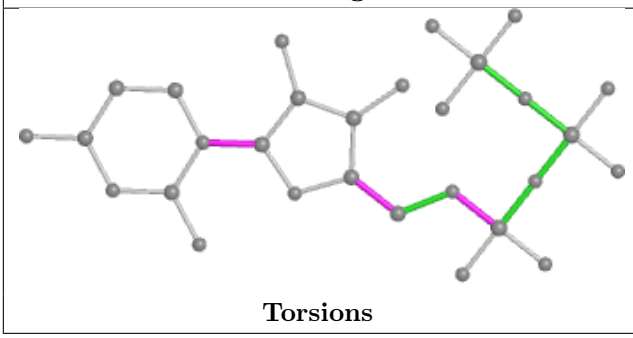


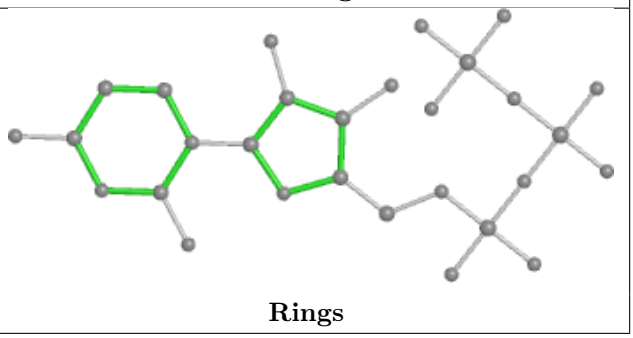
Bond lengths



Bond angles

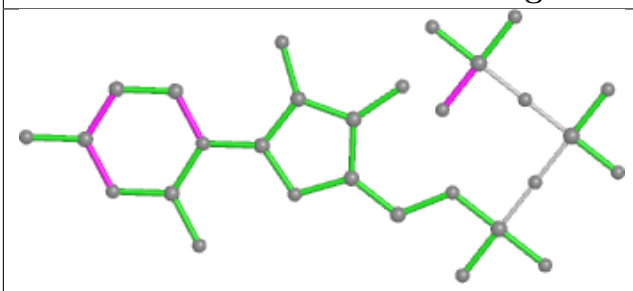


Torsions

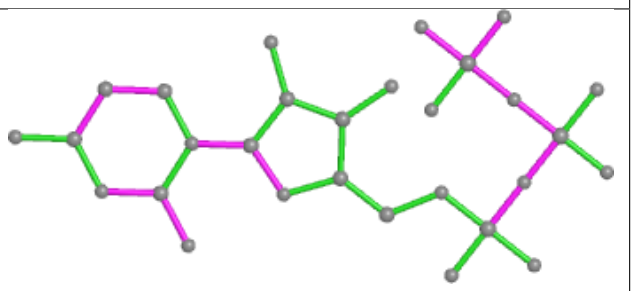


Rings

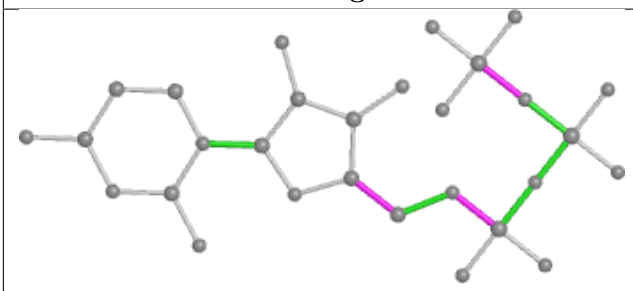
Ligand CTP E 602



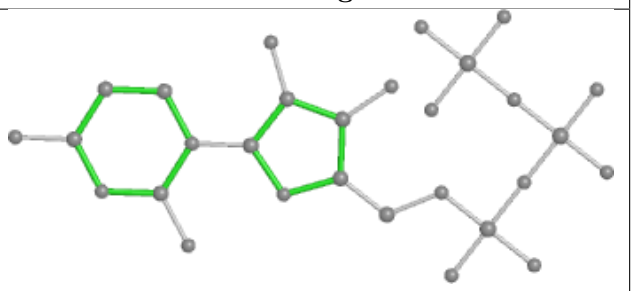
Bond lengths



Bond angles

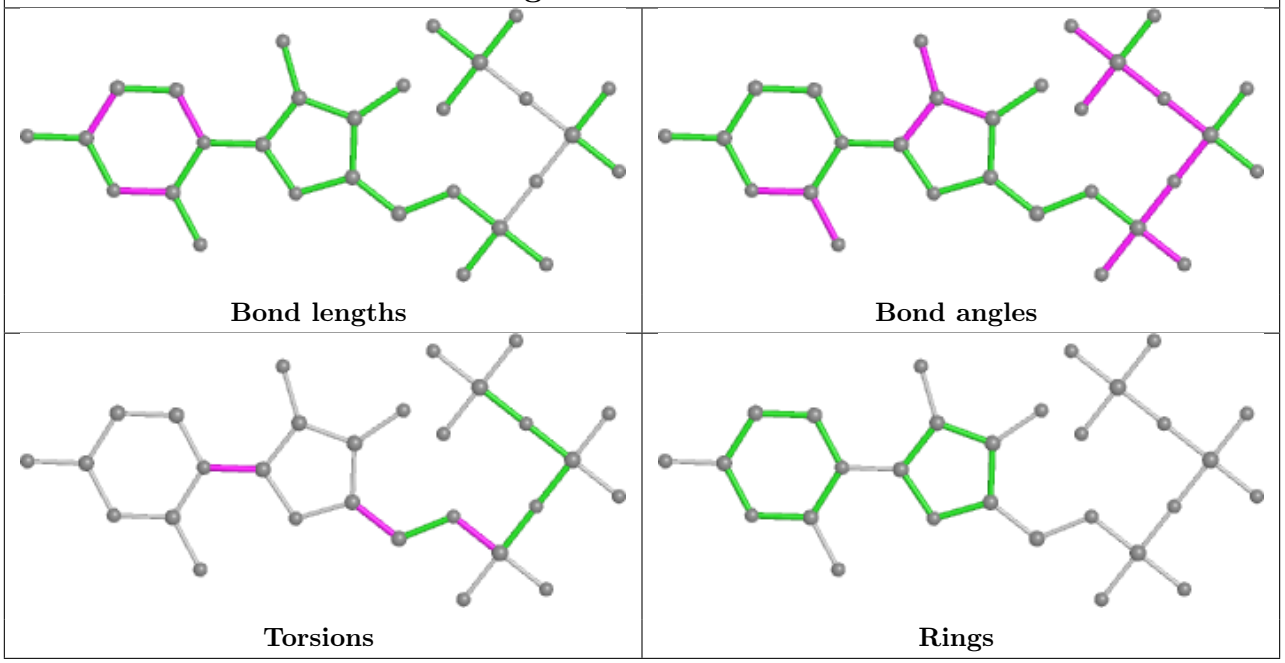


Torsions



Rings

Ligand CTP R 601



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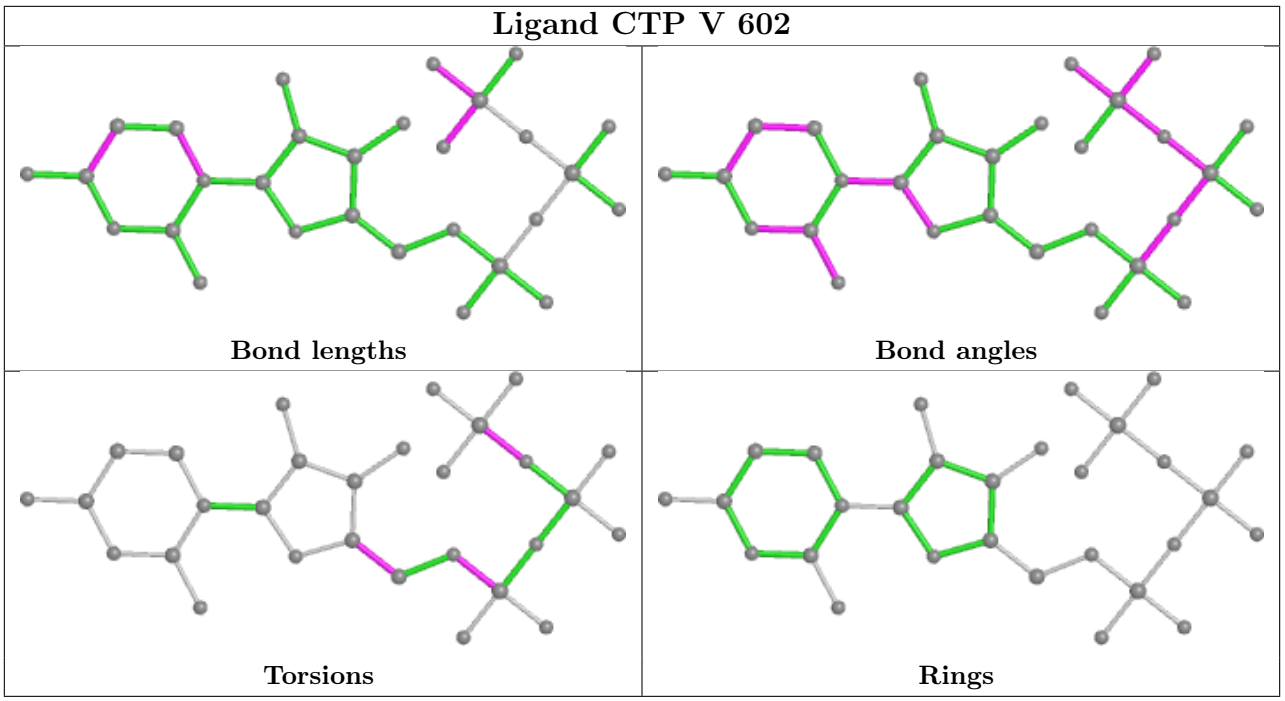

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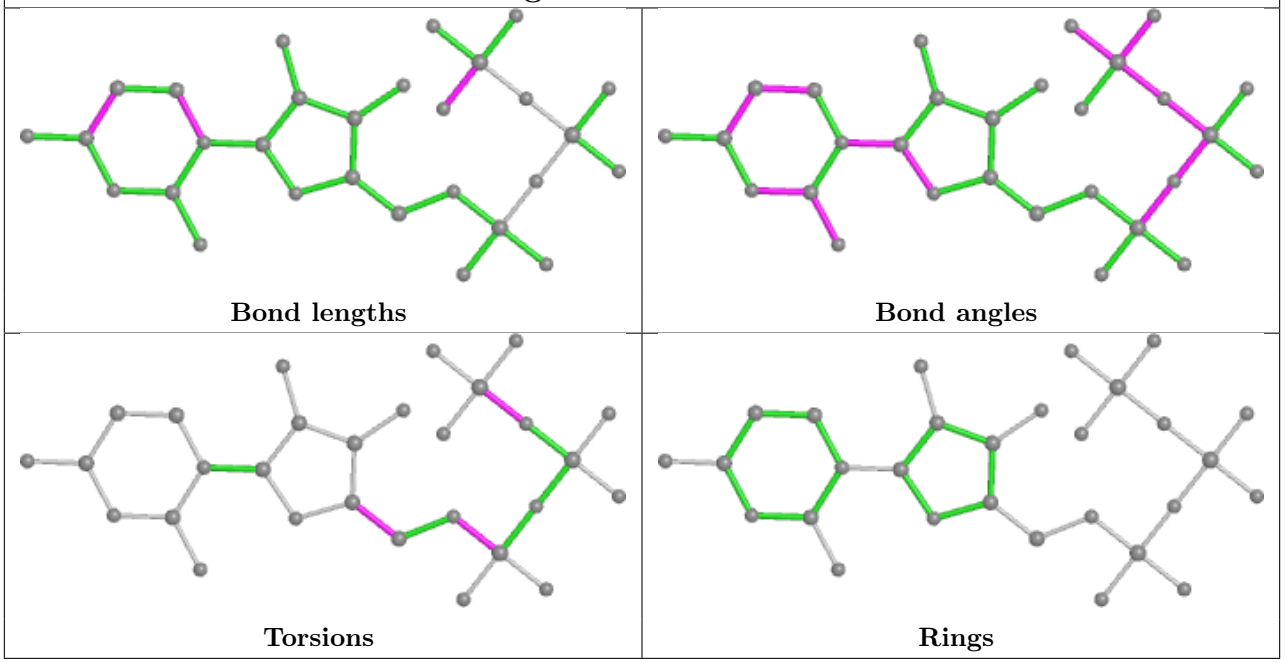

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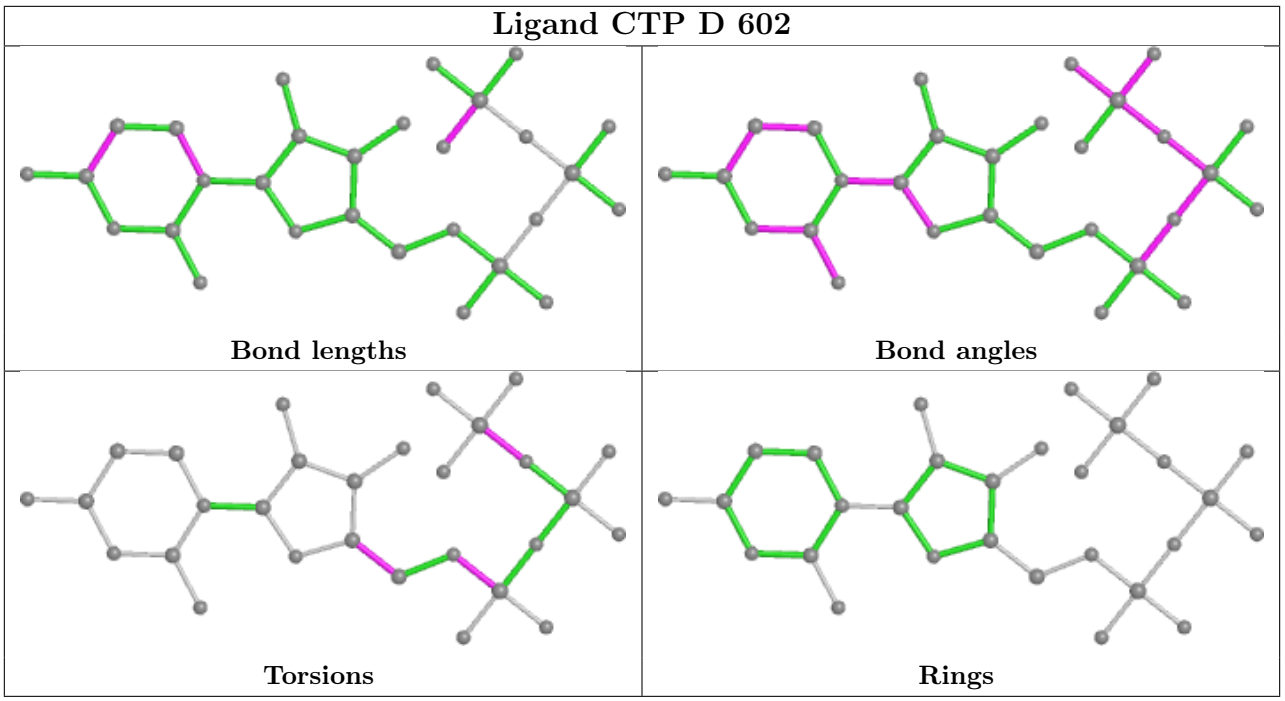

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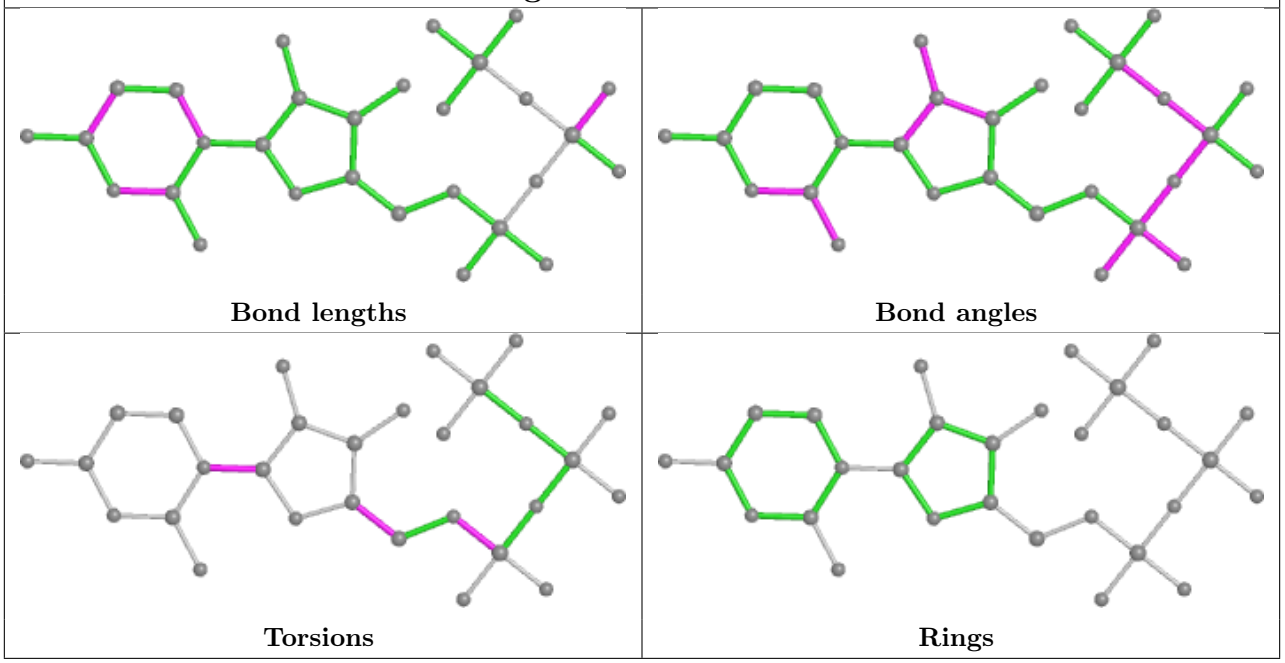

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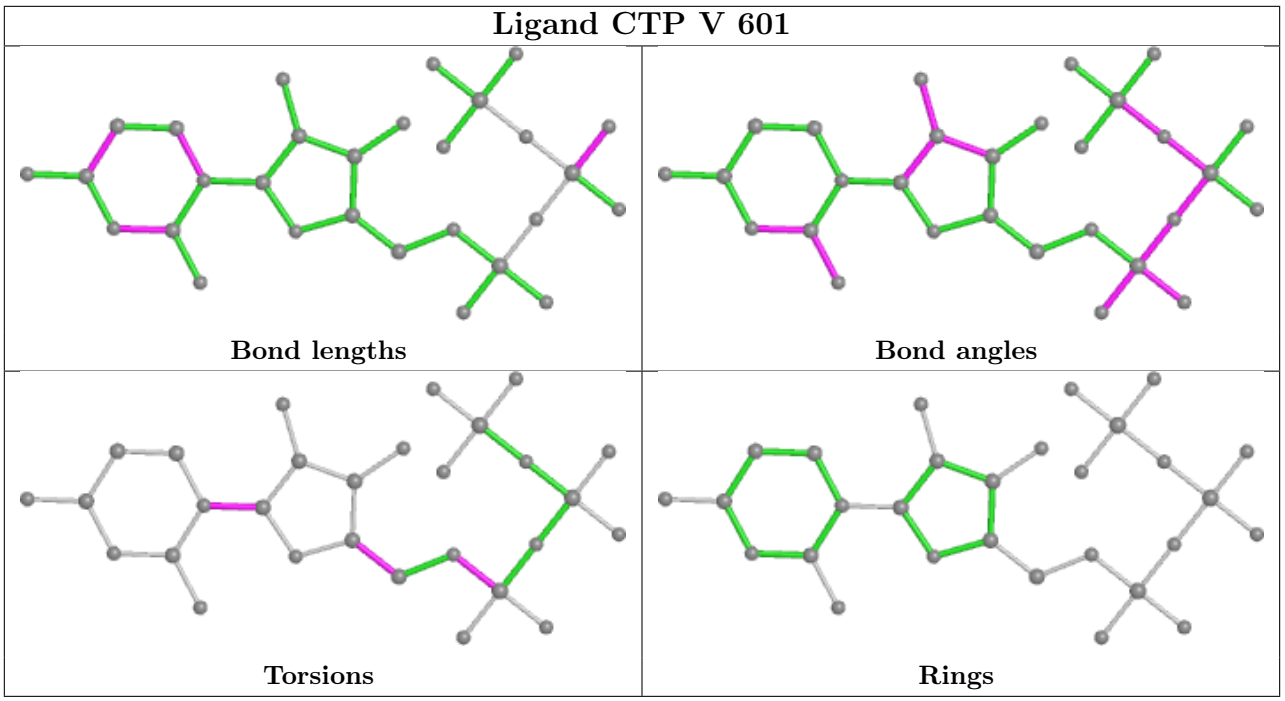

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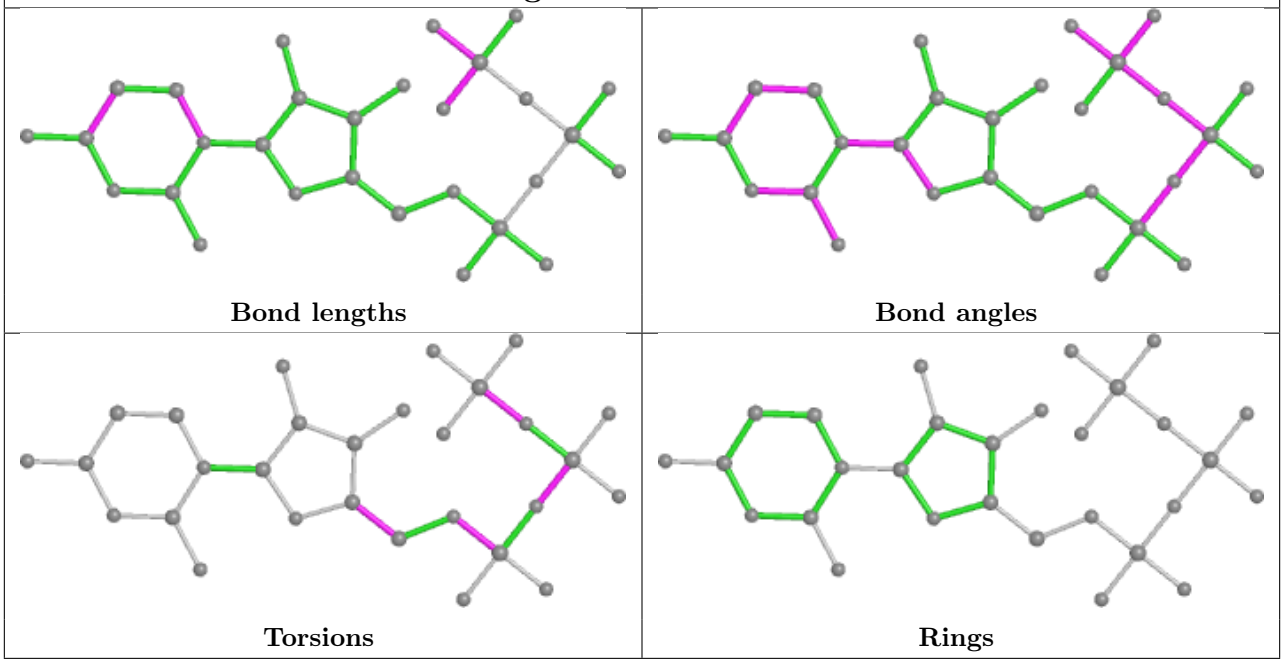
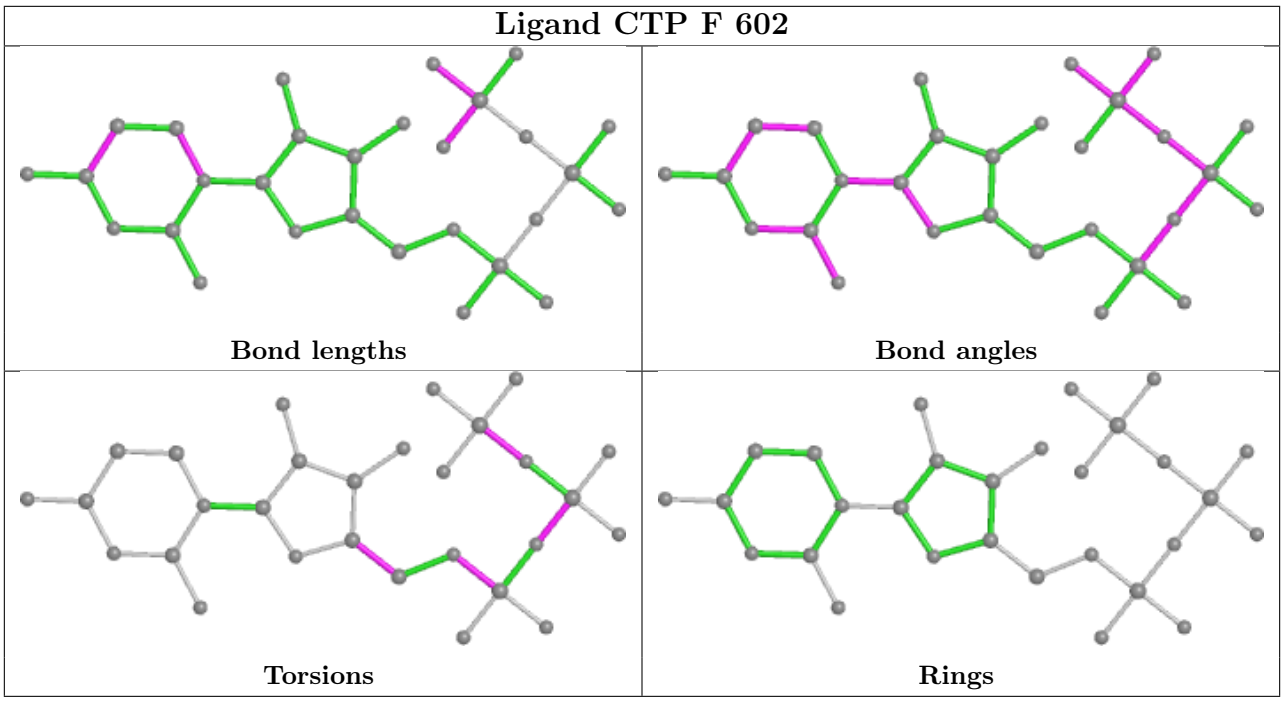


Ligand CTP F 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	V	1
1	D	1
1	E	1
1	F	1
1	g	1
1	Q	1
1	S	1
1	U	1
1	h	1
1	R	1
1	T	1
1	W	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	443:MET	C	455:MET	N	5.62
1	D	443:MET	C	455:MET	N	5.62
1	E	443:MET	C	455:MET	N	5.62
1	F	443:MET	C	455:MET	N	5.62
1	g	443:MET	C	455:MET	N	5.62

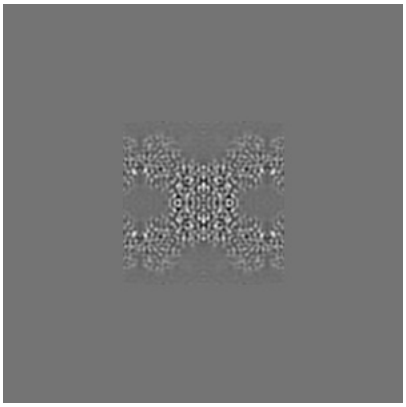
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24560. These allow visual inspection of the internal detail of the map and identification of artifacts.

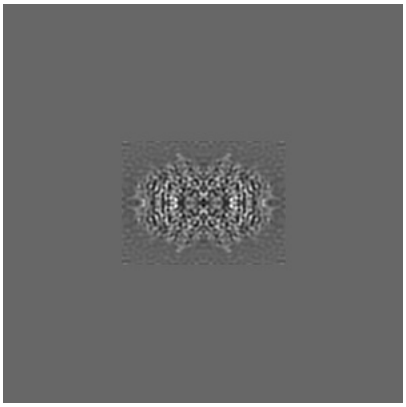
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

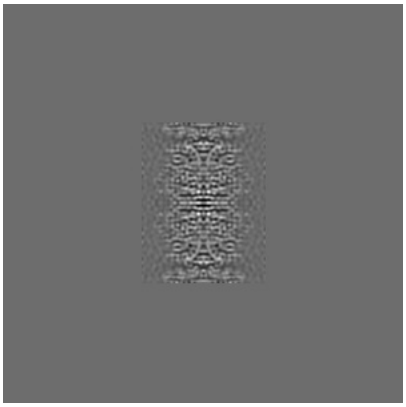
6.1.1 Primary map



X



Y

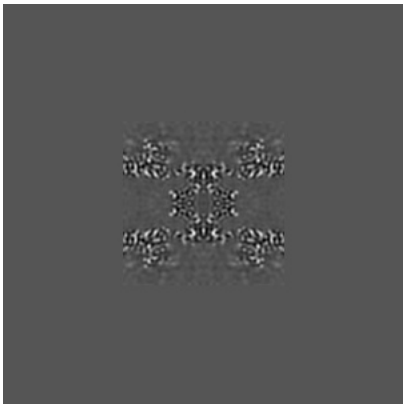


Z

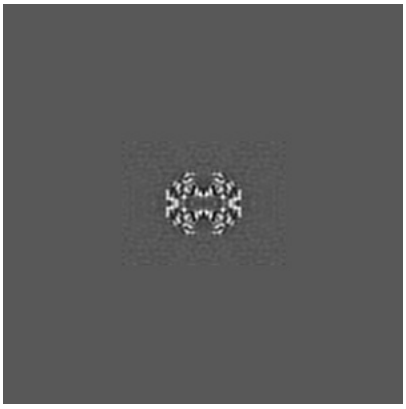
The images above show the map projected in three orthogonal directions.

6.2 Central slices

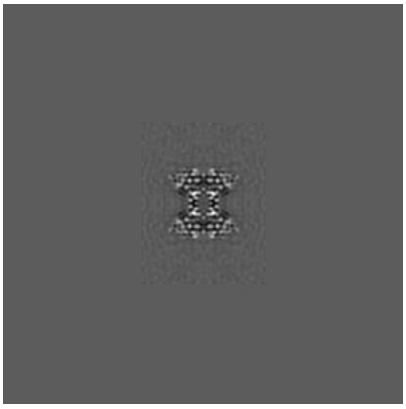
6.2.1 Primary map



X Index: 160



Y Index: 160

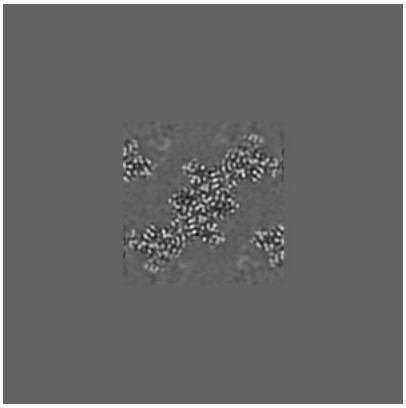


Z Index: 160

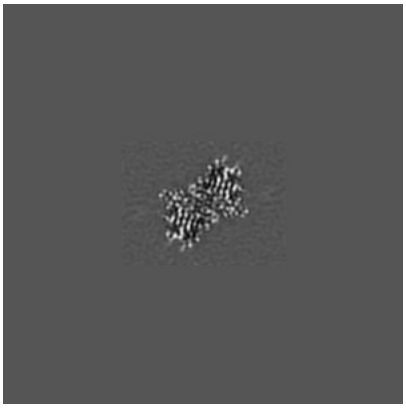
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

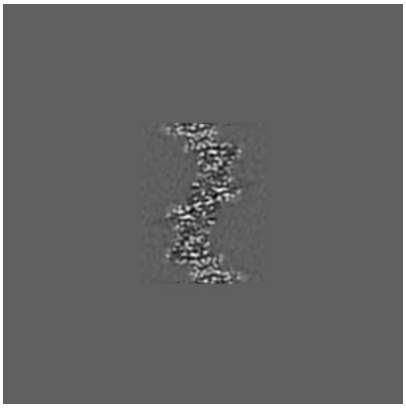
6.3.1 Primary map



X Index: 151



Y Index: 150

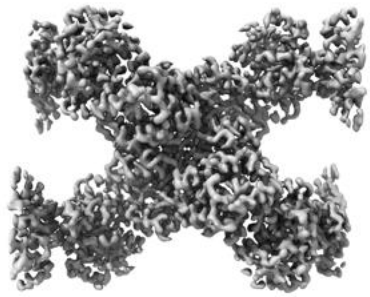


Z Index: 135

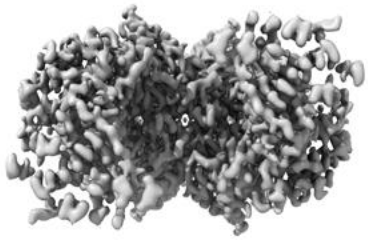
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

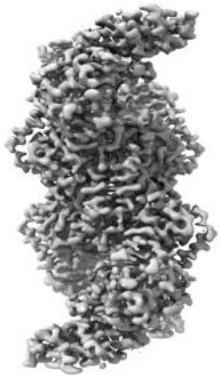
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

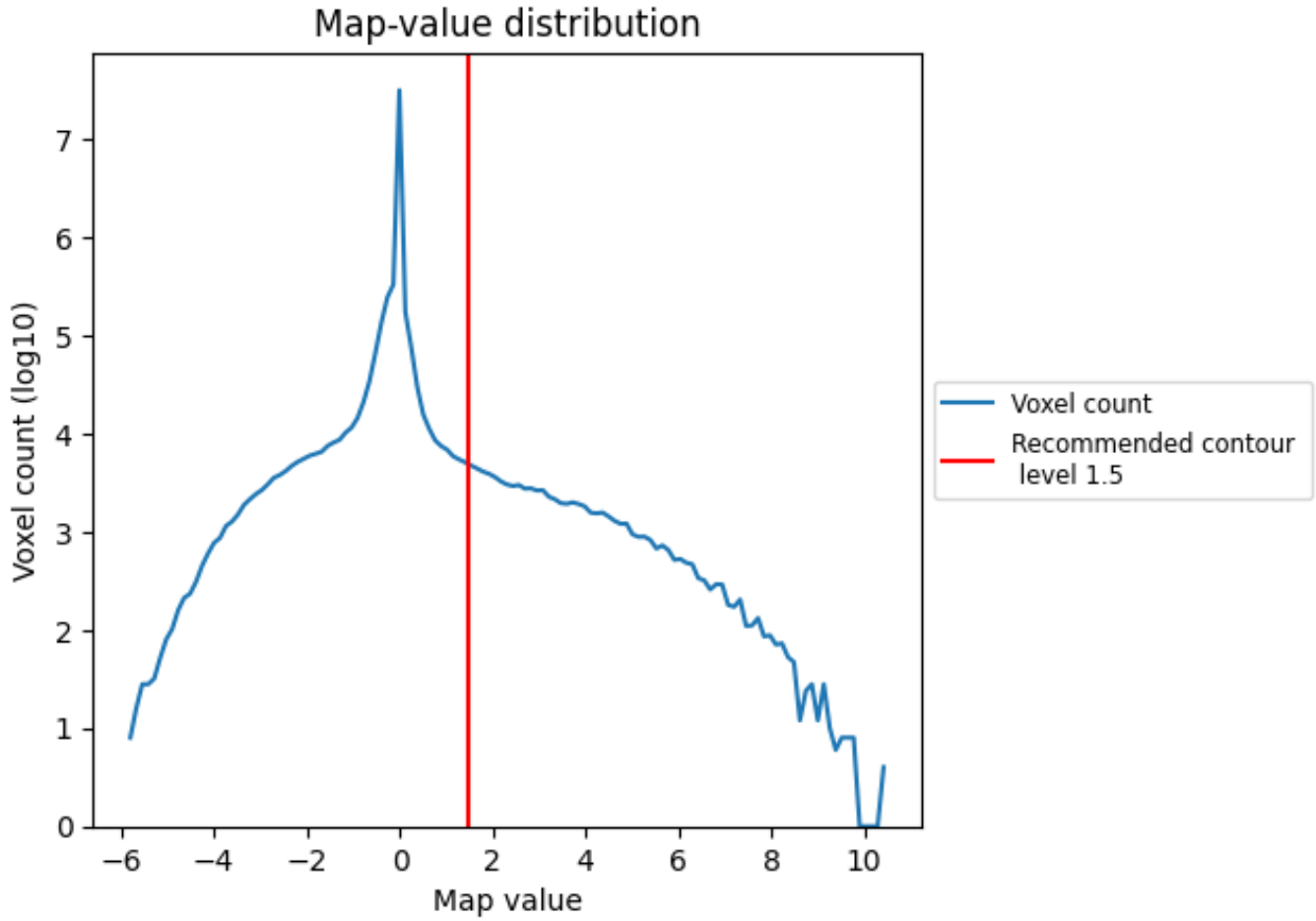
6.5 Mask visualisation (i)

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

7 Map analysis

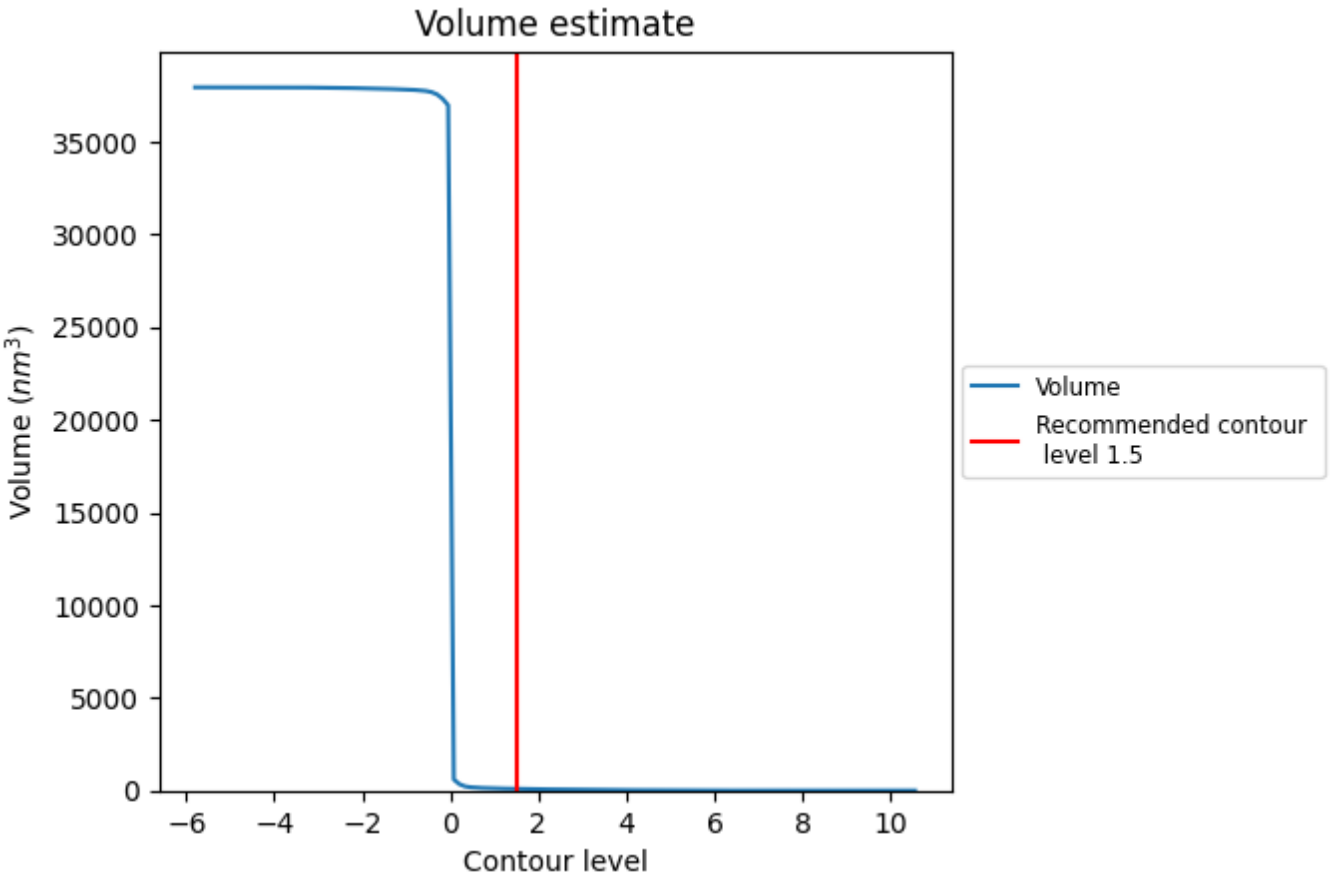
This section contains the results of statistical analysis of the map.

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.

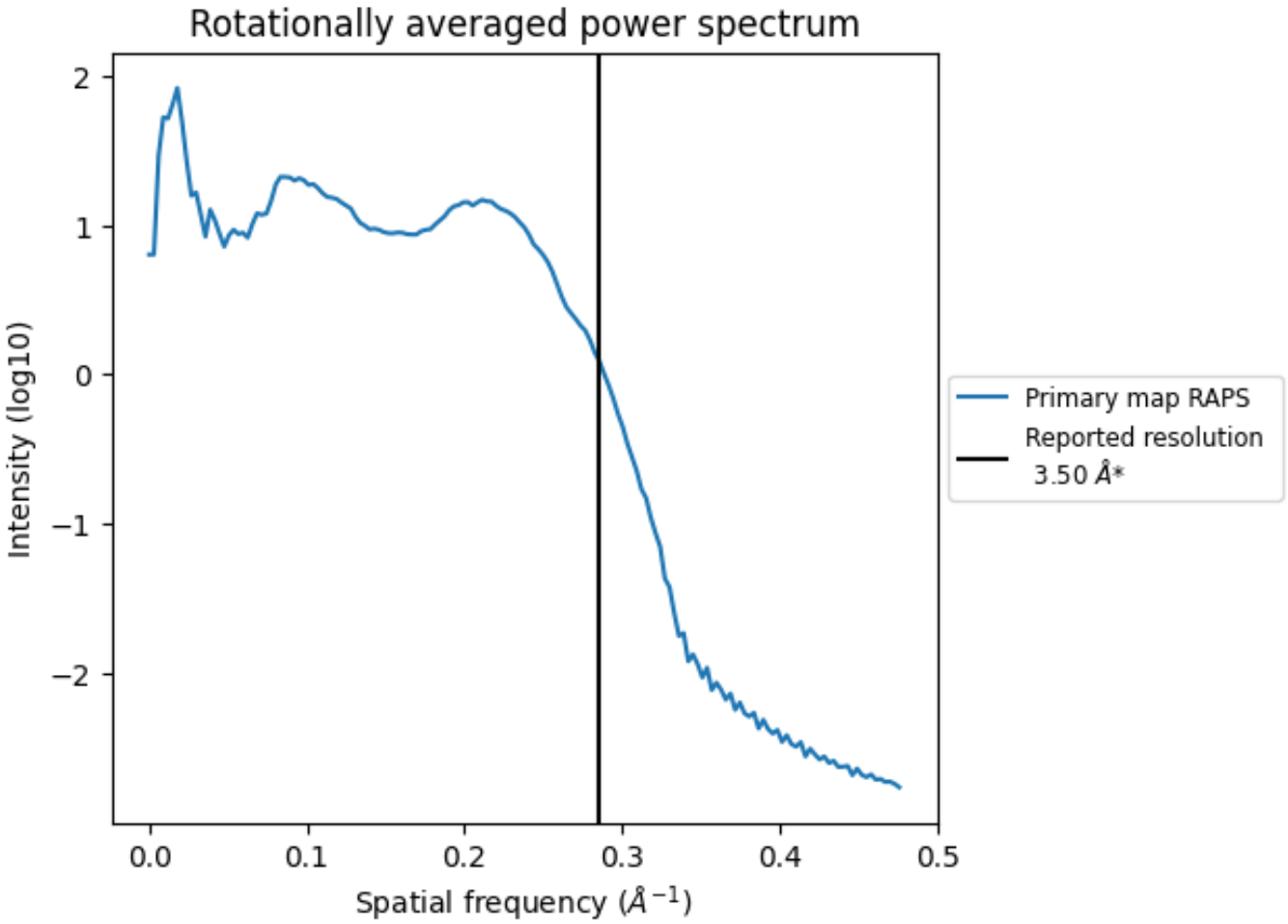
7.2 Volume estimate (i)



The volume at the recommended contour level is 92 nm^3; this corresponds to an approximate mass of 83 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 0.286 Å^{-1}

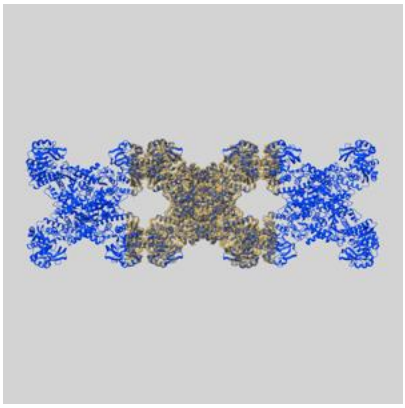
8 Fourier-Shell correlation (i)

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

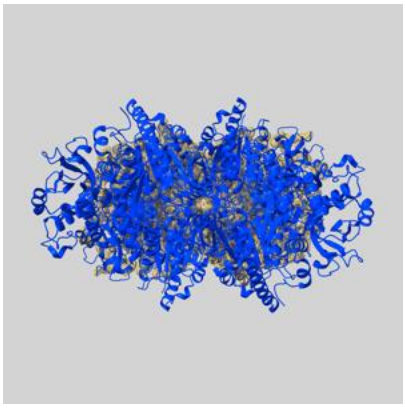
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24560 and PDB model 7RMC. Per-residue inclusion information can be found in section 3 on page 10.

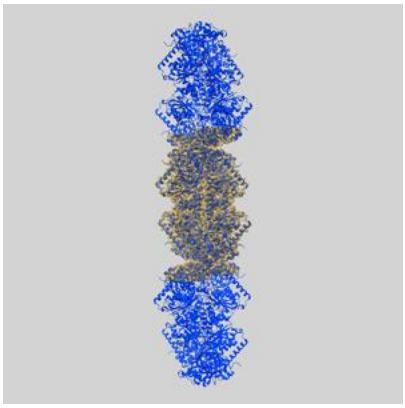
9.1 Map-model overlay



X



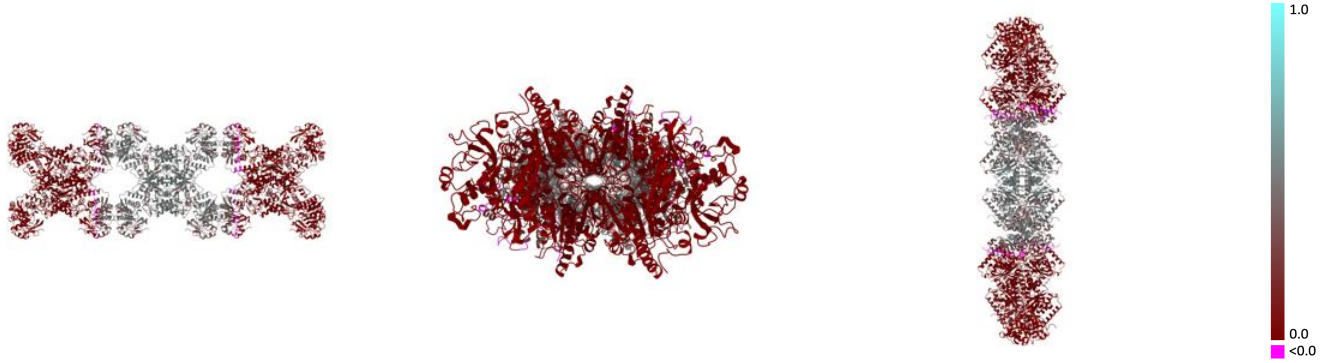
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 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.

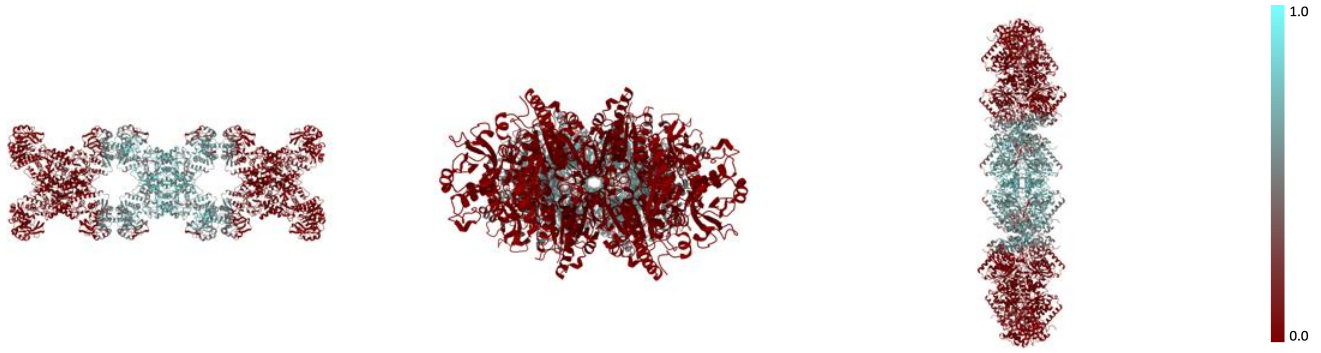
9.2 Q-score mapped to coordinate model



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.

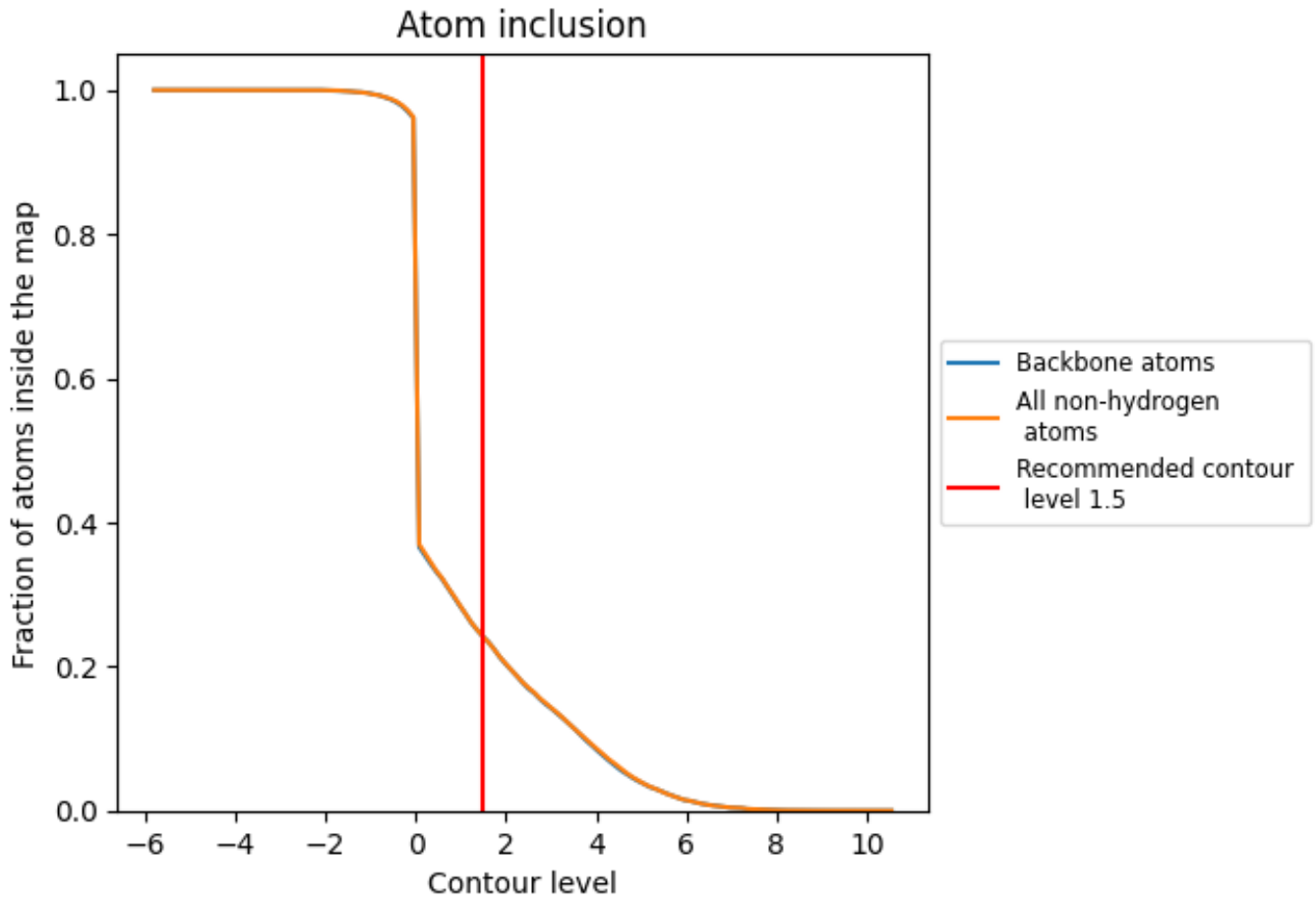
9.3 Atom inclusion mapped to coordinate model



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 (1.5).

9.4 Atom inclusion (i)



At the recommended contour level, 24% of all backbone atoms, 24% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2411	0.1800
D	0.0000	0.0000
E	0.1289	0.0910
F	0.1273	0.0910
Q	0.1203	0.0790
R	0.6045	0.4520
S	0.0000	0.0000
T	0.6076	0.4530
U	0.0000	0.0000
V	0.0000	0.0000
W	0.6081	0.4520
g	0.1296	0.0900
h	0.6074	0.4530