wwPDB EM Validation Summary Report (i)

Aug 4, 2026 – 05:45 PM EDT

PDB ID	:	8SHT / pdb_00008sht
EMDB ID	:	EMD-40494
Title	:	CCT G beta 5 complex closed state 14
Authors	:	Wang, S.; Sass, M.; Willardson, B.M.; Shen, P.S.
Deposited on	:	2023-04-14
Resolution	:	3.00 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 (i) symbol.

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

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

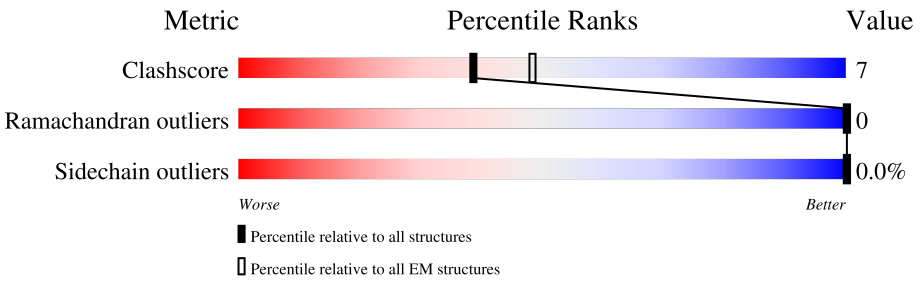
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

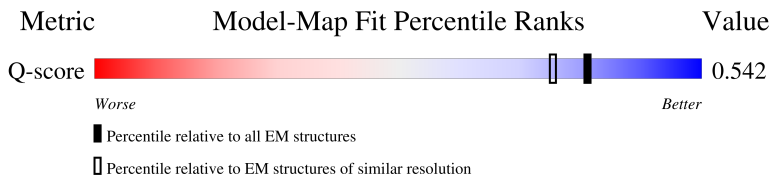
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	536	84% 16%
1	a	536	78% 21% •
2	B	526	84% 16%
2	b	526	83% 17%

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Mol	Chain	Length	Quality of chain
3	D	520	84% 16%
3	d	520	83% 17%
4	E	540	83% 16%
4	e	540	81% 19%
5	G	528	77% 23%
5	g	528	82% 17%
6	H	528	82% 18%
6	h	528	80% 19%
7	Q	538	83% 17%
7	q	538	83% 16%
8	Z	527	78% 21%
8	z	527	81% 19%
9	P	301	30% 46% 16% 38%
10	N	395	42% 12% 46%

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
13	AF3	A	603	-	-	X	-
13	AF3	B	603	-	-	X	-
13	AF3	D	603	-	-	X	-
13	AF3	G	603	-	-	X	-
13	AF3	Q	603	-	-	X	-
13	AF3	a	603	-	-	X	-
13	AF3	b	603	-	-	X	-
13	AF3	d	603	-	-	X	-
13	AF3	g	603	-	-	X	-
13	AF3	z	603	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 68272 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	536	4069	2548	711	787	23	0	0
1	a	532	4041	2533	707	778	23	0	0

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	526	3952	2473	696	764	19	0	0
2	b	525	3943	2467	694	763	19	0	0

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	520	3923	2453	683	764	23	0	0
3	d	520	3917	2450	680	764	23	0	0

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	535	4132	2590	719	792	31	1	0
4	e	540	4169	2610	724	804	31	1	0

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	526	4089	2548	726	785	30	0	0
5	g	523	4063	2532	719	782	30	0	0

- Molecule 6 is a protein called T-complex protein 1 subunit eta, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	528	4054	2561	699	769	25	0	0
6	h	525	4032	2548	696	763	25	0	0

- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Q	538	4086	2579	696	784	27	0	0
7	q	533	4053	2558	690	778	27	0	0

- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Z	525	4022	2528	704	769	21	0	0
8	z	527	4033	2534	706	772	21	0	0

- Molecule 9 is a protein called Phosducin-like protein.

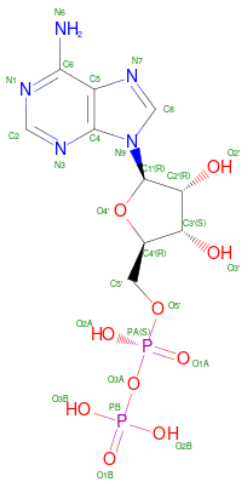
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	P	186	1507	955	256	284	12	0	0

- Molecule 10 is a protein called Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	214	1656	1031	287	326	12	0	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	h	1	Total	C	N	O	P	0
			27	10	5	10	2	

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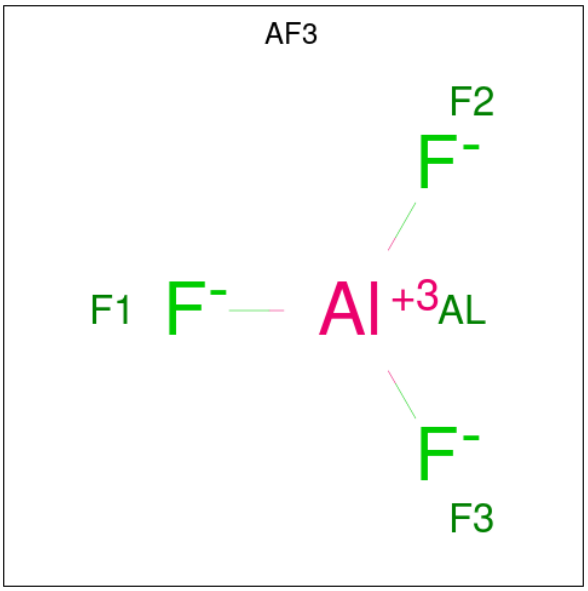
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	q	1	27	10	5	10	2	0
			Total	C	N	O	P	
11	z	1	27	10	5	10	2	0

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
12	A	1	1	1	0
			Total	Mg	
12	B	1	1	1	0
			Total	Mg	
12	D	1	1	1	0
			Total	Mg	
12	E	1	1	1	0
			Total	Mg	
12	G	1	1	1	0
			Total	Mg	
12	H	1	1	1	0
			Total	Mg	
12	Q	1	1	1	0
			Total	Mg	
12	Z	1	1	1	0
			Total	Mg	
12	a	1	1	1	0
			Total	Mg	
12	b	1	1	1	0
			Total	Mg	
12	d	1	1	1	0
			Total	Mg	
12	e	1	1	1	0
			Total	Mg	
12	g	1	1	1	0
			Total	Mg	
12	h	1	1	1	0
			Total	Mg	
12	q	1	1	1	0
			Total	Mg	
12	z	1	1	1	0

- Molecule 13 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
13	A	1	4	1	3	0
13	B	1	4	1	3	0
13	D	1	4	1	3	0
13	E	1	4	1	3	0
13	G	1	4	1	3	0
13	H	1	4	1	3	0
13	Q	1	4	1	3	0
13	Z	1	4	1	3	0
13	a	1	4	1	3	0
13	b	1	4	1	3	0
13	d	1	4	1	3	0
13	e	1	4	1	3	0
13	g	1	4	1	3	0
13	h	1	4	1	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
13	q	1	4	1	3	0
13	z	1	4	1	3	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
14	A	2	2	2	0
14	B	2	2	2	0
14	D	1	1	1	0
14	E	1	1	1	0
14	G	1	1	1	0
14	H	1	1	1	0
14	Q	1	1	1	0
14	Z	1	1	1	0
14	a	2	2	2	0
14	b	1	1	1	0
14	d	1	1	1	0
14	e	1	1	1	0
14	g	1	1	1	0
14	h	1	1	1	0
14	q	1	1	1	0
14	z	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: T-complex protein 1 subunit alpha

Chain A:

E2 R11 M23 S27 I31 V39 K43 M44 D47 D51 T55 N56 D57 G58 A59 D80 K84 T90 G120 E127 M156 N164 A169 N170 M171 I179 I184 R185 G186 Q187 V195 M206 Y214 M225 P226 K227 R228

I229 V230 N231 D238 F239 K245 V252 V253 I254 D261 Q262 I263 R266 K272 I278 T281 T288 T289 Y299 A307 D315 L316 S329 T330 L331 E338 T339 F340 Q347 A348 E349 E350 Q353 E354 R355 D358 D359 E360 L363 N366 T367

K368 I375 E387 C397 R401 G411 Y426 G431 Q435 L436 A437 N450 A456 S460 A474 L483 N498 R526 D529 L530 S537

• Molecule 1: T-complex protein 1 subunit alpha

Chain a:

GLU GLY P4 R11 V22 S34 G37 P38 V39 K43 M44 T55 N56 D57 K73 E77 L78 Q82 D88 D105 E106 L107 H113 I118 S119 G120 Y121 R122 E127 A128 V129 R130 Y131 I132 N133 E134 E142 L143 M156 I163 N164 A169

N170 M171 I179 T182 Y190 V195 R203 S204 Q205 M206 E207 Y214 N217 S222 M225 I229 D238 K245 D261 R266 E273 I278 T281 I292 C296 L297 K298 Y299 E302 M306 D315 R318 K321 S329 T330

L331 F340 E349 E354 L363 N366 R370 M384 E387 M388 C397 R401 V402 L403 G411 L419 L423 Y426 A437 E440 R443 L446 N450 T451 L452 A456 S460 R468 A474 E479 R480 L483 K484 L490

N498 K499 F504 E505 P506 T507 I508 V509 K510 V511 K512 F516 I522 R526 I527 D528 D529 L530 I531 K532 L533 H534 P535 GLU SER

• Molecule 2: T-complex protein 1 subunit beta

Chain B:

A2 E19 R20 F29 I33 A34 I35 L38 V39 P45 K50 L53 S54 A59 V63 T64 N65 D66 G67 A68 L71 P79 V83 L84 V85 V95 G96 D97 G98 T99 T100 E112 A113 W130 R131 A137 D151 K154 L159 M160

S168 K181 V184 K203 K204 I249 K250 I251 F252 G253 S254 R255 V256 R257 V258 D259 S260 T261 A262 K263 I267 E271 K272 K278 I282 H285 R293 Q294 L295 H314 A315 V326 T327 F335 D357 A370 Q381 I382 L383 D384 E385 C395 V396

L397 A398 Q399 Y408 S413 E414 M417 S438 L446 N473 A476 M480 E512 V517 D518 N519 K522 K527

- Molecule 2: T-complex protein 1 subunit beta

Chain b: 83% 17%

A2 L6 I11 F12 E22 T23 L38 V39 T42 P45 K46 G47 K50 S54 R57 D58 A59 N65 P79 V83 V95 T100 E112 A113 H122 P123 Q124 W130 R131 R138 L141 D151 K154 M160 A163 S168

S169 K170 T180 V187 S193 G194 N195 L219 L220 N227 I232 I237 I249 K250 I251 D259 K263 I267 E271 N288 I291 N292 R293 A315 L323 V326 T327 S333 G344 E356 A370 C371 T372 L397 A398 Q399 D403

Y408 S413 E414 M415 L416 M417 T422 N426 E432 M436 E437 S438 M445 L446 L465 R466 A467 E471 L478 D479 M480 E495 Q498 V499 K500 L504 A510 A511 E512 V513 R516 V517 D518 N519 I520 I521 R526 LYS

- Molecule 3: T-complex protein 1 subunit delta

Chain D: 84% 16%

R19 D26 P30 A31 Q32 I38 A45 I48 R49 K55 G56 M57 D58 K59 M60 D67 V68 T69 I70 T71 N72 D73 L78 K79 Q80 P86 R89 V92 T107 S115 S119 C120 T121 M151 S152 R153 P154 S170 S173 V191 I195

V203 V224 E225 G226 L229 L248 I249 Q250 F251 M260 Q263 E278 E279 K291 L299 L305 D311 L312 I322 C337 P344 V345 A346 H347 F351 L374 D407 A408 V411 I412 L415 I430 E431 L432 A453 F454 M458 E459

V460 A469 L480 R483 N494 S501 N502 I503 L504 E505 V508 P511 V514 D533 D534 V535 T538

- Molecule 3: T-complex protein 1 subunit delta

Chain d: 83% 17%

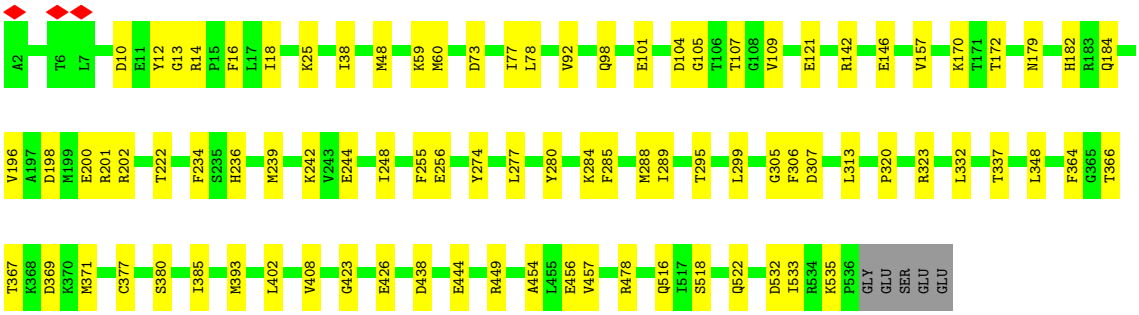
R19 P30 I38 K42 I48 D58 K59 M60 D63 N72 D73 L78 H85 P86 R89 M90 L91 V92 Q98 G103 D104 V110 L117 D118 S119 C120 T121 K122 L123 L124 H129 P130 S134 Q138 S152 R160 S170 S173 K174

V175 Q178 N189 A190 V191 I195 V203 R206 D207 I208 K209 I210 L227 N235 L248 C252 K257 Y269 A270 Q271 M272 D273 R274 V275 L276 R277 R306 I322 I333 T339 K343 S381 V386 T387 I388 D407 C410 V411 I412 R413

C414 L415 K418 I422 A423 L432 R435 A453 M458 N468 T476 L480 I493 I500 I503 P511 I512 L513 V514 R527 K531 I532 D533 D534 V535 T538

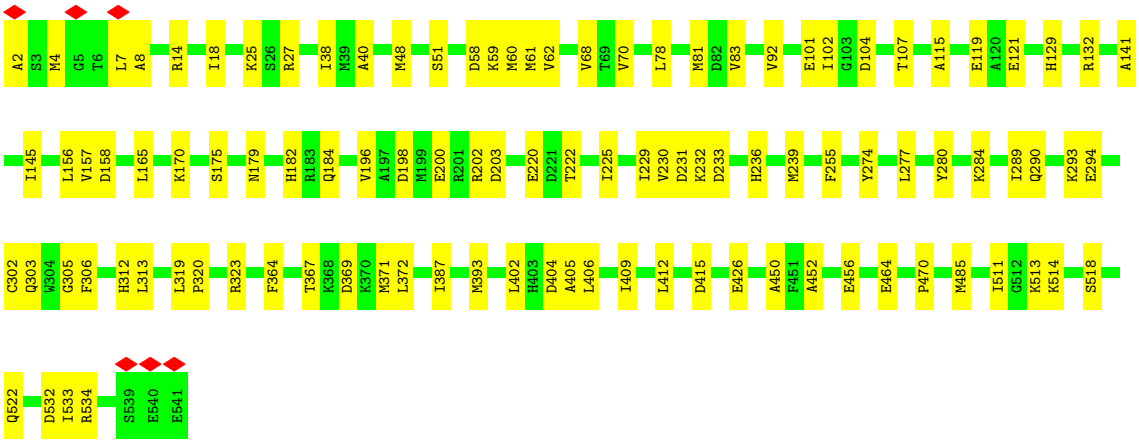
- Molecule 4: T-complex protein 1 subunit epsilon

Chain E:



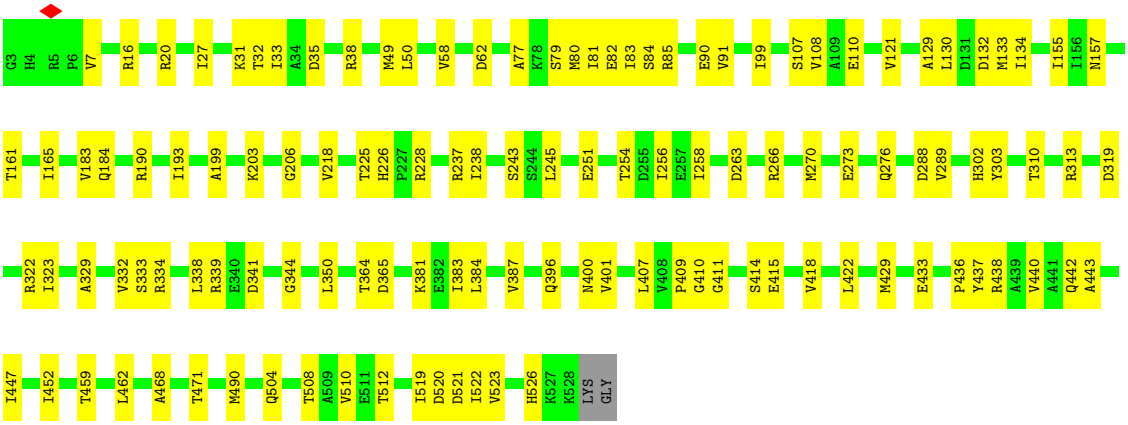
- Molecule 4: T-complex protein 1 subunit epsilon

Chain e:



- Molecule 5: T-complex protein 1 subunit gamma

Chain G:



- Molecule 5: T-complex protein 1 subunit gamma

Chain g:

GLY HIS ARG PRO VAL L8 K21 I27 D35 R38 T39 C40 L41 K48 D62 G63 N64 H74 P75 A76 A77 K78 S79 M80 I81 E82 I83 E90 V91 T95 T96 I99 I100 L101 M105 E110 Y126 R127 L130 D131 D132 M152 I155 I156

N157 T161 M182 D194 K197 K203 G206 G217 V218 K222 D223 V224 M229 D242 S243 S244 L245 E246 E251 I256 E257 I258 D263 R266 M270 V289 T292 E293 K294 H302 D319 R322 I323 E337 L338 R339 L350 E351

I352 T361 P362 I363 C372 L376 L384 V401 G411 E415 W435 P436 Y437 I447 P448 R449 T450 L463 A468 T471 M490 E497 K502 L503 Q504 T508 A509 V510 I519 D520 D521 I522 G530

• Molecule 6: T-complex protein 1 subunit eta, N-terminally processed

Chain H:

M1 M2 P3 K10 S16 P20 Q21 L22 V23 I26 Q30 V31 I32 A33 E34 R37 T38 T39 L40 K47 L48 D70 H73 A76 I82 Q86 D92 V97 T98 L99 A102 E103 F104 L105 K106 Q107 V108 Q130 I136 D147 E150

Q151 R152 L155 E156 K157 M160 L163 L167 I168 A173 V180 D181 A182 V183 M184 M185 L186 D187 D188 L189 L190 Q191 L192 K193 M194 I195 G196 I197 V200 Q201 G202 V242 E243 L244 A269 I273 N335 A336 L337 Q346 I353 G363 C364 A367 K368

R375 T385 E386 M394 I395 V396 I400 E413 M414 E415 L416 I427 P428 G429 Q432 A441 L442 I445 P446 L449 F455 D456 A457 L461 E482 D483 I484 F491 R499 A502 A509 V516 T526 V527 D528

• Molecule 6: T-complex protein 1 subunit eta, N-terminally processed

Chain h:

M1 M2 P5 L8 S16 Q17 G18 Q21 L22 V23 I26 Q30 V31 I32 A33 E34 R37 T38 P42 K47 L48 T57 N60 K67 L68 L69 H73 A76 I82 A83 K84 S85 V90 G91 D92 T95 S96 V97 T98 L99 F104 L105

K106 Q107 V108 K109 V112 R126 I136 K144 R152 E156 M160 S165 I168 A173 D181 M184 M185 L186 D187 D188 L189 L190 Q191 L192 K193 M194 I195 G196 I197 V200 Q201 G202 K218 S221 F225 E249 I255 E279 H283

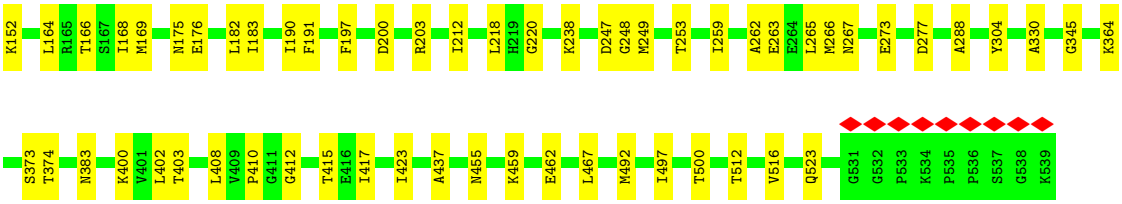
D297 K320 M324 S338 A339 D340 Q346 I353 R357 G363 C364 A367 K368 T369 R375 T385 E386 M394 R398 G408 E413 L416 R421 R425 A441 L442 E443 I444 I445 P446 R447 L461 R465 I479 N487 M497 V498

R499 A502 A509 V516 S525 THR VAL ASP

• Molecule 7: T-complex protein 1 subunit theta

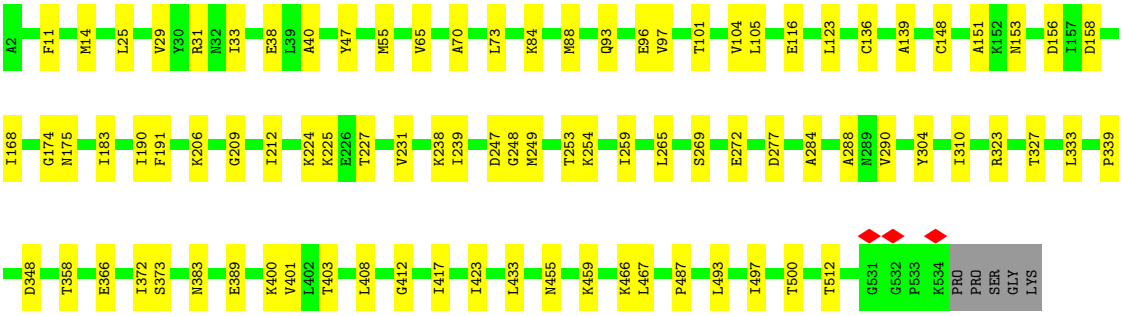
Chain Q:

A2 F11 E26 Y30 R31 N32 I33 E38 T42 Y47 M55 V65 A70 L73 R74 E75 Q79 K84 V87 M88 Q93 D99 G100 T101 N102 L105 E116 E117 L118 I121 G122 L123 I129 E130 G131 C136 A139 A151



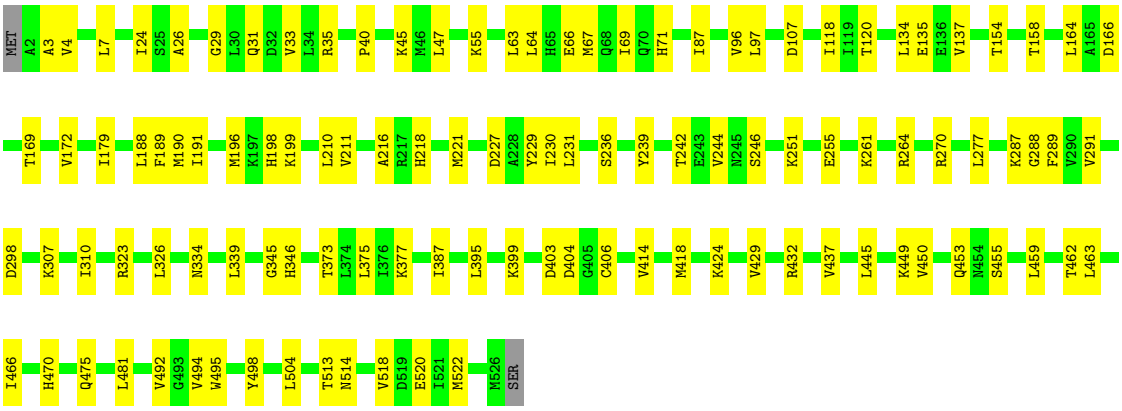
- Molecule 7: T-complex protein 1 subunit theta

Chain q:



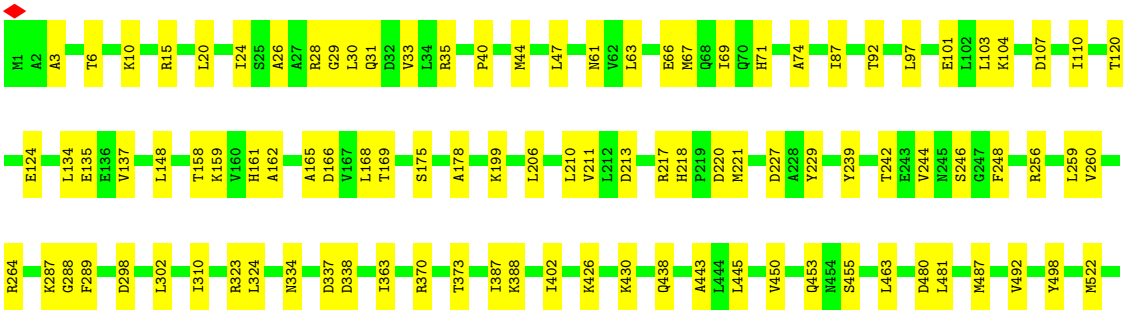
- Molecule 8: T-complex protein 1 subunit zeta

Chain Z:



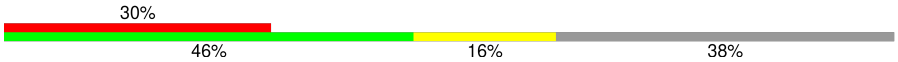
- Molecule 8: T-complex protein 1 subunit zeta

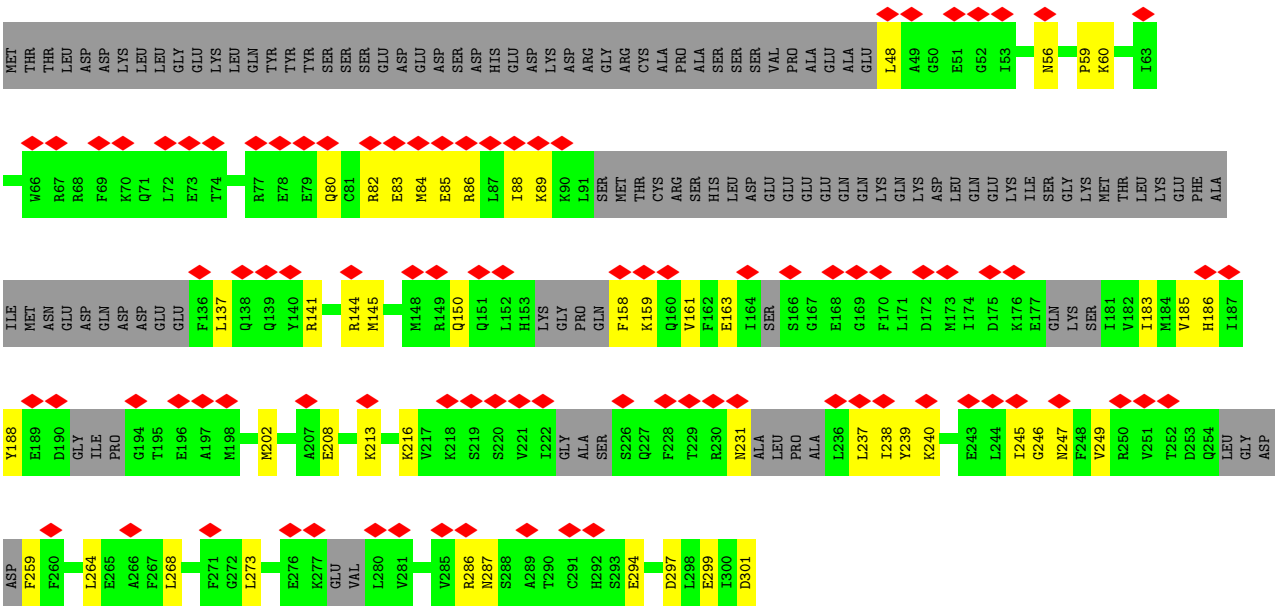
Chain z:



• Molecule 9: Phosducin-like protein

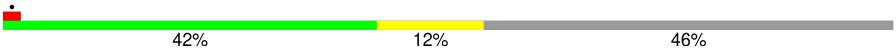
Chain P:

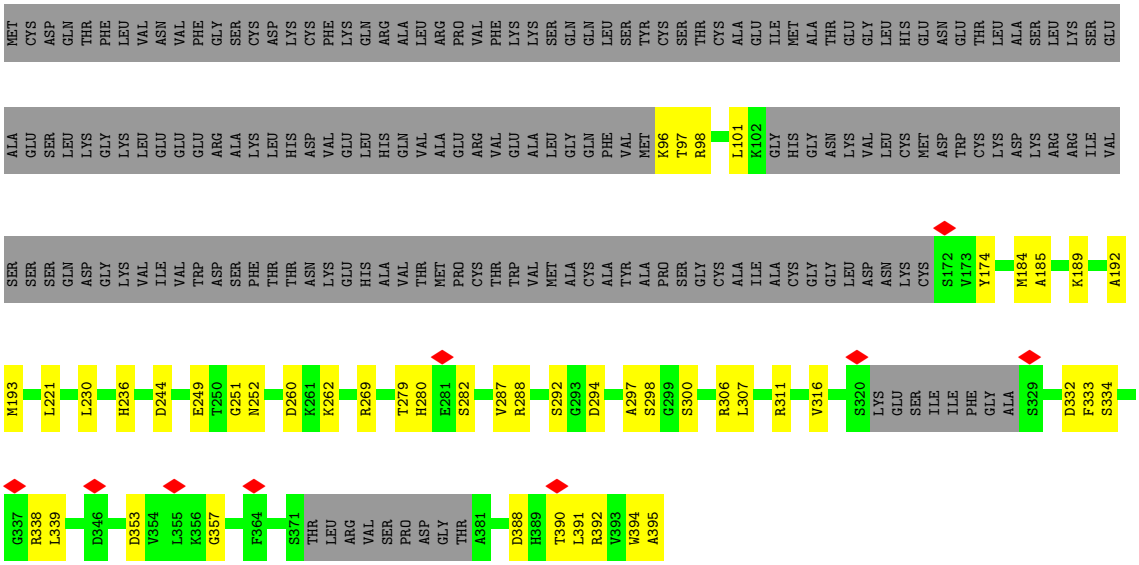




• Molecule 10: Guanine nucleotide-binding protein subunit beta-5

Chain N:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.086	Depositor
Minimum map value	-0.393	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AF3, ADP

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	0.12	0/4109	0.26	0/5548
1	a	0.13	0/4081	0.25	0/5510
2	B	0.13	0/3995	0.25	0/5386
2	b	0.13	0/3986	0.25	0/5375
3	D	0.13	0/3955	0.25	0/5338
3	d	0.13	0/3949	0.25	0/5331
4	E	0.13	0/4183	0.28	0/5635
4	e	0.13	0/4220	0.25	0/5684
5	G	0.13	0/4136	0.25	0/5579
5	g	0.12	0/4108	0.24	0/5539
6	H	0.13	0/4111	0.26	0/5550
6	h	0.13	0/4089	0.26	0/5519
7	Q	0.12	0/4147	0.25	0/5606
7	q	0.12	0/4112	0.25	0/5558
8	Z	0.13	0/4069	0.25	0/5486
8	z	0.13	0/4080	0.26	0/5501
9	P	0.11	0/1521	0.33	0/2024
10	N	0.10	0/1689	0.31	0/2280
All	All	0.13	0/68540	0.26	0/92449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4069	0	4224	54	0
1	a	4041	0	4205	77	0
2	B	3952	0	4070	58	0
2	b	3943	0	4057	66	0
3	D	3923	0	4131	54	0
3	d	3917	0	4120	61	0
4	E	4132	0	4246	65	0
4	e	4169	0	4272	78	0
5	G	4089	0	4224	80	0
5	g	4063	0	4201	60	0
6	H	4054	0	4160	65	0
6	h	4032	0	4140	67	0
7	Q	4086	0	4160	61	0
7	q	4053	0	4125	58	0
8	Z	4022	0	4161	72	0
8	z	4033	0	4171	64	0
9	P	1507	0	1495	35	0
10	N	1656	0	1566	35	0
11	A	27	0	12	1	0
11	B	27	0	12	3	0
11	D	27	0	12	1	0
11	E	27	0	12	0	0
11	G	27	0	12	2	0
11	H	27	0	12	0	0
11	Q	27	0	12	2	0
11	Z	27	0	12	1	0
11	a	27	0	12	3	0
11	b	27	0	12	3	0
11	d	27	0	12	2	0
11	e	27	0	12	1	0
11	g	27	0	12	3	0
11	h	27	0	12	2	0
11	q	27	0	12	3	0
11	z	27	0	12	2	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
12	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1	0	0	0	0
12	a	1	0	0	0	0
12	b	1	0	0	0	0
12	d	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	h	1	0	0	0	0
12	q	1	0	0	0	0
12	z	1	0	0	0	0
13	A	4	0	0	2	0
13	B	4	0	0	3	0
13	D	4	0	0	3	0
13	E	4	0	0	1	0
13	G	4	0	0	2	0
13	H	4	0	0	0	0
13	Q	4	0	0	2	0
13	Z	4	0	0	1	0
13	a	4	0	0	2	0
13	b	4	0	0	2	0
13	d	4	0	0	2	0
13	e	4	0	0	0	0
13	g	4	0	0	3	0
13	h	4	0	0	1	0
13	q	4	0	0	1	0
13	z	4	0	0	2	0
14	A	2	0	0	0	0
14	B	2	0	0	0	0
14	D	1	0	0	0	0
14	E	1	0	0	0	0
14	G	1	0	0	0	0
14	H	1	0	0	0	0
14	Q	1	0	0	0	0
14	Z	1	0	0	0	0
14	a	2	0	0	0	0
14	b	1	0	0	0	0
14	d	1	0	0	1	0
14	e	1	0	0	1	0
14	g	1	0	0	0	0
14	h	1	0	0	0	0
14	q	1	0	0	0	0
14	z	1	0	0	0	0
All	All	68272	0	69920	1003	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 7.

The worst 5 of 1003 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:A:23:MET:HE2	4:e:8:ALA:HA	1.63	0.79
6:h:22:LEU:HD22	6:h:112:VAL:HG11	1.64	0.79
2:B:517:VAL:HG21	4:E:60:MET:HE3	1.65	0.77
5:g:27:ILE:HD13	5:g:110:GLU:HB2	1.67	0.77
3:D:502:ASN:HD22	3:D:505:GLU:HG3	1.49	0.76

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	534/536 (100%)	515 (96%)	19 (4%)	0	100	100
1	a	530/536 (99%)	509 (96%)	21 (4%)	0	100	100
2	B	524/526 (100%)	510 (97%)	14 (3%)	0	100	100
2	b	523/526 (99%)	507 (97%)	16 (3%)	0	100	100
3	D	518/520 (100%)	510 (98%)	8 (2%)	0	100	100
3	d	518/520 (100%)	498 (96%)	20 (4%)	0	100	100
4	E	534/540 (99%)	512 (96%)	22 (4%)	0	100	100
4	e	539/540 (100%)	527 (98%)	12 (2%)	0	100	100
5	G	524/528 (99%)	508 (97%)	16 (3%)	0	100	100
5	g	521/528 (99%)	508 (98%)	13 (2%)	0	100	100
6	H	526/528 (100%)	510 (97%)	16 (3%)	0	100	100
6	h	523/528 (99%)	506 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Q	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
7	q	531/538 (99%)	517 (97%)	14 (3%)	0	100	100
8	Z	523/527 (99%)	509 (97%)	14 (3%)	0	100	100
8	z	525/527 (100%)	511 (97%)	14 (3%)	0	100	100
9	P	166/301 (55%)	150 (90%)	16 (10%)	0	100	100
10	N	206/395 (52%)	182 (88%)	24 (12%)	0	100	100
All	All	8801/9182 (96%)	8511 (97%)	290 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	447/447 (100%)	447 (100%)	0	100	100
1	a	444/447 (99%)	444 (100%)	0	100	100
2	B	418/418 (100%)	418 (100%)	0	100	100
2	b	417/418 (100%)	417 (100%)	0	100	100
3	D	442/442 (100%)	442 (100%)	0	100	100
3	d	441/442 (100%)	441 (100%)	0	100	100
4	E	452/455 (99%)	452 (100%)	0	100	100
4	e	456/455 (100%)	456 (100%)	0	100	100
5	G	456/457 (100%)	456 (100%)	0	100	100
5	g	453/457 (99%)	453 (100%)	0	100	100
6	H	435/435 (100%)	434 (100%)	1 (0%)	87	92
6	h	432/435 (99%)	432 (100%)	0	100	100
7	Q	442/442 (100%)	442 (100%)	0	100	100
7	q	438/442 (99%)	438 (100%)	0	100	100
8	Z	437/439 (100%)	437 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	z	438/439 (100%)	438 (100%)	0	100	100
9	P	166/266 (62%)	166 (100%)	0	100	100
10	N	180/334 (54%)	180 (100%)	0	100	100
All	All	7394/7670 (96%)	7393 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	21	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
6	h	501	ASN
7	q	93	GLN
7	Q	50	ASN
6	H	431	GLN
7	q	219	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	AF3	e	603	11	0,3,3	-	-	-		
13	AF3	H	603	11	0,3,3	-	-	-		
13	AF3	z	603	11	0,3,3	-	-	-		
13	AF3	D	603	11	0,3,3	-	-	-		
13	AF3	q	603	7,11	0,3,3	-	-	-		
11	ADP	h	601	13,12	28,29,29	1.39	4 (14%)	43,45,45	1.85	10 (23%)
11	ADP	Z	601	13,12	28,29,29	1.39	4 (14%)	43,45,45	1.84	9 (20%)
13	AF3	G	603	11	0,3,3	-	-	-		
13	AF3	d	603	11	0,3,3	-	-	-		
11	ADP	D	601	13,12	28,29,29	1.41	4 (14%)	43,45,45	1.81	8 (18%)
13	AF3	g	603	11	0,3,3	-	-	-		
11	ADP	G	601	13,12	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (20%)
11	ADP	A	601	13,12	28,29,29	1.38	4 (14%)	43,45,45	1.83	10 (23%)
13	AF3	Z	603	11	0,3,3	-	-	-		
13	AF3	Q	603	11	0,3,3	-	-	-		
11	ADP	E	601	13,12	28,29,29	1.40	4 (14%)	43,45,45	1.82	9 (20%)
11	ADP	b	601	13,12	28,29,29	1.40	4 (14%)	43,45,45	1.85	10 (23%)
11	ADP	d	601	13,12	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
11	ADP	B	601	13,12	28,29,29	1.40	4 (14%)	43,45,45	1.85	10 (23%)
13	AF3	A	603	11	0,3,3	-	-	-		
11	ADP	g	601	13,12	28,29,29	1.39	5 (17%)	43,45,45	1.81	9 (20%)
13	AF3	h	603	11	0,3,3	-	-	-		
11	ADP	q	601	13,12	28,29,29	1.39	4 (14%)	43,45,45	1.85	9 (20%)
11	ADP	e	601	13,12	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
13	AF3	a	603	11	0,3,3	-	-	-		
13	AF3	E	603	11	0,3,3	-	-	-		
11	ADP	Q	601	13,12	28,29,29	1.38	4 (14%)	43,45,45	1.84	9 (20%)
13	AF3	B	603	11	0,3,3	-	-	-		
11	ADP	z	601	13,12	28,29,29	1.38	4 (14%)	43,45,45	1.84	10 (23%)
11	ADP	H	601	13,12	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
13	AF3	b	603	11	0,3,3	-	-	-		
11	ADP	a	601	13,12	28,29,29	1.39	4 (14%)	43,45,45	1.81	9 (20%)

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
11	ADP	A	601	13,12	-	4/16/32/32	0/3/3/3
11	ADP	E	601	13,12	-	0/16/32/32	0/3/3/3
11	ADP	h	601	13,12	-	3/16/32/32	0/3/3/3
11	ADP	b	601	13,12	-	1/16/32/32	0/3/3/3
11	ADP	d	601	13,12	-	1/16/32/32	0/3/3/3
11	ADP	B	601	13,12	-	3/16/32/32	0/3/3/3
11	ADP	Q	601	13,12	-	7/16/32/32	0/3/3/3
11	ADP	Z	601	13,12	-	4/16/32/32	0/3/3/3
11	ADP	g	601	13,12	-	2/16/32/32	0/3/3/3
11	ADP	q	601	13,12	-	6/16/32/32	0/3/3/3
11	ADP	z	601	13,12	-	3/16/32/32	0/3/3/3
11	ADP	H	601	13,12	-	6/16/32/32	0/3/3/3
11	ADP	D	601	13,12	-	0/16/32/32	0/3/3/3
11	ADP	e	601	13,12	-	1/16/32/32	0/3/3/3
11	ADP	a	601	13,12	-	5/16/32/32	0/3/3/3
11	ADP	G	601	13,12	-	2/16/32/32	0/3/3/3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Z	601	ADP	C5-C4	4.61	1.47	1.39
11	G	601	ADP	C5-C4	4.58	1.47	1.39
11	B	601	ADP	C5-C4	4.57	1.47	1.39
11	d	601	ADP	C5-C4	4.56	1.47	1.39
11	e	601	ADP	C5-C4	4.55	1.47	1.39

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	d	601	ADP	C5-C4-N3	-5.92	118.56	126.72
11	D	601	ADP	C5-C4-N3	-5.87	118.63	126.72
11	b	601	ADP	C5-C4-N3	-5.86	118.64	126.72
11	E	601	ADP	C5-C4-N3	-5.86	118.65	126.72
11	h	601	ADP	C5-C4-N3	-5.86	118.65	126.72

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	601	ADP	C5'-O5'-PA-O1A
11	A	601	ADP	C5'-O5'-PA-O2A
11	A	601	ADP	C5'-O5'-PA-O3A
11	B	601	ADP	C5'-O5'-PA-O1A
11	H	601	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

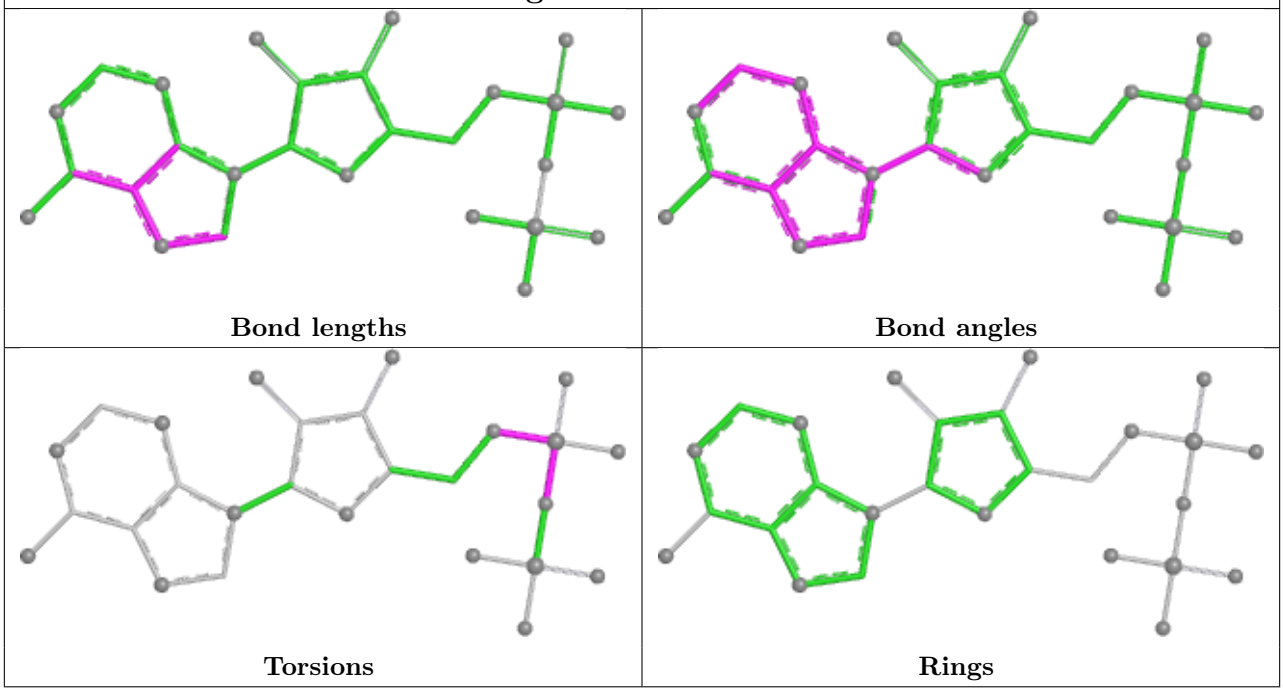
28 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	z	603	AF3	2	0
13	D	603	AF3	3	0
13	q	603	AF3	1	0
11	h	601	ADP	2	0
11	Z	601	ADP	1	0
13	G	603	AF3	2	0
13	d	603	AF3	2	0
11	D	601	ADP	1	0
13	g	603	AF3	3	0
11	G	601	ADP	2	0
11	A	601	ADP	1	0
13	Z	603	AF3	1	0
13	Q	603	AF3	2	0
11	b	601	ADP	3	0
11	d	601	ADP	2	0
11	B	601	ADP	3	0
13	A	603	AF3	2	0
11	g	601	ADP	3	0
13	h	603	AF3	1	0
11	q	601	ADP	3	0
11	e	601	ADP	1	0
13	a	603	AF3	2	0
13	E	603	AF3	1	0
11	Q	601	ADP	2	0
13	B	603	AF3	3	0
11	z	601	ADP	2	0
13	b	603	AF3	2	0
11	a	601	ADP	3	0

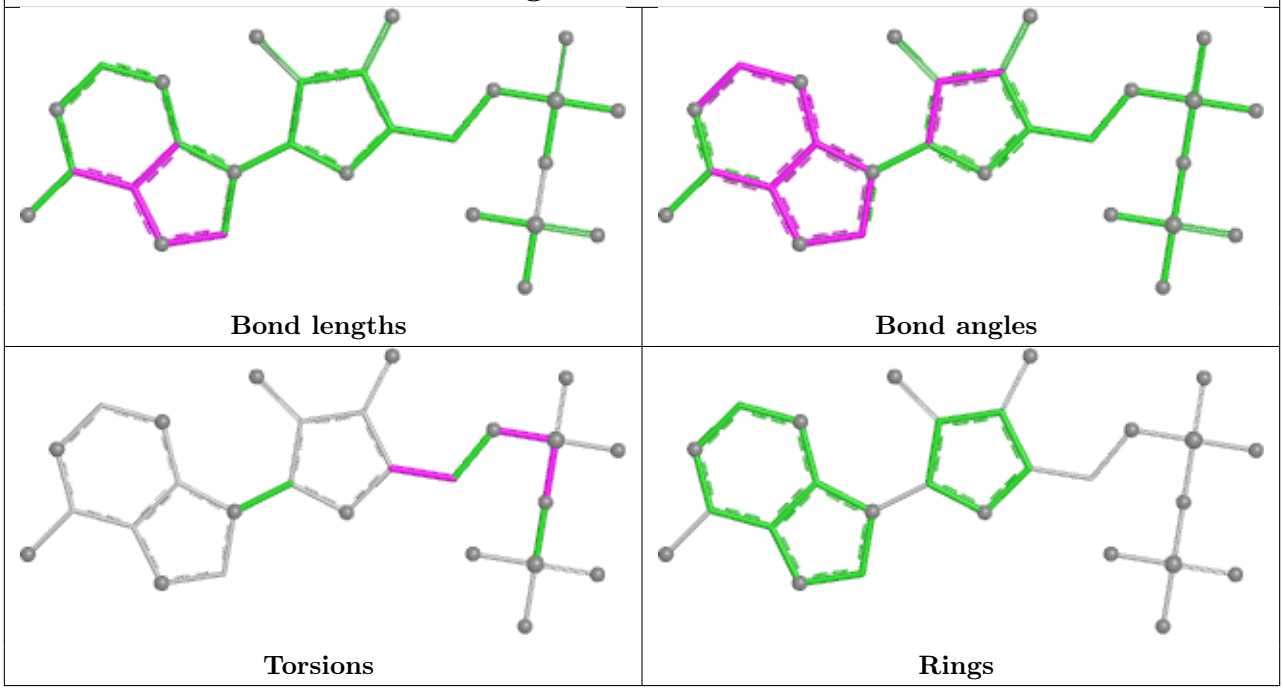
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADP h 601



Ligand ADP Z 601



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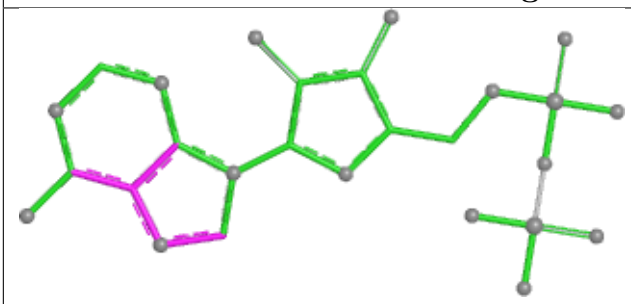
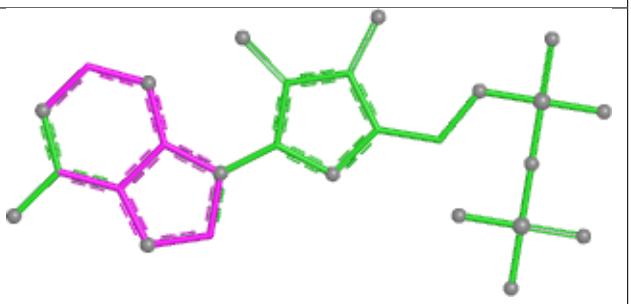
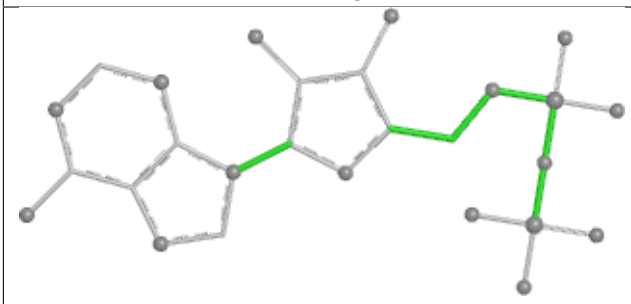
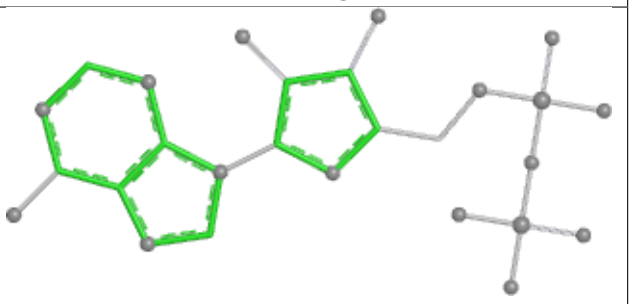
 Bond lengths	 Bond angles
 Torsions	 Rings

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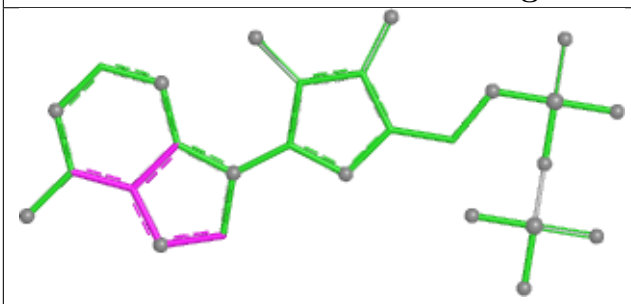
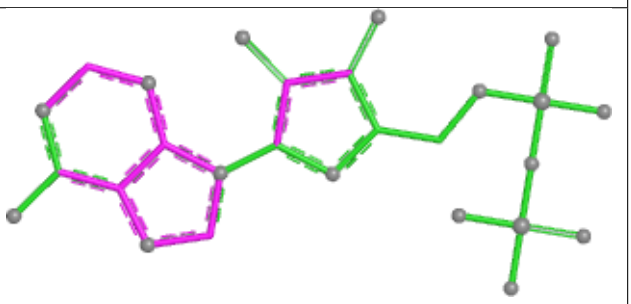
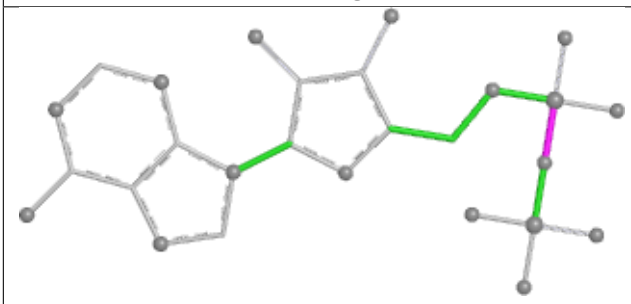
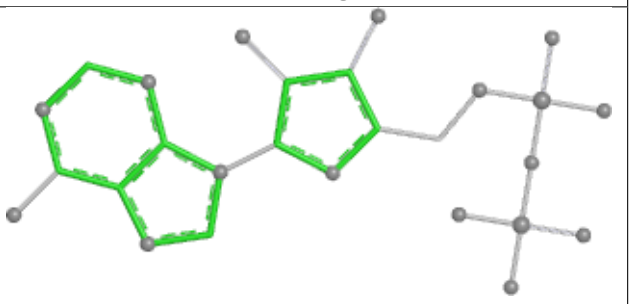
 Bond lengths	 Bond angles
 Torsions	 Rings

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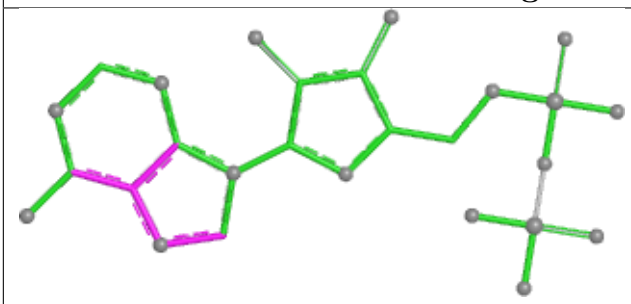
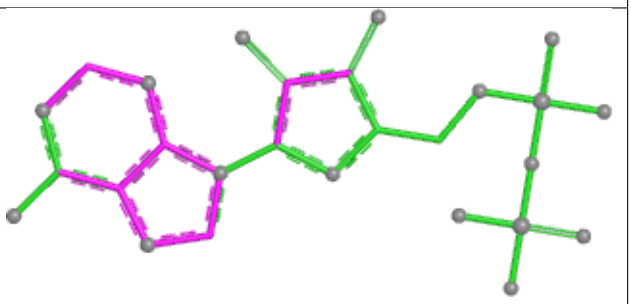
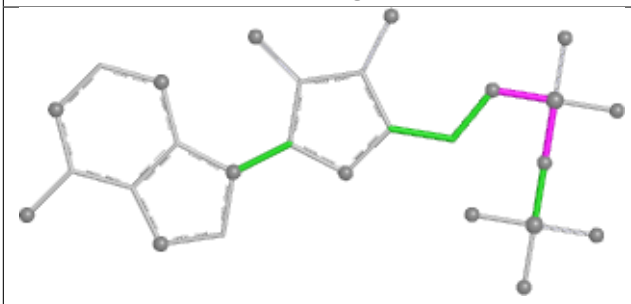
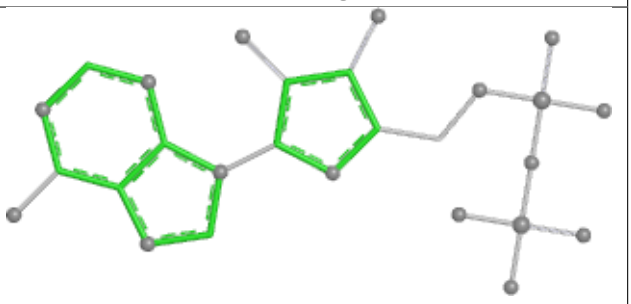
 Bond lengths	 Bond angles
 Torsions	 Rings

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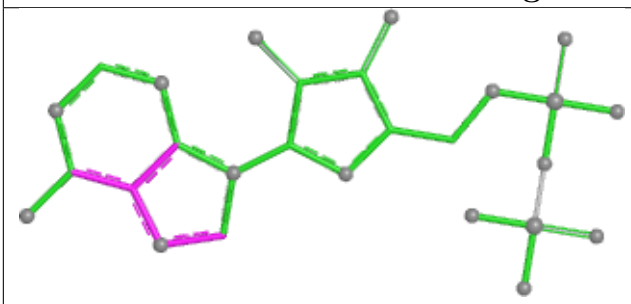
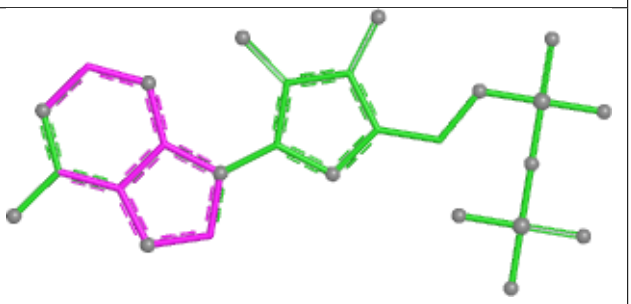
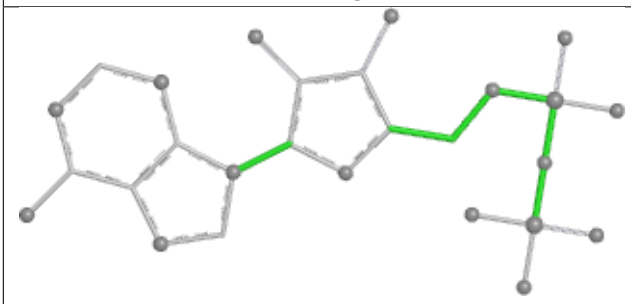
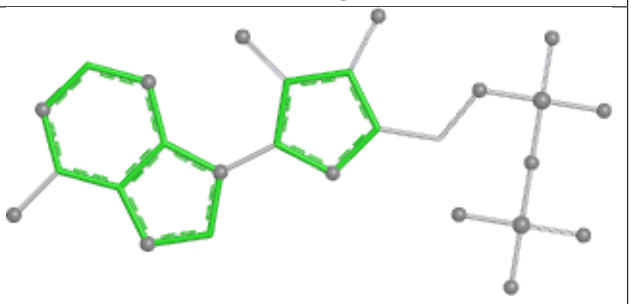
 Bond lengths	 Bond angles
 Torsions	 Rings

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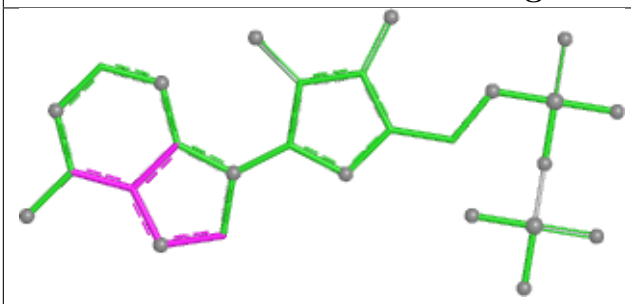
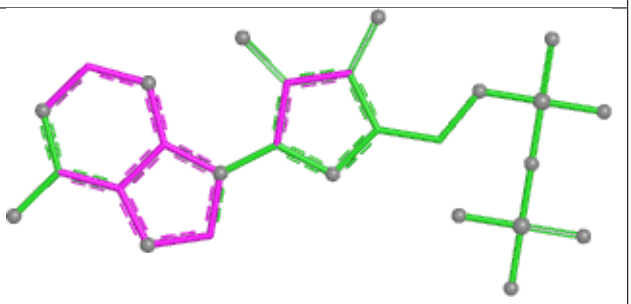
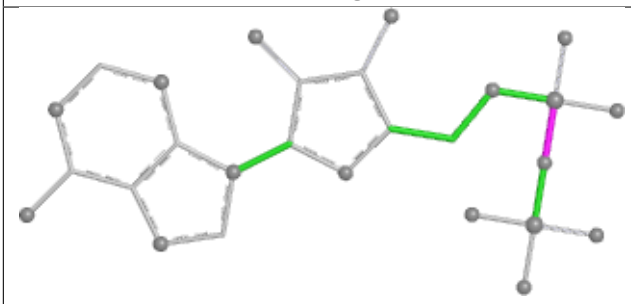
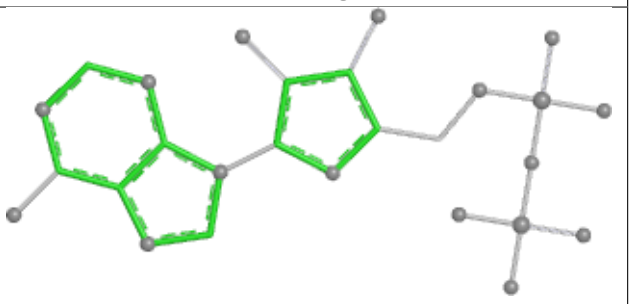
 Bond lengths	 Bond angles
 Torsions	 Rings

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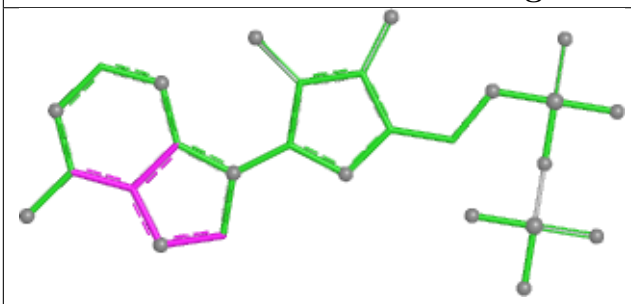
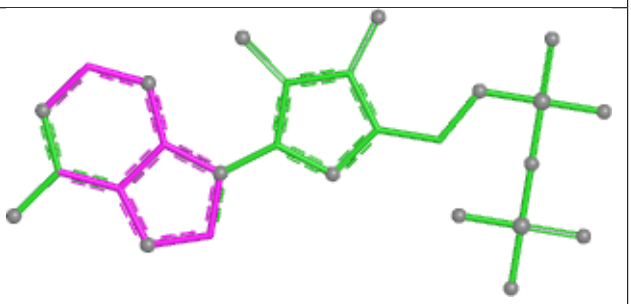
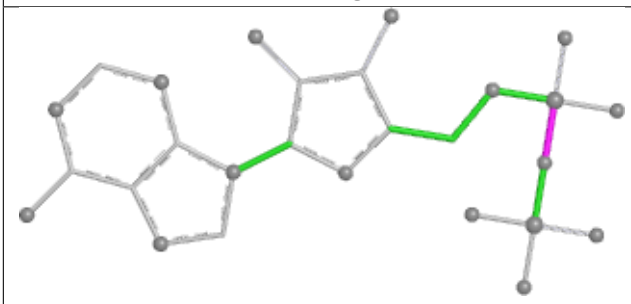
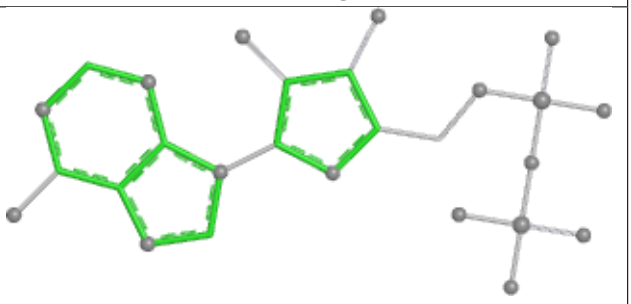
 Bond lengths	 Bond angles
 Torsions	 Rings

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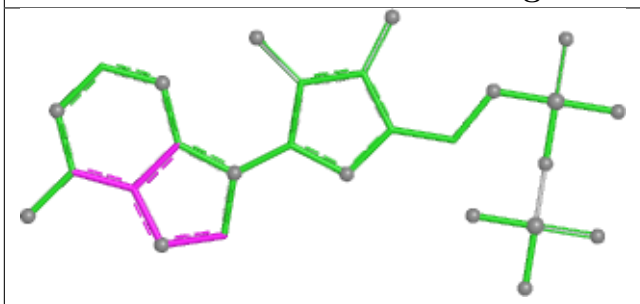
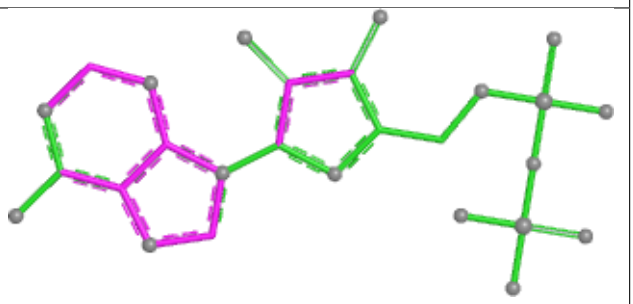
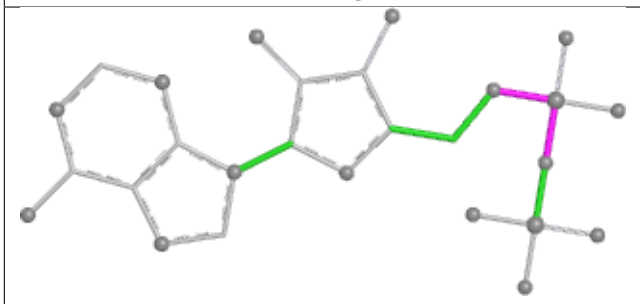
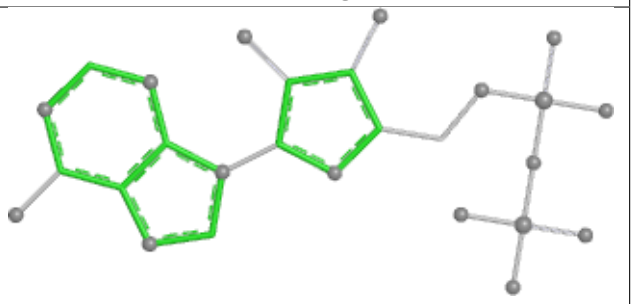
 Bond lengths	 Bond angles
 Torsions	 Rings

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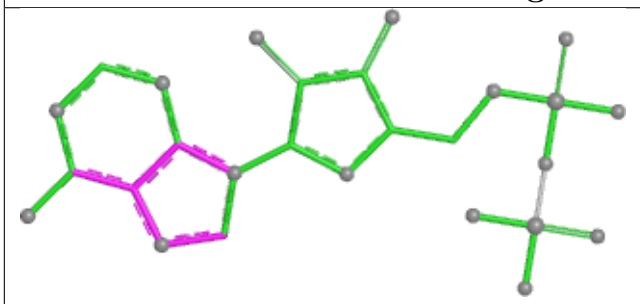
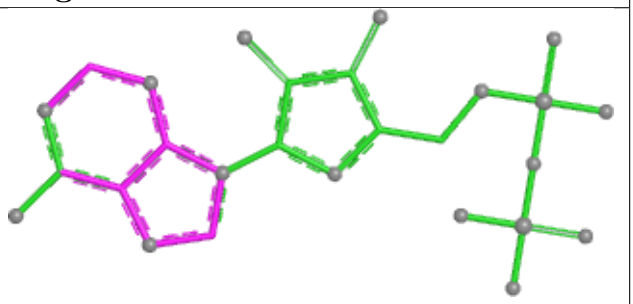
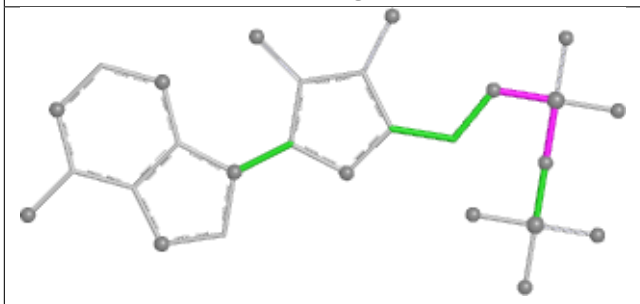
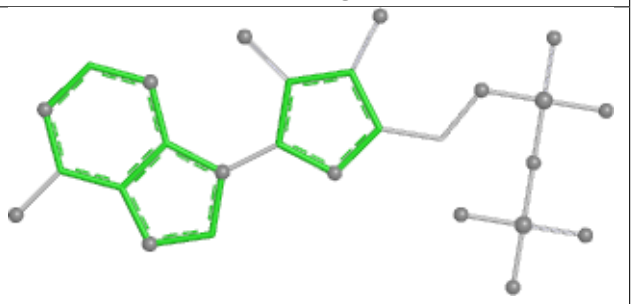
 Bond lengths	 Bond angles
 Torsions	 Rings

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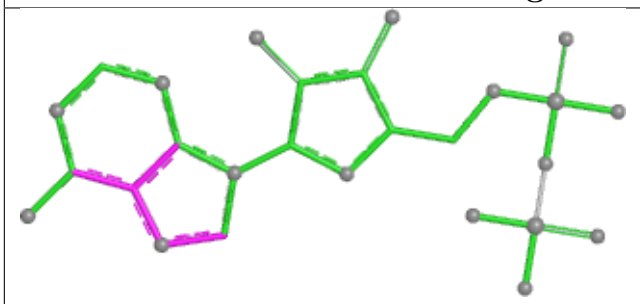
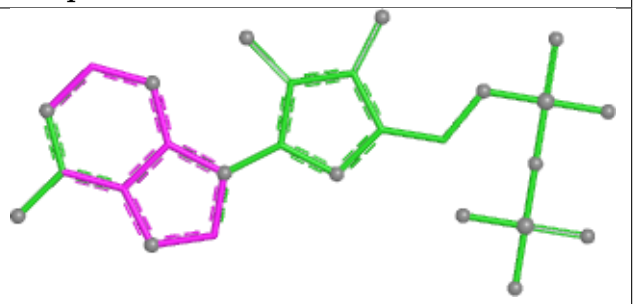
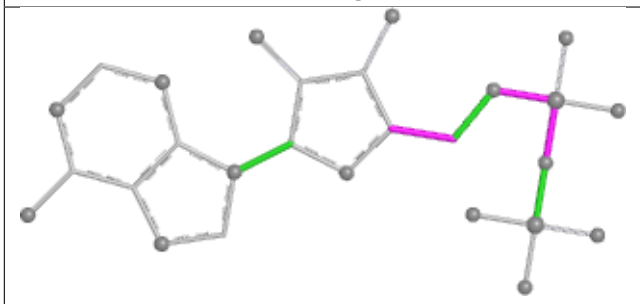
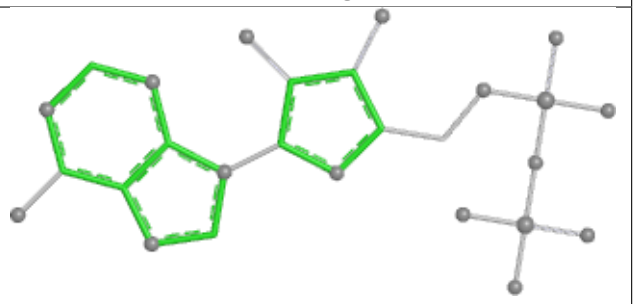
 Bond lengths	 Bond angles
 Torsions	 Rings

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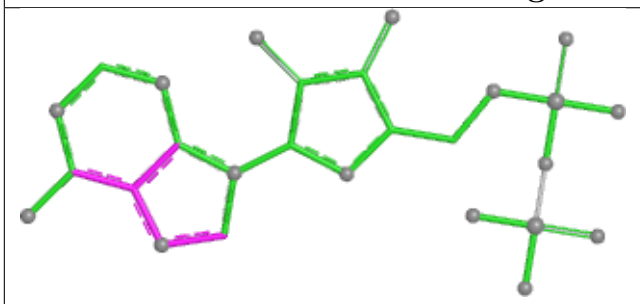
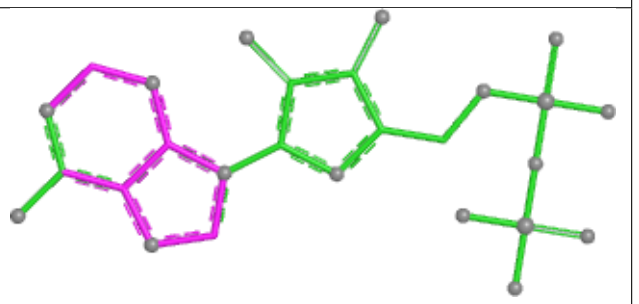
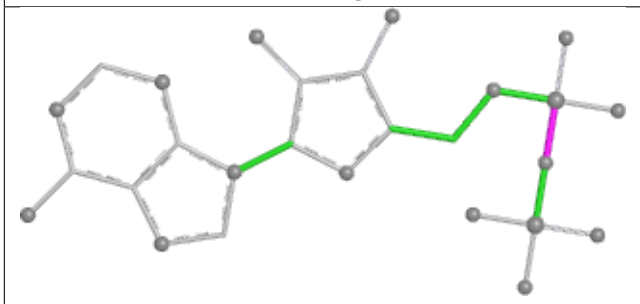
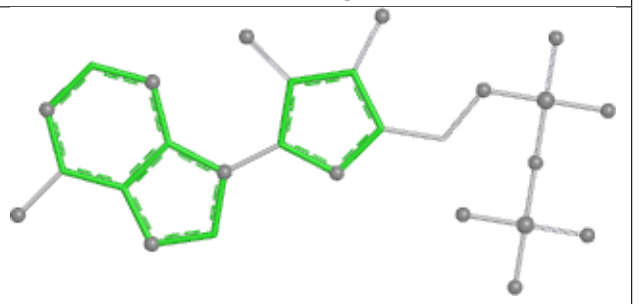
 Bond lengths	 Bond angles
 Torsions	 Rings

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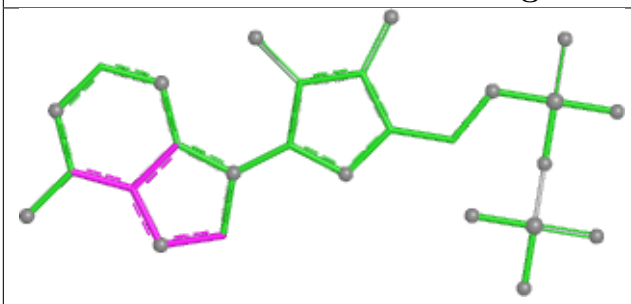
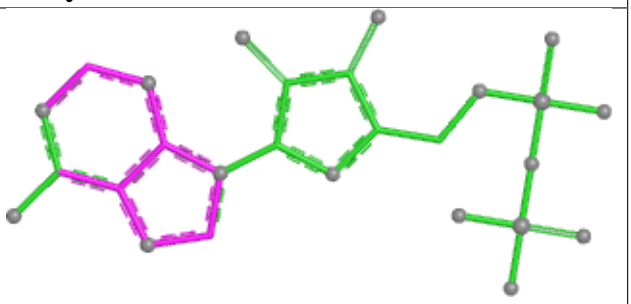
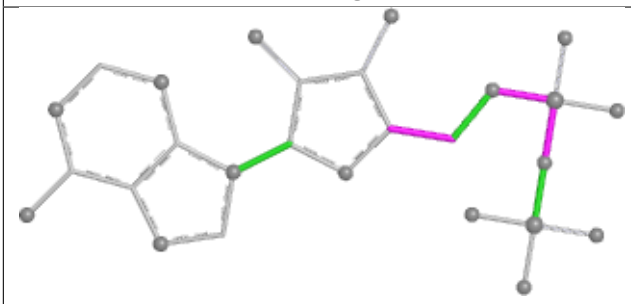
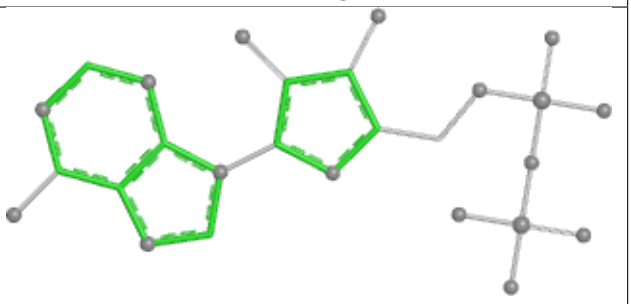
 Bond lengths	 Bond angles
 Torsions	 Rings

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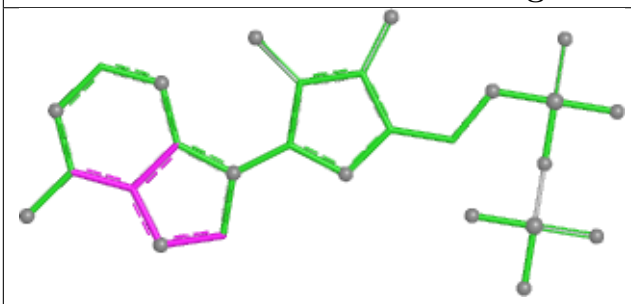
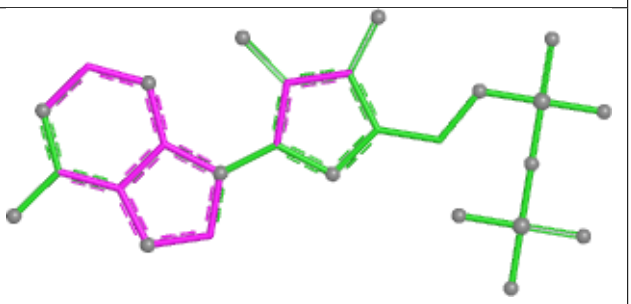
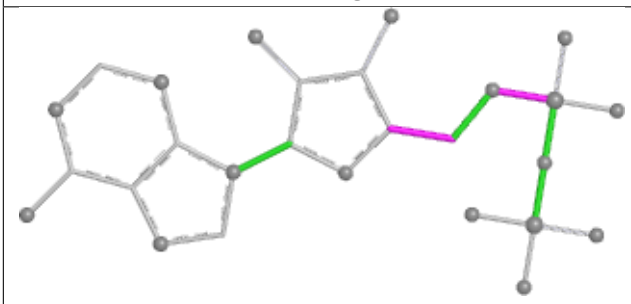
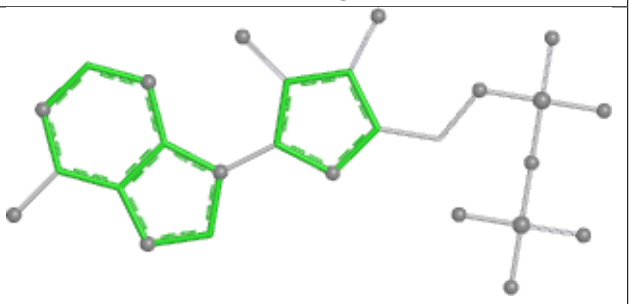
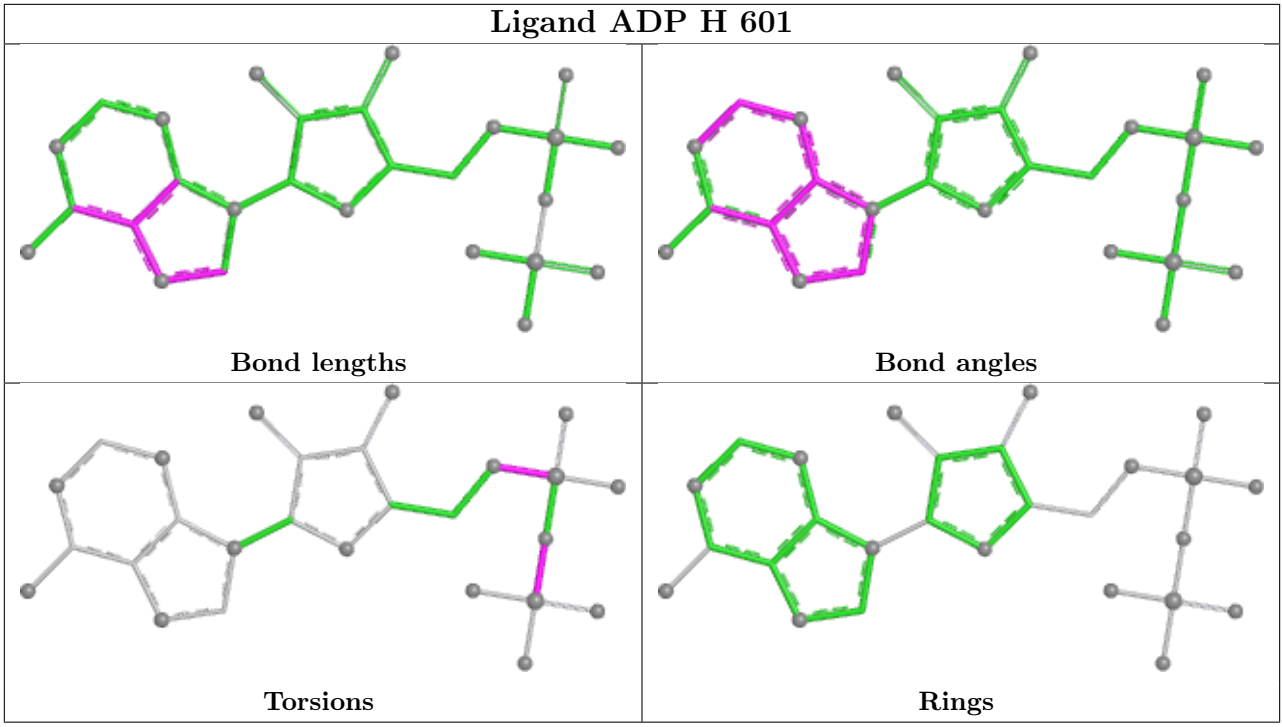
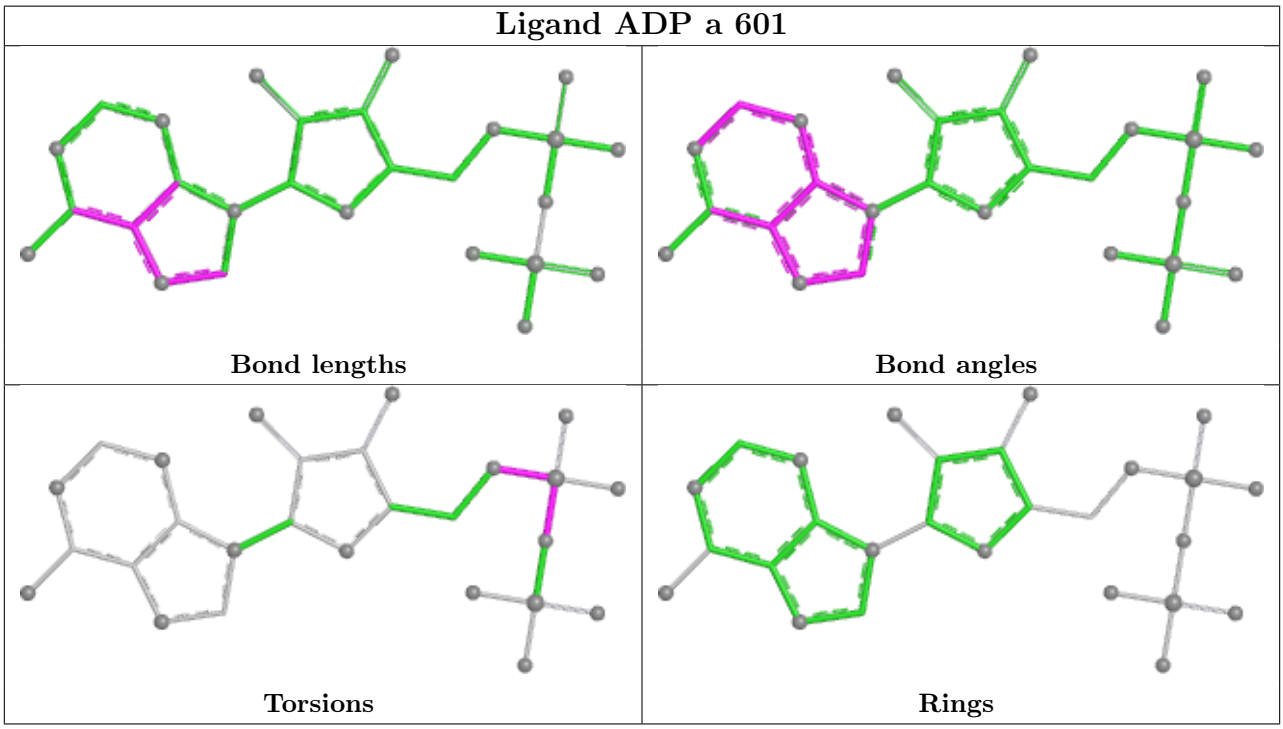
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

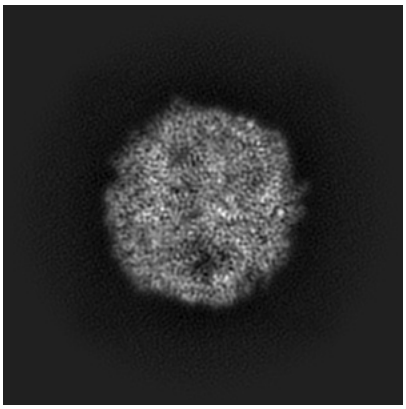
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40494. These allow visual inspection of the internal detail of the map and identification of artifacts.

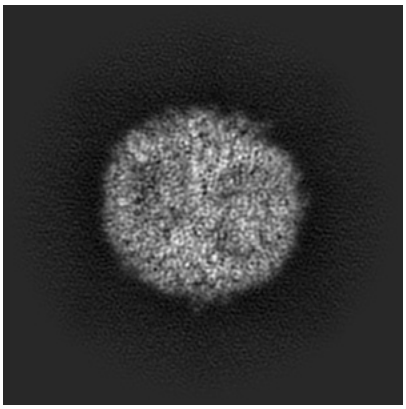
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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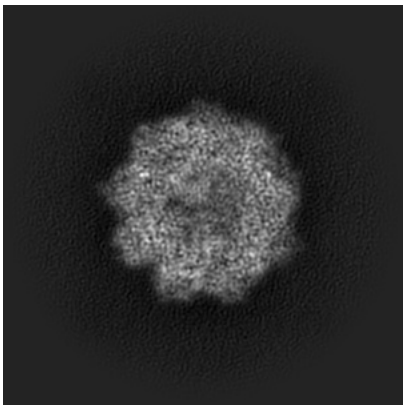
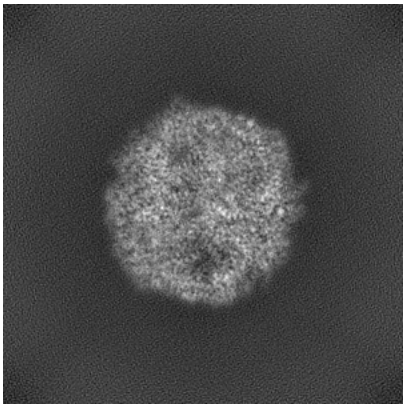
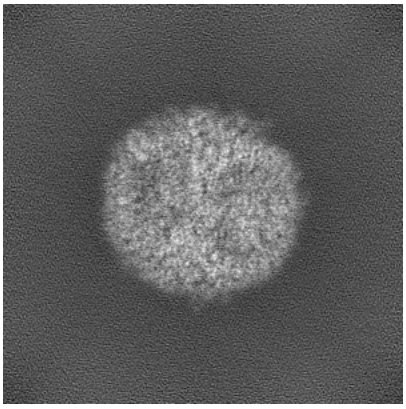


Z

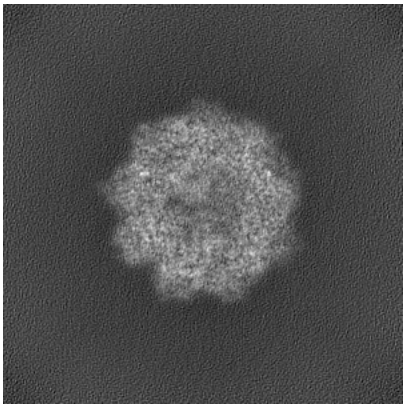
6.1.2 Raw map



X



Y

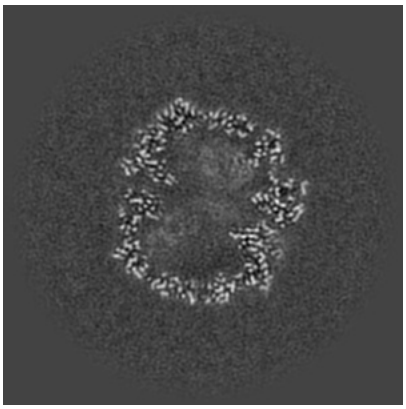


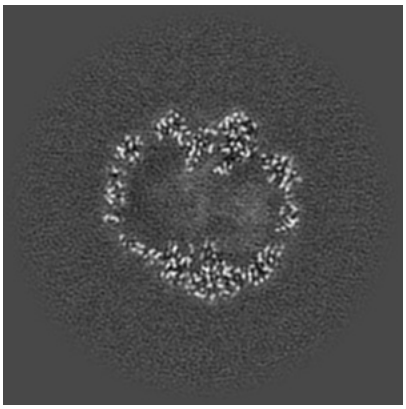
Z

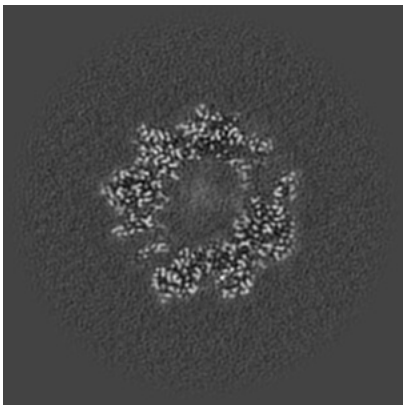
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

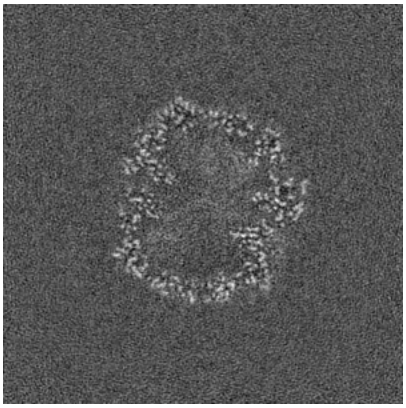
6.2.1 Primary map

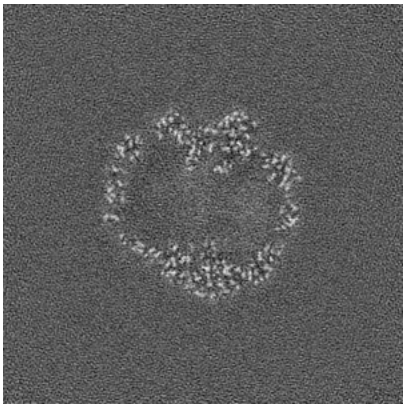

X Index: 150

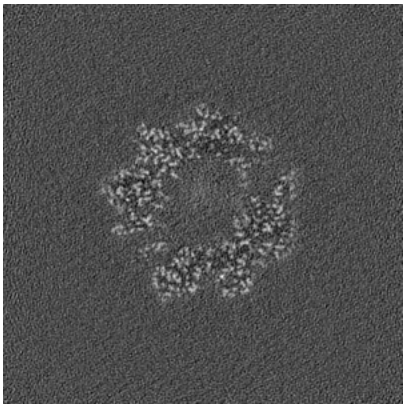

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

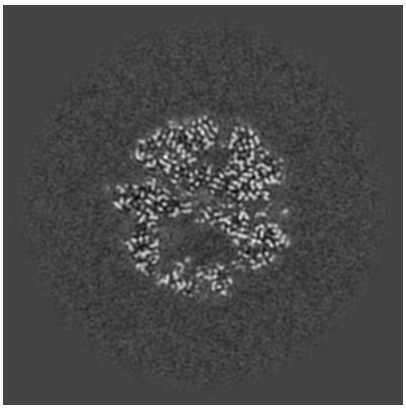

Y Index: 150


Z Index: 150

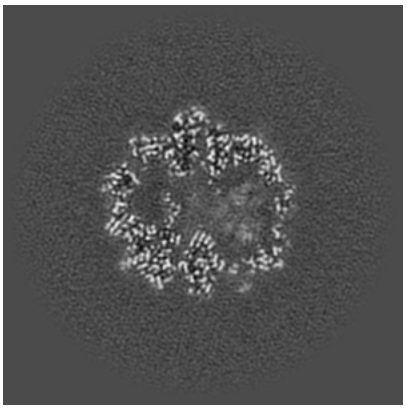
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

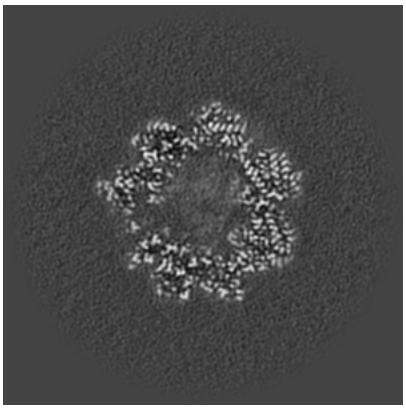
6.3.1 Primary map



X Index: 182

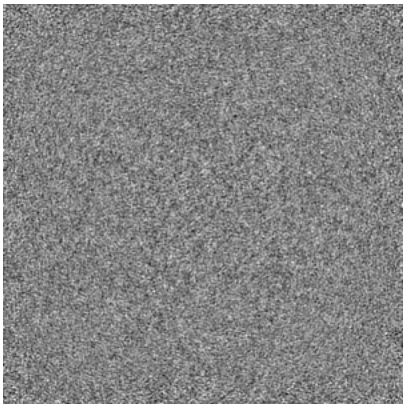


Y Index: 172

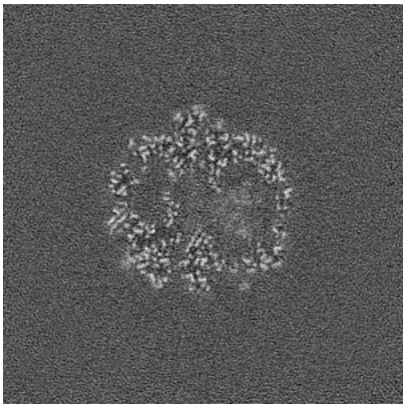


Z Index: 143

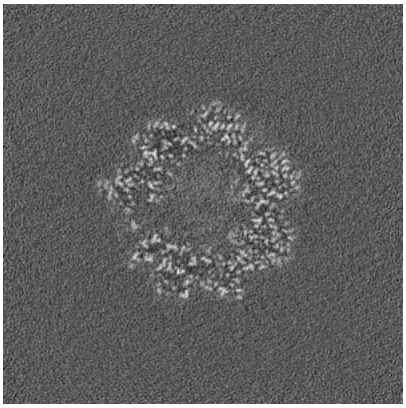
6.3.2 Raw map



X Index: 0



Y Index: 173

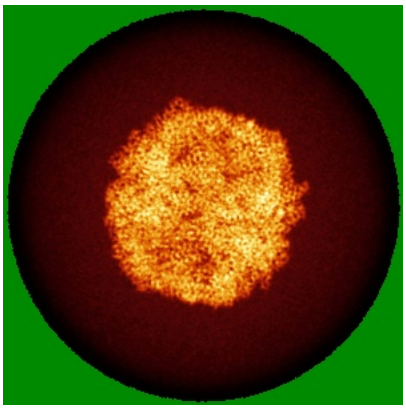


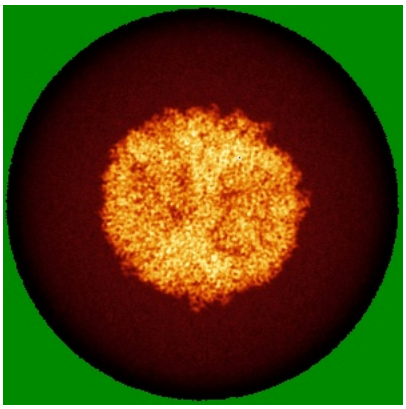
Z Index: 143

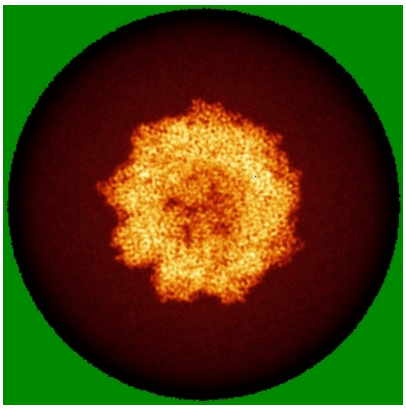
The images above show the largest variance slices of the map in three orthogonal directions.

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

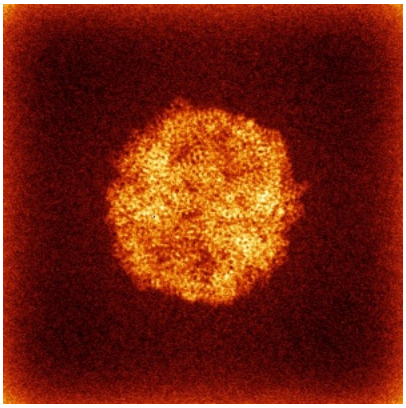
6.4.1 Primary map

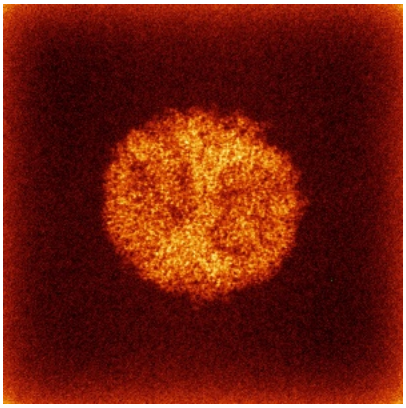

X

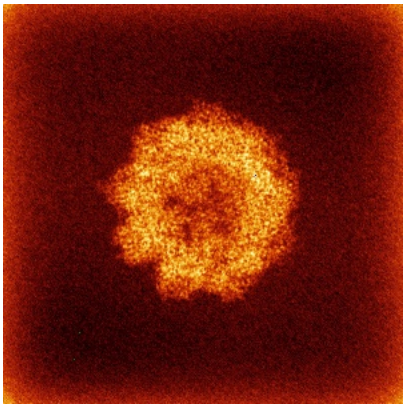

Y


Z

6.4.2 Raw map


X

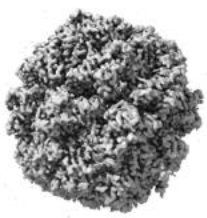

Y


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



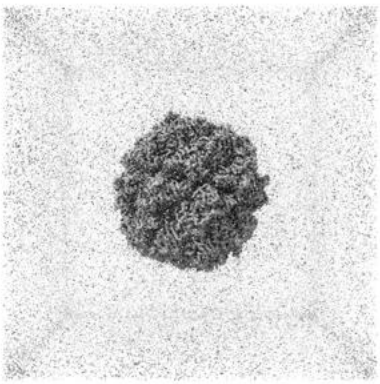
X

Y

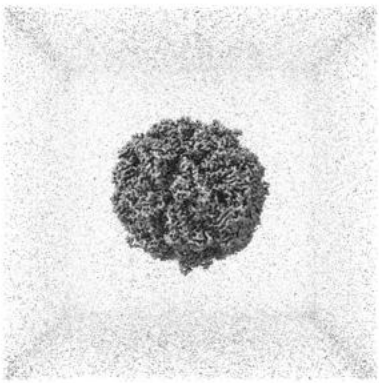
Z

The images above show the 3D surface view of the map at the recommended contour level 0.129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

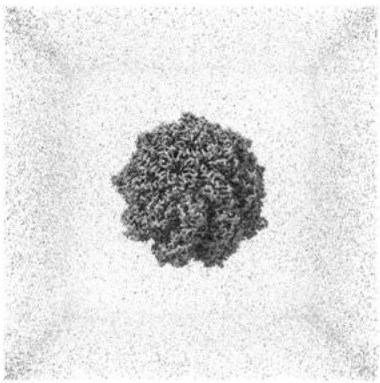
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

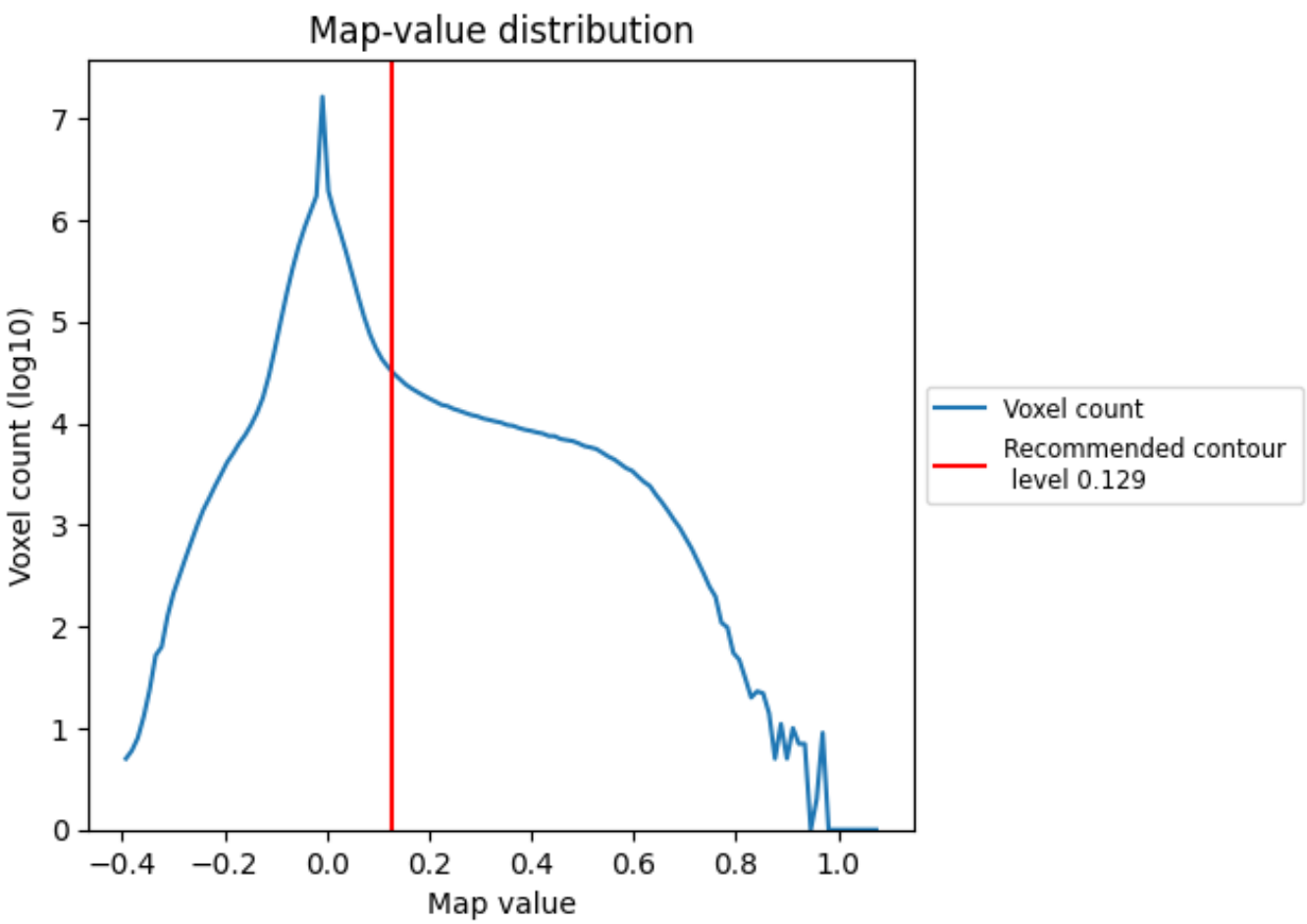
6.6 Mask visualisation (i)

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

7 Map analysis (i)

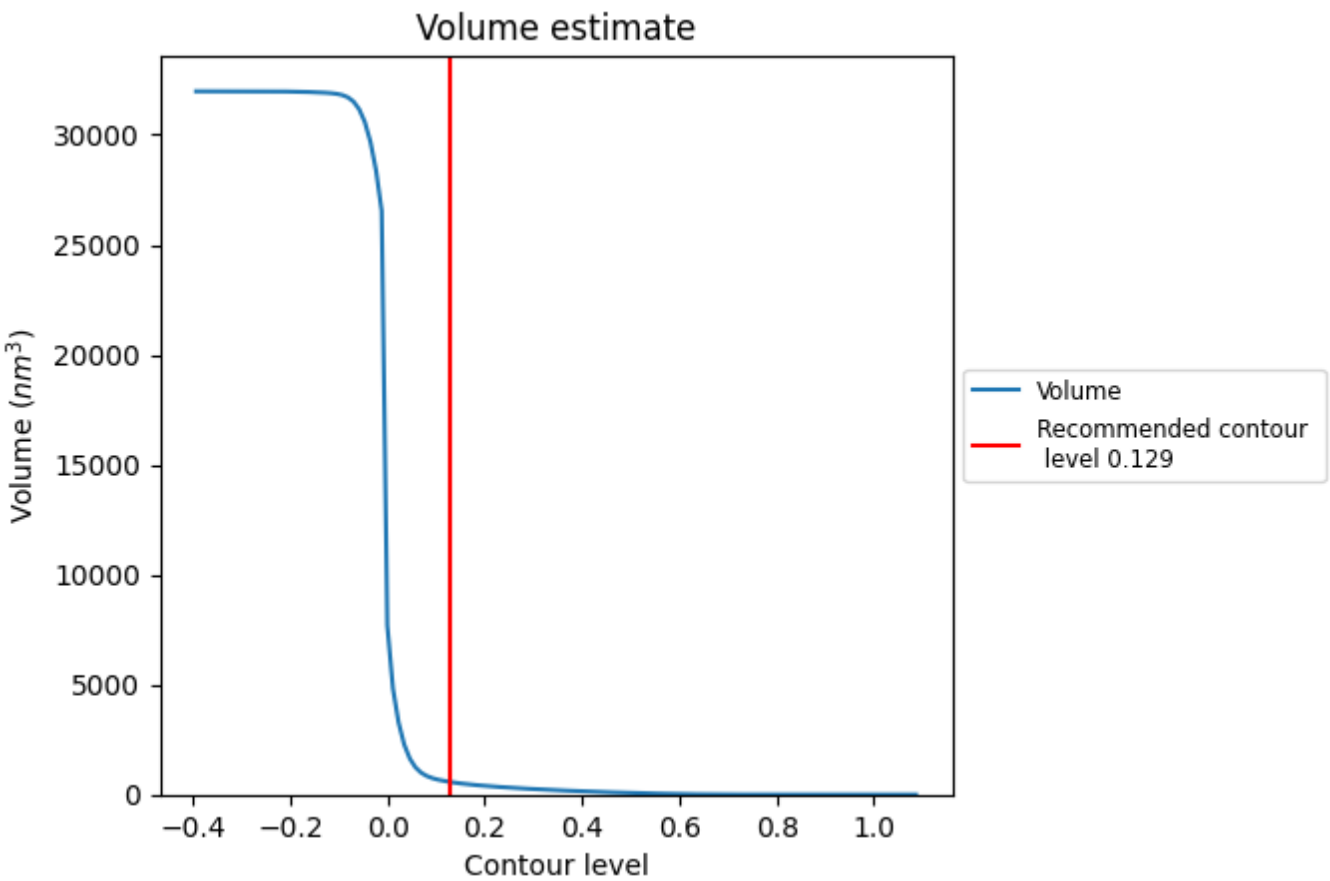
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

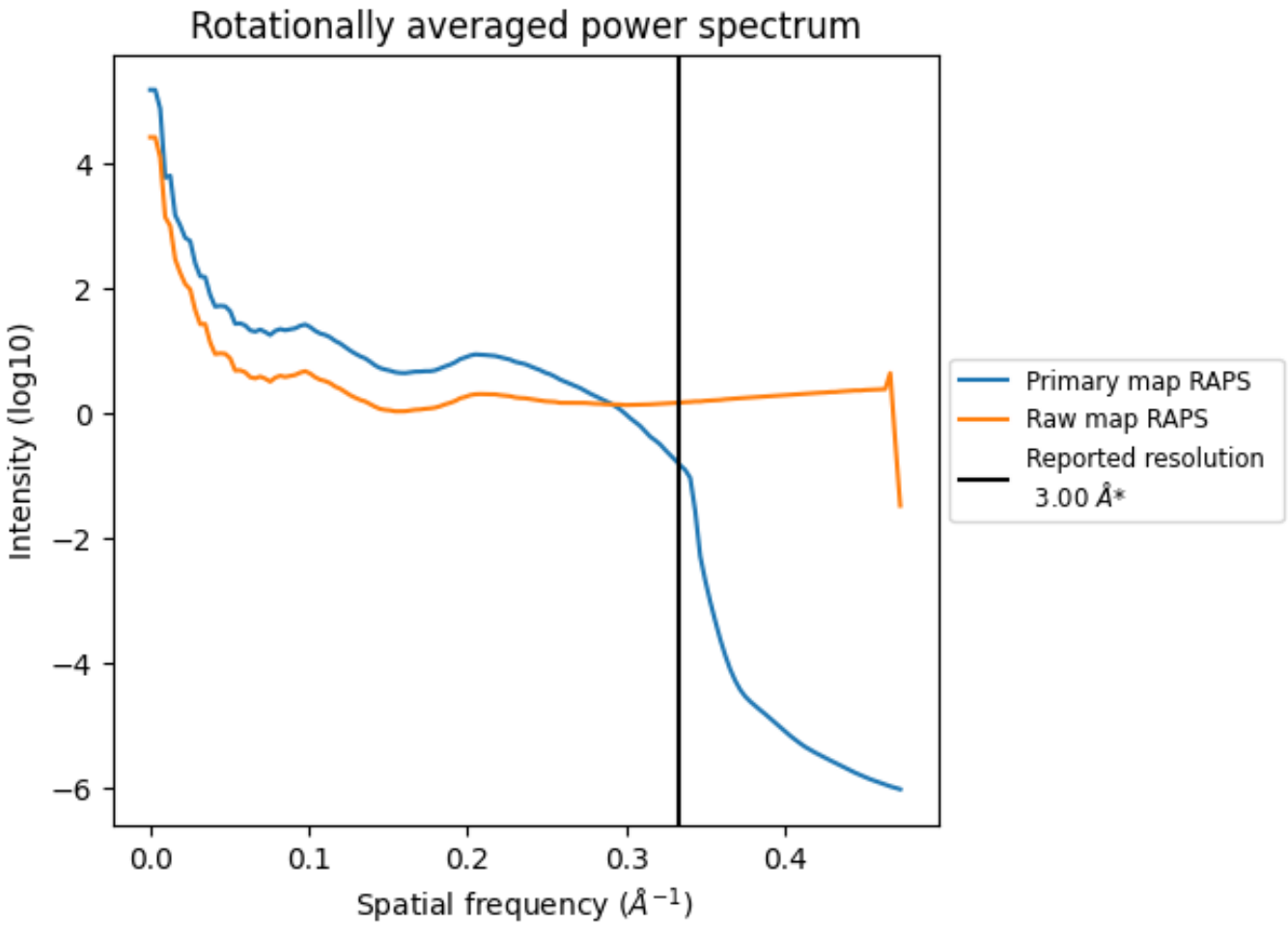
7.2 Volume estimate (i)



The volume at the recommended contour level is 572 nm^3; this corresponds to an approximate mass of 516 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)

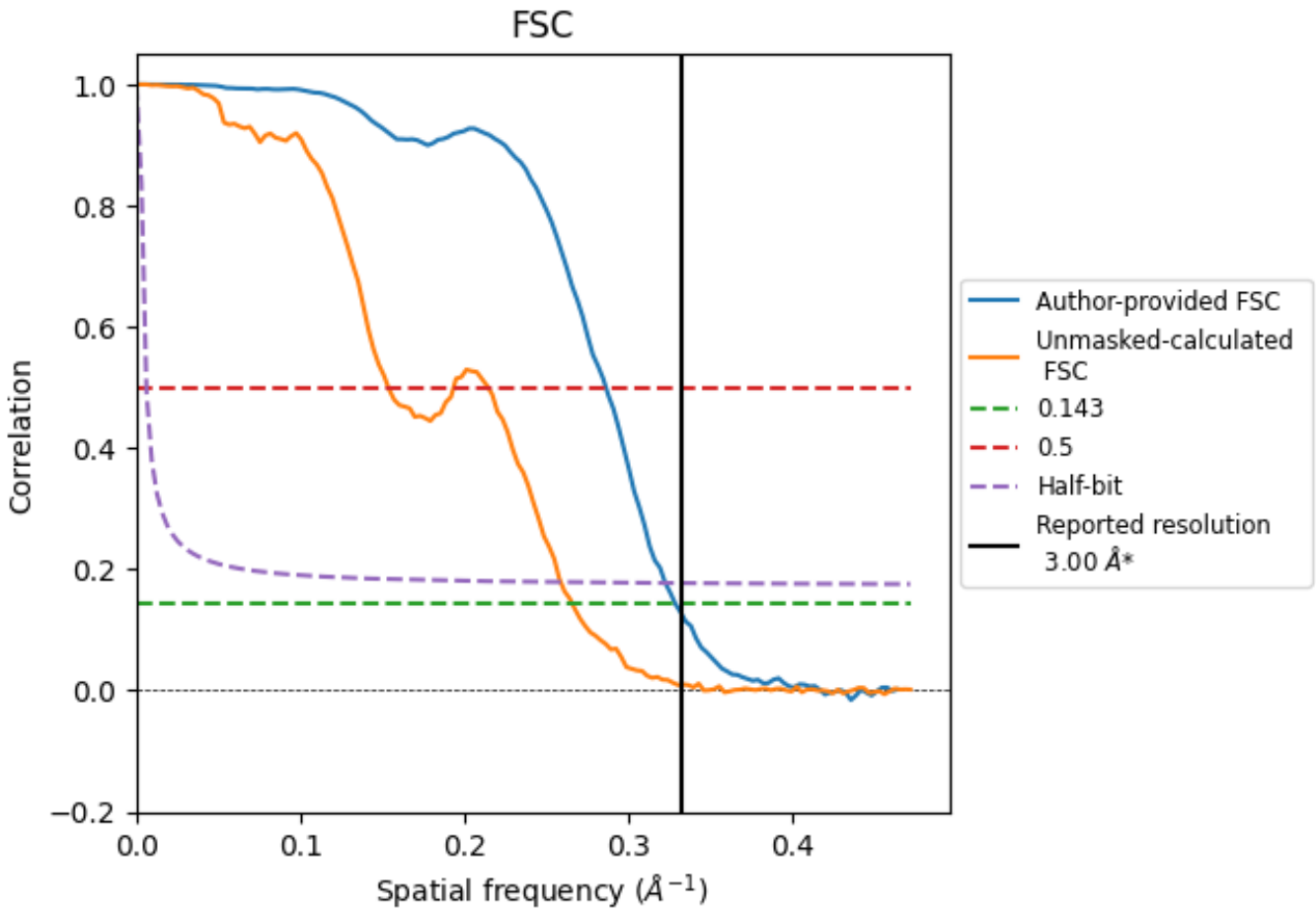


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

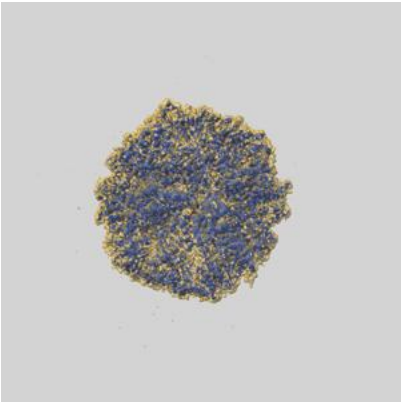
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.49	3.10
Unmasked-calculated*	3.76	6.50	3.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.0 by more than 10 %

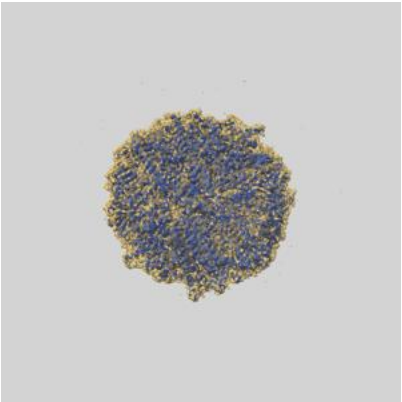
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40494 and PDB model 8SHT. Per-residue inclusion information can be found in section 3 on page 10.

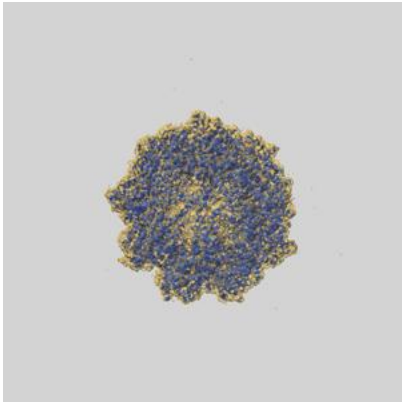
9.1 Map-model overlay (i)



X



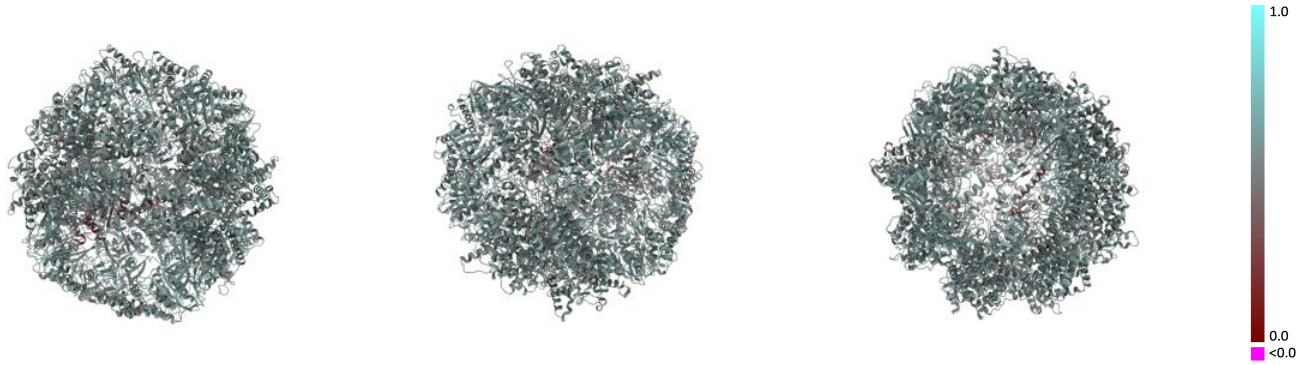
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.129 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.

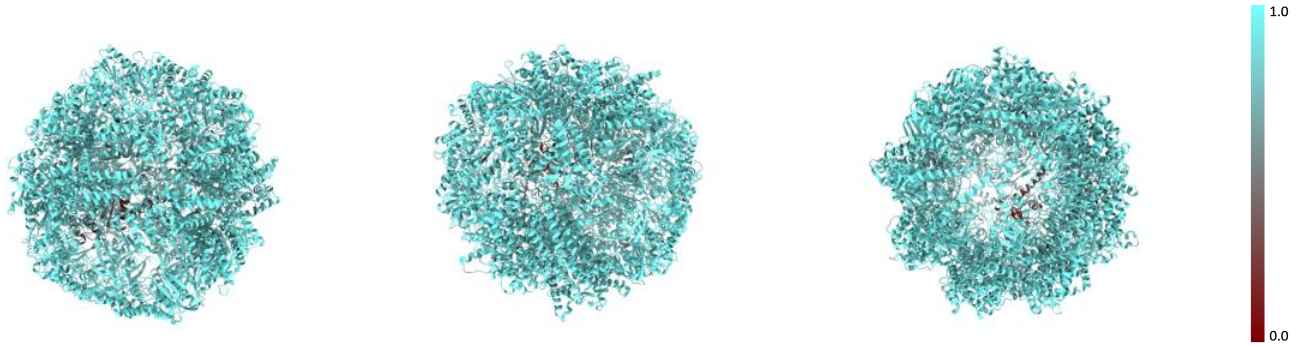
9.2 Q-score mapped to coordinate model (i)



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.

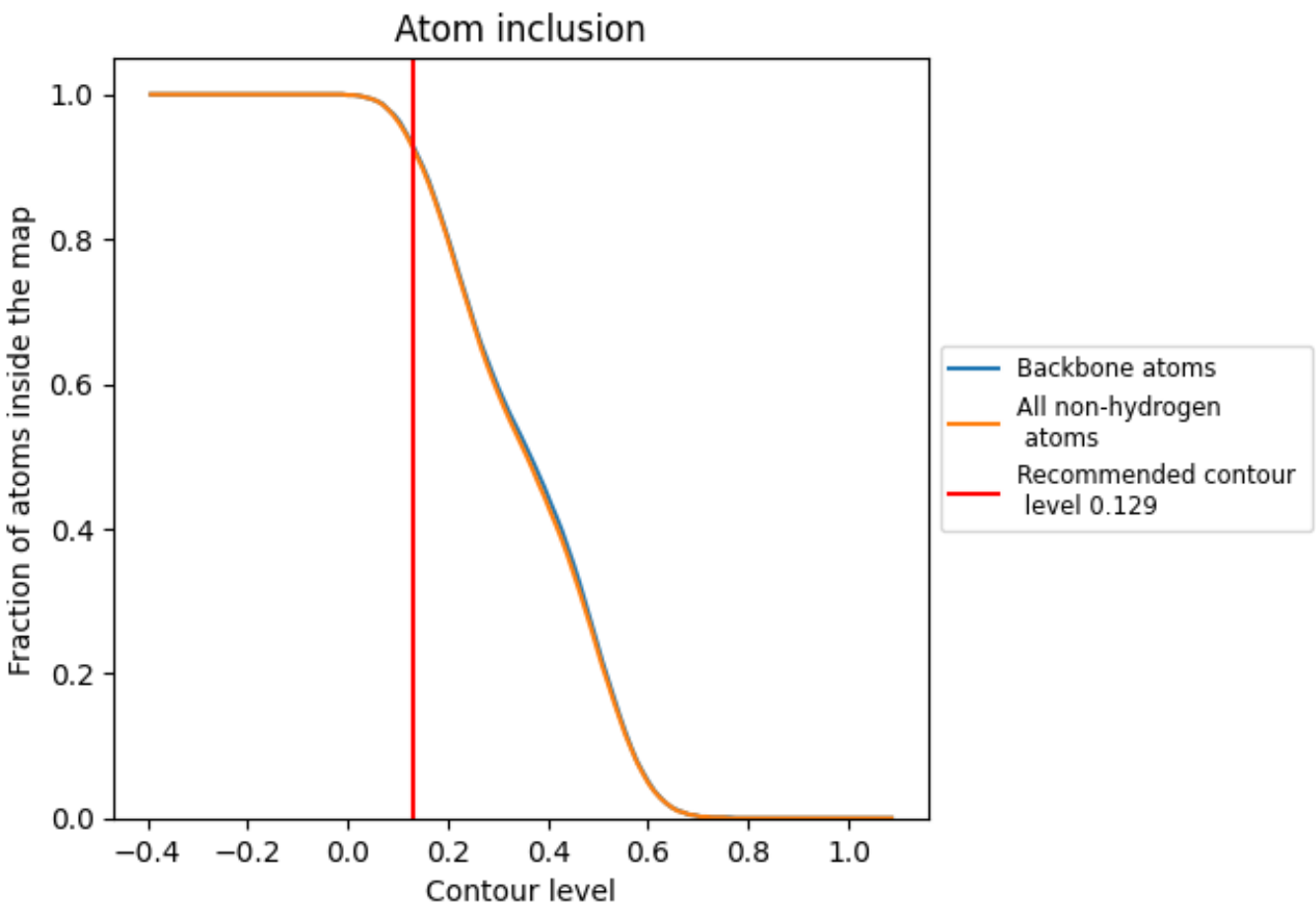
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.129).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.5420
A	0.9420	0.5480
B	0.9500	0.5560
D	0.9500	0.5500
E	0.9410	0.5500
G	0.9430	0.5520
H	0.9470	0.5520
N	0.7870	0.4130
P	0.4160	0.3330
Q	0.9350	0.5460
Z	0.9460	0.5480
a	0.9450	0.5470
b	0.9540	0.5560
d	0.9470	0.5490
e	0.9380	0.5490
g	0.9490	0.5530
h	0.9470	0.5550
q	0.9450	0.5480
z	0.9420	0.5490