



wwPDB EM Validation Summary Report ⓘ

Nov 17, 2025 – 02:29 PM EST

PDB ID : 9YX5 / pdb_00009yx5
EMDB ID : EMD-73596
Title : Structure of the long chain acyl-CoA carboxylase complex from Mycobacterium smegmatis with MSMEG_0435-MSMEG_0436 bound
Authors : Liang, Y.; Rubinstein, J.L.
Deposited on : 2025-10-26
Resolution : 2.90 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:

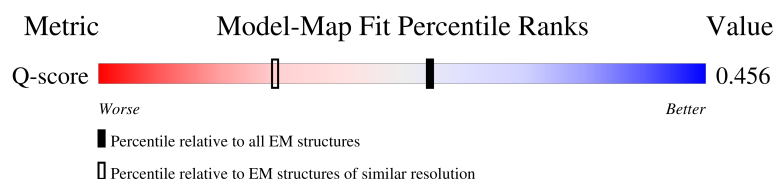
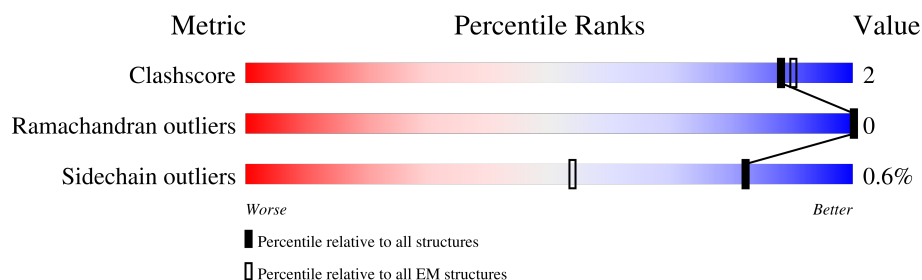
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

1 Overall quality at a glance

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

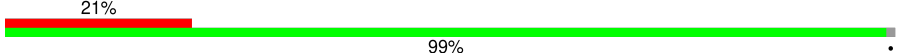
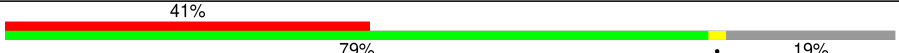


The reported resolution of this entry is 2.90 Å.

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.


















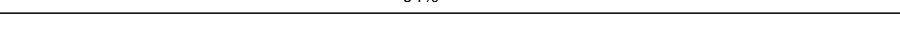
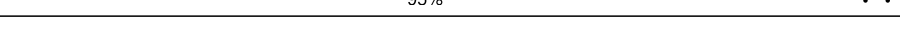
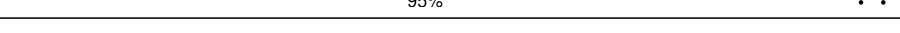
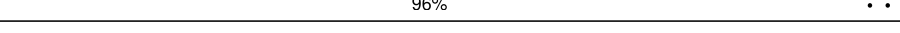
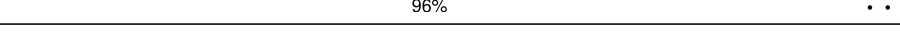
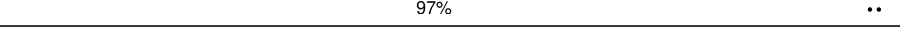
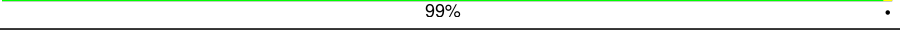
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13054 (2.40 - 3.40)

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 $\leq 5\%$. 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	598	
1	B	598	
1	C	598	
1	D	598	

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Mol	Chain	Length	Quality of chain
1	I	598	
1	J	598	
1	K	598	
1	L	598	
1	Q	598	
1	R	598	
1	S	598	
1	T	598	
1	U	598	
1	X	598	
2	E	94	
2	P	94	
3	F	517	
3	O	517	
4	G	542	
4	H	542	
4	M	542	
4	N	542	
5	V	294	
5	Y	294	
6	W	210	
6	Z	210	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 56321 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 Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	592	Total	C	N	O		0	0
			2894	1710	592	592			
1	I	68	Total	C	N	O	S	0	0
			409	253	73	80	3		
1	J	69	Total	C	N	O	S	0	0
			370	227	72	70	1		
1	K	69	Total	C	N	O	S	0	0
			423	263	76	81	3		
1	L	69	Total	C	N	O	S	0	0
			394	247	74	72	1		
1	Q	592	Total	C	N	O	S	0	0
			3932	2476	730	719	7		
1	X	64	Total	C	N	O	S	0	0
			370	228	67	72	3		
1	U	64	Total	C	N	O	S	0	0
			370	228	67	72	3		
1	B	482	Total	C	N	O		0	0
			2364	1400	482	482			
1	C	482	Total	C	N	O		0	0
			2364	1400	482	482			
1	D	481	Total	C	N	O		0	0
			2359	1397	481	481			
1	R	482	Total	C	N	O	S	0	0
			3656	2303	649	698	6		
1	S	482	Total	C	N	O		0	0
			2364	1400	482	482			
1	T	481	Total	C	N	O		0	0
			2359	1397	481	481			

- Molecule 2 is a protein called Acetyl-/propionyl-coenzyme A carboxylase AccE5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	69	Total	C	N	O	S	0	0
			473	294	97	80	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	70	Total	C	N	O	S	0	0
			510	319	103	85	3		

- Molecule 3 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	516	Total	C	N	O	S	0	0
			3775	2413	674	674	14		
3	O	516	Total	C	N	O	S	0	0
			3797	2424	676	682	15		

- Molecule 4 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	530	Total	C	N	O	S	0	0
			3877	2469	680	713	15		
4	H	538	Total	C	N	O	S	0	0
			3963	2517	694	738	14		
4	M	531	Total	C	N	O	S	0	0
			3887	2477	681	714	15		
4	N	539	Total	C	N	O	S	0	0
			3994	2532	696	752	14		

- Molecule 5 is a protein called Allophanate hydrolase subunit 2.

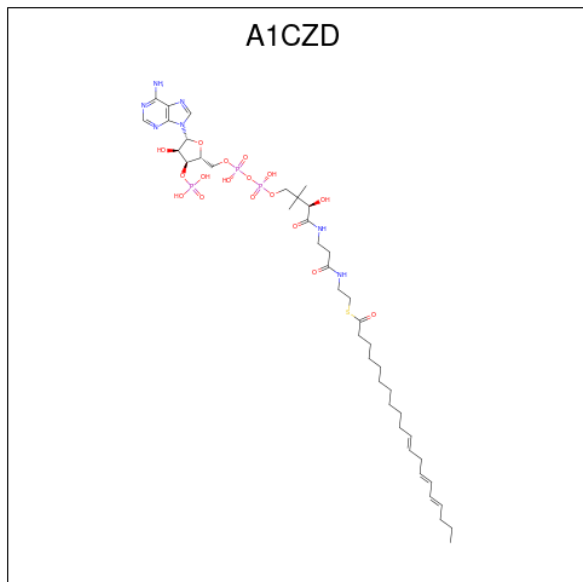
Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	290	Total	C	N	O	S	0	0
			2109	1329	392	384	4		
5	Y	290	Total	C	N	O	S	0	0
			2114	1331	392	387	4		

- Molecule 6 is a protein called Allophanate hydrolase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	210	Total	C	N	O	S	0	0
			1330	862	235	231	2		
6	Z	210	Total	C	N	O	S	0	0
			1371	875	251	243	2		

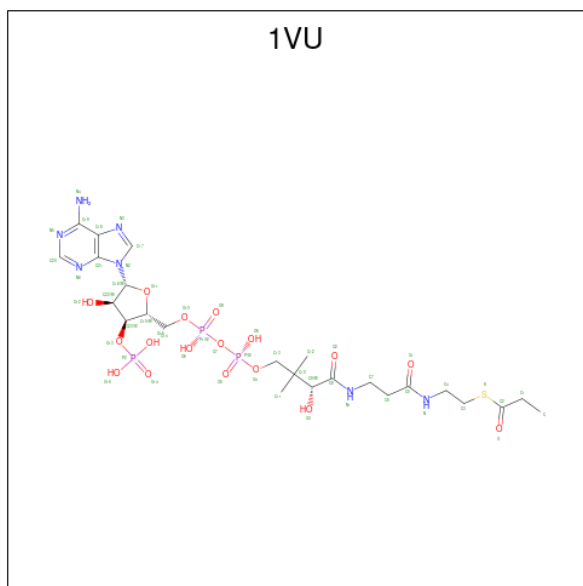
- Molecule 7 is S-{(3S,5S,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)oxolan-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5,10,14-tetraoxo-2,4,6-trioxa-11,15-diazia-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} (11E,14E,16E)-icosa-11,14,16-trie

nethioate (non-preferred name) (CCD ID: A1CZD) (formula: $C_{41}H_{68}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



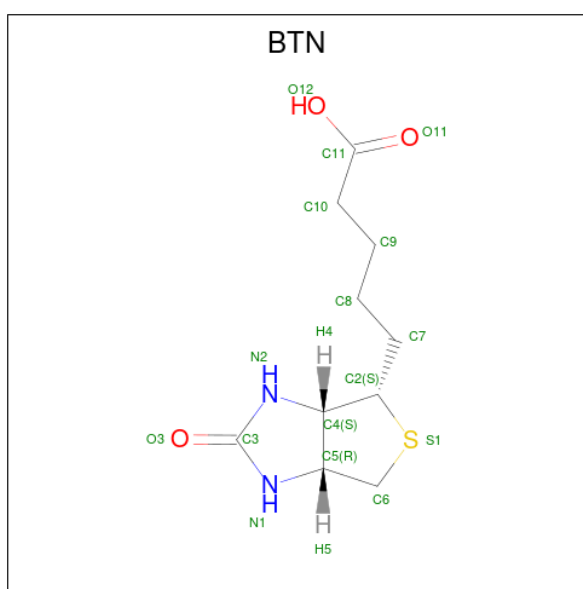
Mol	Chain	Residues	Atoms						AltConf
7	F	1	Total	C	N	O	P	S	0
			69	41	7	17	3	1	
7	O	1	Total	C	N	O	P	S	0
			69	41	7	17	3	1	

- Molecule 8 is propionyl Coenzyme A (CCD ID: 1VU) (formula: $C_{24}H_{40}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



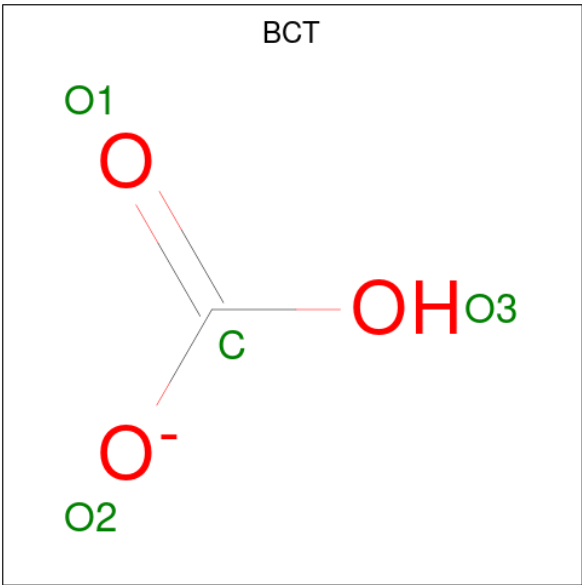
Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	C	N	O	P	S
			52	24	7	17	3	1
8	H	1	Total	C	N	O	P	S
			52	24	7	17	3	1
8	M	1	Total	C	N	O	P	S
			52	24	7	17	3	1
8	N	1	Total	C	N	O	P	S
			52	24	7	17	3	1

- Molecule 9 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



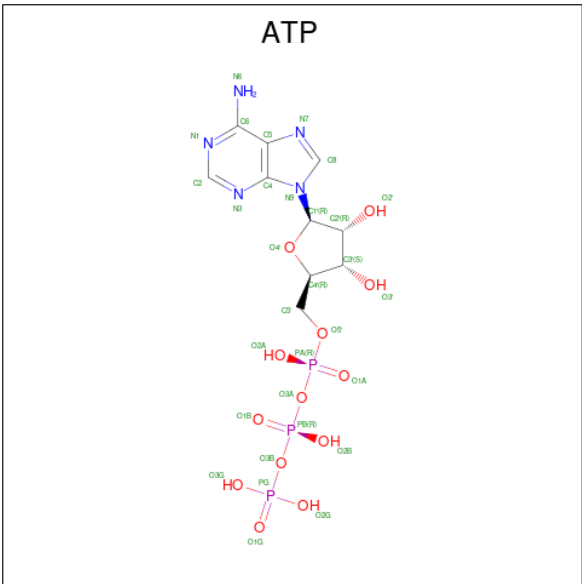
Mol	Chain	Residues	Atoms					AltConf
9	I	1	Total	C	N	O	S	0
			15	10	2	2	1	
9	K	1	Total	C	N	O	S	0
			15	10	2	2	1	
9	Q	1	Total	C	N	O	S	0
			15	10	2	2	1	
9	X	1	Total	C	N	O	S	0
			15	10	2	2	1	
9	U	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 10 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	Q	1	Total	C	O	0
			4	1	3	
10	R	1	Total	C	O	0
			4	1	3	

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	

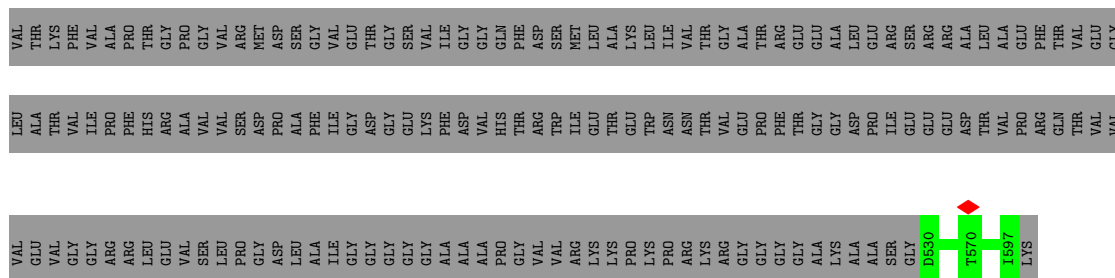
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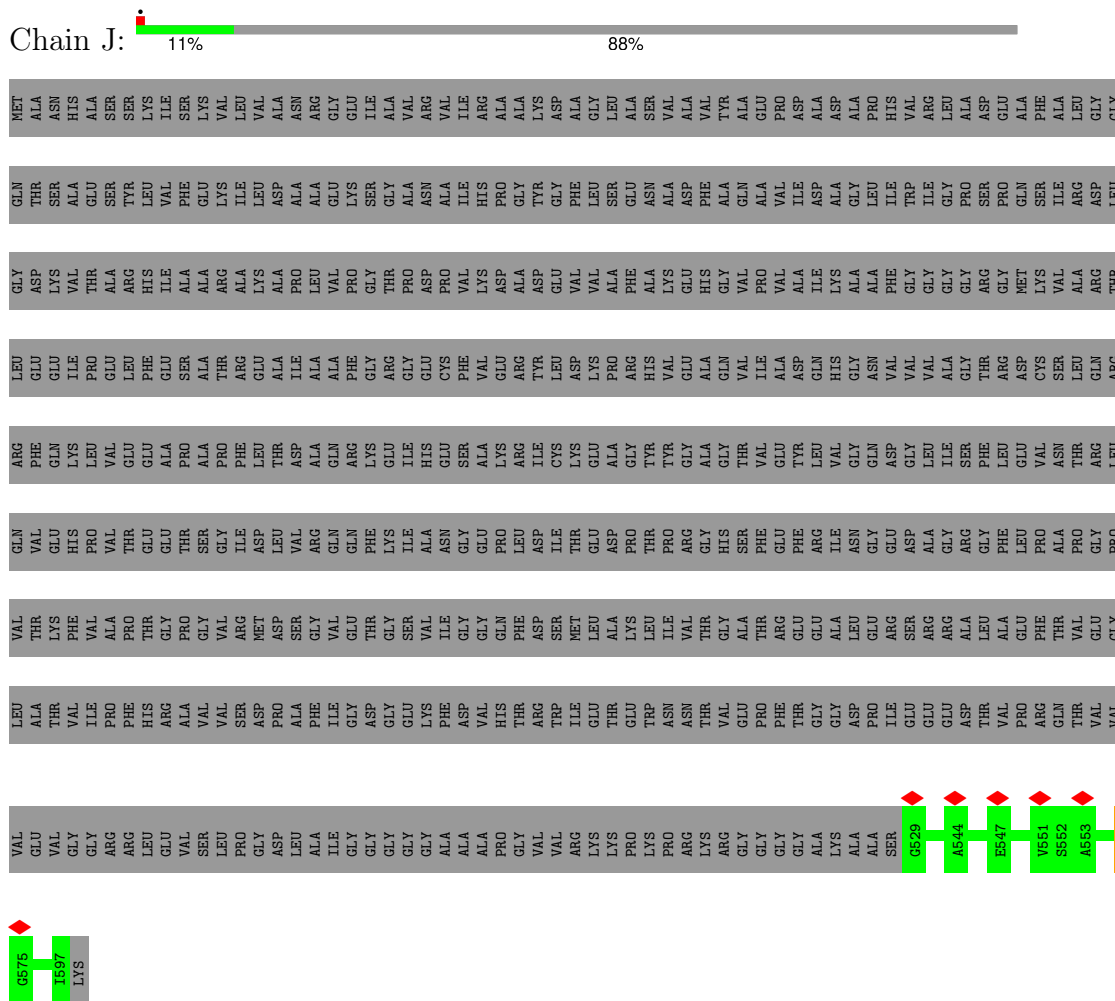
Mol	Chain	Residues	Atoms					AltConf
11	R	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

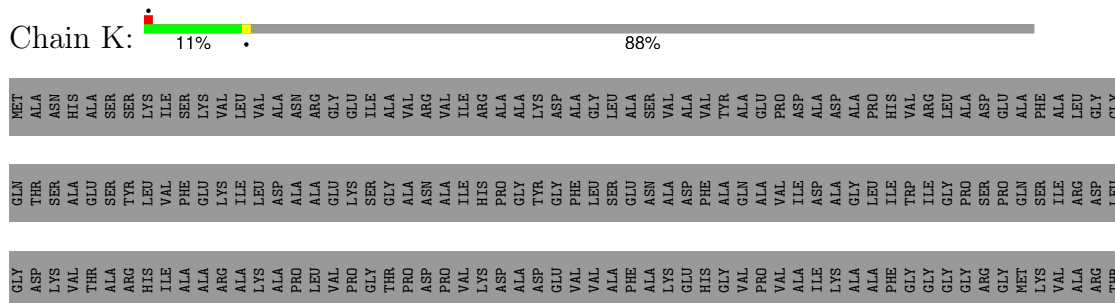
Mol	Chain	Residues	Atoms		AltConf
12	Q	1	Total	Mg	0
			1	1	
12	R	1	Total	Mg	0
			1	1	

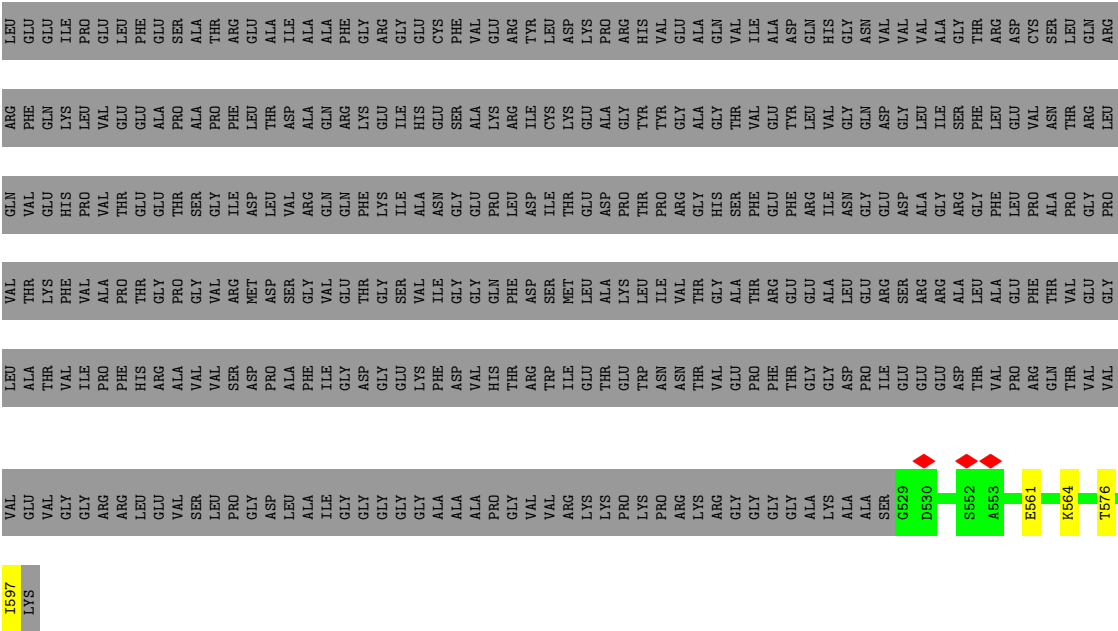


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

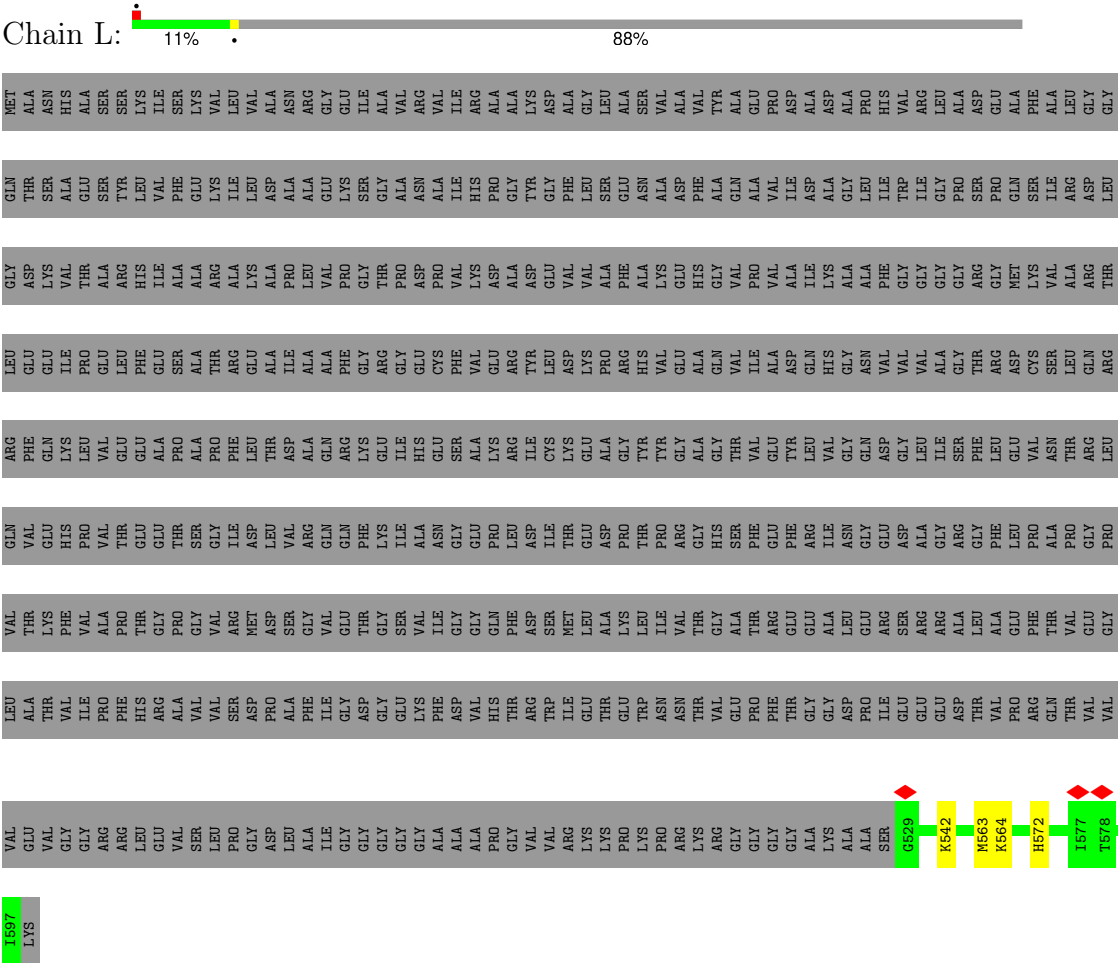


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



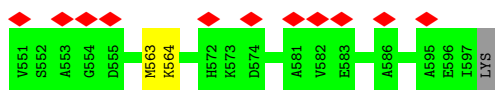


● Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

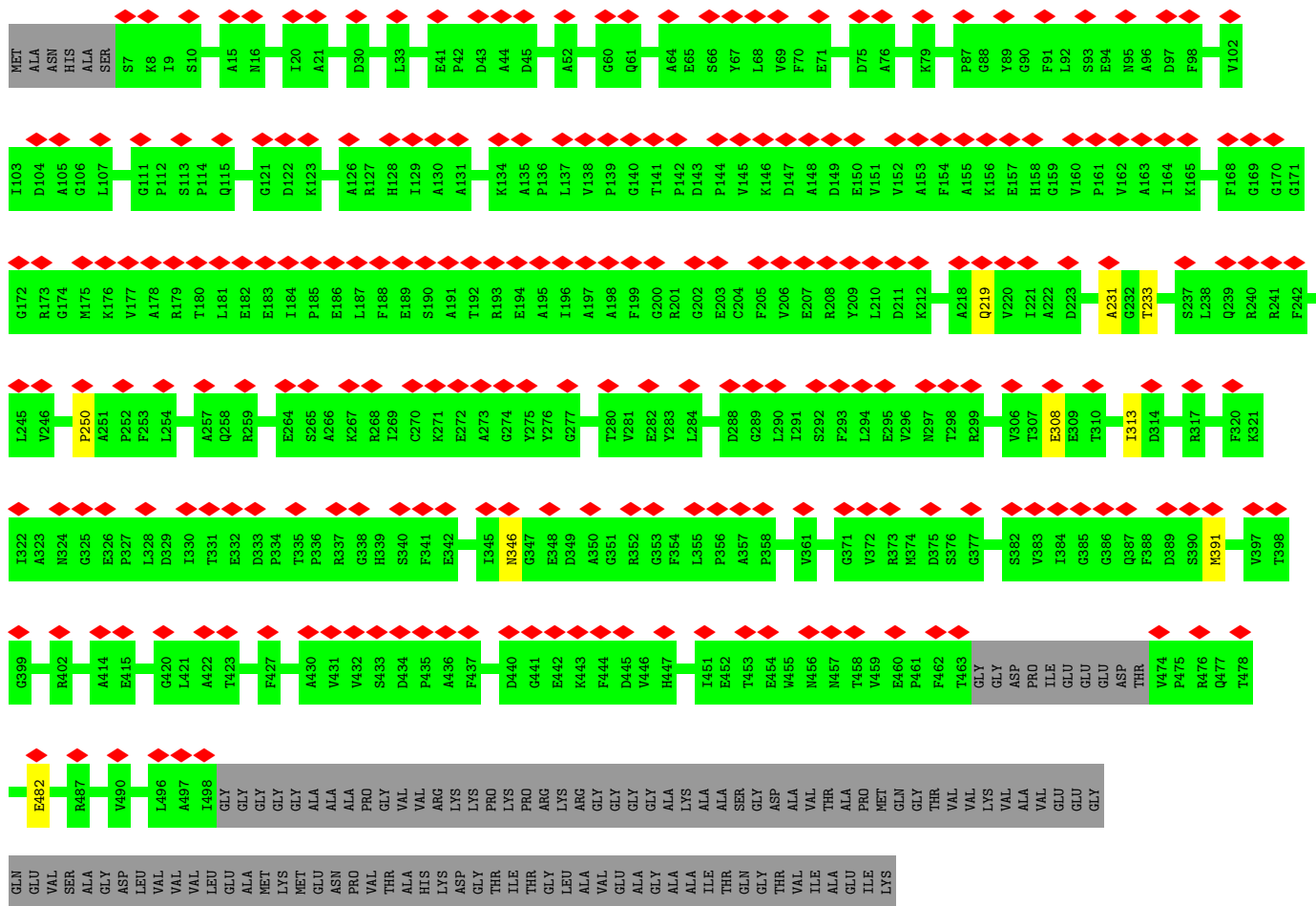


● Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

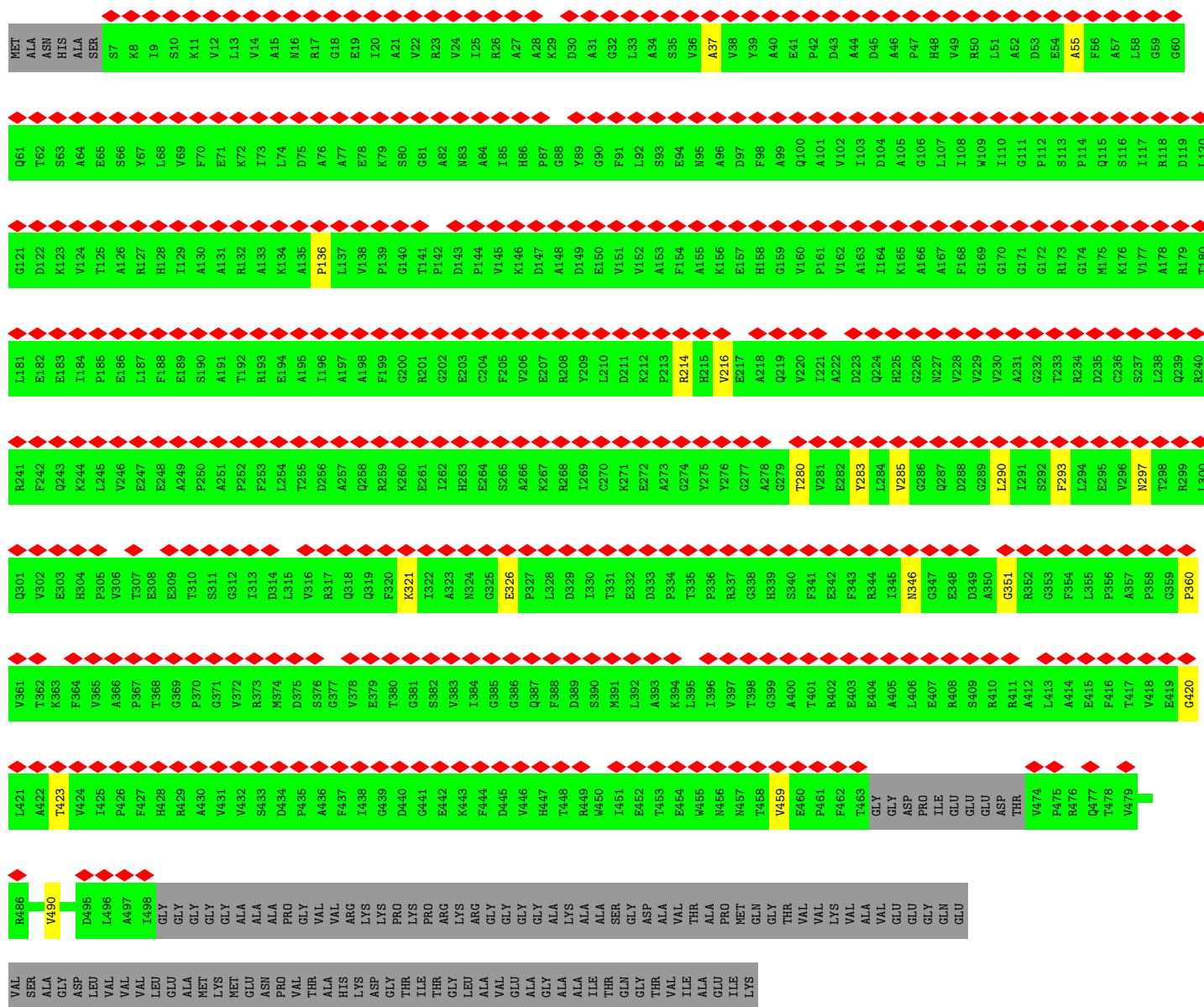
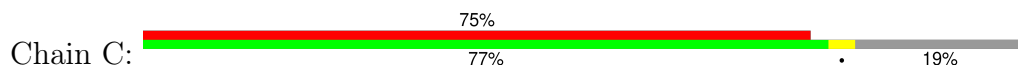


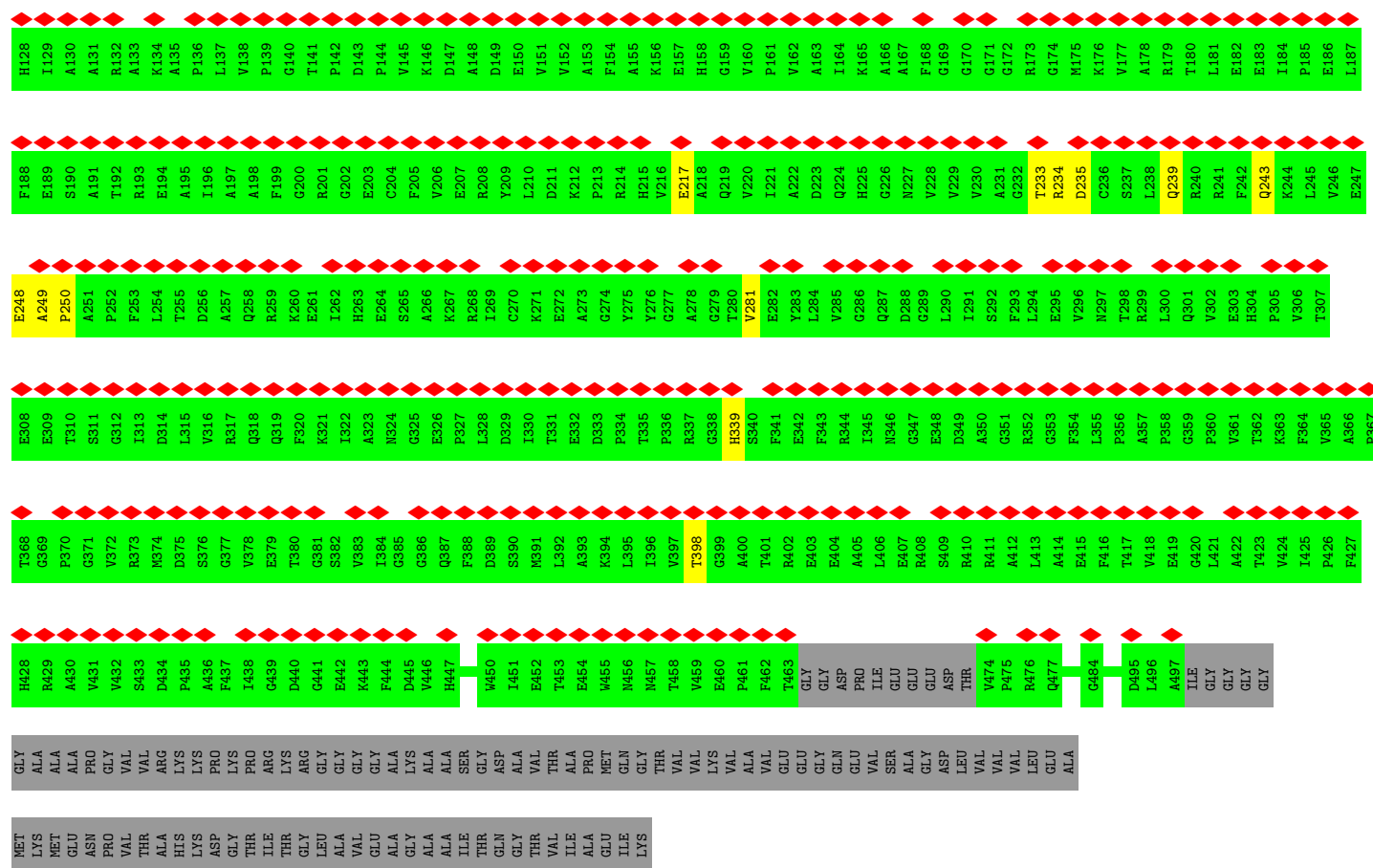


Chain B:

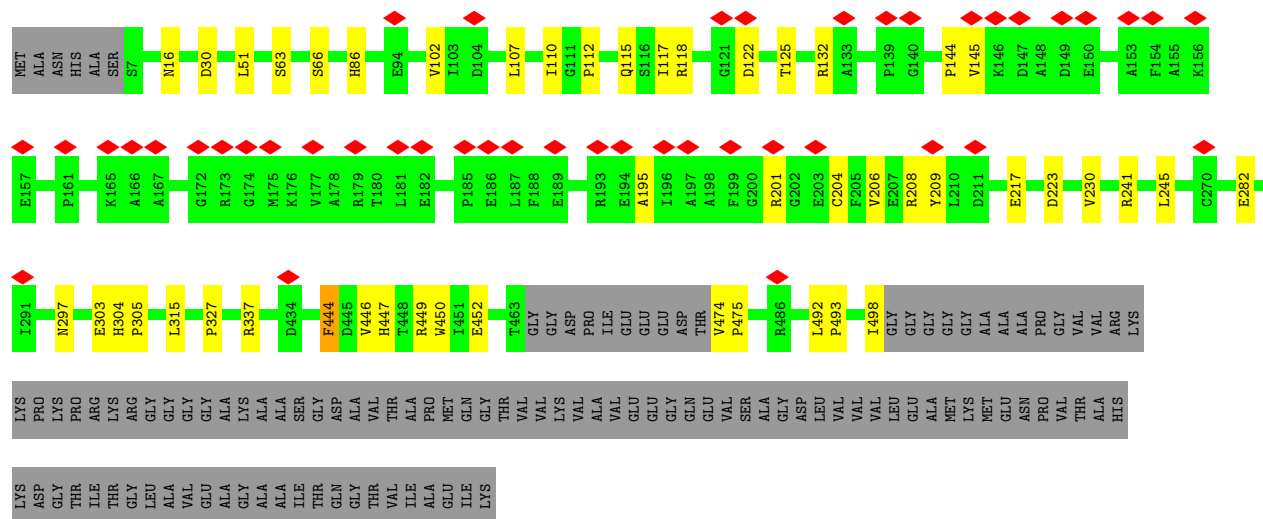
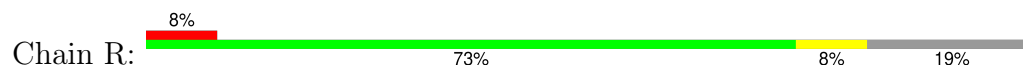


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

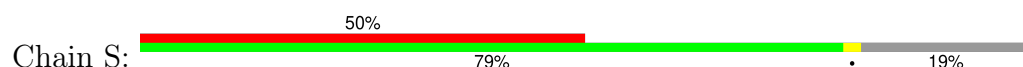


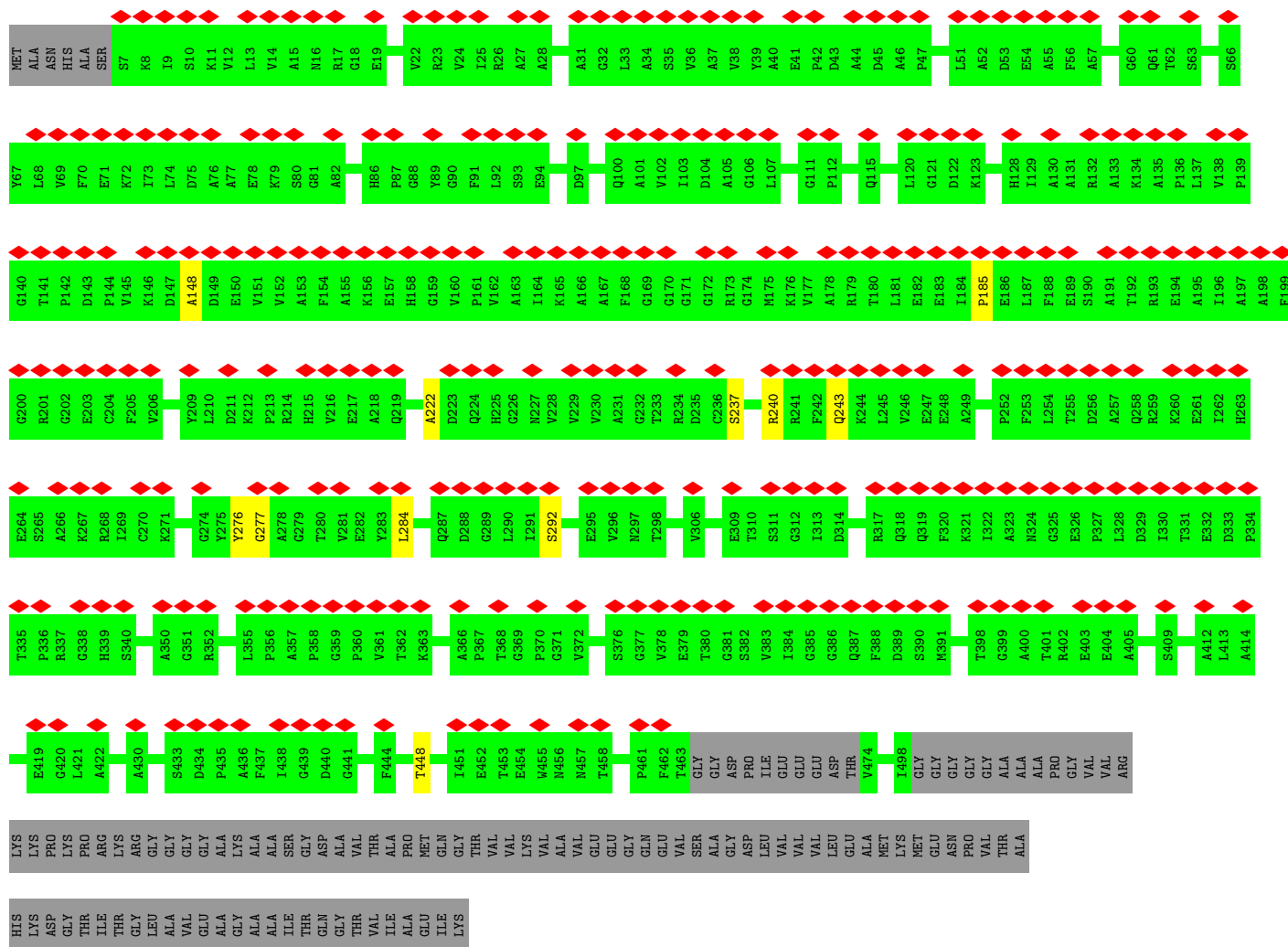


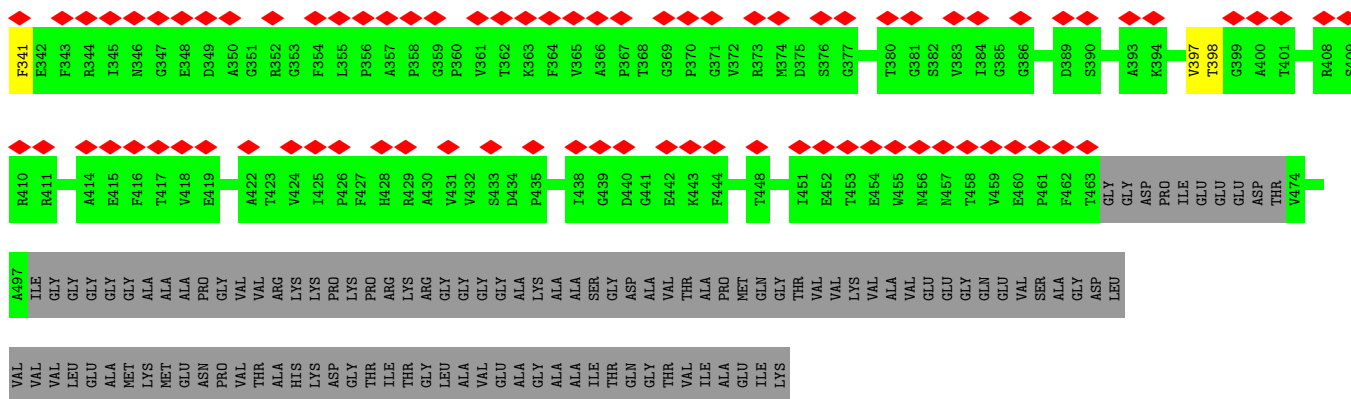
• Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



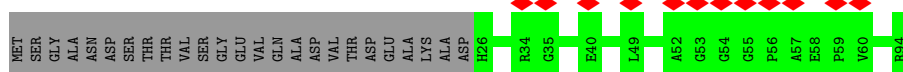
• Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



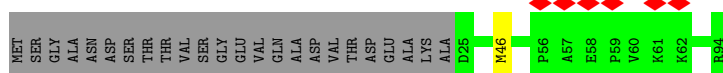




- Molecule 2: Acetyl-/propionyl-coenzyme A carboxylase AccE5



- Molecule 2: Acetyl-/propionyl-coenzyme A carboxylase AccE5



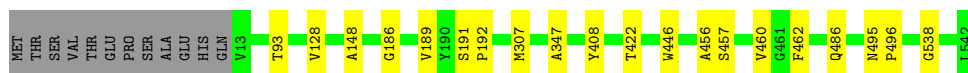
- Molecule 3: Propionyl-CoA carboxylase beta chain



- Molecule 3: Propionyl-CoA carboxylase beta chain



- Molecule 4: Propionyl-CoA carboxylase beta chain



- Molecule 4: Propionyl-CoA carboxylase beta chain

Chain H:  95%



- Molecule 4: Propionyl-CoA carboxylase beta chain

Chain M:  95%



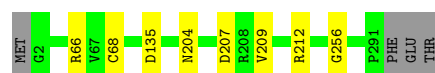
- Molecule 4: Propionyl-CoA carboxylase beta chain

Chain N:  96%



- Molecule 5: Allophanate hydrolase subunit 2

Chain V:  96%



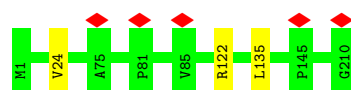
- Molecule 5: Allophanate hydrolase subunit 2

Chain Y:  97%



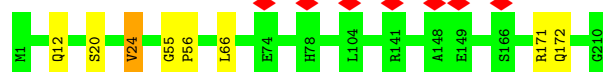
- Molecule 6: Allophanate hydrolase subunit 1

Chain W:  99%



- Molecule 6: Allophanate hydrolase subunit 1

Chain Z:  96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10016	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.983	Depositor
Minimum map value	-0.558	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	446.4, 446.4, 446.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.93, 0.93, 0.93	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, BTN, 1VU, ATP, BCT, A1CZD

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	0.18	0/2893	0.53	0/4009
1	B	0.24	0/2362	0.63	0/3276
1	C	0.32	0/2362	0.76	0/3276
1	D	0.30	0/2357	0.71	0/3269
1	I	0.14	0/411	0.40	0/564
1	J	0.19	0/371	0.46	0/511
1	K	0.14	0/425	0.37	0/582
1	L	0.21	0/396	0.49	0/546
1	Q	0.21	0/4003	0.49	0/5487
1	R	0.19	0/3729	0.51	0/5060
1	S	0.28	0/2362	0.70	0/3276
1	T	0.25	0/2357	0.68	0/3269
1	U	0.24	0/371	0.54	0/509
1	X	0.23	0/371	0.54	0/509
2	E	0.24	0/482	0.54	0/655
2	P	0.21	0/521	0.49	0/706
3	F	0.23	0/3856	0.48	0/5248
3	O	0.22	0/3878	0.47	0/5279
4	G	0.22	0/3953	0.47	0/5390
4	H	0.22	0/4041	0.46	0/5507
4	M	0.21	0/3963	0.45	0/5403
4	N	0.21	0/4072	0.46	0/5548
5	V	0.18	0/2162	0.42	0/2969
5	Y	0.18	0/2167	0.43	0/2975
6	W	0.20	0/1365	0.49	0/1897
6	Z	0.19	0/1403	0.48	0/1937
All	All	0.22	0/56633	0.53	0/77657

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
4	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	402	ARG	Sidechain

5.2 Too-close contacts

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	2894	0	1446	2	0
1	B	2364	0	1160	5	0
1	C	2364	0	1160	11	0
1	D	2359	0	1158	8	0
1	I	409	0	346	0	0
1	J	370	0	272	1	0
1	K	423	0	383	2	0
1	L	394	0	335	1	0
1	Q	3932	0	3592	15	0
1	R	3656	0	3622	31	0
1	S	2364	0	1160	8	0
1	T	2359	0	1158	11	0
1	U	370	0	309	5	0
1	X	370	0	309	1	0
2	E	473	0	401	0	0
2	P	510	0	465	1	0
3	F	3775	0	3698	8	0
3	O	3797	0	3731	14	0
4	G	3877	0	3817	11	0
4	H	3963	0	3898	14	0
4	M	3887	0	3832	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	3994	0	3935	10	0
5	V	2109	0	2072	9	0
5	Y	2114	0	2079	2	0
6	W	1330	0	1127	1	0
6	Z	1371	0	1183	4	0
7	F	69	0	0	2	0
7	O	69	0	0	1	0
8	G	52	0	38	2	0
8	H	52	0	38	5	0
8	M	52	0	38	5	0
8	N	52	0	38	5	0
9	I	15	0	15	0	0
9	K	15	0	15	0	0
9	Q	15	0	15	0	0
9	U	15	0	15	2	0
9	X	15	0	15	1	0
10	Q	4	0	1	0	0
10	R	4	0	1	0	0
11	Q	31	0	12	0	0
11	R	31	0	12	1	0
12	Q	1	0	0	0	0
12	R	1	0	0	0	0
All	All	56321	0	46901	181	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 181 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)
5:V:207:ASP:OD2	1:U:564:LYS:HD3	1.25	1.23
5:V:207:ASP:OD2	1:U:564:LYS:CD	1.88	1.21
5:V:204:ASN:OD1	1:U:537:GLN:NE2	1.91	1.02
6:Z:12:GLN:HE21	6:Z:55:GLY:HA2	1.24	1.02
5:V:212:ARG:NH1	9:U:601:BTN:O11	2.01	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	590/598 (99%)	570 (97%)	20 (3%)	0	100	100
1	B	478/598 (80%)	445 (93%)	33 (7%)	0	100	100
1	C	478/598 (80%)	450 (94%)	28 (6%)	0	100	100
1	D	477/598 (80%)	459 (96%)	18 (4%)	0	100	100
1	I	66/598 (11%)	64 (97%)	2 (3%)	0	100	100
1	J	67/598 (11%)	66 (98%)	1 (2%)	0	100	100
1	K	67/598 (11%)	66 (98%)	1 (2%)	0	100	100
1	L	67/598 (11%)	66 (98%)	1 (2%)	0	100	100
1	Q	590/598 (99%)	559 (95%)	31 (5%)	0	100	100
1	R	478/598 (80%)	455 (95%)	23 (5%)	0	100	100
1	S	478/598 (80%)	458 (96%)	20 (4%)	0	100	100
1	T	477/598 (80%)	450 (94%)	27 (6%)	0	100	100
1	U	62/598 (10%)	59 (95%)	3 (5%)	0	100	100
1	X	62/598 (10%)	59 (95%)	3 (5%)	0	100	100
2	E	67/94 (71%)	62 (92%)	5 (8%)	0	100	100
2	P	68/94 (72%)	61 (90%)	7 (10%)	0	100	100
3	F	514/517 (99%)	500 (97%)	14 (3%)	0	100	100
3	O	514/517 (99%)	498 (97%)	16 (3%)	0	100	100
4	G	528/542 (97%)	511 (97%)	17 (3%)	0	100	100
4	H	536/542 (99%)	520 (97%)	16 (3%)	0	100	100
4	M	529/542 (98%)	513 (97%)	16 (3%)	0	100	100
4	N	537/542 (99%)	520 (97%)	17 (3%)	0	100	100
5	V	288/294 (98%)	281 (98%)	7 (2%)	0	100	100
5	Y	288/294 (98%)	278 (96%)	10 (4%)	0	100	100
6	W	208/210 (99%)	200 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Z	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
All	All	8722/12770 (68%)	8371 (96%)	351 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	I	27/453 (6%)	27 (100%)	0	100	100
1	J	13/453 (3%)	12 (92%)	1 (8%)	10	31
1	K	31/453 (7%)	31 (100%)	0	100	100
1	L	22/453 (5%)	20 (91%)	2 (9%)	7	25
1	Q	315/453 (70%)	313 (99%)	2 (1%)	84	95
1	R	376/453 (83%)	371 (99%)	5 (1%)	65	88
1	U	22/453 (5%)	21 (96%)	1 (4%)	23	56
1	X	22/453 (5%)	21 (96%)	1 (4%)	23	56
2	E	33/76 (43%)	33 (100%)	0	100	100
2	P	42/76 (55%)	42 (100%)	0	100	100
3	F	361/412 (88%)	360 (100%)	1 (0%)	91	97
3	O	369/412 (90%)	367 (100%)	2 (0%)	86	96
4	G	384/436 (88%)	384 (100%)	0	100	100
4	H	397/436 (91%)	394 (99%)	3 (1%)	79	93
4	M	385/436 (88%)	385 (100%)	0	100	100
4	N	406/436 (93%)	405 (100%)	1 (0%)	92	98
5	V	217/237 (92%)	217 (100%)	0	100	100
5	Y	219/237 (92%)	217 (99%)	2 (1%)	75	92
6	W	89/164 (54%)	88 (99%)	1 (1%)	70	90
6	Z	99/164 (60%)	97 (98%)	2 (2%)	50	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3829/7146 (54%)	3805 (99%)	24 (1%)	82	95

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Y	136	VAL
6	Z	66	LEU
6	Z	24	VAL
1	U	546	GLU
1	L	572	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	O	150	HIS
5	V	97	HIS
5	V	93	ASN
6	W	59	GLN
4	H	487	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
8	1VU	M	601	-	48,54,54	0.65	0	60,80,80	0.99	2 (3%)
8	1VU	G	601	-	48,54,54	0.62	0	60,80,80	0.96	2 (3%)
8	1VU	N	601	-	48,54,54	0.63	0	60,80,80	0.98	2 (3%)
7	A1CZD	F	601	-	65,71,71	2.85	20 (30%)	77,97,97	1.85	17 (22%)
9	BTN	K	601	1	15,16,17	6.50	11 (73%)	20,21,23	2.71	7 (35%)
11	ATP	Q	603	12	28,33,33	0.70	0	34,52,52	0.95	2 (5%)
11	ATP	R	601	12	28,33,33	0.62	0	34,52,52	0.94	2 (5%)
9	BTN	U	601	1	15,16,17	6.51	11 (73%)	20,21,23	2.73	9 (45%)
9	BTN	Q	601	1	15,16,17	6.49	11 (73%)	20,21,23	2.76	9 (45%)
8	1VU	H	601	-	48,54,54	0.62	0	60,80,80	1.03	3 (5%)
9	BTN	I	601	1	15,16,17	6.49	11 (73%)	20,21,23	2.78	6 (30%)
10	BCT	R	603	-	3,3,3	1.05	0	2,3,3	3.99	2 (100%)
10	BCT	Q	602	-	3,3,3	1.05	0	2,3,3	4.04	1 (50%)
7	A1CZD	O	601	-	65,71,71	2.93	19 (29%)	77,97,97	1.76	16 (20%)
9	BTN	X	601	1	15,16,17	6.53	11 (73%)	20,21,23	2.73	9 (45%)

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
8	1VU	M	601	-	-	10/49/69/69	0/3/3/3
8	1VU	G	601	-	-	16/49/69/69	0/3/3/3
8	1VU	N	601	-	-	22/49/69/69	0/3/3/3
7	A1CZD	F	601	-	-	33/66/86/86	0/3/3/3
9	BTN	K	601	1	-	1/6/27/28	0/2/2/2
11	ATP	Q	603	12	-	2/18/38/38	0/3/3/3
11	ATP	R	601	12	-	6/18/38/38	0/3/3/3
9	BTN	U	601	1	-	1/6/27/28	0/2/2/2
9	BTN	Q	601	1	-	3/6/27/28	0/2/2/2
8	1VU	H	601	-	-	10/49/69/69	0/3/3/3
9	BTN	I	601	1	-	1/6/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	A1CZD	O	601	-	-	27/66/86/86	0/3/3/3
9	BTN	X	601	1	-	1/6/27/28	0/2/2/2

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	601	A1CZD	P65-O64	14.15	1.84	1.59
7	O	601	A1CZD	P65-O64	14.06	1.84	1.59
9	K	601	BTN	C6-S1	-13.33	1.44	1.81
9	I	601	BTN	C6-S1	-13.28	1.44	1.81
9	U	601	BTN	C6-S1	-13.24	1.44	1.81

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	601	A1CZD	C19-C20-S22	7.82	122.72	113.40
9	I	601	BTN	C6-S1-C2	7.72	106.03	89.98
9	K	601	BTN	C6-S1-C2	7.26	105.08	89.98
7	O	601	A1CZD	C19-C20-S22	7.01	121.75	113.40
9	Q	601	BTN	C6-S1-C2	6.58	103.66	89.98

There are no chirality outliers.

5 of 133 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	601	A1CZD	C17-C18-C19-C20
7	F	601	A1CZD	C33-C31-N30-C29
7	F	601	A1CZD	C31-C33-C34-C35
7	F	601	A1CZD	C31-C33-C34-C36
7	F	601	A1CZD	C31-C33-C34-C37

There are no ring outliers.

9 monomers are involved in 24 short contacts:

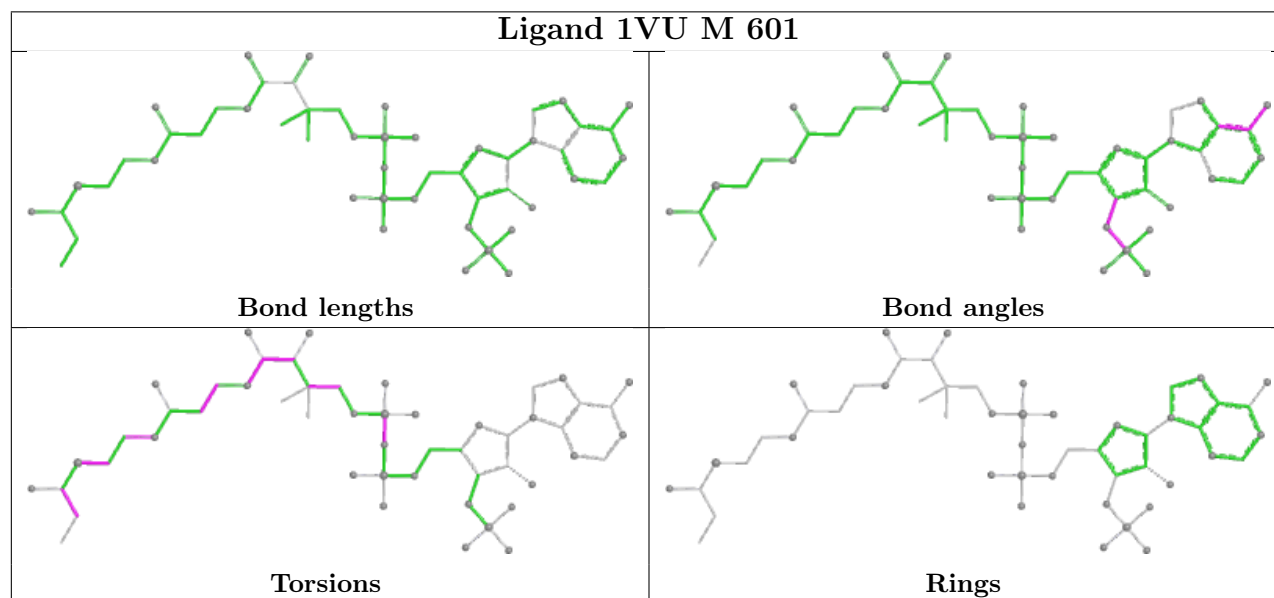
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	601	1VU	5	0
8	G	601	1VU	2	0
8	N	601	1VU	5	0
7	F	601	A1CZD	2	0
11	R	601	ATP	1	0
9	U	601	BTN	2	0

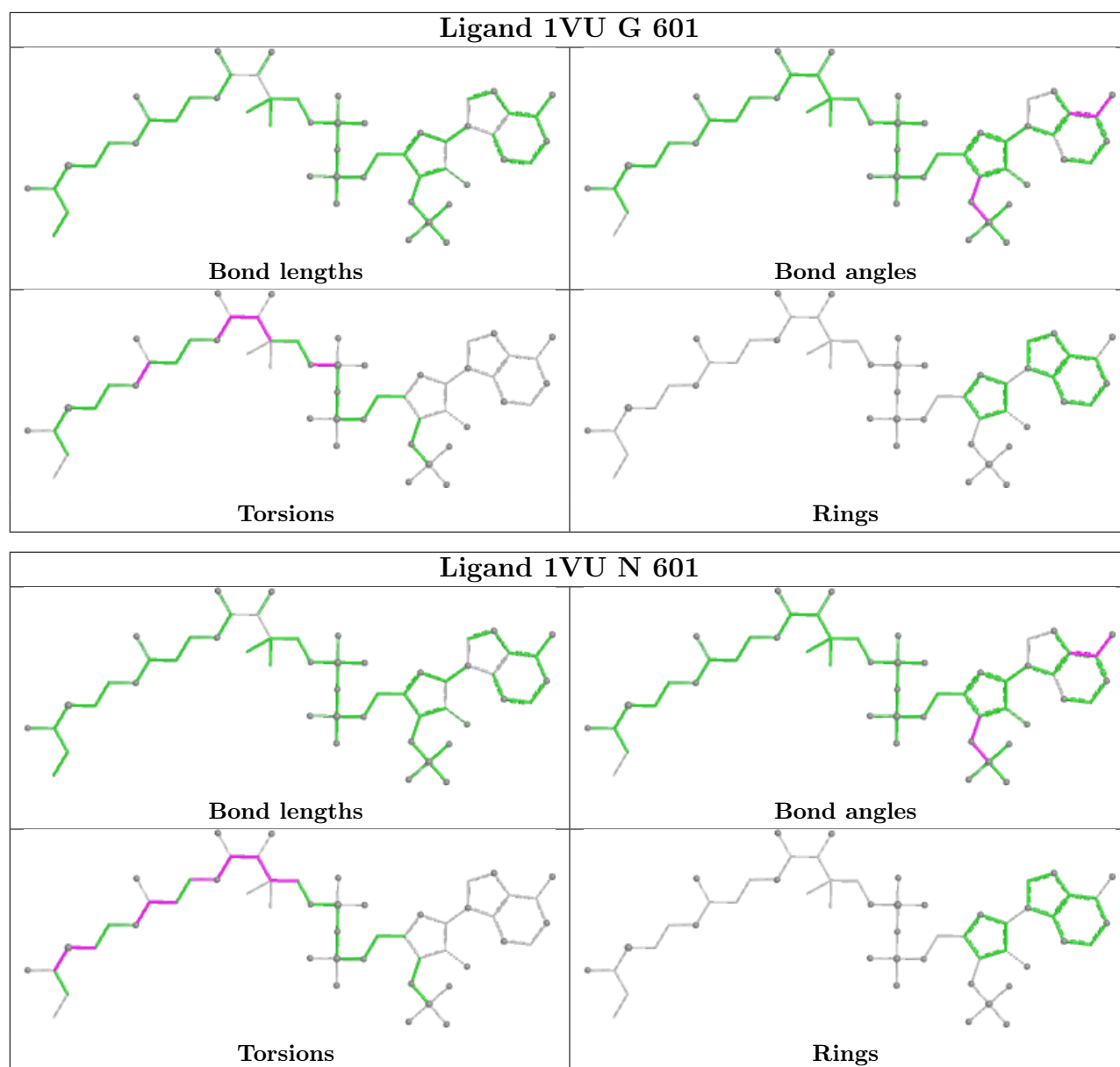
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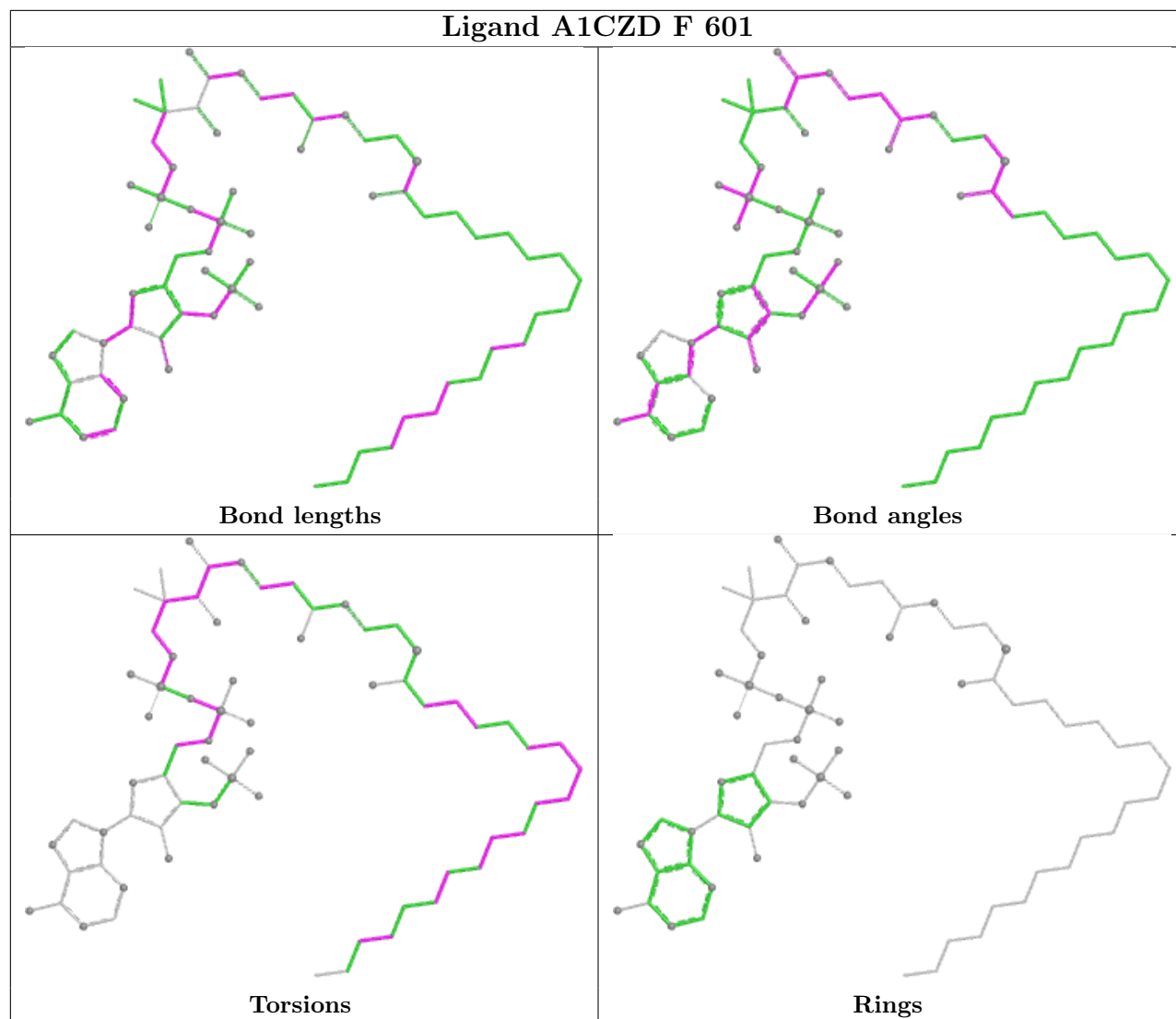
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	601	1VU	5	0
7	O	601	A1CZD	1	0
9	X	601	BTN	1	0

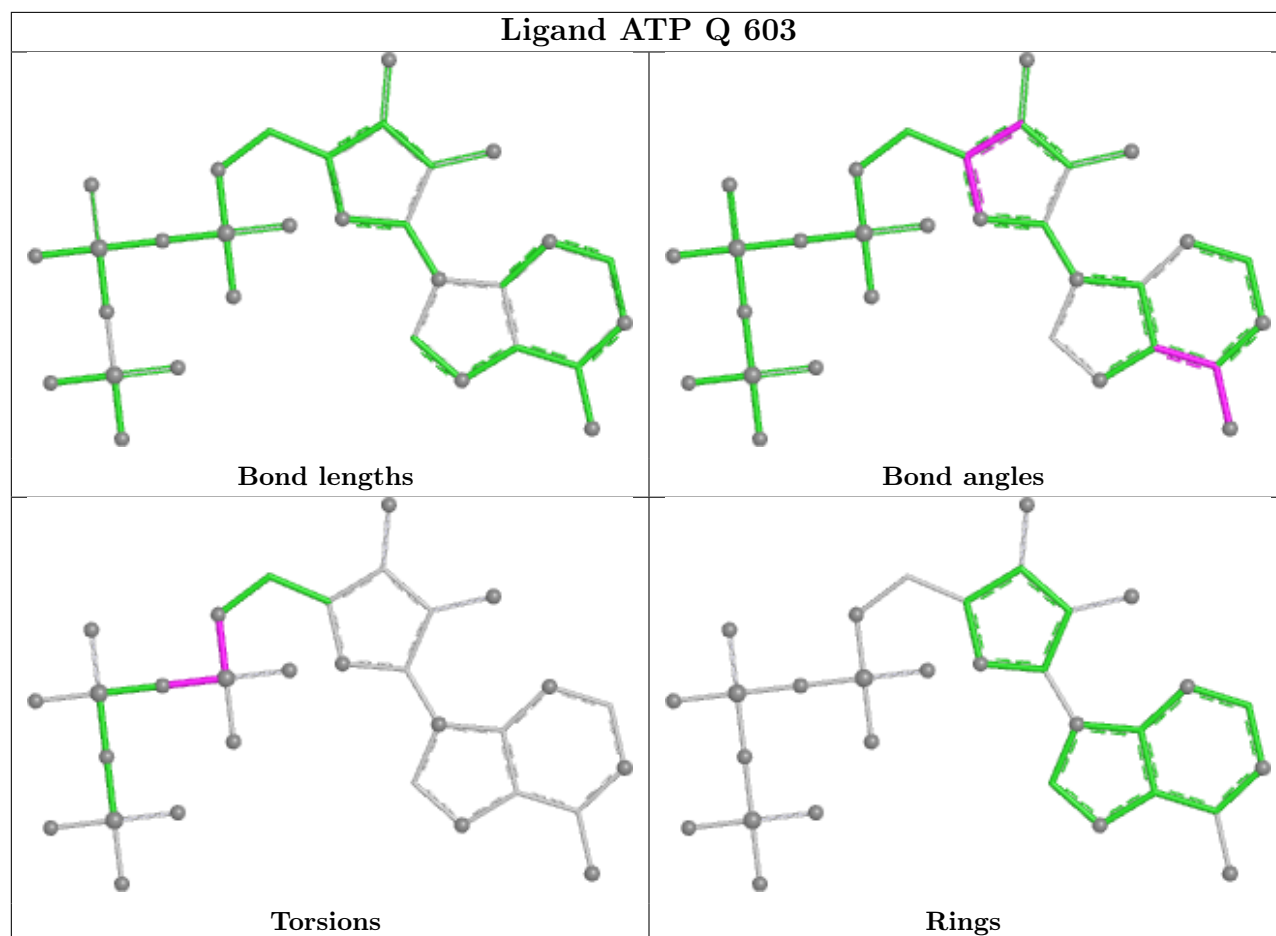
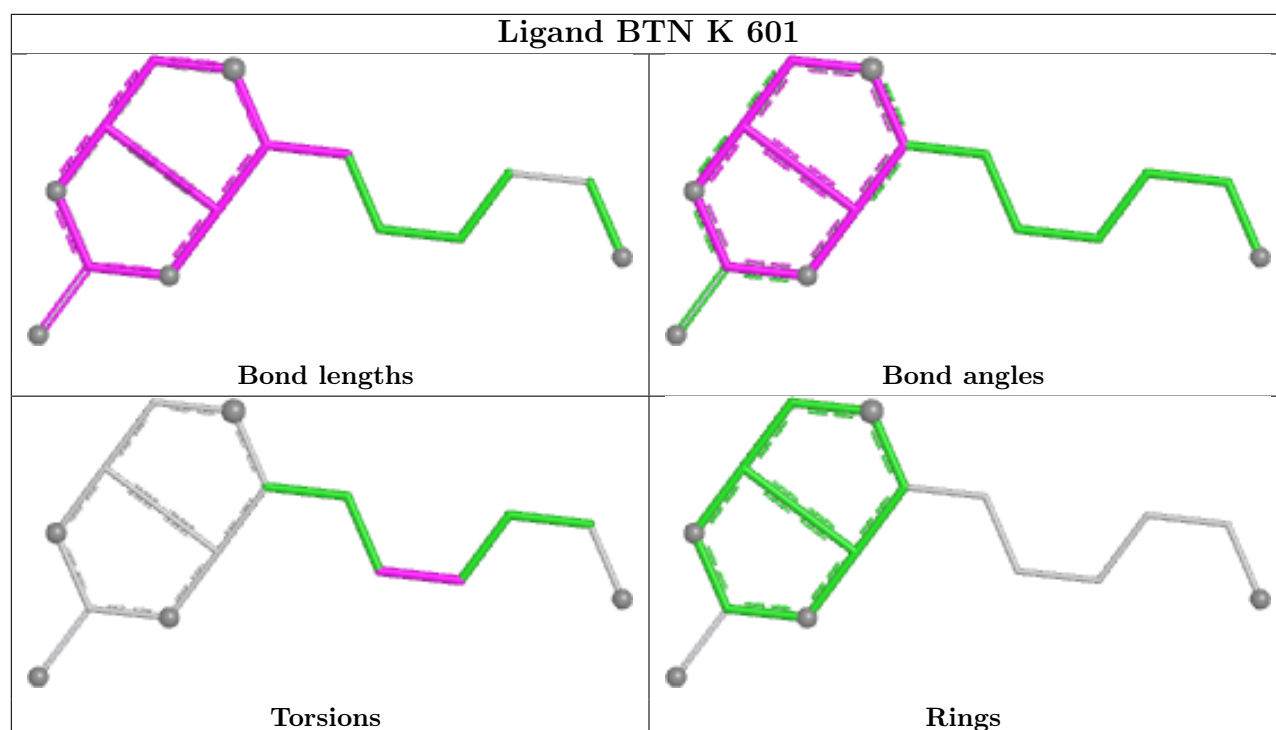
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



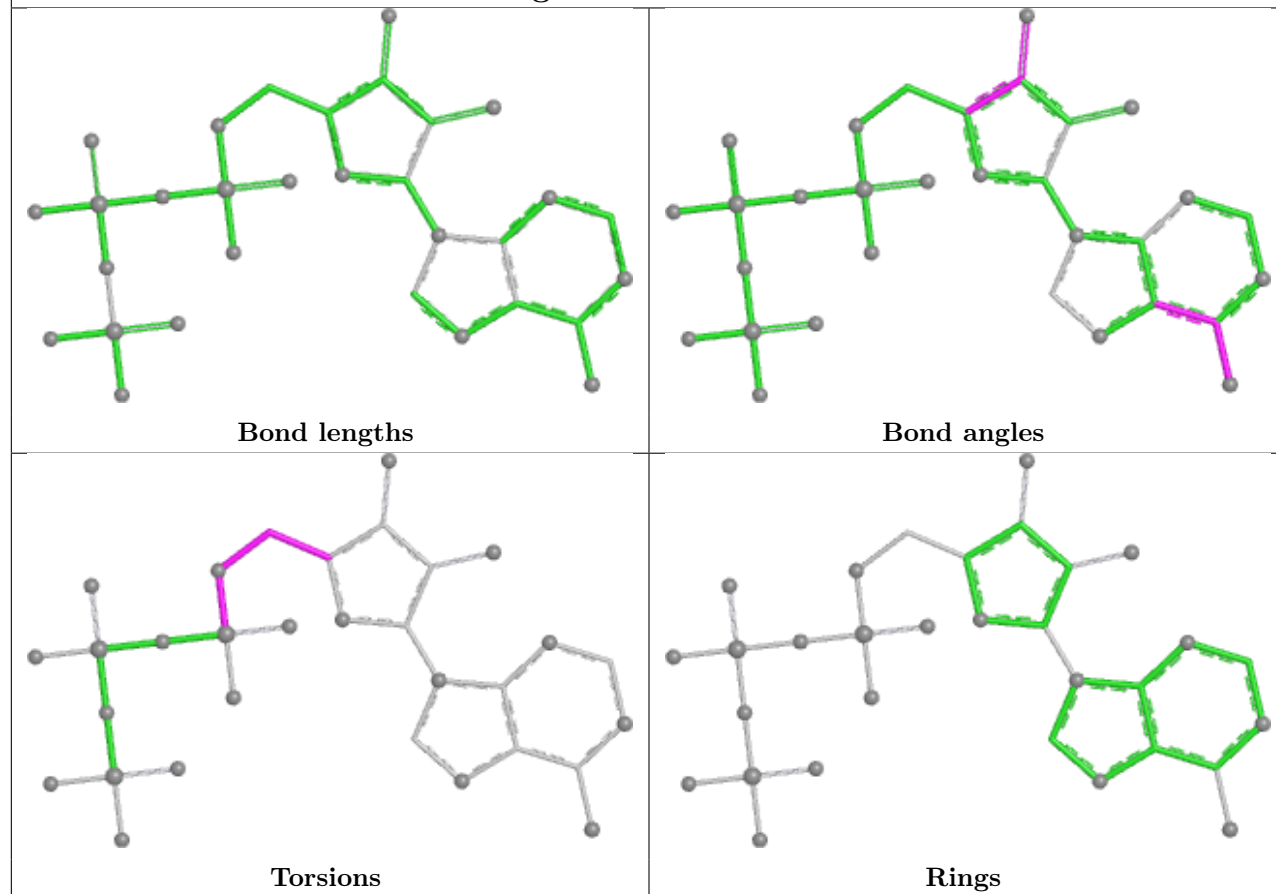


Ligand A1CZD F 601

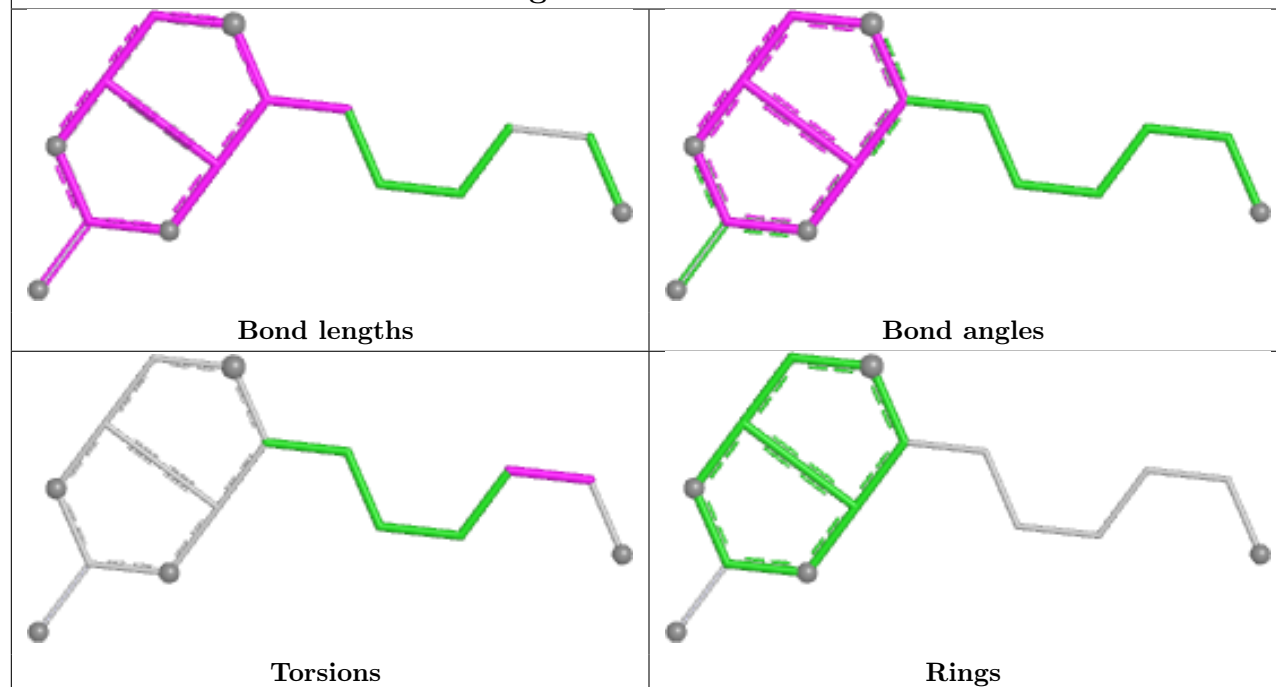


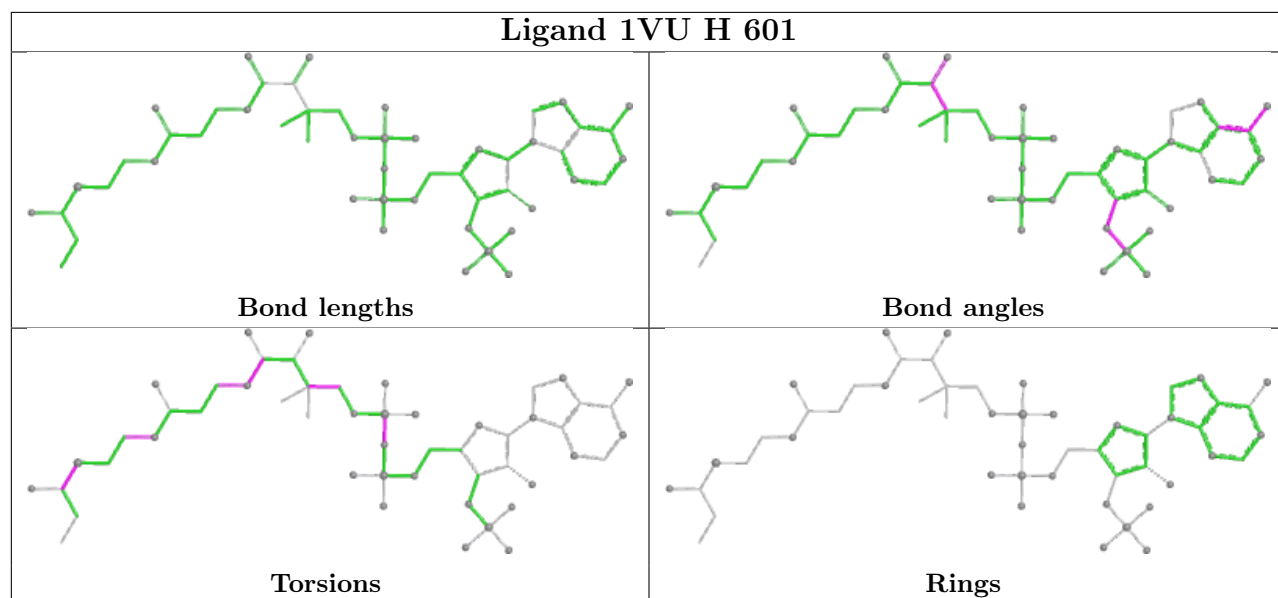
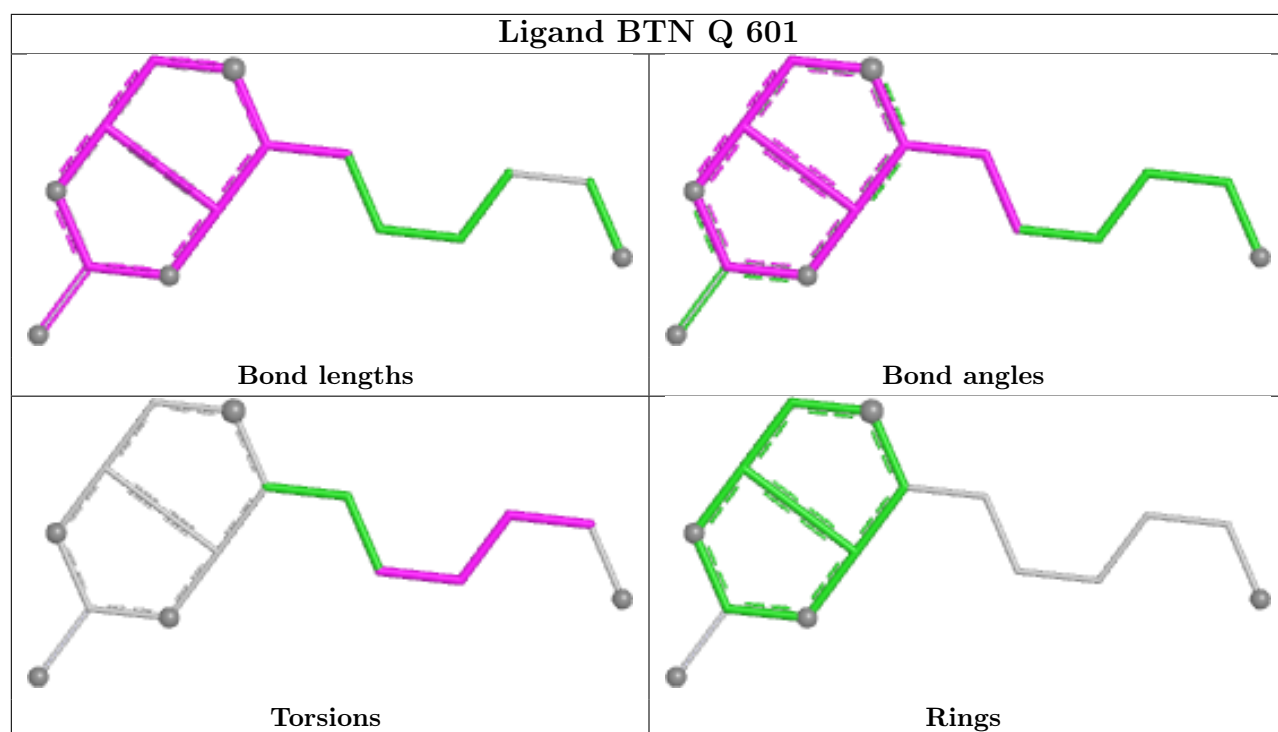


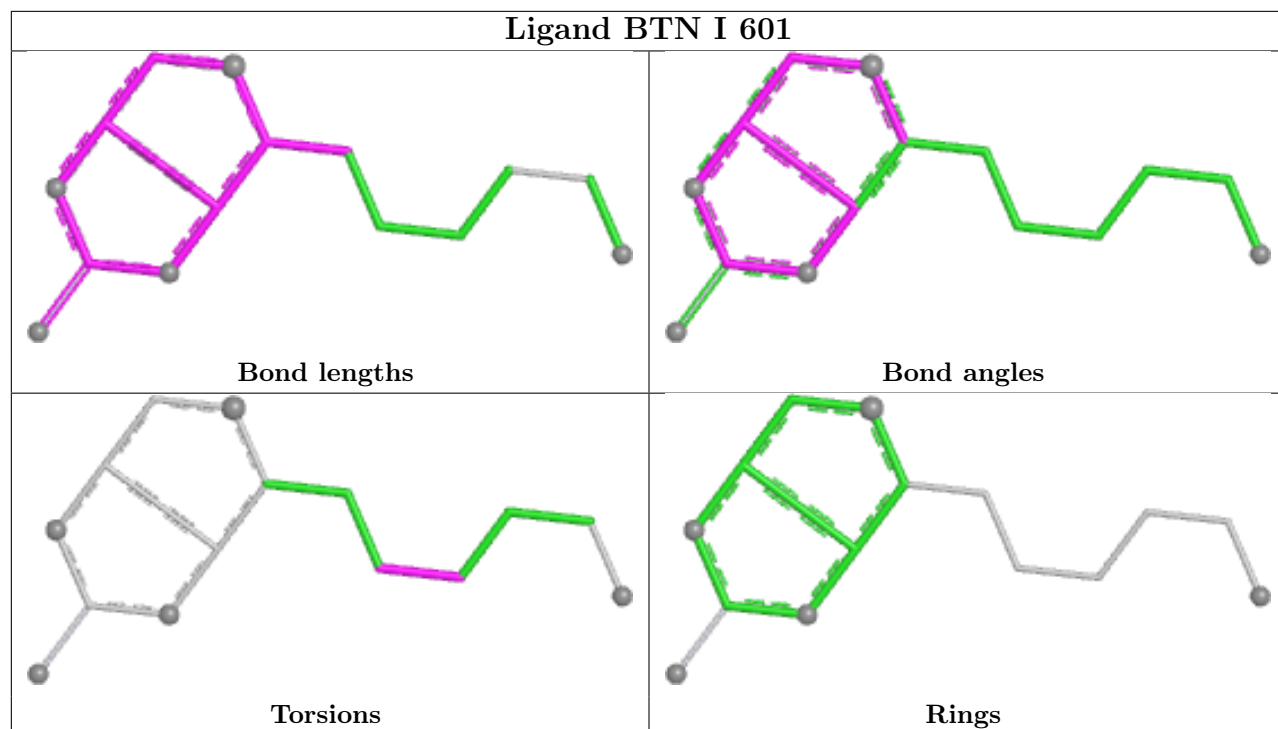
Ligand ATP R 601

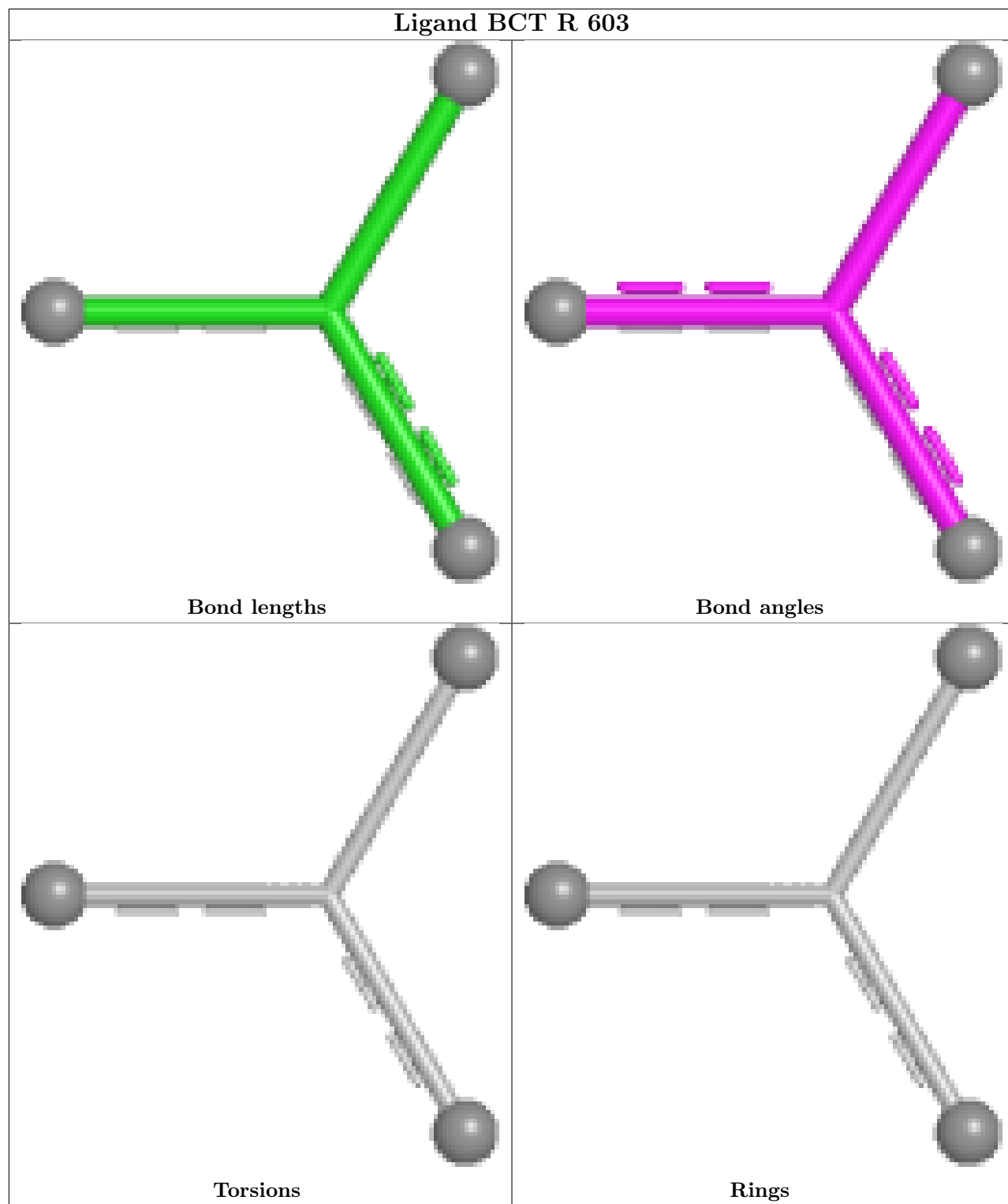


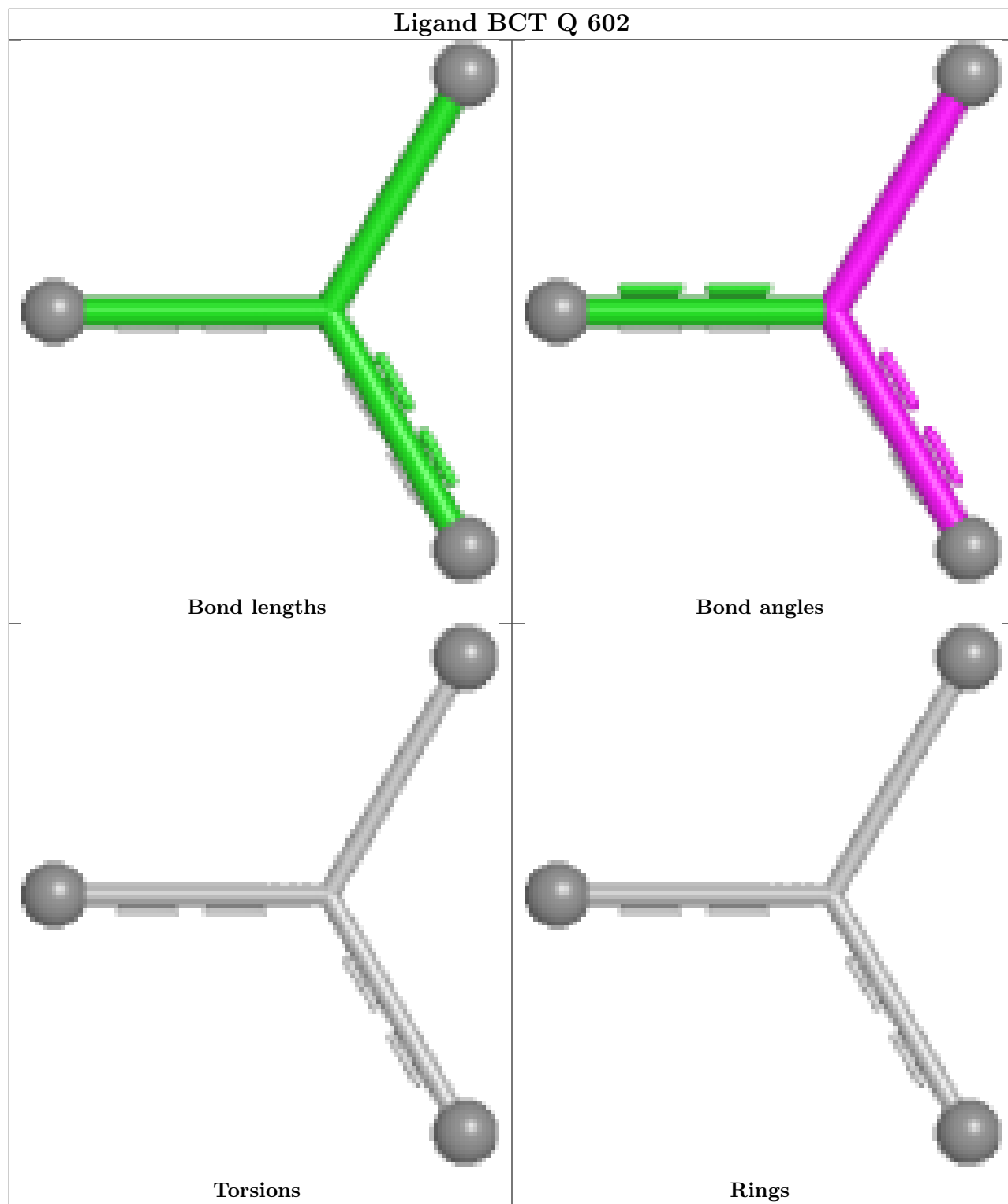
Ligand BTN U 601

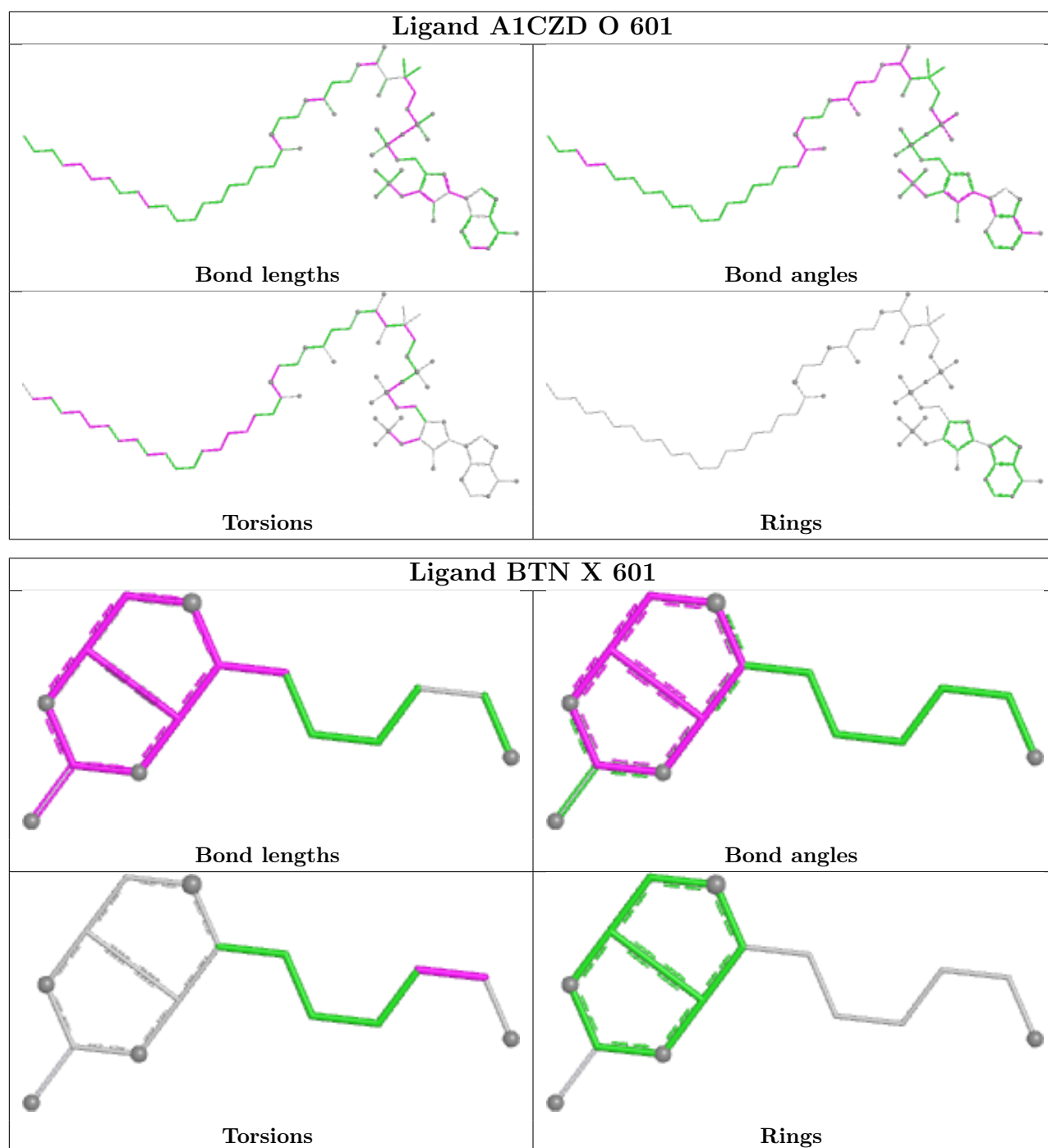












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

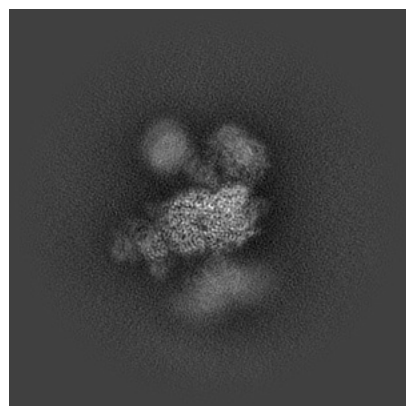
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73596. These allow visual inspection of the internal detail of the map and identification of artifacts.

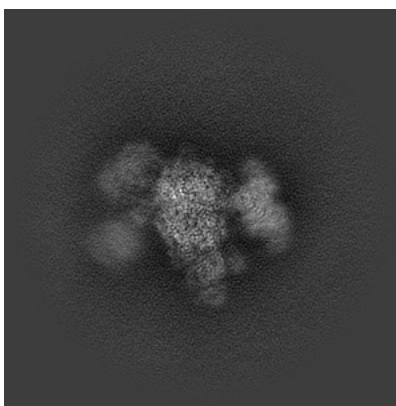
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

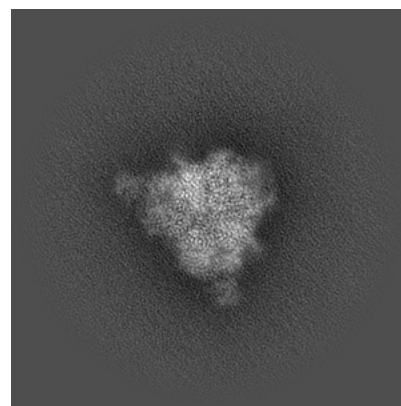
6.1.1 Primary map



X

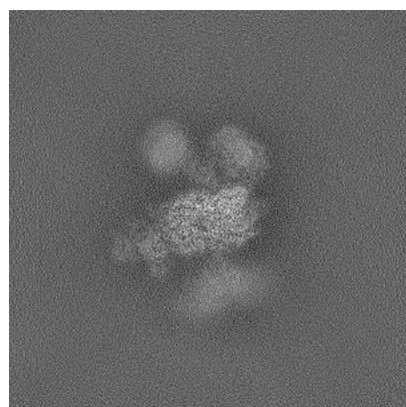


Y

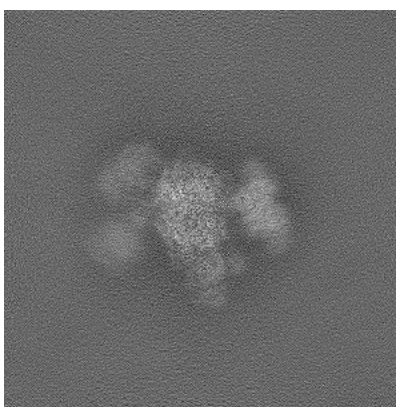


Z

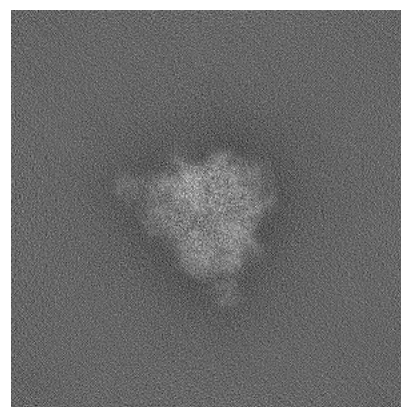
6.1.2 Raw map



X



Y

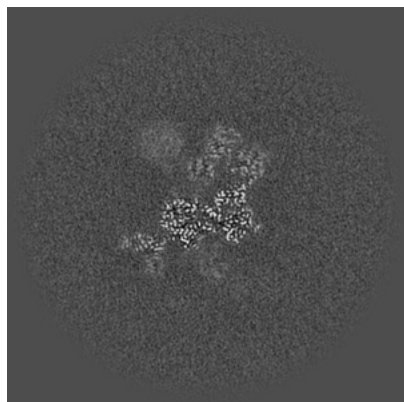


Z

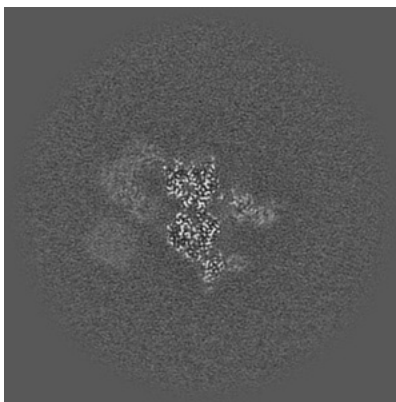
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

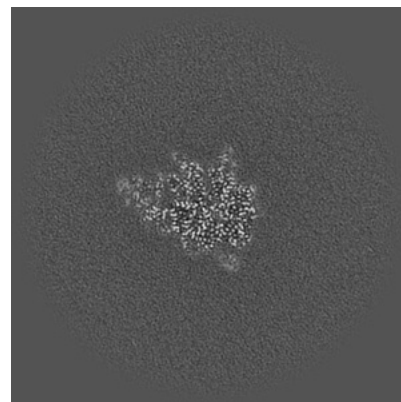
6.2.1 Primary map



X Index: 240

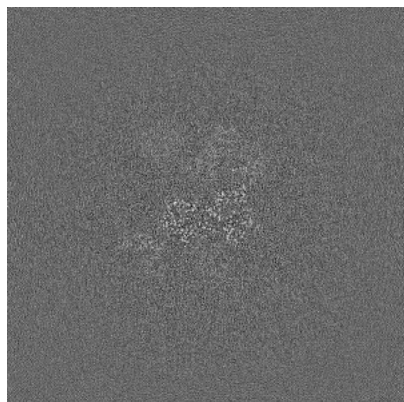


Y Index: 240

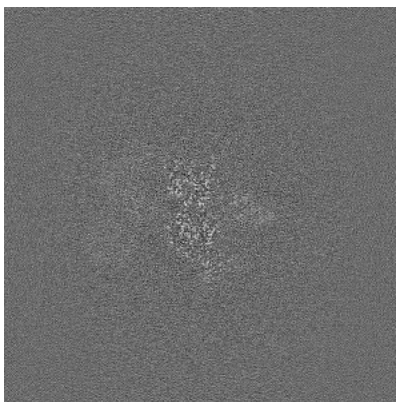


Z Index: 240

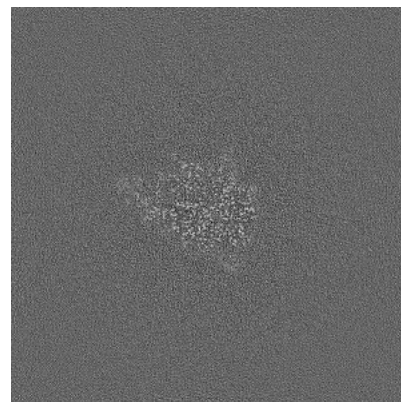
6.2.2 Raw map



X Index: 240



Y Index: 240

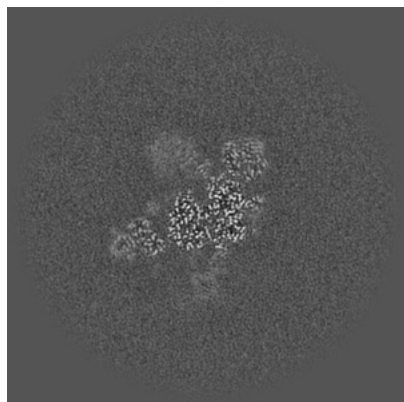


Z Index: 240

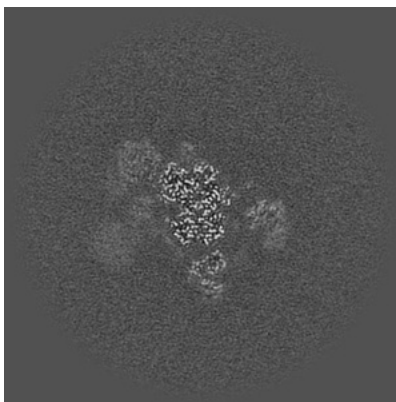
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

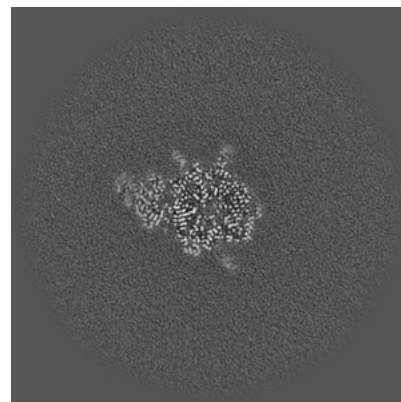
6.3.1 Primary map



X Index: 253

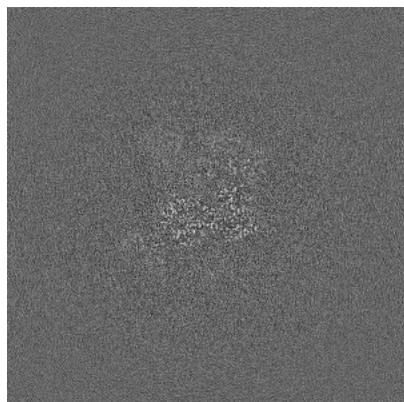


Y Index: 255

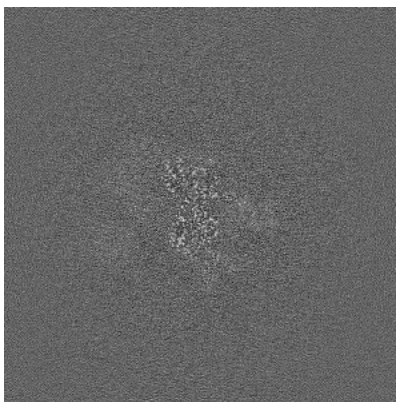


Z Index: 245

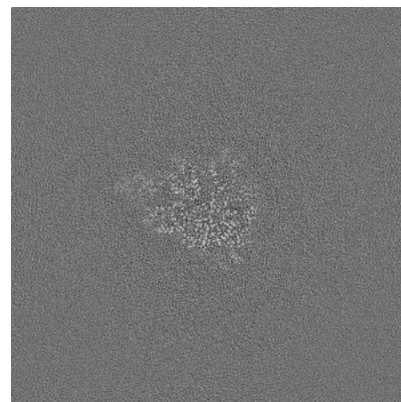
6.3.2 Raw map



X Index: 242



Y Index: 243

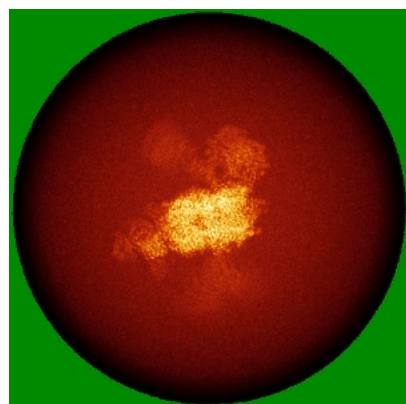


Z Index: 236

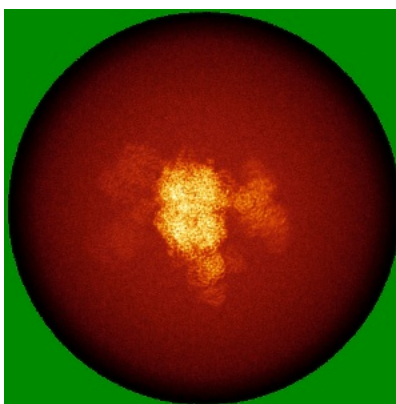
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

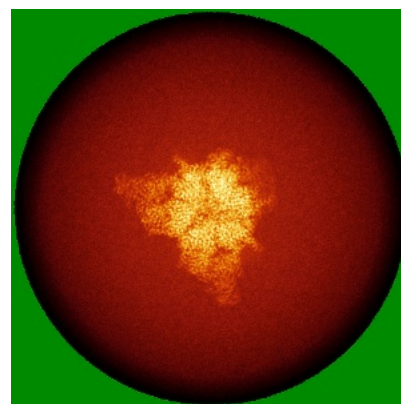
6.4.1 Primary map



X

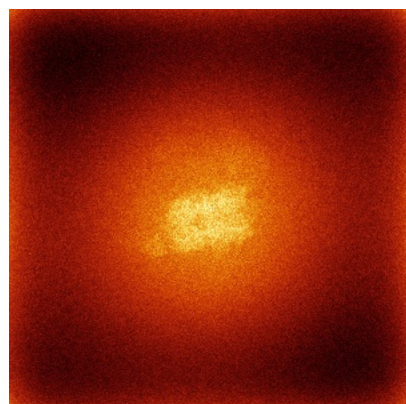


Y

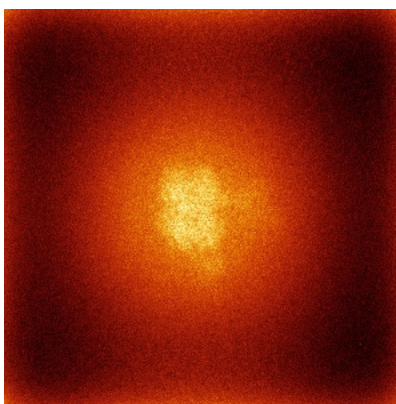


Z

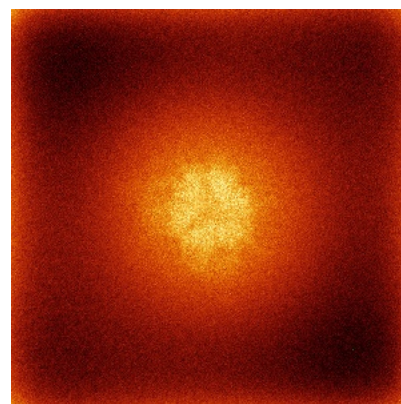
6.4.2 Raw map



X



Y

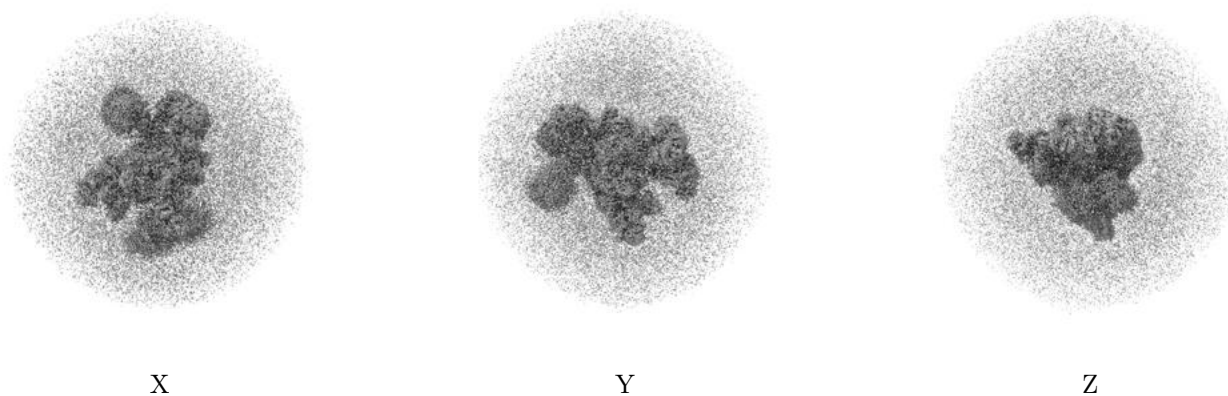


Z

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.

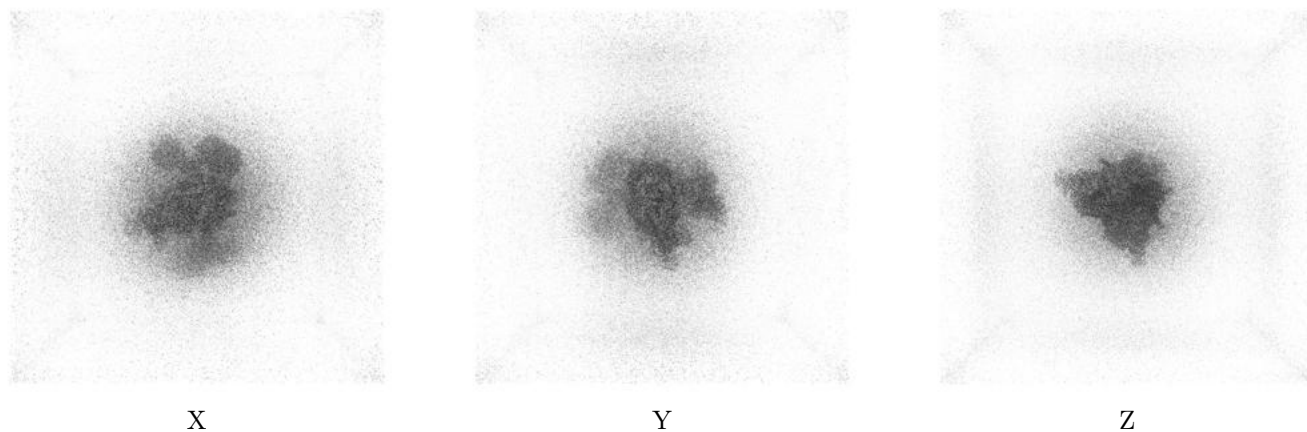
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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



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.

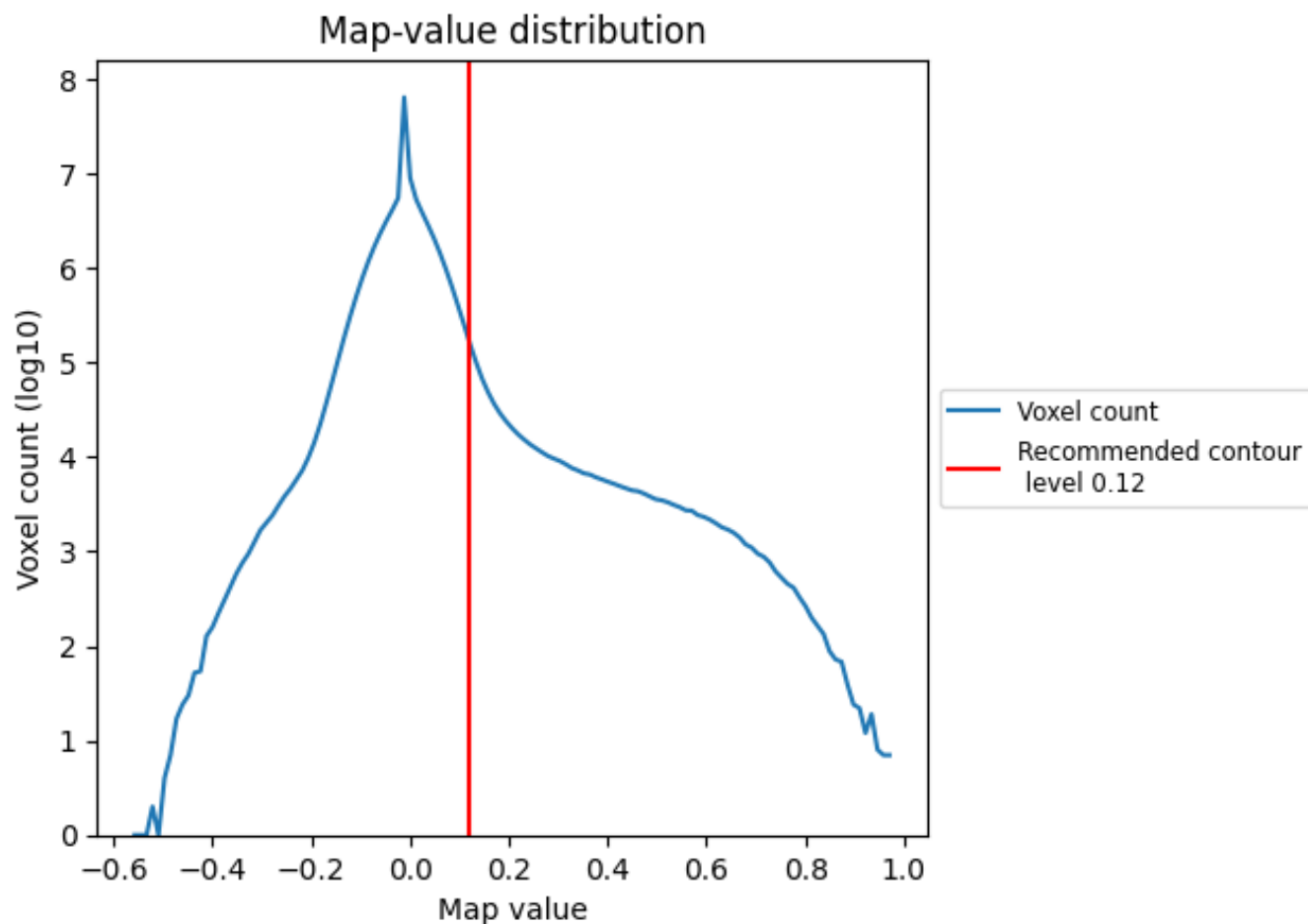
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

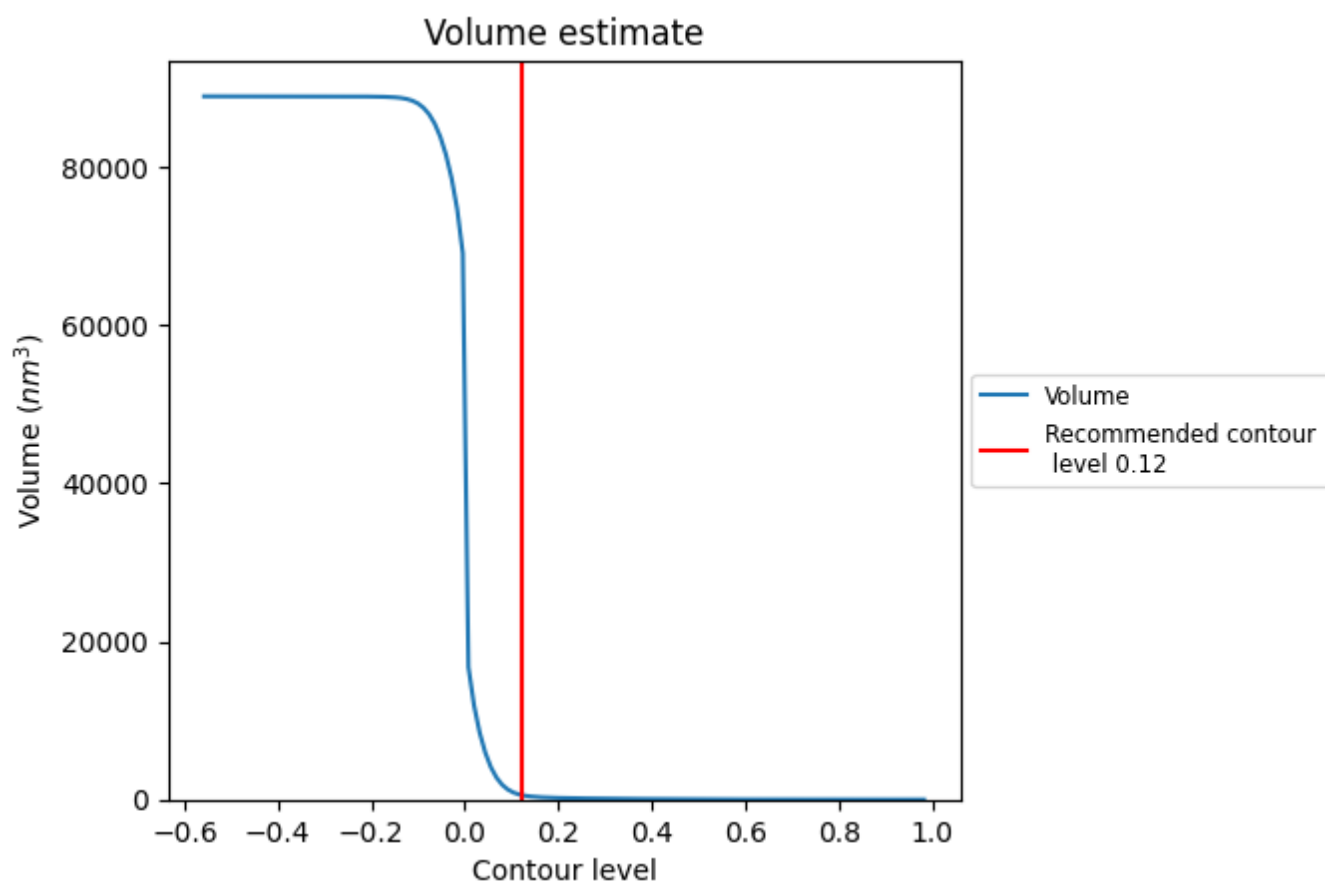
This section contains the results of statistical analysis of the map.

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.

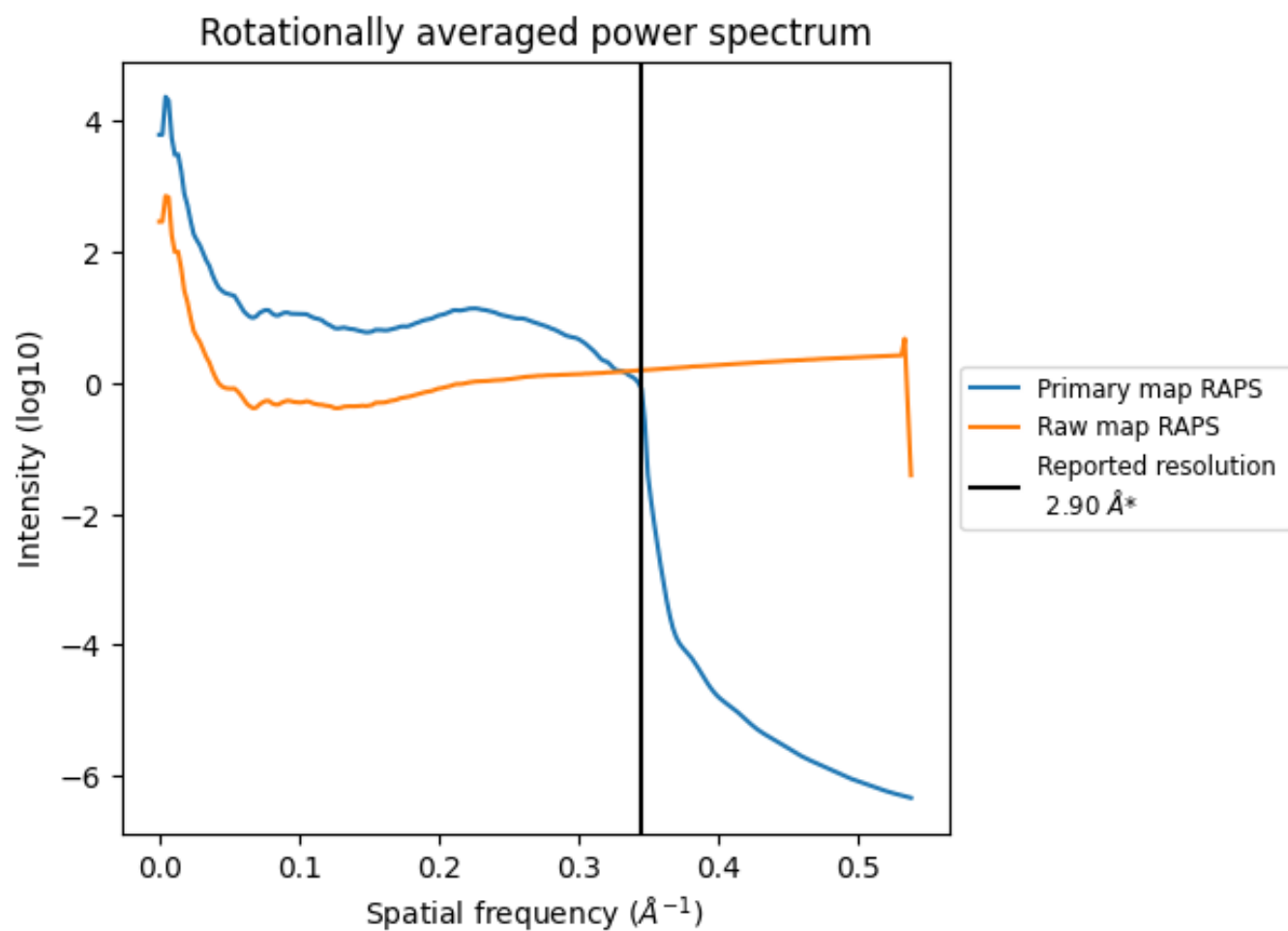
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 597 nm³; this corresponds to an approximate mass of 540 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 ⓘ

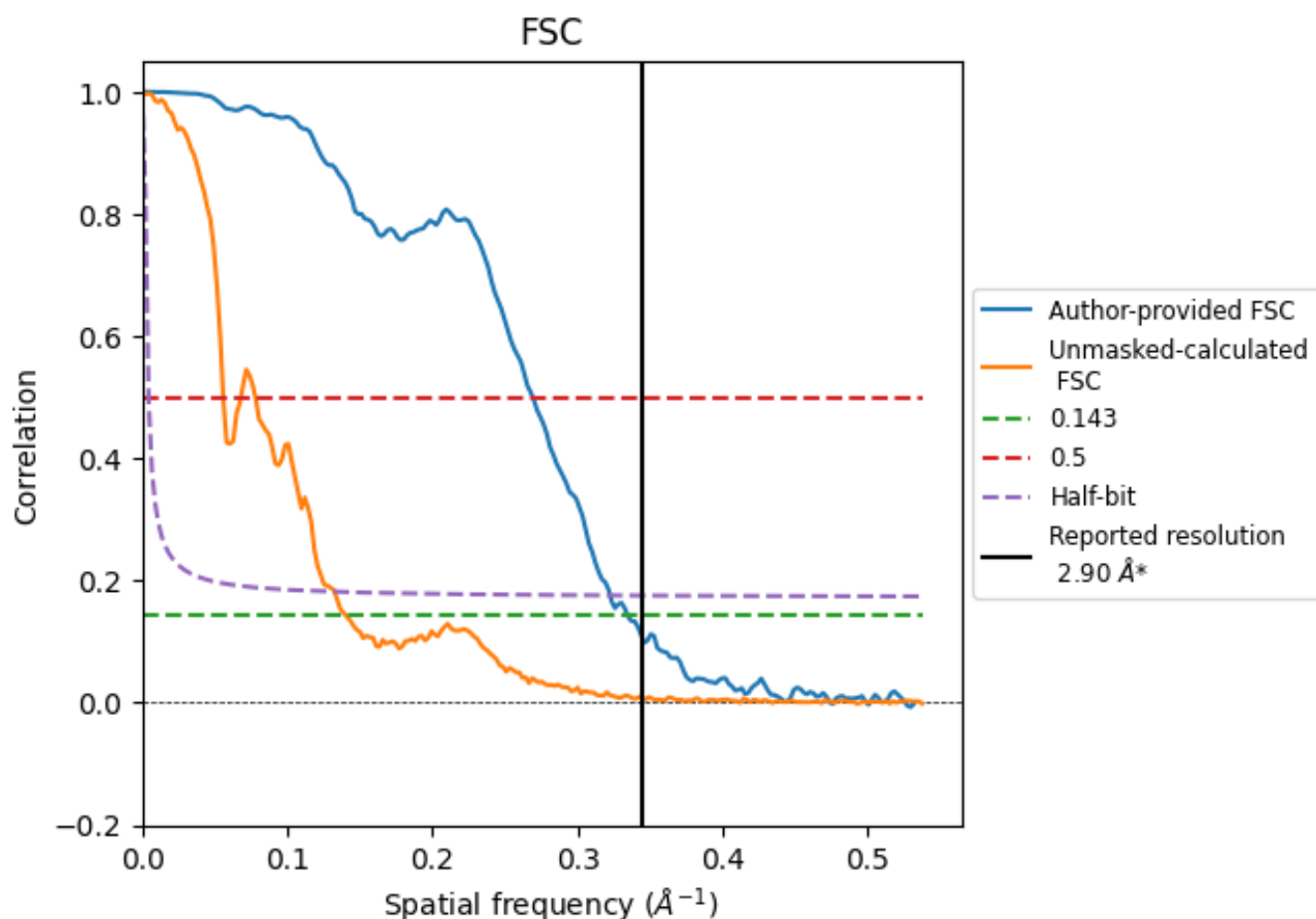


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

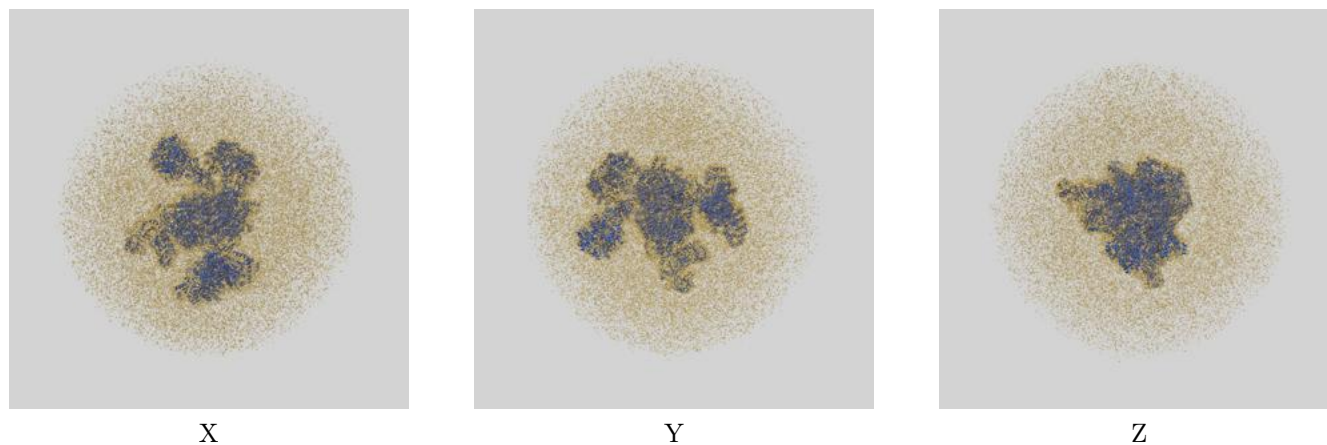
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.99	3.71	3.10
Unmasked-calculated*	7.13	17.92	7.54

*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 7.13 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

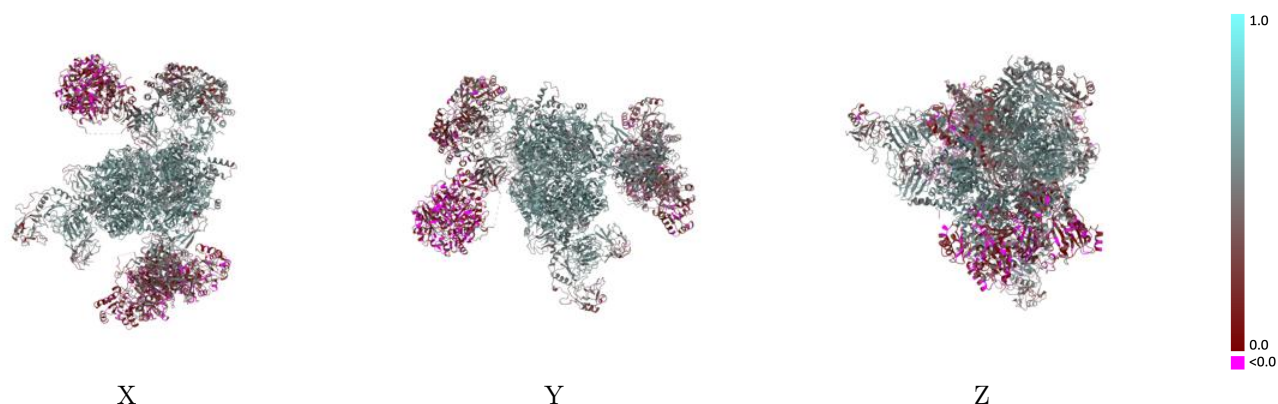
This section contains information regarding the fit between EMDB map EMD-73596 and PDB model 9YX5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



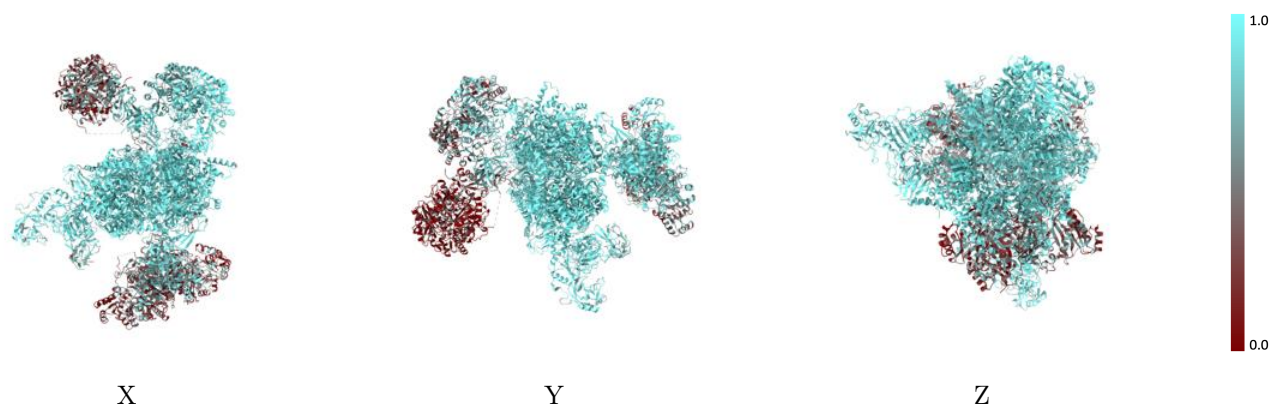
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



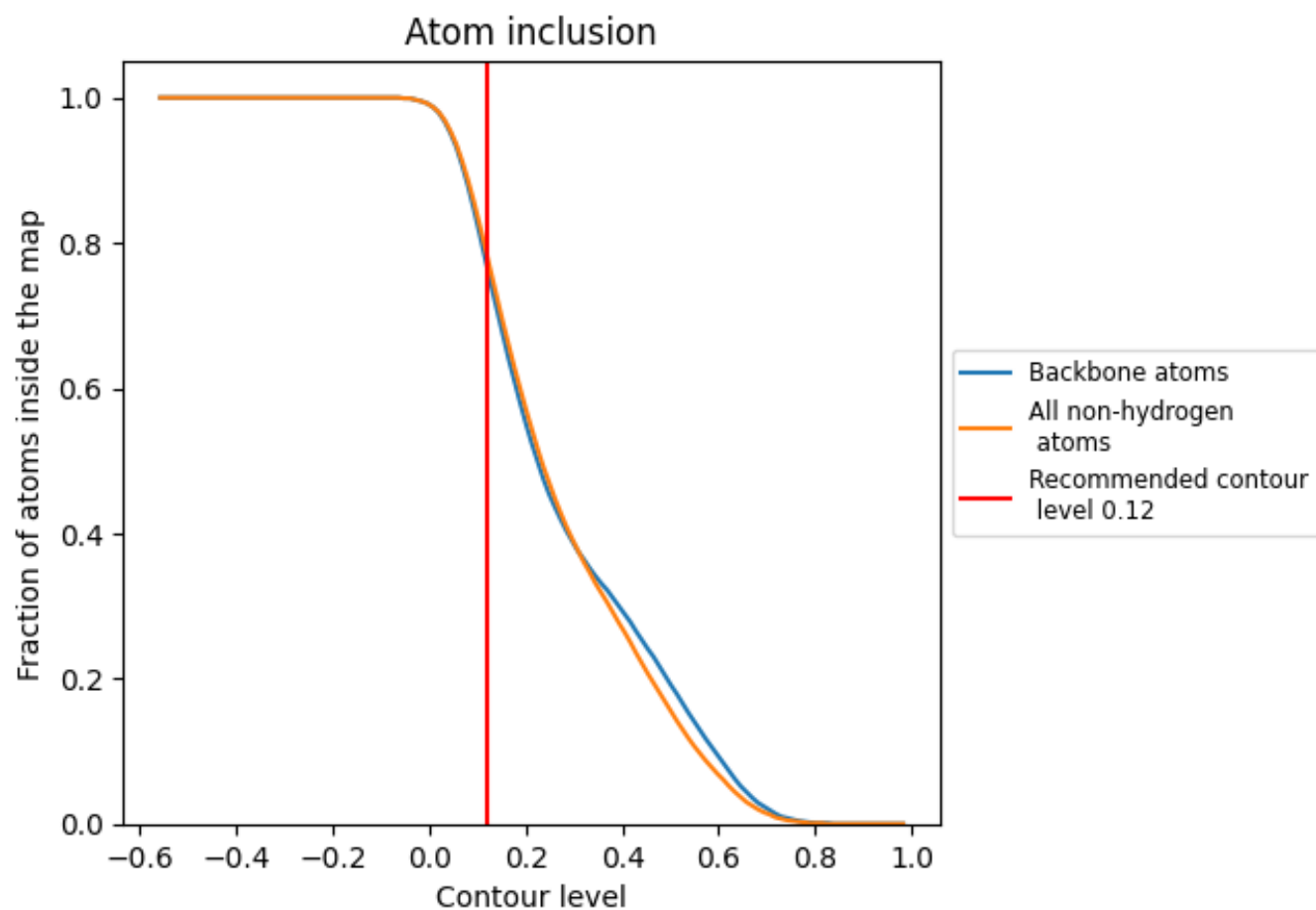
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.12).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.4560
A	 0.6720	 0.3750
B	 0.4670	 0.2550
C	 0.1400	 0.1360
D	 0.2170	 0.1470
E	 0.8210	 0.4990
F	 0.9610	 0.5900
G	 0.9720	 0.5940
H	 0.9590	 0.5910
I	 0.8820	 0.5050
J	 0.7190	 0.4640
K	 0.8330	 0.4670
L	 0.8050	 0.4890
M	 0.9720	 0.5930
N	 0.9620	 0.5920
O	 0.9620	 0.5880
P	 0.9010	 0.5430
Q	 0.9070	 0.5060
R	 0.7360	 0.3590
S	 0.3960	 0.1660
T	 0.4950	 0.1920
U	 0.6730	 0.3350
V	 0.9460	 0.5670
W	 0.8570	 0.4420
X	 0.7460	 0.4020
Y	 0.9380	 0.5630
Z	 0.8570	 0.4450

