



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:53 PM UTC

PDB ID : 8APK / pdb_00008apk
EMDB ID : EMD-15573
Title : rotational state 3 of the Trypanosoma brucei mitochondrial ATP synthase dimer
Authors : Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on : 2022-08-09
Resolution : 3.70 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:

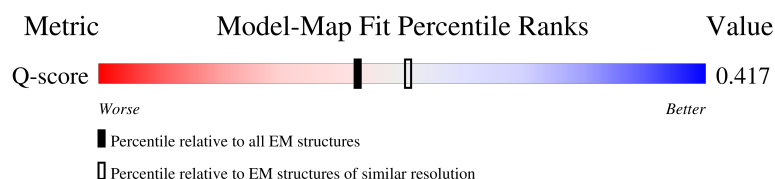
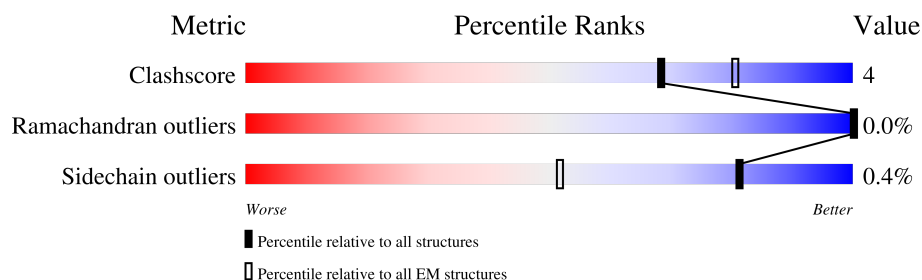
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	L	92	10% 66% 29%
1	l	92	10% 68% 29%
2	M	144	10% 83% 6% 10%
2	m	144	83% 7% 10%

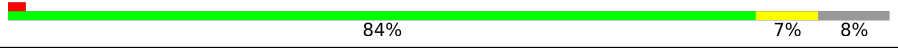
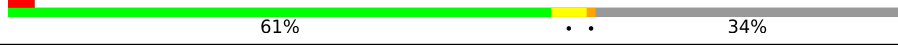
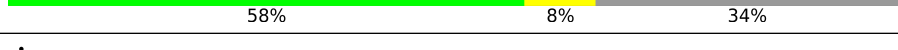
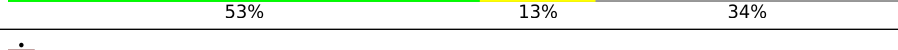
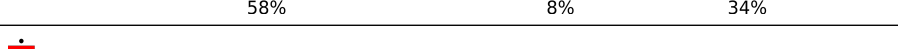
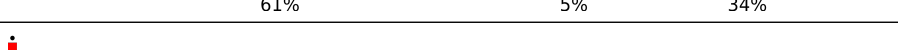
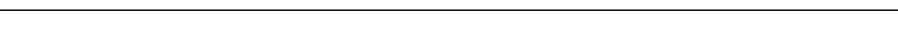
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Mol	Chain	Length	Quality of chain
3	a	231	
4	c	114	
5	d	370	
6	e	396	
7	f	145	
8	g	269	
9	h	157	
10	i	104	
11	j	169	
12	k	124	
13	n	156	
14	o	101	
15	p	105	
16	q	98	
17	r	62	
18	A1	584	
18	B1	584	
18	C1	584	
19	D1	519	
19	E1	519	
19	F1	519	
20	G1	305	
21	H1	182	
22	I1	75	
23	J1	188	

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Mol	Chain	Length	Quality of chain
23	K1	188	
23	L1	188	
24	M1	255	
25	O1	118	
25	P1	118	
25	Q1	118	
25	R1	118	
25	S1	118	
25	T1	118	
25	U1	118	
25	V1	118	
25	W1	118	
25	X1	118	

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
30	Q7G	e	406	X	-	-	-
30	Q7G	n	201	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 129566 atoms, of which 65465 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 subunit-e.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	L	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		
1	l	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		

- Molecule 2 is a protein called subunit-g.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		
2	m	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	a	231	Total	C	H	N	O	S	0	0
			4076	1459	2044	261	284	28		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	23	TRP	-	insertion	UNP P24499
a	180	TRP	-	insertion	UNP P24499

- Molecule 4 is a protein called subunit-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	c	86	Total	C	H	N	O	S	0	0
			1460	494	715	116	130	5		

- Molecule 5 is a protein called subunit-d.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	d	332	Total	C	H	N	O	S	0	0
			5499	1710	2762	505	514	8		

- Molecule 6 is a protein called ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	e	383	Total	C	H	N	O	S	0	0
			6270	2060	3050	558	585	17		

- Molecule 7 is a protein called subunit-f.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	f	135	Total	C	H	N	O	S	0	0
			2256	744	1111	201	195	5		

- Molecule 8 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	268	Total	C	H	N	O	S	0	0
			3953	1211	2020	343	378	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	176	ALA	VAL	conflict	UNP A0A3L6KRX7

- Molecule 9 is a protein called ATPTB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	137	Total	C	H	N	O	S	0	0
			2158	680	1088	184	203	3		

- Molecule 10 is a protein called subunit-i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	i	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		

- Molecule 11 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	j	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		

- Molecule 12 is a protein called subunit-k.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	k	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		

- Molecule 13 is a protein called ATPTB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		

- Molecule 14 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		

- Molecule 15 is a protein called subunit-b.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	80	Total	C	H	N	O	S	0	0
			1335	448	651	108	125	3		

- Molecule 16 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	q	85	Total	C	H	N	O		0	0
			1486	499	720	142	125			

- Molecule 17 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	62	Total	C	H	N	O	S	0	0
			1040	358	498	94	85	5		

- Molecule 18 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	A1	524	Total	C	H	N	O	S	0	0
			8219	2594	4171	703	731	20		
18	B1	522	Total	C	H	N	O	S	0	0
			8174	2578	4146	700	730	20		
18	C1	530	Total	C	H	N	O	S	0	0
			8281	2612	4197	710	742	20		

- Molecule 19 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	D1	487	Total	C	H	N	O	S	0	0
			7431	2329	3742	631	710	19		
19	E1	487	Total	C	H	N	O	S	0	0
			7431	2329	3742	631	710	19		
19	F1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		

- Molecule 20 is a protein called ATP synthase gamma subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G1	300	Total	C	H	N	O	S	0	0
			4774	1507	2387	423	448	9		

- Molecule 21 is a protein called ATP synthase, epsilon chain, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	H1	161	Total	C	H	N	O	S	0	0
			2483	788	1232	211	248	4		

- Molecule 22 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	I1	65	Total	C	H	N	O	S	0	0
			1046	332	513	97	102	2		

- Molecule 23 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	J1	166	Total	C	H	N	O	S	0	0
			2590	822	1276	221	257	14		
23	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
23	L1	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		

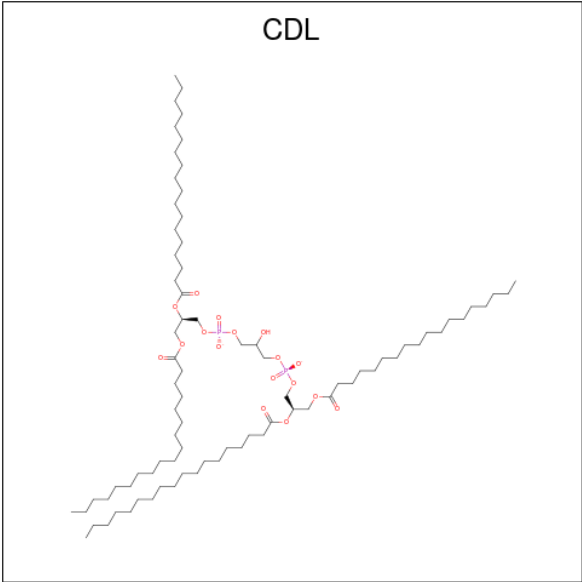
- Molecule 24 is a protein called OSCP.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	M1	234	Total	C	H	N	O	S	0	0
			3750	1212	1873	302	360	3		

- Molecule 25 is a protein called ATPase subunit 9, putative.

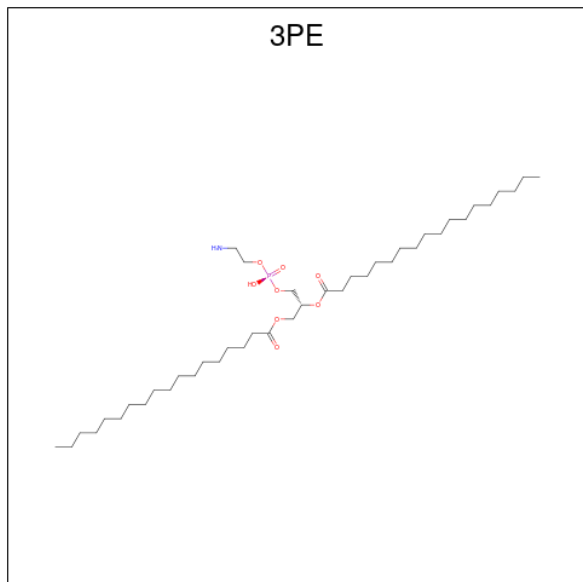
Mol	Chain	Residues	Atoms						AltConf	Trace
25	O1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	P1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	Q1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	R1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	S1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
25	T1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
25	U1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	V1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	W1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	X1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



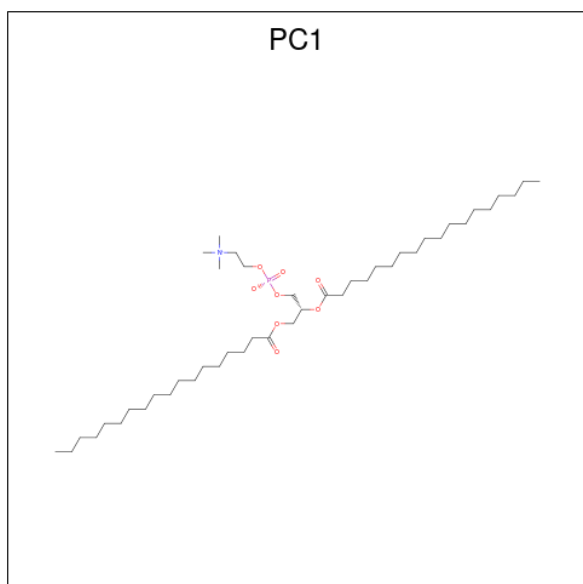
Mol	Chain	Residues	Atoms					AltConf
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	m	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	q	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



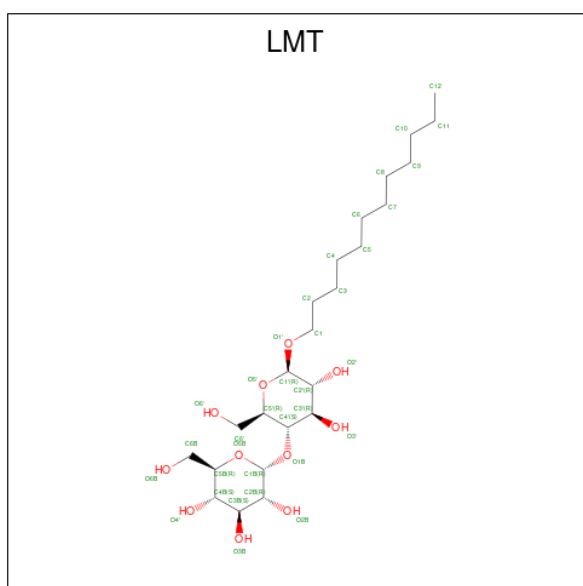
Mol	Chain	Residues	Atoms						AltConf
27	M	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	f	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



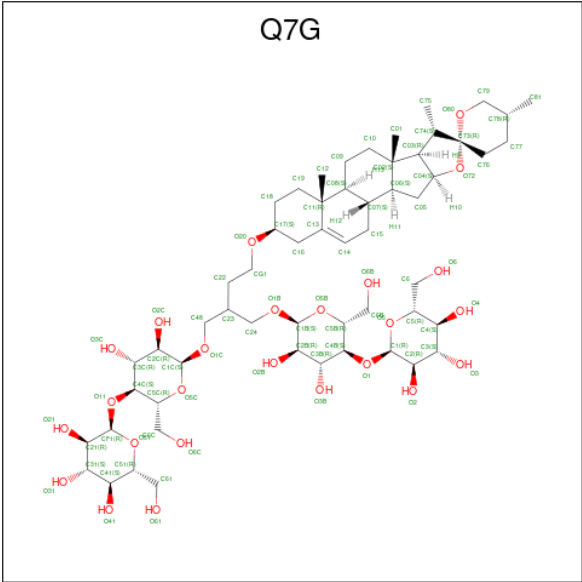
Mol	Chain	Residues	Atoms					AltConf	
28	a	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
28	i	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
28	j	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
28	p	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



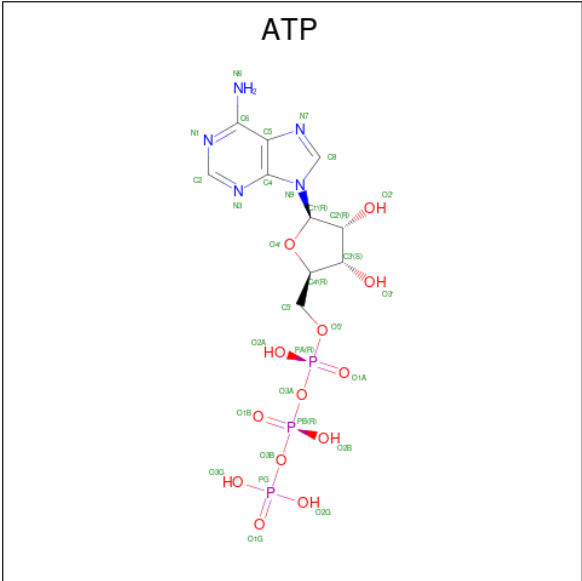
Mol	Chain	Residues	Atoms				AltConf
29	e	1	Total	C	H	O	0
			74	24	39	11	
29	j	1	Total	C	H	O	0
			74	24	39	11	

- Molecule 30 is 2-[[[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula: $C_{56}H_{92}O_{25}$).



Mol	Chain	Residues	Atoms				AltConf
30	e	1	Total	C	H	O	0
			108	38	60	10	
30	n	1	Total	C	H	O	0
			129	44	70	15	

- Molecule 31 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
31	A1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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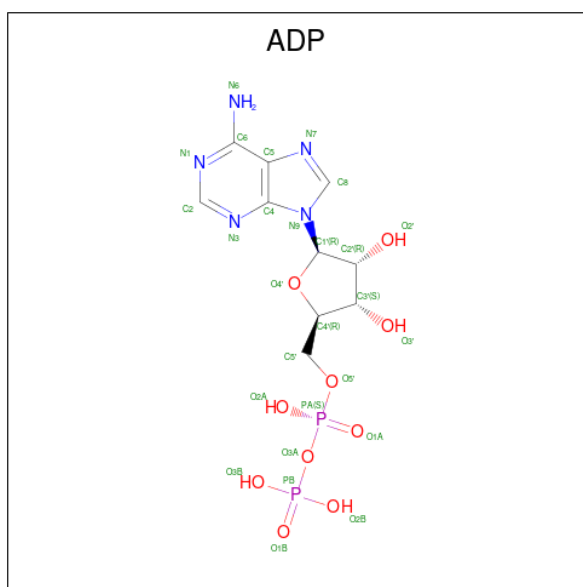
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Mol	Chain	Residues	Atoms					AltConf	
31	B1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
31	C1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
31	E1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

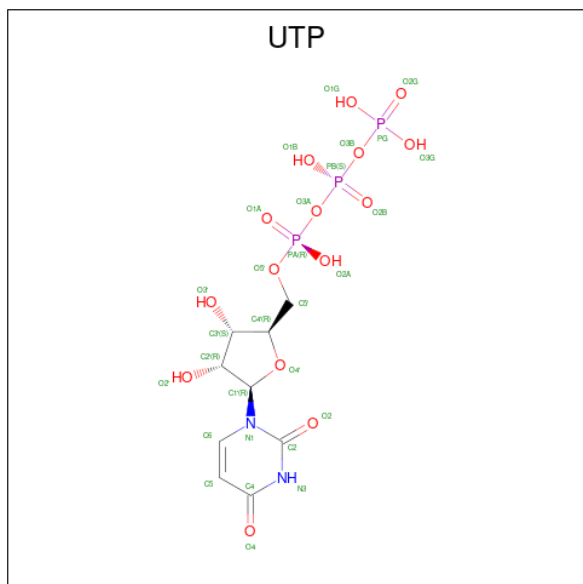
Mol	Chain	Residues	Atoms		AltConf
32	A1	1	Total	Mg	0
			1	1	
32	B1	1	Total	Mg	0
			1	1	
32	C1	1	Total	Mg	0
			1	1	
32	E1	1	Total	Mg	0
			1	1	
32	F1	1	Total	Mg	0
			1	1	

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
33	F1	1	39	10	12	5	10	2	0

- Molecule 34 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).

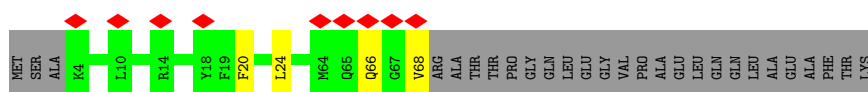


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
34	H1	1	40	9	11	2	15	3	0

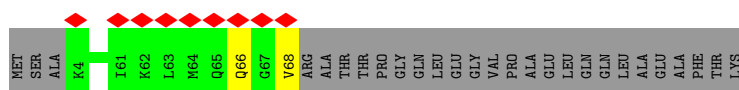
3 Residue-property plots [i](#)

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.

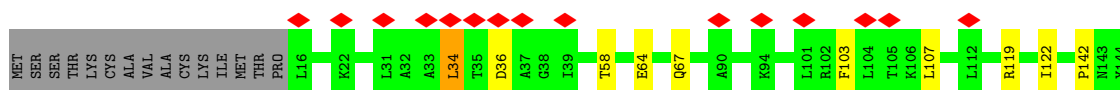
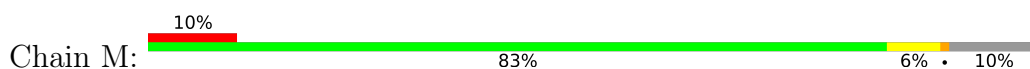
- Molecule 1: subunit-e



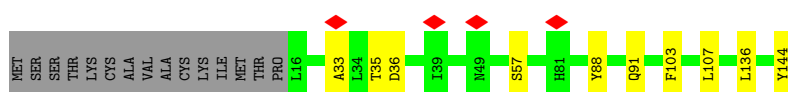
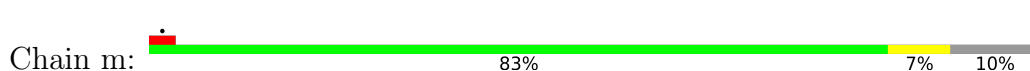
- Molecule 1: subunit-e



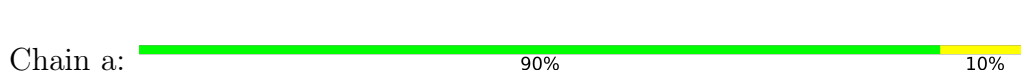
- Molecule 2: subunit-g



- Molecule 2: subunit-g



- Molecule 3: ATP synthase subunit a



- Molecule 4: subunit-8

Chain c:  60% 16% 25%

MET LEU ARG ARG LEU GLY ALA ASN VAL SER ASN MET ALA ARG PRO MET MET ASN LYS TYR VAL VAL THR VAL SER PRO ARG ARG HIS L29 V35 W40 V43 W44 V61 V65 Y66 N67 K68 L69 P70 H73 E77 K78 R79 Q82 K83 V87 L88 T93

M113
I114

• Molecule 5: subunit-d

Chain d:  83% 7% 10%

MET ARG ARG VAL SER PRO ASN THR ILE ILE GLN SER VAL ARG TRP I17 Y25 T30 T31 S32 T33 T34 Q39 N43 R53 E76 K86 D98 L102 D136 R157 R185 V189 D196 L203 K237 K252 R262 P268 E269

E275 L276 E277 V278 I280 T281 W283 Q284 V305 E322 R323 N324 P325 ILE VAL THR GLN THR SER T332 R337 Q348 I351 N352 Q353 R354 ASP GLU VAL GLU PRO SER GLN THR GLU GLN LYS LYS ALA HIS HIS

• Molecule 6: ATPTB1

Chain e:  90% 7% 3%

M1 M11 R39 D58 Y69 D73 Y111 L120 Q144 D158 W170 K184 N185 T210 N223 T226 W229 R232 N235 M262 R285 D325 P326 A327 E335 K338 N339 D350 A351 F352 R378 K383 GLY ASP ASN ALA

ALA VAL GLU GLY ARG HIS THR ALA

• Molecule 7: subunit-f

Chain f:  78% 14% 7%

MET V2 R11 E16 F17 L18 V22 W37 L41 N42 L45 E48 T56 P57 Y62 H63 R64 M80 I81 W84 G85 G86 R101 T36 V102 S113 A114 T128 R136 LYS ALA GLY GLY ALA GLN ALA HIS HIS

• Molecule 8: ATPTB3

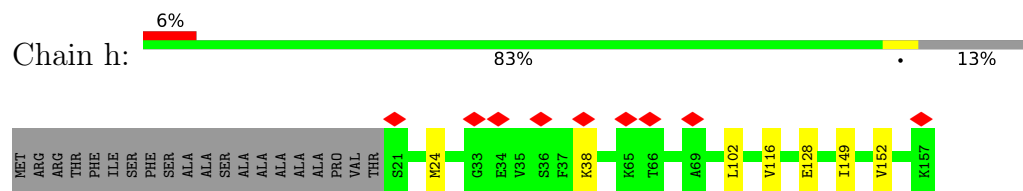
Chain g:  24% 88% 12%

MET S2 K3 L5 T6 G11 A12 T13 A14 Q18 S19 A20 S21 A22 I23 S25 K26 G29 G30 R31 V32 Q33 T34 K35 T36 A37 K38 E39 A40 Q41 R42 H43 A44 T57 A58 V59 T60 E61 V62 P63 K64 S65 A66 S72 G73 V74 S75 V79 R80 A81 V82 L83

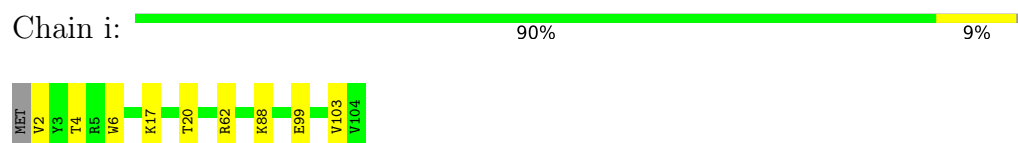
P84 R85 A96 L97 D98 V99 T107 A114 V124 A125 V126 K130 A131 K132 K135 V140 N151 E152 E163 S164 A165 G166 V171 T174 A175 A176 V177 E186 A205 F206 V210 V216 Y217 V220 E221 G222 S230 V234 E241 L242 R243

E244 L245 G246 S249 V254 K260 R263 S267 A268 L269

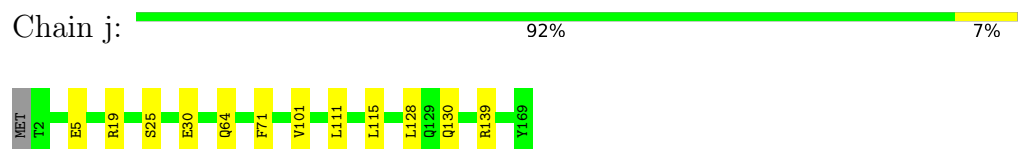
- Molecule 9: ATPTB4



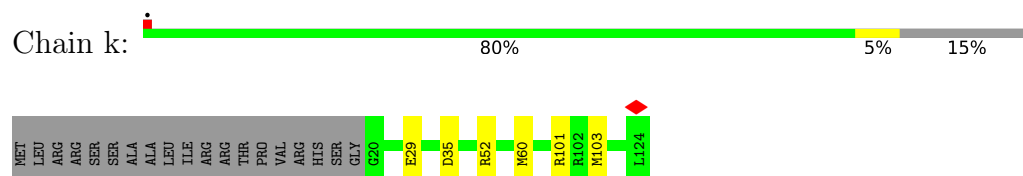
- Molecule 10: subunit-i/j



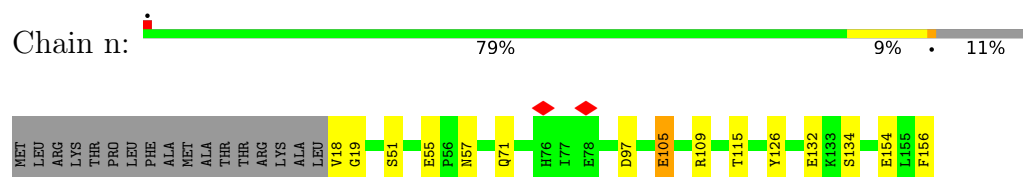
- Molecule 11: ATPTB6



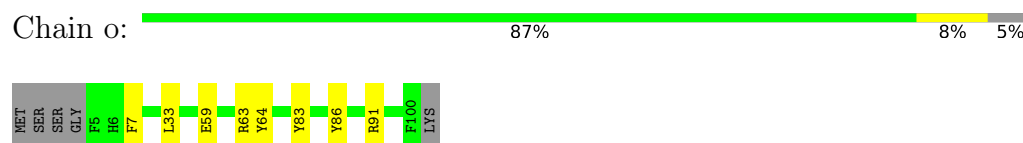
- Molecule 12: subunit-k



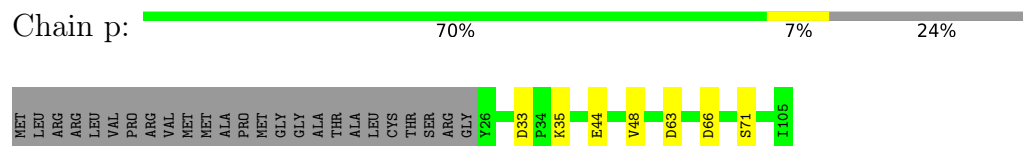
- Molecule 13: ATPTB11



- Molecule 14: ATPTB12

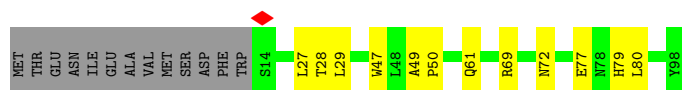


- Molecule 15: subunit-b



- Molecule 16: ATPEG3

Chain q: 



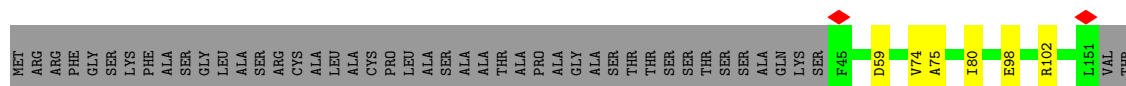
- Molecule 17: ATPEG4

Chain r: 



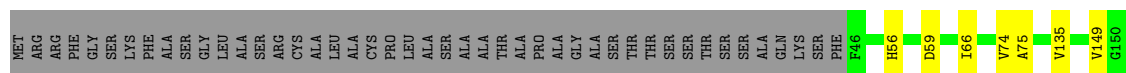
- Molecule 18: ATP synthase subunit alpha, mitochondrial

Chain A1: 



- Molecule 18: ATP synthase subunit alpha, mitochondrial

Chain B1: 



- Molecule 18: ATP synthase subunit alpha, mitochondrial

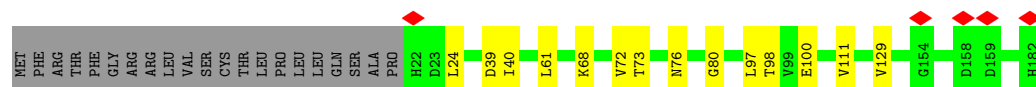
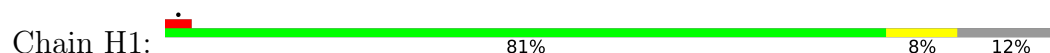
Chain C1: 



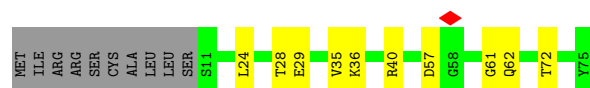
- Molecule 20: ATP synthase gamma subunit



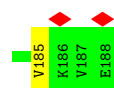
- Molecule 21: ATP synthase, epsilon chain, putative



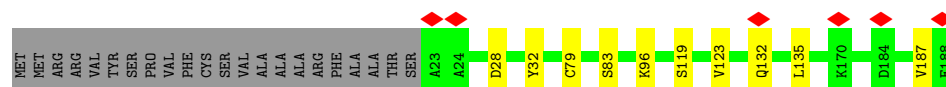
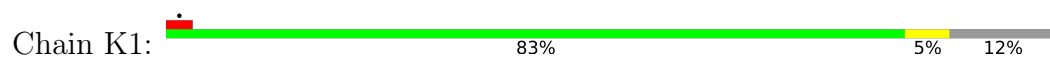
- Molecule 22: ATP synthase subunit epsilon, mitochondrial



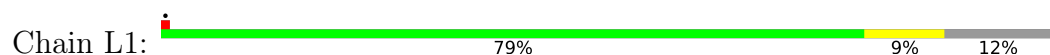
- Molecule 23: ATP synthase subunit p18, mitochondrial



- Molecule 23: ATP synthase subunit p18, mitochondrial

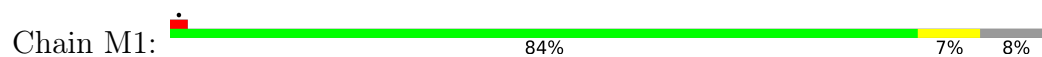


- Molecule 23: ATP synthase subunit p18, mitochondrial

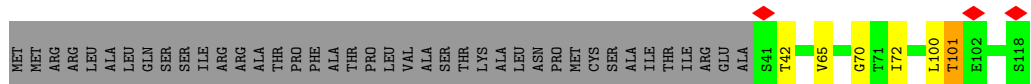




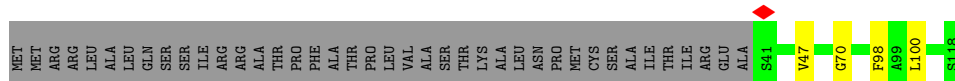
- Molecule 24: OSCP



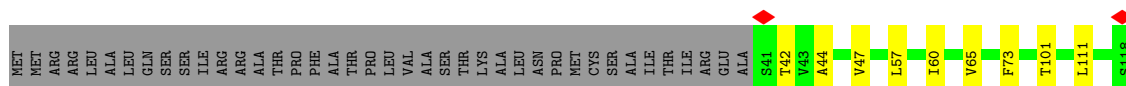
- Molecule 25: ATPase subunit 9, putative



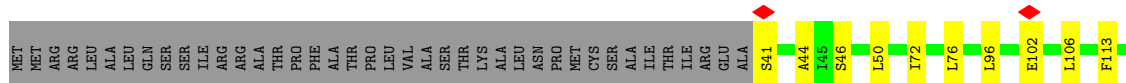
- Molecule 25: ATPase subunit 9, putative



- Molecule 25: ATPase subunit 9, putative

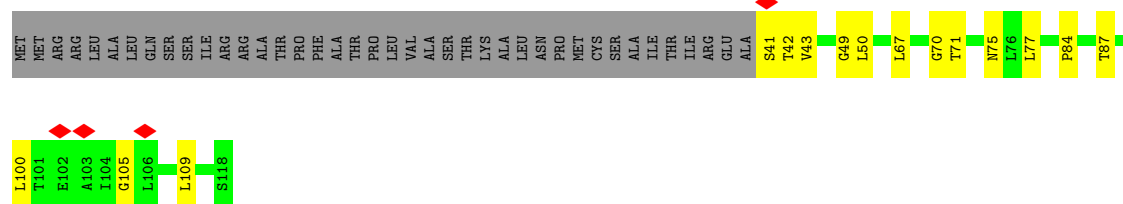


- Molecule 25: ATPase subunit 9, putative



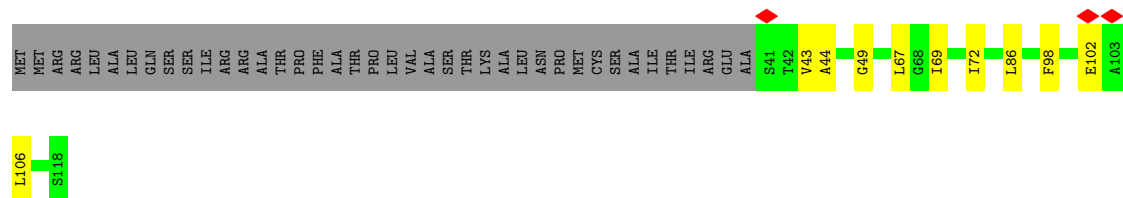
- Molecule 25: ATPase subunit 9, putative

Chain S1: 



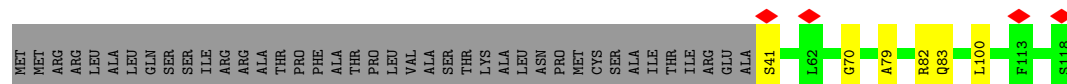
- Molecule 25: ATPase subunit 9, putative

Chain T1: 



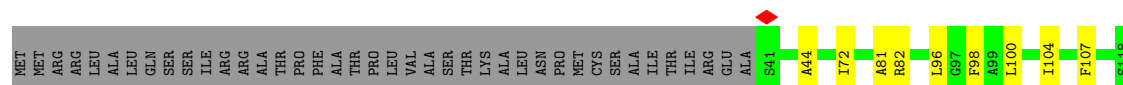
- Molecule 25: ATPase subunit 9, putative

Chain U1: 



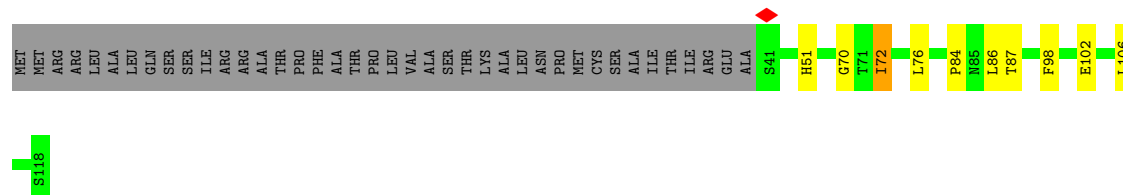
- Molecule 25: ATPase subunit 9, putative

Chain V1: 



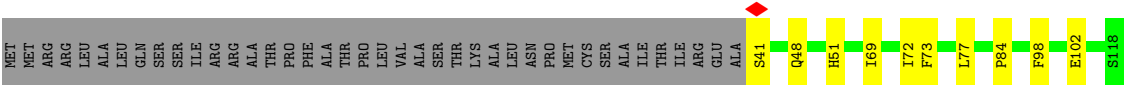
- Molecule 25: ATPase subunit 9, putative

Chain W1: 



- Molecule 25: ATPase subunit 9, putative

Chain X1: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, LMT, 3PE, PC1, ADP, MG, ATP, Q7G, UTP, AME

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	L	0.08	0/547	0.18	0/735
1	l	0.08	0/547	0.16	0/735
2	M	0.09	0/1049	0.19	0/1423
2	m	0.10	0/1049	0.20	0/1423
3	a	0.22	0/2111	0.27	0/2861
4	c	0.21	0/772	0.30	0/1054
5	d	0.13	0/2786	0.21	0/3760
6	e	0.16	0/3305	0.23	0/4482
7	f	0.17	0/1183	0.26	0/1601
8	g	0.08	0/1953	0.19	0/2650
9	h	0.07	0/1088	0.17	0/1466
10	i	0.19	0/913	0.24	0/1240
11	j	0.12	0/1462	0.20	0/1973
12	k	0.12	0/904	0.21	0/1228
13	n	0.18	0/1166	0.25	0/1581
14	o	0.11	0/814	0.19	0/1100
15	p	0.12	0/707	0.22	0/957
16	q	0.16	0/799	0.26	0/1091
17	r	0.15	0/567	0.24	0/767
18	A1	0.14	0/4122	0.24	0/5582
18	B1	0.13	0/4101	0.23	0/5553
18	C1	0.14	0/4159	0.23	0/5632
19	D1	0.13	0/3745	0.23	0/5077
19	E1	0.14	0/3745	0.23	0/5077
19	F1	0.13	0/3753	0.23	0/5088
20	G1	0.14	0/2427	0.24	0/3268
21	H1	0.16	0/1274	0.22	0/1728
22	I1	0.10	0/547	0.21	0/738
23	J1	0.08	0/1341	0.20	0/1810
23	K1	0.09	0/1342	0.20	0/1810
23	L1	0.09	0/1337	0.21	0/1803
24	M1	0.09	0/1916	0.20	0/2591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	O1	0.15	0/574	0.26	0/777
25	P1	0.13	0/574	0.25	0/777
25	Q1	0.12	0/574	0.25	0/777
25	R1	0.14	0/574	0.25	0/777
25	S1	0.14	0/574	0.26	0/777
25	T1	0.14	0/574	0.26	0/777
25	U1	0.15	0/574	0.26	0/777
25	V1	0.16	0/574	0.27	0/777
25	W1	0.18	0/574	0.27	0/777
25	X1	0.16	0/574	0.26	0/777
All	All	0.14	0/63271	0.23	0/85654

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	L	537	545	545	2	0
1	l	537	545	545	1	0
2	M	1027	1042	1042	10	0
2	m	1027	1042	1042	7	0
3	a	2032	2044	2044	17	0
4	c	745	715	715	15	0
5	d	2737	2762	2763	21	0
6	e	3220	3050	3061	20	0
7	f	1145	1111	1111	15	0
8	g	1933	2020	2020	17	0
9	h	1070	1088	1088	6	0
10	i	883	857	857	7	0
11	j	1424	1411	1411	8	0
12	k	873	876	876	6	0
13	n	1128	1082	1082	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	o	789	767	767	4	0
15	p	684	651	651	5	0
16	q	766	720	720	10	0
17	r	542	498	498	9	0
18	A1	4048	4171	4169	43	0
18	B1	4028	4146	4145	41	0
18	C1	4084	4197	4197	28	0
19	D1	3689	3742	3742	32	0
19	E1	3689	3742	3741	54	0
19	F1	3696	3750	3749	30	0
20	G1	2387	2387	2387	15	0
21	H1	1251	1232	1231	12	0
22	I1	533	513	513	9	0
23	J1	1314	1276	1276	14	0
23	K1	1315	1276	1276	8	0
23	L1	1310	1271	1271	11	0
24	M1	1877	1873	1873	15	0
25	O1	565	600	599	5	0
25	P1	565	600	599	4	0
25	Q1	565	600	599	8	0
25	R1	565	600	599	11	0
25	S1	565	601	599	14	0
25	T1	565	601	599	9	0
25	U1	565	600	599	7	0
25	V1	565	600	599	11	0
25	W1	565	600	599	9	0
25	X1	565	600	599	8	0
26	M	200	312	312	0	0
26	a	100	156	156	0	0
26	c	100	156	156	1	0
26	e	400	624	624	2	0
26	f	100	156	156	1	0
26	j	100	156	156	2	0
26	k	100	156	156	1	0
26	l	100	156	156	1	0
26	m	100	156	156	0	0
26	q	100	156	156	1	0
27	M	51	82	82	0	0
27	f	51	82	82	0	0
27	m	51	82	82	0	0
28	a	54	88	88	2	0
28	i	54	88	88	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	j	54	88	88	1	0
28	p	54	88	88	0	0
29	e	35	39	46	0	0
29	j	35	39	46	0	0
30	e	48	60	0	0	0
30	n	59	70	0	0	0
31	A1	31	12	12	0	0
31	B1	31	12	12	2	0
31	C1	31	12	12	0	0
31	E1	31	12	12	2	0
32	A1	1	0	0	0	0
32	B1	1	0	0	0	0
32	C1	1	0	0	0	0
32	E1	1	0	0	0	0
32	F1	1	0	0	0	0
33	F1	27	12	12	1	0
34	H1	29	11	11	3	0
All	All	64101	65465	65343	481	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 4.

The worst 5 of 481 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)
11:j:19:ARG:NH2	16:q:77:GLU:O	2.08	0.85
2:M:119:ARG:NH2	2:M:122:ILE:O	2.18	0.77
2:M:67:GLN:NE2	2:m:36:ASP:OD2	2.19	0.75
19:E1:308:GLN:OE1	19:E1:308:GLN:N	2.21	0.73
25:V1:104:ILE:HD11	25:W1:102:GLU:OE1	1.90	0.72

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	L	63/92 (68%)	63 (100%)	0	0	100	100
1	l	63/92 (68%)	63 (100%)	0	0	100	100
2	M	127/144 (88%)	126 (99%)	1 (1%)	0	100	100
2	m	127/144 (88%)	127 (100%)	0	0	100	100
3	a	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
4	c	84/114 (74%)	80 (95%)	4 (5%)	0	100	100
5	d	328/370 (89%)	325 (99%)	3 (1%)	0	100	100
6	e	381/396 (96%)	373 (98%)	8 (2%)	0	100	100
7	f	133/145 (92%)	129 (97%)	4 (3%)	0	100	100
8	g	266/269 (99%)	262 (98%)	4 (2%)	0	100	100
9	h	135/157 (86%)	133 (98%)	2 (2%)	0	100	100
10	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
11	j	166/169 (98%)	160 (96%)	6 (4%)	0	100	100
12	k	103/124 (83%)	101 (98%)	2 (2%)	0	100	100
13	n	137/156 (88%)	130 (95%)	7 (5%)	0	100	100
14	o	94/101 (93%)	94 (100%)	0	0	100	100
15	p	78/105 (74%)	76 (97%)	2 (3%)	0	100	100
16	q	83/98 (85%)	81 (98%)	2 (2%)	0	100	100
17	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	A1	518/584 (89%)	502 (97%)	16 (3%)	0	100	100
18	B1	516/584 (88%)	506 (98%)	9 (2%)	1 (0%)	43	72
18	C1	526/584 (90%)	513 (98%)	13 (2%)	0	100	100
19	D1	485/519 (93%)	476 (98%)	9 (2%)	0	100	100
19	E1	485/519 (93%)	477 (98%)	7 (1%)	1 (0%)	43	72
19	F1	486/519 (94%)	476 (98%)	9 (2%)	1 (0%)	43	72
20	G1	298/305 (98%)	297 (100%)	1 (0%)	0	100	100
21	H1	159/182 (87%)	156 (98%)	3 (2%)	0	100	100
22	I1	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
23	J1	164/188 (87%)	161 (98%)	3 (2%)	0	100	100
23	K1	164/188 (87%)	157 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	L1	163/188 (87%)	160 (98%)	3 (2%)	0	100	100
24	M1	230/255 (90%)	224 (97%)	6 (3%)	0	100	100
25	O1	76/118 (64%)	76 (100%)	0	0	100	100
25	P1	76/118 (64%)	76 (100%)	0	0	100	100
25	Q1	76/118 (64%)	76 (100%)	0	0	100	100
25	R1	76/118 (64%)	76 (100%)	0	0	100	100
25	S1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
25	T1	76/118 (64%)	76 (100%)	0	0	100	100
25	U1	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
25	V1	76/118 (64%)	76 (100%)	0	0	100	100
25	W1	76/118 (64%)	76 (100%)	0	0	100	100
25	X1	76/118 (64%)	76 (100%)	0	0	100	100
All	All	7775/8943 (87%)	7633 (98%)	139 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	E1	305	VAL
19	F1	305	VAL
18	B1	532	THR

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	L	55/75 (73%)	55 (100%)	0	100	100
1	l	55/75 (73%)	55 (100%)	0	100	100
2	M	111/124 (90%)	110 (99%)	1 (1%)	70	75
2	m	111/124 (90%)	111 (100%)	0	100	100
3	a	225/225 (100%)	223 (99%)	2 (1%)	70	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	c	80/104 (77%)	80 (100%)	0	100	100
5	d	297/334 (89%)	296 (100%)	1 (0%)	86	83
6	e	334/341 (98%)	334 (100%)	0	100	100
7	f	119/124 (96%)	117 (98%)	2 (2%)	53	67
8	g	205/206 (100%)	204 (100%)	1 (0%)	81	80
9	h	110/123 (89%)	110 (100%)	0	100	100
10	i	95/96 (99%)	95 (100%)	0	100	100
11	j	149/150 (99%)	148 (99%)	1 (1%)	76	77
12	k	91/107 (85%)	91 (100%)	0	100	100
13	n	123/137 (90%)	122 (99%)	1 (1%)	73	76
14	o	82/86 (95%)	81 (99%)	1 (1%)	63	72
15	p	75/94 (80%)	75 (100%)	0	100	100
16	q	80/92 (87%)	80 (100%)	0	100	100
17	r	56/56 (100%)	56 (100%)	0	100	100
18	A1	436/479 (91%)	436 (100%)	0	100	100
18	B1	433/479 (90%)	431 (100%)	2 (0%)	81	80
18	C1	439/479 (92%)	438 (100%)	1 (0%)	87	86
19	D1	398/420 (95%)	398 (100%)	0	100	100
19	E1	398/420 (95%)	397 (100%)	1 (0%)	86	83
19	F1	399/420 (95%)	394 (99%)	5 (1%)	61	71
20	G1	253/257 (98%)	252 (100%)	1 (0%)	84	81
21	H1	137/156 (88%)	136 (99%)	1 (1%)	76	77
22	I1	58/67 (87%)	58 (100%)	0	100	100
23	J1	145/162 (90%)	145 (100%)	0	100	100
23	K1	145/162 (90%)	145 (100%)	0	100	100
23	L1	145/162 (90%)	145 (100%)	0	100	100
24	M1	200/215 (93%)	199 (100%)	1 (0%)	81	80
25	O1	56/89 (63%)	55 (98%)	1 (2%)	51	67
25	P1	56/89 (63%)	56 (100%)	0	100	100
25	Q1	56/89 (63%)	56 (100%)	0	100	100
25	R1	56/89 (63%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	S1	56/89 (63%)	56 (100%)	0	100	100
25	T1	56/89 (63%)	55 (98%)	1 (2%)	51	67
25	U1	56/89 (63%)	56 (100%)	0	100	100
25	V1	56/89 (63%)	56 (100%)	0	100	100
25	W1	56/89 (63%)	54 (96%)	2 (4%)	31	54
25	X1	56/89 (63%)	56 (100%)	0	100	100
All	All	6599/7441 (89%)	6573 (100%)	26 (0%)	81	81

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	F1	45	VAL
19	F1	171	LEU
25	W1	51	HIS
19	F1	102	VAL
19	F1	193	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
23	L1	163	GLN
24	M1	112	ASN
25	P1	83	GLN
18	A1	558	GLN
18	A1	525	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	AME	e	1	6	9,10,11	0.29	0	9,11,13	0.41	0

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
6	AME	e	1	6	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	e	1	AME	CT2-CT1-N-CA
6	e	1	AME	OT-CT1-N-CA
6	e	1	AME	CA-CB-CG-SD
6	e	1	AME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 5 are monoatomic - leaving 31 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
26	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	M	201	-	99,99,99	0.29	0	105,111,111	0.25	0
28	PC1	i	201	-	53,53,53	0.28	0	59,61,61	0.29	0
26	CDL	e	402	-	99,99,99	0.28	0	105,111,111	0.26	0
26	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.27	0
29	LMT	e	405	-	36,36,36	0.10	0	47,47,47	0.16	0
30	Q7G	e	406	-	54,54,90	0.14	0	80,84,138	0.25	0
26	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.27	0
28	PC1	a	302	-	53,53,53	0.27	0	59,61,61	0.28	0
28	PC1	p	201	-	53,53,53	0.28	0	59,61,61	0.29	0
30	Q7G	n	201	-	66,66,90	0.13	0	98,102,138	0.28	0
26	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
27	3PE	M	203	-	50,50,50	0.25	0	53,55,55	0.23	0
31	ATP	A1	601	32	32,33,33	0.29	0	48,52,52	0.29	0
31	ATP	E1	601	32	32,33,33	0.29	0	48,52,52	0.28	0
29	LMT	j	203	-	36,36,36	0.11	0	47,47,47	0.19	0
26	CDL	a	301	-	99,99,99	0.29	0	105,111,111	0.26	0
28	PC1	j	202	-	53,53,53	0.28	0	59,61,61	0.28	0
31	ATP	B1	601	32	32,33,33	0.30	0	48,52,52	0.29	0
26	CDL	k	201	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	M	202	-	99,99,99	0.29	0	105,111,111	0.25	0
33	ADP	F1	601	32	28,29,29	0.49	0	43,45,45	0.57	0
26	CDL	m	201	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	e	403	-	99,99,99	0.29	0	105,111,111	0.26	0
27	3PE	f	202	-	50,50,50	0.26	0	53,55,55	0.22	0
31	ATP	C1	601	32	32,33,33	0.30	0	48,52,52	0.31	0
26	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.26	0
27	3PE	m	202	-	50,50,50	0.24	0	53,55,55	0.22	0
26	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.27	0
34	UTP	H1	201	-	29,30,30	0.29	0	43,47,47	0.33	0
26	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.26	0

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
26	CDL	j	201	-	-	22/110/110/110	-
26	CDL	M	201	-	-	14/110/110/110	-
28	PC1	i	201	-	-	8/57/57/57	-
26	CDL	e	402	-	-	24/110/110/110	-
26	CDL	e	401	-	-	18/110/110/110	-
29	LMT	e	405	-	-	1/21/61/61	0/2/2/2
30	Q7G	e	406	-	1/1/19/34	5/15/123/200	0/7/7/10
26	CDL	f	201	-	-	24/110/110/110	-
28	PC1	a	302	-	-	9/57/57/57	-
30	Q7G	n	201	-	2/2/24/34	5/20/148/200	0/8/8/10
28	PC1	p	201	-	-	5/57/57/57	-
26	CDL	q	101	-	-	32/110/110/110	-
27	3PE	M	203	-	-	15/54/54/54	-
31	ATP	A1	601	32	-	7/22/38/38	0/3/3/3
31	ATP	E1	601	32	-	6/22/38/38	0/3/3/3
29	LMT	j	203	-	-	5/21/61/61	0/2/2/2
26	CDL	a	301	-	-	26/110/110/110	-
28	PC1	j	202	-	-	10/57/57/57	-
31	ATP	B1	601	32	-	3/22/38/38	0/3/3/3
26	CDL	k	201	-	-	26/110/110/110	-
26	CDL	M	202	-	-	28/110/110/110	-
33	ADP	F1	601	32	-	2/16/32/32	0/3/3/3
26	CDL	m	201	-	-	24/110/110/110	-
26	CDL	e	403	-	-	28/110/110/110	-
27	3PE	f	202	-	-	11/54/54/54	-
31	ATP	C1	601	32	-	4/22/38/38	0/3/3/3
26	CDL	l	101	-	-	12/110/110/110	-
27	3PE	m	202	-	-	8/54/54/54	-
26	CDL	c	201	-	-	21/110/110/110	-
34	UTP	H1	201	-	-	3/22/38/38	0/2/2/2
26	CDL	e	404	-	-	16/110/110/110	-

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	e	406	Q7G	C1B
30	n	201	Q7G	C1B
30	n	201	Q7G	C1C

5 of 422 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	M	201	CDL	CA3-OA5-PA1-OA2
26	M	202	CDL	CA3-OA5-PA1-OA2
26	M	202	CDL	CA3-OA5-PA1-OA3
26	M	202	CDL	CB2-OB2-PB2-OB3
26	M	202	CDL	CB2-OB2-PB2-OB5

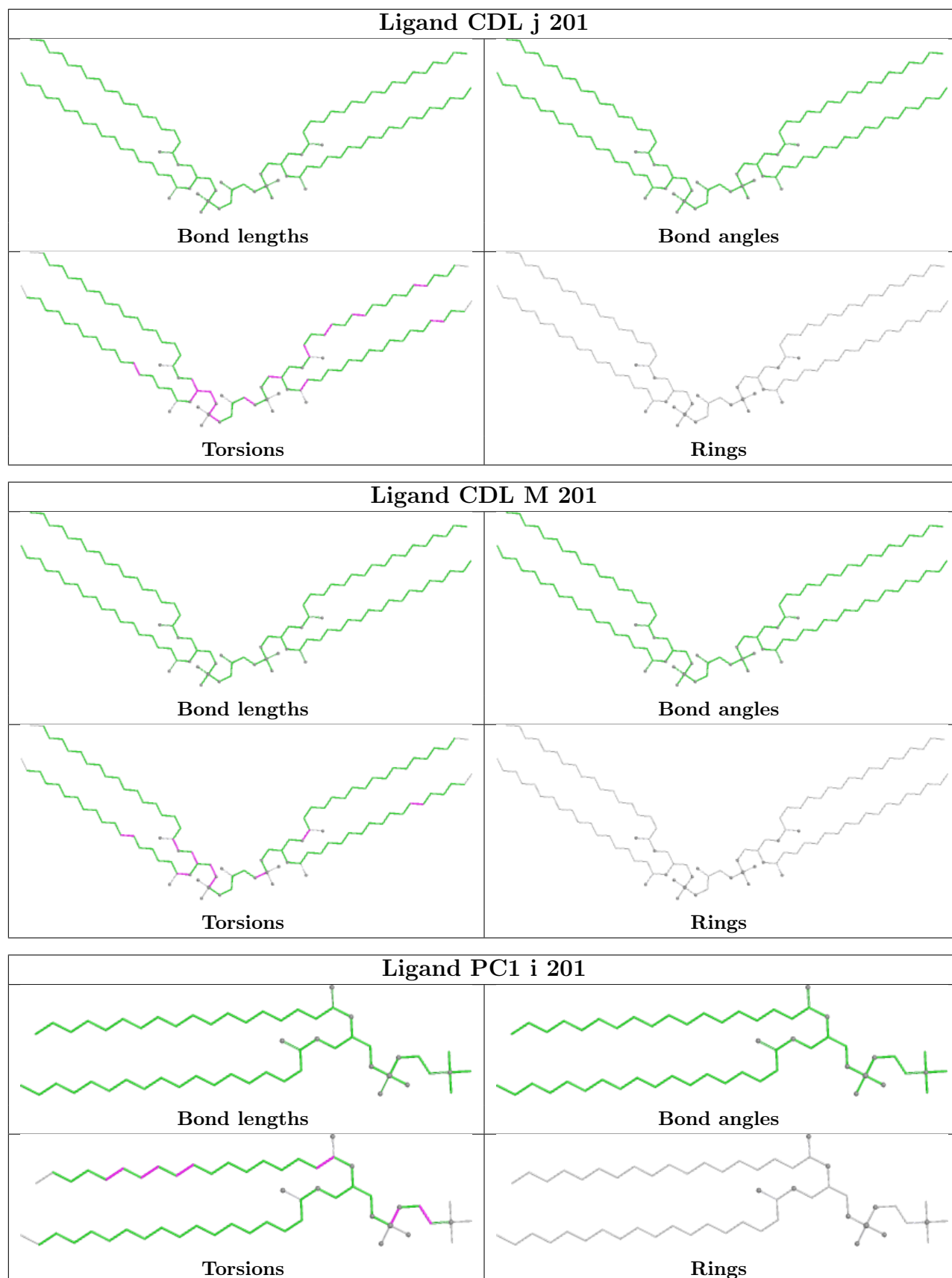
There are no ring outliers.

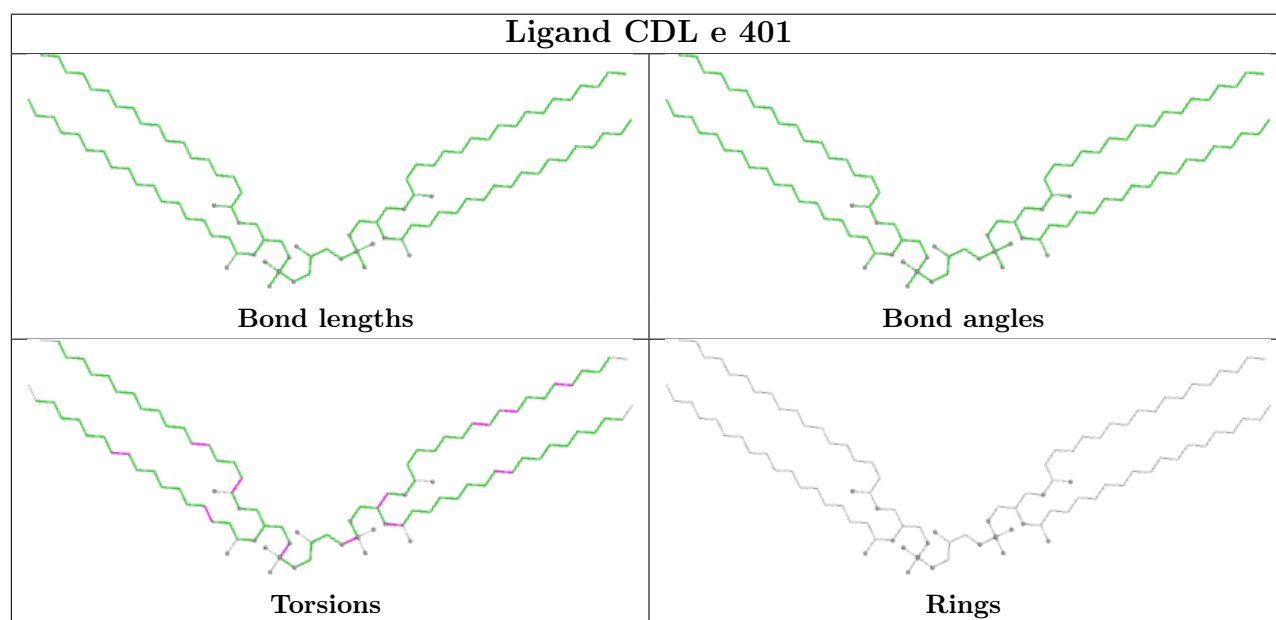
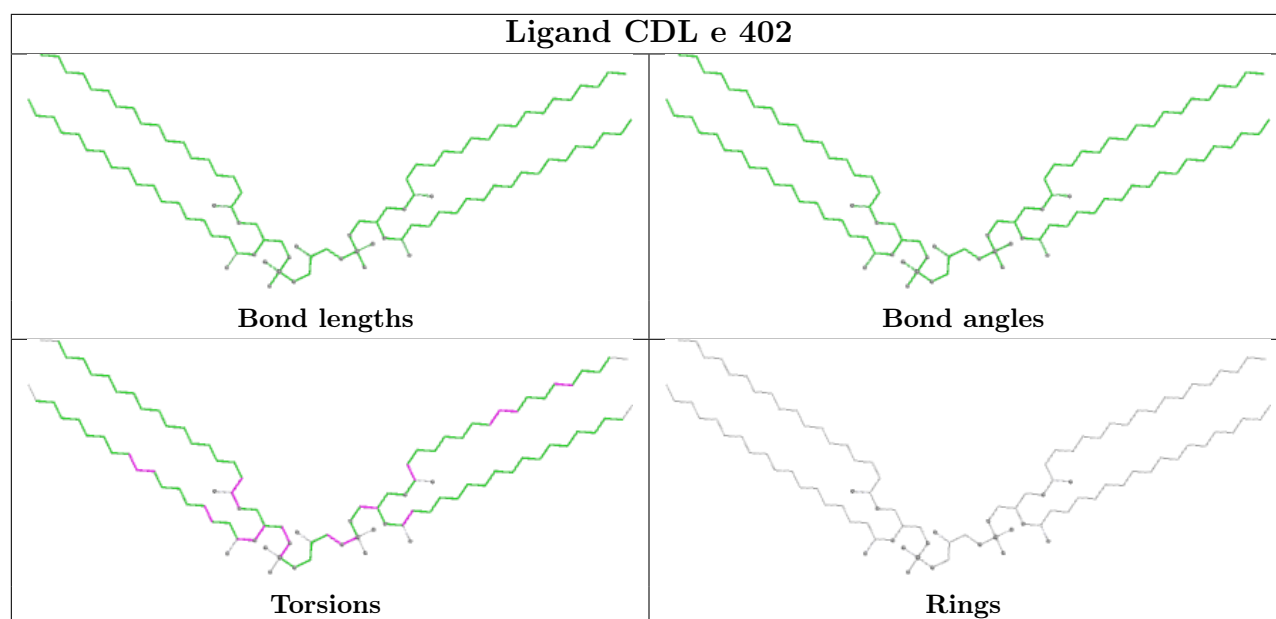
14 monomers are involved in 20 short contacts:

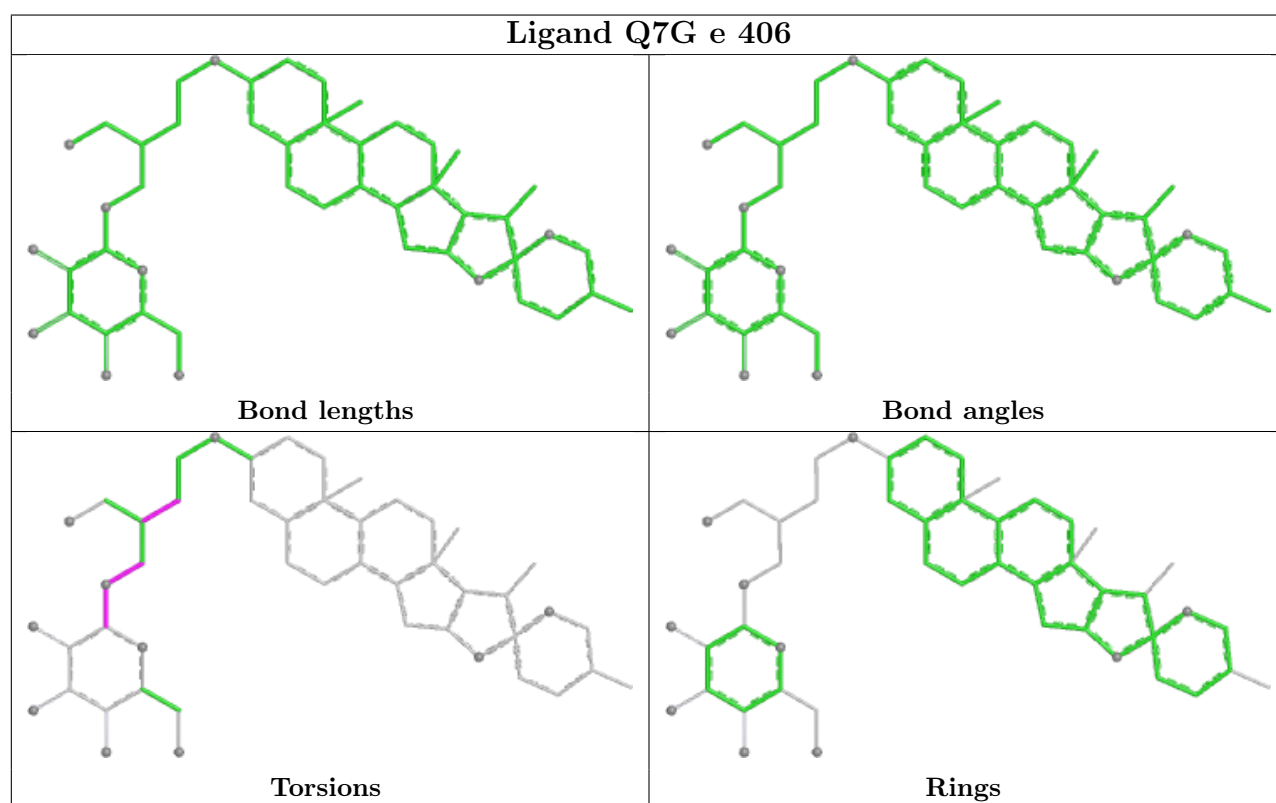
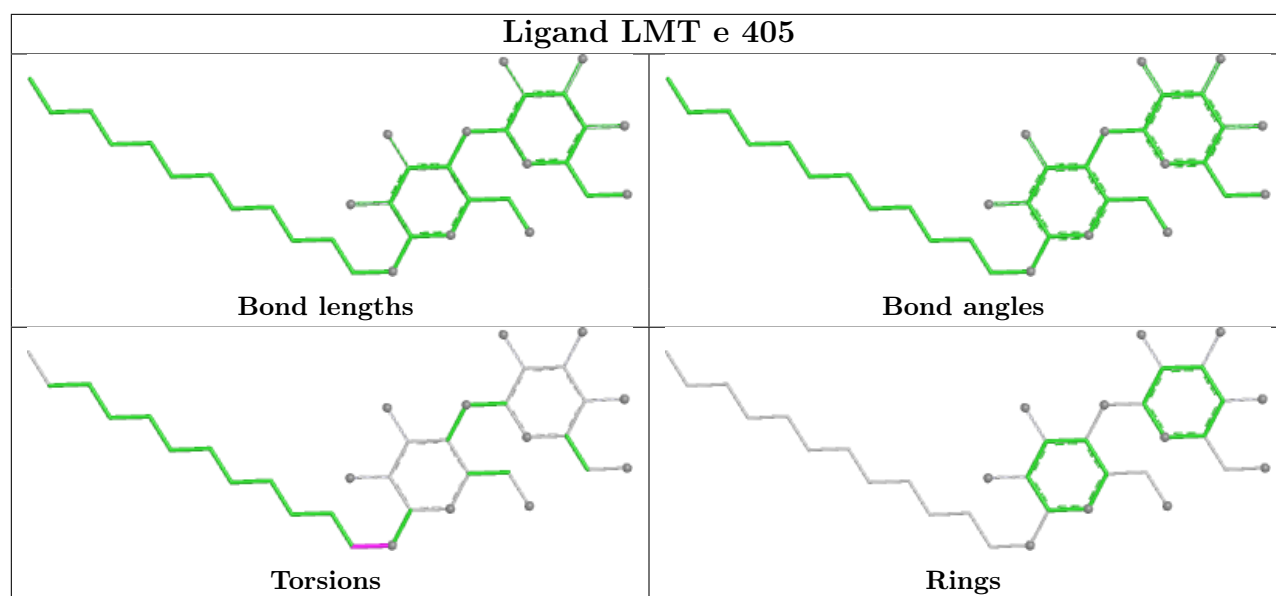
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	j	201	CDL	2	0
26	e	402	CDL	1	0
26	e	401	CDL	1	0
26	f	201	CDL	1	0
28	a	302	PC1	2	0
26	q	101	CDL	1	0
31	E1	601	ATP	2	0
28	j	202	PC1	1	0
31	B1	601	ATP	2	0
26	k	201	CDL	1	0
33	F1	601	ADP	1	0
26	l	101	CDL	1	0
26	c	201	CDL	1	0
34	H1	201	UTP	3	0

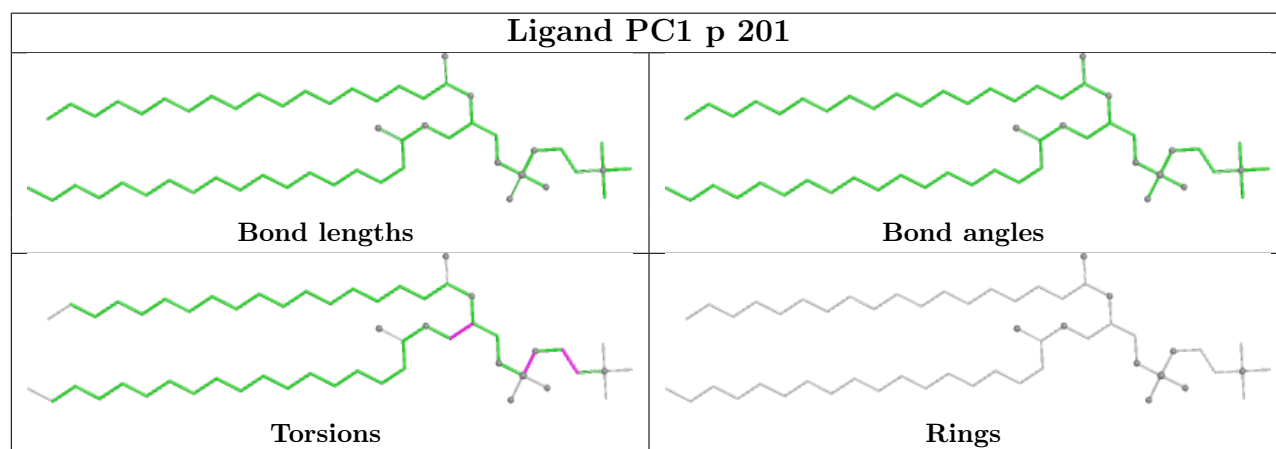
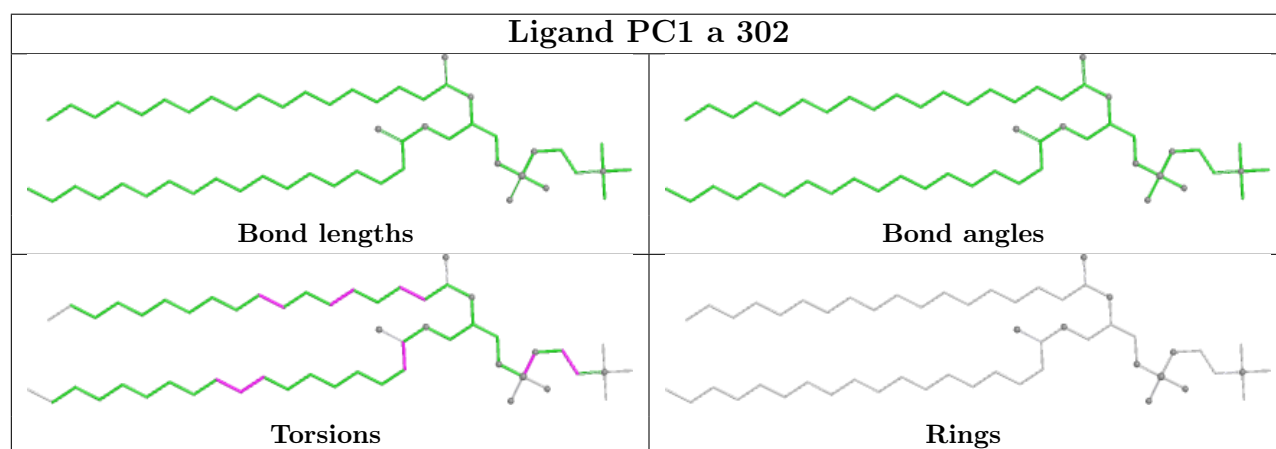
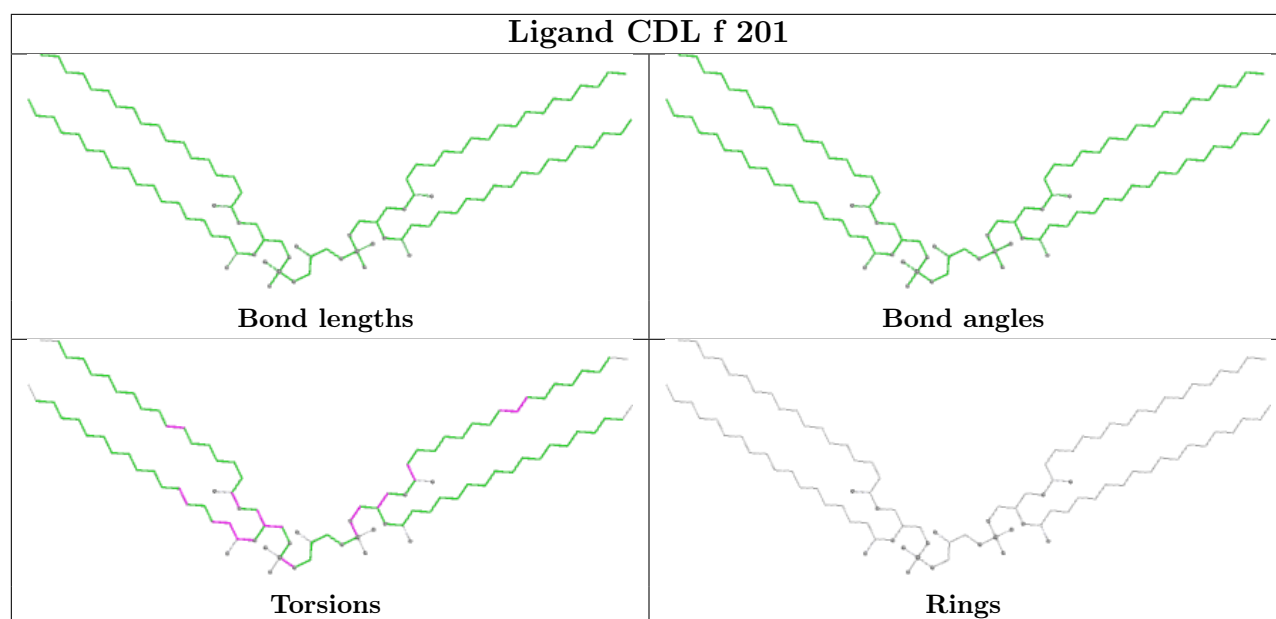
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

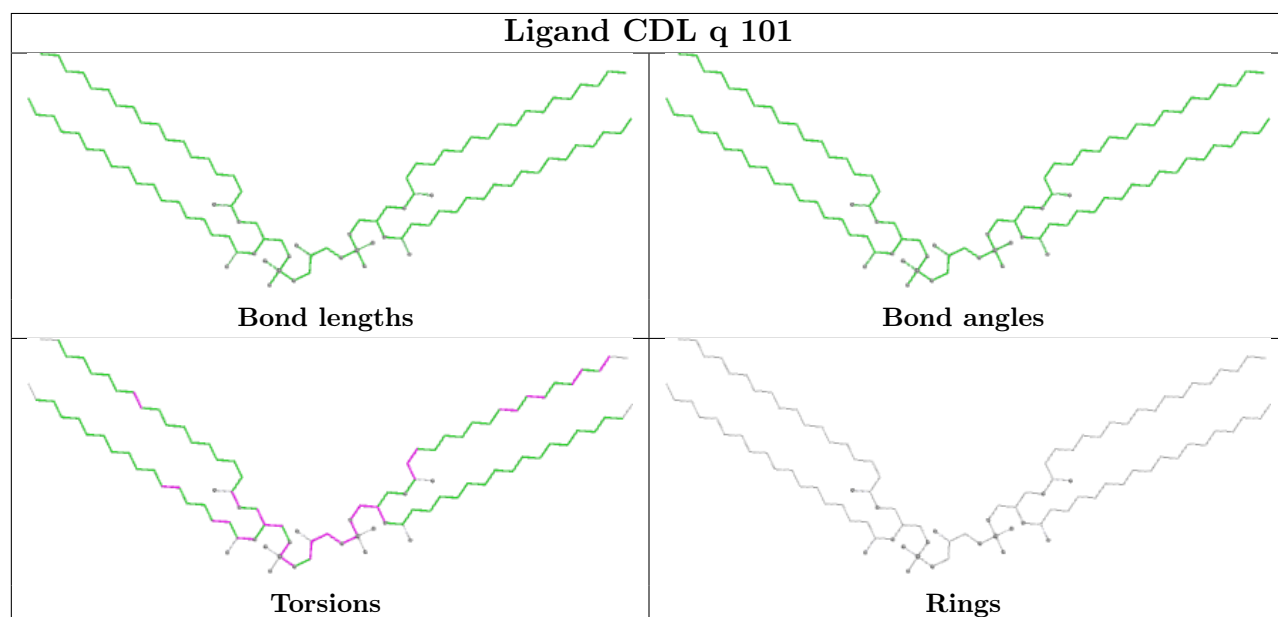
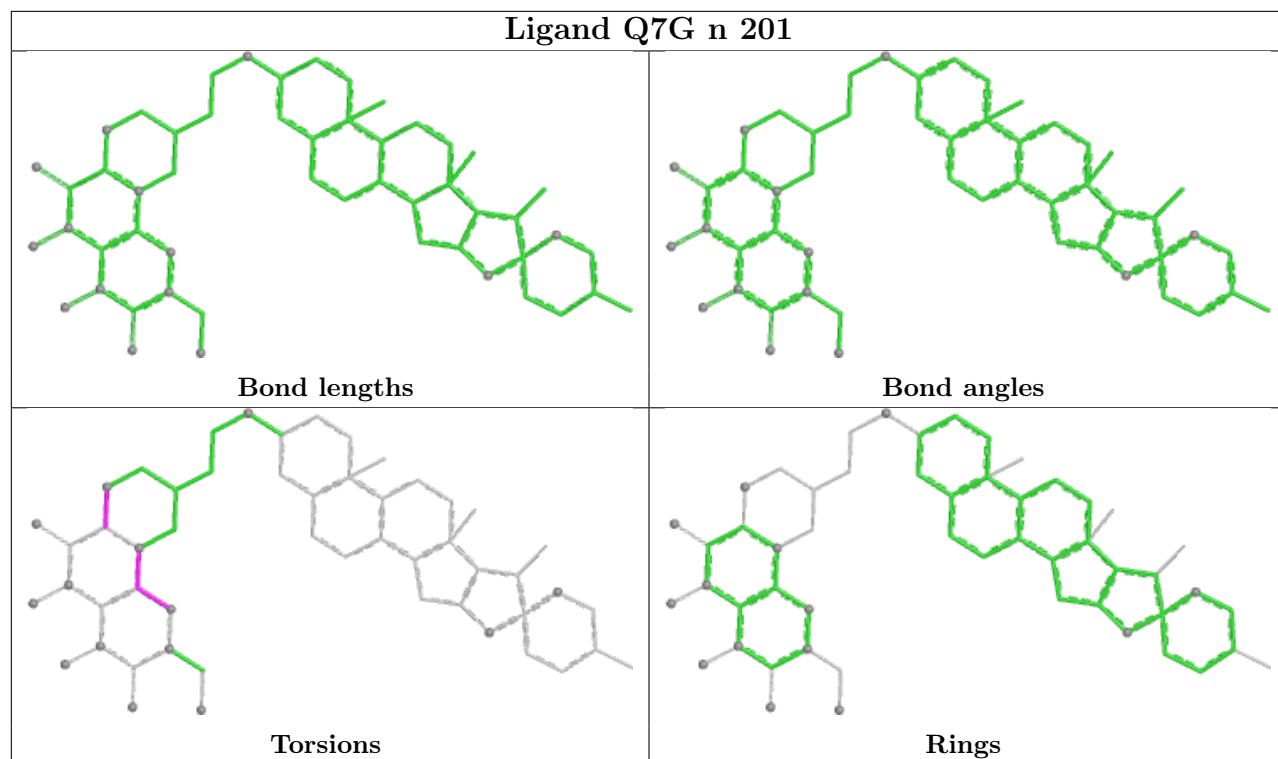
equivalents in the CSD to analyse the geometry.

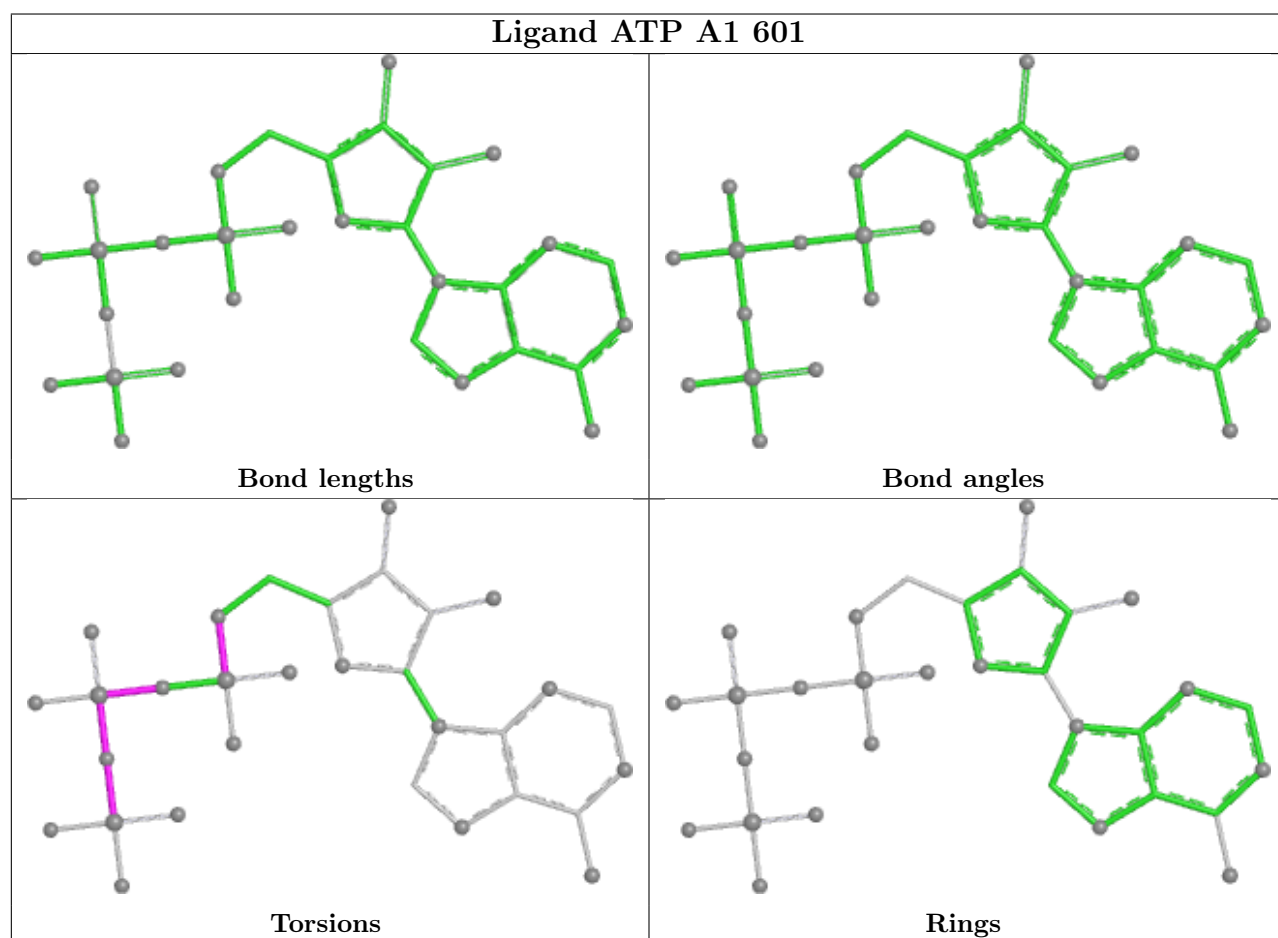
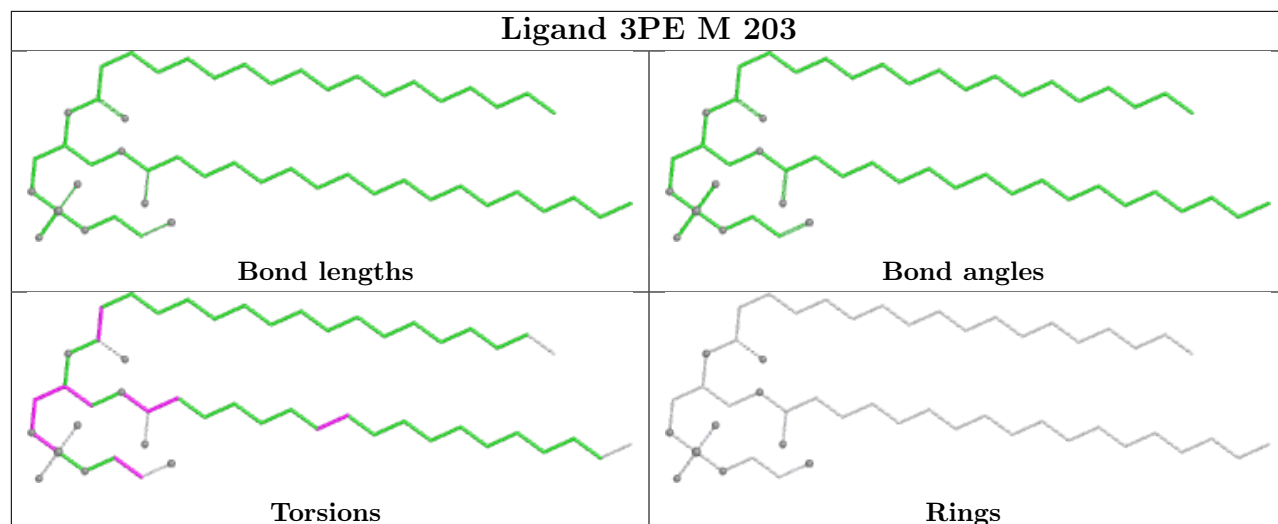


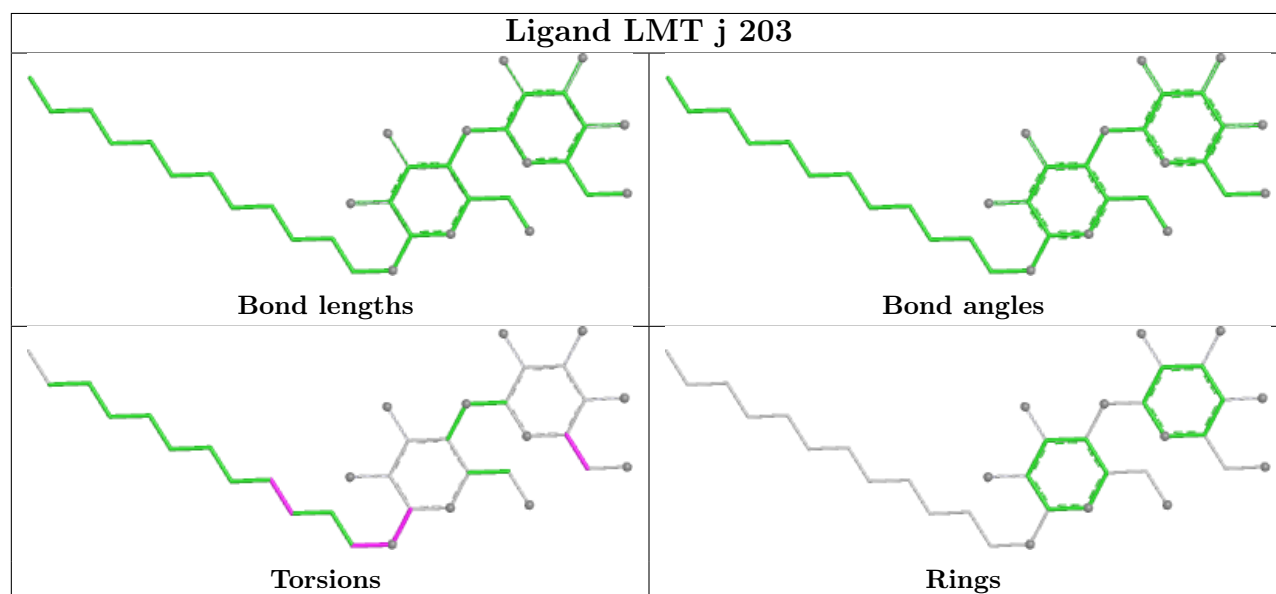
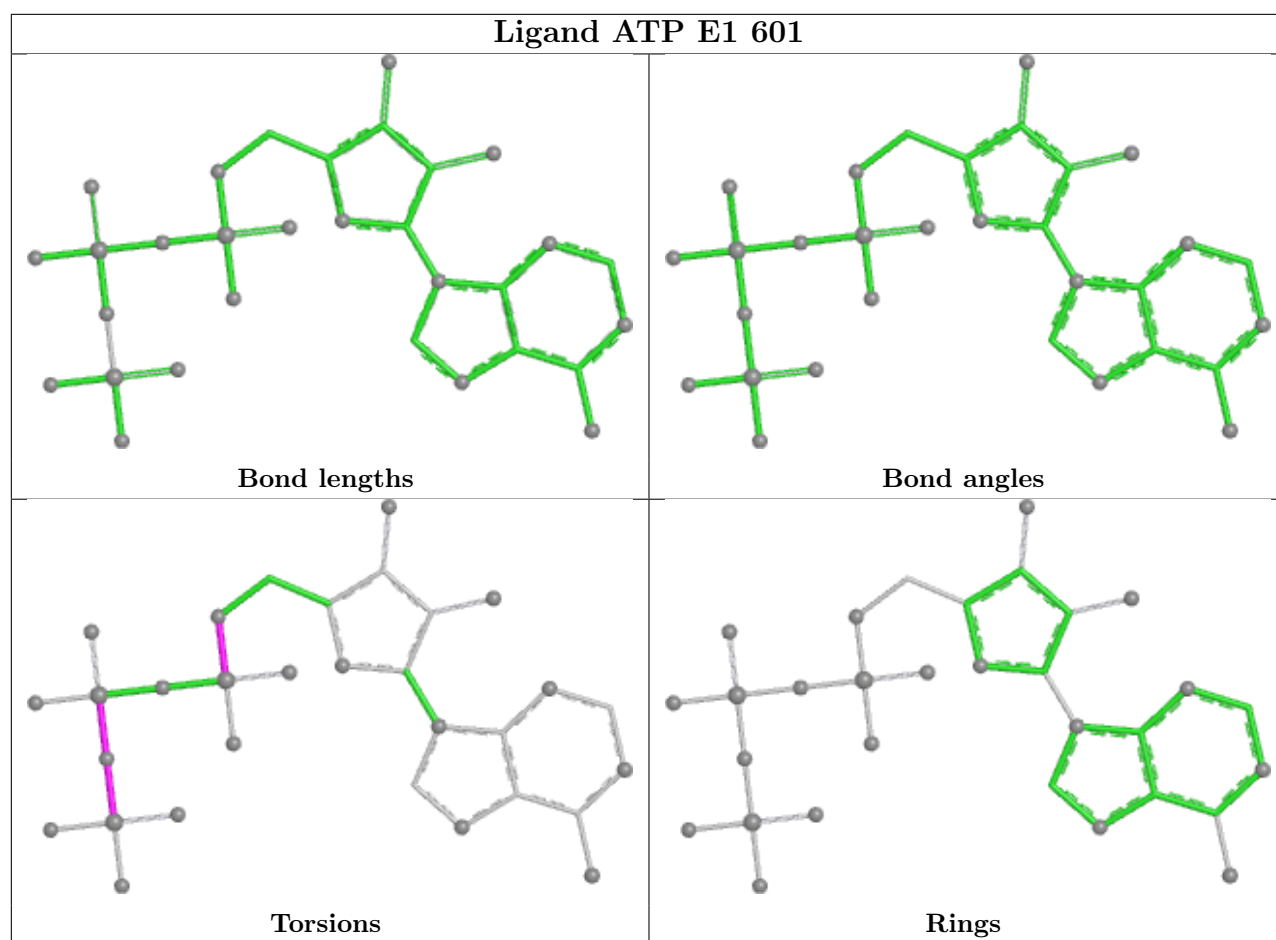


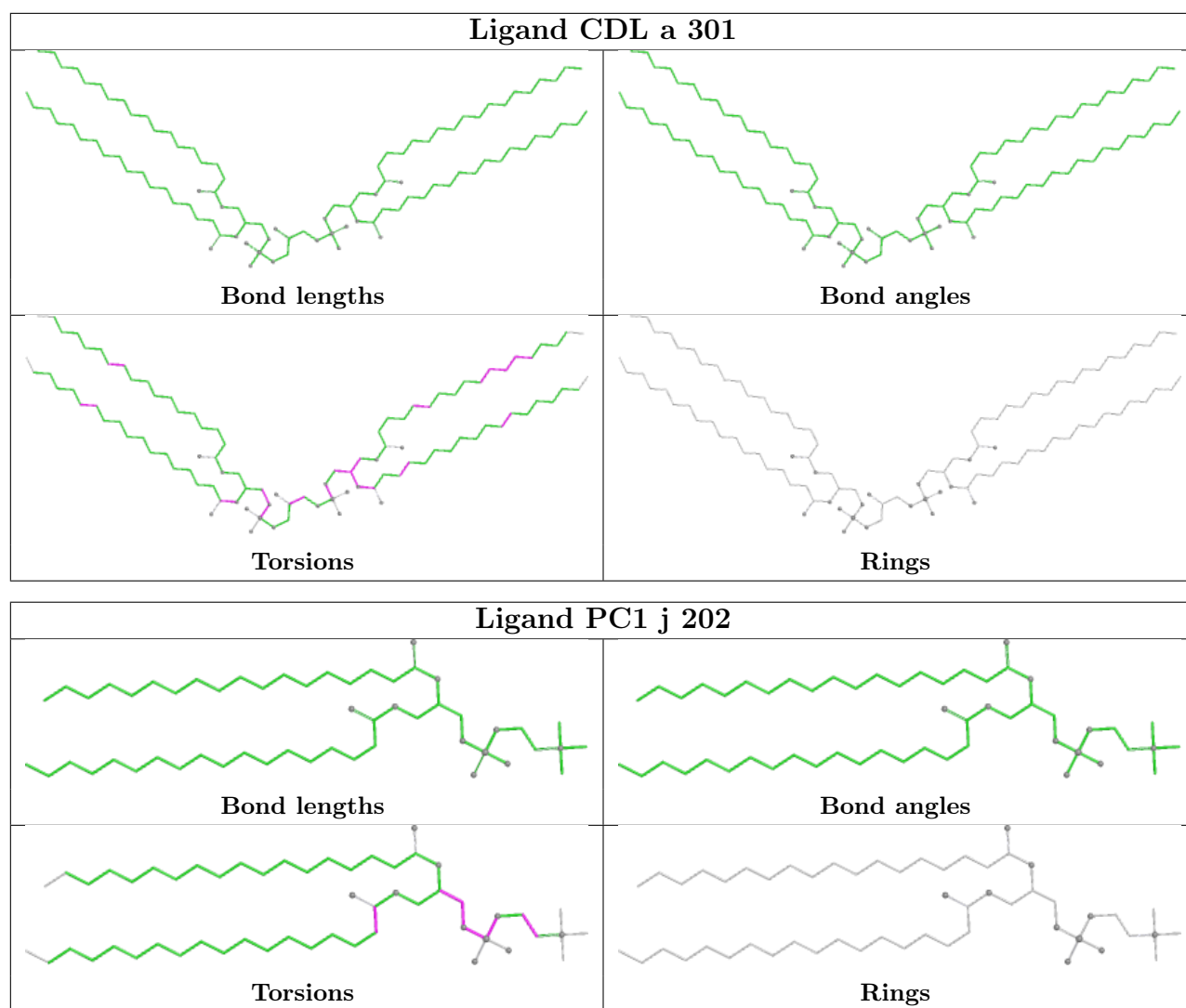


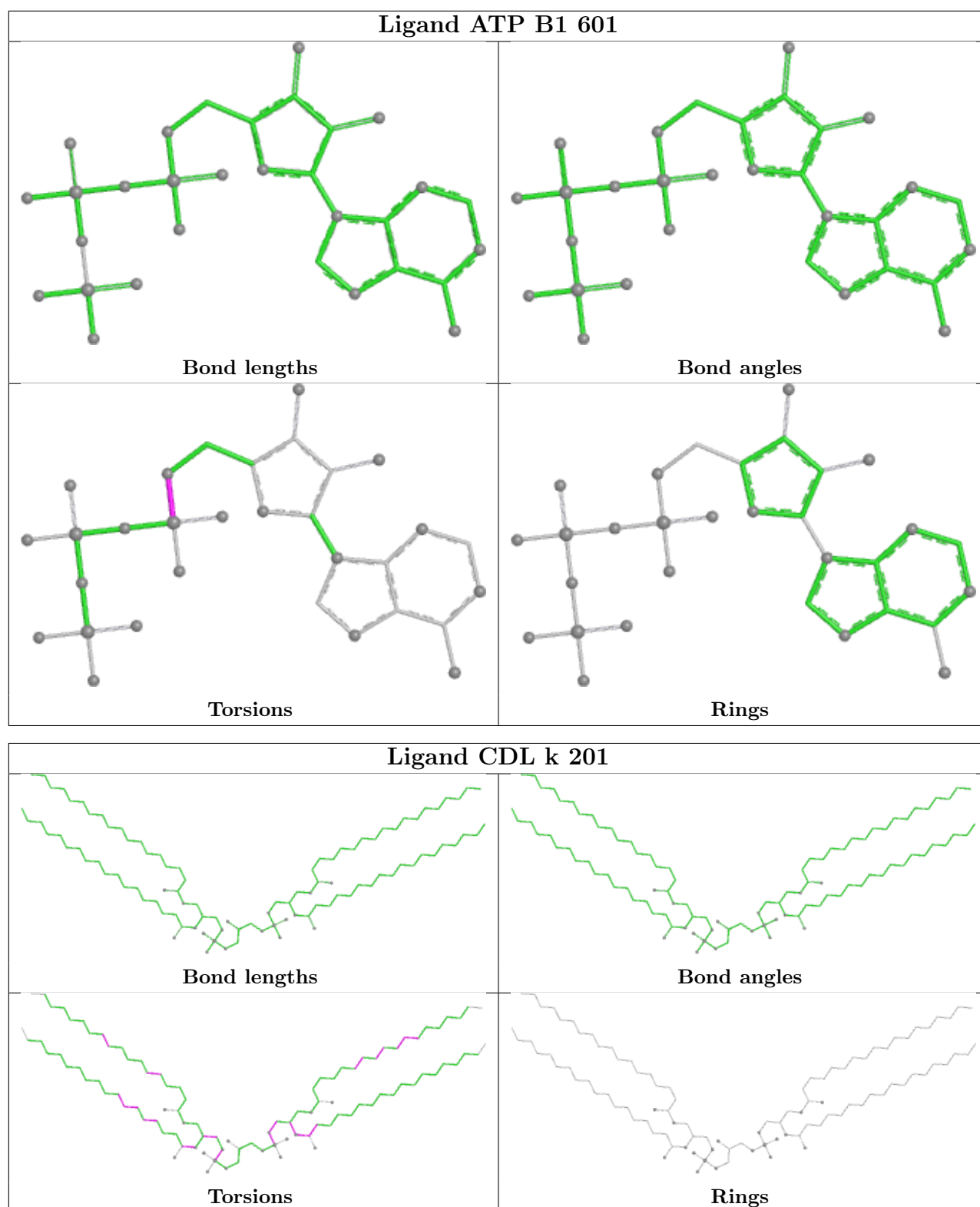


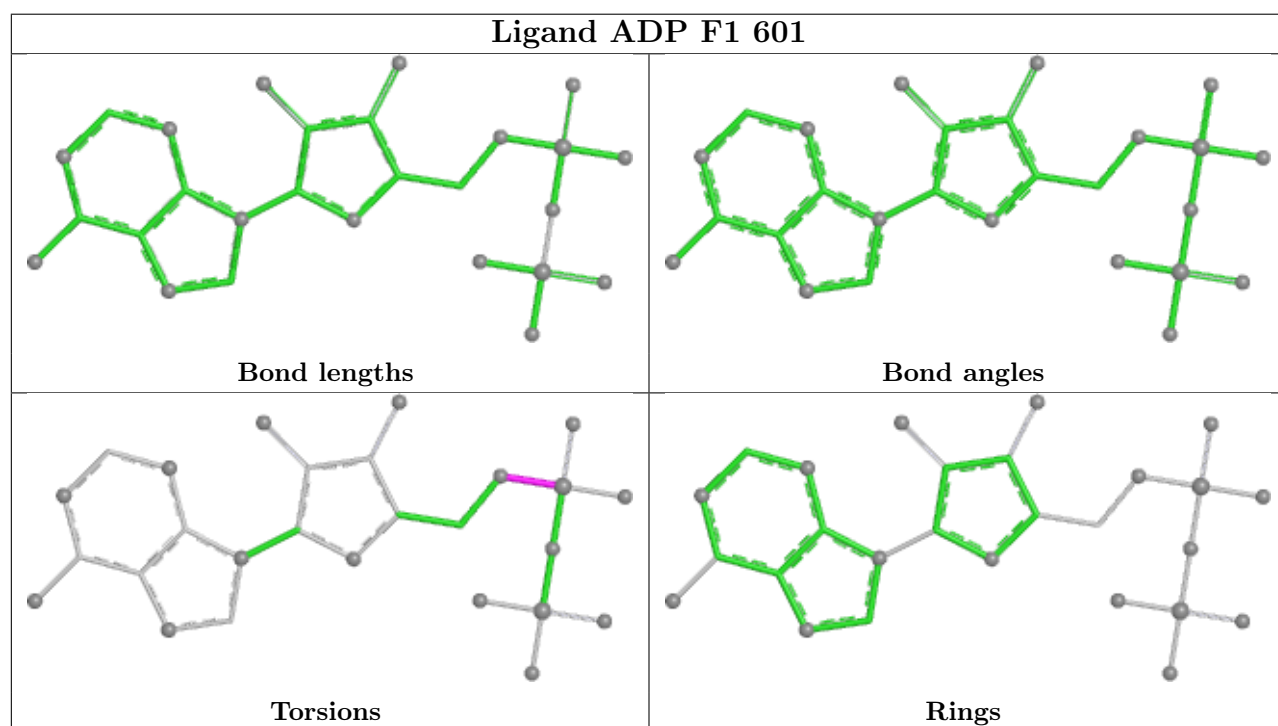
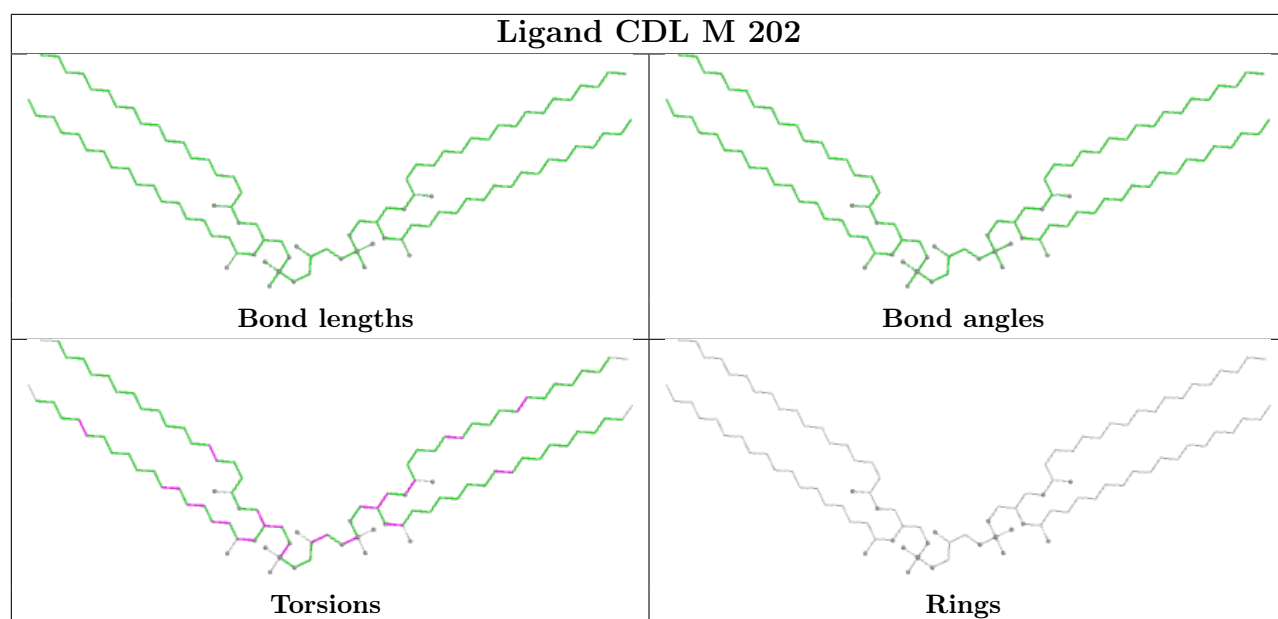


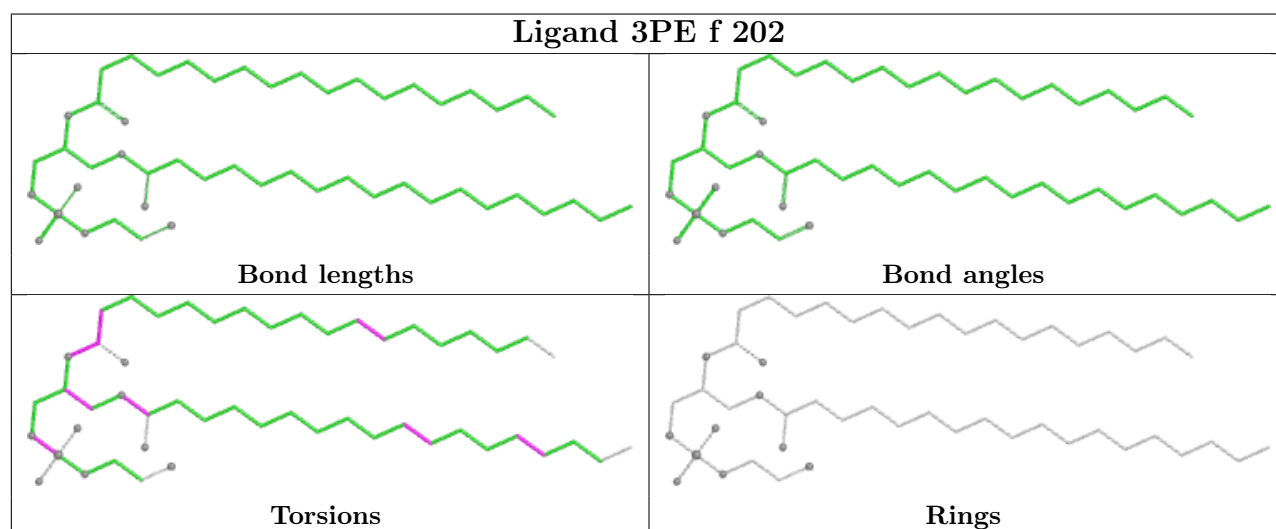
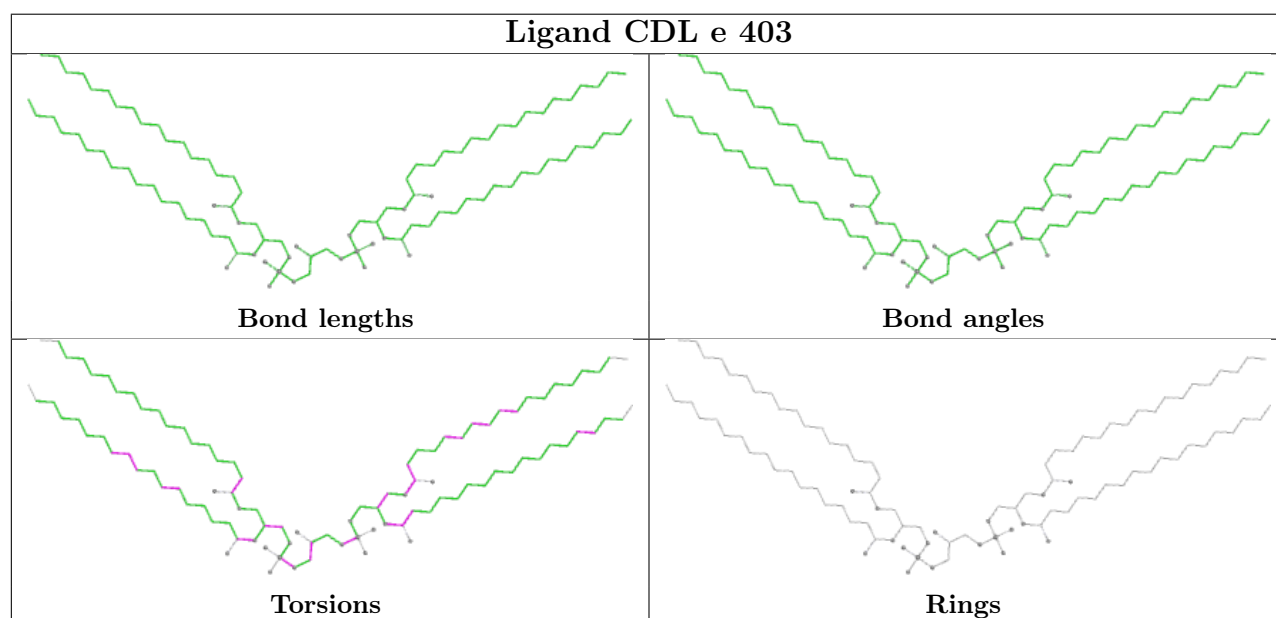
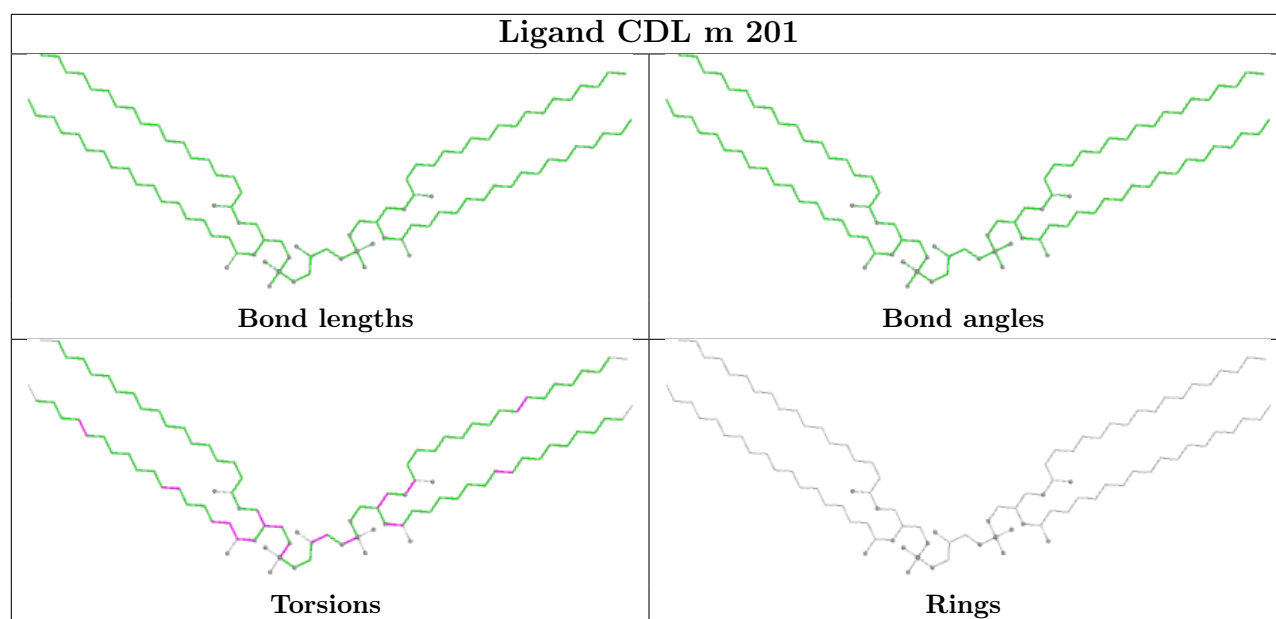


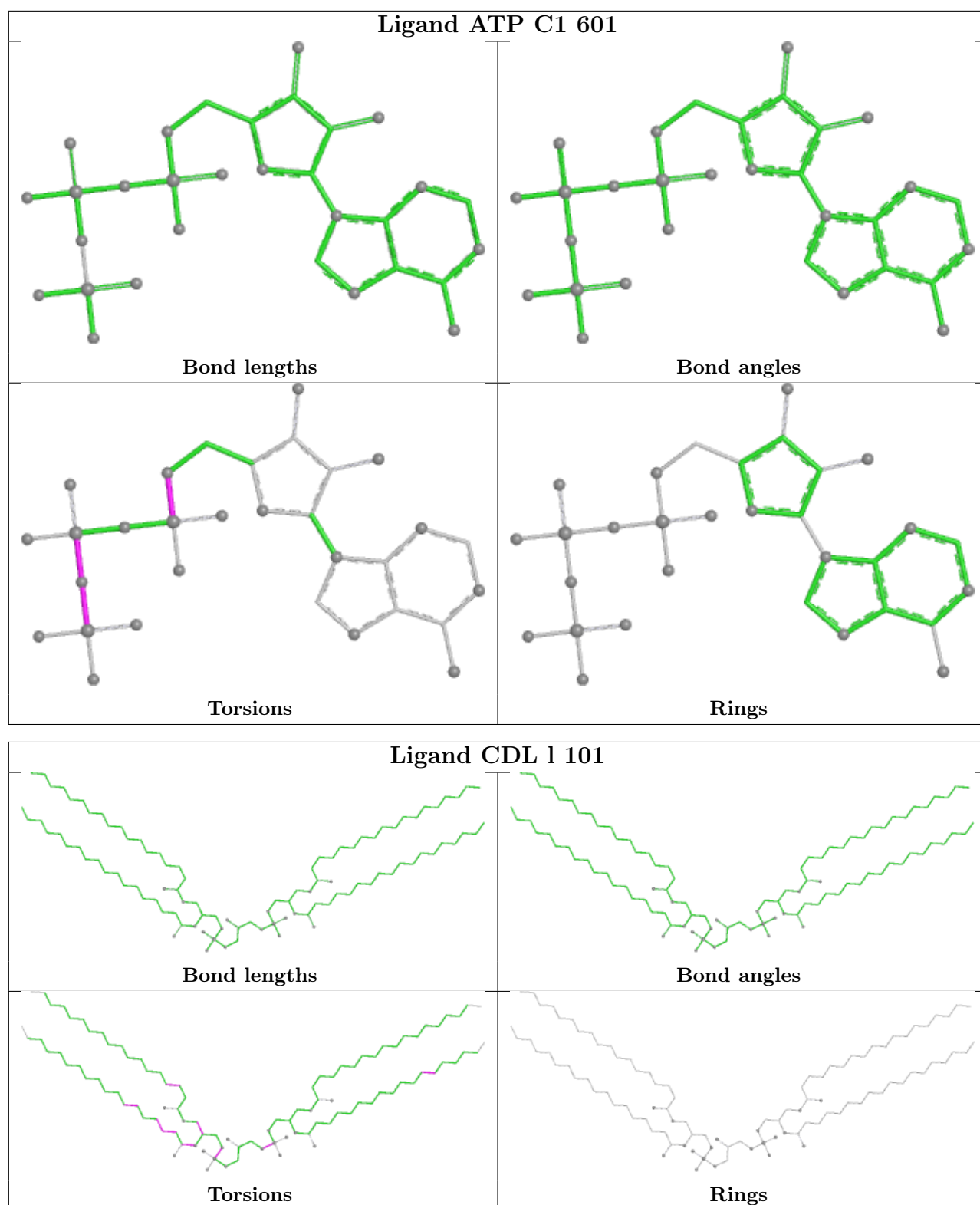


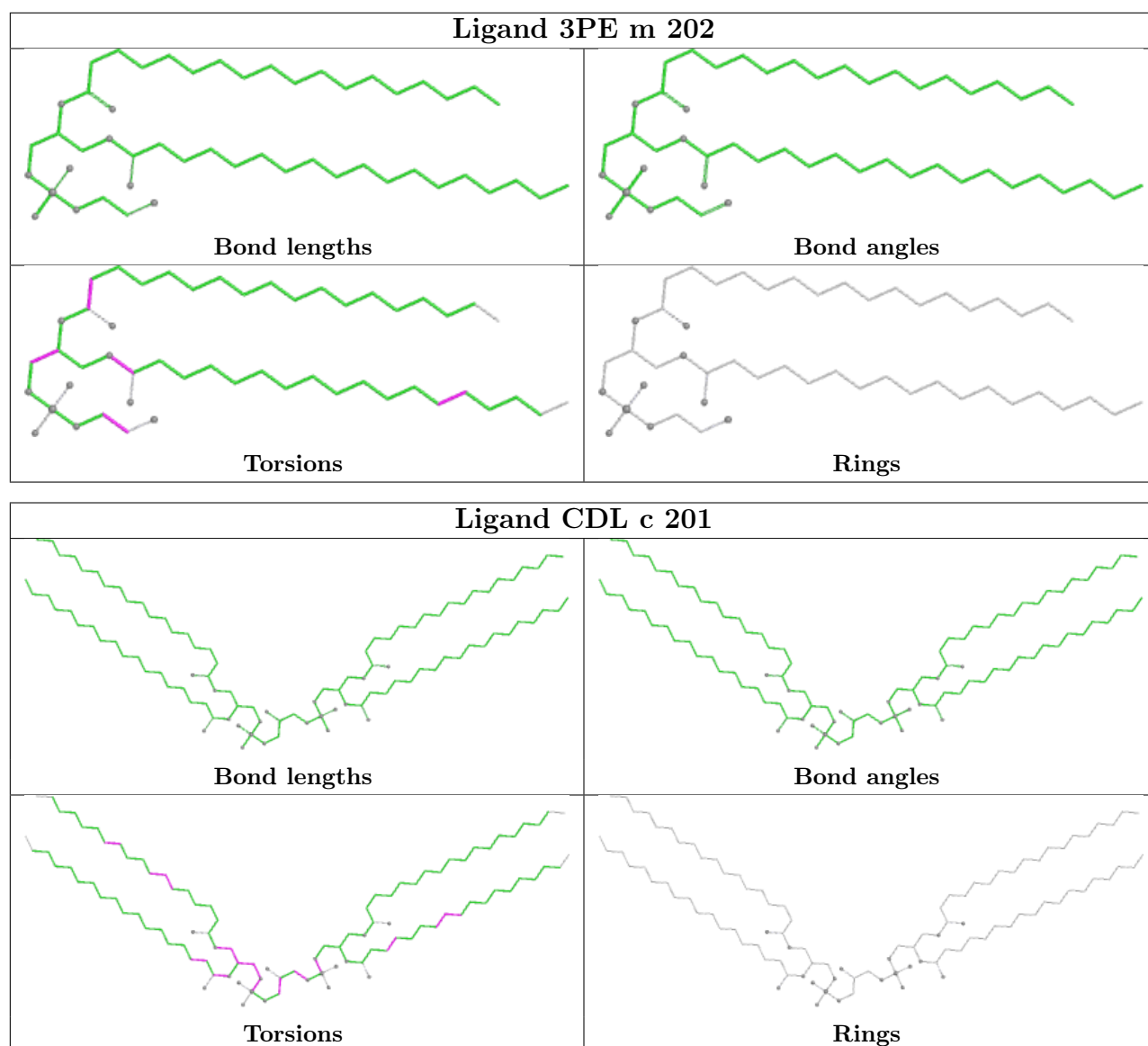


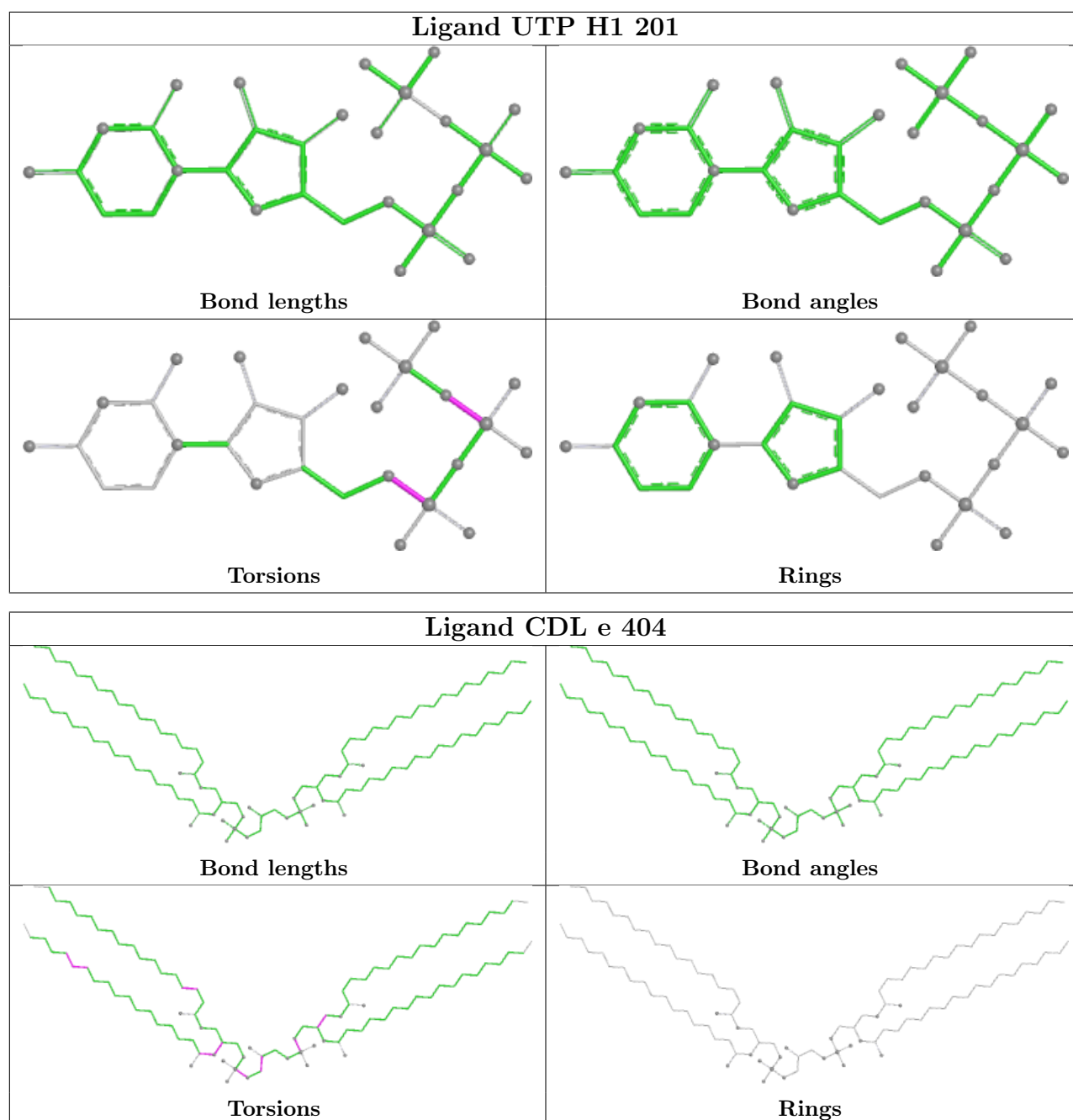












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

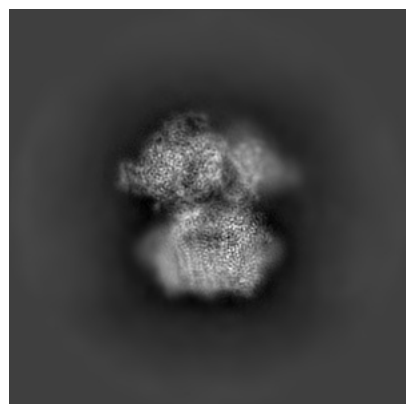
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15573. These allow visual inspection of the internal detail of the map and identification of artifacts.

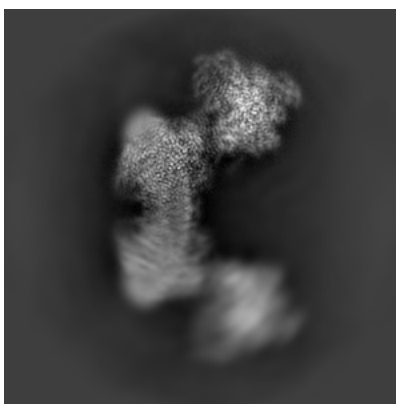
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

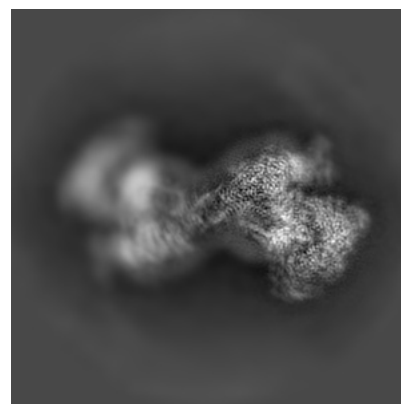
6.1.1 Primary map



X

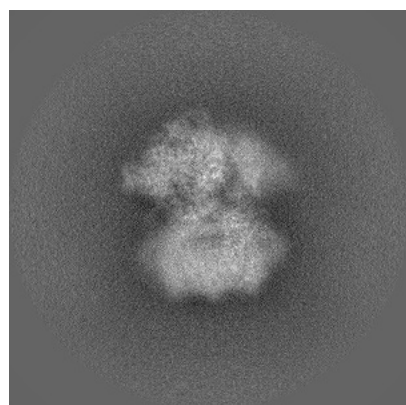


Y

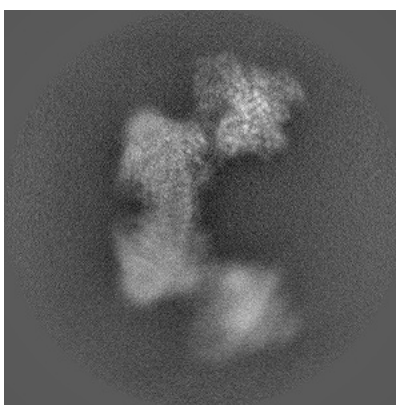


Z

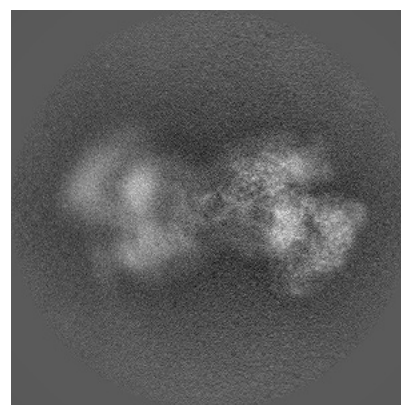
6.1.2 Raw map



X



Y

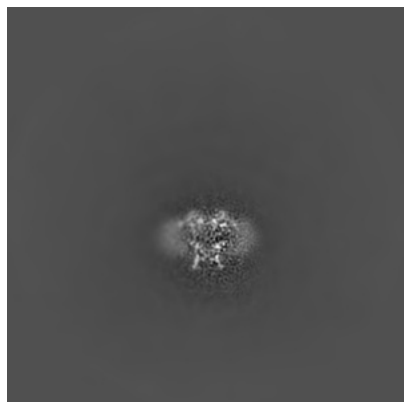


Z

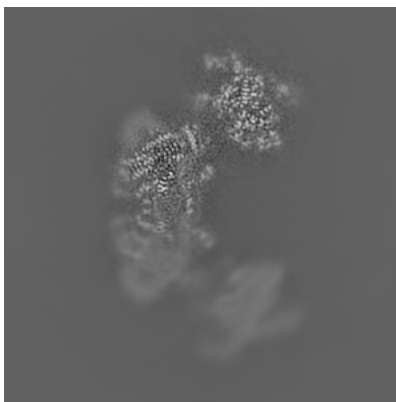
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

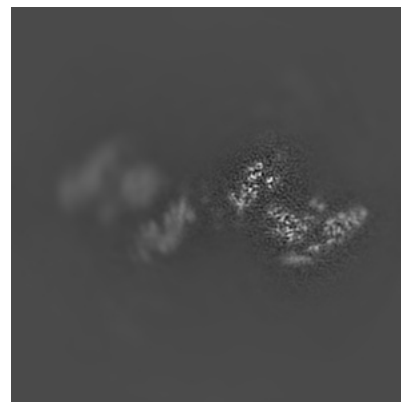
6.2.1 Primary map



X Index: 280

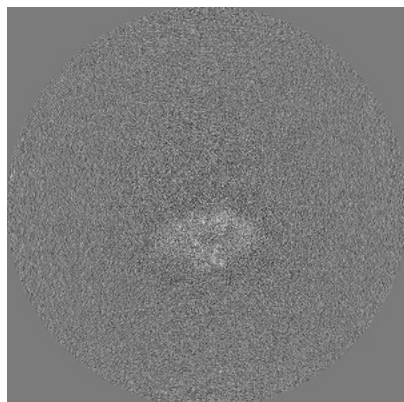


Y Index: 280

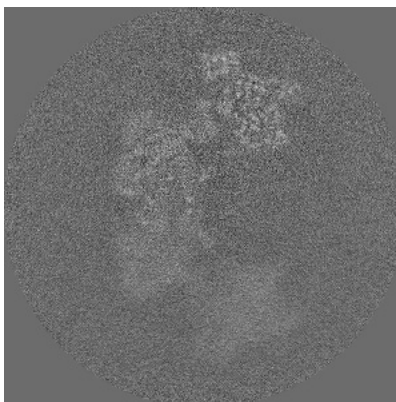


Z Index: 280

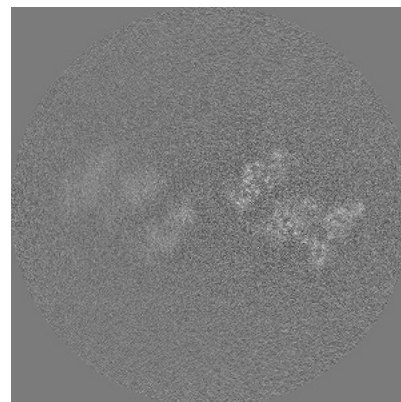
6.2.2 Raw map



X Index: 280



Y Index: 280

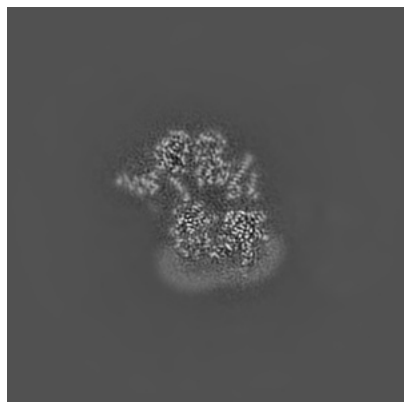


Z Index: 280

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

6.3 Largest variance slices [i](#)

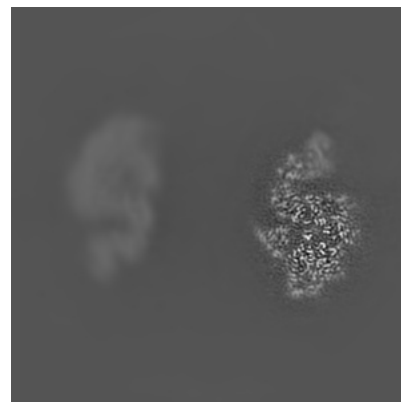
6.3.1 Primary map



X Index: 380

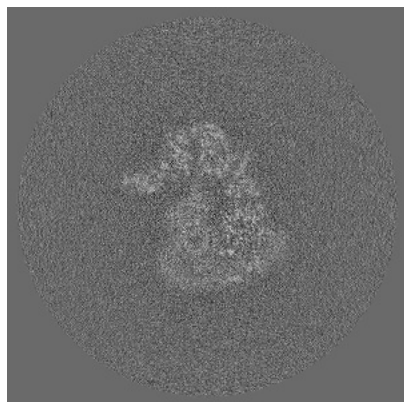


Y Index: 319

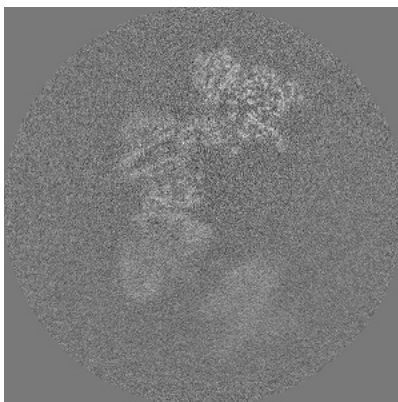


Z Index: 332

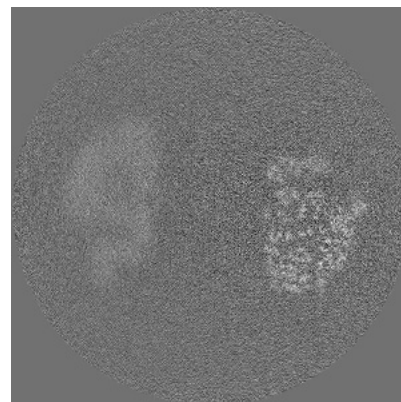
6.3.2 Raw map



X Index: 372



Y Index: 266

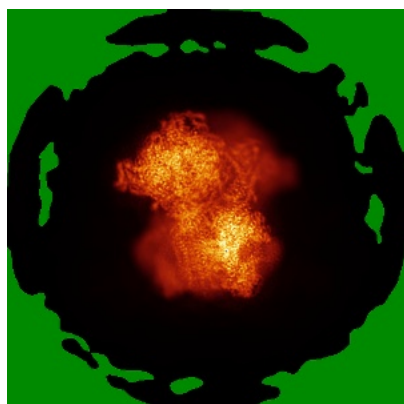


Z Index: 321

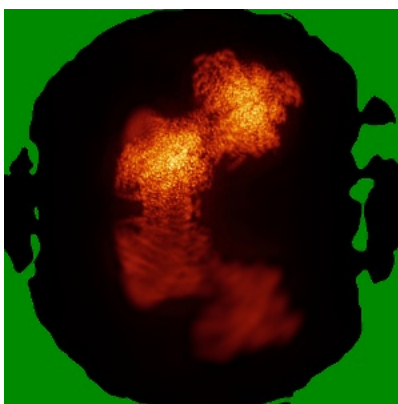
The images above show the largest variance slices of the map in three orthogonal directions.

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

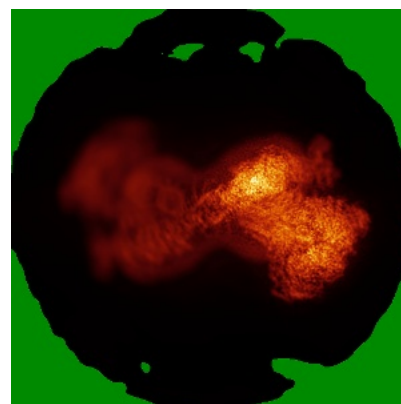
6.4.1 Primary map



X

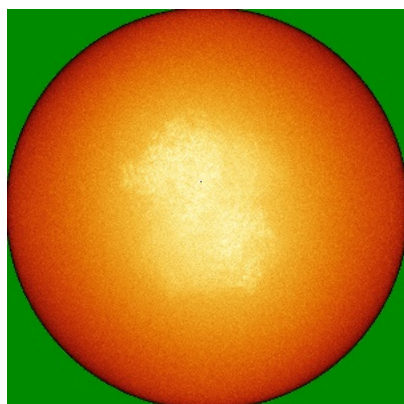


Y

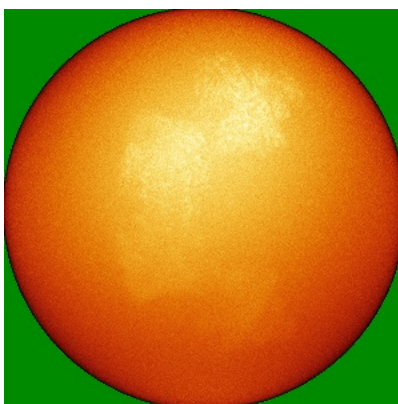


Z

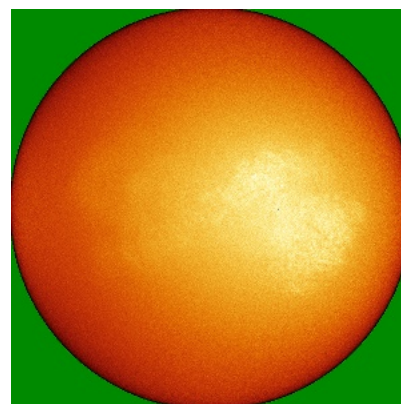
6.4.2 Raw map



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](#)

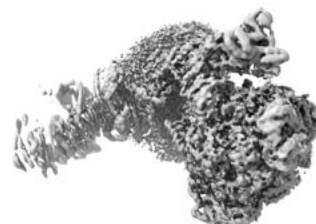
6.5.1 Primary map



X



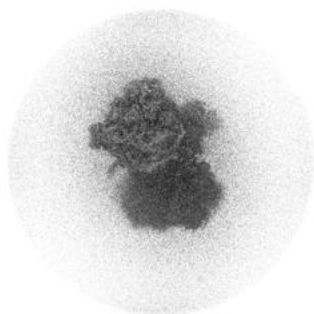
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

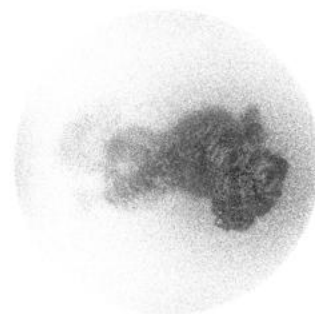
6.5.2 Raw map



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.

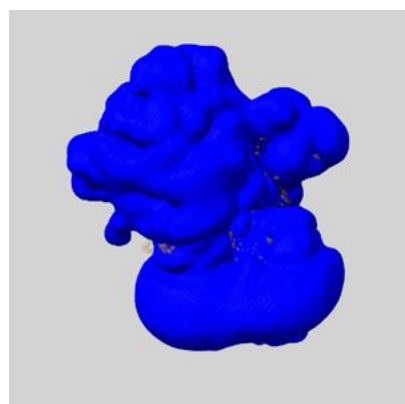
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

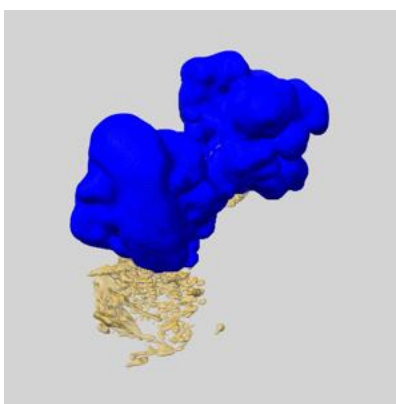
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

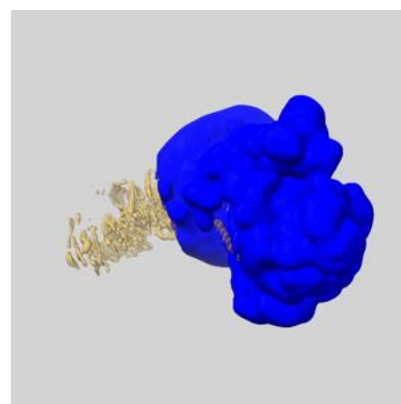
6.6.1 emd_15573_msk_1.map [i](#)



X



Y

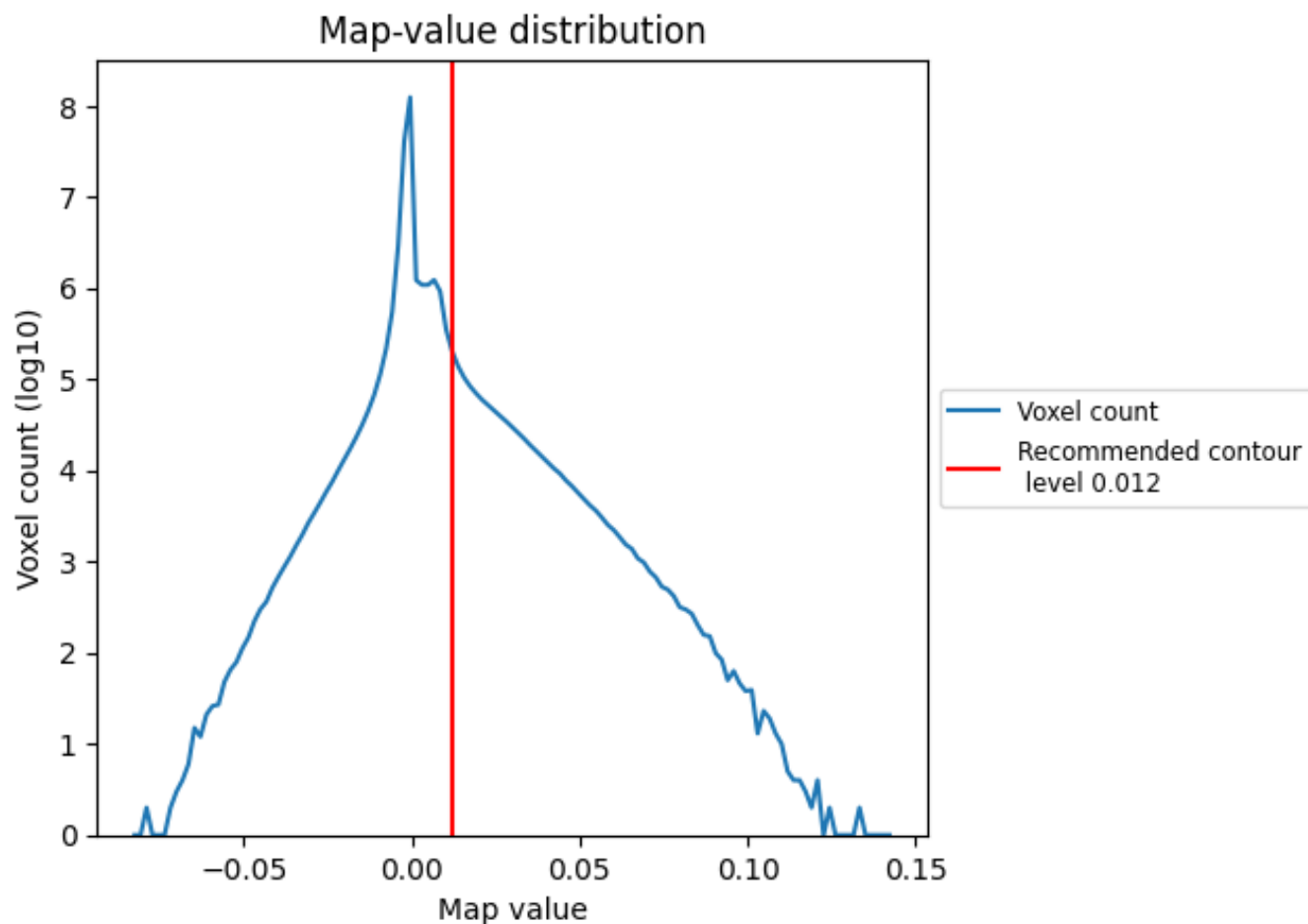


Z

7 Map analysis [i](#)

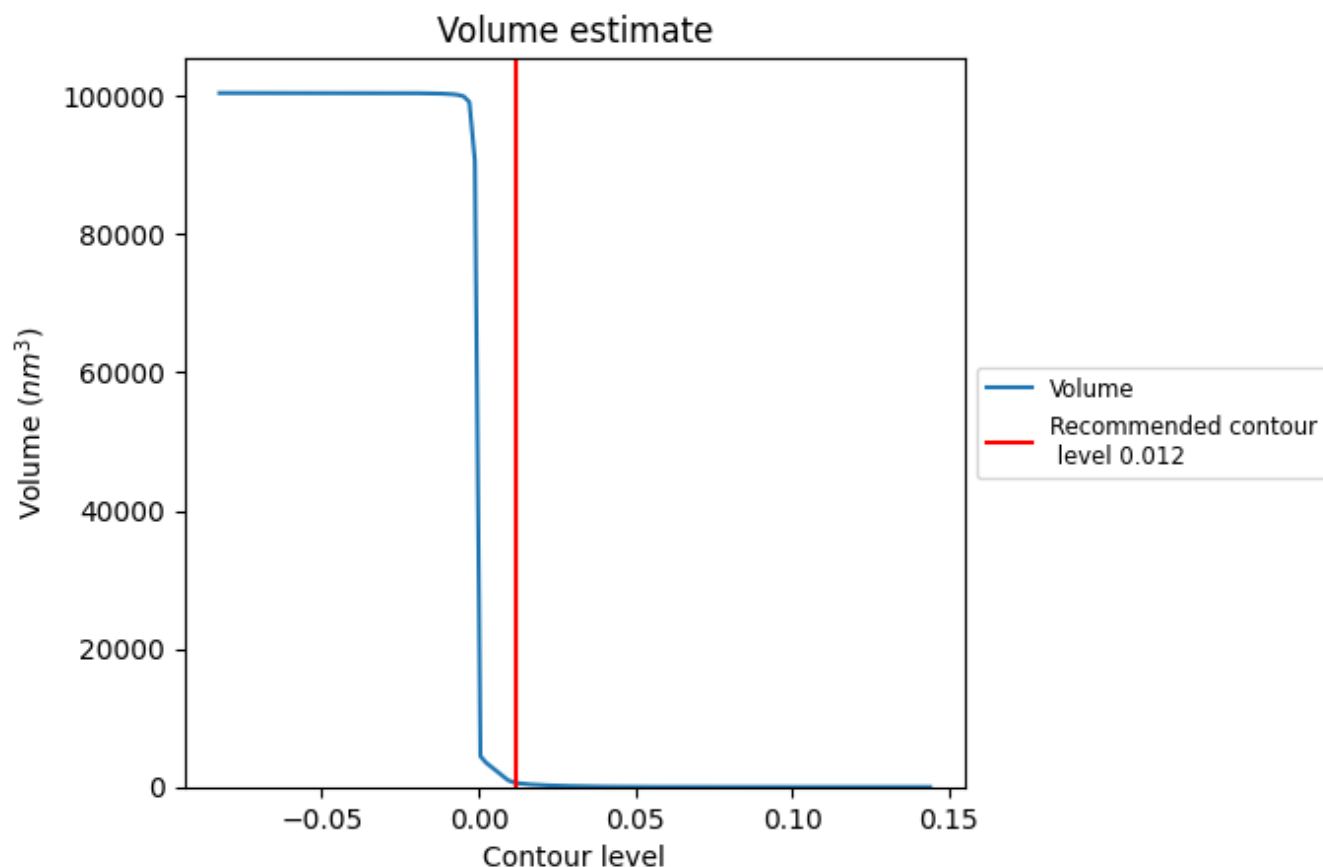
This section contains the results of statistical analysis of the map.

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.

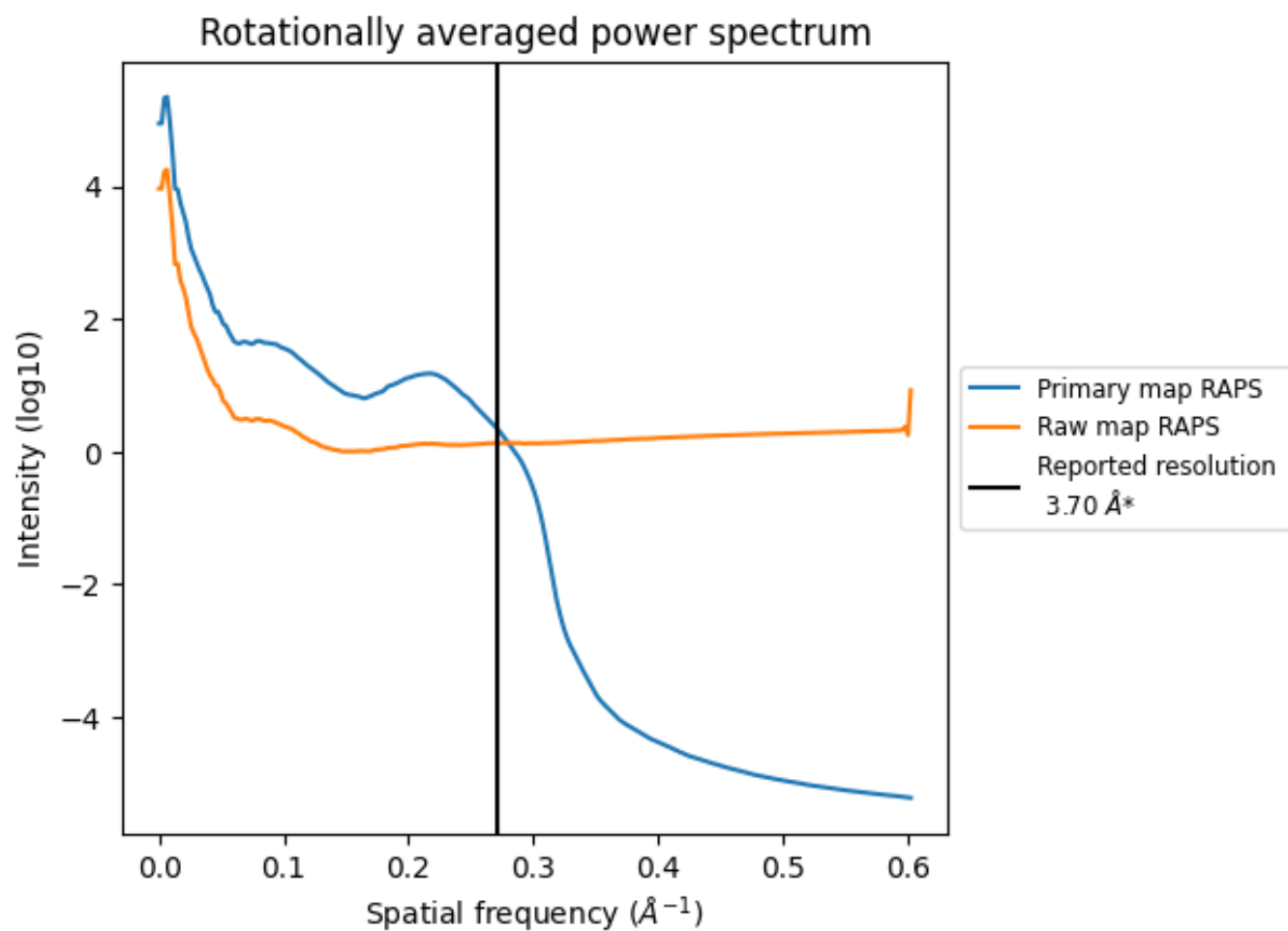
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 607 nm³; this corresponds to an approximate mass of 548 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 ⓘ

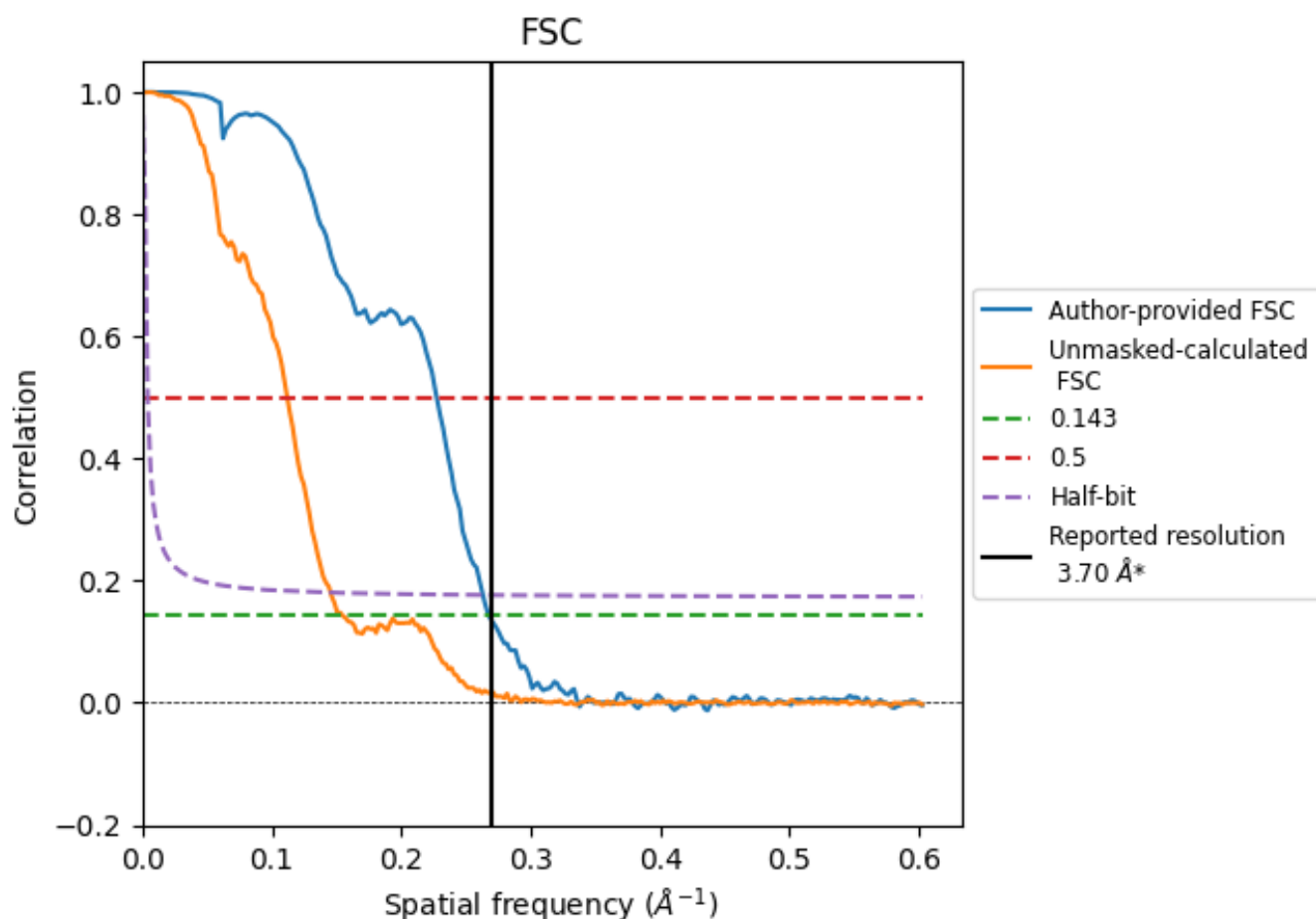


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

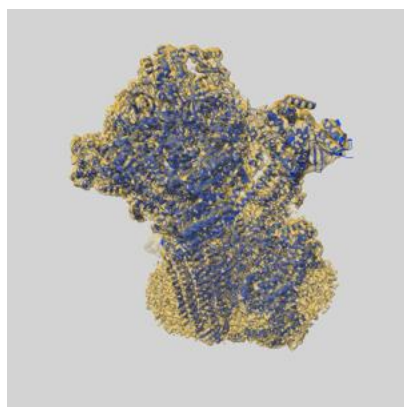
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.40	3.80
Unmasked-calculated*	6.47	8.92	6.87

*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 6.47 differs from the reported value 3.7 by more than 10 %

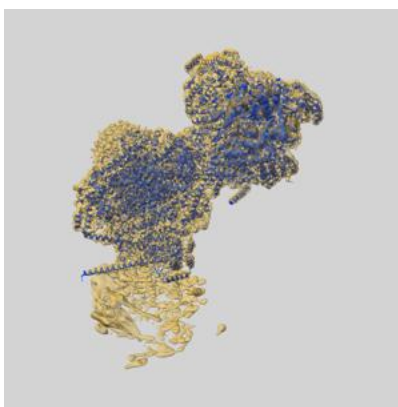
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15573 and PDB model 8APK. Per-residue inclusion information can be found in section [3](#) on page [16](#).

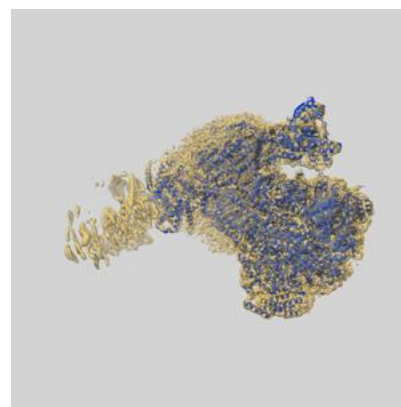
9.1 Map-model overlay [i](#)



X



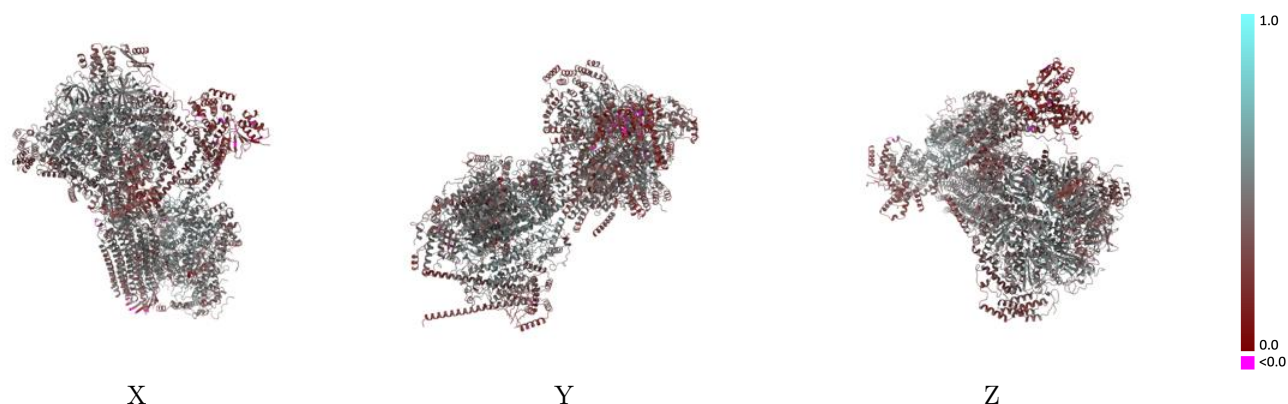
Y



Z

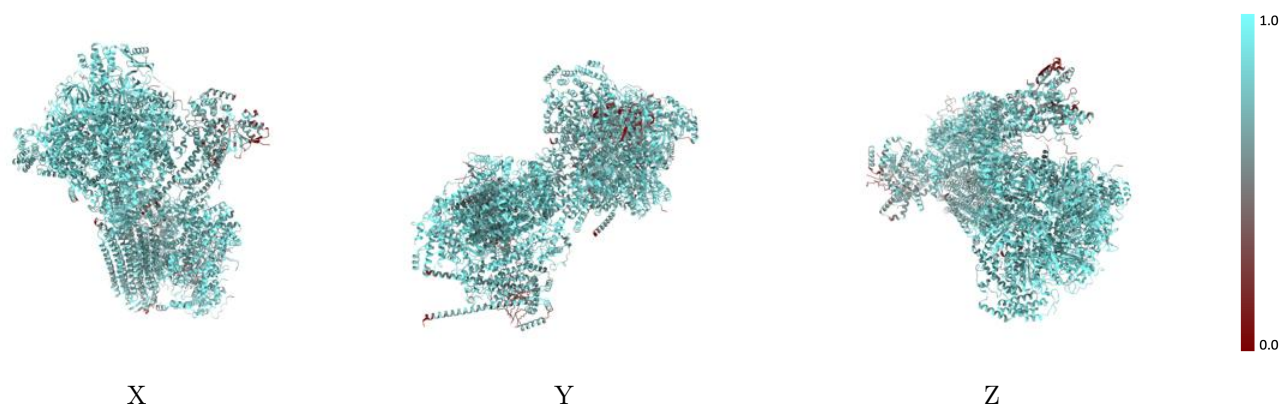
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



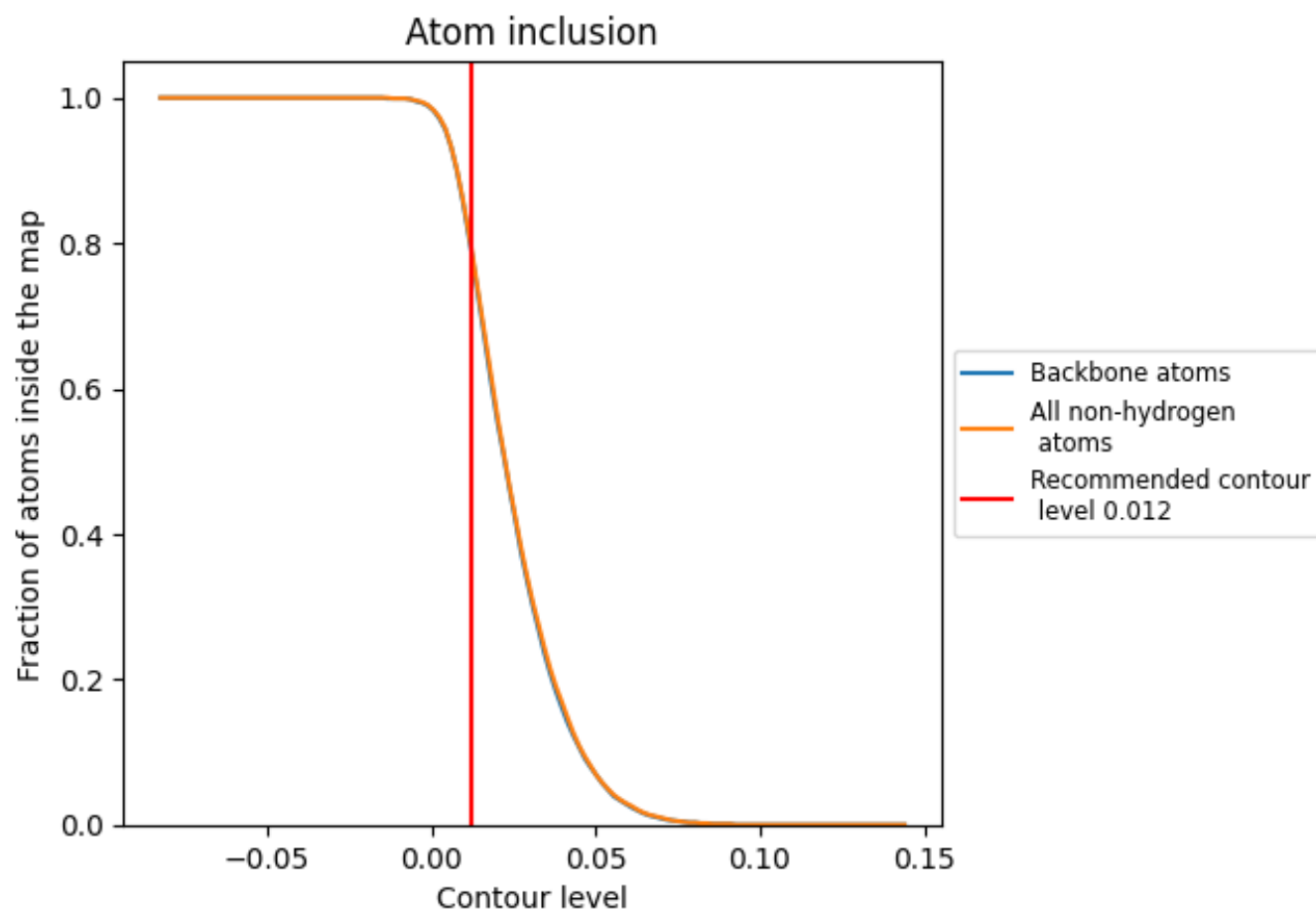
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 80% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7970	 0.4170
A1	 0.8500	 0.4430
B1	 0.8620	 0.4390
C1	 0.8410	 0.4520
D1	 0.8130	 0.4340
E1	 0.8620	 0.4550
F1	 0.8300	 0.4420
G1	 0.8070	 0.4300
H1	 0.8070	 0.4430
I1	 0.8280	 0.4410
J1	 0.7880	 0.3130
K1	 0.7830	 0.3500
L	 0.6500	 0.2890
L1	 0.7960	 0.3310
M	 0.5800	 0.3070
M1	 0.7740	 0.3450
O1	 0.7500	 0.4180
P1	 0.7430	 0.4040
Q1	 0.7540	 0.4090
R1	 0.7470	 0.3830
S1	 0.7360	 0.3910
T1	 0.7150	 0.3960
U1	 0.7380	 0.4210
V1	 0.7750	 0.4450
W1	 0.7950	 0.4480
X1	 0.7950	 0.4440
a	 0.8620	 0.5210
c	 0.8260	 0.4820
d	 0.7720	 0.3830
e	 0.8440	 0.4590
f	 0.8240	 0.4760
g	 0.5720	 0.2170
h	 0.6850	 0.2070
i	 0.8750	 0.4960
j	 0.8230	 0.4260



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Chain	Atom inclusion	Q-score
k	 0.8080	 0.4350
l	 0.5830	 0.3050
m	 0.6670	 0.3160
n	 0.8890	 0.5090
o	 0.8570	 0.4260
p	 0.7990	 0.4560
q	 0.8540	 0.4900
r	 0.8880	 0.4880