



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 09:57 PM UTC

PDB ID : 8APJ / pdb_00008apj
EMDB ID : EMD-15572
Title : rotational state 2d of Trypanosoma brucei mitochondrial ATP synthase
Authors : Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on : 2022-08-09
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation 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:

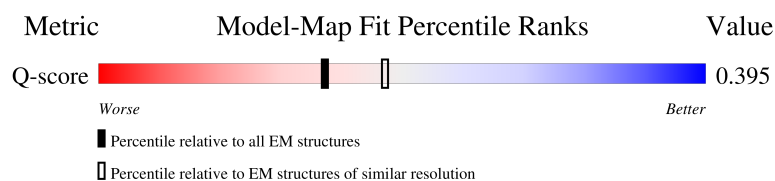
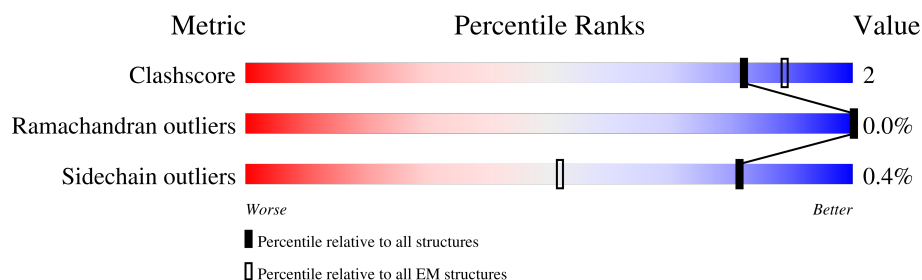
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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.



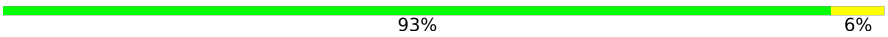
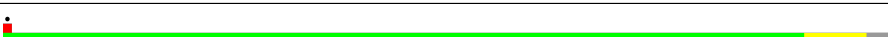
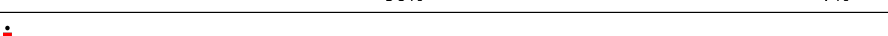
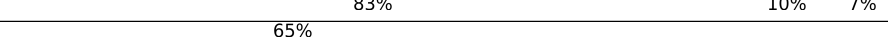
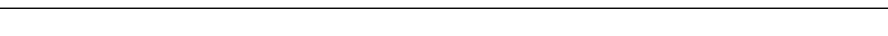
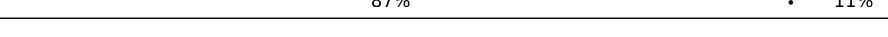
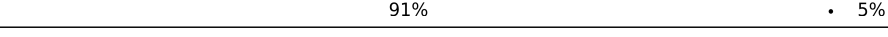
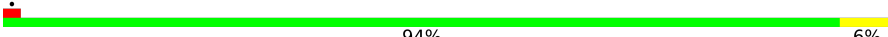
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	15% 64% 7% 29%
1	l	92	17% 65% 5% 29%
2	M	144	18% 83% 6% 10%
2	m	144	6% 81% 8% 10%

Continued on next page...

Continued from previous page...

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	H1	182	
19	I1	75	
20	J1	188	
20	K1	188	
20	L1	188	
21	M1	255	
22	O1	118	
22	P1	118	
22	Q1	118	
22	R1	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
22	S1	118	
22	T1	118	
22	U1	118	
22	V1	118	
22	W1	118	
22	X1	118	
23	G1	305	
24	A1	584	
24	B1	584	
24	C1	584	
25	D1	519	
25	E1	519	
25	F1	519	

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
29	Q7G	e	407	X	-	-	-
29	Q7G	n	201	X	-	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 129563 atoms, of which 65460 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, epsilon chain, putative.

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

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

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

- Molecule 20 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	J1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
20	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
20	L1	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		

- Molecule 21 is a protein called OSCP.

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

- Molecule 22 is a protein called ATPase subunit 9, putative.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	W1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	X1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

- Molecule 23 is a protein called ATP synthase gamma subunit.

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

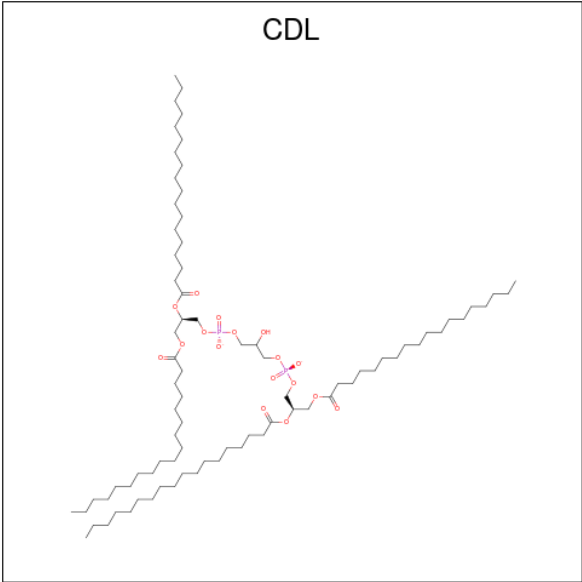
- Molecule 24 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A1	523	Total	C	H	N	O	S	0	0
			8193	2587	4154	701	731	20		
24	B1	529	Total	C	H	N	O	S	0	0
			8260	2603	4187	709	741	20		
24	C1	524	Total	C	H	N	O	S	0	0
			8219	2594	4170	703	732	20		

- Molecule 25 is a protein called ATP synthase subunit beta, mitochondrial.

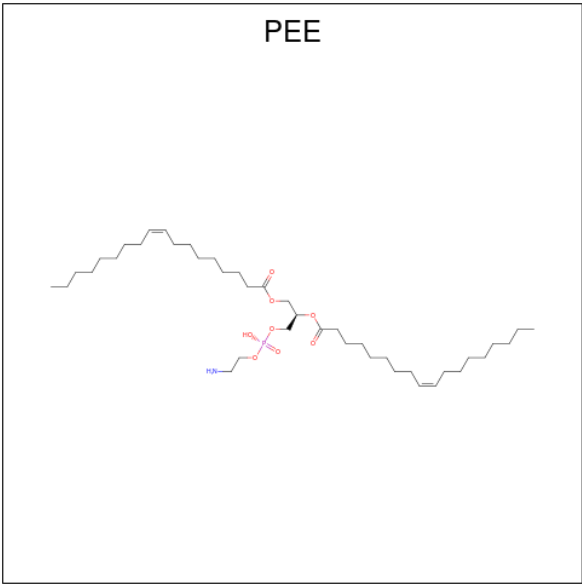
Mol	Chain	Residues	Atoms						AltConf	Trace
25	D1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		
25	E1	486	Total	C	H	N	O	S	0	0
			7414	2324	3732	630	709	19		
25	F1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



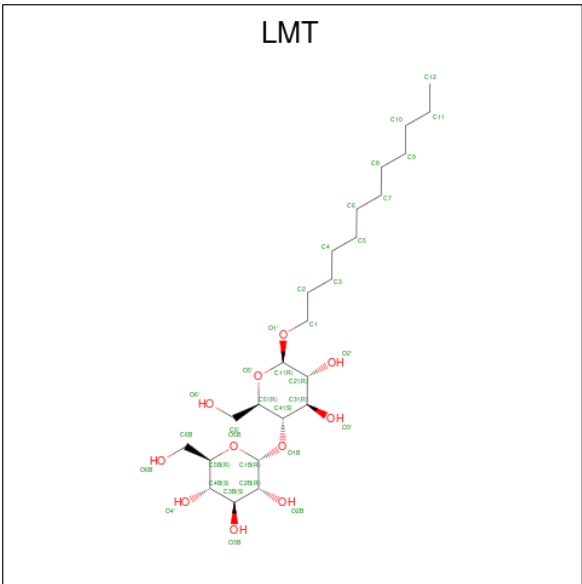
Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	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	j	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-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



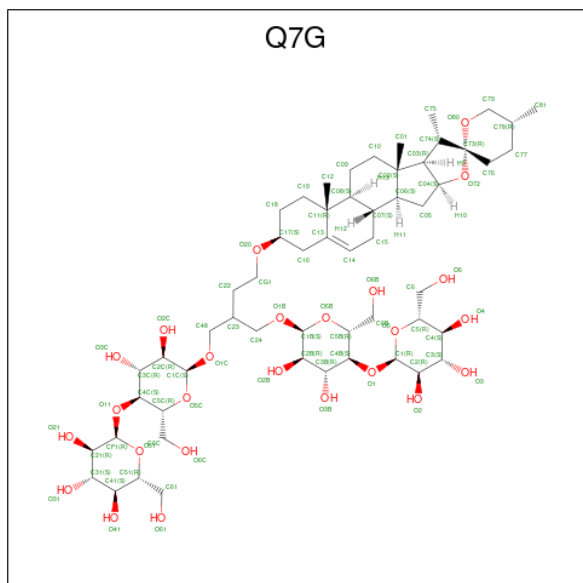
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
27	M	1	Total 133	41	82	1	8	1	0
27	f	1	Total 133	41	82	1	8	1	0
27	m	1	Total 133	41	82	1	8	1	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



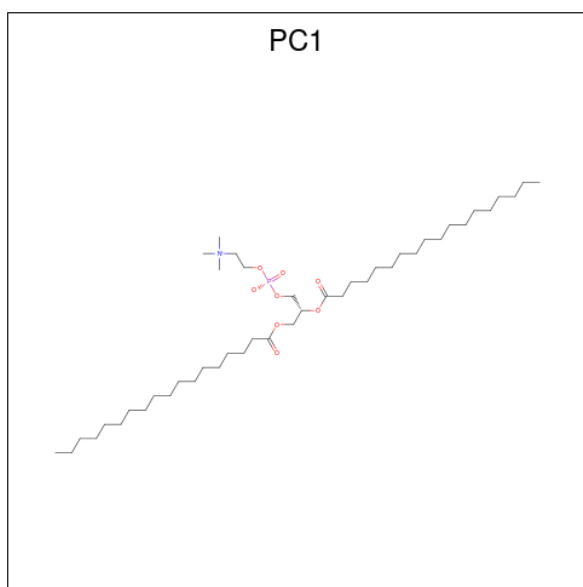
Mol	Chain	Residues	Atoms				AltConf
28	e	1	Total	C	H	O	0
			74	24	39	11	
28	j	1	Total	C	H	O	0
			74	24	39	11	

- Molecule 29 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: C₅₆H₉₂O₂₅).



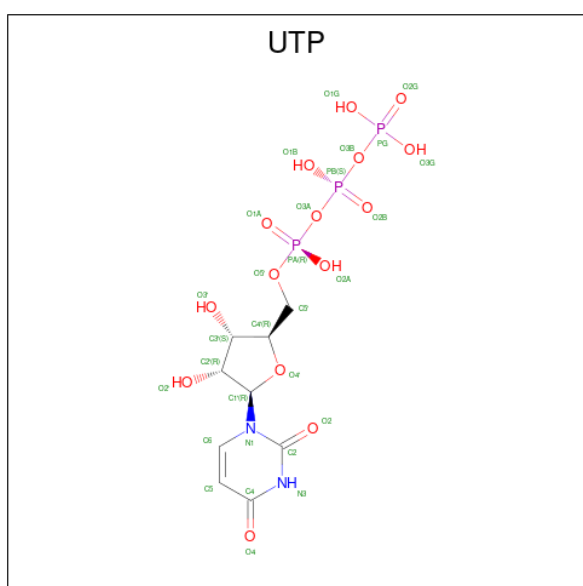
Mol	Chain	Residues	Atoms				AltConf
29	e	1	Total	C	H	O	0
			108	38	60	10	
29	n	1	Total	C	H	O	0
			129	44	70	15	

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



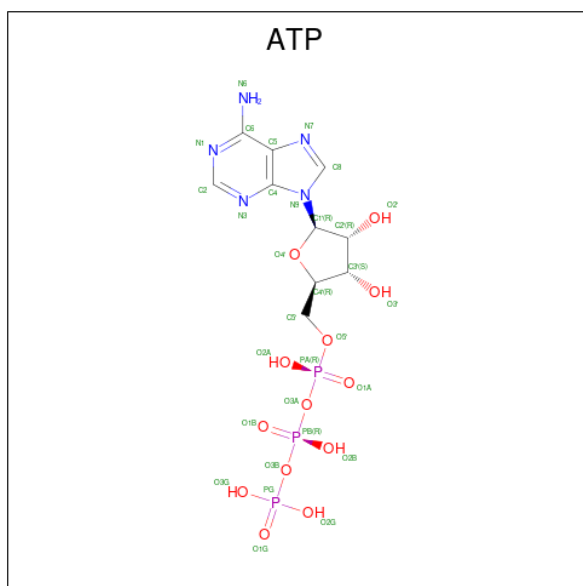
Mol	Chain	Residues	Atoms					AltConf	
30	f	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
30	i	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
30	j	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
30	p	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 31 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
31	H1	1	Total	C	H	N	O	P	0
			40	9	11	2	15	3	

- Molecule 32 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
32	A1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
32	B1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
32	C1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
32	D1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

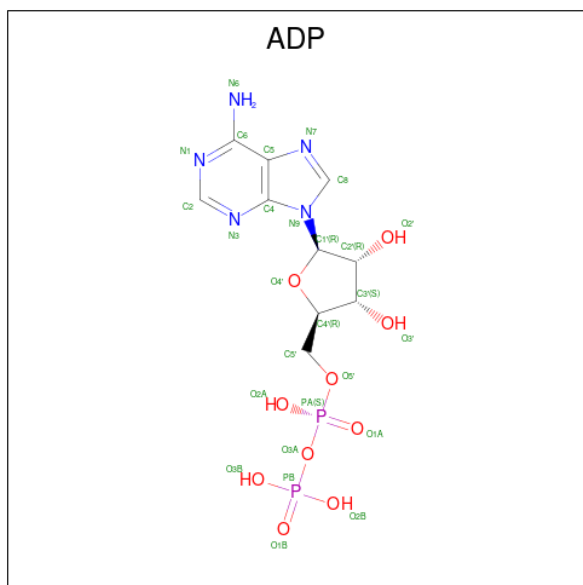
Mol	Chain	Residues	Atoms		AltConf
33	A1	1	Total	Mg	0
			1	1	
33	B1	1	Total	Mg	0
			1	1	
33	C1	1	Total	Mg	0
			1	1	
33	D1	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
33	E1	1	Total	Mg	0
			1	1	

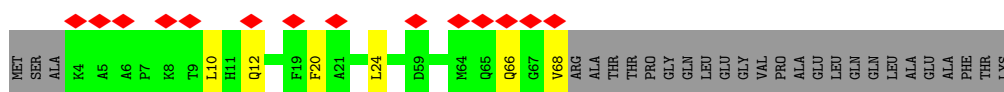
- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



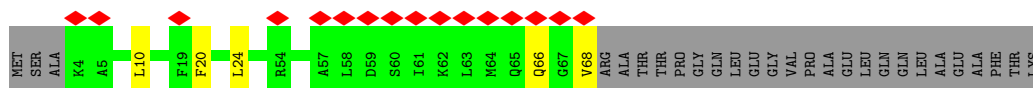
3 Residue-property plots [i](#)

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.

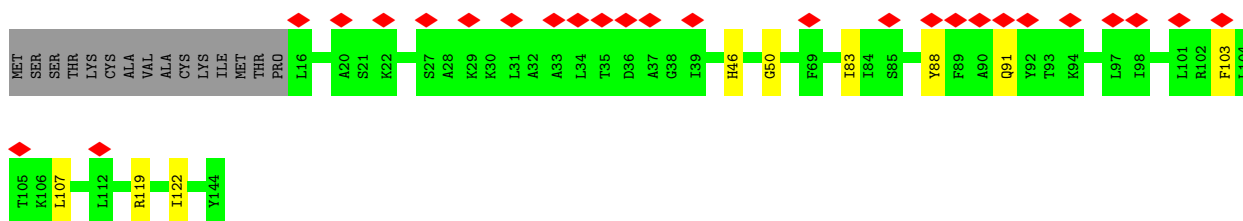
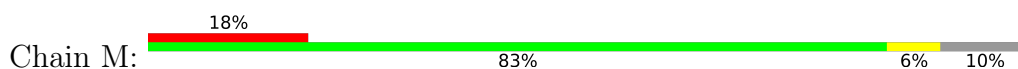
- Molecule 1: subunit-e



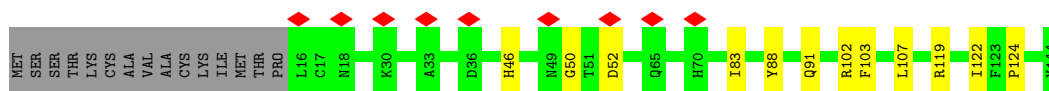
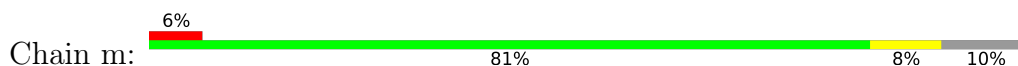
- Molecule 1: subunit-e



- Molecule 2: subunit-g

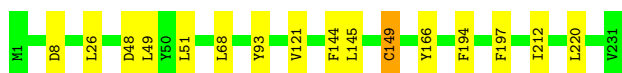


- Molecule 2: subunit-g

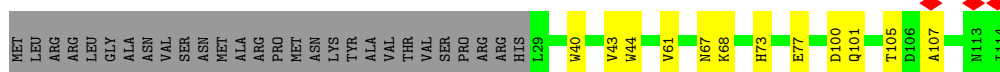


- Molecule 3: ATP synthase subunit a

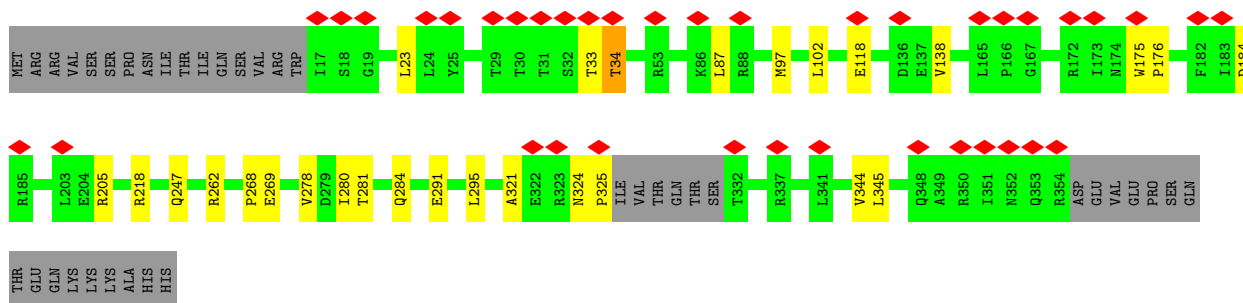
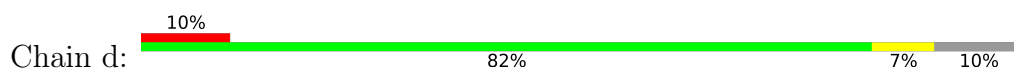




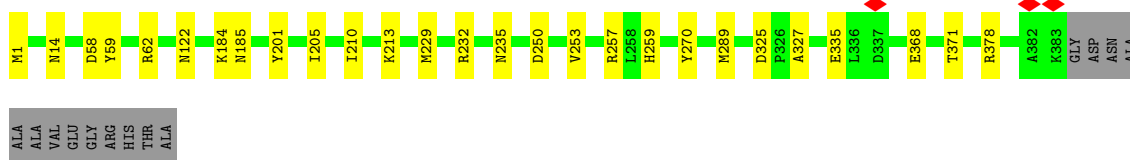
• Molecule 4: subunit-8



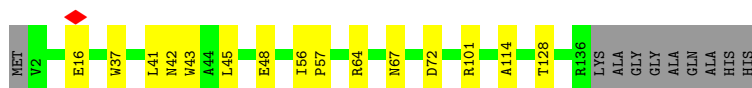
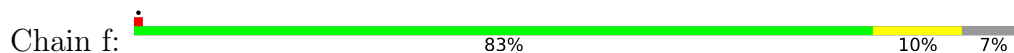
• Molecule 5: subunit-d



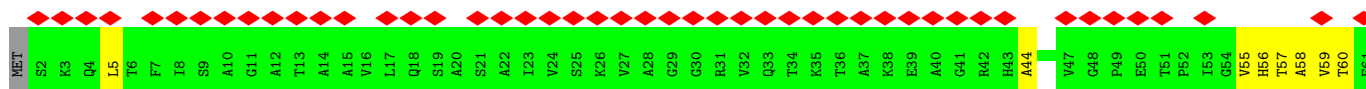
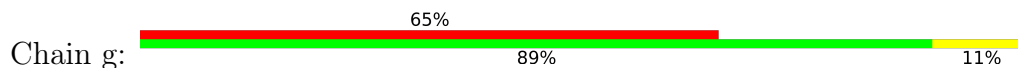
• Molecule 6: ATPTB1

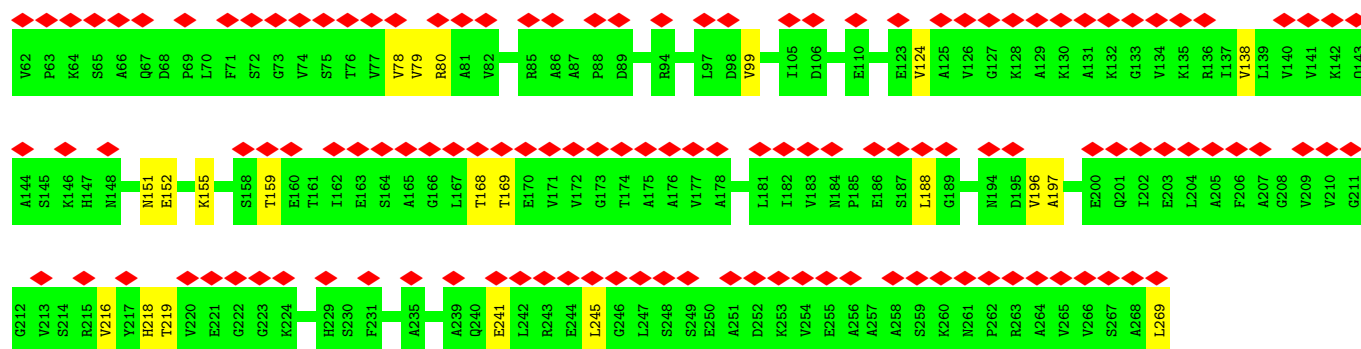


• Molecule 7: subunit-f

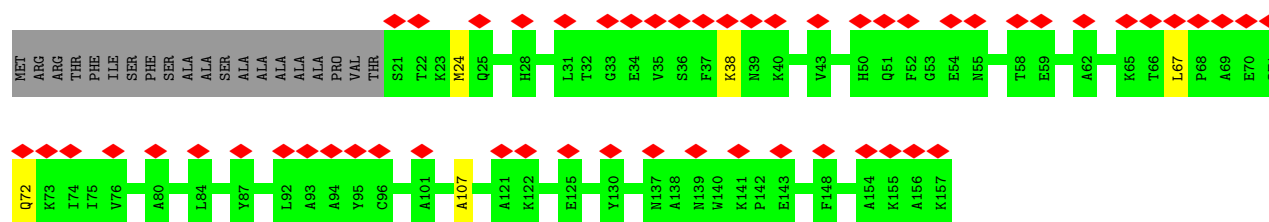
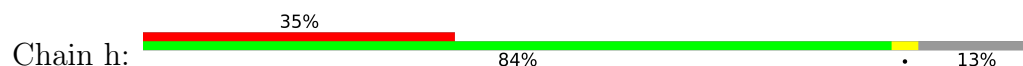


• Molecule 8: ATPTB3

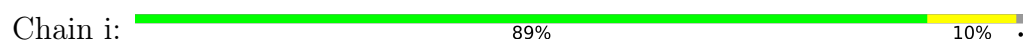




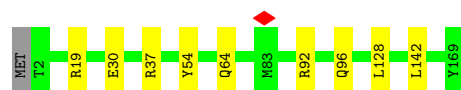
• Molecule 9: ATPTB4



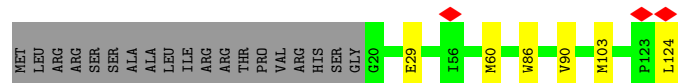
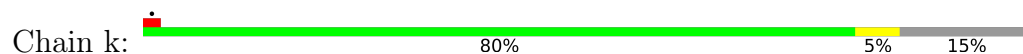
• Molecule 10: subunit-i/j



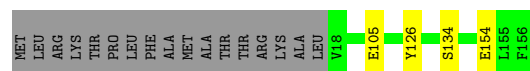
• Molecule 11: ATPTB6



• Molecule 12: subunit-k



• Molecule 13: ATPTB11



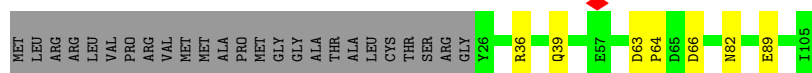
- Molecule 14: ATPTB12

Chain o:  91% 5%



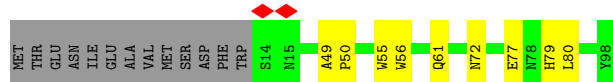
- Molecule 15: subunit-b

Chain p:  70% 7% 24%

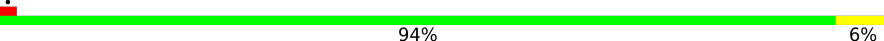


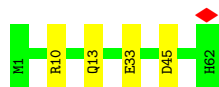
- Molecule 16: ATPEG3

Chain q:  78% 9% 13%



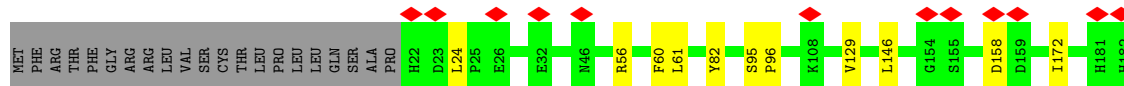
- Molecule 17: ATPEG4

Chain r:  94% 6%



- Molecule 18: ATP synthase, epsilon chain, putative

Chain H1:  7% 82% 6% 12%



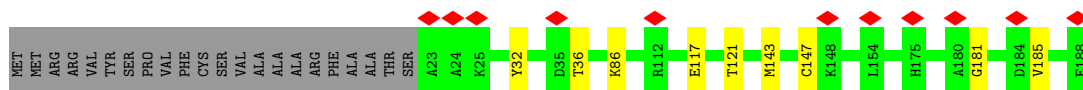
- Molecule 19: ATP synthase subunit epsilon, mitochondrial

Chain I1:  15% 80% 7% 13%

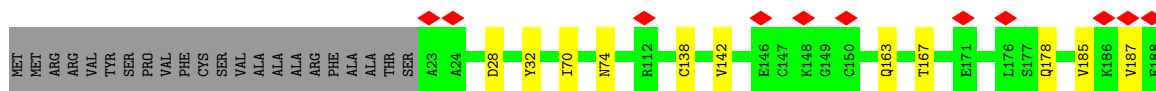
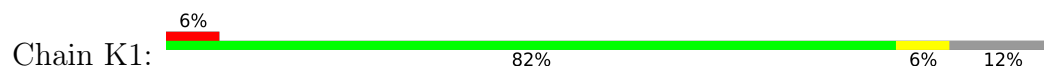


- Molecule 20: ATP synthase subunit p18, mitochondrial

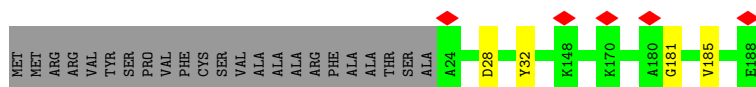
Chain J1:  6% 84% 5% 12%



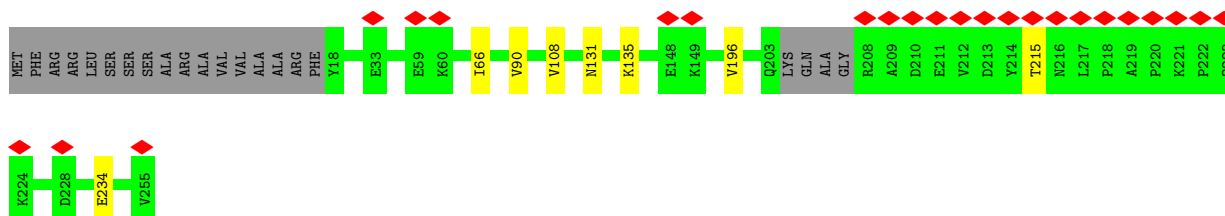
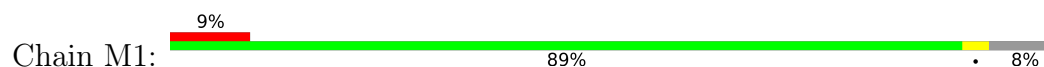
- Molecule 20: ATP synthase subunit p18, mitochondrial



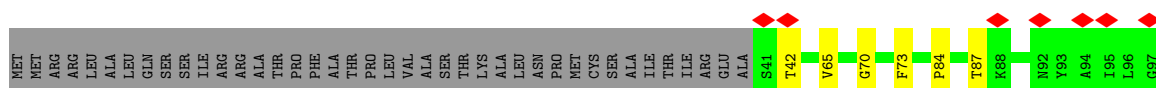
- Molecule 20: ATP synthase subunit p18, mitochondrial



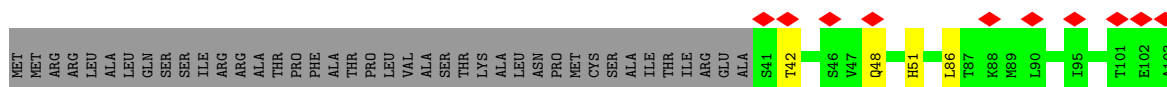
- Molecule 21: OSCP

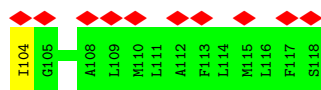


- Molecule 22: ATPase subunit 9, putative

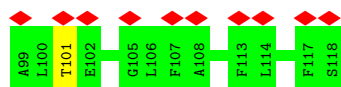
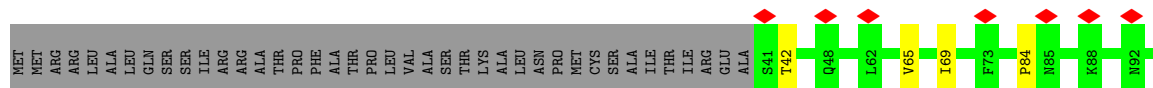


- Molecule 22: ATPase subunit 9, putative

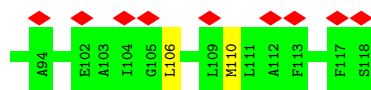
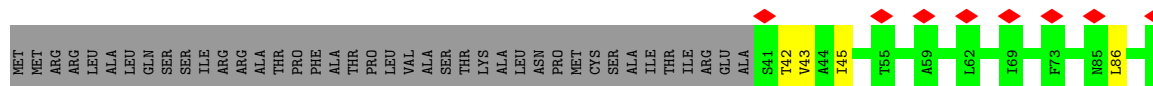




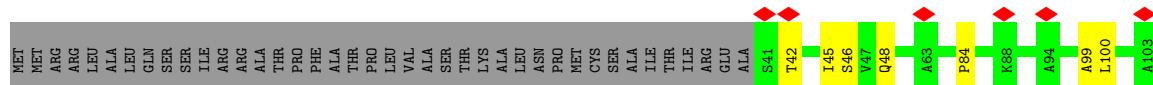
- Molecule 22: ATPase subunit 9, putative



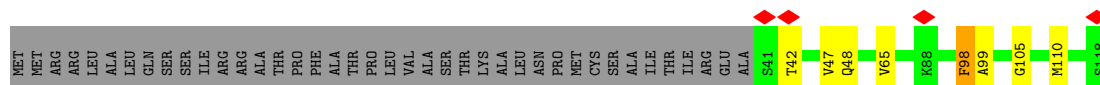
- Molecule 22: ATPase subunit 9, putative



- Molecule 22: ATPase subunit 9, putative

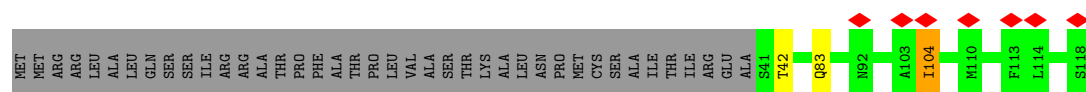


- Molecule 22: ATPase subunit 9, putative

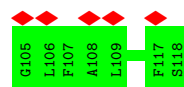
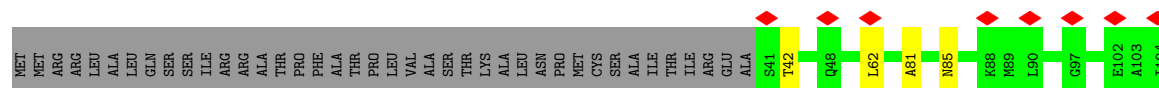


- Molecule 22: ATPase subunit 9, putative

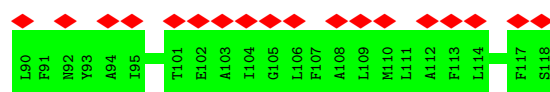
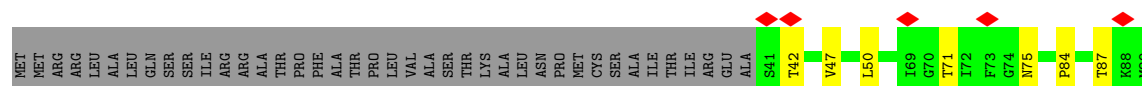




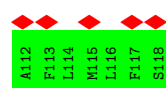
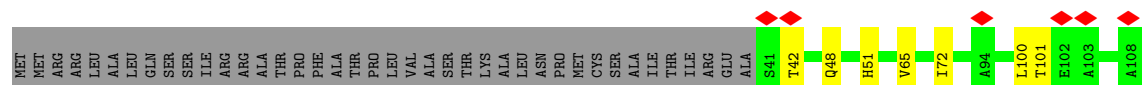
- Molecule 22: ATPase subunit 9, putative



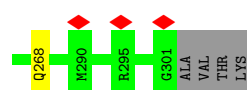
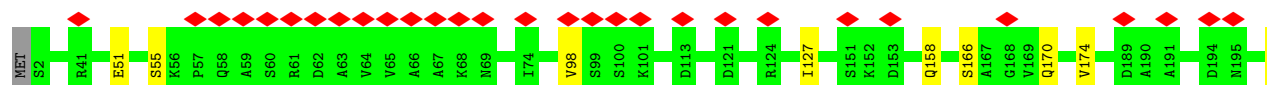
- Molecule 22: ATPase subunit 9, putative



- Molecule 22: ATPase subunit 9, putative

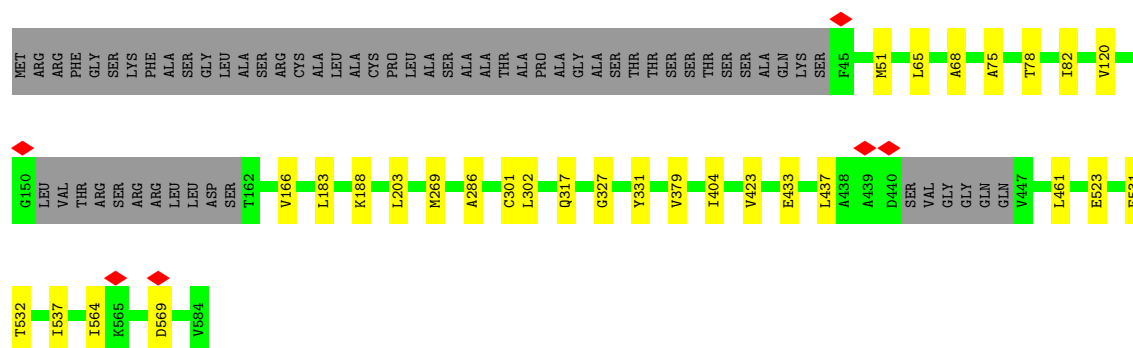


- Molecule 23: ATP synthase gamma subunit



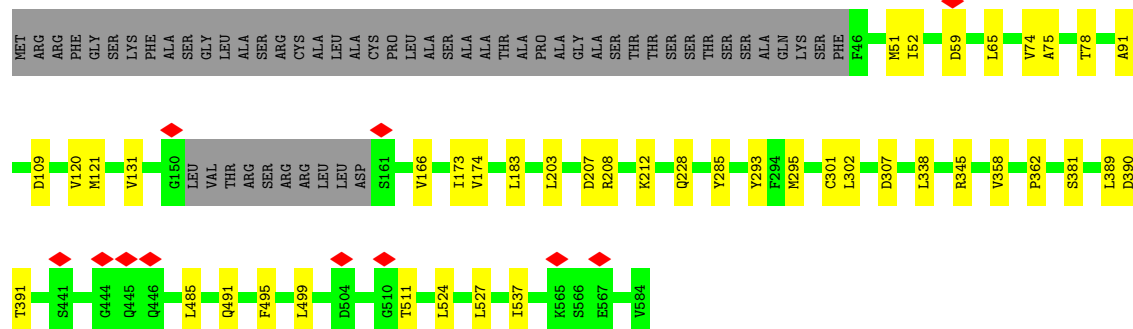
- Molecule 24: ATP synthase subunit alpha, mitochondrial

Chain A1: 



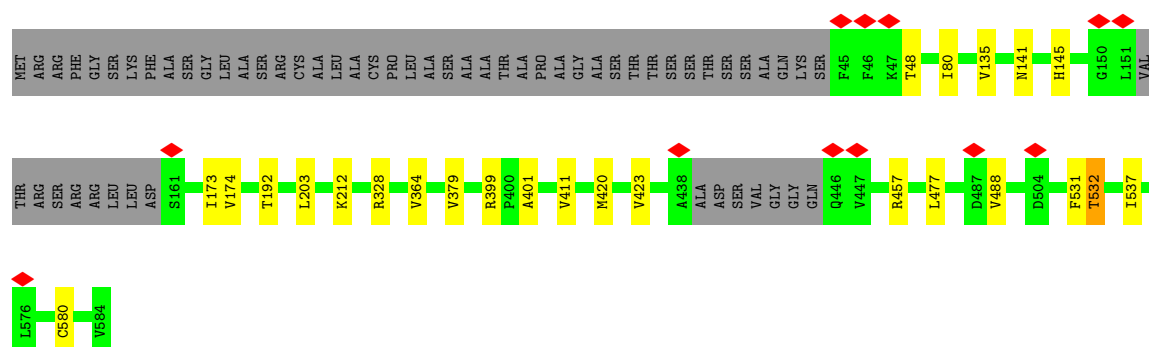
- Molecule 24: ATP synthase subunit alpha, mitochondrial

Chain B1: 



- Molecule 24: ATP synthase subunit alpha, mitochondrial

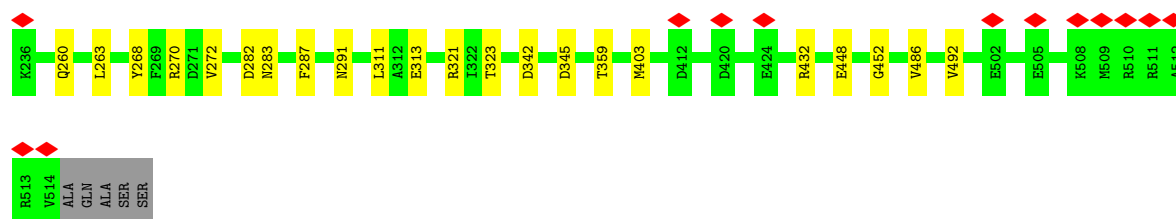
Chain C1: 



- Molecule 25: ATP synthase subunit beta, mitochondrial

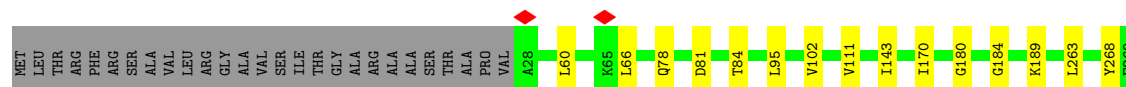
Chain D1: 





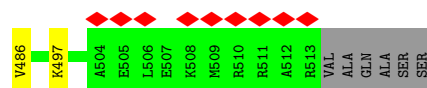
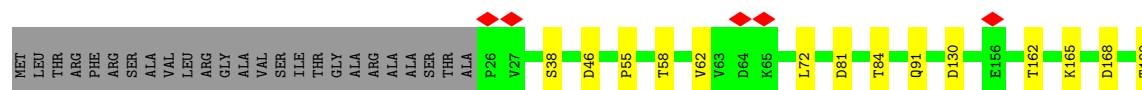
- Molecule 25: ATP synthase subunit beta, mitochondrial

Chain E1: 87% 7% 6%



- Molecule 25: ATP synthase subunit beta, mitochondrial

Chain F1: 6% 87% 8% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17833	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	0.151	Depositor
Minimum map value	-0.089	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	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: PC1, AME, ATP, LMT, MG, CDL, UTP, PEE, ADP, Q7G

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	0.09	0/547	0.16	0/735
1	l	0.09	0/547	0.16	0/735
2	M	0.09	0/1049	0.18	0/1423
2	m	0.09	0/1049	0.19	0/1423
3	a	0.24	0/2111	0.27	0/2861
4	c	0.21	0/772	0.28	0/1054
5	d	0.13	0/2786	0.24	0/3760
6	e	0.17	0/3305	0.22	0/4482
7	f	0.19	0/1183	0.27	0/1601
8	g	0.07	0/1953	0.18	0/2650
9	h	0.06	0/1088	0.17	0/1466
10	i	0.20	0/913	0.23	0/1240
11	j	0.14	0/1462	0.20	0/1973
12	k	0.14	0/904	0.22	0/1228
13	n	0.19	0/1166	0.24	0/1581
14	o	0.13	0/814	0.20	0/1100
15	p	0.14	0/707	0.22	0/957
16	q	0.18	0/799	0.24	0/1091
17	r	0.17	0/567	0.23	0/767
18	H1	0.18	0/1274	0.30	0/1728
19	I1	0.12	0/547	0.30	0/738
20	J1	0.08	0/1342	0.22	0/1810
20	K1	0.08	0/1342	0.20	0/1810
20	L1	0.08	0/1337	0.20	0/1803
21	M1	0.08	0/1916	0.22	0/2591
22	O1	0.09	0/574	0.21	0/777
22	P1	0.09	0/574	0.20	0/777
22	Q1	0.09	0/574	0.17	0/777
22	R1	0.10	0/574	0.18	0/777
22	S1	0.13	0/574	0.27	0/777
22	T1	0.14	0/574	0.23	0/777
22	U1	0.12	0/574	0.23	0/777

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	V1	0.11	0/574	0.18	0/777
22	W1	0.10	0/574	0.19	0/777
22	X1	0.09	0/574	0.17	0/777
23	G1	0.13	0/2427	0.29	0/3268
24	A1	0.14	0/4113	0.22	0/5569
24	B1	0.13	0/4147	0.24	0/5616
24	C1	0.14	0/4123	0.24	0/5582
25	D1	0.14	0/3752	0.24	0/5087
25	E1	0.13	0/3738	0.23	0/5067
25	F1	0.12	0/3753	0.24	0/5088
All	All	0.14	0/63273	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 ⓘ

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	4	0
1	l	537	545	545	3	0
2	M	1027	1042	1042	6	0
2	m	1027	1042	1042	10	0
3	a	2032	2044	2044	18	0
4	c	745	715	715	9	0
5	d	2737	2762	2763	20	0
6	e	3220	3050	3061	18	0
7	f	1145	1111	1111	14	0
8	g	1933	2020	2020	17	0
9	h	1070	1088	1088	4	0
10	i	883	857	857	8	0
11	j	1424	1411	1411	7	0
12	k	873	876	876	6	0
13	n	1128	1082	1082	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	o	789	767	767	3	0
15	p	684	651	651	8	0
16	q	766	720	720	8	0
17	r	542	498	498	5	0
18	H1	1251	1232	1231	8	0
19	I1	533	513	513	5	0
20	J1	1315	1276	1276	6	0
20	K1	1315	1276	1276	8	0
20	L1	1310	1271	1271	2	0
21	M1	1877	1873	1873	6	0
22	O1	565	600	599	5	0
22	P1	565	600	599	3	0
22	Q1	565	600	599	3	0
22	R1	565	600	599	4	0
22	S1	565	601	599	11	0
22	T1	565	601	599	8	0
22	U1	565	600	599	2	0
22	V1	565	600	599	3	0
22	W1	565	600	599	3	0
22	X1	565	600	599	5	0
23	G1	2387	2387	2387	5	0
24	A1	4039	4154	4154	22	0
24	B1	4073	4187	4187	27	0
24	C1	4049	4170	4169	22	0
25	D1	3696	3750	3750	22	0
25	E1	3682	3732	3732	20	0
25	F1	3696	3750	3750	24	0
26	L	100	156	156	0	0
26	M	100	156	156	1	0
26	c	100	156	156	1	0
26	e	500	780	780	2	0
26	f	100	156	156	0	0
26	j	200	312	312	1	0
26	l	100	156	156	0	0
26	m	100	156	156	0	0
26	q	100	156	156	1	0
27	M	51	82	82	1	0
27	f	51	82	82	0	0
27	m	51	82	82	0	0
28	e	35	39	46	0	0
28	j	35	39	46	0	0
29	e	48	60	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	n	59	70	0	0	0
30	f	54	88	88	2	0
30	i	54	88	88	0	0
30	j	54	88	88	1	0
30	p	54	88	88	0	0
31	H1	29	11	11	0	0
32	A1	31	12	12	0	0
32	B1	31	12	12	1	0
32	C1	31	12	12	1	0
32	D1	31	12	12	0	0
33	A1	1	0	0	0	0
33	B1	1	0	0	0	0
33	C1	1	0	0	0	0
33	D1	1	0	0	0	0
33	E1	1	0	0	0	0
34	E1	27	12	12	0	0
All	All	64103	65460	65342	322	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.

All (322) 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	2.15	0.79
25:E1:184:GLY:O	25:E1:189:LYS:NZ	2.19	0.75
7:f:64:ARG:NH2	17:r:33:GLU:OE2	2.20	0.74
6:e:250:ASP:OD1	6:e:270:TYR:OH	2.04	0.74
22:S1:46:SER:OG	22:T1:48:GLN:OE1	2.07	0.71
4:c:73:HIS:NE2	4:c:77:GLU:OE2	2.25	0.69
7:f:16:GLU:OE1	7:f:16:GLU:N	2.25	0.69
12:k:29:GLU:N	12:k:29:GLU:OE1	2.28	0.67
6:e:62:ARG:NH2	26:e:402:CDL:OB4	2.29	0.66
7:f:37:TRP:NE1	7:f:48:GLU:OE1	2.29	0.66
20:K1:28:ASP:OD1	20:K1:32:TYR:N	2.30	0.65
22:X1:48:GLN:O	22:X1:51:HIS:ND1	2.30	0.64
6:e:1:AME:O	6:e:122:ASN:ND2	2.29	0.64
23:G1:166:SER:O	23:G1:170:GLN:NE2	2.29	0.64
3:a:166:TYR:OH	30:f:203:PC1:O12	2.13	0.63
24:C1:328:ARG:NH2	25:D1:345:ASP:OD1	2.32	0.63
10:i:87:PRO:O	10:i:91:GLY:N	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B1:295:MET:HB2	24:B1:358:VAL:HG23	1.82	0.61
13:n:154:GLU:OE1	13:n:154:GLU:N	2.32	0.61
6:e:185:ASN:ND2	6:e:325:ASP:OD1	2.31	0.61
3:a:68:LEU:HD13	7:f:45:LEU:HD11	1.83	0.61
1:l:66:GLN:HG3	1:l:68:VAL:HG23	1.83	0.60
1:L:66:GLN:HG3	1:L:68:VAL:HG23	1.83	0.60
25:E1:347:ALA:HB3	25:E1:348:PRO:HD3	1.85	0.59
4:c:68:LYS:NZ	5:d:284:GLN:O	2.30	0.59
11:j:128:LEU:HD21	11:j:142:LEU:HD12	1.85	0.59
25:F1:263:LEU:HD21	25:F1:321:ARG:HB2	1.83	0.59
22:U1:83:GLN:NE2	22:V1:81:ALA:O	2.35	0.58
2:M:103:PHE:CE2	2:M:107:LEU:HD11	2.38	0.58
5:d:291:GLU:O	5:d:295:LEU:N	2.35	0.58
25:F1:273:GLU:OE1	25:F1:275:GLN:NE2	2.36	0.58
4:c:40:TRP:O	4:c:43:VAL:HG12	2.03	0.58
2:m:103:PHE:CE2	2:m:107:LEU:HD11	2.38	0.58
24:C1:203:LEU:HD13	24:C1:379:VAL:HG11	1.85	0.58
22:O1:84:PRO:O	22:O1:87:THR:HG23	2.02	0.58
24:A1:75:ALA:HB3	24:A1:78:THR:HG21	1.86	0.58
11:j:37:ARG:NH2	26:j:202:CDL:OA3	2.35	0.57
5:d:262:ARG:NH2	6:e:335:GLU:O	2.36	0.57
25:E1:486:VAL:HG21	25:E1:492:VAL:HG22	1.86	0.57
20:J1:86:LYS:NZ	24:B1:228:GLN:O	2.34	0.57
7:f:101:ARG:NH2	2:m:124:PRO:O	2.38	0.56
24:C1:203:LEU:HD11	24:C1:364:VAL:HG23	1.88	0.56
4:c:101:GLN:O	4:c:105:THR:OG1	2.20	0.55
8:g:5:LEU:HD21	8:g:245:LEU:HD11	1.88	0.55
8:g:59:VAL:HG13	8:g:216:VAL:HB	1.89	0.55
22:P1:48:GLN:O	22:P1:51:HIS:ND1	2.39	0.55
5:d:118:GLU:O	5:d:218:ARG:NH2	2.40	0.55
24:A1:51:MET:HE3	24:A1:68:ALA:HB1	1.88	0.55
3:a:8:ASP:OD1	13:n:126:TYR:OH	2.23	0.54
9:h:38:LYS:N	21:M1:215:THR:O	2.40	0.54
24:C1:212:LYS:N	32:C1:601:ATP:O1B	2.40	0.54
25:F1:165:LYS:NZ	25:F1:486:VAL:O	2.38	0.54
3:a:194:PHE:HZ	22:S1:106:LEU:HD22	1.72	0.54
15:p:66:ASP:OD1	17:r:13:GLN:NE2	2.39	0.54
24:C1:328:ARG:NH1	25:D1:342:ASP:OD2	2.41	0.53
24:A1:523:GLU:OE1	24:A1:523:GLU:N	2.40	0.53
6:e:253:VAL:O	6:e:257:ARG:N	2.42	0.53
25:E1:180:GLY:HA3	25:E1:355:LEU:HD13	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C1:80:ILE:C	24:C1:80:ILE:HD12	2.33	0.53
18:H1:129:VAL:CG1	19:I1:28:THR:HG21	2.38	0.53
7:f:41:LEU:HD23	7:f:45:LEU:HD12	1.91	0.52
2:M:103:PHE:CZ	2:M:107:LEU:HD11	2.44	0.52
24:B1:390:ASP:OD1	24:B1:391:THR:N	2.42	0.52
4:c:61:VAL:HG13	5:d:278:VAL:HG11	1.89	0.52
11:j:54:TYR:O	11:j:92:ARG:NH1	2.42	0.52
20:L1:28:ASP:OD1	20:L1:32:TYR:N	2.42	0.52
24:C1:203:LEU:HD13	24:C1:379:VAL:CG1	2.40	0.52
2:m:103:PHE:CZ	2:m:107:LEU:HD11	2.44	0.52
5:d:345:LEU:HD13	25:F1:477:GLN:OE1	2.10	0.52
25:D1:270:ARG:NH1	25:D1:323:THR:O	2.36	0.52
5:d:284:GLN:OE1	5:d:284:GLN:N	2.38	0.52
6:e:62:ARG:NH2	11:j:96:GLN:OE1	2.37	0.52
25:F1:91:GLN:OE1	25:F1:91:GLN:N	2.43	0.52
2:m:119:ARG:NH2	2:m:122:ILE:O	2.43	0.52
26:M:201:CDL:H261	27:M:202:PEE:H44	1.92	0.51
15:p:66:ASP:OD2	17:r:10:ARG:NH1	2.43	0.51
20:J1:117:GLU:O	20:J1:121:THR:HG23	2.11	0.51
20:K1:138:CYS:O	20:K1:142:VAL:HG23	2.10	0.51
20:K1:142:VAL:HG22	24:C1:537:ILE:HD13	1.92	0.51
26:e:403:CDL:H871	16:q:56:TRP:CZ3	2.45	0.51
18:H1:82:TYR:OH	22:V1:85:ASN:ND2	2.44	0.51
20:J1:32:TYR:OH	25:F1:130:ASP:O	2.28	0.51
2:M:119:ARG:NH2	2:M:122:ILE:O	2.43	0.51
24:B1:381:SER:O	25:F1:216:ARG:NH2	2.43	0.51
8:g:155:LYS:O	8:g:159:THR:HG22	2.10	0.51
20:J1:36:THR:HG22	20:J1:36:THR:O	2.12	0.50
6:e:201:TYR:O	6:e:205:ILE:N	2.41	0.50
1:l:10:LEU:HD13	2:m:83:ILE:HD11	1.93	0.50
18:H1:56:ARG:HG2	18:H1:61:LEU:HD11	1.93	0.50
3:a:212:ILE:HD11	22:T1:99:ALA:HB3	1.92	0.50
6:e:58:ASP:OD1	6:e:59:TYR:N	2.42	0.50
5:d:23:LEU:HD11	9:h:107:ALA:HB1	1.93	0.50
20:L1:181:GLY:O	20:L1:185:VAL:HG23	2.11	0.50
24:B1:212:LYS:HG2	24:B1:389:LEU:HD12	1.92	0.50
25:E1:362:ASP:OD1	25:E1:363:ARG:N	2.44	0.50
18:H1:61:LEU:N	18:H1:61:LEU:HD12	2.27	0.50
25:E1:81:ASP:OD1	25:E1:84:THR:N	2.45	0.50
25:E1:469:GLY:HA2	25:E1:472:MET:HE3	1.93	0.50
3:a:145:LEU:HD22	22:T1:110:MET:HE1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Q1:65:VAL:HG13	22:Q1:101:THR:HG22	1.94	0.50
24:B1:212:LYS:N	32:B1:601:ATP:O1B	2.44	0.49
10:i:88:LYS:O	14:o:32:GLN:NE2	2.45	0.49
22:R1:45:ILE:O	22:S1:48:GLN:N	2.45	0.49
25:D1:448:GLU:O	25:D1:452:GLY:N	2.41	0.49
1:L:10:LEU:HD13	2:M:83:ILE:HD11	1.95	0.49
24:B1:166:VAL:O	24:B1:345:ARG:NH1	2.36	0.49
21:M1:90:VAL:CG2	21:M1:108:VAL:HG22	2.43	0.48
24:A1:203:LEU:HD13	24:A1:379:VAL:CG1	2.43	0.48
7:f:64:ARG:NH1	17:r:33:GLU:OE1	2.46	0.48
25:D1:81:ASP:OD1	25:D1:84:THR:N	2.40	0.48
25:F1:81:ASP:OD1	25:F1:84:THR:N	2.43	0.48
24:B1:511:THR:O	24:B1:511:THR:HG22	2.13	0.48
3:a:26:LEU:HD22	7:f:43:TRP:CZ2	2.48	0.48
8:g:44:ALA:N	8:g:241:GLU:OE2	2.46	0.48
23:G1:158:GLN:HG3	23:G1:174:VAL:HG13	1.95	0.48
25:E1:350:THR:HG22	25:E1:350:THR:O	2.13	0.48
24:B1:91:ALA:N	24:B1:109:ASP:OD1	2.47	0.48
20:K1:163:GLN:O	20:K1:167:THR:HG23	2.14	0.48
3:a:26:LEU:O	4:c:67:ASN:ND2	2.44	0.48
3:a:149:CYS:SG	22:T1:110:MET:HE3	2.53	0.48
5:d:280:ILE:O	5:d:280:ILE:HD12	2.13	0.48
8:g:58:ALA:HB3	8:g:80:ARG:HB3	1.96	0.48
16:q:49:ALA:N	16:q:50:PRO:CD	2.77	0.48
18:H1:129:VAL:HG12	19:I1:28:THR:HG21	1.95	0.48
5:d:33:THR:O	5:d:34:THR:C	2.56	0.48
14:o:86:TYR:O	14:o:91:ARG:NE	2.46	0.48
24:A1:203:LEU:HD13	24:A1:379:VAL:HG11	1.95	0.47
22:W1:84:PRO:O	22:W1:87:THR:HG23	2.14	0.47
25:D1:105:THR:O	25:D1:105:THR:HG22	2.14	0.47
25:D1:287:PHE:O	25:D1:291:ASN:ND2	2.43	0.47
25:F1:389:ILE:HD12	25:F1:393:HIS:ND1	2.28	0.47
7:f:101:ARG:NH1	17:r:45:ASP:O	2.47	0.47
22:O1:98:PHE:CD1	22:X1:100:LEU:HD13	2.48	0.47
24:A1:327:GLY:N	24:A1:331:TYR:O	2.45	0.47
25:E1:448:GLU:O	25:E1:452:GLY:N	2.37	0.47
3:a:194:PHE:CZ	22:S1:106:LEU:HD22	2.49	0.47
24:C1:203:LEU:HD11	24:C1:364:VAL:CG2	2.45	0.47
21:M1:131:ASN:O	21:M1:135:LYS:N	2.48	0.47
25:D1:181:LEU:HD23	25:D1:359:THR:HB	1.96	0.47
3:a:194:PHE:CZ	22:S1:106:LEU:HD13	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:20:PHE:CE2	1:l:24:LEU:HD11	2.50	0.47
12:k:103:MET:HE1	16:q:80:LEU:HA	1.96	0.47
25:F1:62:VAL:HG21	25:F1:72:LEU:HD23	1.97	0.47
22:S1:45:ILE:O	22:T1:47:VAL:HA	2.15	0.47
24:C1:531:PHE:O	24:C1:532:THR:CB	2.63	0.47
19:I1:70:ILE:N	19:I1:70:ILE:HD12	2.30	0.46
22:R1:43:VAL:O	22:S1:46:SER:N	2.42	0.46
26:c:201:CDL:H872	26:c:201:CDL:H832	1.96	0.46
11:j:30:GLU:OE1	16:q:72:ASN:ND2	2.49	0.46
2:m:46:HIS:O	2:m:50:GLY:N	2.49	0.46
2:M:88:TYR:O	2:M:91:GLN:NE2	2.49	0.46
2:m:88:TYR:O	2:m:91:GLN:NE2	2.49	0.46
22:X1:65:VAL:HG13	22:X1:101:THR:HG22	1.97	0.46
24:B1:537:ILE:N	24:B1:537:ILE:HD12	2.31	0.46
6:e:229:MET:SD	6:e:235:ASN:ND2	2.86	0.46
18:H1:95:SER:HB3	18:H1:96:PRO:HD2	1.97	0.46
24:B1:524:LEU:HD23	24:B1:527:LEU:HD12	1.98	0.46
10:i:16:LEU:O	10:i:20:THR:HG22	2.16	0.46
10:i:90:THR:O	14:o:36:ARG:NH2	2.49	0.46
1:L:20:PHE:CE2	1:L:24:LEU:HD11	2.50	0.46
19:I1:47:SER:O	19:I1:48:LYS:HB2	2.16	0.46
25:D1:260:GLN:OE1	25:D1:260:GLN:N	2.49	0.46
25:E1:270:ARG:NH1	25:E1:323:THR:O	2.47	0.45
22:O1:73:PHE:CZ	22:X1:100:LEU:HD12	2.51	0.45
24:B1:65:LEU:HD22	24:B1:120:VAL:HG21	1.97	0.45
25:F1:55:PRO:O	25:F1:58:THR:OG1	2.32	0.45
7:f:114:ALA:HB1	22:S1:118:SER:OG	2.17	0.45
8:g:57:THR:HG21	8:g:124:VAL:HG11	1.99	0.45
16:q:77:GLU:OE2	16:q:79:HIS:NE2	2.50	0.45
24:B1:495:PHE:CE2	24:B1:499:LEU:HD11	2.52	0.45
25:D1:268:TYR:CD2	25:D1:272:VAL:HG21	2.52	0.45
25:D1:150:LEU:HD23	25:D1:150:LEU:O	2.16	0.45
25:D1:263:LEU:HD21	25:D1:321:ARG:HB2	1.99	0.45
25:E1:282:ASP:HA	25:E1:283:ASN:HA	1.84	0.45
12:k:103:MET:HE1	16:q:80:LEU:O	2.17	0.45
24:A1:65:LEU:HD22	24:A1:120:VAL:HG21	1.98	0.45
24:B1:285:TYR:OH	24:B1:338:LEU:HD12	2.16	0.45
8:g:56:HIS:NE2	8:g:219:THR:O	2.50	0.44
24:A1:404:ILE:HG22	24:A1:404:ILE:O	2.17	0.44
25:D1:311:LEU:HD23	25:D1:311:LEU:O	2.17	0.44
4:c:43:VAL:HG13	4:c:44:TRP:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:269:GLU:OE1	6:e:184:LYS:NZ	2.43	0.44
10:i:2:VAL:HG22	10:i:3:TYR:N	2.32	0.44
3:a:197:PHE:HE1	22:S1:99:ALA:HB1	1.82	0.44
24:A1:166:VAL:HG12	24:A1:166:VAL:O	2.16	0.44
24:C1:135:VAL:HG12	24:C1:135:VAL:O	2.15	0.44
2:M:46:HIS:O	2:M:50:GLY:N	2.49	0.44
6:e:368:GLU:OE2	15:p:39:GLN:N	2.47	0.44
24:B1:203:LEU:HD12	24:B1:362:PRO:O	2.17	0.44
24:B1:485:LEU:N	24:B1:485:LEU:HD12	2.32	0.44
25:D1:91:GLN:OE1	25:D1:91:GLN:N	2.51	0.44
24:A1:531:PHE:O	24:A1:532:THR:CB	2.65	0.44
25:F1:453:MET:HE1	25:F1:485:MET:HE2	1.99	0.44
5:d:324:ASN:HB2	5:d:325:PRO:HD3	1.98	0.44
10:i:62:ARG:NH2	13:n:134:SER:O	2.49	0.44
11:j:64:GLN:NE2	30:j:203:PC1:O22	2.49	0.44
24:A1:433:GLU:HG2	24:A1:437:LEU:HD13	1.99	0.44
24:B1:207:ASP:OD1	24:B1:208:ARG:N	2.45	0.44
24:C1:173:ILE:HG23	24:C1:174:VAL:HG13	2.00	0.44
20:J1:143:MET:O	20:J1:147:CYS:N	2.51	0.44
20:K1:70:ILE:HG22	20:K1:74:ASN:HD21	1.82	0.44
25:D1:62:VAL:HG21	25:D1:72:LEU:HD23	2.00	0.44
5:d:268:PRO:HB2	6:e:327:ALA:HB3	2.00	0.44
20:K1:187:VAL:HG21	24:C1:580:CYS:SG	2.58	0.44
22:R1:106:LEU:O	22:R1:110:MET:N	2.47	0.44
24:A1:423:VAL:HG12	24:A1:423:VAL:O	2.18	0.44
24:B1:174:VAL:O	24:B1:174:VAL:HG12	2.18	0.44
24:B1:491:GLN:OE1	24:B1:491:GLN:N	2.46	0.44
3:a:51:LEU:HD11	10:i:22:GLU:O	2.18	0.43
20:J1:181:GLY:O	20:J1:185:VAL:HG23	2.18	0.43
21:M1:66:ILE:HD12	21:M1:66:ILE:H	1.82	0.43
24:B1:52:ILE:C	24:B1:52:ILE:HD12	2.43	0.43
25:E1:268:TYR:CE2	25:E1:272:VAL:HG21	2.54	0.43
9:h:67:LEU:O	9:h:72:GLN:NE2	2.52	0.43
2:m:102:ARG:NE	15:p:82:ASN:OD1	2.47	0.43
24:A1:537:ILE:HD12	24:A1:537:ILE:N	2.32	0.43
23:G1:51:GLU:O	23:G1:55:SER:N	2.42	0.43
5:d:321:ALA:O	5:d:325:PRO:HD2	2.19	0.43
6:e:378:ARG:HH22	15:p:63:ASP:CG	2.26	0.43
25:E1:111:VAL:HG23	25:E1:143:ILE:CG2	2.48	0.43
25:D1:120:ARG:NE	25:D1:130:ASP:OD2	2.50	0.43
25:E1:66:LEU:HD12	25:E1:95:LEU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A1:317:GLN:NE2	25:D1:313:GLU:OE1	2.50	0.43
24:B1:307:ASP:OD1	24:B1:307:ASP:N	2.51	0.43
25:D1:282:ASP:HA	25:D1:283:ASN:HA	1.81	0.43
6:e:371:THR:HG23	15:p:64:PRO:CG	2.49	0.43
18:H1:60:PHE:CD1	18:H1:60:PHE:C	2.97	0.43
21:M1:196:VAL:CG2	24:C1:48:THR:HG22	2.49	0.43
24:A1:188:LYS:NZ	24:A1:461:LEU:O	2.46	0.43
3:a:48:ASP:OD2	6:e:213:LYS:NZ	2.44	0.42
7:f:128:THR:O	7:f:128:THR:HG22	2.19	0.42
25:E1:60:LEU:HB3	25:E1:102:VAL:HG12	2.00	0.42
25:F1:250:GLU:O	25:F1:255:ARG:NH1	2.52	0.42
8:g:55:VAL:HG12	8:g:219:THR:HG22	2.01	0.42
2:m:102:ARG:NH1	15:p:89:GLU:OE1	2.52	0.42
22:R1:86:LEU:HD11	22:S1:84:PRO:HB3	2.01	0.42
23:G1:127:ILE:N	23:G1:127:ILE:HD12	2.34	0.42
7:f:56:ILE:HB	7:f:57:PRO:HD3	2.01	0.42
26:q:101:CDL:OB7	26:q:101:CDL:CB3	2.66	0.42
20:K1:185:VAL:HG23	20:K1:185:VAL:O	2.20	0.42
24:C1:411:VAL:HG22	24:C1:411:VAL:O	2.20	0.42
3:a:149:CYS:SG	22:T1:110:MET:HB2	2.60	0.42
5:d:184:ASP:OD1	5:d:184:ASP:N	2.52	0.42
7:f:67:ASN:ND2	7:f:72:ASP:OD2	2.53	0.42
20:K1:178:GLN:NE2	21:M1:234:GLU:OE2	2.49	0.42
6:e:259:HIS:ND1	6:e:289:MET:HE1	2.34	0.42
22:S1:100:LEU:HB3	22:T1:98:PHE:CE1	2.55	0.42
24:A1:301:CYS:SG	24:A1:302:LEU:N	2.93	0.42
5:d:344:VAL:HG22	25:F1:497:LYS:HG3	2.02	0.42
19:I1:48:LYS:O	19:I1:49:PRO:C	2.63	0.42
24:B1:131:VAL:HG11	24:B1:293:TYR:HB2	2.01	0.42
25:D1:486:VAL:HG21	25:D1:492:VAL:HG22	2.02	0.42
22:W1:47:VAL:CG1	22:W1:50:LEU:HG	2.50	0.42
24:B1:301:CYS:SG	24:B1:302:LEU:N	2.92	0.42
25:F1:419:ILE:O	25:F1:419:ILE:HG13	2.20	0.42
16:q:55:TRP:O	16:q:61:GLN:NE2	2.46	0.42
24:C1:399:ARG:HA	24:C1:401:ALA:N	2.35	0.42
25:E1:263:LEU:HD13	25:E1:322:ILE:HG12	2.01	0.42
25:F1:190:THR:HG23	25:F1:191:VAL:N	2.35	0.42
4:c:107:ALA:HB2	8:g:99:VAL:HG21	2.02	0.42
7:f:45:LEU:HD13	30:f:203:PC1:H3I3	2.02	0.42
8:g:57:THR:HB	8:g:218:HIS:HB2	2.02	0.42
25:E1:417:LEU:HD22	25:E1:421:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A1:183:LEU:C	24:A1:183:LEU:HD23	2.46	0.41
24:C1:192:THR:HG22	24:C1:420:MET:SD	2.60	0.41
25:D1:41:ILE:HG22	25:D1:41:ILE:O	2.20	0.41
25:E1:263:LEU:HD21	25:E1:321:ARG:CB	2.50	0.41
24:A1:531:PHE:O	24:A1:532:THR:HB	2.19	0.41
24:A1:564:ILE:HG23	24:A1:569:ASP:HB2	2.02	0.41
24:C1:423:VAL:O	24:C1:423:VAL:HG12	2.21	0.41
5:d:87:LEU:HD22	5:d:247:GLN:HE22	1.85	0.41
8:g:196:VAL:HG12	8:g:197:ALA:N	2.34	0.41
15:p:36:ARG:NH2	15:p:39:GLN:OE1	2.53	0.41
23:G1:268:GLN:NE2	25:F1:342:ASP:OD2	2.54	0.41
25:E1:170:ILE:N	25:E1:170:ILE:HD12	2.36	0.41
24:B1:75:ALA:HB3	24:B1:78:THR:HG21	2.01	0.41
5:d:175:TRP:N	5:d:176:PRO:CD	2.83	0.41
12:k:124:LEU:N	12:k:124:LEU:HD23	2.36	0.41
22:P1:86:LEU:HD11	22:Q1:84:PRO:HB3	2.01	0.41
22:W1:71:THR:O	22:W1:75:ASN:ND2	2.46	0.41
24:C1:192:THR:HG21	24:C1:477:LEU:HD13	2.03	0.41
5:d:324:ASN:CB	5:d:325:PRO:HD3	2.50	0.41
9:h:24:MET:SD	9:h:24:MET:N	2.94	0.41
24:A1:82:ILE:HG12	24:A1:120:VAL:HG22	2.02	0.41
24:A1:564:ILE:HG23	24:A1:569:ASP:CB	2.51	0.41
24:C1:141:ASN:OD1	24:C1:145:HIS:N	2.53	0.41
24:B1:183:LEU:HD23	24:B1:183:LEU:C	2.45	0.41
25:F1:263:LEU:HD21	25:F1:321:ARG:CB	2.51	0.41
3:a:121:VAL:HG11	12:k:60:MET:HB3	2.01	0.41
8:g:59:VAL:HG23	8:g:79:VAL:HG22	2.03	0.41
8:g:269:LEU:HD12	8:g:269:LEU:C	2.45	0.41
22:T1:65:VAL:HG21	22:T1:105:GLY:HA3	2.03	0.41
25:F1:38:SER:N	25:F1:46:ASP:O	2.47	0.41
25:F1:413:ILE:HG21	25:F1:422:LEU:HD21	2.03	0.41
25:F1:462:ASP:OD1	25:F1:466:SER:OG	2.39	0.41
3:a:49:LEU:H	3:a:49:LEU:HD23	1.86	0.41
8:g:168:THR:HG22	8:g:169:THR:N	2.36	0.41
24:A1:269:MET:SD	24:A1:286:ALA:HB3	2.61	0.41
1:L:12:GLN:NE2	2:m:52:ASP:OD2	2.47	0.40
8:g:60:THR:HG22	8:g:78:VAL:O	2.20	0.40
8:g:138:VAL:HG21	8:g:188:LEU:HD22	2.03	0.40
22:O1:65:VAL:HG13	22:O1:101:THR:HG22	2.03	0.40
24:B1:59:ASP:OD1	25:E1:78:GLN:NE2	2.54	0.40
24:C1:531:PHE:O	24:C1:532:THR:HB	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D1:311:LEU:HD23	25:D1:311:LEU:C	2.46	0.40
25:F1:282:ASP:HA	25:F1:283:ASN:HA	1.84	0.40
5:d:97:MET:HE2	5:d:102:LEU:HA	2.03	0.40
12:k:86:TRP:O	12:k:90:VAL:HG23	2.21	0.40
4:c:100:ASP:OD1	4:c:101:GLN:N	2.55	0.40
22:P1:104:ILE:HD12	22:Q1:69:ILE:HD12	2.03	0.40
22:U1:104:ILE:HG23	22:V1:62:LEU:HB3	2.04	0.40
24:B1:51:MET:HB2	24:B1:121:MET:HE1	2.02	0.40
10:i:2:VAL:HG22	10:i:3:TYR:H	1.85	0.40
18:H1:146:LEU:HB2	18:H1:172:ILE:HG21	2.04	0.40
22:O1:70:GLY:HA2	22:X1:72:ILE:HD11	2.02	0.40
24:C1:457:ARG:NH2	24:C1:488:VAL:O	2.42	0.40
25:D1:403:MET:HE1	25:D1:432:ARG:HB3	2.03	0.40
25:F1:162:THR:OG1	25:F1:168:ASP:OD1	2.39	0.40
25:F1:347:ALA:HB3	25:F1:348:PRO:CD	2.51	0.40
3:a:93:TYR:CE2	3:a:220:LEU:HD22	2.56	0.40
6:e:210:ILE:O	6:e:232:ARG:NH2	2.47	0.40
8:g:151:ASN:OD1	8:g:152:GLU:N	2.55	0.40

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%)	127 (100%)	0	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%)	83 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	328/370 (89%)	317 (97%)	10 (3%)	1 (0%)	36	67
6	e	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
7	f	133/145 (92%)	130 (98%)	3 (2%)	0	100	100
8	g	266/269 (99%)	264 (99%)	2 (1%)	0	100	100
9	h	135/157 (86%)	134 (99%)	1 (1%)	0	100	100
10	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
11	j	166/169 (98%)	163 (98%)	3 (2%)	0	100	100
12	k	103/124 (83%)	100 (97%)	3 (3%)	0	100	100
13	n	137/156 (88%)	129 (94%)	8 (6%)	0	100	100
14	o	94/101 (93%)	93 (99%)	1 (1%)	0	100	100
15	p	78/105 (74%)	76 (97%)	2 (3%)	0	100	100
16	q	83/98 (85%)	82 (99%)	1 (1%)	0	100	100
17	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	H1	159/182 (87%)	155 (98%)	3 (2%)	1 (1%)	21	54
19	I1	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
20	J1	164/188 (87%)	160 (98%)	4 (2%)	0	100	100
20	K1	164/188 (87%)	163 (99%)	1 (1%)	0	100	100
20	L1	163/188 (87%)	163 (100%)	0	0	100	100
21	M1	230/255 (90%)	221 (96%)	9 (4%)	0	100	100
22	O1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
22	P1	76/118 (64%)	76 (100%)	0	0	100	100
22	Q1	76/118 (64%)	76 (100%)	0	0	100	100
22	R1	76/118 (64%)	76 (100%)	0	0	100	100
22	S1	76/118 (64%)	76 (100%)	0	0	100	100
22	T1	76/118 (64%)	76 (100%)	0	0	100	100
22	U1	76/118 (64%)	76 (100%)	0	0	100	100
22	V1	76/118 (64%)	76 (100%)	0	0	100	100
22	W1	76/118 (64%)	76 (100%)	0	0	100	100
22	X1	76/118 (64%)	76 (100%)	0	0	100	100
23	G1	298/305 (98%)	290 (97%)	8 (3%)	0	100	100
24	A1	517/584 (88%)	513 (99%)	4 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	B1	525/584 (90%)	515 (98%)	10 (2%)	0	100	100
24	C1	518/584 (89%)	511 (99%)	6 (1%)	1 (0%)	43	73
25	D1	486/519 (94%)	478 (98%)	8 (2%)	0	100	100
25	E1	484/519 (93%)	471 (97%)	13 (3%)	0	100	100
25	F1	486/519 (94%)	473 (97%)	13 (3%)	0	100	100
All	All	7775/8943 (87%)	7644 (98%)	128 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	H1	158	ASP
5	d	34	THR
24	C1	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%)	111 (100%)	0	100	100
2	m	111/124 (90%)	111 (100%)	0	100	100
3	a	225/225 (100%)	223 (99%)	2 (1%)	70	74
4	c	80/104 (77%)	80 (100%)	0	100	100
5	d	297/334 (89%)	294 (99%)	3 (1%)	68	74
6	e	334/341 (98%)	333 (100%)	1 (0%)	86	84
7	f	119/124 (96%)	118 (99%)	1 (1%)	73	76
8	g	205/206 (100%)	205 (100%)	0	100	100
9	h	110/123 (89%)	110 (100%)	0	100	100
10	i	95/96 (99%)	95 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	j	149/150 (99%)	149 (100%)	0	100	100
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%)	82 (100%)	0	100	100
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	H1	137/156 (88%)	136 (99%)	1 (1%)	76	77
19	I1	58/67 (87%)	58 (100%)	0	100	100
20	J1	145/162 (90%)	145 (100%)	0	100	100
20	K1	145/162 (90%)	145 (100%)	0	100	100
20	L1	145/162 (90%)	145 (100%)	0	100	100
21	M1	200/215 (93%)	200 (100%)	0	100	100
22	O1	56/89 (63%)	55 (98%)	1 (2%)	51	67
22	P1	56/89 (63%)	55 (98%)	1 (2%)	51	67
22	Q1	56/89 (63%)	55 (98%)	1 (2%)	51	67
22	R1	56/89 (63%)	55 (98%)	1 (2%)	51	67
22	S1	56/89 (63%)	54 (96%)	2 (4%)	31	54
22	T1	56/89 (63%)	54 (96%)	2 (4%)	31	54
22	U1	56/89 (63%)	54 (96%)	2 (4%)	31	54
22	V1	56/89 (63%)	55 (98%)	1 (2%)	51	67
22	W1	56/89 (63%)	55 (98%)	1 (2%)	51	67
22	X1	56/89 (63%)	55 (98%)	1 (2%)	51	67
23	G1	253/257 (98%)	251 (99%)	2 (1%)	73	76
24	A1	434/479 (91%)	434 (100%)	0	100	100
24	B1	438/479 (91%)	436 (100%)	2 (0%)	81	81
24	C1	436/479 (91%)	436 (100%)	0	100	100
25	D1	399/420 (95%)	397 (100%)	2 (0%)	81	81
25	E1	397/420 (94%)	397 (100%)	0	100	100
25	F1	399/420 (95%)	399 (100%)	0	100	100
All	All	6599/7441 (89%)	6571 (100%)	28 (0%)	81	83

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	144	PHE
3	a	149	CYS
5	d	138	VAL
5	d	205	ARG
5	d	281	THR
6	e	14	ASN
7	f	42	ASN
13	n	105	GLU
18	H1	24	LEU
22	O1	42	THR
22	P1	42	THR
22	Q1	42	THR
22	R1	42	THR
22	S1	42	THR
22	S1	114	LEU
22	T1	42	THR
22	T1	98	PHE
22	U1	42	THR
22	U1	104	ILE
22	V1	42	THR
22	W1	42	THR
22	X1	42	THR
23	G1	98	VAL
23	G1	233	ASN
24	B1	74	VAL
24	B1	173	ILE
25	D1	66	LEU
25	D1	116	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	11	HIS
2	M	47	ASN
3	a	155	HIS
6	e	41	GLN
6	e	166	HIS
7	f	42	ASN
8	g	143	GLN
8	g	218	HIS
1	l	11	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	m	47	ASN
13	n	89	GLN
13	n	91	HIS
13	n	144	HIS
14	o	25	HIS
15	p	95	GLN
18	H1	22	HIS
18	H1	33	HIS
18	H1	41	HIS
18	H1	149	GLN
20	J1	82	GLN
20	J1	93	ASN
20	J1	175	HIS
20	K1	74	ASN
22	V1	85	ASN
23	G1	87	ASN
23	G1	162	ASN
23	G1	176	ASN
24	A1	339	HIS
24	A1	369	ASN
24	A1	502	HIS
24	A1	522	GLN
24	A1	556	HIS
24	A1	558	GLN
24	B1	254	HIS
24	B1	339	HIS
24	B1	398	GLN
24	B1	417	ASN
24	B1	463	ASN
24	B1	472	ASN
24	B1	502	HIS
24	B1	514	ASN
24	B1	551	HIS
24	C1	245	GLN
24	C1	249	ASN
24	C1	463	ASN
25	D1	204	HIS
25	E1	78	GLN
25	E1	83	HIS
25	E1	144	HIS
25	F1	30	HIS
25	F1	398	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	F1	411	GLN

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	0.43	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	-	3/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	e	1	AME	N-CA-CB-CG
6	e	1	AME	C-CA-N-CT1
6	e	1	AME	CB-CA-N-CT1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	e	1	AME	1	0

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	e	401	-	99,99,99	0.28	0	105,111,111	0.25	0
30	PC1	f	203	-	53,53,53	0.27	0	59,61,61	0.28	0
30	PC1	j	203	-	53,53,53	0.28	0	59,61,61	0.27	0
28	LMT	j	204	-	36,36,36	0.10	0	47,47,47	0.18	0
27	PEE	M	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.49	0
26	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	L	101	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	e	405	-	99,99,99	0.28	0	105,111,111	0.26	0
26	CDL	M	201	-	99,99,99	0.29	0	105,111,111	0.34	1 (0%)
28	LMT	e	406	-	36,36,36	0.10	0	47,47,47	0.16	0
26	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
29	Q7G	n	201	-	66,66,90	0.13	0	98,102,138	0.30	0
26	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.28	0
30	PC1	i	201	-	53,53,53	0.28	0	59,61,61	0.28	0
32	ATP	B1	601	33	32,33,33	0.28	0	48,52,52	0.28	0
27	PEE	m	202	-	50,50,50	0.77	2 (4%)	53,55,55	0.48	0
26	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
26	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.26	0
32	ATP	C1	601	33	32,33,33	0.29	0	48,52,52	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PC1	p	201	-	53,53,53	0.28	0	59,61,61	0.28	0
26	CDL	m	201	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.26	0
32	ATP	A1	601	33	32,33,33	0.29	0	48,52,52	0.29	0
26	CDL	j	202	-	99,99,99	0.29	0	105,111,111	0.26	0
29	Q7G	e	407	-	54,54,90	0.13	0	80,84,138	0.25	0
31	UTP	H1	201	-	29,30,30	0.31	0	43,47,47	0.39	0
32	ATP	D1	601	33	32,33,33	0.28	0	48,52,52	0.29	0
34	ADP	E1	601	33	28,29,29	0.40	0	43,45,45	0.48	0
27	PEE	f	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.49	0
26	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.27	0
26	CDL	e	403	-	99,99,99	0.28	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	e	401	-	-	23/110/110/110	-
30	PC1	f	203	-	-	11/57/57/57	-
30	PC1	j	203	-	-	15/57/57/57	-
28	LMT	j	204	-	-	5/21/61/61	0/2/2/2
27	PEE	M	202	-	-	21/54/54/54	-
26	CDL	l	101	-	-	19/110/110/110	-
26	CDL	L	101	-	-	17/110/110/110	-
26	CDL	e	405	-	-	30/110/110/110	-
26	CDL	M	201	-	-	28/110/110/110	-
28	LMT	e	406	-	-	1/21/61/61	0/2/2/2
26	CDL	j	201	-	-	23/110/110/110	-
29	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
26	CDL	f	201	-	-	19/110/110/110	-
30	PC1	i	201	-	-	9/57/57/57	-
32	ATP	B1	601	33	-	6/22/38/38	0/3/3/3
27	PEE	m	202	-	-	22/54/54/54	-
26	CDL	q	101	-	-	24/110/110/110	-
26	CDL	e	404	-	-	20/110/110/110	-
32	ATP	C1	601	33	-	8/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PC1	p	201	-	-	10/57/57/57	-
26	CDL	m	201	-	-	28/110/110/110	-
26	CDL	e	402	-	-	24/110/110/110	-
32	ATP	A1	601	33	-	5/22/38/38	0/3/3/3
26	CDL	j	202	-	-	29/110/110/110	-
29	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
31	UTP	H1	201	-	-	5/22/38/38	0/2/2/2
32	ATP	D1	601	33	-	5/22/38/38	0/3/3/3
34	ADP	E1	601	33	-	2/16/32/32	0/3/3/3
27	PEE	f	202	-	-	17/54/54/54	-
26	CDL	c	201	-	-	23/110/110/110	-
26	CDL	e	403	-	-	24/110/110/110	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	m	202	PEE	C18-C19	3.66	1.52	1.31
27	f	202	PEE	C39-C38	3.65	1.52	1.31
27	M	202	PEE	C18-C19	3.63	1.52	1.31
27	f	202	PEE	C18-C19	3.62	1.52	1.31
27	m	202	PEE	C39-C38	3.59	1.52	1.31
27	M	202	PEE	C39-C38	3.56	1.51	1.31

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	201	CDL	C27-C26-C25	2.39	129.52	113.36

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	e	407	Q7G	C1B
29	n	201	Q7G	C1B
29	n	201	Q7G	C1C

All (484) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	L	101	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	L	101	CDL	CA2-OA2-PA1-OA5
26	L	101	CDL	CA3-OA5-PA1-OA2
26	M	201	CDL	CA2-C1-CB2-OB2
26	M	201	CDL	CA3-OA5-PA1-OA2
26	M	201	CDL	CA3-OA5-PA1-OA3
26	M	201	CDL	CB2-OB2-PB2-OB4
26	M	201	CDL	CB2-OB2-PB2-OB5
26	M	201	CDL	C51-CB5-OB6-CB4
26	c	201	CDL	CB3-OB5-PB2-OB2
26	c	201	CDL	CB3-OB5-PB2-OB4
26	e	401	CDL	CA3-OA5-PA1-OA3
26	e	401	CDL	CB2-OB2-PB2-OB3
26	e	401	CDL	CB2-OB2-PB2-OB4
26	e	401	CDL	CB2-OB2-PB2-OB5
26	e	401	CDL	CB3-OB5-PB2-OB2
26	e	401	CDL	CB3-OB5-PB2-OB3
26	e	402	CDL	CA3-OA5-PA1-OA2
26	e	402	CDL	CA3-OA5-PA1-OA3
26	e	402	CDL	CA3-OA5-PA1-OA4
26	e	403	CDL	CB2-OB2-PB2-OB3
26	e	404	CDL	CA3-OA5-PA1-OA2
26	e	404	CDL	CA3-OA5-PA1-OA4
26	e	404	CDL	CB3-OB5-PB2-OB2
26	e	404	CDL	CB3-OB5-PB2-OB3
26	e	404	CDL	CB3-OB5-PB2-OB4
26	e	405	CDL	CA3-OA5-PA1-OA2
26	e	405	CDL	CA3-OA5-PA1-OA3
26	e	405	CDL	CA3-OA5-PA1-OA4
26	e	405	CDL	CB3-OB5-PB2-OB2
26	f	201	CDL	CA2-OA2-PA1-OA4
26	f	201	CDL	CA2-OA2-PA1-OA5
26	f	201	CDL	CB3-OB5-PB2-OB2
26	j	201	CDL	CA2-OA2-PA1-OA3
26	j	201	CDL	CA3-OA5-PA1-OA2
26	j	201	CDL	CA3-OA5-PA1-OA3
26	j	201	CDL	CA3-OA5-PA1-OA4
26	j	202	CDL	CA2-OA2-PA1-OA4
26	j	202	CDL	CB3-OB5-PB2-OB2
26	j	202	CDL	CB3-OB5-PB2-OB4
26	l	101	CDL	CA2-OA2-PA1-OA3
26	l	101	CDL	CA2-OA2-PA1-OA4
26	l	101	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	l	101	CDL	CA3-OA5-PA1-OA2
26	m	201	CDL	CA2-C1-CB2-OB2
26	m	201	CDL	CA3-OA5-PA1-OA2
26	m	201	CDL	CA3-OA5-PA1-OA3
26	m	201	CDL	OA6-CA4-CA6-OA8
26	m	201	CDL	CB2-OB2-PB2-OB4
26	m	201	CDL	CB2-OB2-PB2-OB5
26	m	201	CDL	C51-CB5-OB6-CB4
26	q	101	CDL	CA2-C1-CB2-OB2
26	q	101	CDL	OA5-CA3-CA4-OA6
26	q	101	CDL	CB2-OB2-PB2-OB3
26	q	101	CDL	CB3-OB5-PB2-OB2
26	q	101	CDL	CB3-OB5-PB2-OB3
27	M	202	PEE	C1-O3P-P-O2P
27	M	202	PEE	C1-O3P-P-O4P
27	M	202	PEE	C4-O4P-P-O3P
27	M	202	PEE	O4P-C4-C5-N
27	f	202	PEE	C4-O4P-P-O2P
27	f	202	PEE	O4P-C4-C5-N
27	m	202	PEE	C1-O3P-P-O2P
27	m	202	PEE	C1-O3P-P-O4P
27	m	202	PEE	C4-O4P-P-O3P
27	m	202	PEE	O4P-C4-C5-N
28	e	406	LMT	C2-C1-O1'-C1'
28	j	204	LMT	C2'-C1'-O1'-C1
28	j	204	LMT	O5'-C1'-O1'-C1
28	j	204	LMT	C2-C1-O1'-C1'
30	f	203	PC1	C11-O13-P-O12
30	f	203	PC1	C11-O13-P-O11
30	f	203	PC1	O13-C11-C12-N
30	i	201	PC1	C11-O13-P-O12
30	i	201	PC1	C11-O13-P-O14
30	i	201	PC1	C11-O13-P-O11
30	i	201	PC1	O13-C11-C12-N
30	j	203	PC1	C11-O13-P-O14
30	j	203	PC1	C1-O11-P-O12
30	j	203	PC1	C1-O11-P-O14
30	j	203	PC1	C1-O11-P-O13
30	p	201	PC1	C11-O13-P-O12
30	p	201	PC1	C11-O13-P-O11
31	H1	201	UTP	C5'-O5'-PA-O1A
31	H1	201	UTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A1	601	ATP	PB-O3B-PG-O2G
32	B1	601	ATP	PB-O3B-PG-O2G
32	C1	601	ATP	PB-O3B-PG-O2G
32	D1	601	ATP	PB-O3B-PG-O2G
26	M	201	CDL	OB7-CB5-OB6-CB4
26	m	201	CDL	OB7-CB5-OB6-CB4
26	M	201	CDL	O1-C1-CB2-OB2
26	e	404	CDL	O1-C1-CA2-OA2
26	m	201	CDL	O1-C1-CB2-OB2
26	q	101	CDL	O1-C1-CB2-OB2
26	e	403	CDL	C11-CA5-OA6-CA4
26	e	403	CDL	C51-CB5-OB6-CB4
26	q	101	CDL	C11-CA5-OA6-CA4
26	q	101	CDL	OA7-CA5-OA6-CA4
29	e	407	Q7G	O5B-C1B-O1B-C24
29	n	201	Q7G	O5B-C1B-O1B-C24
26	e	404	CDL	CB2-C1-CA2-OA2
26	e	402	CDL	C31-CA7-OA8-CA6
27	M	202	PEE	C31-C30-O3-C3
27	m	202	PEE	C31-C30-O3-C3
29	e	407	Q7G	C2B-C1B-O1B-C24
29	n	201	Q7G	C2B-C1B-O1B-C24
26	l	101	CDL	O1-C1-CA2-OA2
26	M	201	CDL	OA6-CA4-CA6-OA8
26	e	402	CDL	OA9-CA7-OA8-CA6
26	e	403	CDL	OA7-CA5-OA6-CA4
26	e	403	CDL	OB7-CB5-OB6-CB4
26	M	201	CDL	CA5-C11-C12-C13
27	m	202	PEE	O5-C30-O3-C3
26	q	101	CDL	C1-CB2-OB2-PB2
26	m	201	CDL	CA5-C11-C12-C13
27	M	202	PEE	O5-C30-O3-C3
29	e	407	Q7G	CG1-C22-C23-C48
26	e	404	CDL	O1-C1-CB2-OB2
26	e	405	CDL	OB5-CB3-CB4-OB6
26	e	405	CDL	C11-CA5-OA6-CA4
26	j	202	CDL	C11-CA5-OA6-CA4
26	j	201	CDL	C13-C14-C15-C16
26	j	202	CDL	C78-C79-C80-C81
27	m	202	PEE	C17-C18-C19-C20
26	L	101	CDL	C31-CA7-OA8-CA6
26	j	202	CDL	C74-C75-C76-C77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	f	203	PC1	C22-C21-O21-C2
26	e	403	CDL	C71-C72-C73-C74
26	e	404	CDL	CA2-C1-CB2-OB2
26	l	101	CDL	C31-CA7-OA8-CA6
27	M	202	PEE	C1-C2-C3-O3
26	c	201	CDL	C55-C56-C57-C58
26	e	404	CDL	C11-CA5-OA6-CA4
26	j	202	CDL	C51-CB5-OB6-CB4
27	f	202	PEE	C11-C10-O2-C2
26	L	101	CDL	OA9-CA7-OA8-CA6
26	e	405	CDL	OA7-CA5-OA6-CA4
26	j	202	CDL	OA7-CA5-OA6-CA4
26	L	101	CDL	C11-CA5-OA6-CA4
26	l	101	CDL	C11-CA5-OA6-CA4
30	p	201	PC1	C22-C21-O21-C2
30	f	203	PC1	O22-C21-O21-C2
26	e	405	CDL	CA7-C31-C32-C33
26	M	201	CDL	C12-C13-C14-C15
26	e	401	CDL	C77-C78-C79-C80
27	M	202	PEE	C17-C18-C19-C20
26	e	403	CDL	C14-C15-C16-C17
26	l	101	CDL	OA9-CA7-OA8-CA6
26	M	201	CDL	C73-C74-C75-C76
26	c	201	CDL	C34-C35-C36-C37
28	j	204	LMT	O5B-C5B-C6B-O6B
26	j	201	CDL	C81-C82-C83-C84
26	e	402	CDL	C11-CA5-OA6-CA4
26	j	201	CDL	CA7-C31-C32-C33
29	n	201	Q7G	O5C-C5C-C6C-O6C
26	e	403	CDL	OB6-CB4-CB6-OB8
26	L	101	CDL	OA7-CA5-OA6-CA4
26	e	405	CDL	C57-C58-C59-C60
26	j	202	CDL	C15-C16-C17-C18
27	f	202	PEE	C42-C43-C44-C45
26	c	201	CDL	CA4-CA6-OA8-CA7
26	e	404	CDL	C17-C18-C19-C20
26	m	201	CDL	C12-C13-C14-C15
26	e	405	CDL	OB5-CB3-CB4-CB6
26	q	101	CDL	OA5-CA3-CA4-CA6
26	e	404	CDL	OA7-CA5-OA6-CA4
26	l	101	CDL	OA7-CA5-OA6-CA4
26	q	101	CDL	CB7-C71-C72-C73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	e	401	CDL	C56-C57-C58-C59
26	m	201	CDL	C73-C74-C75-C76
30	i	201	PC1	C32-C31-O31-C3
26	j	202	CDL	OB7-CB5-OB6-CB4
26	m	201	CDL	CA3-CA4-CA6-OA8
30	f	203	PC1	C1-C2-C3-O31
26	e	402	CDL	C81-C82-C83-C84
26	M	201	CDL	C78-C79-C80-C81
26	m	201	CDL	C78-C79-C80-C81
26	e	402	CDL	C78-C79-C80-C81
26	j	201	CDL	C62-C63-C64-C65
34	E1	601	ADP	PA-O3A-PB-O1B
26	e	402	CDL	CA6-CA4-OA6-CA5
26	e	403	CDL	C78-C79-C80-C81
26	j	201	CDL	C34-C35-C36-C37
26	q	101	CDL	CA5-C11-C12-C13
26	e	404	CDL	OA5-CA3-CA4-OA6
26	e	405	CDL	OA5-CA3-CA4-OA6
26	m	201	CDL	OA5-CA3-CA4-OA6
30	j	203	PC1	O11-C1-C2-O21
26	e	403	CDL	C17-C18-C19-C20
30	f	203	PC1	C32-C31-O31-C3
26	e	401	CDL	C18-C19-C20-C21
26	l	101	CDL	C14-C15-C16-C17
26	e	404	CDL	OB6-CB4-CB6-OB8
26	e	405	CDL	OB6-CB4-CB6-OB8
30	i	201	PC1	O32-C31-O31-C3
26	e	402	CDL	C11-C12-C13-C14
26	c	201	CDL	C39-C40-C41-C42
27	f	202	PEE	O4-C10-O2-C2
30	p	201	PC1	O22-C21-O21-C2
26	c	201	CDL	CA4-CA3-OA5-PA1
26	e	405	CDL	CA4-CA3-OA5-PA1
26	j	201	CDL	CA4-CA3-OA5-PA1
27	M	202	PEE	C2-C1-O3P-P
27	m	202	PEE	C2-C1-O3P-P
26	L	101	CDL	C14-C15-C16-C17
27	M	202	PEE	C22-C23-C24-C25
26	M	201	CDL	OA5-CA3-CA4-CA6
26	c	201	CDL	OA5-CA3-CA4-CA6
26	m	201	CDL	OA5-CA3-CA4-CA6
30	j	203	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	e	403	CDL	O1-C1-CA2-OA2
26	c	201	CDL	CA5-C11-C12-C13
30	i	201	PC1	C2C-C2D-C2E-C2F
26	f	201	CDL	C77-C78-C79-C80
26	e	402	CDL	OA7-CA5-OA6-CA4
27	m	202	PEE	C22-C23-C24-C25
26	M	201	CDL	CA3-CA4-CA6-OA8
26	e	403	CDL	CB3-CB4-CB6-OB8
26	e	404	CDL	CB3-CB4-CB6-OB8
26	e	405	CDL	CB3-CB4-CB6-OB8
26	j	202	CDL	CB3-CB4-CB6-OB8
26	e	402	CDL	C75-C76-C77-C78
26	M	201	CDL	OA5-CA3-CA4-OA6
26	c	201	CDL	OA5-CA3-CA4-OA6
26	f	201	CDL	OA5-CA3-CA4-OA6
26	j	202	CDL	OA5-CA3-CA4-OA6
26	m	201	CDL	C21-C22-C23-C24
26	f	201	CDL	CB4-CB3-OB5-PB2
26	l	101	CDL	CA4-CA3-OA5-PA1
29	n	201	Q7G	C24-C23-C48-O1C
30	f	203	PC1	O32-C31-O31-C3
27	M	202	PEE	C31-C32-C33-C34
26	c	201	CDL	C51-C52-C53-C54
26	L	101	CDL	OA6-CA4-CA6-OA8
26	f	201	CDL	OB6-CB4-CB6-OB8
26	l	101	CDL	OA6-CA4-CA6-OA8
27	f	202	PEE	O2-C2-C3-O3
26	e	405	CDL	C76-C77-C78-C79
27	f	202	PEE	C31-C30-O3-C3
27	M	202	PEE	C11-C10-O2-C2
26	M	201	CDL	C21-C22-C23-C24
26	j	202	CDL	C79-C80-C81-C82
26	j	202	CDL	OA5-CA3-CA4-CA6
26	e	405	CDL	C78-C79-C80-C81
27	f	202	PEE	O5-C30-O3-C3
26	f	201	CDL	C11-CA5-OA6-CA4
29	n	201	Q7G	C16-C17-O20-CG1
29	n	201	Q7G	C18-C17-O20-CG1
26	j	202	CDL	CB3-CB4-OB6-CB5
26	q	101	CDL	CB3-CB4-OB6-CB5
34	E1	601	ADP	PA-O3A-PB-O3B
26	e	403	CDL	C62-C63-C64-C65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	f	201	CDL	C12-C13-C14-C15
26	j	201	CDL	OB5-CB3-CB4-OB6
26	c	201	CDL	CA3-CA4-CA6-OA8
27	f	202	PEE	C1-C2-C3-O3
27	m	202	PEE	C1-C2-C3-O3
30	p	201	PC1	C1-C2-C3-O31
26	c	201	CDL	OA6-CA4-CA6-OA8
26	j	202	CDL	OB6-CB4-CB6-OB8
27	m	202	PEE	O2-C2-C3-O3
30	p	201	PC1	O21-C2-C3-O31
26	e	401	CDL	C51-CB5-OB6-CB4
30	j	203	PC1	O13-C11-C12-N
30	p	201	PC1	O13-C11-C12-N
32	B1	601	ATP	PG-O3B-PB-O2B
32	C1	601	ATP	PA-O3A-PB-O2B
32	D1	601	ATP	PG-O3B-PB-O2B
26	e	405	CDL	OA5-CA3-CA4-CA6
26	j	201	CDL	OB5-CB3-CB4-CB6
30	j	203	PC1	C3C-C3D-C3E-C3F
26	j	201	CDL	C1-CB2-OB2-PB2
26	f	201	CDL	OA7-CA5-OA6-CA4
26	q	101	CDL	OB5-CB3-CB4-OB6
26	c	201	CDL	C83-C84-C85-C86
27	M	202	PEE	O2-C2-C3-O3
30	f	203	PC1	O21-C2-C3-O31
26	j	202	CDL	C76-C77-C78-C79
26	q	101	CDL	C77-C78-C79-C80
29	e	407	Q7G	CG1-C22-C23-C24
29	e	407	Q7G	C23-C24-O1B-C1B
26	j	201	CDL	C55-C56-C57-C58
26	j	201	CDL	C72-C73-C74-C75
27	m	202	PEE	C36-C37-C38-C39
26	e	401	CDL	OB7-CB5-OB6-CB4
27	M	202	PEE	O4-C10-O2-C2
26	L	101	CDL	CA2-OA2-PA1-OA3
26	L	101	CDL	CA3-OA5-PA1-OA3
26	M	201	CDL	CA3-OA5-PA1-OA4
26	M	201	CDL	CB3-OB5-PB2-OB3
26	c	201	CDL	CB2-OB2-PB2-OB3
26	e	401	CDL	CB3-OB5-PB2-OB4
26	e	403	CDL	CB3-OB5-PB2-OB3
26	e	405	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	f	201	CDL	CB3-OB5-PB2-OB3
26	j	201	CDL	CA2-OA2-PA1-OA4
26	j	201	CDL	CA2-OA2-PA1-OA5
26	l	101	CDL	CA3-OA5-PA1-OA3
26	l	101	CDL	CA3-OA5-PA1-OA4
26	m	201	CDL	CA3-OA5-PA1-OA4
26	m	201	CDL	CB3-OB5-PB2-OB3
26	q	101	CDL	CA2-OA2-PA1-OA5
26	q	101	CDL	CA3-OA5-PA1-OA3
26	q	101	CDL	CB2-OB2-PB2-OB4
26	q	101	CDL	CB2-OB2-PB2-OB5
27	f	202	PEE	C4-O4P-P-O3P
27	f	202	PEE	C4-O4P-P-O1P
30	j	203	PC1	C11-O13-P-O12
30	j	203	PC1	C11-O13-P-O11
30	p	201	PC1	C1-O11-P-O12
30	p	201	PC1	C1-O11-P-O14
30	p	201	PC1	C1-O11-P-O13
31	H1	201	UTP	C5'-O5'-PA-O2A
32	A1	601	ATP	C5'-O5'-PA-O1A
32	B1	601	ATP	C5'-O5'-PA-O1A
32	C1	601	ATP	C5'-O5'-PA-O1A
32	D1	601	ATP	C5'-O5'-PA-O1A
26	j	202	CDL	C61-C62-C63-C64
26	L	101	CDL	C31-C32-C33-C34
26	M	201	CDL	C42-C43-C44-C45
26	L	101	CDL	CA4-CA3-OA5-PA1
26	e	402	CDL	CA4-CA3-OA5-PA1
26	j	202	CDL	CB4-CB3-OB5-PB2
30	j	203	PC1	C2-C1-O11-P
26	j	202	CDL	C72-C73-C74-C75
27	m	202	PEE	C41-C42-C43-C44
26	e	404	CDL	CA6-CA4-OA6-CA5
26	l	101	CDL	C31-C32-C33-C34
26	e	404	CDL	OA5-CA3-CA4-CA6
26	e	402	CDL	C74-C75-C76-C77
26	e	402	CDL	C52-C51-CB5-OB6
30	i	201	PC1	C3B-C3C-C3D-C3E
32	A1	601	ATP	PG-O3B-PB-O2B
32	A1	601	ATP	PA-O3A-PB-O2B
32	B1	601	ATP	PA-O3A-PB-O2B
30	f	203	PC1	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	M	202	PEE	C36-C37-C38-C39
27	f	202	PEE	C16-C17-C18-C19
26	l	101	CDL	CB2-C1-CA2-OA2
26	j	202	CDL	C71-CB7-OB8-CB6
26	l	101	CDL	C39-C40-C41-C42
27	f	202	PEE	C18-C19-C20-C21
26	e	405	CDL	C79-C80-C81-C82
28	j	204	LMT	C2-C3-C4-C5
26	e	405	CDL	OB7-CB5-OB6-CB4
26	j	202	CDL	OB9-CB7-OB8-CB6
26	e	403	CDL	OA6-CA4-CA6-OA8
26	e	405	CDL	C51-CB5-OB6-CB4
26	e	405	CDL	C40-C41-C42-C43
26	e	402	CDL	C1-CB2-OB2-PB2
26	f	201	CDL	C37-C38-C39-C40
27	f	202	PEE	C19-C20-C21-C22
26	j	202	CDL	CA2-C1-CB2-OB2
26	j	202	CDL	O1-C1-CB2-OB2
32	A1	601	ATP	PB-O3B-PG-O1G
26	e	401	CDL	C13-C14-C15-C16
26	L	101	CDL	C39-C40-C41-C42
26	c	201	CDL	C35-C36-C37-C38
26	m	201	CDL	C33-C34-C35-C36
27	m	202	PEE	C31-C32-C33-C34
26	j	201	CDL	CA3-CA4-OA6-CA5
30	i	201	PC1	C2A-C2B-C2C-C2D
26	e	405	CDL	C71-C72-C73-C74
26	c	201	CDL	C38-C39-C40-C41
27	M	202	PEE	C16-C17-C18-C19
27	m	202	PEE	C16-C17-C18-C19
26	c	201	CDL	C56-C57-C58-C59
27	M	202	PEE	C38-C39-C40-C41
26	e	404	CDL	C78-C79-C80-C81
26	M	201	CDL	C33-C34-C35-C36
26	M	201	CDL	OA7-CA5-OA6-CA4
26	c	201	CDL	CB2-C1-CA2-OA2
26	j	201	CDL	CB2-C1-CA2-OA2
26	e	404	CDL	C18-C19-C20-C21
26	L	101	CDL	O1-C1-CA2-OA2
32	C1	601	ATP	PG-O3B-PB-O2B
26	e	401	CDL	CB4-CB3-OB5-PB2
26	f	201	CDL	C78-C79-C80-C81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	e	403	CDL	CA3-CA4-CA6-OA8
26	f	201	CDL	C13-C14-C15-C16
26	e	401	CDL	C81-C82-C83-C84
26	m	201	CDL	OA7-CA5-OA6-CA4
30	j	203	PC1	O22-C21-O21-C2
27	m	202	PEE	C38-C39-C40-C41
26	e	401	CDL	C11-C12-C13-C14
26	e	402	CDL	OB5-CB3-CB4-CB6
26	f	201	CDL	OA5-CA3-CA4-CA6
26	q	101	CDL	OB5-CB3-CB4-CB6
27	f	202	PEE	C36-C37-C38-C39
30	f	203	PC1	C37-C38-C39-C3A
26	e	402	CDL	C54-C55-C56-C57
26	c	201	CDL	O1-C1-CA2-OA2
32	B1	601	ATP	PB-O3B-PG-O1G
32	C1	601	ATP	PB-O3B-PG-O1G
26	e	403	CDL	C11-C12-C13-C14
26	m	201	CDL	OB9-CB7-OB8-CB6
26	m	201	CDL	C71-CB7-OB8-CB6
26	m	201	CDL	C42-C43-C44-C45
32	C1	601	ATP	PB-O3B-PG-O3G
27	M	202	PEE	C18-C19-C20-C21
27	m	202	PEE	C18-C19-C20-C21
26	j	201	CDL	O1-C1-CA2-OA2
26	e	401	CDL	C16-C17-C18-C19
26	j	202	CDL	C38-C39-C40-C41
26	e	403	CDL	C1-CA2-OA2-PA1
26	c	201	CDL	C62-C63-C64-C65
26	q	101	CDL	C79-C80-C81-C82
26	f	201	CDL	CB3-CB4-CB6-OB8
26	e	403	CDL	C12-C13-C14-C15
26	L	101	CDL	C60-C61-C62-C63
26	M	201	CDL	C19-C20-C21-C22
26	e	402	CDL	C19-C20-C21-C22
26	e	405	CDL	C12-C11-CA5-OA6
27	f	202	PEE	O2-C10-C11-C12
30	j	203	PC1	C22-C21-O21-C2
31	H1	201	UTP	PG-O3B-PB-O1B
32	B1	601	ATP	PG-O3B-PB-O1B
32	C1	601	ATP	PG-O3B-PB-O1B
32	C1	601	ATP	PA-O3A-PB-O1B
26	M	201	CDL	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	f	201	CDL	C72-C71-CB7-OB8
26	M	201	CDL	C11-CA5-OA6-CA4
26	m	201	CDL	C11-CA5-OA6-CA4
26	M	201	CDL	C12-C11-CA5-OA6
26	e	403	CDL	C32-C31-CA7-OA8
26	m	201	CDL	C12-C11-CA5-OA6
27	m	202	PEE	O3-C30-C31-C32
26	e	405	CDL	C14-C15-C16-C17
26	e	401	CDL	C75-C76-C77-C78
26	e	401	CDL	C32-C31-CA7-OA8
26	e	403	CDL	C52-C51-CB5-OB6
26	j	202	CDL	C12-C11-CA5-OA6
26	L	101	CDL	CA3-CA4-CA6-OA8
26	l	101	CDL	CA3-CA4-CA6-OA8
26	c	201	CDL	C40-C41-C42-C43
26	e	401	CDL	C52-C51-CB5-OB6
26	e	402	CDL	C72-C71-CB7-OB8
26	j	201	CDL	C52-C51-CB5-OB6
27	m	202	PEE	O2-C10-C11-C12
26	c	201	CDL	C53-C54-C55-C56
26	q	101	CDL	C73-C74-C75-C76
32	D1	601	ATP	PB-O3B-PG-O1G
26	e	405	CDL	C32-C31-CA7-OA8
26	q	101	CDL	C72-C71-CB7-OB8
27	M	202	PEE	O2-C10-C11-C12
30	j	203	PC1	O31-C31-C32-C33
26	j	201	CDL	CA6-CA4-OA6-CA5
26	e	401	CDL	C78-C79-C80-C81
26	f	201	CDL	C12-C11-CA5-OA6
26	M	201	CDL	C12-C11-CA5-OA7
26	e	403	CDL	C52-C51-CB5-OB7
26	e	405	CDL	C53-C54-C55-C56
27	m	202	PEE	C23-C24-C25-C26
26	e	402	CDL	OB5-CB3-CB4-OB6
26	e	401	CDL	C32-C31-CA7-OA9
26	f	201	CDL	C72-C71-CB7-OB9
27	f	202	PEE	O4-C10-C11-C12
26	e	405	CDL	C12-C11-CA5-OA7
26	e	402	CDL	C21-C22-C23-C24
27	M	202	PEE	C41-C42-C43-C44
26	m	201	CDL	C12-C11-CA5-OA7
26	m	201	CDL	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	M	201	CDL	C38-C39-C40-C41
26	e	402	CDL	C55-C56-C57-C58
26	l	101	CDL	C60-C61-C62-C63
26	e	401	CDL	C52-C51-CB5-OB7
26	j	201	CDL	C52-C51-CB5-OB7
26	q	101	CDL	C72-C71-CB7-OB9
26	j	202	CDL	C59-C60-C61-C62
26	e	402	CDL	C72-C71-CB7-OB9
27	M	202	PEE	O4-C10-C11-C12
27	m	202	PEE	O5-C30-C31-C32
26	e	403	CDL	C32-C31-CA7-OA9
27	m	202	PEE	O4-C10-C11-C12
26	e	405	CDL	C32-C31-CA7-OA9
26	e	405	CDL	C74-C75-C76-C77
26	j	202	CDL	C37-C38-C39-C40
26	j	202	CDL	C12-C11-CA5-OA7
26	e	403	CDL	OA5-CA3-CA4-CA6
26	e	404	CDL	C32-C31-CA7-OA8
30	j	203	PC1	O32-C31-C32-C33
32	D1	601	ATP	PG-O3B-PB-O1B
31	H1	201	UTP	O4'-C4'-C5'-O5'

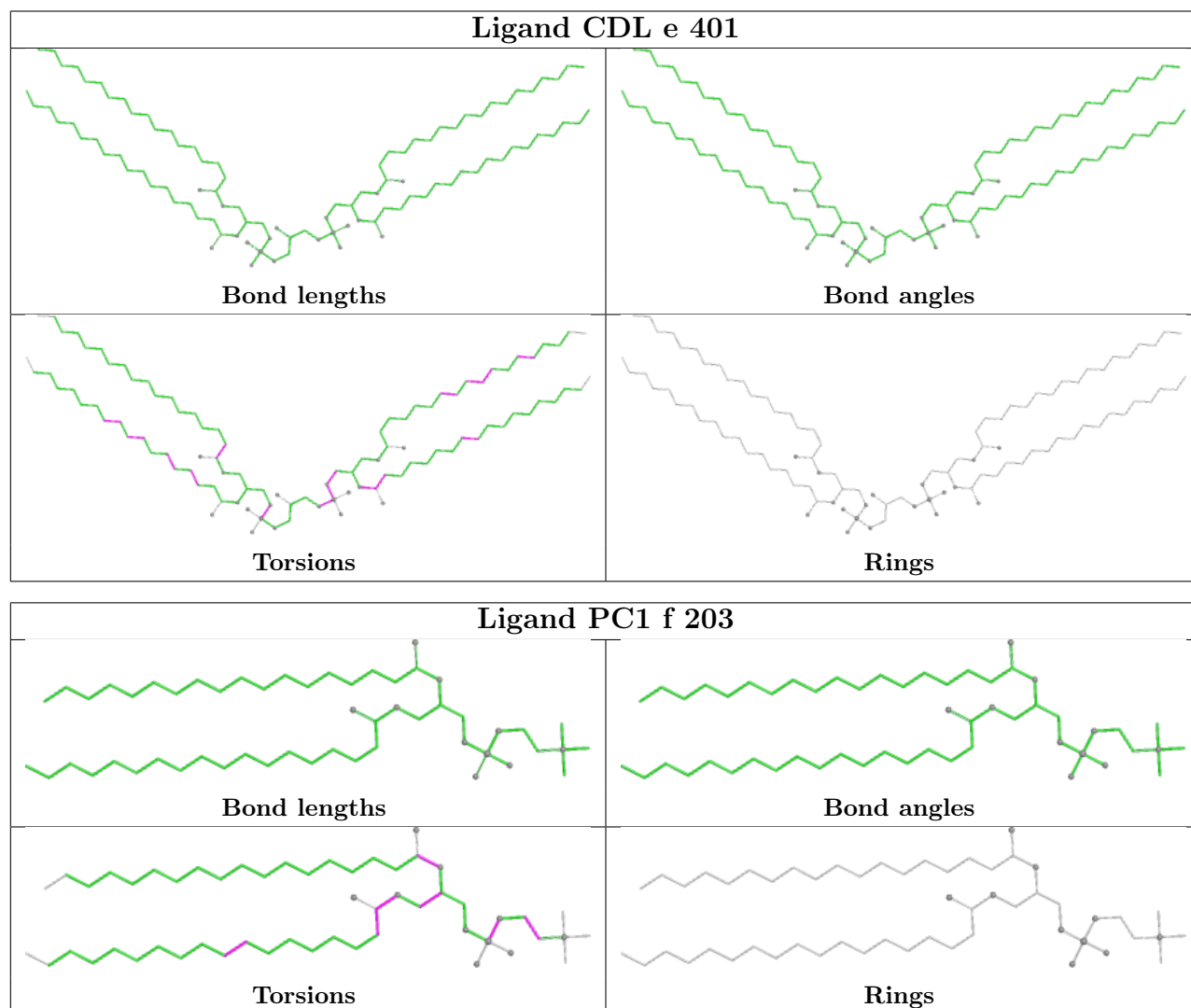
There are no ring outliers.

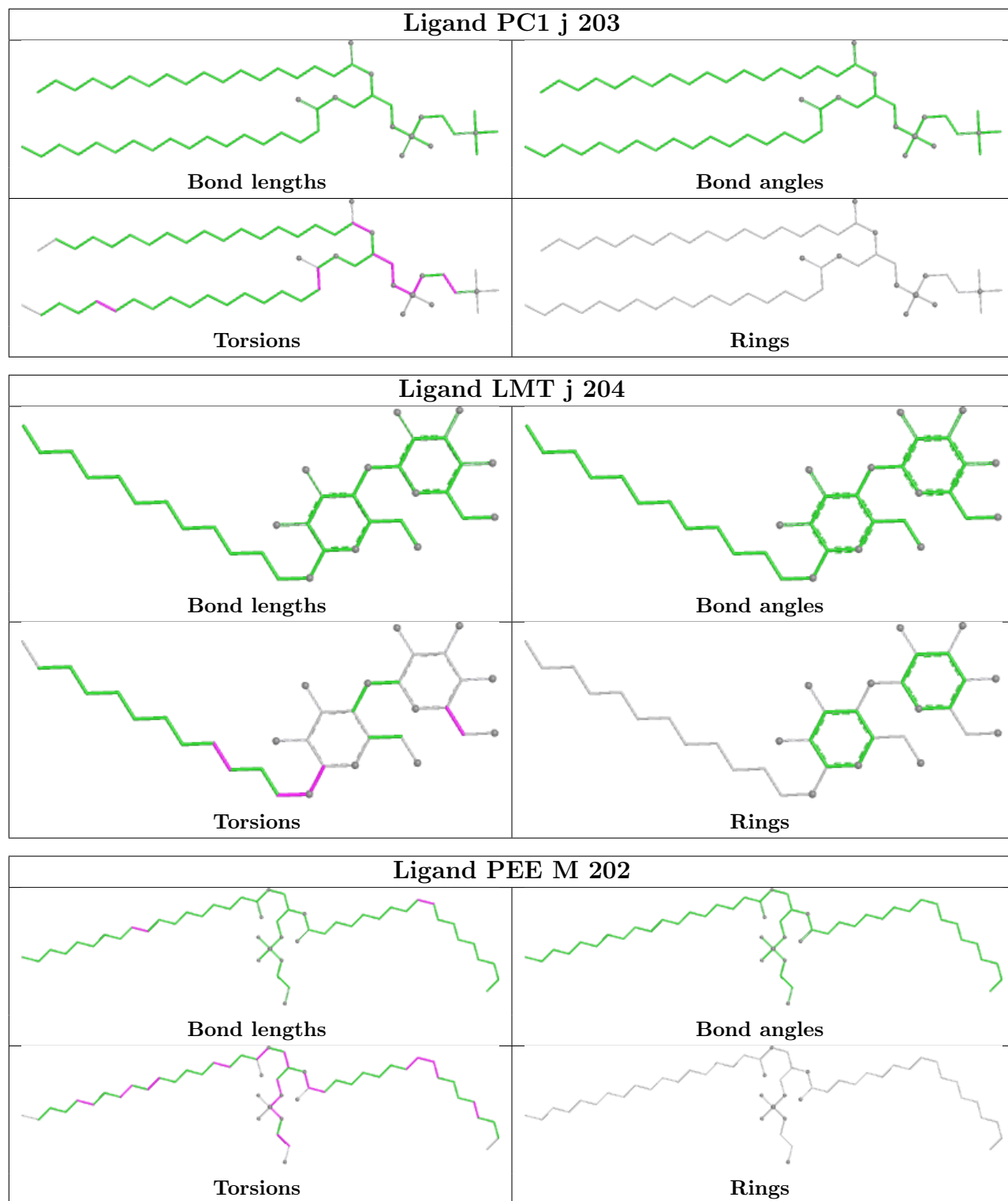
11 monomers are involved in 11 short contacts:

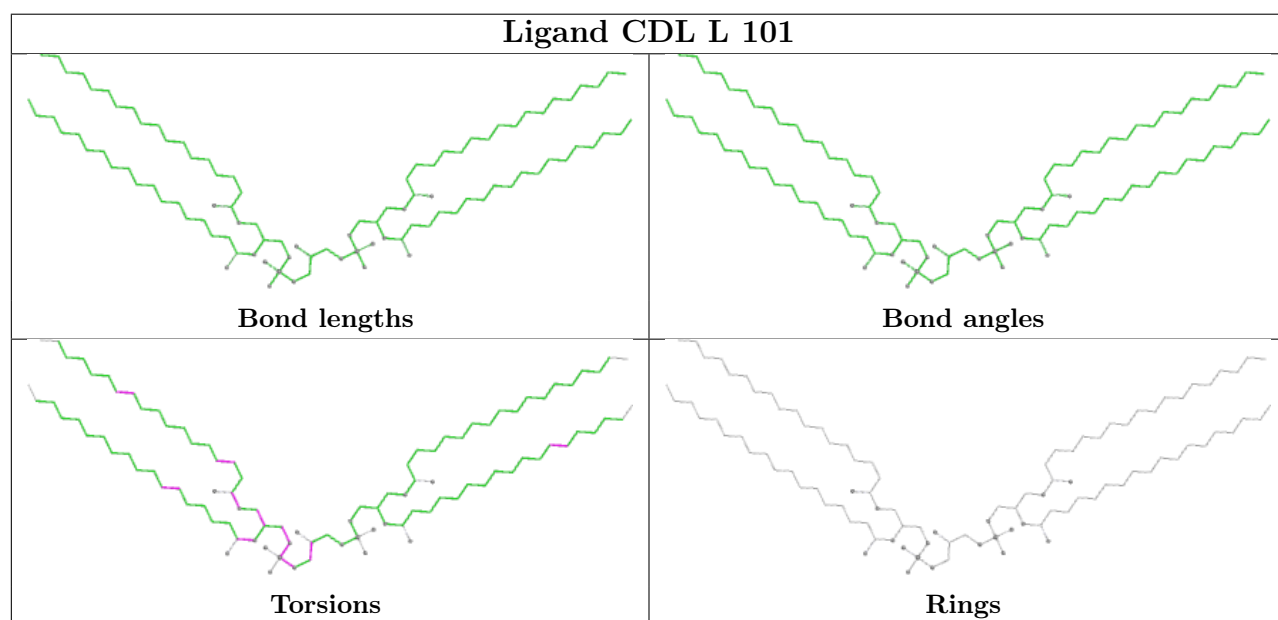
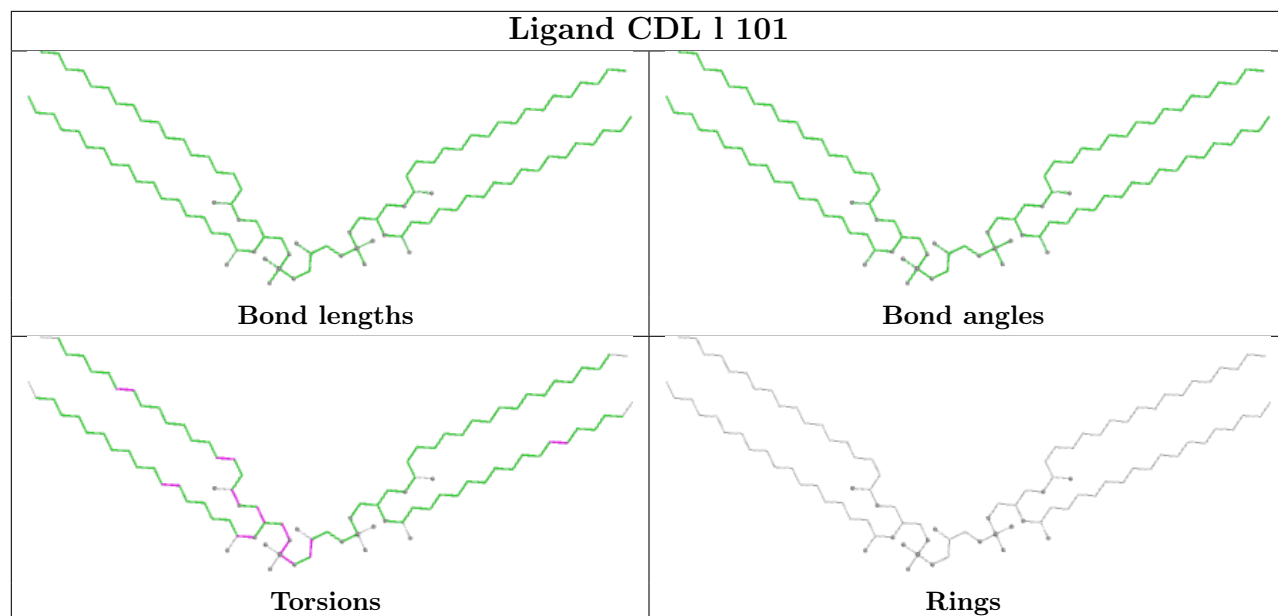
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	f	203	PC1	2	0
30	j	203	PC1	1	0
27	M	202	PEE	1	0
26	M	201	CDL	1	0
32	B1	601	ATP	1	0
26	q	101	CDL	1	0
32	C1	601	ATP	1	0
26	e	402	CDL	1	0
26	j	202	CDL	1	0
26	c	201	CDL	1	0
26	e	403	CDL	1	0

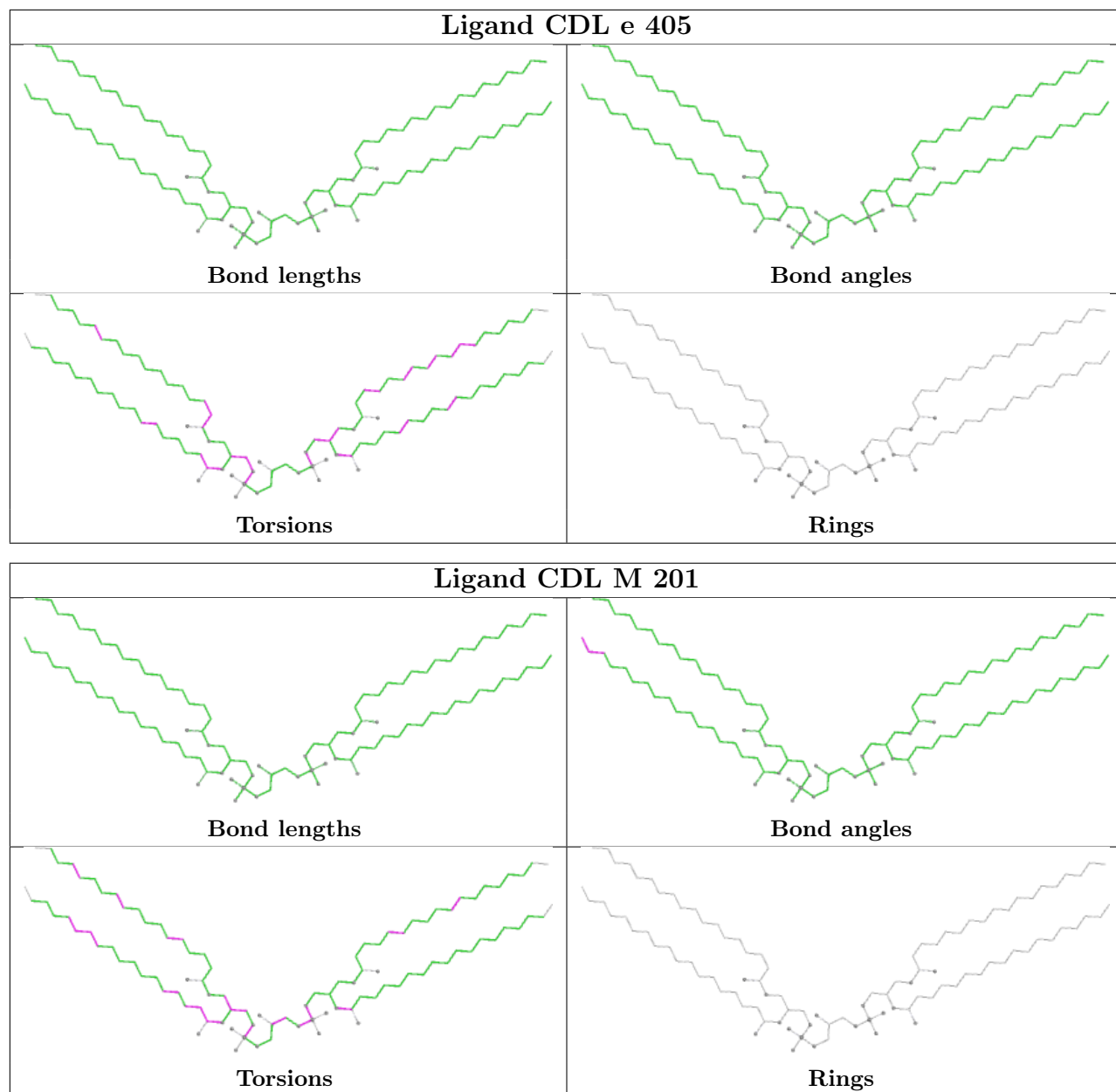
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

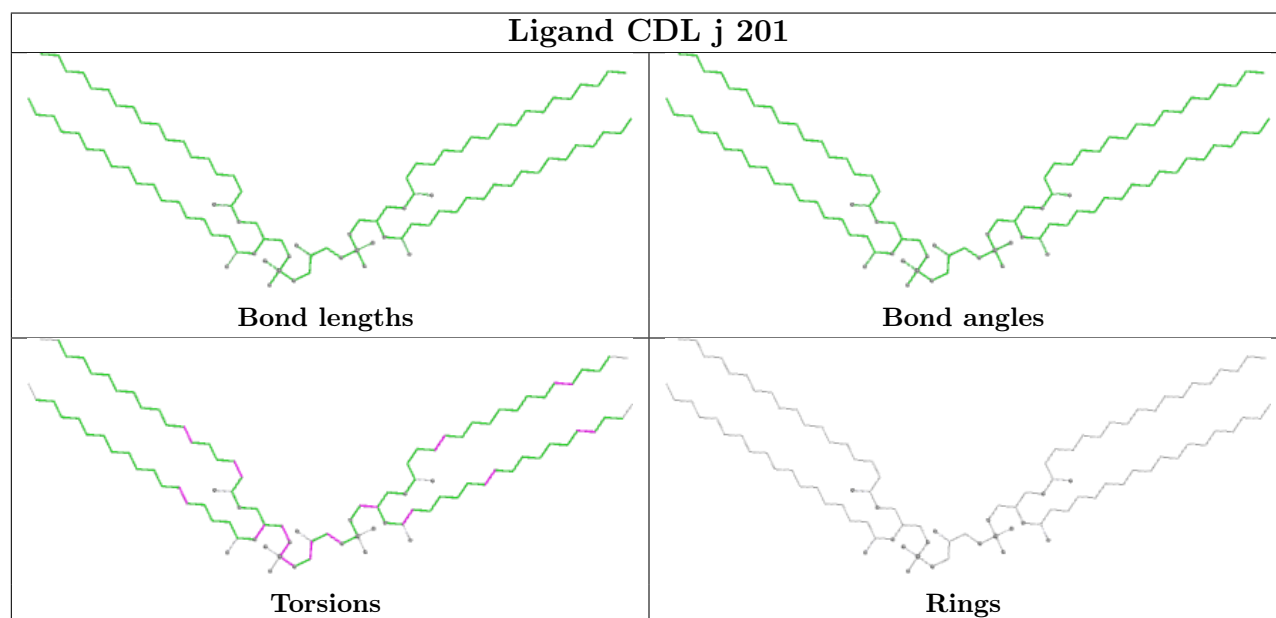
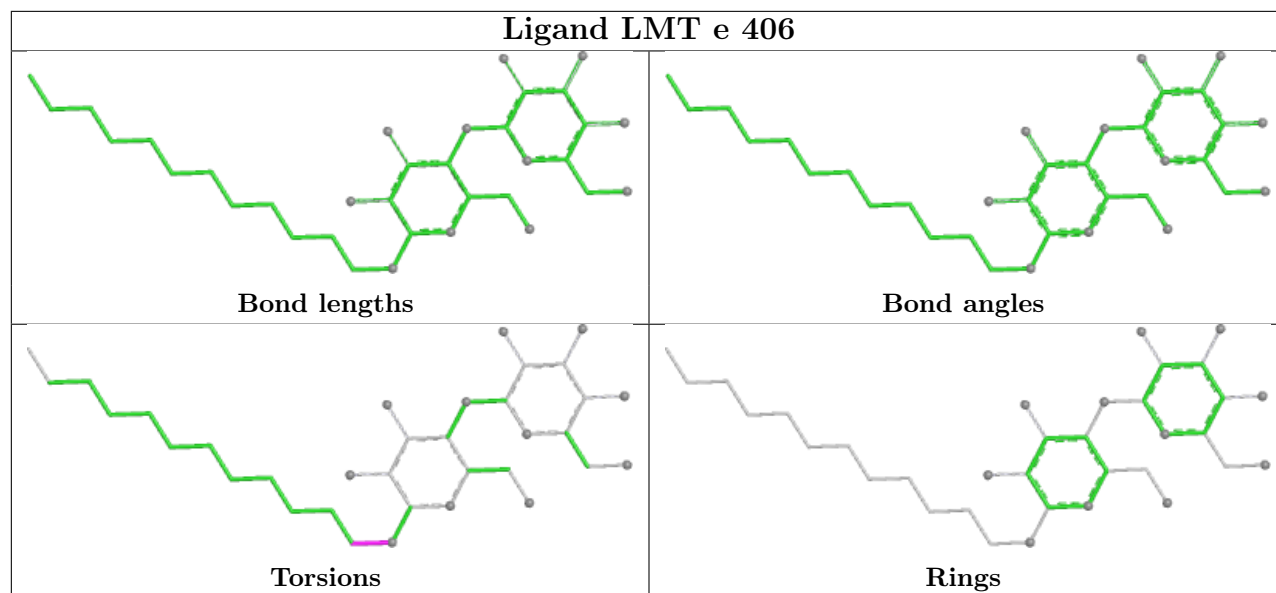
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

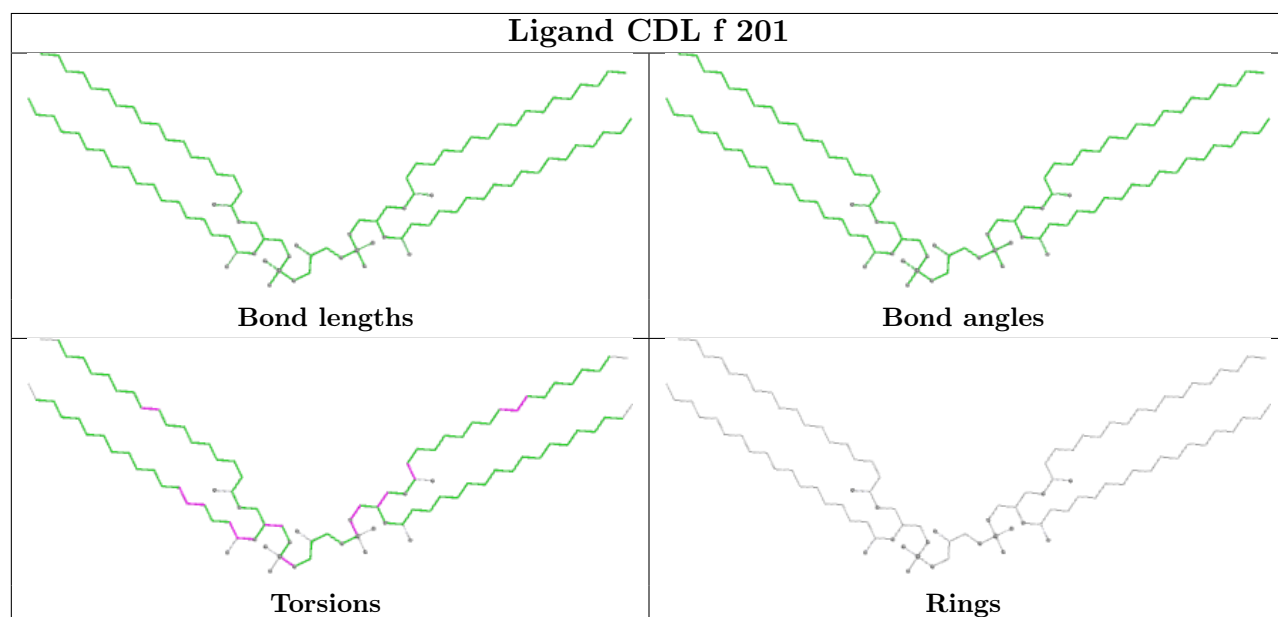
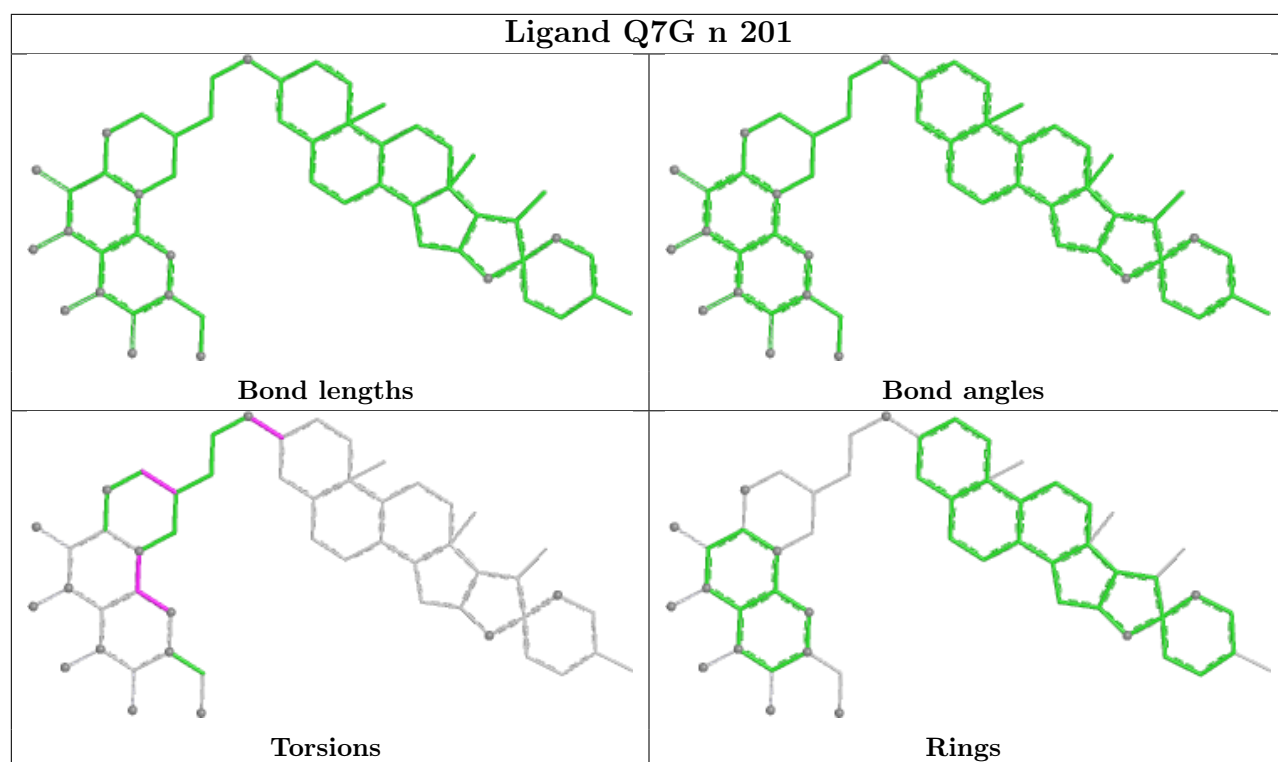


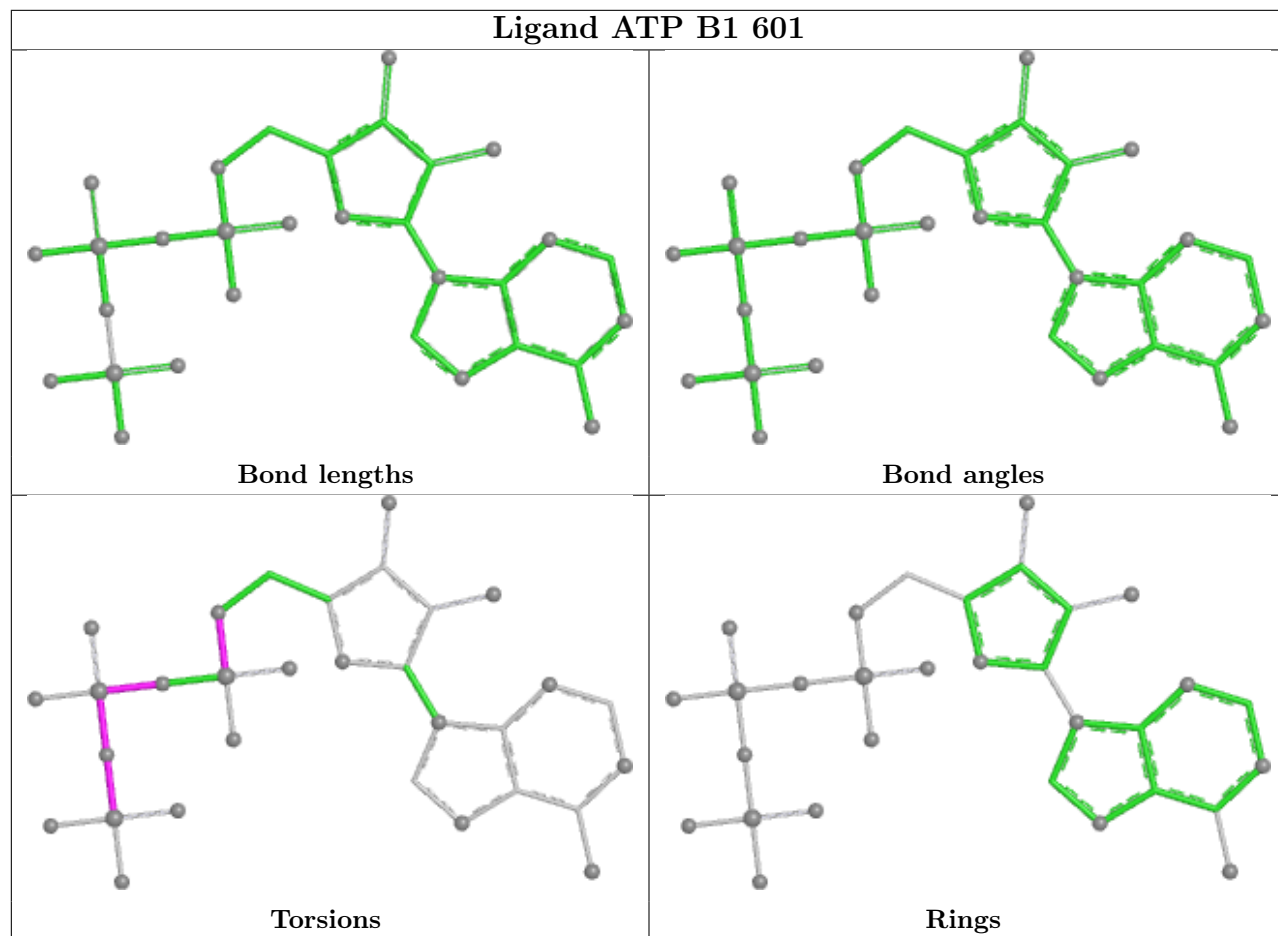
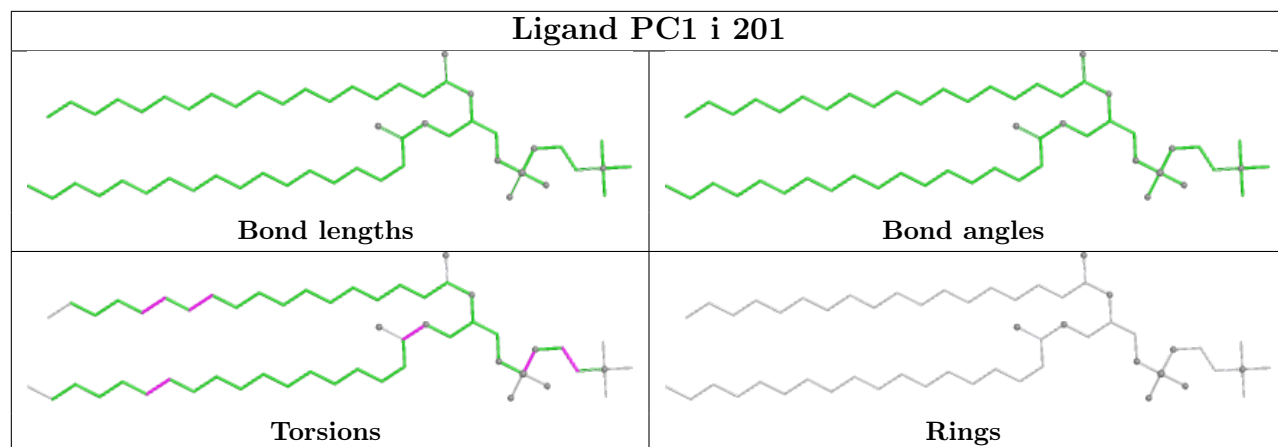


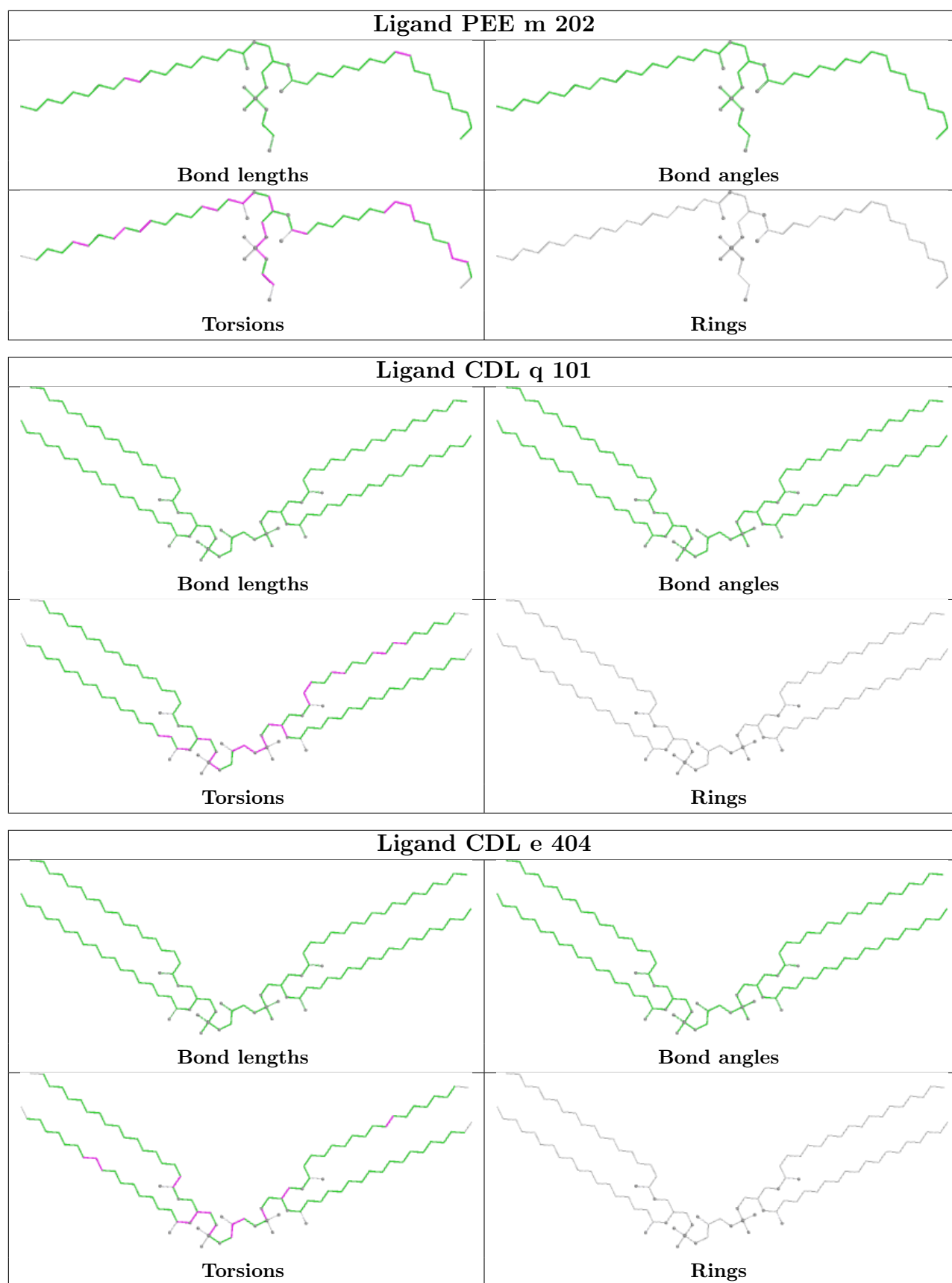


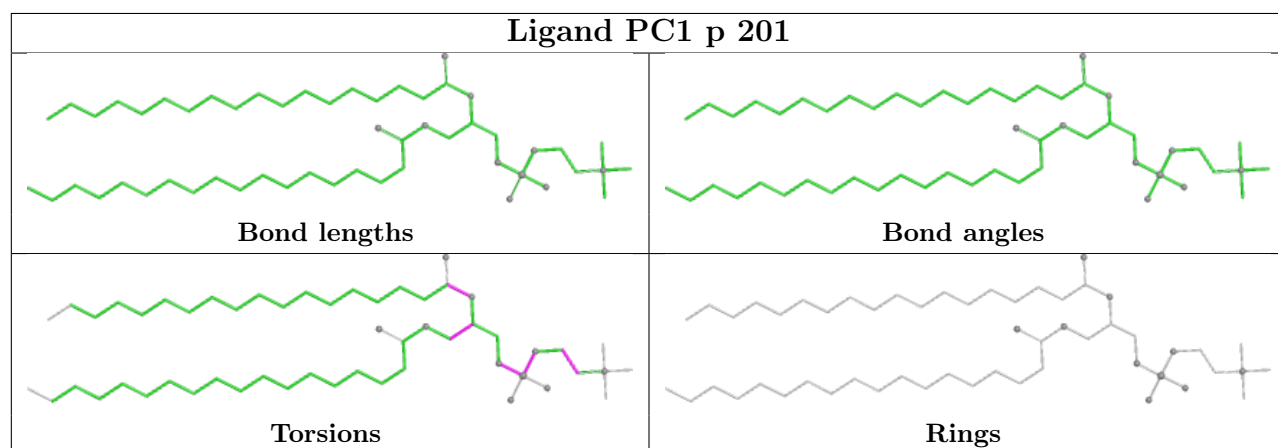
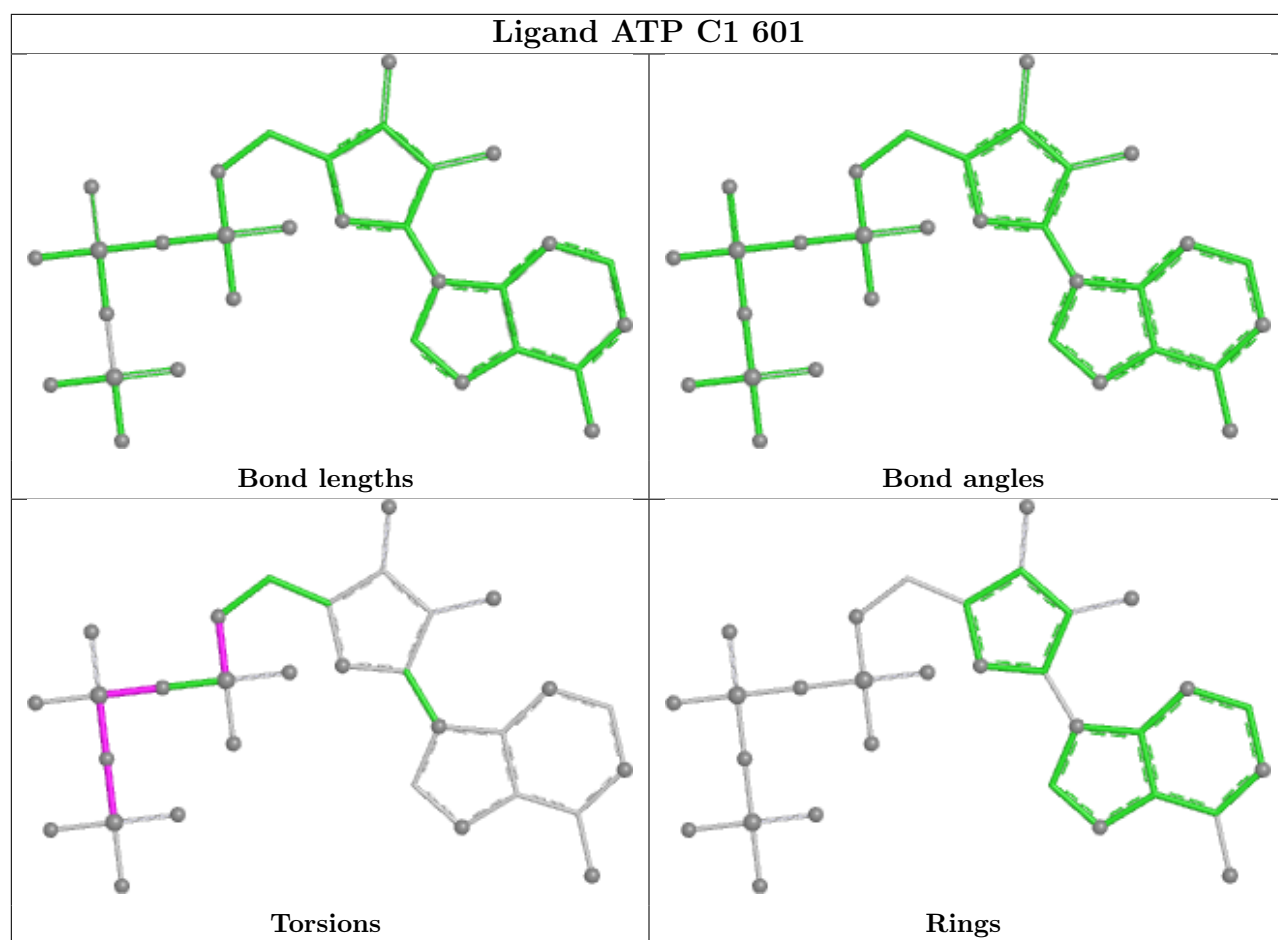


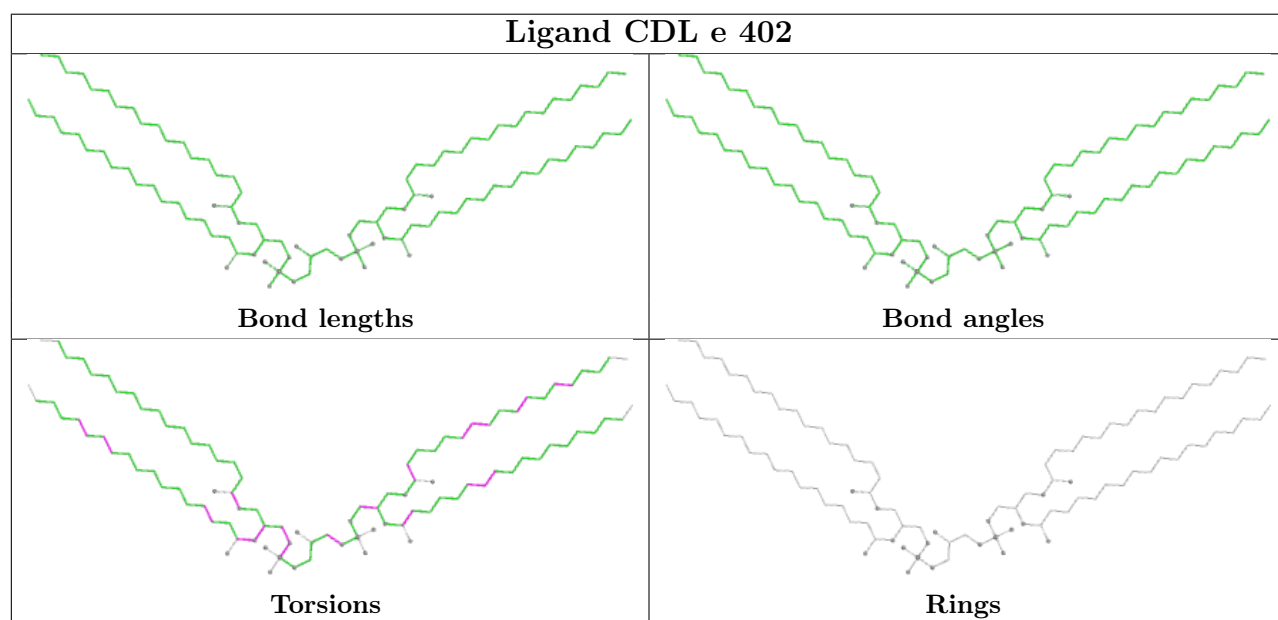
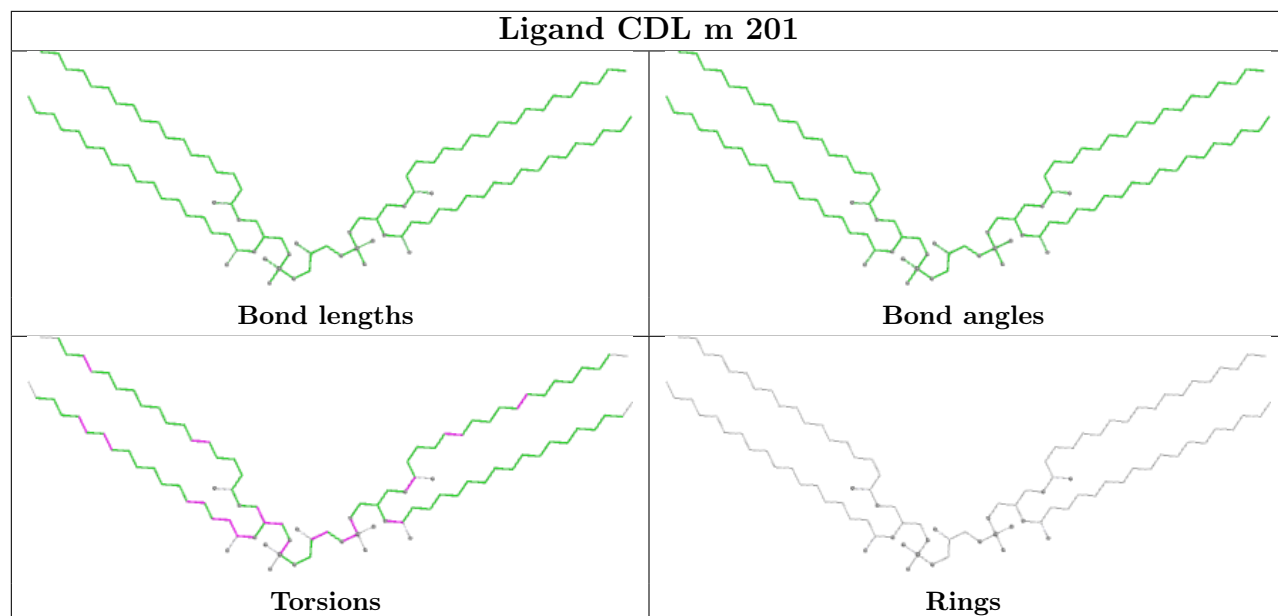


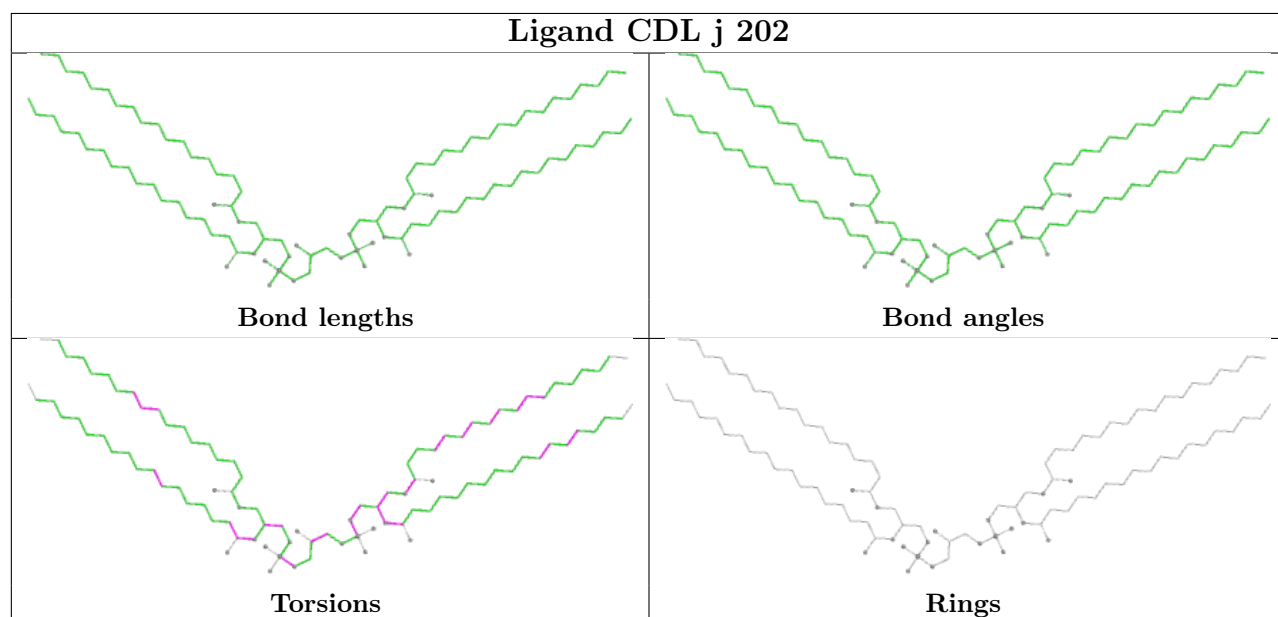
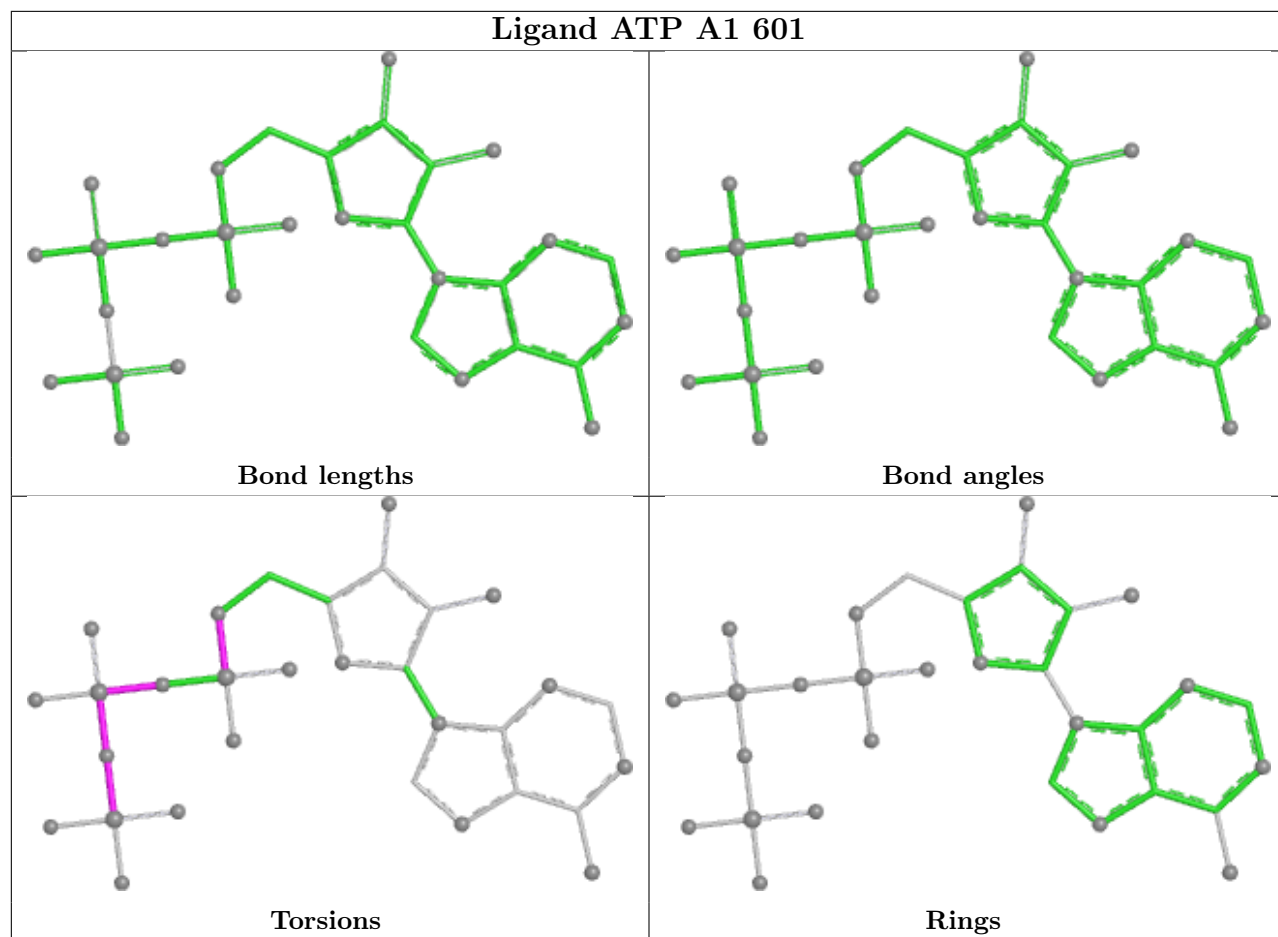


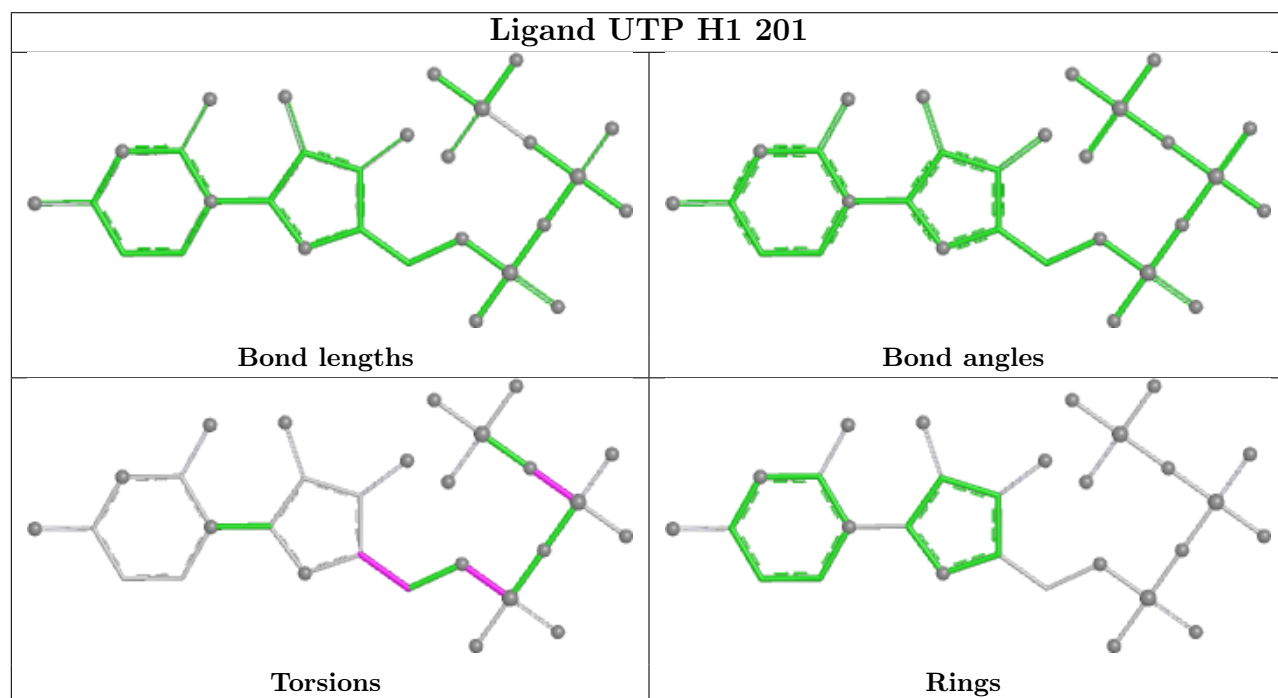
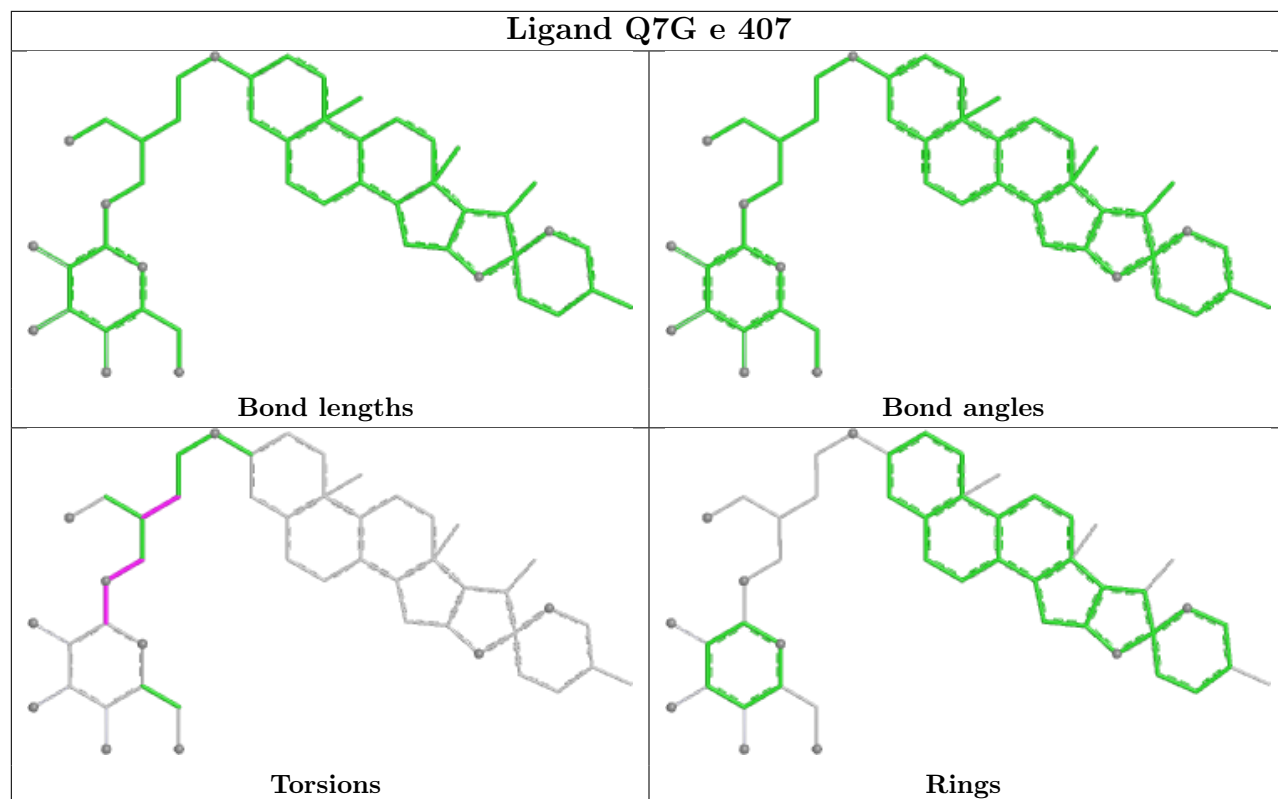




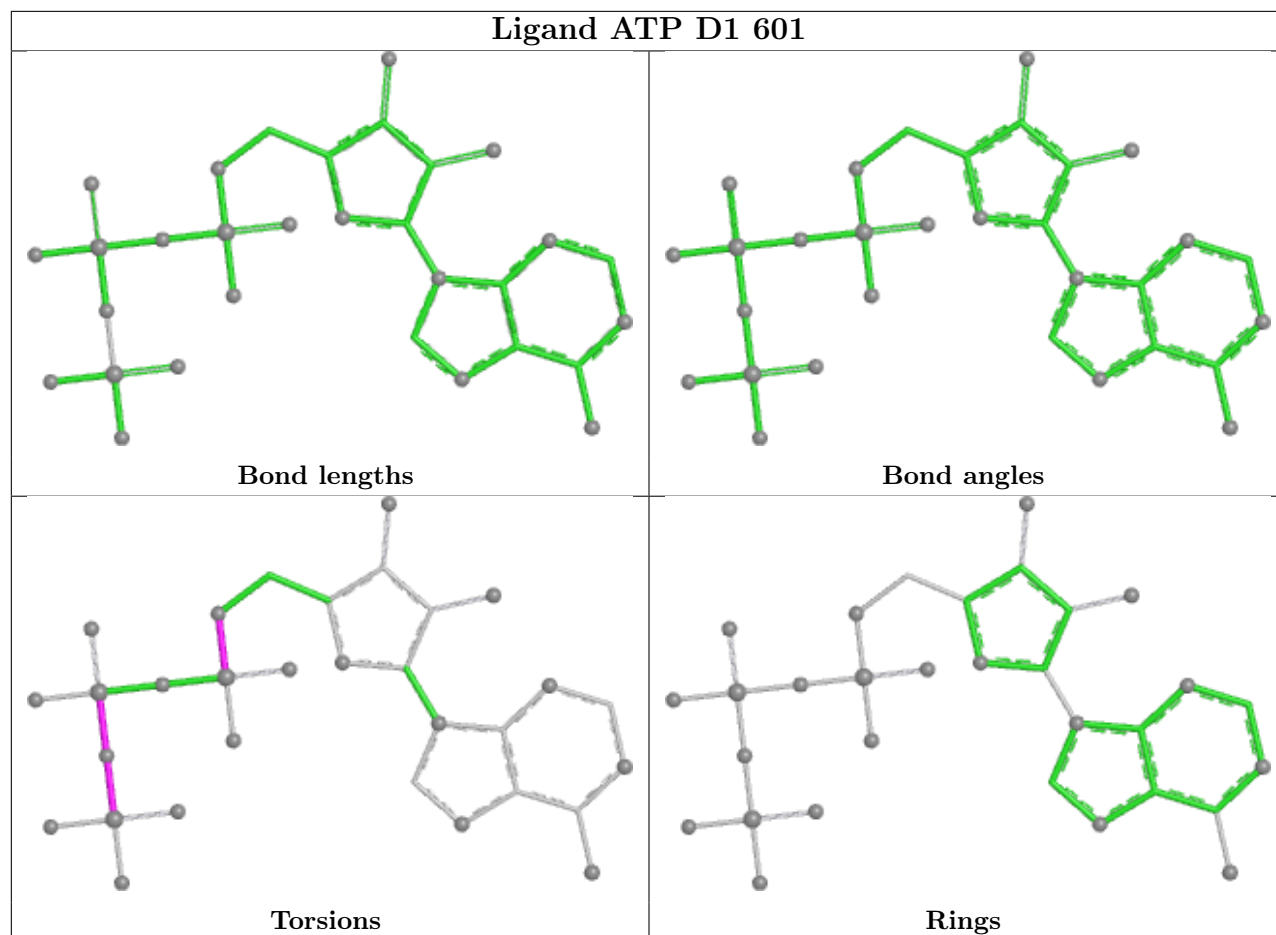




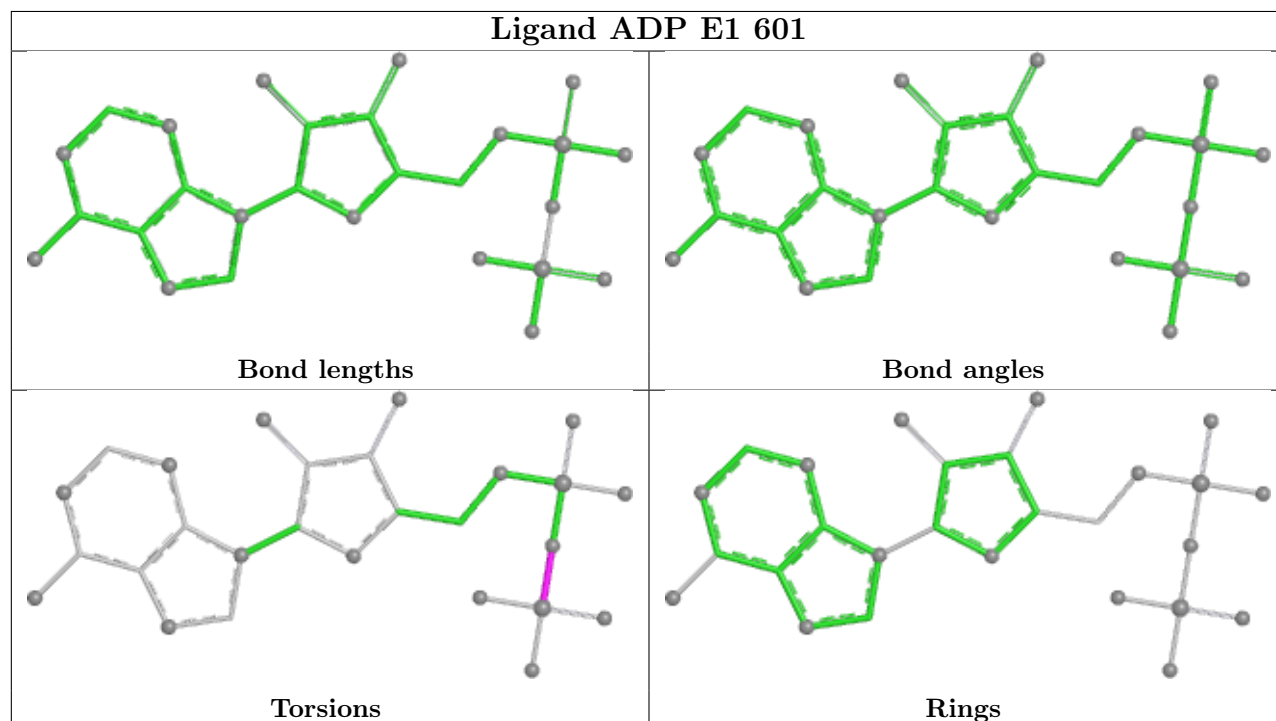


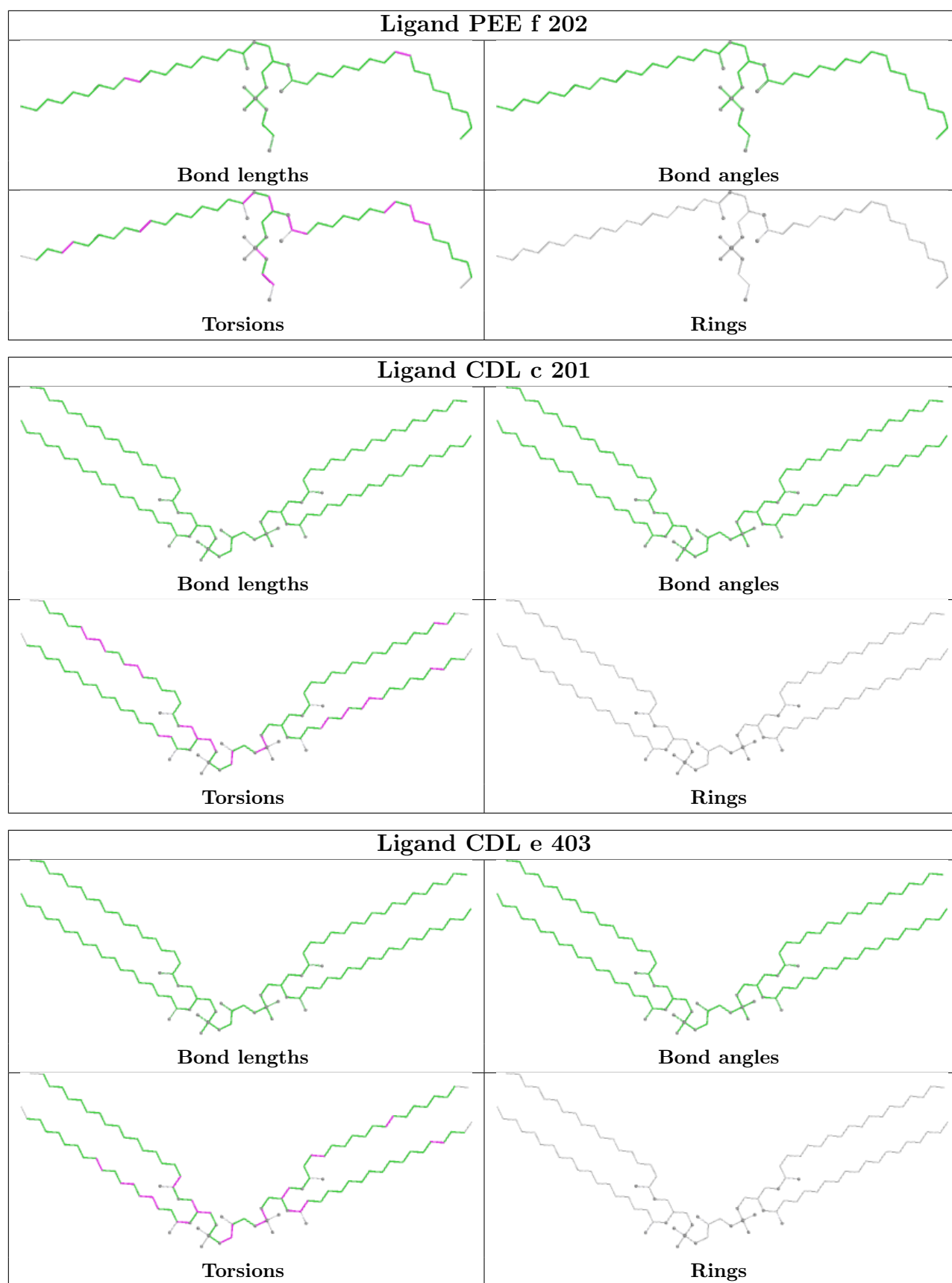


Ligand ATP D1 601



Ligand ADP E1 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.

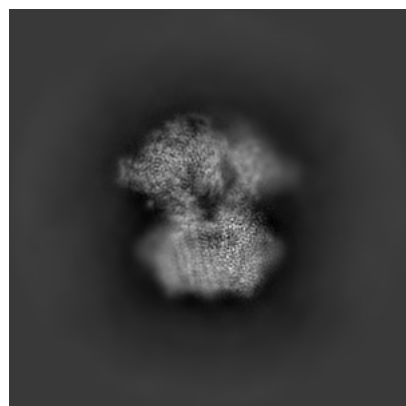
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15572. These allow visual inspection of the internal detail of the map and identification of artifacts.

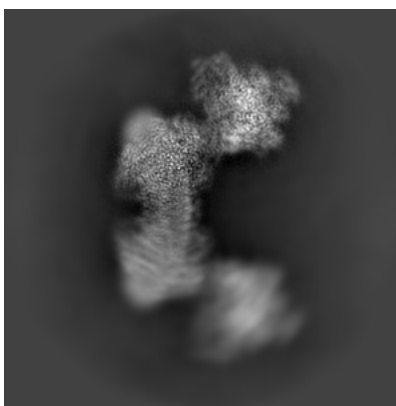
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

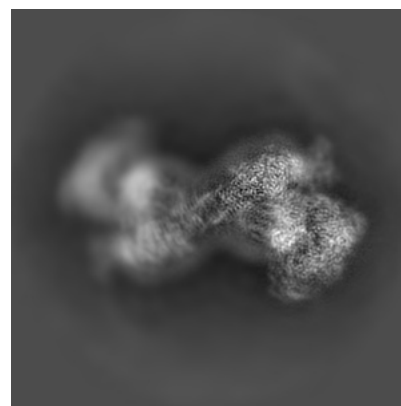
6.1.1 Primary map



X

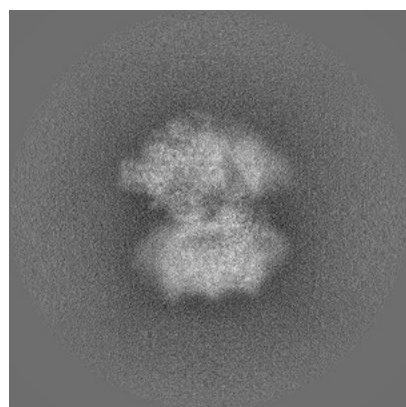


Y

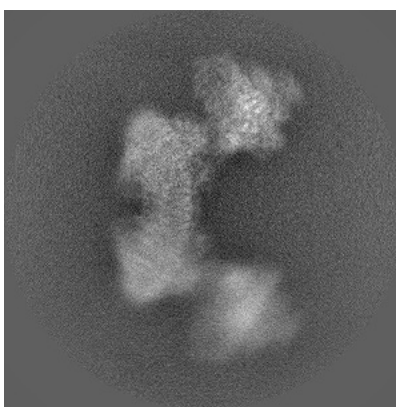


Z

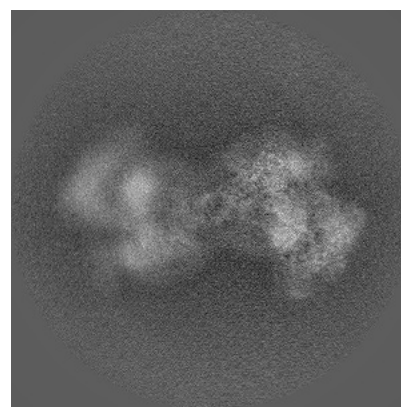
6.1.2 Raw map



X



Y

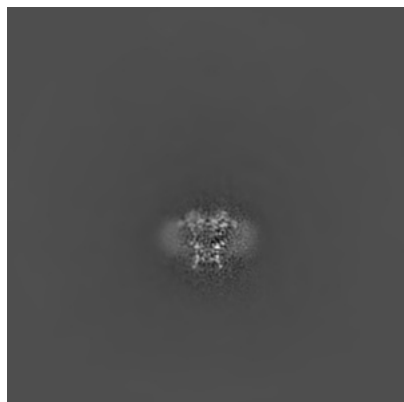


Z

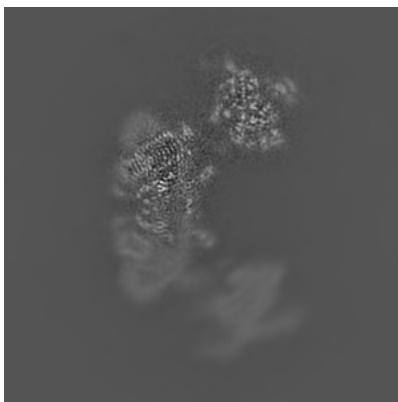
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

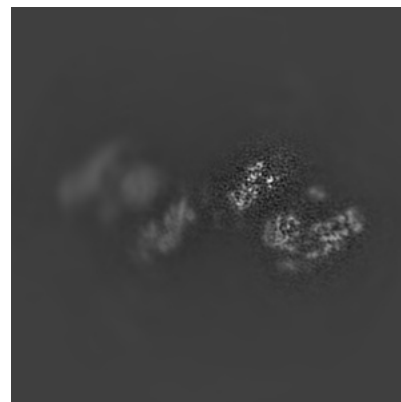
6.2.1 Primary map



X Index: 280

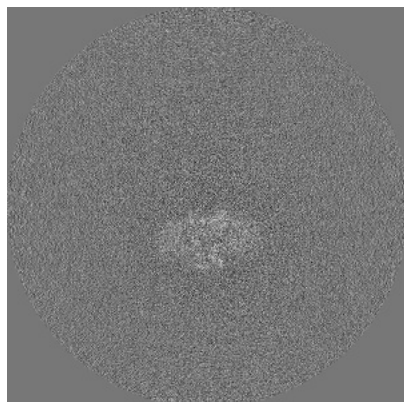


Y Index: 280

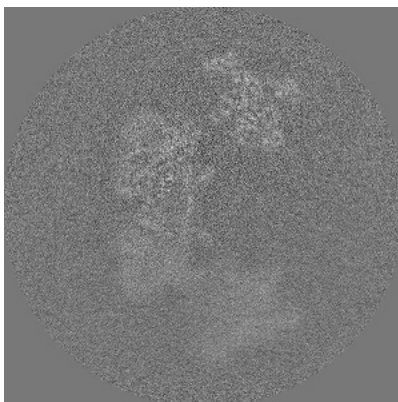


Z Index: 280

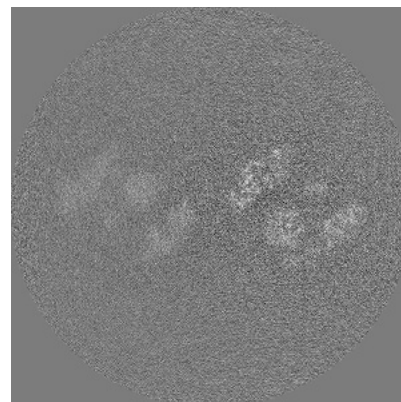
6.2.2 Raw map



X Index: 280



Y Index: 280

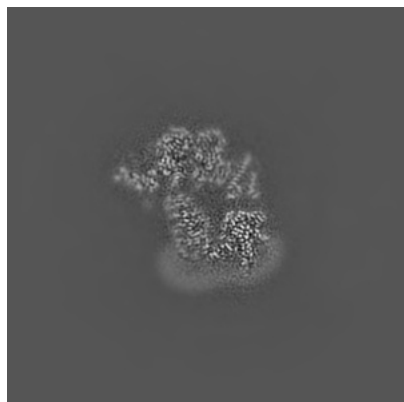


Z Index: 280

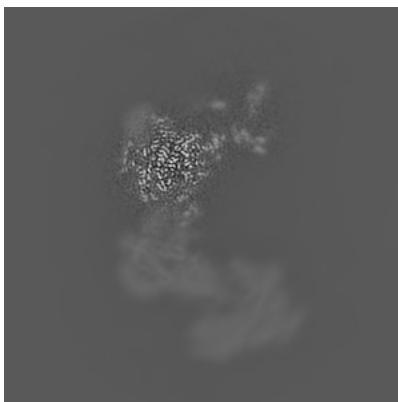
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

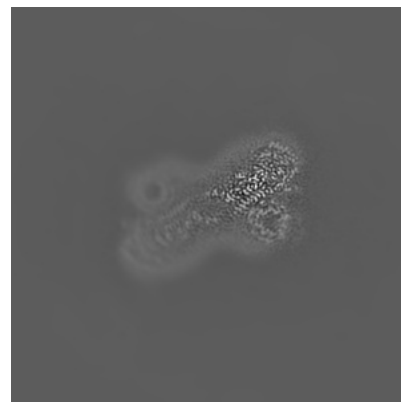
6.3.1 Primary map



X Index: 380

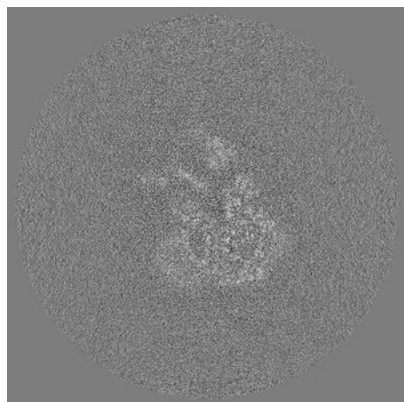


Y Index: 309

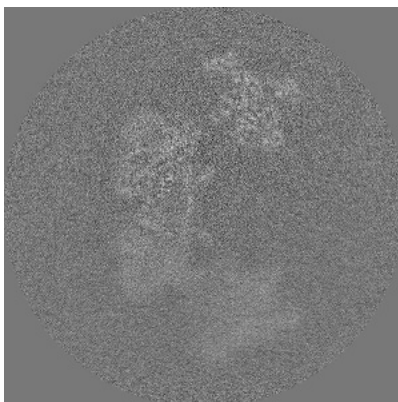


Z Index: 234

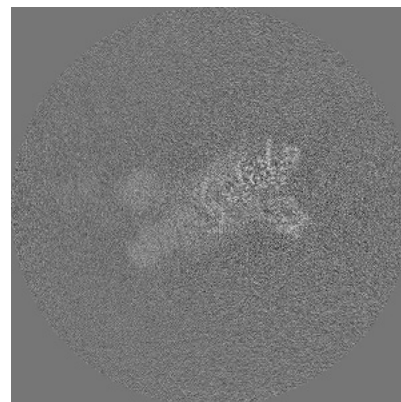
6.3.2 Raw map



X Index: 363



Y Index: 280

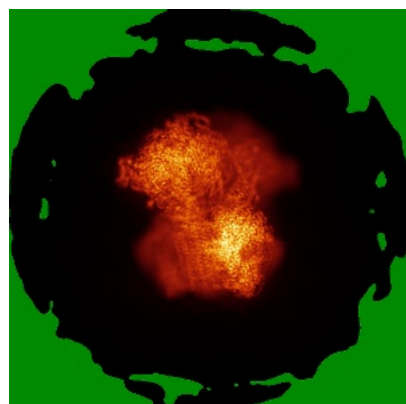


Z Index: 257

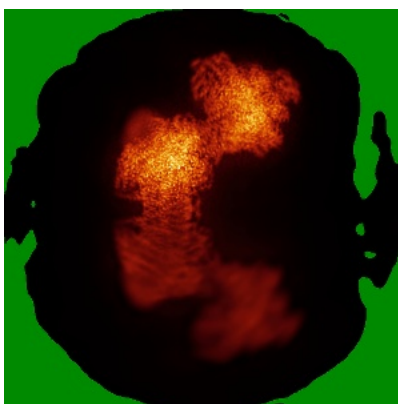
The images above show the largest variance slices of the map in three orthogonal directions.

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

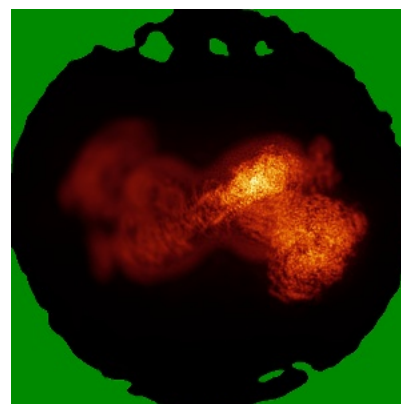
6.4.1 Primary map



X

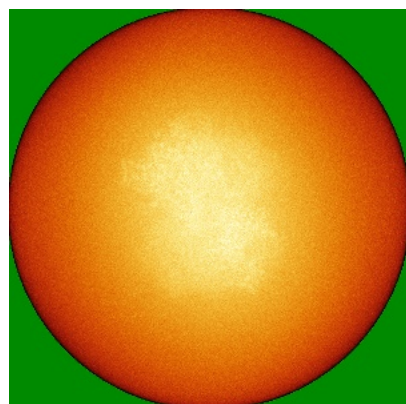


Y

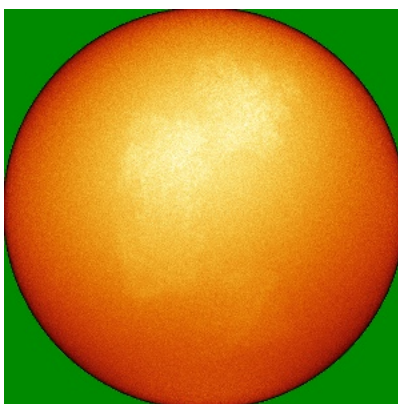


Z

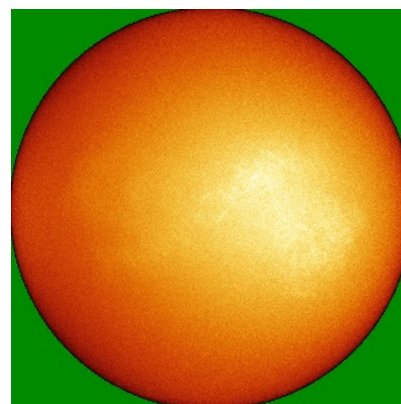
6.4.2 Raw map



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.

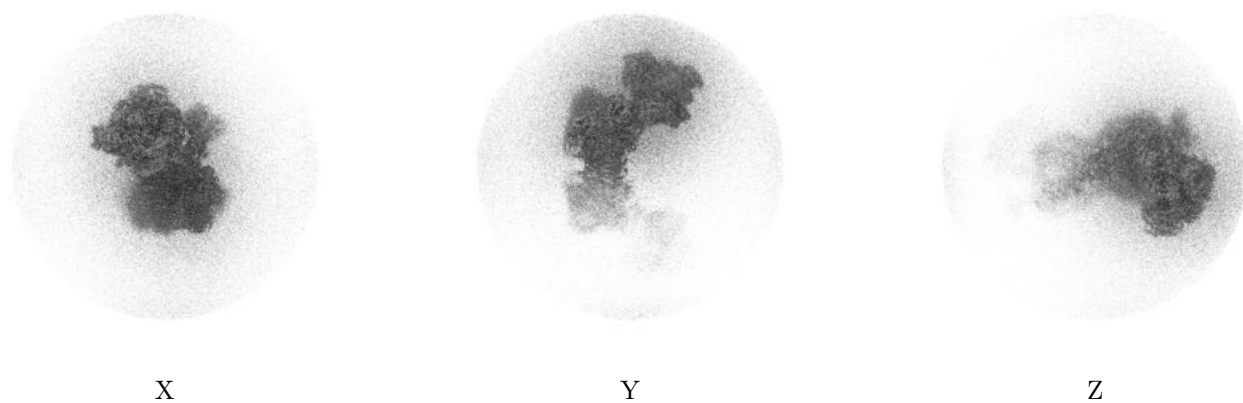
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

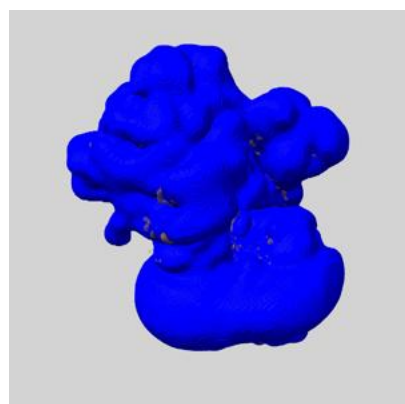
6.6 Mask visualisation [i](#)

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

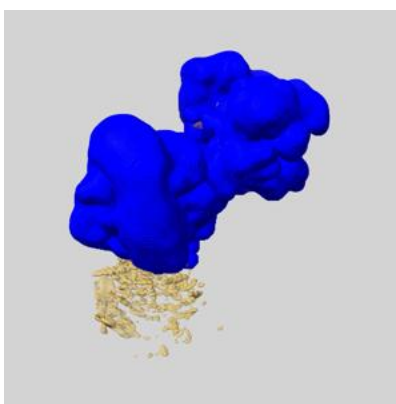
A mask typically either:

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

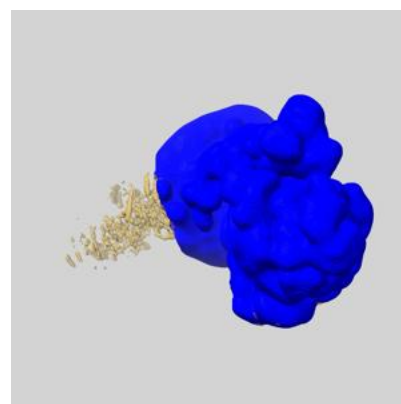
6.6.1 emd_15572_msk_1.map [i](#)



X



Y

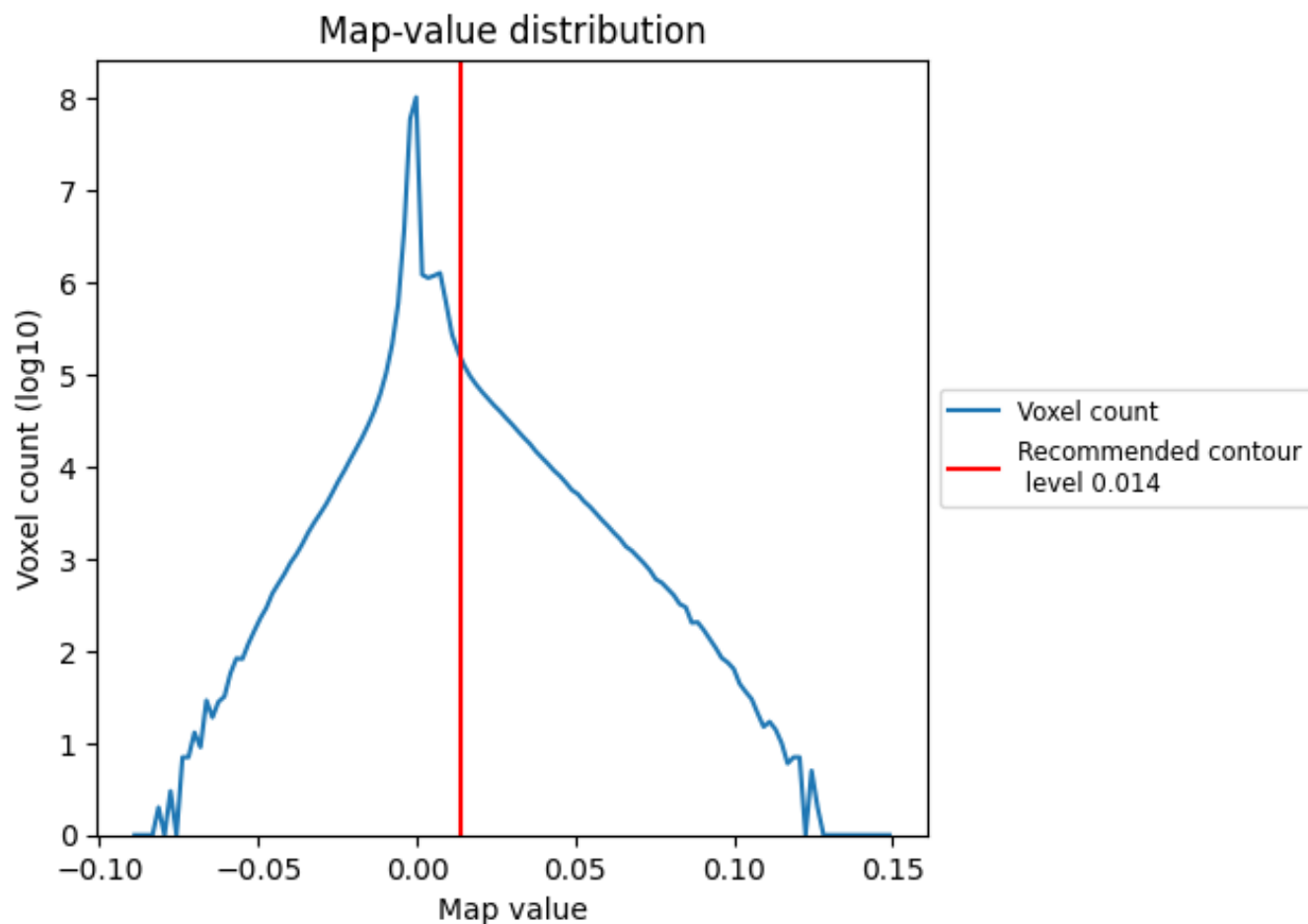


Z

7 Map analysis [i](#)

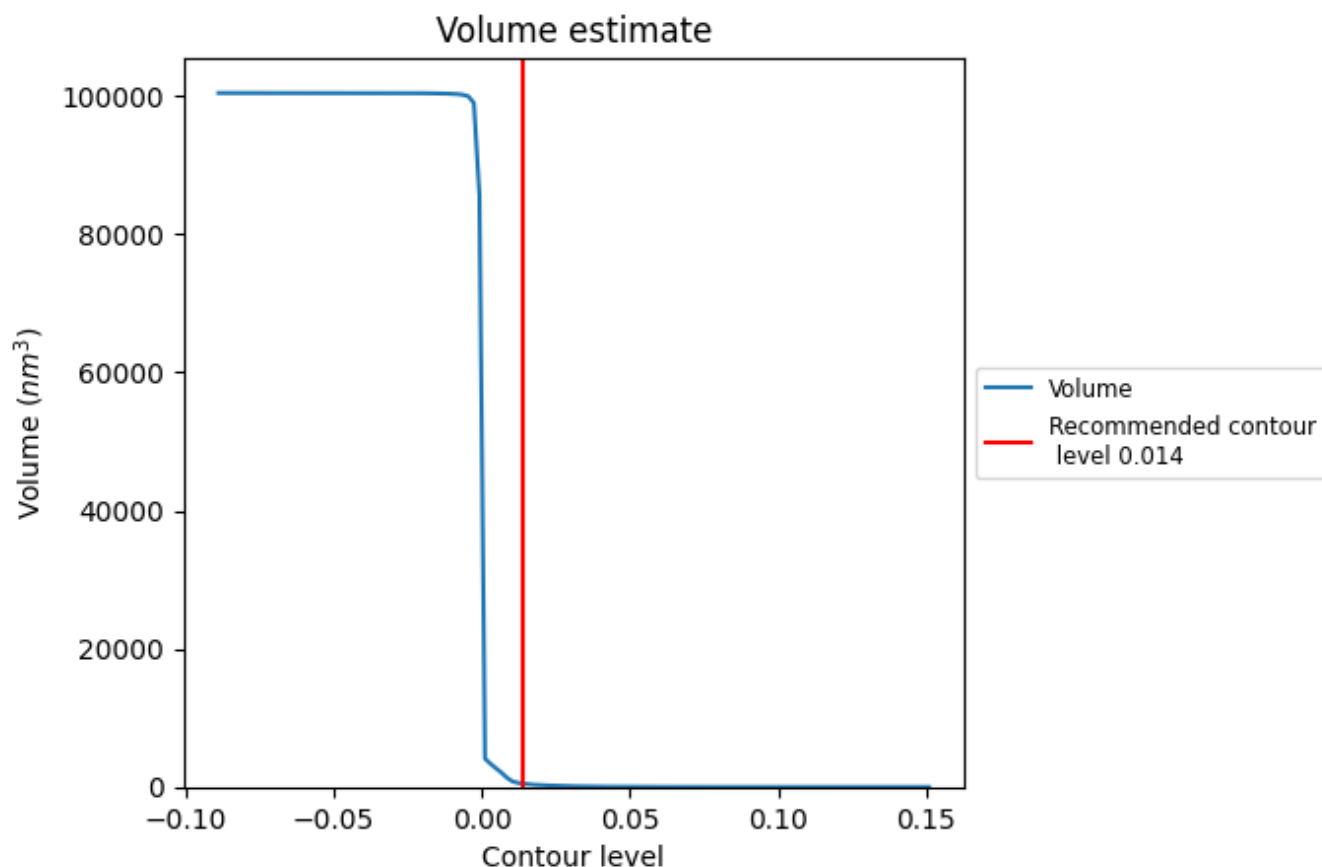
This section contains the results of statistical analysis of the map.

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.

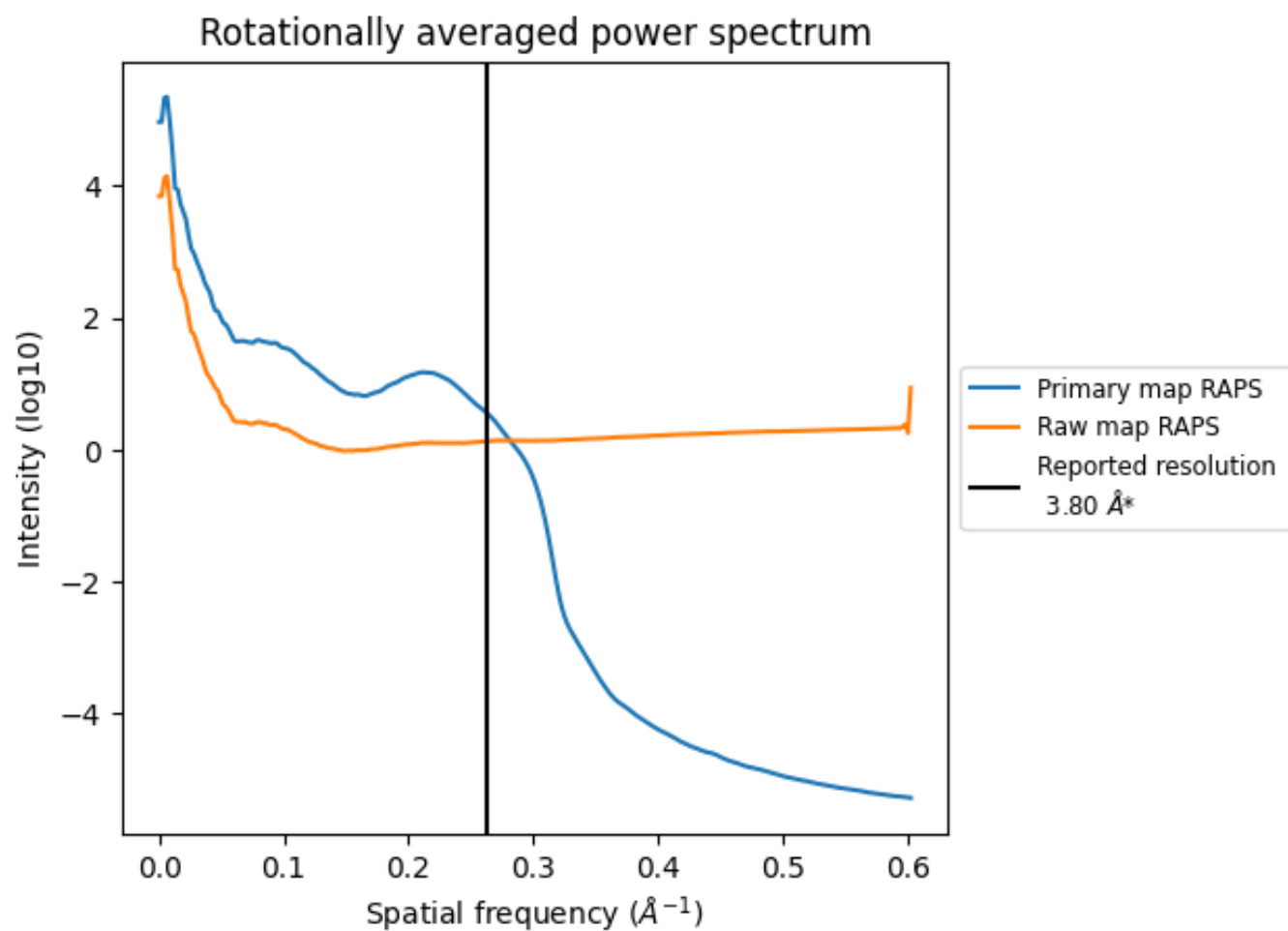
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 470 nm^3 ; this corresponds to an approximate mass of 425 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

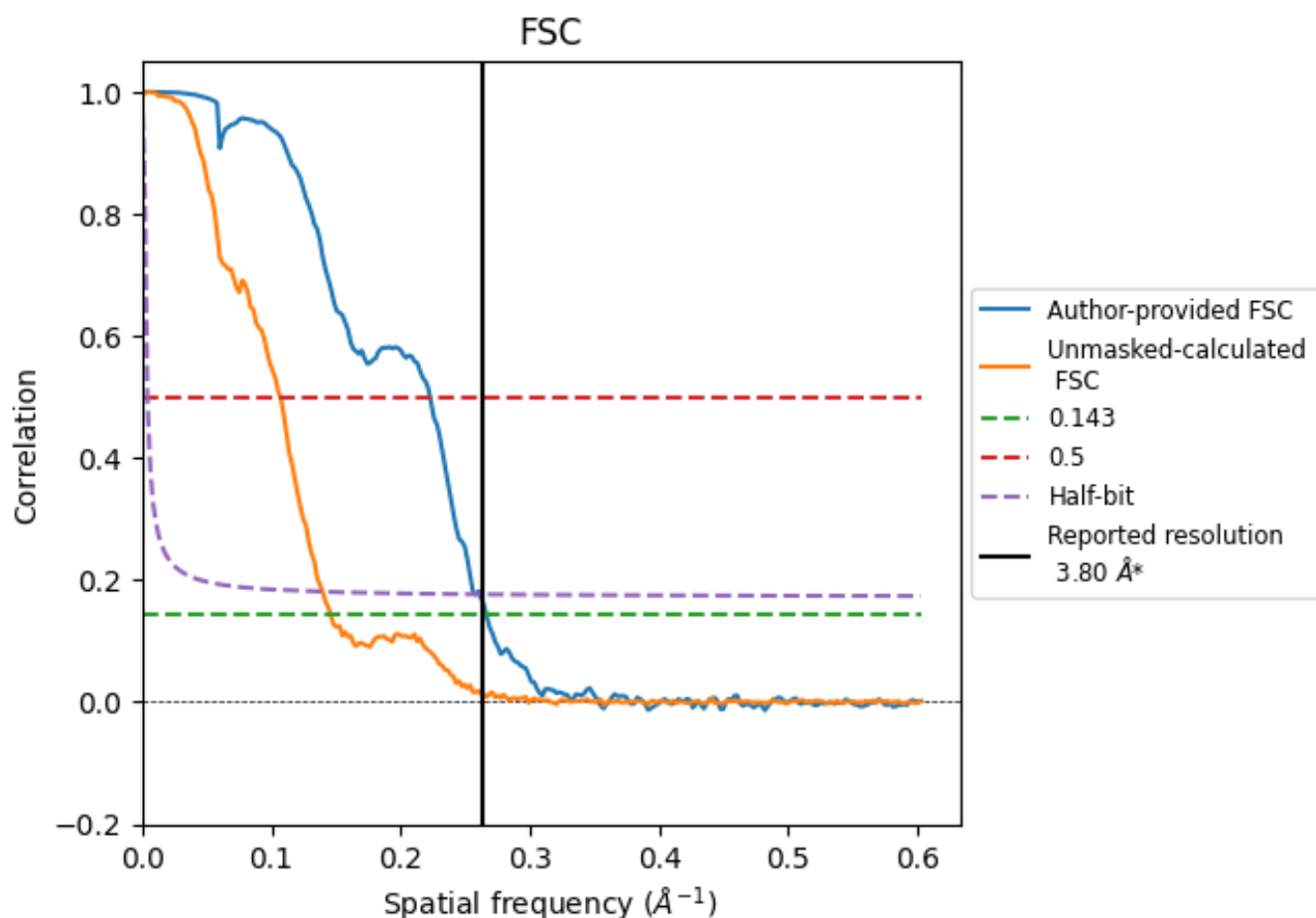


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

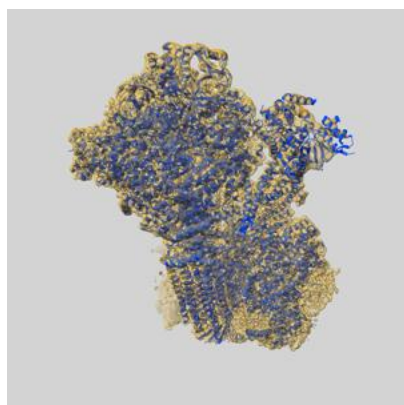
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.49	3.88
Unmasked-calculated*	6.86	9.35	7.15

*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 6.86 differs from the reported value 3.8 by more than 10 %

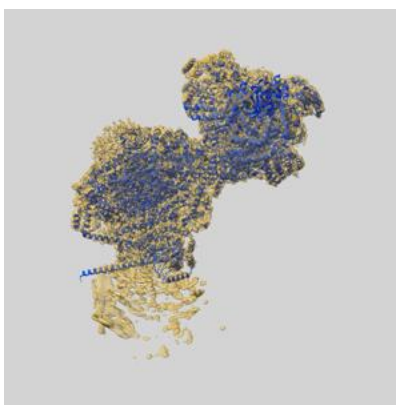
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15572 and PDB model 8APJ. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

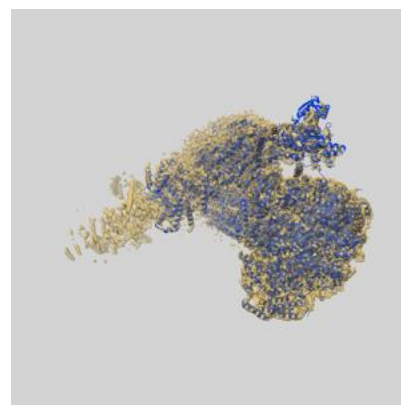
9.1 Map-model overlay [i](#)



X



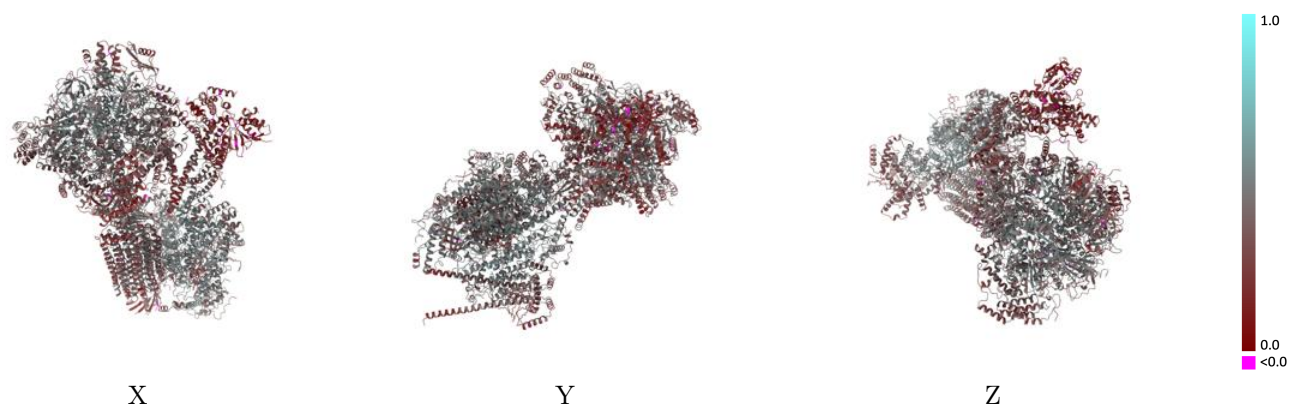
Y



Z

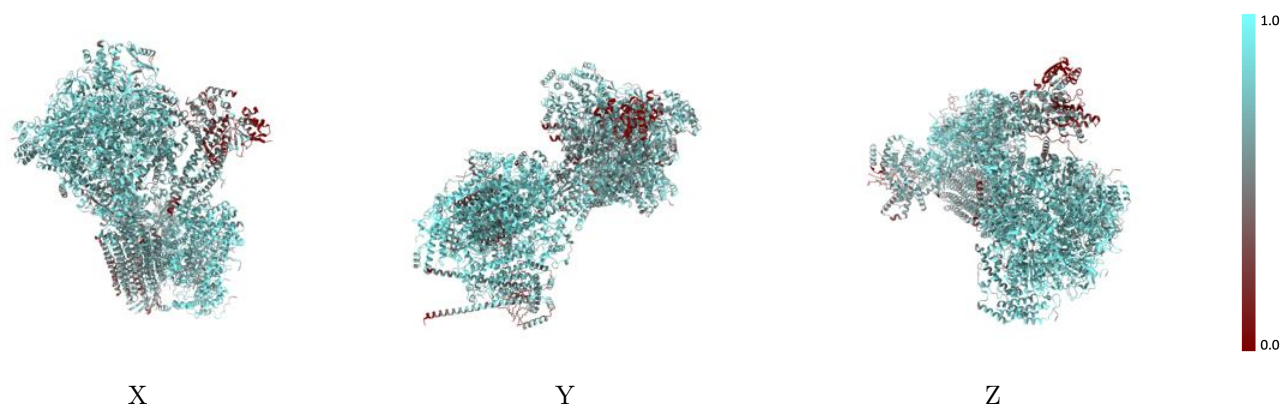
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



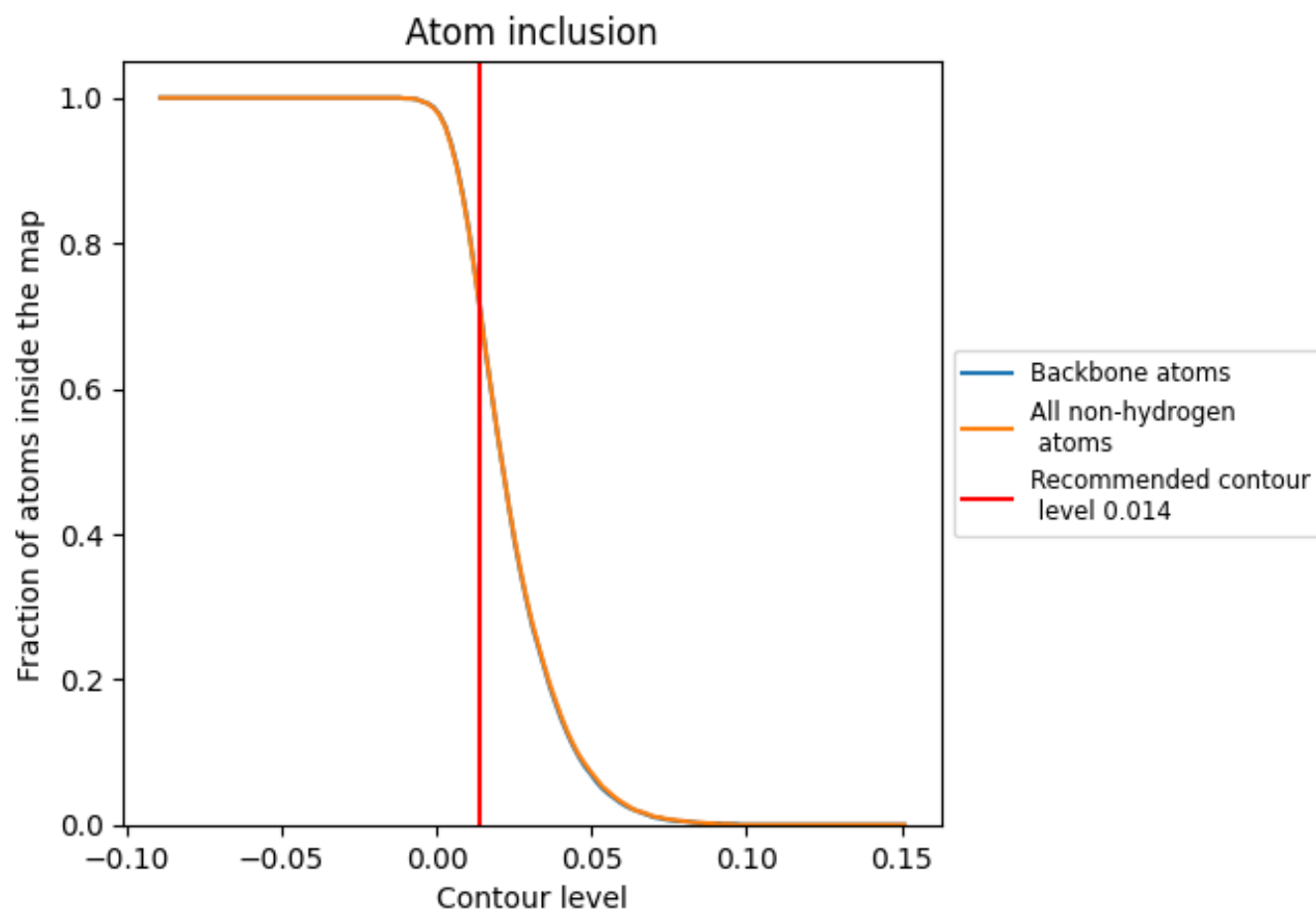
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 71% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.3950
A1	 0.8030	 0.4430
B1	 0.7810	 0.4080
C1	 0.7630	 0.4220
D1	 0.7710	 0.4390
E1	 0.7920	 0.4310
F1	 0.7140	 0.3870
G1	 0.6820	 0.3730
H1	 0.6830	 0.3690
I1	 0.6410	 0.3200
J1	 0.6820	 0.2830
K1	 0.6780	 0.3090
L	 0.5150	 0.3000
L1	 0.7200	 0.3190
M	 0.5320	 0.3200
M1	 0.6290	 0.3090
O1	 0.5760	 0.3270
P1	 0.5720	 0.3300
Q1	 0.5780	 0.3400
R1	 0.5830	 0.3470
S1	 0.6470	 0.3620
T1	 0.7040	 0.3790
U1	 0.6580	 0.3420
V1	 0.6220	 0.3430
W1	 0.5560	 0.3150
X1	 0.5690	 0.3270
a	 0.8630	 0.5340
c	 0.7870	 0.4720
d	 0.6710	 0.3530
e	 0.8290	 0.4700
f	 0.8250	 0.4830
g	 0.2830	 0.1830
h	 0.4330	 0.1840
i	 0.8710	 0.5080
j	 0.7780	 0.4410



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.8120	 0.4560
l	 0.5150	 0.3090
m	 0.6050	 0.3290
n	 0.8670	 0.5110
o	 0.8220	 0.4250
p	 0.7780	 0.4660
q	 0.8460	 0.5040
r	 0.8740	 0.5100