



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:44 AM UTC

PDB ID : 8APF / pdb_00008apf
EMDB ID : EMD-15568
Title : rotational state 2a of the Trypanosoma brucei mitochondrial ATP synthase dimer
Authors : Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on : 2022-08-09
Resolution : 4.30 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:

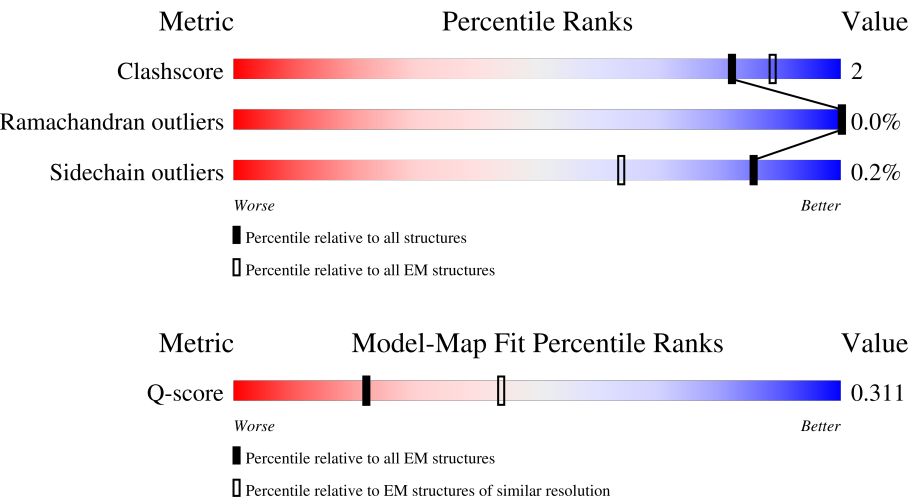
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	H1	182	28% 81%7%12%
2	I1	75	35% 79%8%13%
3	J1	188	16% 80%8%12%
3	K1	188	8% 81%7%12%

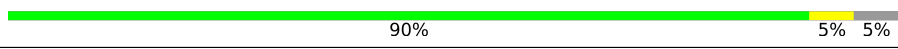
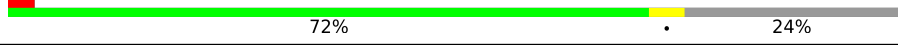
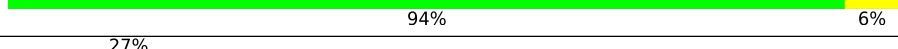
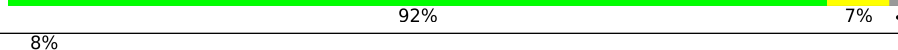
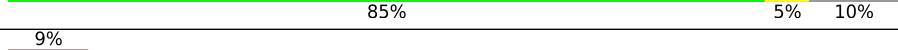
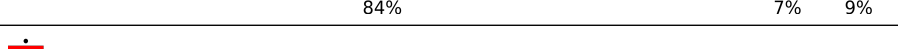
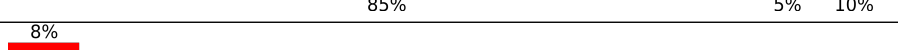
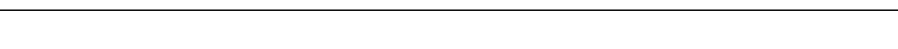
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Mol	Chain	Length	Quality of chain
3	L1	188	
4	L	92	
4	l	92	
5	M	144	
5	m	144	
6	M1	255	
7	O1	118	
7	P1	118	
7	Q1	118	
7	R1	118	
7	S1	118	
7	T1	118	
7	U1	118	
7	V1	118	
7	W1	118	
7	X1	118	
8	a	231	
9	c	114	
10	d	370	
11	e	396	
12	f	145	
13	g	269	
14	h	157	
15	i	104	
16	j	169	

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Mol	Chain	Length	Quality of chain
17	k	124	
18	n	156	
19	o	101	
20	p	105	
21	q	98	
22	r	62	
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 ATP synthase, epsilon chain, putative.

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

- Molecule 2 is a protein called ATP synthase subunit epsilon, mitochondrial.

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

- Molecule 3 is a protein called ATP synthase subunit p18, mitochondrial.

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

- Molecule 4 is a protein called subunit-e.

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

- Molecule 5 is a protein called subunit-g.

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

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

- Molecule 6 is a protein called OSCP.

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

- Molecule 7 is a protein called ATPase subunit 9, putative.

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

- Molecule 8 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	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 9 is a protein called subunit-8.

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

- Molecule 10 is a protein called subunit-d.

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

- Molecule 11 is a protein called ATPTB1.

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

- Molecule 12 is a protein called subunit-f.

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

- Molecule 13 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	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 14 is a protein called ATPTB4.

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

- Molecule 15 is a protein called subunit-i/j.

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

- Molecule 16 is a protein called ATPTB6.

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

- Molecule 17 is a protein called subunit-k.

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

- Molecule 18 is a protein called ATPTB11.

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

- Molecule 19 is a protein called ATPTB12.

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

- Molecule 20 is a protein called subunit-b.

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

- Molecule 21 is a protein called ATPEG3.

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

- Molecule 22 is a protein called ATPEG4.

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

- 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		

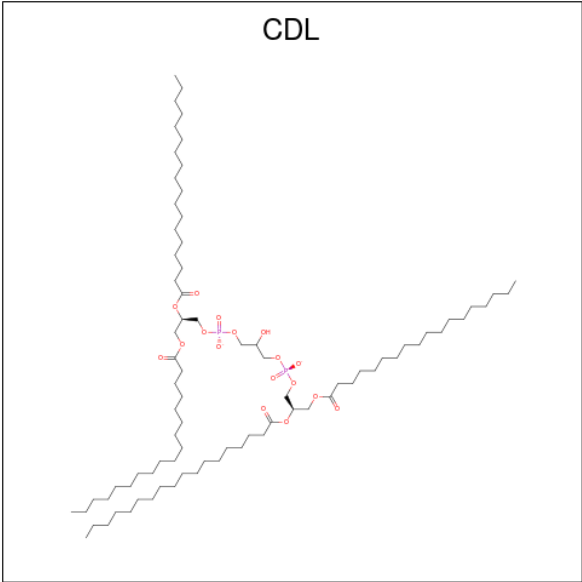
- Molecule 24 is a protein called ATP synthase subunit alpha, mitochondrial.

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.

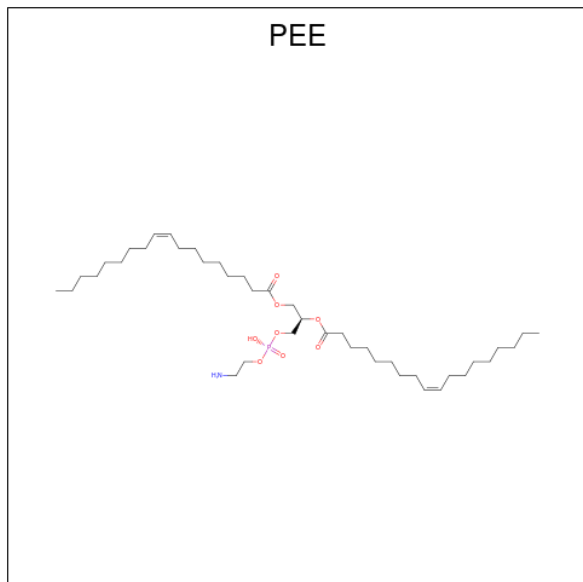
Mol	Chain	Residues	Atoms						AltConf	Trace
25	D1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		
25	E1	486	Total	C	H	N	O	S	0	0
			7414	2324	3732	630	709	19		
25	F1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		

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



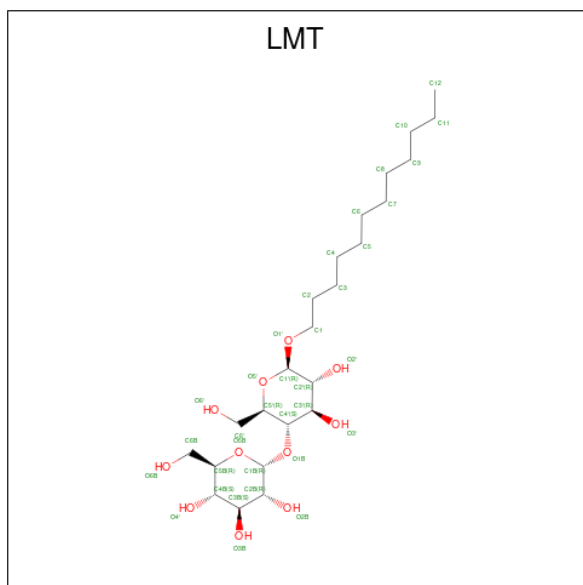
Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	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	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	
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).



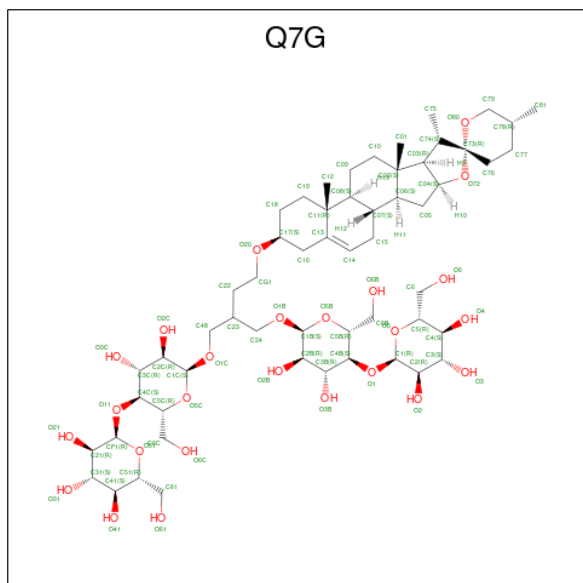
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
27	M	1	Total 133	41	82	1	8	1	0
27	f	1	Total 133	41	82	1	8	1	0
27	m	1	Total 133	41	82	1	8	1	0

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



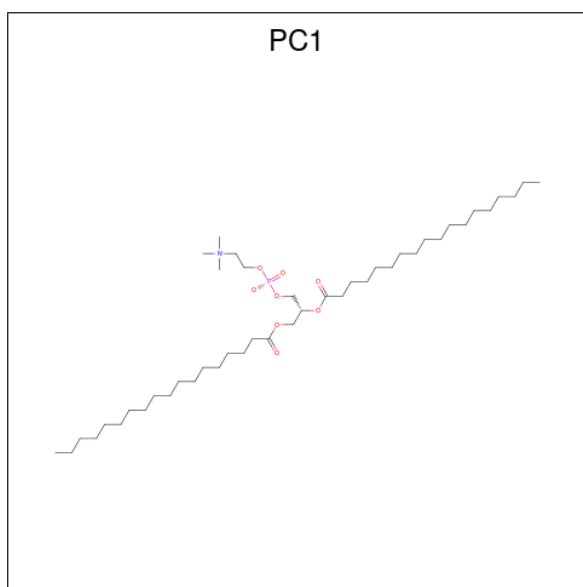
Mol	Chain	Residues	Atoms				AltConf
28	e	1	Total	C	H	O	0
			74	24	39	11	
28	j	1	Total	C	H	O	0
			74	24	39	11	

- 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).



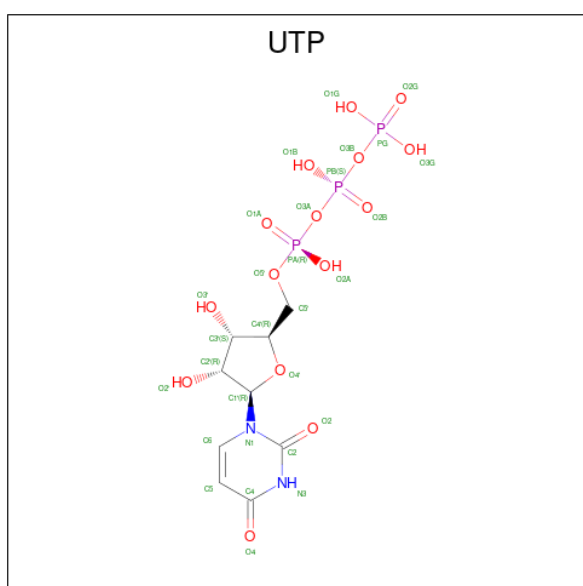
Mol	Chain	Residues	Atoms				AltConf
29	e	1	Total	C	H	O	0
			108	38	60	10	
29	n	1	Total	C	H	O	0
			129	44	70	15	

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



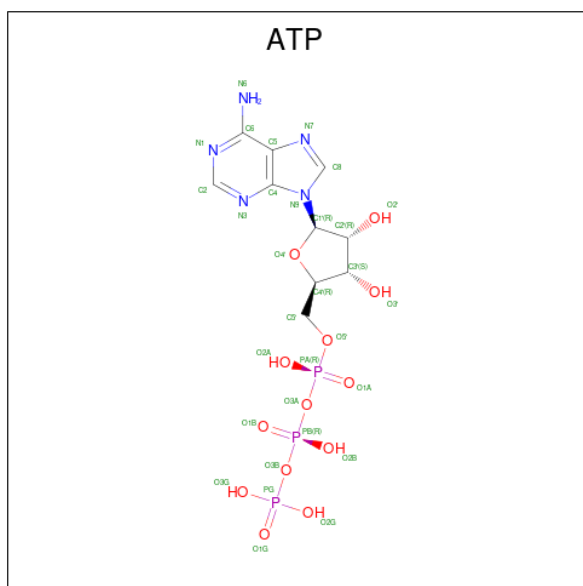
Mol	Chain	Residues	Atoms						AltConf
30	f	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
30	i	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
30	j	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
30	p	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- 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	G1	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).

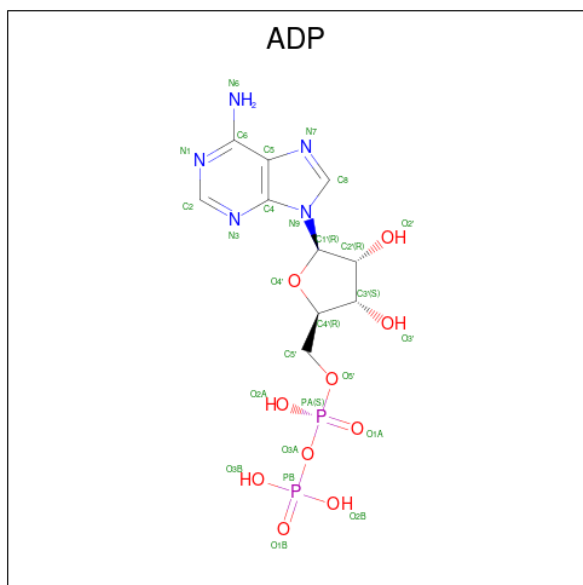
Mol	Chain	Residues	Atoms		AltConf
33	A1	1	Total	Mg	0
			1	1	
33	B1	1	Total	Mg	0
			1	1	
33	C1	1	Total	Mg	0
			1	1	
33	D1	1	Total	Mg	0
			1	1	

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

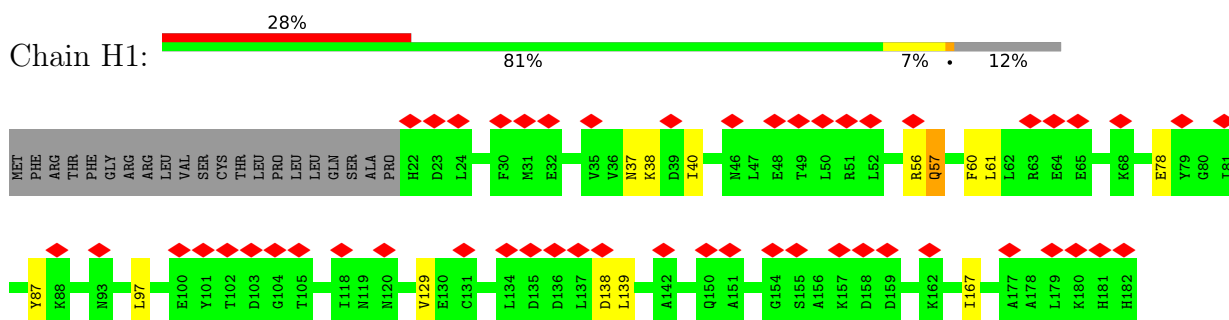
- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



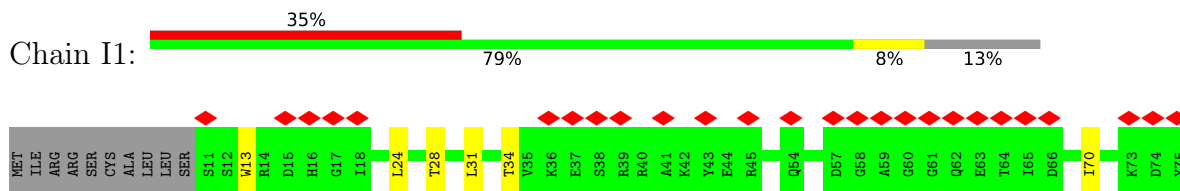
3 Residue-property plots

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.

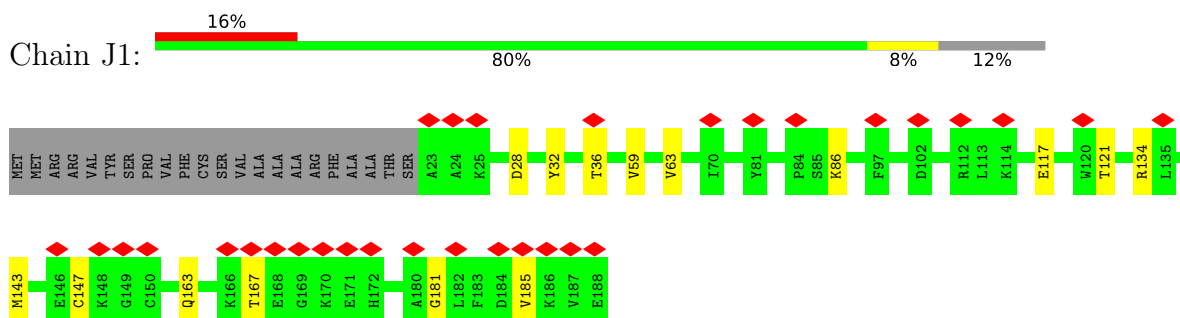
- Molecule 1: ATP synthase, epsilon chain, putative



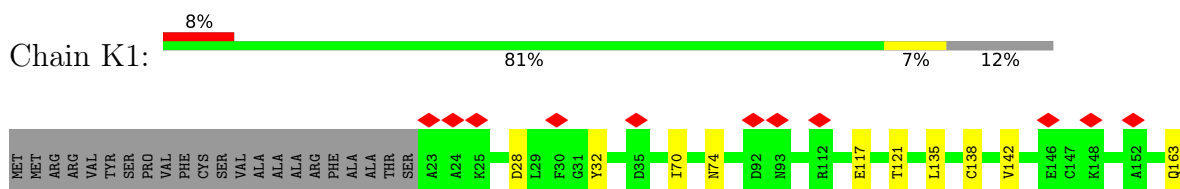
- Molecule 2: ATP synthase subunit epsilon, mitochondrial

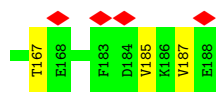


- Molecule 3: ATP synthase subunit p18, mitochondrial

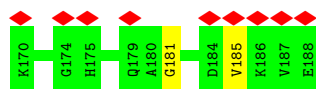
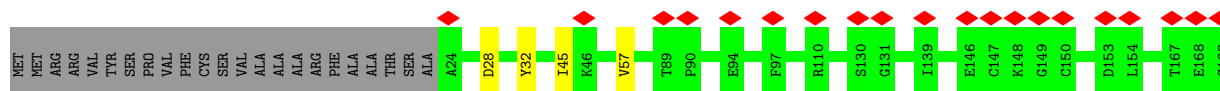
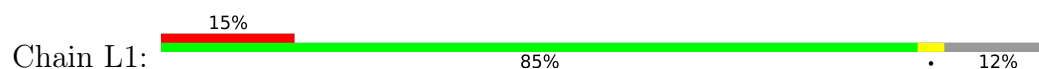


- Molecule 3: ATP synthase subunit p18, mitochondrial

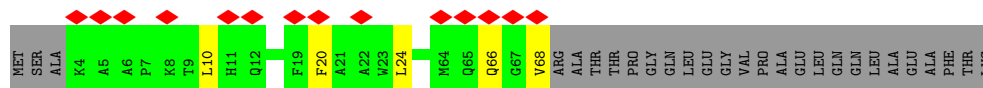




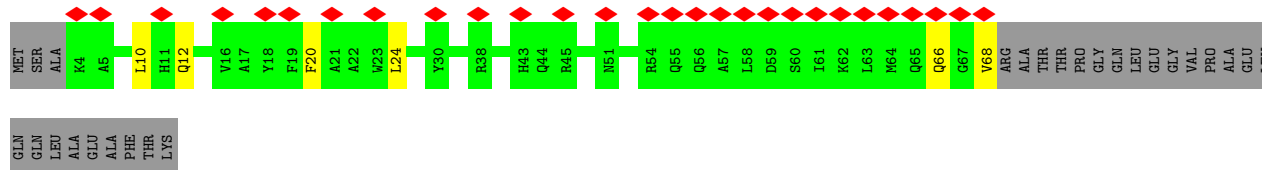
- Molecule 3: ATP synthase subunit p18, mitochondrial



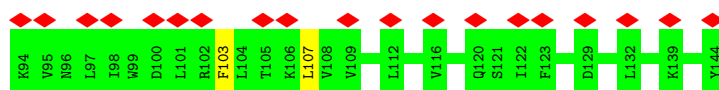
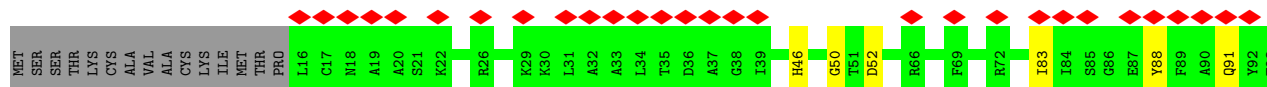
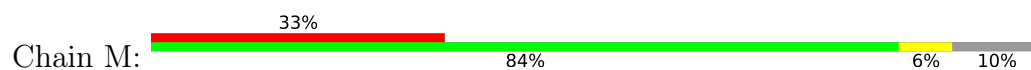
- Molecule 4: subunit-e



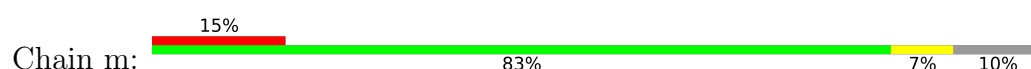
- Molecule 4: subunit-e

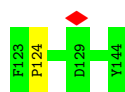


- Molecule 5: subunit-g

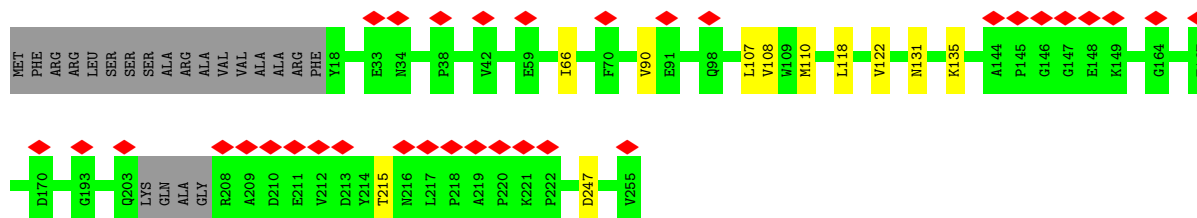


- Molecule 5: subunit-g

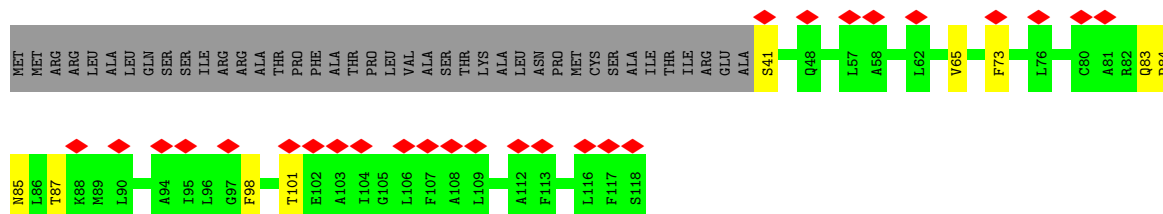




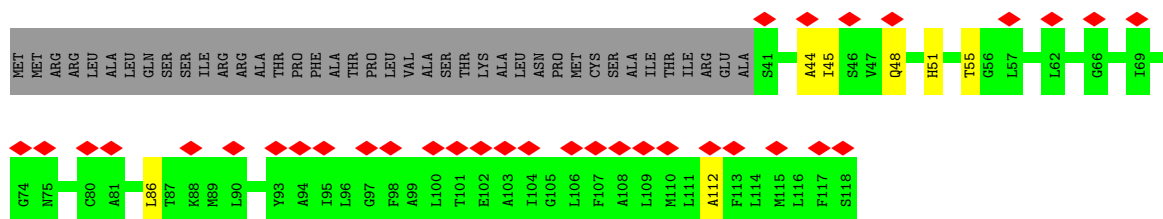
- Molecule 6: OSCP



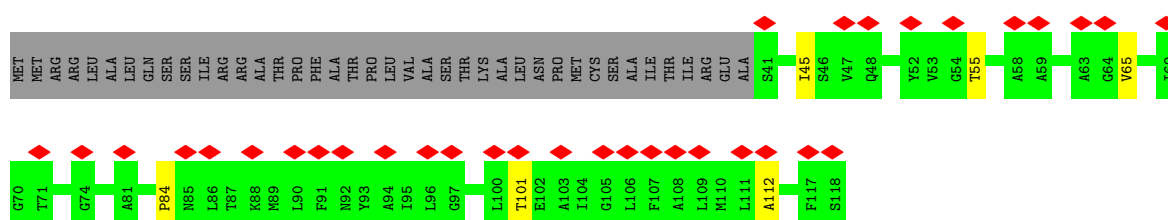
- Molecule 7: ATPase subunit 9, putative



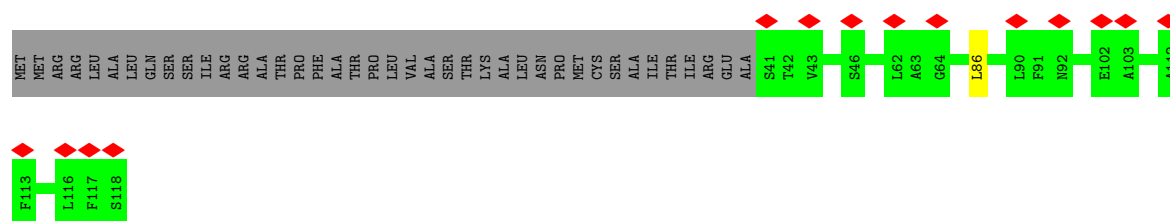
- Molecule 7: ATPase subunit 9, putative



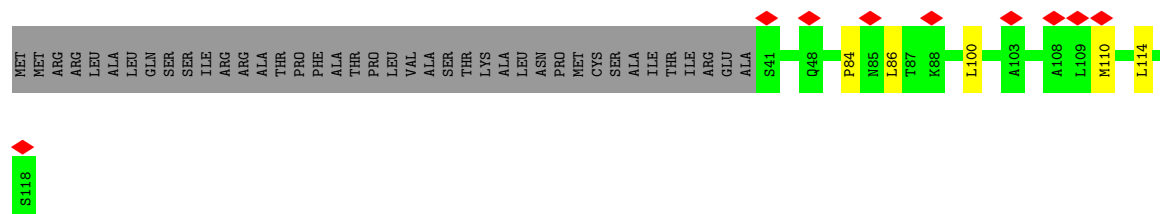
- Molecule 7: ATPase subunit 9, putative



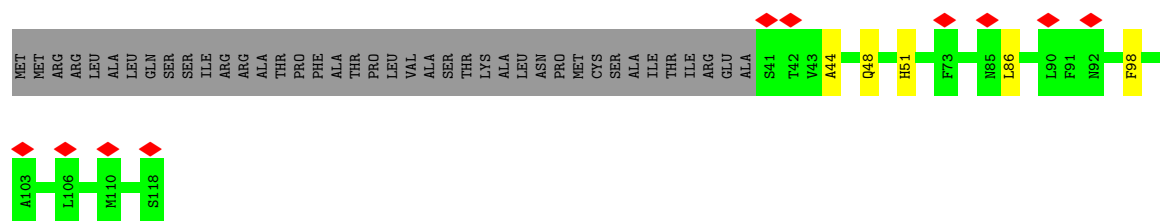
- Molecule 7: ATPase subunit 9, putative



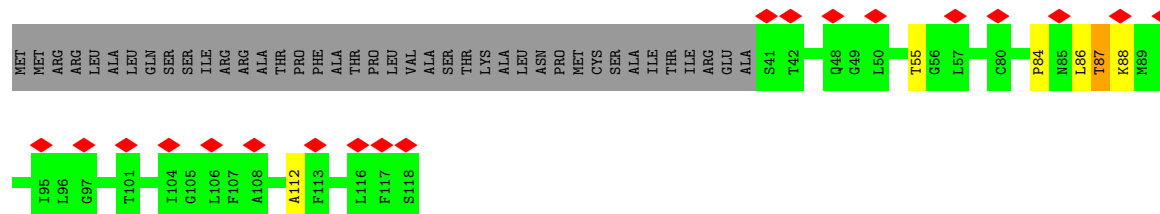
- Molecule 7: ATPase subunit 9, putative



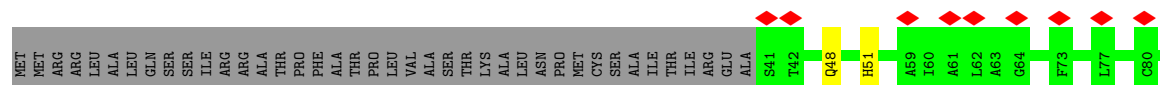
- Molecule 7: ATPase subunit 9, putative

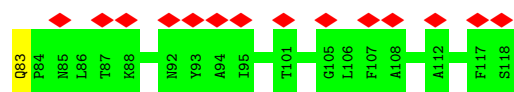


- Molecule 7: ATPase subunit 9, putative

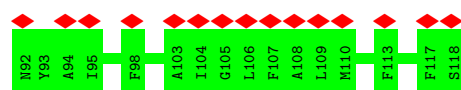
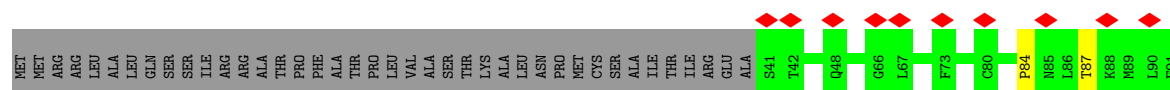


- Molecule 7: ATPase subunit 9, putative

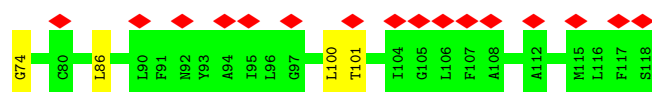
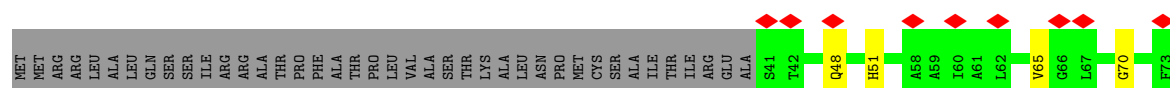




- Molecule 7: ATPase subunit 9, putative



- Molecule 7: ATPase subunit 9, putative



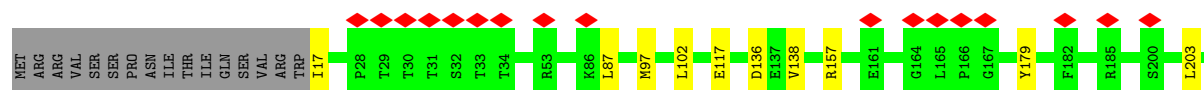
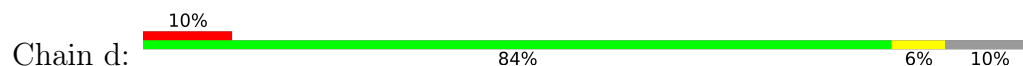
- Molecule 8: ATP synthase subunit a

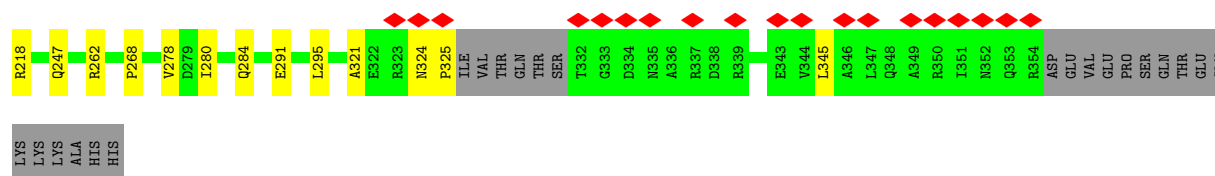


- Molecule 9: subunit-8

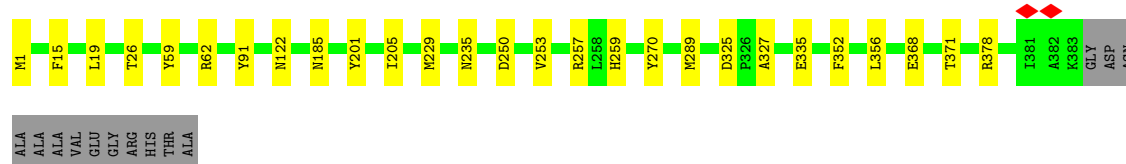


- Molecule 10: subunit-d

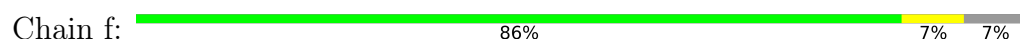




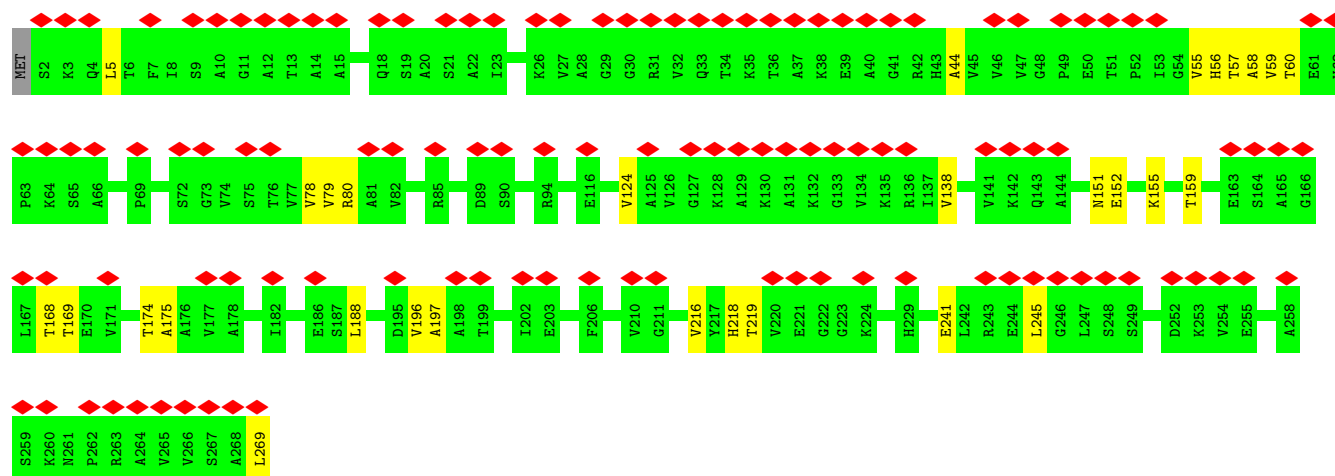
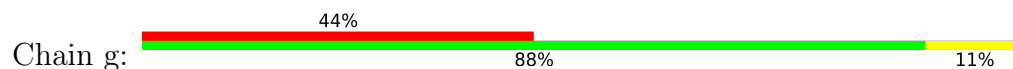
• Molecule 11: ATPTB1



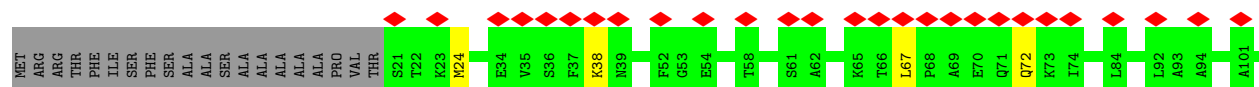
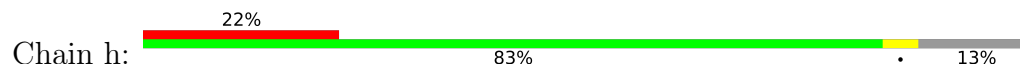
• Molecule 12: subunit-f

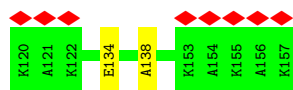


• Molecule 13: ATPTB3



• Molecule 14: ATPTB4





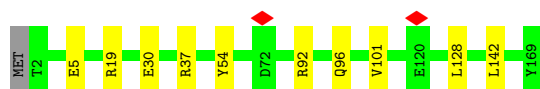
• Molecule 15: subunit-i/j

Chain i: 90% 9%



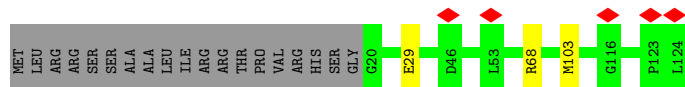
• Molecule 16: ATPTB6

Chain j: 93% 6%



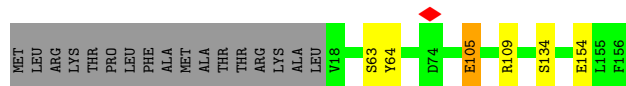
• Molecule 17: subunit-k

Chain k: 82% 15%



• Molecule 18: ATPTB11

Chain n: 85% 11%



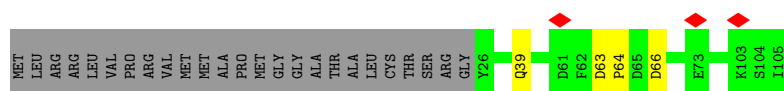
• Molecule 19: ATPTB12

Chain o: 90% 5%



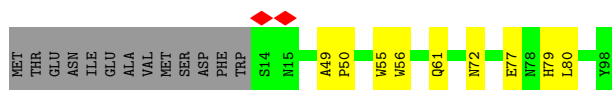
• Molecule 20: subunit-b

Chain p: 72% 24%



• Molecule 21: ATPEG3

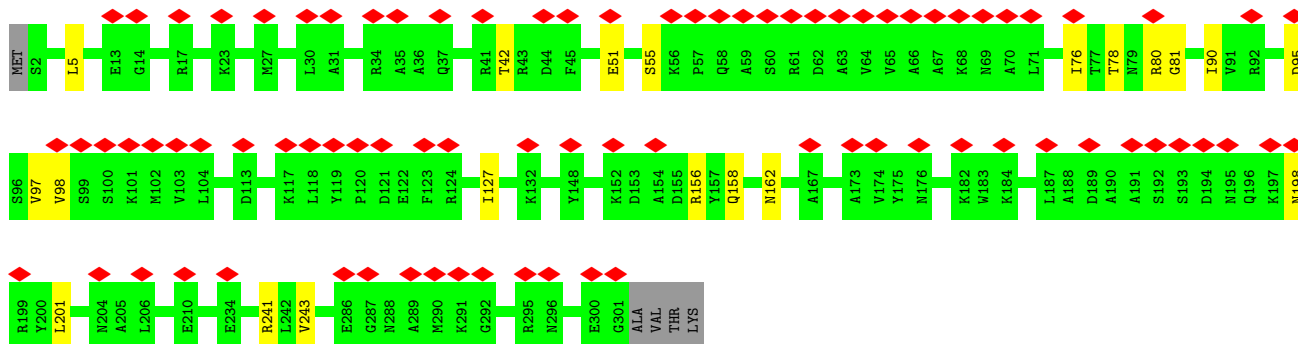
Chain q: 78% 9% 13%



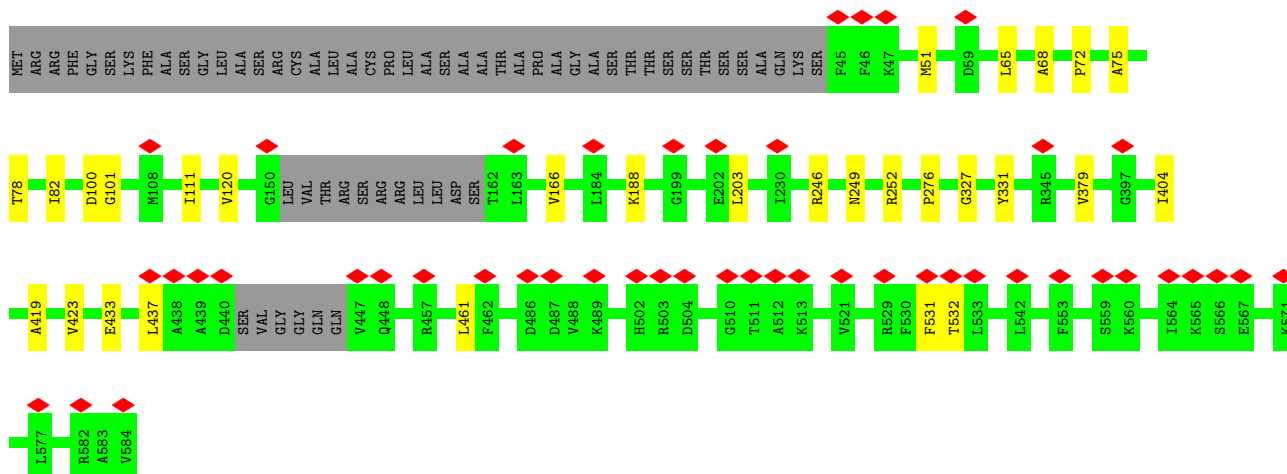
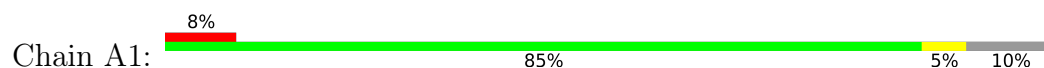
- Molecule 22: ATPEG4



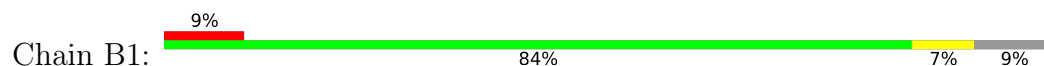
- Molecule 23: ATP synthase gamma subunit

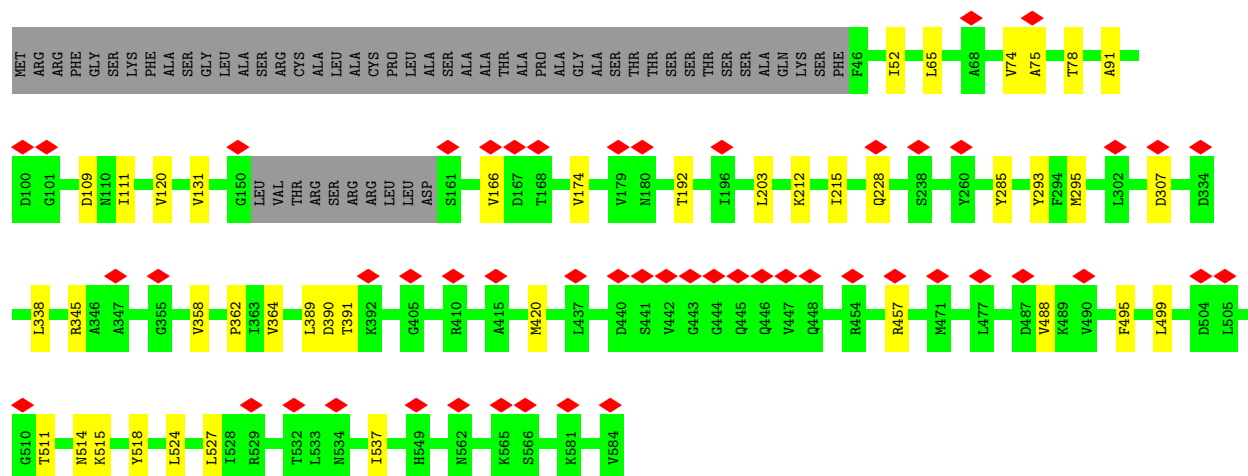


- Molecule 24: ATP synthase subunit alpha, mitochondrial

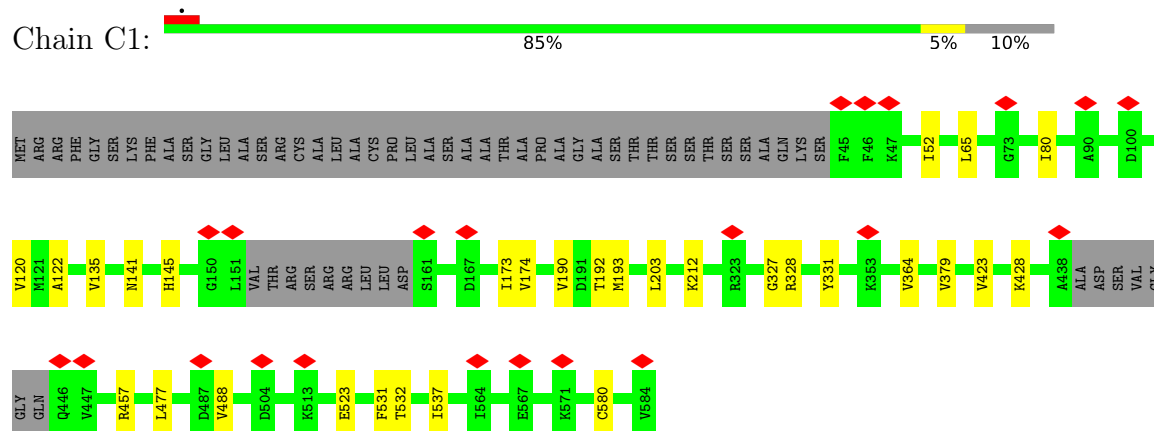


- Molecule 24: ATP synthase subunit alpha, mitochondrial

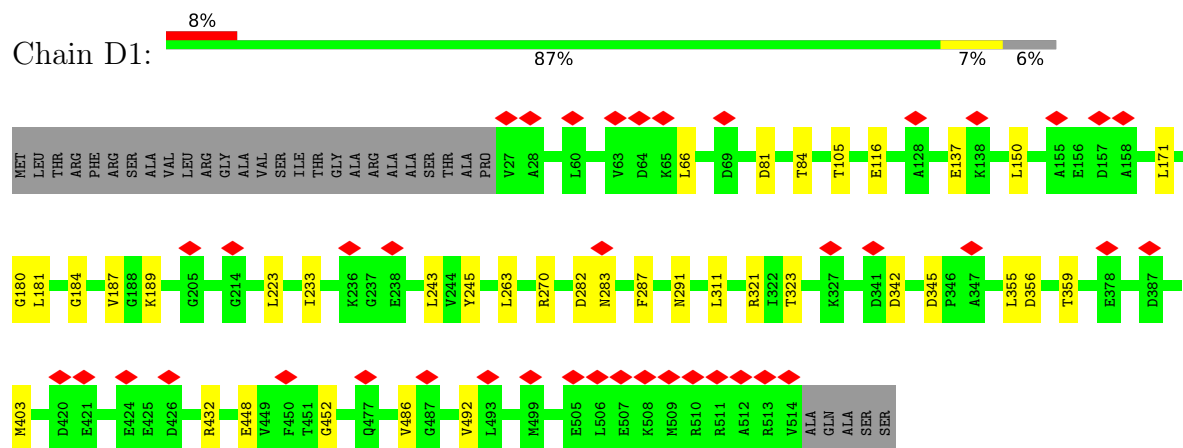




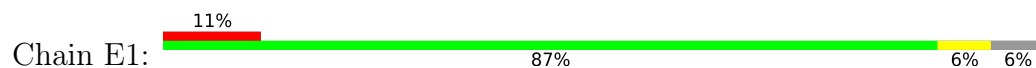
- Molecule 24: ATP synthase subunit alpha, mitochondrial

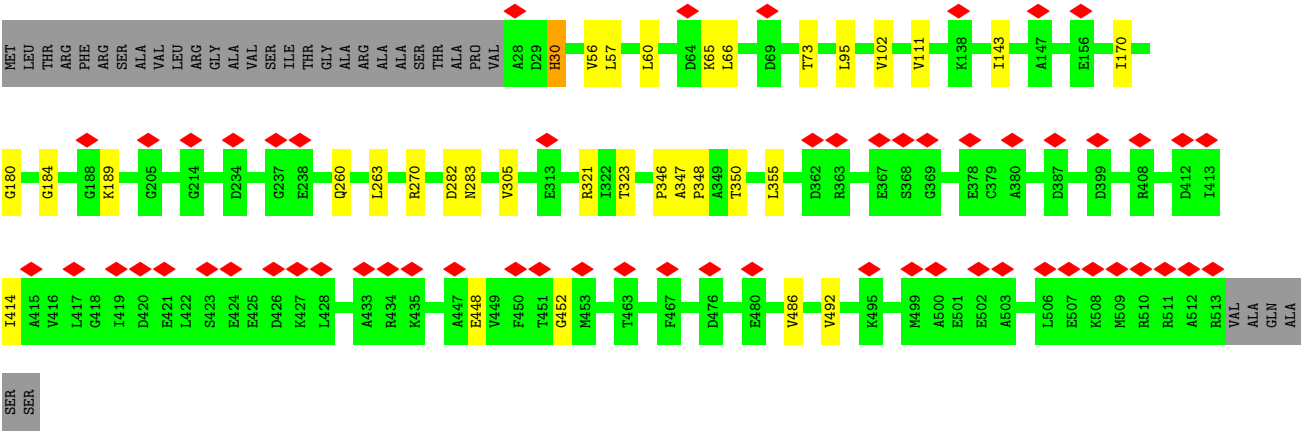


- Molecule 25: ATP synthase subunit beta, mitochondrial

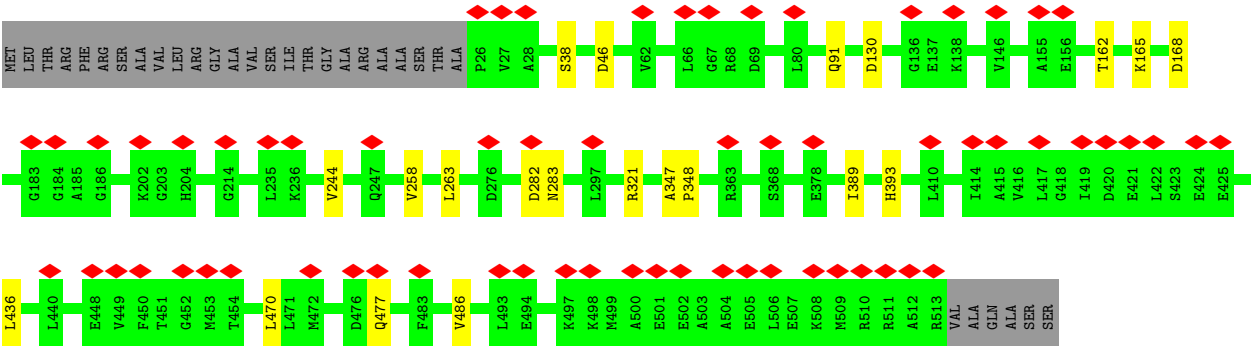
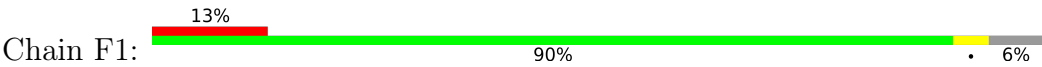


- Molecule 25: ATP synthase subunit beta, mitochondrial





● Molecule 25: ATP synthase subunit beta, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12173	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	0.105	Depositor
Minimum map value	-0.063	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H1	0.13	0/1274	0.21	0/1728
2	I1	0.07	0/547	0.20	0/738
3	J1	0.07	0/1342	0.21	0/1810
3	K1	0.07	0/1342	0.20	0/1810
3	L1	0.06	0/1337	0.21	0/1803
4	L	0.05	0/547	0.14	0/735
4	l	0.07	0/547	0.17	0/735
5	M	0.06	0/1049	0.16	0/1423
5	m	0.08	0/1049	0.20	0/1423
6	M1	0.07	0/1916	0.20	0/2591
7	O1	0.06	0/574	0.16	0/777
7	P1	0.06	0/574	0.16	0/777
7	Q1	0.06	0/574	0.15	0/777
7	R1	0.08	0/574	0.18	0/777
7	S1	0.08	0/574	0.20	0/777
7	T1	0.08	0/574	0.18	0/777
7	U1	0.09	0/574	0.22	0/777
7	V1	0.06	0/574	0.15	0/777
7	W1	0.06	0/574	0.16	0/777
7	X1	0.06	0/574	0.15	0/777
8	a	0.15	0/2111	0.26	0/2861
9	c	0.14	0/772	0.27	0/1054
10	d	0.08	0/2786	0.20	0/3760
11	e	0.11	0/3305	0.22	0/4482
12	f	0.11	0/1183	0.26	0/1601
13	g	0.06	0/1953	0.18	0/2650
14	h	0.06	0/1088	0.16	0/1466
15	i	0.12	0/913	0.22	0/1240
16	j	0.09	0/1462	0.19	0/1973
17	k	0.08	0/904	0.21	0/1228
18	n	0.11	0/1166	0.23	0/1581
19	o	0.08	0/814	0.18	0/1100

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	p	0.08	0/707	0.22	0/957
21	q	0.10	0/799	0.24	0/1091
22	r	0.10	0/567	0.24	0/767
23	G1	0.08	0/2427	0.22	0/3268
24	A1	0.08	0/4113	0.22	0/5569
24	B1	0.08	0/4147	0.24	0/5616
24	C1	0.09	0/4123	0.25	0/5582
25	D1	0.08	0/3752	0.25	0/5087
25	E1	0.09	0/3738	0.24	0/5067
25	F1	0.08	0/3753	0.22	0/5088
All	All	0.09	0/63273	0.22	0/85654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H1	1251	1232	1231	14	0
2	I1	533	513	513	6	0
3	J1	1315	1276	1276	9	0
3	K1	1315	1276	1276	10	0
3	L1	1310	1271	1271	3	0
4	L	537	545	545	3	0
4	l	537	545	545	4	0
5	M	1027	1042	1042	6	0
5	m	1027	1042	1042	7	0
6	M1	1877	1873	1873	8	0
7	O1	565	600	599	7	0
7	P1	565	600	599	5	0
7	Q1	565	600	599	4	0
7	R1	565	600	599	1	0
7	S1	565	601	599	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T1	565	601	599	4	0
7	U1	565	600	599	3	0
7	V1	565	600	599	2	0
7	W1	565	600	599	1	0
7	X1	565	600	599	6	0
8	a	2032	2044	2044	9	0
9	c	745	715	715	9	0
10	d	2737	2762	2763	17	0
11	e	3220	3050	3061	18	0
12	f	1145	1111	1111	9	0
13	g	1933	2020	2020	17	0
14	h	1070	1088	1088	4	0
15	i	883	857	857	6	0
16	j	1424	1411	1411	8	0
17	k	873	876	876	3	0
18	n	1128	1082	1082	4	0
19	o	789	767	767	4	0
20	p	684	651	651	5	0
21	q	766	720	720	7	0
22	r	542	498	498	5	0
23	G1	2387	2387	2387	15	0
24	A1	4039	4154	4154	20	0
24	B1	4073	4187	4187	26	0
24	C1	4049	4170	4170	24	0
25	D1	3696	3750	3750	26	0
25	E1	3682	3732	3732	21	0
25	F1	3696	3750	3750	13	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	4	0
26	f	100	156	156	0	0
26	j	100	156	156	1	0
26	l	100	156	156	0	0
26	m	100	156	156	0	0
26	q	200	312	312	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	n	59	70	0	0	0
30	f	54	88	88	1	0
30	i	54	88	88	0	0
30	j	54	88	88	0	0
30	p	54	88	88	0	0
31	G1	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	1	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	65343	323	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 (323) 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)
16:j:19:ARG:NH2	21:q:77:GLU:O	2.15	0.79
25:E1:260:GLN:N	25:E1:260:GLN:OE1	2.22	0.73
9:c:93:THR:HG21	10:d:136:ASP:OD2	1.89	0.73
12:f:16:GLU:OE1	12:f:16:GLU:N	2.22	0.72
25:E1:184:GLY:O	25:E1:189:LYS:NZ	2.23	0.71
12:f:64:ARG:NH2	22:r:33:GLU:OE2	2.24	0.71
11:e:250:ASP:OD1	11:e:270:TYR:OH	2.09	0.69
1:H1:78:GLU:OE1	7:V1:83:GLN:NE2	2.25	0.69
9:c:73:HIS:NE2	9:c:77:GLU:OE2	2.28	0.66
8:a:166:TYR:OH	30:f:203:PC1:O12	2.12	0.65
1:H1:37:ASN:ND2	23:G1:198:ASN:O	2.29	0.65
11:e:185:ASN:ND2	11:e:325:ASP:OD1	2.29	0.64
25:F1:263:LEU:HD21	25:F1:321:ARG:HB2	1.79	0.64
24:B1:295:MET:HB2	24:B1:358:VAL:HG23	1.80	0.64
3:J1:28:ASP:OD1	3:J1:32:TYR:N	2.30	0.64
6:M1:118:LEU:O	6:M1:122:VAL:HG23	1.97	0.64
25:D1:184:GLY:O	25:D1:189:LYS:NZ	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M1:90:VAL:HG11	6:M1:107:LEU:HB3	1.80	0.64
18:n:154:GLU:OE1	18:n:154:GLU:N	2.31	0.62
7:T1:48:GLN:O	7:T1:51:HIS:ND1	2.32	0.62
7:O1:84:PRO:O	7:O1:87:THR:HG23	2.00	0.62
25:E1:347:ALA:HB3	25:E1:348:PRO:HD3	1.82	0.62
17:k:29:GLU:N	17:k:29:GLU:OE1	2.33	0.62
11:e:62:ARG:NH2	26:e:402:CDL:OB4	2.33	0.61
24:B1:457:ARG:NH2	24:B1:488:VAL:O	2.33	0.61
7:X1:48:GLN:O	7:X1:51:HIS:ND1	2.34	0.61
16:j:128:LEU:HD21	16:j:142:LEU:HD12	1.82	0.61
24:C1:328:ARG:NH1	25:D1:342:ASP:OD2	2.34	0.61
3:J1:134:ARG:NH1	24:B1:515:LYS:O	2.34	0.60
11:e:1:AME:O	11:e:122:ASN:ND2	2.34	0.60
3:K1:117:GLU:O	3:K1:121:THR:HG23	2.02	0.59
4:L:66:GLN:HG3	4:L:68:VAL:HG23	1.84	0.59
25:F1:91:GLN:OE1	25:F1:91:GLN:N	2.36	0.59
25:E1:486:VAL:HG21	25:E1:492:VAL:HG22	1.84	0.59
3:J1:181:GLY:O	3:J1:185:VAL:HG23	2.02	0.58
15:i:87:PRO:O	15:i:91:GLY:N	2.34	0.58
10:d:345:LEU:HD13	25:F1:477:GLN:OE1	2.04	0.58
24:C1:203:LEU:HD11	24:C1:364:VAL:HG23	1.86	0.58
10:d:291:GLU:O	10:d:295:LEU:N	2.35	0.57
24:A1:246:ARG:NH1	25:D1:356:ASP:OD1	2.36	0.57
25:D1:270:ARG:NH1	25:D1:323:THR:O	2.35	0.57
24:C1:212:LYS:N	32:C1:601:ATP:O1B	2.35	0.57
4:l:66:GLN:HG3	4:l:68:VAL:HG23	1.86	0.57
24:B1:215:ILE:HD12	24:B1:389:LEU:HD11	1.87	0.57
24:A1:51:MET:HE3	24:A1:68:ALA:HB1	1.87	0.56
8:a:68:LEU:HD13	12:f:45:LEU:HD11	1.86	0.56
24:B1:285:TYR:OH	24:B1:338:LEU:HD12	2.06	0.56
1:H1:138:ASP:OD1	1:H1:139:LEU:N	2.40	0.55
5:m:103:PHE:CE2	5:m:107:LEU:HD11	2.41	0.55
9:c:61:VAL:HG13	10:d:278:VAL:HG11	1.87	0.55
23:G1:81:GLY:O	23:G1:241:ARG:NH1	2.40	0.55
12:f:37:TRP:NE1	12:f:48:GLU:OE1	2.35	0.55
13:g:59:VAL:HG13	13:g:216:VAL:HB	1.89	0.54
15:i:88:LYS:O	19:o:32:GLN:NE2	2.39	0.54
7:O1:83:GLN:OE1	7:O1:85:ASN:ND2	2.41	0.54
20:p:66:ASP:OD2	22:r:10:ARG:NH1	2.40	0.54
10:d:262:ARG:NH2	11:e:335:GLU:O	2.39	0.54
24:C1:203:LEU:HD13	24:C1:379:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:E1:448:GLU:O	25:E1:452:GLY:N	2.37	0.54
12:f:101:ARG:NH2	5:m:124:PRO:O	2.35	0.54
10:d:284:GLN:OE1	10:d:284:GLN:N	2.39	0.53
24:C1:80:ILE:C	24:C1:80:ILE:HD12	2.33	0.53
20:p:66:ASP:OD1	22:r:13:GLN:NE2	2.38	0.53
24:A1:404:ILE:HG22	24:A1:404:ILE:O	2.09	0.53
25:F1:389:ILE:HD12	25:F1:393:HIS:ND1	2.24	0.53
11:e:229:MET:SD	11:e:235:ASN:ND2	2.82	0.53
13:g:5:LEU:HD21	13:g:245:LEU:HD11	1.90	0.53
25:E1:111:VAL:HG23	25:E1:143:ILE:CG2	2.38	0.53
5:m:103:PHE:CZ	5:m:107:LEU:HD11	2.43	0.53
24:A1:65:LEU:HD22	24:A1:120:VAL:HG21	1.90	0.53
23:G1:97:VAL:HG12	23:G1:97:VAL:O	2.09	0.53
24:B1:75:ALA:HB3	24:B1:78:THR:HG21	1.90	0.53
9:c:40:TRP:O	9:c:43:VAL:HG12	2.09	0.53
26:M:201:CDL:H261	27:M:202:PEE:H44	1.92	0.52
13:g:155:LYS:O	13:g:159:THR:HG22	2.09	0.52
24:C1:173:ILE:HG23	24:C1:174:VAL:HG13	1.91	0.52
1:H1:129:VAL:CG1	2:I1:28:THR:HG21	2.39	0.52
11:e:62:ARG:NH2	16:j:96:GLN:OE1	2.42	0.52
3:J1:163:GLN:O	3:J1:167:THR:HG23	2.10	0.52
5:M:103:PHE:CE2	5:M:107:LEU:HD11	2.45	0.52
1:H1:56:ARG:HG2	1:H1:61:LEU:HD11	1.92	0.51
3:K1:28:ASP:OD1	3:K1:32:TYR:N	2.43	0.51
7:S1:110:MET:SD	8:a:152:LEU:HD23	2.50	0.51
16:j:37:ARG:NH2	26:q:101:CDL:OA3	2.42	0.51
24:A1:75:ALA:HB3	24:A1:78:THR:HG21	1.92	0.51
23:G1:156:ARG:NH2	23:G1:158:GLN:OE1	2.43	0.51
3:L1:181:GLY:O	3:L1:185:VAL:HG23	2.10	0.51
6:M1:110:MET:CE	6:M1:122:VAL:HG21	2.40	0.51
24:B1:166:VAL:O	24:B1:345:ARG:NH1	2.42	0.51
6:M1:215:THR:O	14:h:38:LYS:N	2.43	0.51
7:U1:86:LEU:O	7:U1:88:LYS:N	2.43	0.51
4:L:10:LEU:HD13	5:M:83:ILE:HD11	1.93	0.51
24:B1:514:ASN:O	24:B1:518:TYR:OH	2.21	0.51
8:a:93:TYR:CE2	8:a:220:LEU:HD22	2.45	0.51
6:M1:131:ASN:O	6:M1:135:LYS:N	2.43	0.51
7:Q1:65:VAL:HG13	7:Q1:101:THR:HG22	1.91	0.51
13:g:44:ALA:N	13:g:241:GLU:OE2	2.44	0.51
7:S1:100:LEU:HD22	7:T1:98:PHE:CZ	2.46	0.51
21:q:77:GLU:OE2	21:q:79:HIS:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F1:38:SER:N	25:F1:46:ASP:O	2.42	0.51
3:J1:36:THR:HG22	3:J1:36:THR:O	2.10	0.50
24:B1:65:LEU:HD22	24:B1:120:VAL:HG21	1.94	0.50
16:j:54:TYR:O	16:j:92:ARG:NH1	2.43	0.50
11:e:253:VAL:O	11:e:257:ARG:N	2.45	0.50
21:q:55:TRP:O	21:q:61:GLN:NE2	2.45	0.50
3:K1:142:VAL:HG22	24:C1:537:ILE:HD13	1.94	0.50
9:c:68:LYS:NZ	10:d:284:GLN:O	2.41	0.49
10:d:280:ILE:O	10:d:280:ILE:HD12	2.12	0.49
23:G1:243:VAL:HG12	23:G1:243:VAL:O	2.12	0.49
6:M1:110:MET:HE1	6:M1:122:VAL:HG21	1.95	0.49
25:D1:181:LEU:HD23	25:D1:359:THR:HB	1.93	0.49
3:K1:163:GLN:O	3:K1:167:THR:HG23	2.12	0.49
24:A1:203:LEU:HD13	24:A1:379:VAL:CG1	2.42	0.49
24:C1:135:VAL:HG12	24:C1:135:VAL:O	2.12	0.49
7:X1:70:GLY:O	7:X1:74:GLY:N	2.43	0.49
23:G1:95:ASP:O	23:G1:98:VAL:HG23	2.13	0.49
12:f:101:ARG:NH1	22:r:45:ASP:O	2.45	0.49
25:D1:448:GLU:O	25:D1:452:GLY:N	2.44	0.49
12:f:67:ASN:ND2	12:f:72:ASP:OD2	2.46	0.48
24:C1:203:LEU:HD11	24:C1:364:VAL:CG2	2.42	0.48
24:A1:327:GLY:N	24:A1:331:TYR:O	2.43	0.48
24:C1:203:LEU:HD13	24:C1:379:VAL:CG1	2.42	0.48
1:H1:61:LEU:N	1:H1:61:LEU:HD12	2.28	0.48
7:X1:65:VAL:HG13	7:X1:101:THR:HG22	1.94	0.48
3:K1:138:CYS:O	3:K1:142:VAL:HG23	2.13	0.48
7:V1:48:GLN:O	7:V1:51:HIS:ND1	2.39	0.48
13:g:58:ALA:HB3	13:g:80:ARG:HB3	1.96	0.47
11:e:201:TYR:O	11:e:205:ILE:N	2.41	0.47
23:G1:5:LEU:C	23:G1:5:LEU:HD23	2.39	0.47
25:E1:350:THR:HG22	25:E1:350:THR:O	2.14	0.47
3:J1:86:LYS:NZ	24:B1:228:GLN:O	2.42	0.47
24:A1:249:ASN:OD1	24:A1:252:ARG:NH2	2.41	0.47
25:D1:105:THR:O	25:D1:105:THR:HG22	2.13	0.47
24:C1:192:THR:HG21	24:C1:477:LEU:HD13	1.96	0.47
7:O1:98:PHE:CD1	7:X1:100:LEU:HD13	2.50	0.47
25:E1:180:GLY:HA3	25:E1:355:LEU:HD13	1.96	0.47
15:i:62:ARG:NH2	18:n:134:SER:O	2.46	0.47
21:q:49:ALA:N	21:q:50:PRO:CD	2.78	0.47
4:L:20:PHE:CE2	4:L:24:LEU:HD11	2.49	0.47
25:E1:60:LEU:HB3	25:E1:102:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J1:117:GLU:O	3:J1:121:THR:HG23	2.14	0.46
5:M:88:TYR:O	5:M:91:GLN:NE2	2.48	0.46
24:A1:203:LEU:HD13	24:A1:379:VAL:HG11	1.96	0.46
25:D1:150:LEU:HD23	25:D1:150:LEU:O	2.15	0.46
12:f:41:LEU:HD23	12:f:45:LEU:HD12	1.98	0.46
5:m:46:HIS:O	5:m:50:GLY:N	2.49	0.46
24:B1:212:LYS:HG2	24:B1:389:LEU:HD12	1.98	0.46
24:B1:91:ALA:N	24:B1:109:ASP:OD1	2.48	0.46
24:B1:212:LYS:N	32:B1:601:ATP:O1B	2.46	0.46
25:D1:116:GLU:OE1	25:D1:116:GLU:N	2.43	0.46
25:D1:137:GLU:OE1	25:D1:137:GLU:N	2.46	0.46
10:d:268:PRO:HB2	11:e:327:ALA:HB3	1.97	0.46
24:A1:82:ILE:HG12	24:A1:120:VAL:HG22	1.98	0.46
1:H1:38:LYS:O	23:G1:201:LEU:HD11	2.16	0.46
3:K1:70:ILE:HG22	3:K1:74:ASN:HD21	1.80	0.46
4:l:10:LEU:HD13	5:m:83:ILE:HD11	1.98	0.46
19:o:86:TYR:O	19:o:91:ARG:NE	2.48	0.46
25:E1:305:VAL:HG21	25:E1:346:PRO:CD	2.46	0.46
25:E1:65:LYS:HG2	25:E1:66:LEU:O	2.16	0.46
24:A1:423:VAL:HG12	24:A1:423:VAL:O	2.16	0.45
7:P1:48:GLN:O	7:P1:51:HIS:ND1	2.49	0.45
26:e:403:CDL:H871	21:q:56:TRP:CZ3	2.51	0.45
24:B1:390:ASP:OD1	24:B1:391:THR:N	2.49	0.45
24:C1:531:PHE:O	24:C1:532:THR:HB	2.15	0.45
3:K1:187:VAL:HG21	24:C1:580:CYS:SG	2.56	0.45
25:F1:162:THR:OG1	25:F1:168:ASP:OD1	2.35	0.45
5:M:103:PHE:CZ	5:M:107:LEU:HD11	2.51	0.45
7:T1:44:ALA:HB1	19:o:100:PHE:CD1	2.52	0.45
24:A1:166:VAL:HG12	24:A1:166:VAL:O	2.17	0.45
25:E1:282:ASP:HA	25:E1:283:ASN:HA	1.81	0.45
5:M:52:ASP:OD2	4:l:12:GLN:NE2	2.48	0.45
24:B1:203:LEU:HD12	24:B1:362:PRO:O	2.17	0.45
11:e:371:THR:HG23	20:p:64:PRO:CG	2.47	0.45
24:C1:141:ASN:OD1	24:C1:145:HIS:N	2.49	0.45
10:d:324:ASN:HB2	10:d:325:PRO:HD3	1.99	0.45
23:G1:127:ILE:N	23:G1:127:ILE:HD12	2.32	0.45
25:D1:180:GLY:HA3	25:D1:355:LEU:HD13	1.99	0.45
3:L1:28:ASP:OD1	3:L1:32:TYR:N	2.50	0.44
24:A1:111:ILE:HD12	24:A1:276:PRO:HB3	1.99	0.44
24:B1:174:VAL:HG12	24:B1:174:VAL:O	2.18	0.44
9:c:43:VAL:HG13	9:c:44:TRP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H1:40:ILE:HG21	7:S1:86:LEU:HB2	1.99	0.44
24:C1:190:VAL:O	24:C1:190:VAL:HG12	2.18	0.44
7:P1:55:THR:HG23	7:P1:112:ALA:HB1	2.00	0.44
9:c:30:GLU:N	9:c:31:PRO:CD	2.81	0.44
24:B1:524:LEU:HD23	24:B1:527:LEU:HD12	1.98	0.44
26:c:201:CDL:H872	26:c:201:CDL:H832	1.99	0.44
23:G1:51:GLU:O	23:G1:55:SER:N	2.44	0.44
5:M:46:HIS:O	5:M:50:GLY:N	2.49	0.44
26:e:402:CDL:H522	16:j:101:VAL:HG22	2.00	0.44
7:R1:86:LEU:HD11	7:S1:84:PRO:HB3	2.00	0.43
24:B1:307:ASP:OD1	24:B1:307:ASP:N	2.49	0.43
25:D1:223:LEU:HD23	25:D1:245:TYR:OH	2.18	0.43
25:E1:414:ILE:O	25:E1:414:ILE:HG22	2.18	0.43
25:F1:165:LYS:NZ	25:F1:486:VAL:O	2.48	0.43
1:H1:129:VAL:HG11	2:I1:28:THR:HG21	2.00	0.43
2:I1:31:LEU:O	2:I1:34:THR:OG1	2.34	0.43
7:T1:86:LEU:HD22	7:U1:84:PRO:HB3	1.99	0.43
3:K1:70:ILE:HG22	3:K1:74:ASN:ND2	2.32	0.43
7:O1:65:VAL:HG13	7:O1:101:THR:HG22	2.00	0.43
24:A1:188:LYS:NZ	24:A1:461:LEU:O	2.51	0.43
2:I1:70:ILE:N	2:I1:70:ILE:HD12	2.33	0.43
10:d:321:ALA:O	10:d:325:PRO:HD2	2.17	0.43
5:m:88:TYR:O	5:m:91:GLN:NE2	2.52	0.43
18:n:105:GLU:OE2	18:n:109:ARG:NH2	2.47	0.43
23:G1:78:THR:HG22	23:G1:80:ARG:H	1.84	0.43
13:g:55:VAL:HG12	13:g:219:THR:HG22	2.00	0.43
24:C1:65:LEU:HD22	24:C1:120:VAL:HG21	2.00	0.43
7:Q1:55:THR:HG23	7:Q1:112:ALA:HB1	1.99	0.43
10:d:324:ASN:CB	10:d:325:PRO:HD3	2.48	0.43
24:A1:531:PHE:O	24:A1:532:THR:CB	2.66	0.43
3:K1:185:VAL:HG23	3:K1:185:VAL:O	2.18	0.43
11:e:259:HIS:ND1	11:e:289:MET:HE1	2.33	0.43
11:e:26:THR:HG23	11:e:91:TYR:OH	2.19	0.43
15:i:49:GLU:O	15:i:53:GLY:N	2.48	0.43
23:G1:90:ILE:HD11	23:G1:162:ASN:HD21	1.84	0.43
1:H1:60:PHE:CE2	23:G1:42:THR:HA	2.54	0.42
13:g:57:THR:HG21	13:g:124:VAL:HG11	2.01	0.42
24:B1:52:ILE:C	24:B1:52:ILE:HD12	2.44	0.42
3:J1:59:VAL:O	3:J1:63:VAL:HG23	2.19	0.42
23:G1:76:ILE:O	23:G1:90:ILE:HD13	2.19	0.42
24:A1:68:ALA:HB3	24:A1:72:PRO:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H1:167:ILE:HD11	2:I1:13:TRP:CD1	2.53	0.42
24:B1:537:ILE:N	24:B1:537:ILE:HD12	2.34	0.42
24:C1:193:MET:HE1	24:C1:428:LYS:CD	2.49	0.42
25:E1:30:HIS:CD2	25:E1:30:HIS:N	2.87	0.42
8:a:147:LEU:HD22	8:a:213:PHE:CD2	2.54	0.42
5:m:119:ARG:NH2	5:m:122:ILE:O	2.52	0.42
24:B1:192:THR:HG22	24:B1:420:MET:SD	2.60	0.42
25:D1:189:LYS:N	32:D1:601:ATP:O1B	2.46	0.42
25:D1:486:VAL:HG21	25:D1:492:VAL:HG22	2.02	0.42
25:E1:73:THR:O	25:E1:73:THR:HG23	2.20	0.42
3:L1:45:ILE:HG13	3:L1:57:VAL:HG11	2.02	0.42
10:d:17:ILE:HB	10:d:179:TYR:O	2.20	0.42
16:j:5:GLU:OE1	16:j:5:GLU:N	2.46	0.42
25:D1:403:MET:HE1	25:D1:432:ARG:HB3	2.01	0.42
25:F1:244:VAL:HG12	25:F1:258:VAL:HG23	2.01	0.42
6:M1:66:ILE:HD12	6:M1:66:ILE:H	1.84	0.42
11:e:378:ARG:HH22	20:p:63:ASP:CG	2.27	0.42
26:q:102:CDL:OB7	26:q:102:CDL:CB3	2.66	0.42
8:a:148:PHE:CZ	8:a:152:LEU:HD22	2.55	0.42
10:d:117:GLU:O	10:d:218:ARG:NH1	2.53	0.42
25:D1:233:ILE:HD11	25:D1:243:LEU:HD11	2.02	0.42
7:S1:114:LEU:HD21	9:c:29:LEU:HD11	2.00	0.42
10:d:157:ARG:NH1	10:d:203:LEU:O	2.50	0.42
11:e:368:GLU:OE2	20:p:39:GLN:N	2.49	0.42
4:l:20:PHE:CE2	4:l:24:LEU:HD11	2.55	0.42
24:C1:423:VAL:HG12	24:C1:423:VAL:O	2.20	0.42
24:C1:457:ARG:NH2	24:C1:488:VAL:O	2.45	0.42
25:E1:270:ARG:NH1	25:E1:323:THR:O	2.52	0.42
25:F1:263:LEU:HD21	25:F1:321:ARG:CB	2.47	0.42
25:F1:282:ASP:HA	25:F1:283:ASN:HA	1.83	0.42
7:W1:84:PRO:O	7:W1:87:THR:HG23	2.19	0.42
13:g:56:HIS:NE2	13:g:219:THR:O	2.52	0.42
25:D1:282:ASP:HA	25:D1:283:ASN:HA	1.83	0.42
2:I1:24:LEU:O	2:I1:28:THR:HG23	2.19	0.42
14:h:24:MET:SD	14:h:24:MET:N	2.93	0.42
16:j:30:GLU:OE1	21:q:72:ASN:ND2	2.53	0.42
24:A1:531:PHE:O	24:A1:532:THR:HB	2.19	0.42
8:a:85:LEU:HD22	8:a:147:LEU:HD23	2.02	0.41
14:h:67:LEU:O	14:h:72:GLN:NE2	2.53	0.41
17:k:103:MET:HE1	21:q:80:LEU:O	2.19	0.41
24:B1:203:LEU:HD11	24:B1:364:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:64:ARG:NH1	22:r:33:GLU:OE1	2.48	0.41
24:B1:131:VAL:HG11	24:B1:293:TYR:HB2	2.01	0.41
25:D1:311:LEU:HD23	25:D1:311:LEU:O	2.20	0.41
7:P1:86:LEU:HD11	7:Q1:84:PRO:HB3	2.01	0.41
13:g:57:THR:HB	13:g:218:HIS:HB2	2.02	0.41
15:i:90:THR:O	19:o:36:ARG:NH2	2.53	0.41
25:D1:287:PHE:O	25:D1:291:ASN:ND2	2.45	0.41
25:D1:311:LEU:HD23	25:D1:311:LEU:C	2.45	0.41
10:d:97:MET:HE2	10:d:102:LEU:HA	2.02	0.41
13:g:196:VAL:HG12	13:g:197:ALA:N	2.35	0.41
25:F1:436:LEU:HD23	25:F1:470:LEU:HD23	2.02	0.41
7:P1:45:ILE:HD12	7:Q1:45:ILE:HG23	2.02	0.41
13:g:138:VAL:HG21	13:g:188:LEU:HD22	2.03	0.41
13:g:269:LEU:HD12	13:g:269:LEU:C	2.44	0.41
10:d:87:LEU:HD22	10:d:247:GLN:HE22	1.86	0.41
25:E1:263:LEU:HD21	25:E1:321:ARG:HB2	2.02	0.41
11:e:352:PHE:CE2	11:e:356:LEU:HD11	2.56	0.41
24:B1:511:THR:O	24:B1:511:THR:HG22	2.21	0.41
25:D1:263:LEU:HD21	25:D1:321:ARG:HB2	2.03	0.41
25:E1:56:VAL:HG12	25:E1:57:LEU:N	2.36	0.41
25:E1:263:LEU:HD21	25:E1:321:ARG:CB	2.51	0.41
7:O1:41:SER:O	7:P1:44:ALA:HB3	2.20	0.41
8:a:103:LEU:HD21	11:e:59:TYR:CG	2.55	0.41
24:A1:433:GLU:HG2	24:A1:437:LEU:HD13	2.02	0.41
1:H1:56:ARG:O	1:H1:57:GLN:C	2.63	0.41
1:H1:87:TYR:CD2	23:G1:201:LEU:HB3	2.55	0.41
1:H1:97:LEU:HD23	1:H1:97:LEU:C	2.46	0.41
6:M1:90:VAL:CG2	6:M1:108:VAL:HG22	2.51	0.41
13:g:60:THR:HG22	13:g:78:VAL:O	2.21	0.41
14:h:134:GLU:O	14:h:138:ALA:N	2.54	0.41
25:D1:81:ASP:OD1	25:D1:84:THR:N	2.42	0.41
25:D1:150:LEU:HD23	25:D1:150:LEU:C	2.46	0.41
25:F1:347:ALA:HB3	25:F1:348:PRO:CD	2.51	0.41
3:K1:135:LEU:HD11	24:C1:523:GLU:HG3	2.03	0.41
15:i:16:LEU:O	15:i:20:THR:HG22	2.21	0.41
25:D1:356:ASP:OD1	25:D1:356:ASP:N	2.54	0.41
25:E1:66:LEU:HD12	25:E1:95:LEU:O	2.20	0.41
25:E1:170:ILE:N	25:E1:170:ILE:HD12	2.35	0.41
13:g:151:ASN:OD1	13:g:152:GLU:N	2.54	0.40
13:g:174:THR:HG23	13:g:175:ALA:N	2.36	0.40
24:A1:100:ASP:OD1	24:A1:101:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B1:495:PHE:CE2	24:B1:499:LEU:HD11	2.55	0.40
24:C1:327:GLY:N	24:C1:331:TYR:O	2.50	0.40
7:O1:73:PHE:CZ	7:X1:100:LEU:HD12	2.56	0.40
7:U1:55:THR:HG23	7:U1:112:ALA:HB1	2.03	0.40
11:e:15:PHE:CE2	11:e:19:LEU:HD11	2.55	0.40
26:e:402:CDL:H861	26:e:403:CDL:H673	2.03	0.40
13:g:168:THR:HG22	13:g:169:THR:N	2.37	0.40
24:C1:193:MET:HE1	24:C1:428:LYS:HD3	2.03	0.40
24:C1:328:ARG:NH2	25:D1:345:ASP:OD1	2.55	0.40
8:a:26:LEU:O	9:c:67:ASN:ND2	2.53	0.40
24:A1:419:ALA:HA	24:A1:532:THR:HG23	2.03	0.40
24:B1:174:VAL:HG21	25:F1:130:ASP:HA	2.02	0.40
13:g:59:VAL:HG23	13:g:79:VAL:HG22	2.03	0.40
18:n:63:SER:O	18:n:64:TYR:C	2.64	0.40
24:C1:52:ILE:HG21	24:C1:122:ALA:HB2	2.04	0.40
3:J1:143:MET:O	3:J1:147:CYS:N	2.53	0.40
7:O1:84:PRO:HB3	7:X1:86:LEU:HD11	2.04	0.40
26:j:201:CDL:H1O1	17:k:68:ARG:HH22	1.65	0.40
25:D1:187:VAL:O	25:D1:187:VAL:HG12	2.21	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	H1	159/182 (87%)	156 (98%)	3 (2%)	0	100	100
2	I1	63/75 (84%)	61 (97%)	2 (3%)	0	100	100
3	J1	164/188 (87%)	161 (98%)	3 (2%)	0	100	100
3	K1	164/188 (87%)	163 (99%)	1 (1%)	0	100	100
3	L1	163/188 (87%)	162 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	63/92 (68%)	63 (100%)	0	0	100	100
4	l	63/92 (68%)	63 (100%)	0	0	100	100
5	M	127/144 (88%)	127 (100%)	0	0	100	100
5	m	127/144 (88%)	127 (100%)	0	0	100	100
6	M1	230/255 (90%)	226 (98%)	4 (2%)	0	100	100
7	O1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
7	P1	76/118 (64%)	76 (100%)	0	0	100	100
7	Q1	76/118 (64%)	76 (100%)	0	0	100	100
7	R1	76/118 (64%)	76 (100%)	0	0	100	100
7	S1	76/118 (64%)	76 (100%)	0	0	100	100
7	T1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
7	U1	76/118 (64%)	74 (97%)	1 (1%)	1 (1%)	9	41
7	V1	76/118 (64%)	76 (100%)	0	0	100	100
7	W1	76/118 (64%)	76 (100%)	0	0	100	100
7	X1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
8	a	229/231 (99%)	224 (98%)	5 (2%)	0	100	100
9	c	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
10	d	328/370 (89%)	323 (98%)	5 (2%)	0	100	100
11	e	381/396 (96%)	377 (99%)	4 (1%)	0	100	100
12	f	133/145 (92%)	130 (98%)	3 (2%)	0	100	100
13	g	266/269 (99%)	264 (99%)	2 (1%)	0	100	100
14	h	135/157 (86%)	133 (98%)	2 (2%)	0	100	100
15	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
16	j	166/169 (98%)	161 (97%)	5 (3%)	0	100	100
17	k	103/124 (83%)	99 (96%)	4 (4%)	0	100	100
18	n	137/156 (88%)	130 (95%)	7 (5%)	0	100	100
19	o	94/101 (93%)	93 (99%)	1 (1%)	0	100	100
20	p	78/105 (74%)	77 (99%)	1 (1%)	0	100	100
21	q	83/98 (85%)	81 (98%)	2 (2%)	0	100	100
22	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
23	G1	298/305 (98%)	292 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	A1	517/584 (88%)	509 (98%)	8 (2%)	0	100	100
24	B1	525/584 (90%)	515 (98%)	10 (2%)	0	100	100
24	C1	518/584 (89%)	507 (98%)	11 (2%)	0	100	100
25	D1	486/519 (94%)	476 (98%)	10 (2%)	0	100	100
25	E1	484/519 (93%)	474 (98%)	10 (2%)	0	100	100
25	F1	486/519 (94%)	473 (97%)	13 (3%)	0	100	100
All	All	7775/8943 (87%)	7644 (98%)	130 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	U1	87	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	H1	137/156 (88%)	136 (99%)	1 (1%)	76	79
2	I1	58/67 (87%)	58 (100%)	0	100	100
3	J1	145/162 (90%)	145 (100%)	0	100	100
3	K1	145/162 (90%)	145 (100%)	0	100	100
3	L1	145/162 (90%)	145 (100%)	0	100	100
4	L	55/75 (73%)	55 (100%)	0	100	100
4	l	55/75 (73%)	55 (100%)	0	100	100
5	M	111/124 (90%)	111 (100%)	0	100	100
5	m	111/124 (90%)	111 (100%)	0	100	100
6	M1	200/215 (93%)	199 (100%)	1 (0%)	81	81
7	O1	56/89 (63%)	56 (100%)	0	100	100
7	P1	56/89 (63%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Q1	56/89 (63%)	56 (100%)	0	100	100
7	R1	56/89 (63%)	56 (100%)	0	100	100
7	S1	56/89 (63%)	56 (100%)	0	100	100
7	T1	56/89 (63%)	56 (100%)	0	100	100
7	U1	56/89 (63%)	55 (98%)	1 (2%)	51	67
7	V1	56/89 (63%)	56 (100%)	0	100	100
7	W1	56/89 (63%)	56 (100%)	0	100	100
7	X1	56/89 (63%)	56 (100%)	0	100	100
8	a	225/225 (100%)	224 (100%)	1 (0%)	84	82
9	c	80/104 (77%)	80 (100%)	0	100	100
10	d	297/334 (89%)	296 (100%)	1 (0%)	86	84
11	e	334/341 (98%)	334 (100%)	0	100	100
12	f	119/124 (96%)	118 (99%)	1 (1%)	73	77
13	g	205/206 (100%)	205 (100%)	0	100	100
14	h	110/123 (89%)	110 (100%)	0	100	100
15	i	95/96 (99%)	95 (100%)	0	100	100
16	j	149/150 (99%)	149 (100%)	0	100	100
17	k	91/107 (85%)	91 (100%)	0	100	100
18	n	123/137 (90%)	122 (99%)	1 (1%)	73	77
19	o	82/86 (95%)	82 (100%)	0	100	100
20	p	75/94 (80%)	75 (100%)	0	100	100
21	q	80/92 (87%)	80 (100%)	0	100	100
22	r	56/56 (100%)	56 (100%)	0	100	100
23	G1	253/257 (98%)	253 (100%)	0	100	100
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%)	396 (100%)	1 (0%)	86	84
25	F1	399/420 (95%)	399 (100%)	0	100	100
All	All	6599/7441 (89%)	6587 (100%)	12 (0%)	85	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H1	57	GLN
6	M1	247	ASP
7	U1	87	THR
8	a	144	PHE
10	d	138	VAL
12	f	42	ASN
18	n	105	GLU
24	B1	74	VAL
24	B1	111	ILE
25	D1	66	LEU
25	D1	171	LEU
25	E1	30	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	H1	33	HIS
3	J1	82	GLN
3	J1	172	HIS
3	K1	74	ASN
3	K1	132	GLN
3	K1	175	HIS
8	a	155	HIS
11	e	41	GLN
12	f	38	ASN
12	f	42	ASN
13	g	143	GLN
13	g	218	HIS
4	l	11	HIS
18	n	89	GLN
18	n	91	HIS
19	o	25	HIS
20	p	95	GLN
23	G1	136	HIS
23	G1	162	ASN
23	G1	233	ASN
24	A1	71	ASN
24	A1	115	GLN
24	A1	296	ASN
24	A1	339	HIS
24	A1	539	HIS

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Mol	Chain	Res	Type
24	A1	558	GLN
24	B1	56	HIS
24	B1	254	HIS
24	B1	296	ASN
24	B1	339	HIS
24	B1	398	GLN
24	B1	417	ASN
24	B1	463	ASN
24	B1	551	HIS
24	C1	228	GLN
24	C1	245	GLN
24	C1	463	ASN
25	D1	39	GLN
25	D1	144	HIS
25	D1	204	HIS
25	D1	490	ASN
25	E1	30	HIS
25	E1	39	GLN
25	E1	79	HIS
25	E1	83	HIS
25	F1	30	HIS
25	F1	36	HIS
25	F1	78	GLN
25	F1	398	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
11	AME	e	1	11	9,10,11	0.26	0	9,11,13	0.45	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
11	AME	e	1	11	-	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
11	e	1	AME	N-CA-CB-CG
11	e	1	AME	C-CA-N-CT1
11	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
11	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	$\# Z > 2$
28	LMT	e	406	-	36,36,36	0.10	0	47,47,47	0.16	0
26	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	e	405	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.27	0
29	Q7G	e	407	-	54,54,90	0.13	0	80,84,138	0.25	0
32	ATP	C1	601	33	32,33,33	0.28	0	48,52,52	0.29	0
26	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.26	0
30	PC1	f	203	-	53,53,53	0.27	0	59,61,61	0.30	0
34	ADP	E1	601	33	28,29,29	0.41	0	43,45,45	0.49	0
26	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	q	102	-	99,99,99	0.29	0	105,111,111	0.28	0
30	PC1	p	201	-	53,53,53	0.28	0	59,61,61	0.29	0
26	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.26	0
32	ATP	A1	601	33	32,33,33	0.28	0	48,52,52	0.29	0
31	UTP	G1	401	-	29,30,30	0.29	0	43,47,47	0.30	0
26	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	e	403	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	m	202	-	99,99,99	0.29	0	105,111,111	0.25	0
27	PEE	M	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.49	0
26	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.25	0
29	Q7G	n	201	-	66,66,90	0.13	0	98,102,138	0.29	0
27	PEE	m	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.48	0
28	LMT	j	203	-	36,36,36	0.11	0	47,47,47	0.18	0
30	PC1	j	202	-	53,53,53	0.28	0	59,61,61	0.27	0
26	CDL	M	201	-	99,99,99	0.29	0	105,111,111	0.34	1 (0%)
32	ATP	B1	601	33	32,33,33	0.28	0	48,52,52	0.28	0
26	CDL	L	101	-	99,99,99	0.29	0	105,111,111	0.25	0
30	PC1	i	201	-	53,53,53	0.29	0	59,61,61	0.28	0
27	PEE	f	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.47	0
32	ATP	D1	601	33	32,33,33	0.28	0	48,52,52	0.28	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
28	LMT	e	406	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	l	101	-	-	19/110/110/110	-
26	CDL	e	405	-	-	32/110/110/110	-
29	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
26	CDL	f	201	-	-	21/110/110/110	-
32	ATP	C1	601	33	-	8/22/38/38	0/3/3/3
26	CDL	e	402	-	-	22/110/110/110	-
30	PC1	f	203	-	-	12/57/57/57	-
34	ADP	E1	601	33	-	1/16/32/32	0/3/3/3
26	CDL	q	101	-	-	30/110/110/110	-
26	CDL	q	102	-	-	24/110/110/110	-
30	PC1	p	201	-	-	10/57/57/57	-
26	CDL	e	404	-	-	19/110/110/110	-
32	ATP	A1	601	33	-	6/22/38/38	0/3/3/3
31	UTP	G1	401	-	-	0/22/38/38	0/2/2/2
26	CDL	e	401	-	-	24/110/110/110	-
26	CDL	e	403	-	-	25/110/110/110	-
26	CDL	c	201	-	-	25/110/110/110	-
26	CDL	m	202	-	-	28/110/110/110	-
27	PEE	M	202	-	-	25/54/54/54	-
29	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
26	CDL	j	201	-	-	24/110/110/110	-
27	PEE	m	201	-	-	23/54/54/54	-
28	LMT	j	203	-	-	5/21/61/61	0/2/2/2
30	PC1	j	202	-	-	15/57/57/57	-
26	CDL	M	201	-	-	27/110/110/110	-
32	ATP	B1	601	33	-	6/22/38/38	0/3/3/3
26	CDL	L	101	-	-	17/110/110/110	-
30	PC1	i	201	-	-	9/57/57/57	-
27	PEE	f	202	-	-	17/54/54/54	-
32	ATP	D1	601	33	-	3/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	202	PEE	C39-C38	3.66	1.52	1.31
27	m	201	PEE	C18-C19	3.66	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	202	PEE	C18-C19	3.64	1.52	1.31
27	f	202	PEE	C18-C19	3.63	1.52	1.31
27	m	201	PEE	C39-C38	3.58	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	2.38	129.44	113.36

All (3) chirality outliers are listed below:

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

All (489) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	L	101	CDL	CA2-OA2-PA1-OA3
26	L	101	CDL	CA2-OA2-PA1-OA4
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	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	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

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Mol	Chain	Res	Type	Atoms
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	e	405	CDL	OB5-CB3-CB4-OB6
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	l	101	CDL	CA2-OA2-PA1-OA3
26	l	101	CDL	CA2-OA2-PA1-OA4
26	l	101	CDL	CA2-OA2-PA1-OA5
26	l	101	CDL	CA3-OA5-PA1-OA2
26	m	202	CDL	CA2-C1-CB2-OB2
26	m	202	CDL	CA3-OA5-PA1-OA2
26	m	202	CDL	CA3-OA5-PA1-OA3
26	m	202	CDL	OA6-CA4-CA6-OA8
26	m	202	CDL	CB2-OB2-PB2-OB4
26	m	202	CDL	CB2-OB2-PB2-OB5
26	m	202	CDL	C51-CB5-OB6-CB4
26	q	101	CDL	CA2-OA2-PA1-OA4
26	q	101	CDL	CB3-OB5-PB2-OB2
26	q	101	CDL	CB3-OB5-PB2-OB4
26	q	102	CDL	CA2-C1-CB2-OB2
26	q	102	CDL	OA5-CA3-CA4-OA6
26	q	102	CDL	CB3-OB5-PB2-OB2
26	q	102	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-O2P
27	M	202	PEE	O4P-C4-C5-N
27	f	202	PEE	C4-O4P-P-O2P
27	f	202	PEE	C4-O4P-P-O1P
27	m	201	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
27	m	201	PEE	C1-O3P-P-O4P
27	m	201	PEE	C4-O4P-P-O2P
27	m	201	PEE	O4P-C4-C5-N
28	j	203	LMT	C2'-C1'-O1'-C1
28	j	203	LMT	O5'-C1'-O1'-C1
28	j	203	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	202	PC1	C11-O13-P-O14
30	j	202	PC1	C11-O13-P-O11
30	j	202	PC1	C1-O11-P-O12
30	j	202	PC1	C1-O11-P-O14
30	j	202	PC1	C1-O11-P-O13
30	p	201	PC1	C11-O13-P-O12
30	p	201	PC1	C11-O13-P-O11
32	A1	601	ATP	PB-O3B-PG-O2G
32	B1	601	ATP	PB-O3B-PG-O2G
32	C1	601	ATP	PB-O3B-PG-O2G
26	M	201	CDL	OB7-CB5-OB6-CB4
26	m	202	CDL	OB7-CB5-OB6-CB4
26	M	201	CDL	O1-C1-CB2-OB2
26	e	404	CDL	O1-C1-CA2-OA2
26	m	202	CDL	O1-C1-CB2-OB2
26	q	102	CDL	O1-C1-CB2-OB2
29	e	407	Q7G	O5B-C1B-O1B-C24
29	n	201	Q7G	O5B-C1B-O1B-C24
27	m	201	PEE	C31-C30-O3-C3
26	e	403	CDL	C11-CA5-OA6-CA4
26	e	402	CDL	C31-CA7-OA8-CA6
29	e	407	Q7G	C2B-C1B-O1B-C24
29	n	201	Q7G	C2B-C1B-O1B-C24
26	l	101	CDL	O1-C1-CA2-OA2
27	M	202	PEE	C31-C30-O3-C3
26	M	201	CDL	CA5-C11-C12-C13
26	m	202	CDL	CA5-C11-C12-C13
26	e	402	CDL	OA9-CA7-OA8-CA6
26	e	403	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
27	m	201	PEE	O5-C30-O3-C3
27	M	202	PEE	O5-C30-O3-C3
26	e	403	CDL	C51-CB5-OB6-CB4
26	q	102	CDL	C11-CA5-OA6-CA4
26	e	403	CDL	OB7-CB5-OB6-CB4
26	q	102	CDL	OA7-CA5-OA6-CA4
29	e	407	Q7G	CG1-C22-C23-C48
26	e	404	CDL	O1-C1-CB2-OB2
26	q	101	CDL	C78-C79-C80-C81
27	m	201	PEE	C17-C18-C19-C20
26	j	201	CDL	C13-C14-C15-C16
28	e	406	LMT	C2-C1-O1'-C1'
26	q	101	CDL	C74-C75-C76-C77
26	e	405	CDL	C11-CA5-OA6-CA4
26	q	101	CDL	C11-CA5-OA6-CA4
26	c	201	CDL	O1-C1-CA2-OA2
26	e	403	CDL	O1-C1-CA2-OA2
26	q	101	CDL	O1-C1-CB2-OB2
26	q	102	CDL	CA5-C11-C12-C13
26	q	101	CDL	CA2-C1-CB2-OB2
27	M	202	PEE	C31-C32-C33-C34
26	e	403	CDL	C71-C72-C73-C74
26	e	405	CDL	OA7-CA5-OA6-CA4
26	q	101	CDL	OA7-CA5-OA6-CA4
26	e	405	CDL	CA7-C31-C32-C33
26	c	201	CDL	C55-C56-C57-C58
26	f	201	CDL	O1-C1-CB2-OB2
26	L	101	CDL	C11-CA5-OA6-CA4
26	e	404	CDL	C11-CA5-OA6-CA4
26	q	101	CDL	C51-CB5-OB6-CB4
27	f	202	PEE	C11-C10-O2-C2
30	f	203	PC1	C22-C21-O21-C2
30	f	203	PC1	O22-C21-O21-C2
26	M	201	CDL	C12-C13-C14-C15
26	L	101	CDL	C31-CA7-OA8-CA6
27	M	202	PEE	C17-C18-C19-C20
26	e	401	CDL	C77-C78-C79-C80
26	j	201	CDL	C81-C82-C83-C84
26	M	201	CDL	C73-C74-C75-C76
28	j	203	LMT	O5B-C5B-C6B-O6B
26	e	403	CDL	C14-C15-C16-C17
26	j	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	m	202	CDL	C73-C74-C75-C76
29	n	201	Q7G	O5C-C5C-C6C-O6C
26	m	202	CDL	C12-C13-C14-C15
26	j	201	CDL	CA4-CA3-OA5-PA1
26	q	101	CDL	C15-C16-C17-C18
26	e	404	CDL	CB2-C1-CA2-OA2
26	e	404	CDL	CA2-C1-CB2-OB2
27	f	202	PEE	C42-C43-C44-C45
26	e	404	CDL	C17-C18-C19-C20
26	c	201	CDL	C34-C35-C36-C37
26	e	405	CDL	C57-C58-C59-C60
26	M	201	CDL	OA5-CA3-CA4-CA6
26	c	201	CDL	OA5-CA3-CA4-CA6
26	q	102	CDL	OA5-CA3-CA4-CA6
26	e	404	CDL	OA7-CA5-OA6-CA4
27	f	202	PEE	O4-C10-O2-C2
27	m	201	PEE	C31-C32-C33-C34
26	l	101	CDL	C31-CA7-OA8-CA6
30	i	201	PC1	C32-C31-O31-C3
26	e	402	CDL	C81-C82-C83-C84
26	M	201	CDL	CA3-CA4-CA6-OA8
26	e	403	CDL	CB3-CB4-CB6-OB8
26	q	101	CDL	CB3-CB4-CB6-OB8
27	M	202	PEE	C1-C2-C3-O3
30	p	201	PC1	C1-C2-C3-O31
26	e	403	CDL	C17-C18-C19-C20
26	j	201	CDL	C62-C63-C64-C65
26	m	202	CDL	C78-C79-C80-C81
26	L	101	CDL	OA9-CA7-OA8-CA6
26	e	405	CDL	CA4-CA3-OA5-PA1
26	e	401	CDL	C56-C57-C58-C59
26	j	201	CDL	C34-C35-C36-C37
26	e	402	CDL	C11-C12-C13-C14
26	c	201	CDL	CB2-C1-CA2-OA2
26	M	201	CDL	OA5-CA3-CA4-OA6
26	e	405	CDL	OA5-CA3-CA4-OA6
26	j	201	CDL	OB5-CB3-CB4-OB6
26	m	202	CDL	OA5-CA3-CA4-OA6
26	e	403	CDL	C78-C79-C80-C81
26	q	102	CDL	CB7-C71-C72-C73
26	M	201	CDL	C78-C79-C80-C81
26	e	402	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
26	l	101	CDL	C14-C15-C16-C17
26	e	403	CDL	OB6-CB4-CB6-OB8
26	f	201	CDL	OB6-CB4-CB6-OB8
26	j	201	CDL	O1-C1-CA2-OA2
26	e	401	CDL	C18-C19-C20-C21
26	c	201	CDL	CA4-CA6-OA8-CA7
32	D1	601	ATP	PG-O3B-PB-O1B
26	l	101	CDL	C11-CA5-OA6-CA4
26	c	201	CDL	C39-C40-C41-C42
26	L	101	CDL	OA7-CA5-OA6-CA4
26	q	101	CDL	OB7-CB5-OB6-CB4
26	c	201	CDL	CA4-CA3-OA5-PA1
26	q	102	CDL	C1-CB2-OB2-PB2
27	m	201	PEE	C2-C1-O3P-P
26	l	101	CDL	OA9-CA7-OA8-CA6
26	L	101	CDL	C14-C15-C16-C17
26	e	405	CDL	OB5-CB3-CB4-CB6
30	p	201	PC1	C22-C21-O21-C2
30	i	201	PC1	O32-C31-O31-C3
26	c	201	CDL	C51-C52-C53-C54
27	M	202	PEE	C22-C23-C24-C25
26	f	201	CDL	C77-C78-C79-C80
27	m	201	PEE	C22-C23-C24-C25
26	c	201	CDL	CA3-CA4-CA6-OA8
26	e	404	CDL	CB3-CB4-CB6-OB8
26	m	202	CDL	CA3-CA4-CA6-OA8
27	m	201	PEE	C1-C2-C3-O3
26	e	405	CDL	C76-C77-C78-C79
26	c	201	CDL	OA5-CA3-CA4-OA6
26	f	201	CDL	OA5-CA3-CA4-OA6
26	q	101	CDL	OA5-CA3-CA4-OA6
30	i	201	PC1	C2C-C2D-C2E-C2F
26	L	101	CDL	CA4-CA3-OA5-PA1
26	f	201	CDL	CB4-CB3-OB5-PB2
26	l	101	CDL	CA4-CA3-OA5-PA1
27	M	202	PEE	C2-C1-O3P-P
29	n	201	Q7G	C24-C23-C48-O1C
26	e	402	CDL	C75-C76-C77-C78
26	L	101	CDL	OA6-CA4-CA6-OA8
26	e	404	CDL	OB6-CB4-CB6-OB8
26	l	101	CDL	OA6-CA4-CA6-OA8
27	f	202	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	p	201	PC1	O21-C2-C3-O31
29	e	407	Q7G	CG1-C22-C23-C24
26	m	202	CDL	C21-C22-C23-C24
26	e	402	CDL	C11-CA5-OA6-CA4
26	q	101	CDL	C79-C80-C81-C82
26	e	405	CDL	OA5-CA3-CA4-CA6
26	m	202	CDL	OA5-CA3-CA4-CA6
26	q	101	CDL	OA5-CA3-CA4-CA6
26	e	405	CDL	C78-C79-C80-C81
26	q	101	CDL	C72-C73-C74-C75
26	l	101	CDL	OA7-CA5-OA6-CA4
29	n	201	Q7G	C16-C17-O20-CG1
29	n	201	Q7G	C18-C17-O20-CG1
26	c	201	CDL	CA5-C11-C12-C13
26	e	402	CDL	CA6-CA4-OA6-CA5
26	q	101	CDL	CB3-CB4-OB6-CB5
26	q	102	CDL	CB3-CB4-OB6-CB5
27	f	202	PEE	C31-C30-O3-C3
26	M	201	CDL	C21-C22-C23-C24
26	e	405	CDL	CB3-CB4-CB6-OB8
27	f	202	PEE	C1-C2-C3-O3
30	f	203	PC1	C1-C2-C3-O31
26	e	403	CDL	C62-C63-C64-C65
26	l	101	CDL	C31-C32-C33-C34
26	c	201	CDL	OA6-CA4-CA6-OA8
26	q	101	CDL	OB6-CB4-CB6-OB8
30	f	203	PC1	O21-C2-C3-O31
26	L	101	CDL	C31-C32-C33-C34
30	j	202	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
26	f	201	CDL	C12-C13-C14-C15
26	e	402	CDL	OA7-CA5-OA6-CA4
30	p	201	PC1	O22-C21-O21-C2
26	j	201	CDL	CB2-C1-CA2-OA2
30	f	203	PC1	C32-C31-O31-C3
27	f	202	PEE	O5-C30-O3-C3
30	j	202	PC1	C3C-C3D-C3E-C3F
26	e	402	CDL	C74-C75-C76-C77
26	c	201	CDL	C83-C84-C85-C86
26	e	405	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
30	f	203	PC1	O32-C31-O31-C3
30	j	202	PC1	O11-C1-C2-C3
26	L	101	CDL	O1-C1-CA2-OA2
26	e	402	CDL	CA4-CA3-OA5-PA1
26	j	201	CDL	C1-CB2-OB2-PB2
26	q	101	CDL	CB4-CB3-OB5-PB2
26	e	404	CDL	OA5-CA3-CA4-OA6
26	q	102	CDL	OB5-CB3-CB4-OB6
30	j	202	PC1	O11-C1-C2-O21
27	M	202	PEE	C11-C10-O2-C2
26	q	102	CDL	C77-C78-C79-C80
27	m	201	PEE	C36-C37-C38-C39
26	q	101	CDL	C76-C77-C78-C79
26	e	405	CDL	OB6-CB4-CB6-OB8
27	M	202	PEE	O2-C2-C3-O3
27	m	201	PEE	O2-C2-C3-O3
26	M	201	CDL	C42-C43-C44-C45
29	e	407	Q7G	C23-C24-O1B-C1B
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	CA3-OA5-PA1-OA2
26	e	401	CDL	CB3-OB5-PB2-OB4
26	e	403	CDL	CB2-OB2-PB2-OB3
26	e	403	CDL	CB3-OB5-PB2-OB3
26	e	405	CDL	CB3-OB5-PB2-OB3
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	202	CDL	CA3-OA5-PA1-OA4
26	m	202	CDL	CB3-OB5-PB2-OB3
26	q	101	CDL	CA2-OA2-PA1-OA5
26	q	102	CDL	CA2-OA2-PA1-OA5
26	q	102	CDL	CA3-OA5-PA1-OA3
26	q	102	CDL	CB2-OB2-PB2-OB3
26	q	102	CDL	CB2-OB2-PB2-OB4
26	q	102	CDL	CB2-OB2-PB2-OB5
27	M	202	PEE	C4-O4P-P-O3P
27	M	202	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
27	f	202	PEE	C1-O3P-P-O1P
27	f	202	PEE	C4-O4P-P-O3P
27	m	201	PEE	C4-O4P-P-O3P
27	m	201	PEE	C4-O4P-P-O1P
30	j	202	PC1	C11-O13-P-O12
30	p	201	PC1	C1-O11-P-O12
30	p	201	PC1	C1-O11-P-O14
30	p	201	PC1	C1-O11-P-O13
32	A1	601	ATP	C5'-O5'-PA-O1A
32	B1	601	ATP	C5'-O5'-PA-O1A
32	C1	601	ATP	C5'-O5'-PA-O1A
30	j	202	PC1	C2-C1-O11-P
26	q	101	CDL	C61-C62-C63-C64
26	j	201	CDL	C72-C73-C74-C75
32	D1	601	ATP	PB-O3B-PG-O1G
34	E1	601	ADP	PA-O3A-PB-O1B
26	e	404	CDL	CA6-CA4-OA6-CA5
26	j	201	CDL	C55-C56-C57-C58
26	j	201	CDL	OB5-CB3-CB4-CB6
26	e	402	CDL	C52-C51-CB5-OB6
26	e	401	CDL	C13-C14-C15-C16
26	f	201	CDL	CB3-CB4-CB6-OB8
32	A1	601	ATP	PA-O3A-PB-O2B
32	B1	601	ATP	PA-O3A-PB-O2B
32	D1	601	ATP	PG-O3B-PB-O2B
26	m	202	CDL	C33-C34-C35-C36
27	f	202	PEE	C18-C19-C20-C21
26	M	201	CDL	C33-C34-C35-C36
26	e	401	CDL	C81-C82-C83-C84
26	m	202	CDL	C42-C43-C44-C45
27	M	202	PEE	C39-C40-C41-C42
27	m	201	PEE	C23-C24-C25-C26
26	l	101	CDL	CB2-C1-CA2-OA2
30	f	203	PC1	C37-C38-C39-C3A
28	j	203	LMT	C2-C3-C4-C5
27	m	201	PEE	C41-C42-C43-C44
26	e	404	CDL	C18-C19-C20-C21
26	m	202	CDL	C71-CB7-OB8-CB6
27	f	202	PEE	C16-C17-C18-C19
26	e	404	CDL	OA5-CA3-CA4-CA6
26	f	201	CDL	C13-C14-C15-C16
26	l	101	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
27	M	202	PEE	O4-C10-O2-C2
27	M	202	PEE	C36-C37-C38-C39
26	c	201	CDL	C35-C36-C37-C38
26	f	201	CDL	C78-C79-C80-C81
26	e	405	CDL	C71-C72-C73-C74
26	L	101	CDL	C39-C40-C41-C42
26	c	201	CDL	C53-C54-C55-C56
30	i	201	PC1	C2A-C2B-C2C-C2D
26	j	201	CDL	CA3-CA4-OA6-CA5
26	m	202	CDL	OB9-CB7-OB8-CB6
26	e	405	CDL	C53-C54-C55-C56
30	f	203	PC1	O31-C31-C32-C33
26	e	405	CDL	C79-C80-C81-C82
26	e	401	CDL	OB5-CB3-CB4-OB6
26	c	201	CDL	C38-C39-C40-C41
26	e	403	CDL	CB5-C51-C52-C53
26	e	404	CDL	C78-C79-C80-C81
27	M	202	PEE	C16-C17-C18-C19
27	m	201	PEE	C16-C17-C18-C19
26	e	403	CDL	OA6-CA4-CA6-OA8
27	M	202	PEE	C43-C44-C45-C46
27	f	202	PEE	C19-C20-C21-C22
26	c	201	CDL	C62-C63-C64-C65
26	q	101	CDL	C71-CB7-OB8-CB6
26	e	401	CDL	C16-C17-C18-C19
26	e	403	CDL	C11-C12-C13-C14
26	f	201	CDL	OA7-CA5-OA6-CA4
26	e	402	CDL	C54-C55-C56-C57
26	e	401	CDL	CB4-CB3-OB5-PB2
26	e	402	CDL	C1-CB2-OB2-PB2
26	e	403	CDL	CA3-CA4-CA6-OA8
26	M	201	CDL	C19-C20-C21-C22
26	q	101	CDL	OB9-CB7-OB8-CB6
27	m	201	PEE	C38-C39-C40-C41
26	L	101	CDL	C60-C61-C62-C63
26	e	401	CDL	OB5-CB3-CB4-CB6
26	q	102	CDL	OB5-CB3-CB4-CB6
27	M	202	PEE	C38-C39-C40-C41
26	M	201	CDL	C20-C21-C22-C23
26	e	402	CDL	C55-C56-C57-C58
26	c	201	CDL	C56-C57-C58-C59
27	f	202	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
32	B1	601	ATP	PB-O3B-PG-O1G
32	C1	601	ATP	PB-O3B-PG-O1G
32	C1	601	ATP	PB-O3B-PG-O3G
27	M	202	PEE	C18-C19-C20-C21
26	c	201	CDL	C1-CB2-OB2-PB2
26	e	403	CDL	C1-CA2-OA2-PA1
26	c	201	CDL	C42-C43-C44-C45
26	L	101	CDL	CA3-CA4-CA6-OA8
26	l	101	CDL	CA3-CA4-CA6-OA8
26	q	102	CDL	C73-C74-C75-C76
26	e	405	CDL	C56-C57-C58-C59
26	e	405	CDL	C12-C11-CA5-OA6
26	c	201	CDL	C40-C41-C42-C43
26	q	102	CDL	C71-C72-C73-C74
26	e	403	CDL	C32-C31-CA7-OA8
26	e	402	CDL	OB5-CB3-CB4-CB6
26	e	403	CDL	OA5-CA3-CA4-CA6
26	e	401	CDL	C11-C12-C13-C14
26	M	201	CDL	C12-C11-CA5-OA6
26	f	201	CDL	C12-C11-CA5-OA6
26	e	405	CDL	OB7-CB5-OB6-CB4
27	M	202	PEE	C23-C24-C25-C26
26	m	202	CDL	C12-C11-CA5-OA6
27	f	202	PEE	O2-C10-C11-C12
32	A1	601	ATP	PG-O3B-PB-O2B
32	B1	601	ATP	PG-O3B-PB-O1B
32	C1	601	ATP	PG-O3B-PB-O1B
32	C1	601	ATP	PG-O3B-PB-O2B
32	C1	601	ATP	PA-O3A-PB-O1B
26	f	201	CDL	C72-C71-CB7-OB8
27	m	201	PEE	C18-C19-C20-C21
26	e	405	CDL	C51-CB5-OB6-CB4
26	f	201	CDL	C11-CA5-OA6-CA4
27	m	201	PEE	C34-C35-C36-C37
26	e	403	CDL	C52-C51-CB5-OB6
26	f	201	CDL	C37-C38-C39-C40
26	q	101	CDL	C12-C11-CA5-OA6
26	q	102	CDL	C79-C80-C81-C82
26	q	101	CDL	C38-C39-C40-C41
30	j	202	PC1	O31-C31-C32-C33
26	j	201	CDL	C52-C51-CB5-OB6
27	M	202	PEE	O2-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	e	405	CDL	OA6-CA4-CA6-OA8
26	e	403	CDL	C12-C13-C14-C15
26	e	405	CDL	C74-C75-C76-C77
26	e	401	CDL	C32-C31-CA7-OA8
27	m	201	PEE	O2-C10-C11-C12
26	e	401	CDL	C43-C44-C45-C46
32	A1	601	ATP	PB-O3B-PG-O1G
30	f	203	PC1	C2B-C2C-C2D-C2E
26	f	201	CDL	OA5-CA3-CA4-CA6
26	e	405	CDL	C32-C31-CA7-OA8
26	j	201	CDL	CA6-CA4-OA6-CA5
30	j	202	PC1	O22-C21-O21-C2
26	l	101	CDL	C60-C61-C62-C63
26	M	201	CDL	C12-C11-CA5-OA7
26	e	405	CDL	C11-C12-C13-C14
26	e	402	CDL	C32-C31-CA7-OA8
26	m	202	CDL	C12-C11-CA5-OA7
26	m	202	CDL	C19-C20-C21-C22
26	e	402	CDL	C53-C54-C55-C56
30	i	201	PC1	C3B-C3C-C3D-C3E
26	e	401	CDL	C75-C76-C77-C78
26	e	405	CDL	C12-C11-CA5-OA7
26	f	201	CDL	C12-C11-CA5-OA7
30	j	202	PC1	O32-C31-C32-C33
26	M	201	CDL	OA7-CA5-OA6-CA4
26	e	401	CDL	OB7-CB5-OB6-CB4
26	m	202	CDL	OA7-CA5-OA6-CA4
26	e	403	CDL	C32-C31-CA7-OA9
27	f	202	PEE	O4-C10-C11-C12
26	q	101	CDL	C59-C60-C61-C62
26	e	401	CDL	C52-C51-CB5-OB6
26	j	201	CDL	C77-C78-C79-C80
26	e	401	CDL	C32-C31-CA7-OA9
26	f	201	CDL	C72-C71-CB7-OB9
26	e	403	CDL	C52-C51-CB5-OB7
26	e	405	CDL	C32-C31-CA7-OA9
26	q	101	CDL	C12-C11-CA5-OA7
26	M	201	CDL	C38-C39-C40-C41
27	m	201	PEE	O4-C10-C11-C12
26	e	402	CDL	C32-C31-CA7-OA9
26	q	102	CDL	C72-C71-CB7-OB8
30	j	202	PC1	C22-C21-O21-C2

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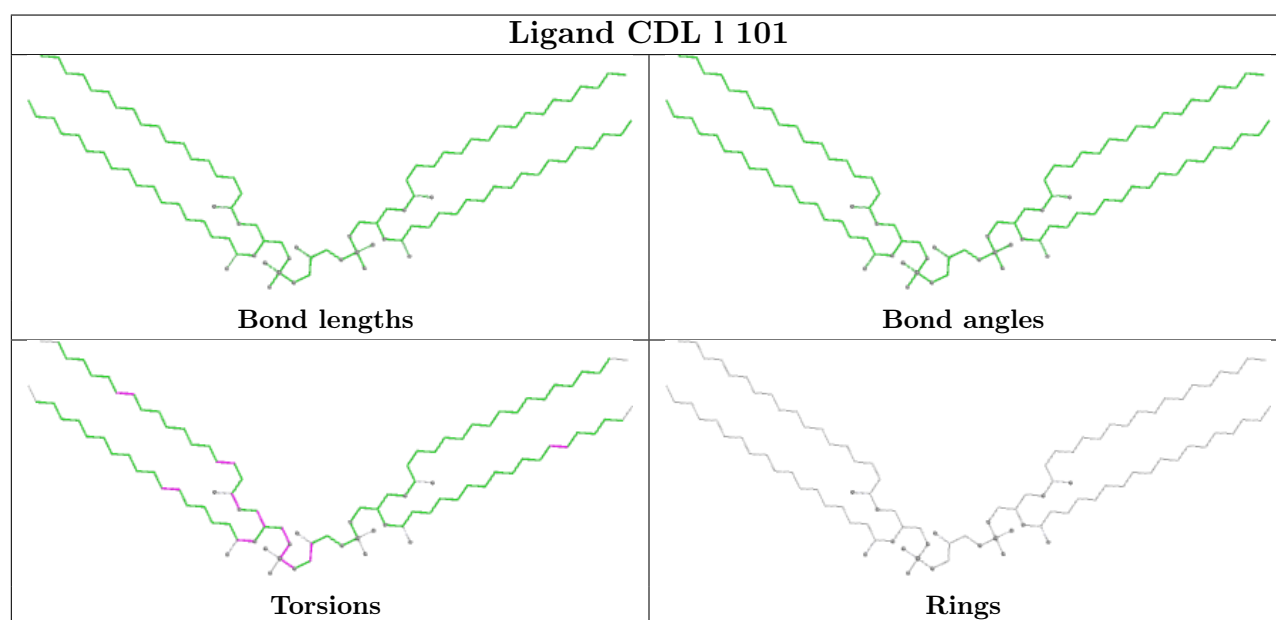
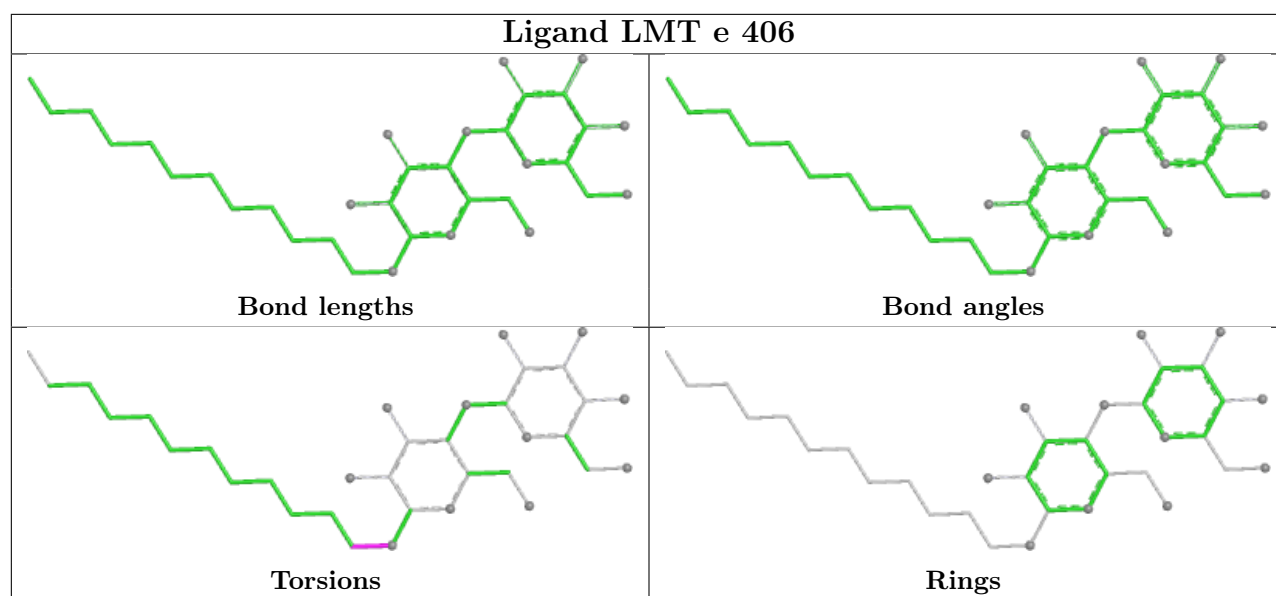
Mol	Chain	Res	Type	Atoms
32	A1	601	ATP	PG-O3B-PB-O1B
26	q	101	CDL	C73-C74-C75-C76
26	m	202	CDL	C72-C71-CB7-OB8
26	j	201	CDL	C52-C51-CB5-OB7
27	M	202	PEE	O4-C10-C11-C12

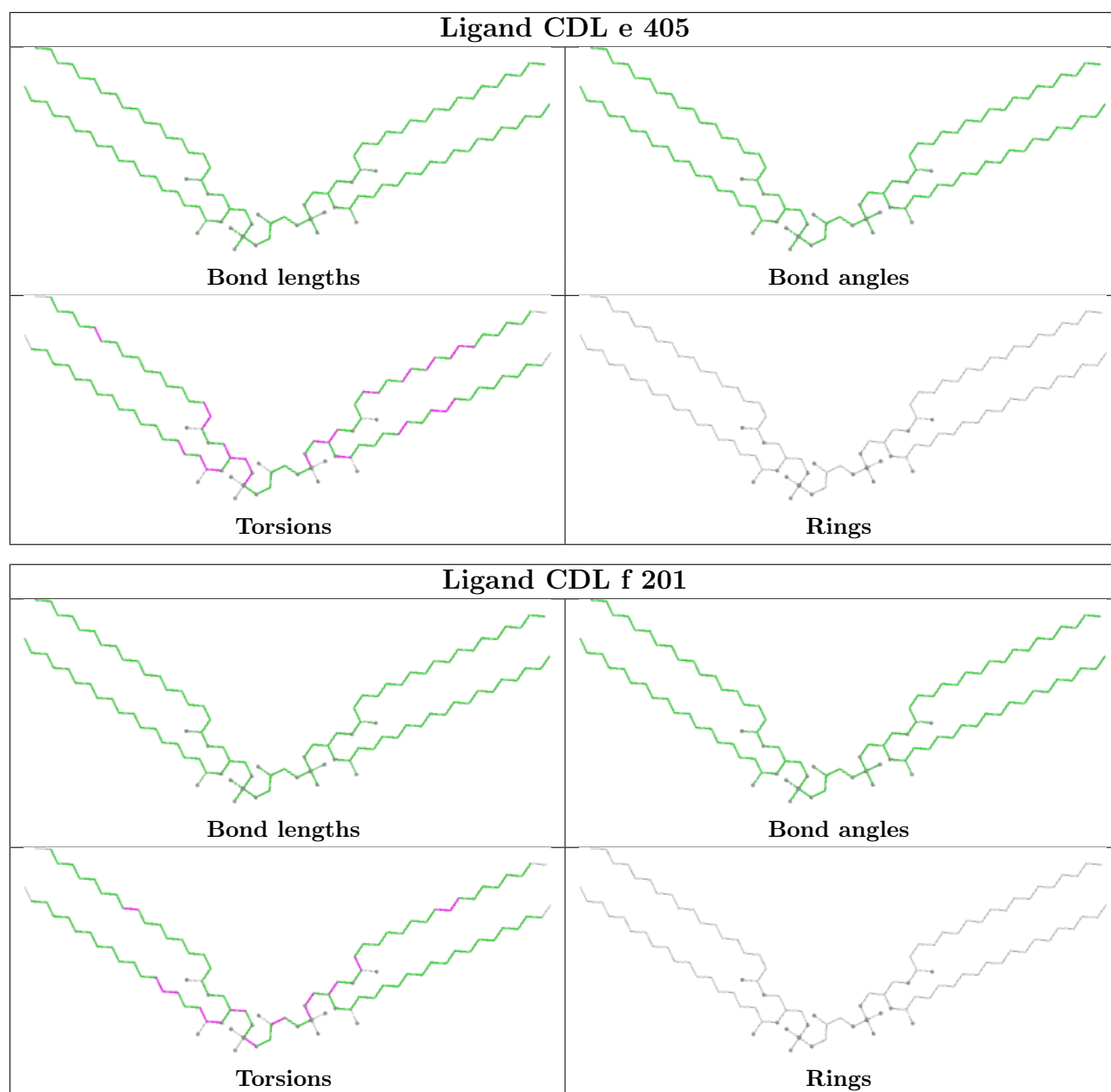
There are no ring outliers.

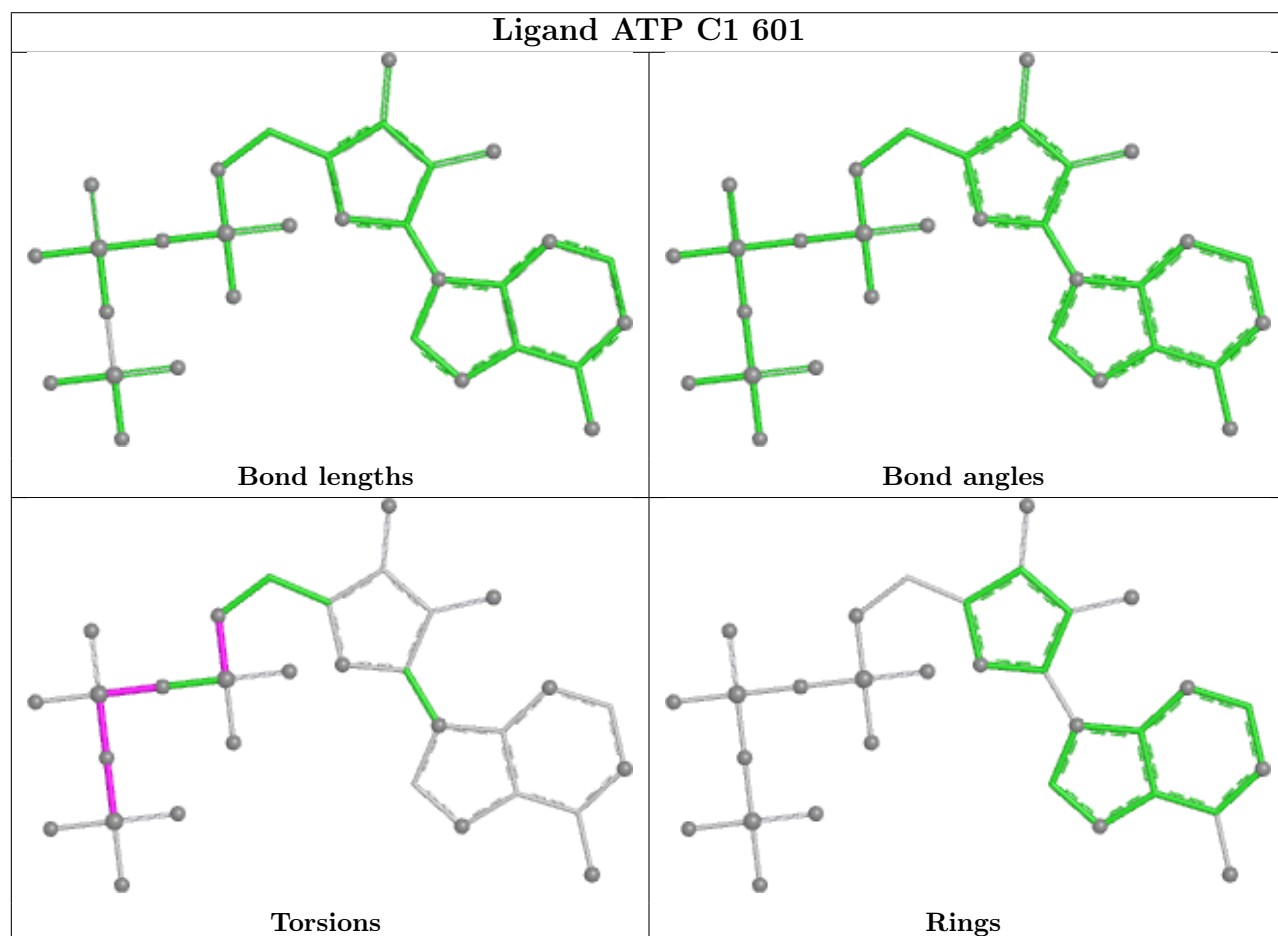
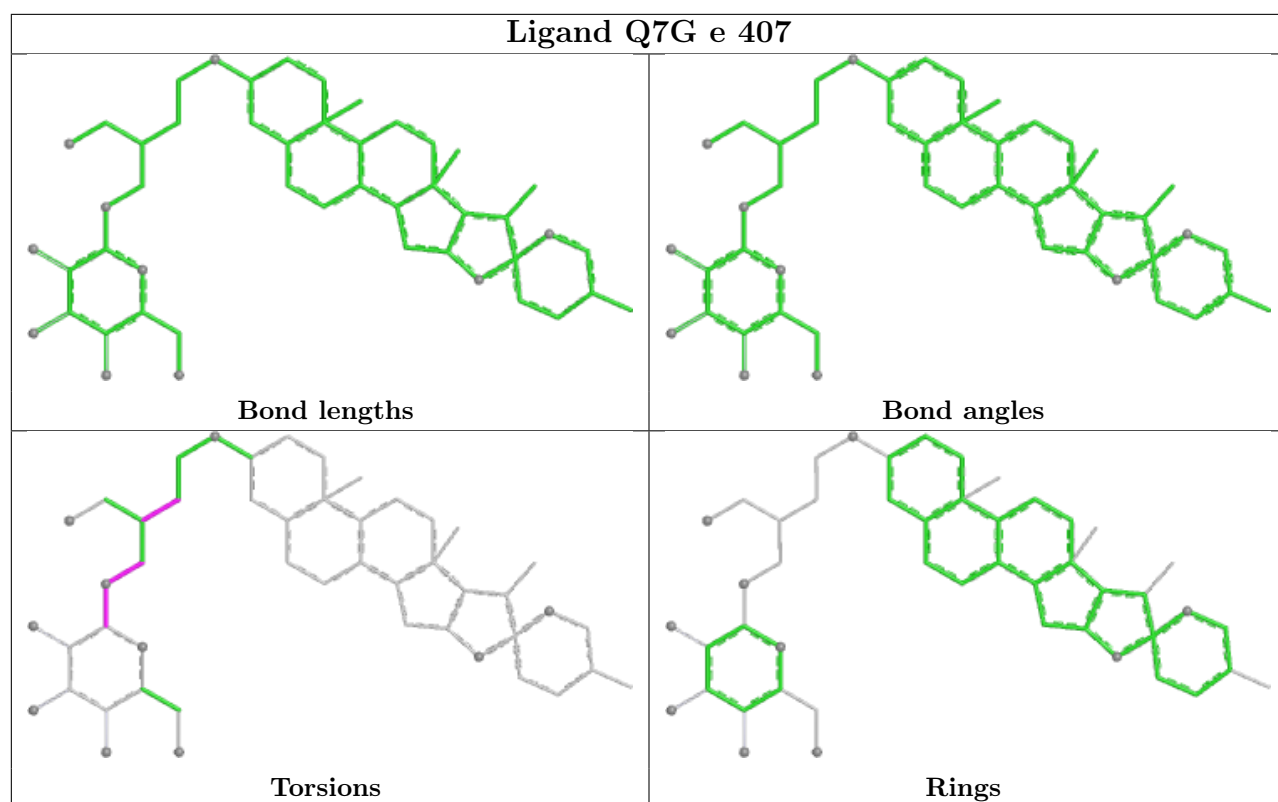
12 monomers are involved in 13 short contacts:

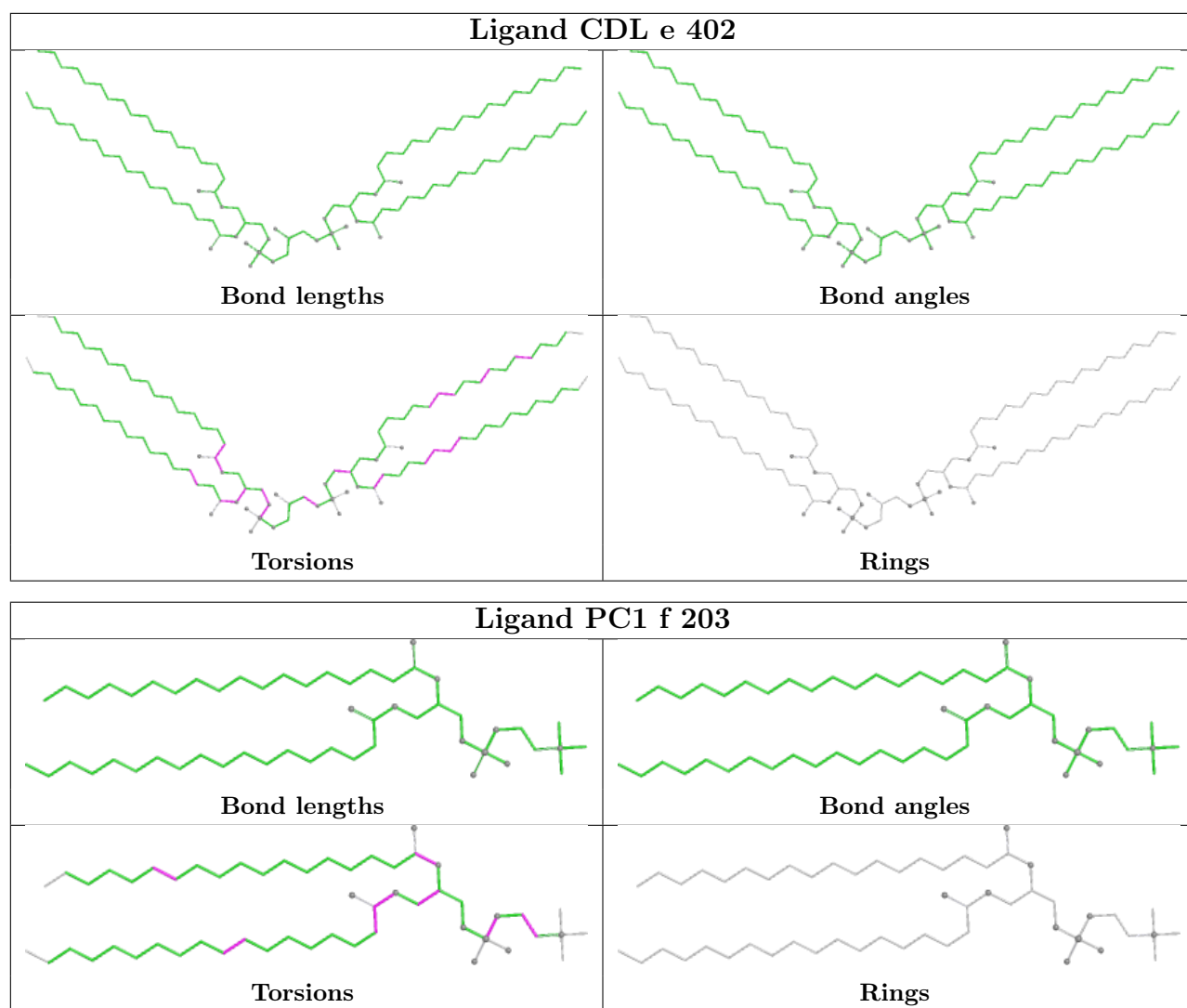
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	C1	601	ATP	1	0
26	e	402	CDL	3	0
30	f	203	PC1	1	0
26	q	101	CDL	1	0
26	q	102	CDL	1	0
26	e	403	CDL	2	0
26	c	201	CDL	1	0
27	M	202	PEE	1	0
26	j	201	CDL	1	0
26	M	201	CDL	1	0
32	B1	601	ATP	1	0
32	D1	601	ATP	1	0

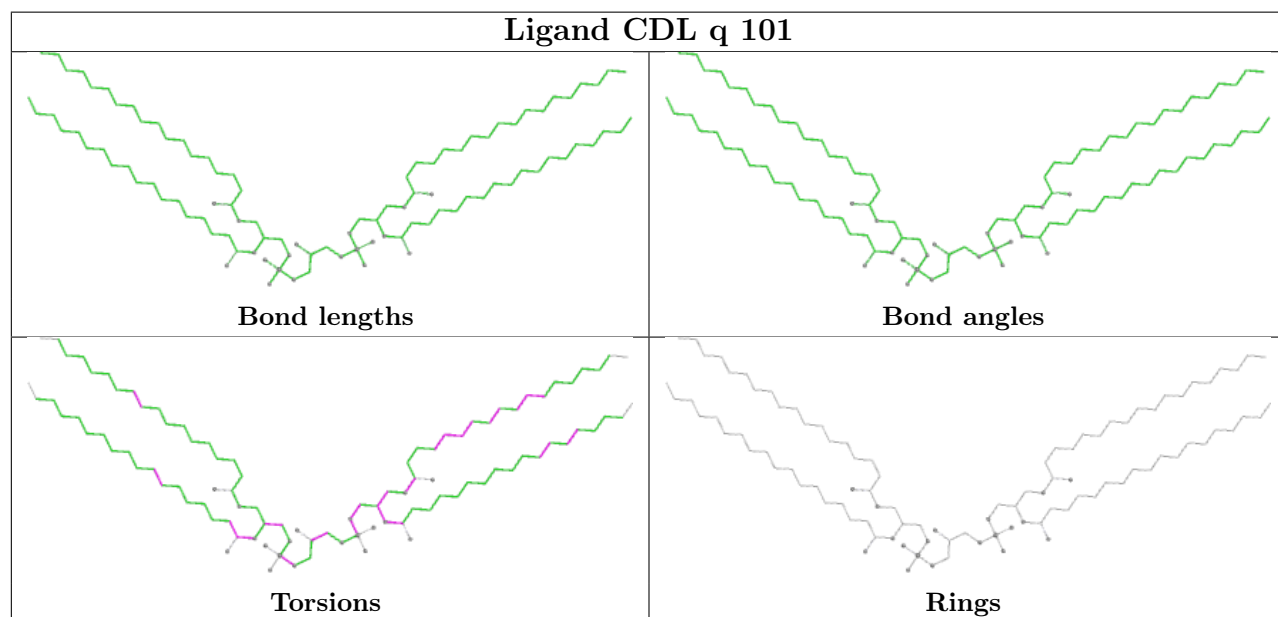
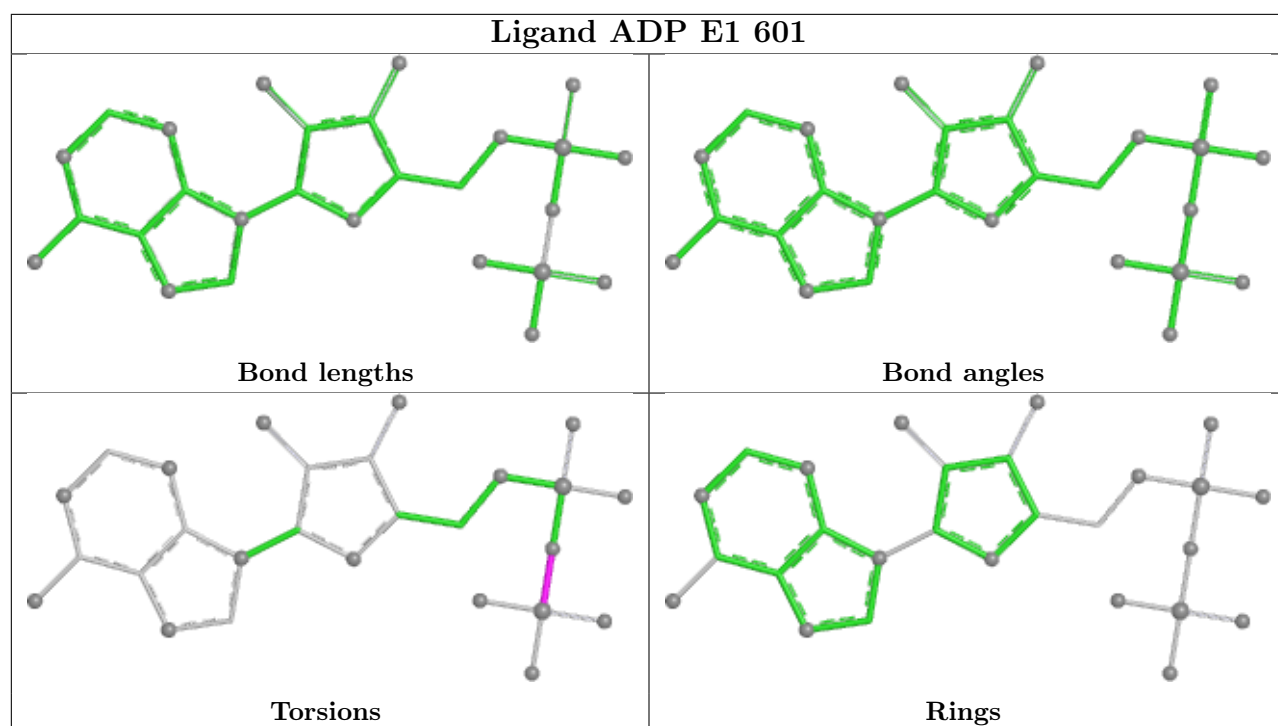
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

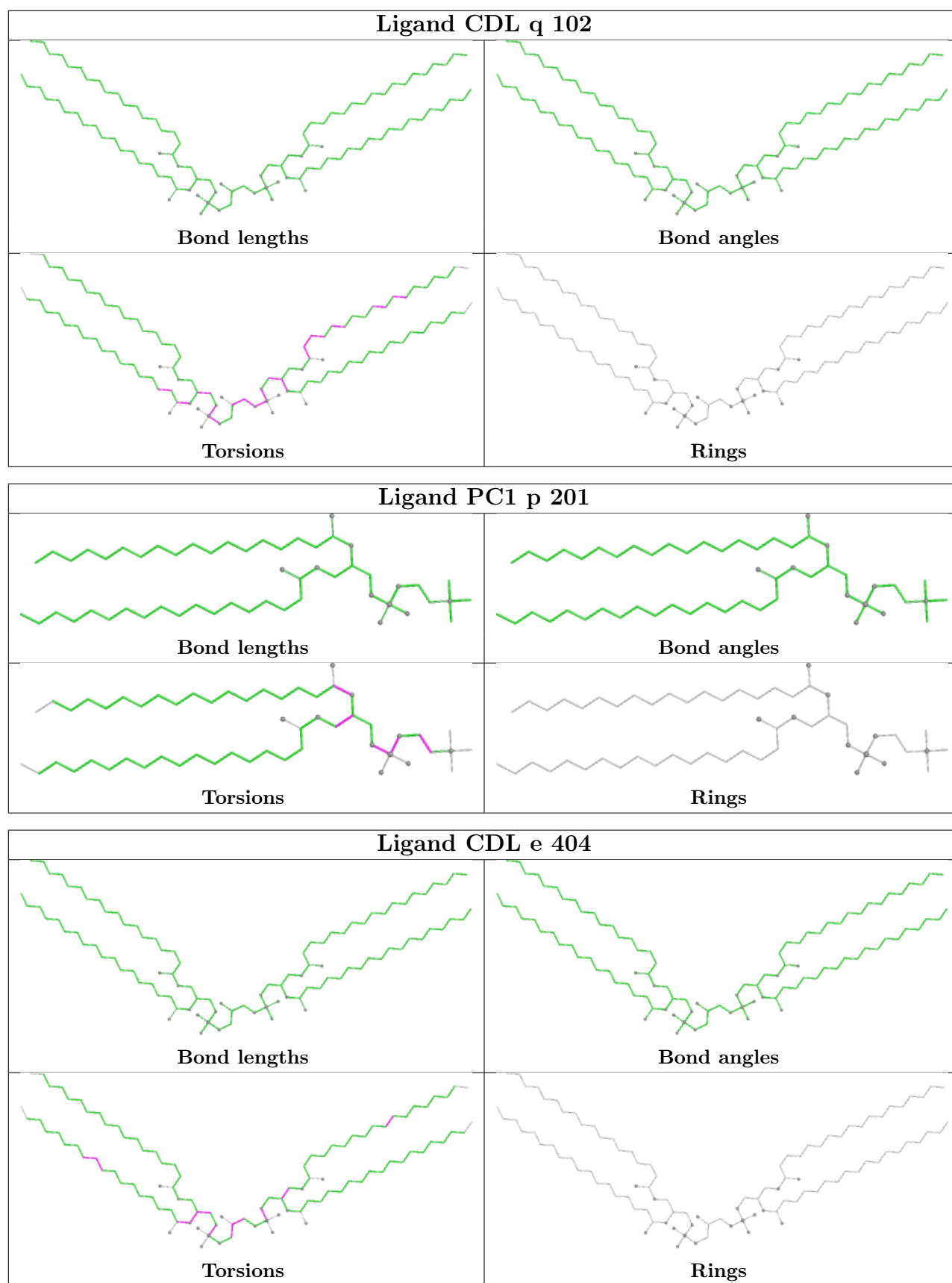


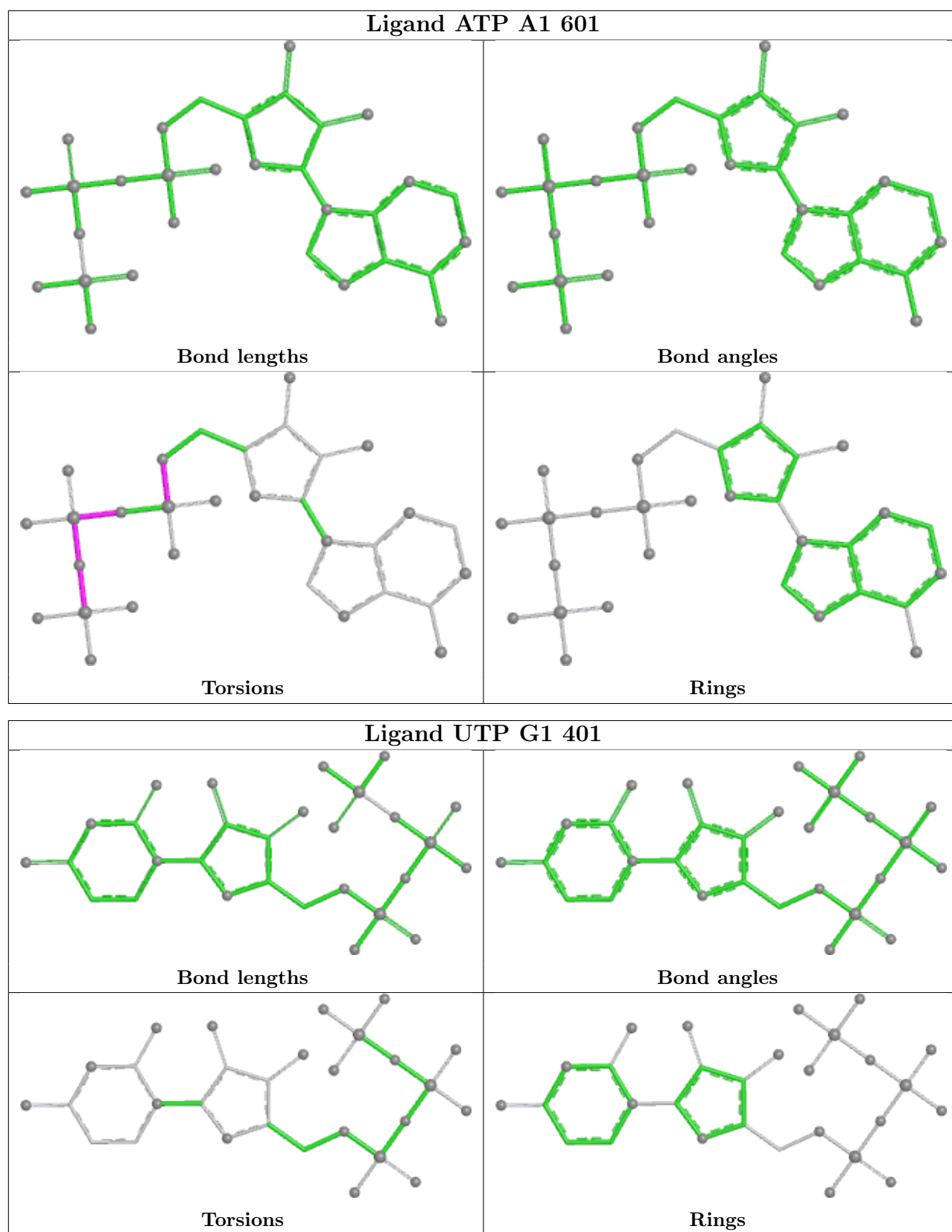


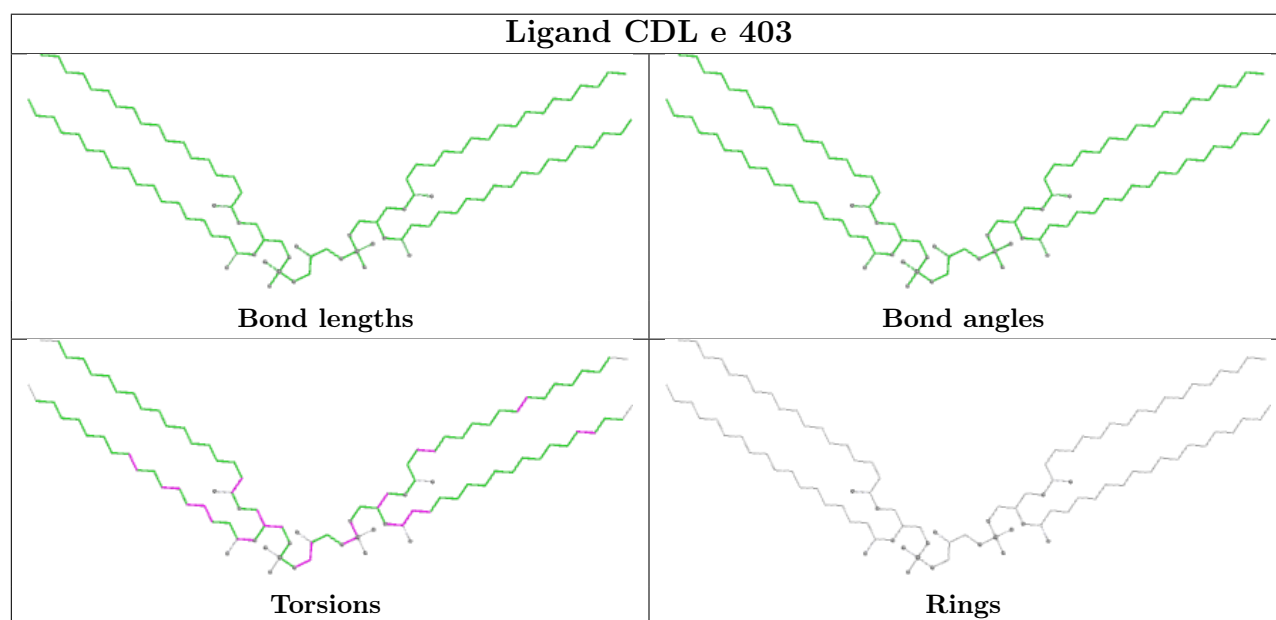
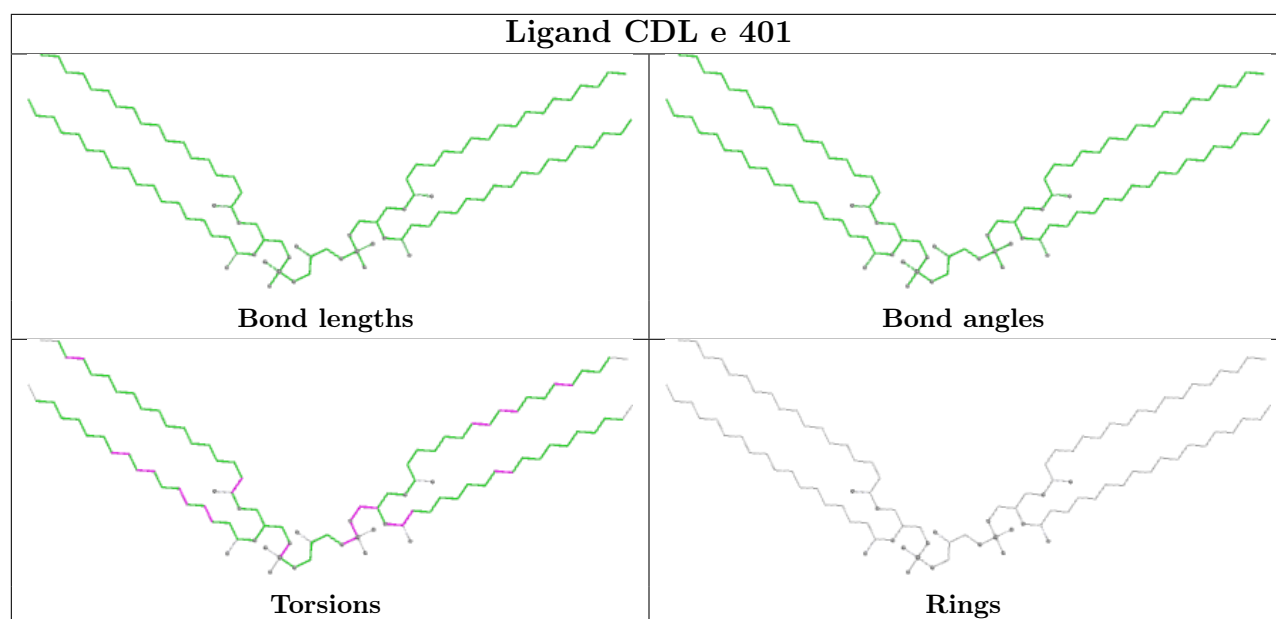


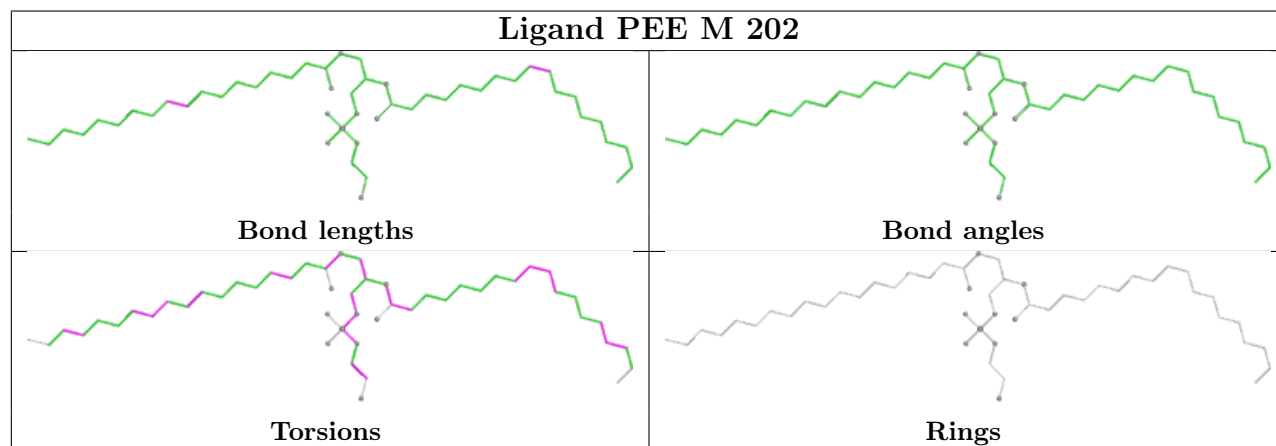
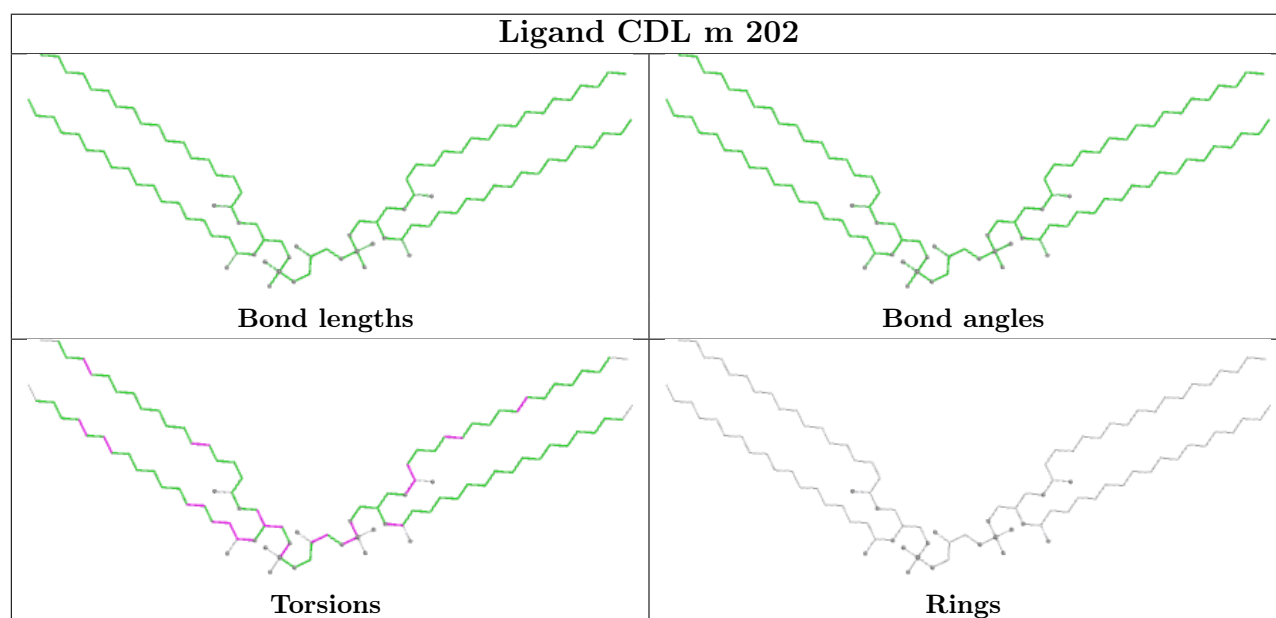
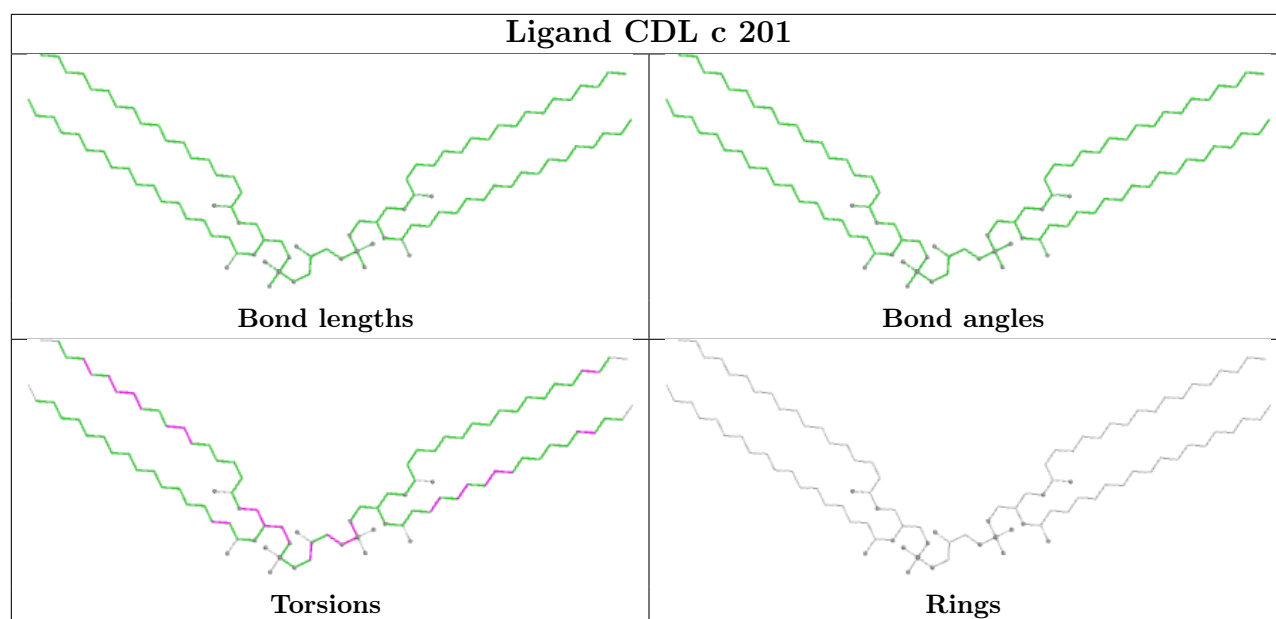


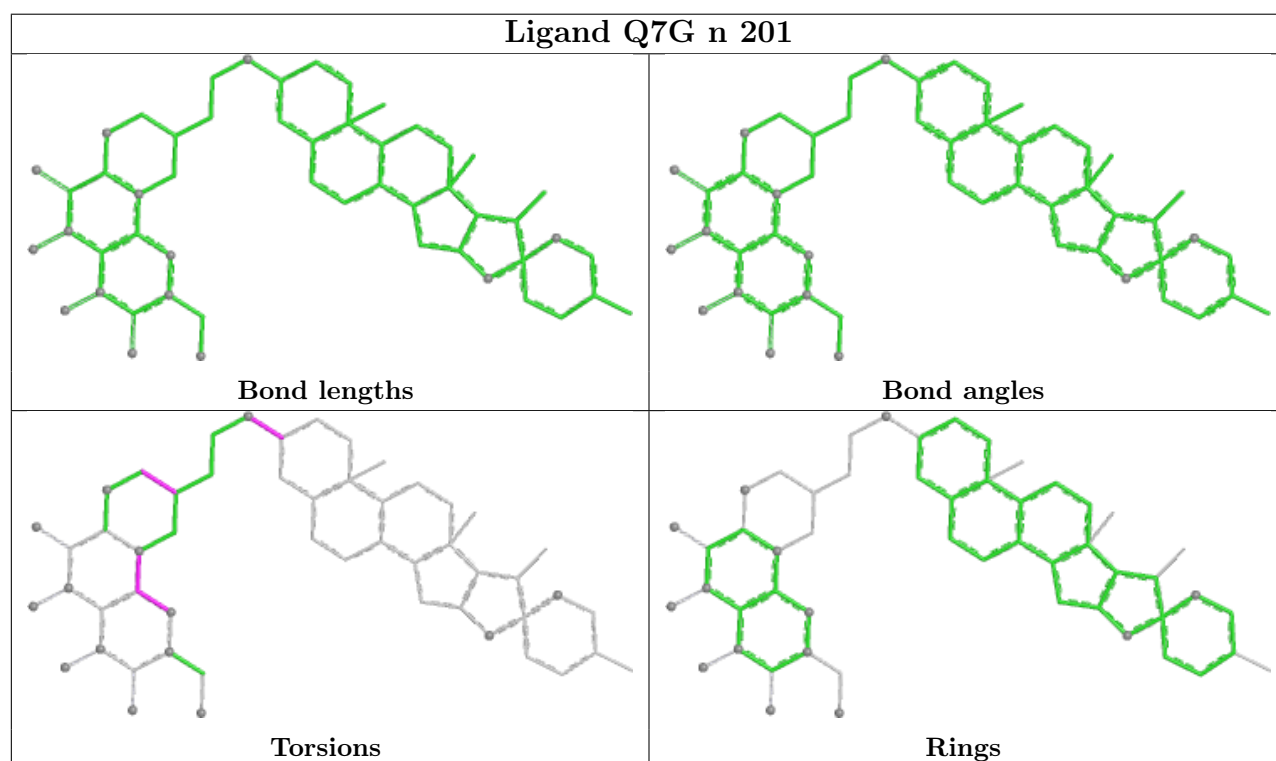
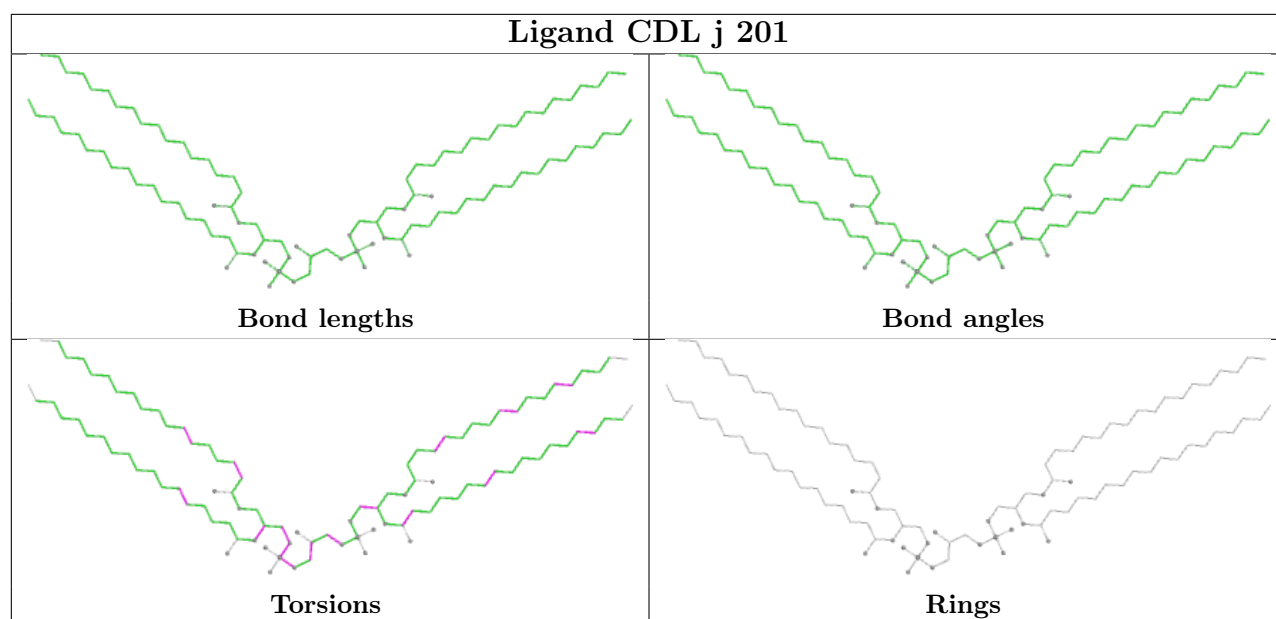


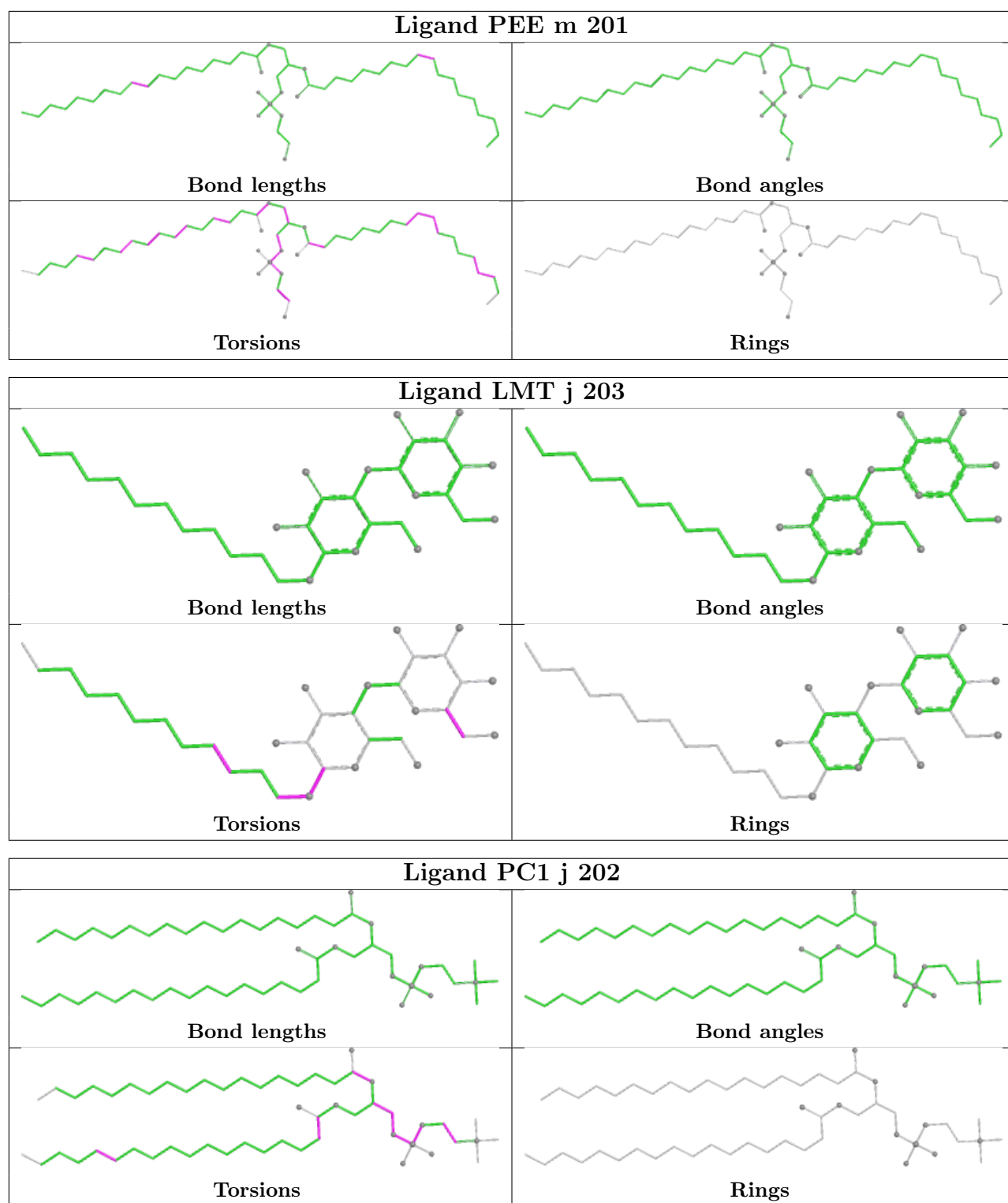


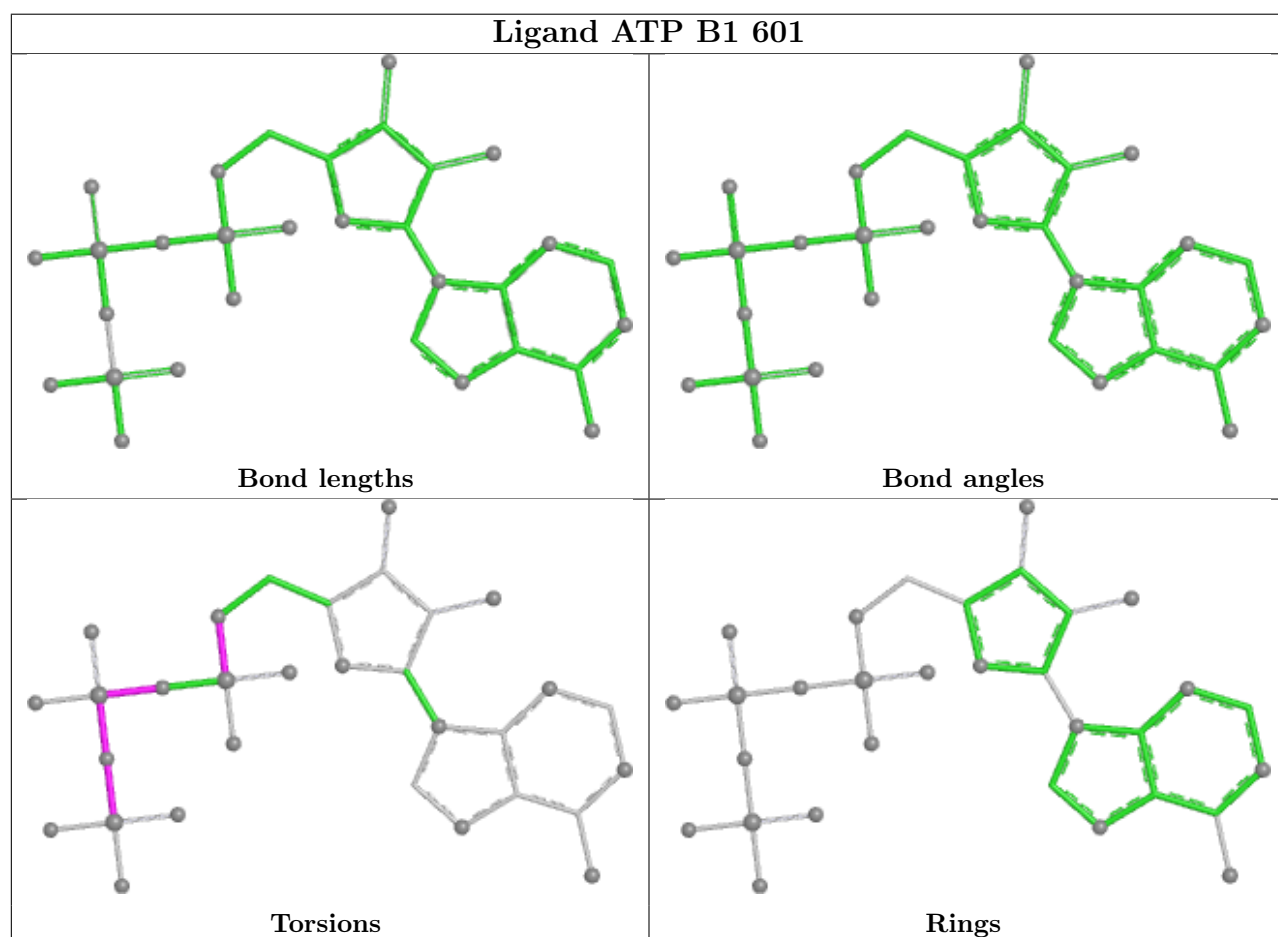
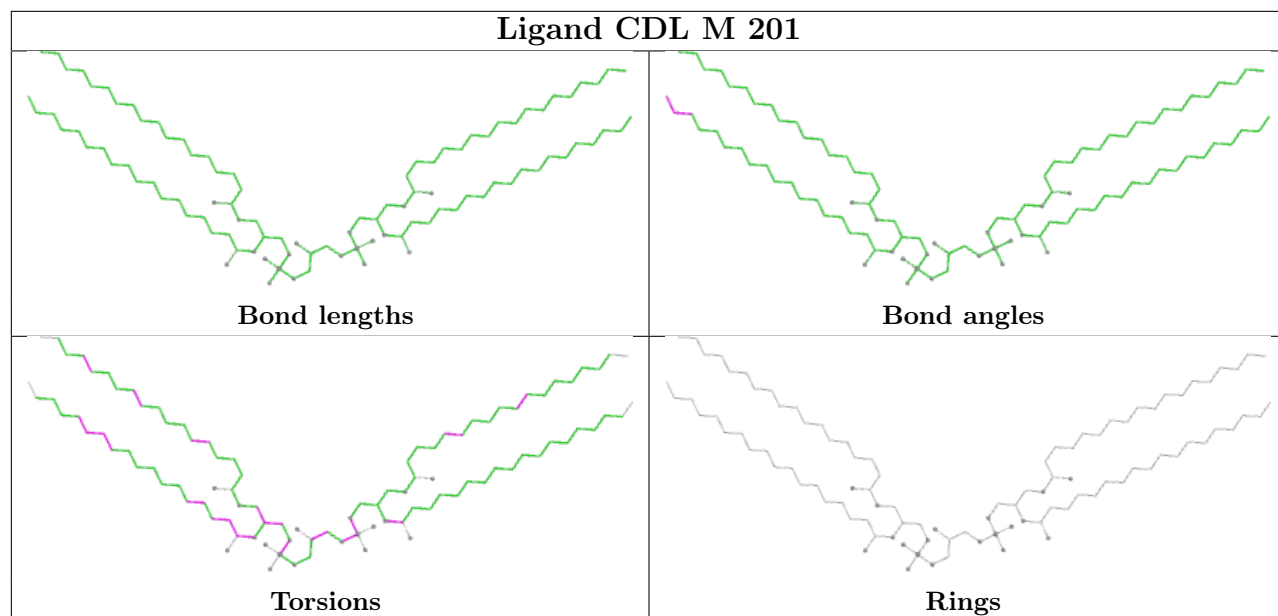


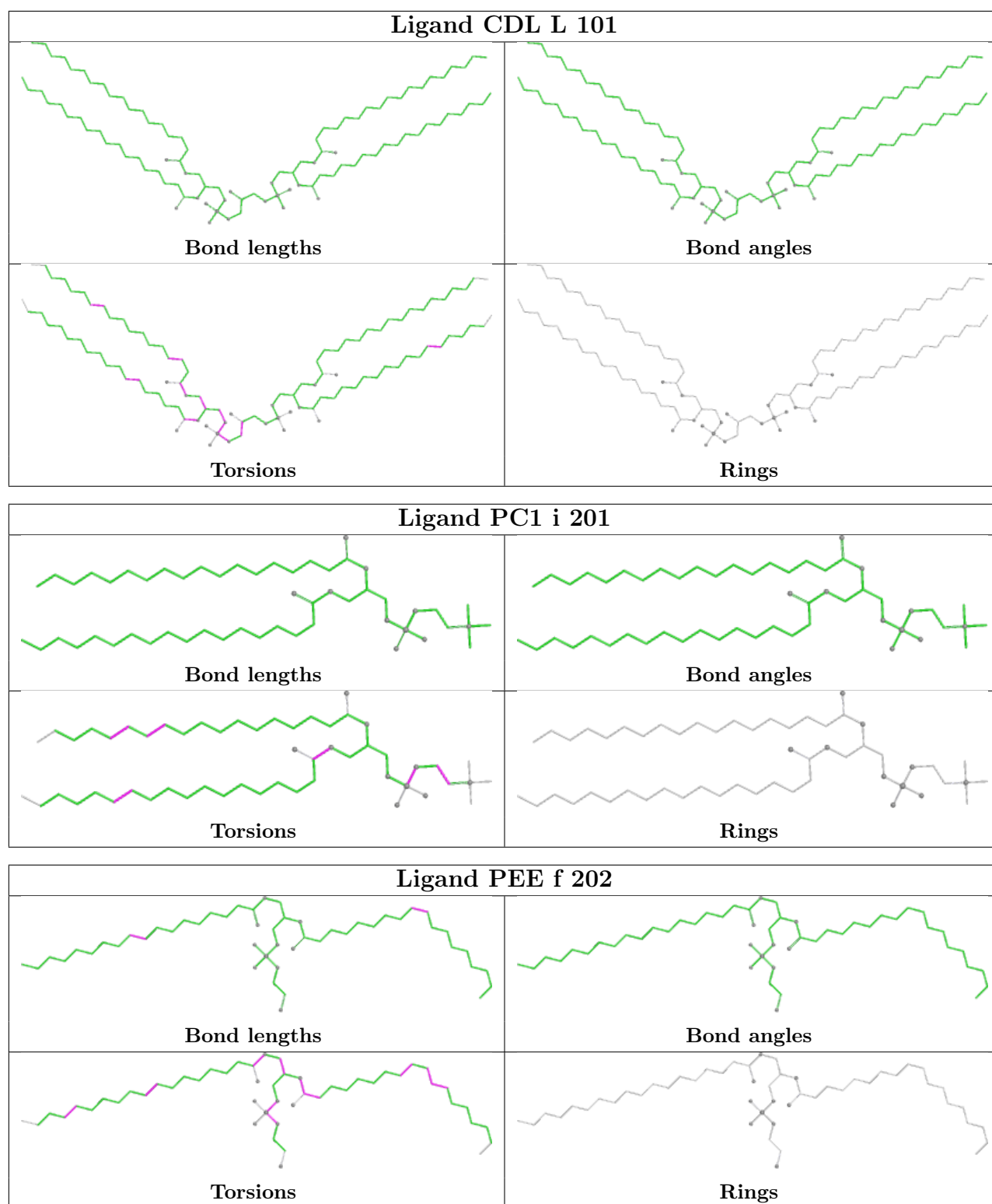


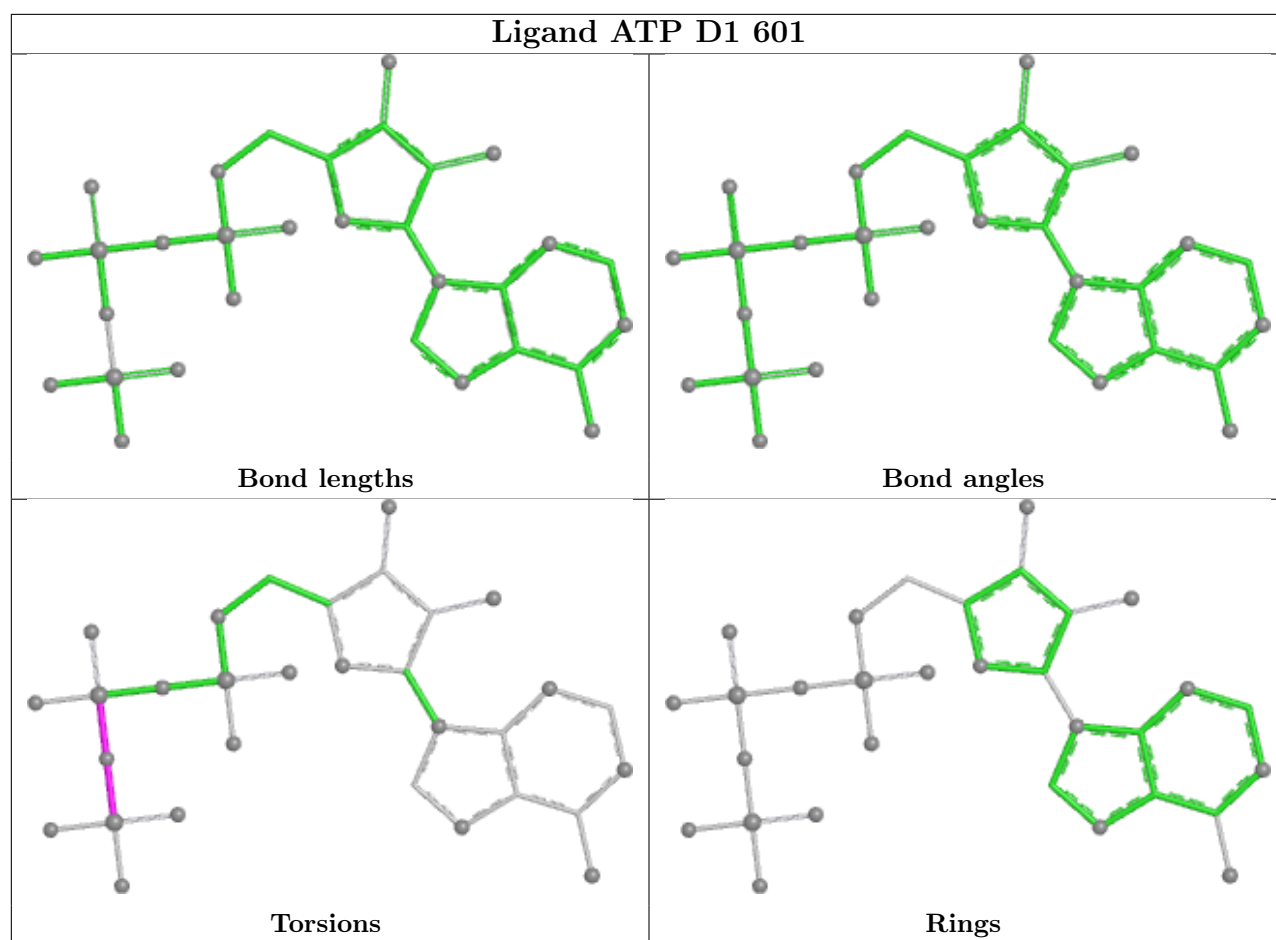












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

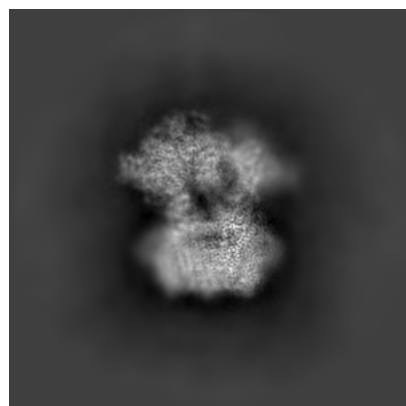
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15568. These allow visual inspection of the internal detail of the map and identification of artifacts.

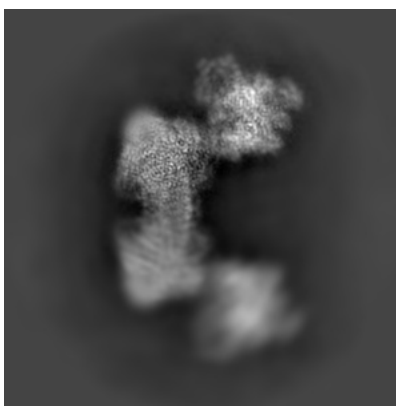
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

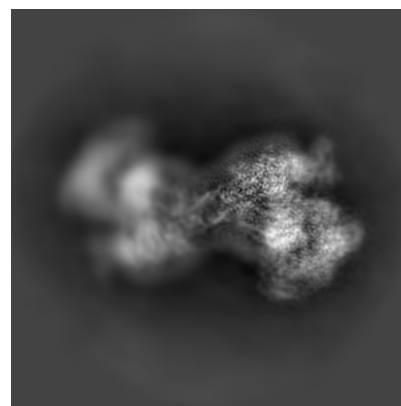
6.1.1 Primary map



X

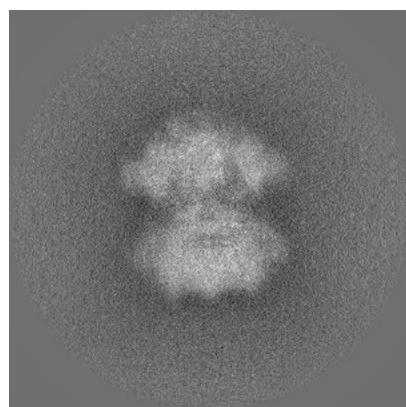


Y

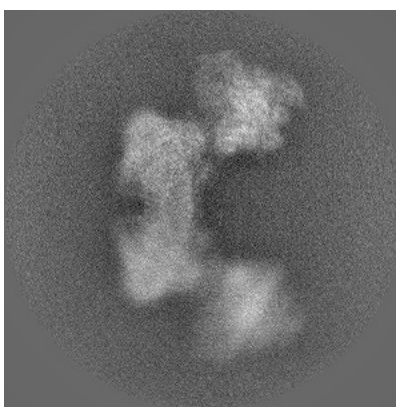


Z

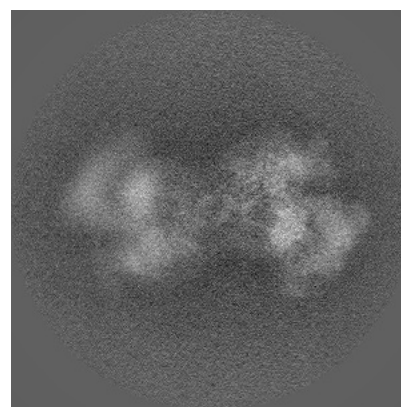
6.1.2 Raw map



X



Y

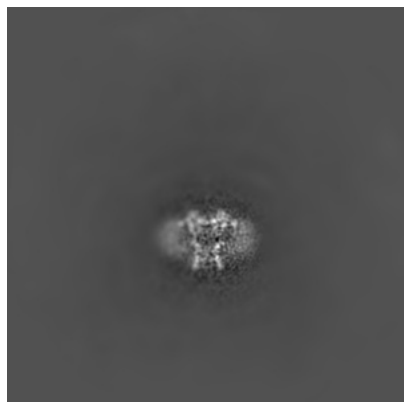


Z

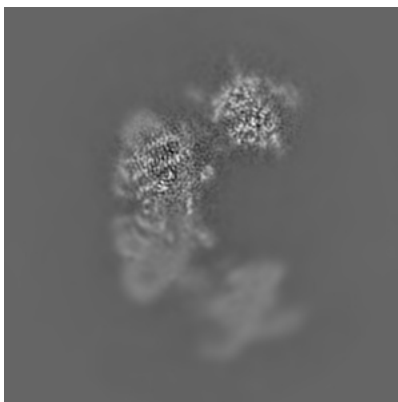
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

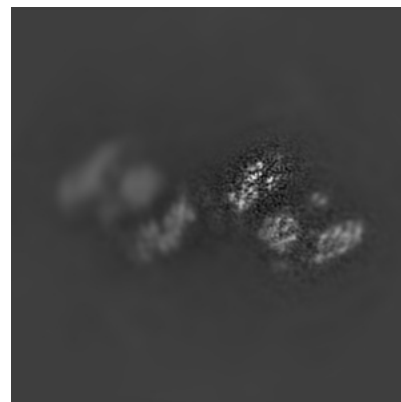
6.2.1 Primary map



X Index: 280

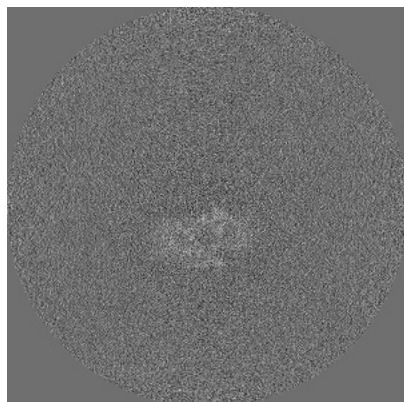


Y Index: 280

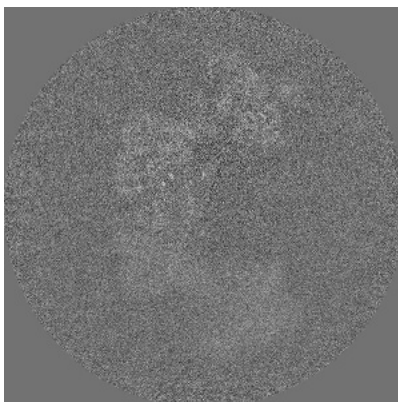


Z Index: 280

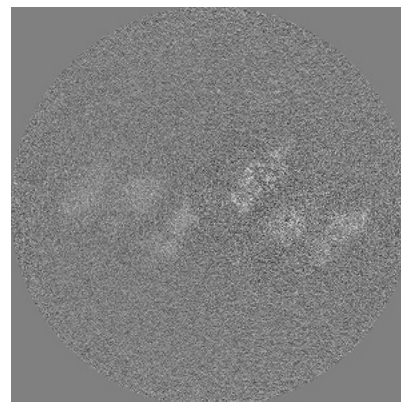
6.2.2 Raw map



X Index: 280



Y Index: 280

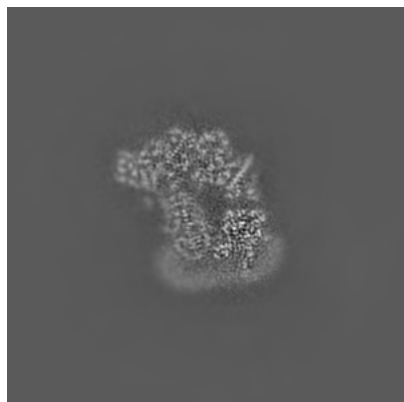


Z Index: 280

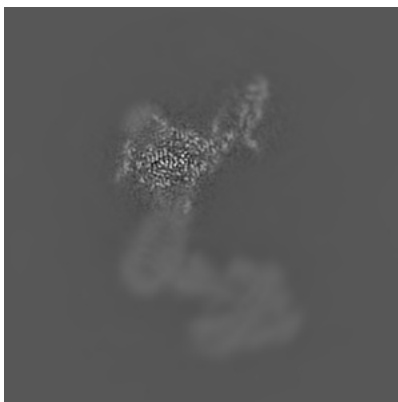
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

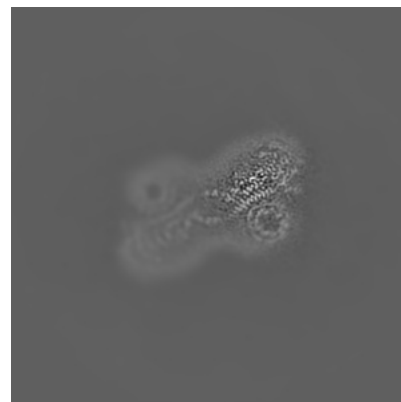
6.3.1 Primary map



X Index: 378

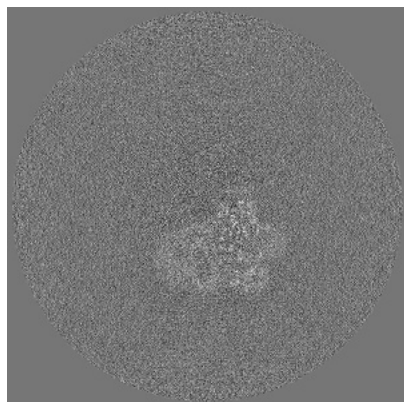


Y Index: 319

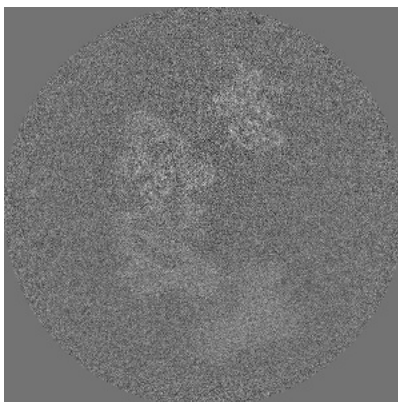


Z Index: 233

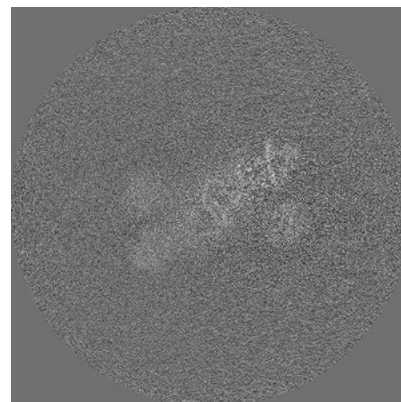
6.3.2 Raw map



X Index: 347



Y Index: 288

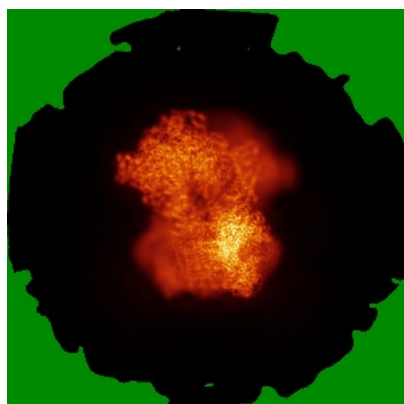


Z Index: 259

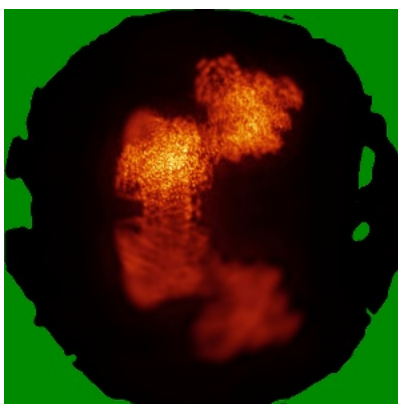
The images above show the largest variance slices of the map in three orthogonal directions.

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

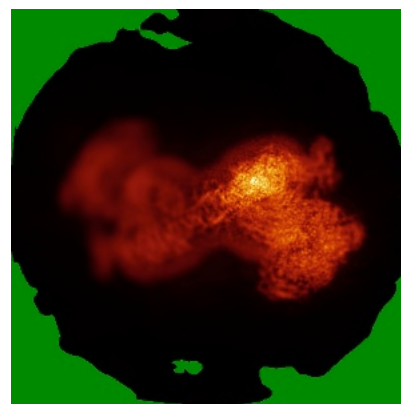
6.4.1 Primary map



X

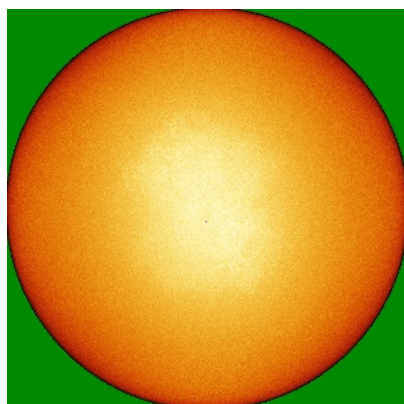


Y

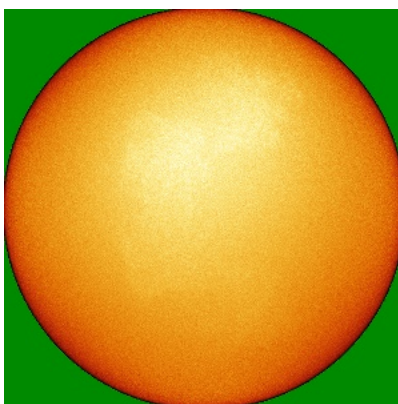


Z

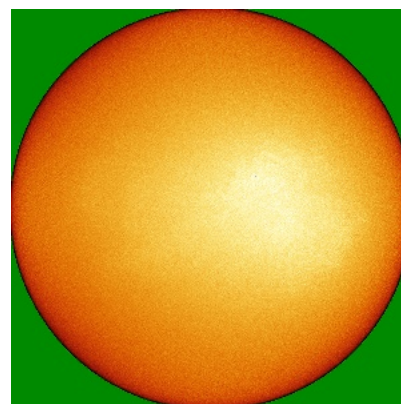
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

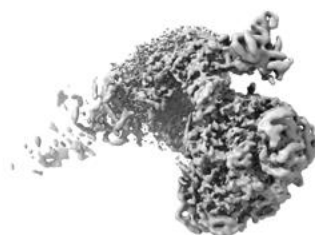
6.5.1 Primary map



X



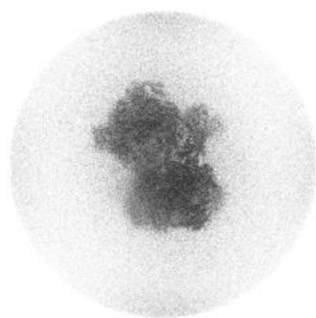
Y



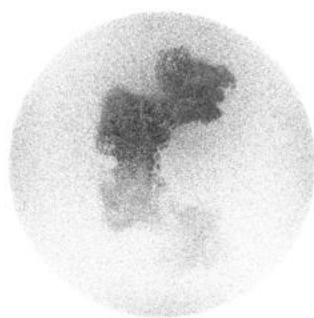
Z

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

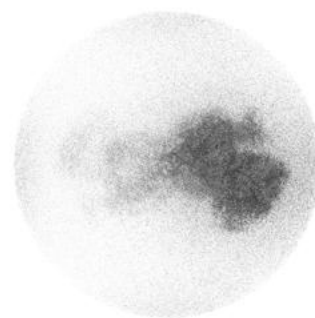
6.5.2 Raw map



X



Y



Z

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

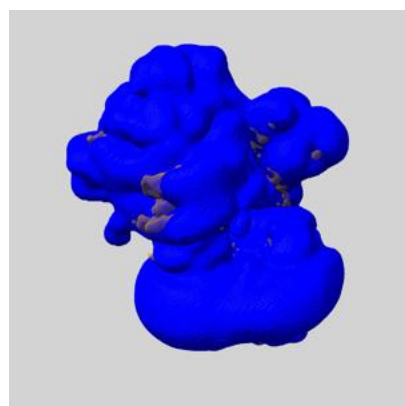
6.6 Mask visualisation [i](#)

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

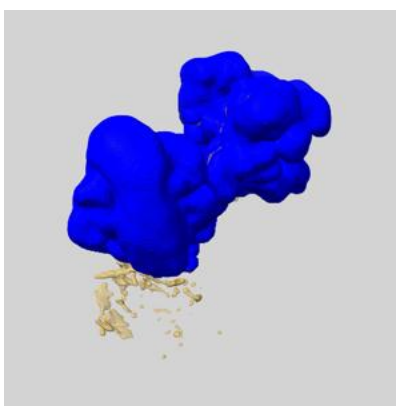
A mask typically either:

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

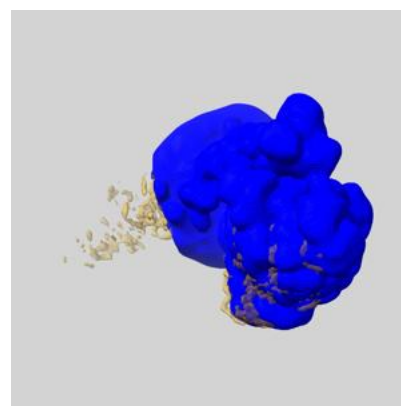
6.6.1 emd_15568_msk_1.map [i](#)



X



Y

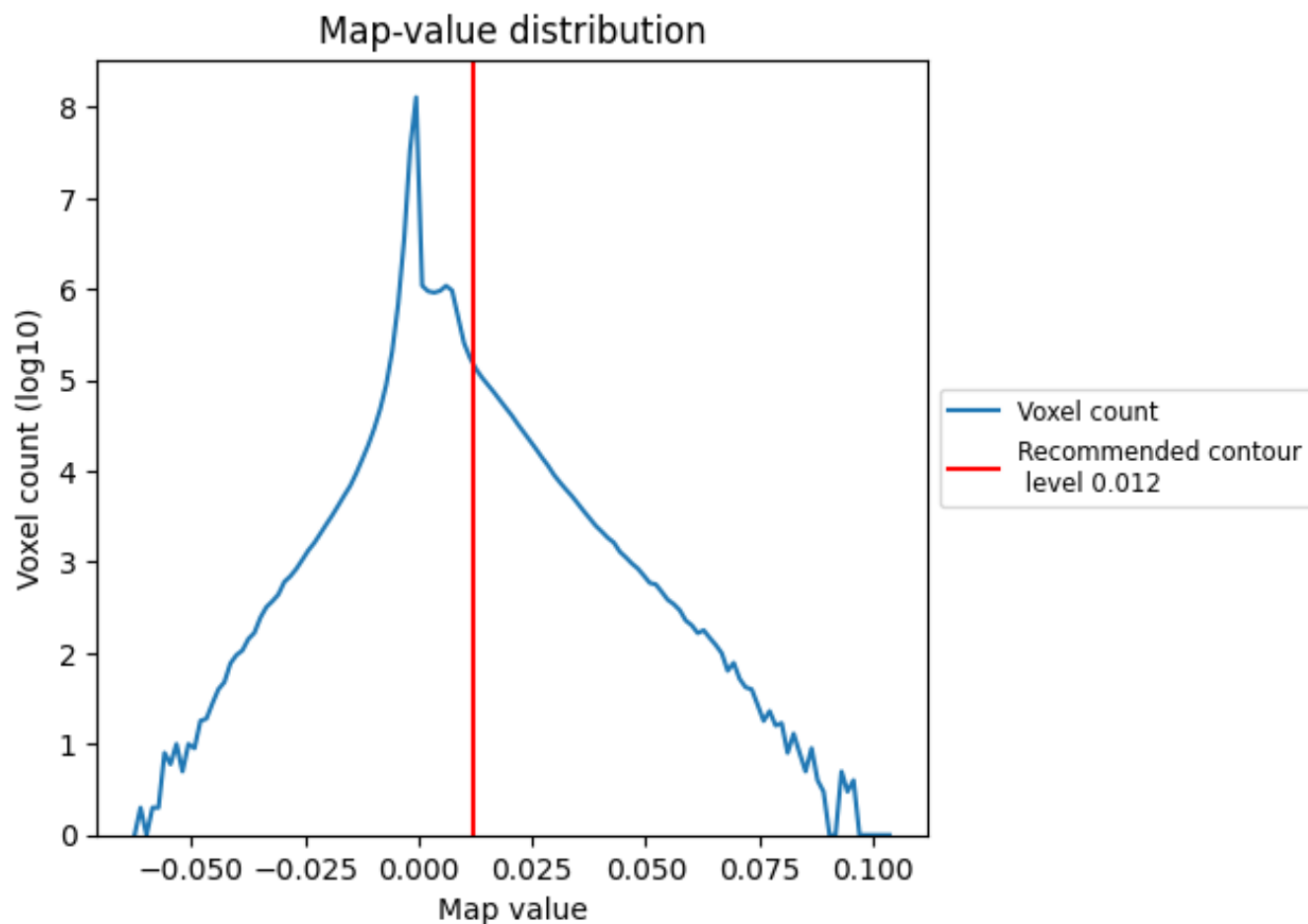


Z

7 Map analysis [i](#)

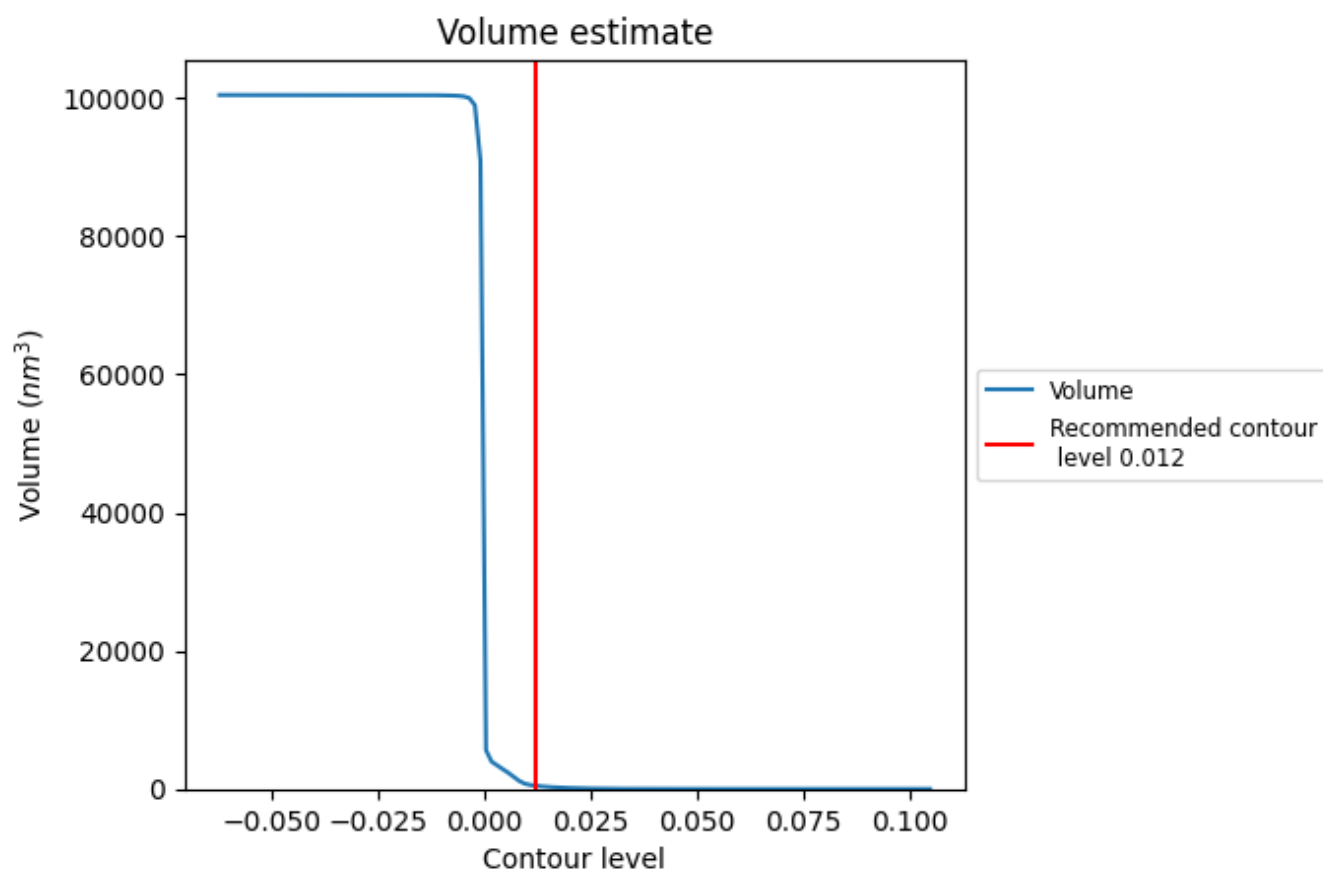
This section contains the results of statistical analysis of the map.

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.

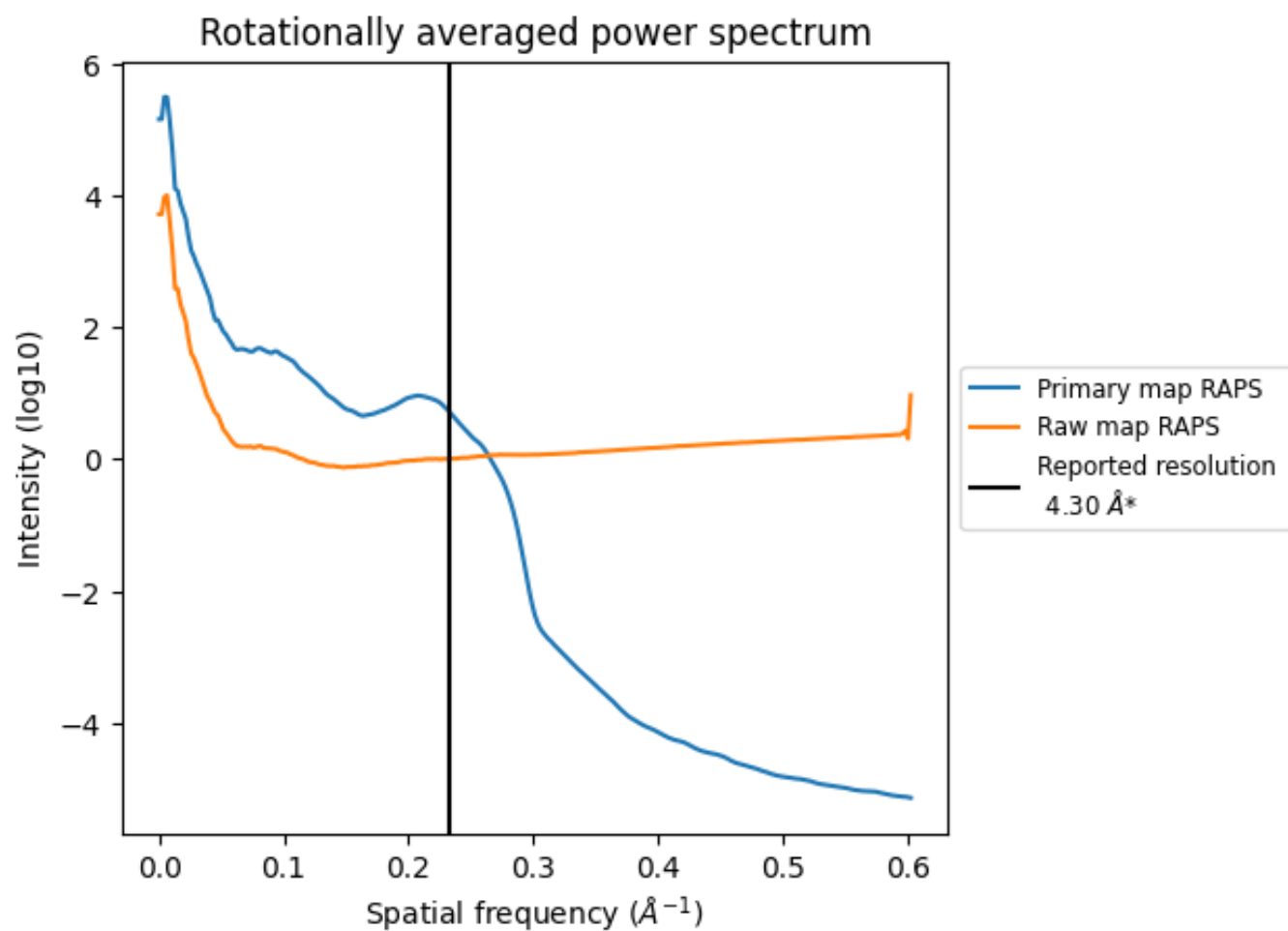
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 465 nm³; this corresponds to an approximate mass of 420 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

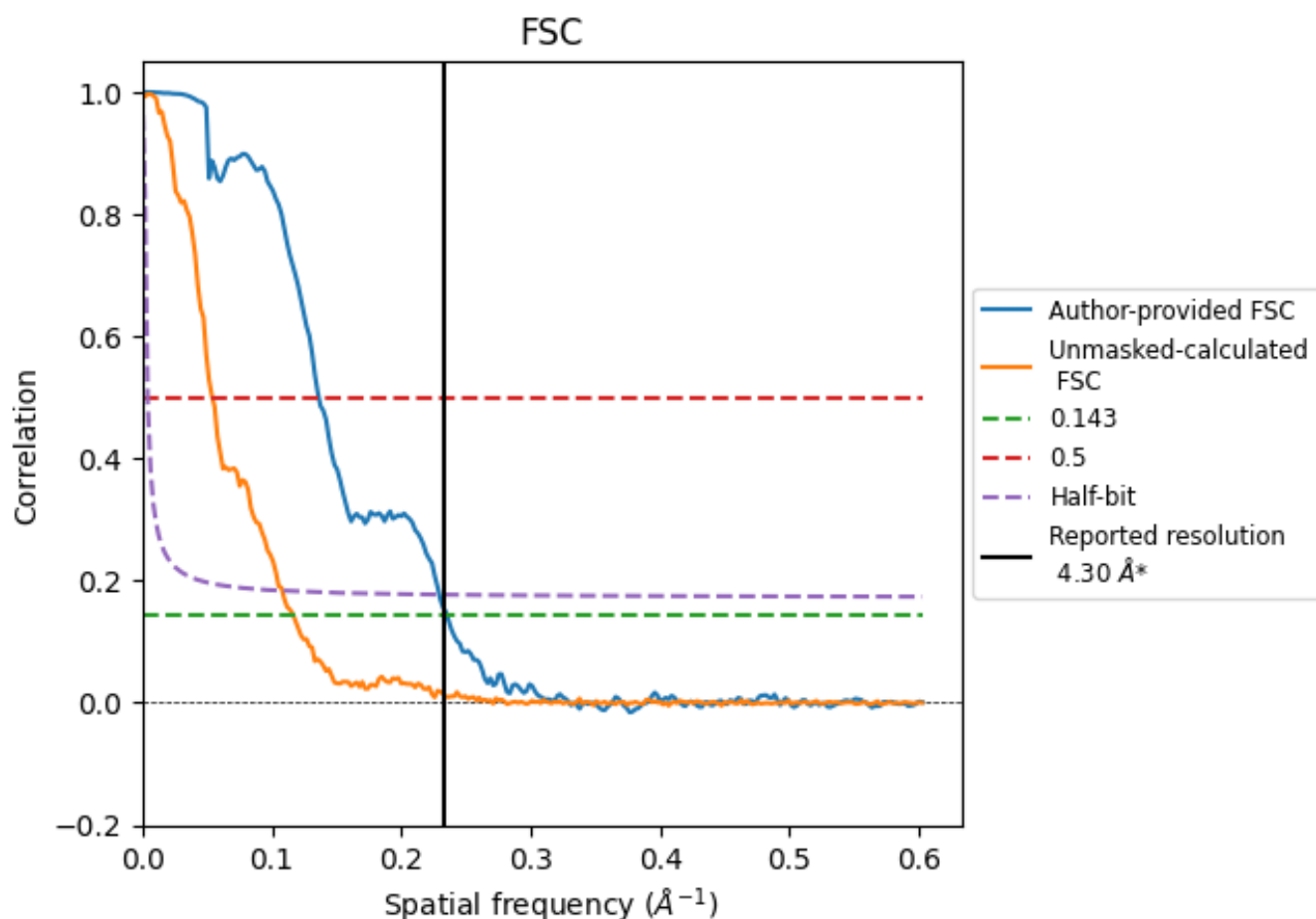


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

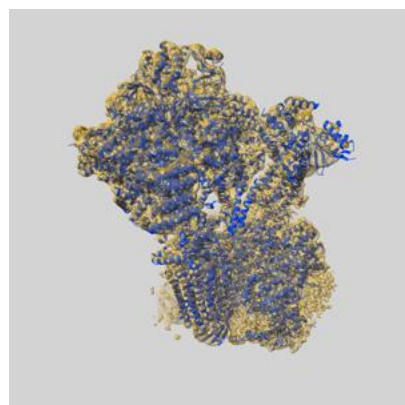
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.25	7.33	4.36
Unmasked-calculated*	8.57	18.48	9.24

*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 8.57 differs from the reported value 4.3 by more than 10 %

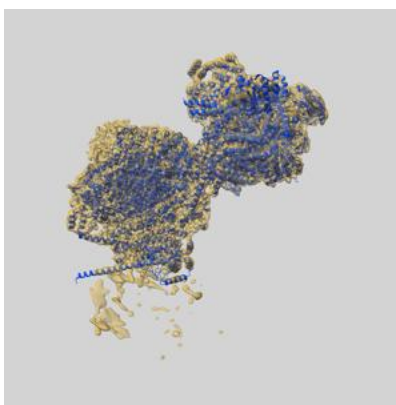
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15568 and PDB model 8APF. Per-residue inclusion information can be found in section 3 on page 16.

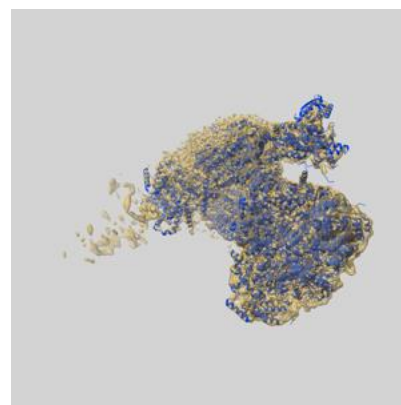
9.1 Map-model overlay [i](#)



X



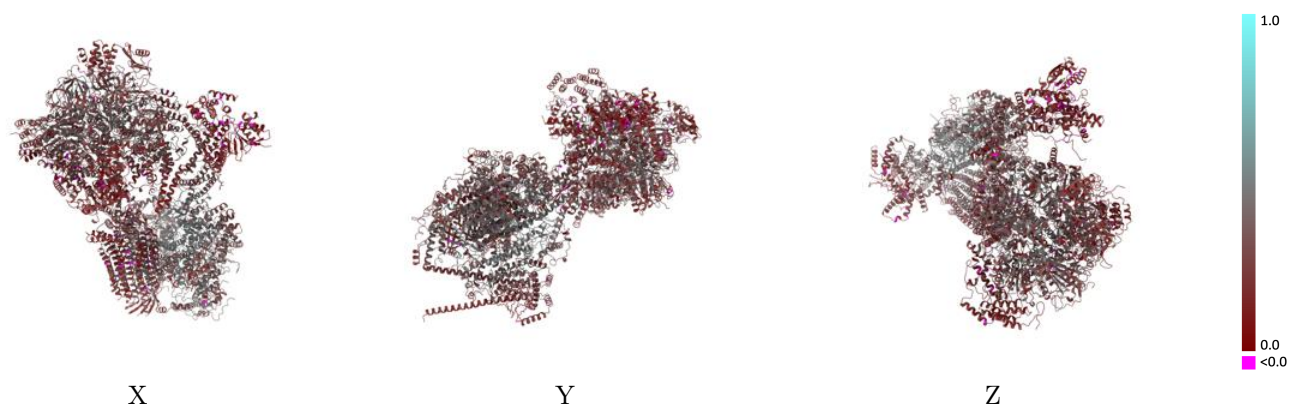
Y



Z

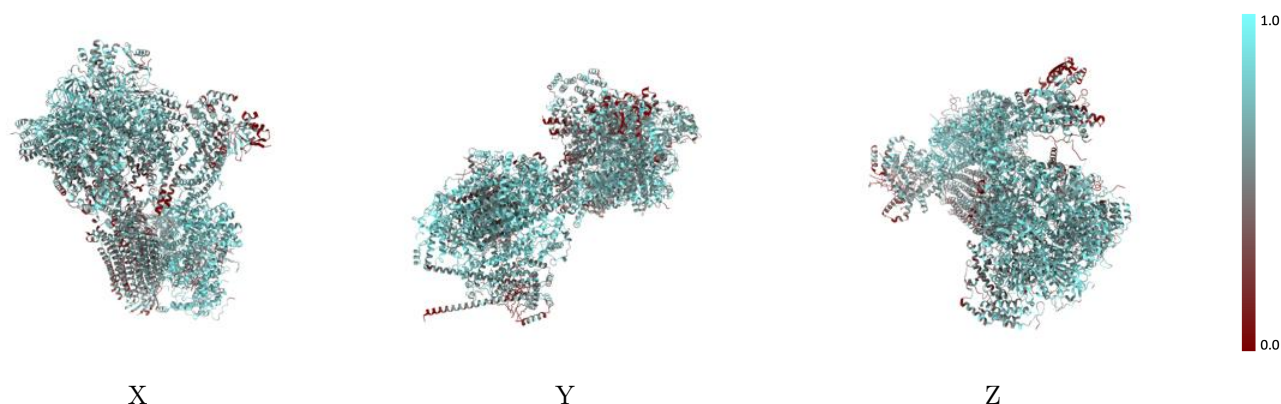
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



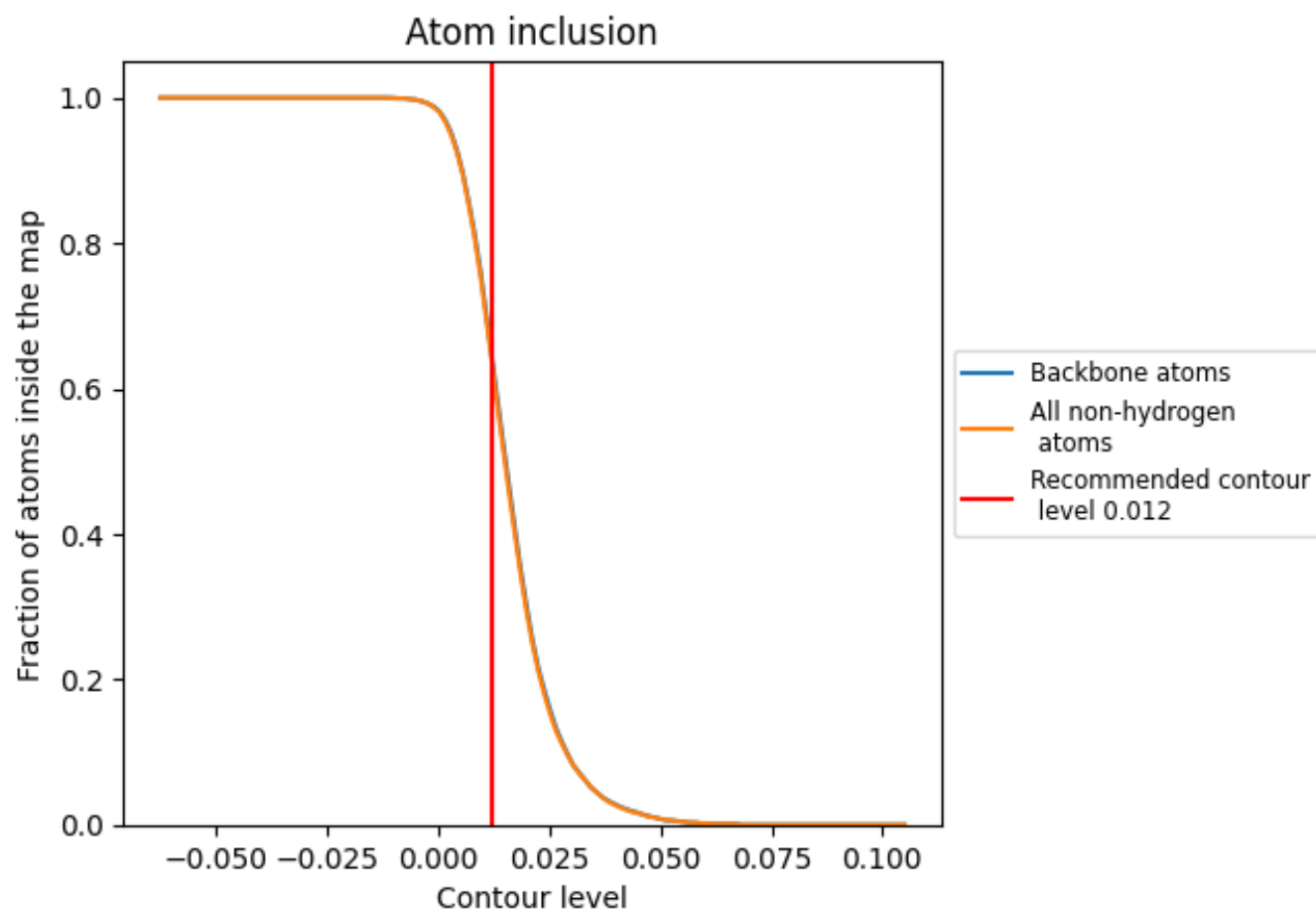
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6410	 0.3110
A1	 0.6600	 0.3130
B1	 0.6630	 0.2880
C1	 0.7210	 0.3610
D1	 0.6690	 0.3330
E1	 0.6620	 0.3110
F1	 0.6360	 0.3040
G1	 0.5510	 0.2790
H1	 0.5040	 0.2720
I1	 0.4840	 0.2510
J1	 0.5820	 0.1870
K1	 0.6450	 0.2780
L	 0.4560	 0.2210
L1	 0.5800	 0.2050
M	 0.4150	 0.2180
M1	 0.5820	 0.2460
O1	 0.5100	 0.2250
P1	 0.4530	 0.2220
Q1	 0.4690	 0.2350
R1	 0.5760	 0.2820
S1	 0.6240	 0.2880
T1	 0.6100	 0.2720
U1	 0.5360	 0.2300
V1	 0.5170	 0.2320
W1	 0.4900	 0.2460
X1	 0.5200	 0.2330
a	 0.7970	 0.4560
c	 0.7590	 0.4300
d	 0.6780	 0.3120
e	 0.7640	 0.3970
f	 0.7730	 0.4300
g	 0.4380	 0.1670
h	 0.5430	 0.1680
i	 0.8280	 0.4400
j	 0.7500	 0.3590



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.7530	 0.3780
l	 0.3980	 0.2110
m	 0.5280	 0.2420
n	 0.8240	 0.4540
o	 0.7820	 0.3610
p	 0.7000	 0.3800
q	 0.7500	 0.4110
r	 0.7660	 0.3940