



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

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

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

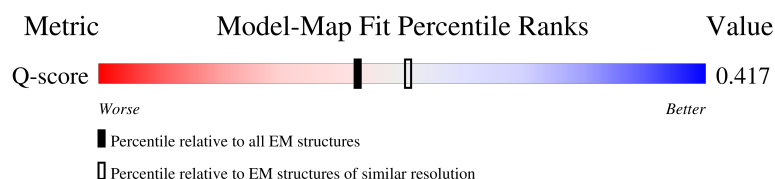
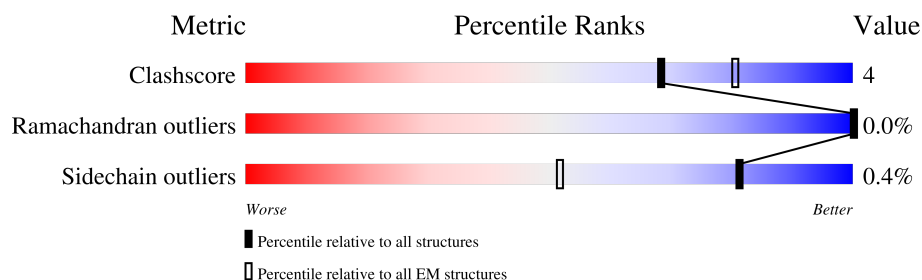
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

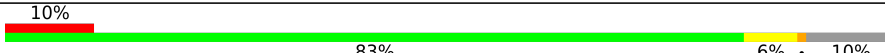
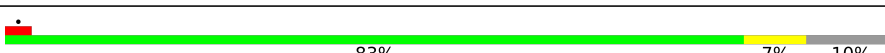
The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	92	
1	l	92	
2	M	144	
2	m	144	

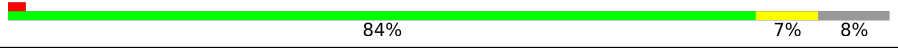
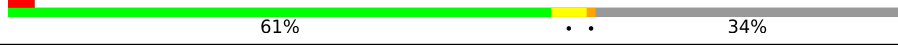
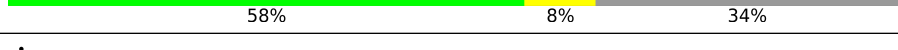
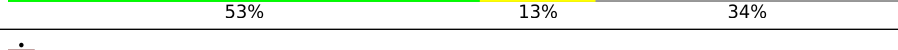
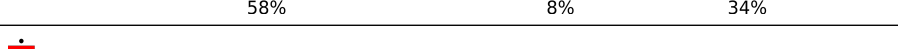
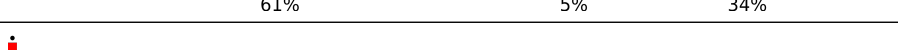
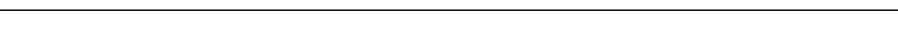
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	Q7G	e	406	X	-	-	-
30	Q7G	n	201	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 129566 atoms, of which 65465 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called subunit-e.

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

- Molecule 2 is a protein called subunit-g.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called subunit-8.

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

- Molecule 5 is a protein called subunit-d.

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

- Molecule 6 is a protein called ATPTB1.

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

- Molecule 7 is a protein called subunit-f.

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

- Molecule 8 is a protein called ATPTB3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 9 is a protein called ATPTB4.

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

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

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

- Molecule 11 is a protein called ATPTB6.

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

- Molecule 12 is a protein called subunit-k.

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

- Molecule 13 is a protein called ATPTB11.

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

- Molecule 14 is a protein called ATPTB12.

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

- Molecule 15 is a protein called subunit-b.

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

- Molecule 16 is a protein called ATPEG3.

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

- Molecule 17 is a protein called ATPEG4.

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

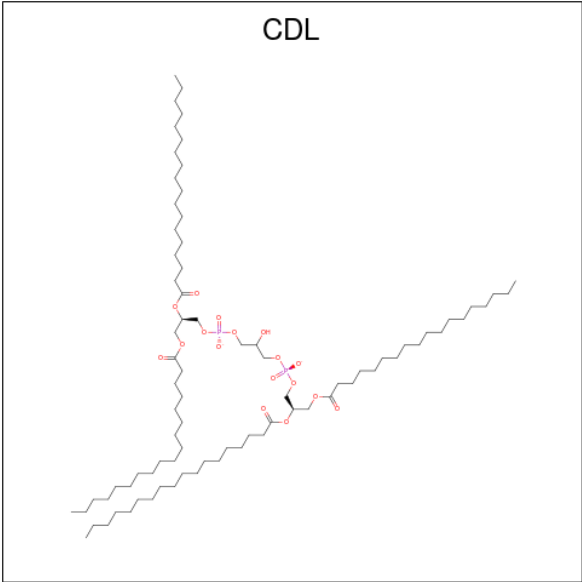
- Molecule 24 is a protein called OSCP.

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

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

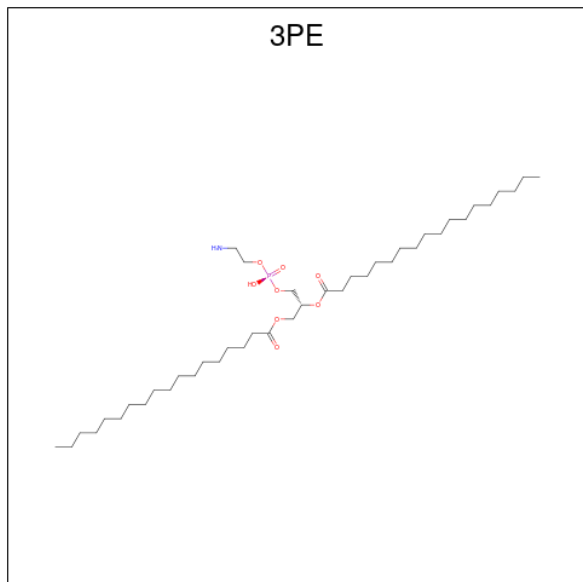
Mol	Chain	Residues	Atoms						AltConf	Trace
25	O1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	P1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	Q1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	R1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	S1	78	Total	C	H	N	O	S	0	0
			1166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

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



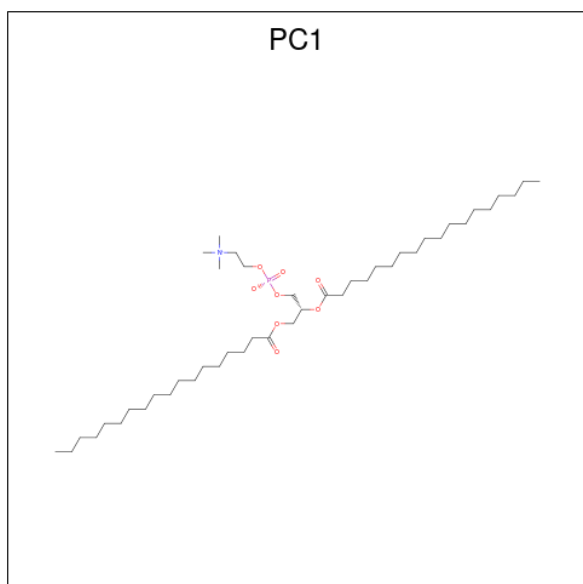
Mol	Chain	Residues	Atoms					AltConf
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1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

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



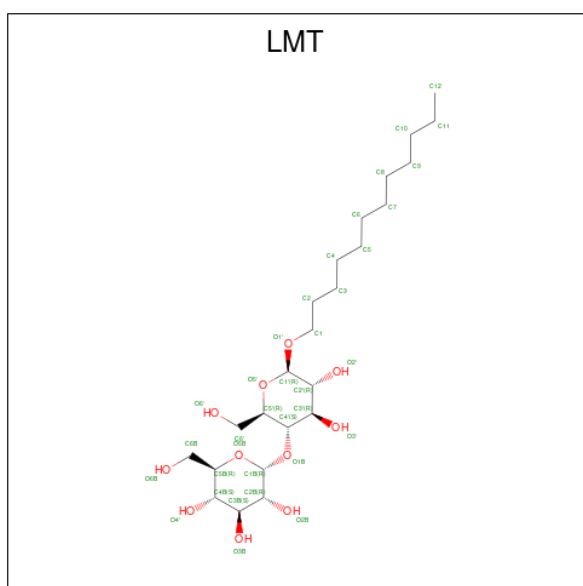
Mol	Chain	Residues	Atoms						AltConf
27	M	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	f	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

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



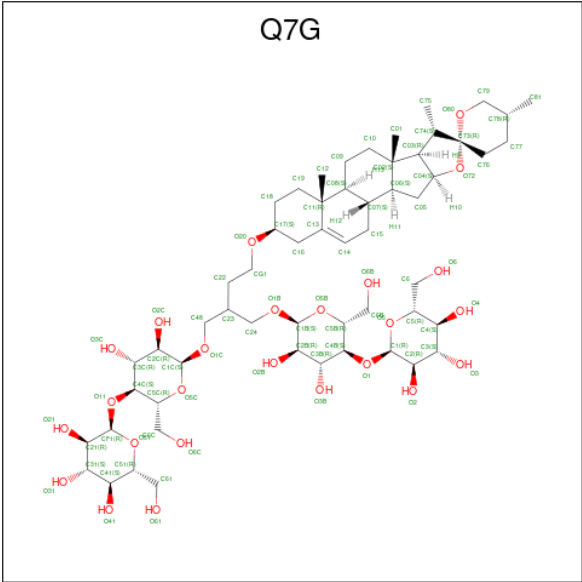
Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total	C	H	N	O	P
			142	44	88	1	8	1
28	i	1	Total	C	H	N	O	P
			142	44	88	1	8	1
28	j	1	Total	C	H	N	O	P
			142	44	88	1	8	1
28	p	1	Total	C	H	N	O	P
			142	44	88	1	8	1

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



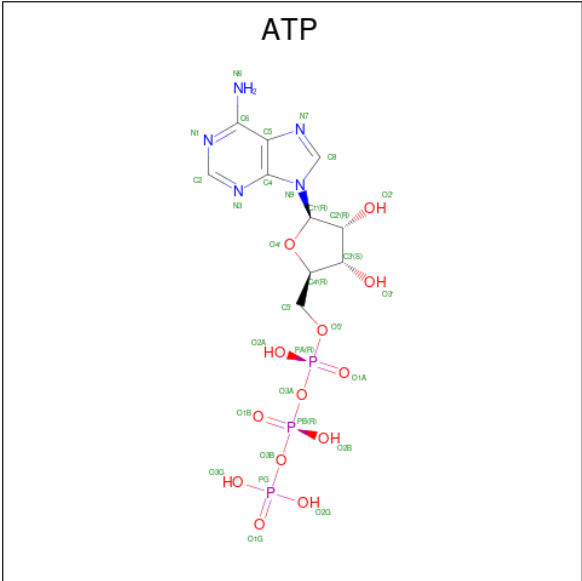
Mol	Chain	Residues	Atoms				AltConf
29	e	1	Total	C	H	O	0
			74	24	39	11	
29	j	1	Total	C	H	O	0
			74	24	39	11	

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



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

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



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

Continued on next page...

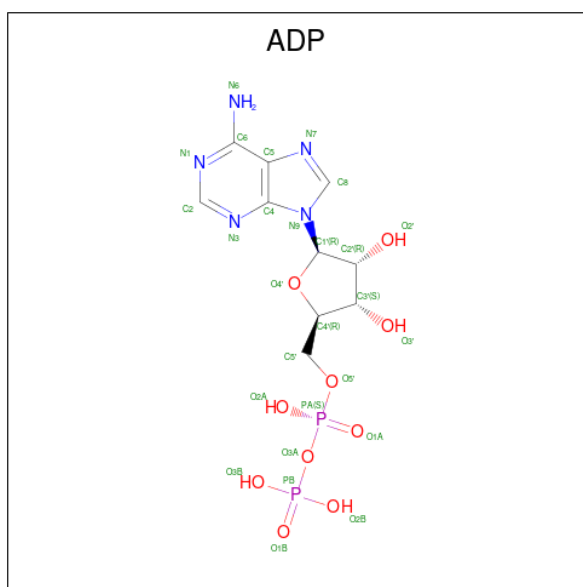
Continued from previous page...

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

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

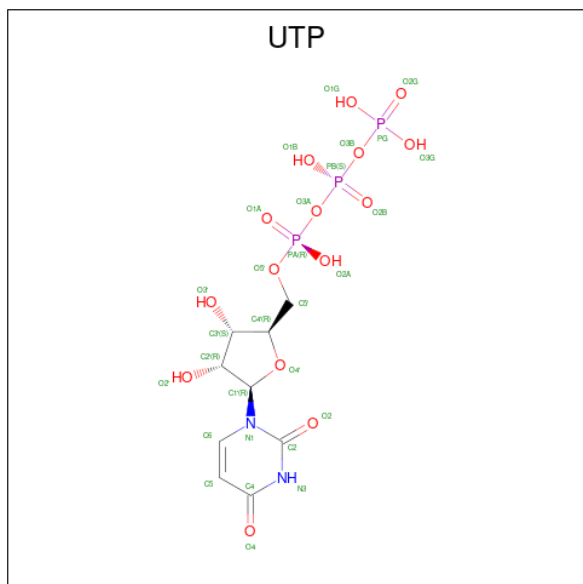
Mol	Chain	Residues	Atoms		AltConf
32	A1	1	Total	Mg	0
			1	1	
32	B1	1	Total	Mg	0
			1	1	
32	C1	1	Total	Mg	0
			1	1	
32	E1	1	Total	Mg	0
			1	1	
32	F1	1	Total	Mg	0
			1	1	

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



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

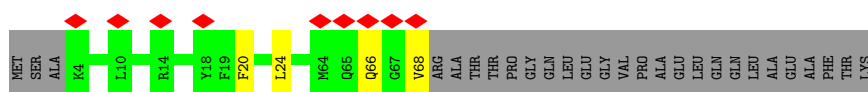
- Molecule 34 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



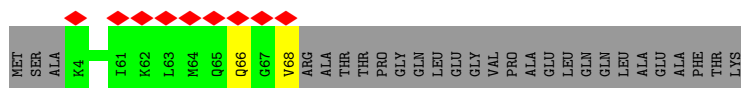
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

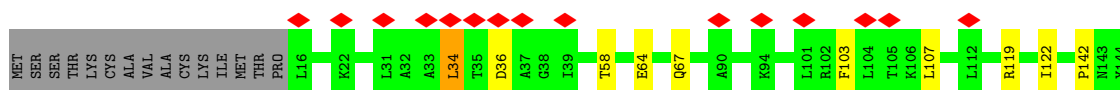
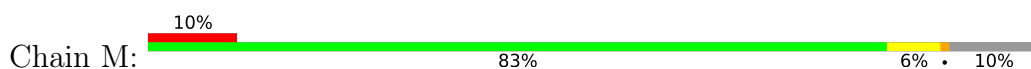
- Molecule 1: subunit-e



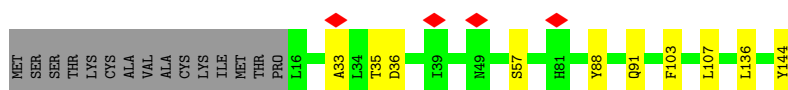
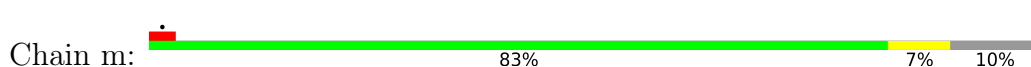
- Molecule 1: subunit-e



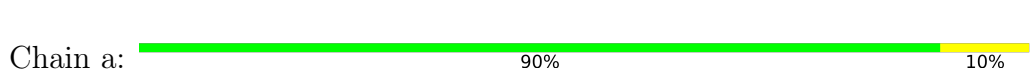
- Molecule 2: subunit-g



- Molecule 2: subunit-g

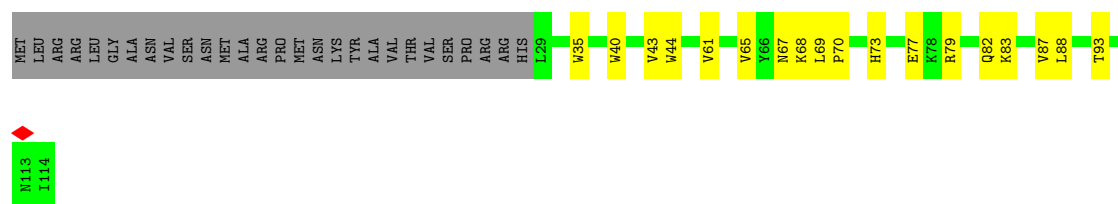


- Molecule 3: ATP synthase subunit a



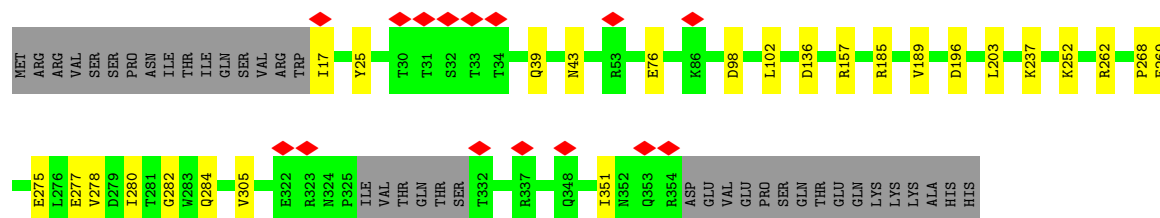
- Molecule 4: subunit-8

Chain c: 



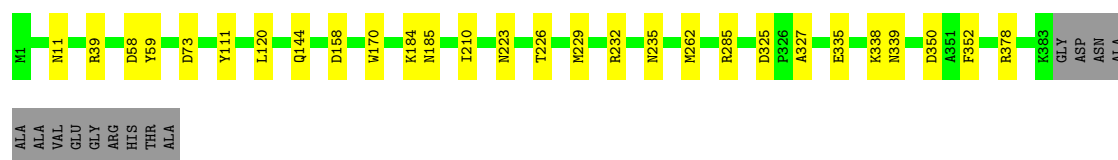
- Molecule 5: subunit-d

Chain d: 



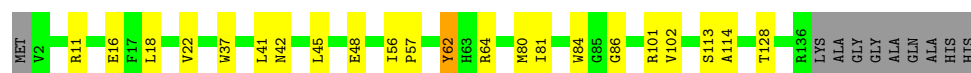
- Molecule 6: ATPTB1

Chain e: 



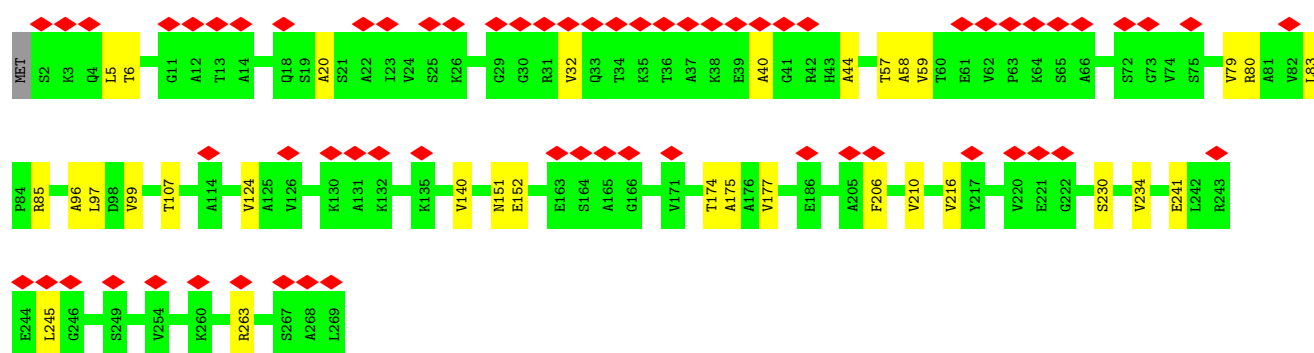
- Molecule 7: subunit-f

Chain f: 

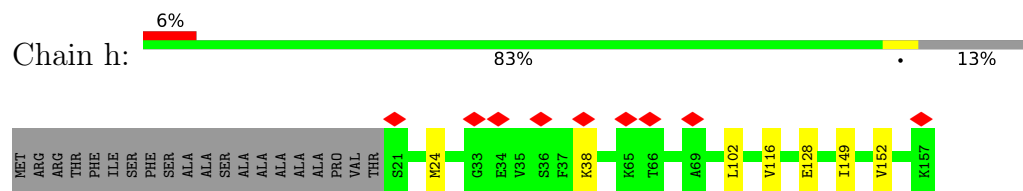


- Molecule 8: ATPTB3

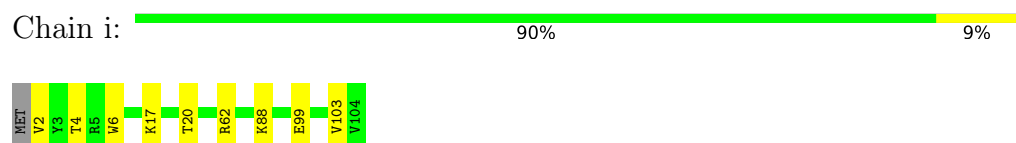
Chain g: 



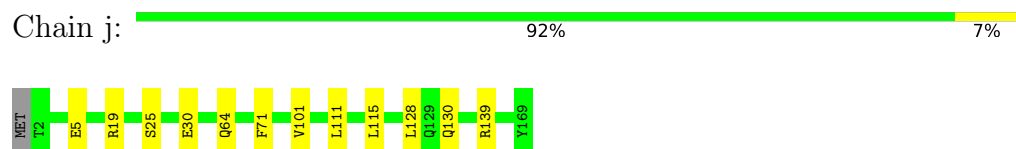
- Molecule 9: ATPTB4



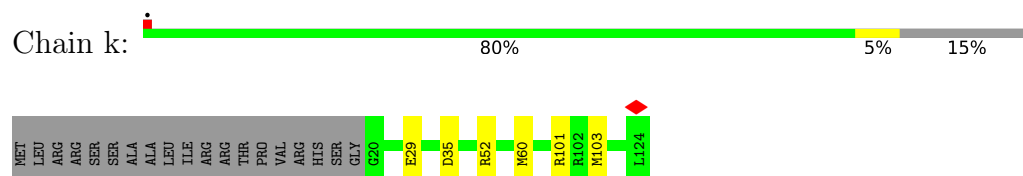
- Molecule 10: subunit-i/j



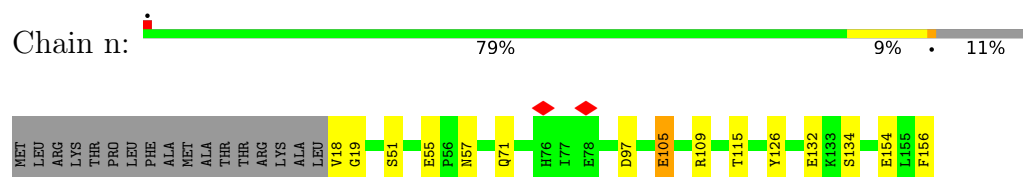
- Molecule 11: ATPTB6



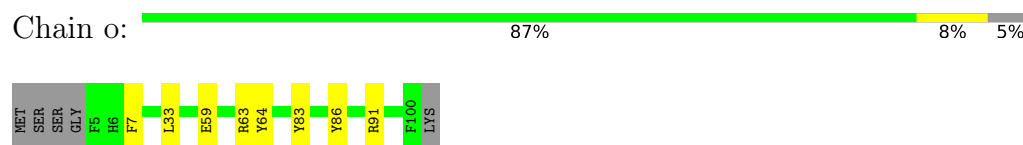
- Molecule 12: subunit-k



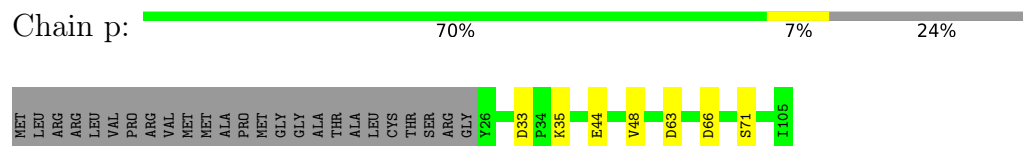
- Molecule 13: ATPTB11



- Molecule 14: ATPTB12

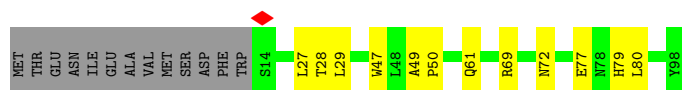


- Molecule 15: subunit-b



- Molecule 16: ATPEG3

Chain q:  74% 12% 13%



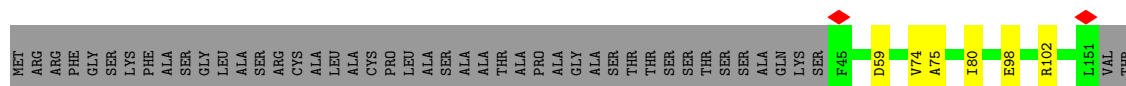
- Molecule 17: ATPEG4

Chain r:  87% 13%



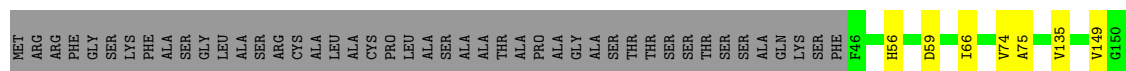
- Molecule 18: ATP synthase subunit alpha, mitochondrial

Chain A1:  79% 11% 10%



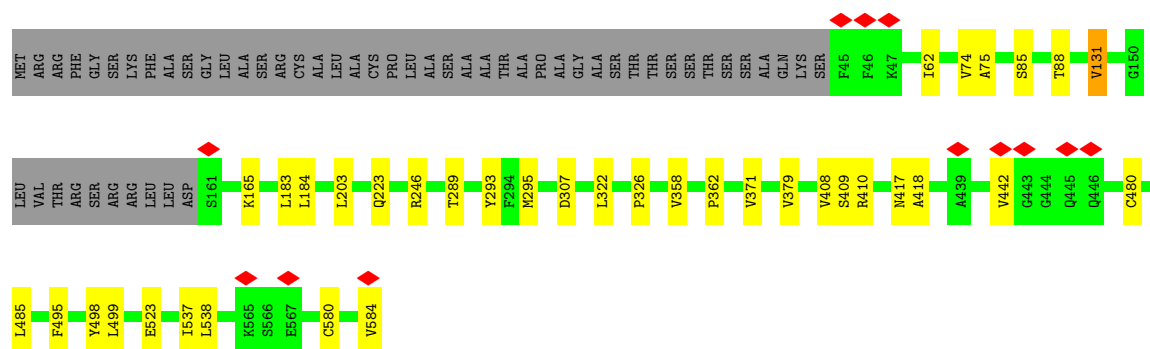
- Molecule 18: ATP synthase subunit alpha, mitochondrial

Chain B1:  79% 10% 11%



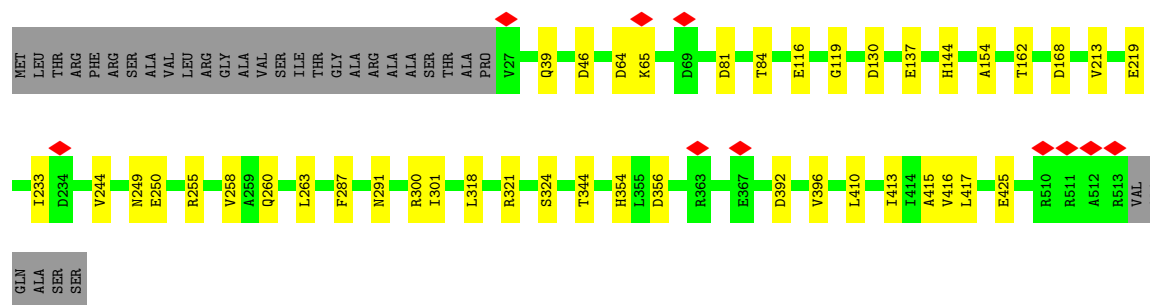
- Molecule 18: ATP synthase subunit alpha, mitochondrial

Chain C1:  84% 6% 9%



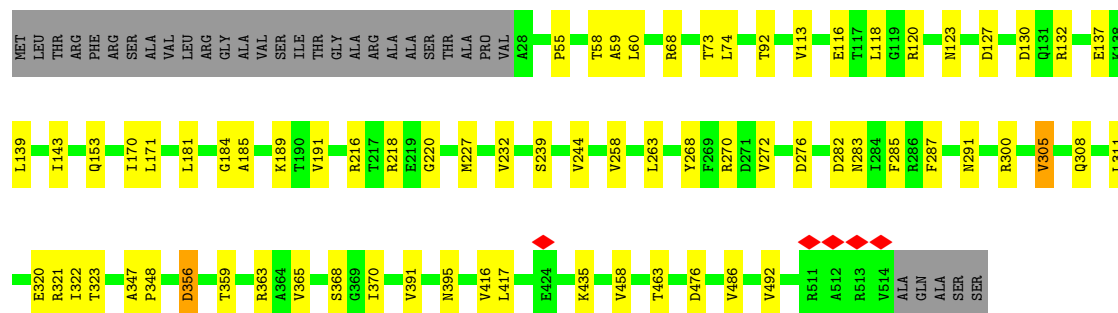
- Molecule 19: ATP synthase subunit beta, mitochondrial

Chain D1: 86% 8% 6%



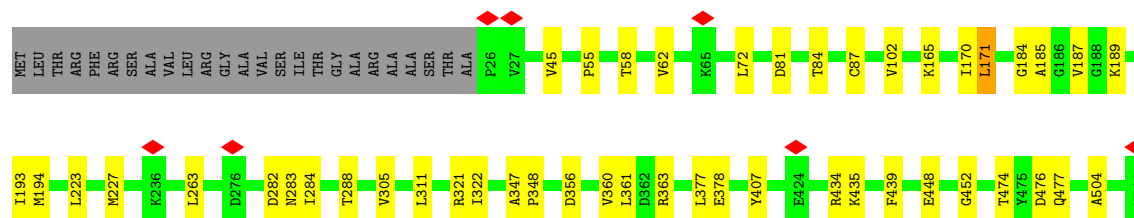
- Molecule 19: ATP synthase subunit beta, mitochondrial

Chain E1: 80% 13% 6%



- Molecule 19: ATP synthase subunit beta, mitochondrial

Chain F1: 85% 9% 6%

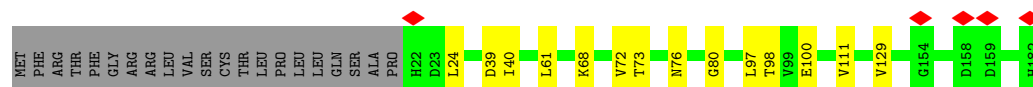
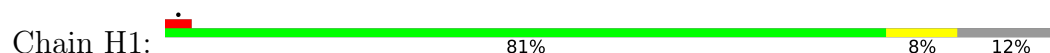




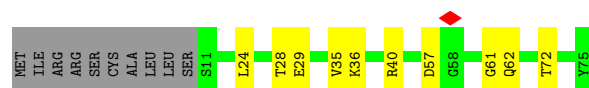
- Molecule 20: ATP synthase gamma subunit



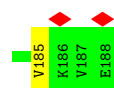
- Molecule 21: ATP synthase, epsilon chain, putative



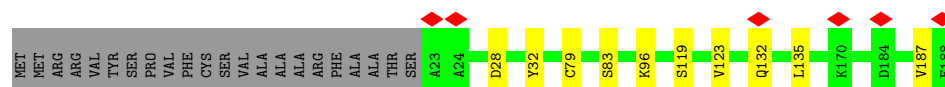
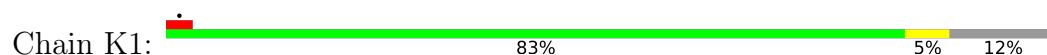
- Molecule 22: ATP synthase subunit epsilon, mitochondrial



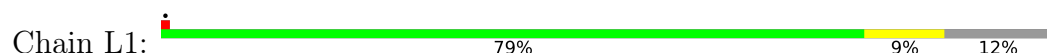
- Molecule 23: ATP synthase subunit p18, mitochondrial



- Molecule 23: ATP synthase subunit p18, mitochondrial

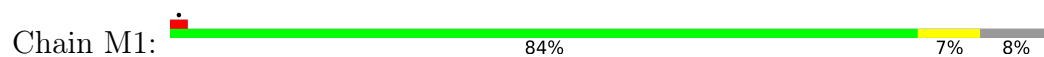


- Molecule 23: ATP synthase subunit p18, mitochondrial

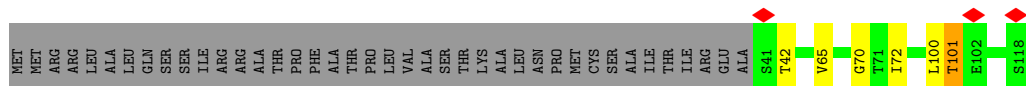




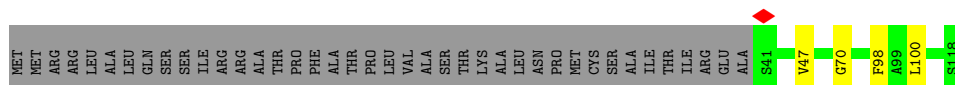
- Molecule 24: OSCP



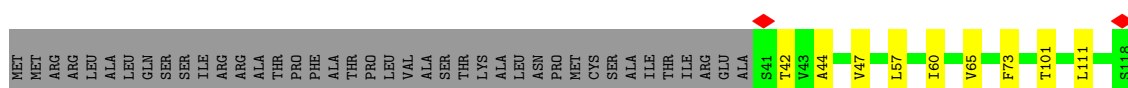
- Molecule 25: ATPase subunit 9, putative



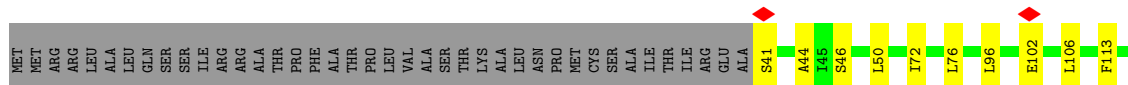
- Molecule 25: ATPase subunit 9, putative



- Molecule 25: ATPase subunit 9, putative

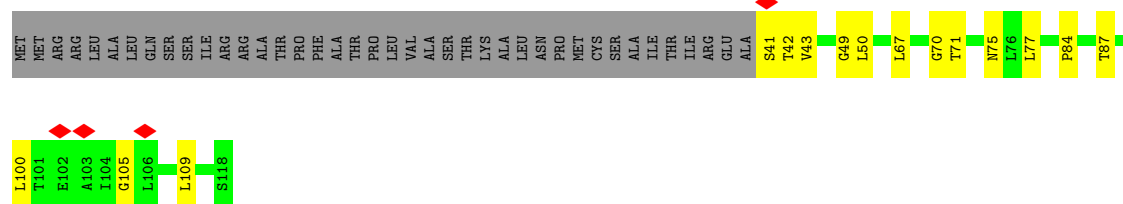


- Molecule 25: ATPase subunit 9, putative



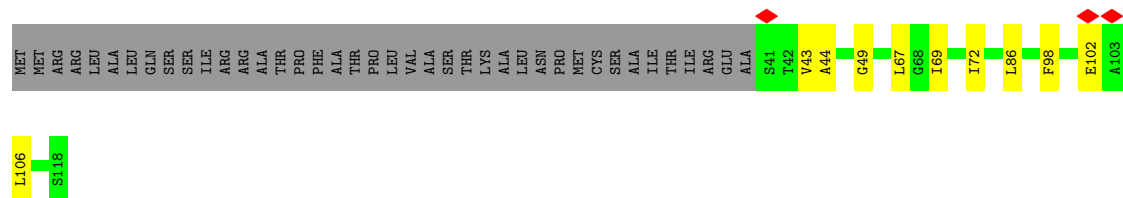
- Molecule 25: ATPase subunit 9, putative

Chain S1: 



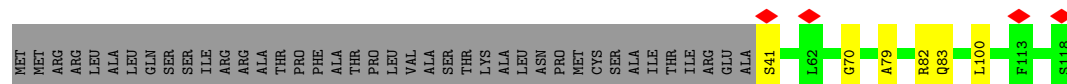
- Molecule 25: ATPase subunit 9, putative

Chain T1: 



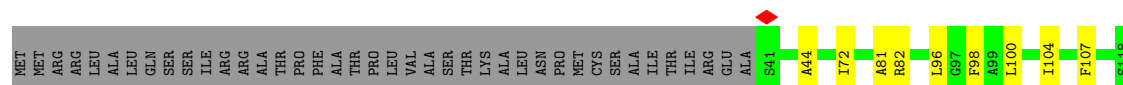
- Molecule 25: ATPase subunit 9, putative

Chain U1: 



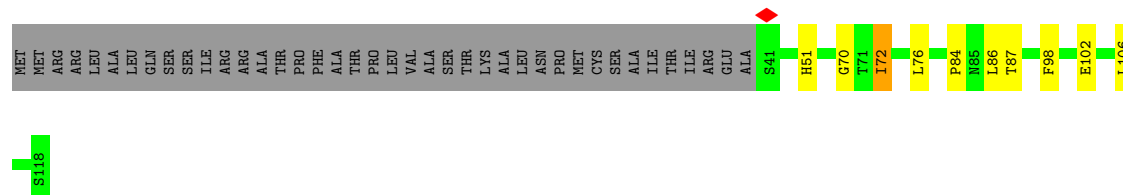
- Molecule 25: ATPase subunit 9, putative

Chain V1: 



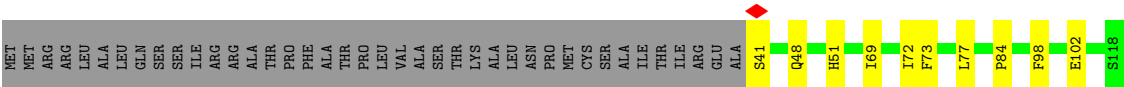
- Molecule 25: ATPase subunit 9, putative

Chain W1: 



- Molecule 25: ATPase subunit 9, putative

Chain X1: 



4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (481) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:j:19:ARG:NH2	16:q:77:GLU:O	2.08	0.85
2:M:119:ARG:NH2	2:M:122:ILE:O	2.18	0.77
2:M:67:GLN:NE2	2:m:36:ASP:OD2	2.19	0.75
19:E1:308:GLN:OE1	19:E1:308:GLN:N	2.21	0.73
25:V1:104:ILE:HD11	25:W1:102:GLU:OE1	1.90	0.72
5:d:76:GLU:OE2	5:d:237:LYS:NZ	2.22	0.71
18:A1:285:TYR:OH	18:A1:338:LEU:HD12	1.89	0.71
15:p:44:GLU:O	15:p:48:VAL:HG23	1.91	0.70
11:j:30:GLU:OE1	16:q:72:ASN:ND2	2.25	0.70
21:H1:80:GLY:O	25:U1:83:GLN:NE2	2.25	0.69
4:c:79:ARG:NH1	4:c:82:GLN:OE1	2.24	0.69
19:D1:81:ASP:OD1	19:D1:84:THR:N	2.26	0.69
5:d:252:LYS:NZ	6:e:339:ASN:OD1	2.25	0.69
5:d:262:ARG:NH2	6:e:335:GLU:O	2.25	0.69
26:j:201:CDL:OB3	26:j:201:CDL:O1	2.10	0.69
23:K1:28:ASP:OD1	23:K1:32:TYR:N	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:5:LEU:HD21	8:g:245:LEU:HD11	1.76	0.68
19:D1:162:THR:OG1	19:D1:168:ASP:OD1	2.09	0.68
18:C1:417:ASN:OD1	18:C1:418:ALA:N	2.27	0.68
19:F1:194:MET:SD	19:F1:223:LEU:HD13	2.34	0.67
5:d:157:ARG:NH1	5:d:203:LEU:O	2.28	0.67
18:B1:523:GLU:N	18:B1:523:GLU:OE1	2.28	0.67
19:E1:189:LYS:N	31:E1:601:ATP:O1B	2.25	0.67
25:W1:86:LEU:HD21	25:X1:84:PRO:HB3	1.76	0.67
18:B1:508:MET:O	23:J1:179:GLN:NE2	2.27	0.67
18:B1:529:ARG:NH1	23:J1:105:GLU:OE1	2.28	0.67
19:D1:213:VAL:HG22	19:D1:258:VAL:CG1	2.25	0.67
4:c:61:VAL:HG13	5:d:278:VAL:HG11	1.78	0.66
2:m:88:TYR:O	2:m:91:GLN:NE2	2.29	0.66
7:f:16:GLU:OE1	7:f:16:GLU:N	2.29	0.66
5:d:280:ILE:O	5:d:280:ILE:HD12	1.96	0.66
19:D1:263:LEU:HD21	19:D1:321:ARG:HB2	1.79	0.65
18:B1:223:GLN:O	18:B1:227:ASN:ND2	2.30	0.65
18:A1:192:THR:HG22	18:A1:420:MET:SD	2.37	0.65
19:F1:81:ASP:OD1	19:F1:84:THR:N	2.30	0.65
13:n:132:GLU:OE1	16:q:28:THR:OG1	2.12	0.65
11:j:64:GLN:NE2	28:j:202:PC1:O22	2.31	0.64
3:a:150:ASN:HA	25:W1:106:LEU:HD13	1.79	0.64
19:D1:137:GLU:N	19:D1:137:GLU:OE1	2.31	0.64
10:i:2:VAL:N	13:n:97:ASP:OD1	2.31	0.64
24:M1:45:ASP:OD2	24:M1:115:MET:HE1	1.97	0.64
19:E1:184:GLY:O	19:E1:189:LYS:NZ	2.31	0.63
15:p:71:SER:O	17:r:16:ARG:NH1	2.32	0.63
23:J1:58:LEU:O	23:J1:62:ASN:ND2	2.30	0.63
18:A1:203:LEU:HD13	18:A1:379:VAL:HG11	1.81	0.63
23:J1:157:ALA:O	23:J1:161:ASN:ND2	2.31	0.63
1:L:66:GLN:HG3	1:L:68:VAL:HG23	1.78	0.63
18:B1:192:THR:HG22	18:B1:420:MET:HE3	1.81	0.62
18:B1:537:ILE:HD13	23:J1:142:VAL:HG22	1.80	0.62
18:A1:495:PHE:CE2	18:A1:499:LEU:HD11	2.34	0.62
25:O1:72:ILE:HD11	25:P1:70:GLY:HA2	1.81	0.62
25:S1:100:LEU:HD13	25:T1:98:PHE:CE1	2.35	0.62
15:p:66:ASP:OD1	17:r:13:GLN:NE2	2.32	0.62
16:q:27:LEU:HD21	16:q:29:LEU:HD21	1.82	0.62
1:l:66:GLN:HG3	1:l:68:VAL:HG23	1.80	0.62
6:e:111:TYR:OH	16:q:47:TRP:O	2.14	0.61
19:E1:435:LYS:NZ	19:E1:476:ASP:O	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U1:100:LEU:HD13	25:V1:98:PHE:CE1	2.35	0.61
19:E1:185:ALA:O	19:E1:363:ARG:NH2	2.33	0.61
6:e:185:ASN:ND2	6:e:325:ASP:OD1	2.34	0.61
19:F1:347:ALA:HB3	19:F1:348:PRO:HD3	1.82	0.61
24:M1:88:ALA:HB1	24:M1:93:ILE:HD11	1.82	0.61
25:O1:65:VAL:HG13	25:O1:101:THR:HG22	1.83	0.60
14:o:86:TYR:O	14:o:91:ARG:NE	2.32	0.60
18:A1:454:ARG:NH2	18:A1:482:ASN:O	2.33	0.60
19:F1:448:GLU:O	19:F1:452:GLY:N	2.32	0.60
18:B1:527:LEU:HD23	23:J1:101:MET:HE2	1.83	0.60
13:n:154:GLU:N	13:n:154:GLU:OE1	2.32	0.60
18:C1:184:LEU:O	18:C1:223:GLN:NE2	2.35	0.60
18:B1:247:CYS:SG	19:E1:153:GLN:NE2	2.75	0.59
19:D1:425:GLU:N	19:D1:425:GLU:OE1	2.36	0.59
34:H1:201:UTP:O1B	25:U1:82:ARG:NH1	2.35	0.59
6:e:226:THR:OG1	26:e:401:CDL:OA4	2.20	0.59
6:e:210:ILE:O	6:e:232:ARG:NH2	2.36	0.58
19:F1:263:LEU:HD13	19:F1:322:ILE:HG12	1.85	0.58
26:c:201:CDL:H872	26:c:201:CDL:H832	1.84	0.58
18:A1:301:CYS:SG	18:A1:302:LEU:N	2.76	0.58
19:E1:268:TYR:CE2	19:E1:272:VAL:HG21	2.38	0.58
23:J1:181:GLY:O	23:J1:185:VAL:HG23	2.03	0.58
7:f:64:ARG:NH2	17:r:33:GLU:OE2	2.36	0.58
5:d:269:GLU:OE1	6:e:184:LYS:NZ	2.33	0.58
3:a:85:LEU:HD12	3:a:148:PHE:HB2	1.84	0.58
11:j:111:LEU:HD11	11:j:115:LEU:HD11	1.86	0.57
25:U1:41:SER:O	25:V1:44:ALA:O	2.22	0.57
25:V1:100:LEU:HD13	25:W1:98:PHE:CE1	2.39	0.57
9:h:116:VAL:HG23	9:h:152:VAL:HG23	1.86	0.57
19:F1:171:LEU:HD23	19:F1:171:LEU:N	2.20	0.57
25:R1:41:SER:N	25:S1:43:VAL:HA	2.19	0.57
13:n:51:SER:OG	13:n:55:GLU:OE2	2.23	0.57
19:E1:320:GLU:O	19:E1:323:THR:HG22	2.05	0.57
11:j:128:LEU:O	11:j:139:ARG:NH1	2.37	0.57
19:D1:119:GLY:HA2	19:D1:233:ILE:HG23	1.86	0.57
20:G1:195:ASN:OD1	20:G1:196:GLN:N	2.37	0.56
18:A1:527:LEU:HD23	23:L1:101:MET:HE2	1.88	0.56
19:D1:130:ASP:O	23:K1:32:TYR:OH	2.23	0.56
22:I1:29:GLU:OE1	22:I1:72:THR:HG21	2.05	0.56
18:C1:410:ARG:NH1	19:D1:219:GLU:OE2	2.38	0.56
2:m:103:PHE:CZ	2:m:107:LEU:HD11	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W1:84:PRO:O	25:W1:87:THR:HG23	2.05	0.56
6:e:229:MET:SD	6:e:235:ASN:ND2	2.79	0.56
18:A1:212:LYS:HG2	18:A1:389:LEU:HD12	1.88	0.56
6:e:58:ASP:OD1	6:e:59:TYR:N	2.37	0.56
8:g:83:LEU:O	8:g:85:ARG:NH1	2.39	0.56
20:G1:97:VAL:HG12	20:G1:97:VAL:O	2.06	0.56
24:M1:33:GLU:OE1	24:M1:33:GLU:N	2.36	0.56
23:K1:119:SER:O	23:K1:123:VAL:HG23	2.05	0.55
19:F1:185:ALA:O	19:F1:363:ARG:NH2	2.38	0.55
9:h:128:GLU:HG2	9:h:149:ILE:HD11	1.88	0.55
18:C1:580:CYS:O	18:C1:584:VAL:HG22	2.06	0.55
19:E1:287:PHE:O	19:E1:291:ASN:ND2	2.38	0.55
25:X1:48:GLN:O	25:X1:51:HIS:ND1	2.39	0.55
19:E1:486:VAL:HG21	19:E1:492:VAL:HG22	1.88	0.55
18:A1:173:ILE:HD11	19:E1:220:GLY:C	2.32	0.55
18:B1:209:GLN:NE2	31:B1:601:ATP:O3G	2.39	0.55
23:J1:28:ASP:OD1	23:J1:32:TYR:N	2.40	0.55
24:M1:212:VAL:HG13	24:M1:214:TYR:CZ	2.42	0.55
7:f:64:ARG:NH1	17:r:33:GLU:OE1	2.40	0.54
19:F1:189:LYS:NZ	33:F1:601:ADP:O3B	2.35	0.54
8:g:20:ALA:HB2	8:g:234:VAL:HG11	1.89	0.54
19:E1:143:ILE:O	19:E1:321:ARG:NH1	2.39	0.54
25:W1:72:ILE:HD11	25:X1:73:PHE:HB2	1.90	0.54
18:A1:246:ARG:NH1	19:D1:356:ASP:OD1	2.37	0.54
19:E1:416:VAL:HG23	19:E1:417:LEU:N	2.22	0.54
20:G1:54:PHE:O	20:G1:56:LYS:NZ	2.28	0.54
19:D1:116:GLU:OE1	19:D1:116:GLU:N	2.37	0.54
25:Q1:65:VAL:HG13	25:Q1:101:THR:HG22	1.88	0.54
19:E1:55:PRO:O	19:E1:58:THR:OG1	2.26	0.54
3:a:63:PHE:HB3	3:a:210:LEU:HD21	1.89	0.54
25:T1:72:ILE:HD11	25:U1:70:GLY:HA2	1.89	0.54
7:f:101:ARG:NH1	17:r:45:ASP:O	2.42	0.53
19:D1:39:GLN:NE2	19:D1:46:ASP:OD2	2.41	0.53
21:H1:39:ASP:OD1	21:H1:40:ILE:N	2.42	0.53
18:B1:495:PHE:CE2	18:B1:499:LEU:HD11	2.44	0.53
19:D1:263:LEU:HD21	19:D1:321:ARG:CB	2.37	0.53
19:E1:244:VAL:HG12	19:E1:258:VAL:HG23	1.91	0.53
20:G1:122:GLU:N	20:G1:122:GLU:OE1	2.42	0.53
3:a:14:LEU:HG	13:n:115:THR:HG23	1.91	0.53
15:p:33:ASP:OD2	15:p:35:LYS:NZ	2.31	0.53
18:A1:98:GLU:OE1	18:A1:102:ARG:NH1	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H1:129:VAL:CG1	22:I1:28:THR:HG21	2.39	0.52
18:A1:561:MET:HA	18:A1:564:ILE:HD12	1.91	0.52
6:e:144:GLN:OE1	6:e:223:ASN:ND2	2.41	0.52
18:A1:246:ARG:NH1	19:D1:354:HIS:O	2.42	0.52
18:A1:489:LYS:O	18:A1:493:VAL:HG23	2.09	0.52
18:C1:498:TYR:CE1	23:K1:187:VAL:HG22	2.44	0.52
25:S1:100:LEU:HD13	25:T1:98:PHE:CD1	2.43	0.52
3:a:12:LEU:HD13	3:a:65:LEU:HD22	1.92	0.52
2:M:58:THR:OG1	26:l:101:CDL:OA3	2.16	0.52
5:d:280:ILE:HD13	6:e:158:ASP:HA	1.90	0.52
18:A1:566:SER:O	18:A1:570:VAL:HG23	2.09	0.52
19:F1:288:THR:HG23	19:F1:311:LEU:HD13	1.92	0.52
3:a:26:LEU:O	4:c:67:ASN:ND2	2.41	0.52
18:A1:203:LEU:HD13	18:A1:379:VAL:CG1	2.40	0.52
18:A1:228:GLN:O	23:L1:86:LYS:NZ	2.37	0.52
8:g:59:VAL:HG13	8:g:216:VAL:HB	1.92	0.52
8:g:206:PHE:O	8:g:210:VAL:HG23	2.09	0.52
25:O1:42:THR:O	25:X1:41:SER:N	2.43	0.52
21:H1:97:LEU:HD23	21:H1:98:THR:N	2.25	0.52
4:c:93:THR:HG21	5:d:136:ASP:OD2	2.10	0.52
18:B1:514:ASN:O	18:B1:518:TYR:OH	2.21	0.52
19:F1:477:GLN:N	19:F1:477:GLN:OE1	2.40	0.52
18:A1:293:TYR:O	18:A1:297:ARG:NH1	2.40	0.51
18:B1:210:THR:N	31:B1:601:ATP:O1B	2.43	0.51
2:M:103:PHE:CE2	2:M:107:LEU:HD11	2.45	0.51
18:B1:184:LEU:O	18:B1:223:GLN:NE2	2.43	0.51
19:D1:244:VAL:HG12	19:D1:258:VAL:HG23	1.92	0.51
22:I1:29:GLU:CD	22:I1:72:THR:HG21	2.35	0.51
5:d:284:GLN:OE1	5:d:284:GLN:N	2.37	0.51
20:G1:196:GLN:OE1	20:G1:199:ARG:NH2	2.42	0.51
25:S1:71:THR:O	25:S1:75:ASN:ND2	2.44	0.51
28:a:302:PC1:O14	17:r:30:TRP:NE1	2.42	0.51
22:I1:24:LEU:O	22:I1:28:THR:HG23	2.10	0.51
24:M1:148:GLU:O	24:M1:151:VAL:HG13	2.11	0.51
8:g:6:THR:HG21	8:g:40:ALA:HB2	1.93	0.51
19:F1:377:LEU:HD22	19:F1:377:LEU:H	1.75	0.51
23:L1:153:ASP:OD1	23:L1:154:LEU:N	2.44	0.51
25:S1:41:SER:O	25:T1:43:VAL:HG13	2.11	0.51
18:A1:343:LEU:HD12	18:A1:382:ILE:HG21	1.91	0.51
20:G1:26:LYS:HB2	20:G1:245:VAL:HG11	1.92	0.51
18:B1:527:LEU:HD23	23:J1:101:MET:CE	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:8:ASP:OD1	13:n:126:TYR:OH	2.26	0.50
5:d:39:GLN:NE2	5:d:43:ASN:OD1	2.44	0.50
19:E1:311:LEU:C	19:E1:311:LEU:HD23	2.36	0.50
22:I1:62:GLN:N	22:I1:62:GLN:OE1	2.44	0.50
11:j:25:SER:OG	11:j:130:GLN:NE2	2.44	0.50
18:A1:495:PHE:CZ	18:A1:499:LEU:HD11	2.46	0.50
19:D1:410:LEU:HD23	19:D1:413:ILE:HD12	1.92	0.50
3:a:1:MET:HE1	4:c:35:TRP:CZ3	2.46	0.50
3:a:1:MET:HE1	4:c:35:TRP:HZ3	1.76	0.50
19:F1:170:ILE:HB	19:F1:171:LEU:HD23	1.93	0.50
25:S1:42:THR:HA	25:T1:44:ALA:O	2.11	0.50
10:i:62:ARG:NH2	13:n:134:SER:O	2.43	0.50
16:q:77:GLU:OE2	16:q:79:HIS:NE2	2.45	0.50
18:C1:246:ARG:NH1	19:F1:356:ASP:OD1	2.44	0.50
19:D1:244:VAL:HG12	19:D1:258:VAL:CG2	2.42	0.50
19:F1:435:LYS:NZ	19:F1:476:ASP:O	2.44	0.50
19:D1:287:PHE:O	19:D1:291:ASN:ND2	2.38	0.50
12:k:29:GLU:N	12:k:29:GLU:OE1	2.43	0.50
19:E1:244:VAL:HG12	19:E1:258:VAL:CG2	2.42	0.50
18:B1:269:MET:SD	18:B1:286:ALA:HB3	2.51	0.50
25:O1:70:GLY:HA2	25:X1:72:ILE:HD11	1.93	0.50
18:C1:442:VAL:HB	20:G1:24:THR:HG21	1.94	0.50
18:A1:478:TYR:O	18:A1:482:ASN:ND2	2.40	0.49
18:C1:485:LEU:HD12	18:C1:485:LEU:N	2.27	0.49
23:K1:79:CYS:O	23:K1:83:SER:OG	2.16	0.49
2:M:34:LEU:HD12	2:M:36:ASP:H	1.77	0.49
2:M:103:PHE:CZ	2:M:107:LEU:HD11	2.47	0.49
23:J1:163:GLN:O	23:J1:167:THR:HG23	2.12	0.49
18:B1:489:LYS:O	18:B1:493:VAL:HG23	2.12	0.49
8:g:57:THR:HG21	8:g:124:VAL:HG11	1.93	0.49
26:k:201:CDL:OB5	16:q:69:ARG:NH2	2.45	0.49
18:A1:269:MET:HE1	18:A1:286:ALA:CB	2.42	0.49
18:A1:381:SER:O	19:E1:216:ARG:NH2	2.45	0.49
19:E1:270:ARG:NH1	19:E1:323:THR:O	2.46	0.49
4:c:40:TRP:O	4:c:43:VAL:HG12	2.12	0.49
19:D1:263:LEU:HD22	19:D1:318:LEU:HD12	1.94	0.49
23:K1:132:GLN:OE1	23:K1:135:LEU:HD12	2.12	0.49
25:R1:102:GLU:O	25:R1:106:LEU:HD13	2.13	0.49
25:V1:100:LEU:HD13	25:W1:98:PHE:CD1	2.47	0.49
23:L1:187:VAL:HG12	23:L1:187:VAL:O	2.13	0.49
26:j:201:CDL:H1O1	26:j:201:CDL:PB2	2.35	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:105:GLU:OE2	13:n:109:ARG:NH1	2.42	0.49
19:E1:170:ILE:HB	19:E1:171:LEU:HD23	1.94	0.49
23:L1:173:PRO:HD2	23:L1:176:LEU:HD12	1.94	0.49
18:B1:183:LEU:HD23	18:B1:183:LEU:C	2.38	0.48
25:S1:84:PRO:O	25:S1:87:THR:OG1	2.28	0.48
8:g:59:VAL:HG23	8:g:79:VAL:HG22	1.95	0.48
13:n:57:ASN:ND2	13:n:71:GLN:O	2.40	0.48
5:d:268:PRO:HB2	6:e:327:ALA:HB3	1.95	0.48
19:D1:392:ASP:O	19:D1:396:VAL:HG23	2.14	0.48
22:I1:35:VAL:O	22:I1:40:ARG:NH2	2.45	0.48
24:M1:239:TYR:CE2	24:M1:243:LEU:HD11	2.49	0.48
3:a:157:LEU:HD22	25:V1:107:PHE:CE1	2.48	0.48
18:B1:192:THR:CG2	18:B1:420:MET:HE3	2.43	0.48
12:k:35:ASP:OD1	12:k:52:ARG:NH2	2.44	0.48
2:M:34:LEU:HD12	2:M:34:LEU:C	2.39	0.48
25:T1:69:ILE:HD12	25:T1:98:PHE:HD1	1.79	0.48
18:A1:207:ASP:OD1	18:A1:208:ARG:N	2.43	0.47
3:a:166:TYR:CE2	28:a:302:PC1:H152	2.50	0.47
18:B1:423:VAL:HG21	18:B1:474:ILE:HD11	1.95	0.47
18:C1:326:PRO:HD2	20:G1:282:MET:HE1	1.96	0.47
18:A1:226:ILE:N	18:A1:226:ILE:HD12	2.29	0.47
18:C1:183:LEU:HD23	18:C1:184:LEU:N	2.29	0.47
19:D1:144:HIS:ND1	19:D1:260:GLN:OE1	2.47	0.47
4:c:43:VAL:HG13	4:c:44:TRP:N	2.29	0.47
19:E1:116:GLU:OE1	19:E1:116:GLU:N	2.41	0.47
18:C1:495:PHE:CE2	18:C1:499:LEU:HD11	2.50	0.47
19:E1:365:VAL:O	19:E1:368:SER:OG	2.31	0.47
18:C1:203:LEU:HD13	18:C1:379:VAL:CG1	2.44	0.47
19:D1:249:ASN:OD1	19:D1:250:GLU:N	2.48	0.47
19:E1:59:ALA:C	19:E1:60:LEU:HD12	2.40	0.47
19:E1:123:ASN:OD1	19:E1:127:ASP:N	2.46	0.47
19:F1:360:VAL:HG11	19:F1:378:GLU:OE1	2.15	0.47
25:O1:100:LEU:HD23	25:P1:98:PHE:CD1	2.50	0.47
25:P1:47:VAL:HG23	25:Q1:47:VAL:HG13	1.97	0.47
8:g:96:ALA:HA	8:g:99:VAL:HG12	1.95	0.47
16:q:49:ALA:N	16:q:50:PRO:CD	2.78	0.47
19:D1:250:GLU:O	19:D1:255:ARG:NH1	2.48	0.47
19:E1:120:ARG:NE	19:E1:130:ASP:OD2	2.44	0.47
19:F1:407:TYR:OH	19:F1:434:ARG:NH1	2.48	0.47
25:R1:76:LEU:HA	25:S1:77:LEU:HD13	1.96	0.47
6:e:350:ASP:OD1	6:e:352:PHE:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B1:293:TYR:O	18:B1:297:ARG:NH1	2.42	0.47
19:E1:347:ALA:HB3	19:E1:348:PRO:CD	2.46	0.47
24:M1:118:LEU:O	24:M1:122:VAL:HG23	2.15	0.47
21:H1:97:LEU:HD23	21:H1:97:LEU:C	2.40	0.46
25:R1:50:LEU:HD12	25:S1:49:GLY:C	2.41	0.46
8:g:151:ASN:OD1	8:g:152:GLU:N	2.48	0.46
18:A1:485:LEU:HD12	18:A1:485:LEU:N	2.29	0.46
18:B1:531:PHE:O	18:B1:532:THR:CB	2.62	0.46
1:L:20:PHE:CE2	1:L:24:LEU:HD11	2.51	0.46
22:I1:35:VAL:HG12	22:I1:36:LYS:N	2.31	0.46
19:E1:139:LEU:C	19:E1:139:LEU:HD12	2.40	0.46
6:e:226:THR:O	6:e:229:MET:N	2.49	0.46
18:B1:503:ARG:NH1	23:J1:185:VAL:HG13	2.31	0.46
3:a:67:ASN:O	3:a:70:SER:OG	2.21	0.46
7:f:11:ARG:NE	26:f:201:CDL:OB3	2.44	0.46
19:E1:263:LEU:HD21	19:E1:321:ARG:CB	2.46	0.46
23:L1:143:MET:O	23:L1:147:CYS:N	2.49	0.46
18:B1:457:ARG:NH2	18:B1:488:VAL:O	2.38	0.46
19:D1:119:GLY:CA	19:D1:233:ILE:HG23	2.46	0.46
19:E1:68:ARG:NH1	19:E1:92:THR:O	2.48	0.46
19:F1:184:GLY:O	19:F1:189:LYS:NZ	2.49	0.46
18:A1:311:GLN:HE21	18:A1:338:LEU:HD11	1.81	0.46
18:A1:379:VAL:O	18:A1:383:THR:HG23	2.16	0.46
18:A1:532:THR:HG23	18:A1:535:SER:H	1.82	0.46
25:S1:105:GLY:O	25:S1:109:LEU:HD23	2.16	0.46
8:g:58:ALA:HB3	8:g:80:ARG:HB3	1.99	0.45
5:d:277:GLU:O	5:d:282:GLY:N	2.48	0.45
18:A1:307:ASP:N	18:A1:307:ASP:OD1	2.48	0.45
21:H1:24:LEU:H	21:H1:24:LEU:HD12	1.80	0.45
21:H1:129:VAL:HG11	22:I1:28:THR:HG21	1.98	0.45
25:X1:69:ILE:HD12	25:X1:98:PHE:HD1	1.81	0.45
25:T1:102:GLU:O	25:T1:106:LEU:HD23	2.16	0.45
17:r:45:ASP:OD1	17:r:45:ASP:N	2.50	0.45
23:J1:120:TRP:CZ3	23:J1:142:VAL:HG11	2.52	0.45
24:M1:90:VAL:HA	24:M1:93:ILE:HD12	1.98	0.45
7:f:18:LEU:O	7:f:22:VAL:HG23	2.17	0.45
20:G1:2:SER:OG	20:G1:3:GLY:N	2.49	0.45
24:M1:115:MET:HE2	24:M1:118:LEU:CD1	2.46	0.45
19:E1:132:ARG:NH2	23:L1:30:PHE:O	2.44	0.45
19:E1:356:ASP:N	19:E1:356:ASP:OD1	2.48	0.45
19:E1:370:ILE:HD12	19:E1:370:ILE:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:39:ARG:NE	6:e:73:ASP:OD2	2.49	0.45
7:f:81:ILE:O	7:f:86:GLY:N	2.41	0.45
18:C1:183:LEU:HD23	18:C1:183:LEU:C	2.42	0.45
18:C1:537:ILE:HB	18:C1:538:LEU:HD12	1.98	0.45
19:F1:263:LEU:HD21	19:F1:321:ARG:CB	2.46	0.45
20:G1:201:LEU:HD22	20:G1:201:LEU:H	1.82	0.45
21:H1:72:VAL:HG22	21:H1:73:THR:N	2.32	0.45
19:E1:73:THR:C	19:E1:74:LEU:HD23	2.42	0.44
19:E1:391:VAL:HG12	19:E1:395:ASN:HD21	1.82	0.44
19:F1:55:PRO:O	19:F1:58:THR:OG1	2.29	0.44
19:F1:171:LEU:HD23	19:F1:171:LEU:H	1.81	0.44
21:H1:68:LYS:N	21:H1:100:GLU:O	2.50	0.44
21:H1:76:ASN:ND2	34:H1:201:UTP:O1G	2.43	0.44
3:a:146:ARG:NH2	25:X1:102:GLU:OE2	2.51	0.44
18:B1:295:MET:HB2	18:B1:358:VAL:HG23	2.00	0.44
19:D1:154:ALA:N	19:D1:324:SER:O	2.49	0.44
19:F1:187:VAL:HG23	19:F1:361:LEU:HD23	1.98	0.44
8:g:174:THR:HG23	8:g:175:ALA:N	2.32	0.44
19:F1:223:LEU:HD11	19:F1:227:MET:HE3	2.00	0.44
34:H1:201:UTP:O2G	25:V1:82:ARG:NH1	2.47	0.44
19:D1:64:ASP:OD1	19:D1:65:LYS:N	2.50	0.44
19:E1:227:MET:HE3	19:E1:232:VAL:HB	2.00	0.44
4:c:61:VAL:O	4:c:65:VAL:HG23	2.17	0.44
18:B1:277:ALA:HB1	18:B1:314:ALA:HB1	1.99	0.44
18:B1:301:CYS:SG	18:B1:302:LEU:N	2.90	0.44
12:k:103:MET:HE1	16:q:80:LEU:HA	1.99	0.44
18:A1:530:PHE:O	23:L1:109:HIS:NE2	2.50	0.44
18:B1:59:ASP:OD1	19:E1:300:ARG:NH2	2.47	0.44
18:C1:295:MET:SD	18:C1:358:VAL:HG23	2.57	0.44
25:Q1:57:LEU:HA	25:Q1:60:ILE:HD12	2.00	0.44
18:C1:62:ILE:HD12	18:C1:322:LEU:HD23	1.99	0.44
23:K1:83:SER:O	23:K1:96:LYS:NZ	2.41	0.44
4:c:88:LEU:HD21	5:d:305:VAL:HG21	2.00	0.43
6:e:378:ARG:HH22	15:p:63:ASP:CG	2.25	0.43
18:B1:149:VAL:HG21	18:B1:254:HIS:CE1	2.53	0.43
18:B1:246:ARG:NH1	19:E1:356:ASP:OD1	2.51	0.43
18:B1:343:LEU:HD12	18:B1:382:ILE:HG21	2.00	0.43
19:E1:191:VAL:HG23	31:E1:601:ATP:O2A	2.17	0.43
25:U1:100:LEU:HD13	25:V1:98:PHE:CZ	2.53	0.43
25:W1:76:LEU:HA	25:X1:77:LEU:HD13	2.01	0.43
9:h:38:LYS:N	24:M1:215:THR:O	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A1:188:LYS:O	18:A1:192:THR:HG23	2.19	0.43
19:E1:276:ASP:OD1	19:E1:276:ASP:N	2.50	0.43
25:Q1:111:LEU:HD21	25:R1:113:PHE:CE1	2.53	0.43
25:R1:72:ILE:HD11	25:S1:70:GLY:HA2	2.01	0.43
25:S1:50:LEU:HD12	25:T1:49:GLY:C	2.42	0.43
7:f:84:TRP:NE1	17:r:49:ASP:OD2	2.46	0.43
11:j:5:GLU:OE1	11:j:5:GLU:N	2.45	0.43
25:V1:72:ILE:HD11	25:W1:70:GLY:HA2	1.99	0.43
18:A1:292:GLU:O	18:A1:296:ASN:ND2	2.50	0.43
19:E1:73:THR:O	19:E1:74:LEU:HD23	2.18	0.43
4:c:61:VAL:HG11	10:i:6:TRP:CD2	2.54	0.43
4:c:83:LYS:O	4:c:87:VAL:HG23	2.18	0.43
8:g:263:ARG:HH11	9:h:102:LEU:HD13	1.83	0.43
3:a:49:LEU:HD23	3:a:49:LEU:H	1.83	0.43
19:E1:181:LEU:HD23	19:E1:359:THR:HB	1.99	0.43
23:L1:36:THR:O	23:L1:36:THR:HG22	2.18	0.43
5:d:102:LEU:HD23	5:d:102:LEU:C	2.43	0.43
2:m:33:ALA:O	2:m:35:THR:HG23	2.19	0.43
18:A1:199:GLY:N	18:A1:357:SER:OG	2.51	0.43
18:A1:384:ASP:OD1	19:E1:218:ARG:NE	2.47	0.43
25:P1:100:LEU:HD12	25:Q1:73:PHE:CZ	2.53	0.43
18:B1:56:HIS:HB2	18:B1:66:ILE:HG23	2.01	0.43
18:B1:246:ARG:NH2	19:E1:356:ASP:OD1	2.50	0.43
18:C1:203:LEU:HD12	18:C1:362:PRO:HG2	1.99	0.43
19:E1:305:VAL:HG12	19:E1:305:VAL:O	2.19	0.43
19:E1:416:VAL:HG23	19:E1:417:LEU:H	1.83	0.43
2:M:64:GLU:OE1	2:m:57:SER:OG	2.28	0.43
7:f:128:THR:HG22	7:f:128:THR:O	2.19	0.43
8:g:44:ALA:N	8:g:241:GLU:OE2	2.52	0.43
23:J1:151:PRO:HG2	23:J1:154:LEU:HD12	2.01	0.43
23:L1:70:ILE:O	23:L1:74:ASN:ND2	2.41	0.43
25:V1:96:LEU:C	25:V1:96:LEU:HD23	2.44	0.43
5:d:275:GLU:HB3	10:i:4:THR:HG21	2.01	0.43
26:e:402:CDL:H673	16:q:61:GLN:HB3	2.01	0.43
18:A1:532:THR:OG1	18:A1:533:LEU:N	2.51	0.43
19:F1:282:ASP:HA	19:F1:283:ASN:HA	1.84	0.43
22:I1:57:ASP:OD1	22:I1:61:GLY:N	2.51	0.43
25:Q1:42:THR:HA	25:R1:44:ALA:O	2.19	0.43
25:Q1:44:ALA:HA	25:R1:46:SER:O	2.18	0.43
4:c:68:LYS:O	4:c:69:LEU:C	2.62	0.42
18:C1:131:VAL:HG11	18:C1:293:TYR:CB	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:J1:138:CYS:O	23:J1:142:VAL:HG23	2.19	0.42
25:R1:96:LEU:HD23	25:R1:96:LEU:C	2.44	0.42
19:D1:301:ILE:HG22	20:G1:279:LEU:HD22	2.00	0.42
19:F1:263:LEU:HD21	19:F1:321:ARG:HB3	2.00	0.42
25:U1:79:ALA:HB1	25:V1:81:ALA:HB2	2.01	0.42
7:f:113:SER:OG	7:f:114:ALA:N	2.52	0.42
18:A1:243:ILE:N	18:A1:306:ASP:O	2.42	0.42
21:H1:61:LEU:N	21:H1:61:LEU:HD12	2.34	0.42
24:M1:38:PRO:C	24:M1:39:LEU:HD12	2.44	0.42
3:a:37:LEU:HD12	3:a:37:LEU:N	2.34	0.42
5:d:185:ARG:O	5:d:189:VAL:HG23	2.19	0.42
6:e:262:MET:O	6:e:285:ARG:NH2	2.48	0.42
11:j:71:PHE:O	12:k:52:ARG:NH1	2.50	0.42
14:o:7:PHE:CE1	14:o:33:LEU:HD23	2.54	0.42
19:E1:268:TYR:CD2	19:E1:272:VAL:HG21	2.55	0.42
5:d:351:ILE:HD12	19:F1:504:ALA:N	2.34	0.42
7:f:80:MET:HG2	7:f:102:VAL:HG11	2.02	0.42
10:i:17:LYS:HA	10:i:20:THR:HG22	2.02	0.42
12:k:101:ARG:O	14:o:83:TYR:OH	2.33	0.42
19:F1:165:LYS:NZ	19:F1:439:PHE:O	2.31	0.42
19:F1:283:ASN:OD1	19:F1:284:ILE:N	2.52	0.42
3:a:231:VAL:O	6:e:170:TRP:NE1	2.45	0.42
4:c:69:LEU:HB2	4:c:70:PRO:HD3	2.02	0.42
18:C1:165:LYS:O	18:C1:289:THR:OG1	2.33	0.42
19:D1:344:THR:O	19:D1:344:THR:HG22	2.20	0.42
19:D1:416:VAL:HG12	19:D1:417:LEU:HD22	2.02	0.42
8:g:97:LEU:HD12	8:g:107:THR:HG21	2.01	0.42
18:B1:295:MET:SD	18:B1:358:VAL:HG23	2.60	0.42
18:B1:542:LEU:HD11	18:B1:546:LEU:HD11	2.01	0.42
18:C1:538:LEU:HD12	18:C1:538:LEU:N	2.35	0.42
24:M1:115:MET:HE2	24:M1:118:LEU:HD11	2.02	0.42
4:c:73:HIS:NE2	4:c:77:GLU:OE2	2.52	0.42
26:q:101:CDL:OB7	26:q:101:CDL:CB3	2.66	0.42
18:C1:74:VAL:HG22	18:C1:75:ALA:N	2.34	0.42
23:L1:73:TYR:OH	23:L1:111:ASN:ND2	2.53	0.42
25:Q1:111:LEU:HD21	25:R1:113:PHE:HE1	1.84	0.42
5:d:17:ILE:O	5:d:17:ILE:HG23	2.20	0.42
18:A1:184:LEU:O	18:A1:223:GLN:NE2	2.53	0.42
18:A1:449:THR:HG23	18:A1:451:PRO:HD2	2.02	0.42
19:E1:283:ASN:OD1	19:E1:285:PHE:N	2.42	0.42
19:F1:288:THR:CG2	19:F1:311:LEU:HD13	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B1:292:GLU:O	18:B1:296:ASN:ND2	2.49	0.41
7:f:41:LEU:HD23	7:f:45:LEU:HD12	2.02	0.41
7:f:62:TYR:CD1	7:f:62:TYR:C	2.98	0.41
2:M:142:PRO:HB2	2:m:136:LEU:HD13	2.02	0.41
8:g:140:VAL:CG2	8:g:177:VAL:HG21	2.50	0.41
19:E1:113:VAL:HG21	19:E1:268:TYR:CD2	2.55	0.41
2:M:119:ARG:O	2:m:144:TYR:OH	2.24	0.41
3:a:121:VAL:HG11	12:k:60:MET:HB3	2.01	0.41
5:d:252:LYS:NZ	6:e:338:LYS:O	2.51	0.41
14:o:59:GLU:O	14:o:63:ARG:HG2	2.21	0.41
18:B1:220:ILE:HG23	18:B1:238:SER:OG	2.21	0.41
25:S1:67:LEU:HD23	25:T1:67:LEU:HD13	2.01	0.41
7:f:37:TRP:NE1	7:f:48:GLU:OE1	2.52	0.41
18:A1:80:ILE:C	18:A1:80:ILE:HD12	2.45	0.41
18:C1:408:VAL:HG22	18:C1:409:SER:N	2.35	0.41
24:M1:45:ASP:N	24:M1:45:ASP:OD1	2.53	0.41
18:B1:74:VAL:HG12	18:B1:75:ALA:N	2.35	0.41
18:C1:523:GLU:OE1	23:K1:135:LEU:HD11	2.20	0.41
18:B1:183:LEU:HD23	18:B1:184:LEU:N	2.35	0.41
19:E1:458:VAL:HG12	19:E1:463:THR:HG23	2.02	0.41
19:F1:62:VAL:HG21	19:F1:72:LEU:HD23	2.02	0.41
10:i:88:LYS:NZ	13:n:156:PHE:OXT	2.42	0.41
19:E1:282:ASP:HA	19:E1:283:ASN:HA	1.83	0.41
7:f:56:ILE:HB	7:f:57:PRO:HD3	2.03	0.41
18:A1:74:VAL:HG22	18:A1:75:ALA:N	2.35	0.41
18:B1:180:ASN:N	18:B1:180:ASN:OD1	2.54	0.41
18:B1:471:MET:O	18:B1:475:VAL:HG23	2.21	0.41
19:E1:263:LEU:HD13	19:E1:322:ILE:HG12	2.03	0.41
20:G1:201:LEU:HD11	21:H1:40:ILE:HD11	2.03	0.41
6:e:11:ASN:ND2	6:e:120:LEU:O	2.45	0.41
9:h:24:MET:N	9:h:24:MET:SD	2.94	0.41
10:i:99:GLU:O	10:i:103:VAL:HG23	2.21	0.41
18:A1:329:GLU:O	18:A1:330:ALA:HB3	2.20	0.41
19:E1:137:GLU:OE1	19:E1:137:GLU:N	2.41	0.41
8:g:230:SER:O	8:g:234:VAL:HG23	2.20	0.40
19:E1:59:ALA:O	19:E1:60:LEU:HD12	2.21	0.40
5:d:25:TYR:OH	5:d:196:ASP:OD2	2.32	0.40
13:n:18:VAL:HG22	13:n:19:GLY:N	2.37	0.40
18:C1:85:SER:OG	18:C1:88:THR:N	2.52	0.40
19:D1:415:ALA:O	20:G1:34:ARG:NH1	2.55	0.40
24:M1:211:GLU:C	24:M1:212:VAL:HG12	2.45	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M1:213:ASP:O	24:M1:214:TYR:HB2	2.21	0.40
9:h:149:ILE:HA	9:h:152:VAL:HG12	2.02	0.40
18:B1:135:VAL:O	18:B1:135:VAL:HG12	2.21	0.40
18:C1:131:VAL:HG11	18:C1:293:TYR:HB2	2.04	0.40
18:C1:371:VAL:HG12	18:C1:371:VAL:O	2.21	0.40
19:D1:416:VAL:HG13	20:G1:30:LEU:HD13	2.03	0.40
19:E1:118:LEU:HD13	19:E1:239:SER:O	2.22	0.40
25:R1:41:SER:N	25:S1:42:THR:O	2.55	0.40
17:r:34:TYR:HB2	17:r:35:PRO:HD3	2.03	0.40
18:A1:59:ASP:OD1	19:D1:300:ARG:NH2	2.55	0.40
18:C1:307:ASP:N	18:C1:307:ASP:OD1	2.54	0.40
18:C1:480:CYS:HA	18:C1:485:LEU:HD13	2.03	0.40
19:F1:474:THR:O	19:F1:474:THR:HG22	2.21	0.40
20:G1:129:ASN:OD1	20:G1:130:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	63/92 (68%)	63 (100%)	0	0	100	100
1	l	63/92 (68%)	63 (100%)	0	0	100	100
2	M	127/144 (88%)	126 (99%)	1 (1%)	0	100	100
2	m	127/144 (88%)	127 (100%)	0	0	100	100
3	a	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
4	c	84/114 (74%)	80 (95%)	4 (5%)	0	100	100
5	d	328/370 (89%)	325 (99%)	3 (1%)	0	100	100
6	e	381/396 (96%)	373 (98%)	8 (2%)	0	100	100
7	f	133/145 (92%)	129 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	g	266/269 (99%)	262 (98%)	4 (2%)	0	100	100
9	h	135/157 (86%)	133 (98%)	2 (2%)	0	100	100
10	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
11	j	166/169 (98%)	160 (96%)	6 (4%)	0	100	100
12	k	103/124 (83%)	101 (98%)	2 (2%)	0	100	100
13	n	137/156 (88%)	130 (95%)	7 (5%)	0	100	100
14	o	94/101 (93%)	94 (100%)	0	0	100	100
15	p	78/105 (74%)	76 (97%)	2 (3%)	0	100	100
16	q	83/98 (85%)	81 (98%)	2 (2%)	0	100	100
17	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	A1	518/584 (89%)	502 (97%)	16 (3%)	0	100	100
18	B1	516/584 (88%)	506 (98%)	9 (2%)	1 (0%)	43	72
18	C1	526/584 (90%)	513 (98%)	13 (2%)	0	100	100
19	D1	485/519 (93%)	476 (98%)	9 (2%)	0	100	100
19	E1	485/519 (93%)	477 (98%)	7 (1%)	1 (0%)	43	72
19	F1	486/519 (94%)	476 (98%)	9 (2%)	1 (0%)	43	72
20	G1	298/305 (98%)	297 (100%)	1 (0%)	0	100	100
21	H1	159/182 (87%)	156 (98%)	3 (2%)	0	100	100
22	I1	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
23	J1	164/188 (87%)	161 (98%)	3 (2%)	0	100	100
23	K1	164/188 (87%)	157 (96%)	7 (4%)	0	100	100
23	L1	163/188 (87%)	160 (98%)	3 (2%)	0	100	100
24	M1	230/255 (90%)	224 (97%)	6 (3%)	0	100	100
25	O1	76/118 (64%)	76 (100%)	0	0	100	100
25	P1	76/118 (64%)	76 (100%)	0	0	100	100
25	Q1	76/118 (64%)	76 (100%)	0	0	100	100
25	R1	76/118 (64%)	76 (100%)	0	0	100	100
25	S1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
25	T1	76/118 (64%)	76 (100%)	0	0	100	100
25	U1	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
25	V1	76/118 (64%)	76 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	W1	76/118 (64%)	76 (100%)	0	0	100	100
25	X1	76/118 (64%)	76 (100%)	0	0	100	100
All	All	7775/8943 (87%)	7633 (98%)	139 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	55/75 (73%)	55 (100%)	0	100	100
1	l	55/75 (73%)	55 (100%)	0	100	100
2	M	111/124 (90%)	110 (99%)	1 (1%)	70	75
2	m	111/124 (90%)	111 (100%)	0	100	100
3	a	225/225 (100%)	223 (99%)	2 (1%)	70	75
4	c	80/104 (77%)	80 (100%)	0	100	100
5	d	297/334 (89%)	296 (100%)	1 (0%)	86	83
6	e	334/341 (98%)	334 (100%)	0	100	100
7	f	119/124 (96%)	117 (98%)	2 (2%)	53	67
8	g	205/206 (100%)	204 (100%)	1 (0%)	81	80
9	h	110/123 (89%)	110 (100%)	0	100	100
10	i	95/96 (99%)	95 (100%)	0	100	100
11	j	149/150 (99%)	148 (99%)	1 (1%)	76	77
12	k	91/107 (85%)	91 (100%)	0	100	100
13	n	123/137 (90%)	122 (99%)	1 (1%)	73	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	o	82/86 (95%)	81 (99%)	1 (1%)	63	72
15	p	75/94 (80%)	75 (100%)	0	100	100
16	q	80/92 (87%)	80 (100%)	0	100	100
17	r	56/56 (100%)	56 (100%)	0	100	100
18	A1	436/479 (91%)	436 (100%)	0	100	100
18	B1	433/479 (90%)	431 (100%)	2 (0%)	81	80
18	C1	439/479 (92%)	438 (100%)	1 (0%)	87	86
19	D1	398/420 (95%)	398 (100%)	0	100	100
19	E1	398/420 (95%)	397 (100%)	1 (0%)	86	83
19	F1	399/420 (95%)	394 (99%)	5 (1%)	61	71
20	G1	253/257 (98%)	252 (100%)	1 (0%)	84	81
21	H1	137/156 (88%)	136 (99%)	1 (1%)	76	77
22	I1	58/67 (87%)	58 (100%)	0	100	100
23	J1	145/162 (90%)	145 (100%)	0	100	100
23	K1	145/162 (90%)	145 (100%)	0	100	100
23	L1	145/162 (90%)	145 (100%)	0	100	100
24	M1	200/215 (93%)	199 (100%)	1 (0%)	81	80
25	O1	56/89 (63%)	55 (98%)	1 (2%)	51	67
25	P1	56/89 (63%)	56 (100%)	0	100	100
25	Q1	56/89 (63%)	56 (100%)	0	100	100
25	R1	56/89 (63%)	56 (100%)	0	100	100
25	S1	56/89 (63%)	56 (100%)	0	100	100
25	T1	56/89 (63%)	55 (98%)	1 (2%)	51	67
25	U1	56/89 (63%)	56 (100%)	0	100	100
25	V1	56/89 (63%)	56 (100%)	0	100	100
25	W1	56/89 (63%)	54 (96%)	2 (4%)	31	54
25	X1	56/89 (63%)	56 (100%)	0	100	100
All	All	6599/7441 (89%)	6573 (100%)	26 (0%)	81	81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	a	190	PHE
3	a	212	ILE
5	d	98	ASP
7	f	42	ASN
7	f	62	TYR
8	g	32	VAL
11	j	101	VAL
13	n	105	GLU
14	o	64	TYR
18	B1	288	VAL
18	B1	384	ASP
18	C1	131	VAL
19	E1	356	ASP
19	F1	45	VAL
19	F1	87	CYS
19	F1	102	VAL
19	F1	171	LEU
19	F1	193	ILE
20	G1	237	GLU
21	H1	111	VAL
24	M1	212	VAL
25	O1	101	THR
25	T1	86	LEU
25	W1	51	HIS
25	W1	72	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	11	HIS
2	M	47	ASN
2	M	49	ASN
2	M	67	GLN
2	M	70	HIS
5	d	39	GLN
5	d	43	ASN
5	d	222	GLN
6	e	41	GLN
6	e	166	HIS
8	g	143	GLN
8	g	218	HIS
9	h	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	l	43	HIS
2	m	96	ASN
14	o	25	HIS
15	p	95	GLN
16	q	42	HIS
18	A1	56	HIS
18	A1	296	ASN
18	A1	311	GLN
18	A1	386	GLN
18	A1	491	GLN
18	A1	525	ASN
18	A1	558	GLN
18	A1	562	ASN
18	B1	56	HIS
18	B1	115	GLN
18	B1	209	GLN
18	B1	472	ASN
18	B1	556	HIS
18	B1	558	GLN
18	C1	56	HIS
18	C1	83	GLN
18	C1	254	HIS
18	C1	339	HIS
18	C1	369	ASN
18	C1	525	ASN
19	D1	459	GLN
19	E1	30	HIS
19	E1	83	HIS
19	E1	153	GLN
19	E1	247	GLN
19	E1	275	GLN
19	E1	354	HIS
19	F1	48	HIS
19	F1	79	HIS
19	F1	108	ASN
19	F1	229	GLN
19	F1	260	GLN
19	F1	398	GLN
20	G1	207	GLN
20	G1	256	GLN
23	J1	175	HIS
23	K1	109	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	L1	78	GLN
23	L1	111	ASN
23	L1	163	GLN
24	M1	65	ASN
24	M1	112	ASN
24	M1	131	ASN
24	M1	197	ASN
25	O1	51	HIS
25	O1	83	GLN
25	P1	51	HIS
25	P1	83	GLN
25	R1	83	GLN
25	T1	85	ASN
25	U1	75	ASN
25	V1	48	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AME	e	1	6	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 5 are monoatomic - leaving 31 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	M	201	-	99,99,99	0.29	0	105,111,111	0.25	0
28	PC1	i	201	-	53,53,53	0.28	0	59,61,61	0.29	0
26	CDL	e	402	-	99,99,99	0.28	0	105,111,111	0.26	0
26	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.27	0
29	LMT	e	405	-	36,36,36	0.10	0	47,47,47	0.16	0
30	Q7G	e	406	-	54,54,90	0.14	0	80,84,138	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.27	0
28	PC1	a	302	-	53,53,53	0.27	0	59,61,61	0.28	0
28	PC1	p	201	-	53,53,53	0.28	0	59,61,61	0.29	0
30	Q7G	n	201	-	66,66,90	0.13	0	98,102,138	0.28	0
26	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
27	3PE	M	203	-	50,50,50	0.25	0	53,55,55	0.23	0
31	ATP	A1	601	32	32,33,33	0.29	0	48,52,52	0.29	0
31	ATP	E1	601	32	32,33,33	0.29	0	48,52,52	0.28	0
29	LMT	j	203	-	36,36,36	0.11	0	47,47,47	0.19	0
26	CDL	a	301	-	99,99,99	0.29	0	105,111,111	0.26	0
28	PC1	j	202	-	53,53,53	0.28	0	59,61,61	0.28	0
31	ATP	B1	601	32	32,33,33	0.30	0	48,52,52	0.29	0
26	CDL	k	201	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	M	202	-	99,99,99	0.29	0	105,111,111	0.25	0
33	ADP	F1	601	32	28,29,29	0.49	0	43,45,45	0.57	0
26	CDL	m	201	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	e	403	-	99,99,99	0.29	0	105,111,111	0.26	0
27	3PE	f	202	-	50,50,50	0.26	0	53,55,55	0.22	0
31	ATP	C1	601	32	32,33,33	0.30	0	48,52,52	0.31	0
26	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.26	0
27	3PE	m	202	-	50,50,50	0.24	0	53,55,55	0.22	0
26	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.27	0
34	UTP	H1	201	-	29,30,30	0.29	0	43,47,47	0.33	0
26	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	j	201	-	-	22/110/110/110	-
26	CDL	M	201	-	-	14/110/110/110	-
28	PC1	i	201	-	-	8/57/57/57	-
26	CDL	e	402	-	-	24/110/110/110	-
26	CDL	e	401	-	-	18/110/110/110	-
29	LMT	e	405	-	-	1/21/61/61	0/2/2/2
30	Q7G	e	406	-	1/1/19/34	5/15/123/200	0/7/7/10
26	CDL	f	201	-	-	24/110/110/110	-
28	PC1	a	302	-	-	9/57/57/57	-
30	Q7G	n	201	-	2/2/24/34	5/20/148/200	0/8/8/10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PC1	p	201	-	-	5/57/57/57	-
26	CDL	q	101	-	-	32/110/110/110	-
27	3PE	M	203	-	-	15/54/54/54	-
31	ATP	A1	601	32	-	7/22/38/38	0/3/3/3
31	ATP	E1	601	32	-	6/22/38/38	0/3/3/3
29	LMT	j	203	-	-	5/21/61/61	0/2/2/2
26	CDL	a	301	-	-	26/110/110/110	-
28	PC1	j	202	-	-	10/57/57/57	-
31	ATP	B1	601	32	-	3/22/38/38	0/3/3/3
26	CDL	k	201	-	-	26/110/110/110	-
26	CDL	M	202	-	-	28/110/110/110	-
33	ADP	F1	601	32	-	2/16/32/32	0/3/3/3
26	CDL	m	201	-	-	24/110/110/110	-
26	CDL	e	403	-	-	28/110/110/110	-
27	3PE	f	202	-	-	11/54/54/54	-
31	ATP	C1	601	32	-	4/22/38/38	0/3/3/3
26	CDL	l	101	-	-	12/110/110/110	-
27	3PE	m	202	-	-	8/54/54/54	-
26	CDL	c	201	-	-	21/110/110/110	-
34	UTP	H1	201	-	-	3/22/38/38	0/2/2/2
26	CDL	e	404	-	-	16/110/110/110	-

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

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

All (422) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	M	201	CDL	CA3-OA5-PA1-OA2
26	M	202	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	M	202	CDL	CA3-OA5-PA1-OA3
26	M	202	CDL	CB2-OB2-PB2-OB3
26	M	202	CDL	CB2-OB2-PB2-OB5
26	M	202	CDL	C51-CB5-OB6-CB4
26	a	301	CDL	CA3-OA5-PA1-OA2
26	a	301	CDL	CA3-OA5-PA1-OA3
26	a	301	CDL	CB3-OB5-PB2-OB2
26	c	201	CDL	CB3-OB5-PB2-OB2
26	c	201	CDL	CB3-OB5-PB2-OB4
26	e	401	CDL	CA3-OA5-PA1-OA2
26	e	401	CDL	CA3-OA5-PA1-OA3
26	e	401	CDL	CB2-OB2-PB2-OB4
26	e	402	CDL	CA3-OA5-PA1-OA2
26	e	402	CDL	CB2-OB2-PB2-OB5
26	e	403	CDL	CA2-OA2-PA1-OA3
26	e	403	CDL	CA2-OA2-PA1-OA5
26	e	403	CDL	CB2-OB2-PB2-OB3
26	e	403	CDL	CB2-OB2-PB2-OB5
26	e	403	CDL	OB6-CB4-CB6-OB8
26	e	403	CDL	C51-CB5-OB6-CB4
26	e	404	CDL	CA2-OA2-PA1-OA3
26	e	404	CDL	CA2-OA2-PA1-OA4
26	e	404	CDL	CA2-OA2-PA1-OA5
26	e	404	CDL	C11-CA5-OA6-CA4
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	f	201	CDL	CA2-OA2-PA1-OA3
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	CA2-OA2-PA1-OA5
26	j	201	CDL	CA3-OA5-PA1-OA3
26	k	201	CDL	CA3-OA5-PA1-OA2
26	k	201	CDL	CA3-OA5-PA1-OA4
26	k	201	CDL	C11-CA5-OA6-CA4
26	k	201	CDL	CB3-OB5-PB2-OB2
26	k	201	CDL	CB3-OB5-PB2-OB3
26	l	101	CDL	CA3-OA5-PA1-OA2
26	l	101	CDL	OA6-CA4-CA6-OA8
26	l	101	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	m	201	CDL	CA2-C1-CB2-OB2
26	m	201	CDL	CA3-OA5-PA1-OA2
26	m	201	CDL	CA3-OA5-PA1-OA3
26	m	201	CDL	CB2-OB2-PB2-OB4
26	m	201	CDL	CB2-OB2-PB2-OB5
26	m	201	CDL	OB7-CB5-OB6-CB4
26	m	201	CDL	C51-CB5-OB6-CB4
26	q	101	CDL	CA3-OA5-PA1-OA3
26	q	101	CDL	OA5-CA3-CA4-OA6
26	q	101	CDL	C11-CA5-OA6-CA4
26	q	101	CDL	CB2-OB2-PB2-OB3
26	q	101	CDL	CB2-OB2-PB2-OB5
26	q	101	CDL	CB3-OB5-PB2-OB2
26	q	101	CDL	CB3-OB5-PB2-OB3
27	M	203	3PE	C1-O11-P-O12
27	M	203	3PE	C1-O11-P-O13
27	M	203	3PE	C1-O11-P-O14
27	M	203	3PE	O13-C11-C12-N
27	f	202	3PE	C1-O11-P-O12
28	a	302	PC1	C11-O13-P-O12
28	a	302	PC1	C11-O13-P-O11
28	a	302	PC1	O13-C11-C12-N
28	i	201	PC1	C11-O13-P-O11
28	i	201	PC1	O13-C11-C12-N
28	j	202	PC1	C11-O13-P-O14
28	j	202	PC1	C11-O13-P-O11
28	j	202	PC1	C1-O11-P-O12
28	j	202	PC1	C1-O11-P-O14
28	j	202	PC1	C1-O11-P-O13
28	p	201	PC1	C11-O13-P-O12
28	p	201	PC1	C11-O13-P-O11
29	j	203	LMT	C2'-C1'-O1'-C1
29	j	203	LMT	O5'-C1'-O1'-C1
29	j	203	LMT	C2-C1-O1'-C1'
30	e	406	Q7G	CG1-C22-C23-C48
31	A1	601	ATP	PB-O3B-PG-O2G
31	C1	601	ATP	PB-O3B-PG-O3G
31	E1	601	ATP	PB-O3B-PG-O2G
31	E1	601	ATP	C5'-O5'-PA-O1A
33	F1	601	ADP	C5'-O5'-PA-O2A
33	F1	601	ADP	C5'-O5'-PA-O3A
34	H1	201	UTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	H1	201	UTP	C5'-O5'-PA-O3A
26	M	202	CDL	OB7-CB5-OB6-CB4
26	e	403	CDL	OB7-CB5-OB6-CB4
26	e	404	CDL	OA7-CA5-OA6-CA4
26	k	201	CDL	OB7-CB5-OB6-CB4
26	q	101	CDL	OA7-CA5-OA6-CA4
27	M	203	3PE	C32-C31-O31-C3
27	M	203	3PE	O32-C31-O31-C3
26	a	301	CDL	OB7-CB5-OB6-CB4
26	k	201	CDL	OA7-CA5-OA6-CA4
26	e	403	CDL	O1-C1-CA2-OA2
26	m	201	CDL	O1-C1-CB2-OB2
26	a	301	CDL	C51-CB5-OB6-CB4
26	k	201	CDL	C51-CB5-OB6-CB4
27	M	203	3PE	C2-C1-O11-P
30	e	406	Q7G	O5B-C1B-O1B-C24
30	n	201	Q7G	O5B-C1B-O1B-C24
26	a	301	CDL	C11-CA5-OA6-CA4
26	c	201	CDL	CB2-C1-CA2-OA2
26	M	201	CDL	C31-CA7-OA8-CA6
26	e	402	CDL	C31-CA7-OA8-CA6
30	e	406	Q7G	C2B-C1B-O1B-C24
30	n	201	Q7G	C2B-C1B-O1B-C24
26	M	202	CDL	O1-C1-CB2-OB2
26	a	301	CDL	O1-C1-CB2-OB2
26	M	201	CDL	OA9-CA7-OA8-CA6
26	e	402	CDL	OA9-CA7-OA8-CA6
28	p	201	PC1	O21-C2-C3-O31
26	c	201	CDL	CA5-C11-C12-C13
26	f	201	CDL	CA5-C11-C12-C13
28	a	302	PC1	C21-C22-C23-C24
26	c	201	CDL	O1-C1-CA2-OA2
26	a	301	CDL	OA7-CA5-OA6-CA4
26	e	404	CDL	O1-C1-CA2-OA2
26	l	101	CDL	CA5-C11-C12-C13
26	e	403	CDL	C11-CA5-OA6-CA4
26	l	101	CDL	C11-CA5-OA6-CA4
26	j	201	CDL	C13-C14-C15-C16
26	c	201	CDL	C55-C56-C57-C58
26	e	402	CDL	C11-CA5-OA6-CA4
26	M	202	CDL	CA5-C11-C12-C13
26	m	201	CDL	CA5-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	l	101	CDL	OA7-CA5-OA6-CA4
26	q	101	CDL	C1-CB2-OB2-PB2
26	e	402	CDL	C11-C12-C13-C14
26	e	402	CDL	OA7-CA5-OA6-CA4
26	e	403	CDL	OA7-CA5-OA6-CA4
26	M	202	CDL	C71-CB7-OB8-CB6
26	M	201	CDL	C11-CA5-OA6-CA4
26	e	401	CDL	C51-CB5-OB6-CB4
26	f	201	CDL	C11-CA5-OA6-CA4
27	f	202	3PE	C22-C21-O21-C2
26	k	201	CDL	C78-C79-C80-C81
29	j	203	LMT	O5B-C5B-C6B-O6B
26	e	403	CDL	C62-C63-C64-C65
27	f	202	3PE	O22-C21-O21-C2
26	M	202	CDL	OA5-CA3-CA4-OA6
26	a	301	CDL	OB5-CB3-CB4-OB6
26	M	202	CDL	C11-CA5-OA6-CA4
26	c	201	CDL	C11-CA5-OA6-CA4
30	n	201	Q7G	O5C-C5C-C6C-O6C
26	e	404	CDL	OB6-CB4-CB6-OB8
26	j	201	CDL	C81-C82-C83-C84
26	M	201	CDL	OA7-CA5-OA6-CA4
26	q	101	CDL	CA2-C1-CB2-OB2
26	e	403	CDL	C71-CB7-OB8-CB6
26	e	402	CDL	C81-C82-C83-C84
26	M	202	CDL	OB9-CB7-OB8-CB6
26	M	202	CDL	OA5-CA3-CA4-CA6
26	c	201	CDL	OA5-CA3-CA4-CA6
26	q	101	CDL	OA5-CA3-CA4-CA6
26	e	401	CDL	OB7-CB5-OB6-CB4
27	f	202	3PE	C3D-C3E-C3F-C3G
27	f	202	3PE	C2A-C2B-C2C-C2D
26	q	101	CDL	CB7-C71-C72-C73
26	j	201	CDL	C62-C63-C64-C65
26	l	101	CDL	CA3-CA4-CA6-OA8
26	m	201	CDL	CB3-CB4-CB6-OB8
26	q	101	CDL	CA3-CA4-CA6-OA8
28	p	201	PC1	C1-C2-C3-O31
26	M	202	CDL	C78-C79-C80-C81
26	a	301	CDL	C59-C60-C61-C62
28	i	201	PC1	C2C-C2D-C2E-C2F
26	e	403	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	c	201	CDL	C35-C36-C37-C38
26	m	201	CDL	C71-CB7-OB8-CB6
26	e	402	CDL	CA6-CA4-OA6-CA5
26	c	201	CDL	C39-C40-C41-C42
26	k	201	CDL	C79-C80-C81-C82
26	a	301	CDL	CA2-C1-CB2-OB2
26	e	401	CDL	C11-C12-C13-C14
27	m	202	3PE	C3C-C3D-C3E-C3F
27	f	202	3PE	C32-C31-O31-C3
26	m	201	CDL	C78-C79-C80-C81
26	f	201	CDL	OB6-CB4-CB6-OB8
26	a	301	CDL	C79-C80-C81-C82
26	e	403	CDL	C17-C18-C19-C20
31	A1	601	ATP	PG-O3B-PB-O1B
26	M	201	CDL	C71-CB7-OB8-CB6
26	f	201	CDL	C31-CA7-OA8-CA6
26	k	201	CDL	C74-C75-C76-C77
26	e	403	CDL	C14-C15-C16-C17
26	j	201	CDL	C72-C73-C74-C75
26	m	201	CDL	C21-C22-C23-C24
26	c	201	CDL	OA7-CA5-OA6-CA4
26	f	201	CDL	OA7-CA5-OA6-CA4
26	k	201	CDL	C15-C16-C17-C18
26	j	201	CDL	C1-CB2-OB2-PB2
30	n	201	Q7G	C2C-C1C-O1C-C48
28	a	302	PC1	C24-C25-C26-C27
26	M	202	CDL	OB5-CB3-CB4-CB6
26	a	301	CDL	OB5-CB3-CB4-CB6
27	m	202	3PE	O11-C1-C2-C3
26	e	401	CDL	C18-C19-C20-C21
26	e	403	CDL	C77-C78-C79-C80
26	M	202	CDL	C21-C22-C23-C24
26	M	202	CDL	OA7-CA5-OA6-CA4
26	M	202	CDL	CB3-CB4-CB6-OB8
26	c	201	CDL	CA3-CA4-CA6-OA8
26	e	403	CDL	CB3-CB4-CB6-OB8
27	f	202	3PE	C1-C2-C3-O31
26	m	201	CDL	OB9-CB7-OB8-CB6
26	c	201	CDL	C56-C57-C58-C59
26	k	201	CDL	C76-C77-C78-C79
26	j	201	CDL	OB5-CB3-CB4-OB6
26	q	101	CDL	O1-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	M	201	CDL	CA4-CA3-OA5-PA1
26	a	301	CDL	CA4-CA3-OA5-PA1
28	j	202	PC1	C2-C1-O11-P
26	M	201	CDL	OA6-CA4-CA6-OA8
26	M	202	CDL	OA6-CA4-CA6-OA8
26	m	201	CDL	OA6-CA4-CA6-OA8
27	M	203	3PE	O21-C2-C3-O31
27	f	202	3PE	O21-C2-C3-O31
27	f	202	3PE	O32-C31-O31-C3
26	a	301	CDL	C78-C79-C80-C81
30	n	201	Q7G	O5C-C1C-O1C-C48
26	e	401	CDL	C56-C57-C58-C59
26	q	101	CDL	C77-C78-C79-C80
26	m	201	CDL	C11-CA5-OA6-CA4
26	e	403	CDL	CB2-C1-CA2-OA2
26	m	201	CDL	C14-C15-C16-C17
26	f	201	CDL	OA9-CA7-OA8-CA6
26	c	201	CDL	CA4-CA6-OA8-CA7
26	e	402	CDL	C77-C78-C79-C80
31	A1	601	ATP	PB-O3B-PG-O1G
26	f	201	CDL	C77-C78-C79-C80
26	M	202	CDL	C56-C57-C58-C59
26	M	201	CDL	OB9-CB7-OB8-CB6
26	M	202	CDL	OB5-CB3-CB4-OB6
27	M	203	3PE	O11-C1-C2-O21
26	a	301	CDL	CB3-CB4-CB6-OB8
26	e	404	CDL	CB3-CB4-CB6-OB8
27	M	203	3PE	C1-C2-C3-O31
26	e	402	CDL	C17-C18-C19-C20
26	M	202	CDL	OB6-CB4-CB6-OB8
26	m	201	CDL	OB6-CB4-CB6-OB8
26	q	101	CDL	OA6-CA4-CA6-OA8
27	M	203	3PE	C36-C37-C38-C39
26	q	101	CDL	C31-CA7-OA8-CA6
26	e	401	CDL	C81-C82-C83-C84
26	c	201	CDL	CA4-CA3-OA5-PA1
28	j	202	PC1	O13-C11-C12-N
28	p	201	PC1	O13-C11-C12-N
31	E1	601	ATP	PG-O3B-PB-O2B
26	a	301	CDL	C73-C74-C75-C76
26	l	101	CDL	C14-C15-C16-C17
29	e	405	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	m	202	3PE	C32-C31-O31-C3
26	e	402	CDL	C52-C51-CB5-OB6
26	j	201	CDL	OB5-CB3-CB4-CB6
26	k	201	CDL	OA5-CA3-CA4-CA6
27	M	203	3PE	O11-C1-C2-C3
26	m	201	CDL	OA7-CA5-OA6-CA4
26	k	201	CDL	OA5-CA3-CA4-OA6
26	q	101	CDL	OB5-CB3-CB4-OB6
27	m	202	3PE	O11-C1-C2-O21
26	a	301	CDL	C39-C40-C41-C42
27	m	202	3PE	O32-C31-O31-C3
26	a	301	CDL	OB6-CB4-CB6-OB8
26	c	201	CDL	OA6-CA4-CA6-OA8
26	j	201	CDL	OA6-CA4-CA6-OA8
26	j	201	CDL	CA3-CA4-CA6-OA8
30	e	406	Q7G	CG1-C22-C23-C24
26	q	101	CDL	OA9-CA7-OA8-CA6
28	i	201	PC1	C28-C29-C2A-C2B
26	M	201	CDL	CA3-OA5-PA1-OA3
26	M	201	CDL	CB2-OB2-PB2-OB3
26	M	202	CDL	CA3-OA5-PA1-OA4
26	a	301	CDL	CA3-OA5-PA1-OA4
26	a	301	CDL	CB3-OB5-PB2-OB3
26	c	201	CDL	CA3-OA5-PA1-OA3
26	e	401	CDL	CA3-OA5-PA1-OA4
26	e	401	CDL	CB2-OB2-PB2-OB3
26	e	401	CDL	CB2-OB2-PB2-OB5
26	e	402	CDL	CA3-OA5-PA1-OA3
26	e	402	CDL	CB2-OB2-PB2-OB3
26	e	402	CDL	CB2-OB2-PB2-OB4
26	f	201	CDL	CB3-OB5-PB2-OB3
26	j	201	CDL	CA2-OA2-PA1-OA4
26	j	201	CDL	CA3-OA5-PA1-OA2
26	j	201	CDL	CA3-OA5-PA1-OA4
26	k	201	CDL	CA3-OA5-PA1-OA3
26	k	201	CDL	CB3-OB5-PB2-OB4
26	l	101	CDL	CA3-OA5-PA1-OA3
26	m	201	CDL	CA3-OA5-PA1-OA4
26	q	101	CDL	CA2-OA2-PA1-OA5
26	q	101	CDL	CB2-OB2-PB2-OB4
27	m	202	3PE	O13-C11-C12-N
28	i	201	PC1	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A1	601	ATP	C5'-O5'-PA-O1A
31	B1	601	ATP	C5'-O5'-PA-O1A
31	B1	601	ATP	C5'-O5'-PA-O2A
31	B1	601	ATP	C5'-O5'-PA-O3A
31	C1	601	ATP	C5'-O5'-PA-O1A
26	c	201	CDL	C1-CB2-OB2-PB2
26	f	201	CDL	CB4-CB3-OB5-PB2
26	a	301	CDL	CB6-CB4-OB6-CB5
26	q	101	CDL	CB3-CB4-OB6-CB5
26	l	101	CDL	C11-C12-C13-C14
26	c	201	CDL	OA5-CA3-CA4-OA6
26	k	201	CDL	C33-C34-C35-C36
26	j	201	CDL	CA4-CA3-OA5-PA1
34	H1	201	UTP	PG-O3B-PB-O1B
26	q	101	CDL	C14-C15-C16-C17
26	e	401	CDL	C77-C78-C79-C80
28	a	302	PC1	C37-C38-C39-C3A
26	e	401	CDL	OB6-CB4-CB6-OB8
28	i	201	PC1	C2A-C2B-C2C-C2D
26	c	201	CDL	C51-C52-C53-C54
26	k	201	CDL	C14-C15-C16-C17
26	e	403	CDL	C73-C74-C75-C76
26	e	404	CDL	CB2-C1-CA2-OA2
26	l	101	CDL	C31-C32-C33-C34
29	j	203	LMT	C2-C3-C4-C5
26	e	404	CDL	CA3-CA4-OA6-CA5
26	j	201	CDL	CA6-CA4-OA6-CA5
26	k	201	CDL	CB3-CB4-OB6-CB5
26	f	201	CDL	C13-C14-C15-C16
28	a	302	PC1	C38-C39-C3A-C3B
26	M	202	CDL	C73-C74-C75-C76
31	C1	601	ATP	PG-O3B-PB-O1B
26	a	301	CDL	C80-C81-C82-C83
26	e	402	CDL	CA4-CA3-OA5-PA1
28	a	302	PC1	O31-C31-C32-C33
26	f	201	CDL	C78-C79-C80-C81
26	m	201	CDL	OA5-CA3-CA4-OA6
26	q	101	CDL	CB2-C1-CA2-OA2
26	e	402	CDL	C76-C77-C78-C79
26	q	101	CDL	OB5-CB3-CB4-CB6
28	j	202	PC1	O11-C1-C2-C3
26	f	201	CDL	OA6-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	q	101	CDL	CB4-CB3-OB5-PB2
26	e	401	CDL	C75-C76-C77-C78
26	k	201	CDL	CB6-CB4-OB6-CB5
31	E1	601	ATP	PB-O3B-PG-O3G
26	k	201	CDL	CB4-CB3-OB5-PB2
26	M	201	CDL	CA3-CA4-CA6-OA8
26	M	202	CDL	CA3-CA4-CA6-OA8
26	f	201	CDL	CA3-CA4-CA6-OA8
26	f	201	CDL	CB3-CB4-CB6-OB8
26	m	201	CDL	CA3-CA4-CA6-OA8
26	c	201	CDL	C34-C35-C36-C37
26	m	201	CDL	C56-C57-C58-C59
26	e	402	CDL	C16-C17-C18-C19
26	e	404	CDL	C31-C32-C33-C34
26	M	201	CDL	C60-C61-C62-C63
26	e	403	CDL	C72-C71-CB7-OB8
26	q	101	CDL	C79-C80-C81-C82
26	M	202	CDL	C14-C15-C16-C17
26	k	201	CDL	C12-C13-C14-C15
31	A1	601	ATP	PG-O3B-PB-O2B
31	C1	601	ATP	PG-O3B-PB-O2B
31	E1	601	ATP	PG-O3B-PB-O1B
26	e	403	CDL	C52-C51-CB5-OB6
26	k	201	CDL	C52-C51-CB5-OB6
26	M	201	CDL	C14-C15-C16-C17
26	a	301	CDL	C81-C82-C83-C84
28	i	201	PC1	O21-C21-C22-C23
26	f	201	CDL	OA5-CA3-CA4-OA6
26	q	101	CDL	C82-C83-C84-C85
26	e	401	CDL	C32-C31-CA7-OA8
26	e	403	CDL	C32-C31-CA7-OA8
26	e	401	CDL	C33-C34-C35-C36
26	M	202	CDL	C12-C13-C14-C15
26	k	201	CDL	C38-C39-C40-C41
26	l	101	CDL	C60-C61-C62-C63
26	e	403	CDL	C75-C76-C77-C78
26	e	402	CDL	C32-C31-CA7-OA8
26	j	201	CDL	C72-C71-CB7-OB8
27	M	203	3PE	O21-C21-C22-C23
28	j	202	PC1	O31-C31-C32-C33
26	e	404	CDL	C20-C21-C22-C23
27	f	202	3PE	C39-C3A-C3B-C3C

Continued on next page...

Continued from previous page...

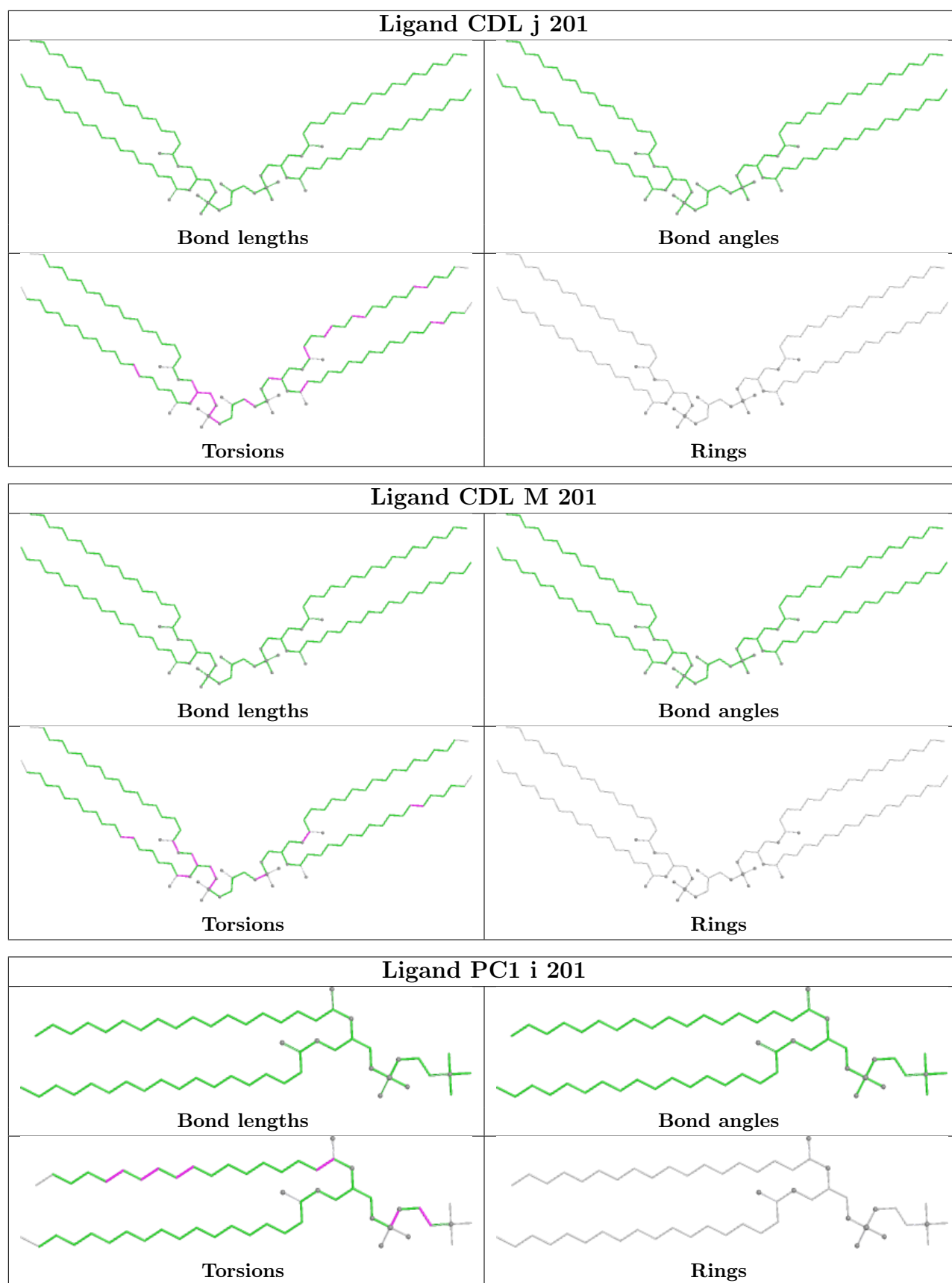
Mol	Chain	Res	Type	Atoms
26	f	201	CDL	C12-C11-CA5-OA6
26	f	201	CDL	C72-C71-CB7-OB8
31	E1	601	ATP	PB-O3B-PG-O1G
26	f	201	CDL	C35-C36-C37-C38
26	j	201	CDL	C52-C51-CB5-OB6
28	a	302	PC1	C27-C28-C29-C2A
27	m	202	3PE	O21-C21-C22-C23
26	a	301	CDL	C51-C52-C53-C54
26	q	101	CDL	CA5-C11-C12-C13
26	e	403	CDL	C18-C19-C20-C21
26	j	201	CDL	C75-C76-C77-C78
26	e	402	CDL	C72-C71-CB7-OB8
26	e	403	CDL	C52-C51-CB5-OB7
26	j	201	CDL	C72-C71-CB7-OB9
27	M	203	3PE	O31-C31-C32-C33
26	k	201	CDL	C52-C51-CB5-OB7
26	q	101	CDL	C84-C85-C86-C87
26	a	301	CDL	C20-C21-C22-C23
26	M	202	CDL	C32-C33-C34-C35
26	e	401	CDL	C32-C31-CA7-OA9
26	e	403	CDL	C72-C71-CB7-OB9
28	i	201	PC1	O22-C21-C22-C23
27	m	202	3PE	O22-C21-C22-C23
27	f	202	3PE	O21-C21-C22-C23
26	f	201	CDL	C12-C11-CA5-OA7
26	f	201	CDL	C72-C71-CB7-OB9
27	M	203	3PE	O22-C21-C22-C23
26	e	402	CDL	C1-CB2-OB2-PB2
30	e	406	Q7G	C23-C24-O1B-C1B
26	q	101	CDL	C72-C71-CB7-OB8
28	j	202	PC1	O32-C31-C32-C33
26	q	101	CDL	C38-C39-C40-C41
26	e	402	CDL	OB5-CB3-CB4-CB6
26	e	403	CDL	OA5-CA3-CA4-CA6
26	j	201	CDL	OA5-CA3-CA4-CA6
26	e	404	CDL	C21-C22-C23-C24
26	e	402	CDL	C32-C31-CA7-OA9
26	e	403	CDL	C32-C31-CA7-OA9
26	m	201	CDL	C12-C11-CA5-OA6
31	A1	601	ATP	PA-O3A-PB-O1B
31	A1	601	ATP	PA-O3A-PB-O2B
26	e	402	CDL	C72-C71-CB7-OB9

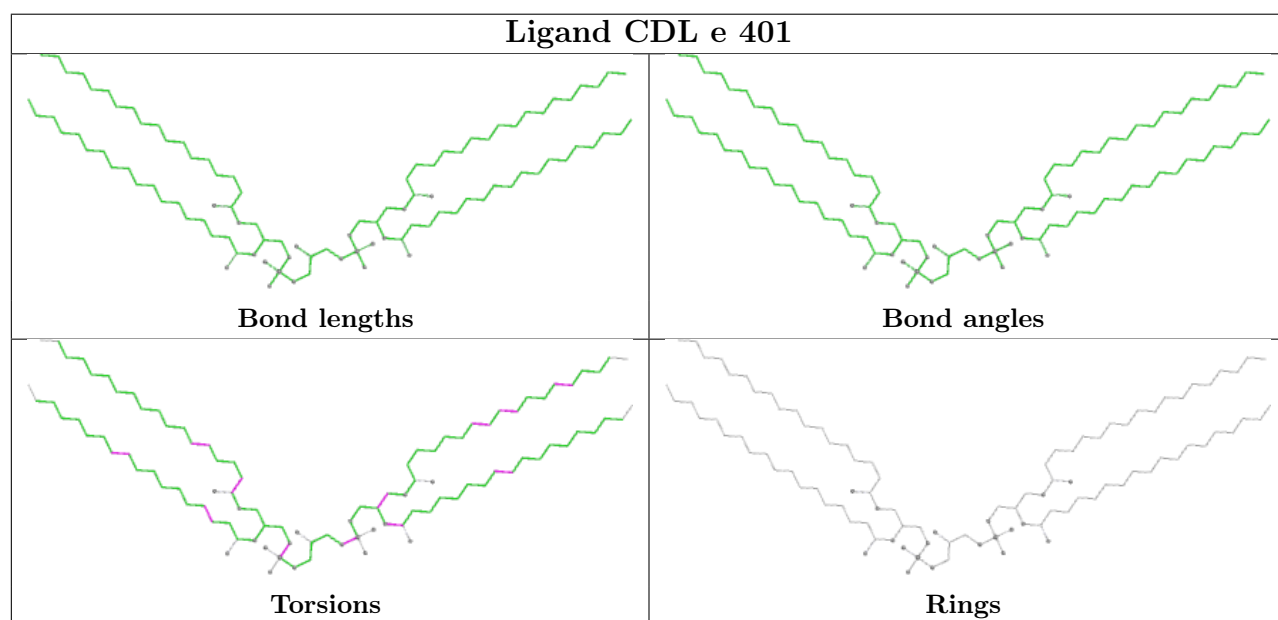
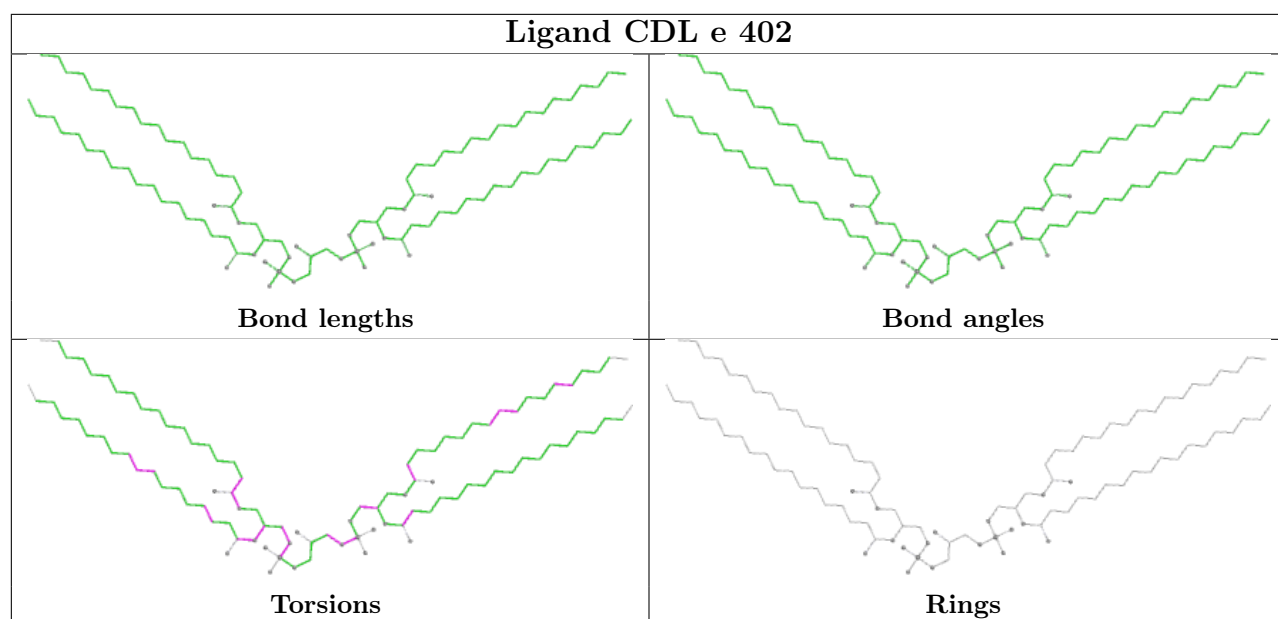
There are no ring outliers.

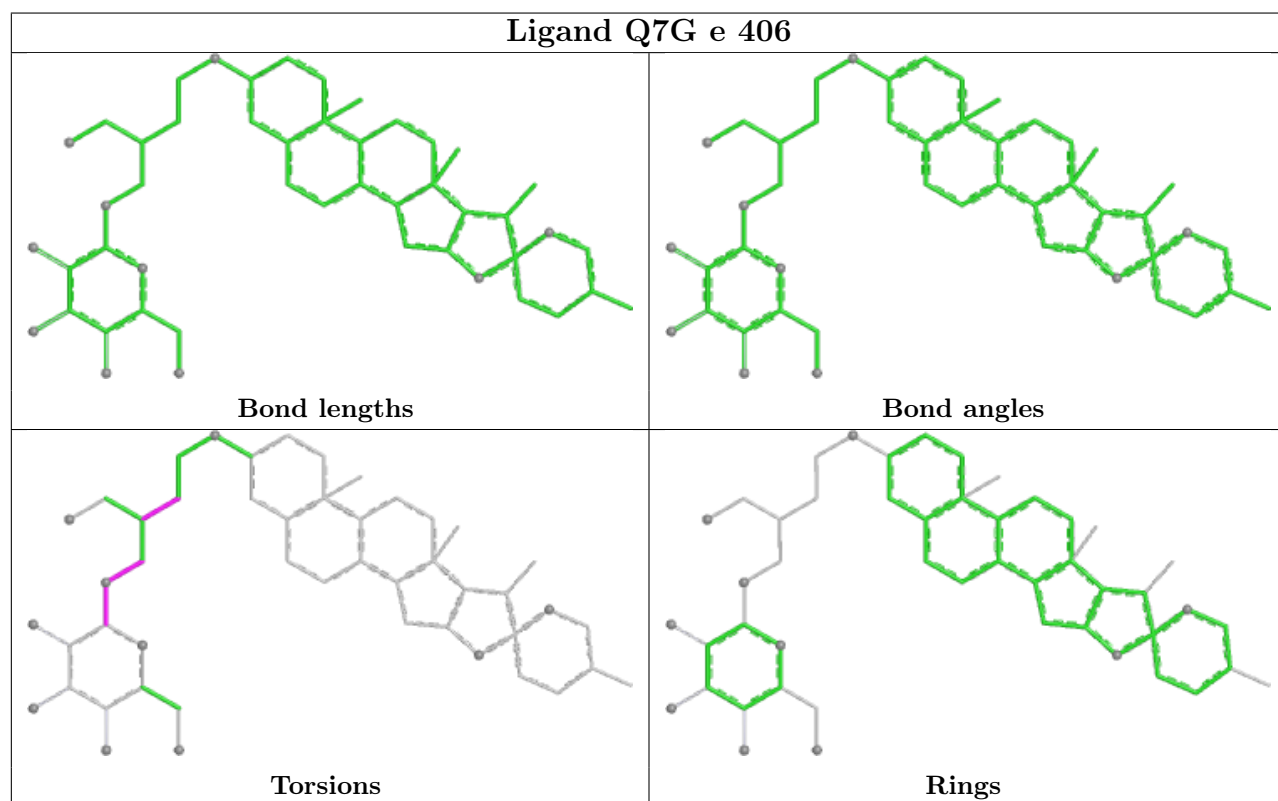
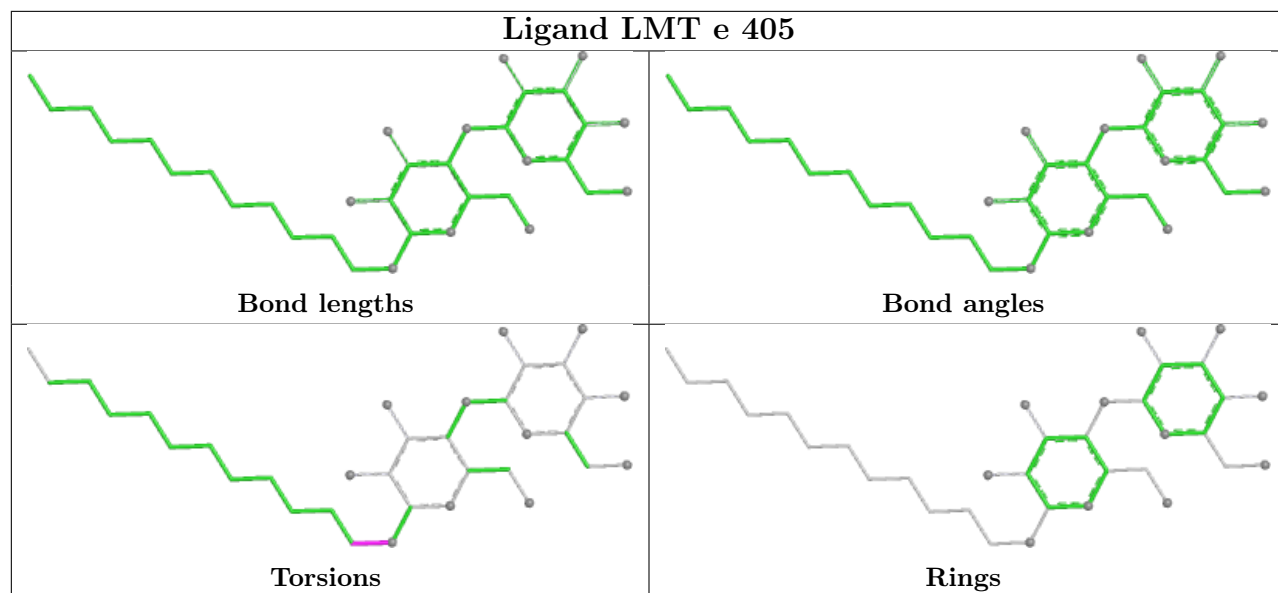
14 monomers are involved in 20 short contacts:

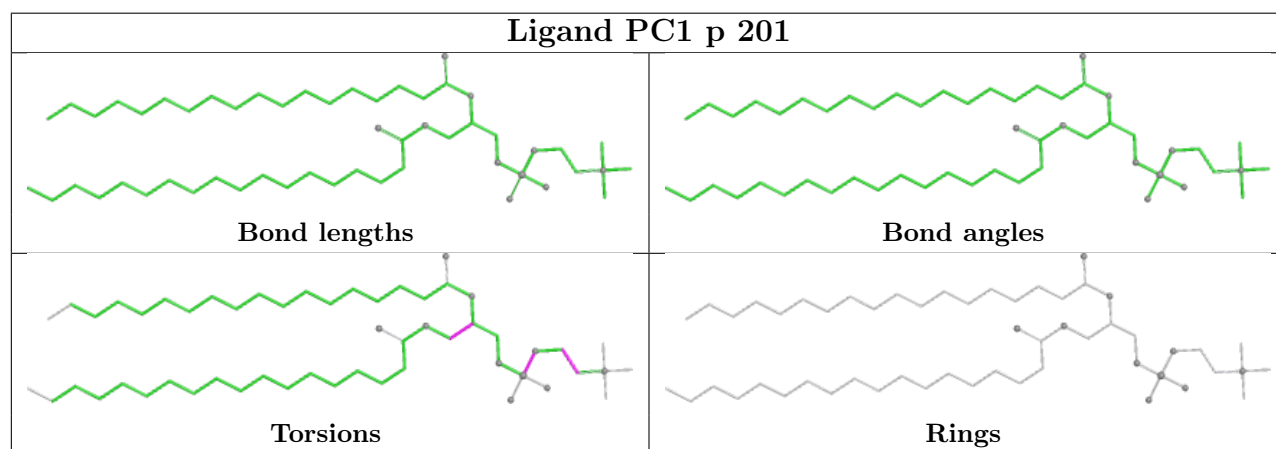
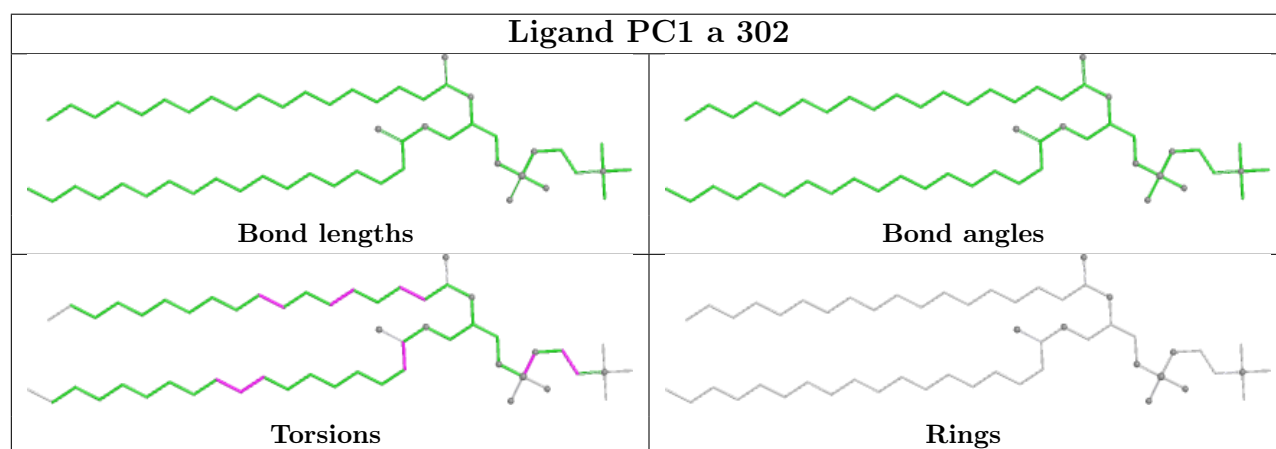
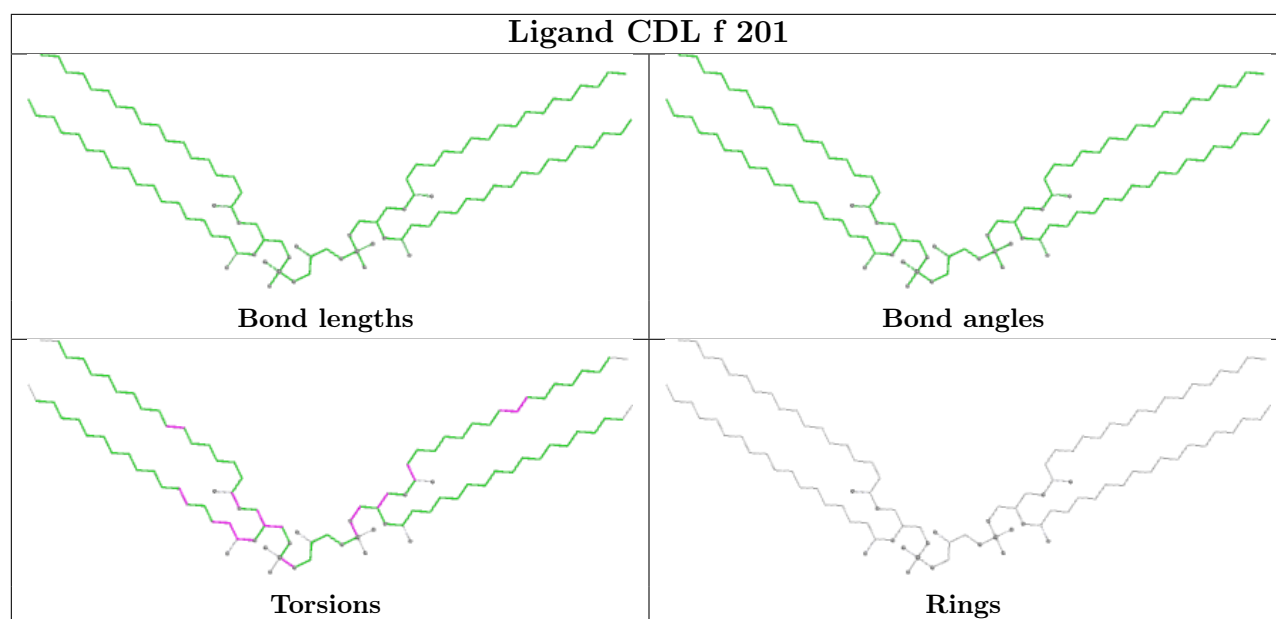
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	j	201	CDL	2	0
26	e	402	CDL	1	0
26	e	401	CDL	1	0
26	f	201	CDL	1	0
28	a	302	PC1	2	0
26	q	101	CDL	1	0
31	E1	601	ATP	2	0
28	j	202	PC1	1	0
31	B1	601	ATP	2	0
26	k	201	CDL	1	0
33	F1	601	ADP	1	0
26	l	101	CDL	1	0
26	c	201	CDL	1	0
34	H1	201	UTP	3	0

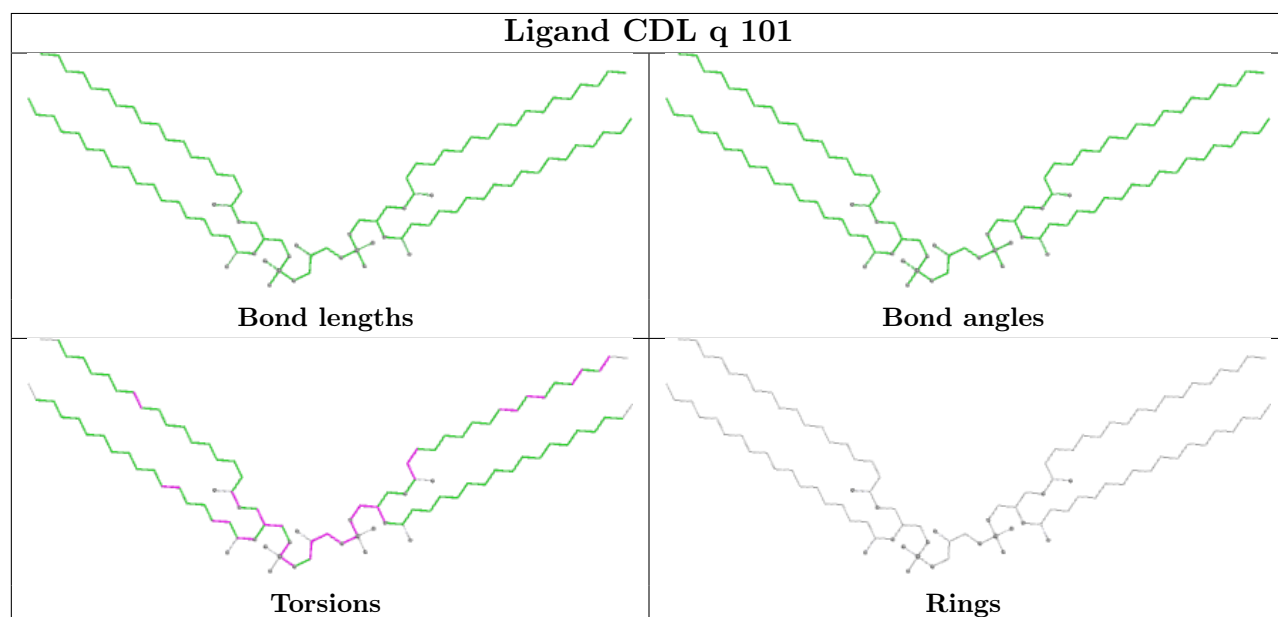
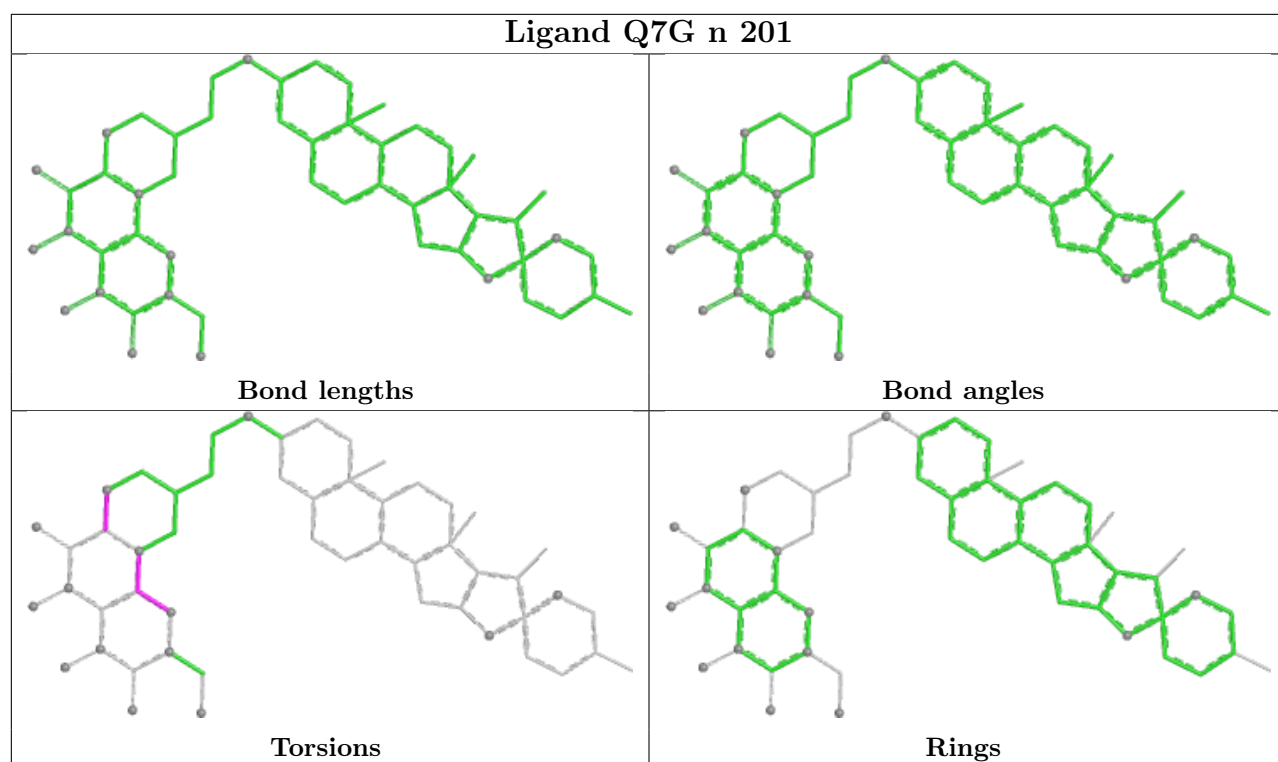
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



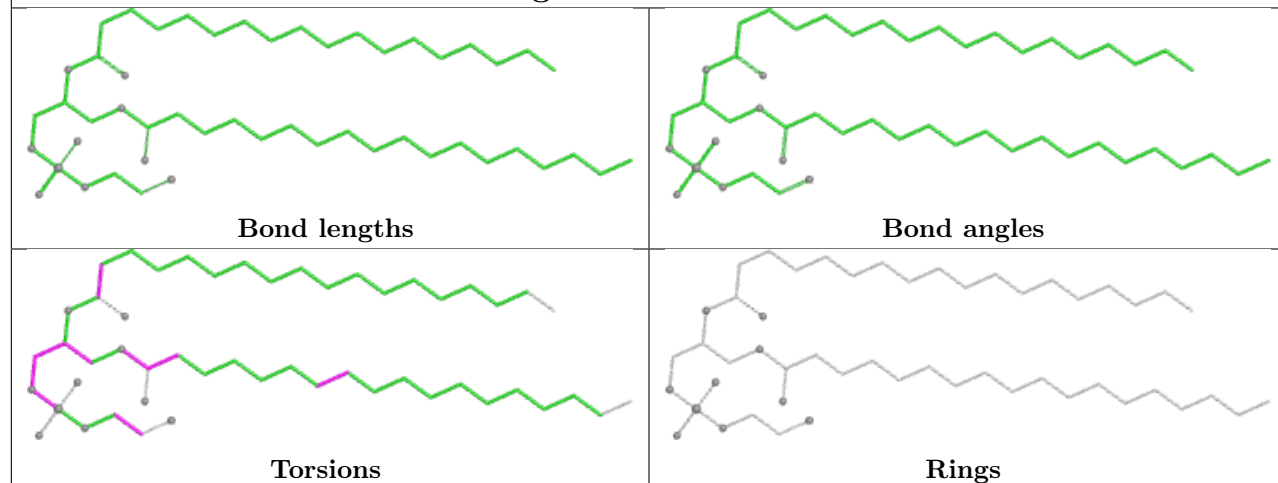




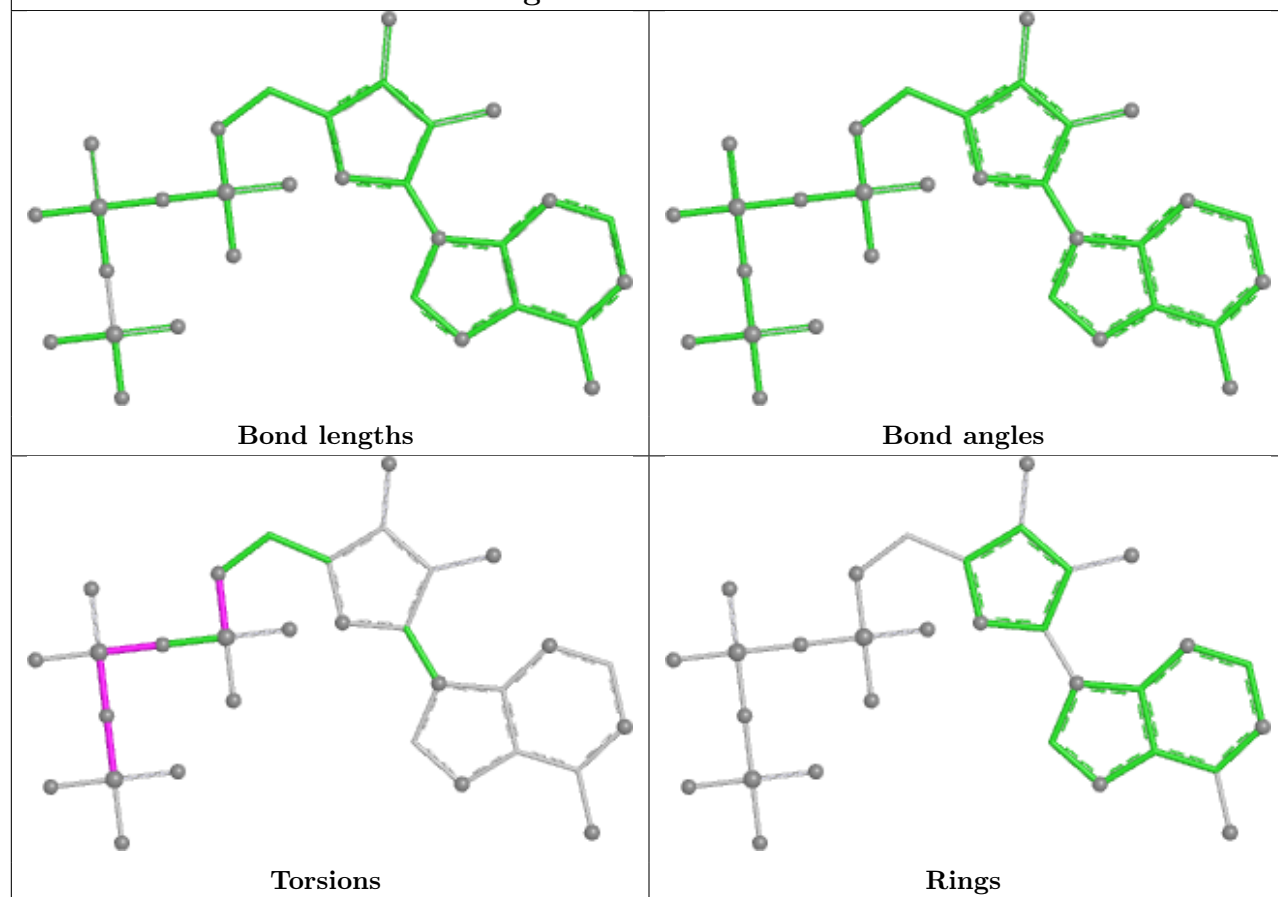


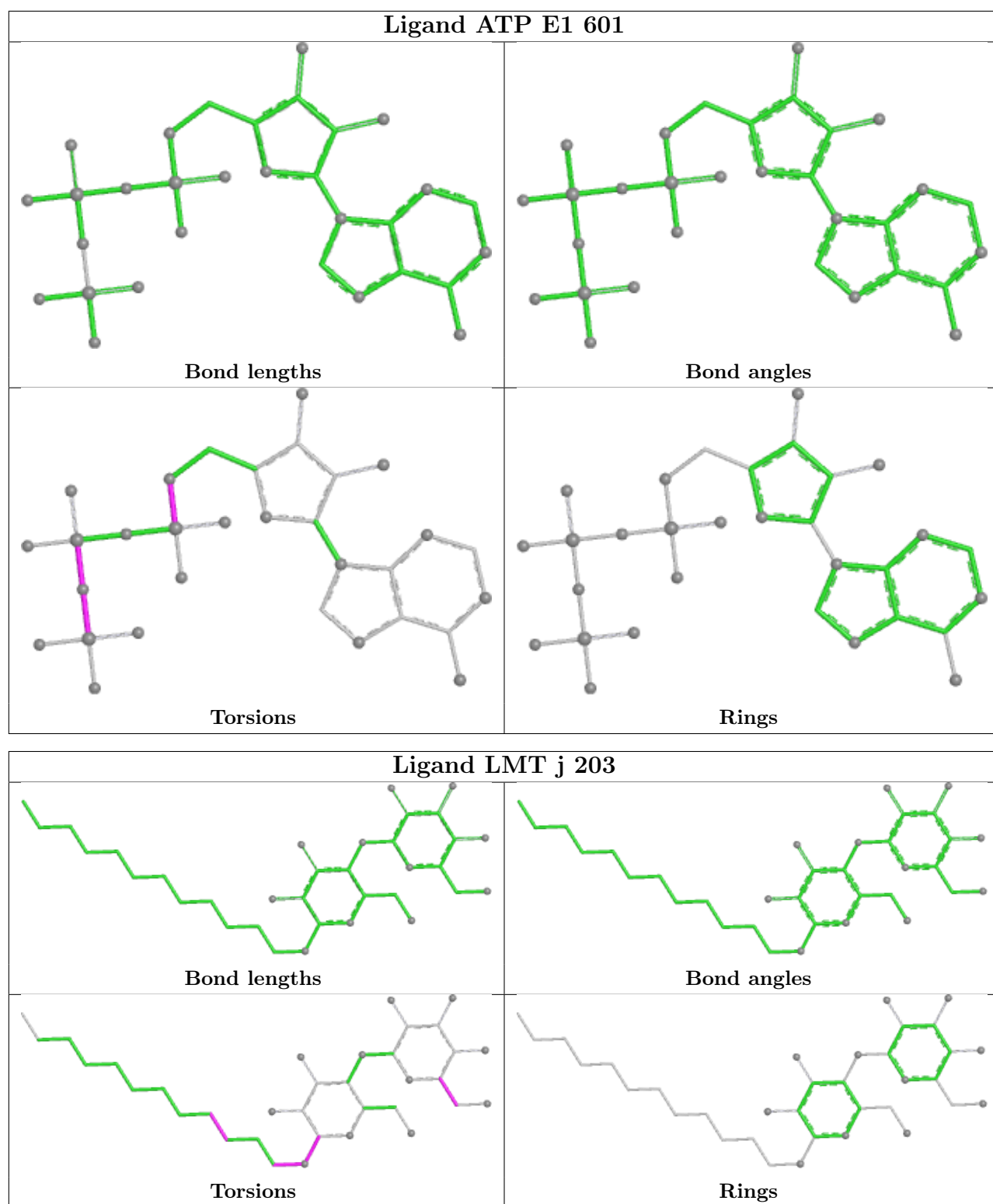


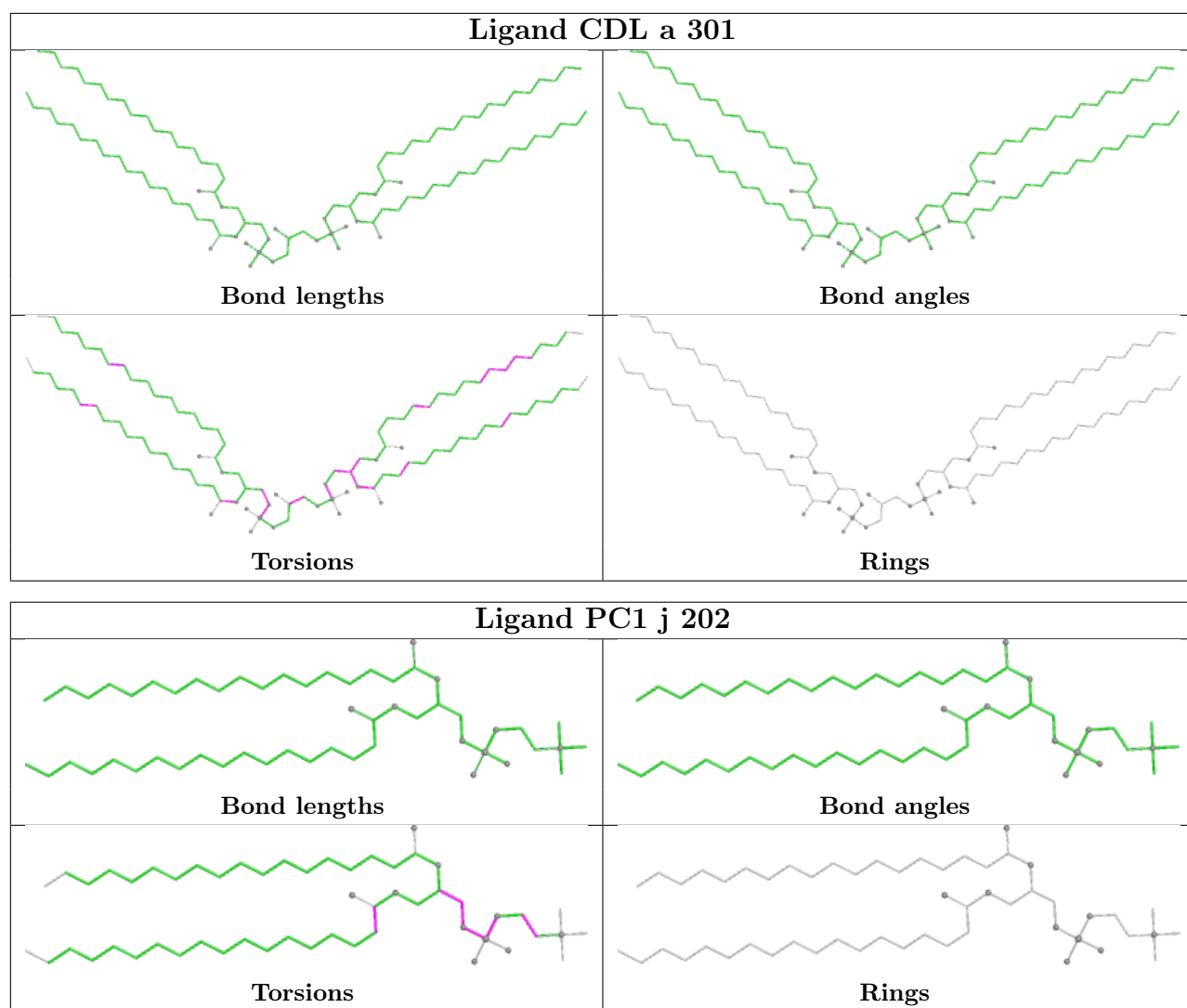
Ligand 3PE M 203

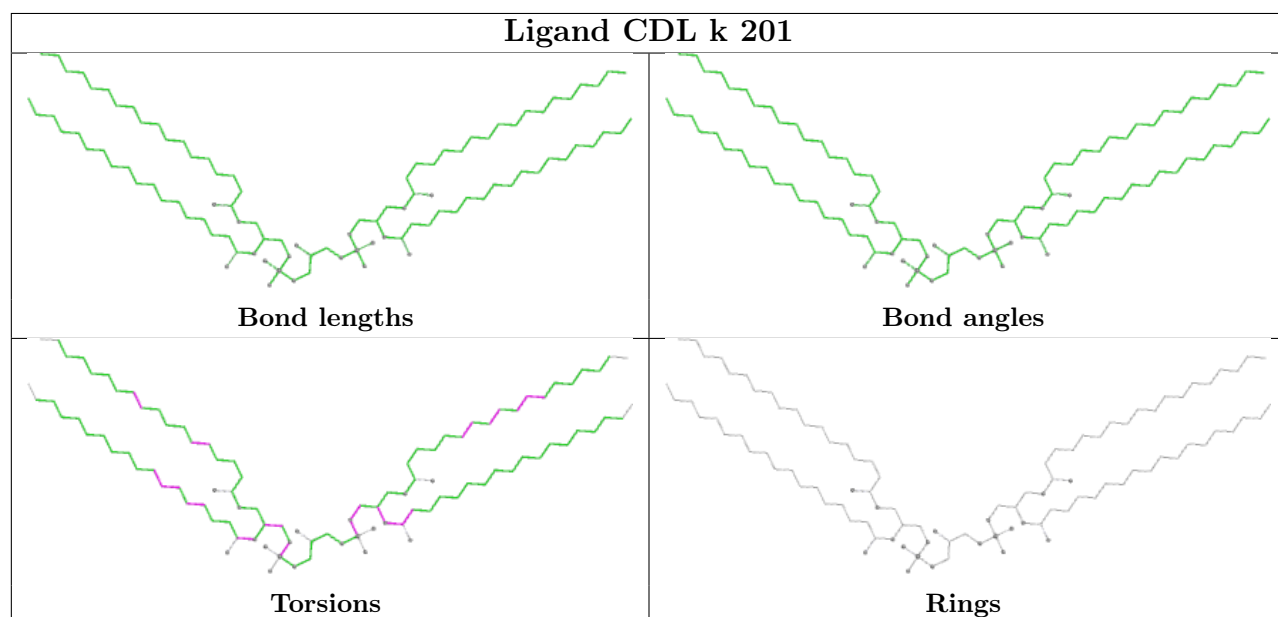
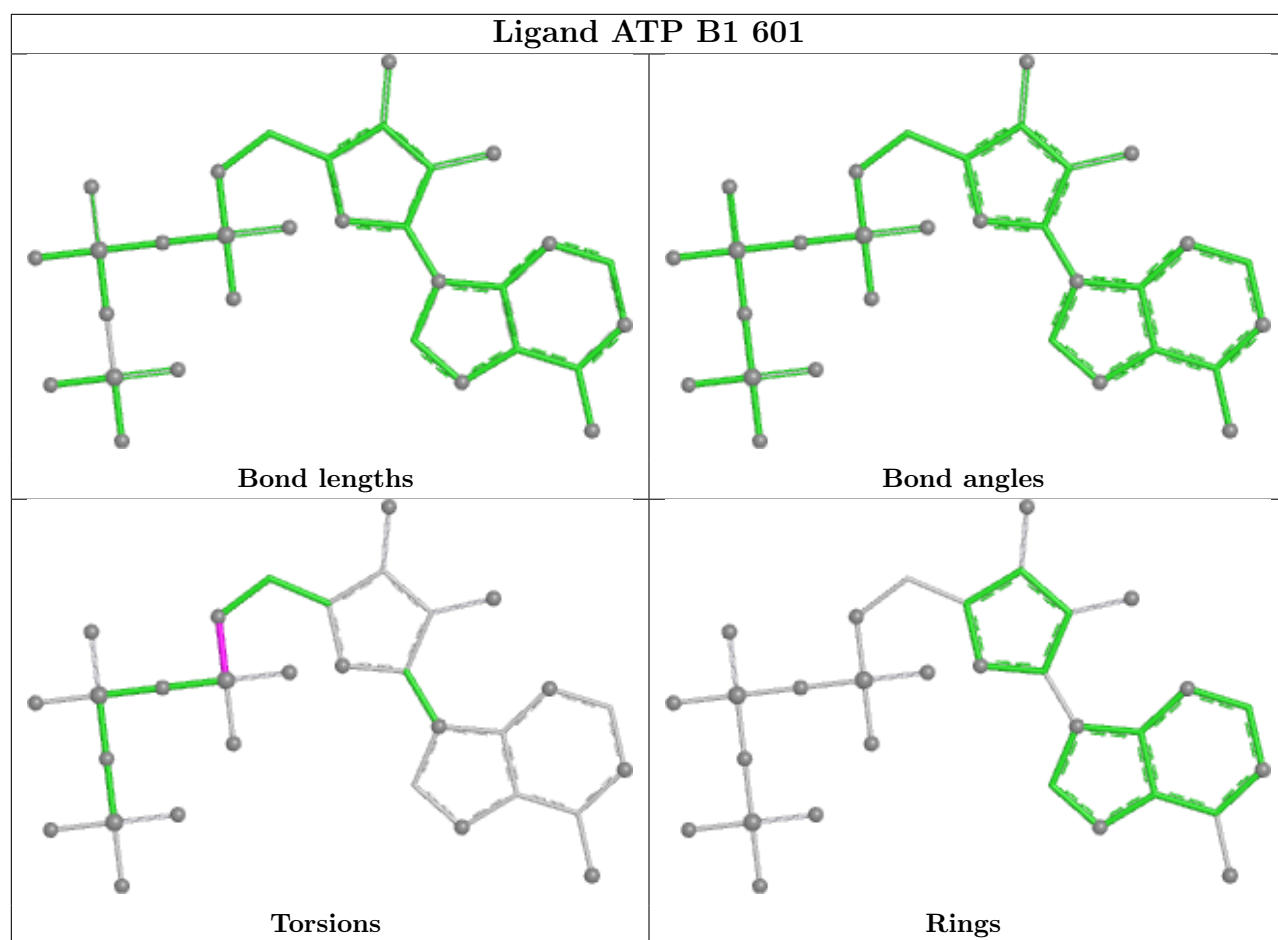


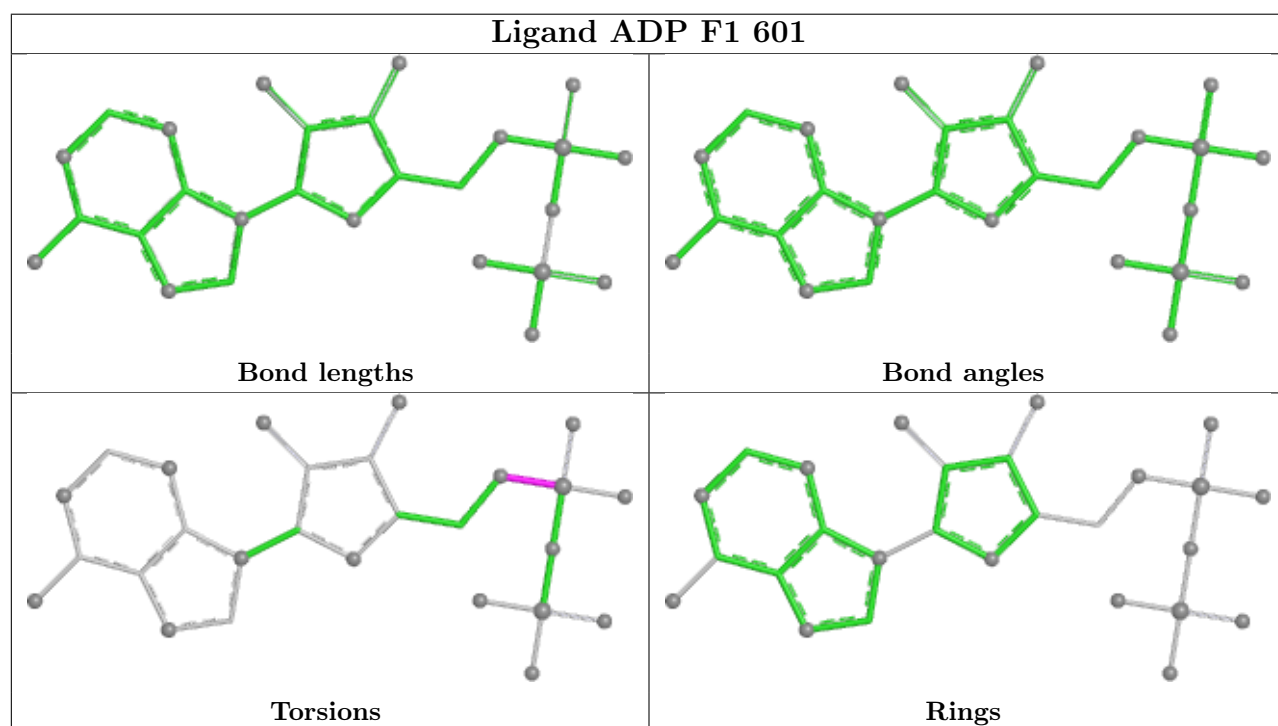
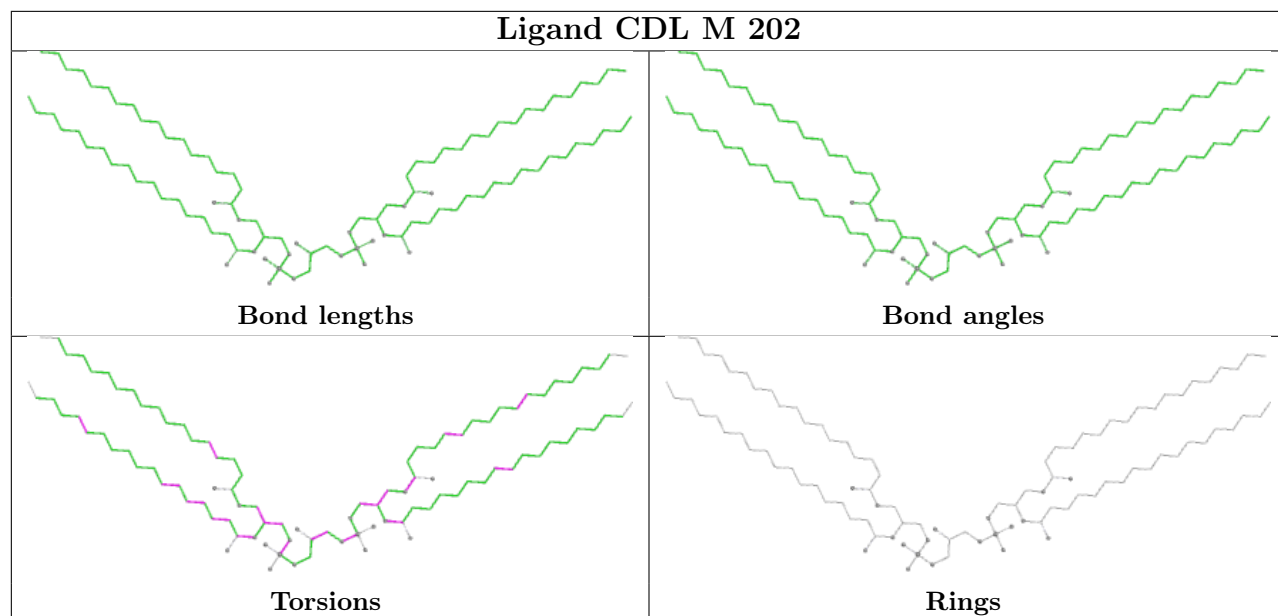
Ligand ATP A1 601

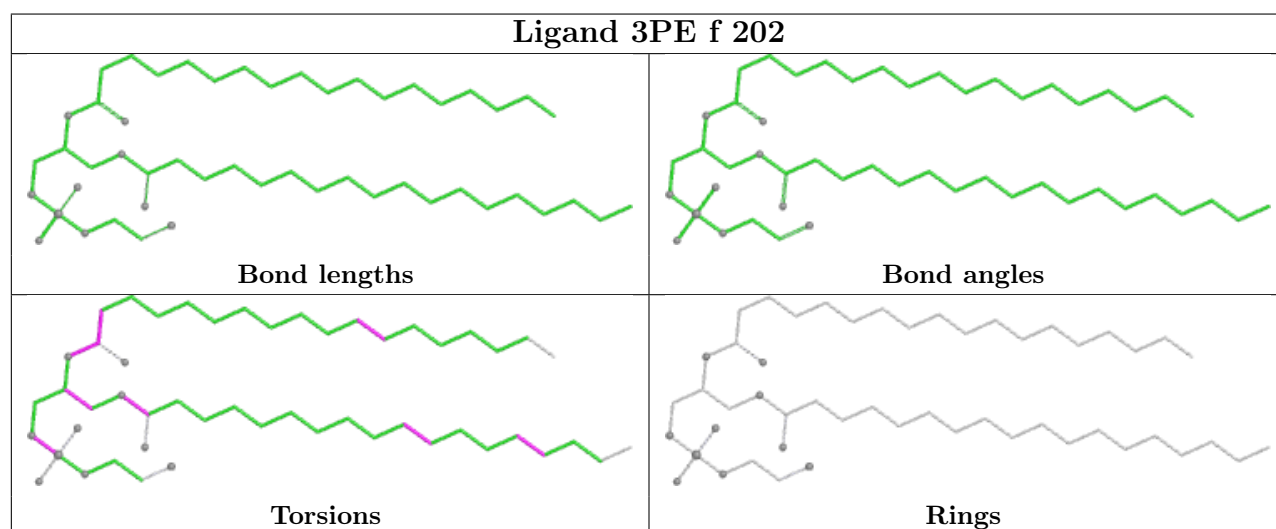
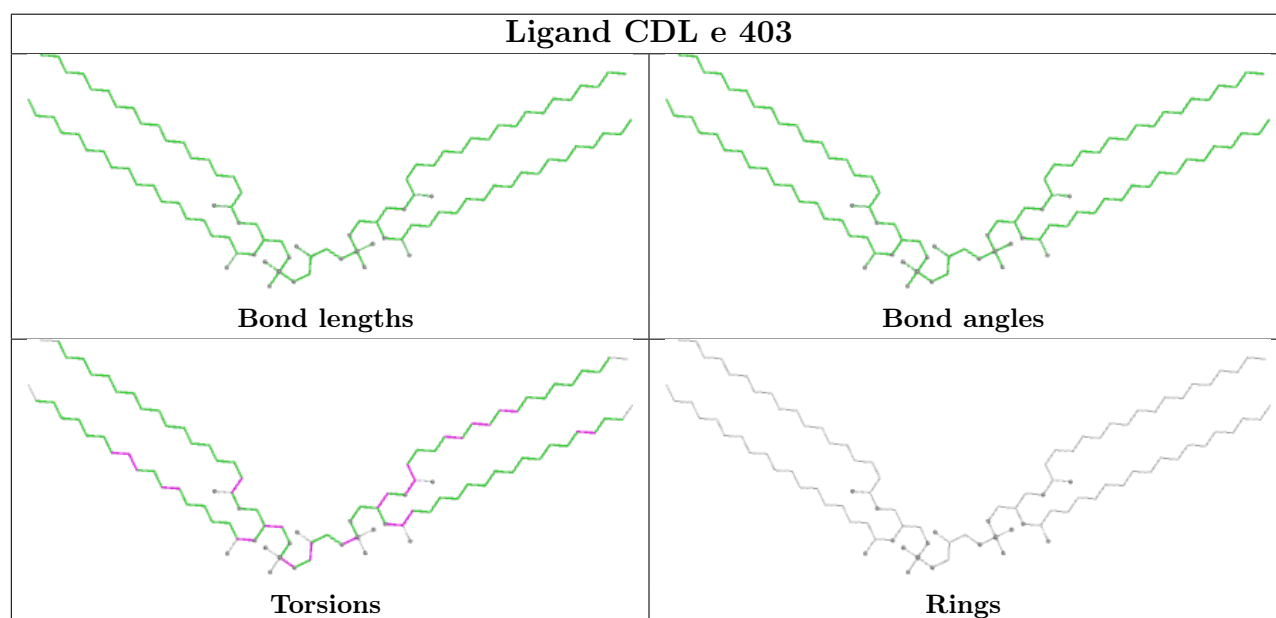
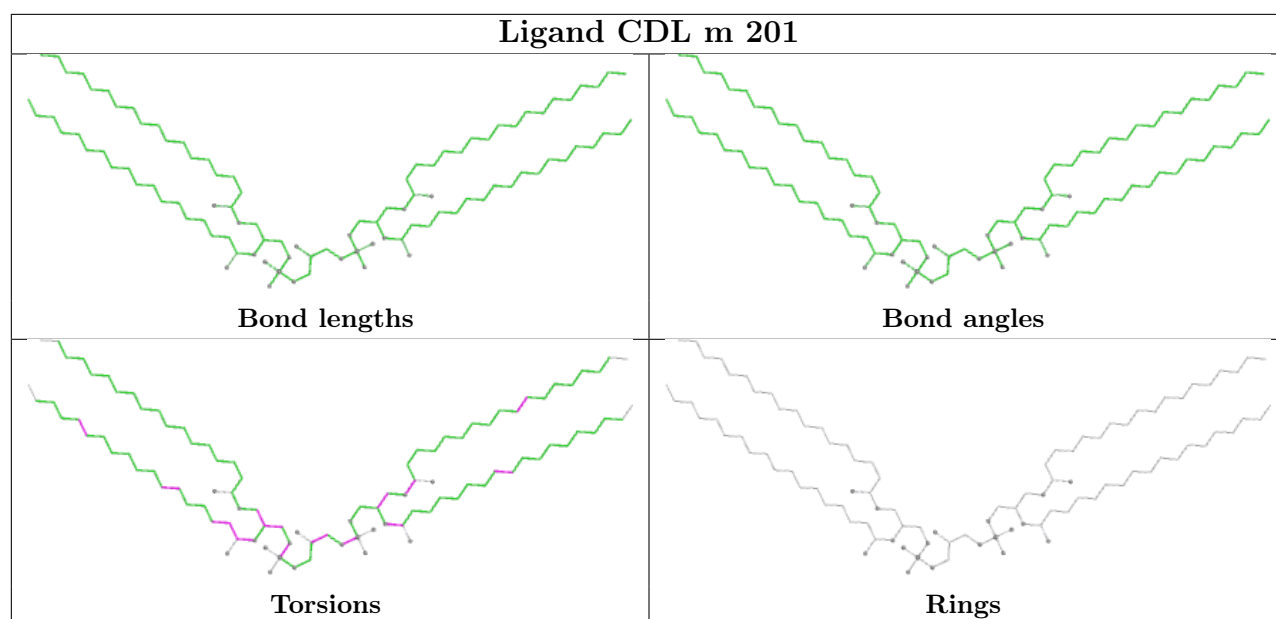


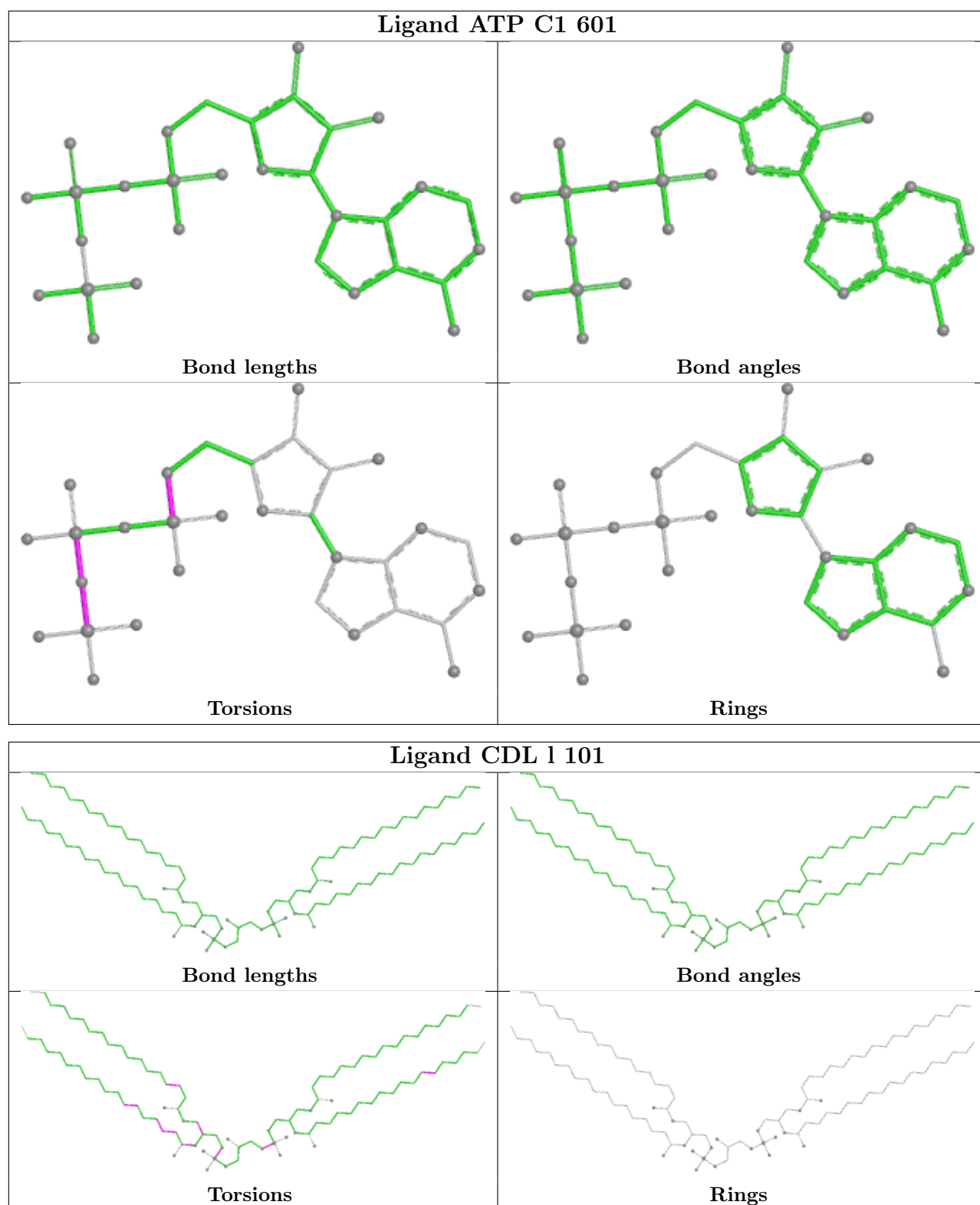


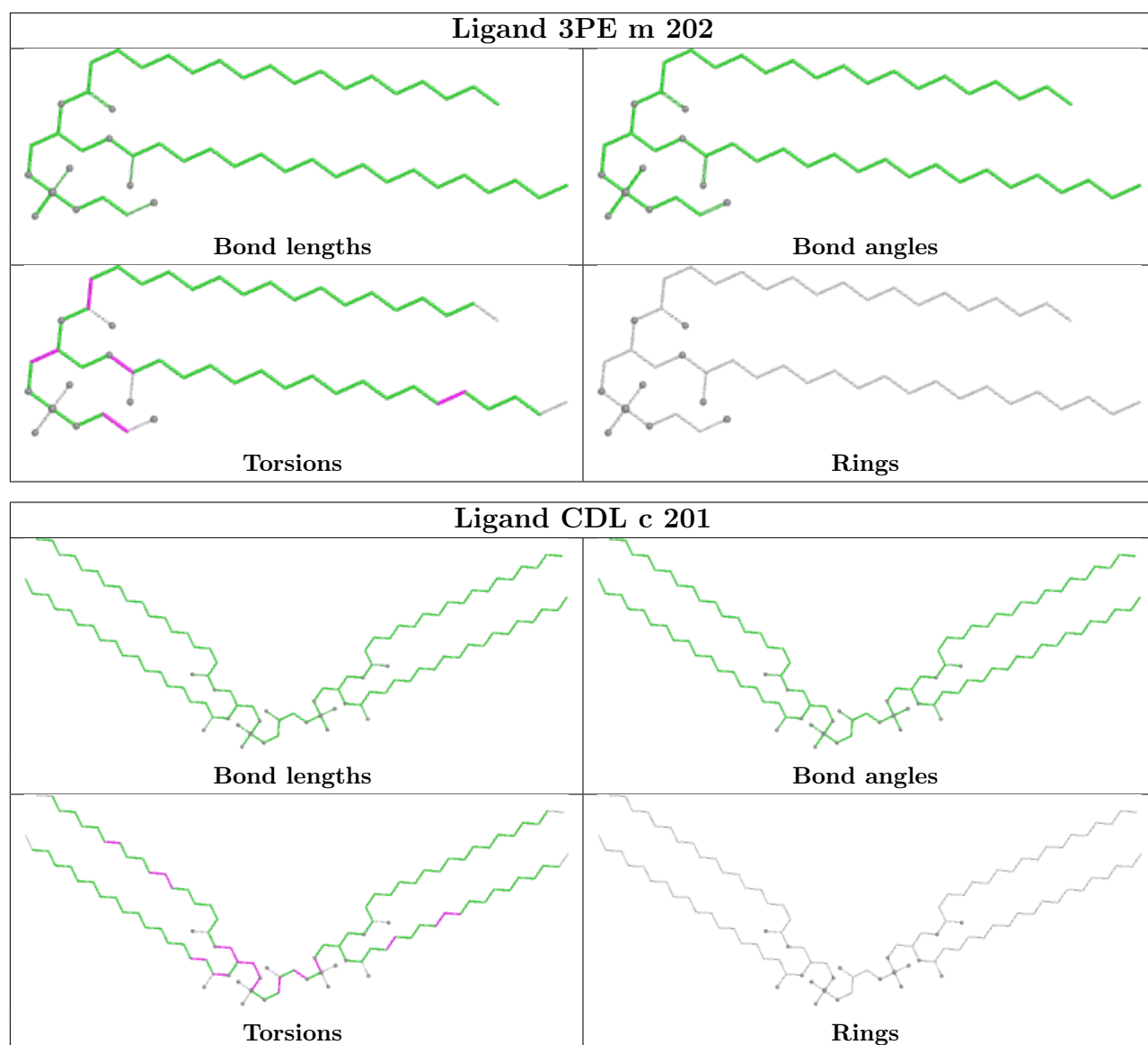


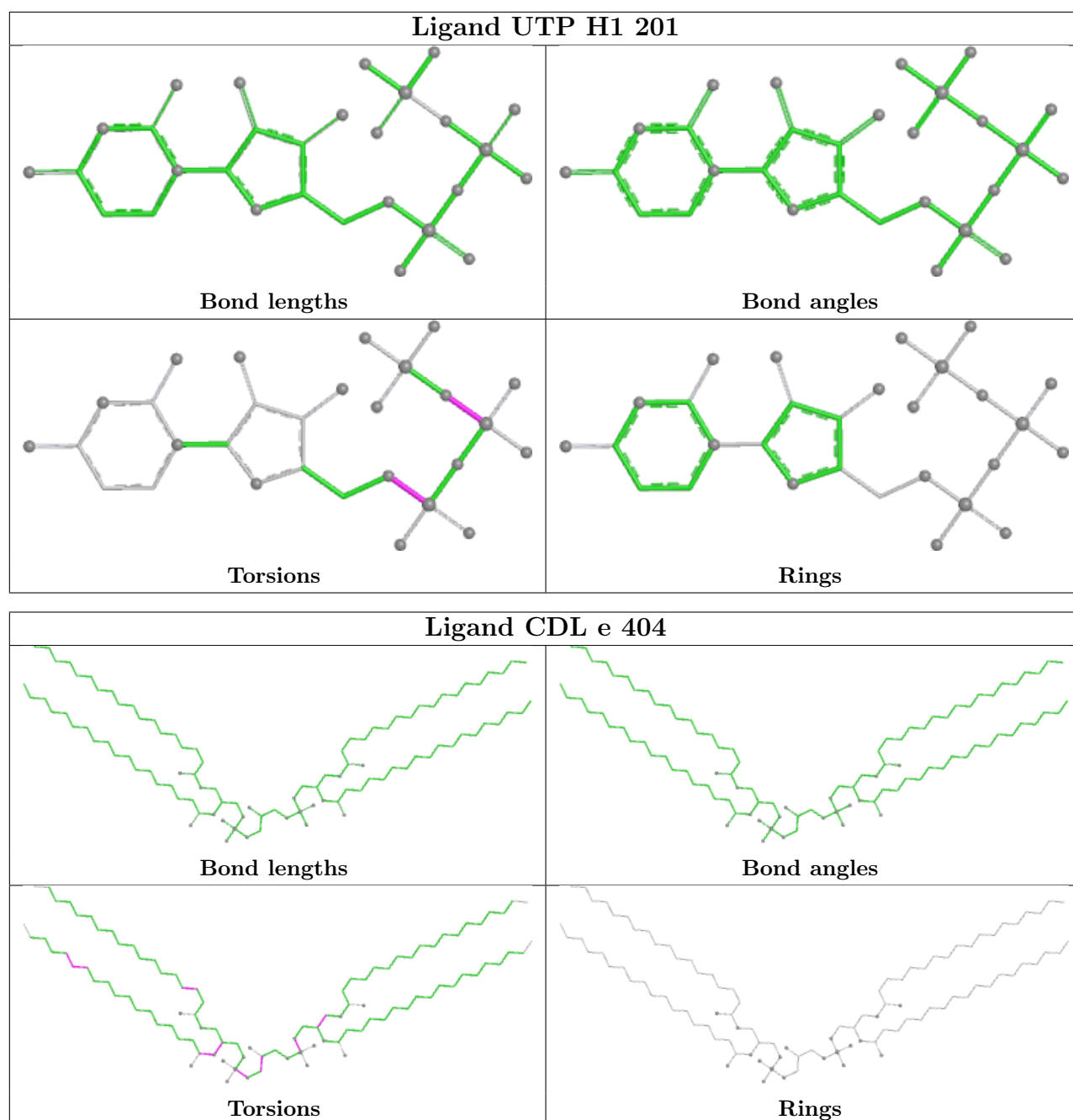












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

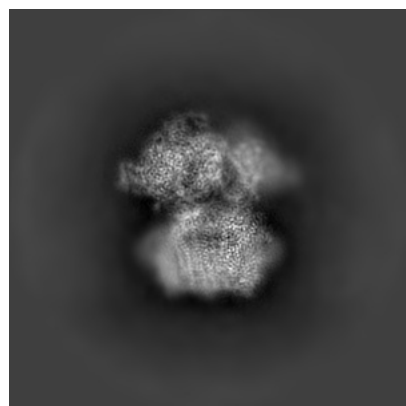
6 Map visualisation [i](#)

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

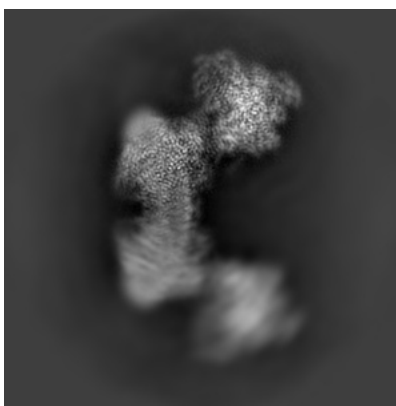
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

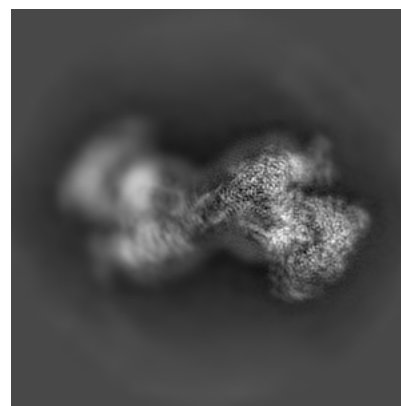
6.1.1 Primary map



X

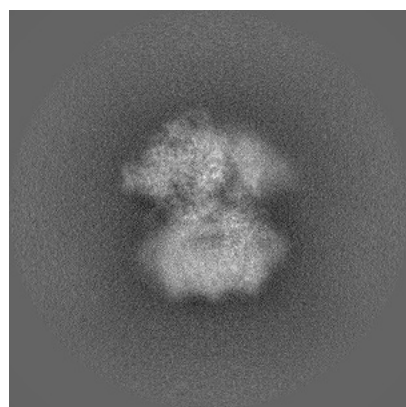


Y

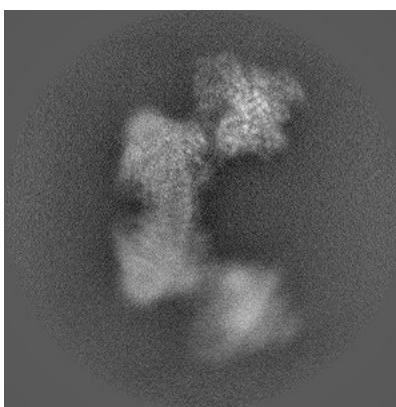


Z

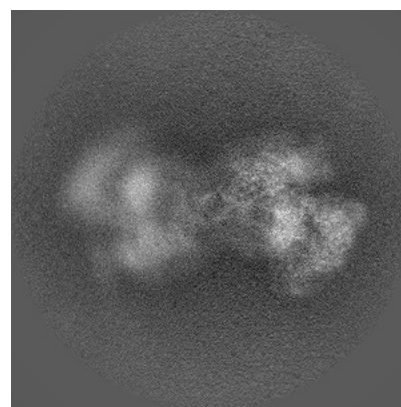
6.1.2 Raw map



X



Y

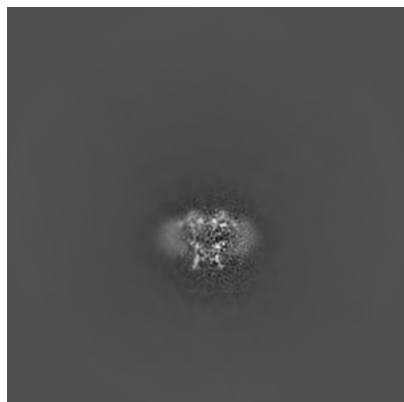


Z

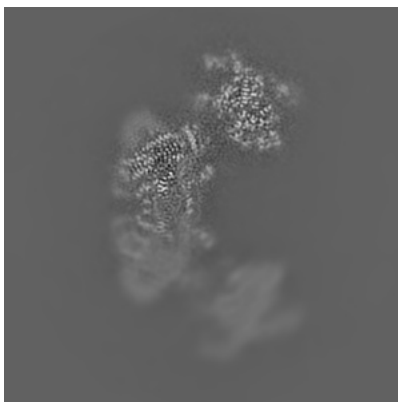
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

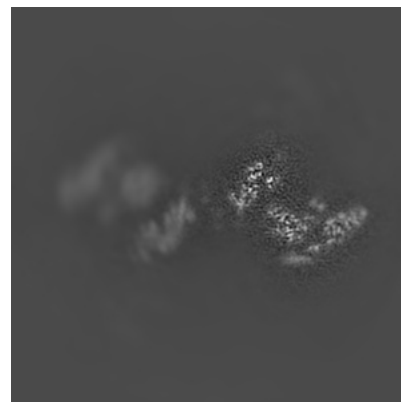
6.2.1 Primary map



X Index: 280

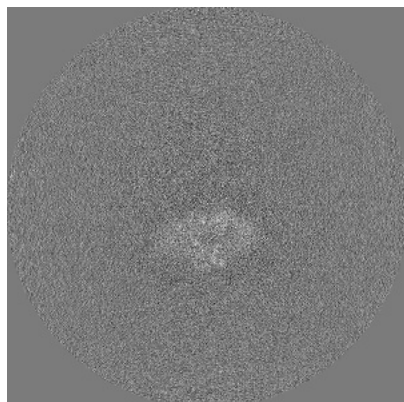


Y Index: 280

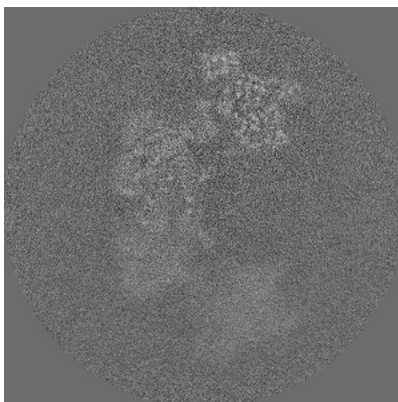


Z Index: 280

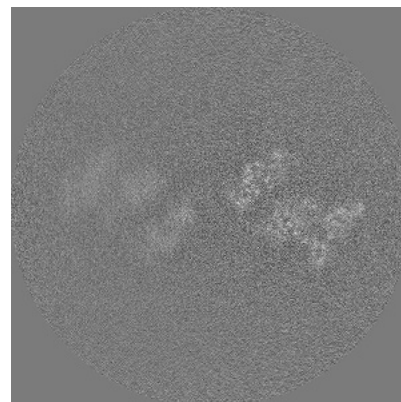
6.2.2 Raw map



X Index: 280



Y Index: 280

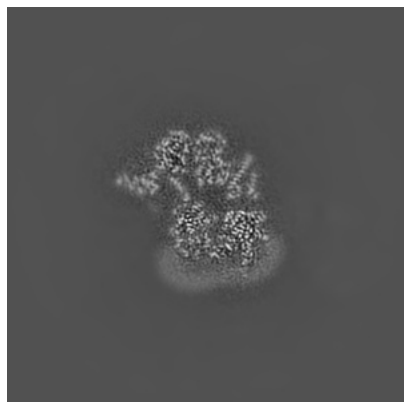


Z Index: 280

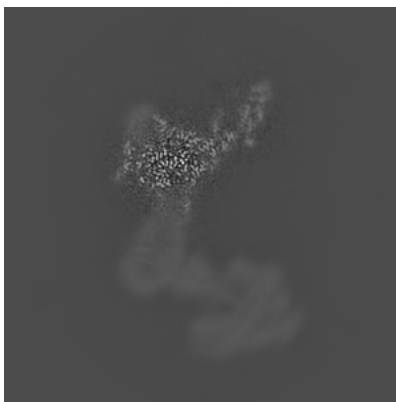
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

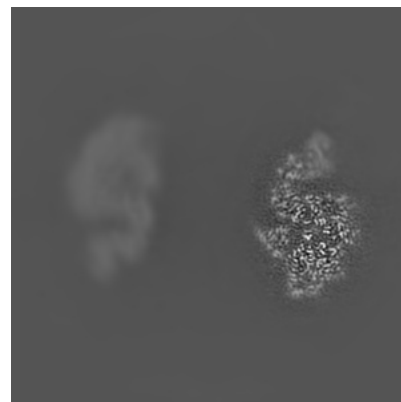
6.3.1 Primary map



X Index: 380

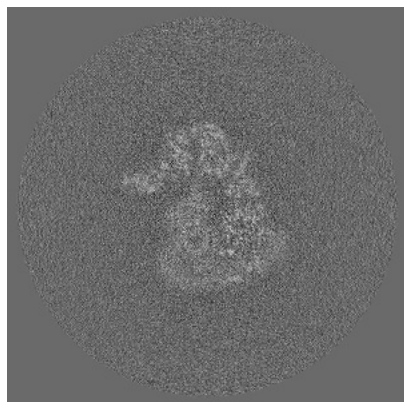


Y Index: 319

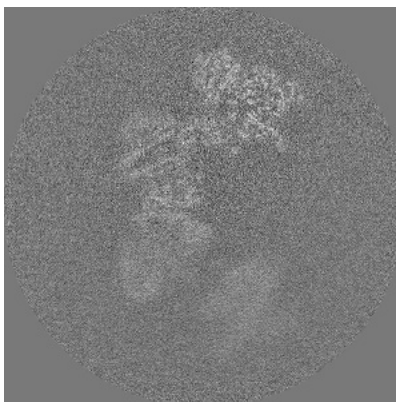


Z Index: 332

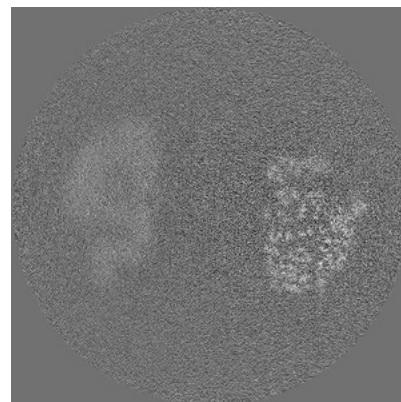
6.3.2 Raw map



X Index: 372



Y Index: 266

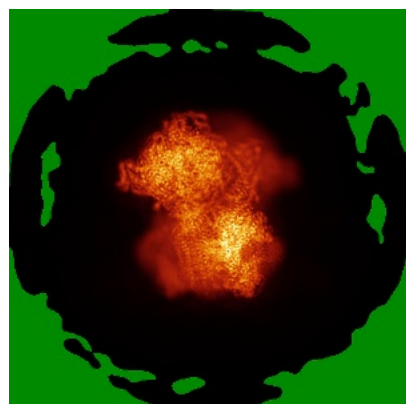


Z Index: 321

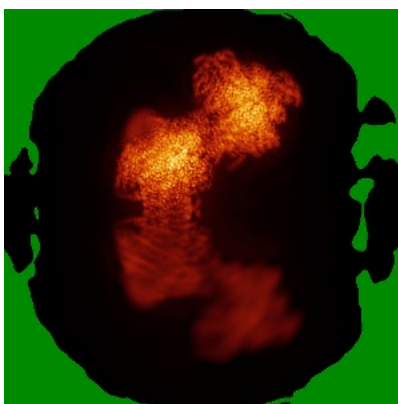
The images above show the largest variance slices of the map in three orthogonal directions.

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

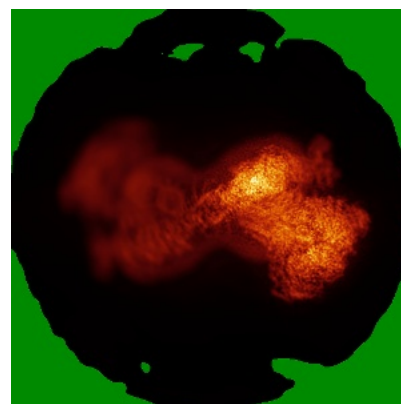
6.4.1 Primary map



X

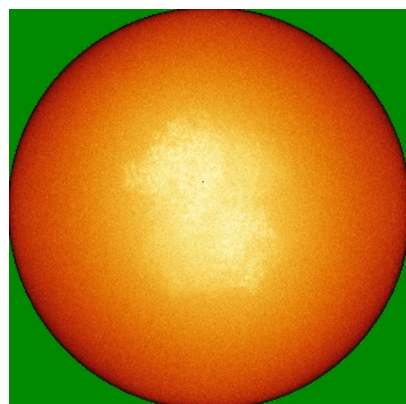


Y

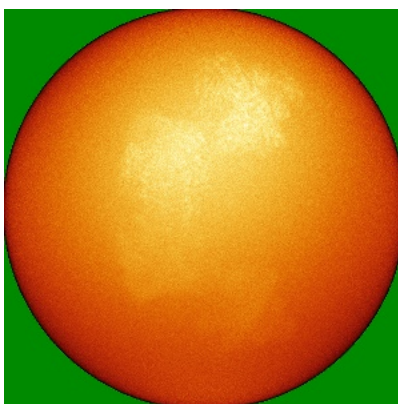


Z

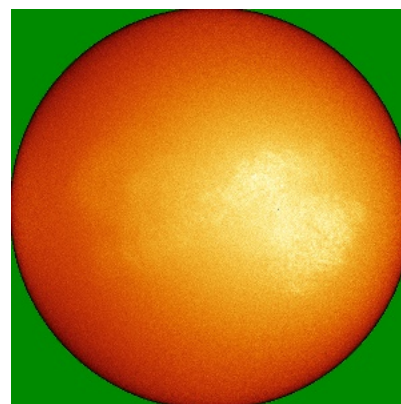
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

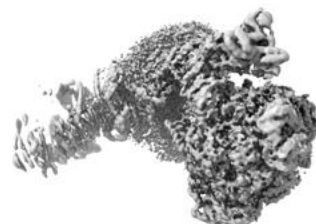
6.5.1 Primary map



X



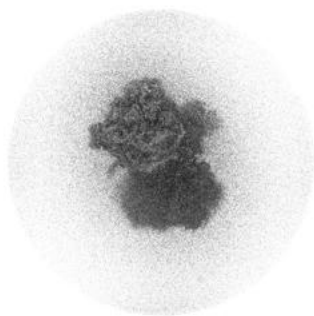
Y



Z

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

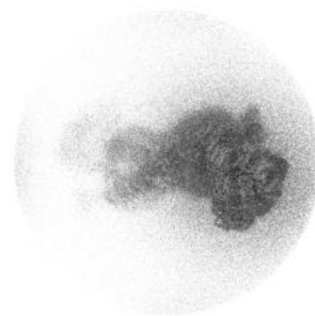
6.5.2 Raw map



X



Y



Z

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

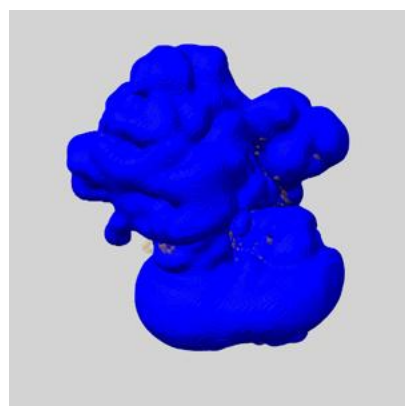
6.6 Mask visualisation [i](#)

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

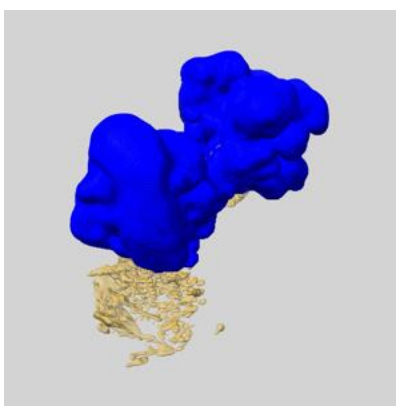
A mask typically either:

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

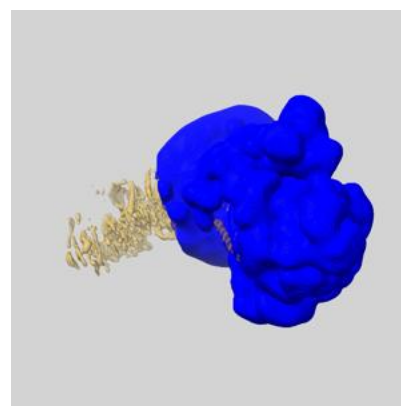
6.6.1 emd_15573_msk_1.map [i](#)



X



Y

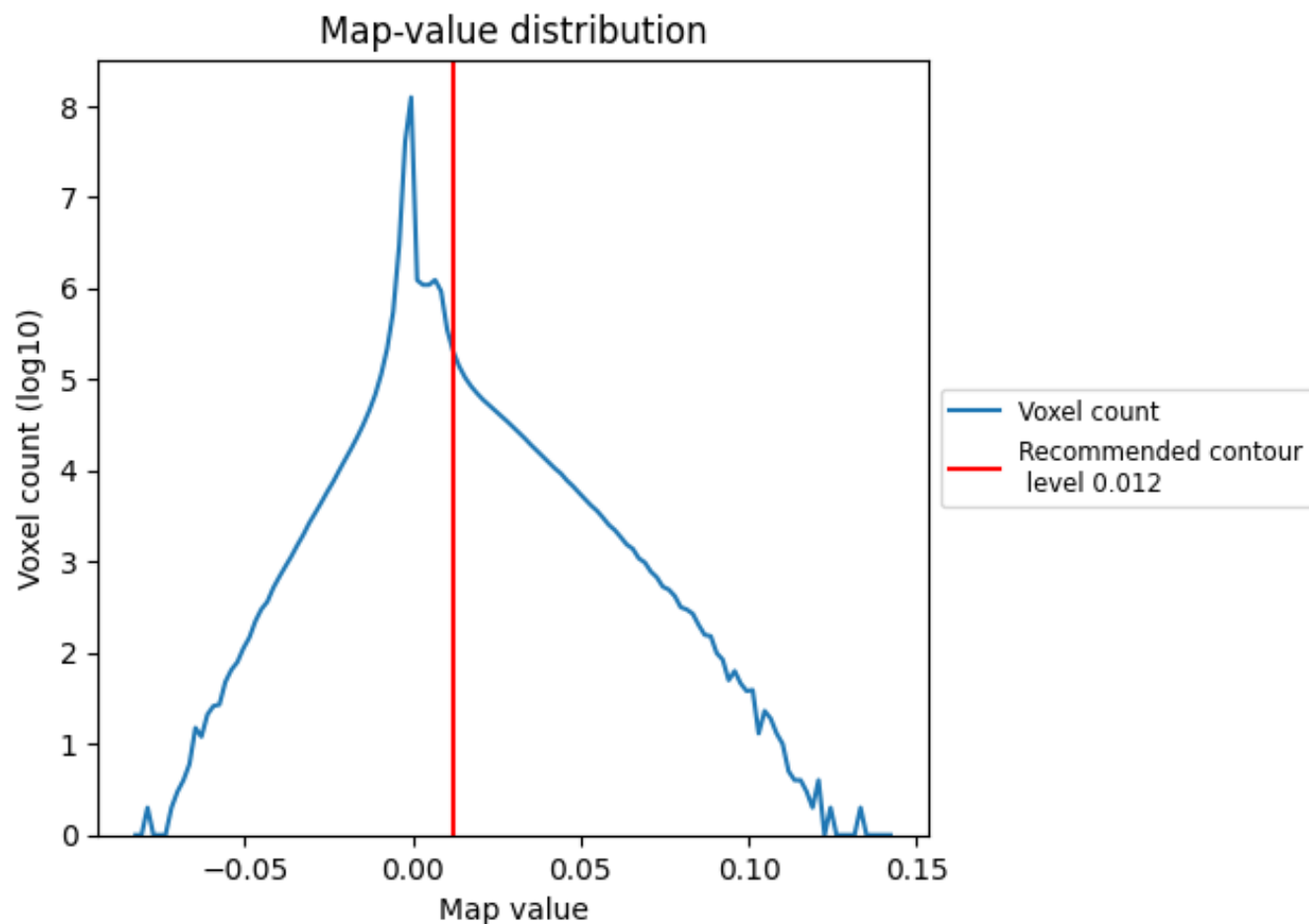


Z

7 Map analysis [i](#)

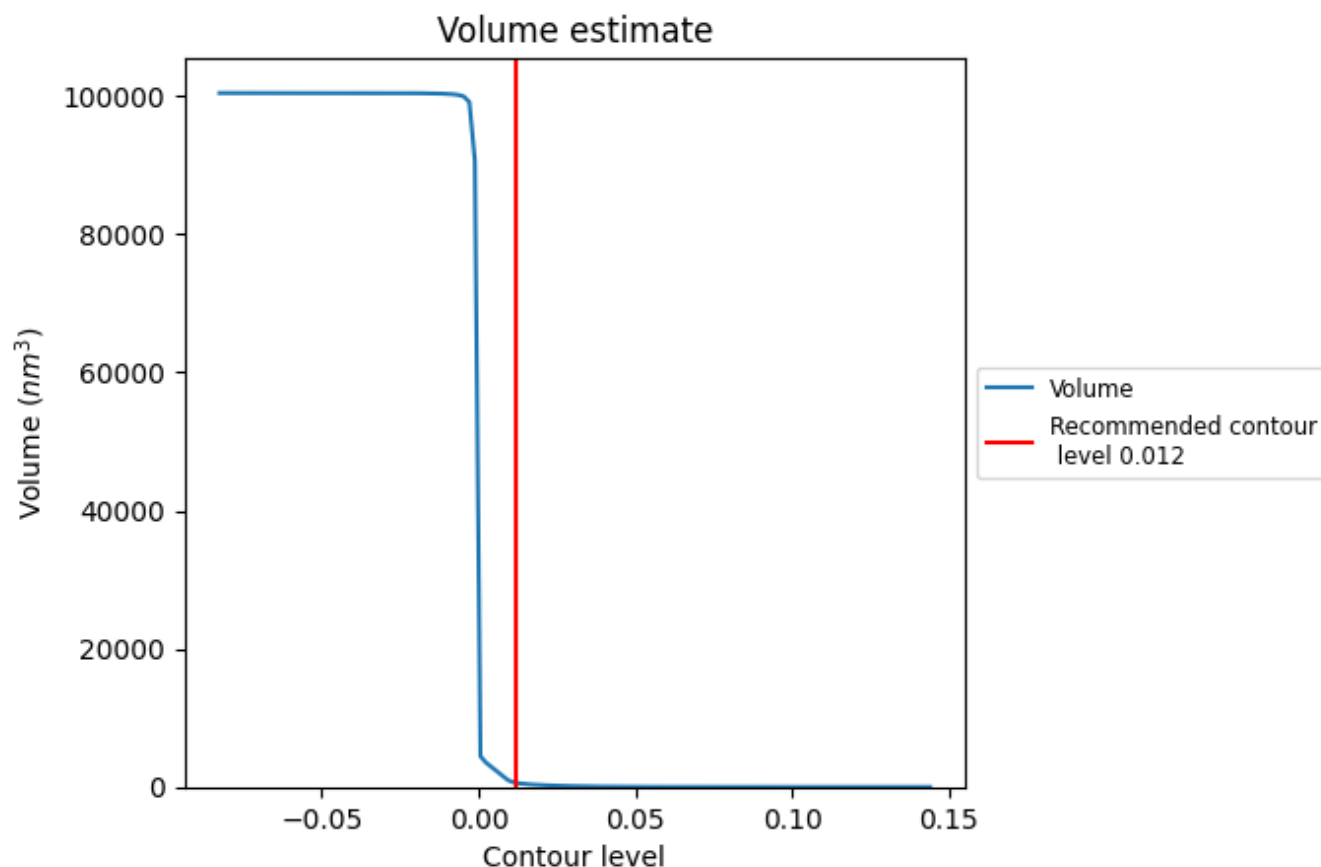
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

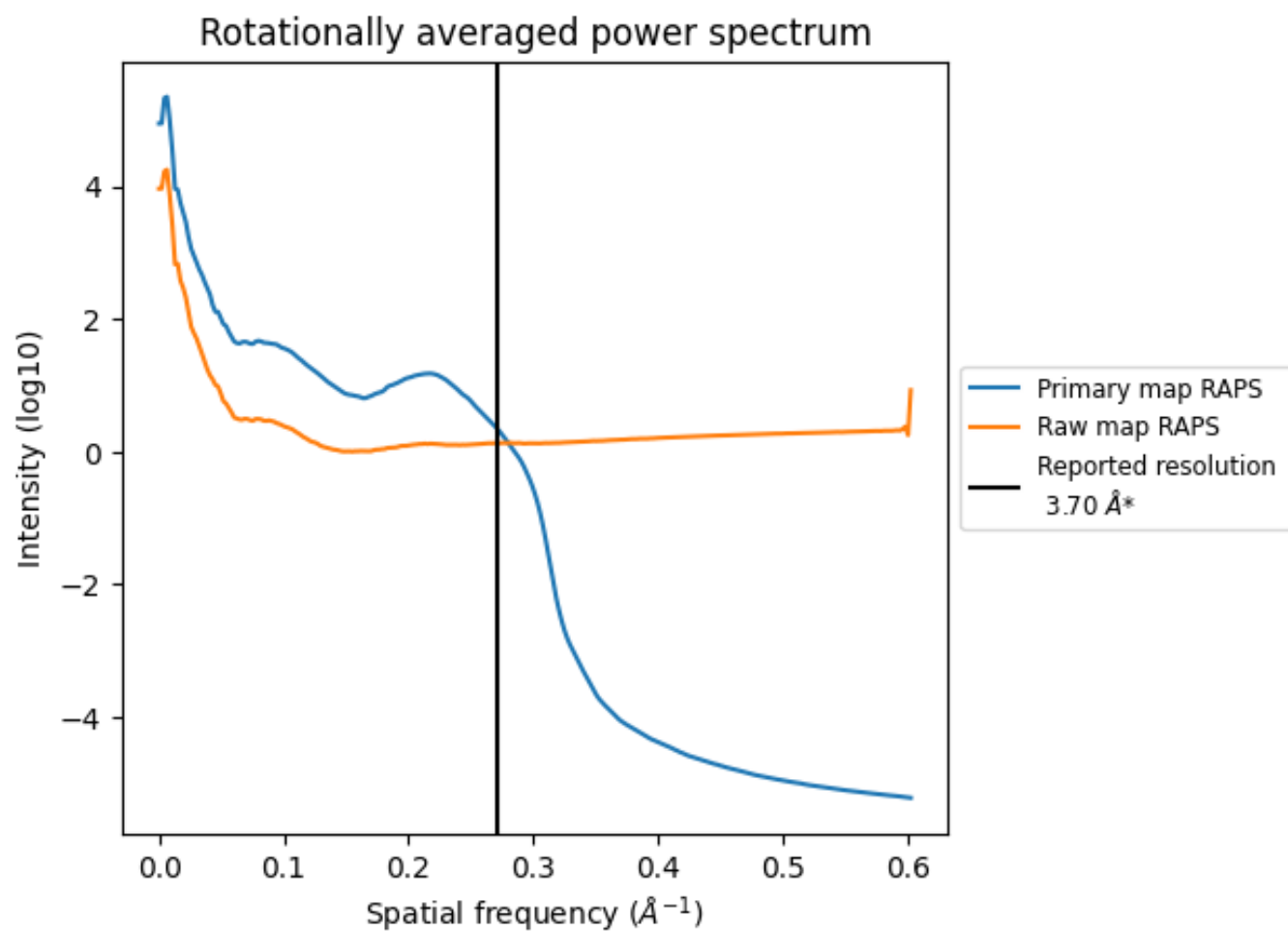
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 607 nm^3 ; this corresponds to an approximate mass of 548 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

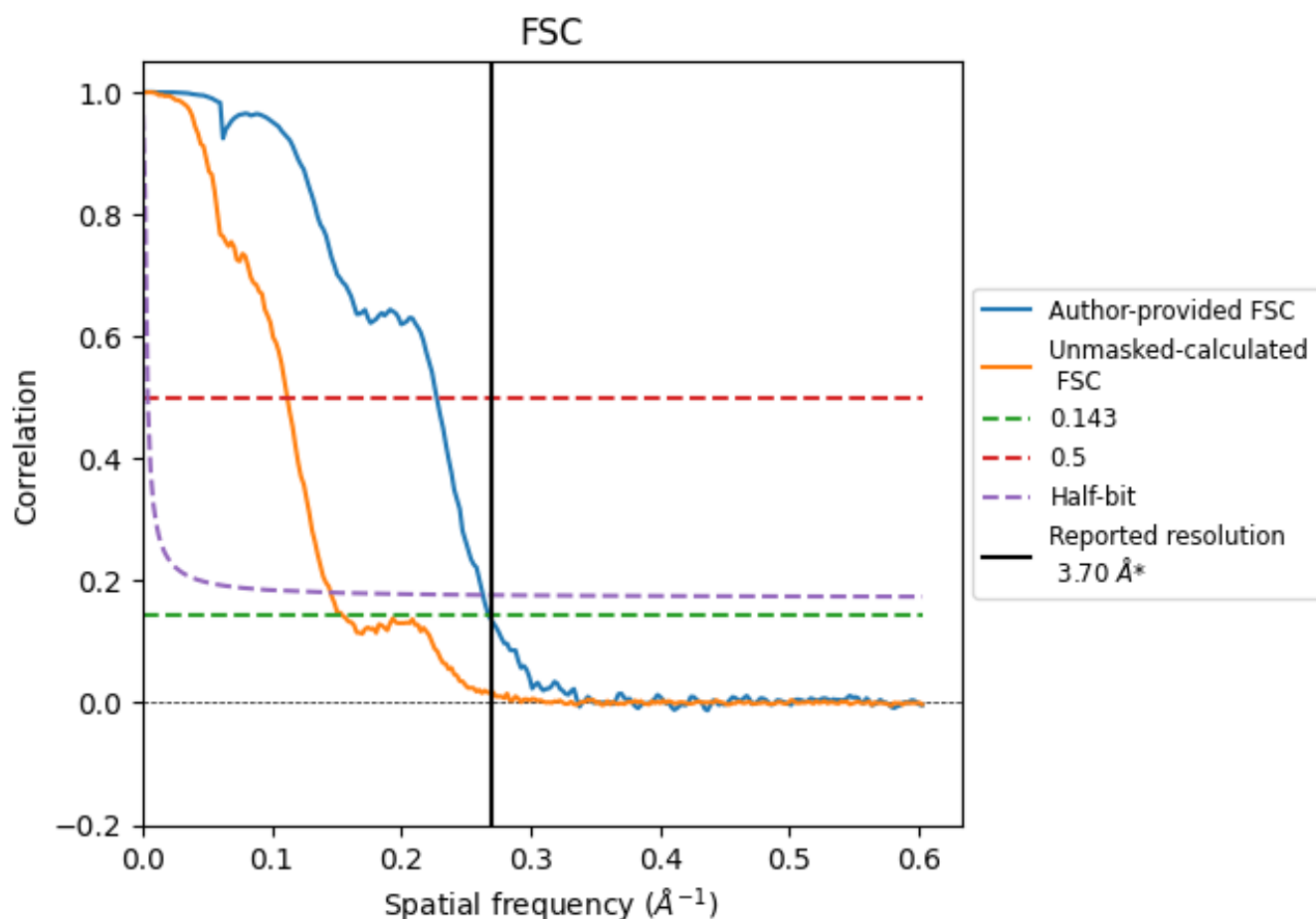


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

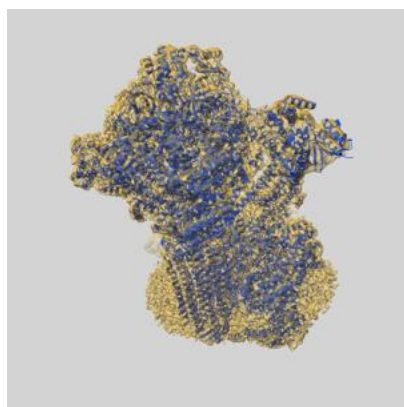
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.40	3.80
Unmasked-calculated*	6.47	8.92	6.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.47 differs from the reported value 3.7 by more than 10 %

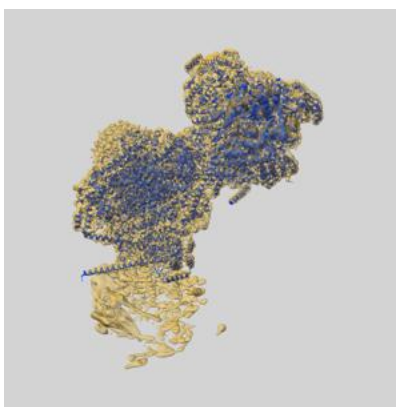
9 Map-model fit [i](#)

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

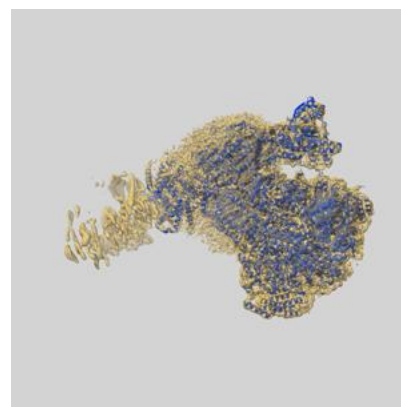
9.1 Map-model overlay [i](#)



X



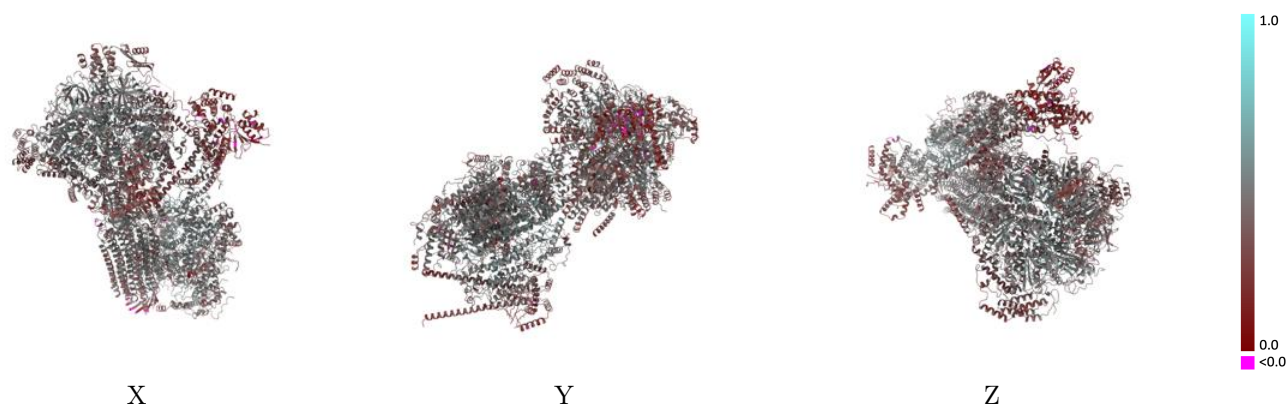
Y



Z

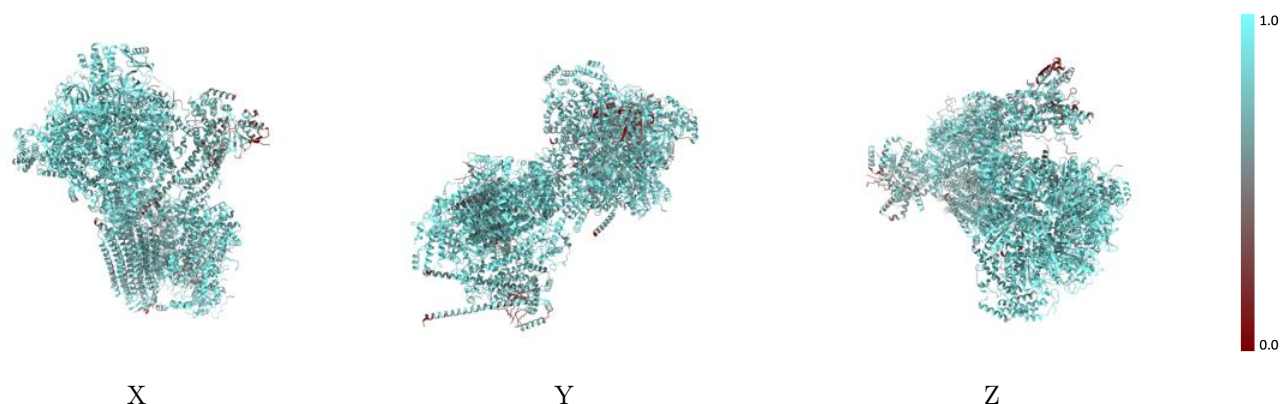
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



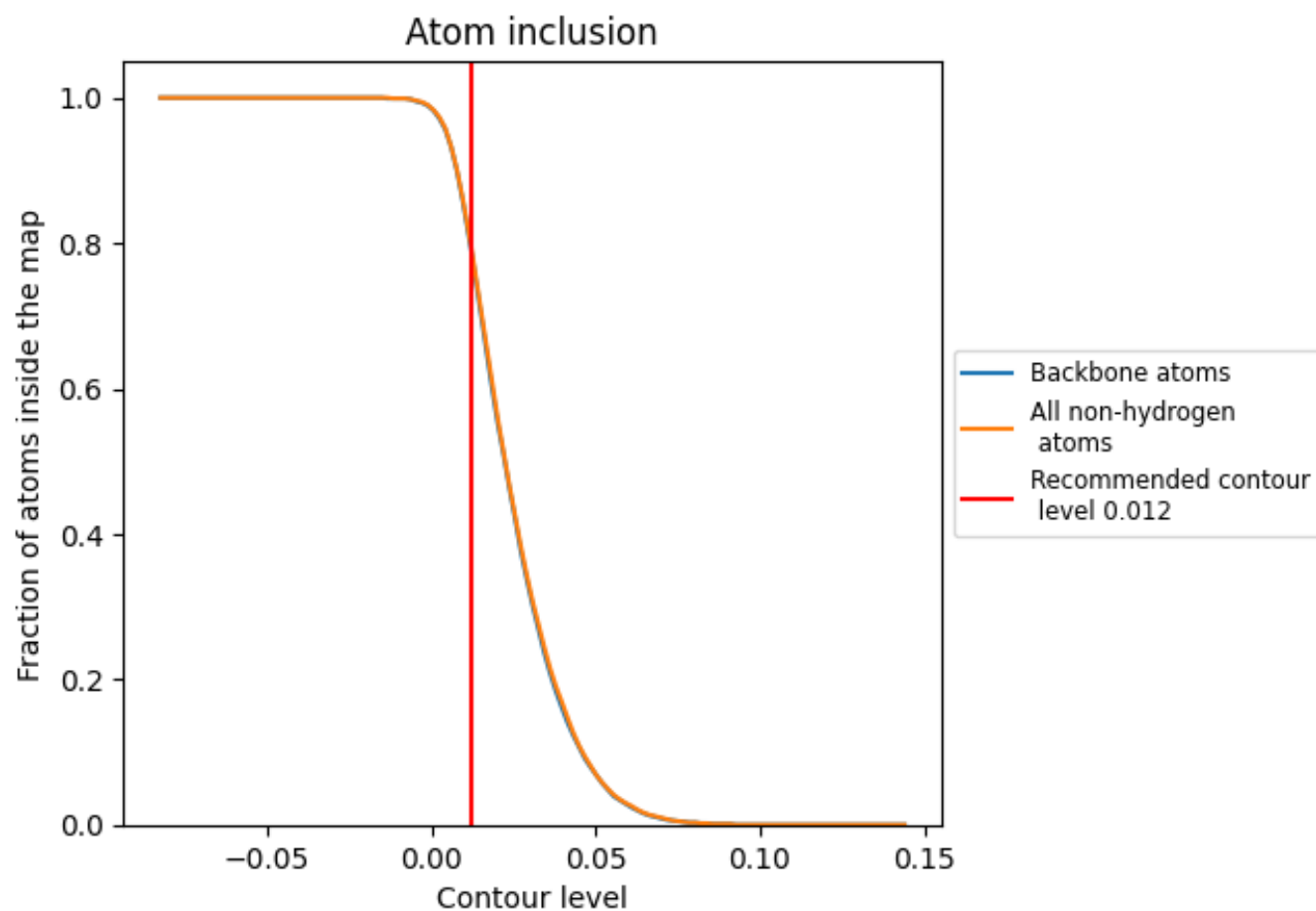
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

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



Continued on next page...

Continued from previous page...

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