



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:52 PM UTC

PDB ID : 8APD / pdb_00008apd
EMDB ID : EMD-15566
Title : rotational state 1d 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:

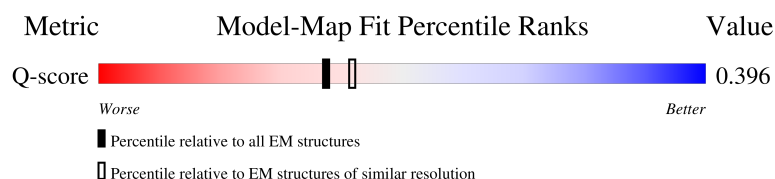
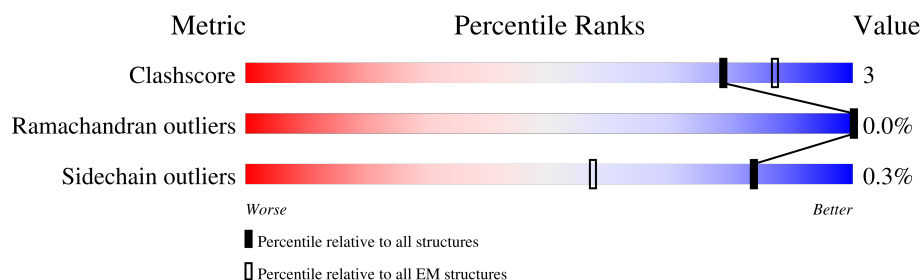
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

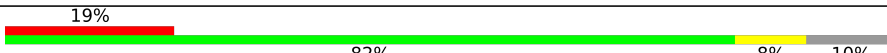
The reported resolution of this entry is 3.70 Å.

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.



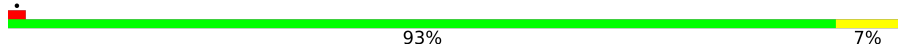
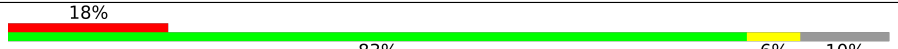
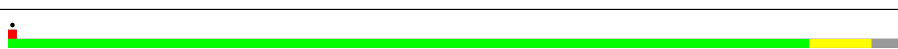
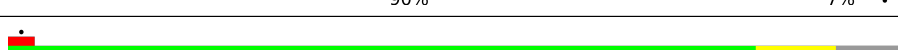
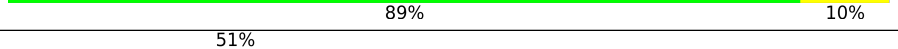
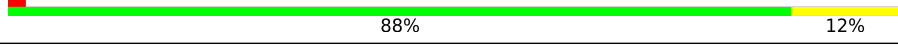
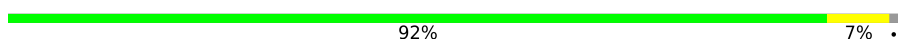
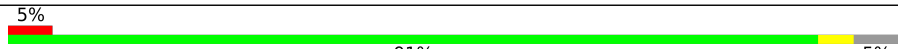
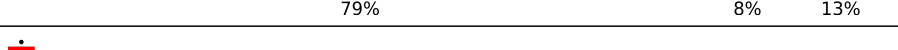
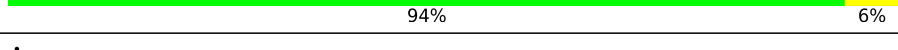
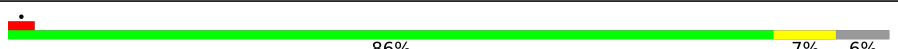
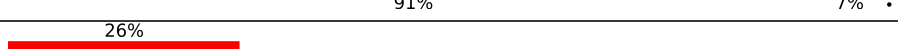
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	

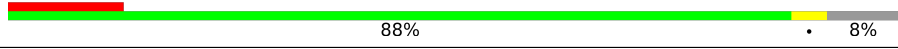
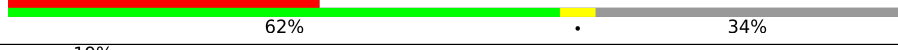
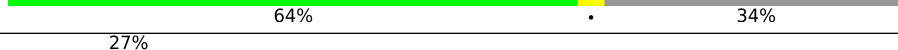
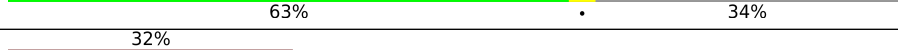
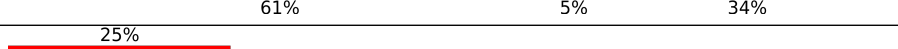
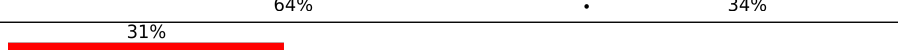
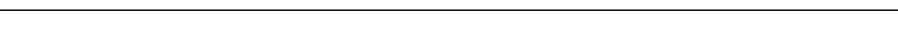
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Mol	Chain	Length	Quality of chain
3	a	231	
4	c	114	
5	d	370	
6	e	396	
7	f	145	
8	g	269	
9	h	157	
10	i	104	
11	j	169	
12	k	124	
13	n	156	
14	o	101	
15	p	105	
16	q	98	
17	r	62	
18	A1	584	
18	B1	584	
18	C1	584	
19	D1	519	
19	E1	519	
19	F1	519	
20	G1	305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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	Q7G	e	407	X	-	-	-
30	Q7G	n	201	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 129568 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	530	Total	C	H	N	O	S	0	0
			8281	2612	4197	710	742	20		
18	B1	523	Total	C	H	N	O	S	0	0
			8200	2585	4162	702	731	20		
18	C1	523	Total	C	H	N	O	S	0	0
			8194	2587	4155	701	731	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	486	Total	C	H	N	O	S	0	0
			7415	2324	3733	630	709	19		
19	F1	489	Total	C	H	N	O	S	0	0
			7462	2339	3759	633	712	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
			2591	822	1276	221	258	14		
23	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		

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

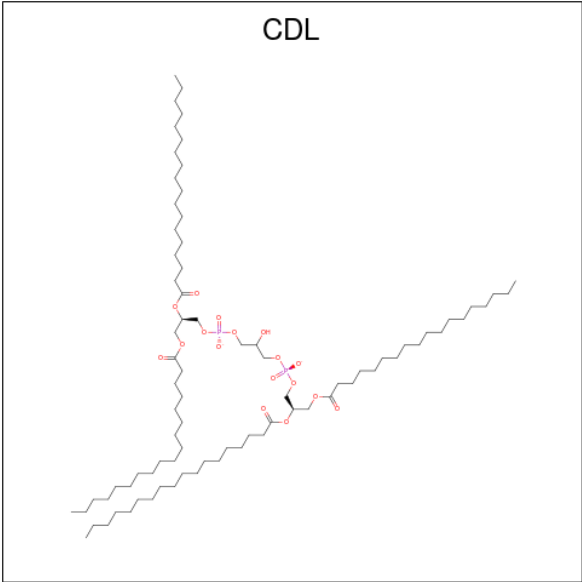
- Molecule 24 is a protein called OSCP.

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

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

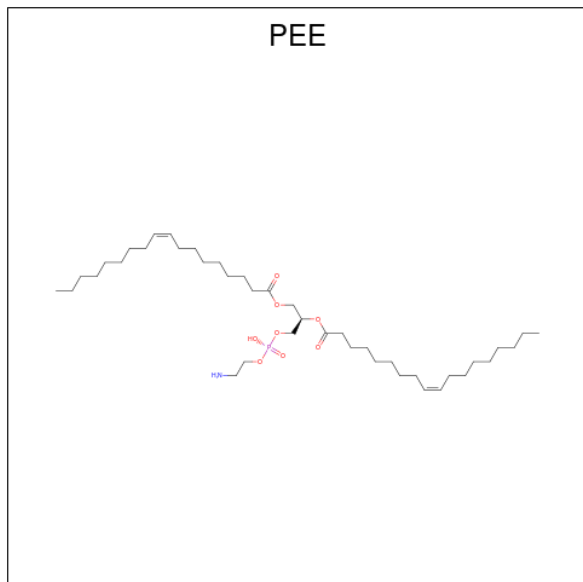
Mol	Chain	Residues	Atoms						AltConf	Trace
25	O1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	P1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	Q1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	R1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	S1	78	Total	C	H	N	O	S	0	0
			1166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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



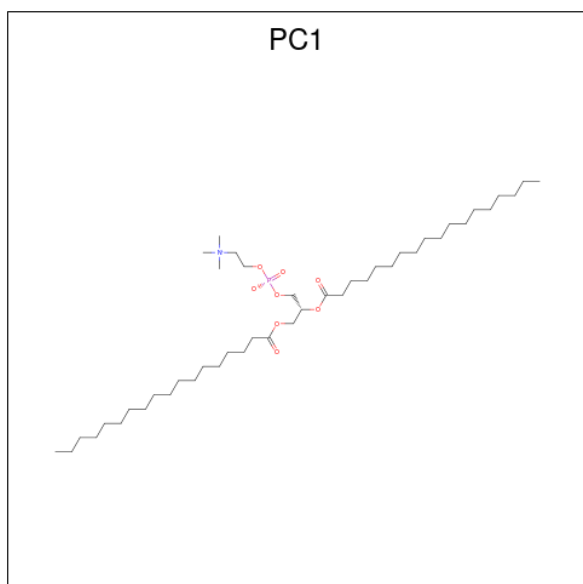
Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1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

- Molecule 27 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



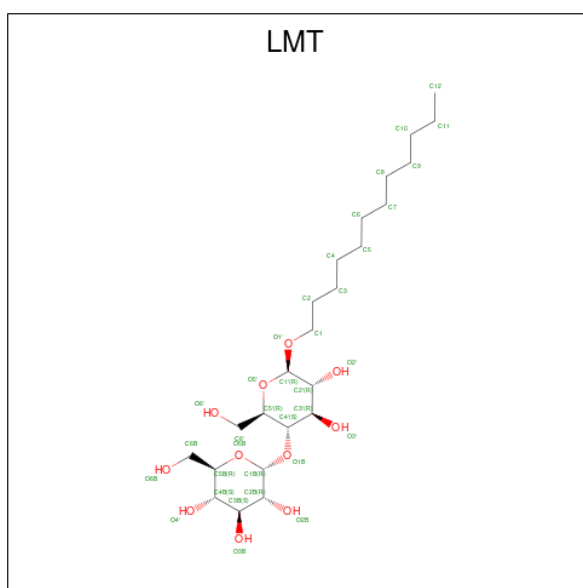
Mol	Chain	Residues	Atoms						AltConf
27	M	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	f	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



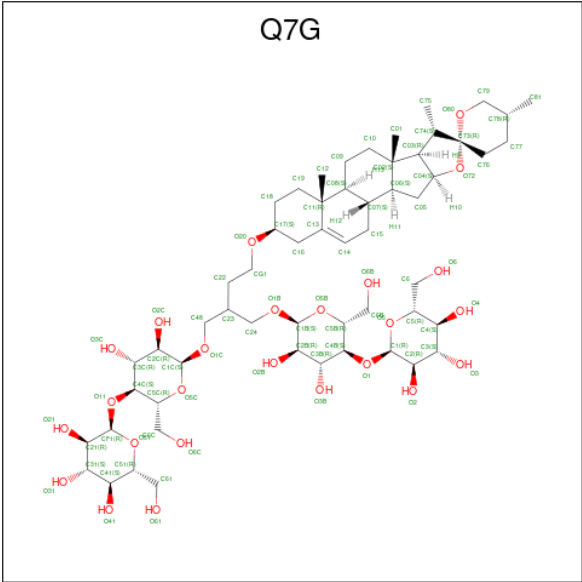
Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total	C	H	N	O	P
			142	44	88	1	8	1
28	f	1	Total	C	H	N	O	P
			142	44	88	1	8	1
28	f	1	Total	C	H	N	O	P
			142	44	88	1	8	1
28	i	1	Total	C	H	N	O	P
			142	44	88	1	8	1

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



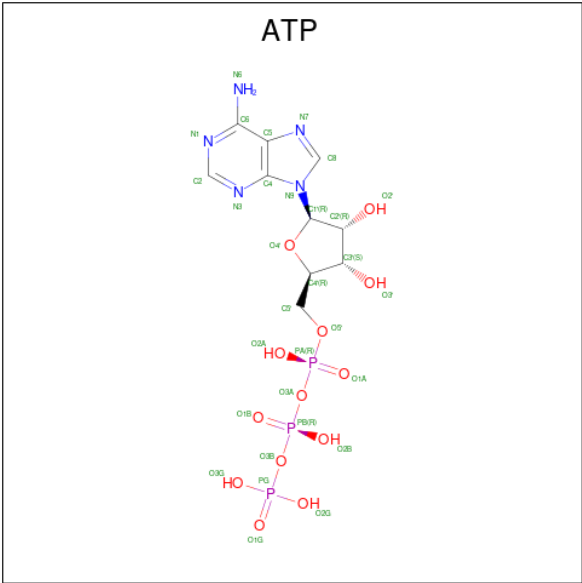
Mol	Chain	Residues	Atoms				AltConf
29	e	1	Total	C	H	O	0
			74	24	39	11	
29	j	1	Total	C	H	O	0
			74	24	39	11	

- 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: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
31	A1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
31	B1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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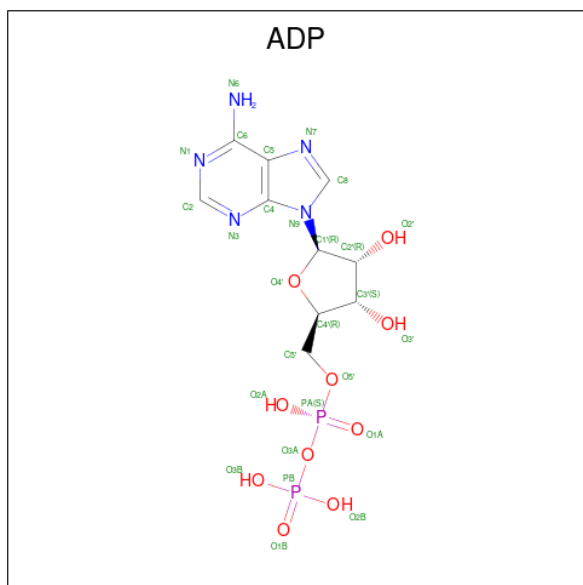
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Mol	Chain	Residues	Atoms						AltConf
31	C1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
31	F1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

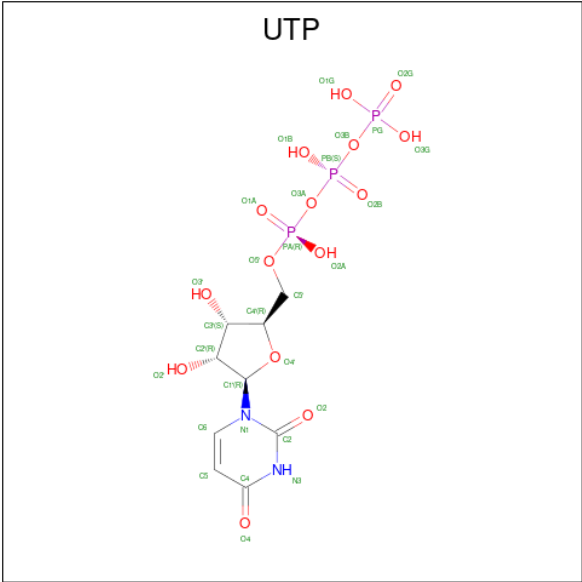
Mol	Chain	Residues	Atoms		AltConf
32	A1	1	Total	Mg	0
			1	1	
32	B1	1	Total	Mg	0
			1	1	
32	C1	1	Total	Mg	0
			1	1	
32	D1	1	Total	Mg	0
			1	1	
32	F1	1	Total	Mg	0
			1	1	

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						AltConf
33	D1	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 34 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).

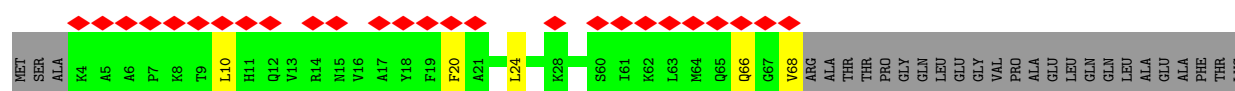


Mol	Chain	Residues	Atoms						AltConf
34	H1	1	Total	C	H	N	O	P	0
			40	9	11	2	15	3	

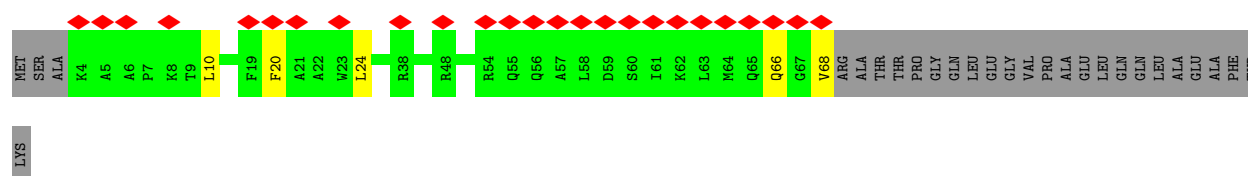
3 Residue-property plots [i](#)

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

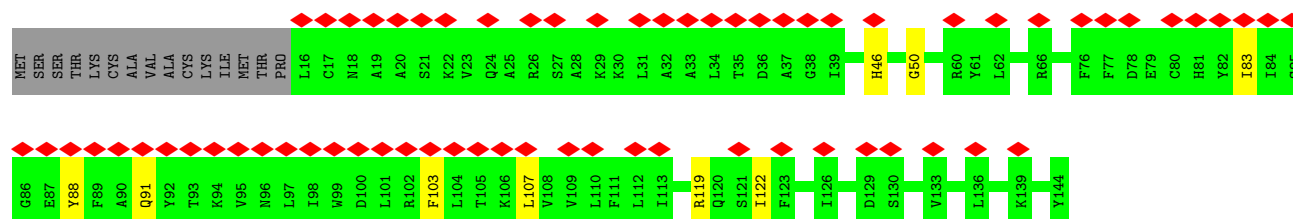
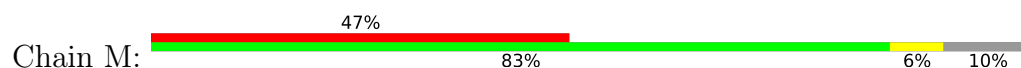
- Molecule 1: subunit-e



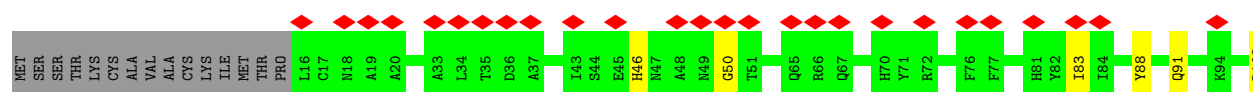
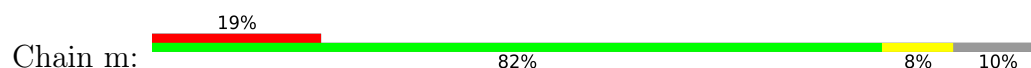
- Molecule 1: subunit-e



- Molecule 2: subunit-g

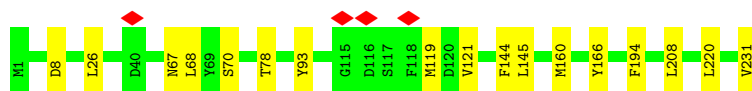


- Molecule 2: subunit-g

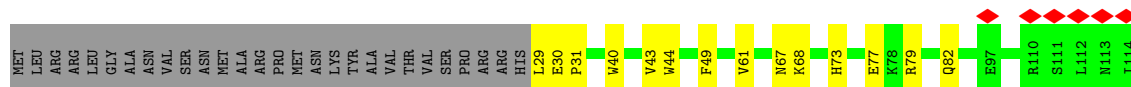




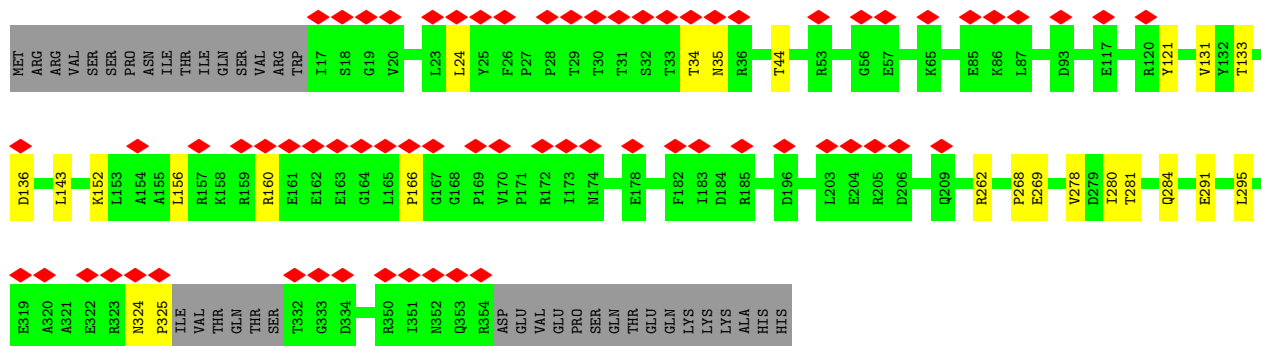
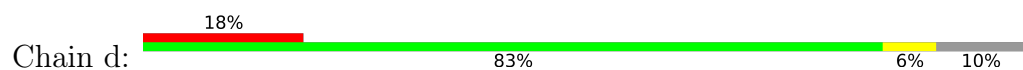
- Molecule 3: ATP synthase subunit a



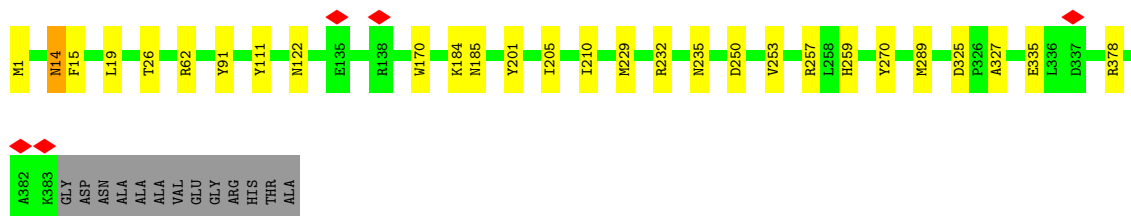
- Molecule 4: subunit-8



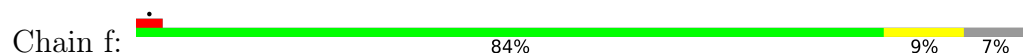
- Molecule 5: subunit-d

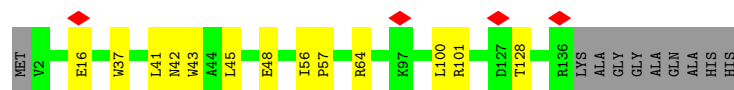


- Molecule 6: ATPTB1

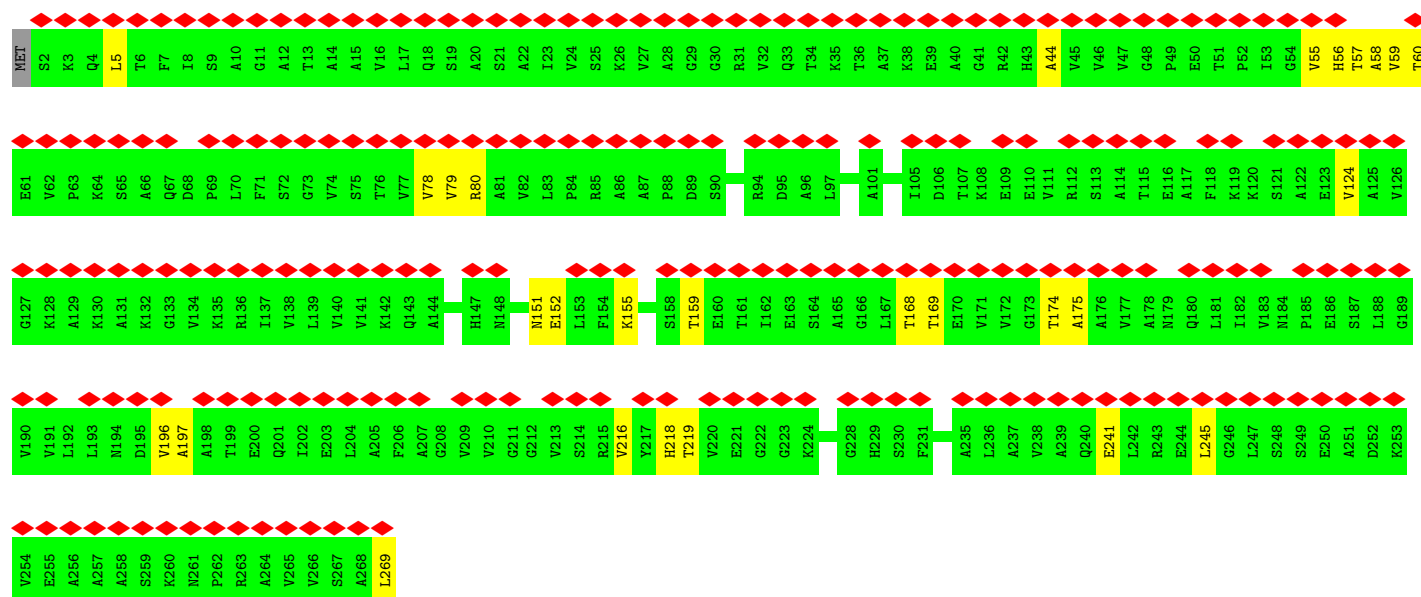
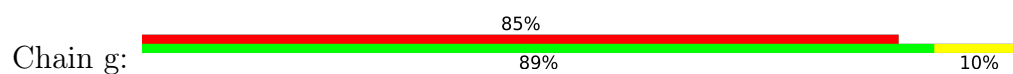


- Molecule 7: subunit-f

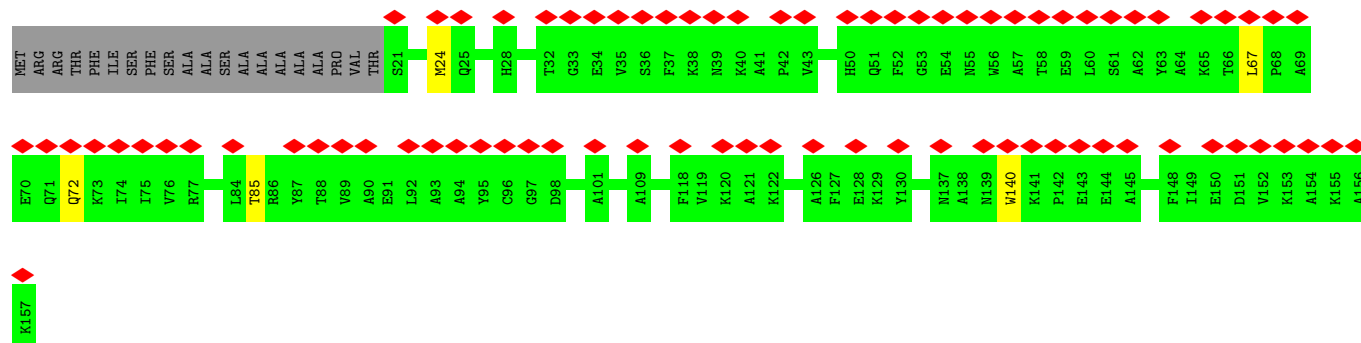
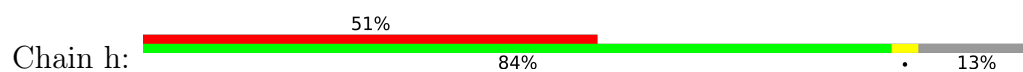




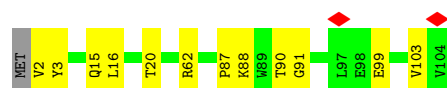
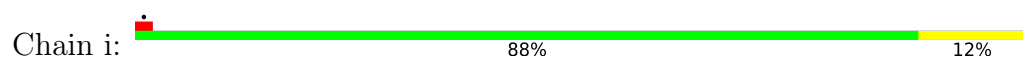
• Molecule 8: ATPTB3



• Molecule 9: ATPTB4



• Molecule 10: subunit-i/j



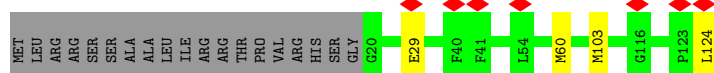
• Molecule 11: ATPTB6

Chain j:  92% 7%



• Molecule 12: subunit-k

Chain k:  6% 81% 15%

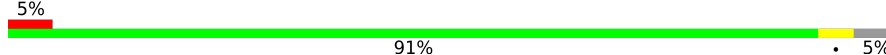


• Molecule 13: ATPTB11

Chain n:  85% 11%



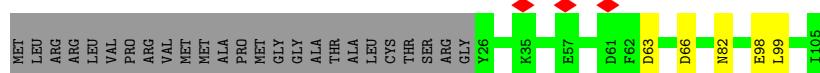
• Molecule 14: ATPTB12

Chain o:  5% 91% 5%



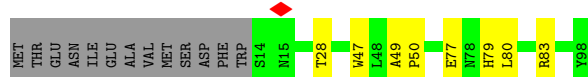
• Molecule 15: subunit-b

Chain p:  71% 5% 24%

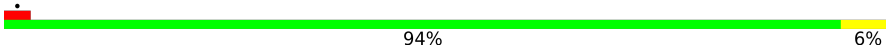


• Molecule 16: ATPEG3

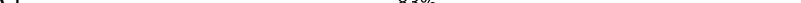
Chain q:  79% 8% 13%

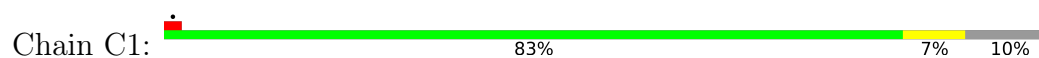
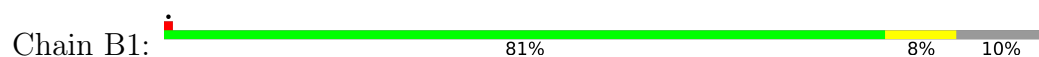


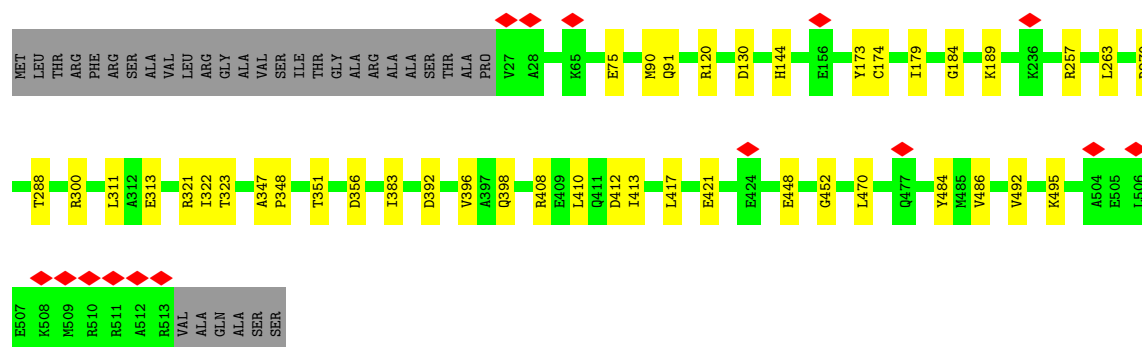
• Molecule 17: ATPEG4

Chain r:  94% 6%



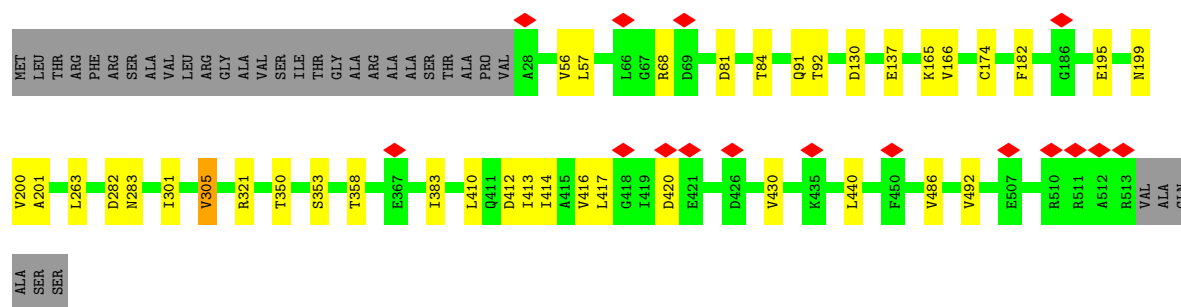
- Chain A1:  83% 7% 9%





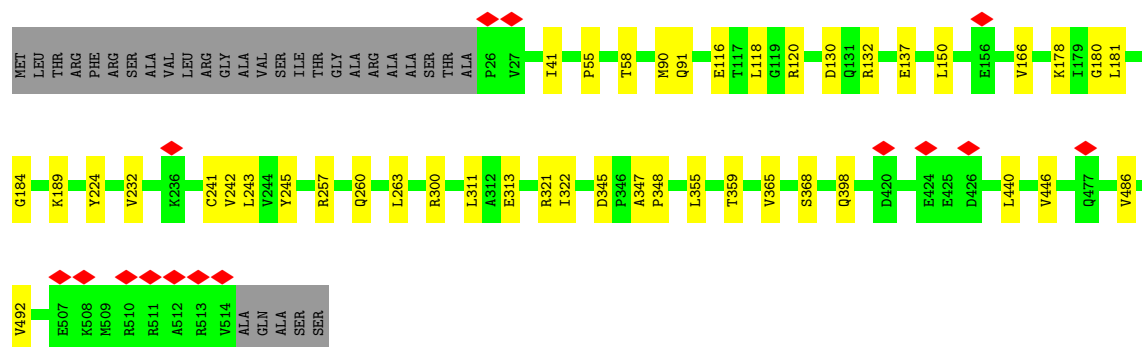
- Molecule 19: ATP synthase subunit beta, mitochondrial

Chain E1: 86% 7% 6%



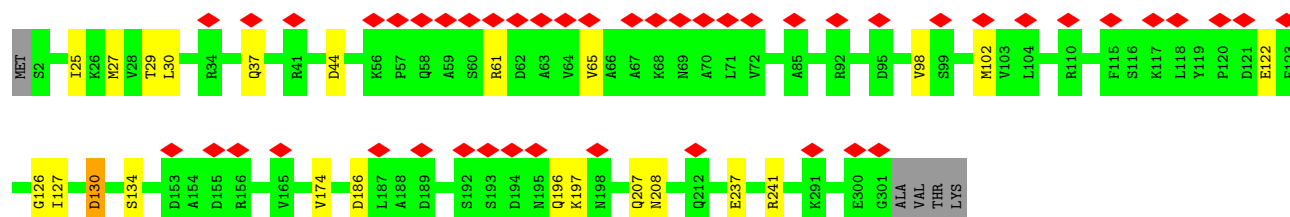
- Molecule 19: ATP synthase subunit beta, mitochondrial

Chain F1: 86% 8% 6%

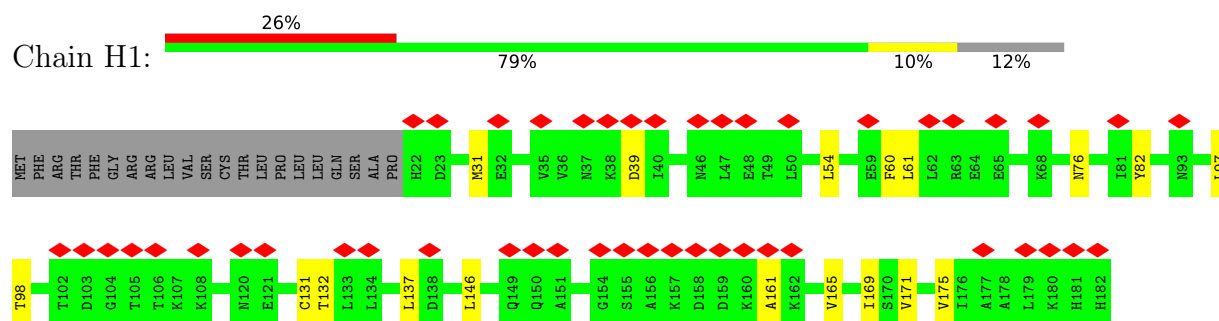


- Molecule 20: ATP synthase gamma subunit

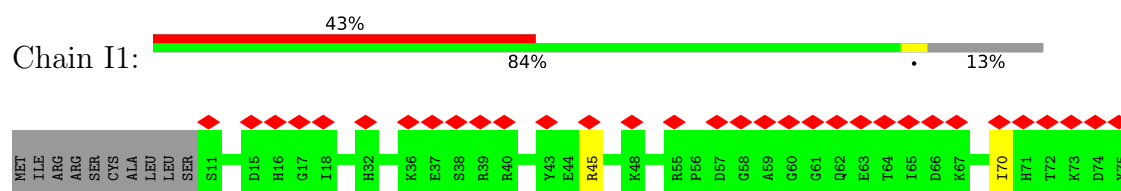
Chain G1: 15% 91% 7%



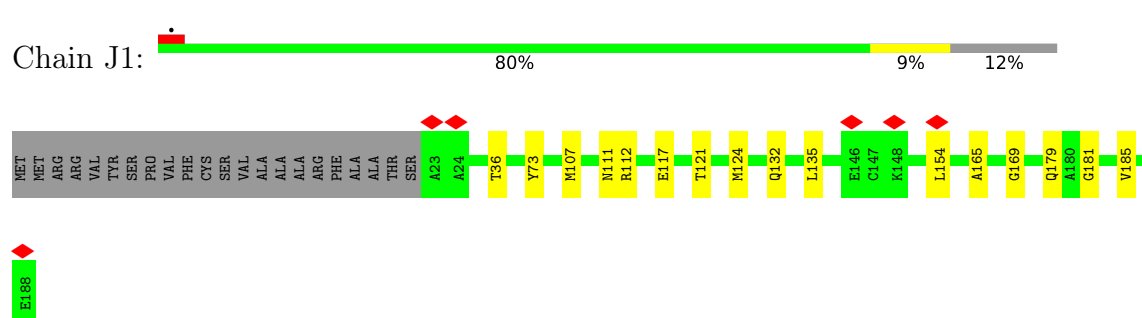
- Molecule 21: ATP synthase, epsilon chain, putative



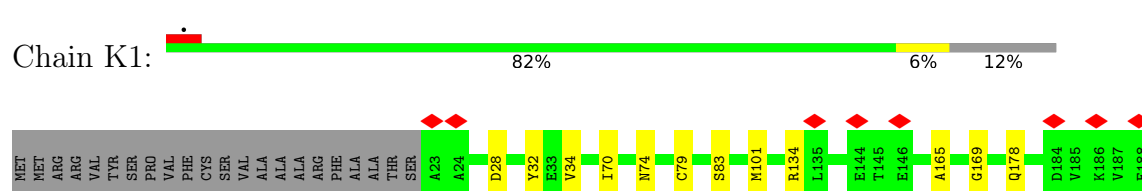
- Molecule 22: ATP synthase subunit epsilon, mitochondrial



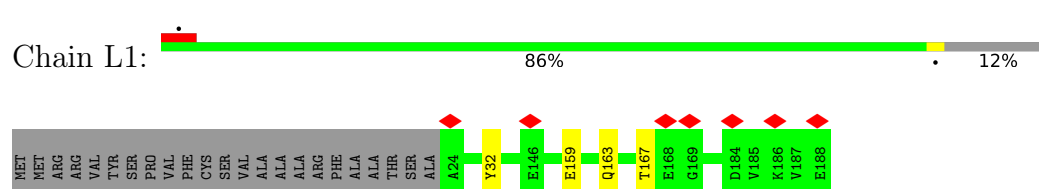
- Molecule 23: ATP synthase subunit p18, mitochondrial



- Molecule 23: ATP synthase subunit p18, mitochondrial

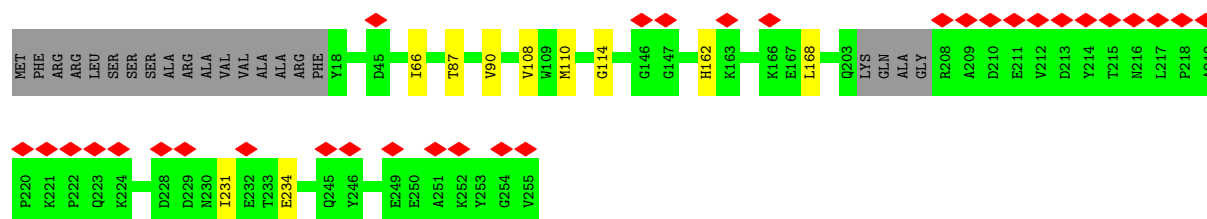


- Molecule 23: ATP synthase subunit p18, mitochondrial

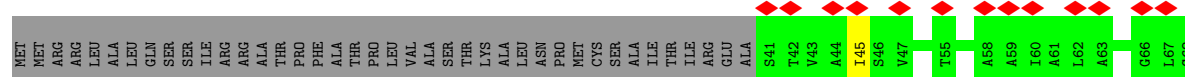


- Molecule 24: OSCP

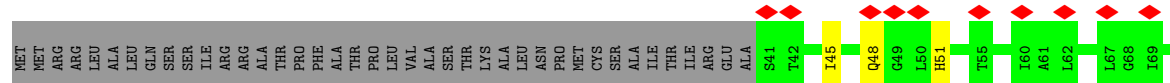




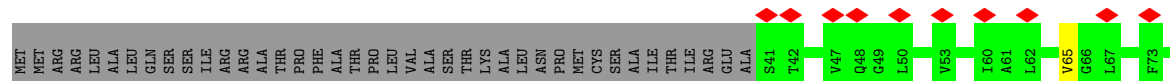
- Molecule 25: ATPase subunit 9, putative



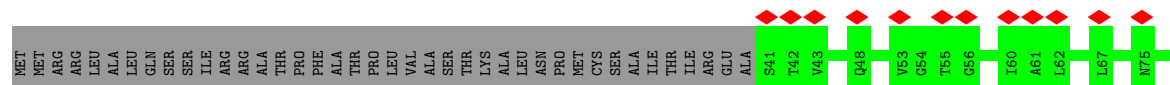
- Molecule 25: ATPase subunit 9, putative

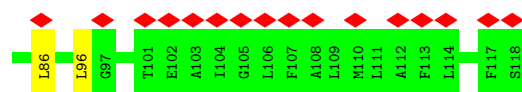


- Molecule 25: ATPase subunit 9, putative

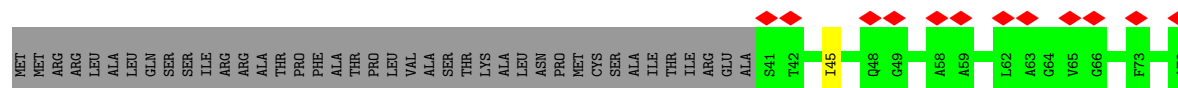


- Molecule 25: ATPase subunit 9, putative

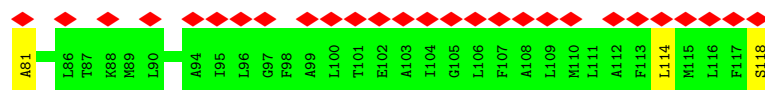
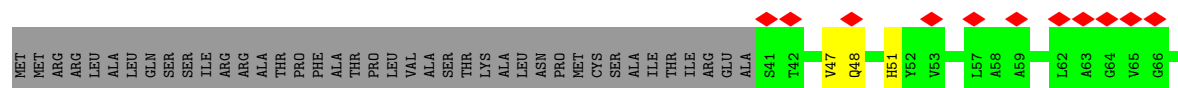




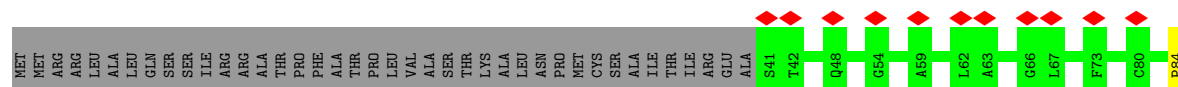
- Molecule 25: ATPase subunit 9, putative



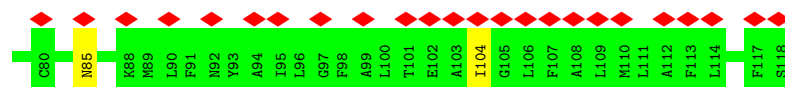
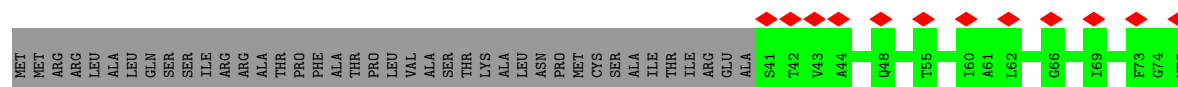
- Molecule 25: ATPase subunit 9, putative



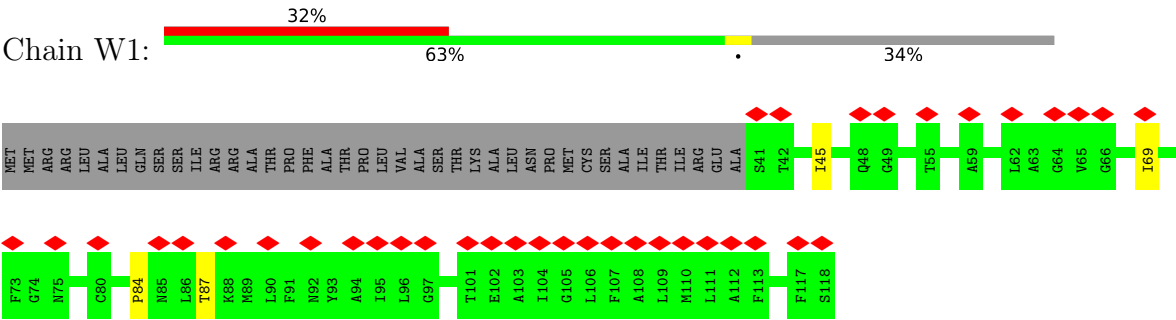
- Molecule 25: ATPase subunit 9, putative



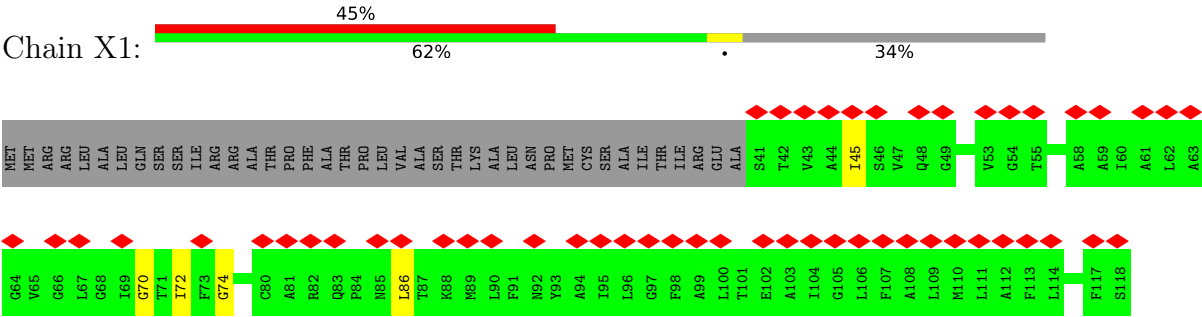
- Molecule 25: ATPase subunit 9, putative



- Molecule 25: ATPase subunit 9, putative



• Molecule 25: ATPase subunit 9, putative



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23019	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	0.111	Depositor
Minimum map value	-0.063	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	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: UTP, PC1, ATP, ADP, AME, CDL, PEE, MG, LMT, Q7G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.07	0/547	0.16	0/735
1	l	0.07	0/547	0.16	0/735
2	M	0.08	0/1049	0.18	0/1423
2	m	0.08	0/1049	0.18	0/1423
3	a	0.22	0/2111	0.26	0/2861
4	c	0.19	0/772	0.28	0/1054
5	d	0.12	0/2786	0.22	0/3760
6	e	0.15	0/3305	0.22	0/4482
7	f	0.16	0/1183	0.27	0/1601
8	g	0.07	0/1953	0.18	0/2650
9	h	0.06	0/1088	0.17	0/1466
10	i	0.18	0/913	0.22	0/1240
11	j	0.12	0/1462	0.20	0/1973
12	k	0.13	0/904	0.22	0/1228
13	n	0.17	0/1166	0.23	0/1581
14	o	0.11	0/814	0.19	0/1100
15	p	0.11	0/707	0.21	0/957
16	q	0.17	0/799	0.24	0/1091
17	r	0.15	0/567	0.24	0/767
18	A1	0.16	0/4159	0.22	0/5632
18	B1	0.15	0/4111	0.23	0/5566
18	C1	0.16	0/4113	0.22	0/5569
19	D1	0.16	0/3745	0.23	0/5077
19	E1	0.15	0/3738	0.24	0/5067
19	F1	0.15	0/3760	0.22	0/5098
20	G1	0.12	0/2427	0.22	0/3268
21	H1	0.14	0/1274	0.24	0/1728
22	I1	0.08	0/547	0.20	0/738
23	J1	0.08	0/1342	0.19	0/1810
23	K1	0.09	0/1342	0.20	0/1810
23	L1	0.09	0/1337	0.19	0/1803
24	M1	0.09	0/1916	0.19	0/2591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	O1	0.09	0/574	0.20	0/777
25	P1	0.10	0/574	0.19	0/777
25	Q1	0.11	0/574	0.19	0/777
25	R1	0.09	0/574	0.18	0/777
25	S1	0.08	0/574	0.23	0/777
25	T1	0.07	0/574	0.17	0/777
25	U1	0.07	0/574	0.17	0/777
25	V1	0.08	0/574	0.17	0/777
25	W1	0.08	0/574	0.16	0/777
25	X1	0.07	0/574	0.18	0/777
All	All	0.14	0/63273	0.22	0/85654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	537	545	545	3	0
1	l	537	545	545	3	0
2	M	1027	1042	1042	6	0
2	m	1027	1042	1042	9	0
3	a	2032	2044	2044	16	0
4	c	745	715	715	11	0
5	d	2737	2762	2763	19	0
6	e	3220	3050	3061	19	0
7	f	1145	1111	1111	12	0
8	g	1933	2020	2020	16	0
9	h	1070	1088	1088	4	0
10	i	883	857	857	9	0
11	j	1424	1411	1411	8	0
12	k	873	876	876	5	0
13	n	1128	1082	1082	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	o	789	767	767	3	0
15	p	684	651	651	6	0
16	q	766	720	720	8	0
17	r	542	498	498	5	0
18	A1	4084	4197	4196	29	0
18	B1	4038	4162	4160	31	0
18	C1	4039	4155	4154	27	0
19	D1	3689	3742	3741	27	0
19	E1	3682	3733	3733	23	0
19	F1	3703	3759	3758	30	0
20	G1	2387	2387	2387	15	0
21	H1	1251	1232	1231	13	0
22	I1	533	513	513	2	0
23	J1	1315	1276	1276	9	0
23	K1	1315	1276	1276	8	0
23	L1	1310	1271	1271	2	0
24	M1	1877	1873	1873	7	0
25	O1	565	600	599	8	0
25	P1	565	600	599	7	0
25	Q1	565	600	599	7	0
25	R1	565	600	599	3	0
25	S1	565	601	599	4	0
25	T1	565	601	599	4	0
25	U1	565	600	599	1	0
25	V1	565	600	599	2	0
25	W1	565	600	599	3	0
25	X1	565	600	599	4	0
26	L	100	156	156	0	0
26	M	100	156	156	0	0
26	c	100	156	156	1	0
26	e	500	780	780	2	0
26	f	100	156	156	0	0
26	j	200	312	312	1	0
26	l	100	156	156	0	0
26	m	100	156	156	0	0
26	q	100	156	156	1	0
27	M	51	82	82	0	0
27	f	51	82	82	0	0
27	m	51	82	82	0	0
28	a	54	88	88	0	0
28	f	108	176	176	1	0
28	i	54	88	88	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
31	C1	31	12	12	1	0
31	F1	31	12	12	0	0
32	A1	1	0	0	0	0
32	B1	1	0	0	0	0
32	C1	1	0	0	0	0
32	D1	1	0	0	0	0
32	F1	1	0	0	0	0
33	D1	27	12	12	0	0
34	H1	29	11	11	1	0
All	All	64103	65465	65342	360	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 3.

All (360) 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)
18:B1:531:PHE:O	18:B1:532:THR:OG1	1.93	0.86
11:j:19:ARG:NH2	16:q:77:GLU:O	2.12	0.83
6:e:250:ASP:OD1	6:e:270:TYR:OH	2.00	0.79
18:A1:398:GLN:NE2	18:A1:463:ASN:OD1	2.16	0.78
4:c:49:PHE:O	10:i:15:GLN:NE2	2.18	0.76
6:e:62:ARG:NH2	26:e:402:CDL:OB4	2.21	0.74
7:f:64:ARG:NH2	17:r:33:GLU:OE2	2.21	0.73
18:A1:75:ALA:HB3	18:A1:78:THR:HG21	1.72	0.70
23:K1:178:GLN:NE2	24:M1:234:GLU:OE2	2.23	0.70
6:e:185:ASN:ND2	6:e:325:ASP:OD1	2.28	0.67
18:C1:533:LEU:HD22	18:C1:542:LEU:HD22	1.75	0.67
19:D1:184:GLY:O	19:D1:189:LYS:NZ	2.29	0.64
18:B1:328:ARG:NH2	19:F1:345:ASP:OD1	2.31	0.64
6:e:1:AME:O	6:e:122:ASN:ND2	2.30	0.63
6:e:201:TYR:O	6:e:205:ILE:N	2.30	0.63
20:G1:237:GLU:OE2	20:G1:241:ARG:NH2	2.32	0.62
5:d:262:ARG:NH2	6:e:335:GLU:O	2.31	0.62
4:c:61:VAL:HG13	5:d:278:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:68:LYS:NZ	5:d:284:GLN:O	2.32	0.62
25:O1:84:PRO:O	25:O1:87:THR:HG23	2.00	0.62
19:F1:486:VAL:HG21	19:F1:492:VAL:HG22	1.81	0.61
4:c:73:HIS:NE2	4:c:77:GLU:OE2	2.33	0.61
11:j:128:LEU:HD21	11:j:142:LEU:HD12	1.81	0.61
19:E1:165:LYS:NZ	19:E1:486:VAL:O	2.28	0.61
20:G1:98:VAL:HG22	20:G1:102:MET:HE1	1.83	0.61
3:a:160:MET:HE2	25:P1:117:PHE:CE2	2.37	0.60
18:C1:523:GLU:N	18:C1:523:GLU:OE1	2.33	0.60
18:B1:420:MET:HE2	18:B1:470:PHE:CE1	2.37	0.60
19:E1:412:ASP:O	19:E1:416:VAL:HG23	2.01	0.60
1:l:66:GLN:HG3	1:l:68:VAL:HG23	1.83	0.59
23:K1:79:CYS:O	23:K1:83:SER:OG	2.14	0.59
19:F1:184:GLY:O	19:F1:189:LYS:NZ	2.34	0.59
23:K1:28:ASP:OD1	23:K1:32:TYR:N	2.36	0.59
1:L:66:GLN:HG3	1:L:68:VAL:HG23	1.83	0.59
3:a:26:LEU:HD22	7:f:43:TRP:CZ2	2.38	0.59
3:a:68:LEU:HD13	7:f:45:LEU:HD11	1.86	0.58
5:d:284:GLN:OE1	5:d:284:GLN:N	2.32	0.58
1:l:10:LEU:HD13	2:m:83:ILE:HD11	1.86	0.58
25:T1:48:GLN:O	25:T1:51:HIS:ND1	2.35	0.58
18:A1:438:ALA:O	18:A1:441:SER:OG	2.16	0.57
21:H1:39:ASP:OD1	21:H1:39:ASP:N	2.38	0.57
18:B1:180:ASN:OD1	18:B1:181:TYR:N	2.37	0.57
1:L:10:LEU:HD13	2:M:83:ILE:HD11	1.86	0.57
7:f:41:LEU:HD23	7:f:45:LEU:HD12	1.87	0.56
20:G1:27:MET:SD	20:G1:27:MET:N	2.78	0.56
12:k:29:GLU:N	12:k:29:GLU:OE1	2.38	0.56
19:D1:347:ALA:HB3	19:D1:348:PRO:HD3	1.86	0.56
19:E1:130:ASP:O	23:L1:32:TYR:OH	2.23	0.56
23:J1:117:GLU:O	23:J1:121:THR:HG23	2.05	0.56
20:G1:126:GLY:C	20:G1:127:ILE:HD12	2.31	0.56
4:c:29:LEU:HD12	25:Q1:117:PHE:CZ	2.41	0.56
19:E1:263:LEU:HD21	19:E1:321:ARG:HB2	1.88	0.56
5:d:291:GLU:O	5:d:295:LEU:N	2.38	0.55
19:E1:68:ARG:NH1	19:E1:92:THR:O	2.39	0.55
21:H1:132:THR:HG21	21:H1:137:LEU:HD21	1.88	0.55
18:C1:59:ASP:OD1	19:F1:300:ARG:NH2	2.39	0.55
8:g:5:LEU:HD21	8:g:245:LEU:HD11	1.88	0.55
4:c:40:TRP:O	4:c:43:VAL:HG12	2.06	0.55
2:M:103:PHE:CE2	2:M:107:LEU:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:37:TRP:NE1	7:f:48:GLU:OE1	2.38	0.55
20:G1:102:MET:HE2	20:G1:122:GLU:OE1	2.06	0.55
23:K1:70:ILE:O	23:K1:74:ASN:ND2	2.40	0.55
2:m:103:PHE:CE2	2:m:107:LEU:HD11	2.42	0.54
8:g:59:VAL:HG13	8:g:216:VAL:HB	1.90	0.54
18:C1:168:THR:OG1	18:C1:345:ARG:NH2	2.40	0.54
6:e:253:VAL:O	6:e:257:ARG:N	2.41	0.54
21:H1:54:LEU:HD21	21:H1:131:CYS:SG	2.47	0.54
18:B1:301:CYS:SG	18:B1:302:LEU:N	2.82	0.53
5:d:121:TYR:CD1	5:d:143:LEU:HD21	2.44	0.53
19:D1:90:MET:HE1	19:D1:257:ARG:HG3	1.91	0.53
19:F1:120:ARG:NE	19:F1:130:ASP:OD2	2.40	0.53
8:g:155:LYS:O	8:g:159:THR:HG22	2.09	0.53
10:i:88:LYS:O	14:o:32:GLN:NE2	2.42	0.53
18:B1:75:ALA:HB3	18:B1:78:THR:HG21	1.90	0.53
13:n:154:GLU:OE1	13:n:154:GLU:N	2.37	0.53
18:A1:212:LYS:HG2	18:A1:389:LEU:HD12	1.91	0.53
3:a:26:LEU:O	4:c:67:ASN:ND2	2.42	0.52
25:O1:70:GLY:HA2	25:X1:72:ILE:HD11	1.92	0.52
19:D1:91:GLN:OE1	19:D1:91:GLN:N	2.42	0.52
24:M1:162:HIS:NE2	24:M1:168:LEU:O	2.38	0.52
7:f:101:ARG:NH2	2:m:124:PRO:O	2.38	0.52
19:E1:410:LEU:O	19:E1:414:ILE:HG23	2.10	0.52
19:F1:90:MET:HE1	19:F1:257:ARG:HG3	1.90	0.52
19:F1:178:LYS:HG2	19:F1:355:LEU:HD23	1.92	0.52
3:a:208:LEU:HD21	25:P1:100:LEU:HD21	1.92	0.52
6:e:229:MET:SD	6:e:235:ASN:ND2	2.80	0.52
25:R1:86:LEU:HD11	25:S1:84:PRO:HB3	1.90	0.52
19:D1:417:LEU:CD2	20:G1:25:ILE:HD11	2.39	0.52
7:f:101:ARG:NH1	17:r:45:ASP:O	2.42	0.52
18:B1:52:ILE:C	18:B1:52:ILE:HD12	2.36	0.52
18:B1:508:MET:O	23:J1:179:GLN:NE2	2.43	0.51
19:F1:118:LEU:HA	19:F1:242:VAL:HG22	1.91	0.51
3:a:8:ASP:OD1	13:n:126:TYR:OH	2.25	0.51
14:o:86:TYR:O	14:o:91:ARG:NE	2.44	0.51
21:H1:76:ASN:ND2	34:H1:201:UTP:O2'	2.43	0.51
5:d:280:ILE:O	5:d:280:ILE:HD12	2.10	0.51
18:A1:524:LEU:HD23	18:A1:527:LEU:HD12	1.93	0.51
18:C1:203:LEU:HD13	18:C1:379:VAL:CG1	2.40	0.51
2:M:103:PHE:CZ	2:M:107:LEU:HD11	2.45	0.51
18:C1:62:ILE:HD12	18:C1:62:ILE:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:C1:140:VAL:HG21	18:C1:290:MET:HE1	1.93	0.51
18:C1:447:VAL:HG12	18:C1:449:THR:HG23	1.92	0.50
2:m:103:PHE:CZ	2:m:107:LEU:HD11	2.45	0.50
18:A1:51:MET:HE3	18:A1:68:ALA:HB1	1.92	0.50
18:C1:515:LYS:O	23:K1:134:ARG:NH1	2.42	0.50
2:m:102:ARG:NH2	15:p:82:ASN:OD1	2.43	0.50
18:A1:166:VAL:HG12	18:A1:166:VAL:O	2.12	0.50
20:G1:29:THR:HG21	20:G1:241:ARG:HD2	1.94	0.50
11:j:54:TYR:O	11:j:92:ARG:NH1	2.42	0.50
18:B1:173:ILE:HG23	18:B1:174:VAL:HG13	1.92	0.50
25:X1:70:GLY:O	25:X1:74:GLY:N	2.42	0.50
19:D1:120:ARG:NE	19:D1:130:ASP:OD2	2.42	0.50
21:H1:171:VAL:O	21:H1:175:VAL:HG23	2.12	0.50
18:C1:454:ARG:NH1	18:C1:481:LEU:O	2.45	0.50
21:H1:161:ALA:O	21:H1:165:VAL:HG23	2.11	0.50
11:j:120:GLU:OE2	11:j:123:ARG:NH2	2.45	0.49
11:j:37:ARG:NH2	26:j:202:CDL:OA3	2.43	0.49
5:d:133:THR:O	5:d:136:ASP:N	2.44	0.49
6:e:62:ARG:NH2	11:j:96:GLN:OE1	2.41	0.49
8:g:44:ALA:N	8:g:241:GLU:OE2	2.45	0.49
18:B1:80:ILE:HD12	18:B1:80:ILE:C	2.38	0.49
18:C1:203:LEU:HD13	18:C1:379:VAL:HG11	1.95	0.49
20:G1:44:ASP:HA	21:H1:31:MET:HE2	1.93	0.49
10:i:87:PRO:O	10:i:91:GLY:N	2.34	0.49
18:A1:457:ARG:NH2	18:A1:488:VAL:O	2.40	0.49
2:M:88:TYR:O	2:M:91:GLN:NE2	2.46	0.49
18:B1:239:ILE:HG23	18:B1:267:THR:HG23	1.95	0.49
25:O1:45:ILE:HD12	25:P1:45:ILE:HG21	1.95	0.49
2:m:88:TYR:O	2:m:91:GLN:NE2	2.46	0.49
18:B1:500:LEU:HD11	18:B1:545:MET:HE1	1.94	0.49
19:F1:263:LEU:HD21	19:F1:321:ARG:HB2	1.95	0.49
25:T1:114:LEU:O	25:T1:118:SER:OG	2.26	0.49
19:D1:417:LEU:HD13	19:D1:421:GLU:HG2	1.95	0.48
23:K1:165:ALA:O	23:K1:169:GLY:N	2.45	0.48
4:c:43:VAL:HG13	4:c:44:TRP:N	2.28	0.48
16:q:49:ALA:N	16:q:50:PRO:CD	2.76	0.48
23:J1:165:ALA:O	23:J1:169:GLY:N	2.46	0.48
19:D1:263:LEU:HD21	19:D1:321:ARG:HB2	1.95	0.48
19:D1:408:ARG:NH1	19:D1:412:ASP:OD1	2.46	0.48
25:Q1:106:LEU:O	25:Q1:110:MET:N	2.41	0.48
5:d:131:VAL:HG22	5:d:136:ASP:OD1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F1:166:VAL:HG12	19:F1:440:LEU:HD22	1.95	0.48
18:A1:292:GLU:O	18:A1:296:ASN:ND2	2.47	0.48
18:B1:532:THR:HG22	18:B1:533:LEU:N	2.28	0.48
18:A1:59:ASP:OD1	19:D1:300:ARG:NH2	2.47	0.48
3:a:231:VAL:O	6:e:170:TRP:NE1	2.44	0.48
6:e:210:ILE:O	6:e:232:ARG:NH2	2.40	0.48
18:C1:531:PHE:O	18:C1:532:THR:CB	2.62	0.48
19:D1:470:LEU:HD23	19:D1:470:LEU:O	2.14	0.48
8:g:58:ALA:HB3	8:g:80:ARG:HB3	1.96	0.48
19:D1:270:ARG:NH1	19:D1:323:THR:O	2.47	0.48
19:F1:116:GLU:OE1	19:F1:116:GLU:N	2.42	0.48
20:G1:197:LYS:HD3	20:G1:197:LYS:C	2.39	0.48
18:B1:111:ILE:HD12	18:B1:276:PRO:HB3	1.95	0.47
20:G1:61:ARG:O	20:G1:65:VAL:HG23	2.14	0.47
11:j:137:GLN:NE2	11:j:148:GLU:O	2.46	0.47
5:d:34:THR:O	5:d:35:ASN:C	2.57	0.47
16:q:77:GLU:OE2	16:q:79:HIS:NE2	2.48	0.47
4:c:30:GLU:N	4:c:31:PRO:CD	2.77	0.47
18:A1:61:THR:HG22	18:A1:111:ILE:CD1	2.44	0.47
18:B1:199:GLY:N	18:B1:357:SER:OG	2.48	0.47
19:D1:484:TYR:O	19:D1:495:LYS:NZ	2.46	0.47
5:d:121:TYR:HD1	5:d:143:LEU:HD21	1.80	0.47
9:h:67:LEU:O	9:h:72:GLN:NE2	2.48	0.47
10:i:2:VAL:HG22	10:i:3:TYR:H	1.80	0.47
25:P1:48:GLN:O	25:P1:51:HIS:ND1	2.48	0.47
12:k:103:MET:HE1	16:q:80:LEU:HA	1.96	0.46
18:A1:398:GLN:NE2	18:A1:459:VAL:O	2.48	0.46
18:B1:141:ASN:OD1	18:B1:145:HIS:N	2.48	0.46
23:J1:181:GLY:O	23:J1:185:VAL:HG23	2.15	0.46
26:c:201:CDL:H872	26:c:201:CDL:H832	1.96	0.46
6:e:259:HIS:ND1	6:e:289:MET:HE1	2.31	0.46
18:B1:285:TYR:OH	18:B1:338:LEU:HD12	2.16	0.46
18:A1:537:ILE:HD12	18:A1:537:ILE:N	2.31	0.46
19:D1:130:ASP:O	23:K1:32:TYR:OH	2.29	0.46
19:E1:81:ASP:OD1	19:E1:84:THR:N	2.44	0.46
5:d:269:GLU:OE1	6:e:184:LYS:NZ	2.43	0.46
2:m:119:ARG:NH2	2:m:122:ILE:O	2.49	0.46
18:C1:108:MET:HE3	18:C1:282:LEU:HD11	1.98	0.46
19:F1:260:GLN:OE1	19:F1:260:GLN:N	2.49	0.46
10:i:62:ARG:NH2	13:n:134:SER:O	2.48	0.46
2:m:46:HIS:O	2:m:50:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B1:532:THR:HG22	18:B1:533:LEU:H	1.81	0.46
19:E1:410:LEU:HD13	19:E1:430:VAL:HG23	1.98	0.46
19:F1:41:ILE:HG23	19:F1:41:ILE:O	2.15	0.46
21:H1:82:TYR:OH	25:V1:85:ASN:ND2	2.49	0.46
10:i:2:VAL:HG22	10:i:3:TYR:N	2.31	0.46
18:C1:301:CYS:SG	18:C1:302:LEU:N	2.89	0.45
19:D1:486:VAL:HG21	19:D1:492:VAL:HG22	1.97	0.45
19:F1:91:GLN:OE1	19:F1:91:GLN:N	2.49	0.45
18:A1:399:ARG:NH2	19:D1:398:GLN:OE1	2.49	0.45
18:C1:52:ILE:HD12	18:C1:52:ILE:C	2.41	0.45
3:a:119:MET:HE2	25:S1:91:PHE:CZ	2.52	0.45
5:d:156:LEU:HD23	5:d:156:LEU:O	2.17	0.45
6:e:111:TYR:OH	16:q:47:TRP:O	2.28	0.45
19:D1:174:CYS:HB3	19:D1:383:ILE:HG21	1.98	0.45
5:d:35:ASN:N	5:d:35:ASN:OD1	2.49	0.45
2:M:119:ARG:NH2	2:M:122:ILE:O	2.49	0.45
19:E1:305:VAL:HG12	19:E1:305:VAL:O	2.16	0.45
25:O1:84:PRO:HB3	25:X1:86:LEU:HD11	1.98	0.45
10:i:90:THR:O	14:o:36:ARG:NH2	2.50	0.45
18:B1:110:ASN:O	18:B1:114:VAL:HG23	2.16	0.45
19:D1:392:ASP:O	19:D1:396:VAL:HG23	2.17	0.45
22:I1:70:ILE:N	22:I1:70:ILE:HD12	2.32	0.45
18:B1:109:ASP:OD1	18:B1:109:ASP:N	2.50	0.45
18:C1:80:ILE:C	18:C1:80:ILE:HD12	2.41	0.45
19:F1:243:LEU:HD22	19:F1:245:TYR:HE2	1.82	0.45
7:f:64:ARG:NH1	17:r:33:GLU:OE1	2.48	0.44
18:A1:75:ALA:O	18:A1:78:THR:OG1	2.30	0.44
19:E1:350:THR:O	19:E1:353:SER:OG	2.35	0.44
23:J1:73:TYR:OH	23:J1:111:ASN:OD1	2.36	0.44
3:a:145:LEU:HB2	25:Q1:106:LEU:HD13	2.00	0.44
6:e:26:THR:HG23	6:e:91:TYR:OH	2.17	0.44
10:i:16:LEU:O	10:i:20:THR:HG22	2.17	0.44
18:A1:61:THR:HG22	18:A1:111:ILE:HD13	1.98	0.44
19:F1:311:LEU:C	19:F1:311:LEU:HD23	2.43	0.44
5:d:160:ARG:HD3	5:d:166:PRO:O	2.17	0.44
18:A1:246:ARG:NH1	19:D1:356:ASP:OD1	2.50	0.44
18:C1:527:LEU:HD23	23:K1:101:MET:HE2	1.99	0.44
19:D1:351:THR:HG22	19:D1:351:THR:O	2.17	0.44
19:E1:182:PHE:CD1	19:E1:358:THR:HG23	2.52	0.44
20:G1:208:ASN:OD1	25:R1:82:ARG:NE	2.44	0.44
25:W1:45:ILE:HD12	25:X1:45:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:100:LEU:HD21	15:p:99:LEU:HD23	1.99	0.44
21:H1:97:LEU:C	21:H1:97:LEU:HD23	2.43	0.44
18:C1:166:VAL:HG12	18:C1:166:VAL:O	2.17	0.44
18:C1:317:GLN:NE2	19:F1:313:GLU:OE1	2.45	0.44
19:D1:448:GLU:O	19:D1:452:GLY:N	2.40	0.44
19:F1:150:LEU:HD23	19:F1:150:LEU:O	2.17	0.44
18:A1:188:LYS:NZ	18:A1:461:LEU:O	2.39	0.44
18:C1:225:ARG:NH2	18:C1:522:GLN:OE1	2.51	0.44
18:C1:514:ASN:O	18:C1:518:TYR:OH	2.19	0.44
3:a:166:TYR:OH	28:f:204:PC1:O12	2.28	0.43
1:l:20:PHE:CE2	1:l:24:LEU:HD11	2.53	0.43
19:F1:180:GLY:HA3	19:F1:355:LEU:HD13	2.00	0.43
19:F1:347:ALA:HB3	19:F1:348:PRO:CD	2.48	0.43
25:S1:45:ILE:O	25:T1:47:VAL:HA	2.18	0.43
3:a:93:TYR:CE1	3:a:220:LEU:HD22	2.53	0.43
13:n:132:GLU:OE1	16:q:28:THR:OG1	2.26	0.43
18:A1:131:VAL:HG11	18:A1:293:TYR:HB2	2.00	0.43
21:H1:60:PHE:O	21:H1:60:PHE:CD1	2.71	0.43
8:g:56:HIS:NE2	8:g:219:THR:O	2.51	0.43
18:C1:52:ILE:HD12	18:C1:53:GLY:N	2.34	0.43
2:M:46:HIS:O	2:M:50:GLY:N	2.49	0.43
4:c:79:ARG:NH1	4:c:82:GLN:OE1	2.48	0.43
16:q:77:GLU:OE1	16:q:83:ARG:NH2	2.47	0.43
18:B1:323:ARG:HA	19:E1:301:ILE:HD12	1.99	0.43
18:C1:399:ARG:NH2	19:F1:398:GLN:OE1	2.51	0.43
19:F1:137:GLU:OE1	19:F1:137:GLU:N	2.42	0.43
19:F1:232:VAL:HG11	19:F1:241:CYS:SG	2.58	0.43
18:A1:285:TYR:OH	18:A1:338:LEU:HD12	2.18	0.43
18:A1:514:ASN:O	18:A1:518:TYR:OH	2.21	0.43
19:E1:174:CYS:HB3	19:E1:383:ILE:HD13	2.00	0.43
21:H1:61:LEU:HD12	21:H1:61:LEU:H	1.84	0.43
25:O1:107:PHE:CD1	25:O1:107:PHE:N	2.86	0.43
18:B1:295:MET:HB2	18:B1:358:VAL:HG23	2.01	0.43
18:B1:56:HIS:HB2	18:B1:66:ILE:HG23	2.01	0.43
19:E1:195:GLU:OE2	19:E1:199:ASN:ND2	2.50	0.43
5:d:152:LYS:HB2	24:M1:231:ILE:HG12	2.01	0.43
18:C1:537:ILE:N	18:C1:537:ILE:HD12	2.33	0.42
24:M1:66:ILE:HD12	24:M1:66:ILE:N	2.34	0.42
15:p:98:GLU:OE2	17:r:40:LYS:NZ	2.47	0.42
1:L:20:PHE:CE2	1:L:24:LEU:HD11	2.53	0.42
6:e:378:ARG:HH22	15:p:63:ASP:CG	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:402:CDL:H522	11:j:101:VAL:HG22	2.01	0.42
15:p:66:ASP:OD2	17:r:10:ARG:NH1	2.53	0.42
18:A1:511:THR:HG22	18:A1:511:THR:O	2.19	0.42
19:F1:181:LEU:HD23	19:F1:359:THR:HB	2.02	0.42
23:J1:107:MET:O	23:J1:112:ARG:N	2.53	0.42
23:J1:124:MET:HB3	23:J1:154:LEU:HD23	2.00	0.42
3:a:67:ASN:O	3:a:70:SER:OG	2.30	0.42
8:g:269:LEU:HD12	8:g:269:LEU:C	2.45	0.42
19:E1:410:LEU:HD23	19:E1:413:ILE:HD12	2.02	0.42
3:a:78:THR:O	4:c:40:TRP:NE1	2.37	0.42
18:A1:100:ASP:OD1	18:A1:100:ASP:N	2.52	0.42
19:F1:132:ARG:NH1	19:F1:224:TYR:OH	2.53	0.42
3:a:121:VAL:HG11	12:k:60:MET:HB3	2.00	0.42
8:g:57:THR:HB	8:g:218:HIS:HB2	2.02	0.42
18:B1:307:ASP:OD1	18:B1:307:ASP:N	2.52	0.42
19:E1:282:ASP:HA	19:E1:283:ASN:HA	1.87	0.42
19:F1:55:PRO:O	19:F1:58:THR:OG1	2.34	0.42
25:P1:86:LEU:HD11	25:Q1:84:PRO:HB3	2.02	0.42
25:U1:84:PRO:O	25:U1:87:THR:HG23	2.19	0.42
18:A1:273:ALA:O	18:A1:274:ALA:HB3	2.20	0.42
21:H1:97:LEU:HD23	21:H1:98:THR:N	2.35	0.42
7:f:128:THR:HG22	7:f:128:THR:O	2.20	0.42
8:g:151:ASN:OD1	8:g:152:GLU:N	2.53	0.42
19:E1:166:VAL:HG22	19:E1:440:LEU:HB3	2.02	0.42
7:f:16:GLU:OE1	7:f:16:GLU:N	2.53	0.41
9:h:24:MET:SD	9:h:24:MET:N	2.93	0.41
18:B1:420:MET:HE2	18:B1:470:PHE:HE1	1.83	0.41
19:D1:173:TYR:CD2	19:D1:179:ILE:HD13	2.55	0.41
7:f:56:ILE:HB	7:f:57:PRO:HD3	2.02	0.41
18:B1:203:LEU:HD13	18:B1:379:VAL:HG11	2.02	0.41
19:E1:137:GLU:OE1	19:E1:137:GLU:N	2.42	0.41
21:H1:146:LEU:CD1	21:H1:169:ILE:HG23	2.50	0.41
23:J1:36:THR:HG22	23:J1:36:THR:O	2.19	0.41
10:i:99:GLU:O	10:i:103:VAL:HG23	2.20	0.41
19:E1:91:GLN:N	19:E1:91:GLN:OE1	2.53	0.41
20:G1:130:ASP:OD1	20:G1:130:ASP:N	2.53	0.41
5:d:268:PRO:HB2	6:e:327:ALA:HB3	2.01	0.41
6:e:14:ASN:OD1	6:e:14:ASN:N	2.54	0.41
8:g:57:THR:HG21	8:g:124:VAL:HG11	2.02	0.41
8:g:196:VAL:HG12	8:g:197:ALA:N	2.35	0.41
12:k:124:LEU:N	12:k:124:LEU:HD23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A1:61:THR:HG21	19:D1:313:GLU:OE2	2.20	0.41
19:E1:416:VAL:HB	19:E1:417:LEU:HD12	2.02	0.41
19:E1:486:VAL:HG21	19:E1:492:VAL:HG22	2.01	0.41
20:G1:207:GLN:O	25:Q1:82:ARG:NH2	2.53	0.41
5:d:324:ASN:HB2	5:d:325:PRO:CD	2.50	0.41
8:g:60:THR:HG22	8:g:78:VAL:O	2.20	0.41
18:B1:215:ILE:HG23	18:B1:216:ALA:N	2.36	0.41
24:M1:90:VAL:HG21	24:M1:108:VAL:HG22	2.03	0.41
6:e:15:PHE:CE2	6:e:19:LEU:HD11	2.55	0.41
19:D1:75:GLU:OE2	19:D1:144:HIS:NE2	2.44	0.41
19:D1:263:LEU:HD13	19:D1:322:ILE:HG12	2.02	0.41
19:D1:410:LEU:HD23	19:D1:413:ILE:HD12	2.02	0.41
20:G1:134:SER:OG	22:I1:45:ARG:NH2	2.53	0.41
25:V1:104:ILE:HD12	25:W1:69:ILE:HD12	2.02	0.41
18:A1:269:MET:SD	18:A1:286:ALA:HB3	2.61	0.41
18:B1:184:LEU:O	18:B1:223:GLN:NE2	2.50	0.41
18:B1:454:ARG:NH1	18:B1:481:LEU:O	2.53	0.41
18:B1:471:MET:HE1	18:B1:522:GLN:HA	2.03	0.41
18:C1:212:LYS:N	31:C1:601:ATP:O1B	2.51	0.41
25:P1:104:ILE:HD11	25:Q1:102:GLU:OE1	2.20	0.41
8:g:168:THR:HG22	8:g:169:THR:N	2.36	0.41
8:g:174:THR:HG23	8:g:175:ALA:N	2.36	0.41
2:m:102:ARG:NE	15:p:82:ASN:OD1	2.53	0.41
18:A1:203:LEU:HD13	18:A1:379:VAL:CG1	2.51	0.41
18:C1:135:VAL:HG12	18:C1:135:VAL:O	2.21	0.41
3:a:194:PHE:CE1	25:O1:107:PHE:CE1	3.09	0.41
12:k:103:MET:HE1	16:q:80:LEU:O	2.20	0.41
19:D1:288:THR:HG23	19:D1:311:LEU:HD13	2.02	0.41
19:F1:178:LYS:NZ	19:F1:322:ILE:O	2.38	0.41
19:F1:446:VAL:HG12	19:F1:446:VAL:O	2.20	0.41
23:J1:132:GLN:OE1	23:J1:135:LEU:HD12	2.20	0.41
23:L1:159:GLU:OE2	23:L1:163:GLN:NE2	2.54	0.41
18:B1:107:LEU:HD12	18:B1:111:ILE:HG23	2.02	0.41
19:E1:56:VAL:HG12	19:E1:57:LEU:N	2.36	0.41
20:G1:186:ASP:OD1	20:G1:196:GLN:NE2	2.54	0.40
25:Q1:65:VAL:HG13	25:Q1:101:THR:HG22	2.02	0.40
3:a:194:PHE:HE1	25:O1:107:PHE:CE1	2.39	0.40
8:g:59:VAL:HG23	8:g:79:VAL:HG22	2.03	0.40
13:n:105:GLU:OE2	13:n:109:ARG:NH1	2.50	0.40
26:q:101:CDL:OB7	26:q:101:CDL:CB3	2.68	0.40
18:C1:576:LEU:O	18:C1:579:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R1:96:LEU:O	25:R1:96:LEU:HD23	2.21	0.40
25:S1:82:ARG:HG3	25:T1:81:ALA:HB1	2.03	0.40
25:W1:84:PRO:O	25:W1:87:THR:HG23	2.22	0.40
8:g:55:VAL:HG12	8:g:219:THR:HG22	2.02	0.40
18:A1:491:GLN:OE1	18:A1:491:GLN:N	2.48	0.40
19:F1:365:VAL:O	19:F1:368:SER:OG	2.38	0.40
9:h:85:THR:O	9:h:85:THR:HG22	2.21	0.40
19:E1:200:VAL:HG13	19:E1:201:ALA:N	2.35	0.40
24:M1:90:VAL:CG2	24:M1:108:VAL:HG22	2.51	0.40
24:M1:110:MET:O	24:M1:114:GLY:N	2.54	0.40
5:d:24:LEU:HD11	9:h:140:TRP:CZ3	2.57	0.40
18:A1:131:VAL:HG12	18:A1:132:GLY:N	2.36	0.40
19:F1:150:LEU:HD23	19:F1:150:LEU:C	2.46	0.40
25:O1:45:ILE:HD12	25:P1:45:ILE:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	63/92 (68%)	63 (100%)	0	0	100	100
1	l	63/92 (68%)	63 (100%)	0	0	100	100
2	M	127/144 (88%)	127 (100%)	0	0	100	100
2	m	127/144 (88%)	127 (100%)	0	0	100	100
3	a	229/231 (99%)	225 (98%)	4 (2%)	0	100	100
4	c	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
5	d	328/370 (89%)	315 (96%)	13 (4%)	0	100	100
6	e	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
7	f	133/145 (92%)	129 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	g	266/269 (99%)	264 (99%)	2 (1%)	0	100	100
9	h	135/157 (86%)	134 (99%)	1 (1%)	0	100	100
10	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
11	j	166/169 (98%)	163 (98%)	3 (2%)	0	100	100
12	k	103/124 (83%)	100 (97%)	3 (3%)	0	100	100
13	n	137/156 (88%)	130 (95%)	7 (5%)	0	100	100
14	o	94/101 (93%)	94 (100%)	0	0	100	100
15	p	78/105 (74%)	77 (99%)	1 (1%)	0	100	100
16	q	83/98 (85%)	80 (96%)	3 (4%)	0	100	100
17	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	A1	526/584 (90%)	521 (99%)	5 (1%)	0	100	100
18	B1	517/584 (88%)	507 (98%)	10 (2%)	0	100	100
18	C1	517/584 (88%)	512 (99%)	5 (1%)	0	100	100
19	D1	485/519 (93%)	478 (99%)	7 (1%)	0	100	100
19	E1	484/519 (93%)	475 (98%)	8 (2%)	1 (0%)	43	72
19	F1	487/519 (94%)	477 (98%)	10 (2%)	0	100	100
20	G1	298/305 (98%)	291 (98%)	7 (2%)	0	100	100
21	H1	159/182 (87%)	156 (98%)	3 (2%)	0	100	100
22	I1	63/75 (84%)	63 (100%)	0	0	100	100
23	J1	164/188 (87%)	163 (99%)	1 (1%)	0	100	100
23	K1	164/188 (87%)	160 (98%)	4 (2%)	0	100	100
23	L1	163/188 (87%)	162 (99%)	1 (1%)	0	100	100
24	M1	230/255 (90%)	226 (98%)	4 (2%)	0	100	100
25	O1	76/118 (64%)	75 (99%)	1 (1%)	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%)	76 (100%)	0	0	100	100
25	T1	76/118 (64%)	76 (100%)	0	0	100	100
25	U1	76/118 (64%)	76 (100%)	0	0	100	100
25	V1	76/118 (64%)	76 (100%)	0	0	100	100

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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%)	7658 (98%)	116 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	E1	305	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	55/75 (73%)	55 (100%)	0	100	100
1	l	55/75 (73%)	55 (100%)	0	100	100
2	M	111/124 (90%)	111 (100%)	0	100	100
2	m	111/124 (90%)	111 (100%)	0	100	100
3	a	225/225 (100%)	224 (100%)	1 (0%)	84	81
4	c	80/104 (77%)	80 (100%)	0	100	100
5	d	297/334 (89%)	295 (99%)	2 (1%)	76	77
6	e	334/341 (98%)	333 (100%)	1 (0%)	86	83
7	f	119/124 (96%)	118 (99%)	1 (1%)	73	76
8	g	205/206 (100%)	205 (100%)	0	100	100
9	h	110/123 (89%)	110 (100%)	0	100	100
10	i	95/96 (99%)	95 (100%)	0	100	100
11	j	149/150 (99%)	149 (100%)	0	100	100
12	k	91/107 (85%)	91 (100%)	0	100	100
13	n	123/137 (90%)	121 (98%)	2 (2%)	55	68
14	o	82/86 (95%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	439/479 (92%)	438 (100%)	1 (0%)	87	86
18	B1	435/479 (91%)	434 (100%)	1 (0%)	87	86
18	C1	434/479 (91%)	434 (100%)	0	100	100
19	D1	398/420 (95%)	398 (100%)	0	100	100
19	E1	397/420 (94%)	396 (100%)	1 (0%)	86	83
19	F1	400/420 (95%)	400 (100%)	0	100	100
20	G1	253/257 (98%)	249 (98%)	4 (2%)	55	68
21	H1	137/156 (88%)	137 (100%)	0	100	100
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%)	144 (99%)	1 (1%)	76	77
23	L1	145/162 (90%)	144 (99%)	1 (1%)	76	77
24	M1	200/215 (93%)	199 (100%)	1 (0%)	81	80
25	O1	56/89 (63%)	56 (100%)	0	100	100
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%)	56 (100%)	0	100	100
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%)	56 (100%)	0	100	100
25	X1	56/89 (63%)	56 (100%)	0	100	100
All	All	6599/7441 (89%)	6582 (100%)	17 (0%)	84	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	144	PHE
5	d	44	THR

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Mol	Chain	Res	Type
5	d	281	THR
6	e	14	ASN
7	f	42	ASN
13	n	105	GLU
13	n	132	GLU
18	A1	267	THR
18	B1	181	TYR
19	E1	420	ASP
20	G1	30	LEU
20	G1	37	GLN
20	G1	130	ASP
20	G1	174	VAL
23	K1	34	VAL
23	L1	167	THR
24	M1	87	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	47	ASN
3	a	155	HIS
4	c	113	ASN
6	e	166	HIS
7	f	19	HIS
8	g	143	GLN
8	g	218	HIS
13	n	89	GLN
13	n	91	HIS
14	o	6	HIS
14	o	25	HIS
15	p	95	GLN
16	q	42	HIS
18	A1	56	HIS
18	A1	339	HIS
18	A1	398	GLN
18	A1	463	ASN
18	A1	472	ASN
18	A1	551	HIS
18	B1	56	HIS
18	B1	245	GLN
18	B1	296	ASN
18	B1	339	HIS

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Mol	Chain	Res	Type
18	B1	463	ASN
18	B1	562	ASN
18	C1	339	HIS
18	C1	416	GLN
18	C1	551	HIS
18	C1	558	GLN
19	D1	39	GLN
19	D1	48	HIS
19	D1	411	GLN
19	E1	48	HIS
19	E1	275	GLN
19	E1	354	HIS
19	E1	398	GLN
19	E1	411	GLN
19	F1	36	HIS
19	F1	48	HIS
19	F1	108	ASN
19	F1	354	HIS
20	G1	16	ASN
20	G1	176	ASN
20	G1	296	ASN
21	H1	76	ASN
21	H1	149	GLN
22	I1	16	HIS
22	I1	54	GLN
22	I1	71	HIS
23	J1	111	ASN
23	K1	82	GLN
23	K1	109	HIS
23	K1	178	GLN
23	L1	140	GLN
23	L1	175	HIS
24	M1	65	ASN
25	Q1	51	HIS
25	R1	51	HIS
25	T1	85	ASN
25	V1	75	ASN
25	V1	85	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	AME	e	1	6	9,10,11	0.28	0	9,11,13	0.44	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	O-C-CA-CB
6	e	1	AME	N-CA-CB-CG
6	e	1	AME	C-CA-N-CT1
6	e	1	AME	CB-CA-N-CT1

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
29	LMT	e	406	-	36,36,36	0.09	0	47,47,47	0.15	0
26	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
31	ATP	A1	601	32	32,33,33	0.30	0	48,52,52	0.28	0
30	Q7G	e	407	-	54,54,90	0.13	0	80,84,138	0.25	0
28	PC1	i	201	-	53,53,53	0.28	0	59,61,61	0.29	0
34	UTP	H1	201	-	29,30,30	0.50	0	43,47,47	0.70	0
33	ADP	D1	601	32	28,29,29	0.40	0	43,45,45	0.48	0
26	CDL	e	403	-	99,99,99	0.28	0	105,111,111	0.26	0
26	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.27	0
31	ATP	F1	601	32	32,33,33	0.29	0	48,52,52	0.28	0
26	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.26	0
30	Q7G	n	201	-	66,66,90	0.13	0	98,102,138	0.28	0
27	PEE	m	202	-	50,50,50	0.77	2 (4%)	53,55,55	0.49	0
27	PEE	f	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.48	0
28	PC1	f	204	-	53,53,53	0.27	0	59,61,61	0.28	0
29	LMT	j	203	-	36,36,36	0.11	0	47,47,47	0.19	0
26	CDL	L	101	-	99,99,99	0.29	0	105,111,111	0.25	0
31	ATP	C1	601	32	32,33,33	0.29	0	48,52,52	0.28	0
26	CDL	m	201	-	99,99,99	0.29	0	105,111,111	0.25	0
27	PEE	M	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.49	0
28	PC1	a	301	-	53,53,53	0.28	0	59,61,61	0.28	0
26	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.26	0
31	ATP	B1	601	32	32,33,33	0.29	0	48,52,52	0.28	0
28	PC1	f	203	-	53,53,53	0.28	0	59,61,61	0.29	0
26	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	e	405	-	99,99,99	0.29	0	105,111,111	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	M	201	-	99,99,99	0.42	0	105,111,111	0.29	0
26	CDL	j	202	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.27	0
26	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	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
29	LMT	e	406	-	-	1/21/61/61	0/2/2/2
26	CDL	j	201	-	-	21/110/110/110	-
31	ATP	A1	601	32	-	3/22/38/38	0/3/3/3
30	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
28	PC1	i	201	-	-	8/57/57/57	-
34	UTP	H1	201	-	-	4/22/38/38	0/2/2/2
33	ADP	D1	601	32	-	2/16/32/32	0/3/3/3
26	CDL	e	403	-	-	26/110/110/110	-
26	CDL	f	201	-	-	20/110/110/110	-
31	ATP	F1	601	32	-	5/22/38/38	0/3/3/3
26	CDL	e	401	-	-	22/110/110/110	-
30	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
27	PEE	m	202	-	-	23/54/54/54	-
27	PEE	f	202	-	-	17/54/54/54	-
28	PC1	f	204	-	-	7/57/57/57	-
29	LMT	j	203	-	-	5/21/61/61	0/2/2/2
26	CDL	L	101	-	-	17/110/110/110	-
31	ATP	C1	601	32	-	7/22/38/38	0/3/3/3
26	CDL	m	201	-	-	27/110/110/110	-
27	PEE	M	202	-	-	25/54/54/54	-
28	PC1	a	301	-	-	10/57/57/57	-
26	CDL	l	101	-	-	16/110/110/110	-
31	ATP	B1	601	32	-	7/22/38/38	0/3/3/3
28	PC1	f	203	-	-	7/57/57/57	-
26	CDL	e	402	-	-	24/110/110/110	-
26	CDL	e	404	-	-	22/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	e	405	-	-	27/110/110/110	-
26	CDL	M	201	-	-	17/110/110/110	-
26	CDL	j	202	-	-	26/110/110/110	-
26	CDL	c	201	-	-	25/110/110/110	-
26	CDL	q	101	-	-	23/110/110/110	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	202	PEE	C18-C19	3.66	1.52	1.31
27	f	202	PEE	C39-C38	3.66	1.52	1.31
27	m	202	PEE	C18-C19	3.66	1.52	1.31
27	f	202	PEE	C18-C19	3.63	1.52	1.31
27	m	202	PEE	C39-C38	3.59	1.52	1.31
27	M	202	PEE	C39-C38	3.53	1.51	1.31

There are no bond angle outliers.

All (3) chirality outliers are listed below:

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

All (455) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
26	e	402	CDL	CA3-OA5-PA1-OA4
26	e	403	CDL	CB2-OB2-PB2-OB3
26	e	403	CDL	CB3-OB5-PB2-OB3
26	e	404	CDL	CA3-OA5-PA1-OA2
26	e	404	CDL	CA3-OA5-PA1-OA3
26	e	404	CDL	CA3-OA5-PA1-OA4
26	e	404	CDL	CB3-OB5-PB2-OB2
26	e	404	CDL	CB3-OB5-PB2-OB3
26	e	404	CDL	CB3-OB5-PB2-OB4
26	e	405	CDL	CA3-OA5-PA1-OA2
26	e	405	CDL	CA3-OA5-PA1-OA3
26	e	405	CDL	CA3-OA5-PA1-OA4
26	e	405	CDL	CB3-OB5-PB2-OB2
26	f	201	CDL	CA2-OA2-PA1-OA4
26	f	201	CDL	CA2-OA2-PA1-OA5
26	f	201	CDL	CB3-OB5-PB2-OB2
26	j	201	CDL	CA2-OA2-PA1-OA3
26	j	201	CDL	CA3-OA5-PA1-OA3
26	j	201	CDL	CA3-OA5-PA1-OA4
26	j	202	CDL	CB3-OB5-PB2-OB2
26	j	202	CDL	CB3-OB5-PB2-OB4
26	l	101	CDL	CA2-OA2-PA1-OA4
26	l	101	CDL	CA2-OA2-PA1-OA5
26	l	101	CDL	CA3-OA5-PA1-OA2
26	m	201	CDL	CA2-C1-CB2-OB2
26	m	201	CDL	CA3-OA5-PA1-OA2
26	m	201	CDL	CA3-OA5-PA1-OA3
26	m	201	CDL	OA6-CA4-CA6-OA8
26	m	201	CDL	CB2-OB2-PB2-OB4
26	m	201	CDL	CB2-OB2-PB2-OB5
26	m	201	CDL	C51-CB5-OB6-CB4
26	q	101	CDL	CA2-C1-CB2-OB2
26	q	101	CDL	OA5-CA3-CA4-OA6
26	q	101	CDL	CB2-OB2-PB2-OB3
26	q	101	CDL	CB2-OB2-PB2-OB4
27	M	202	PEE	C1-O3P-P-O2P
27	M	202	PEE	C1-O3P-P-O4P
27	M	202	PEE	C4-O4P-P-O2P
27	M	202	PEE	O4P-C4-C5-N
27	f	202	PEE	C4-O4P-P-O2P
27	m	202	PEE	C1-O3P-P-O2P
27	m	202	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
27	m	202	PEE	C4-O4P-P-O2P
27	m	202	PEE	O4P-C4-C5-N
28	a	301	PC1	C11-O13-P-O14
28	a	301	PC1	C11-O13-P-O11
28	a	301	PC1	C1-O11-P-O12
28	a	301	PC1	C1-O11-P-O14
28	a	301	PC1	C1-O11-P-O13
28	f	203	PC1	C11-O13-P-O12
28	f	203	PC1	C11-O13-P-O11
28	f	203	PC1	C1-O11-P-O14
28	f	203	PC1	C1-O11-P-O13
28	f	204	PC1	C11-O13-P-O12
28	f	204	PC1	C11-O13-P-O11
28	f	204	PC1	O13-C11-C12-N
28	i	201	PC1	C11-O13-P-O12
28	i	201	PC1	C11-O13-P-O14
28	i	201	PC1	C11-O13-P-O11
28	i	201	PC1	O13-C11-C12-N
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	n	201	Q7G	C2B-C1B-O1B-C24
31	A1	601	ATP	PB-O3B-PG-O2G
31	A1	601	ATP	C5'-O5'-PA-O1A
31	B1	601	ATP	PB-O3B-PG-O2G
31	C1	601	ATP	PB-O3B-PG-O2G
31	F1	601	ATP	PB-O3B-PG-O2G
34	H1	201	UTP	PB-O3A-PA-O5'
34	H1	201	UTP	C5'-O5'-PA-O1A
34	H1	201	UTP	C5'-O5'-PA-O2A
34	H1	201	UTP	C5'-O5'-PA-O3A
26	M	201	CDL	OB7-CB5-OB6-CB4
26	e	403	CDL	OA7-CA5-OA6-CA4
26	m	201	CDL	OB7-CB5-OB6-CB4
26	e	403	CDL	C11-CA5-OA6-CA4
26	q	101	CDL	OA7-CA5-OA6-CA4
26	M	201	CDL	O1-C1-CB2-OB2
26	e	403	CDL	O1-C1-CA2-OA2
26	e	404	CDL	O1-C1-CA2-OA2
26	j	201	CDL	O1-C1-CA2-OA2
26	m	201	CDL	O1-C1-CB2-OB2
26	q	101	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
30	e	407	Q7G	O5B-C1B-O1B-C24
26	e	402	CDL	C31-CA7-OA8-CA6
27	M	202	PEE	C31-C30-O3-C3
27	m	202	PEE	C31-C30-O3-C3
30	e	407	Q7G	C2B-C1B-O1B-C24
26	q	101	CDL	O1-C1-CB2-OB2
26	e	402	CDL	OA9-CA7-OA8-CA6
26	e	405	CDL	OB5-CB3-CB4-OB6
26	m	201	CDL	CA5-C11-C12-C13
27	M	202	PEE	O5-C30-O3-C3
27	m	202	PEE	O5-C30-O3-C3
26	j	201	CDL	CA4-CA3-OA5-PA1
30	n	201	Q7G	O5B-C1B-O1B-C24
26	e	404	CDL	CB2-C1-CA2-OA2
26	e	405	CDL	CA7-C31-C32-C33
26	e	403	CDL	C51-CB5-OB6-CB4
26	e	405	CDL	C11-CA5-OA6-CA4
26	e	403	CDL	OB7-CB5-OB6-CB4
26	e	405	CDL	OA7-CA5-OA6-CA4
30	e	407	Q7G	CG1-C22-C23-C48
26	e	404	CDL	O1-C1-CB2-OB2
26	M	201	CDL	C71-CB7-OB8-CB6
26	e	401	CDL	C77-C78-C79-C80
26	j	202	CDL	C11-CA5-OA6-CA4
26	M	201	CDL	C74-C75-C76-C77
29	e	406	LMT	C2-C1-O1'-C1'
26	j	202	CDL	C74-C75-C76-C77
26	j	201	CDL	OB5-CB3-CB4-CB6
26	e	403	CDL	C71-C72-C73-C74
26	j	202	CDL	OA7-CA5-OA6-CA4
26	j	201	CDL	C13-C14-C15-C16
26	e	404	CDL	CA2-C1-CB2-OB2
26	j	201	CDL	CB2-C1-CA2-OA2
26	l	101	CDL	C31-CA7-OA8-CA6
26	j	202	CDL	C78-C79-C80-C81
26	M	201	CDL	OB9-CB7-OB8-CB6
26	e	404	CDL	C11-CA5-OA6-CA4
26	j	202	CDL	C51-CB5-OB6-CB4
26	l	101	CDL	C11-CA5-OA6-CA4
27	f	202	PEE	C11-C10-O2-C2
26	L	101	CDL	C31-CA7-OA8-CA6
26	e	403	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	M	201	CDL	C33-C34-C35-C36
26	L	101	CDL	C11-CA5-OA6-CA4
26	M	201	CDL	C11-CA5-OA6-CA4
26	e	402	CDL	C11-CA5-OA6-CA4
26	f	201	CDL	C11-CA5-OA6-CA4
27	M	202	PEE	C31-C32-C33-C34
26	c	201	CDL	C55-C56-C57-C58
27	m	202	PEE	C17-C18-C19-C20
26	e	405	CDL	C57-C58-C59-C60
26	M	201	CDL	C22-C23-C24-C25
26	m	201	CDL	C12-C13-C14-C15
26	j	201	CDL	C81-C82-C83-C84
26	l	101	CDL	OA9-CA7-OA8-CA6
29	j	203	LMT	O5B-C5B-C6B-O6B
26	j	201	CDL	CA7-C31-C32-C33
30	n	201	Q7G	O5C-C5C-C6C-O6C
26	c	201	CDL	C34-C35-C36-C37
26	c	201	CDL	CA4-CA3-OA5-PA1
26	M	201	CDL	OA7-CA5-OA6-CA4
26	j	202	CDL	C15-C16-C17-C18
26	m	201	CDL	C73-C74-C75-C76
27	f	202	PEE	C42-C43-C44-C45
26	L	101	CDL	OA9-CA7-OA8-CA6
26	q	101	CDL	OA5-CA3-CA4-CA6
26	e	404	CDL	OA7-CA5-OA6-CA4
26	j	202	CDL	OB7-CB5-OB6-CB4
26	l	101	CDL	OA7-CA5-OA6-CA4
26	e	402	CDL	C11-C12-C13-C14
26	e	402	CDL	C81-C82-C83-C84
27	M	202	PEE	C17-C18-C19-C20
26	e	403	CDL	CB3-CB4-CB6-OB8
26	m	201	CDL	CA3-CA4-CA6-OA8
27	M	202	PEE	C1-C2-C3-O3
27	m	202	PEE	C1-C2-C3-O3
26	j	201	CDL	C62-C63-C64-C65
26	M	201	CDL	C78-C79-C80-C81
26	e	403	CDL	C17-C18-C19-C20
26	e	401	CDL	C56-C57-C58-C59
26	m	201	CDL	C78-C79-C80-C81
27	M	202	PEE	C22-C23-C24-C25
26	L	101	CDL	OA7-CA5-OA6-CA4
27	f	202	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
26	M	201	CDL	C72-C73-C74-C75
26	e	404	CDL	C17-C18-C19-C20
26	q	101	CDL	CB7-C71-C72-C73
26	q	101	CDL	CA5-C11-C12-C13
26	e	404	CDL	OA5-CA3-CA4-OA6
26	m	201	CDL	OA5-CA3-CA4-OA6
26	e	403	CDL	C78-C79-C80-C81
26	j	202	CDL	C79-C80-C81-C82
26	e	402	CDL	C78-C79-C80-C81
26	L	101	CDL	C14-C15-C16-C17
26	e	403	CDL	OB6-CB4-CB6-OB8
26	f	201	CDL	OB6-CB4-CB6-OB8
28	f	203	PC1	O21-C2-C3-O31
26	l	101	CDL	C14-C15-C16-C17
27	m	202	PEE	C22-C23-C24-C25
26	f	201	CDL	C77-C78-C79-C80
26	c	201	CDL	C51-C52-C53-C54
28	f	204	PC1	C21-C22-C23-C24
26	e	402	CDL	C75-C76-C77-C78
26	e	401	CDL	C18-C19-C20-C21
26	e	402	CDL	OA7-CA5-OA6-CA4
26	f	201	CDL	OA7-CA5-OA6-CA4
26	e	405	CDL	CA4-CA3-OA5-PA1
27	M	202	PEE	C2-C1-O3P-P
27	m	202	PEE	C2-C1-O3P-P
26	e	405	CDL	OB5-CB3-CB4-CB6
26	m	201	CDL	OA5-CA3-CA4-CA6
26	c	201	CDL	CA4-CA6-OA8-CA7
26	j	202	CDL	C76-C77-C78-C79
26	e	404	CDL	CB3-CB4-CB6-OB8
26	e	405	CDL	CB3-CB4-CB6-OB8
28	f	203	PC1	C1-C2-C3-O31
27	m	202	PEE	C31-C32-C33-C34
26	c	201	CDL	C39-C40-C41-C42
26	e	403	CDL	C12-C13-C14-C15
26	c	201	CDL	OA5-CA3-CA4-OA6
26	j	201	CDL	OB5-CB3-CB4-OB6
26	j	202	CDL	OA5-CA3-CA4-OA6
26	l	101	CDL	CA4-CA3-OA5-PA1
28	a	301	PC1	C2-C1-O11-P
26	e	405	CDL	C78-C79-C80-C81
30	n	201	Q7G	C24-C23-C48-O1C

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Mol	Chain	Res	Type	Atoms
26	j	201	CDL	C34-C35-C36-C37
26	L	101	CDL	OA6-CA4-CA6-OA8
26	l	101	CDL	OA6-CA4-CA6-OA8
28	i	201	PC1	C2C-C2D-C2E-C2F
26	q	101	CDL	C77-C78-C79-C80
26	M	201	CDL	C42-C43-C44-C45
26	e	405	CDL	C76-C77-C78-C79
30	e	407	Q7G	CG1-C22-C23-C24
26	e	403	CDL	C62-C63-C64-C65
26	m	201	CDL	C21-C22-C23-C24
26	q	101	CDL	CB2-C1-CA2-OA2
26	c	201	CDL	OA5-CA3-CA4-CA6
26	j	202	CDL	OA5-CA3-CA4-CA6
26	e	402	CDL	CA6-CA4-OA6-CA5
26	q	101	CDL	CB3-CB4-OB6-CB5
31	B1	601	ATP	PB-O3B-PG-O3G
26	f	201	CDL	OA5-CA3-CA4-OA6
26	f	201	CDL	C12-C13-C14-C15
26	e	404	CDL	OB6-CB4-CB6-OB8
26	e	405	CDL	OB6-CB4-CB6-OB8
27	f	202	PEE	O2-C2-C3-O3
27	m	202	PEE	O2-C2-C3-O3
26	e	401	CDL	C81-C82-C83-C84
28	a	301	PC1	O13-C11-C12-N
28	f	203	PC1	O13-C11-C12-N
31	C1	601	ATP	PG-O3B-PB-O2B
26	j	202	CDL	O1-C1-CB2-OB2
26	f	201	CDL	C13-C14-C15-C16
26	l	101	CDL	C31-C32-C33-C34
26	e	404	CDL	OA5-CA3-CA4-CA6
26	L	101	CDL	C31-C32-C33-C34
26	e	405	CDL	OA5-CA3-CA4-OA6
26	e	405	CDL	C40-C41-C42-C43
27	M	202	PEE	O2-C2-C3-O3
26	c	201	CDL	CA3-CA4-CA6-OA8
26	j	202	CDL	CB3-CB4-CB6-OB8
27	f	202	PEE	C1-C2-C3-O3
30	e	407	Q7G	C23-C24-O1B-C1B
27	m	202	PEE	C36-C37-C38-C39
26	M	201	CDL	C54-C55-C56-C57
26	L	101	CDL	CA2-OA2-PA1-OA3
26	L	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
26	c	201	CDL	CB2-OB2-PB2-OB3
26	e	401	CDL	CB2-OB2-PB2-OB5
26	e	401	CDL	CB3-OB5-PB2-OB2
26	e	401	CDL	CB3-OB5-PB2-OB4
26	e	405	CDL	CB3-OB5-PB2-OB3
26	f	201	CDL	CB3-OB5-PB2-OB3
26	j	201	CDL	CA3-OA5-PA1-OA2
26	l	101	CDL	CA2-OA2-PA1-OA3
26	l	101	CDL	CA3-OA5-PA1-OA3
26	m	201	CDL	CA3-OA5-PA1-OA4
26	m	201	CDL	CB3-OB5-PB2-OB3
26	q	101	CDL	CA3-OA5-PA1-OA3
26	q	101	CDL	CB2-OB2-PB2-OB5
26	q	101	CDL	CB3-OB5-PB2-OB3
27	M	202	PEE	C4-O4P-P-O3P
27	M	202	PEE	C4-O4P-P-O1P
27	f	202	PEE	C1-O3P-P-O1P
27	f	202	PEE	C4-O4P-P-O3P
27	f	202	PEE	C4-O4P-P-O1P
27	m	202	PEE	C4-O4P-P-O3P
27	m	202	PEE	C4-O4P-P-O1P
31	B1	601	ATP	C5'-O5'-PA-O1A
31	C1	601	ATP	C5'-O5'-PA-O1A
31	F1	601	ATP	C5'-O5'-PA-O1A
26	L	101	CDL	CA4-CA3-OA5-PA1
26	e	402	CDL	CA4-CA3-OA5-PA1
26	f	201	CDL	CB4-CB3-OB5-PB2
26	j	202	CDL	CB4-CB3-OB5-PB2
26	j	202	CDL	C61-C62-C63-C64
30	n	201	Q7G	C16-C17-O20-CG1
26	e	404	CDL	CA6-CA4-OA6-CA5
26	j	202	CDL	CB3-CB4-OB6-CB5
26	c	201	CDL	C83-C84-C85-C86
26	e	401	CDL	C13-C14-C15-C16
26	M	201	CDL	CA2-C1-CB2-OB2
26	e	403	CDL	CB2-C1-CA2-OA2
29	j	203	LMT	C2-C3-C4-C5
26	e	402	CDL	C1-CB2-OB2-PB2
26	j	201	CDL	C1-CB2-OB2-PB2
26	L	101	CDL	O1-C1-CA2-OA2
26	j	201	CDL	C55-C56-C57-C58
26	e	402	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
27	f	202	PEE	O5-C30-O3-C3
27	M	202	PEE	C39-C40-C41-C42
26	f	201	CDL	CB3-CB4-CB6-OB8
31	A1	601	ATP	PG-O3B-PB-O2B
31	B1	601	ATP	PA-O3A-PB-O2B
31	F1	601	ATP	PG-O3B-PB-O1B
31	F1	601	ATP	PG-O3B-PB-O2B
27	M	202	PEE	C36-C37-C38-C39
27	f	202	PEE	C18-C19-C20-C21
28	f	204	PC1	C37-C38-C39-C3A
26	c	201	CDL	C38-C39-C40-C41
28	i	201	PC1	C2A-C2B-C2C-C2D
26	j	202	CDL	CA2-C1-CB2-OB2
27	f	202	PEE	C31-C30-O3-C3
26	e	402	CDL	OB5-CB3-CB4-OB6
26	e	403	CDL	OA6-CA4-CA6-OA8
26	c	201	CDL	C56-C57-C58-C59
26	q	101	CDL	C1-CB2-OB2-PB2
26	j	201	CDL	C77-C78-C79-C80
27	m	202	PEE	C41-C42-C43-C44
26	e	402	CDL	C53-C54-C55-C56
26	j	202	CDL	CA3-CA4-CA6-OA8
26	m	201	CDL	C42-C43-C44-C45
30	n	201	Q7G	C18-C17-O20-CG1
26	m	201	CDL	C71-CB7-OB8-CB6
26	j	201	CDL	C72-C73-C74-C75
26	j	201	CDL	CA3-CA4-OA6-CA5
26	e	401	CDL	OB5-CB3-CB4-OB6
26	c	201	CDL	C40-C41-C42-C43
27	f	202	PEE	C16-C17-C18-C19
27	f	202	PEE	C19-C20-C21-C22
27	m	202	PEE	C23-C24-C25-C26
27	M	202	PEE	C23-C24-C25-C26
26	e	405	CDL	OA5-CA3-CA4-CA6
26	m	201	CDL	C33-C34-C35-C36
27	m	202	PEE	C16-C17-C18-C19
26	j	202	CDL	OA6-CA4-CA6-OA8
26	l	101	CDL	C39-C40-C41-C42
26	L	101	CDL	C39-C40-C41-C42
26	e	402	CDL	C52-C51-CB5-OB6
26	m	201	CDL	OB9-CB7-OB8-CB6
26	e	404	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
26	e	404	CDL	C18-C19-C20-C21
26	c	201	CDL	C42-C43-C44-C45
26	e	403	CDL	CA3-CA4-CA6-OA8
28	f	204	PC1	O31-C31-C32-C33
26	q	101	CDL	OB5-CB3-CB4-OB6
26	e	403	CDL	CB5-C51-C52-C53
26	m	201	CDL	OA7-CA5-OA6-CA4
26	c	201	CDL	CB2-C1-CA2-OA2
26	e	401	CDL	OB5-CB3-CB4-CB6
26	e	402	CDL	OB5-CB3-CB4-CB6
28	a	301	PC1	O11-C1-C2-C3
26	c	201	CDL	OA6-CA4-CA6-OA8
27	M	202	PEE	C16-C17-C18-C19
27	M	202	PEE	C38-C39-C40-C41
27	f	202	PEE	C36-C37-C38-C39
26	f	201	CDL	C37-C38-C39-C40
26	f	201	CDL	C78-C79-C80-C81
27	m	202	PEE	C38-C39-C40-C41
31	B1	601	ATP	PB-O3B-PG-O1G
31	C1	601	ATP	PB-O3B-PG-O1G
26	e	405	CDL	C79-C80-C81-C82
26	c	201	CDL	CA5-C11-C12-C13
27	m	202	PEE	C18-C19-C20-C21
26	e	401	CDL	C63-C64-C65-C66
26	M	201	CDL	C71-C72-C73-C74
26	e	401	CDL	C16-C17-C18-C19
26	l	101	CDL	CA3-CA4-CA6-OA8
26	j	202	CDL	C38-C39-C40-C41
26	f	201	CDL	C12-C11-CA5-OA6
28	i	201	PC1	O21-C21-C22-C23
26	e	405	CDL	C32-C31-CA7-OA8
27	f	202	PEE	O2-C10-C11-C12
26	f	201	CDL	OA5-CA3-CA4-CA6
26	q	101	CDL	OB5-CB3-CB4-CB6
26	e	405	CDL	C12-C11-CA5-OA6
26	M	201	CDL	C35-C36-C37-C38
26	e	401	CDL	CB4-CB3-OB5-PB2
28	f	204	PC1	C24-C25-C26-C27
31	B1	601	ATP	PG-O3B-PB-O1B
31	B1	601	ATP	PG-O3B-PB-O2B
31	C1	601	ATP	PG-O3B-PB-O1B
31	C1	601	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
31	C1	601	ATP	PA-O3A-PB-O2B
33	D1	601	ADP	PB-O3A-PA-O1A
26	e	403	CDL	C32-C31-CA7-OA8
26	j	202	CDL	C12-C11-CA5-OA6
27	M	202	PEE	O2-C10-C11-C12
27	M	202	PEE	C18-C19-C20-C21
26	e	405	CDL	C53-C54-C55-C56
26	m	201	CDL	C11-CA5-OA6-CA4
26	c	201	CDL	C35-C36-C37-C38
27	M	202	PEE	C41-C42-C43-C44
26	f	201	CDL	C72-C71-CB7-OB8
26	m	201	CDL	C12-C11-CA5-OA6
26	e	403	CDL	C11-C12-C13-C14
26	e	405	CDL	C56-C57-C58-C59
26	e	401	CDL	C32-C31-CA7-OA8
27	m	202	PEE	O2-C10-C11-C12
26	L	101	CDL	CA3-CA4-CA6-OA8
26	e	402	CDL	C19-C20-C21-C22
26	e	402	CDL	C72-C71-CB7-OB8
26	e	401	CDL	C52-C51-CB5-OB6
26	e	403	CDL	C52-C51-CB5-OB6
26	j	201	CDL	C52-C51-CB5-OB6
31	F1	601	ATP	PB-O3B-PG-O1G
27	m	202	PEE	C34-C35-C36-C37
26	e	402	CDL	C54-C55-C56-C57
26	j	201	CDL	CA6-CA4-OA6-CA5
26	c	201	CDL	C62-C63-C64-C65
26	l	101	CDL	C60-C61-C62-C63
26	e	401	CDL	OB7-CB5-OB6-CB4
26	e	404	CDL	C13-C14-C15-C16
27	M	202	PEE	C34-C35-C36-C37
26	e	405	CDL	C32-C31-CA7-OA9
27	f	202	PEE	O4-C10-C11-C12
26	q	101	CDL	C71-C72-C73-C74
26	e	403	CDL	C32-C31-CA7-OA9
26	j	202	CDL	C12-C11-CA5-OA7
26	e	403	CDL	OB9-CB7-OB8-CB6
26	e	405	CDL	C14-C15-C16-C17
28	a	301	PC1	O11-C1-C2-O21
26	j	202	CDL	C59-C60-C61-C62
26	m	201	CDL	C12-C11-CA5-OA7
26	L	101	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
26	e	401	CDL	C51-CB5-OB6-CB4
26	e	403	CDL	C71-CB7-OB8-CB6
26	c	201	CDL	O1-C1-CA2-OA2
26	q	101	CDL	O1-C1-CA2-OA2
26	e	405	CDL	C12-C11-CA5-OA7
26	f	201	CDL	C72-C71-CB7-OB9
28	i	201	PC1	O22-C21-C22-C23
28	a	301	PC1	C23-C24-C25-C26
26	e	404	CDL	C32-C31-CA7-OA8
27	M	202	PEE	C11-C10-O2-C2
26	f	201	CDL	C12-C11-CA5-OA7
27	m	202	PEE	O4-C10-C11-C12
27	M	202	PEE	O4-C10-C11-C12
26	j	202	CDL	C72-C73-C74-C75
26	e	401	CDL	C32-C31-CA7-OA9
26	q	101	CDL	C72-C71-CB7-OB8
26	e	403	CDL	C52-C51-CB5-OB7
26	q	101	CDL	C79-C80-C81-C82
26	e	401	CDL	C52-C51-CB5-OB7
26	e	402	CDL	C32-C31-CA7-OA8
33	D1	601	ADP	PB-O3A-PA-O2A
26	e	402	CDL	C72-C71-CB7-OB9

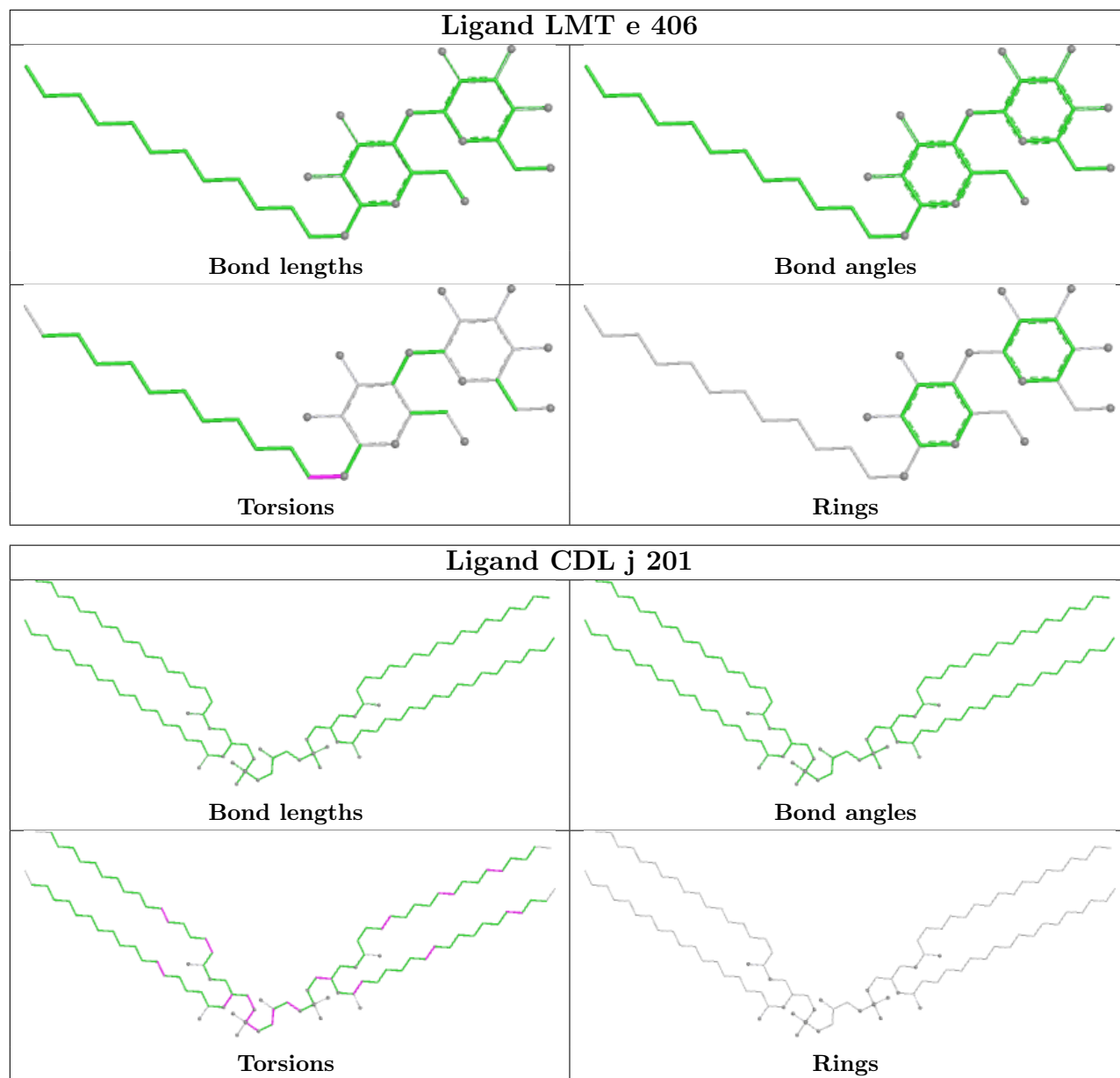
There are no ring outliers.

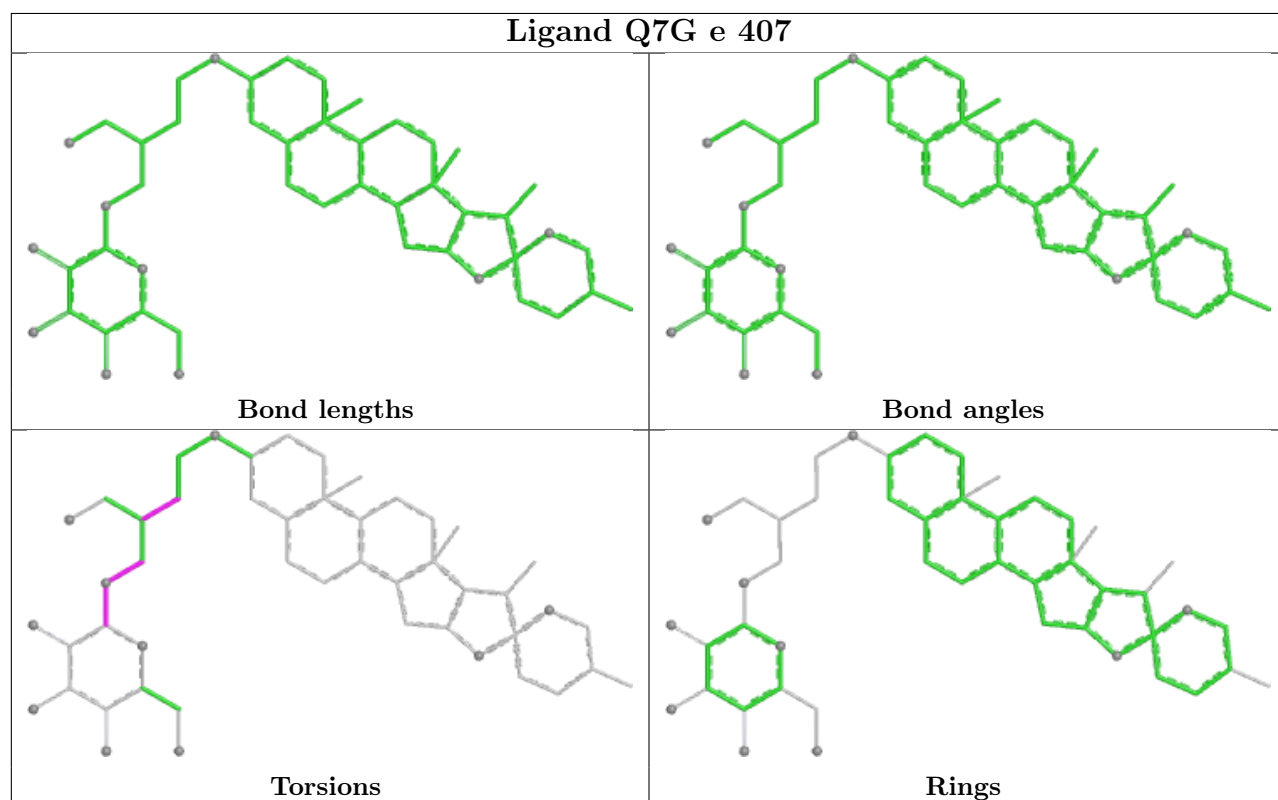
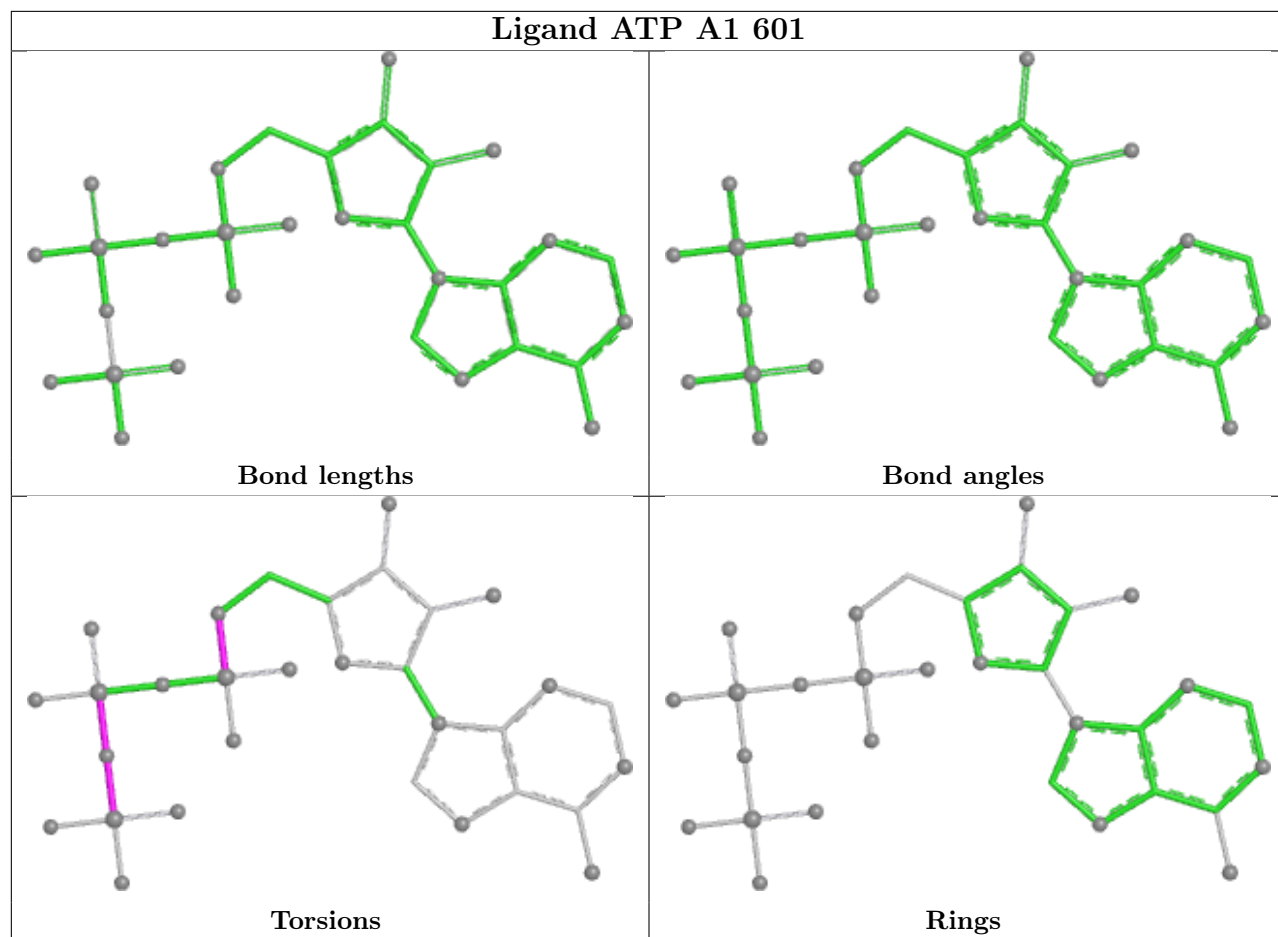
7 monomers are involved in 8 short contacts:

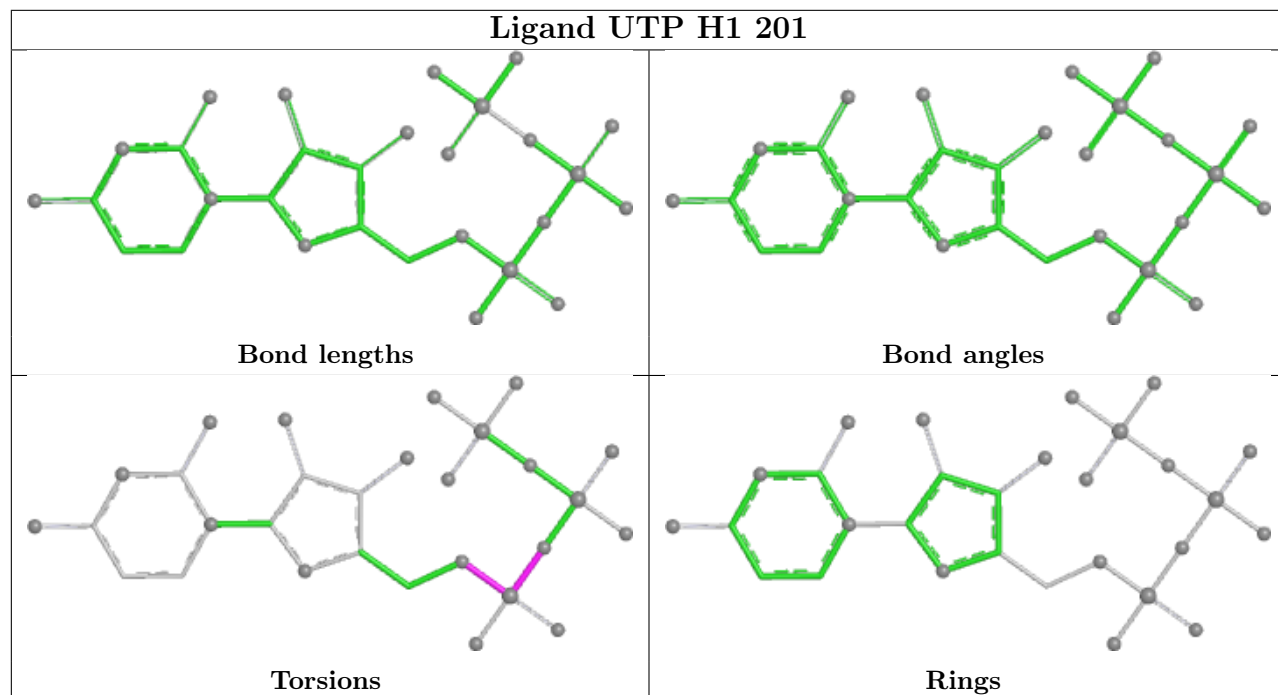
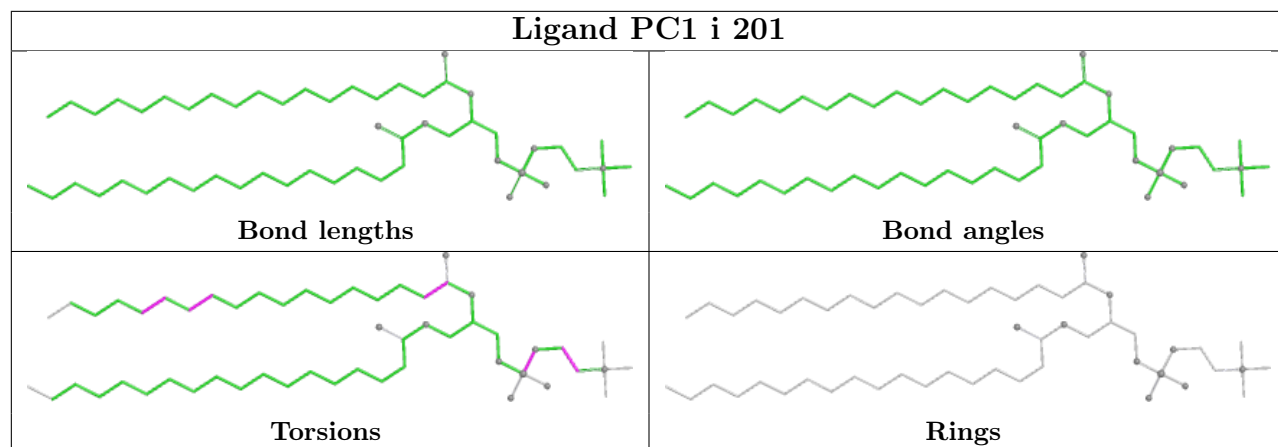
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	H1	201	UTP	1	0
28	f	204	PC1	1	0
31	C1	601	ATP	1	0
26	e	402	CDL	2	0
26	j	202	CDL	1	0
26	c	201	CDL	1	0
26	q	101	CDL	1	0

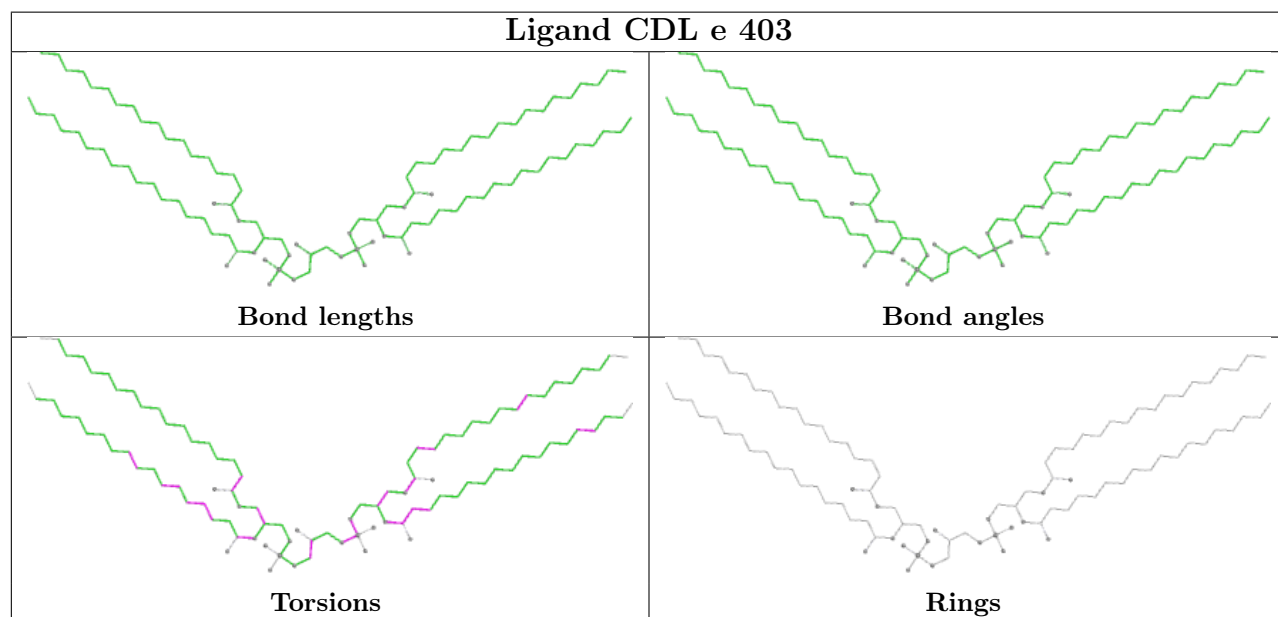
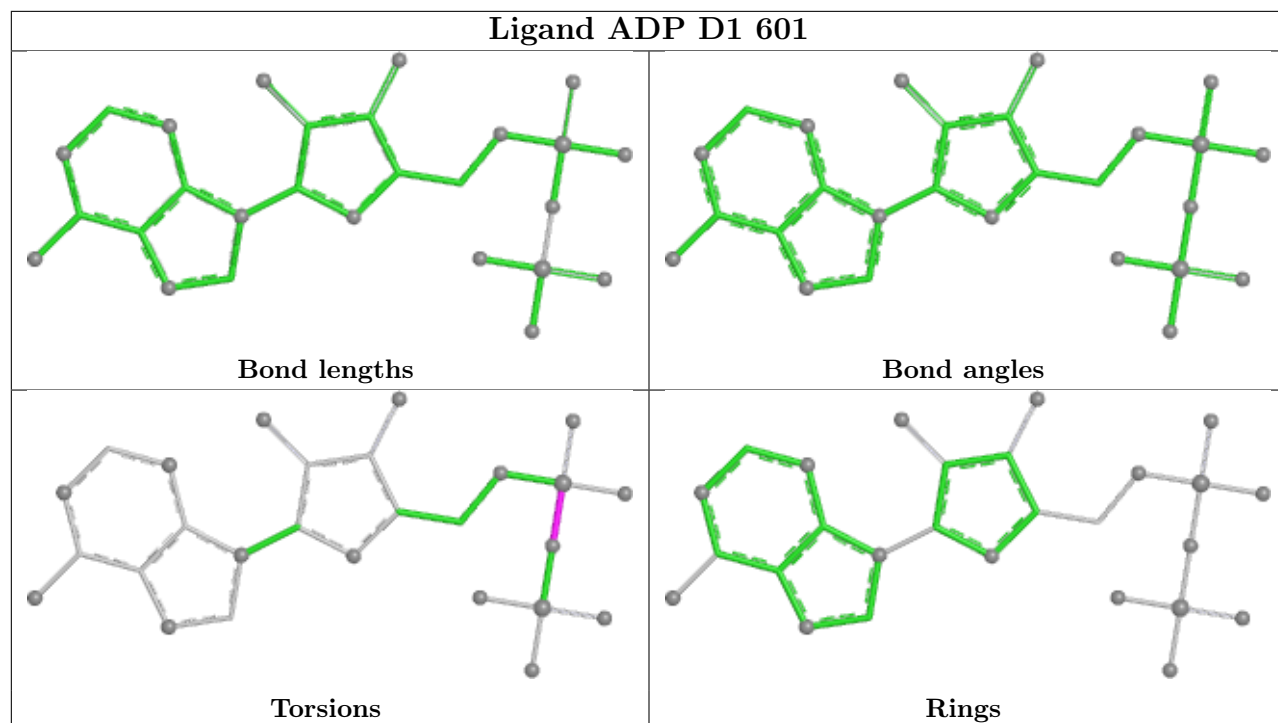
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

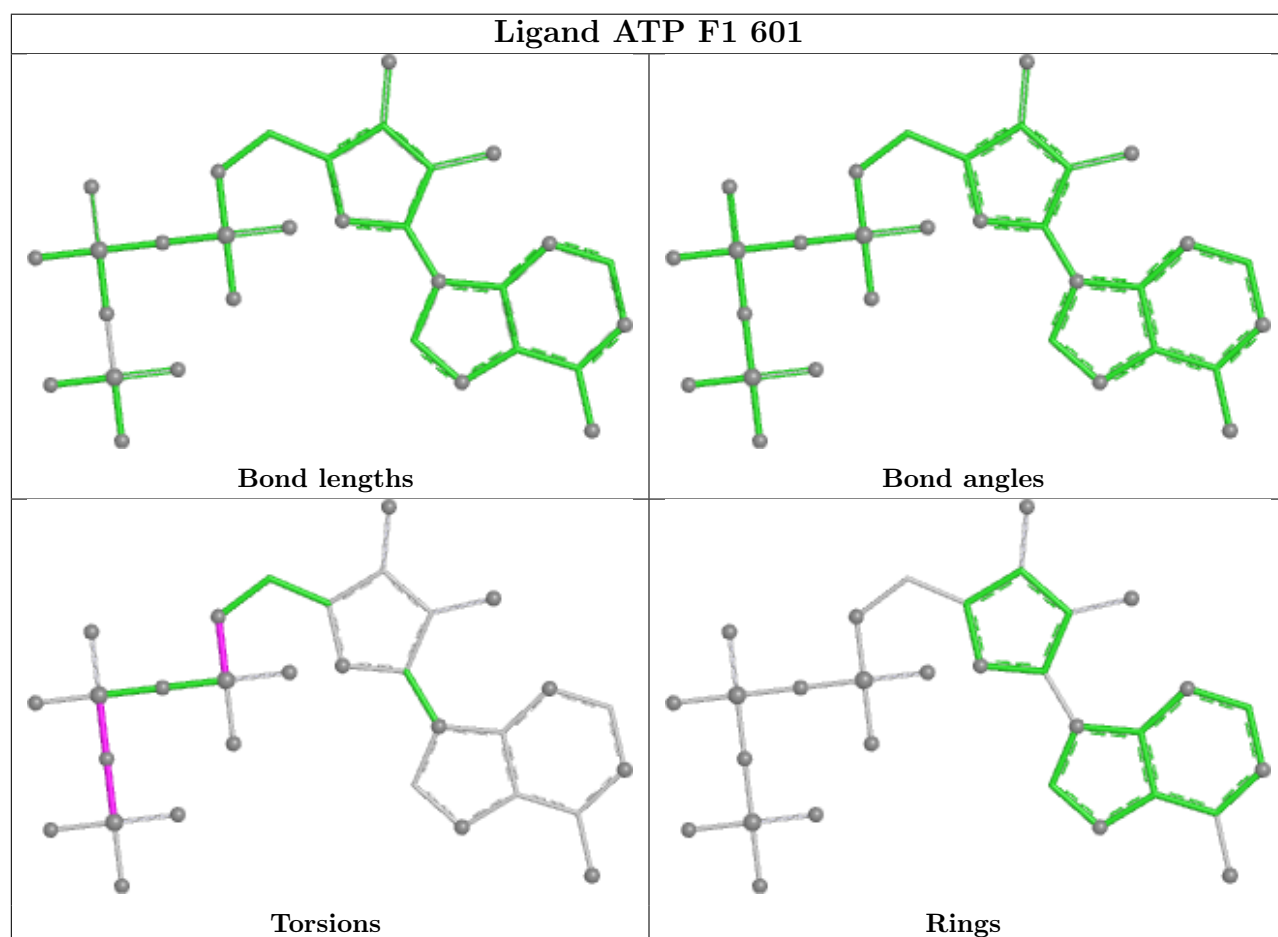
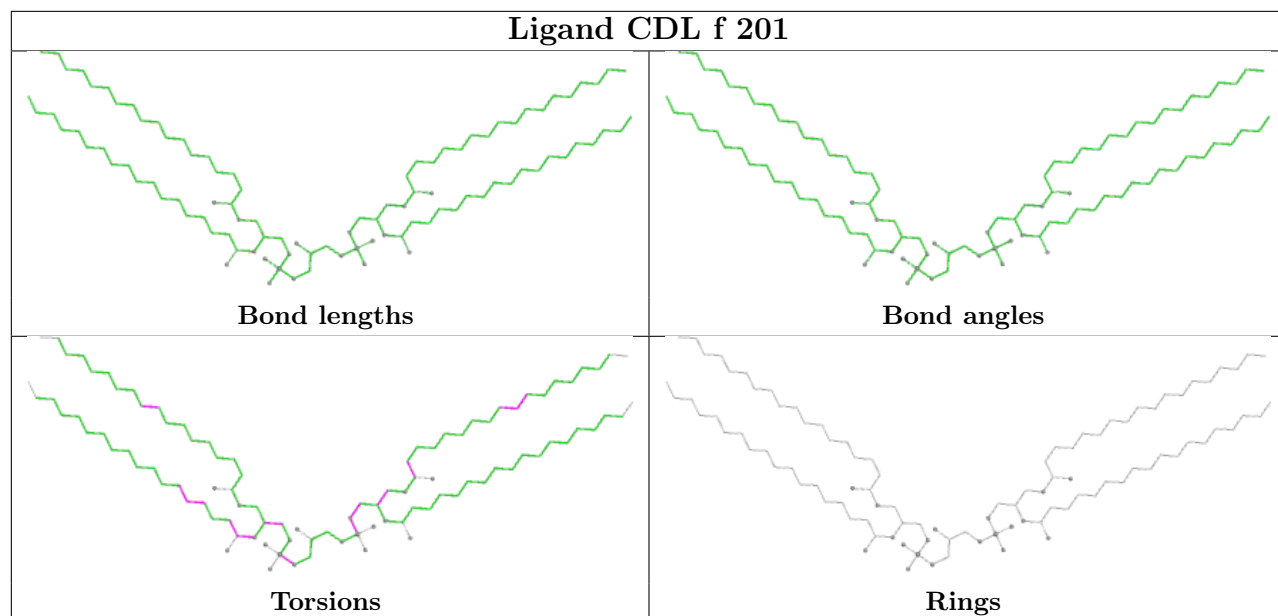
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

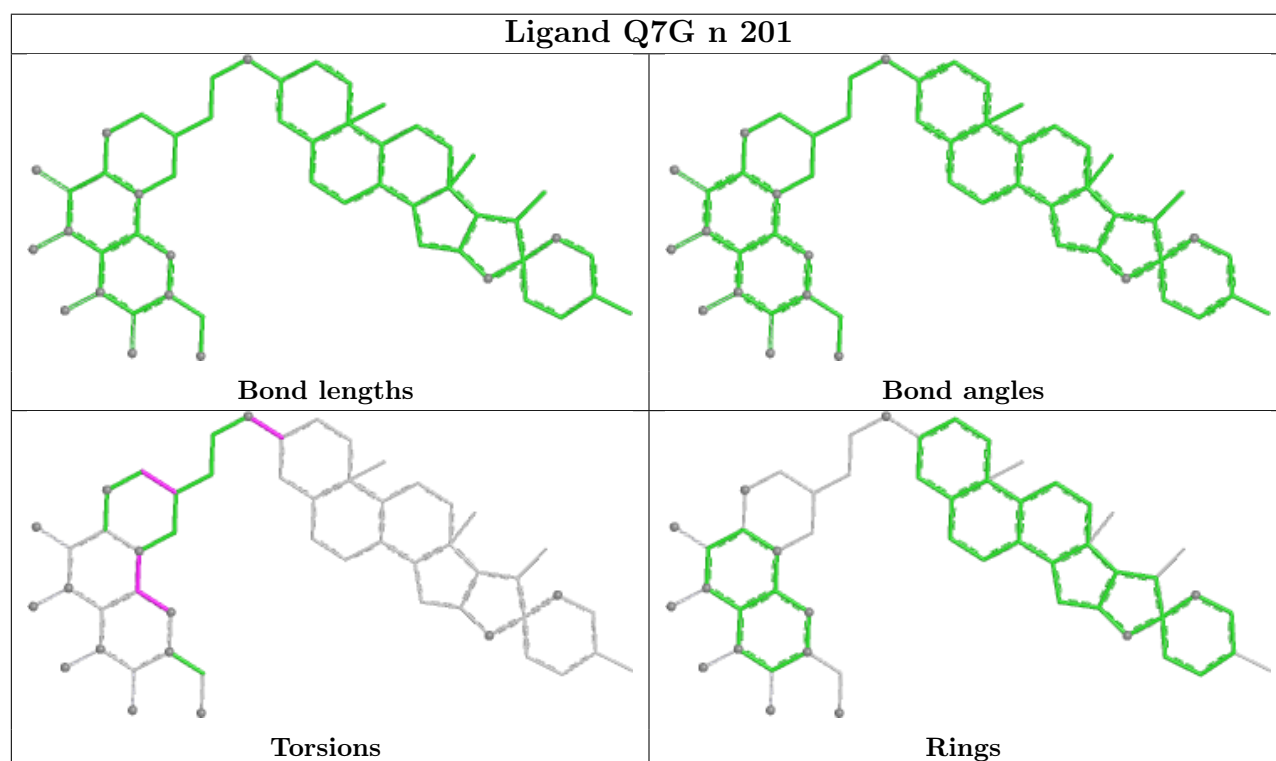
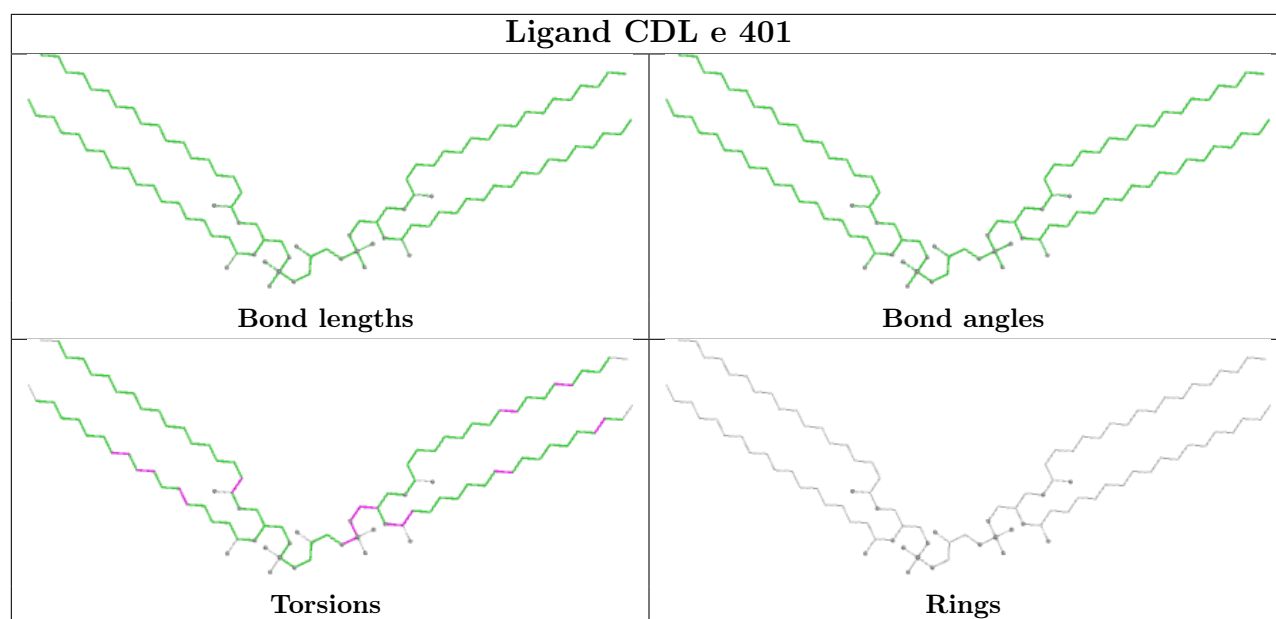


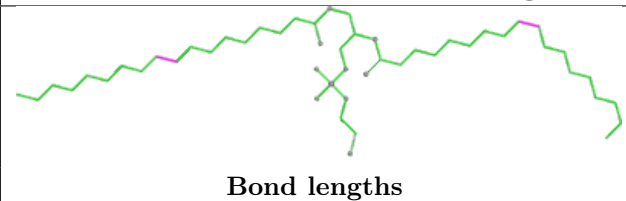
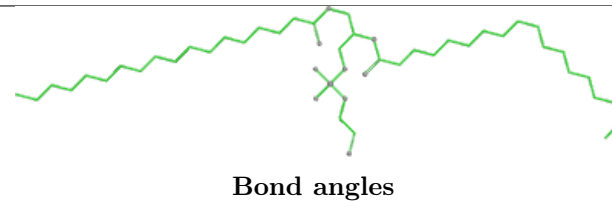
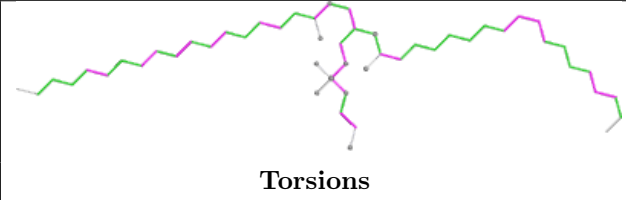
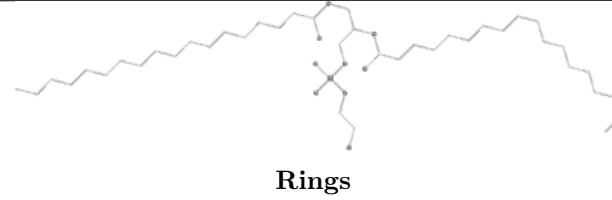


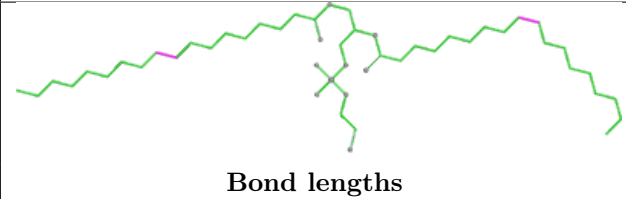
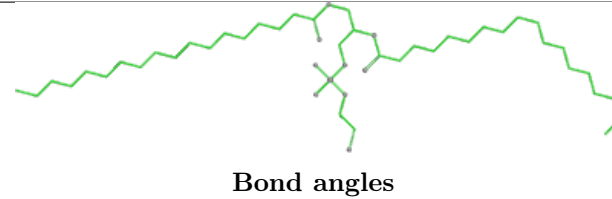
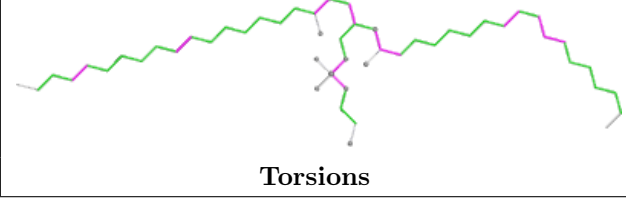
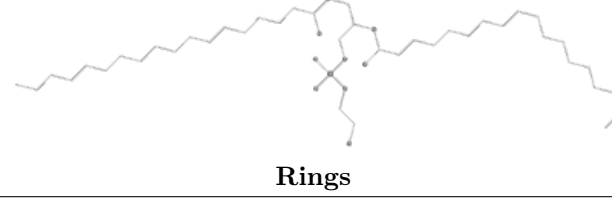


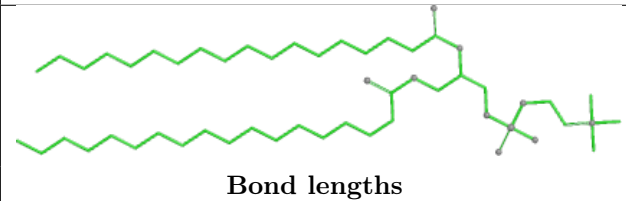
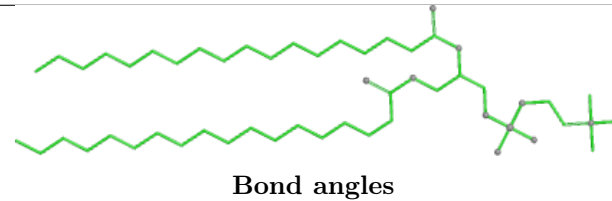
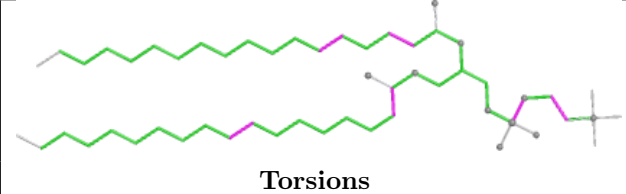
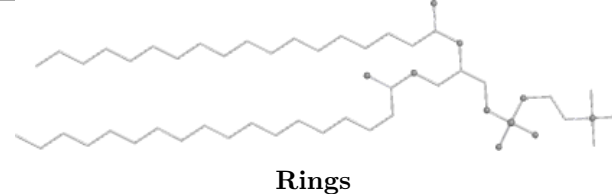


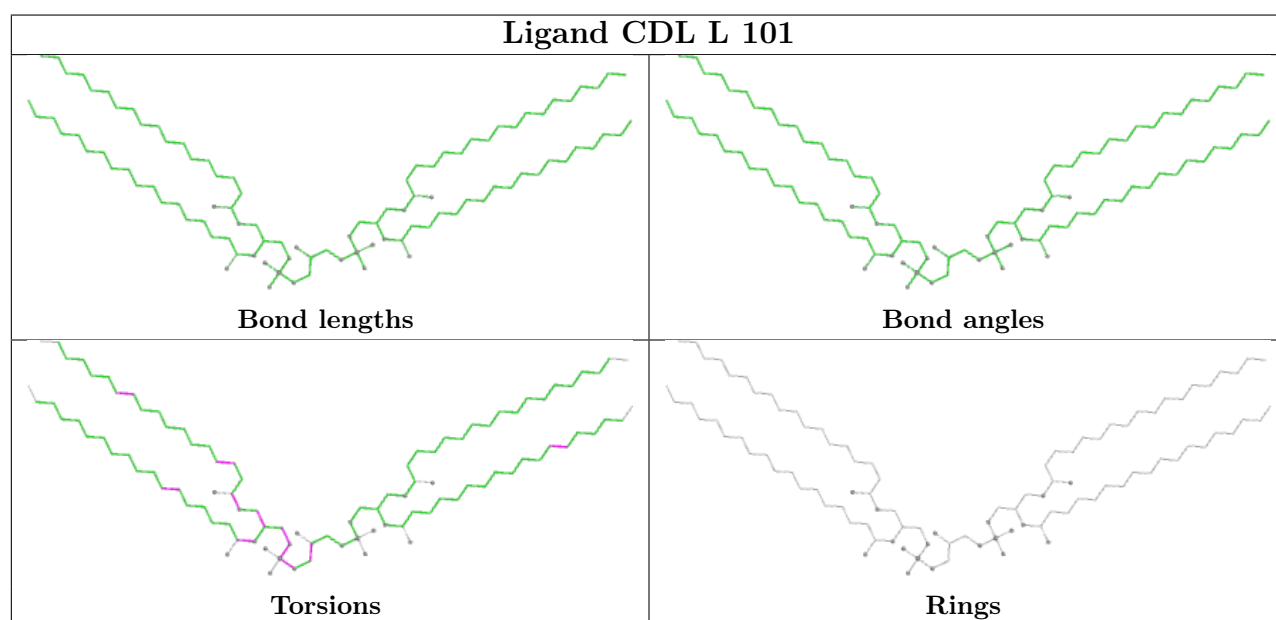
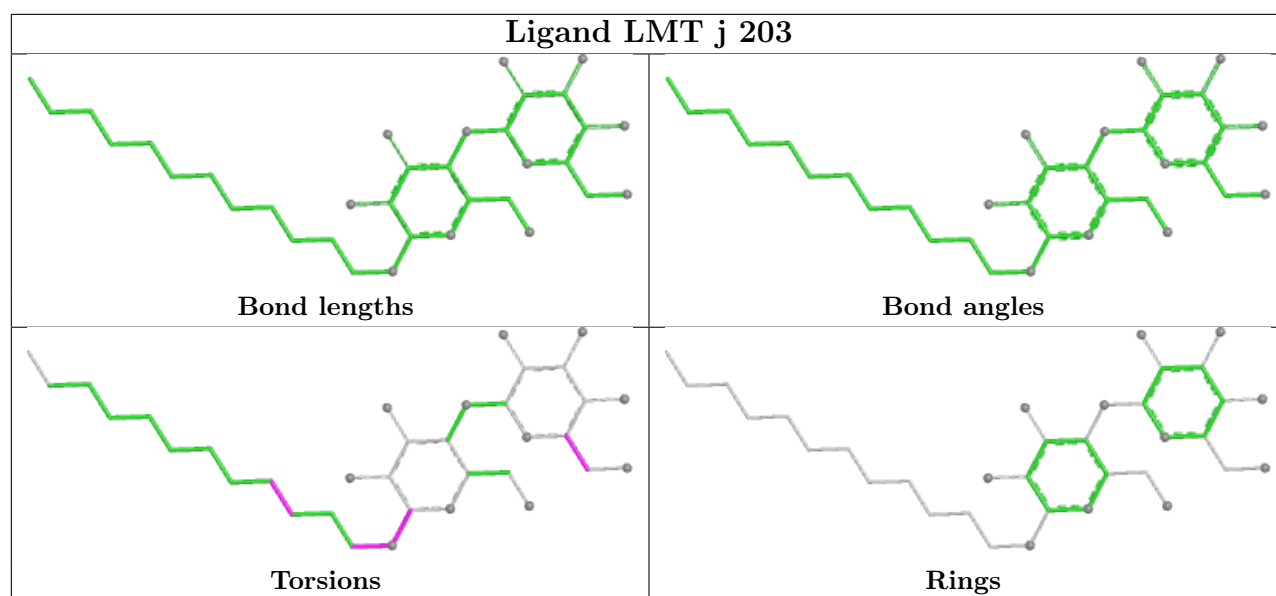


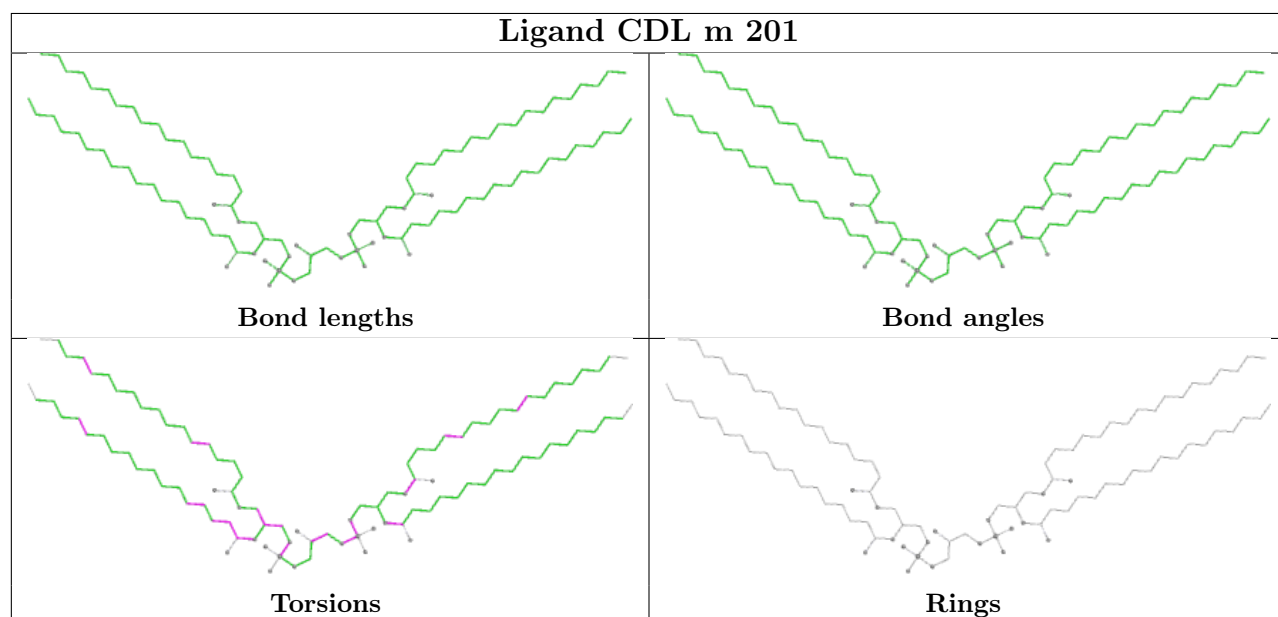
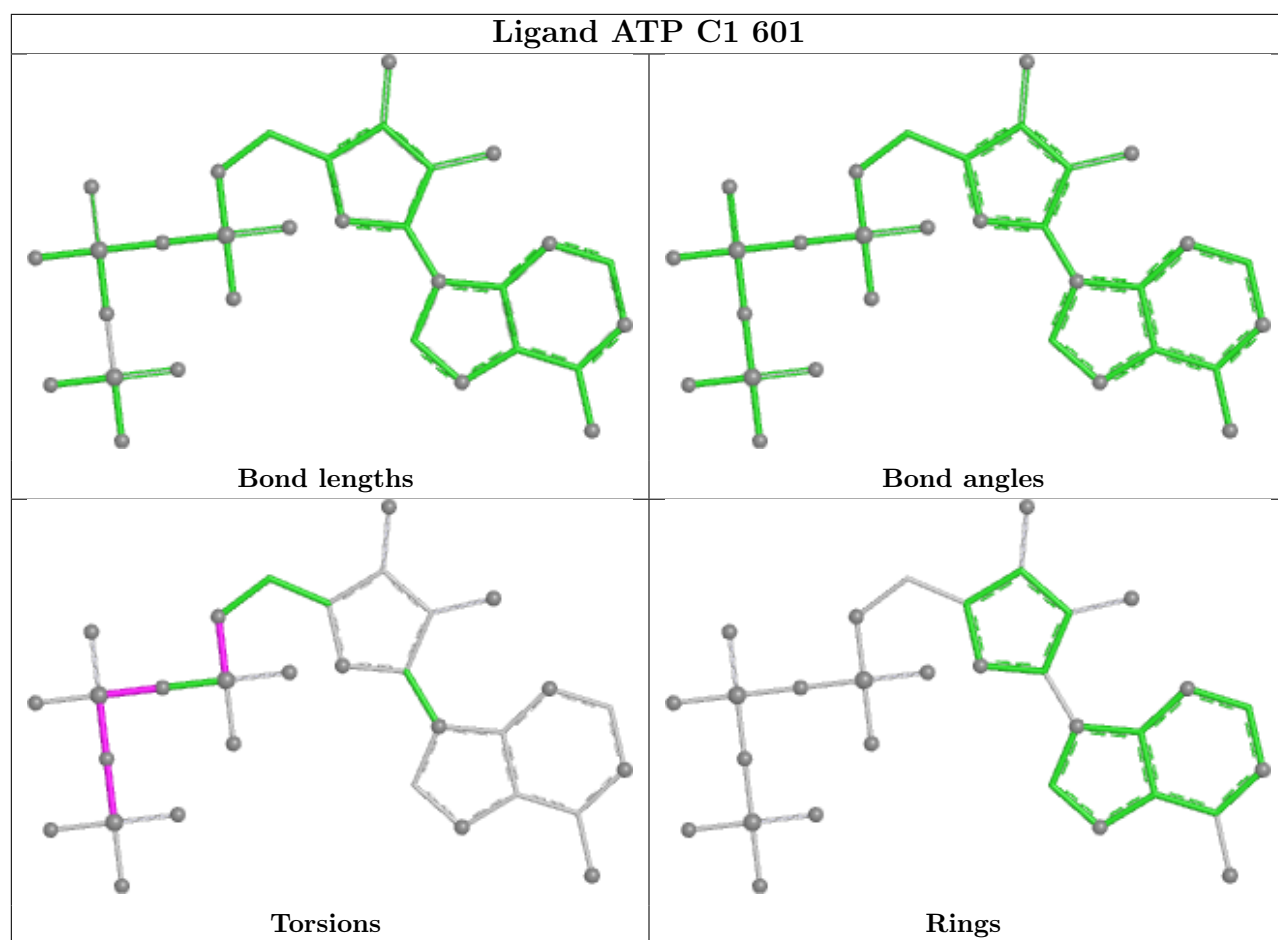


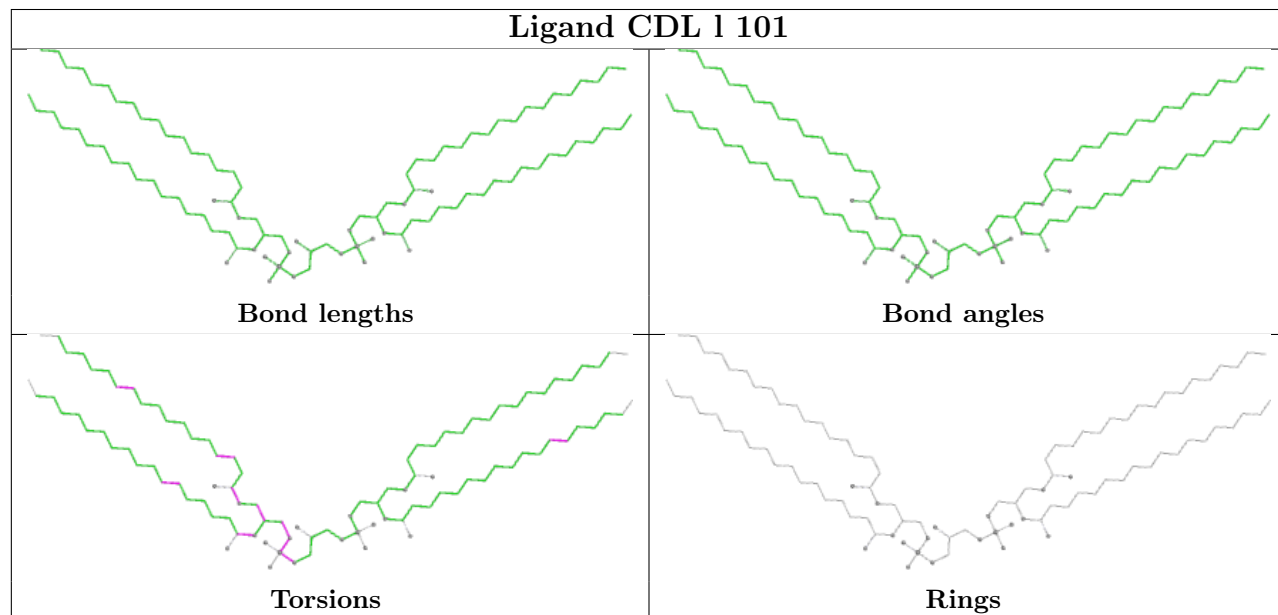
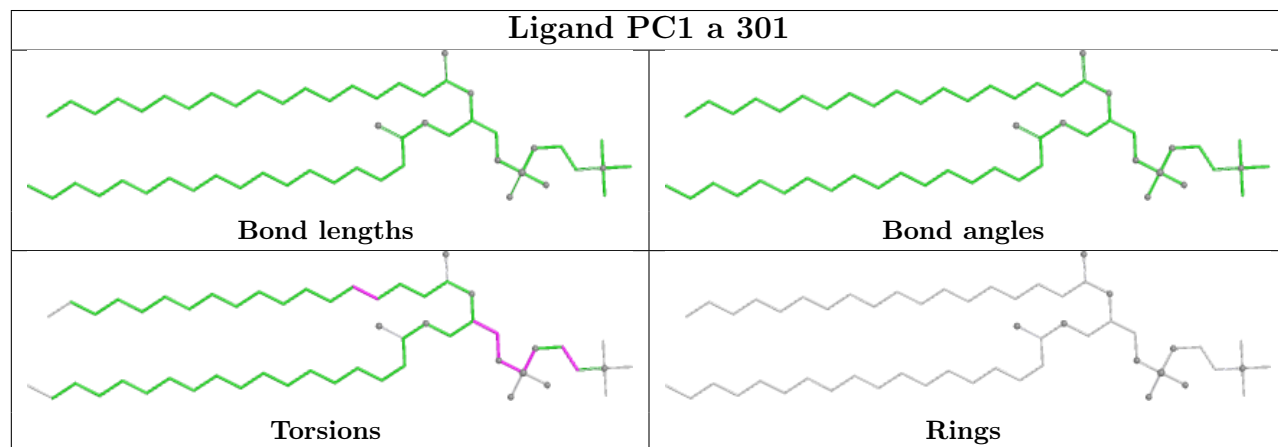
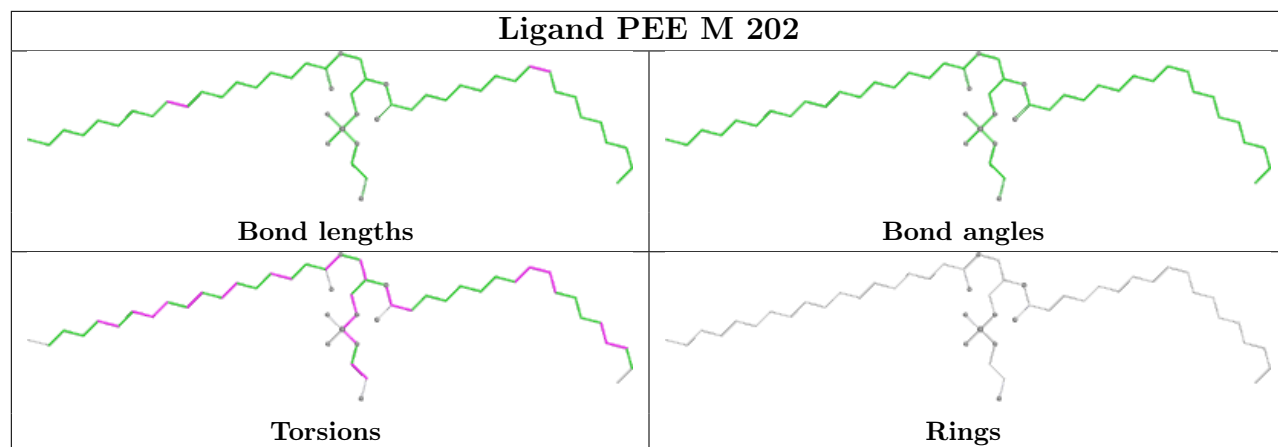
Ligand PEE m 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

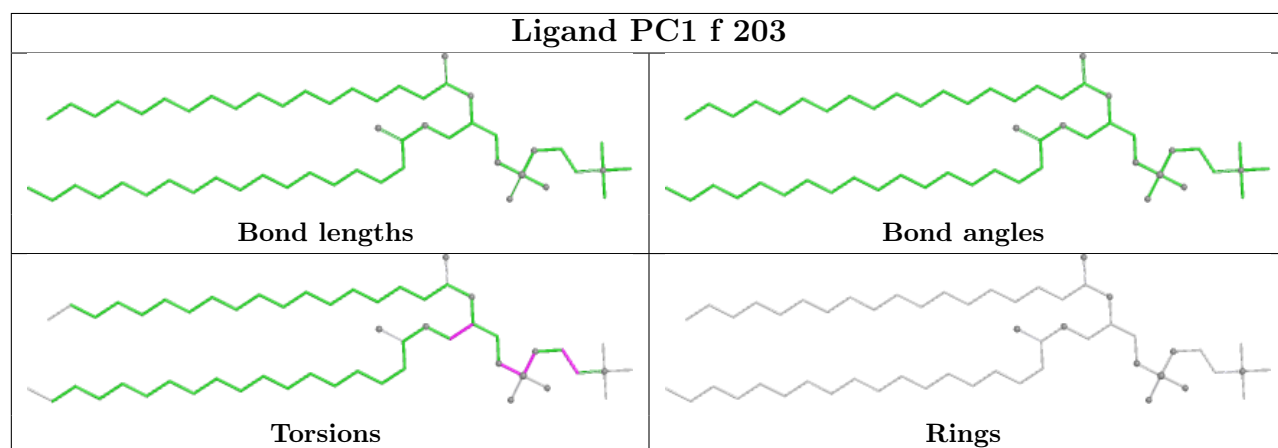
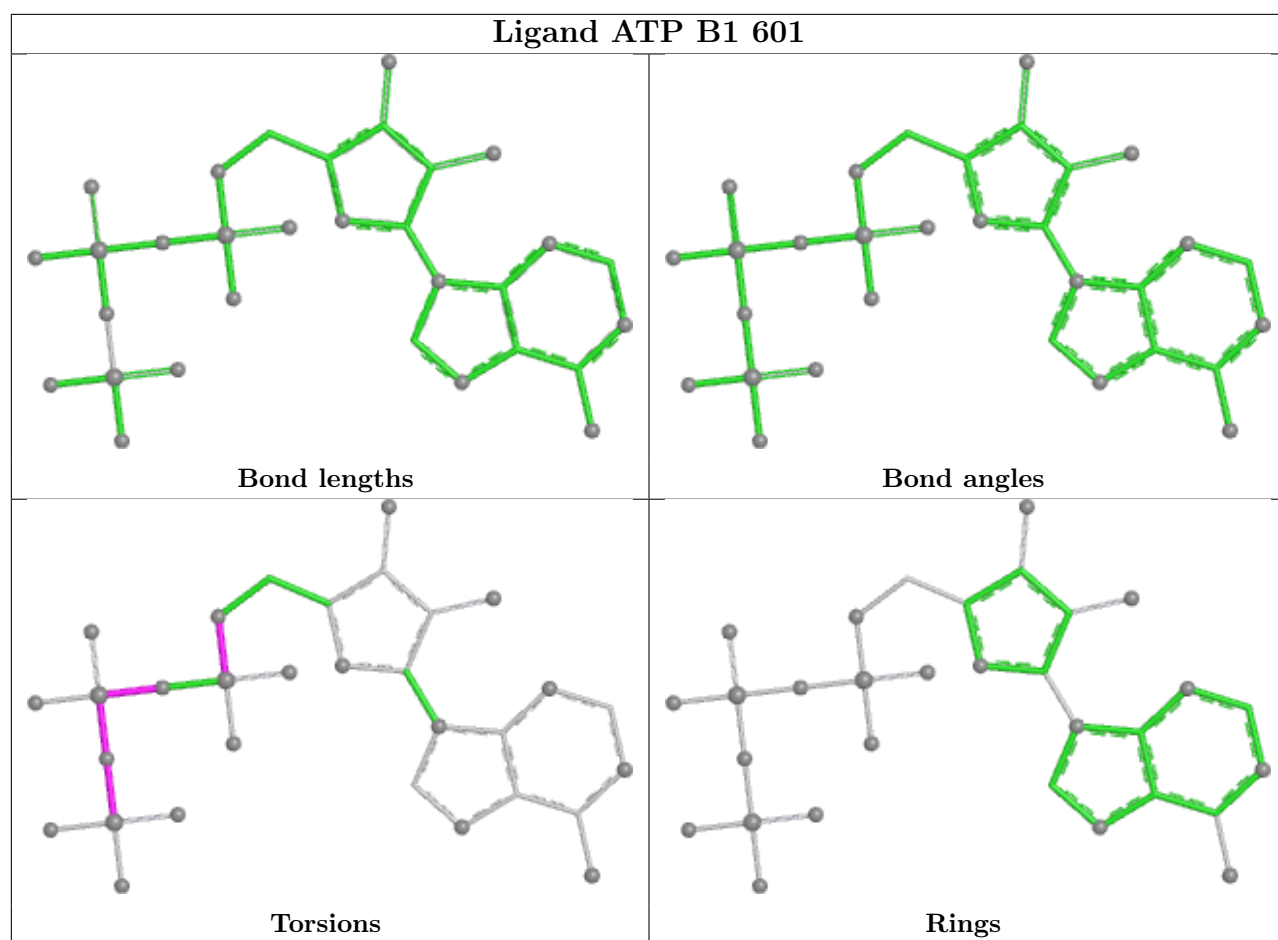
Ligand PEE f 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

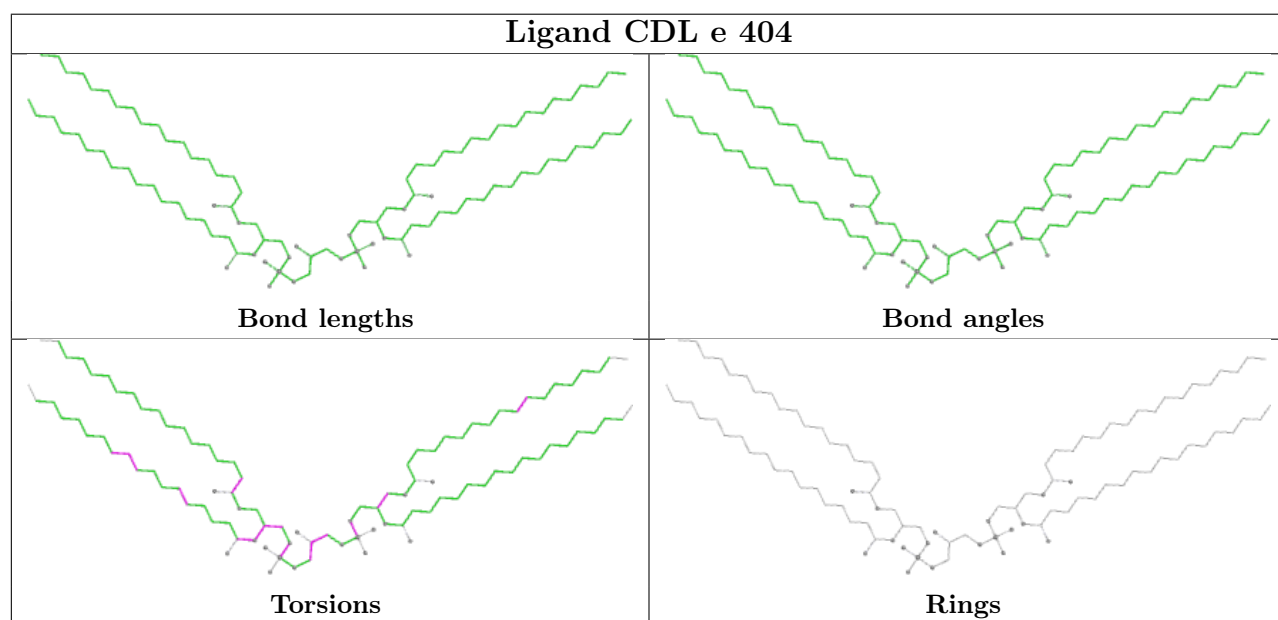
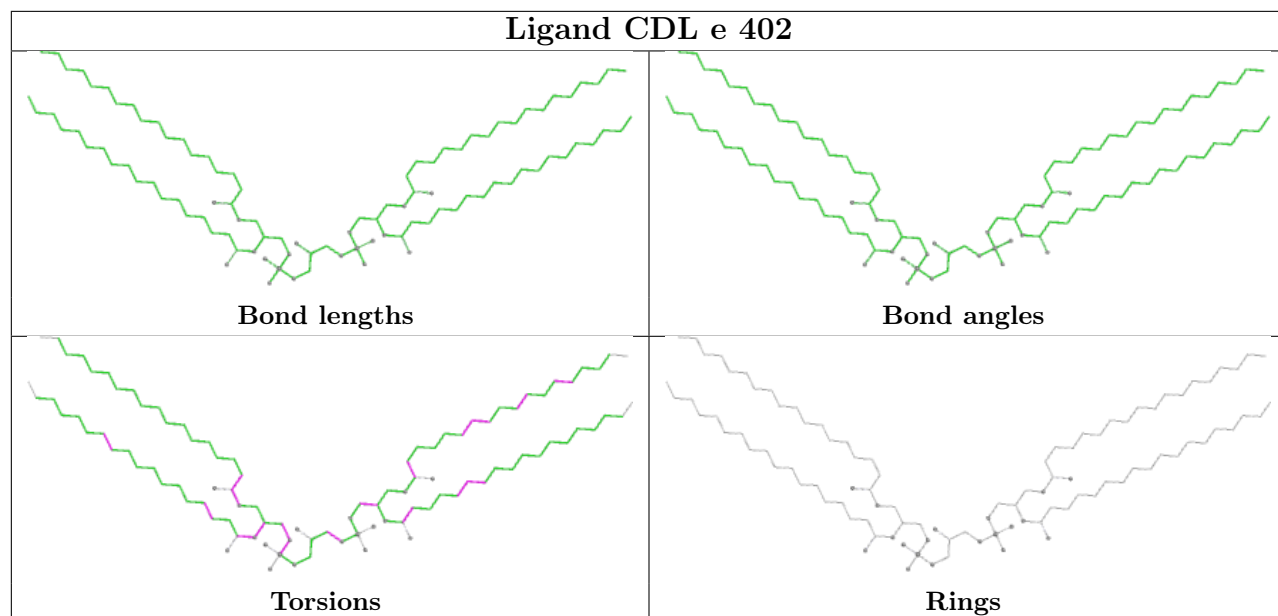
Ligand PC1 f 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

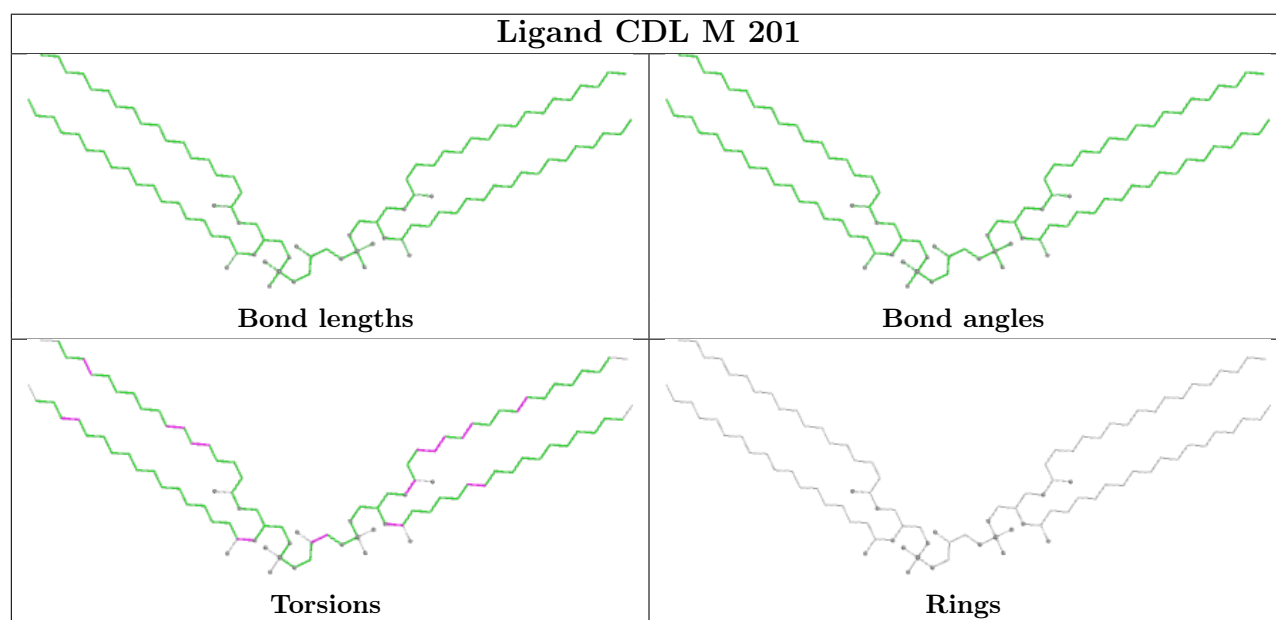
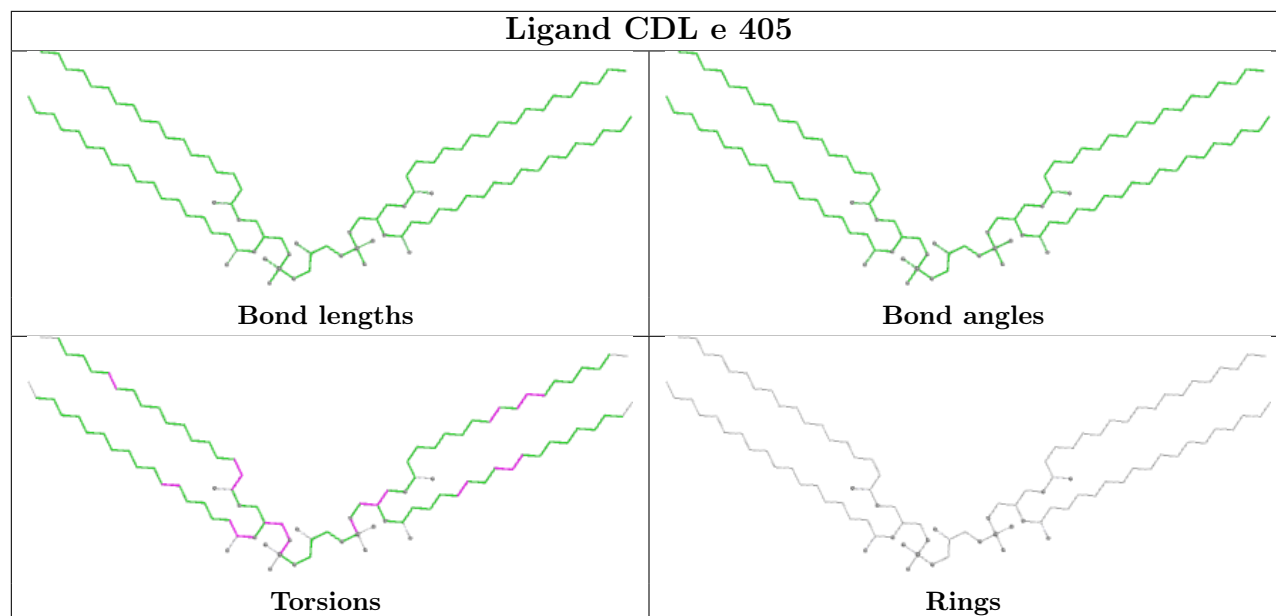


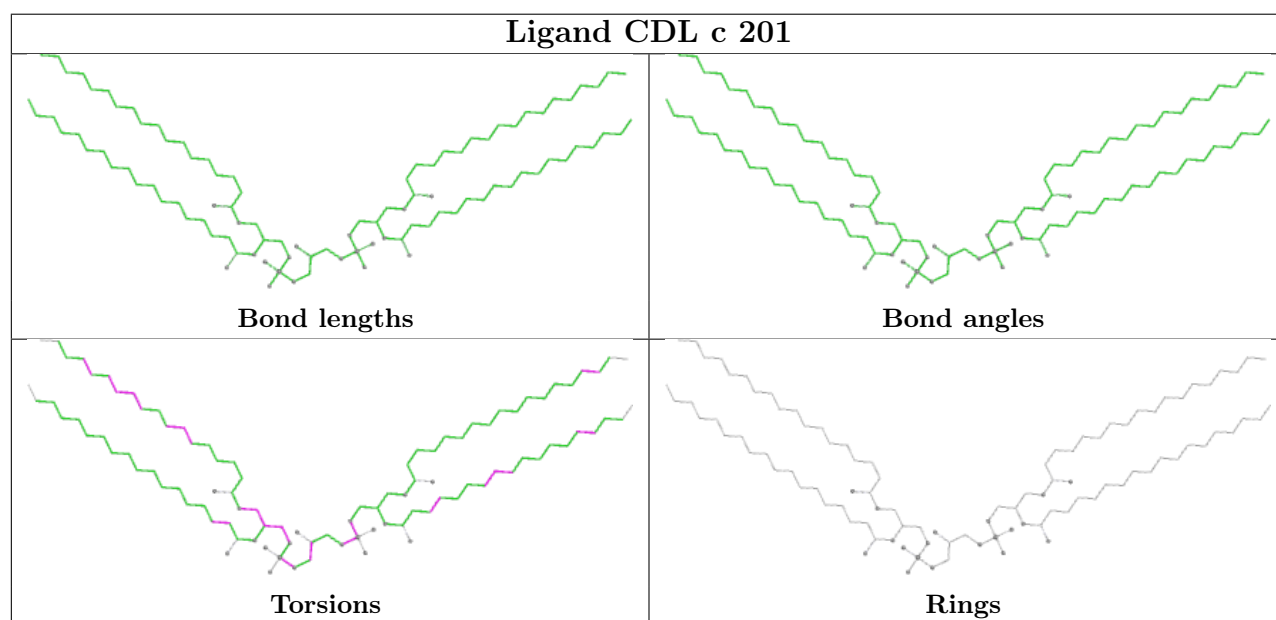
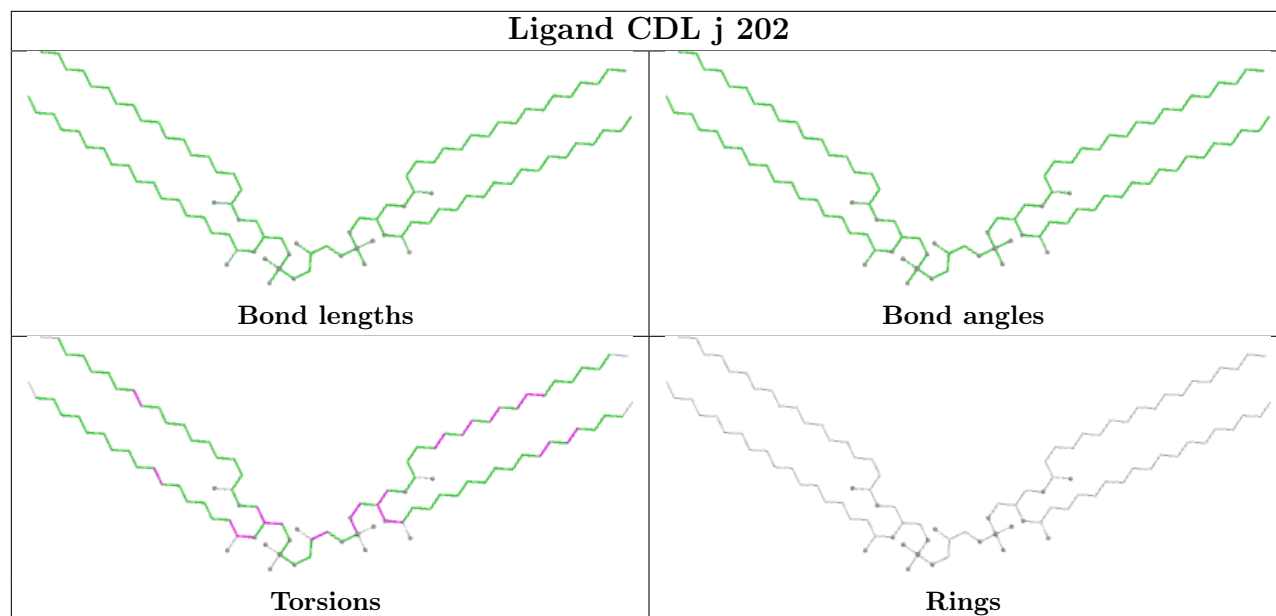


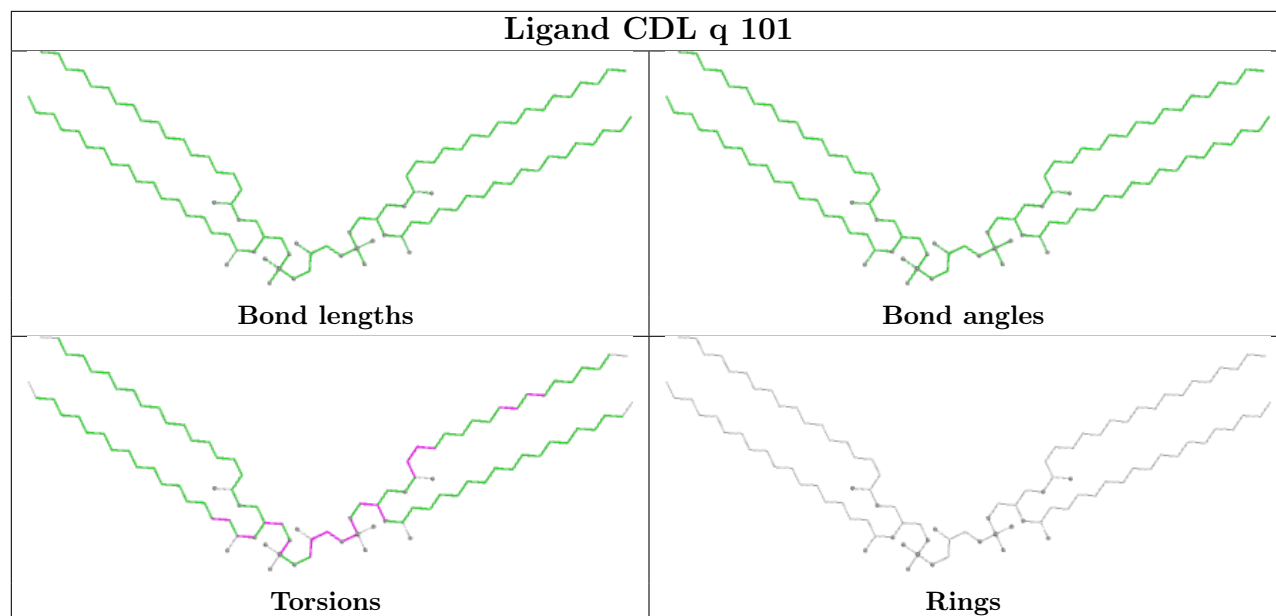












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

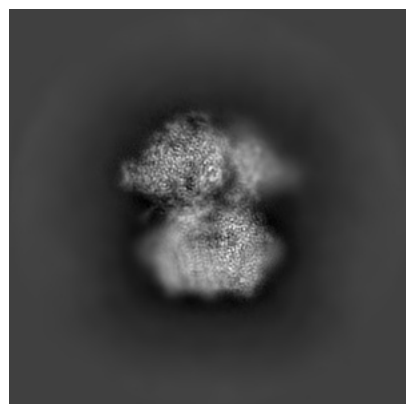
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15566. These allow visual inspection of the internal detail of the map and identification of artifacts.

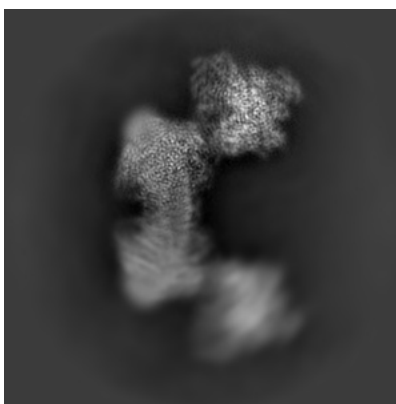
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

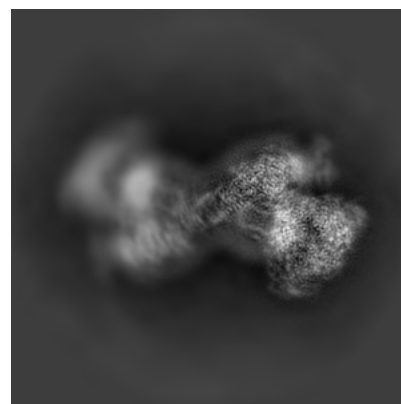
6.1.1 Primary map



X

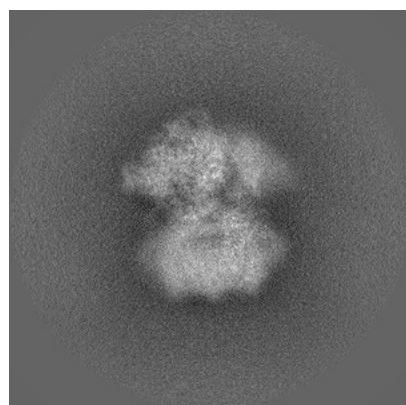


Y

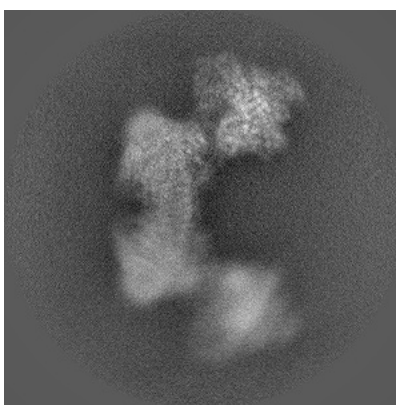


Z

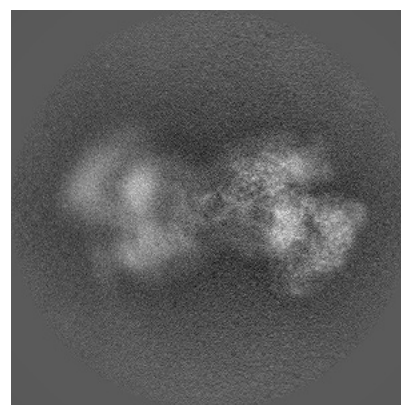
6.1.2 Raw map



X



Y

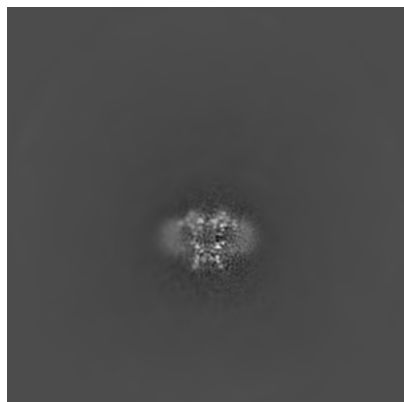


Z

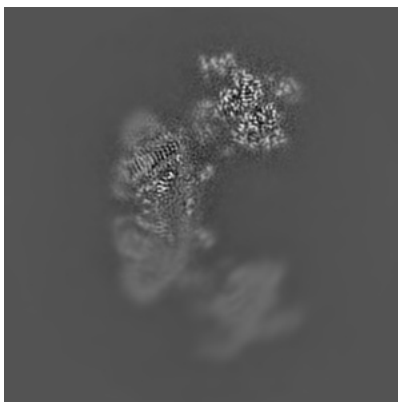
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

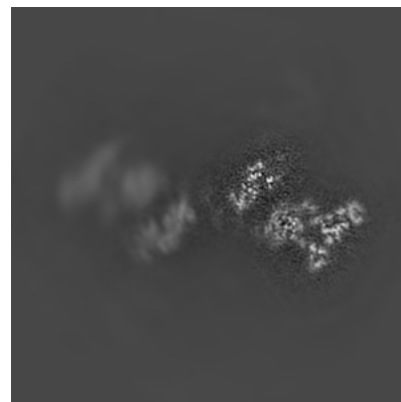
6.2.1 Primary map



X Index: 280

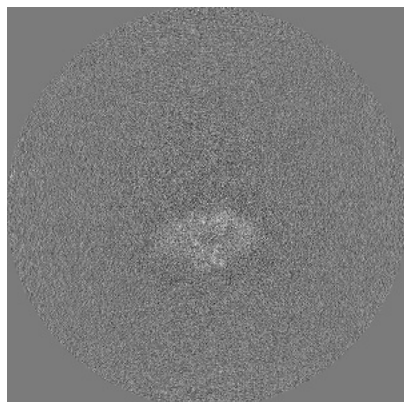


Y Index: 280

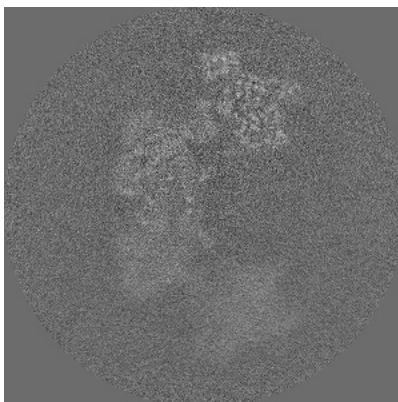


Z Index: 280

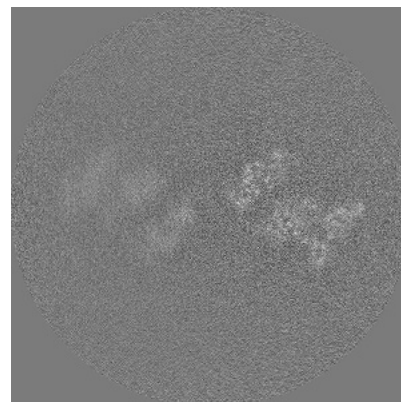
6.2.2 Raw map



X Index: 280



Y Index: 280

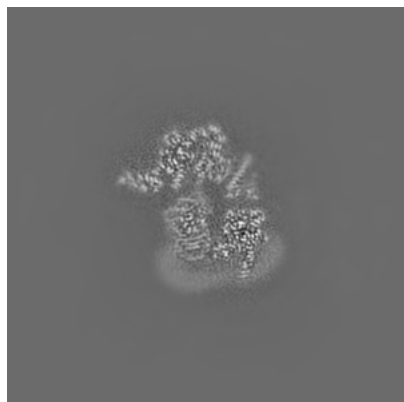


Z Index: 280

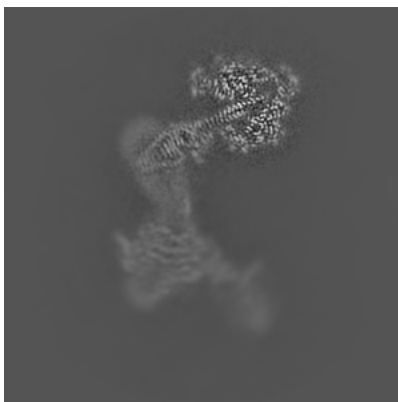
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 377

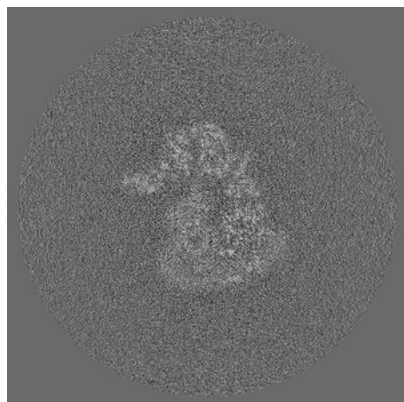


Y Index: 242

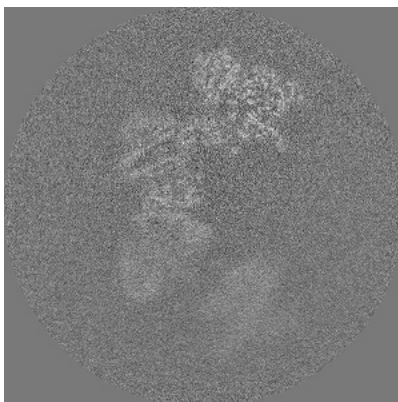


Z Index: 338

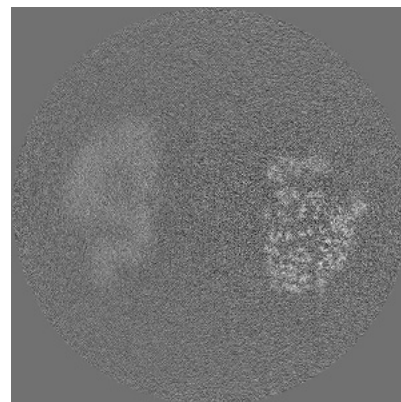
6.3.2 Raw map



X Index: 372



Y Index: 266

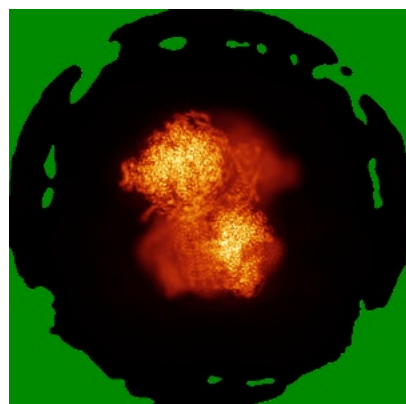


Z Index: 321

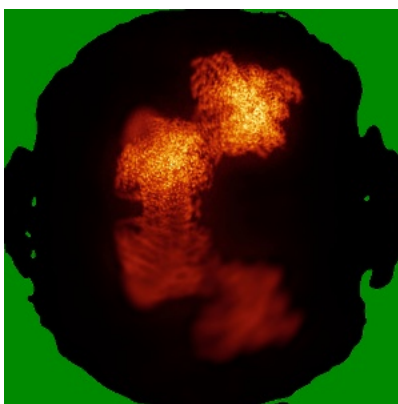
The images above show the largest variance slices of the map in three orthogonal directions.

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

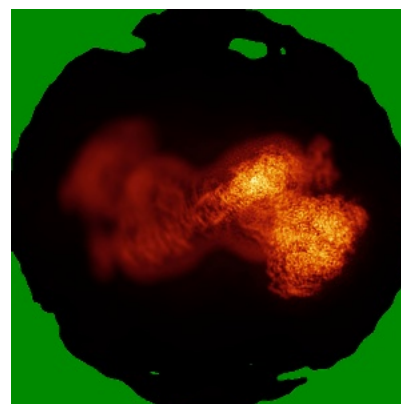
6.4.1 Primary map



X

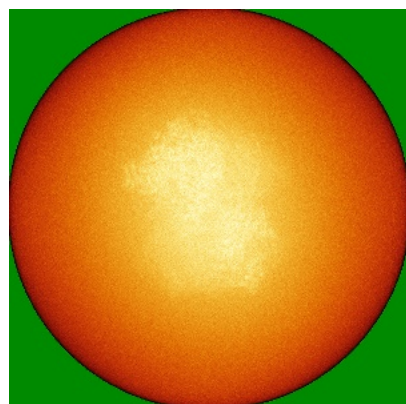


Y

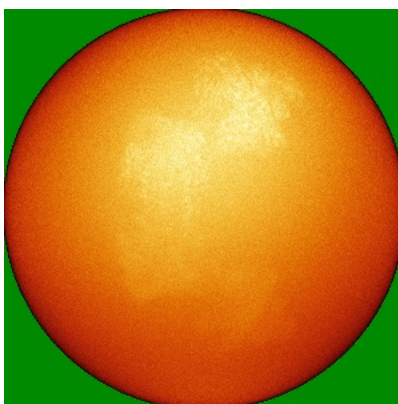


Z

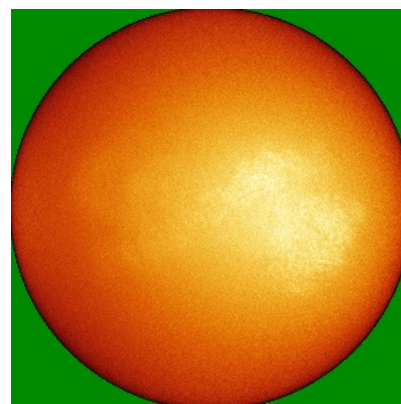
6.4.2 Raw map



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](#)

This section was not generated.

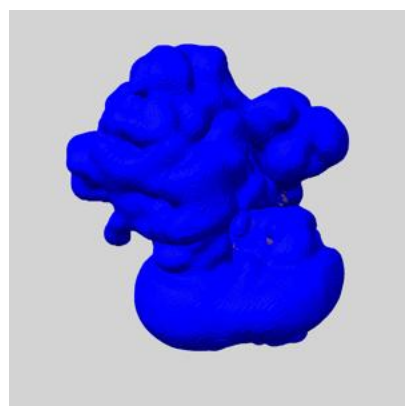
6.6 Mask visualisation [i](#)

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

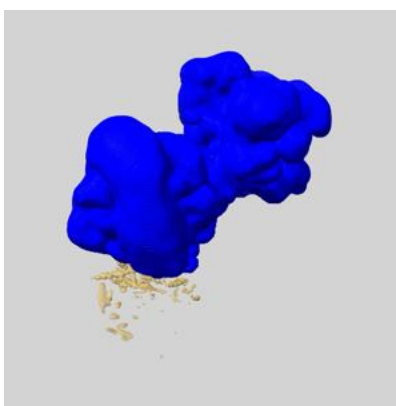
A mask typically either:

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

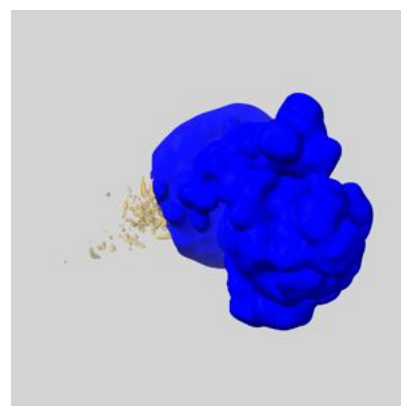
6.6.1 emd_15566_msk_1.map [i](#)



X



Y

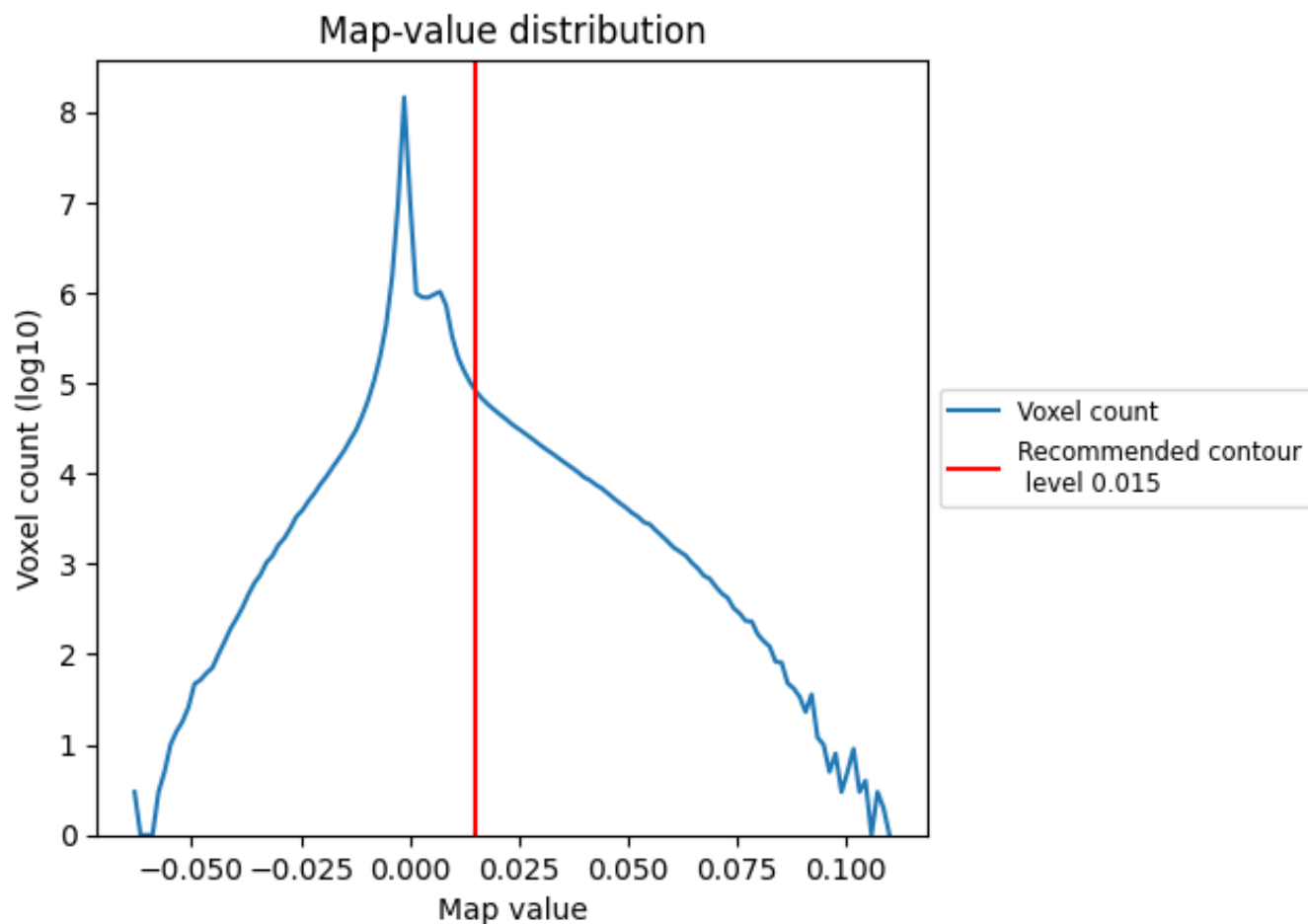


Z

7 Map analysis [i](#)

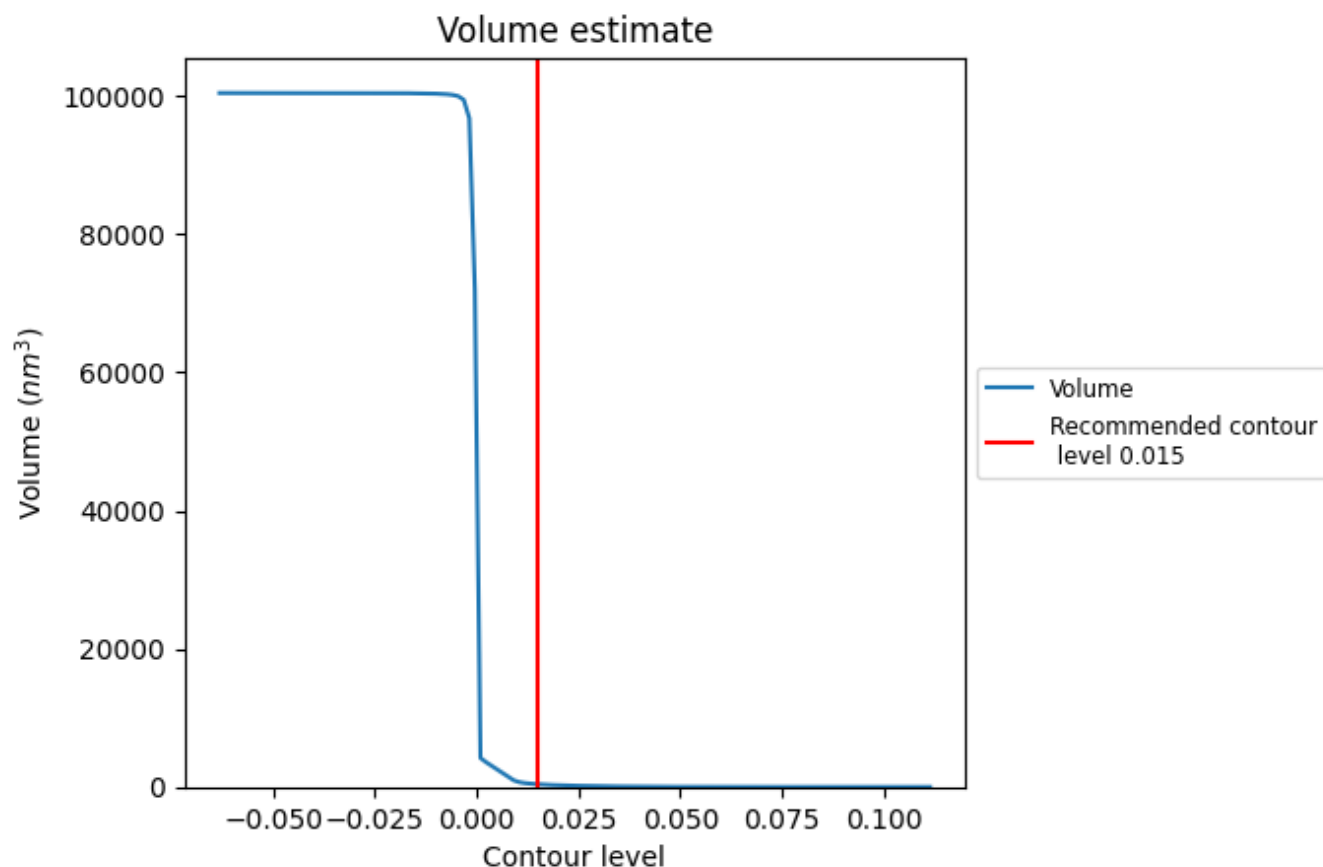
This section contains the results of statistical analysis of the map.

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.

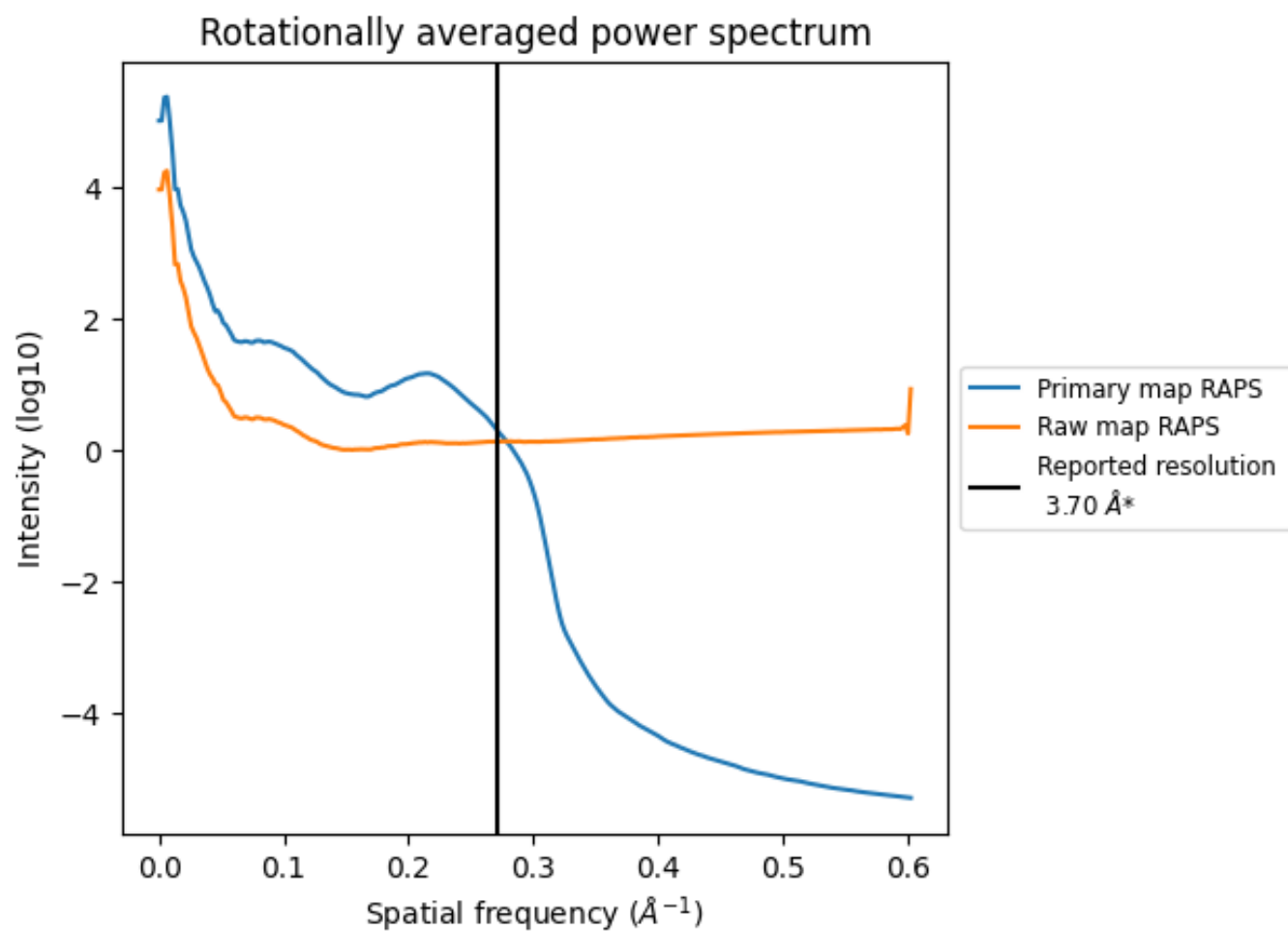
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 393 nm³; this corresponds to an approximate mass of 355 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

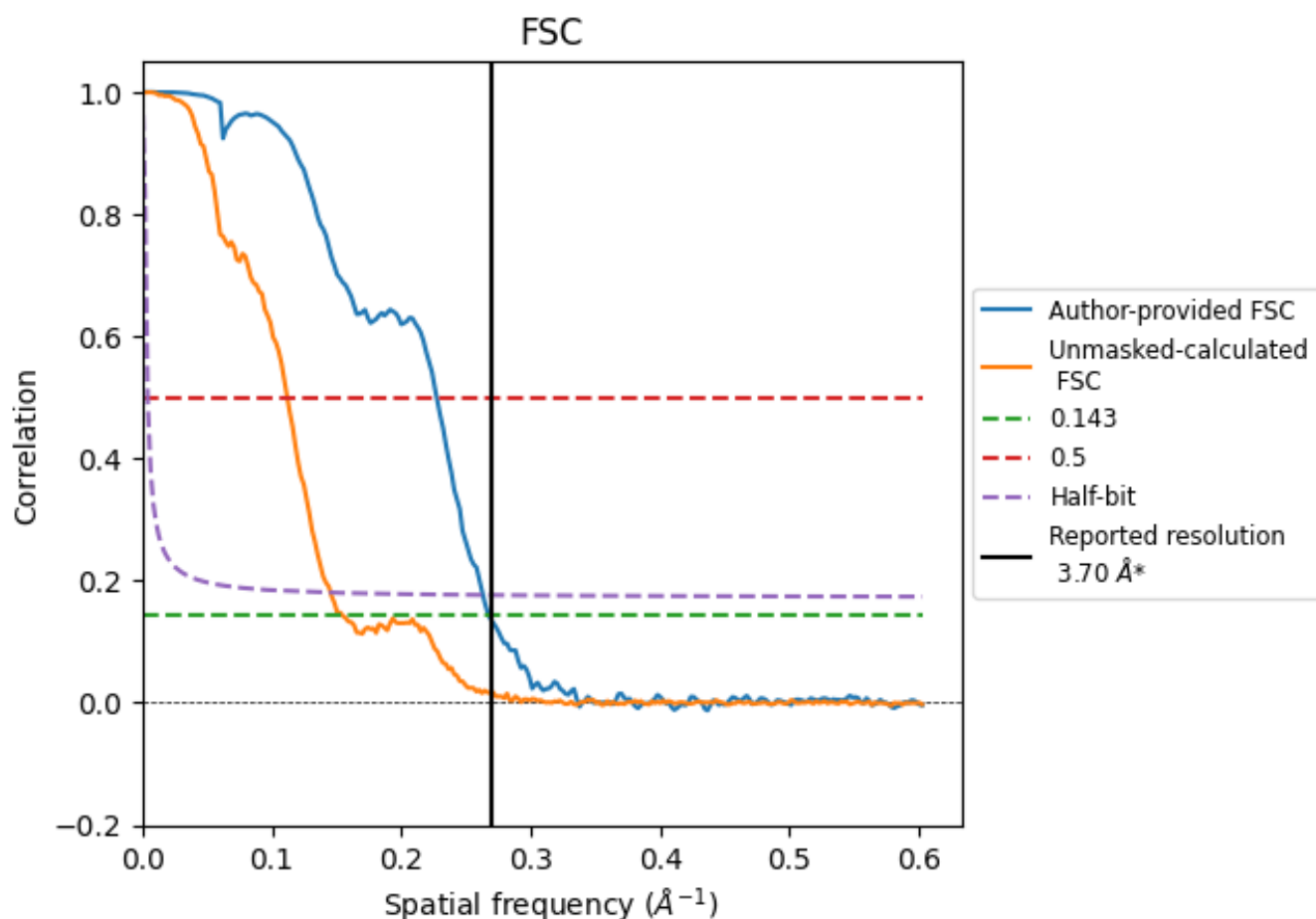


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

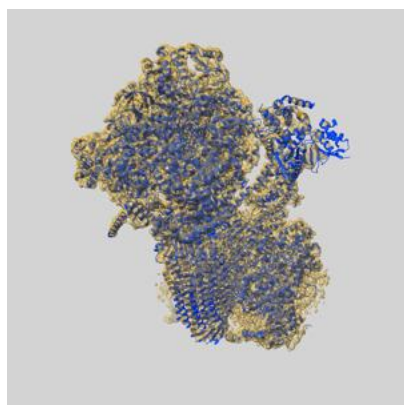
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.40	3.80
Unmasked-calculated*	6.47	8.92	6.87

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

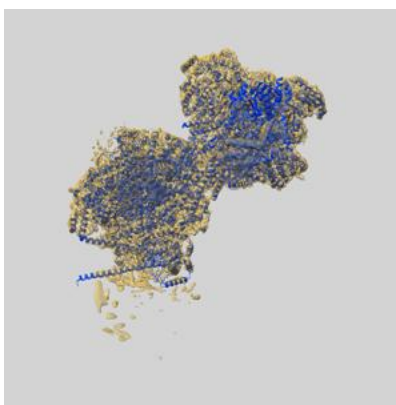
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15566 and PDB model 8APD. Per-residue inclusion information can be found in section 3 on page 16.

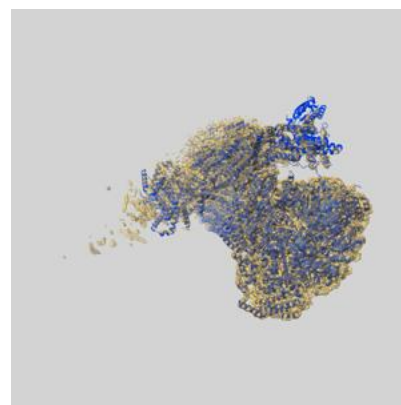
9.1 Map-model overlay [i](#)



X



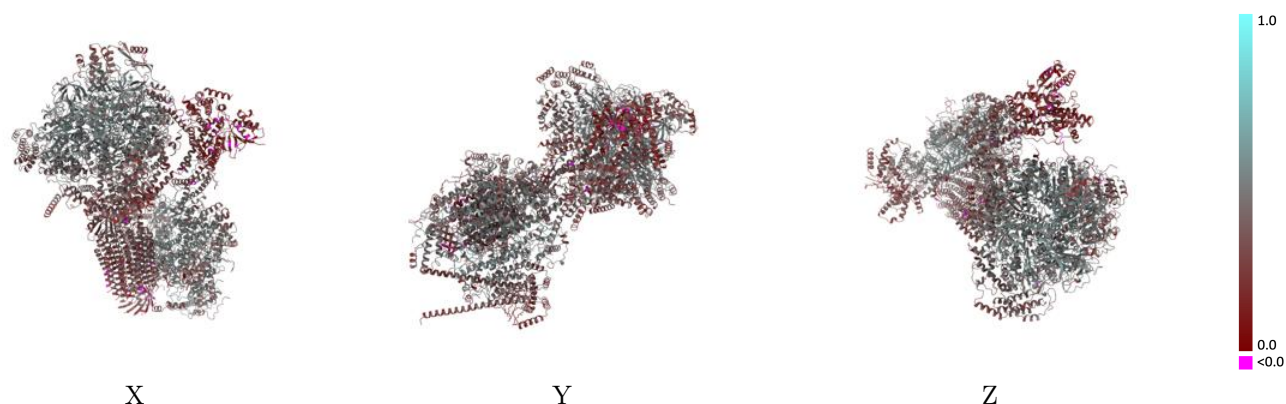
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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](#)

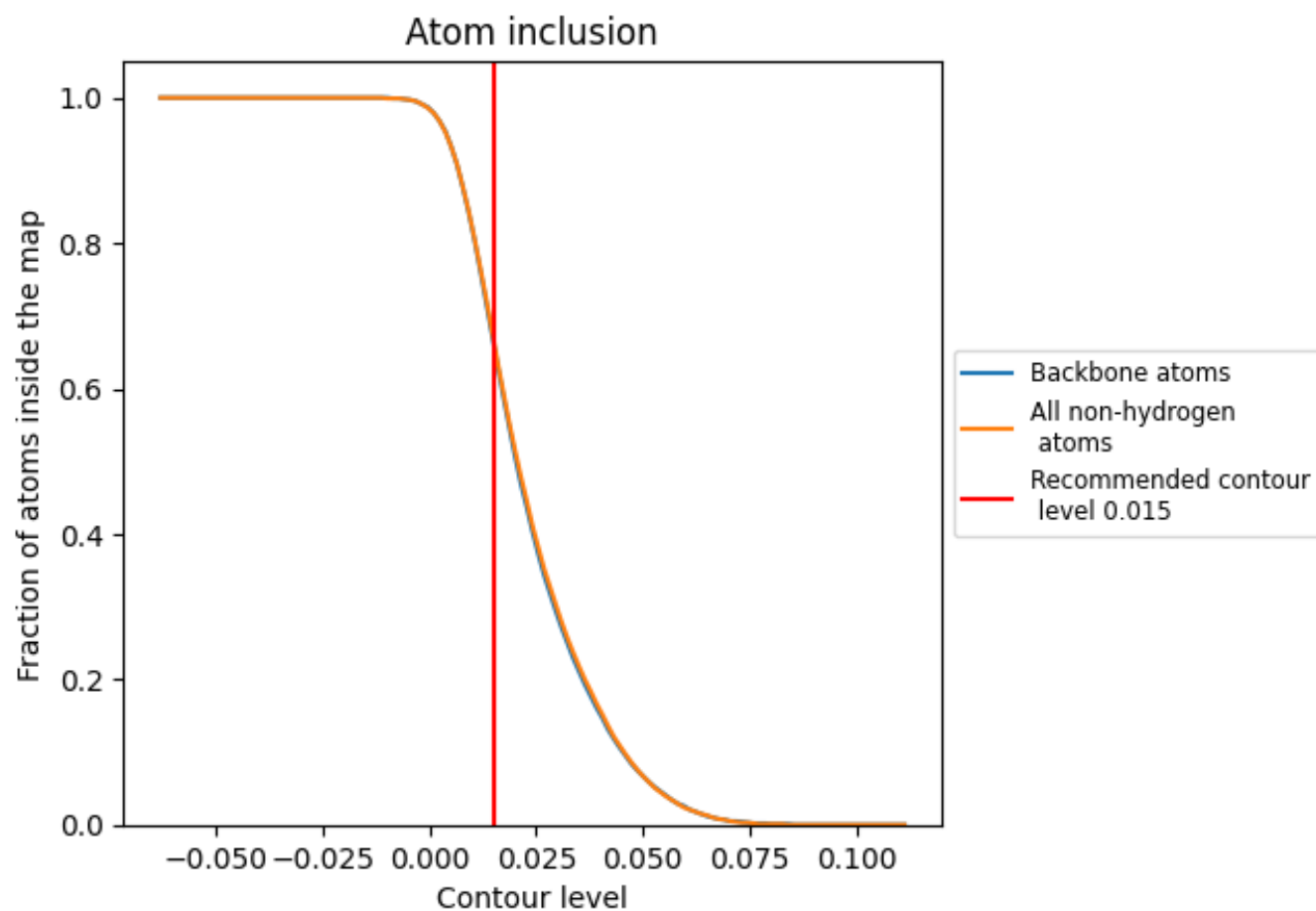


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 67% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.3960
A1	 0.8100	 0.4690
B1	 0.7910	 0.4440
C1	 0.7850	 0.4610
D1	 0.7930	 0.4720
E1	 0.7890	 0.4490
F1	 0.7690	 0.4500
G1	 0.6410	 0.3670
H1	 0.5360	 0.3130
I1	 0.4440	 0.2870
J1	 0.7090	 0.3360
K1	 0.7010	 0.3590
L	 0.3770	 0.2700
L1	 0.7370	 0.3690
M	 0.3620	 0.2810
M1	 0.6430	 0.3370
O1	 0.3710	 0.2360
P1	 0.5120	 0.2920
Q1	 0.5360	 0.2730
R1	 0.4740	 0.2730
S1	 0.4390	 0.2700
T1	 0.3980	 0.2670
U1	 0.4370	 0.2720
V1	 0.4030	 0.2420
W1	 0.3800	 0.2670
X1	 0.3190	 0.2550
a	 0.7830	 0.4990
c	 0.6990	 0.4510
d	 0.5980	 0.3350
e	 0.7700	 0.4530
f	 0.7450	 0.4650
g	 0.1550	 0.1760
h	 0.3020	 0.1660
i	 0.8280	 0.4860
j	 0.7480	 0.4270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.7250	 0.4260
l	 0.3880	 0.2990
m	 0.4770	 0.2940
n	 0.8230	 0.4970
o	 0.7570	 0.4170
p	 0.7070	 0.4240
q	 0.8360	 0.4960
r	 0.8020	 0.4840