



Full wwPDB EM Validation Report ⓘ

Apr 7, 2026 – 06:27 PM UTC

PDB ID : 6TMK / pdb_00006tmk
EMDB ID : EMD-10524
Title : Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase dimer, composite model
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2019-12-04
Resolution : 2.90 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

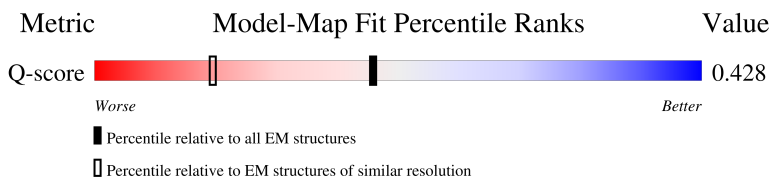
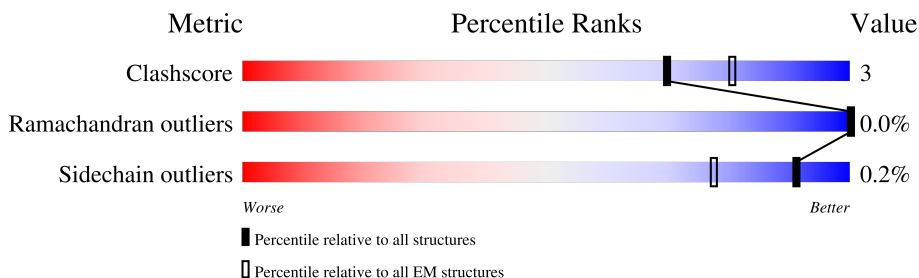
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	Q	134	 86% 13% .
1	q	134	 88% 11% .
2	I	236	 36% 62%
2	i	236	 36% 62%

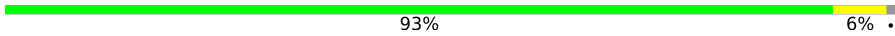
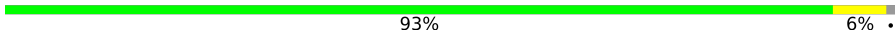
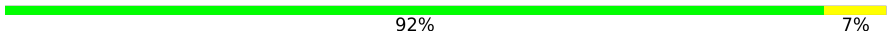
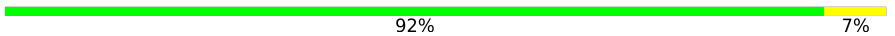
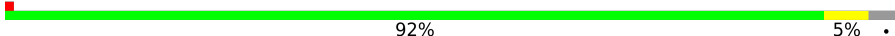
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Mol	Chain	Length	Quality of chain
3	T	133	
3	t	133	
4	G	252	
4	g	252	
5	O	157	
5	o	157	
6	K	224	
6	k	224	
7	J	229	
7	j	229	
8	S	128	
8	s	128	
9	U	126	
9	u	126	
10	H	239	
10	h	239	
11	E	325	
11	e	325	
12	X	83	
12	x	83	
13	B	571	
13	b	571	
14	R	134	
14	r	134	
15	P	138	

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Mol	Chain	Length	Quality of chain
15	p	138	
16	V	111	
16	v	111	
17	L	208	
17	l	208	
18	C	398	
18	c	398	
19	D	310	
19	d	310	
20	M	205	
20	m	205	
21	N	166	
21	n	166	
22	F	267	
22	f	267	
23	W	106	
23	w	106	
24	A	536	
24	a	536	
25	i1	145	
25	i2	145	
26	A1	565	
26	A2	565	
26	C1	565	
26	C2	565	

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Mol	Chain	Length	Quality of chain
26	E1	565	
26	E2	565	
27	B1	560	
27	B2	560	
27	D1	560	
27	D2	560	
27	F1	560	
27	F2	560	
28	g1	314	
28	g2	314	
29	d1	183	
29	d2	183	
30	e1	73	
30	e2	73	
31	G1	252	
31	G2	252	
32	H1	166	
32	H2	166	
32	I1	166	
32	I2	166	
32	J1	166	
32	J2	166	
32	K1	166	
32	K2	166	
32	L1	166	

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Mol	Chain	Length	Quality of chain
32	L2	166	
32	M1	166	
32	M2	166	
32	N1	166	
32	N2	166	
32	O1	166	
32	O2	166	
32	P1	166	
32	P2	166	
32	Q1	166	
32	Q2	166	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 266834 atoms, of which 134048 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 ATPTG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	Q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		

- Molecule 2 is a protein called ATPTG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	i	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		

- Molecule 3 is a protein called ATPTG14.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	t	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	T	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		

- Molecule 4 is a protein called ATPTG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	g	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	G	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	51	VAL	PHE	conflict	UNP S7WD71

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Chain	Residue	Modelled	Actual	Comment	Reference
g	73	CYS	SER	conflict	UNP S7WD71
g	110	LYS	GLU	conflict	UNP S7WD71
g	233	THR	MET	conflict	UNP S7WD71
G	51	VAL	PHE	conflict	UNP S7WD71
G	73	CYS	SER	conflict	UNP S7WD71
G	110	LYS	GLU	conflict	UNP S7WD71
G	233	THR	MET	conflict	UNP S7WD71

- Molecule 5 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	o	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		
5	O	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		

- Molecule 6 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	K	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		

- Molecule 7 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	j	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		

- Molecule 8 is a protein called ATPTG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	s	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		

- Molecule 9 is a protein called ATPTG15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	u	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		

- Molecule 10 is a protein called ATPTG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	h	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	89	ASN	HIS	conflict	UNP A0A125YLR0
H	89	ASN	HIS	conflict	UNP A0A125YLR0

- Molecule 11 is a protein called ATPTG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	e	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	LYS	deletion	UNP A0A125YLR0
e	63	PRO	SER	conflict	UNP A0A125YLR0
e	99	LEU	PRO	conflict	UNP A0A125YLR0
e	312	ALA	THR	conflict	UNP A0A125YLR0
E	?	-	LYS	deletion	UNP A0A125YLR0
E	63	PRO	SER	conflict	UNP A0A125YLR0
E	99	LEU	PRO	conflict	UNP A0A125YLR0
E	312	ALA	THR	conflict	UNP A0A125YLR0

- Molecule 12 is a protein called ATPTG17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	x	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	X	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	77	TRP	-	expression tag	UNP S7W180
x	78	MET	-	expression tag	UNP S7W180
x	79	PHE	-	expression tag	UNP S7W180
x	80	GLY	-	expression tag	UNP S7W180
x	81	ASN	-	expression tag	UNP S7W180
x	82	SER	-	expression tag	UNP S7W180
x	83	TYR	-	expression tag	UNP S7W180
X	77	TRP	-	expression tag	UNP S7W180
X	78	MET	-	expression tag	UNP S7W180
X	79	PHE	-	expression tag	UNP S7W180
X	80	GLY	-	expression tag	UNP S7W180
X	81	ASN	-	expression tag	UNP S7W180
X	82	SER	-	expression tag	UNP S7W180
X	83	TYR	-	expression tag	UNP S7W180

- Molecule 13 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b	484	Total	C	H	N	O	S	0	0
			7841	2525	3909	652	740	15		
13	B	484	Total	C	H	N	O	S	0	0
			7841	2525	3909	652	740	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	48	LEU	SER	conflict	UNP S7V2T0
b	472	THR	ALA	conflict	UNP S7V2T0
B	48	LEU	SER	conflict	UNP S7V2T0
B	472	THR	ALA	conflict	UNP S7V2T0

- Molecule 14 is a protein called ATPTG12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	r	133	Total	C	H	N	O	S	0	0
			2144	681	1073	182	202	6		
14	R	133	Total	C	H	N	O	S	0	0
			2144	681	1073	182	202	6		

- Molecule 15 is a protein called ATPTG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	P	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		

- Molecule 16 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	v	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	V	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	54	ALA	VAL	conflict	UNP S7UQT7
V	54	ALA	VAL	conflict	UNP S7UQT7

- Molecule 17 is a protein called ATPTG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	l	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	L	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		

- Molecule 18 is a protein called ATPTG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	C	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		

- Molecule 19 is a protein called ATPTG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	d	255	Total	C	H	N	O	S	0	0
			4056	1326	1975	366	381	8		
19	D	255	Total	C	H	N	O	S	0	0
			4056	1326	1975	366	381	8		

- Molecule 20 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	m	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	M	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		

- Molecule 21 is a protein called ATPTG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	n	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		
21	N	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	140	SER	ALA	conflict	UNP A0A125YUZ2
N	140	SER	ALA	conflict	UNP A0A125YUZ2

- Molecule 22 is a protein called ATPTG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	f	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	F	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		

- Molecule 23 is a protein called ATPTG16.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w	97	Total	C	H	N	O	S	0	0
			1520	497	760	128	131	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	97	Total	C	H	N	O	S	0	0
			1520	497	760	128	131	4		

- Molecule 24 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	467	Total	C	H	N	O	S	0	0
			7396	2405	3616	656	698	21		
24	A	467	Total	C	H	N	O	S	0	0
			7396	2405	3616	656	698	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	351	THR	ALA	conflict	UNP S7V493
A	351	THR	ALA	conflict	UNP S7V493

- Molecule 25 is a protein called Inhibitor of F1.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	i2	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		
25	i1	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		

- Molecule 26 is a protein called ATP synthase subunit alpha,subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	A2	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
26	E2	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
26	C2	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
26	A1	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
26	E1	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
26	C1	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		

- Molecule 27 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	B2	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
27	F2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	D2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	B1	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
27	F1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	D1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		

- Molecule 28 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	g2	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
28	g1	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		

- Molecule 29 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	d2	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		
29	d1	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		

- Molecule 30 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e2	65	Total	C	H	N	O	S	0	0
			1077	337	539	99	98	4		
30	e1	65	Total	C	H	N	O	S	0	0
			1077	337	539	99	98	4		

- Molecule 31 is a protein called Oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	G2	180	Total	C	H	N	O	S	0	0
			2901	895	1486	255	261	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
31	G1	180	Total	C	H	N	O	S	0	0
			2901	895	1486	255	261	4		

- Molecule 32 is a protein called subunit c.

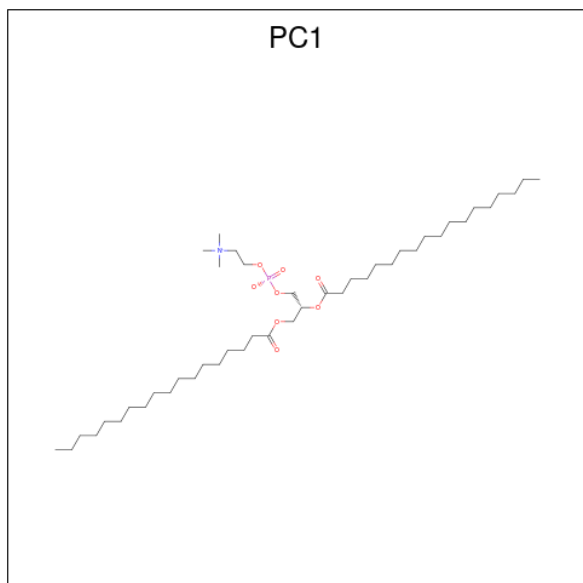
Mol	Chain	Residues	Atoms						AltConf	Trace
32	H2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	I2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	J2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	K2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	L2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	M2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	N2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	O2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	P2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	H1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	I1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	J1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	K1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	L1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	M1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	N1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	O1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

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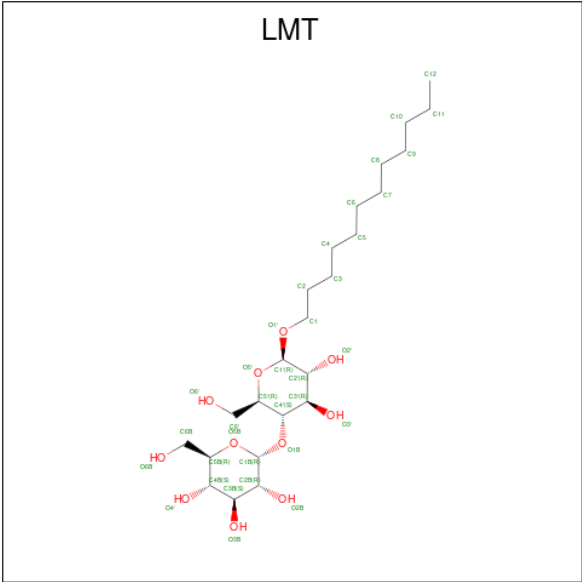
Mol	Chain	Residues	Atoms						AltConf	Trace
32	P1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



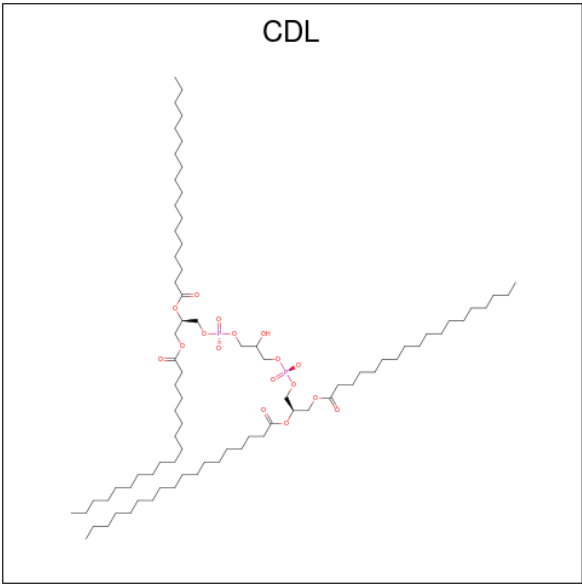
Mol	Chain	Residues	Atoms						AltConf
33	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	v	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	O	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	O	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	V	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
34	o	1	Total	C	H	O	0
			81	24	46	11	
34	h	1	Total	C	H	O	0
			81	24	46	11	
34	x	1	Total	C	H	O	0
			81	24	46	11	
34	c	1	Total	C	H	O	0
			81	24	46	11	
34	c	1	Total	C	H	O	0
			81	24	46	11	
34	d	1	Total	C	H	O	0
			81	24	46	11	
34	d	1	Total	C	H	O	0
			81	24	46	11	
34	O	1	Total	C	H	O	0
			81	24	46	11	
34	H	1	Total	C	H	O	0
			81	24	46	11	
34	X	1	Total	C	H	O	0
			81	24	46	11	
34	C	1	Total	C	H	O	0
			81	24	46	11	
34	C	1	Total	C	H	O	0
			81	24	46	11	
34	D	1	Total	C	H	O	0
			81	24	46	11	
34	D	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 35 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



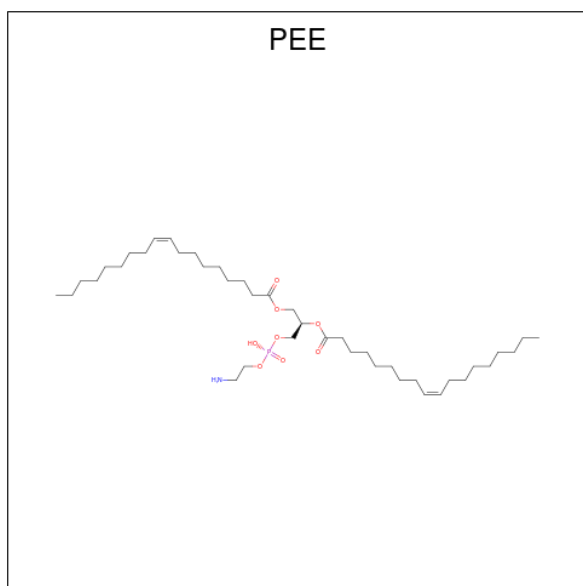
Mol	Chain	Residues	Atoms					AltConf
35	o	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	u	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	h	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	v	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	d	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	O	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	U	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	H	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	V	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	D	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 36 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



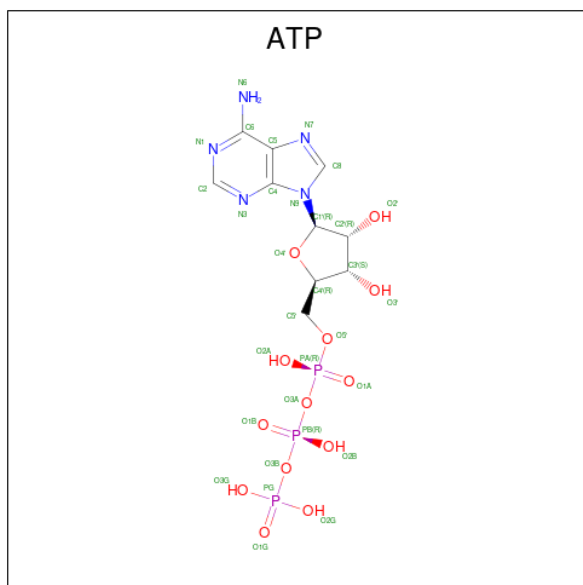
Mol	Chain	Residues	Atoms					AltConf	
36	j	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	j	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	c	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	J	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	J	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

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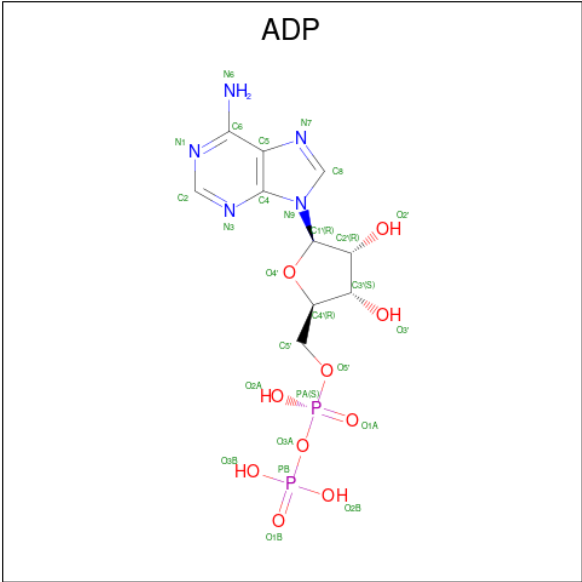
Mol	Chain	Residues	Atoms					AltConf	
36	C	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
37	A2	1	Total 42	C 10	H 11	N 5	O 13	P 3	0
37	E2	1	Total 42	C 10	H 11	N 5	O 13	P 3	0
37	C2	1	Total 42	C 10	H 11	N 5	O 13	P 3	0
37	A1	1	Total 42	C 10	H 11	N 5	O 13	P 3	0
37	E1	1	Total 42	C 10	H 11	N 5	O 13	P 3	0
37	C1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

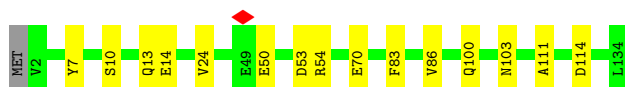
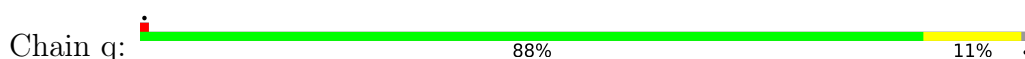


Mol	Chain	Residues	Atoms						AltConf
38	B2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
38	D2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	B1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	D1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

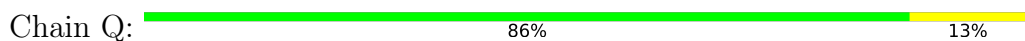
3 Residue-property plots [i](#)

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.

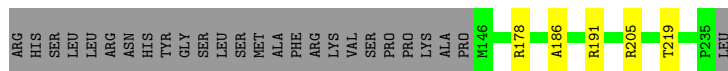
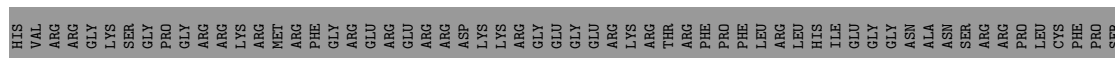
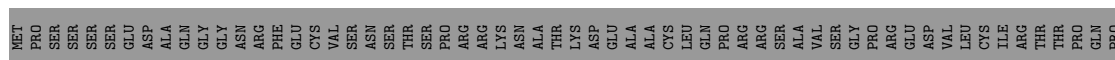
- Molecule 1: ATPTG11



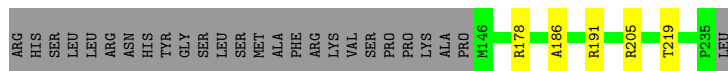
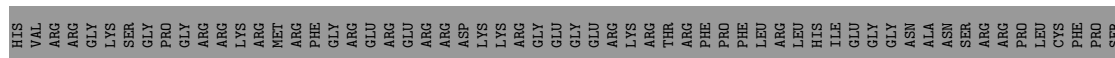
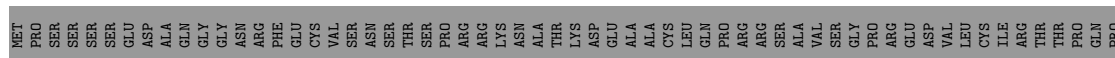
- Molecule 1: ATPTG11



- Molecule 2: ATPTG7



- Molecule 2: ATPTG7

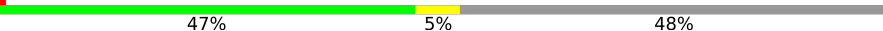


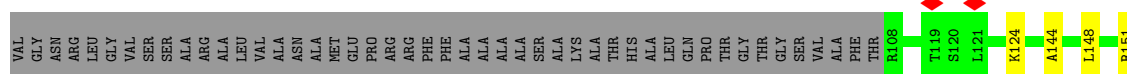
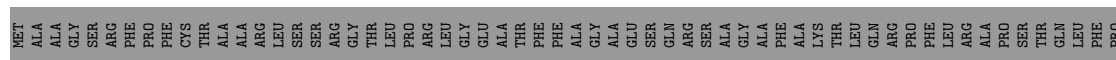
- Molecule 5: subunit k

Chain O: 

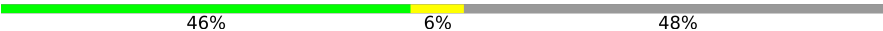


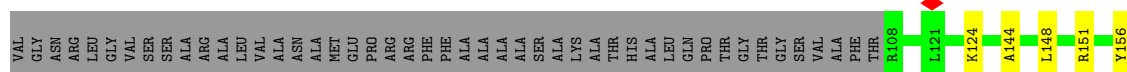
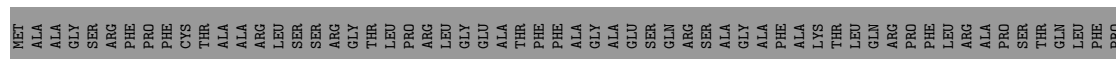
- Molecule 6: subunit a

Chain k: 



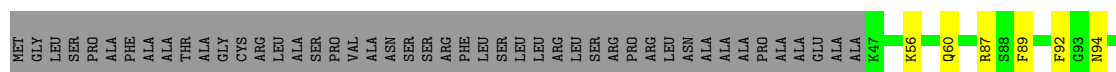
- Molecule 6: subunit a

Chain K: 



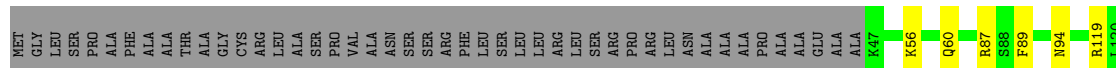
- Molecule 7: subunit i/j

Chain j: 



- Molecule 7: subunit i/j

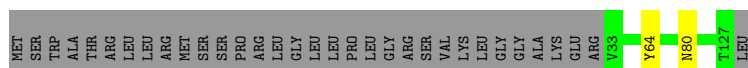
Chain J: 





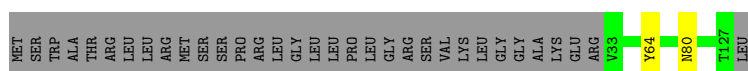
• Molecule 8: ATPTG13

Chain s: 73% 26%



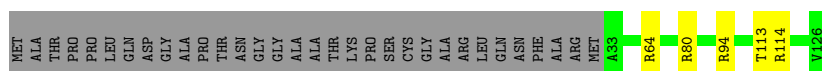
• Molecule 8: ATPTG13

Chain S: 73% 26%



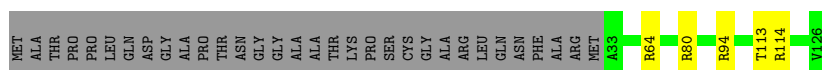
• Molecule 9: ATPTG15

Chain u: 71% 25%



• Molecule 9: ATPTG15

Chain U: 71% 25%



• Molecule 10: ATPTG6

Chain h: 91% 5%



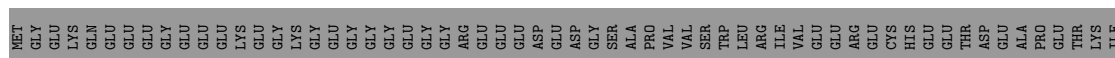
• Molecule 10: ATPTG6

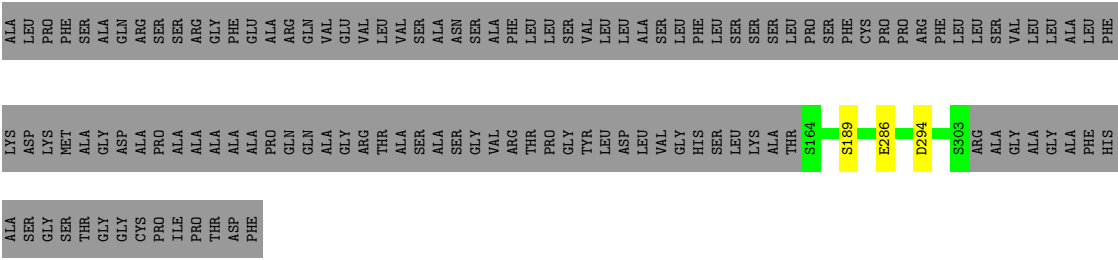
Chain H: 90% 5%



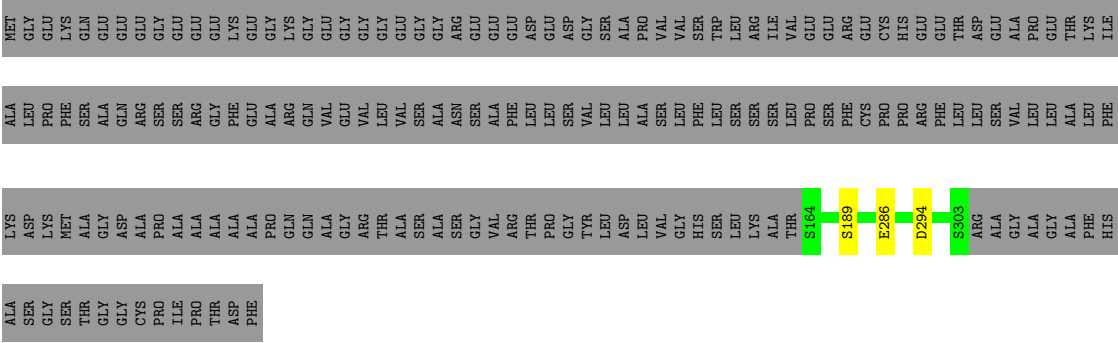
• Molecule 11: ATPTG3

Chain e: 42% 57%





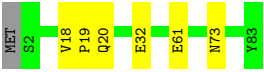
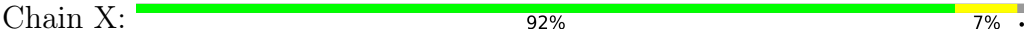
• Molecule 11: ATPTG3



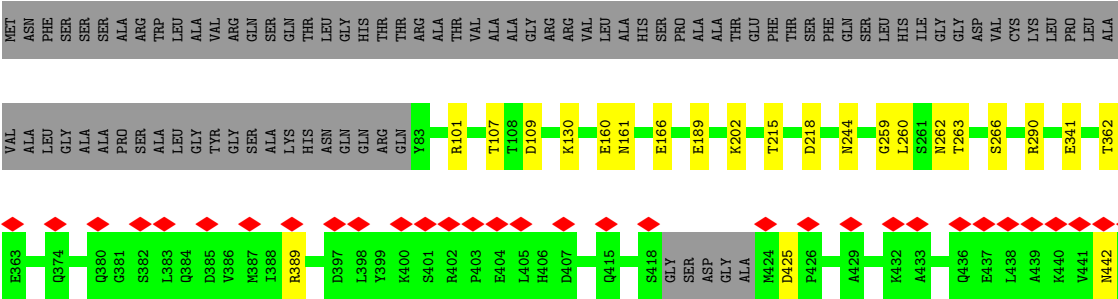
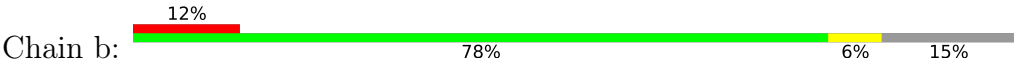
• Molecule 12: ATPTG17

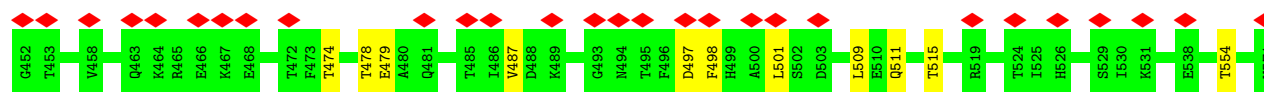


• Molecule 12: ATPTG17

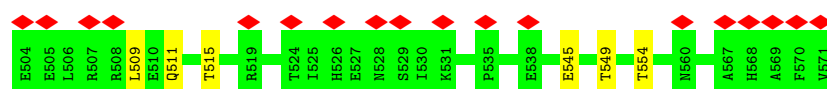
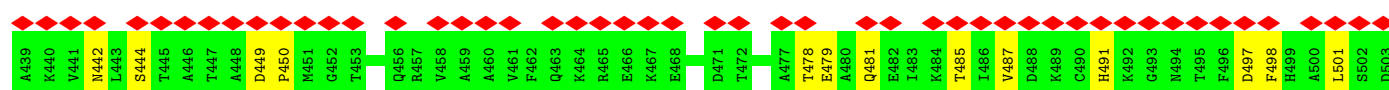
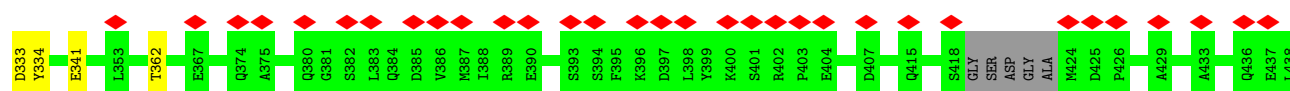
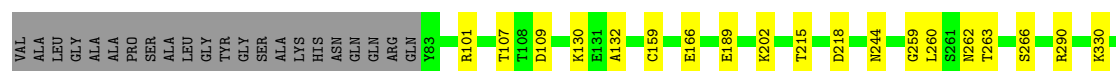
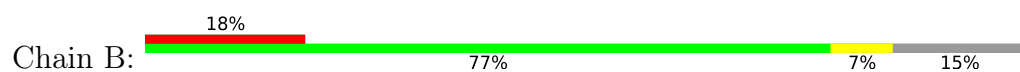


• Molecule 13: subunit b

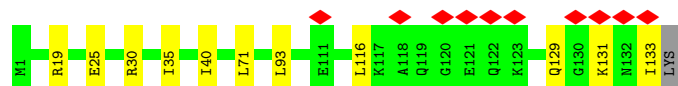
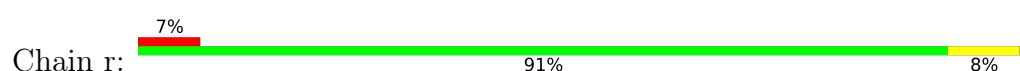




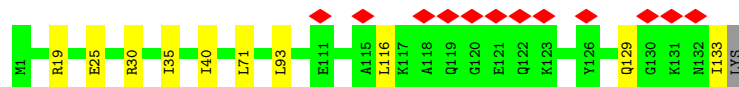
• Molecule 13: subunit b



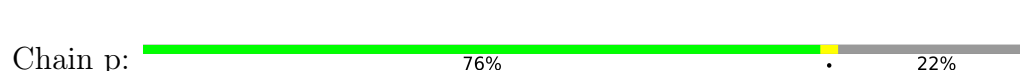
• Molecule 14: ATPTG12



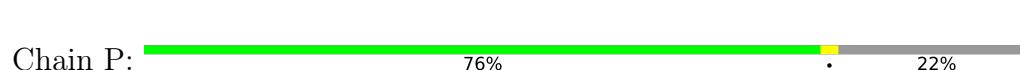
• Molecule 14: ATPTG12



• Molecule 15: ATPTG10

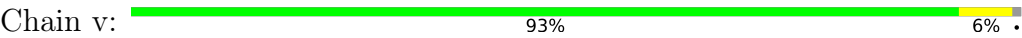


• Molecule 15: ATPTG10





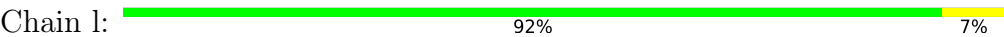
• Molecule 16: subunit f



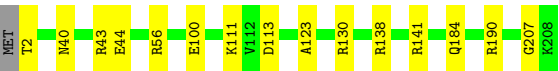
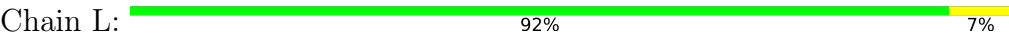
• Molecule 16: subunit f



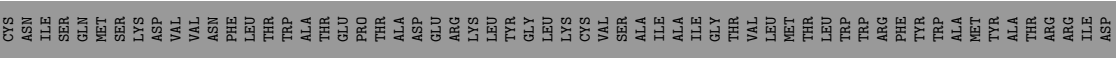
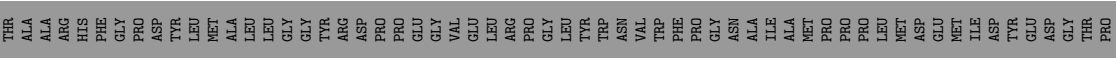
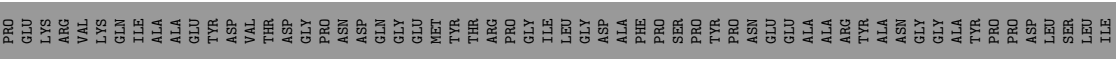
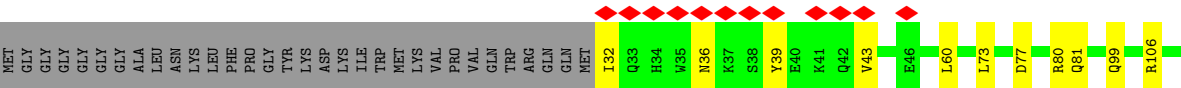
• Molecule 17: ATPTG8



• Molecule 17: ATPTG8

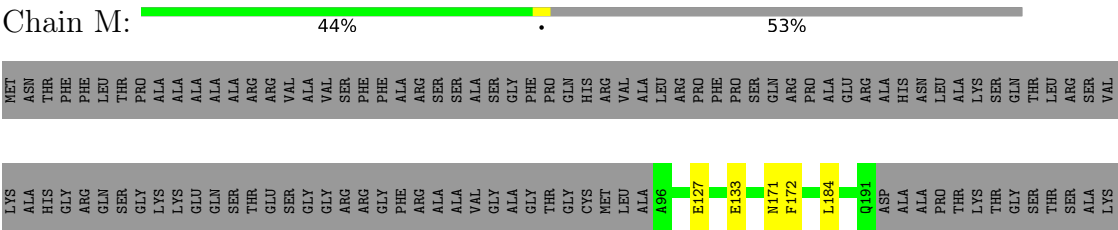


• Molecule 18: ATPTG1



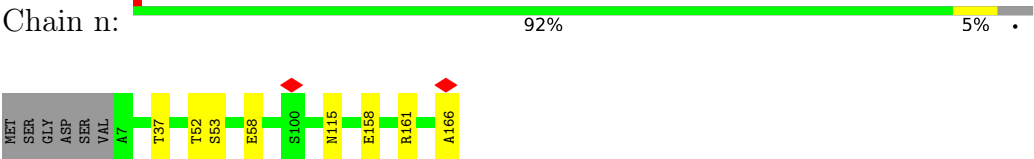
ALA
LYS
LYS

• Molecule 20: subunit 8

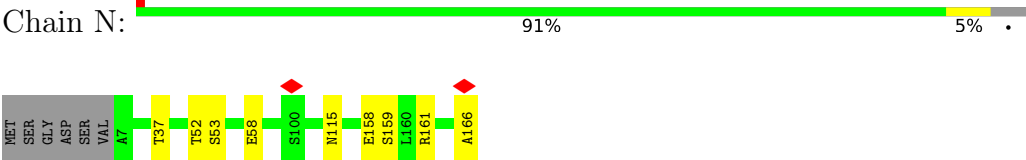


LYS

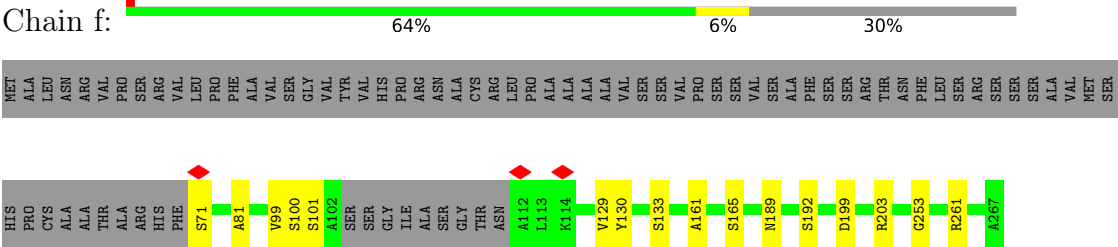
• Molecule 21: ATPTG9



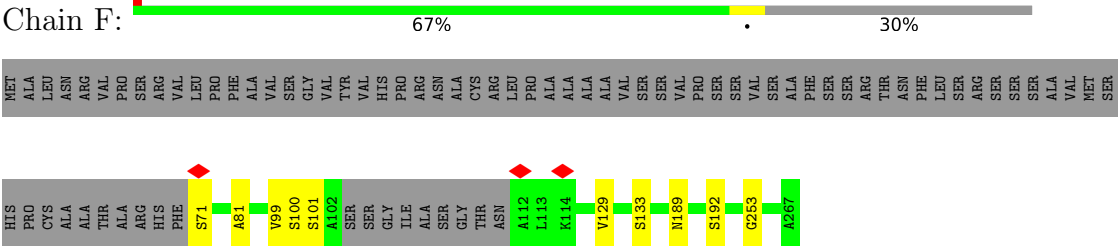
• Molecule 21: ATPTG9



• Molecule 22: ATPTG4

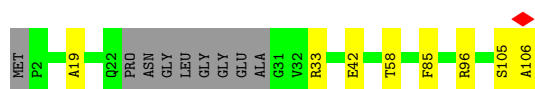


• Molecule 22: ATPTG4



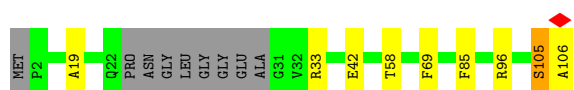
• Molecule 23: ATPTG16

Chain w:  84% 8% 8%



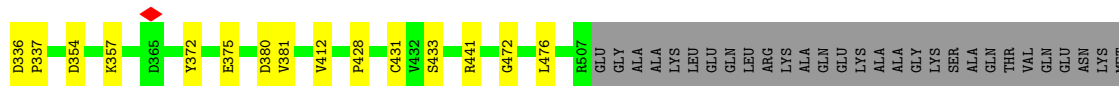
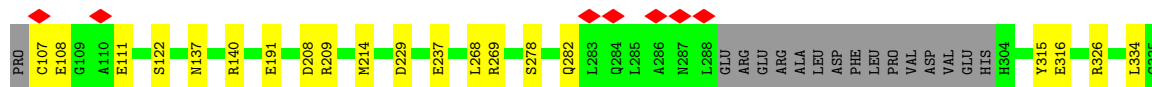
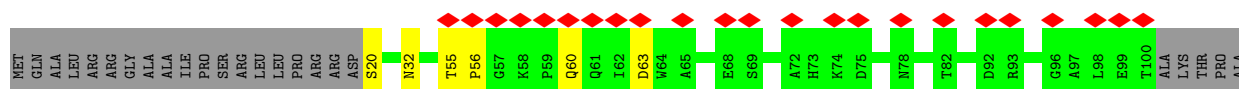
- Molecule 23: ATPTG16

Chain W:  83% 8% 8%



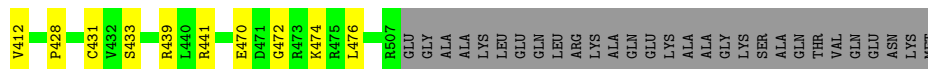
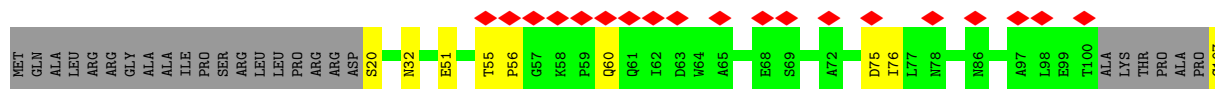
- Molecule 24: subunit d

Chain a:  6% 79% 8% 13%



- Molecule 24: subunit d

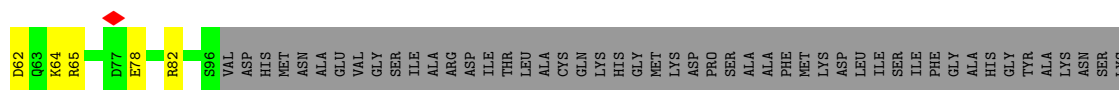
Chain A:  5% 79% 8% 13%



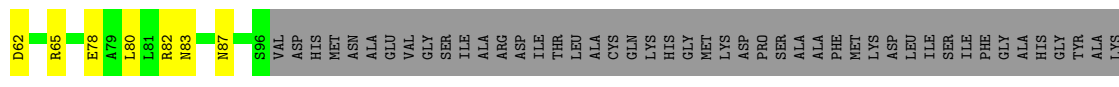
- Molecule 25: Inhibitor of F1

Chain i2:  24% 72% 4%

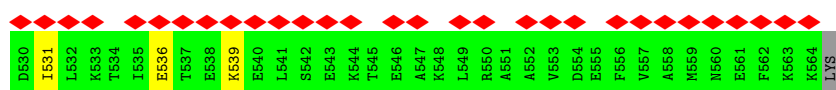
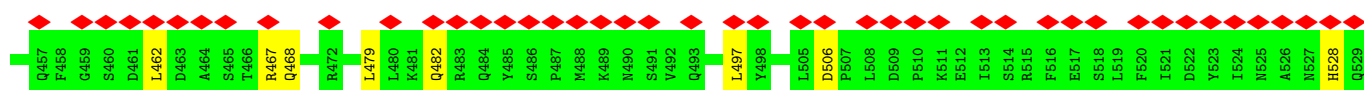
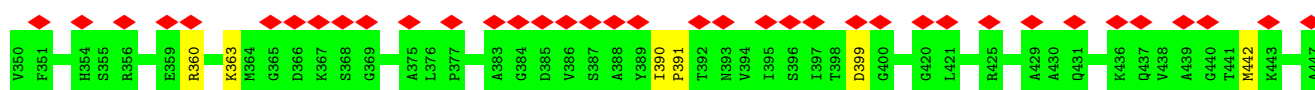
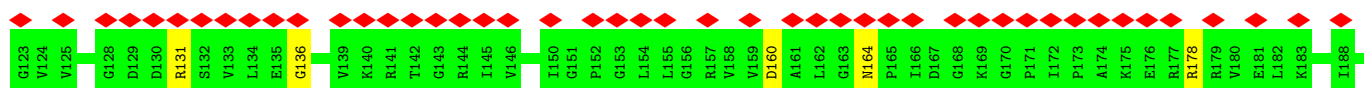
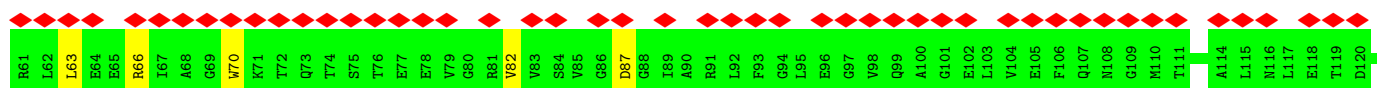
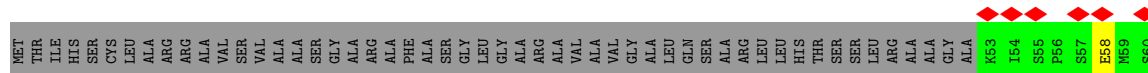
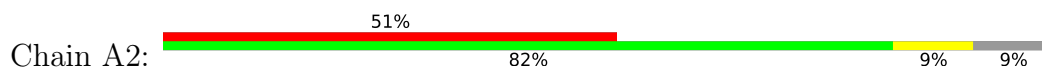




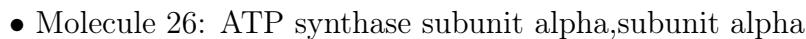
• Molecule 25: Inhibitor of F1

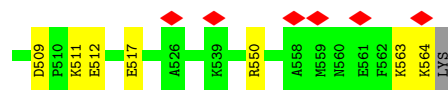


• Molecule 26: ATP synthase subunit alpha,subunit alpha

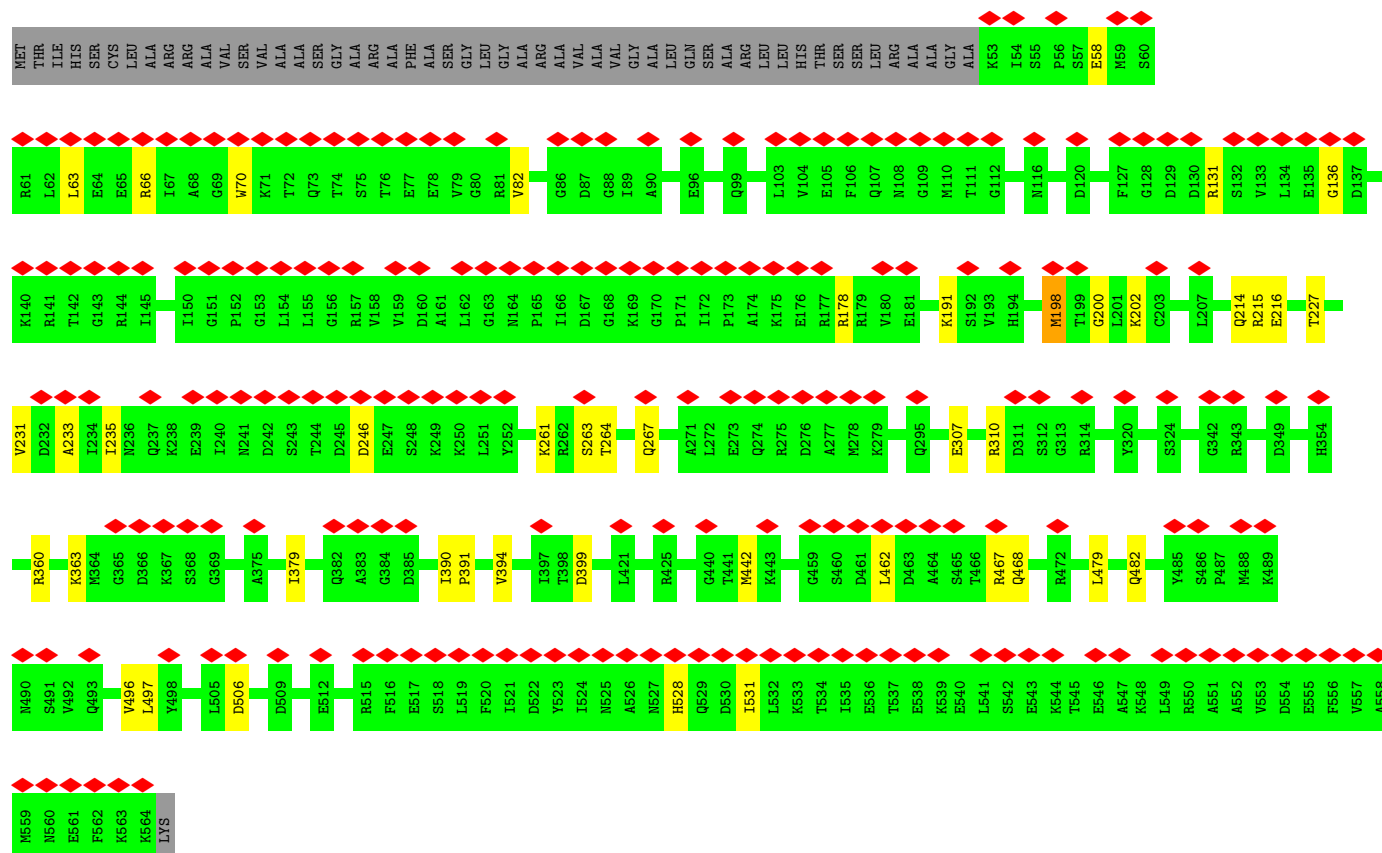
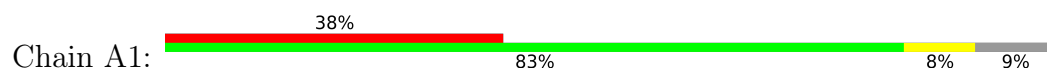


• Molecule 26: ATP synthase subunit alpha,subunit alpha

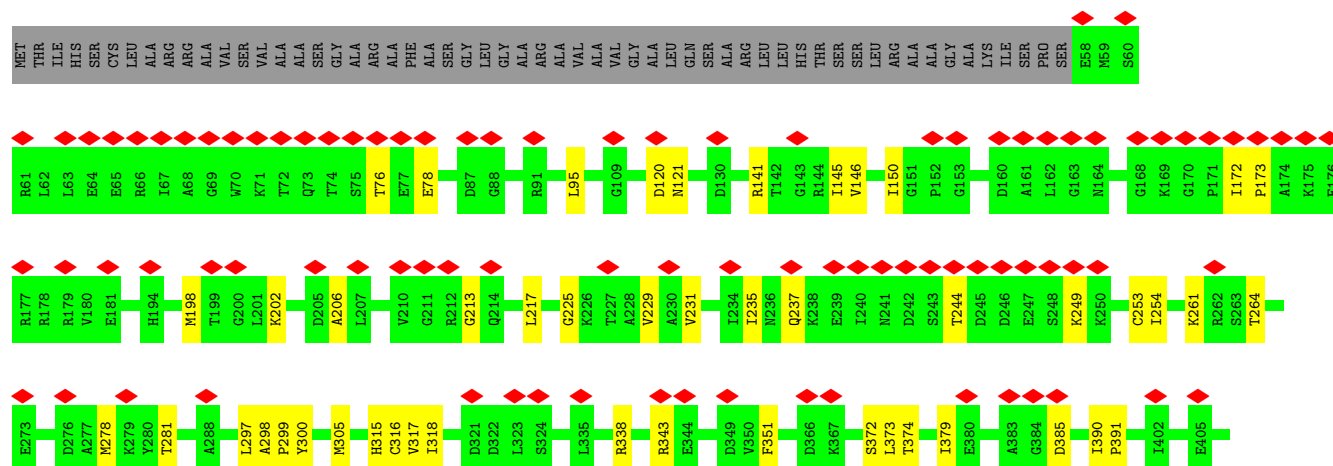
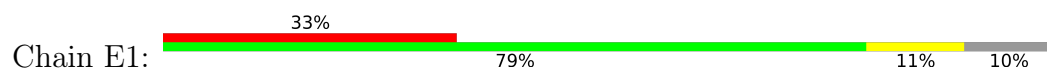


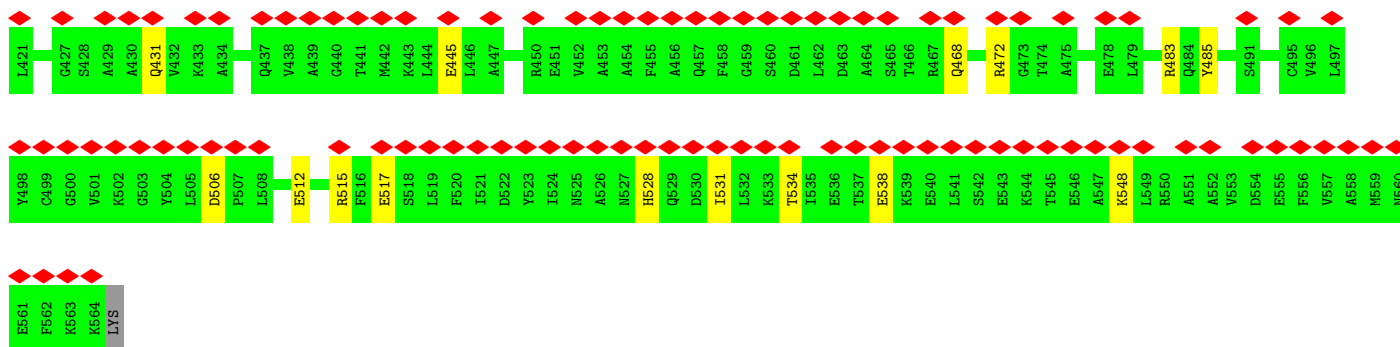


- Molecule 26: ATP synthase subunit alpha,subunit alpha

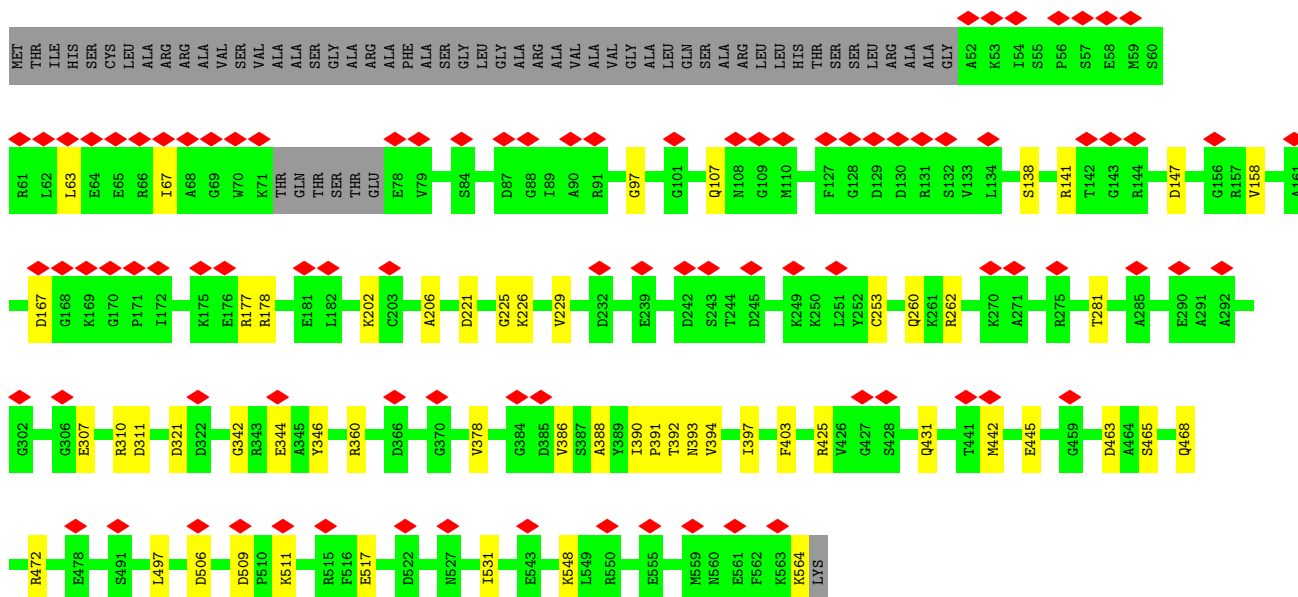
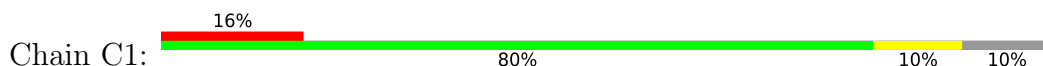


- Molecule 26: ATP synthase subunit alpha,subunit alpha

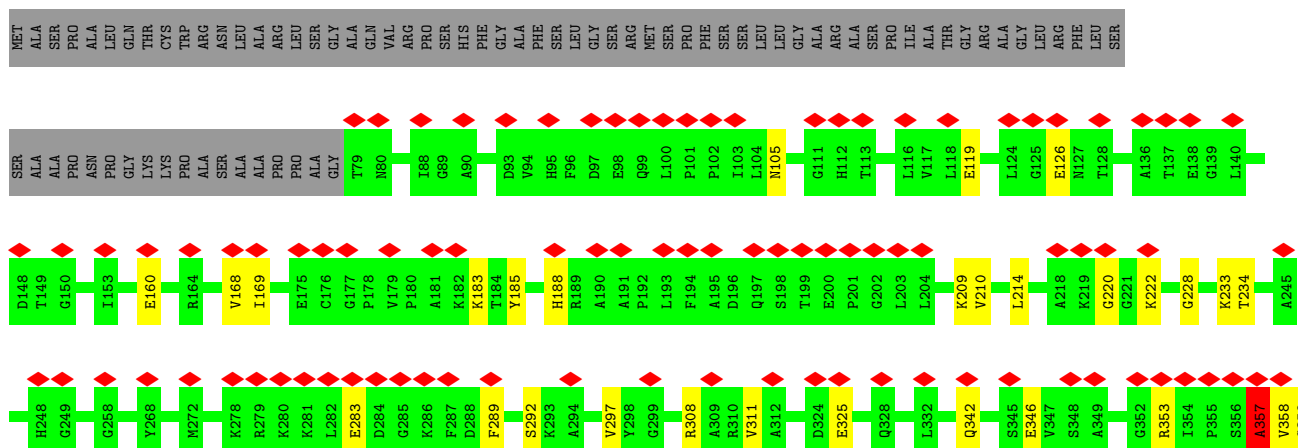
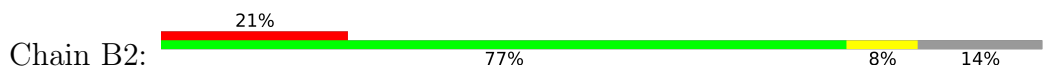


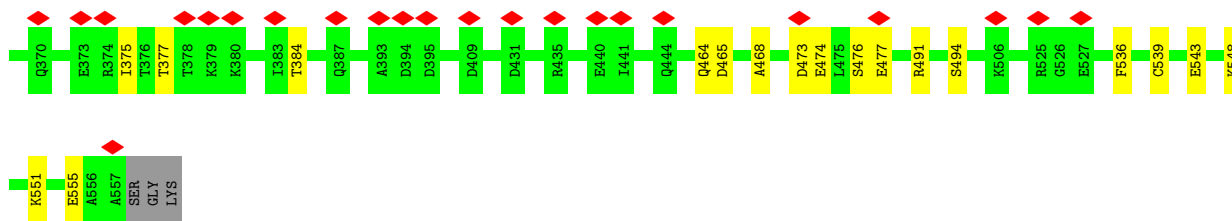


- Molecule 26: ATP synthase subunit alpha,subunit alpha

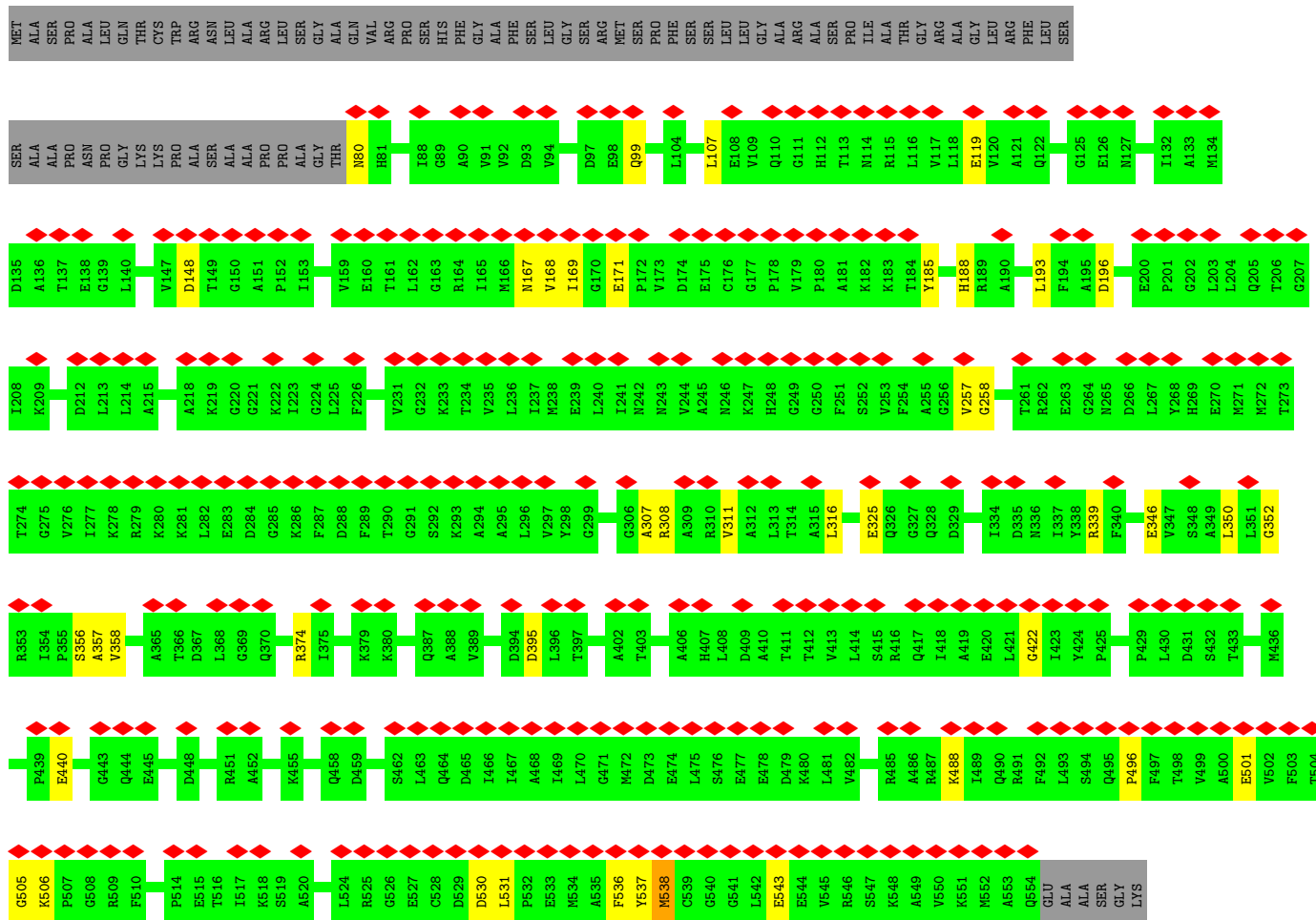
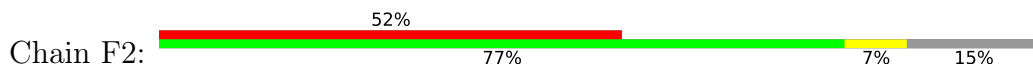


- Molecule 27: ATP synthase subunit beta

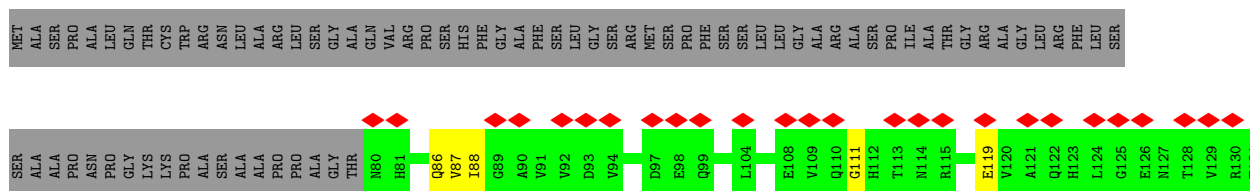
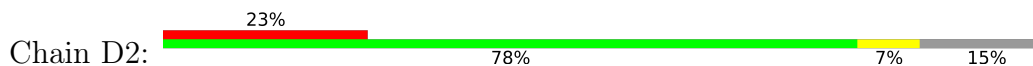


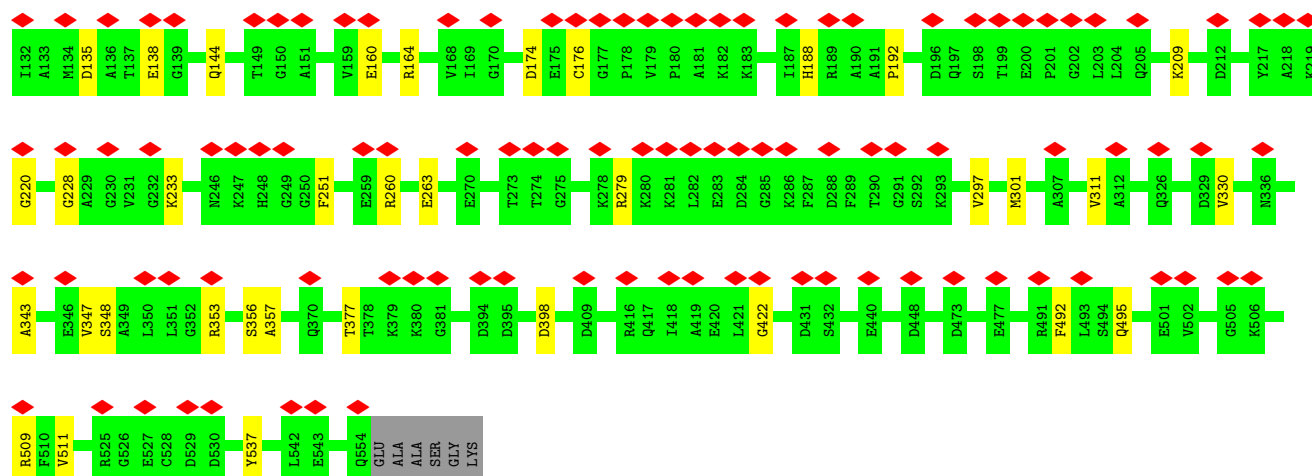


• Molecule 27: ATP synthase subunit beta

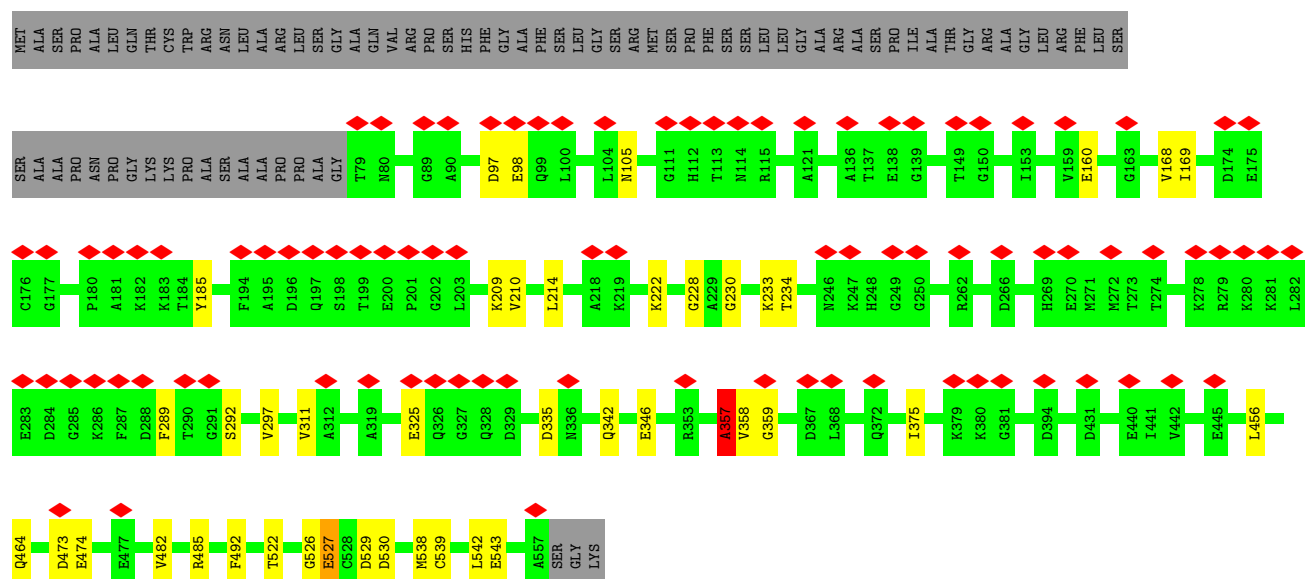
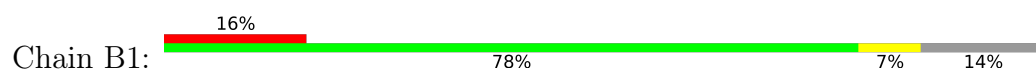


• Molecule 27: ATP synthase subunit beta

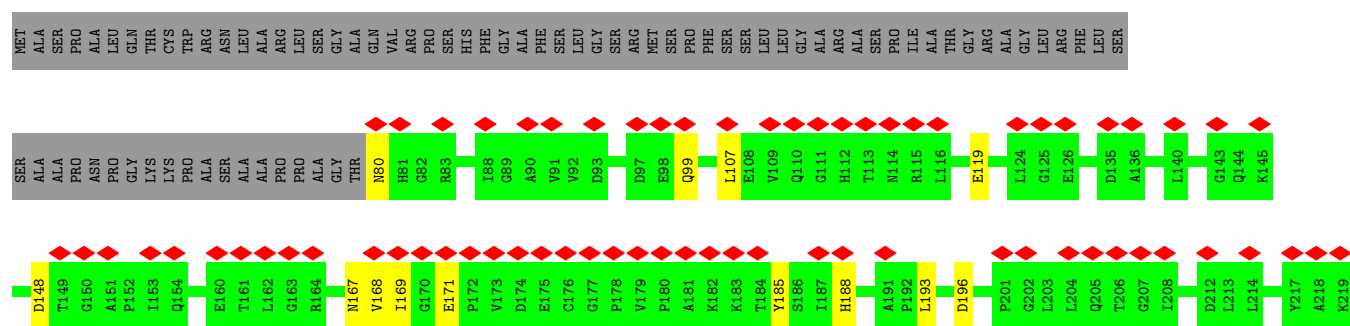
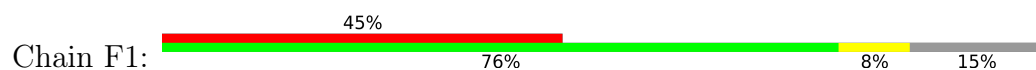


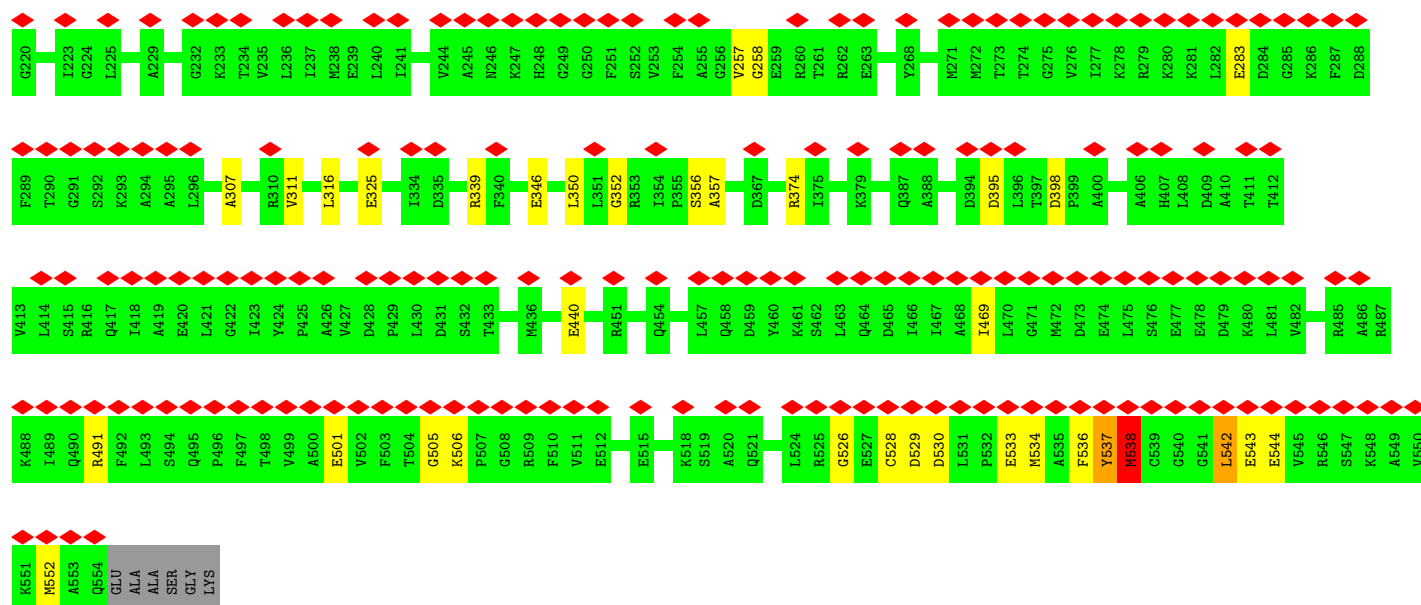


• Molecule 27: ATP synthase subunit beta

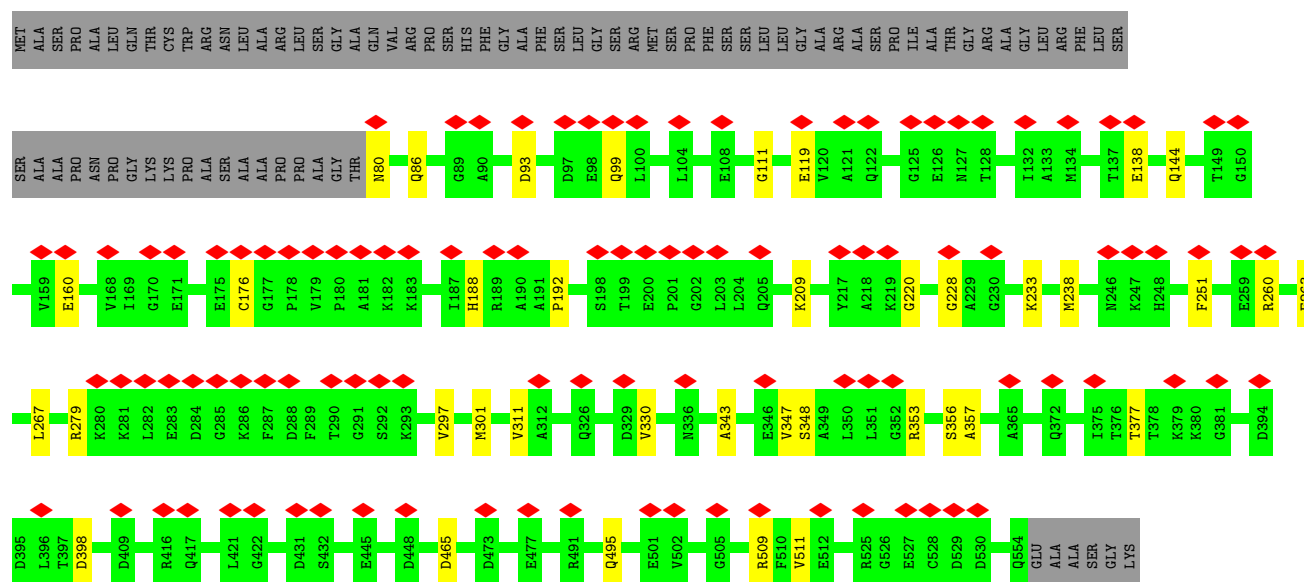
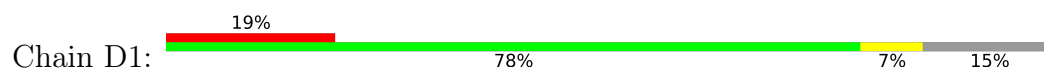


• Molecule 27: ATP synthase subunit beta

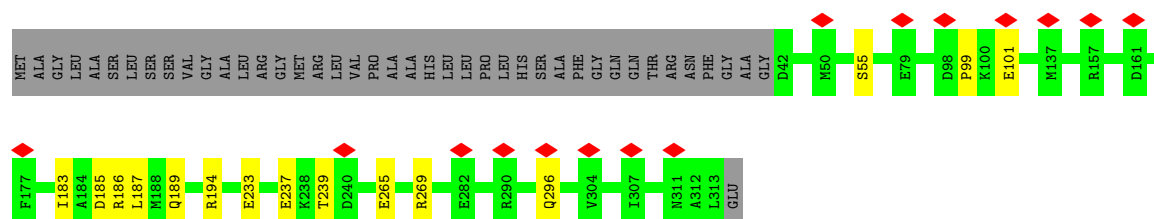
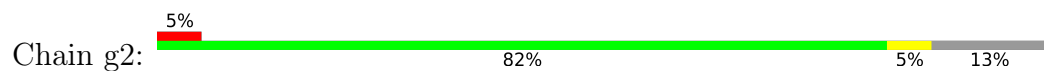




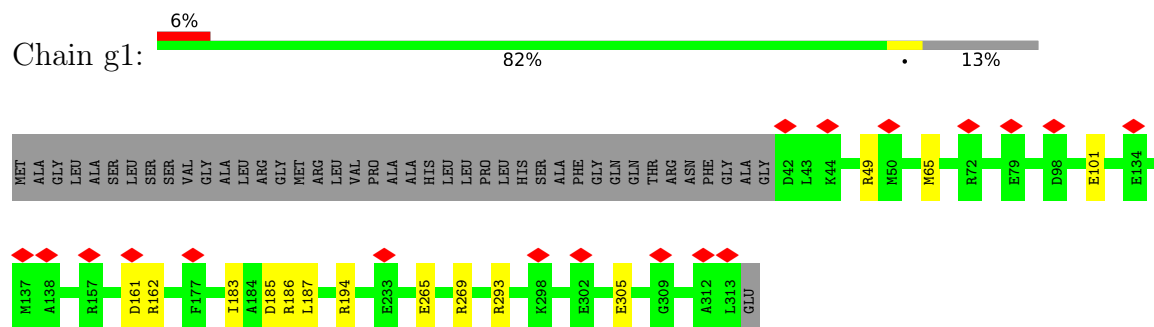
• Molecule 27: ATP synthase subunit beta



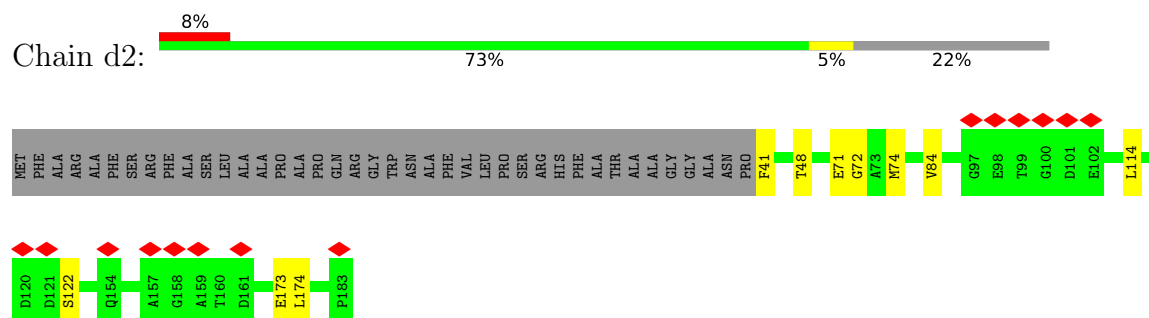
• Molecule 28: ATP synthase subunit gamma



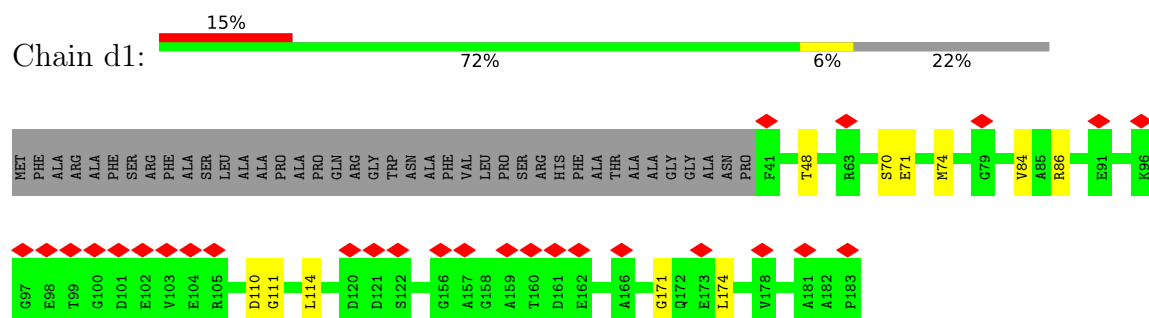
- Molecule 28: ATP synthase subunit gamma



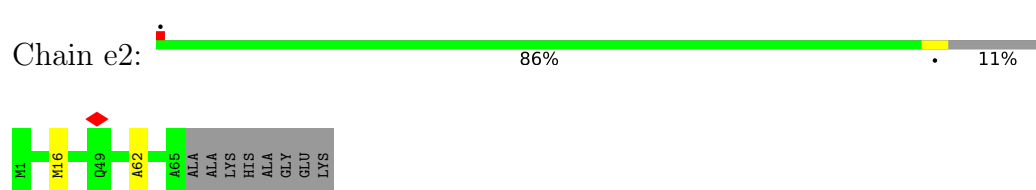
- Molecule 29: ATP synthase subunit delta



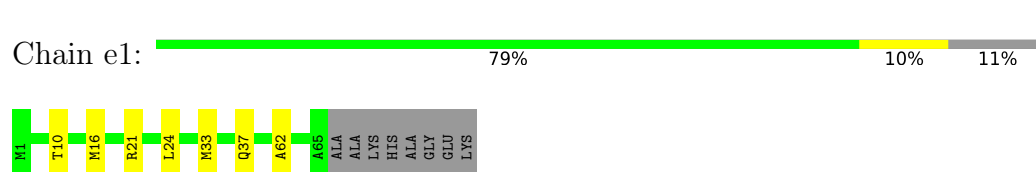
- Molecule 29: ATP synthase subunit delta



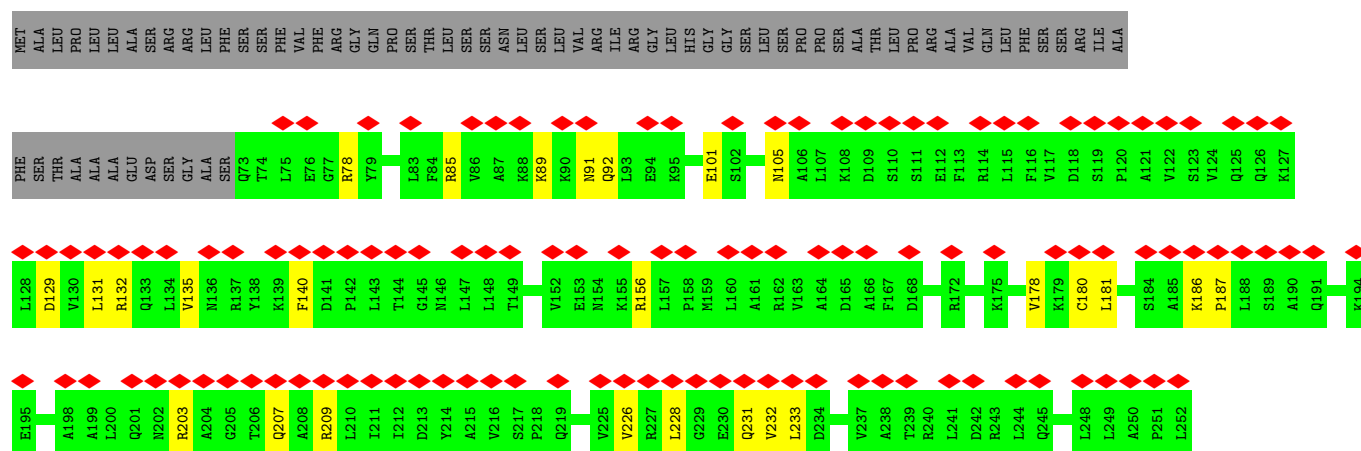
- Molecule 30: ATP synthase subunit epsilon



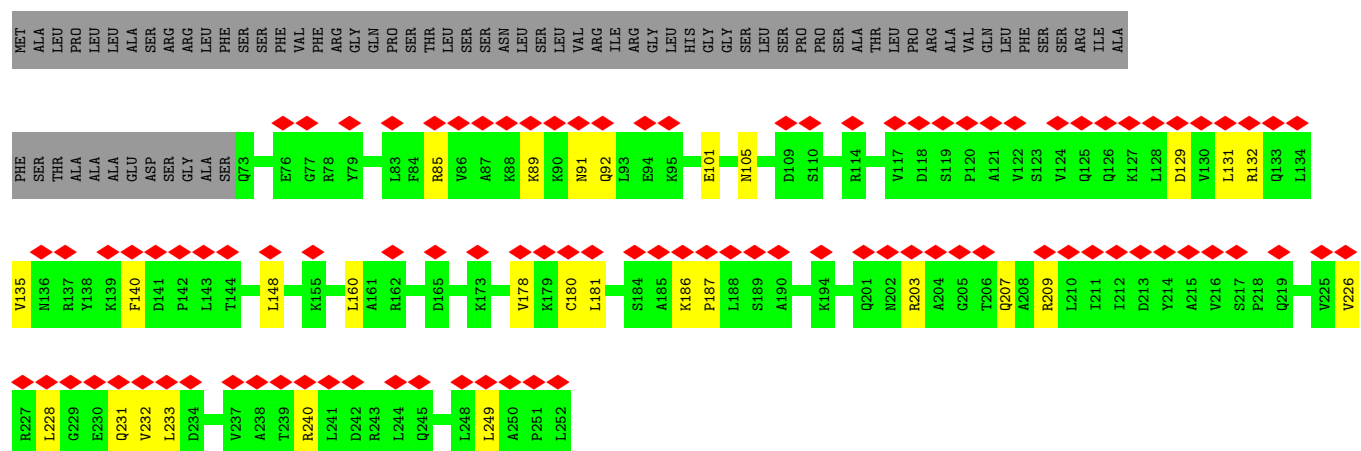
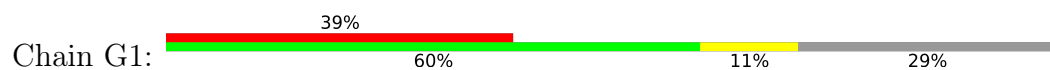
- Molecule 30: ATP synthase subunit epsilon



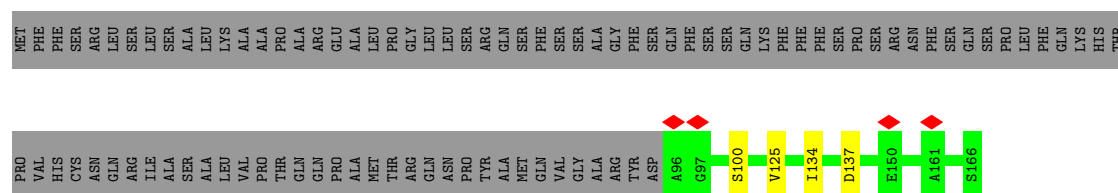
- Molecule 31: Oligomycin sensitivity conferring protein (OSCP)



• Molecule 31: Oligomycin sensitivity conferring protein (OSCP)

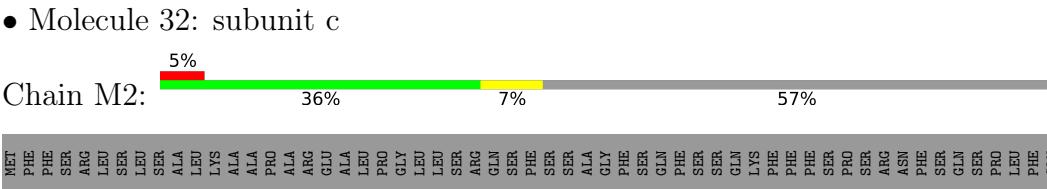
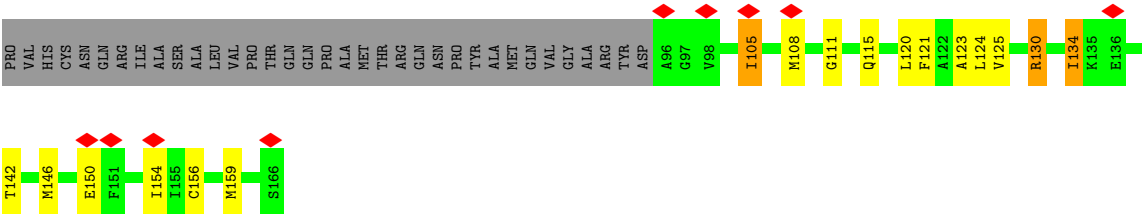
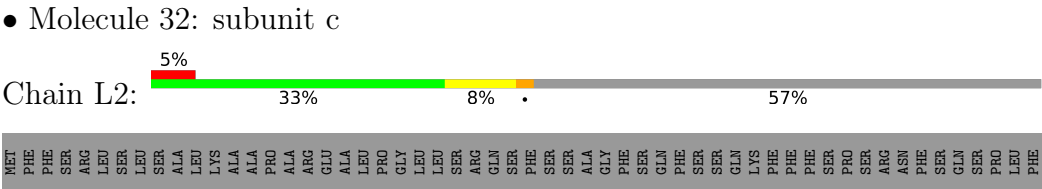
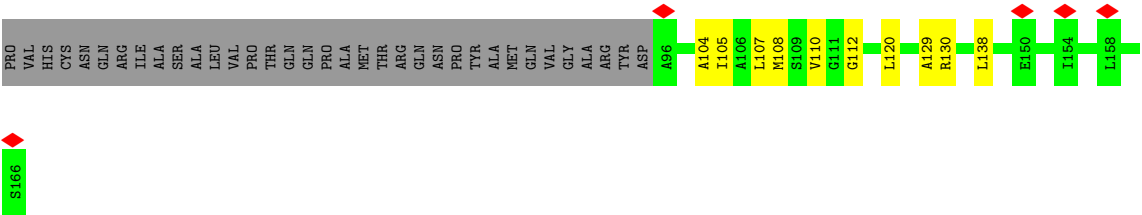
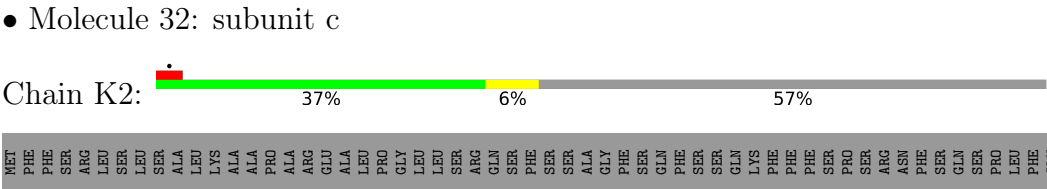
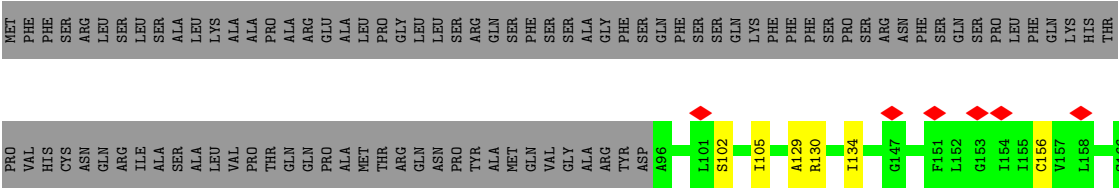
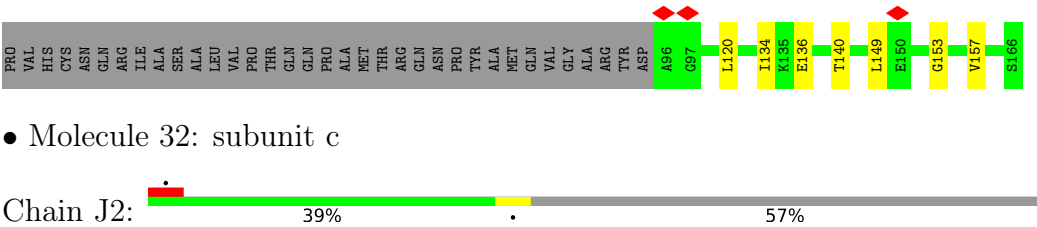


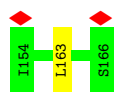
• Molecule 32: subunit c



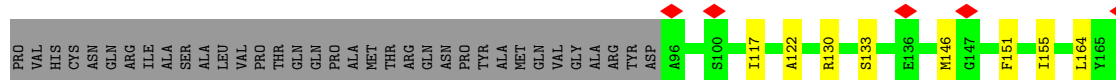
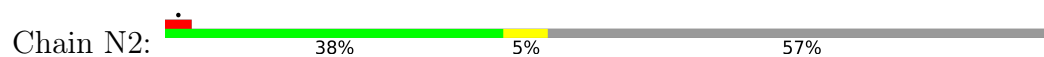
• Molecule 32: subunit c



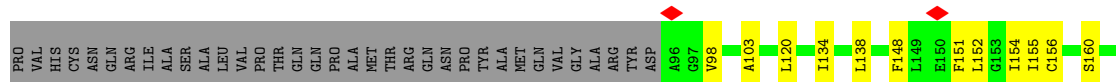
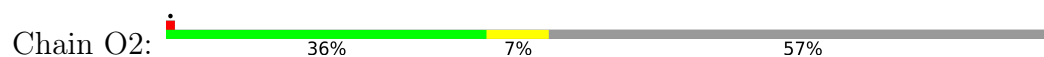




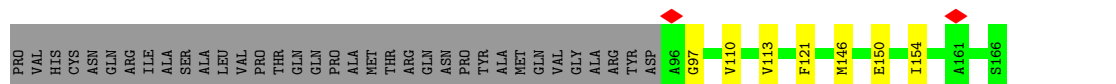
• Molecule 32: subunit c



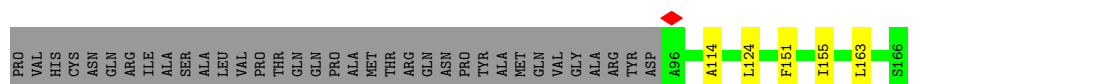
• Molecule 32: subunit c



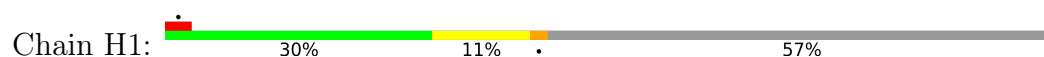
• Molecule 32: subunit c

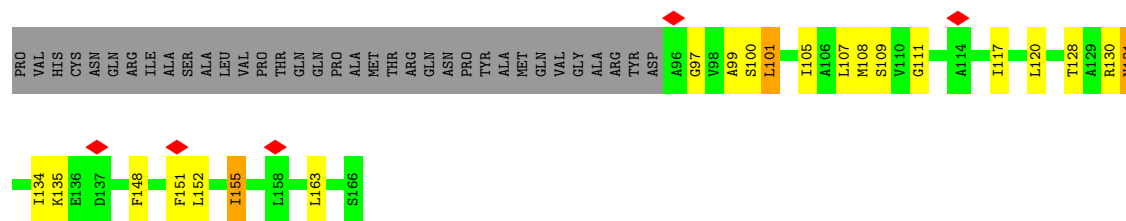


• Molecule 32: subunit c

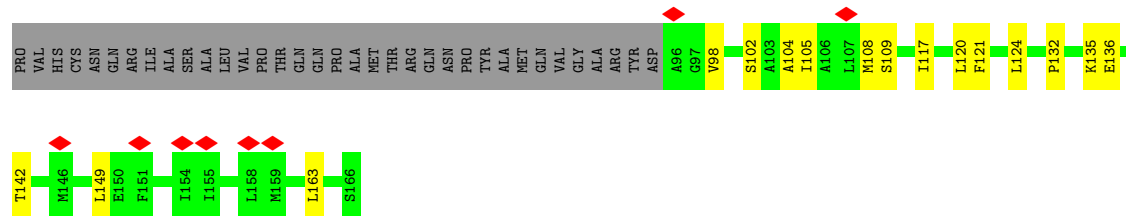
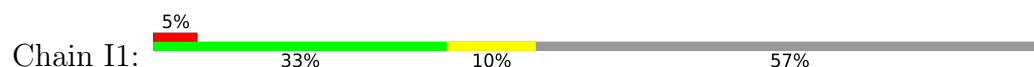


• Molecule 32: subunit c

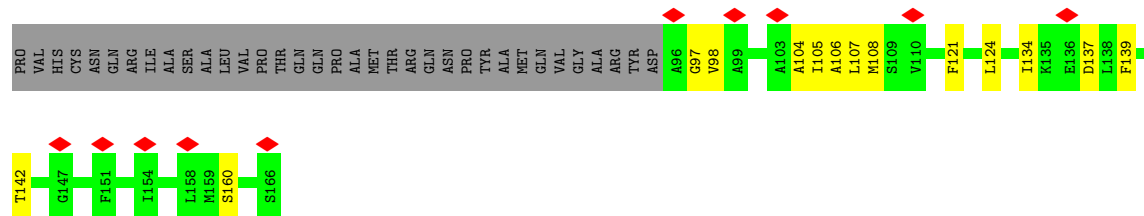
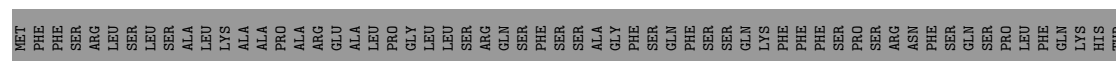
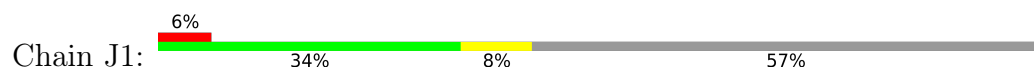




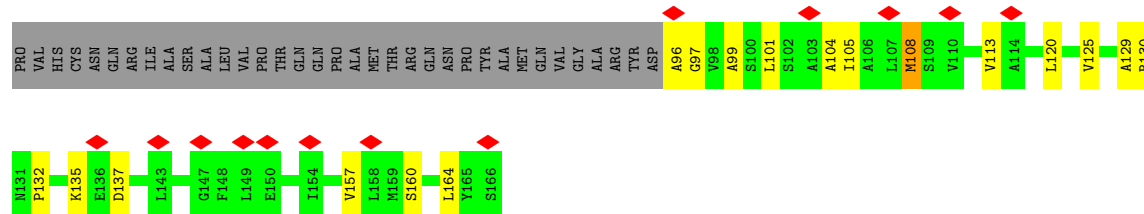
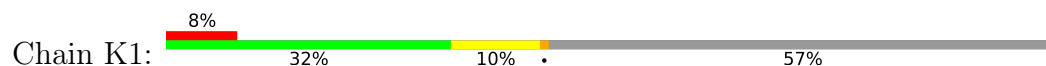
- Molecule 32: subunit c



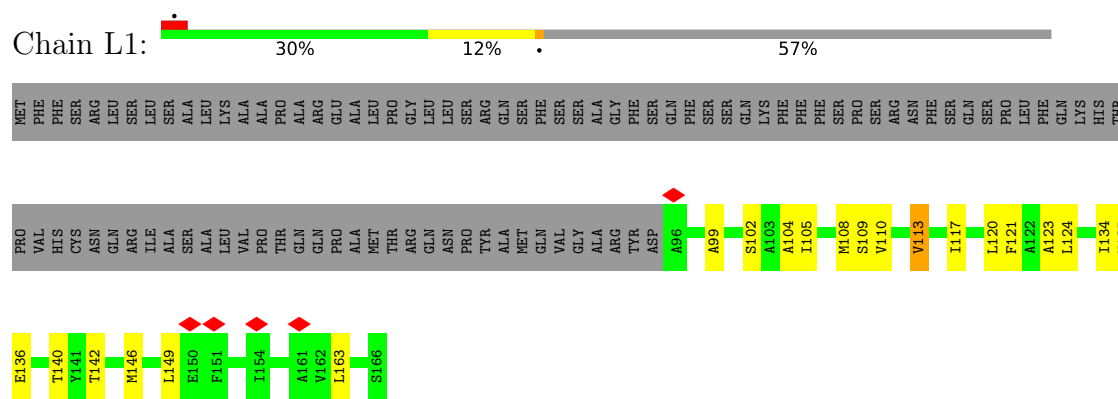
- Molecule 32: subunit c



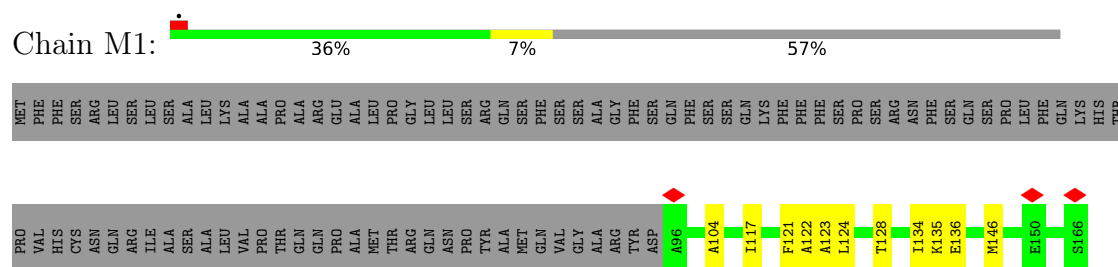
- Molecule 32: subunit c



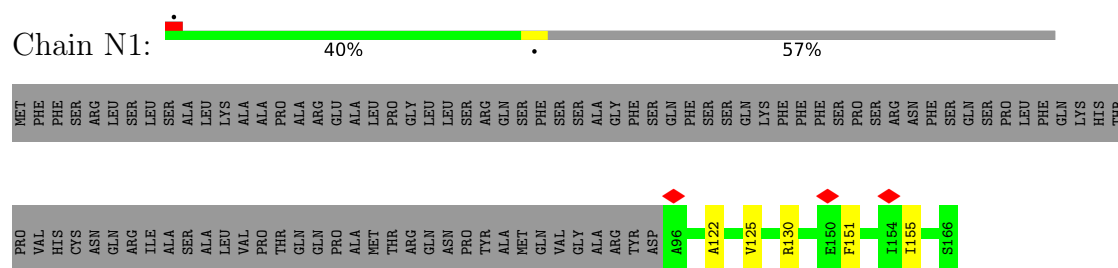
- Molecule 32: subunit c



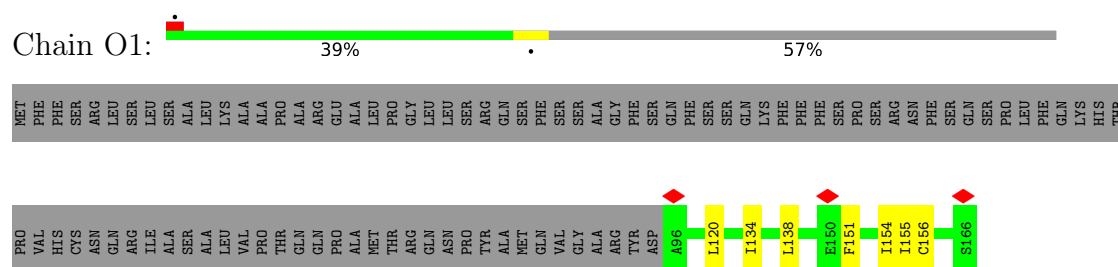
• Molecule 32: subunit c



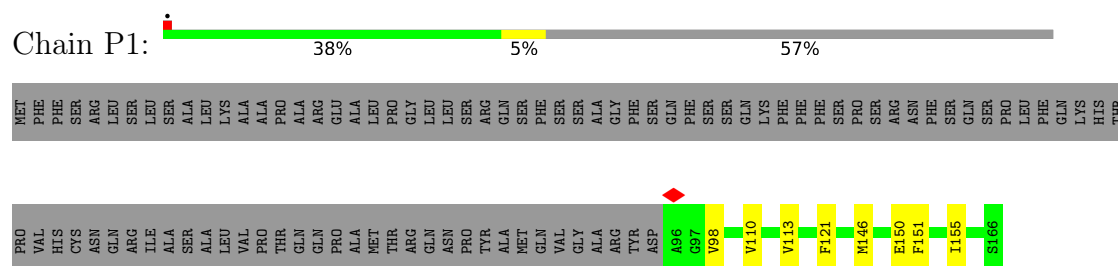
• Molecule 32: subunit c



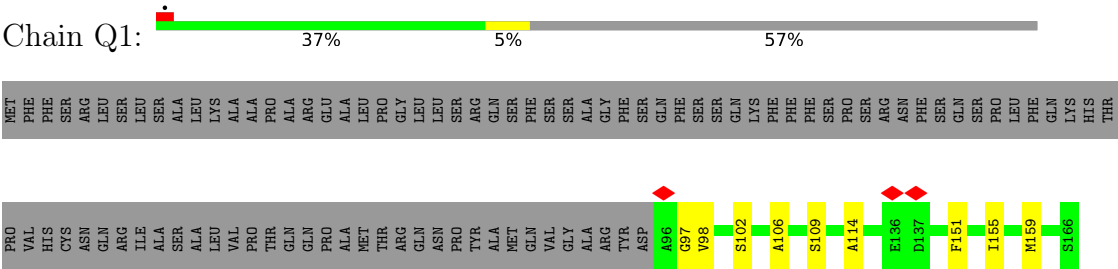
• Molecule 32: subunit c



• Molecule 32: subunit c



● Molecule 32: subunit c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101505	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	Q	0.22	0/1103	0.39	0/1496
1	q	0.21	0/1103	0.39	0/1496
2	I	0.23	0/719	0.33	0/962
2	i	0.23	0/719	0.33	0/962
3	T	0.22	0/741	0.33	0/1007
3	t	0.22	0/741	0.33	0/1007
4	G	0.26	0/896	0.33	0/1216
4	g	0.26	0/896	0.33	0/1216
5	O	0.29	0/1250	0.33	0/1682
5	o	0.29	0/1250	0.33	0/1682
6	K	0.25	0/981	0.32	0/1321
6	k	0.25	0/981	0.31	0/1321
7	J	0.38	0/1573	0.38	0/2137
7	j	0.38	0/1573	0.38	0/2137
8	S	0.28	0/826	0.30	0/1119
8	s	0.27	0/826	0.30	0/1119
9	U	0.32	0/770	0.37	0/1040
9	u	0.32	0/770	0.37	0/1040
10	H	0.33	0/1902	0.37	0/2575
10	h	0.34	0/1902	0.37	0/2575
11	E	0.31	0/1154	0.34	0/1572
11	e	0.31	0/1154	0.34	0/1572
12	X	0.27	0/678	0.32	0/923
12	x	0.27	0/678	0.32	0/923
13	B	0.23	0/4016	0.34	0/5422
13	b	0.24	0/4016	0.34	0/5422
14	R	0.24	0/1092	0.32	0/1470
14	r	0.25	0/1092	0.37	0/1470
15	P	0.28	0/888	0.33	0/1202
15	p	0.28	0/888	0.33	0/1202
16	V	0.35	0/944	0.39	0/1280
16	v	0.35	0/944	0.39	0/1280

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	L	0.31	0/1651	0.33	0/2227
17	l	0.31	0/1651	0.32	0/2227
18	C	0.30	0/1057	0.38	0/1428
18	c	0.30	0/1057	0.40	0/1428
19	D	0.33	0/2143	0.34	0/2912
19	d	0.33	0/2143	0.34	0/2912
20	M	0.29	0/789	0.33	0/1065
20	m	0.29	0/789	0.33	0/1065
21	N	0.23	0/1280	0.32	0/1734
21	n	0.23	0/1280	0.32	0/1734
22	F	0.24	0/1475	0.33	0/2009
22	f	0.24	0/1475	0.33	0/2009
23	W	0.30	0/784	0.31	0/1064
23	w	0.30	0/784	0.32	0/1064
24	A	0.22	0/3883	0.31	0/5262
24	a	0.22	0/3883	0.32	0/5262
25	i1	0.15	0/343	0.28	0/459
25	i2	0.15	0/343	0.27	0/459
26	A1	0.12	0/3979	0.34	0/5372
26	A2	0.12	0/3979	0.34	0/5372
26	C1	0.12	0/3938	0.30	0/5314
26	C2	0.12	0/3938	0.30	0/5314
26	E1	0.11	0/3942	0.31	0/5322
26	E2	0.11	0/3942	0.31	0/5322
27	B1	0.14	0/3698	0.37	0/5016
27	B2	0.13	0/3698	0.34	0/5016
27	D1	0.11	0/3672	0.30	0/4980
27	D2	0.11	0/3672	0.30	0/4980
27	F1	0.12	0/3672	0.37	2/4980 (0.0%)
27	F2	0.12	0/3672	0.33	0/4980
28	g1	0.14	0/2145	0.28	0/2890
28	g2	0.14	0/2145	0.31	0/2890
29	d1	0.12	0/1083	0.29	0/1466
29	d2	0.13	0/1083	0.28	0/1466
30	e1	0.15	0/547	0.34	0/733
30	e2	0.15	0/547	0.34	0/733
31	G1	0.13	0/1431	0.37	0/1929
31	G2	0.13	0/1431	0.37	0/1929
32	H1	0.23	0/507	0.59	0/686
32	H2	0.16	0/507	0.36	0/686
32	I1	0.21	0/507	0.53	0/686
32	I2	0.16	0/507	0.33	0/686
32	J1	0.19	0/507	0.46	0/686

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	J2	0.18	0/507	0.40	0/686
32	K1	0.21	0/507	0.49	0/686
32	K2	0.15	0/507	0.31	0/686
32	L1	0.23	0/507	0.57	0/686
32	L2	0.21	0/507	0.56	0/686
32	M1	0.22	0/507	0.43	0/686
32	M2	0.17	0/507	0.35	0/686
32	N1	0.16	0/507	0.28	0/686
32	N2	0.16	0/507	0.26	0/686
32	O1	0.18	0/507	0.32	0/686
32	O2	0.18	0/507	0.33	0/686
32	P1	0.22	0/507	0.39	0/686
32	P2	0.22	0/507	0.40	0/686
32	Q1	0.21	0/507	0.46	0/686
32	Q2	0.22	0/507	0.41	0/686
All	All	0.22	0/132230	0.34	2/178892 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	J	0	1
7	j	0	1
26	A1	0	1
26	A2	0	1
27	B1	0	1
27	B2	0	1
27	F1	1	0
All	All	1	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F1	538	MET	N-CA-CB	6.24	121.55	112.13
27	F1	538	MET	CB-CA-C	5.16	119.06	111.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	F1	538	MET	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A1	198	MET	Peptide
26	A2	198	MET	Peptide
27	B1	357	ALA	Peptide
27	B2	357	ALA	Peptide
7	J	89	PHE	Peptide
7	j	89	PHE	Peptide

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	Q	1075	1044	1044	12	0
1	q	1075	1044	1044	11	0
2	I	708	678	678	6	0
2	i	708	678	678	6	0
3	T	723	716	728	9	0
3	t	723	716	728	8	0
4	G	876	856	856	6	0
4	g	876	856	856	8	0
5	O	1220	1195	1195	11	0
5	o	1220	1195	1195	11	0
6	K	952	952	952	13	0
6	k	952	952	952	12	0
7	J	1512	1469	1469	12	0
7	j	1512	1469	1469	13	0
8	S	800	770	770	2	0
8	s	800	770	770	2	0
9	U	751	741	741	5	0
9	u	751	741	741	5	0
10	H	1848	1741	1741	8	0
10	h	1848	1741	1741	7	0
11	E	1115	1064	1064	4	0
11	e	1115	1064	1064	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	659	639	639	7	0
12	x	659	639	639	6	0
13	B	3932	3909	3909	32	0
13	b	3932	3909	3909	29	0
14	R	1071	1073	1073	9	0
14	r	1071	1073	1073	9	0
15	P	864	847	847	3	0
15	p	864	847	847	3	0
16	V	913	888	888	7	0
16	v	913	888	888	7	0
17	L	1626	1647	1647	11	0
17	l	1626	1647	1647	11	0
18	C	1030	999	999	9	0
18	c	1030	999	999	9	0
19	D	2081	1975	1975	10	0
19	d	2081	1975	1975	9	0
20	M	765	744	744	4	0
20	m	765	744	744	5	0
21	N	1247	1202	1200	8	0
21	n	1247	1202	1200	7	0
22	F	1442	1425	1425	7	0
22	f	1442	1425	1425	10	0
23	W	760	760	760	9	0
23	w	760	760	760	8	0
24	A	3780	3616	3615	29	0
24	a	3780	3616	3615	29	0
25	i1	336	324	324	5	0
25	i2	336	324	324	4	0
26	A1	3922	4003	4003	24	0
26	A2	3922	4003	4003	29	0
26	C1	3882	3967	3967	32	0
26	C2	3882	3967	3967	30	0
26	E1	3886	3962	3962	37	0
26	E2	3886	3962	3962	41	0
27	B1	3638	3676	3676	25	0
27	B2	3638	3676	3676	31	0
27	D1	3612	3653	3653	22	0
27	D2	3612	3653	3653	25	0
27	F1	3612	3653	3653	29	0
27	F2	3612	3653	3653	25	0
28	g1	2116	2173	2173	10	0
28	g2	2116	2173	2173	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	d1	1069	1076	1076	8	0
29	d2	1069	1076	1076	8	0
30	e1	538	539	539	6	0
30	e2	538	539	539	2	0
31	G1	1415	1486	1486	18	0
31	G2	1415	1486	1486	18	0
32	H1	501	527	527	16	0
32	H2	501	527	527	3	0
32	I1	501	527	527	19	0
32	I2	501	527	527	4	0
32	J1	501	527	527	19	0
32	J2	501	527	527	6	0
32	K1	501	527	527	23	0
32	K2	501	527	527	10	0
32	L1	501	527	527	22	0
32	L2	501	527	527	17	0
32	M1	501	527	527	8	0
32	M2	501	527	527	9	0
32	N1	501	527	527	5	0
32	N2	501	527	527	8	0
32	O1	501	527	527	6	0
32	O2	501	527	527	10	0
32	P1	501	527	527	10	0
32	P2	501	527	527	12	0
32	Q1	501	527	527	9	0
32	Q2	501	527	527	5	0
33	O	108	176	176	2	0
33	V	54	88	88	0	0
33	o	108	176	176	2	0
33	v	54	88	88	0	0
34	C	70	92	92	1	0
34	D	70	92	92	1	0
34	H	35	46	46	2	0
34	O	35	46	46	1	0
34	X	35	46	46	1	0
34	c	70	92	92	0	0
34	d	70	92	92	1	0
34	h	35	46	46	2	0
34	o	35	46	46	1	0
34	x	35	46	46	1	0
35	B	200	312	312	5	0
35	C	100	156	156	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	100	156	156	0	0
35	E	100	156	156	0	0
35	H	100	156	156	0	0
35	O	100	156	156	1	0
35	U	100	156	156	1	0
35	V	100	156	156	7	0
35	b	200	312	312	5	0
35	c	100	156	156	7	0
35	d	100	156	156	0	0
35	e	100	156	156	0	0
35	h	100	156	156	0	0
35	o	100	156	156	0	0
35	u	100	156	156	1	0
35	v	100	156	156	6	0
36	C	51	82	82	0	0
36	J	102	164	164	2	0
36	c	51	82	82	0	0
36	j	102	164	164	4	0
37	A1	31	11	12	1	0
37	A2	31	11	12	0	0
37	C1	31	12	12	0	0
37	C2	31	11	12	0	0
37	E1	31	11	12	0	0
37	E2	31	11	12	0	0
38	B1	27	11	12	3	0
38	B2	27	12	12	1	0
38	D1	27	11	11	0	0
38	D2	27	11	12	1	0
All	All	132786	134048	134073	902	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 (902) 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)
32:K1:137:ASP:OD1	32:L1:135:LYS:NZ	2.06	0.89
14:r:93:LEU:O	24:a:32:ASN:ND2	2.10	0.85
18:C:77:ASP:OD2	18:C:80:ARG:NH1	2.10	0.85
27:D2:111:GLY:O	27:D2:144:GLN:NE2	2.10	0.84
6:k:163:GLN:NE2	32:P1:150:GLU:OE2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:d:61:ALA:O	23:w:96:ARG:NH2	2.10	0.84
32:K1:105:ILE:HG22	32:L1:108:MET:HE3	1.57	0.84
26:E2:315:HIS:HD1	26:E2:372:SER:HG	1.12	0.84
7:J:153:GLU:OE1	23:W:58:THR:OG1	1.96	0.83
7:j:153:GLU:OE1	23:w:58:THR:OG1	1.96	0.83
19:D:61:ALA:O	23:W:96:ARG:NH2	2.12	0.83
27:D1:111:GLY:O	27:D1:144:GLN:NE2	2.12	0.83
18:c:77:ASP:OD2	18:c:80:ARG:NH1	2.11	0.83
10:H:50:ILE:O	10:H:55:ARG:NH1	2.11	0.83
14:R:93:LEU:O	24:A:32:ASN:ND2	2.11	0.83
10:h:50:ILE:O	10:h:55:ARG:NH1	2.12	0.81
27:B2:357:ALA:O	27:B2:359:GLY:N	2.14	0.80
27:B1:357:ALA:O	27:B1:359:GLY:N	2.14	0.80
10:h:223:ARG:O	34:h:301:LMT:O3B	2.00	0.80
10:H:223:ARG:O	34:H:301:LMT:O3B	2.00	0.79
26:C2:97:GLY:O	26:C2:141:ARG:NH1	2.15	0.79
8:S:64:TYR:OH	12:X:32:GLU:OE1	2.01	0.79
26:A1:202:LYS:NZ	26:A1:479:LEU:O	2.16	0.79
24:a:278:SER:O	24:a:282:GLN:NE2	2.16	0.78
24:a:357:LYS:O	24:a:372:TYR:OH	2.02	0.78
24:A:268:LEU:HD22	24:A:412:VAL:HG23	1.66	0.77
3:T:73:ASP:OD1	24:A:441:ARG:NH1	2.18	0.77
29:d2:71:GLU:OE1	32:N2:130:ARG:NH2	2.16	0.77
26:C1:97:GLY:O	26:C1:141:ARG:NH1	2.17	0.77
5:o:39:SER:OG	33:o:201:PC1:O22	2.02	0.77
26:E1:315:HIS:HD1	26:E1:372:SER:HG	0.97	0.76
7:J:121:ASP:OD1	7:J:159:ARG:NH2	2.19	0.76
24:a:268:LEU:HD22	24:a:412:VAL:HG23	1.68	0.76
7:J:119:ARG:NH2	10:H:226:LYS:O	2.19	0.76
7:j:121:ASP:OD1	7:j:159:ARG:NH2	2.18	0.76
26:C1:178:ARG:NH1	26:C1:307:GLU:OE1	2.19	0.76
24:A:357:LYS:O	24:A:372:TYR:OH	2.02	0.76
26:A2:468:GLN:NE2	26:A2:506:ASP:OD2	2.19	0.76
7:j:119:ARG:NH2	10:h:226:LYS:O	2.19	0.75
3:t:73:ASP:OD1	24:a:441:ARG:NH1	2.18	0.75
26:E2:483:ARG:NH2	27:F2:440:GLU:OE2	2.20	0.75
27:B1:185:TYR:OH	27:B1:325:GLU:OE2	2.04	0.74
26:A2:263:SER:O	26:A2:267:GLN:NE2	2.20	0.74
26:A1:468:GLN:NE2	26:A1:506:ASP:OD2	2.21	0.74
32:I1:136:GLU:N	32:I1:136:GLU:OE1	2.20	0.74
4:g:213:ARG:NH2	4:g:217:GLU:OE1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:205:ARG:NH2	15:p:82:ALA:O	2.20	0.74
2:I:205:ARG:NH2	15:P:82:ALA:O	2.21	0.73
7:j:212:SER:N	7:J:192:PRO:O	2.20	0.73
26:A1:263:SER:O	26:A1:267:GLN:NE2	2.21	0.73
7:j:192:PRO:O	7:J:212:SER:N	2.21	0.73
7:J:155:ARG:NH1	7:J:169:GLU:OE2	2.22	0.73
27:F2:185:TYR:OH	27:F2:325:GLU:OE2	2.03	0.72
31:G1:129:ASP:OD1	31:G1:132:ARG:NH2	2.23	0.72
26:E2:445:GLU:OE2	26:E2:472:ARG:NH1	2.22	0.72
4:G:213:ARG:NH2	4:G:217:GLU:OE1	2.22	0.72
17:l:40:ASN:OD1	17:l:43:ARG:NH2	2.23	0.72
26:A2:178:ARG:NH1	26:A2:307:GLU:OE1	2.23	0.72
29:d2:74:MET:SD	32:K2:130:ARG:NH2	2.63	0.72
7:j:155:ARG:NH1	7:j:169:GLU:OE2	2.22	0.71
8:s:64:TYR:OH	12:x:32:GLU:OE1	2.06	0.71
26:C1:445:GLU:OE2	26:C1:472:ARG:NH1	2.23	0.71
16:v:86:ARG:NH2	21:n:158:GLU:OE1	2.23	0.71
21:N:161:ARG:NH2	21:N:166:ALA:OXT	2.24	0.71
32:J1:137:ASP:OD2	32:K1:135:LYS:NZ	2.21	0.71
35:v:202:CDL:H671	35:B:601:CDL:H811	1.72	0.71
24:A:137:ASN:OD1	24:A:140:ARG:NH1	2.24	0.71
26:E1:445:GLU:OE2	26:E1:472:ARG:NH1	2.24	0.71
21:n:161:ARG:NH2	21:n:166:ALA:OXT	2.24	0.70
13:B:130:LYS:NZ	13:B:202:LYS:O	2.24	0.70
13:B:554:THR:HG23	14:R:116:LEU:HD21	1.72	0.70
26:E2:261:LYS:O	26:E2:264:THR:OG1	2.10	0.70
27:B2:185:TYR:OH	27:B2:325:GLU:OE2	2.09	0.70
3:T:82:ARG:NH1	24:A:316:GLU:OE2	2.25	0.70
25:i2:78:GLU:OE2	25:i2:82:ARG:NH1	2.24	0.70
13:b:130:LYS:NZ	13:b:202:LYS:O	2.24	0.70
27:F1:185:TYR:OH	27:F1:325:GLU:OE2	2.04	0.70
27:F1:307:ALA:O	27:F1:311:VAL:HG23	1.91	0.70
29:d2:173:GLU:OE2	32:N2:133:SER:OG	2.08	0.70
35:V:202:CDL:OA4	21:N:159:SER:OG	2.08	0.70
35:b:601:CDL:H811	35:V:202:CDL:H671	1.73	0.69
27:F2:307:ALA:O	27:F2:311:VAL:HG23	1.92	0.69
3:t:82:ARG:NH1	24:a:316:GLU:OE2	2.24	0.69
25:i1:78:GLU:OE2	25:i1:82:ARG:NH1	2.25	0.69
3:T:19:ARG:O	3:T:22:ARG:NH1	2.26	0.69
26:E1:261:LYS:O	26:E1:264:THR:OG1	2.09	0.69
24:a:137:ASN:OD1	24:a:140:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:40:ASN:OD1	17:L:43:ARG:NH2	2.25	0.69
26:E2:318:ILE:HD11	26:E2:373:LEU:HD11	1.75	0.69
32:L2:111:GLY:O	32:L2:115:GLN:NE2	2.26	0.69
26:A1:227:THR:OG1	37:A1:601:ATP:O1B	2.07	0.69
14:r:25:GLU:OE1	14:r:30:ARG:NH2	2.26	0.69
16:V:90:LYS:NZ	35:V:202:CDL:OB3	2.21	0.69
4:G:147:GLN:OE1	4:G:179:ARG:NH2	2.26	0.69
3:t:19:ARG:O	3:t:22:ARG:NH1	2.27	0.68
26:C2:202:LYS:NZ	26:C2:517:GLU:OE2	2.26	0.68
28:g1:265:GLU:OE2	28:g1:269:ARG:NH2	2.26	0.68
16:V:86:ARG:NH2	21:N:158:GLU:OE1	2.26	0.68
26:C1:63:LEU:O	26:C1:67:ILE:HG23	1.94	0.68
26:E1:213:GLY:H	26:E1:374:THR:HG22	1.58	0.68
14:R:25:GLU:OE1	14:R:30:ARG:NH2	2.26	0.68
13:b:215:THR:OG1	13:b:218:ASP:OD1	2.13	0.68
26:C2:509:ASP:OD1	26:C2:511:LYS:NZ	2.27	0.68
19:d:172:GLN:OE1	19:d:175:ARG:NH1	2.27	0.67
26:C2:63:LEU:O	26:C2:67:ILE:HG23	1.93	0.67
9:u:113:THR:O	17:l:56:ARG:NH1	2.27	0.67
31:G1:135:VAL:HG22	31:G1:140:PHE:CD2	2.30	0.67
26:A2:202:LYS:NZ	26:A2:479:LEU:O	2.27	0.67
22:F:101:SER:OG	24:A:428:PRO:O	2.08	0.67
26:E2:213:GLY:H	26:E2:374:THR:HG22	1.58	0.67
31:G2:129:ASP:OD1	31:G2:132:ARG:NH2	2.27	0.67
24:a:107:CYS:SG	24:a:108:GLU:N	2.68	0.67
10:H:222:ARG:NH1	34:H:301:LMT:O4'	2.28	0.67
13:B:215:THR:OG1	13:B:218:ASP:OD1	2.13	0.67
9:U:113:THR:O	17:L:56:ARG:NH1	2.27	0.67
24:A:107:CYS:SG	24:A:108:GLU:N	2.66	0.67
32:K1:105:ILE:CG2	32:L1:108:MET:HE3	2.24	0.66
16:v:90:LYS:NZ	35:v:202:CDL:OB3	2.21	0.66
26:C2:468:GLN:NE2	26:C2:506:ASP:OD2	2.28	0.66
4:g:147:GLN:OE1	4:g:179:ARG:NH2	2.27	0.66
8:S:80:ASN:OD1	9:U:80:ARG:NH2	2.29	0.66
10:h:222:ARG:NH1	34:h:301:LMT:O4'	2.28	0.66
19:D:172:GLN:OE1	19:D:175:ARG:NH1	2.28	0.66
26:E1:468:GLN:NE2	26:E1:506:ASP:OD2	2.29	0.66
28:g2:265:GLU:OE2	28:g2:269:ARG:NH2	2.29	0.65
6:k:224:PHE:OXT	7:j:87:ARG:NE	2.30	0.65
26:E2:238:LYS:NZ	26:E2:276:ASP:OD2	2.28	0.65
32:L2:124:LEU:HD22	32:L2:142:THR:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:s:80:ASN:OD1	9:u:80:ARG:NH2	2.30	0.65
6:K:224:PHE:OXT	7:J:87:ARG:NE	2.29	0.65
28:g2:185:ASP:OD1	28:g2:189:GLN:NE2	2.29	0.65
31:G2:186:LYS:NZ	31:G2:187:PRO:O	2.22	0.65
26:E1:206:ALA:O	26:E1:431:GLN:NE2	2.30	0.65
13:b:425:ASP:OD2	31:G1:240:ARG:NH2	2.30	0.64
13:b:554:THR:HG23	14:r:116:LEU:HD21	1.79	0.64
31:G2:135:VAL:HG22	31:G2:140:PHE:CD2	2.32	0.64
26:C1:260:GLN:NE2	26:C1:321:ASP:OD2	2.31	0.64
26:E2:316:CYS:HB3	26:E2:373:LEU:HD12	1.78	0.64
32:L1:99:ALA:O	32:L1:102:SER:OG	2.13	0.64
27:B2:126:GLU:OE1	31:G2:78:ARG:NH2	2.31	0.64
27:F1:544:GLU:N	27:F1:544:GLU:OE1	2.31	0.64
27:D2:176:CYS:SG	27:D2:279:ARG:NH1	2.70	0.64
27:F1:543:GLU:OE1	27:F1:543:GLU:N	2.30	0.64
3:T:104:LEU:O	24:A:315:TYR:OH	2.16	0.64
26:E2:118:GLU:OE1	27:D2:86:GLN:NE2	2.31	0.64
26:E1:315:HIS:CG	26:E1:372:SER:HG	2.15	0.64
26:A2:191:LYS:N	26:A2:363:LYS:O	2.32	0.63
26:C1:509:ASP:OD1	26:C1:511:LYS:NZ	2.31	0.63
7:j:122:ARG:NH1	20:m:127:GLU:OE2	2.32	0.63
26:E2:206:ALA:O	26:E2:431:GLN:NE2	2.31	0.63
27:F2:543:GLU:N	27:F2:543:GLU:OE1	2.31	0.63
26:A1:178:ARG:NH1	26:A1:307:GLU:OE1	2.31	0.63
27:D1:176:CYS:SG	27:D1:279:ARG:NH1	2.72	0.63
32:H1:111:GLY:HA3	32:Q1:109:SER:OG	1.98	0.63
3:t:104:LEU:O	24:a:315:TYR:OH	2.17	0.63
26:C2:260:GLN:NE2	26:C2:321:ASP:OD2	2.32	0.63
32:L2:146:MET:HE2	32:L2:146:MET:HA	1.79	0.63
27:F1:80:ASN:ND2	27:F1:99:GLN:O	2.32	0.63
35:c:401:CDL:H431	35:c:401:CDL:H392	1.81	0.63
36:J:302:PEE:H59	35:C:401:CDL:H271	1.80	0.62
17:l:113:ASP:OD1	17:l:141:ARG:NH1	2.32	0.62
28:g2:186:ARG:NH2	30:e2:62:ALA:O	2.32	0.62
7:J:122:ARG:NH1	20:M:127:GLU:OE2	2.32	0.62
6:k:215:PHE:CZ	32:P1:146:MET:HE1	2.34	0.62
26:C2:206:ALA:O	26:C2:431:GLN:NE2	2.32	0.62
26:A1:214:GLN:NE2	26:A1:216:GLU:OE1	2.33	0.62
31:G1:101:GLU:O	31:G1:105:ASN:ND2	2.32	0.62
26:E2:468:GLN:NE2	26:E2:506:ASP:OD2	2.33	0.62
32:K2:138:LEU:HD22	32:L2:125:VAL:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:472:GLY:O	24:a:476:LEU:N	2.32	0.62
28:g1:101:GLU:O	28:g1:194:ARG:NH1	2.33	0.62
26:C2:342:GLY:N	26:C2:346:TYR:O	2.33	0.62
26:E1:198:MET:O	26:E1:237:GLN:NE2	2.32	0.62
28:g1:161:ASP:OD1	28:g1:162:ARG:NH1	2.33	0.62
17:L:113:ASP:OD1	17:L:141:ARG:NH1	2.32	0.61
22:F:129:VAL:O	22:F:133:SER:OG	2.13	0.61
26:C1:342:GLY:N	26:C1:346:TYR:O	2.31	0.61
26:A2:442:MET:HE1	26:A2:497:LEU:HD22	1.82	0.61
26:C1:202:LYS:NZ	26:C1:517:GLU:OE2	2.33	0.61
13:B:511:GLN:O	13:B:515:THR:HG23	2.00	0.61
31:G2:101:GLU:O	31:G2:105:ASN:ND2	2.33	0.61
26:A1:528:HIS:HB3	26:A1:531:ILE:HD12	1.83	0.61
32:K2:107:LEU:C	32:K2:108:MET:HE2	2.26	0.61
25:i2:65:ARG:NE	27:B2:464:GLN:OE1	2.33	0.61
26:C2:225:GLY:O	26:C2:229:VAL:HG23	2.00	0.61
32:K1:157:VAL:O	32:K1:160:SER:OG	2.15	0.61
32:N1:151:PHE:CZ	32:N1:155:ILE:HD11	2.35	0.61
26:A2:260:GLN:NE2	26:A2:321:ASP:OD2	2.34	0.61
5:o:59:ARG:NH2	12:x:20:GLN:OE1	2.34	0.60
35:b:601:CDL:OA3	13:B:101:ARG:NH1	2.32	0.60
13:b:511:GLN:O	13:b:515:THR:HG23	2.01	0.60
27:F2:80:ASN:ND2	27:F2:99:GLN:O	2.34	0.60
26:E1:385:ASP:OD2	28:g1:293:ARG:NH1	2.35	0.60
5:O:59:ARG:NH2	12:X:20:GLN:OE1	2.34	0.60
26:C2:262:ARG:NH1	27:D2:192:PRO:O	2.34	0.60
27:B2:222:LYS:NZ	27:B2:375:ILE:O	2.29	0.60
32:J2:105:ILE:O	32:K2:108:MET:HE1	2.01	0.60
26:C1:468:GLN:NE2	26:C1:506:ASP:OD2	2.34	0.60
13:b:101:ARG:NH1	35:B:601:CDL:OA3	2.33	0.60
32:L1:136:GLU:O	32:L1:140:THR:HG23	2.02	0.60
9:u:94:ARG:NH2	23:w:42:GLU:OE2	2.35	0.59
2:I:186:ALA:HB1	11:E:286:GLU:HG3	1.83	0.59
26:A1:442:MET:HE1	26:A1:497:LEU:HD22	1.84	0.59
26:E2:76:THR:O	26:E2:95:LEU:N	2.34	0.59
24:A:472:GLY:O	24:A:476:LEU:N	2.31	0.59
28:g2:237:GLU:OE1	28:g2:239:THR:N	2.30	0.59
26:C1:225:GLY:O	26:C1:229:VAL:HG23	2.01	0.59
32:P1:113:VAL:HG22	32:Q1:114:ALA:CB	2.32	0.59
13:B:244:ASN:OD1	16:V:14:ARG:NH2	2.36	0.59
28:g2:101:GLU:O	28:g2:194:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:84:CYS:HB3	24:A:334:LEU:HD21	1.85	0.59
27:B2:228:GLY:O	27:B2:233:LYS:NZ	2.35	0.59
26:A2:528:HIS:HB3	26:A2:531:ILE:HD12	1.83	0.59
10:H:162:ASP:O	17:L:138:ARG:NH2	2.36	0.59
27:D2:220:GLY:O	27:D2:377:THR:OG1	2.21	0.58
27:D2:348:SER:OG	27:D2:353:ARG:NH2	2.36	0.58
26:E1:483:ARG:NH2	27:F1:440:GLU:OE2	2.35	0.58
22:f:101:SER:OG	24:a:428:PRO:O	2.10	0.58
24:A:111:GLU:N	24:A:111:GLU:OE1	2.36	0.58
13:b:260:LEU:O	13:B:266:SER:OG	2.20	0.58
3:t:84:CYS:HB3	24:a:334:LEU:HD21	1.85	0.58
31:G2:135:VAL:HG22	31:G2:140:PHE:CE2	2.39	0.58
27:B1:228:GLY:O	27:B1:233:LYS:NZ	2.36	0.58
31:G2:203:ARG:NH2	31:G2:207:GLN:O	2.37	0.58
1:q:70:GLU:OE2	1:q:70:GLU:N	2.37	0.58
23:w:106:ALA:HB2	24:a:214:MET:CE	2.33	0.58
1:Q:70:GLU:OE2	1:Q:70:GLU:N	2.37	0.58
13:b:244:ASN:OD1	16:v:14:ARG:NH2	2.35	0.58
1:Q:111:ALA:O	4:G:225:LYS:NZ	2.37	0.58
9:U:94:ARG:NH2	23:W:42:GLU:OE2	2.34	0.58
24:a:111:GLU:N	24:a:111:GLU:OE1	2.37	0.58
24:A:354:ASP:OD1	24:A:375:GLU:N	2.36	0.58
27:D2:422:GLY:O	27:D2:537:TYR:OH	2.17	0.58
27:D1:348:SER:OG	27:D1:353:ARG:NH2	2.36	0.58
27:F2:119:GLU:OE2	27:F2:188:HIS:NE2	2.36	0.57
24:a:336:ASP:OD1	24:a:337:PRO:HA	2.04	0.57
26:C1:253:CYS:HB2	26:C1:281:THR:HG22	1.85	0.57
26:C2:178:ARG:NH1	26:C2:307:GLU:OE1	2.37	0.57
18:c:106:ARG:NH1	18:c:109:GLU:O	2.37	0.57
24:a:354:ASP:OD1	24:a:375:GLU:N	2.36	0.57
26:E2:198:MET:O	26:E2:237:GLN:NE2	2.36	0.57
10:h:162:ASP:O	17:l:138:ARG:NH2	2.36	0.57
3:T:95:LEU:O	24:A:326:ARG:NH2	2.38	0.57
6:K:162:PHE:CD2	32:P2:154:ILE:HD11	2.39	0.57
28:g2:233:GLU:OE1	32:J2:130:ARG:NH2	2.38	0.57
16:v:78:ALA:HB2	35:v:202:CDL:H672	1.87	0.57
5:O:39:SER:OG	33:O:201:PC1:O22	2.10	0.57
17:L:100:GLU:N	17:L:100:GLU:OE1	2.38	0.57
27:F1:506:LYS:NZ	27:F1:538:MET:O	2.38	0.57
29:d1:110:ASP:OD1	29:d1:111:GLY:N	2.38	0.57
3:t:95:LEU:O	24:a:326:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:78:ALA:HB2	35:V:202:CDL:H672	1.86	0.57
27:B2:220:GLY:N	27:B2:384:THR:OG1	2.38	0.56
26:E1:318:ILE:HD11	26:E1:373:LEU:HD11	1.86	0.56
27:D1:356:SER:OG	27:D1:357:ALA:N	2.37	0.56
2:i:186:ALA:HB1	11:e:286:GLU:HG3	1.85	0.56
32:K2:105:ILE:O	32:L2:108:MET:HE1	2.06	0.56
17:l:100:GLU:OE1	17:l:100:GLU:N	2.38	0.56
26:C2:107:GLN:NE2	26:C2:137:ASP:OD2	2.38	0.56
27:D1:80:ASN:ND2	27:D1:99:GLN:O	2.39	0.56
23:w:106:ALA:HB2	24:a:214:MET:HE1	1.87	0.56
32:H1:105:ILE:HB	32:I1:104:ALA:HB1	1.88	0.56
26:C2:388:ALA:O	26:C2:392:THR:OG1	2.15	0.56
31:G1:186:LYS:NZ	31:G1:187:PRO:O	2.23	0.56
27:B2:543:GLU:N	27:B2:543:GLU:OE1	2.36	0.56
5:o:35:SER:O	5:o:39:SER:OG	2.23	0.56
35:b:601:CDL:H472	35:B:601:CDL:H472	1.87	0.56
26:C2:253:CYS:HB2	26:C2:281:THR:HG22	1.87	0.56
26:C1:262:ARG:NH1	27:D1:192:PRO:O	2.38	0.56
6:K:215:PHE:CZ	32:P2:146:MET:HE1	2.40	0.55
18:C:106:ARG:NH1	18:C:109:GLU:O	2.39	0.55
29:d1:71:GLU:OE1	32:N1:130:ARG:NH2	2.38	0.55
5:o:128:ARG:NH1	10:h:208:ASP:OD2	2.39	0.55
17:L:44:GLU:OE2	17:L:190:ARG:NH2	2.40	0.55
26:C2:315:HIS:HD1	26:C2:372:SER:HG	1.53	0.55
26:C1:509:ASP:OD2	26:C1:564:LYS:NZ	2.39	0.55
5:O:35:SER:O	5:O:39:SER:OG	2.25	0.55
27:F1:283:GLU:OE2	27:F1:283:GLU:N	2.36	0.55
1:q:111:ALA:O	4:g:225:LYS:NZ	2.39	0.55
27:B1:209:LYS:NZ	27:B1:539:CYS:O	2.39	0.55
32:J1:105:ILE:HB	32:K1:104:ALA:HB1	1.89	0.55
32:M1:123:ALA:HB2	32:N1:122:ALA:HB1	1.88	0.55
22:f:71:SER:N	24:a:208:ASP:OD1	2.39	0.55
18:C:99:GLN:O	18:C:106:ARG:NH2	2.39	0.55
13:b:266:SER:OG	13:B:260:LEU:O	2.24	0.55
32:O2:103:ALA:O	32:O2:160:SER:OG	2.23	0.55
27:B2:465:ASP:OD2	28:g2:55:SER:OG	2.25	0.54
27:B2:491:ARG:O	27:B2:494:SER:OG	2.24	0.54
32:J1:134:ILE:HD13	32:K1:132:PRO:HG3	1.89	0.54
5:O:128:ARG:NH1	10:H:208:ASP:OD2	2.40	0.54
9:u:64:ARG:NH1	35:u:201:CDL:OA4	2.39	0.54
18:c:99:GLN:O	18:c:106:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C1:388:ALA:O	26:C1:392:THR:OG1	2.21	0.54
26:C2:221:ASP:O	26:C2:226:LYS:NZ	2.38	0.54
27:D2:356:SER:OG	27:D2:357:ALA:N	2.38	0.54
26:E1:217:LEU:HD11	26:E1:379:ILE:HD12	1.88	0.54
27:D1:86:GLN:NE2	27:D1:93:ASP:OD2	2.41	0.54
27:D1:220:GLY:O	27:D1:377:THR:OG1	2.25	0.54
32:K1:120:LEU:HD21	32:L1:121:PHE:HB2	1.90	0.54
1:q:83:PHE:O	1:q:86:VAL:HG22	2.08	0.54
22:f:130:TYR:OH	22:f:261:ARG:NH1	2.39	0.54
32:I1:117:ILE:HG13	32:I1:149:LEU:HD13	1.89	0.54
26:A1:200:GLY:O	26:A1:482:GLN:NE2	2.41	0.54
13:B:330:LYS:O	13:B:333:ASP:OD1	2.26	0.54
2:I:186:ALA:HB1	11:E:286:GLU:CG	2.38	0.54
26:E2:244:THR:HG21	26:E2:249:LYS:HB2	1.90	0.54
29:d2:174:LEU:HD13	30:e2:16:MET:HE3	1.90	0.54
27:F1:257:VAL:O	27:F1:339:ARG:NE	2.34	0.54
13:b:487:VAL:HG11	13:b:509:LEU:HD12	1.90	0.54
17:l:207:GLY:O	2:I:191:ARG:NH1	2.41	0.54
7:J:191:PHE:HA	7:J:194:VAL:O	2.08	0.53
27:B2:539:CYS:SG	27:B2:548:LYS:NZ	2.72	0.53
13:b:160:GLU:OE1	13:b:161:ASN:ND2	2.41	0.53
31:G1:135:VAL:HG22	31:G1:140:PHE:CE2	2.43	0.53
1:Q:83:PHE:O	1:Q:86:VAL:HG22	2.08	0.53
26:E2:315:HIS:CG	26:E2:372:SER:HG	2.25	0.53
25:i2:62:ASP:OD2	25:i2:65:ARG:NH2	2.41	0.53
32:K2:120:LEU:HD21	32:L2:121:PHE:HB2	1.91	0.53
26:A1:215:ARG:NH2	26:A1:399:ASP:OD1	2.40	0.53
17:l:44:GLU:OE2	17:l:190:ARG:NH2	2.40	0.53
2:i:178:ARG:NH1	11:e:294:ASP:OD1	2.41	0.53
13:B:487:VAL:HG11	13:B:509:LEU:HD12	1.90	0.53
27:F1:537:TYR:OH	27:F1:538:MET:HE2	2.09	0.53
22:F:71:SER:N	24:A:208:ASP:OD2	2.41	0.53
27:D2:495:GLN:NE2	27:D2:509:ARG:O	2.41	0.53
32:N2:151:PHE:CZ	32:N2:155:ILE:HD11	2.44	0.53
26:E1:343:ARG:NH2	27:D1:398:ASP:OD2	2.41	0.53
32:K1:105:ILE:HG21	32:L1:104:ALA:HB1	1.91	0.53
18:C:47:SER:OG	19:D:49:ARG:NH1	2.40	0.53
27:D2:119:GLU:OE2	27:D2:188:HIS:NE2	2.40	0.53
1:Q:10:SER:O	1:Q:14:GLU:HG3	2.08	0.53
26:C1:221:ASP:O	26:C1:226:LYS:NZ	2.42	0.53
2:i:186:ALA:HB1	11:e:286:GLU:CG	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F2:258:GLY:O	27:F2:339:ARG:NE	2.42	0.52
6:k:148:LEU:O	6:k:151:ARG:NH2	2.41	0.52
24:a:237:GLU:OE1	24:a:269:ARG:NH1	2.43	0.52
13:B:333:ASP:OD1	13:B:334:TYR:N	2.42	0.52
13:B:442:ASN:OD1	13:B:444:SER:OG	2.27	0.52
26:E2:231:VAL:HG12	26:E2:235:ILE:HD12	1.92	0.52
27:F2:257:VAL:O	27:F2:339:ARG:NE	2.36	0.52
26:E1:76:THR:O	26:E1:95:LEU:N	2.43	0.52
26:E2:78:GLU:OE2	26:E2:141:ARG:NH1	2.42	0.52
35:C:401:CDL:H511	35:C:401:CDL:H151	1.90	0.52
32:O1:156:CYS:SG	32:P1:110:VAL:HG11	2.49	0.52
7:j:191:PHE:HA	7:j:194:VAL:O	2.08	0.52
14:R:35:ILE:HG21	14:R:40:ILE:HD11	1.90	0.52
21:N:115:ASN:OD1	23:W:33:ARG:NH2	2.42	0.52
32:L2:108:MET:HE2	32:L2:108:MET:HA	1.91	0.52
32:L1:105:ILE:HB	32:M1:104:ALA:HB1	1.92	0.52
24:a:191:GLU:OE1	24:a:191:GLU:N	2.41	0.52
5:O:31:ARG:NH2	18:C:73:LEU:HD12	2.23	0.52
32:L1:123:ALA:HB2	32:M1:122:ALA:HB1	1.92	0.52
22:f:129:VAL:O	22:f:133:SER:OG	2.14	0.52
32:H1:100:SER:OG	32:Q1:102:SER:CB	2.58	0.52
32:H1:101:LEU:HD11	32:Q1:98:VAL:HG13	1.92	0.52
14:r:35:ILE:HG21	14:r:40:ILE:HD11	1.91	0.52
32:I2:120:LEU:HD12	32:I2:149:LEU:HD12	1.92	0.52
27:D1:495:GLN:NE2	27:D1:509:ARG:O	2.43	0.52
5:o:31:ARG:NH2	18:c:73:LEU:HD12	2.25	0.52
9:U:64:ARG:NH1	35:U:201:CDL:OA4	2.42	0.52
3:T:30:VAL:HG23	3:T:30:VAL:O	2.10	0.52
4:G:149:ASP:OD2	4:G:155:ARG:NH2	2.43	0.52
27:F1:356:SER:OG	27:F1:357:ALA:N	2.42	0.52
25:i1:65:ARG:NE	27:B1:464:GLN:OE1	2.43	0.51
27:B2:119:GLU:OE2	27:B2:188:HIS:NE2	2.40	0.51
32:H1:107:LEU:HD21	32:Q1:159:MET:HB2	1.91	0.51
26:E2:343:ARG:NH2	27:D2:398:ASP:OD2	2.42	0.51
27:B2:209:LYS:NZ	27:B2:539:CYS:O	2.26	0.51
27:D2:164:ARG:NH1	27:D2:174:ASP:OD2	2.44	0.51
1:q:50:GLU:HA	1:q:53:ASP:OD1	2.10	0.51
27:B2:342:GLN:O	27:B2:346:GLU:HG3	2.11	0.51
32:J1:134:ILE:HD11	32:K1:129:ALA:HA	1.92	0.51
2:I:178:ARG:NH1	11:E:294:ASP:OD1	2.43	0.51
26:A2:200:GLY:O	26:A2:482:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:E1:244:THR:HG21	26:E1:249:LYS:HB2	1.93	0.51
32:I1:120:LEU:HD12	32:I1:149:LEU:HD12	1.93	0.51
16:v:25:TRP:O	19:d:117:ARG:NH1	2.44	0.51
19:D:230:ASN:ND2	23:W:19:ALA:O	2.44	0.51
31:G2:178:VAL:HA	31:G2:209:ARG:O	2.10	0.51
32:O2:98:VAL:HG11	32:P2:97:GLY:HA3	1.92	0.51
27:F1:119:GLU:OE2	27:F1:188:HIS:NE2	2.40	0.51
31:G1:178:VAL:HA	31:G1:209:ARG:O	2.11	0.51
26:C1:147:ASP:O	26:C1:177:ARG:NH2	2.44	0.51
32:H1:107:LEU:HD22	32:Q1:106:ALA:HB1	1.92	0.51
32:I1:102:SER:OG	32:I1:163:LEU:HD13	2.11	0.51
26:C2:445:GLU:OE2	26:C2:472:ARG:NH1	2.44	0.50
16:V:25:TRP:O	19:D:117:ARG:NH1	2.44	0.50
27:B2:283:GLU:OE2	27:B2:283:GLU:N	2.42	0.50
27:F2:356:SER:OG	27:F2:357:ALA:N	2.42	0.50
26:A1:58:GLU:HA	26:A1:63:LEU:HD21	1.93	0.50
32:H1:148:PHE:O	32:H1:152:LEU:HD13	2.11	0.50
6:K:148:LEU:O	6:K:151:ARG:NH2	2.43	0.50
12:X:18:VAL:HG22	12:X:19:PRO:HD3	1.92	0.50
26:E1:78:GLU:OE2	26:E1:141:ARG:NH1	2.45	0.50
11:E:189:SER:O	21:N:161:ARG:NH1	2.42	0.50
32:I1:120:LEU:HD21	32:J1:121:PHE:HB2	1.93	0.50
6:k:174:PHE:CE2	32:O1:154:ILE:HG21	2.46	0.50
32:J1:98:VAL:HG11	32:K1:97:GLY:HA2	1.94	0.50
4:g:149:ASP:OD2	4:g:155:ARG:NH2	2.43	0.50
21:n:115:ASN:OD1	23:w:33:ARG:NH2	2.43	0.50
1:Q:114:ASP:O	4:G:225:LYS:NZ	2.45	0.50
27:B1:342:GLN:O	27:B1:346:GLU:HG3	2.11	0.50
27:F1:530:ASP:N	27:F1:530:ASP:OD2	2.44	0.50
1:q:114:ASP:O	4:g:225:LYS:NZ	2.45	0.50
3:t:30:VAL:O	3:t:30:VAL:HG23	2.11	0.50
4:g:208:LYS:O	4:g:209:ASP:OD1	2.30	0.50
12:x:18:VAL:HG22	12:x:19:PRO:HD3	1.93	0.50
26:A1:82:VAL:O	26:A1:136:GLY:HA2	2.11	0.50
26:E1:120:ASP:OD1	26:E1:121:ASN:N	2.45	0.50
19:d:230:ASN:ND2	23:w:19:ALA:O	2.45	0.50
27:B2:551:LYS:O	27:B2:555:GLU:OE1	2.30	0.50
32:J2:134:ILE:HD11	32:K2:129:ALA:HA	1.94	0.50
27:F1:107:LEU:HD23	27:F1:148:ASP:HA	1.94	0.50
27:F2:193:LEU:N	27:F2:196:ASP:OD1	2.45	0.49
26:E1:231:VAL:HG12	26:E1:235:ILE:HD12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F1:193:LEU:N	27:F1:196:ASP:OD2	2.45	0.49
17:L:2:THR:N	19:D:192:GLU:OE1	2.44	0.49
24:A:237:GLU:OE1	24:A:269:ARG:NH1	2.45	0.49
13:b:166:GLU:OE2	13:b:166:GLU:N	2.43	0.49
24:A:191:GLU:OE1	24:A:191:GLU:N	2.41	0.49
27:B2:160:GLU:N	27:B2:160:GLU:OE1	2.45	0.49
27:F2:308:ARG:NH2	27:F2:346:GLU:OE2	2.44	0.49
26:A1:191:LYS:N	26:A1:363:LYS:O	2.45	0.49
26:C1:425:ARG:NH2	38:B1:601:ADP:O3B	2.45	0.49
27:F2:107:LEU:HD23	27:F2:148:ASP:HA	1.93	0.49
27:B1:160:GLU:N	27:B1:160:GLU:OE1	2.45	0.49
27:B1:297:VAL:HG12	27:B1:311:VAL:CG2	2.43	0.49
17:l:2:THR:N	19:d:192:GLU:OE1	2.45	0.49
24:a:431:CYS:SG	24:a:433:SER:OG	2.67	0.49
26:A2:215:ARG:H	26:A2:399:ASP:HB2	1.77	0.49
26:E1:512:GLU:OE1	26:E1:515:ARG:NE	2.44	0.49
29:d1:74:MET:SD	32:K1:130:ARG:NH2	2.84	0.49
6:K:162:PHE:HD2	32:P2:154:ILE:HD11	1.77	0.49
26:E2:120:ASP:OD1	26:E2:121:ASN:N	2.45	0.49
26:E1:297:LEU:O	26:E1:300:TYR:N	2.46	0.49
17:l:123:ALA:O	17:l:130:ARG:NH1	2.46	0.49
26:A2:310:ARG:NH1	26:A2:360:ARG:O	2.46	0.49
6:K:156:TYR:OH	23:W:105:SER:OG	2.29	0.49
26:A2:215:ARG:NH2	26:A2:399:ASP:OD1	2.46	0.49
32:O2:156:CYS:SG	32:P2:110:VAL:HG11	2.52	0.49
27:B1:230:GLY:N	38:B1:601:ADP:O3B	2.44	0.49
32:I1:120:LEU:CD1	32:I1:149:LEU:HD12	2.43	0.49
26:C2:120:ASP:OD2	26:C2:121:ASN:N	2.44	0.48
27:B2:220:GLY:O	27:B2:377:THR:OG1	2.30	0.48
32:M2:123:ALA:HB2	32:N2:122:ALA:HB1	1.95	0.48
32:Q1:151:PHE:CZ	32:Q1:155:ILE:HD11	2.48	0.48
5:O:87:ASP:OD1	5:O:87:ASP:N	2.46	0.48
26:A2:231:VAL:HG12	26:A2:235:ILE:HD12	1.95	0.48
26:C2:158:VAL:N	26:C2:167:ASP:OD2	2.46	0.48
26:E1:316:CYS:HB3	26:E1:373:LEU:HD12	1.95	0.48
29:d1:174:LEU:HD13	30:e1:16:MET:HE3	1.94	0.48
32:O1:134:ILE:HD12	32:O1:138:LEU:HD21	1.94	0.48
1:q:100:GLN:HA	1:q:103:ASN:OD1	2.14	0.48
32:I2:134:ILE:HD11	32:J2:129:ALA:HA	1.95	0.48
32:H1:131:ASN:HB3	32:H1:134:ILE:HG22	1.95	0.48
17:L:123:ALA:O	17:L:130:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C2:509:ASP:OD2	26:C2:564:LYS:NZ	2.46	0.48
27:F2:530:ASP:OD2	27:F2:531:LEU:HD22	2.13	0.48
26:C1:344:GLU:N	28:g1:305:GLU:OE2	2.46	0.48
13:b:290:ARG:NH1	13:B:107:THR:O	2.47	0.48
7:J:56:LYS:O	7:J:60:GLN:NE2	2.47	0.48
26:C2:147:ASP:O	26:C2:177:ARG:NH2	2.46	0.48
26:A1:198:MET:HE2	26:A1:233:ALA:HB2	1.96	0.48
27:B1:234:THR:HG22	38:B1:601:ADP:O2A	2.12	0.48
27:B1:209:LYS:NZ	27:B1:492:PHE:O	2.35	0.48
31:G1:203:ARG:NH2	31:G1:207:GLN:O	2.47	0.48
13:b:189:GLU:OE1	14:r:19:ARG:NH2	2.46	0.48
26:E2:217:LEU:HD11	26:E2:379:ILE:HD12	1.95	0.48
26:E1:172:ILE:HG22	26:E1:173:PRO:O	2.14	0.48
26:E1:534:THR:O	26:E1:538:GLU:OE1	2.31	0.48
27:F1:258:GLY:O	27:F1:339:ARG:NE	2.46	0.48
31:G1:232:VAL:O	31:G1:232:VAL:HG13	2.13	0.48
1:q:10:SER:O	1:q:14:GLU:HG3	2.14	0.48
26:A2:82:VAL:O	26:A2:136:GLY:HA2	2.14	0.48
26:E2:531:ILE:HD11	26:E2:548:LYS:HB3	1.95	0.48
27:B2:297:VAL:HG12	27:B2:311:VAL:CG2	2.43	0.48
26:C1:393:ASN:O	26:C1:397:ILE:HG12	2.13	0.48
32:I1:98:VAL:HG11	32:J1:97:GLY:CA	2.44	0.48
7:j:56:LYS:O	7:j:60:GLN:NE2	2.46	0.48
26:C2:442:MET:HE1	26:C2:497:LEU:HD22	1.95	0.48
1:Q:100:GLN:HA	1:Q:103:ASN:OD1	2.14	0.48
26:A2:58:GLU:HA	26:A2:63:LEU:HD21	1.95	0.48
26:A2:462:LEU:O	26:A2:467:ARG:NH2	2.46	0.48
26:E2:338:ARG:NH1	27:F2:352:GLY:O	2.46	0.48
26:E1:202:LYS:NZ	26:E1:517:GLU:OE2	2.40	0.48
26:C1:206:ALA:O	26:C1:431:GLN:NE2	2.45	0.47
27:B1:456:LEU:HD21	27:B1:485:ARG:HB3	1.96	0.47
32:L1:117:ILE:HG13	32:L1:149:LEU:HD13	1.95	0.47
13:B:259:GLY:O	13:B:262:ASN:ND2	2.44	0.47
26:E2:231:VAL:HG11	26:E2:485:TYR:HE2	1.79	0.47
27:D2:233:LYS:N	38:D2:601:ADP:O1A	2.47	0.47
32:J1:105:ILE:CG2	32:K1:108:MET:HG3	2.44	0.47
32:P1:151:PHE:CZ	32:P1:155:ILE:HD11	2.49	0.47
5:o:87:ASP:OD1	5:o:87:ASP:N	2.46	0.47
32:L2:134:ILE:HG23	32:L2:134:ILE:O	2.13	0.47
32:L2:156:CYS:SG	32:M2:110:VAL:HG11	2.54	0.47
32:L1:110:VAL:O	32:L1:113:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:j:127:SER:OG	20:m:133:GLU:OE2	2.32	0.47
26:A2:214:GLN:NE2	26:A2:216:GLU:OE1	2.48	0.47
32:L2:146:MET:HE2	32:L2:146:MET:CA	2.43	0.47
32:N2:151:PHE:CE2	32:N2:155:ILE:HD11	2.49	0.47
13:B:189:GLU:OE1	14:R:19:ARG:NH2	2.46	0.47
26:E2:512:GLU:OE1	26:E2:515:ARG:NE	2.45	0.47
31:G2:232:VAL:HG13	31:G2:232:VAL:O	2.14	0.47
26:A1:462:LEU:O	26:A1:467:ARG:NH2	2.47	0.47
26:E1:231:VAL:HG11	26:E1:485:TYR:HE2	1.79	0.47
32:L1:124:LEU:HB2	32:L1:142:THR:HG21	1.96	0.47
5:o:141:ARG:NH2	10:h:220:GLU:OE2	2.44	0.47
35:b:601:CDL:H762	35:V:202:CDL:H673	1.96	0.47
35:v:202:CDL:H673	35:B:601:CDL:H762	1.96	0.47
5:O:84:ASN:ND2	5:O:87:ASP:OD1	2.48	0.47
31:G2:180:CYS:SG	31:G2:181:LEU:N	2.87	0.47
26:E1:278:MET:SD	26:E1:281:THR:OG1	2.73	0.47
26:E1:528:HIS:ND1	26:E1:531:ILE:HD12	2.30	0.47
26:C1:463:ASP:OD1	26:C1:465:SER:OG	2.27	0.47
31:G1:85:ARG:O	31:G1:89:LYS:HG3	2.15	0.47
32:H1:97:GLY:O	32:H1:101:LEU:HD13	2.14	0.47
32:H1:99:ALA:HB1	32:H1:163:LEU:O	2.14	0.47
32:I1:98:VAL:HG11	32:J1:97:GLY:HA2	1.96	0.47
6:k:217:THR:O	6:k:221:THR:OG1	2.29	0.47
9:u:114:ARG:NE	17:l:184:GLN:OE1	2.44	0.47
22:f:161:ALA:O	22:f:165:SER:OG	2.18	0.47
26:E2:150:ILE:HG22	26:E2:305:MET:HA	1.97	0.47
27:F2:395:ASP:OD2	28:g2:296:GLN:NE2	2.47	0.47
27:D2:209:LYS:NZ	27:D2:492:PHE:O	2.44	0.47
27:F1:526:GLY:O	27:F1:529:ASP:OD1	2.33	0.47
2:i:191:ARG:NH1	17:L:207:GLY:O	2.44	0.47
5:o:84:ASN:ND2	5:o:87:ASP:OD1	2.48	0.47
13:b:107:THR:O	13:B:290:ARG:NH1	2.48	0.47
13:b:362:THR:HG21	24:a:60:GLN:HB3	1.97	0.47
26:E2:351:PHE:HZ	27:D2:301:MET:HE2	1.80	0.47
29:d2:48:THR:HG23	29:d2:48:THR:O	2.15	0.47
27:F1:501:GLU:O	27:F1:505:GLY:N	2.39	0.47
36:j:302:PEE:C37	35:c:401:CDL:H271	2.44	0.47
1:Q:7:TYR:CG	1:Q:14:GLU:HG2	2.50	0.47
26:E2:172:ILE:HG22	26:E2:173:PRO:O	2.15	0.47
14:r:131:LYS:N	14:r:131:LYS:HD2	2.30	0.46
9:U:114:ARG:NE	17:L:184:GLN:OE1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D2:297:VAL:HG12	27:D2:311:VAL:HG13	1.96	0.46
27:D1:297:VAL:HG12	27:D1:311:VAL:HG13	1.97	0.46
31:G1:233:LEU:HD23	31:G1:233:LEU:H	1.81	0.46
32:L1:120:LEU:HD13	32:M1:121:PHE:HB3	1.97	0.46
26:C2:390:ILE:HB	26:C2:391:PRO:HD3	1.97	0.46
28:g1:185:ASP:OD2	30:e1:10:THR:OG1	2.33	0.46
26:A2:58:GLU:OE2	31:G2:156:ARG:NE	2.47	0.46
26:C2:512:GLU:OE2	26:C2:563:LYS:NZ	2.45	0.46
27:D2:160:GLU:N	27:D2:160:GLU:OE1	2.49	0.46
32:Q2:151:PHE:CE2	32:Q2:155:ILE:HD11	2.51	0.46
6:k:215:PHE:HZ	32:P1:146:MET:HE1	1.79	0.46
36:j:301:PEE:H46	23:w:85:PHE:HB3	1.98	0.46
32:O2:120:LEU:HD21	32:P2:121:PHE:HB2	1.97	0.46
32:I1:108:MET:HE3	32:J1:108:MET:HG2	1.97	0.46
32:K1:99:ALA:HB1	32:K1:164:LEU:HA	1.96	0.46
32:Q1:151:PHE:CE2	32:Q1:155:ILE:HD11	2.50	0.46
21:n:58:GLU:N	21:n:58:GLU:OE1	2.47	0.46
32:L2:134:ILE:HD13	32:M2:132:PRO:HB3	1.98	0.46
26:C1:394:VAL:HA	26:C1:397:ILE:HG12	1.95	0.46
32:M1:134:ILE:HG22	32:M1:136:GLU:H	1.80	0.46
26:A2:66:ARG:NH2	26:A2:70:TRP:O	2.37	0.46
26:C1:390:ILE:HB	26:C1:391:PRO:HD3	1.98	0.46
27:D1:138:GLU:N	27:D1:138:GLU:OE1	2.48	0.46
28:g1:186:ARG:NH2	30:e1:62:ALA:O	2.49	0.46
32:H1:109:SER:OG	32:I1:108:MET:HA	2.16	0.46
13:b:109:ASP:OD1	13:b:109:ASP:N	2.49	0.46
13:b:501:LEU:O	13:b:501:LEU:HG	2.16	0.46
1:Q:7:TYR:HD1	1:Q:13:GLN:HG2	1.79	0.46
26:E2:202:LYS:NZ	26:E2:517:GLU:OE2	2.43	0.46
26:E1:150:ILE:HG22	26:E1:305:MET:HA	1.97	0.46
27:B1:530:ASP:OD1	27:B1:530:ASP:N	2.46	0.46
14:R:71:LEU:HD21	20:M:184:LEU:HD22	1.98	0.46
24:A:431:CYS:SG	24:A:433:SER:OG	2.67	0.46
31:G1:228:LEU:HD21	31:G1:231:GLN:HB2	1.98	0.46
14:r:129:GLN:HA	14:r:133:ILE:HD12	1.97	0.46
27:F2:496:PRO:HD3	27:F2:506:LYS:HZ3	1.81	0.46
27:B1:526:GLY:O	27:B1:529:ASP:OD1	2.33	0.46
26:A1:310:ARG:NH1	26:A1:360:ARG:O	2.47	0.46
27:D1:465:ASP:OD1	28:g1:49:ARG:NH2	2.44	0.46
6:k:144:ALA:O	6:k:148:LEU:HD23	2.16	0.45
36:j:302:PEE:H60	35:c:401:CDL:H271	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:l:100:GLU:OE1	17:l:111:LYS:NZ	2.49	0.45
7:j:127:SER:OG	20:m:133:GLU:OE2	2.34	0.45
36:j:301:PEE:H46	23:w:85:PHE:HB3	1.98	0.45
28:g1:183:ILE:O	28:g1:187:LEU:HD23	2.17	0.45
29:d1:48:THR:O	29:d1:48:THR:HG23	2.15	0.45
31:G1:91:ASN:O	31:G1:92:GLN:HG2	2.16	0.45
32:L1:117:ILE:HG23	32:L1:121:PHE:CZ	2.51	0.45
26:E2:278:MET:SD	26:E2:281:THR:OG1	2.74	0.45
29:d2:41:PHE:N	29:d2:122:SER:O	2.49	0.45
31:G2:85:ARG:O	31:G2:89:LYS:HG3	2.16	0.45
31:G1:148:LEU:HD23	31:G1:160:LEU:HD21	1.98	0.45
13:B:166:GLU:OE2	13:B:166:GLU:N	2.44	0.45
26:A1:131:ARG:NH2	27:B1:105:ASN:OD1	2.48	0.45
13:b:497:ASP:OD1	13:b:498:PHE:N	2.48	0.45
27:D1:119:GLU:OE2	27:D1:188:HIS:NE2	2.43	0.45
32:M1:124:LEU:HA	32:N1:125:VAL:HG11	1.98	0.45
6:K:174:PHE:CE2	32:O2:154:ILE:HG21	2.52	0.45
21:N:58:GLU:OE1	21:N:58:GLU:N	2.47	0.45
31:G2:226:VAL:HG13	31:G2:226:VAL:O	2.17	0.45
25:i1:62:ASP:OD2	25:i1:65:ARG:NH2	2.47	0.45
6:K:215:PHE:CE2	32:P2:146:MET:HE1	2.52	0.45
17:L:100:GLU:OE1	17:L:111:LYS:NZ	2.50	0.45
26:E2:297:LEU:O	26:E2:300:TYR:N	2.49	0.45
27:F1:469:ILE:HD13	28:g1:65:MET:HE2	1.99	0.45
29:d1:84:VAL:HG22	29:d1:114:LEU:HD23	1.99	0.45
16:v:111:ARG:HB3	19:d:257:ILE:HD13	1.99	0.45
13:B:497:ASP:OD1	13:B:498:PHE:N	2.48	0.45
26:C2:442:MET:HE1	26:C2:497:LEU:HD13	1.99	0.45
27:D2:138:GLU:OE1	27:D2:138:GLU:N	2.49	0.45
32:L2:120:LEU:HD23	32:L2:146:MET:CE	2.47	0.45
27:D1:160:GLU:N	27:D1:160:GLU:OE1	2.49	0.45
32:L1:134:ILE:HD11	32:M1:135:LYS:HD3	1.98	0.45
26:C2:107:GLN:OE1	26:C2:138:SER:N	2.44	0.45
31:G2:233:LEU:HD23	31:G2:233:LEU:H	1.81	0.45
26:C1:107:GLN:OE1	26:C1:138:SER:N	2.45	0.45
1:q:7:TYR:CG	1:q:14:GLU:HG2	2.52	0.45
13:B:554:THR:CG2	14:R:116:LEU:HD21	2.46	0.45
35:C:401:CDL:H431	35:C:401:CDL:H392	1.98	0.45
26:A2:131:ARG:NH2	27:B2:105:ASN:OD1	2.49	0.45
26:A2:536:GLU:O	26:A2:539:LYS:NZ	2.37	0.45
27:F2:167:ASN:OD1	27:F2:171:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D2:87:VAL:O	27:D2:88:ILE:HD13	2.17	0.45
27:F1:167:ASN:OD1	27:F1:171:GLU:N	2.50	0.45
32:N1:151:PHE:CE2	32:N1:155:ILE:HD11	2.52	0.45
11:e:189:SER:O	21:n:161:ARG:NH1	2.46	0.44
24:A:470:GLU:O	24:A:474:LYS:NZ	2.48	0.44
28:g2:183:ILE:O	28:g2:187:LEU:HD23	2.17	0.44
26:A1:390:ILE:HB	26:A1:391:PRO:HD3	1.99	0.44
26:E1:145:ILE:HG22	26:E1:146:VAL:N	2.32	0.44
27:B1:168:VAL:HG13	27:B1:169:ILE:HG23	1.98	0.44
7:j:92:PHE:O	7:j:98:SER:OG	2.24	0.44
13:b:389:ARG:HH12	31:G1:249:LEU:HD11	1.83	0.44
26:C2:504:TYR:OH	26:C2:550:ARG:NH1	2.46	0.44
27:B1:522:THR:HG23	27:B1:527:GLU:HB2	2.00	0.44
32:P1:98:VAL:HG11	32:Q1:97:GLY:HA3	1.99	0.44
2:i:219:THR:HG23	15:p:23:LEU:HD13	2.00	0.44
12:x:61:GLU:O	12:x:73:ASN:ND2	2.50	0.44
13:b:259:GLY:O	13:b:262:ASN:ND2	2.45	0.44
13:B:109:ASP:OD2	13:B:109:ASP:N	2.49	0.44
18:C:73:LEU:HD13	19:D:60:HIS:ND1	2.32	0.44
26:C1:442:MET:HE1	26:C1:497:LEU:HD22	1.98	0.44
31:G1:226:VAL:HG13	31:G1:226:VAL:O	2.18	0.44
32:K1:120:LEU:CD2	32:L1:121:PHE:HB2	2.47	0.44
22:f:189:ASN:O	22:f:192:SER:OG	2.35	0.44
6:K:144:ALA:O	6:K:148:LEU:HD23	2.17	0.44
13:B:341:GLU:OE2	24:A:20:SER:N	2.51	0.44
13:B:501:LEU:HG	13:B:501:LEU:O	2.16	0.44
27:D2:251:PHE:HB2	27:D2:330:VAL:HG12	1.99	0.44
26:A1:66:ARG:NH2	26:A1:70:TRP:O	2.39	0.44
32:I1:105:ILE:HB	32:J1:104:ALA:HB1	1.98	0.44
32:K1:105:ILE:CG2	32:L1:104:ALA:HB1	2.48	0.44
32:O1:120:LEU:HD21	32:P1:121:PHE:CB	2.47	0.44
35:C:401:CDL:H452	34:C:404:LMT:H22	1.98	0.44
26:E2:145:ILE:HG22	26:E2:146:VAL:N	2.32	0.44
31:G2:91:ASN:O	31:G2:92:GLN:HG2	2.16	0.44
31:G1:131:LEU:O	31:G1:135:VAL:HG23	2.17	0.44
3:t:59:ARG:NH1	22:f:81:ALA:O	2.51	0.44
33:O:201:PC1:H153	33:O:201:PC1:O13	2.18	0.44
13:B:481:GLN:O	13:B:485:THR:OG1	2.29	0.44
35:V:202:CDL:OB5	35:V:202:CDL:O1	2.34	0.44
14:r:71:LEU:HD21	20:m:184:LEU:HD22	1.99	0.44
16:V:111:ARG:HB3	19:D:257:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:E2:103:LEU:O	26:E2:142:THR:OG1	2.34	0.44
26:E1:531:ILE:HD11	26:E1:548:LYS:HB3	1.98	0.44
27:F1:395:ASP:OD1	27:F1:398:ASP:N	2.51	0.44
32:L1:108:MET:N	32:L1:108:MET:HE2	2.32	0.44
24:a:55:THR:OG1	24:a:56:PRO:HD3	2.18	0.44
16:V:82:ILE:HD11	35:V:202:CDL:C63	2.48	0.44
25:i2:64:LYS:NZ	27:B2:468:ALA:O	2.46	0.44
26:A2:261:LYS:HG3	26:A2:264:THR:HG22	2.00	0.44
26:E2:225:GLY:O	26:E2:229:VAL:HG23	2.17	0.44
32:J2:156:CYS:SG	32:K2:110:VAL:HG11	2.58	0.44
26:E1:225:GLY:O	26:E1:229:VAL:HG23	2.17	0.44
1:Q:99:ARG:O	1:Q:103:ASN:OD1	2.36	0.44
28:g2:99:PRO:O	28:g2:194:ARG:NH2	2.46	0.44
32:M2:163:LEU:HD21	32:N2:164:LEU:HD22	1.99	0.44
32:P2:113:VAL:HG22	32:Q2:114:ALA:CB	2.47	0.44
32:N2:117:ILE:HD13	32:N2:146:MET:HE1	1.99	0.43
32:O1:151:PHE:O	32:O1:155:ILE:HG12	2.18	0.43
33:o:201:PC1:H153	33:o:201:PC1:O13	2.18	0.43
32:H2:134:ILE:HD11	32:H2:137:ASP:OD2	2.18	0.43
7:J:94:ASN:OD1	7:J:94:ASN:N	2.51	0.43
26:E1:253:CYS:SG	26:E1:254:ILE:N	2.92	0.43
32:H1:120:LEU:HD21	32:I1:121:PHE:HB2	1.99	0.43
32:H1:151:PHE:CZ	32:H1:155:ILE:HD11	2.53	0.43
1:q:7:TYR:HD1	1:q:13:GLN:HG2	1.84	0.43
22:F:189:ASN:O	22:F:192:SER:OG	2.35	0.43
26:A2:390:ILE:HB	26:A2:391:PRO:HD3	2.00	0.43
27:D2:260:ARG:HB2	27:D2:263:GLU:HG2	2.01	0.43
32:H2:125:VAL:HG11	32:Q2:124:LEU:HA	2.01	0.43
27:F1:168:VAL:HG13	27:F1:169:ILE:HG23	2.01	0.43
30:e1:21:ARG:HA	30:e1:24:LEU:HD12	2.01	0.43
32:J1:98:VAL:HG11	32:K1:97:GLY:CA	2.48	0.43
13:b:442:ASN:OD1	13:b:444:SER:OG	2.31	0.43
18:c:73:LEU:HD13	19:d:60:HIS:ND1	2.33	0.43
6:K:124:LYS:HB2	18:C:60:LEU:HD11	2.00	0.43
27:B2:168:VAL:HG13	27:B2:169:ILE:HG23	1.99	0.43
27:B2:476:SER:OG	27:B2:477:GLU:N	2.52	0.43
29:d2:72:GLY:O	32:L2:130:ARG:NH2	2.50	0.43
32:Q2:151:PHE:CZ	32:Q2:155:ILE:HD11	2.53	0.43
26:E1:351:PHE:HZ	27:D1:301:MET:HE2	1.83	0.43
26:C1:310:ARG:NH1	26:C1:360:ARG:O	2.48	0.43
27:B2:183:LYS:NZ	27:B2:325:GLU:OE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:O2:148:PHE:CZ	32:P2:146:MET:SD	3.11	0.43
25:i1:83:ASN:O	25:i1:87:ASN:ND2	2.49	0.43
27:B1:97:ASP:HB3	27:B1:98:GLU:OE1	2.18	0.43
32:I1:105:ILE:HG23	32:J1:108:MET:SD	2.58	0.43
24:a:209:ARG:NH1	24:a:229:ASP:OD2	2.52	0.43
2:I:219:THR:HG23	15:P:23:LEU:HD13	1.99	0.43
26:E2:396:SER:O	27:D2:301:MET:HE1	2.18	0.43
31:G2:131:LEU:O	31:G2:135:VAL:HG23	2.18	0.43
32:M2:148:PHE:CG	32:N2:146:MET:HE2	2.53	0.43
26:C1:158:VAL:N	26:C1:167:ASP:OD2	2.51	0.43
27:F1:537:TYR:CZ	27:F1:538:MET:HE2	2.54	0.43
31:G1:180:CYS:SG	31:G1:181:LEU:N	2.92	0.43
32:L1:109:SER:O	32:L1:113:VAL:HG13	2.19	0.43
26:A1:246:ASP:OD2	26:A1:246:ASP:O	2.37	0.43
27:F1:542:LEU:HD22	27:F1:542:LEU:O	2.18	0.43
13:b:341:GLU:OE2	24:a:20:SER:N	2.52	0.43
35:c:401:CDL:OA7	35:c:401:CDL:HA61	2.17	0.43
21:n:52:THR:HG22	21:n:53:SER:N	2.34	0.43
20:M:171:ASN:O	20:M:172:PHE:HB2	2.19	0.43
27:F2:506:LYS:NZ	27:F2:538:MET:O	2.43	0.43
26:A1:261:LYS:HG3	26:A1:264:THR:HG22	2.01	0.43
20:m:171:ASN:O	20:m:172:PHE:HB2	2.19	0.43
21:n:37:THR:HG22	21:n:37:THR:O	2.19	0.43
12:X:32:GLU:OE2	34:X:101:LMT:H52	2.19	0.43
13:B:132:ALA:HB2	13:B:159:CYS:SG	2.59	0.43
13:B:487:VAL:O	13:B:491:HIS:ND1	2.51	0.43
21:N:52:THR:HG22	21:N:53:SER:N	2.33	0.43
27:F2:168:VAL:HG13	27:F2:169:ILE:HG23	2.01	0.43
27:D1:251:PHE:HB2	27:D1:330:VAL:HG12	2.01	0.43
1:q:53:ASP:OD1	1:q:54:ARG:N	2.52	0.42
5:O:141:ARG:NH2	10:H:220:GLU:OE2	2.45	0.42
13:B:554:THR:HG23	14:R:116:LEU:CD2	2.46	0.42
21:N:37:THR:O	21:N:37:THR:HG22	2.19	0.42
26:E1:338:ARG:NH1	27:F1:352:GLY:O	2.52	0.42
32:I1:124:LEU:HD22	32:I1:142:THR:HG21	2.01	0.42
13:b:474:THR:HG21	14:r:133:ILE:HD11	2.00	0.42
18:c:81:GLN:NE2	22:f:253:GLY:O	2.52	0.42
12:X:61:GLU:O	12:X:73:ASN:ND2	2.52	0.42
13:B:545:GLU:O	13:B:549:THR:HG23	2.19	0.42
35:C:401:CDL:H582	23:W:69:PHE:HB3	2.01	0.42
26:C2:472:ARG:NH1	26:C2:501:VAL:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:234:THR:HG22	38:B2:601:ADP:PA	2.59	0.42
27:F2:422:GLY:O	27:F2:537:TYR:OH	2.31	0.42
29:d2:84:VAL:HG22	29:d2:114:LEU:HD23	2.01	0.42
32:I2:153:GLY:O	32:I2:157:VAL:HG23	2.19	0.42
27:F1:534:MET:HE1	27:F1:552:MET:SD	2.59	0.42
32:J1:124:LEU:HA	32:K1:125:VAL:HG11	2.01	0.42
32:K1:96:ALA:HB1	32:K1:99:ALA:HB3	2.00	0.42
5:o:149:ARG:NH2	19:d:256:PRO:O	2.48	0.42
35:v:202:CDL:H1O1	35:v:202:CDL:PB2	2.41	0.42
14:R:129:GLN:HA	14:R:133:ILE:HD12	2.01	0.42
27:D2:209:LYS:HG2	27:D2:511:VAL:HG11	2.01	0.42
4:g:193:GLU:OE2	4:g:193:GLU:N	2.47	0.42
18:C:39:TYR:O	18:C:43:VAL:HG23	2.18	0.42
18:C:81:GLN:NE2	22:F:253:GLY:O	2.53	0.42
27:B2:210:VAL:HG23	27:B2:214:LEU:HD12	2.01	0.42
32:J2:102:SER:HB2	32:K2:104:ALA:HB2	2.02	0.42
32:M2:103:ALA:O	32:M2:107:LEU:HG	2.20	0.42
32:O2:134:ILE:HD12	32:O2:138:LEU:HD21	2.00	0.42
32:L1:99:ALA:HB1	32:L1:163:LEU:O	2.19	0.42
12:x:32:GLU:OE2	34:x:101:LMT:H52	2.19	0.42
13:b:478:THR:HG23	13:b:479:GLU:N	2.34	0.42
26:A2:87:ASP:OD1	27:B2:353:ARG:NH2	2.52	0.42
27:F2:316:LEU:HD21	27:F2:374:ARG:HB2	2.02	0.42
27:F2:488:LYS:HB3	27:F2:536:PHE:CE1	2.54	0.42
32:L2:105:ILE:HG22	32:M2:104:ALA:HB1	2.01	0.42
32:L2:150:GLU:O	32:L2:154:ILE:HG12	2.20	0.42
27:B1:222:LYS:NZ	27:B1:375:ILE:O	2.48	0.42
6:k:215:PHE:CE2	32:P1:146:MET:HE1	2.55	0.42
5:O:149:ARG:NH2	19:D:256:PRO:O	2.46	0.42
32:H1:108:MET:HE3	32:I1:108:MET:CG	2.49	0.42
32:H1:128:THR:HG23	32:H1:135:LYS:CG	2.50	0.42
1:q:24:VAL:HG12	15:p:41:PRO:HB3	2.02	0.42
6:k:124:LYS:HB2	18:c:60:LEU:HD11	2.01	0.42
35:c:401:CDL:H511	35:c:401:CDL:H151	2.00	0.42
35:c:401:CDL:H731	35:c:401:CDL:OB9	2.19	0.42
3:T:59:ARG:NH1	22:F:81:ALA:O	2.52	0.42
13:B:478:THR:HG23	13:B:479:GLU:N	2.34	0.42
26:E2:253:CYS:SG	26:E2:254:ILE:N	2.93	0.42
6:k:204:TYR:OH	32:O1:151:PHE:HB2	2.19	0.42
36:j:302:PEE:C38	35:c:401:CDL:H271	2.49	0.42
16:v:82:ILE:HD11	35:v:202:CDL:C63	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B2:473:ASP:OD2	27:B2:474:GLU:N	2.53	0.42
26:A1:231:VAL:HG12	26:A1:235:ILE:HD12	2.00	0.42
27:B1:473:ASP:OD2	27:B1:474:GLU:N	2.52	0.42
32:J1:139:PHE:O	32:J1:142:THR:OG1	2.30	0.42
22:f:199:ASP:O	22:f:203:ARG:NH2	2.47	0.42
1:Q:24:VAL:HG12	15:P:41:PRO:HB3	2.01	0.42
12:X:61:GLU:OE1	12:X:61:GLU:N	2.50	0.42
26:A2:198:MET:HE2	26:A2:233:ALA:HB2	2.01	0.42
26:C1:386:VAL:HG11	26:C1:403:PHE:HE2	1.85	0.42
27:D1:228:GLY:O	27:D1:233:LYS:NZ	2.49	0.42
18:c:32:ILE:O	18:c:36:ASN:ND2	2.53	0.42
6:K:166:ARG:NH2	32:P2:150:GLU:OE2	2.53	0.42
24:A:55:THR:OG1	24:A:56:PRO:HD3	2.19	0.42
32:K2:112:GLY:CA	32:L2:115:GLN:OE1	2.68	0.42
27:B1:210:VAL:HG23	27:B1:214:LEU:HD12	2.02	0.42
32:L1:136:GLU:O	32:L1:136:GLU:HG3	2.20	0.42
35:b:601:CDL:H832	13:B:260:LEU:HD21	2.02	0.41
24:a:63:ASP:OD1	24:a:63:ASP:N	2.48	0.41
19:D:259:ASP:HB3	34:D:403:LMT:H4B	2.01	0.41
26:E2:298:ALA:HB3	26:E2:299:PRO:HD3	2.02	0.41
32:P2:146:MET:HE3	32:P2:146:MET:HB3	1.96	0.41
26:C1:226:LYS:HD2	26:C1:378:VAL:HG13	2.01	0.41
27:B1:289:PHE:O	27:B1:292:SER:OG	2.26	0.41
27:F1:491:ARG:HB3	27:F1:537:TYR:HB2	2.02	0.41
27:D1:209:LYS:HG2	27:D1:511:VAL:HG11	2.02	0.41
27:D1:260:ARG:HB2	27:D1:263:GLU:HG2	2.02	0.41
30:e1:33:MET:O	30:e1:37:GLN:HG3	2.20	0.41
32:K1:97:GLY:O	32:K1:101:LEU:HG	2.20	0.41
7:j:94:ASN:OD1	7:j:94:ASN:N	2.51	0.41
5:O:100:ASP:OD2	34:O:202:LMT:O6B	2.38	0.41
23:W:106:ALA:HB2	24:A:214:MET:HE1	2.02	0.41
26:E1:317:VAL:HG23	26:E1:374:THR:OG1	2.21	0.41
27:B1:526:GLY:HA2	27:B1:529:ASP:OD1	2.20	0.41
32:J1:106:ALA:CB	32:J1:160:SER:OG	2.68	0.41
6:k:214:THR:O	6:k:217:THR:HG22	2.21	0.41
18:c:39:TYR:O	18:c:43:VAL:HG23	2.20	0.41
24:A:268:LEU:HD22	24:A:412:VAL:CG2	2.44	0.41
26:E2:500:GLY:HA2	26:E2:505:LEU:HD12	2.02	0.41
28:g2:237:GLU:OE1	28:g2:239:THR:OG1	2.33	0.41
32:M2:134:ILE:HG22	32:M2:136:GLU:H	1.84	0.41
27:B1:526:GLY:CA	27:B1:529:ASP:OD1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H1:97:GLY:O	32:H1:101:LEU:CD1	2.68	0.41
24:a:268:LEU:HD22	24:a:412:VAL:CG2	2.45	0.41
4:G:193:GLU:OE2	4:G:193:GLU:N	2.47	0.41
32:O2:151:PHE:O	32:O2:155:ILE:HG12	2.20	0.41
26:A1:379:ILE:HD11	26:A1:394:VAL:HG21	2.02	0.41
6:K:214:THR:O	6:K:217:THR:HG22	2.21	0.41
13:B:362:THR:HG21	24:A:60:GLN:HB3	2.02	0.41
24:A:209:ARG:NH1	24:A:229:ASP:OD2	2.53	0.41
27:F2:346:GLU:O	27:F2:350:LEU:HG	2.20	0.41
26:A1:479:LEU:HD21	26:A1:496:VAL:HG12	2.02	0.41
29:d1:70:SER:N	29:d1:86:ARG:O	2.54	0.41
32:I1:109:SER:OG	32:J1:107:LEU:O	2.25	0.41
32:M1:117:ILE:HG12	32:M1:146:MET:SD	2.60	0.41
5:o:100:ASP:OD2	34:o:202:LMT:O6B	2.38	0.41
12:x:18:VAL:N	12:x:19:PRO:CD	2.84	0.41
19:d:259:ASP:HB3	34:d:403:LMT:H4B	2.02	0.41
22:f:99:VAL:HG12	22:f:100:SER:N	2.36	0.41
26:E2:528:HIS:ND1	26:E2:531:ILE:HD12	2.36	0.41
27:B2:289:PHE:O	27:B2:292:SER:OG	2.33	0.41
26:E1:298:ALA:HB3	26:E1:299:PRO:HD3	2.02	0.41
32:P1:151:PHE:CE2	32:P1:155:ILE:HD11	2.55	0.41
13:b:449:ASP:HB2	13:b:450:PRO:HD3	2.02	0.41
12:X:18:VAL:N	12:X:19:PRO:CD	2.84	0.41
24:A:51:GLU:O	24:A:55:THR:HG23	2.21	0.41
27:F2:501:GLU:O	27:F2:505:GLY:N	2.40	0.41
32:L2:123:ALA:HB2	32:M2:122:ALA:HB1	2.01	0.41
32:O2:152:LEU:HD22	32:P2:110:VAL:HG13	2.02	0.41
26:A2:225:GLY:O	26:A2:229:VAL:HG23	2.20	0.41
1:Q:124:ARG:NH2	5:O:156:ASN:OD1	2.54	0.41
35:O:203:CDL:H472	35:C:401:CDL:C27	2.51	0.41
6:K:204:TYR:OH	32:O2:151:PHE:HB2	2.20	0.41
13:B:449:ASP:HB2	13:B:450:PRO:HD3	2.02	0.41
24:A:287:ASN:O	24:A:288:LEU:HD23	2.20	0.41
26:E2:178:ARG:NH2	26:E2:311:ASP:OD2	2.54	0.41
31:G2:228:LEU:HD21	31:G2:231:GLN:HB2	2.02	0.41
26:E1:390:ILE:HB	26:E1:391:PRO:HD3	2.03	0.41
26:C1:178:ARG:NH2	26:C1:311:ASP:OD2	2.54	0.41
27:F1:316:LEU:HD21	27:F1:374:ARG:HB2	2.03	0.41
29:d1:171:GLY:HA2	30:e1:16:MET:HE1	2.03	0.41
4:g:134:SER:O	4:g:137:ASN:ND2	2.54	0.41
3:T:83:GLU:OE1	24:A:439:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A2:199:THR:OG1	26:A2:236:ASN:OD1	2.25	0.41
32:I2:136:GLU:O	32:I2:140:THR:OG1	2.31	0.41
32:K1:105:ILE:O	32:K1:108:MET:HB2	2.20	0.41
13:b:260:LEU:HD21	35:B:601:CDL:H832	2.03	0.40
26:A2:160:ASP:OD1	26:A2:164:ASN:N	2.54	0.40
27:D2:343:ALA:O	27:D2:347:VAL:HG23	2.21	0.40
27:F1:346:GLU:O	27:F1:350:LEU:HG	2.21	0.40
13:b:487:VAL:HG11	13:b:509:LEU:CD1	2.52	0.40
1:Q:50:GLU:HA	1:Q:53:ASP:OD1	2.21	0.40
26:A2:215:ARG:NE	26:A2:399:ASP:OD2	2.49	0.40
27:B2:491:ARG:HB3	27:B2:536:PHE:O	2.21	0.40
32:K1:105:ILE:HB	32:L1:104:ALA:HB1	2.03	0.40
5:o:97:TYR:OH	20:m:113:GLU:OE2	2.39	0.40
26:C2:54:ILE:HG22	26:C2:56:PRO:CD	2.51	0.40
26:C2:393:ASN:O	26:C2:397:ILE:HG12	2.22	0.40
27:B2:308:ARG:NH2	27:B2:346:GLU:OE2	2.54	0.40
27:F2:358:VAL:O	27:F2:358:VAL:HG12	2.22	0.40
26:C1:531:ILE:HD11	26:C1:548:LYS:HB3	2.03	0.40
27:D1:238:MET:HE1	27:D1:267:LEU:HD13	2.03	0.40
32:J1:105:ILE:HG23	32:K1:108:MET:HG3	2.01	0.40
13:b:263:THR:O	13:b:263:THR:HG22	2.22	0.40
24:a:380:ASP:OD1	24:a:381:VAL:N	2.54	0.40
10:H:26:SER:O	10:H:28:VAL:N	2.54	0.40
24:A:75:ASP:OD1	24:A:76:ILE:N	2.52	0.40
31:G2:228:LEU:H	31:G2:228:LEU:HD23	1.86	0.40
32:H2:100:SER:HB2	32:Q2:163:LEU:HD22	2.04	0.40
26:C1:442:MET:HE1	26:C1:497:LEU:HD13	2.04	0.40
27:D1:343:ALA:O	27:D1:347:VAL:HG23	2.21	0.40
32:I1:108:MET:CE	32:J1:108:MET:HE3	2.52	0.40
32:I1:132:PRO:O	32:I1:135:LYS:HB3	2.22	0.40
13:B:263:THR:HG22	13:B:263:THR:O	2.22	0.40
22:F:99:VAL:HG12	22:F:100:SER:N	2.36	0.40
26:E2:88:GLY:N	26:E2:130:ASP:OD2	2.45	0.40
26:E2:310:ARG:NH1	26:E2:360:ARG:O	2.55	0.40
27:D2:228:GLY:O	27:D2:233:LYS:NZ	2.50	0.40
25:i1:80:LEU:HD13	27:B1:530:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	Q	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	q	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
2	I	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	i	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
3	T	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
4	G	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	g	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
5	O	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
5	o	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
6	K	115/224 (51%)	112 (97%)	3 (3%)	0	100	100
6	k	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
7	J	174/229 (76%)	166 (95%)	8 (5%)	0	100	100
7	j	174/229 (76%)	166 (95%)	8 (5%)	0	100	100
8	S	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
9	U	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
10	H	224/239 (94%)	216 (96%)	8 (4%)	0	100	100
10	h	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
11	E	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
11	e	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
12	X	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
13	B	480/571 (84%)	466 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	b	480/571 (84%)	465 (97%)	15 (3%)	0	100	100
14	R	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
14	r	131/134 (98%)	124 (95%)	7 (5%)	0	100	100
15	P	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
16	V	108/111 (97%)	108 (100%)	0	0	100	100
16	v	108/111 (97%)	108 (100%)	0	0	100	100
17	L	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	l	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
18	C	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
18	c	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
19	D	251/310 (81%)	246 (98%)	5 (2%)	0	100	100
19	d	251/310 (81%)	246 (98%)	5 (2%)	0	100	100
20	M	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	m	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
21	N	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	n	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
22	F	184/267 (69%)	173 (94%)	11 (6%)	0	100	100
22	f	184/267 (69%)	173 (94%)	11 (6%)	0	100	100
23	W	93/106 (88%)	87 (94%)	6 (6%)	0	100	100
23	w	93/106 (88%)	88 (95%)	5 (5%)	0	100	100
24	A	461/536 (86%)	445 (96%)	16 (4%)	0	100	100
24	a	461/536 (86%)	445 (96%)	16 (4%)	0	100	100
25	i1	38/145 (26%)	38 (100%)	0	0	100	100
25	i2	38/145 (26%)	38 (100%)	0	0	100	100
26	A1	510/565 (90%)	488 (96%)	22 (4%)	0	100	100
26	A2	510/565 (90%)	489 (96%)	21 (4%)	0	100	100
26	C1	503/565 (89%)	487 (97%)	16 (3%)	0	100	100
26	C2	503/565 (89%)	485 (96%)	18 (4%)	0	100	100
26	E1	505/565 (89%)	482 (95%)	23 (5%)	0	100	100
26	E2	505/565 (89%)	485 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	B1	477/560 (85%)	453 (95%)	22 (5%)	2 (0%)	30	60
27	B2	477/560 (85%)	454 (95%)	21 (4%)	2 (0%)	30	60
27	D1	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
27	D2	473/560 (84%)	452 (96%)	21 (4%)	0	100	100
27	F1	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
27	F2	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
28	g1	270/314 (86%)	260 (96%)	10 (4%)	0	100	100
28	g2	270/314 (86%)	260 (96%)	10 (4%)	0	100	100
29	d1	141/183 (77%)	136 (96%)	5 (4%)	0	100	100
29	d2	141/183 (77%)	137 (97%)	4 (3%)	0	100	100
30	e1	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
30	e2	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	G1	178/252 (71%)	159 (89%)	19 (11%)	0	100	100
31	G2	178/252 (71%)	159 (89%)	19 (11%)	0	100	100
32	H1	69/166 (42%)	69 (100%)	0	0	100	100
32	H2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	I1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	I2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	J1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	J2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	L1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	M1	69/166 (42%)	63 (91%)	6 (9%)	0	100	100
32	M2	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	N1	69/166 (42%)	69 (100%)	0	0	100	100
32	N2	69/166 (42%)	69 (100%)	0	0	100	100
32	O1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	O2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	P1	69/166 (42%)	66 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	P2	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	Q1	69/166 (42%)	69 (100%)	0	0	100	100
32	Q2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
All	All	16388/22836 (72%)	15771 (96%)	613 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	B1	358	VAL
27	B2	357	ALA
27	B2	358	VAL
27	B1	357	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	119/120 (99%)	117 (98%)	2 (2%)	56	83
1	q	119/120 (99%)	119 (100%)	0	100	100
2	I	71/197 (36%)	71 (100%)	0	100	100
2	i	71/197 (36%)	71 (100%)	0	100	100
3	T	77/106 (73%)	77 (100%)	0	100	100
3	t	77/106 (73%)	77 (100%)	0	100	100
4	G	93/214 (44%)	93 (100%)	0	100	100
4	g	93/214 (44%)	93 (100%)	0	100	100
5	O	127/129 (98%)	127 (100%)	0	100	100
5	o	127/129 (98%)	127 (100%)	0	100	100
6	K	100/175 (57%)	100 (100%)	0	100	100
6	k	100/175 (57%)	100 (100%)	0	100	100
7	J	160/195 (82%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	j	160/195 (82%)	160 (100%)	0	100	100
8	S	86/113 (76%)	86 (100%)	0	100	100
8	s	86/113 (76%)	86 (100%)	0	100	100
9	U	76/98 (78%)	76 (100%)	0	100	100
9	u	76/98 (78%)	76 (100%)	0	100	100
10	H	197/204 (97%)	197 (100%)	0	100	100
10	h	197/204 (97%)	197 (100%)	0	100	100
11	E	118/258 (46%)	118 (100%)	0	100	100
11	e	118/258 (46%)	118 (100%)	0	100	100
12	X	70/71 (99%)	70 (100%)	0	100	100
12	x	70/71 (99%)	70 (100%)	0	100	100
13	B	428/491 (87%)	428 (100%)	0	100	100
13	b	428/491 (87%)	428 (100%)	0	100	100
14	R	116/117 (99%)	116 (100%)	0	100	100
14	r	116/117 (99%)	116 (100%)	0	100	100
15	P	91/113 (80%)	91 (100%)	0	100	100
15	p	91/113 (80%)	91 (100%)	0	100	100
16	V	86/87 (99%)	86 (100%)	0	100	100
16	v	86/87 (99%)	86 (100%)	0	100	100
17	L	177/178 (99%)	177 (100%)	0	100	100
17	l	177/178 (99%)	177 (100%)	0	100	100
18	C	107/338 (32%)	107 (100%)	0	100	100
18	c	107/338 (32%)	107 (100%)	0	100	100
19	D	218/259 (84%)	218 (100%)	0	100	100
19	d	218/259 (84%)	217 (100%)	1 (0%)	86	96
20	M	77/156 (49%)	77 (100%)	0	100	100
20	m	77/156 (49%)	77 (100%)	0	100	100
21	N	138/144 (96%)	138 (100%)	0	100	100
21	n	138/144 (96%)	138 (100%)	0	100	100
22	F	155/218 (71%)	155 (100%)	0	100	100
22	f	155/218 (71%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	84/89 (94%)	83 (99%)	1 (1%)	67	89
23	w	84/89 (94%)	83 (99%)	1 (1%)	67	89
24	A	392/447 (88%)	392 (100%)	0	100	100
24	a	392/447 (88%)	391 (100%)	1 (0%)	91	97
25	i1	37/125 (30%)	37 (100%)	0	100	100
25	i2	37/125 (30%)	37 (100%)	0	100	100
26	A1	421/454 (93%)	421 (100%)	0	100	100
26	A2	421/454 (93%)	421 (100%)	0	100	100
26	C1	415/454 (91%)	415 (100%)	0	100	100
26	C2	415/454 (91%)	415 (100%)	0	100	100
26	E1	416/454 (92%)	416 (100%)	0	100	100
26	E2	416/454 (92%)	416 (100%)	0	100	100
27	B1	390/447 (87%)	384 (98%)	6 (2%)	60	85
27	B2	390/447 (87%)	390 (100%)	0	100	100
27	D1	388/447 (87%)	388 (100%)	0	100	100
27	D2	388/447 (87%)	387 (100%)	1 (0%)	91	97
27	F1	388/447 (87%)	382 (98%)	6 (2%)	60	85
27	F2	388/447 (87%)	387 (100%)	1 (0%)	91	97
28	g1	228/257 (89%)	228 (100%)	0	100	100
28	g2	228/257 (89%)	228 (100%)	0	100	100
29	d1	118/144 (82%)	118 (100%)	0	100	100
29	d2	118/144 (82%)	118 (100%)	0	100	100
30	e1	57/61 (93%)	57 (100%)	0	100	100
30	e2	57/61 (93%)	57 (100%)	0	100	100
31	G1	154/212 (73%)	154 (100%)	0	100	100
31	G2	154/212 (73%)	154 (100%)	0	100	100
32	H1	52/133 (39%)	47 (90%)	5 (10%)	7	22
32	H2	52/133 (39%)	52 (100%)	0	100	100
32	I1	52/133 (39%)	52 (100%)	0	100	100
32	I2	52/133 (39%)	52 (100%)	0	100	100
32	J1	52/133 (39%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	J2	52/133 (39%)	52 (100%)	0	100	100
32	K1	52/133 (39%)	50 (96%)	2 (4%)	28	63
32	K2	52/133 (39%)	52 (100%)	0	100	100
32	L1	52/133 (39%)	50 (96%)	2 (4%)	28	63
32	L2	52/133 (39%)	48 (92%)	4 (8%)	10	31
32	M1	52/133 (39%)	51 (98%)	1 (2%)	52	81
32	M2	52/133 (39%)	52 (100%)	0	100	100
32	N1	52/133 (39%)	52 (100%)	0	100	100
32	N2	52/133 (39%)	52 (100%)	0	100	100
32	O1	52/133 (39%)	52 (100%)	0	100	100
32	O2	52/133 (39%)	52 (100%)	0	100	100
32	P1	52/133 (39%)	52 (100%)	0	100	100
32	P2	52/133 (39%)	52 (100%)	0	100	100
32	Q1	52/133 (39%)	52 (100%)	0	100	100
32	Q2	52/133 (39%)	52 (100%)	0	100	100
All	All	13790/18698 (74%)	13756 (100%)	34 (0%)	91	98

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	d	42	LYS
23	w	105	SER
24	a	122	SER
1	Q	15	ILE
1	Q	17	LEU
23	W	105	SER
27	F2	538	MET
27	D2	135	ASP
32	L2	105	ILE
32	L2	130	ARG
32	L2	134	ILE
32	L2	159	MET
27	B1	335	ASP
27	B1	482	VAL
27	B1	527	GLU
27	B1	538	MET
27	B1	542	LEU

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Mol	Chain	Res	Type
27	B1	543	GLU
27	F1	528	CYS
27	F1	533	GLU
27	F1	536	PHE
27	F1	537	TYR
27	F1	538	MET
27	F1	542	LEU
32	H1	101	LEU
32	H1	117	ILE
32	H1	130	ARG
32	H1	131	ASN
32	H1	155	ILE
32	K1	108	MET
32	K1	113	VAL
32	L1	113	VAL
32	L1	146	MET
32	M1	128	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	q	25	GLN
1	q	133	HIS
2	i	206	HIS
7	j	137	HIS
7	j	190	GLN
7	j	210	HIS
10	h	33	GLN
10	h	39	HIS
10	h	67	ASN
12	x	74	HIS
13	b	119	GLN
13	b	528	ASN
14	r	54	HIS
15	p	67	ASN
16	v	80	HIS
17	l	77	ASN
18	c	33	GLN
18	c	36	ASN
20	m	132	ASN
22	f	155	GLN
22	f	166	ASN

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Mol	Chain	Res	Type
22	f	242	GLN
23	w	49	GLN
24	a	155	ASN
24	a	321	GLN
1	Q	71	GLN
1	Q	133	HIS
2	I	206	HIS
6	K	116	GLN
7	J	210	HIS
7	J	216	GLN
10	H	33	GLN
10	H	39	HIS
13	B	119	GLN
13	B	526	HIS
13	B	568	HIS
14	R	54	HIS
15	P	67	ASN
16	V	80	HIS
17	L	77	ASN
18	C	34	HIS
20	M	132	ASN
21	N	91	HIS
22	F	155	GLN
22	F	166	ASN
22	F	242	GLN
23	W	49	GLN
24	A	155	ASN
26	A2	267	GLN
26	C2	99	GLN
26	C2	382	GLN
27	B2	86	GLN
27	B2	265	ASN
27	B2	269	HIS
27	B2	328	GLN
27	F2	80	ASN
27	F2	86	GLN
27	F2	248	HIS
27	F2	265	ASN
27	F2	269	HIS
27	F2	326	GLN
27	F2	521	GLN
27	D2	81	HIS

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Mol	Chain	Res	Type
27	D2	144	GLN
27	D2	154	GLN
27	D2	197	GLN
27	D2	205	GLN
27	D2	248	HIS
27	D2	269	HIS
28	g2	135	ASN
28	g2	140	ASN
28	g2	143	GLN
29	d2	44	GLN
30	e2	39	HIS
30	e2	57	ASN
31	G2	192	GLN
31	G2	247	GLN
32	N2	115	GLN
26	A1	267	GLN
26	C1	382	GLN
27	B1	205	GLN
27	B1	265	ASN
27	B1	269	HIS
27	B1	328	GLN
27	F1	86	GLN
27	F1	123	HIS
27	F1	248	HIS
27	F1	265	ASN
27	F1	269	HIS
27	F1	326	GLN
27	F1	521	GLN
27	D1	86	GLN
27	D1	144	GLN
27	D1	154	GLN
27	D1	197	GLN
27	D1	248	HIS
27	D1	269	HIS
27	D1	342	GLN
28	g1	179	GLN
28	g1	223	GLN
29	d1	172	GLN
30	e1	39	HIS
30	e1	57	ASN
31	G1	91	ASN
32	N1	115	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

54 ligands are 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$
34	LMT	h	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.04	2 (4%)
37	ATP	A1	601	-	28,33,33	3.86	9 (32%)	34,52,52	2.49	5 (14%)
35	CDL	d	402	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	3 (2%)
35	CDL	B	602	-	99,99,99	0.89	8 (8%)	105,111,111	0.98	4 (3%)
34	LMT	X	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.05	3 (6%)
35	CDL	b	601	-	99,99,99	0.88	8 (8%)	105,111,111	1.00	5 (4%)
38	ADP	D2	601	-	24,29,29	3.94	9 (37%)	29,45,45	3.73	6 (20%)
34	LMT	d	403	-	36,36,36	1.11	2 (5%)	47,47,47	0.86	1 (2%)
37	ATP	C1	601	-	28,33,33	3.83	10 (35%)	34,52,52	2.66	6 (17%)
33	PC1	o	204	-	53,53,53	0.97	4 (7%)	59,61,61	1.05	2 (3%)
35	CDL	c	401	-	99,99,99	0.90	7 (7%)	105,111,111	0.92	4 (3%)
36	PEE	J	302	-	50,50,50	1.16	6 (12%)	53,55,55	1.16	3 (5%)
35	CDL	v	202	-	99,99,99	0.89	7 (7%)	105,111,111	0.99	4 (3%)
35	CDL	H	302	-	99,99,99	0.88	7 (7%)	105,111,111	0.99	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMT	D	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.88	1 (2%)
35	CDL	V	202	-	99,99,99	0.89	7 (7%)	105,111,111	0.98	4 (3%)
35	CDL	O	203	-	99,99,99	0.89	7 (7%)	105,111,111	1.01	5 (4%)
35	CDL	e	401	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
38	ADP	D1	601	-	24,29,29	3.93	9 (37%)	29,45,45	3.67	7 (24%)
35	CDL	h	302	-	99,99,99	0.88	6 (6%)	105,111,111	0.98	4 (3%)
33	PC1	v	201	-	53,53,53	1.01	3 (5%)	59,61,61	1.00	2 (3%)
34	LMT	c	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.08	2 (4%)
38	ADP	B2	601	-	24,29,29	3.93	9 (37%)	29,45,45	3.92	7 (24%)
35	CDL	B	601	-	99,99,99	0.88	8 (8%)	105,111,111	1.00	5 (4%)
34	LMT	O	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.95	2 (4%)
33	PC1	V	201	-	53,53,53	1.01	3 (5%)	59,61,61	0.99	2 (3%)
34	LMT	d	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.91	1 (2%)
36	PEE	j	301	-	50,50,50	1.14	6 (12%)	53,55,55	1.09	3 (5%)
37	ATP	E2	601	-	28,33,33	3.86	10 (35%)	34,52,52	2.45	6 (17%)
35	CDL	u	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.02	4 (3%)
34	LMT	D	403	-	36,36,36	1.11	2 (5%)	47,47,47	0.91	1 (2%)
34	LMT	H	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.04	2 (4%)
35	CDL	D	402	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	3 (2%)
36	PEE	J	301	-	50,50,50	1.14	6 (12%)	53,55,55	1.08	3 (5%)
37	ATP	E1	601	-	28,33,33	3.86	9 (32%)	34,52,52	2.44	6 (17%)
37	ATP	C2	601	-	28,33,33	3.85	10 (35%)	34,52,52	2.56	6 (17%)
35	CDL	U	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.01	4 (3%)
33	PC1	O	201	-	53,53,53	0.98	4 (7%)	59,61,61	1.06	3 (5%)
36	PEE	C	403	-	50,50,50	1.17	5 (10%)	53,55,55	1.01	2 (3%)
34	LMT	c	402	-	36,36,36	1.09	2 (5%)	47,47,47	1.02	1 (2%)
35	CDL	E	401	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
35	CDL	o	203	-	99,99,99	0.89	7 (7%)	105,111,111	1.00	5 (4%)
33	PC1	o	201	-	53,53,53	0.98	4 (7%)	59,61,61	1.05	3 (5%)
38	ADP	B1	601	-	24,29,29	3.94	9 (37%)	29,45,45	3.75	6 (20%)
34	LMT	C	402	-	36,36,36	1.10	2 (5%)	47,47,47	1.01	1 (2%)
35	CDL	b	602	-	99,99,99	0.89	8 (8%)	105,111,111	0.98	4 (3%)
36	PEE	c	403	-	50,50,50	1.17	5 (10%)	53,55,55	1.02	2 (3%)
33	PC1	O	204	-	53,53,53	0.97	4 (7%)	59,61,61	1.05	2 (3%)
34	LMT	C	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.15	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	CDL	C	401	-	99,99,99	0.89	6 (6%)	105,111,111	0.86	4 (3%)
34	LMT	x	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	3 (6%)
34	LMT	o	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.92	1 (2%)
37	ATP	A2	601	-	28,33,33	3.83	9 (32%)	34,52,52	2.52	6 (17%)
36	PEE	j	302	-	50,50,50	1.16	6 (12%)	53,55,55	1.09	3 (5%)

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
34	LMT	h	301	-	-	9/21/61/61	0/2/2/2
37	ATP	A1	601	-	-	0/18/38/38	0/3/3/3
35	CDL	d	402	-	-	45/110/110/110	-
35	CDL	B	602	-	-	49/110/110/110	-
34	LMT	X	101	-	-	12/21/61/61	0/2/2/2
35	CDL	b	601	-	-	39/110/110/110	-
38	ADP	D2	601	-	-	2/12/32/32	0/3/3/3
34	LMT	d	403	-	-	6/21/61/61	0/2/2/2
37	ATP	C1	601	-	-	5/18/38/38	0/3/3/3
33	PC1	o	204	-	-	24/57/57/57	-
35	CDL	c	401	-	-	63/110/110/110	-
36	PEE	J	302	-	-	19/54/54/54	-
35	CDL	v	202	-	-	37/110/110/110	-
35	CDL	H	302	-	-	44/110/110/110	-
34	LMT	D	401	-	-	11/21/61/61	0/2/2/2
35	CDL	V	202	-	-	38/110/110/110	-
35	CDL	O	203	-	-	39/110/110/110	-
35	CDL	e	401	-	-	49/110/110/110	-
38	ADP	D1	601	-	-	0/12/32/32	0/3/3/3
35	CDL	h	302	-	-	45/110/110/110	-
33	PC1	v	201	-	-	28/57/57/57	-
34	LMT	c	404	-	-	7/21/61/61	0/2/2/2
38	ADP	B2	601	-	-	4/12/32/32	0/3/3/3
35	CDL	B	601	-	-	39/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	O	202	-	-	4/21/61/61	0/2/2/2
33	PC1	V	201	-	-	29/57/57/57	-
34	LMT	d	401	-	-	9/21/61/61	0/2/2/2
36	PEE	j	301	-	-	20/54/54/54	-
37	ATP	E2	601	-	-	4/18/38/38	0/3/3/3
35	CDL	u	201	-	-	38/110/110/110	-
34	LMT	D	403	-	-	6/21/61/61	0/2/2/2
34	LMT	H	301	-	-	9/21/61/61	0/2/2/2
35	CDL	D	402	-	-	45/110/110/110	-
36	PEE	J	301	-	-	20/54/54/54	-
37	ATP	E1	601	-	-	4/18/38/38	0/3/3/3
37	ATP	C2	601	-	-	5/18/38/38	0/3/3/3
35	CDL	U	201	-	-	38/110/110/110	-
33	PC1	O	201	-	-	23/57/57/57	-
36	PEE	C	403	-	-	21/54/54/54	-
34	LMT	c	402	-	-	8/21/61/61	0/2/2/2
35	CDL	E	401	-	-	49/110/110/110	-
35	CDL	o	203	-	-	39/110/110/110	-
33	PC1	o	201	-	-	23/57/57/57	-
38	ADP	B1	601	-	-	4/12/32/32	0/3/3/3
34	LMT	C	402	-	-	8/21/61/61	0/2/2/2
35	CDL	b	602	-	-	50/110/110/110	-
36	PEE	c	403	-	-	21/54/54/54	-
33	PC1	O	204	-	-	24/57/57/57	-
34	LMT	C	404	-	-	7/21/61/61	0/2/2/2
35	CDL	C	401	-	-	60/110/110/110	-
34	LMT	x	101	-	-	12/21/61/61	0/2/2/2
34	LMT	o	202	-	-	4/21/61/61	0/2/2/2
37	ATP	A2	601	-	-	0/18/38/38	0/3/3/3
36	PEE	j	302	-	-	20/54/54/54	-

All (309) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E1	601	ATP	O4'-C1'	12.06	1.56	1.40
37	A1	601	ATP	O4'-C1'	12.02	1.56	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E2	601	ATP	O4'-C1'	12.01	1.56	1.40
37	C2	601	ATP	O4'-C1'	12.00	1.56	1.40
37	A2	601	ATP	O4'-C1'	11.89	1.56	1.40
37	C1	601	ATP	O4'-C1'	11.84	1.56	1.40
38	B1	601	ADP	C2'-C3'	-10.76	1.24	1.53
38	D2	601	ADP	C2'-C3'	-10.69	1.24	1.53
38	D1	601	ADP	C2'-C3'	-10.62	1.24	1.53
38	B2	601	ADP	C2'-C3'	-10.50	1.24	1.53
37	A1	601	ATP	C3'-C4'	-9.42	1.29	1.53
37	E1	601	ATP	C3'-C4'	-9.41	1.29	1.53
37	A2	601	ATP	C3'-C4'	-9.39	1.29	1.53
37	C2	601	ATP	C3'-C4'	-9.38	1.29	1.53
37	E2	601	ATP	C3'-C4'	-9.38	1.29	1.53
37	C1	601	ATP	C3'-C4'	-9.35	1.29	1.53
38	D2	601	ADP	O4'-C1'	8.56	1.52	1.40
38	B1	601	ADP	O4'-C1'	8.47	1.52	1.40
38	D1	601	ADP	O4'-C1'	8.42	1.51	1.40
38	B2	601	ADP	O4'-C1'	8.25	1.51	1.40
38	B2	601	ADP	C1'-N9	-7.28	1.31	1.49
38	D1	601	ADP	C1'-N9	-6.91	1.32	1.49
38	B1	601	ADP	C1'-N9	-6.91	1.32	1.49
38	D2	601	ADP	C1'-N9	-6.87	1.32	1.49
38	B2	601	ADP	O4'-C4'	-6.67	1.30	1.45
38	D1	601	ADP	O4'-C4'	-6.32	1.30	1.45
38	B1	601	ADP	O4'-C4'	-6.25	1.31	1.45
38	D2	601	ADP	O4'-C4'	-6.20	1.31	1.45
37	A1	601	ATP	PB-O3A	6.10	1.66	1.59
37	A1	601	ATP	PA-O3A	6.07	1.66	1.59
37	E1	601	ATP	PB-O3A	6.06	1.66	1.59
37	E2	601	ATP	PB-O3A	6.04	1.66	1.59
37	C1	601	ATP	PA-O3A	6.02	1.66	1.59
37	C2	601	ATP	PB-O3A	6.01	1.66	1.59
37	E1	601	ATP	PA-O3A	6.01	1.66	1.59
37	E2	601	ATP	PA-O3A	6.00	1.66	1.59
38	B1	601	ADP	C3'-C4'	5.99	1.68	1.53
37	A2	601	ATP	PB-O3A	5.99	1.66	1.59
37	C2	601	ATP	PA-O3A	5.98	1.66	1.59
37	C1	601	ATP	PB-O3A	5.97	1.65	1.59
38	D2	601	ADP	C3'-C4'	5.96	1.68	1.53
38	D1	601	ADP	C3'-C4'	5.94	1.68	1.53
37	A2	601	ATP	PA-O3A	5.89	1.65	1.59
38	B2	601	ADP	C3'-C4'	5.81	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E2	601	ATP	PB-O3B	5.49	1.65	1.59
37	A2	601	ATP	PB-O3B	5.46	1.65	1.59
37	E1	601	ATP	PB-O3B	5.46	1.65	1.59
37	A1	601	ATP	PB-O3B	5.43	1.65	1.59
37	C1	601	ATP	PB-O3B	5.43	1.65	1.59
37	C2	601	ATP	PB-O3B	5.39	1.65	1.59
37	C1	601	ATP	C2'-C3'	4.93	1.66	1.53
37	E2	601	ATP	C2'-C3'	4.86	1.66	1.53
37	A2	601	ATP	C2'-C3'	4.86	1.66	1.53
37	E1	601	ATP	C2'-C3'	4.81	1.66	1.53
37	C2	601	ATP	C2'-C3'	4.78	1.66	1.53
37	C2	601	ATP	O4'-C4'	4.74	1.55	1.45
37	A1	601	ATP	C2'-C3'	4.74	1.66	1.53
37	A1	601	ATP	O4'-C4'	4.70	1.55	1.45
37	E2	601	ATP	O4'-C4'	4.69	1.55	1.45
37	E1	601	ATP	O4'-C4'	4.68	1.55	1.45
37	A2	601	ATP	O4'-C4'	4.60	1.55	1.45
38	D1	601	ADP	PA-O3A	4.54	1.64	1.59
37	C1	601	ATP	O4'-C4'	4.50	1.55	1.45
38	D2	601	ADP	PA-O3A	4.44	1.64	1.59
38	B1	601	ADP	PA-O3A	4.38	1.64	1.59
38	B2	601	ADP	PA-O3A	4.29	1.64	1.59
36	J	302	PEE	C39-C38	3.83	1.53	1.31
36	j	302	PEE	C39-C38	3.83	1.53	1.31
36	C	403	PEE	C18-C19	3.81	1.53	1.31
36	c	403	PEE	C39-C38	3.80	1.53	1.31
36	c	403	PEE	C18-C19	3.80	1.53	1.31
36	C	403	PEE	C39-C38	3.79	1.53	1.31
36	J	302	PEE	C18-C19	3.75	1.53	1.31
36	J	301	PEE	C39-C38	3.74	1.53	1.31
36	j	301	PEE	C39-C38	3.73	1.52	1.31
36	j	302	PEE	C18-C19	3.73	1.52	1.31
38	D1	601	ADP	O2'-C2'	3.70	1.52	1.43
36	J	301	PEE	C18-C19	3.68	1.52	1.31
38	D2	601	ADP	O2'-C2'	3.68	1.52	1.43
36	j	301	PEE	C18-C19	3.67	1.52	1.31
38	B2	601	ADP	O2'-C2'	3.66	1.52	1.43
38	B1	601	ADP	O2'-C2'	3.63	1.51	1.43
34	D	401	LMT	O5B-C1B	3.44	1.50	1.41
34	d	401	LMT	O5B-C1B	3.43	1.50	1.41
34	x	101	LMT	O5B-C1B	3.41	1.50	1.41
34	X	101	LMT	O5B-C1B	3.40	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	o	202	LMT	O5B-C1B	3.39	1.50	1.41
34	O	202	LMT	O5B-C1B	3.38	1.50	1.41
37	E2	601	ATP	C6-N6	3.34	1.46	1.34
37	A2	601	ATP	C6-N6	3.34	1.46	1.34
37	E1	601	ATP	C6-N6	3.33	1.46	1.34
37	C2	601	ATP	C6-N6	3.32	1.46	1.34
34	h	301	LMT	O5'-C1'	3.32	1.50	1.41
34	H	301	LMT	O5B-C1B	3.32	1.50	1.41
37	A1	601	ATP	C6-N6	3.31	1.45	1.34
34	H	301	LMT	O5'-C1'	3.30	1.50	1.41
37	C1	601	ATP	C6-N6	3.30	1.45	1.34
34	h	301	LMT	O5B-C1B	3.29	1.50	1.41
34	d	403	LMT	O5B-C1B	3.26	1.50	1.41
34	c	402	LMT	O5B-C1B	3.25	1.50	1.41
34	D	403	LMT	O5B-C1B	3.25	1.50	1.41
34	C	402	LMT	O5B-C1B	3.23	1.50	1.41
34	D	401	LMT	O5'-C1'	3.23	1.50	1.41
34	C	404	LMT	O5B-C1B	3.23	1.50	1.41
34	c	404	LMT	O5B-C1B	3.22	1.50	1.41
34	d	401	LMT	O5'-C1'	3.20	1.50	1.41
38	D1	601	ADP	C6-N6	3.20	1.45	1.34
38	D2	601	ADP	C6-N6	3.20	1.45	1.34
34	X	101	LMT	O5'-C1'	3.19	1.50	1.41
34	x	101	LMT	O5'-C1'	3.19	1.50	1.41
38	B1	601	ADP	C6-N6	3.16	1.45	1.34
38	B2	601	ADP	C6-N6	3.16	1.45	1.34
33	O	201	PC1	O21-C2	-3.10	1.39	1.46
33	o	201	PC1	O21-C2	-3.07	1.39	1.46
34	d	403	LMT	O5'-C1'	3.03	1.49	1.41
35	O	203	CDL	OA6-CA4	-3.01	1.39	1.46
34	D	403	LMT	O5'-C1'	3.00	1.49	1.41
34	O	202	LMT	O5'-C1'	2.98	1.49	1.41
34	C	404	LMT	O5'-C1'	2.97	1.49	1.41
35	o	203	CDL	OA6-CA4	-2.97	1.39	1.46
35	E	401	CDL	OA6-CA4	-2.97	1.39	1.46
34	C	402	LMT	O5'-C1'	2.97	1.49	1.41
34	c	404	LMT	O5'-C1'	2.95	1.49	1.41
35	e	401	CDL	OA6-CA4	-2.95	1.39	1.46
35	u	201	CDL	OA6-CA4	-2.95	1.39	1.46
34	c	402	LMT	O5'-C1'	2.94	1.49	1.41
34	o	202	LMT	O5'-C1'	2.93	1.49	1.41
35	U	201	CDL	OA6-CA4	-2.93	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	401	CDL	OB6-CB4	-2.92	1.39	1.46
35	V	202	CDL	OB6-CB4	-2.92	1.39	1.46
36	c	403	PEE	O2-C2	-2.91	1.39	1.46
35	U	201	CDL	OB6-CB4	-2.91	1.39	1.46
35	v	202	CDL	OB6-CB4	-2.91	1.39	1.46
35	b	601	CDL	OB6-CB4	-2.90	1.39	1.46
36	C	403	PEE	O2-C2	-2.90	1.39	1.46
35	h	302	CDL	OA6-CA4	-2.88	1.39	1.46
35	H	302	CDL	OA6-CA4	-2.87	1.39	1.46
35	u	201	CDL	OB6-CB4	-2.87	1.39	1.46
35	B	601	CDL	OB6-CB4	-2.87	1.39	1.46
35	B	601	CDL	OA6-CA4	-2.81	1.40	1.46
35	H	302	CDL	OB6-CB4	-2.80	1.40	1.46
35	b	601	CDL	OA6-CA4	-2.80	1.40	1.46
35	h	302	CDL	OB6-CB4	-2.80	1.40	1.46
35	c	401	CDL	OB6-CB4	-2.79	1.40	1.46
35	D	402	CDL	OB6-CB4	-2.79	1.40	1.46
35	d	402	CDL	OB6-CB4	-2.78	1.40	1.46
35	B	602	CDL	OB6-CB4	-2.75	1.40	1.46
35	V	202	CDL	OA6-CA4	-2.75	1.40	1.46
35	v	202	CDL	OA6-CA4	-2.75	1.40	1.46
35	o	203	CDL	OB6-CB4	-2.75	1.40	1.46
35	b	602	CDL	OB6-CB4	-2.74	1.40	1.46
35	O	203	CDL	OB6-CB4	-2.72	1.40	1.46
36	j	301	PEE	O2-C2	-2.72	1.40	1.46
36	j	302	PEE	O2-C2	-2.72	1.40	1.46
36	J	302	PEE	O2-C2	-2.71	1.40	1.46
36	J	301	PEE	O2-C2	-2.70	1.40	1.46
35	C	401	CDL	OA6-CA4	-2.70	1.40	1.46
35	c	401	CDL	OA6-CA4	-2.70	1.40	1.46
35	E	401	CDL	OB6-CB4	-2.69	1.40	1.46
35	e	401	CDL	OB6-CB4	-2.67	1.40	1.46
33	o	204	PC1	O21-C2	-2.66	1.40	1.46
33	V	201	PC1	O21-C2	-2.61	1.40	1.46
33	O	204	PC1	O21-C2	-2.61	1.40	1.46
35	C	401	CDL	OA8-CA7	2.60	1.40	1.33
33	v	201	PC1	O21-C2	-2.60	1.40	1.46
35	d	402	CDL	OA6-CA4	-2.57	1.40	1.46
35	c	401	CDL	OA8-CA7	2.57	1.40	1.33
35	b	602	CDL	OA6-CA4	-2.56	1.40	1.46
35	E	401	CDL	OB8-CB7	2.56	1.40	1.33
35	D	402	CDL	OA6-CA4	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	602	CDL	OA6-CA4	-2.55	1.40	1.46
35	e	401	CDL	OB8-CB7	2.54	1.40	1.33
35	b	602	CDL	OB8-CB7	2.51	1.40	1.33
35	c	401	CDL	OB8-CB7	2.51	1.40	1.33
33	V	201	PC1	O31-C31	2.49	1.40	1.33
33	v	201	PC1	O31-C31	2.48	1.40	1.33
35	b	602	CDL	OA8-CA7	2.48	1.40	1.33
35	C	401	CDL	OB8-CB7	2.48	1.40	1.33
35	B	602	CDL	OB8-CB7	2.48	1.40	1.33
35	V	202	CDL	OA8-CA7	2.48	1.40	1.33
35	B	602	CDL	OA8-CA7	2.47	1.40	1.33
35	v	202	CDL	OA8-CA7	2.47	1.40	1.33
36	C	403	PEE	O3-C30	2.46	1.40	1.33
33	O	201	PC1	O31-C3	-2.46	1.39	1.45
35	U	201	CDL	OA8-CA7	2.46	1.40	1.33
36	c	403	PEE	O3-C30	2.45	1.40	1.33
35	U	201	CDL	OB8-CB7	2.45	1.40	1.33
33	o	201	PC1	O31-C3	-2.45	1.39	1.45
35	H	302	CDL	OA8-CA7	2.45	1.40	1.33
35	u	201	CDL	OB8-CB7	2.44	1.40	1.33
35	h	302	CDL	OA8-CA7	2.44	1.40	1.33
35	O	203	CDL	OB8-CB7	2.44	1.40	1.33
33	o	204	PC1	O31-C31	2.44	1.40	1.33
35	u	201	CDL	OA8-CA7	2.43	1.40	1.33
35	v	202	CDL	OB8-CB6	-2.43	1.39	1.45
33	O	204	PC1	O31-C31	2.43	1.40	1.33
35	D	402	CDL	OA8-CA6	-2.42	1.39	1.45
35	d	402	CDL	OB8-CB7	2.42	1.40	1.33
35	O	203	CDL	OA8-CA7	2.42	1.40	1.33
35	D	402	CDL	OB8-CB7	2.41	1.40	1.33
35	o	203	CDL	OB8-CB7	2.41	1.40	1.33
35	d	402	CDL	OA8-CA6	-2.41	1.39	1.45
36	j	302	PEE	O3-C30	2.40	1.40	1.33
36	J	302	PEE	O3-C30	2.39	1.40	1.33
35	b	601	CDL	OA8-CA6	-2.38	1.39	1.45
35	B	601	CDL	OA8-CA6	-2.38	1.39	1.45
36	J	301	PEE	O3-C3	-2.38	1.39	1.45
35	V	202	CDL	OB8-CB6	-2.38	1.39	1.45
35	o	203	CDL	OA8-CA7	2.37	1.40	1.33
35	E	401	CDL	OA8-CA7	2.35	1.40	1.33
35	B	601	CDL	OA8-CA7	2.34	1.40	1.33
35	c	401	CDL	OB8-CB6	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	401	CDL	OA8-CA7	2.33	1.40	1.33
35	v	202	CDL	OB8-CB7	2.33	1.40	1.33
36	j	301	PEE	O3-C3	-2.33	1.40	1.45
35	b	601	CDL	OA8-CA7	2.33	1.40	1.33
35	h	302	CDL	OB8-CB7	2.31	1.40	1.33
35	V	202	CDL	OB8-CB7	2.31	1.40	1.33
35	b	601	CDL	OB8-CB7	2.30	1.40	1.33
36	j	301	PEE	O3-C30	2.30	1.40	1.33
35	C	401	CDL	OB8-CB6	-2.30	1.40	1.45
35	H	302	CDL	OB8-CB7	2.30	1.40	1.33
35	B	601	CDL	OB8-CB6	-2.29	1.40	1.45
35	B	601	CDL	OB8-CB7	2.28	1.40	1.33
35	O	203	CDL	OA8-CA6	-2.28	1.40	1.45
35	d	402	CDL	OA8-CA7	2.28	1.40	1.33
35	D	402	CDL	OA8-CA7	2.27	1.40	1.33
35	b	601	CDL	OB8-CB6	-2.27	1.40	1.45
35	B	602	CDL	OA6-CA5	2.27	1.40	1.34
35	o	203	CDL	OA8-CA6	-2.27	1.40	1.45
35	b	602	CDL	OA6-CA5	2.25	1.40	1.34
35	O	203	CDL	OB8-CB6	-2.24	1.40	1.45
36	J	301	PEE	O3-C30	2.23	1.39	1.33
33	O	201	PC1	O31-C31	2.23	1.39	1.33
33	o	201	PC1	O31-C31	2.23	1.39	1.33
36	j	302	PEE	O3-C3	-2.22	1.40	1.45
35	H	302	CDL	OB8-CB6	-2.22	1.40	1.45
35	c	401	CDL	OA6-CA5	2.21	1.40	1.34
35	D	402	CDL	OB8-CB6	-2.21	1.40	1.45
35	E	401	CDL	OA8-CA6	-2.20	1.40	1.45
38	D2	601	ADP	C2-N3	2.20	1.35	1.32
35	o	203	CDL	OB8-CB6	-2.20	1.40	1.45
36	C	403	PEE	O3-C3	-2.20	1.40	1.45
35	U	201	CDL	OA8-CA6	-2.19	1.40	1.45
35	h	302	CDL	OB8-CB6	-2.19	1.40	1.45
33	v	201	PC1	O21-C21	2.18	1.40	1.34
33	o	204	PC1	O21-C21	2.18	1.40	1.34
35	u	201	CDL	OA8-CA6	-2.18	1.40	1.45
35	h	302	CDL	OA8-CA6	-2.18	1.40	1.45
35	e	401	CDL	OA8-CA6	-2.18	1.40	1.45
33	O	204	PC1	O21-C21	2.18	1.40	1.34
35	d	402	CDL	OA6-CA5	2.17	1.40	1.34
33	V	201	PC1	O21-C21	2.17	1.40	1.34
37	C1	601	ATP	C5'-C4'	2.17	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	401	CDL	OA6-CA5	2.17	1.40	1.34
36	J	302	PEE	O2-C10	2.16	1.40	1.34
35	b	602	CDL	OB8-CB6	-2.16	1.40	1.45
35	B	602	CDL	OA8-CA6	-2.16	1.40	1.45
37	E2	601	ATP	C5'-C4'	2.16	1.58	1.51
35	e	401	CDL	OB8-CB6	-2.16	1.40	1.45
35	B	602	CDL	OB8-CB6	-2.15	1.40	1.45
36	c	403	PEE	O3-C3	-2.15	1.40	1.45
35	U	201	CDL	OB8-CB6	-2.15	1.40	1.45
35	H	302	CDL	OA8-CA6	-2.15	1.40	1.45
35	d	402	CDL	OB6-CB5	2.15	1.40	1.34
35	d	402	CDL	OB8-CB6	-2.15	1.40	1.45
37	C2	601	ATP	C5'-C4'	2.14	1.58	1.51
35	E	401	CDL	OB8-CB6	-2.14	1.40	1.45
37	E1	601	ATP	C5'-C4'	2.14	1.58	1.51
36	j	302	PEE	O2-C10	2.14	1.40	1.34
35	b	602	CDL	OA8-CA6	-2.14	1.40	1.45
36	J	302	PEE	O3-C3	-2.14	1.40	1.45
35	v	202	CDL	OA8-CA6	-2.12	1.40	1.45
35	D	402	CDL	OA6-CA5	2.12	1.40	1.34
35	D	402	CDL	OB6-CB5	2.12	1.40	1.34
35	U	201	CDL	OA6-CA5	2.12	1.40	1.34
35	u	201	CDL	OA6-CA5	2.12	1.40	1.34
35	e	401	CDL	OB6-CB5	2.11	1.40	1.34
35	V	202	CDL	OA8-CA6	-2.11	1.40	1.45
35	o	203	CDL	OB6-CB5	2.11	1.40	1.34
38	B2	601	ADP	C2-N3	2.11	1.35	1.32
38	B1	601	ADP	C2-N3	2.10	1.35	1.32
35	E	401	CDL	OB6-CB5	2.10	1.40	1.34
33	O	204	PC1	O31-C3	-2.09	1.40	1.45
37	C1	601	ATP	C2-N3	2.09	1.35	1.32
36	j	301	PEE	O2-C10	2.09	1.40	1.34
35	B	602	CDL	OB6-CB5	2.08	1.40	1.34
35	V	202	CDL	OA6-CA5	2.08	1.40	1.34
35	O	203	CDL	OB6-CB5	2.07	1.40	1.34
35	u	201	CDL	OB8-CB6	-2.07	1.40	1.45
38	D1	601	ADP	C2-N3	2.07	1.35	1.32
35	v	202	CDL	OA6-CA5	2.07	1.40	1.34
35	b	602	CDL	OB6-CB5	2.06	1.40	1.34
37	A2	601	ATP	C5'-C4'	2.06	1.57	1.51
33	o	204	PC1	O31-C3	-2.06	1.40	1.45
36	J	301	PEE	O2-C10	2.05	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	b	601	CDL	OA6-CA5	2.05	1.40	1.34
37	A1	601	ATP	C5'-C4'	2.04	1.57	1.51
35	e	401	CDL	OA6-CA5	2.04	1.40	1.34
37	E2	601	ATP	C2-N3	2.04	1.35	1.32
35	B	601	CDL	OA6-CA5	2.03	1.40	1.34
35	E	401	CDL	OA6-CA5	2.03	1.40	1.34
35	H	302	CDL	OA6-CA5	2.03	1.40	1.34
35	b	601	CDL	OB6-CB5	2.02	1.40	1.34
35	c	401	CDL	OA8-CA6	-2.02	1.40	1.45
33	o	201	PC1	O21-C21	2.02	1.40	1.34
37	C2	601	ATP	C2-N3	2.01	1.35	1.32
35	B	601	CDL	OB6-CB5	2.01	1.40	1.34
33	O	201	PC1	O21-C21	2.00	1.39	1.34

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	B2	601	ADP	C1'-N9-C4	15.61	154.07	126.64
38	D1	601	ADP	C1'-N9-C4	14.69	152.45	126.64
38	D2	601	ADP	C1'-N9-C4	14.02	151.28	126.64
38	B1	601	ADP	C1'-N9-C4	13.90	151.06	126.64
37	C1	601	ATP	C4'-O4'-C1'	-7.90	102.69	109.92
38	B2	601	ADP	C4'-O4'-C1'	-7.71	102.86	109.92
37	E1	601	ATP	C5-C6-N6	7.57	131.84	120.31
37	A1	601	ATP	C5-C6-N6	7.56	131.82	120.31
37	C2	601	ATP	C5-C6-N6	7.56	131.82	120.31
38	D1	601	ADP	C5-C6-N6	7.55	131.81	120.31
37	E2	601	ATP	C5-C6-N6	7.53	131.77	120.31
38	D2	601	ADP	C5-C6-N6	7.52	131.76	120.31
37	A2	601	ATP	C5-C6-N6	7.48	131.71	120.31
37	C1	601	ATP	C5-C6-N6	7.45	131.66	120.31
38	B2	601	ADP	C5-C6-N6	7.44	131.64	120.31
38	B1	601	ADP	C5-C6-N6	7.43	131.63	120.31
37	C2	601	ATP	C4'-O4'-C1'	-6.88	103.62	109.92
37	A2	601	ATP	C4'-O4'-C1'	-6.52	103.95	109.92
38	B1	601	ADP	N3-C2-N1	-6.44	119.92	128.67
38	D2	601	ADP	N3-C2-N1	-6.43	119.95	128.67
37	C1	601	ATP	N3-C2-N1	-6.38	120.01	128.67
38	B1	601	ADP	C4'-O4'-C1'	-6.36	104.10	109.92
37	E1	601	ATP	N3-C2-N1	-6.34	120.06	128.67
38	D1	601	ADP	N3-C2-N1	-6.34	120.07	128.67
38	B2	601	ADP	N3-C2-N1	-6.33	120.08	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A1	601	ATP	N3-C2-N1	-6.33	120.08	128.67
37	C2	601	ATP	N3-C2-N1	-6.32	120.09	128.67
37	E2	601	ATP	N3-C2-N1	-6.29	120.13	128.67
37	A2	601	ATP	N3-C2-N1	-6.28	120.15	128.67
37	A1	601	ATP	C4'-O4'-C1'	-6.22	104.23	109.92
38	B1	601	ADP	O4'-C1'-N9	6.01	116.71	108.75
38	D2	601	ADP	C4'-O4'-C1'	-5.83	104.58	109.92
37	C1	601	ATP	C1'-N9-C4	5.75	136.74	126.64
38	D2	601	ADP	O4'-C1'-N9	5.71	116.31	108.75
37	E2	601	ATP	C1'-N9-C4	5.66	136.59	126.64
37	E1	601	ATP	C1'-N9-C4	5.66	136.59	126.64
37	A2	601	ATP	C1'-N9-C4	5.56	136.41	126.64
37	C2	601	ATP	C1'-N9-C4	5.56	136.40	126.64
37	E2	601	ATP	C4'-O4'-C1'	-5.50	104.89	109.92
37	A1	601	ATP	C1'-N9-C4	5.45	136.21	126.64
37	E1	601	ATP	C4'-O4'-C1'	-5.20	105.16	109.92
38	D1	601	ADP	N6-C6-N1	-4.82	108.03	118.33
38	D2	601	ADP	N6-C6-N1	-4.82	108.03	118.33
37	C2	601	ATP	N6-C6-N1	-4.79	108.09	118.33
37	A1	601	ATP	N6-C6-N1	-4.78	108.13	118.33
38	B1	601	ADP	N6-C6-N1	-4.75	108.19	118.33
37	E1	601	ATP	N6-C6-N1	-4.73	108.22	118.33
38	B2	601	ADP	N6-C6-N1	-4.72	108.25	118.33
37	C1	601	ATP	N6-C6-N1	-4.71	108.27	118.33
37	E2	601	ATP	N6-C6-N1	-4.71	108.27	118.33
37	A2	601	ATP	N6-C6-N1	-4.70	108.30	118.33
33	O	204	PC1	O21-C21-C22	4.62	121.47	111.48
33	o	204	PC1	O21-C21-C22	4.59	121.42	111.48
38	D1	601	ADP	C4'-O4'-C1'	-4.38	105.91	109.92
35	d	402	CDL	OB6-CB5-C51	4.20	120.58	111.48
33	v	201	PC1	O21-C21-C22	4.20	120.58	111.48
33	V	201	PC1	O21-C21-C22	4.19	120.56	111.48
33	O	201	PC1	O21-C21-C22	4.14	120.44	111.48
35	D	402	CDL	OB6-CB5-C51	4.14	120.43	111.48
35	o	203	CDL	OB6-CB5-C51	4.08	120.30	111.48
33	o	201	PC1	O21-C21-C22	4.05	120.24	111.48
35	O	203	CDL	OB6-CB5-C51	4.04	120.22	111.48
35	b	602	CDL	OB6-CB5-C51	4.01	120.16	111.48
35	B	602	CDL	OB6-CB5-C51	3.99	120.10	111.48
36	J	302	PEE	O2-C10-C11	3.95	120.03	111.48
35	h	302	CDL	OB6-CB5-C51	3.92	119.97	111.48
35	H	302	CDL	OB6-CB5-C51	3.91	119.95	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	j	301	PEE	O2-C10-C11	3.75	119.60	111.48
36	j	302	PEE	O2-C10-C11	3.75	119.59	111.48
35	D	402	CDL	OA6-CA5-C11	3.71	119.50	111.48
36	J	301	PEE	O2-C10-C11	3.70	119.49	111.48
35	d	402	CDL	OA6-CA5-C11	3.70	119.48	111.48
35	e	401	CDL	OB6-CB5-C51	3.63	119.33	111.48
35	B	601	CDL	OB6-CB5-C51	3.61	119.29	111.48
35	u	201	CDL	OA6-CA5-C11	3.60	119.27	111.48
35	b	601	CDL	OB6-CB5-C51	3.60	119.26	111.48
35	E	401	CDL	OB6-CB5-C51	3.57	119.20	111.48
35	b	601	CDL	OA6-CA5-C11	3.54	119.15	111.48
35	U	201	CDL	OA6-CA5-C11	3.52	119.10	111.48
35	B	601	CDL	OA6-CA5-C11	3.52	119.09	111.48
34	x	101	LMT	O5'-C5'-C4'	3.42	116.79	109.72
35	e	401	CDL	OA6-CA5-C11	3.42	118.88	111.48
34	X	101	LMT	O5'-C5'-C4'	3.41	116.77	109.72
35	E	401	CDL	OA6-CA5-C11	3.39	118.82	111.48
35	b	602	CDL	OA6-CA5-C11	3.38	118.79	111.48
35	u	201	CDL	OB6-CB5-C51	3.36	118.75	111.48
35	B	602	CDL	OA6-CA5-C11	3.35	118.72	111.48
35	U	201	CDL	OB6-CB5-C51	3.31	118.64	111.48
35	c	401	CDL	OA6-CA5-C11	3.25	118.51	111.48
35	C	401	CDL	OA6-CA5-C11	3.22	118.45	111.48
38	D1	601	ADP	O4'-C1'-N9	3.20	112.99	108.75
35	c	401	CDL	OB6-CB5-C51	3.18	118.37	111.48
35	o	203	CDL	OA6-CA5-C11	3.16	118.31	111.48
35	O	203	CDL	OA6-CA5-C11	3.11	118.20	111.48
35	v	202	CDL	OB6-CB5-C51	3.10	118.20	111.48
35	V	202	CDL	OB6-CB5-C51	3.06	118.11	111.48
35	C	401	CDL	OB6-CB5-C51	3.06	118.10	111.48
35	V	202	CDL	OA6-CA5-C11	3.04	118.05	111.48
35	h	302	CDL	OA6-CA5-C11	3.02	118.01	111.48
35	u	201	CDL	OA8-CA7-C31	3.00	120.97	111.83
35	v	202	CDL	OA6-CA5-C11	2.98	117.93	111.48
36	c	403	PEE	O2-C10-C11	2.98	117.92	111.48
36	C	403	PEE	O2-C10-C11	2.96	117.89	111.48
33	v	201	PC1	O31-C31-C32	2.94	120.80	111.83
35	U	201	CDL	OA8-CA7-C31	2.94	120.79	111.83
34	d	401	LMT	C1B-O1B-C4'	-2.93	111.02	117.98
33	V	201	PC1	O31-C31-C32	2.93	120.77	111.83
38	D1	601	ADP	C2'-C3'-C4'	2.93	108.27	102.61
34	C	404	LMT	C1B-O1B-C4'	-2.93	111.04	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	401	LMT	C1B-O1B-C4'	-2.90	111.11	117.98
35	O	203	CDL	OA8-CA7-C31	2.87	120.59	111.83
35	v	202	CDL	OA8-CA7-C31	2.86	120.55	111.83
35	H	302	CDL	OA6-CA5-C11	2.86	117.67	111.48
35	o	203	CDL	OA8-CA7-C31	2.83	120.48	111.83
35	V	202	CDL	OA8-CA7-C31	2.83	120.46	111.83
35	e	401	CDL	OA8-CA7-C31	2.77	120.28	111.83
35	E	401	CDL	OA8-CA7-C31	2.73	120.15	111.83
34	c	404	LMT	C1B-O1B-C4'	-2.71	111.56	117.98
33	o	204	PC1	O31-C31-C32	2.71	120.09	111.83
35	C	401	CDL	OA8-CA7-C31	2.71	120.09	111.83
35	D	402	CDL	OB8-CB7-C71	2.70	120.07	111.83
36	J	302	PEE	O3-C30-C31	2.70	120.06	111.83
35	d	402	CDL	OB8-CB7-C71	2.69	120.05	111.83
35	h	302	CDL	OB8-CB7-C71	2.64	119.89	111.83
37	A2	601	ATP	C2'-C3'-C4'	2.64	107.71	102.61
35	H	302	CDL	OB8-CB7-C71	2.64	119.87	111.83
36	C	403	PEE	O3-C30-C31	2.63	119.86	111.83
33	O	204	PC1	O31-C31-C32	2.63	119.85	111.83
35	E	401	CDL	OB8-CB7-C71	2.62	119.82	111.83
36	c	403	PEE	O3-C30-C31	2.61	119.81	111.83
33	O	201	PC1	C2-O21-C21	-2.61	111.56	117.80
35	e	401	CDL	OB8-CB7-C71	2.59	119.74	111.83
33	o	201	PC1	C2-O21-C21	-2.55	111.69	117.80
37	C1	601	ATP	C2'-C3'-C4'	2.55	107.53	102.61
38	B2	601	ADP	O4'-C1'-N9	2.53	112.10	108.75
35	b	602	CDL	OB8-CB7-C71	2.51	119.48	111.83
37	E1	601	ATP	C2'-C3'-C4'	2.46	107.36	102.61
35	B	602	CDL	OB8-CB7-C71	2.44	119.28	111.83
34	X	101	LMT	C3'-C4'-C5'	2.42	116.30	110.93
34	x	101	LMT	C3'-C4'-C5'	2.42	116.29	110.93
35	u	201	CDL	OB8-CB7-C71	2.42	119.20	111.83
36	j	301	PEE	O3-C30-C31	2.40	119.15	111.83
38	B2	601	ADP	C2'-C3'-C4'	2.39	107.23	102.61
35	b	601	CDL	OB8-CB7-C71	2.38	119.09	111.83
33	O	201	PC1	O31-C31-C32	2.38	119.09	111.83
35	B	601	CDL	OB8-CB7-C71	2.37	119.07	111.83
35	B	602	CDL	OA8-CA7-C31	2.36	119.04	111.83
35	U	201	CDL	OB8-CB7-C71	2.34	118.98	111.83
37	E2	601	ATP	C2'-C3'-C4'	2.34	107.14	102.61
33	o	201	PC1	O31-C31-C32	2.34	118.96	111.83
36	J	301	PEE	O3-C30-C31	2.33	118.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	602	CDL	OA8-CA7-C31	2.31	118.87	111.83
35	O	203	CDL	CA4-OA6-CA5	-2.27	112.37	117.80
35	v	202	CDL	OB8-CB7-C71	2.24	118.66	111.83
34	D	403	LMT	C1B-O5B-C5B	-2.23	109.36	113.72
34	x	101	LMT	C1B-O1B-C4'	-2.23	112.69	117.98
35	H	302	CDL	OA8-CA7-C31	2.23	118.62	111.83
36	J	302	PEE	C17-C18-C19	-2.23	108.15	124.83
36	j	302	PEE	C17-C18-C19	-2.21	108.28	124.83
34	H	301	LMT	O5'-C1'-C2'	2.21	114.90	110.37
34	h	301	LMT	O1B-C4'-C3'	2.19	112.80	107.23
34	h	301	LMT	O5'-C1'-C2'	2.19	114.87	110.37
34	O	202	LMT	O5'-C5'-C4'	2.19	114.25	109.72
34	d	403	LMT	C1B-O5B-C5B	-2.19	109.45	113.72
35	c	401	CDL	OB8-CB7-C71	2.18	118.49	111.83
35	V	202	CDL	OB8-CB7-C71	2.18	118.48	111.83
34	X	101	LMT	C1B-O1B-C4'	-2.17	112.83	117.98
35	c	401	CDL	C42-C41-C40	2.17	125.35	114.37
36	j	302	PEE	O3-C30-C31	2.16	118.43	111.83
34	C	402	LMT	C1B-O1B-C4'	-2.16	112.86	117.98
35	o	203	CDL	CA4-OA6-CA5	-2.16	112.63	117.80
34	H	301	LMT	O1B-C4'-C3'	2.15	112.71	107.23
35	O	203	CDL	OB8-CB7-C71	2.14	118.37	111.83
34	c	402	LMT	C1B-O1B-C4'	-2.14	112.91	117.98
35	h	302	CDL	OA8-CA7-C31	2.13	118.34	111.83
34	o	202	LMT	O5'-C5'-C4'	2.13	114.12	109.72
35	o	203	CDL	OB8-CB7-C71	2.12	118.31	111.83
34	C	404	LMT	C3'-C4'-C5'	2.11	115.61	110.93
35	b	601	CDL	OA8-CA7-C31	2.10	118.24	111.83
34	c	404	LMT	O5'-C5'-C4'	2.10	114.07	109.72
34	C	404	LMT	O5'-C5'-C4'	2.10	114.06	109.72
37	C2	601	ATP	C2'-C3'-C4'	2.09	106.65	102.61
36	j	301	PEE	C20-C19-C18	-2.09	109.19	124.83
36	J	301	PEE	C20-C19-C18	-2.09	109.20	124.83
35	B	601	CDL	OA8-CA7-C31	2.07	118.15	111.83
35	C	401	CDL	OB8-CB7-C71	2.06	118.12	111.83
35	B	601	CDL	CB4-OB6-CB5	-2.02	112.97	117.80
35	b	601	CDL	CB4-OB6-CB5	-2.02	112.97	117.80
34	O	202	LMT	C1B-O5B-C5B	-2.00	109.81	113.72

There are no chirality outliers.

All (1218) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	o	201	PC1	C1-O11-P-O14
33	o	201	PC1	C1-O11-P-O13
33	o	201	PC1	O13-C11-C12-N
33	o	201	PC1	C22-C21-O21-C2
33	o	204	PC1	C11-O13-P-O14
33	o	204	PC1	C22-C21-O21-C2
33	v	201	PC1	C1-O11-P-O12
33	v	201	PC1	C1-O11-P-O14
33	v	201	PC1	C1-O11-P-O13
33	v	201	PC1	C12-C11-O13-P
33	v	201	PC1	O13-C11-C12-N
33	v	201	PC1	O22-C21-O21-C2
33	O	201	PC1	C1-O11-P-O14
33	O	201	PC1	C1-O11-P-O13
33	O	201	PC1	O13-C11-C12-N
33	O	201	PC1	C22-C21-O21-C2
33	O	204	PC1	C11-O13-P-O14
33	O	204	PC1	C22-C21-O21-C2
33	V	201	PC1	C1-O11-P-O12
33	V	201	PC1	C1-O11-P-O14
33	V	201	PC1	C1-O11-P-O13
33	V	201	PC1	C12-C11-O13-P
33	V	201	PC1	O13-C11-C12-N
33	V	201	PC1	O22-C21-O21-C2
34	h	301	LMT	O5'-C1'-O1'-C1
34	x	101	LMT	C2'-C1'-O1'-C1
34	x	101	LMT	O5'-C1'-O1'-C1
34	d	403	LMT	C2-C1-O1'-C1'
34	H	301	LMT	O5'-C1'-O1'-C1
34	X	101	LMT	C2'-C1'-O1'-C1
34	X	101	LMT	O5'-C1'-O1'-C1
34	D	403	LMT	C2-C1-O1'-C1'
35	o	203	CDL	C11-CA5-OA6-CA4
35	o	203	CDL	CB3-OB5-PB2-OB2
35	o	203	CDL	CB3-OB5-PB2-OB3
35	u	201	CDL	CA3-OA5-PA1-OA2
35	u	201	CDL	CA3-OA5-PA1-OA3
35	u	201	CDL	CA3-OA5-PA1-OA4
35	u	201	CDL	CB2-OB2-PB2-OB3
35	h	302	CDL	CB2-C1-CA2-OA2
35	h	302	CDL	CA2-OA2-PA1-OA4
35	h	302	CDL	CA2-OA2-PA1-OA5
35	h	302	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
35	h	302	CDL	CB2-OB2-PB2-OB5
35	h	302	CDL	OB7-CB5-OB6-CB4
35	e	401	CDL	CA3-OA5-PA1-OA2
35	e	401	CDL	CA3-OA5-PA1-OA4
35	e	401	CDL	CB2-OB2-PB2-OB3
35	e	401	CDL	CB2-OB2-PB2-OB4
35	e	401	CDL	CB2-OB2-PB2-OB5
35	e	401	CDL	CB3-OB5-PB2-OB2
35	e	401	CDL	CB3-OB5-PB2-OB3
35	e	401	CDL	CB3-OB5-PB2-OB4
35	b	601	CDL	OB7-CB5-OB6-CB4
35	b	601	CDL	C51-CB5-OB6-CB4
35	b	602	CDL	CA2-OA2-PA1-OA3
35	b	602	CDL	CA2-OA2-PA1-OA4
35	b	602	CDL	CA2-OA2-PA1-OA5
35	b	602	CDL	CA3-OA5-PA1-OA3
35	b	602	CDL	C51-CB5-OB6-CB4
35	v	202	CDL	O1-C1-CB2-OB2
35	v	202	CDL	CA2-C1-CB2-OB2
35	v	202	CDL	C1-CB2-OB2-PB2
35	c	401	CDL	CA3-OA5-PA1-OA2
35	c	401	CDL	CA3-OA5-PA1-OA3
35	c	401	CDL	CA3-OA5-PA1-OA4
35	c	401	CDL	CB3-OB5-PB2-OB2
35	c	401	CDL	CB3-OB5-PB2-OB3
35	c	401	CDL	CB3-OB5-PB2-OB4
35	d	402	CDL	O1-C1-CB2-OB2
35	d	402	CDL	CA2-C1-CB2-OB2
35	d	402	CDL	CA2-OA2-PA1-OA3
35	d	402	CDL	CB2-OB2-PB2-OB3
35	d	402	CDL	CB2-OB2-PB2-OB5
35	d	402	CDL	CB3-OB5-PB2-OB2
35	d	402	CDL	CB3-OB5-PB2-OB4
35	d	402	CDL	C51-CB5-OB6-CB4
35	O	203	CDL	C11-CA5-OA6-CA4
35	O	203	CDL	CB3-OB5-PB2-OB2
35	O	203	CDL	CB3-OB5-PB2-OB3
35	O	203	CDL	CB3-OB5-PB2-OB4
35	U	201	CDL	CA3-OA5-PA1-OA2
35	U	201	CDL	CA3-OA5-PA1-OA3
35	U	201	CDL	CA3-OA5-PA1-OA4
35	U	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
35	H	302	CDL	CB2-C1-CA2-OA2
35	H	302	CDL	CA2-OA2-PA1-OA4
35	H	302	CDL	CA2-OA2-PA1-OA5
35	H	302	CDL	CB2-OB2-PB2-OB3
35	H	302	CDL	CB2-OB2-PB2-OB5
35	H	302	CDL	OB7-CB5-OB6-CB4
35	E	401	CDL	CA3-OA5-PA1-OA2
35	E	401	CDL	CA3-OA5-PA1-OA4
35	E	401	CDL	CB2-OB2-PB2-OB3
35	E	401	CDL	CB2-OB2-PB2-OB4
35	E	401	CDL	CB2-OB2-PB2-OB5
35	E	401	CDL	CB3-OB5-PB2-OB2
35	E	401	CDL	CB3-OB5-PB2-OB3
35	E	401	CDL	CB3-OB5-PB2-OB4
35	B	601	CDL	OB7-CB5-OB6-CB4
35	B	601	CDL	C51-CB5-OB6-CB4
35	B	602	CDL	CA2-OA2-PA1-OA3
35	B	602	CDL	CA2-OA2-PA1-OA4
35	B	602	CDL	CA2-OA2-PA1-OA5
35	B	602	CDL	CA3-OA5-PA1-OA3
35	B	602	CDL	C51-CB5-OB6-CB4
35	V	202	CDL	O1-C1-CB2-OB2
35	V	202	CDL	CA2-C1-CB2-OB2
35	V	202	CDL	CA3-OA5-PA1-OA2
35	V	202	CDL	C1-CB2-OB2-PB2
35	C	401	CDL	O1-C1-CA2-OA2
35	C	401	CDL	C1-CA2-OA2-PA1
35	C	401	CDL	CB3-OB5-PB2-OB2
35	D	402	CDL	O1-C1-CB2-OB2
35	D	402	CDL	CA2-C1-CB2-OB2
35	D	402	CDL	CA2-OA2-PA1-OA3
35	D	402	CDL	CB2-OB2-PB2-OB3
35	D	402	CDL	CB2-OB2-PB2-OB5
35	D	402	CDL	CB3-OB5-PB2-OB2
35	D	402	CDL	C51-CB5-OB6-CB4
36	j	302	PEE	O4P-C4-C5-N
36	c	403	PEE	C17-C18-C19-C20
36	c	403	PEE	C1-O3P-P-O1P
36	c	403	PEE	C1-O3P-P-O4P
36	c	403	PEE	O4P-C4-C5-N
36	J	302	PEE	O4P-C4-C5-N
36	C	403	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
36	C	403	PEE	C1-O3P-P-O1P
36	C	403	PEE	C1-O3P-P-O4P
36	C	403	PEE	O4P-C4-C5-N
37	E2	601	ATP	C5'-O5'-PA-O1A
37	C2	601	ATP	C5'-O5'-PA-O1A
37	C2	601	ATP	C5'-O5'-PA-O2A
37	C2	601	ATP	C5'-O5'-PA-O3A
37	E1	601	ATP	C5'-O5'-PA-O1A
37	C1	601	ATP	C5'-O5'-PA-O1A
37	C1	601	ATP	C5'-O5'-PA-O2A
37	C1	601	ATP	C5'-O5'-PA-O3A
38	B2	601	ADP	C5'-O5'-PA-O3A
38	B1	601	ADP	C5'-O5'-PA-O3A
35	e	401	CDL	OA9-CA7-OA8-CA6
35	E	401	CDL	OA9-CA7-OA8-CA6
35	h	302	CDL	OB9-CB7-OB8-CB6
35	b	601	CDL	OB9-CB7-OB8-CB6
35	c	401	CDL	OA9-CA7-OA8-CA6
35	H	302	CDL	OB9-CB7-OB8-CB6
35	B	601	CDL	OB9-CB7-OB8-CB6
35	C	401	CDL	OA9-CA7-OA8-CA6
33	o	201	PC1	O22-C21-O21-C2
33	O	201	PC1	O22-C21-O21-C2
35	o	203	CDL	OA7-CA5-OA6-CA4
35	b	602	CDL	OB7-CB5-OB6-CB4
35	d	402	CDL	OB7-CB5-OB6-CB4
35	O	203	CDL	OA7-CA5-OA6-CA4
35	B	602	CDL	OB7-CB5-OB6-CB4
35	D	402	CDL	OB7-CB5-OB6-CB4
35	h	302	CDL	C71-CB7-OB8-CB6
35	e	401	CDL	C31-CA7-OA8-CA6
35	b	601	CDL	C71-CB7-OB8-CB6
35	c	401	CDL	C31-CA7-OA8-CA6
35	H	302	CDL	C71-CB7-OB8-CB6
35	E	401	CDL	C31-CA7-OA8-CA6
35	B	601	CDL	C71-CB7-OB8-CB6
35	C	401	CDL	C31-CA7-OA8-CA6
33	v	201	PC1	C22-C21-O21-C2
33	V	201	PC1	C22-C21-O21-C2
35	h	302	CDL	C51-CB5-OB6-CB4
35	H	302	CDL	C51-CB5-OB6-CB4
34	h	301	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
34	H	301	LMT	C3'-C4'-O1B-C1B
34	X	101	LMT	O5B-C5B-C6B-O6B
35	B	602	CDL	C31-CA7-OA8-CA6
36	j	301	PEE	C37-C38-C39-C40
36	J	301	PEE	C37-C38-C39-C40
35	o	203	CDL	OA9-CA7-OA8-CA6
35	O	203	CDL	OA9-CA7-OA8-CA6
33	o	204	PC1	O22-C21-O21-C2
33	O	204	PC1	O22-C21-O21-C2
34	D	403	LMT	O5B-C5B-C6B-O6B
35	h	302	CDL	O1-C1-CA2-OA2
35	H	302	CDL	O1-C1-CA2-OA2
35	b	602	CDL	C31-CA7-OA8-CA6
34	d	403	LMT	C4B-C5B-C6B-O6B
34	D	403	LMT	C4B-C5B-C6B-O6B
34	d	403	LMT	O5B-C5B-C6B-O6B
38	D2	601	ADP	O4'-C4'-C5'-O5'
38	D2	601	ADP	C3'-C4'-C5'-O5'
38	B1	601	ADP	C3'-C4'-C5'-O5'
35	o	203	CDL	C31-CA7-OA8-CA6
35	O	203	CDL	C31-CA7-OA8-CA6
35	b	601	CDL	C31-C32-C33-C34
35	b	602	CDL	OA9-CA7-OA8-CA6
35	B	602	CDL	OA9-CA7-OA8-CA6
34	x	101	LMT	O5B-C5B-C6B-O6B
34	C	404	LMT	O5'-C5'-C6'-O6'
35	B	601	CDL	C31-C32-C33-C34
34	X	101	LMT	C4B-C5B-C6B-O6B
34	c	404	LMT	O5'-C1'-O1'-C1
34	d	401	LMT	O5B-C5B-C6B-O6B
35	o	203	CDL	CB7-C71-C72-C73
35	O	203	CDL	CB7-C71-C72-C73
34	H	301	LMT	O5'-C5'-C6'-O6'
34	D	401	LMT	O5B-C5B-C6B-O6B
34	X	101	LMT	O5B-C1B-O1B-C4'
35	C	401	CDL	CB2-C1-CA2-OA2
35	v	202	CDL	C71-CB7-OB8-CB6
35	V	202	CDL	C71-CB7-OB8-CB6
34	C	404	LMT	C4'-C5'-C6'-O6'
35	c	401	CDL	C40-C41-C42-C43
34	x	101	LMT	C4B-C5B-C6B-O6B
34	d	401	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
33	o	201	PC1	C31-C32-C33-C34
33	O	201	PC1	C31-C32-C33-C34
34	h	301	LMT	O5B-C5B-C6B-O6B
34	D	401	LMT	C4B-C5B-C6B-O6B
35	C	401	CDL	C51-CB5-OB6-CB4
35	D	402	CDL	C71-CB7-OB8-CB6
35	c	401	CDL	CA5-C11-C12-C13
34	x	101	LMT	O5B-C1B-O1B-C4'
34	h	301	LMT	O5'-C5'-C6'-O6'
34	H	301	LMT	O5B-C5B-C6B-O6B
35	h	302	CDL	C20-C21-C22-C23
35	d	402	CDL	C71-CB7-OB8-CB6
35	H	302	CDL	C20-C21-C22-C23
35	h	302	CDL	CB5-C51-C52-C53
35	U	201	CDL	CA7-C31-C32-C33
35	H	302	CDL	CB5-C51-C52-C53
34	H	301	LMT	C4'-C5'-C6'-O6'
35	u	201	CDL	CA7-C31-C32-C33
35	v	202	CDL	OB9-CB7-OB8-CB6
35	V	202	CDL	OB9-CB7-OB8-CB6
35	h	302	CDL	CA4-CA3-OA5-PA1
35	H	302	CDL	CA4-CA3-OA5-PA1
35	h	302	CDL	CA5-C11-C12-C13
35	e	401	CDL	CB5-C51-C52-C53
35	c	401	CDL	CB5-C51-C52-C53
35	H	302	CDL	CA5-C11-C12-C13
35	C	401	CDL	CA5-C11-C12-C13
34	C	404	LMT	O5'-C1'-O1'-C1
35	c	401	CDL	O1-C1-CB2-OB2
35	u	201	CDL	CB5-C51-C52-C53
35	b	601	CDL	CA7-C31-C32-C33
35	U	201	CDL	CB5-C51-C52-C53
35	E	401	CDL	CB5-C51-C52-C53
35	B	601	CDL	CA7-C31-C32-C33
35	c	401	CDL	C71-CB7-OB8-CB6
35	C	401	CDL	C71-CB7-OB8-CB6
35	v	202	CDL	CB7-C71-C72-C73
35	V	202	CDL	CB7-C71-C72-C73
35	C	401	CDL	OB7-CB5-OB6-CB4
35	c	401	CDL	CA2-C1-CB2-OB2
33	O	201	PC1	C32-C31-O31-C3
38	B2	601	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
33	o	201	PC1	C32-C31-O31-C3
35	u	201	CDL	C11-CA5-OA6-CA4
35	c	401	CDL	C51-CB5-OB6-CB4
35	U	201	CDL	C11-CA5-OA6-CA4
35	u	201	CDL	OA7-CA5-OA6-CA4
35	c	401	CDL	OB7-CB5-OB6-CB4
35	U	201	CDL	OA7-CA5-OA6-CA4
35	e	401	CDL	O1-C1-CA2-OA2
35	E	401	CDL	O1-C1-CA2-OA2
33	o	201	PC1	C21-C22-C23-C24
35	d	402	CDL	C1-CB2-OB2-PB2
35	D	402	CDL	C1-CB2-OB2-PB2
35	C	401	CDL	OB9-CB7-OB8-CB6
35	v	202	CDL	C63-C64-C65-C66
35	V	202	CDL	C63-C64-C65-C66
35	c	401	CDL	OB9-CB7-OB8-CB6
35	d	402	CDL	OB9-CB7-OB8-CB6
35	D	402	CDL	OB9-CB7-OB8-CB6
33	O	201	PC1	C21-C22-C23-C24
35	b	602	CDL	C71-CB7-OB8-CB6
35	B	602	CDL	C71-CB7-OB8-CB6
36	c	403	PEE	C31-C30-O3-C3
36	C	403	PEE	C31-C30-O3-C3
34	c	404	LMT	C1-C2-C3-C4
35	h	302	CDL	C71-C72-C73-C74
35	b	602	CDL	C38-C39-C40-C41
35	v	202	CDL	C57-C58-C59-C60
35	B	602	CDL	C38-C39-C40-C41
35	V	202	CDL	C57-C58-C59-C60
35	C	401	CDL	C35-C36-C37-C38
33	o	204	PC1	C3A-C3B-C3C-C3D
33	O	204	PC1	C3A-C3B-C3C-C3D
35	c	401	CDL	C17-C18-C19-C20
35	d	402	CDL	C42-C43-C44-C45
35	V	202	CDL	C35-C36-C37-C38
33	o	201	PC1	C3D-C3E-C3F-C3G
35	o	203	CDL	C16-C17-C18-C19
35	b	602	CDL	C22-C23-C24-C25
35	v	202	CDL	C35-C36-C37-C38
35	H	302	CDL	C71-C72-C73-C74
35	B	602	CDL	C22-C23-C24-C25
35	D	402	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
36	j	302	PEE	C31-C30-O3-C3
36	J	302	PEE	C31-C30-O3-C3
33	v	201	PC1	C35-C36-C37-C38
33	V	201	PC1	C35-C36-C37-C38
35	o	203	CDL	C12-C13-C14-C15
35	e	401	CDL	C31-C32-C33-C34
35	b	602	CDL	C77-C78-C79-C80
35	c	401	CDL	C53-C54-C55-C56
35	O	203	CDL	C12-C13-C14-C15
35	O	203	CDL	C16-C17-C18-C19
35	E	401	CDL	C31-C32-C33-C34
35	B	602	CDL	C77-C78-C79-C80
35	C	401	CDL	C21-C22-C23-C24
33	O	201	PC1	C3D-C3E-C3F-C3G
35	d	402	CDL	C60-C61-C62-C63
35	e	401	CDL	C78-C79-C80-C81
35	c	401	CDL	C52-C53-C54-C55
35	o	203	CDL	C51-C52-C53-C54
35	u	201	CDL	C41-C42-C43-C44
35	O	203	CDL	C51-C52-C53-C54
35	E	401	CDL	C78-C79-C80-C81
35	D	402	CDL	C60-C61-C62-C63
35	d	402	CDL	C11-CA5-OA6-CA4
35	D	402	CDL	C11-CA5-OA6-CA4
35	v	202	CDL	C72-C73-C74-C75
33	o	204	PC1	C27-C28-C29-C2A
33	O	204	PC1	C27-C28-C29-C2A
33	V	201	PC1	C25-C26-C27-C28
35	o	203	CDL	C38-C39-C40-C41
35	U	201	CDL	C41-C42-C43-C44
33	V	201	PC1	C21-C22-C23-C24
35	B	602	CDL	CA7-C31-C32-C33
33	v	201	PC1	C25-C26-C27-C28
35	u	201	CDL	C62-C63-C64-C65
35	b	601	CDL	C18-C19-C20-C21
35	b	602	CDL	C40-C41-C42-C43
35	c	401	CDL	C74-C75-C76-C77
35	O	203	CDL	C38-C39-C40-C41
35	U	201	CDL	C75-C76-C77-C78
35	B	601	CDL	C18-C19-C20-C21
35	B	602	CDL	C40-C41-C42-C43
35	B	602	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
35	V	202	CDL	C72-C73-C74-C75
35	C	401	CDL	C11-C12-C13-C14
35	u	201	CDL	C75-C76-C77-C78
35	b	602	CDL	C52-C53-C54-C55
35	H	302	CDL	C56-C57-C58-C59
35	C	401	CDL	C33-C34-C35-C36
34	C	404	LMT	C1-C2-C3-C4
35	c	401	CDL	C32-C33-C34-C35
35	C	401	CDL	C22-C23-C24-C25
33	v	201	PC1	C21-C22-C23-C24
34	X	101	LMT	O5'-C5'-C6'-O6'
33	o	201	PC1	O32-C31-O31-C3
33	O	201	PC1	O32-C31-O31-C3
35	h	302	CDL	C56-C57-C58-C59
35	b	601	CDL	C74-C75-C76-C77
35	U	201	CDL	C62-C63-C64-C65
35	B	602	CDL	C56-C57-C58-C59
35	D	402	CDL	C52-C53-C54-C55
34	d	401	LMT	C3-C4-C5-C6
35	b	602	CDL	C56-C57-C58-C59
35	O	203	CDL	C61-C62-C63-C64
35	H	302	CDL	C22-C23-C24-C25
35	B	601	CDL	C74-C75-C76-C77
35	e	401	CDL	CB2-C1-CA2-OA2
35	E	401	CDL	CB2-C1-CA2-OA2
35	h	302	CDL	C22-C23-C24-C25
35	e	401	CDL	C81-C82-C83-C84
35	b	602	CDL	C80-C81-C82-C83
35	c	401	CDL	C21-C22-C23-C24
35	c	401	CDL	C22-C23-C24-C25
35	d	402	CDL	C82-C83-C84-C85
35	U	201	CDL	C77-C78-C79-C80
35	b	602	CDL	CA7-C31-C32-C33
33	o	204	PC1	C32-C33-C34-C35
33	O	204	PC1	C32-C33-C34-C35
34	o	202	LMT	C7-C8-C9-C10
34	O	202	LMT	C7-C8-C9-C10
35	o	203	CDL	C23-C24-C25-C26
35	o	203	CDL	C37-C38-C39-C40
35	o	203	CDL	C61-C62-C63-C64
35	u	201	CDL	C23-C24-C25-C26
35	u	201	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
35	e	401	CDL	C37-C38-C39-C40
35	e	401	CDL	C40-C41-C42-C43
35	e	401	CDL	C58-C59-C60-C61
35	c	401	CDL	C55-C56-C57-C58
35	d	402	CDL	C52-C53-C54-C55
35	O	203	CDL	C23-C24-C25-C26
35	O	203	CDL	C37-C38-C39-C40
35	O	203	CDL	C83-C84-C85-C86
35	U	201	CDL	C23-C24-C25-C26
35	U	201	CDL	C35-C36-C37-C38
35	E	401	CDL	C40-C41-C42-C43
35	E	401	CDL	C81-C82-C83-C84
35	B	602	CDL	C80-C81-C82-C83
35	D	402	CDL	C82-C83-C84-C85
35	B	602	CDL	OB9-CB7-OB8-CB6
36	j	302	PEE	O5-C30-O3-C3
36	C	403	PEE	O5-C30-O3-C3
35	o	203	CDL	C83-C84-C85-C86
35	u	201	CDL	C77-C78-C79-C80
35	E	401	CDL	C37-C38-C39-C40
35	C	401	CDL	C63-C64-C65-C66
35	c	401	CDL	C19-C20-C21-C22
35	H	302	CDL	C59-C60-C61-C62
35	u	201	CDL	C79-C80-C81-C82
35	b	602	CDL	C73-C74-C75-C76
35	E	401	CDL	C58-C59-C60-C61
35	B	602	CDL	C73-C74-C75-C76
35	b	602	CDL	OB9-CB7-OB8-CB6
36	c	403	PEE	O5-C30-O3-C3
34	x	101	LMT	C7-C8-C9-C10
34	X	101	LMT	C5-C6-C7-C8
35	h	302	CDL	C59-C60-C61-C62
35	e	401	CDL	C23-C24-C25-C26
35	E	401	CDL	C23-C24-C25-C26
35	C	401	CDL	C54-C55-C56-C57
34	X	101	LMT	C7-C8-C9-C10
35	U	201	CDL	C79-C80-C81-C82
36	C	403	PEE	C23-C24-C25-C26
34	D	401	LMT	C11-C10-C9-C8
35	h	302	CDL	C80-C81-C82-C83
35	H	302	CDL	C80-C81-C82-C83
36	c	403	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
36	J	302	PEE	O5-C30-O3-C3
34	x	101	LMT	C5-C6-C7-C8
35	c	401	CDL	C72-C73-C74-C75
36	j	301	PEE	C14-C15-C16-C17
35	d	402	CDL	OA7-CA5-OA6-CA4
35	D	402	CDL	OA7-CA5-OA6-CA4
36	J	301	PEE	C14-C15-C16-C17
35	u	201	CDL	C14-C15-C16-C17
35	c	401	CDL	C82-C83-C84-C85
35	C	401	CDL	C32-C33-C34-C35
35	c	401	CDL	C39-C40-C41-C42
35	U	201	CDL	C14-C15-C16-C17
36	J	301	PEE	C23-C24-C25-C26
33	V	201	PC1	C33-C34-C35-C36
36	j	301	PEE	C23-C24-C25-C26
36	J	301	PEE	C34-C35-C36-C37
33	V	201	PC1	C3B-C3C-C3D-C3E
35	C	401	CDL	C14-C15-C16-C17
36	j	301	PEE	C34-C35-C36-C37
33	v	201	PC1	C3B-C3C-C3D-C3E
34	X	101	LMT	C3-C4-C5-C6
35	C	401	CDL	C74-C75-C76-C77
35	h	302	CDL	C53-C54-C55-C56
34	D	401	LMT	C5-C6-C7-C8
35	H	302	CDL	C53-C54-C55-C56
36	c	403	PEE	C22-C23-C24-C25
36	C	403	PEE	C22-C23-C24-C25
35	u	201	CDL	C51-CB5-OB6-CB4
35	b	601	CDL	C11-CA5-OA6-CA4
35	U	201	CDL	C51-CB5-OB6-CB4
35	B	601	CDL	C11-CA5-OA6-CA4
33	v	201	PC1	C33-C34-C35-C36
35	u	201	CDL	OB7-CB5-OB6-CB4
35	U	201	CDL	OB7-CB5-OB6-CB4
35	B	601	CDL	OA7-CA5-OA6-CA4
35	e	401	CDL	C74-C75-C76-C77
35	B	601	CDL	C72-C73-C74-C75
35	B	602	CDL	C11-C12-C13-C14
35	E	401	CDL	C74-C75-C76-C77
36	C	403	PEE	C21-C22-C23-C24
34	x	101	LMT	C3-C4-C5-C6
35	b	601	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
35	b	602	CDL	C11-C12-C13-C14
36	c	403	PEE	C21-C22-C23-C24
38	B1	601	ADP	O4'-C4'-C5'-O5'
35	O	203	CDL	C31-C32-C33-C34
34	d	401	LMT	C7-C8-C9-C10
35	o	203	CDL	C31-C32-C33-C34
34	d	401	LMT	C1-C2-C3-C4
35	b	601	CDL	C36-C37-C38-C39
35	d	402	CDL	C80-C81-C82-C83
35	B	601	CDL	C36-C37-C38-C39
35	b	602	CDL	C62-C63-C64-C65
35	D	402	CDL	C80-C81-C82-C83
34	c	402	LMT	C1-C2-C3-C4
35	b	601	CDL	OA7-CA5-OA6-CA4
35	B	602	CDL	C62-C63-C64-C65
35	C	401	CDL	C41-C42-C43-C44
34	C	402	LMT	C1-C2-C3-C4
36	j	301	PEE	C10-C11-C12-C13
36	J	301	PEE	C10-C11-C12-C13
35	D	402	CDL	C73-C74-C75-C76
35	V	202	CDL	OA6-CA4-CA6-OA8
33	O	201	PC1	C26-C27-C28-C29
35	B	601	CDL	C41-C42-C43-C44
35	C	401	CDL	C58-C59-C60-C61
34	D	401	LMT	C1-C2-C3-C4
35	b	601	CDL	C16-C17-C18-C19
35	b	601	CDL	C78-C79-C80-C81
35	B	601	CDL	C78-C79-C80-C81
35	V	202	CDL	C61-C62-C63-C64
35	V	202	CDL	C62-C63-C64-C65
33	o	201	PC1	C26-C27-C28-C29
35	v	202	CDL	C62-C63-C64-C65
35	d	402	CDL	C73-C74-C75-C76
35	B	601	CDL	C16-C17-C18-C19
36	c	403	PEE	C36-C37-C38-C39
36	C	403	PEE	C36-C37-C38-C39
35	b	601	CDL	C41-C42-C43-C44
35	v	202	CDL	C61-C62-C63-C64
35	v	202	CDL	C55-C56-C57-C58
33	v	201	PC1	C23-C24-C25-C26
35	d	402	CDL	C40-C41-C42-C43
35	V	202	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
35	C	401	CDL	C15-C16-C17-C18
35	C	401	CDL	C20-C21-C22-C23
35	D	402	CDL	C40-C41-C42-C43
33	V	201	PC1	C23-C24-C25-C26
36	J	302	PEE	C17-C18-C19-C20
33	o	204	PC1	C39-C3A-C3B-C3C
33	O	204	PC1	C39-C3A-C3B-C3C
35	u	201	CDL	C60-C61-C62-C63
35	c	401	CDL	C43-C44-C45-C46
35	c	401	CDL	C81-C82-C83-C84
35	b	601	CDL	C58-C59-C60-C61
35	U	201	CDL	C60-C61-C62-C63
35	c	401	CDL	C51-C52-C53-C54
35	B	601	CDL	C58-C59-C60-C61
35	d	402	CDL	C63-C64-C65-C66
36	c	403	PEE	C19-C20-C21-C22
36	C	403	PEE	C19-C20-C21-C22
34	D	401	LMT	C3-C4-C5-C6
35	C	401	CDL	OB5-CB3-CB4-CB6
34	c	402	LMT	C3-C4-C5-C6
34	d	401	LMT	C4-C5-C6-C7
34	C	402	LMT	C3-C4-C5-C6
35	B	601	CDL	C56-C57-C58-C59
34	C	404	LMT	C3-C4-C5-C6
35	b	601	CDL	C56-C57-C58-C59
34	D	401	LMT	O5'-C5'-C6'-O6'
38	B2	601	ADP	O4'-C4'-C5'-O5'
36	C	403	PEE	C13-C14-C15-C16
34	h	301	LMT	C4'-C5'-C6'-O6'
35	b	601	CDL	C62-C63-C64-C65
35	B	601	CDL	C62-C63-C64-C65
35	D	402	CDL	C63-C64-C65-C66
36	c	403	PEE	C13-C14-C15-C16
35	D	402	CDL	C36-C37-C38-C39
35	c	401	CDL	C44-C45-C46-C47
35	C	401	CDL	C55-C56-C57-C58
35	c	401	CDL	CA7-C31-C32-C33
34	c	404	LMT	C2-C3-C4-C5
35	o	203	CDL	C63-C64-C65-C66
35	h	302	CDL	C58-C59-C60-C61
35	d	402	CDL	C36-C37-C38-C39
36	j	302	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	o	203	CDL	CB3-CB4-CB6-OB8
35	v	202	CDL	CA3-CA4-CA6-OA8
35	V	202	CDL	CA3-CA4-CA6-OA8
35	C	401	CDL	CB3-CB4-CB6-OB8
35	O	203	CDL	C63-C64-C65-C66
35	H	302	CDL	C58-C59-C60-C61
33	o	204	PC1	C37-C38-C39-C3A
33	O	204	PC1	C37-C38-C39-C3A
35	h	302	CDL	C74-C75-C76-C77
35	B	601	CDL	C43-C44-C45-C46
34	C	404	LMT	C2-C3-C4-C5
35	b	602	CDL	C51-C52-C53-C54
35	H	302	CDL	C74-C75-C76-C77
35	B	602	CDL	C51-C52-C53-C54
35	o	203	CDL	C71-CB7-OB8-CB6
35	O	203	CDL	C71-CB7-OB8-CB6
34	d	401	LMT	O5'-C5'-C6'-O6'
34	c	404	LMT	C3-C4-C5-C6
35	b	601	CDL	C43-C44-C45-C46
35	e	401	CDL	C53-C54-C55-C56
35	H	302	CDL	C76-C77-C78-C79
35	h	302	CDL	C76-C77-C78-C79
35	c	401	CDL	C12-C13-C14-C15
35	E	401	CDL	C14-C15-C16-C17
35	E	401	CDL	C53-C54-C55-C56
35	e	401	CDL	C14-C15-C16-C17
35	e	401	CDL	CA7-C31-C32-C33
35	b	601	CDL	C31-CA7-OA8-CA6
35	d	402	CDL	C31-CA7-OA8-CA6
35	B	601	CDL	C31-CA7-OA8-CA6
35	D	402	CDL	C31-CA7-OA8-CA6
35	h	302	CDL	CB3-CB4-OB6-CB5
35	d	402	CDL	CA6-CA4-OA6-CA5
35	H	302	CDL	CB3-CB4-OB6-CB5
35	D	402	CDL	CA6-CA4-OA6-CA5
34	D	401	LMT	C7-C8-C9-C10
35	E	401	CDL	CA7-C31-C32-C33
33	V	201	PC1	O11-C1-C2-O21
35	b	601	CDL	OA5-CA3-CA4-OA6
35	b	602	CDL	OA5-CA3-CA4-OA6
35	B	601	CDL	OA5-CA3-CA4-OA6
35	b	601	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
36	j	302	PEE	C40-C41-C42-C43
36	J	302	PEE	C40-C41-C42-C43
35	h	302	CDL	C14-C15-C16-C17
35	B	601	CDL	C80-C81-C82-C83
36	J	302	PEE	C23-C24-C25-C26
35	U	201	CDL	C84-C85-C86-C87
35	H	302	CDL	C14-C15-C16-C17
36	j	301	PEE	C41-C42-C43-C44
36	J	301	PEE	C41-C42-C43-C44
36	C	403	PEE	C42-C43-C44-C45
33	o	201	PC1	C37-C38-C39-C3A
33	O	201	PC1	C37-C38-C39-C3A
35	B	601	CDL	C63-C64-C65-C66
36	j	302	PEE	C23-C24-C25-C26
36	c	403	PEE	C42-C43-C44-C45
35	u	201	CDL	C84-C85-C86-C87
34	x	101	LMT	C2-C3-C4-C5
34	X	101	LMT	C2-C3-C4-C5
35	o	203	CDL	OB6-CB4-CB6-OB8
35	e	401	CDL	OA6-CA4-CA6-OA8
35	v	202	CDL	OA6-CA4-CA6-OA8
35	O	203	CDL	OB6-CB4-CB6-OB8
35	E	401	CDL	OA6-CA4-CA6-OA8
35	v	202	CDL	C59-C60-C61-C62
35	B	602	CDL	C44-C45-C46-C47
35	b	601	CDL	C32-C33-C34-C35
35	b	601	CDL	C63-C64-C65-C66
35	v	202	CDL	C74-C75-C76-C77
35	c	401	CDL	C31-C32-C33-C34
35	V	202	CDL	C59-C60-C61-C62
33	O	204	PC1	C3E-C3F-C3G-C3H
35	B	602	CDL	C58-C59-C60-C61
33	o	204	PC1	C3E-C3F-C3G-C3H
35	b	602	CDL	C44-C45-C46-C47
34	x	101	LMT	O5'-C5'-C6'-O6'
33	V	201	PC1	C36-C37-C38-C39
34	D	403	LMT	C3-C4-C5-C6
35	V	202	CDL	C74-C75-C76-C77
35	V	202	CDL	C44-C45-C46-C47
34	d	403	LMT	C3-C4-C5-C6
35	B	601	CDL	C32-C33-C34-C35
35	C	401	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
33	v	201	PC1	C36-C37-C38-C39
34	h	301	LMT	C4B-C5B-C6B-O6B
35	H	302	CDL	C34-C35-C36-C37
35	h	302	CDL	C34-C35-C36-C37
35	v	202	CDL	C44-C45-C46-C47
35	b	602	CDL	C58-C59-C60-C61
35	u	201	CDL	C38-C39-C40-C41
35	U	201	CDL	C38-C39-C40-C41
35	c	401	CDL	C15-C16-C17-C18
35	C	401	CDL	C19-C20-C21-C22
35	v	202	CDL	C1-CA2-OA2-PA1
33	V	201	PC1	C38-C39-C3A-C3B
34	d	401	LMT	C5-C6-C7-C8
35	b	601	CDL	C52-C53-C54-C55
35	U	201	CDL	C58-C59-C60-C61
35	B	601	CDL	C17-C18-C19-C20
35	C	401	CDL	C34-C35-C36-C37
33	v	201	PC1	C38-C39-C3A-C3B
35	u	201	CDL	C58-C59-C60-C61
36	j	302	PEE	C21-C22-C23-C24
34	D	401	LMT	C6-C7-C8-C9
35	E	401	CDL	C42-C43-C44-C45
35	C	401	CDL	C60-C61-C62-C63
36	J	302	PEE	C21-C22-C23-C24
35	h	302	CDL	C64-C65-C66-C67
35	e	401	CDL	OB5-CB3-CB4-CB6
35	E	401	CDL	OB5-CB3-CB4-CB6
35	e	401	CDL	C42-C43-C44-C45
35	H	302	CDL	C64-C65-C66-C67
35	h	302	CDL	C24-C25-C26-C27
35	H	302	CDL	C24-C25-C26-C27
34	c	402	LMT	O1'-C1-C2-C3
34	C	402	LMT	O1'-C1-C2-C3
35	b	601	CDL	C17-C18-C19-C20
35	b	601	CDL	C83-C84-C85-C86
35	u	201	CDL	C64-C65-C66-C67
35	c	401	CDL	C13-C14-C15-C16
35	c	401	CDL	C14-C15-C16-C17
36	J	302	PEE	C13-C14-C15-C16
35	B	601	CDL	C52-C53-C54-C55
35	B	601	CDL	C83-C84-C85-C86
35	c	401	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
35	U	201	CDL	C64-C65-C66-C67
36	j	302	PEE	C13-C14-C15-C16
35	b	601	CDL	OA9-CA7-OA8-CA6
35	B	601	CDL	OA9-CA7-OA8-CA6
35	O	203	CDL	C35-C36-C37-C38
35	o	203	CDL	C35-C36-C37-C38
35	B	602	CDL	C31-C32-C33-C34
35	C	401	CDL	CA7-C31-C32-C33
34	c	404	LMT	C4'-C5'-C6'-O6'
35	C	401	CDL	C75-C76-C77-C78
35	o	203	CDL	CA3-CA4-CA6-OA8
35	b	602	CDL	CB3-CB4-CB6-OB8
35	c	401	CDL	CB3-CB4-CB6-OB8
35	O	203	CDL	CA3-CA4-CA6-OA8
35	O	203	CDL	CB3-CB4-CB6-OB8
35	B	602	CDL	CB3-CB4-CB6-OB8
35	b	602	CDL	C31-C32-C33-C34
35	c	401	CDL	C63-C64-C65-C66
34	D	401	LMT	O1'-C1-C2-C3
35	O	203	CDL	C59-C60-C61-C62
35	V	202	CDL	C11-C12-C13-C14
35	o	203	CDL	C59-C60-C61-C62
35	v	202	CDL	C11-C12-C13-C14
35	o	203	CDL	OB9-CB7-OB8-CB6
35	O	203	CDL	OB9-CB7-OB8-CB6
35	c	401	CDL	C59-C60-C61-C62
33	o	201	PC1	O11-C1-C2-O21
33	o	204	PC1	O11-C1-C2-O21
33	v	201	PC1	O11-C1-C2-O21
33	O	201	PC1	O11-C1-C2-O21
33	O	204	PC1	O11-C1-C2-O21
35	b	602	CDL	OB5-CB3-CB4-OB6
35	c	401	CDL	OB5-CB3-CB4-OB6
35	B	602	CDL	OB5-CB3-CB4-OB6
35	C	401	CDL	C13-C14-C15-C16
35	C	401	CDL	C61-C62-C63-C64
35	V	202	CDL	C1-CA2-OA2-PA1
35	V	202	CDL	C52-C53-C54-C55
35	v	202	CDL	C52-C53-C54-C55
35	V	202	CDL	C15-C16-C17-C18
34	H	301	LMT	C5'-C4'-O1B-C1B
33	O	204	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
36	c	403	PEE	C34-C35-C36-C37
36	C	403	PEE	C34-C35-C36-C37
33	o	204	PC1	C26-C27-C28-C29
35	D	402	CDL	C71-C72-C73-C74
35	e	401	CDL	C32-C33-C34-C35
35	d	402	CDL	C71-C72-C73-C74
35	E	401	CDL	C32-C33-C34-C35
35	D	402	CDL	C56-C57-C58-C59
36	J	302	PEE	C30-C31-C32-C33
35	d	402	CDL	OA9-CA7-OA8-CA6
33	V	201	PC1	C2B-C2C-C2D-C2E
35	c	401	CDL	C20-C21-C22-C23
35	d	402	CDL	C56-C57-C58-C59
35	v	202	CDL	C15-C16-C17-C18
35	V	202	CDL	C33-C34-C35-C36
35	C	401	CDL	C62-C63-C64-C65
33	O	201	PC1	C34-C35-C36-C37
35	v	202	CDL	C33-C34-C35-C36
34	h	301	LMT	C5'-C4'-O1B-C1B
34	H	301	LMT	C4B-C5B-C6B-O6B
33	v	201	PC1	C2B-C2C-C2D-C2E
35	D	402	CDL	OA9-CA7-OA8-CA6
36	j	302	PEE	C30-C31-C32-C33
33	o	201	PC1	C34-C35-C36-C37
35	c	401	CDL	OB5-CB3-CB4-CB6
35	c	401	CDL	C34-C35-C36-C37
35	h	302	CDL	C36-C37-C38-C39
35	e	401	CDL	C71-C72-C73-C74
35	E	401	CDL	C71-C72-C73-C74
35	b	602	CDL	C63-C64-C65-C66
35	H	302	CDL	C36-C37-C38-C39
35	B	602	CDL	C63-C64-C65-C66
35	C	401	CDL	C31-C32-C33-C34
35	b	602	CDL	CB6-CB4-OB6-CB5
35	B	602	CDL	CB6-CB4-OB6-CB5
34	C	402	LMT	C3'-C4'-O1B-C1B
35	c	401	CDL	C75-C76-C77-C78
35	o	203	CDL	C44-C45-C46-C47
35	O	203	CDL	C44-C45-C46-C47
35	h	302	CDL	C78-C79-C80-C81
35	e	401	CDL	OB5-CB3-CB4-OB6
35	b	601	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
35	v	202	CDL	OA5-CA3-CA4-OA6
35	B	602	CDL	OA5-CA3-CA4-OA6
35	C	401	CDL	OB5-CB3-CB4-OB6
35	O	203	CDL	C72-C73-C74-C75
35	o	203	CDL	C72-C73-C74-C75
35	V	202	CDL	CB3-CB4-CB6-OB8
34	x	101	LMT	C9-C10-C11-C12
35	H	302	CDL	C78-C79-C80-C81
35	b	601	CDL	C61-C62-C63-C64
33	o	204	PC1	C12-C11-O13-P
33	O	204	PC1	C12-C11-O13-P
35	u	201	CDL	C11-C12-C13-C14
35	h	302	CDL	OB6-CB4-CB6-OB8
35	b	602	CDL	OB6-CB4-CB6-OB8
35	v	202	CDL	OB6-CB4-CB6-OB8
35	c	401	CDL	OB6-CB4-CB6-OB8
35	H	302	CDL	OB6-CB4-CB6-OB8
35	B	602	CDL	OB6-CB4-CB6-OB8
34	C	402	LMT	C11-C10-C9-C8
35	E	401	CDL	C17-C18-C19-C20
34	c	402	LMT	C6-C7-C8-C9
34	C	402	LMT	C6-C7-C8-C9
35	U	201	CDL	C11-C12-C13-C14
35	H	302	CDL	C16-C17-C18-C19
35	B	601	CDL	C61-C62-C63-C64
35	C	401	CDL	C56-C57-C58-C59
34	X	101	LMT	C9-C10-C11-C12
35	d	402	CDL	CA7-C31-C32-C33
35	D	402	CDL	CA7-C31-C32-C33
33	O	204	PC1	C23-C24-C25-C26
33	o	204	PC1	C23-C24-C25-C26
34	c	402	LMT	C11-C10-C9-C8
35	h	302	CDL	C16-C17-C18-C19
35	d	402	CDL	C38-C39-C40-C41
35	e	401	CDL	C59-C60-C61-C62
35	D	402	CDL	C38-C39-C40-C41
33	o	204	PC1	O13-C11-C12-N
33	O	204	PC1	O13-C11-C12-N
35	E	401	CDL	C59-C60-C61-C62
35	O	203	CDL	C43-C44-C45-C46
34	c	402	LMT	C3'-C4'-O1B-C1B
36	c	403	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
35	o	203	CDL	C43-C44-C45-C46
36	J	301	PEE	C12-C13-C14-C15
36	j	302	PEE	C44-C45-C46-C47
35	D	402	CDL	C41-C42-C43-C44
35	e	401	CDL	C17-C18-C19-C20
35	d	402	CDL	C41-C42-C43-C44
36	j	301	PEE	C12-C13-C14-C15
36	J	302	PEE	C44-C45-C46-C47
35	B	602	CDL	C71-C72-C73-C74
33	v	201	PC1	O11-C1-C2-C3
33	V	201	PC1	O11-C1-C2-C3
35	v	202	CDL	OA5-CA3-CA4-CA6
35	V	202	CDL	OA5-CA3-CA4-CA6
34	D	401	LMT	C4-C5-C6-C7
36	C	403	PEE	C40-C41-C42-C43
35	b	602	CDL	C71-C72-C73-C74
34	x	101	LMT	C4-C5-C6-C7
34	X	101	LMT	C4-C5-C6-C7
35	D	402	CDL	C11-C12-C13-C14
35	V	202	CDL	OA5-CA3-CA4-OA6
35	d	402	CDL	C11-C12-C13-C14
34	C	402	LMT	C5'-C4'-O1B-C1B
33	o	201	PC1	C38-C39-C3A-C3B
34	d	403	LMT	O1'-C1-C2-C3
34	D	403	LMT	O1'-C1-C2-C3
33	O	201	PC1	C38-C39-C3A-C3B
35	E	401	CDL	C20-C21-C22-C23
36	j	302	PEE	C16-C17-C18-C19
36	J	302	PEE	C16-C17-C18-C19
35	e	401	CDL	C20-C21-C22-C23
36	j	302	PEE	C14-C15-C16-C17
35	o	203	CDL	OA6-CA4-CA6-OA8
35	O	203	CDL	OA6-CA4-CA6-OA8
35	V	202	CDL	OB6-CB4-CB6-OB8
35	C	401	CDL	OB6-CB4-CB6-OB8
35	C	401	CDL	C17-C18-C19-C20
35	C	401	CDL	C43-C44-C45-C46
36	J	302	PEE	C14-C15-C16-C17
35	v	202	CDL	CB3-CB4-CB6-OB8
35	c	401	CDL	C54-C55-C56-C57
35	B	602	CDL	C59-C60-C61-C62
35	B	602	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	o	204	PC1	C3B-C3C-C3D-C3E
35	b	602	CDL	C59-C60-C61-C62
33	O	204	PC1	C3B-C3C-C3D-C3E
33	O	201	PC1	C2D-C2E-C2F-C2G
35	b	602	CDL	C15-C16-C17-C18
36	j	302	PEE	C41-C42-C43-C44
33	o	201	PC1	C11-O13-P-O14
33	o	201	PC1	C1-O11-P-O12
33	v	201	PC1	C11-O13-P-O14
33	v	201	PC1	C11-O13-P-O11
33	O	201	PC1	C11-O13-P-O14
33	O	201	PC1	C1-O11-P-O12
33	V	201	PC1	C11-O13-P-O14
33	V	201	PC1	C11-O13-P-O11
35	o	203	CDL	CB3-OB5-PB2-OB4
35	u	201	CDL	CB2-OB2-PB2-OB5
35	h	302	CDL	CA2-OA2-PA1-OA3
35	h	302	CDL	CB2-OB2-PB2-OB4
35	e	401	CDL	CA3-OA5-PA1-OA3
35	v	202	CDL	CA2-OA2-PA1-OA3
35	U	201	CDL	CB2-OB2-PB2-OB5
35	H	302	CDL	CA2-OA2-PA1-OA3
35	H	302	CDL	CB2-OB2-PB2-OB4
35	E	401	CDL	CA3-OA5-PA1-OA3
35	V	202	CDL	CA2-OA2-PA1-OA3
35	C	401	CDL	CA3-OA5-PA1-OA2
35	C	401	CDL	CA3-OA5-PA1-OA3
35	C	401	CDL	CA3-OA5-PA1-OA4
35	C	401	CDL	CB3-OB5-PB2-OB3
35	D	402	CDL	CB3-OB5-PB2-OB4
37	E2	601	ATP	C5'-O5'-PA-O2A
37	E2	601	ATP	C5'-O5'-PA-O3A
37	E1	601	ATP	C5'-O5'-PA-O2A
37	E1	601	ATP	C5'-O5'-PA-O3A
38	B2	601	ADP	C5'-O5'-PA-O1A
38	B1	601	ADP	C5'-O5'-PA-O1A
33	o	201	PC1	C2D-C2E-C2F-C2G
35	U	201	CDL	C18-C19-C20-C21
35	H	302	CDL	C84-C85-C86-C87
35	h	302	CDL	C1-CA2-OA2-PA1
35	O	203	CDL	CA4-CA3-OA5-PA1
35	H	302	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
36	J	302	PEE	C41-C42-C43-C44
35	u	201	CDL	C18-C19-C20-C21
35	C	401	CDL	C53-C54-C55-C56
33	v	201	PC1	C26-C27-C28-C29
35	h	302	CDL	C84-C85-C86-C87
35	b	601	CDL	O1-C1-CA2-OA2
35	B	601	CDL	O1-C1-CA2-OA2
34	c	402	LMT	C5'-C4'-O1B-C1B
33	V	201	PC1	C26-C27-C28-C29
35	b	601	CDL	C60-C61-C62-C63
35	B	602	CDL	C83-C84-C85-C86
35	b	602	CDL	CA3-CA4-OA6-CA5
35	v	202	CDL	CA3-CA4-OA6-CA5
35	b	602	CDL	C83-C84-C85-C86
35	V	202	CDL	C37-C38-C39-C40
35	O	203	CDL	C19-C20-C21-C22
35	U	201	CDL	C16-C17-C18-C19
33	o	204	PC1	O11-C1-C2-C3
33	O	204	PC1	O11-C1-C2-C3
35	o	203	CDL	OA5-CA3-CA4-CA6
35	b	601	CDL	OA5-CA3-CA4-CA6
35	B	601	CDL	OA5-CA3-CA4-CA6
35	D	402	CDL	OA5-CA3-CA4-CA6
35	u	201	CDL	C33-C34-C35-C36
35	v	202	CDL	C37-C38-C39-C40
35	c	401	CDL	C23-C24-C25-C26
35	U	201	CDL	C33-C34-C35-C36
36	J	301	PEE	C20-C21-C22-C23
35	E	401	CDL	OB5-CB3-CB4-OB6
35	u	201	CDL	C16-C17-C18-C19
35	V	202	CDL	C81-C82-C83-C84
36	j	301	PEE	C20-C21-C22-C23
35	v	202	CDL	C81-C82-C83-C84
35	u	201	CDL	C36-C37-C38-C39
35	C	401	CDL	C83-C84-C85-C86
35	B	601	CDL	C60-C61-C62-C63
36	j	301	PEE	O4-C10-O2-C2
35	o	203	CDL	CA4-CA3-OA5-PA1
35	c	401	CDL	C1-CA2-OA2-PA1
35	d	402	CDL	OB6-CB4-CB6-OB8
35	D	402	CDL	OB6-CB4-CB6-OB8
33	O	204	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
33	o	204	PC1	O31-C31-C32-C33
35	o	203	CDL	C19-C20-C21-C22
36	J	301	PEE	O4-C10-O2-C2
35	U	201	CDL	C36-C37-C38-C39
35	H	302	CDL	C39-C40-C41-C42
35	d	402	CDL	C74-C75-C76-C77
35	D	402	CDL	C74-C75-C76-C77
35	c	401	CDL	C80-C81-C82-C83
36	j	301	PEE	O5-C30-O3-C3
33	v	201	PC1	C2F-C2G-C2H-C2I
33	V	201	PC1	C2F-C2G-C2H-C2I
35	v	202	CDL	C24-C25-C26-C27
33	v	201	PC1	O32-C31-O31-C3
33	V	201	PC1	O32-C31-O31-C3
33	V	201	PC1	C32-C31-O31-C3
35	V	202	CDL	C24-C25-C26-C27
35	h	302	CDL	C39-C40-C41-C42
33	v	201	PC1	C32-C31-O31-C3
36	J	301	PEE	O5-C30-O3-C3
35	e	401	CDL	OA5-CA3-CA4-OA6
35	B	601	CDL	OB5-CB3-CB4-OB6
33	O	204	PC1	C2B-C2C-C2D-C2E
36	j	301	PEE	C21-C22-C23-C24
35	B	601	CDL	C76-C77-C78-C79
36	J	301	PEE	C21-C22-C23-C24
35	C	401	CDL	C39-C40-C41-C42
33	o	204	PC1	C2B-C2C-C2D-C2E
35	c	401	CDL	C35-C36-C37-C38
35	B	601	CDL	C15-C16-C17-C18
35	b	601	CDL	C76-C77-C78-C79
34	d	401	LMT	O1'-C1-C2-C3
33	O	201	PC1	C39-C3A-C3B-C3C
35	b	601	CDL	C15-C16-C17-C18
35	b	602	CDL	C13-C14-C15-C16
36	C	403	PEE	C33-C34-C35-C36
36	J	302	PEE	C34-C35-C36-C37
33	O	204	PC1	C25-C26-C27-C28
35	V	202	CDL	C76-C77-C78-C79
33	o	201	PC1	C39-C3A-C3B-C3C
35	e	401	CDL	C1-CB2-OB2-PB2
35	E	401	CDL	C1-CB2-OB2-PB2
33	o	204	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
36	J	302	PEE	C11-C12-C13-C14
36	c	403	PEE	C33-C34-C35-C36
36	J	301	PEE	C11-C10-O2-C2
35	u	201	CDL	C44-C45-C46-C47
35	O	203	CDL	C17-C18-C19-C20
35	U	201	CDL	C44-C45-C46-C47
35	B	602	CDL	C13-C14-C15-C16
35	o	203	CDL	C17-C18-C19-C20
35	v	202	CDL	C76-C77-C78-C79
34	O	202	LMT	C5-C6-C7-C8
36	j	302	PEE	C11-C12-C13-C14
35	e	401	CDL	C62-C63-C64-C65
36	j	302	PEE	C34-C35-C36-C37
36	j	301	PEE	C31-C30-O3-C3
35	c	401	CDL	C11-C12-C13-C14
35	h	302	CDL	CA3-CA4-OA6-CA5
35	h	302	CDL	CA6-CA4-OA6-CA5
35	c	401	CDL	CA6-CA4-OA6-CA5
35	d	402	CDL	CB3-CB4-OB6-CB5
35	H	302	CDL	CA3-CA4-OA6-CA5
35	B	602	CDL	CA3-CA4-OA6-CA5
35	V	202	CDL	CA3-CA4-OA6-CA5
35	D	402	CDL	CB3-CB4-OB6-CB5
35	h	302	CDL	C63-C64-C65-C66
33	O	201	PC1	C3A-C3B-C3C-C3D
33	v	201	PC1	C39-C3A-C3B-C3C
33	o	201	PC1	C3A-C3B-C3C-C3D
34	o	202	LMT	C5-C6-C7-C8
34	c	402	LMT	C7-C8-C9-C10
35	E	401	CDL	C62-C63-C64-C65
34	c	404	LMT	O5'-C5'-C6'-O6'
36	C	403	PEE	C11-C12-C13-C14
33	V	201	PC1	C39-C3A-C3B-C3C
35	d	402	CDL	C75-C76-C77-C78
34	C	402	LMT	C7-C8-C9-C10
35	E	401	CDL	OA5-CA3-CA4-OA6
33	o	204	PC1	C24-C25-C26-C27
35	d	402	CDL	C16-C17-C18-C19
36	j	301	PEE	C11-C10-O2-C2
35	H	302	CDL	C63-C64-C65-C66
36	J	301	PEE	C31-C30-O3-C3
33	o	204	PC1	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
33	O	204	PC1	C29-C2A-C2B-C2C
35	D	402	CDL	C16-C17-C18-C19
35	D	402	CDL	C75-C76-C77-C78
35	e	401	CDL	C55-C56-C57-C58
35	b	601	CDL	OB5-CB3-CB4-CB6
35	d	402	CDL	OA5-CA3-CA4-CA6
35	O	203	CDL	OA5-CA3-CA4-CA6
35	d	402	CDL	C32-C33-C34-C35
36	c	403	PEE	C11-C12-C13-C14
35	b	602	CDL	C17-C18-C19-C20
36	c	403	PEE	C38-C39-C40-C41
36	C	403	PEE	C38-C39-C40-C41
35	B	602	CDL	C17-C18-C19-C20
35	D	402	CDL	C32-C33-C34-C35
33	O	204	PC1	C24-C25-C26-C27
36	j	301	PEE	C22-C23-C24-C25
35	E	401	CDL	C55-C56-C57-C58
35	d	402	CDL	C64-C65-C66-C67
35	D	402	CDL	C64-C65-C66-C67
35	e	401	CDL	OB7-CB5-OB6-CB4
35	E	401	CDL	OB7-CB5-OB6-CB4
36	J	301	PEE	C22-C23-C24-C25
37	C1	601	ATP	PB-O3A-PA-O2A
35	D	402	CDL	C24-C25-C26-C27
35	C	401	CDL	C16-C17-C18-C19
35	e	401	CDL	C84-C85-C86-C87
36	J	301	PEE	C13-C14-C15-C16
36	j	301	PEE	C2-C1-O3P-P
36	J	301	PEE	C2-C1-O3P-P
35	o	203	CDL	C52-C51-CB5-OB6
36	j	301	PEE	C13-C14-C15-C16
36	c	403	PEE	C12-C13-C14-C15
36	j	301	PEE	C42-C43-C44-C45
35	C	401	CDL	CB5-C51-C52-C53
35	d	402	CDL	CB3-CB4-CB6-OB8
35	D	402	CDL	CB3-CB4-CB6-OB8
36	C	403	PEE	C12-C13-C14-C15
35	C	401	CDL	C36-C37-C38-C39
35	C	401	CDL	CB7-C71-C72-C73
35	B	602	CDL	C21-C22-C23-C24
36	J	301	PEE	C19-C20-C21-C22
35	O	203	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
35	c	401	CDL	C83-C84-C85-C86
34	o	202	LMT	C2-C1-O1'-C1'
34	O	202	LMT	C2-C1-O1'-C1'
36	J	301	PEE	C42-C43-C44-C45
35	e	401	CDL	C35-C36-C37-C38
35	b	602	CDL	C21-C22-C23-C24
35	c	401	CDL	C41-C42-C43-C44
35	d	402	CDL	C24-C25-C26-C27
35	u	201	CDL	C32-C31-CA7-OA8
35	U	201	CDL	C32-C31-CA7-OA8
35	E	401	CDL	C84-C85-C86-C87
35	E	401	CDL	OA7-CA5-OA6-CA4
36	j	301	PEE	C19-C20-C21-C22
35	C	401	CDL	C82-C83-C84-C85
35	E	401	CDL	C35-C36-C37-C38
33	o	201	PC1	O11-C1-C2-C3
33	O	201	PC1	O11-C1-C2-C3
35	e	401	CDL	OA5-CA3-CA4-CA6
35	b	602	CDL	OA5-CA3-CA4-CA6
35	b	602	CDL	OB5-CB3-CB4-CB6
35	E	401	CDL	OA5-CA3-CA4-CA6
35	B	601	CDL	OB5-CB3-CB4-CB6
35	B	602	CDL	OA5-CA3-CA4-CA6
35	B	602	CDL	OB5-CB3-CB4-CB6
35	V	202	CDL	C34-C35-C36-C37
35	h	302	CDL	OA6-CA4-CA6-OA8
34	c	404	LMT	C5-C6-C7-C8
35	v	202	CDL	C34-C35-C36-C37
34	H	301	LMT	C5-C6-C7-C8
35	u	201	CDL	C43-C44-C45-C46
34	h	301	LMT	C5-C6-C7-C8
36	j	301	PEE	C36-C37-C38-C39
36	J	301	PEE	C36-C37-C38-C39
35	U	201	CDL	C43-C44-C45-C46
34	C	404	LMT	C5-C6-C7-C8
35	b	602	CDL	C60-C61-C62-C63
35	O	203	CDL	C32-C31-CA7-OA8
35	c	401	CDL	CA3-CA4-OA6-CA5
35	H	302	CDL	CA6-CA4-OA6-CA5
35	C	401	CDL	CA6-CA4-OA6-CA5
36	j	302	PEE	C3-C2-O2-C10
35	o	203	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
35	O	203	CDL	C34-C35-C36-C37
36	j	301	PEE	C32-C33-C34-C35
35	o	203	CDL	C34-C35-C36-C37
35	U	201	CDL	C54-C55-C56-C57
35	e	401	CDL	CA3-CA4-CA6-OA8
33	O	201	PC1	C2F-C2G-C2H-C2I
35	u	201	CDL	C54-C55-C56-C57
36	J	301	PEE	C32-C33-C34-C35
35	H	302	CDL	CB7-C71-C72-C73
36	c	403	PEE	C18-C19-C20-C21
36	C	403	PEE	C18-C19-C20-C21
34	o	202	LMT	C9-C10-C11-C12
35	B	602	CDL	C60-C61-C62-C63
33	v	201	PC1	C32-C33-C34-C35
33	V	201	PC1	C32-C33-C34-C35
35	h	302	CDL	CB7-C71-C72-C73
35	b	602	CDL	C72-C71-CB7-OB8
35	B	602	CDL	C72-C71-CB7-OB8
33	o	201	PC1	C2F-C2G-C2H-C2I
35	H	302	CDL	OA6-CA4-CA6-OA8
34	O	202	LMT	C9-C10-C11-C12
35	o	203	CDL	C77-C78-C79-C80
35	v	202	CDL	C82-C83-C84-C85
35	e	401	CDL	C51-CB5-OB6-CB4
35	u	201	CDL	C52-C51-CB5-OB6
35	U	201	CDL	C52-C51-CB5-OB6
35	e	401	CDL	OA7-CA5-OA6-CA4
35	C	401	CDL	C81-C82-C83-C84
35	V	202	CDL	C82-C83-C84-C85
37	C2	601	ATP	PB-O3A-PA-O2A
37	C1	601	ATP	PB-O3A-PA-O1A
35	B	602	CDL	C41-C42-C43-C44
33	o	204	PC1	C28-C29-C2A-C2B
35	E	401	CDL	C51-CB5-OB6-CB4
35	O	203	CDL	C80-C81-C82-C83
35	b	602	CDL	C41-C42-C43-C44
35	O	203	CDL	C77-C78-C79-C80
35	V	202	CDL	C83-C84-C85-C86
35	b	601	CDL	C40-C41-C42-C43
35	c	401	CDL	C56-C57-C58-C59
35	v	202	CDL	C83-C84-C85-C86
35	H	302	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
35	C	401	CDL	C80-C81-C82-C83
35	o	203	CDL	C80-C81-C82-C83
33	o	204	PC1	C2C-C2D-C2E-C2F
35	E	401	CDL	CA3-CA4-CA6-OA8
36	c	403	PEE	C41-C42-C43-C44
36	C	403	PEE	C41-C42-C43-C44
33	O	204	PC1	C28-C29-C2A-C2B
36	j	302	PEE	O3-C30-C31-C32
35	h	302	CDL	C42-C43-C44-C45
35	e	401	CDL	C15-C16-C17-C18
35	B	602	CDL	C19-C20-C21-C22
35	E	401	CDL	C36-C37-C38-C39
35	b	602	CDL	C19-C20-C21-C22
35	B	601	CDL	C40-C41-C42-C43
35	D	402	CDL	C31-C32-C33-C34
36	J	302	PEE	O3-C30-C31-C32
35	d	402	CDL	C31-C32-C33-C34
34	h	301	LMT	O1'-C1-C2-C3
35	e	401	CDL	C36-C37-C38-C39
35	e	401	CDL	C80-C81-C82-C83
35	U	201	CDL	OA5-CA3-CA4-CA6
34	H	301	LMT	O1'-C1-C2-C3
35	E	401	CDL	C15-C16-C17-C18
35	E	401	CDL	C80-C81-C82-C83
35	b	602	CDL	CA6-CA4-OA6-CA5
36	j	302	PEE	C1-C2-O2-C10
36	J	302	PEE	C3-C2-O2-C10
35	O	203	CDL	C79-C80-C81-C82
33	V	201	PC1	C11-C12-N-C15
35	E	401	CDL	C72-C73-C74-C75
35	o	203	CDL	C79-C80-C81-C82
35	b	601	CDL	C32-C31-CA7-OA8
35	b	602	CDL	C32-C31-CA7-OA8
35	B	602	CDL	C32-C31-CA7-OA8
33	o	204	PC1	C22-C23-C24-C25
35	B	601	CDL	C32-C31-CA7-OA8
33	O	204	PC1	C2C-C2D-C2E-C2F
35	D	402	CDL	C33-C34-C35-C36
33	V	201	PC1	C28-C29-C2A-C2B
36	j	302	PEE	C42-C43-C44-C45
33	O	204	PC1	C22-C23-C24-C25
35	U	201	CDL	C72-C71-CB7-OB8

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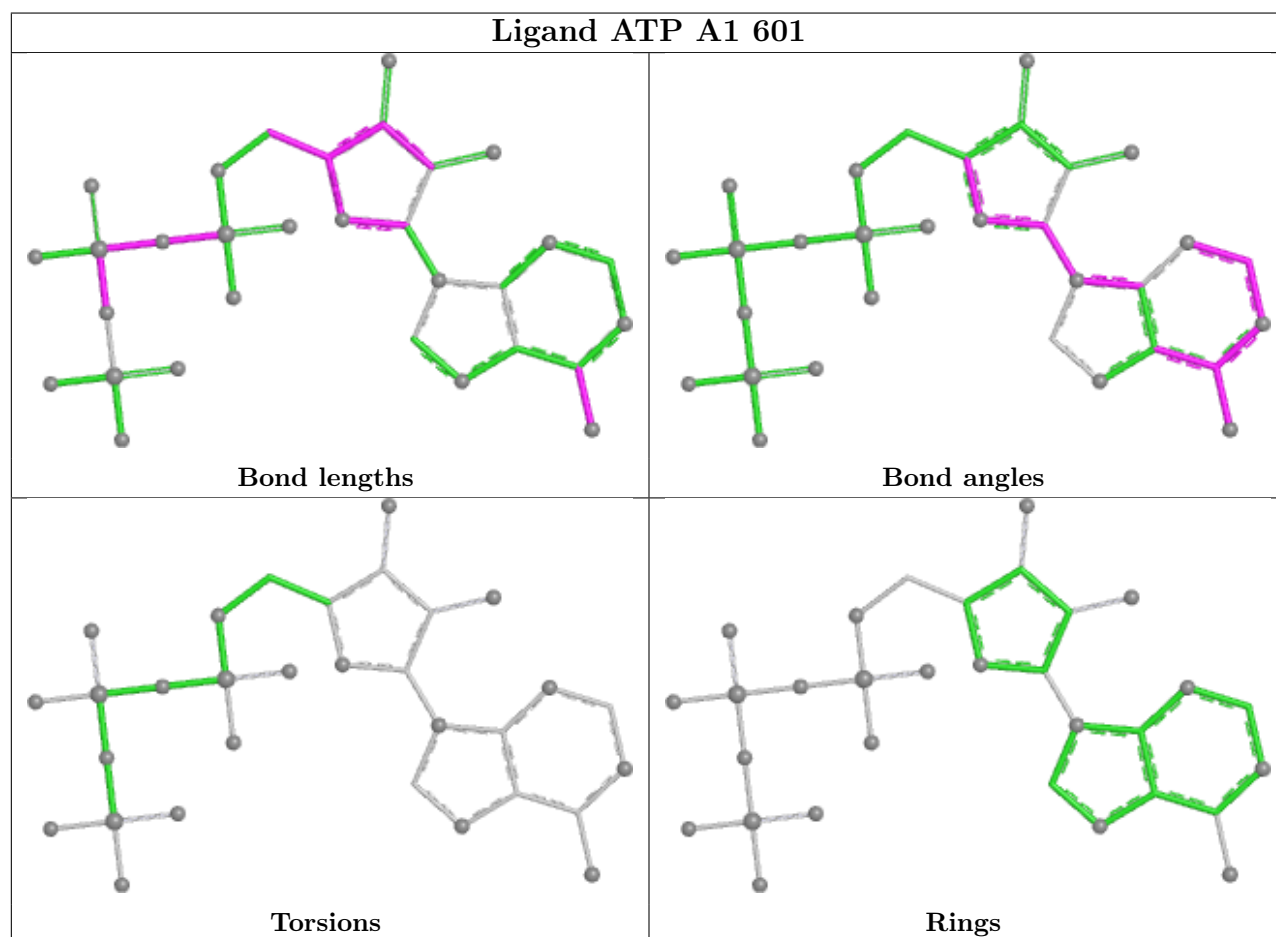
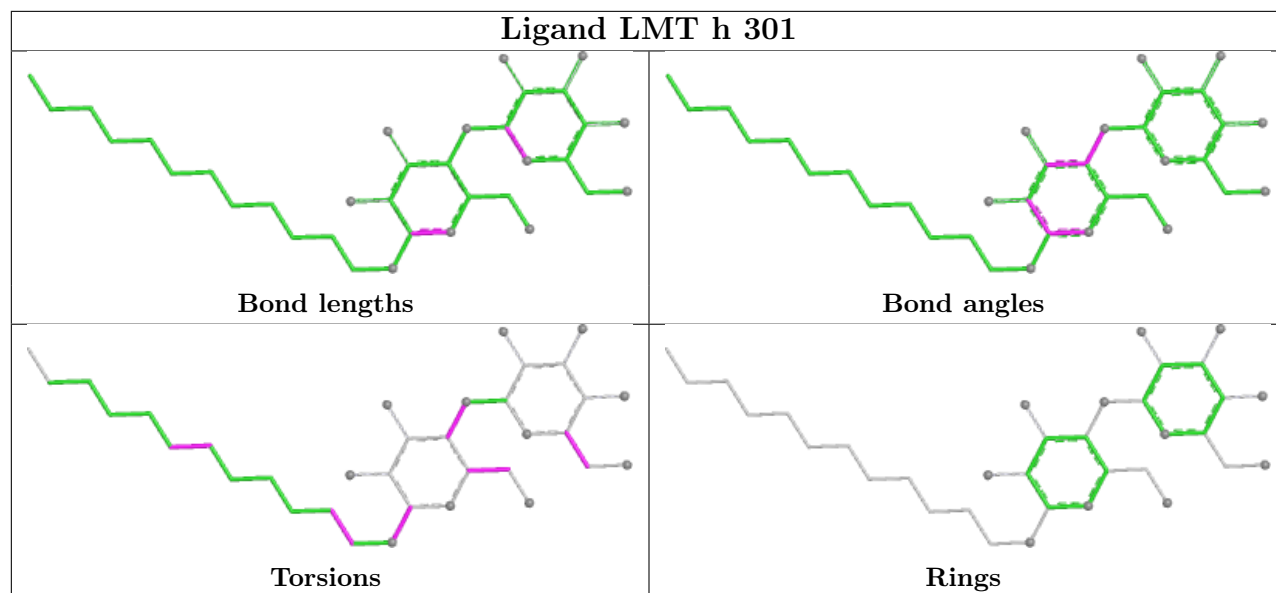
Mol	Chain	Res	Type	Atoms
35	u	201	CDL	C52-C51-CB5-OB7
36	J	302	PEE	O5-C30-C31-C32
35	e	401	CDL	C72-C73-C74-C75
35	B	602	CDL	C72-C71-CB7-OB9
36	J	302	PEE	C42-C43-C44-C45
35	C	401	CDL	C37-C38-C39-C40
33	v	201	PC1	C28-C29-C2A-C2B
35	h	302	CDL	C43-C44-C45-C46
35	d	402	CDL	C33-C34-C35-C36
35	b	602	CDL	C72-C71-CB7-OB9
35	U	201	CDL	C52-C51-CB5-OB7
35	C	401	CDL	C64-C65-C66-C67
35	D	402	CDL	C12-C13-C14-C15
35	c	401	CDL	C16-C17-C18-C19
35	H	302	CDL	C43-C44-C45-C46
36	j	302	PEE	O5-C30-C31-C32
35	u	201	CDL	C72-C71-CB7-OB8
33	V	201	PC1	C1-C2-C3-O31
33	v	201	PC1	C11-C12-N-C14
33	o	201	PC1	C3E-C3F-C3G-C3H
35	u	201	CDL	OA5-CA3-CA4-CA6
35	c	401	CDL	C58-C59-C60-C61
35	c	401	CDL	C60-C61-C62-C63
35	h	302	CDL	C72-C71-CB7-OB8
35	d	402	CDL	C12-C13-C14-C15
33	O	201	PC1	C3E-C3F-C3G-C3H
37	E2	601	ATP	PG-O3B-PB-O2B
37	C2	601	ATP	PB-O3A-PA-O1A
37	E1	601	ATP	PG-O3B-PB-O2B
35	b	601	CDL	C32-C31-CA7-OA9
35	b	602	CDL	C32-C31-CA7-OA9
34	D	403	LMT	C2-C3-C4-C5
35	b	602	CDL	C18-C19-C20-C21
34	d	403	LMT	C2-C3-C4-C5
35	B	602	CDL	C18-C19-C20-C21
35	v	202	CDL	CA7-C31-C32-C33
35	V	202	CDL	CA7-C31-C32-C33
35	u	201	CDL	C72-C71-CB7-OB9
35	U	201	CDL	C72-C71-CB7-OB9
35	B	601	CDL	C32-C31-CA7-OA9
35	B	602	CDL	C32-C31-CA7-OA9

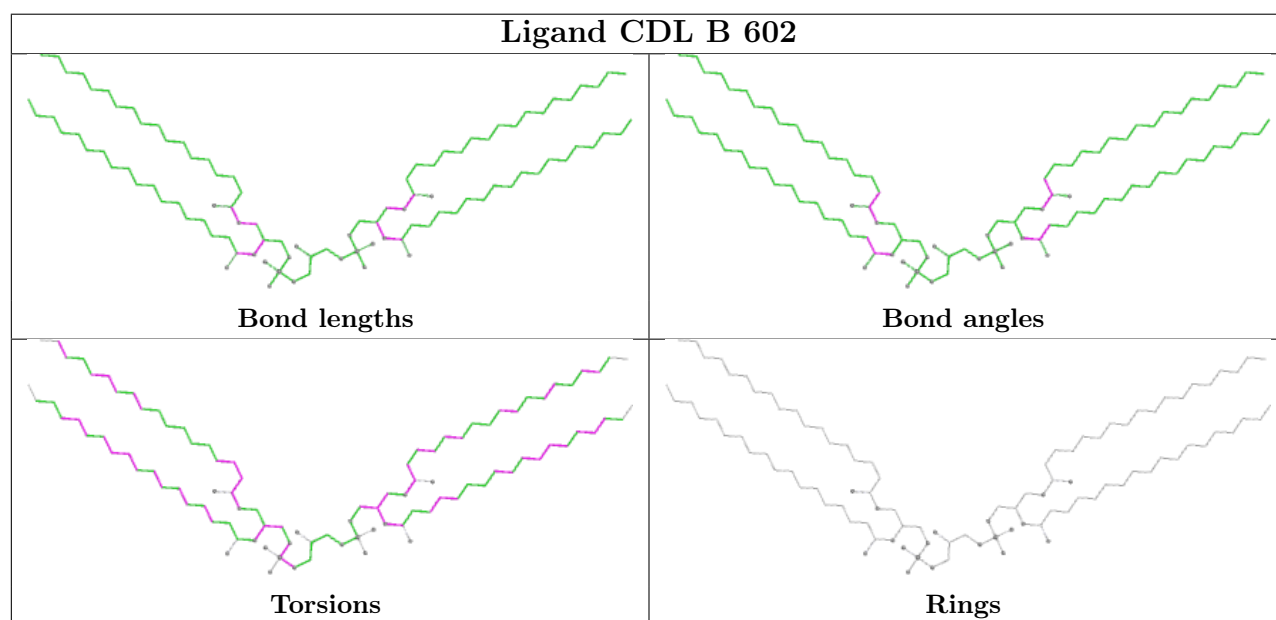
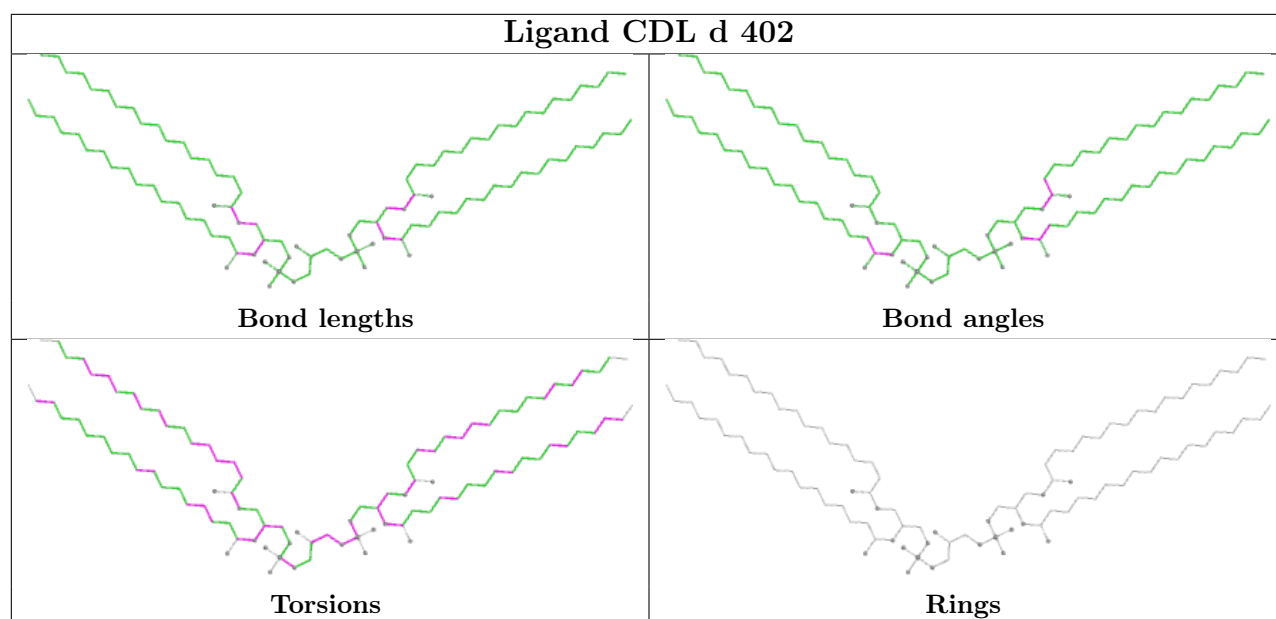
There are no ring outliers.

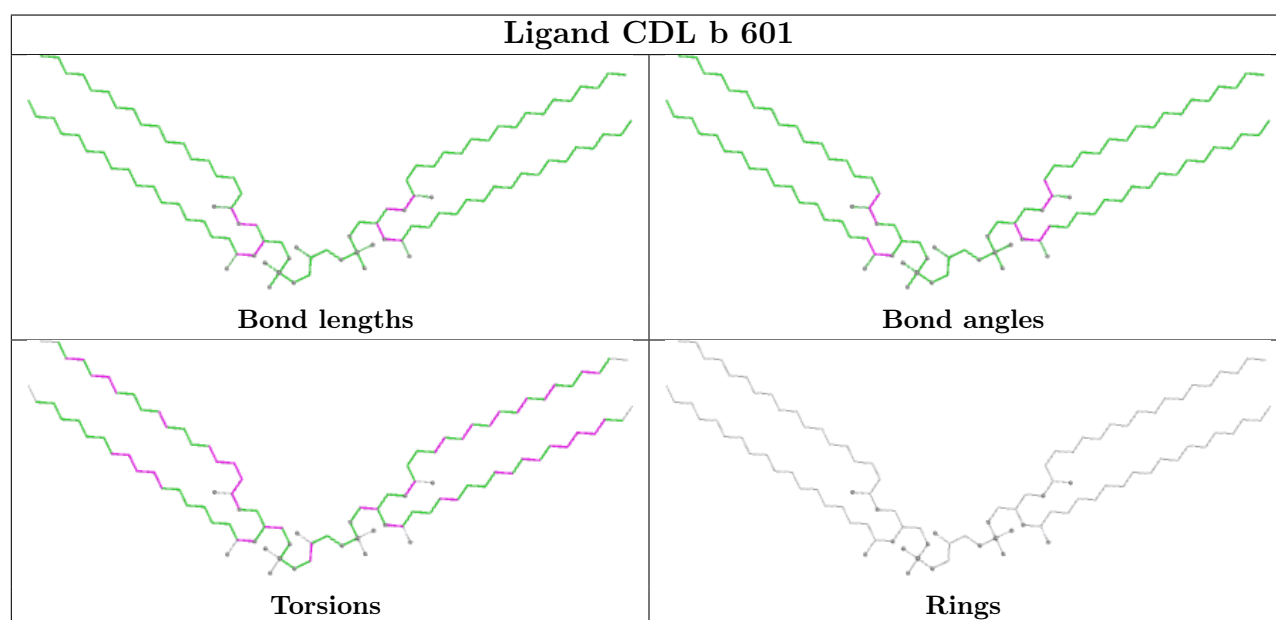
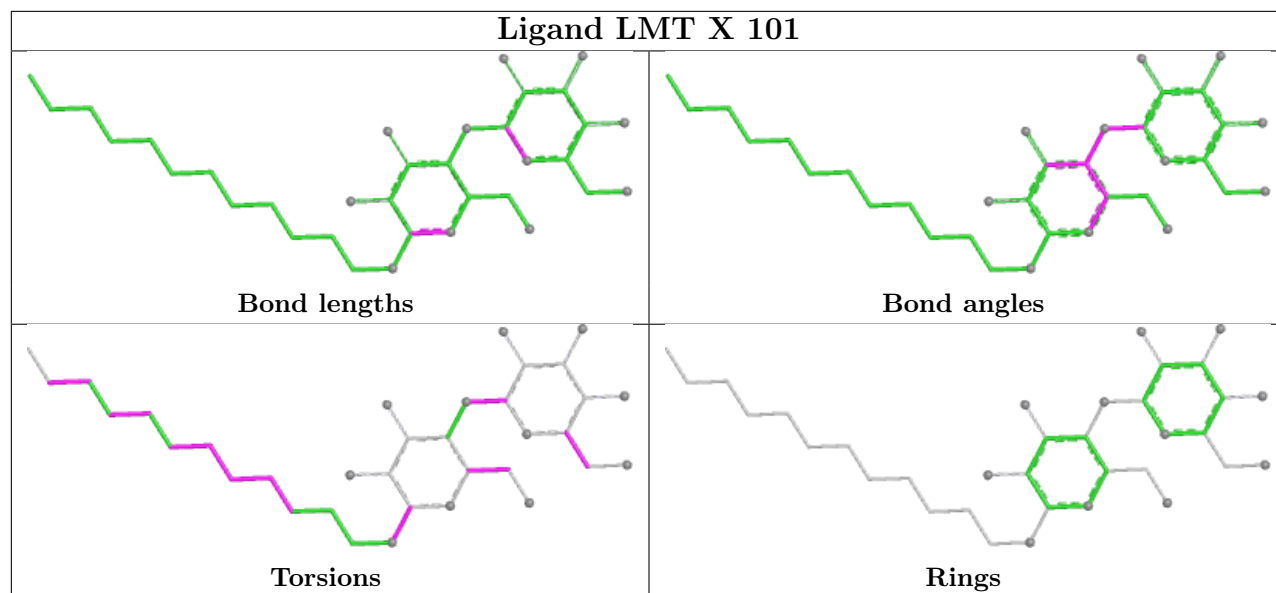
28 monomers are involved in 55 short contacts:

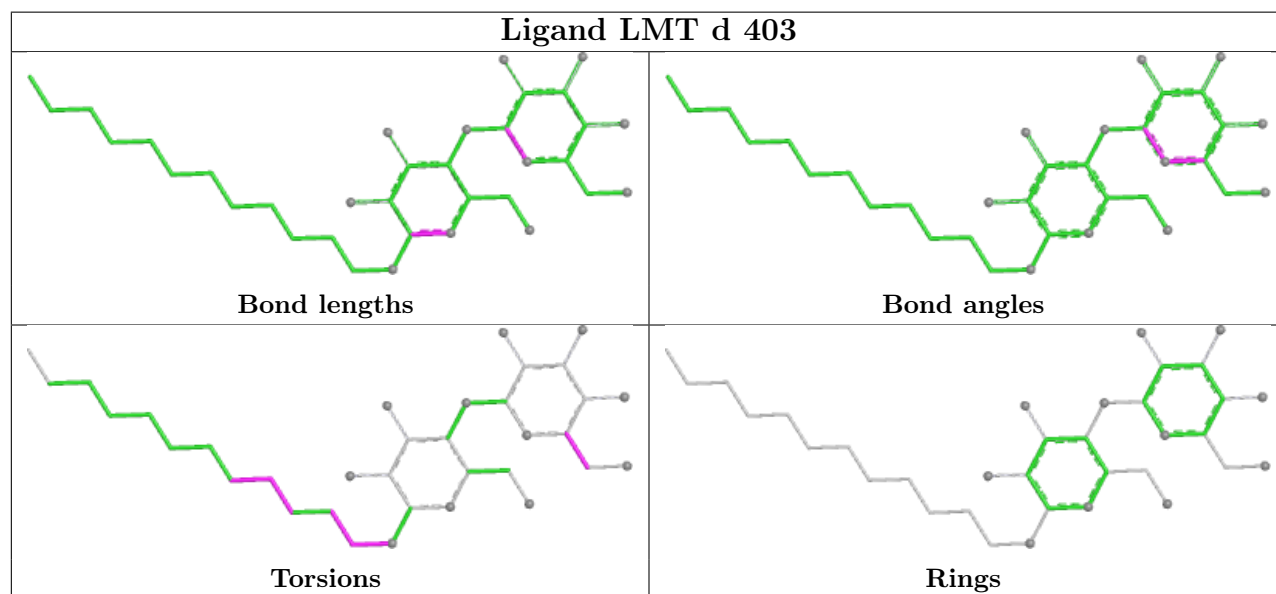
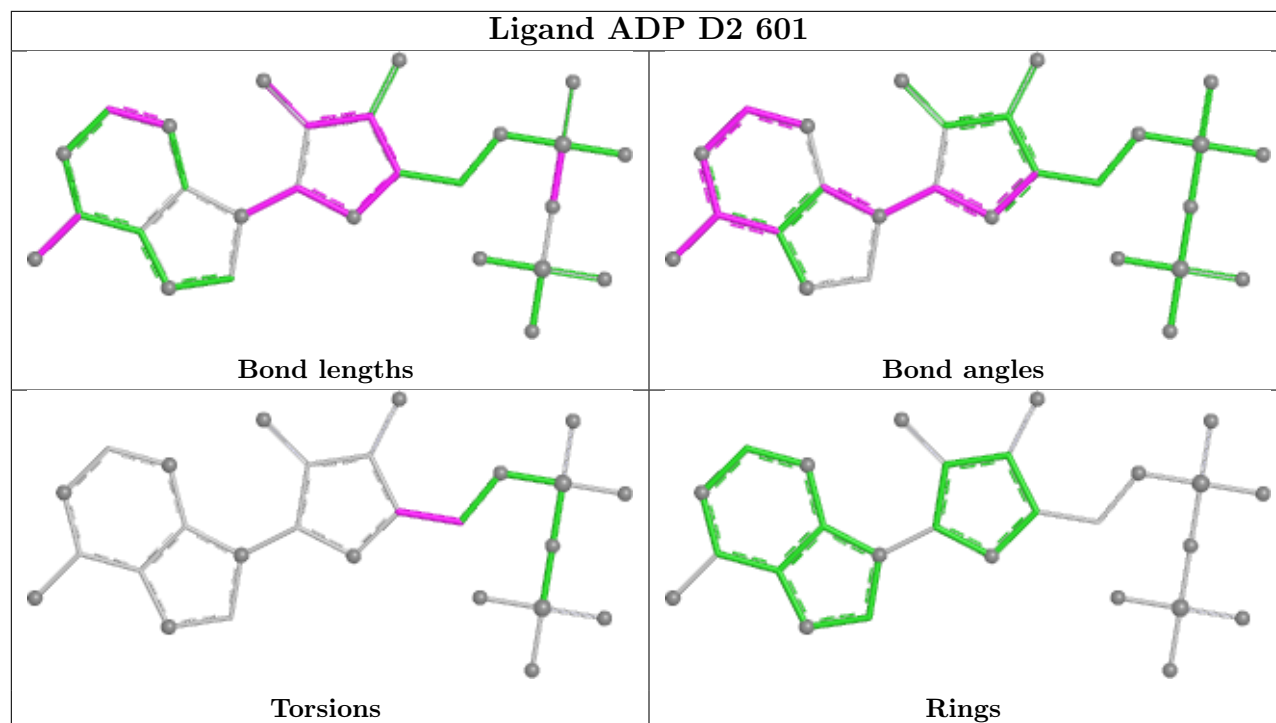
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	h	301	LMT	2	0
37	A1	601	ATP	1	0
34	X	101	LMT	1	0
35	b	601	CDL	5	0
38	D2	601	ADP	1	0
34	d	403	LMT	1	0
35	c	401	CDL	7	0
36	J	302	PEE	1	0
35	v	202	CDL	6	0
35	V	202	CDL	7	0
35	O	203	CDL	1	0
38	B2	601	ADP	1	0
35	B	601	CDL	5	0
34	O	202	LMT	1	0
36	j	301	PEE	1	0
35	u	201	CDL	1	0
34	D	403	LMT	1	0
34	H	301	LMT	2	0
36	J	301	PEE	1	0
35	U	201	CDL	1	0
33	O	201	PC1	2	0
33	o	201	PC1	2	0
38	B1	601	ADP	3	0
34	C	404	LMT	1	0
35	C	401	CDL	6	0
34	x	101	LMT	1	0
34	o	202	LMT	1	0
36	j	302	PEE	3	0

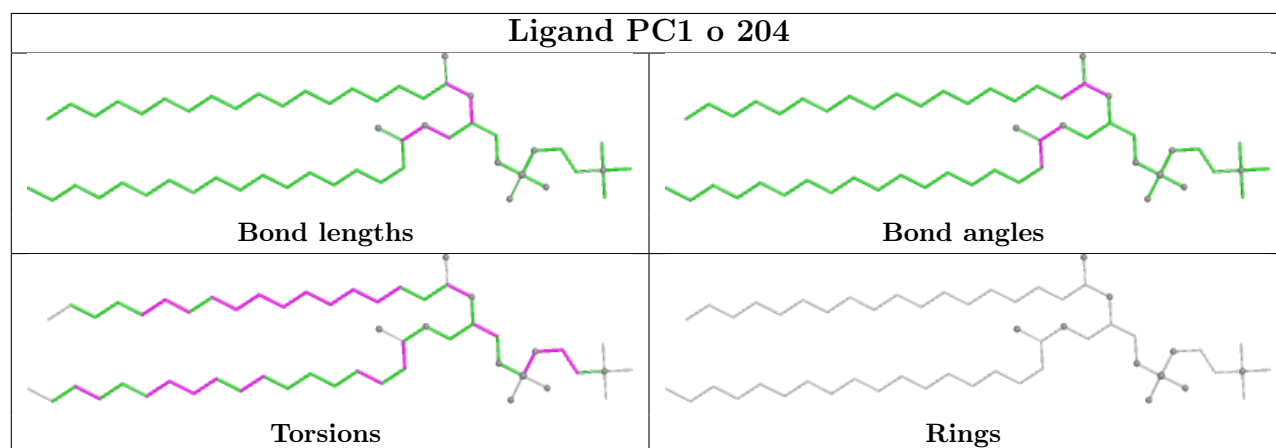
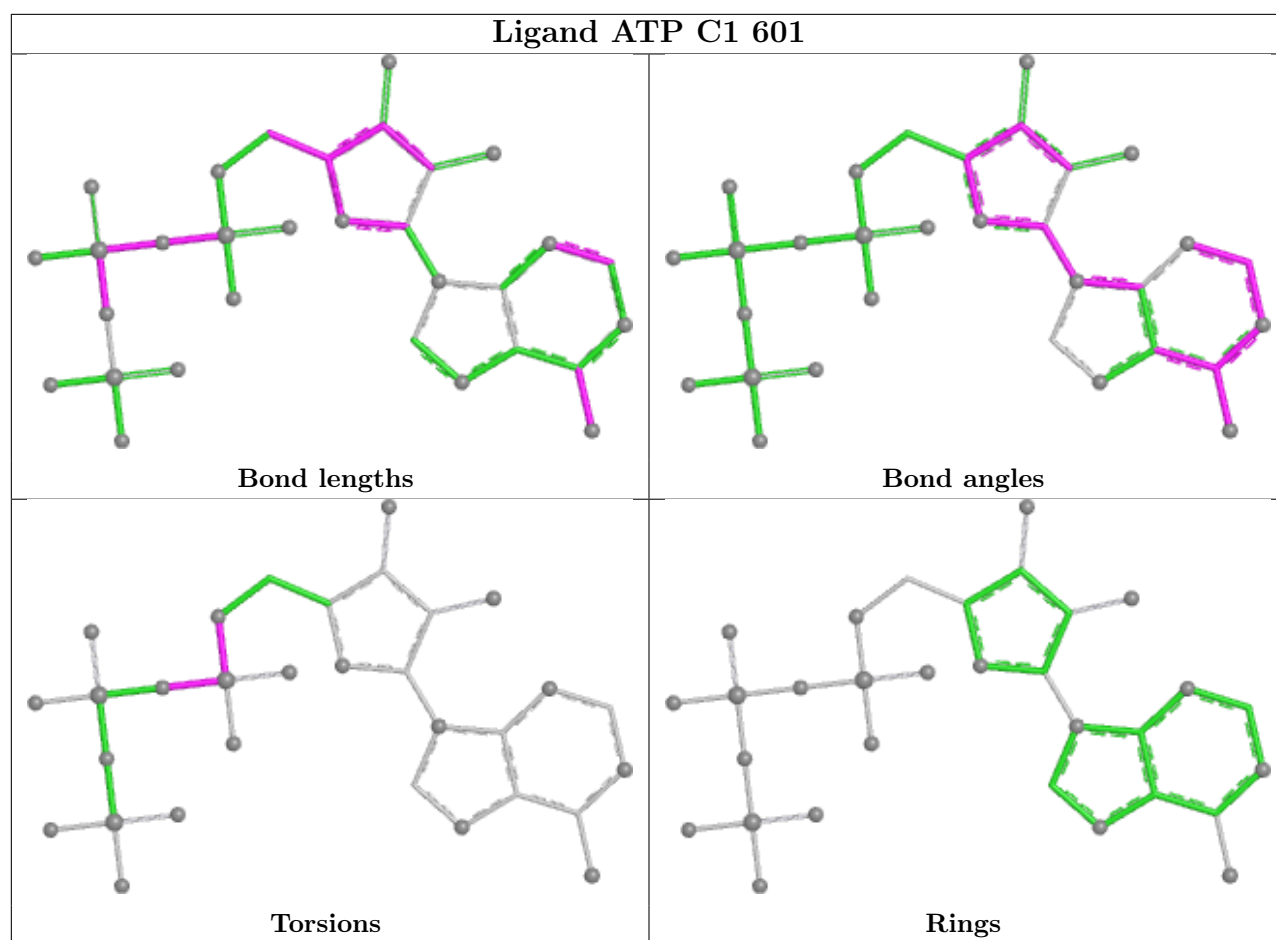
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

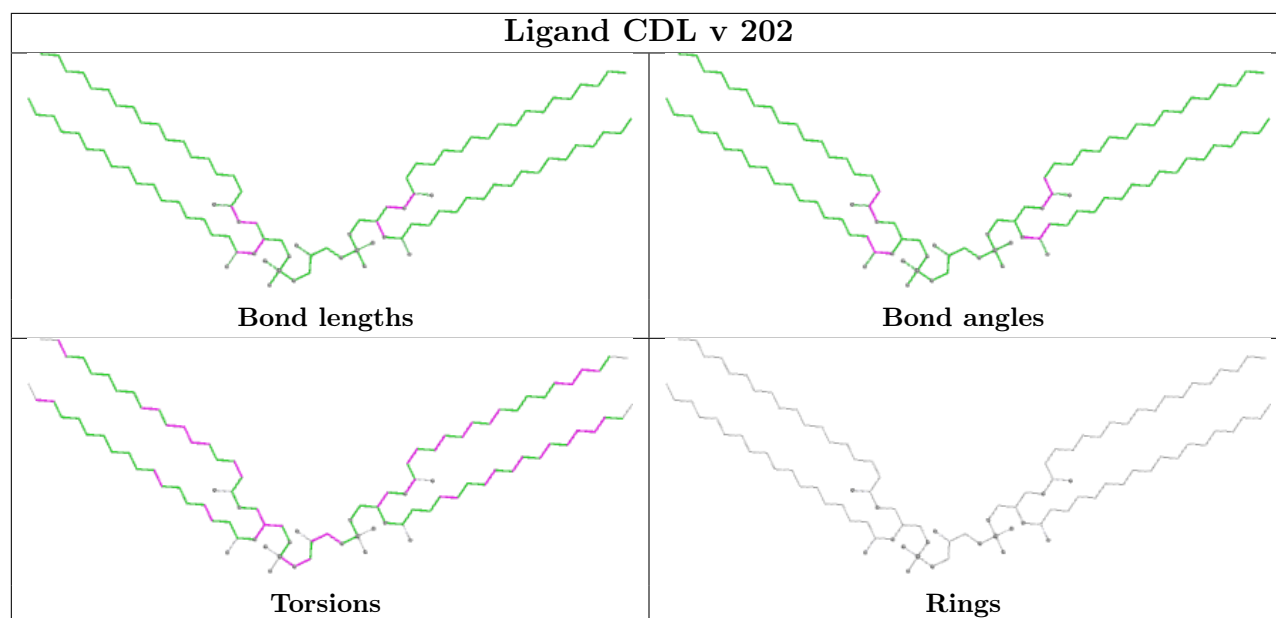
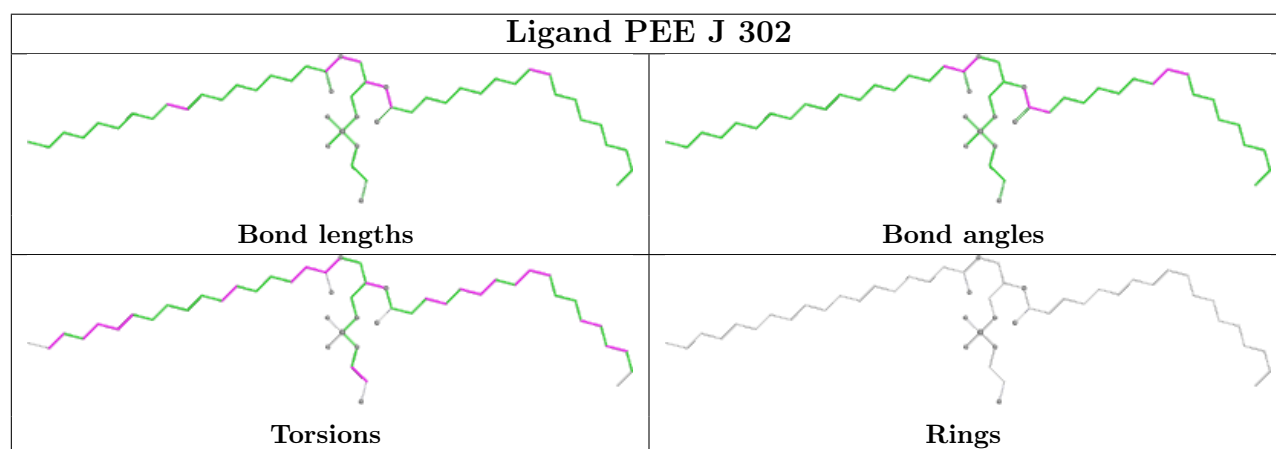
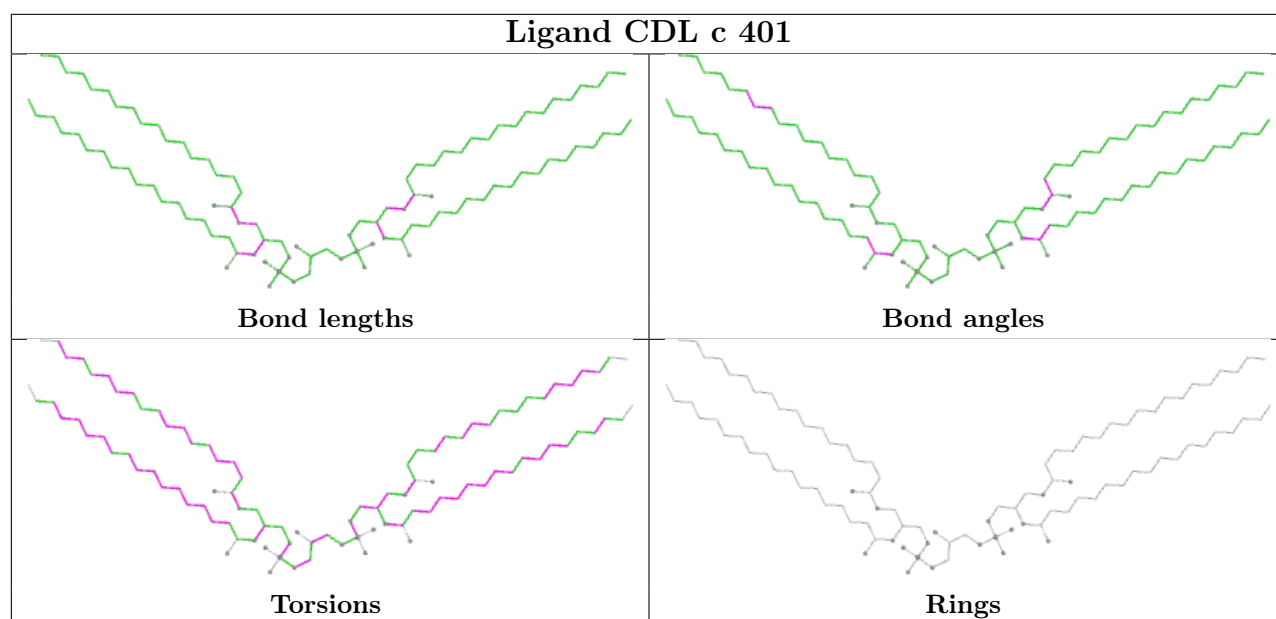


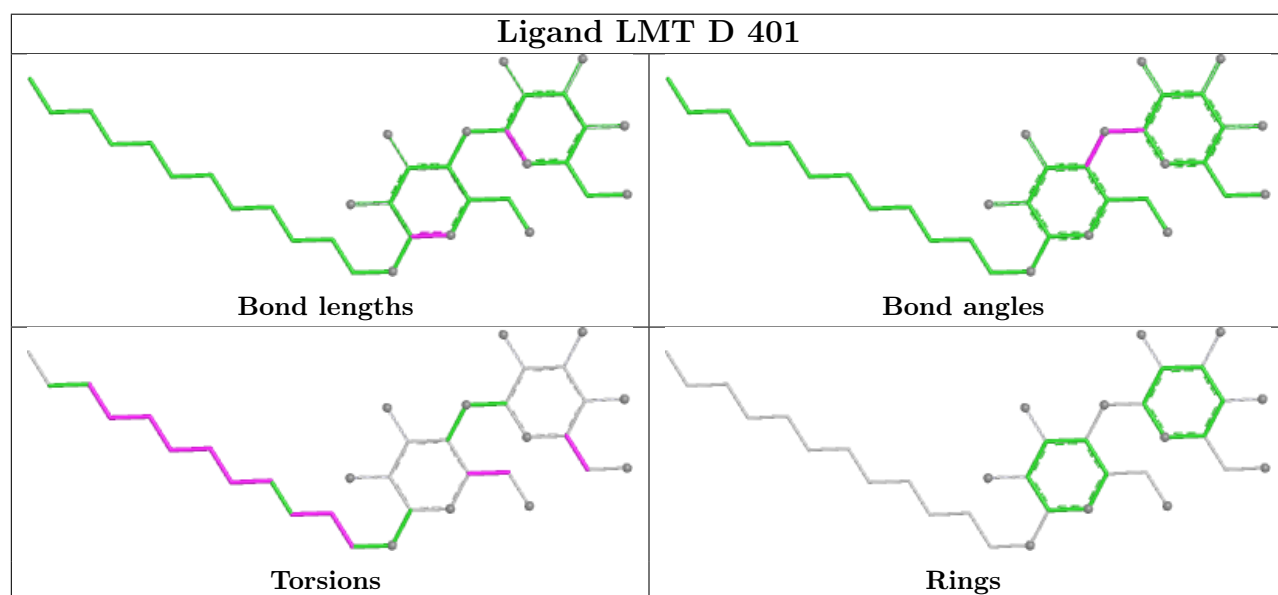
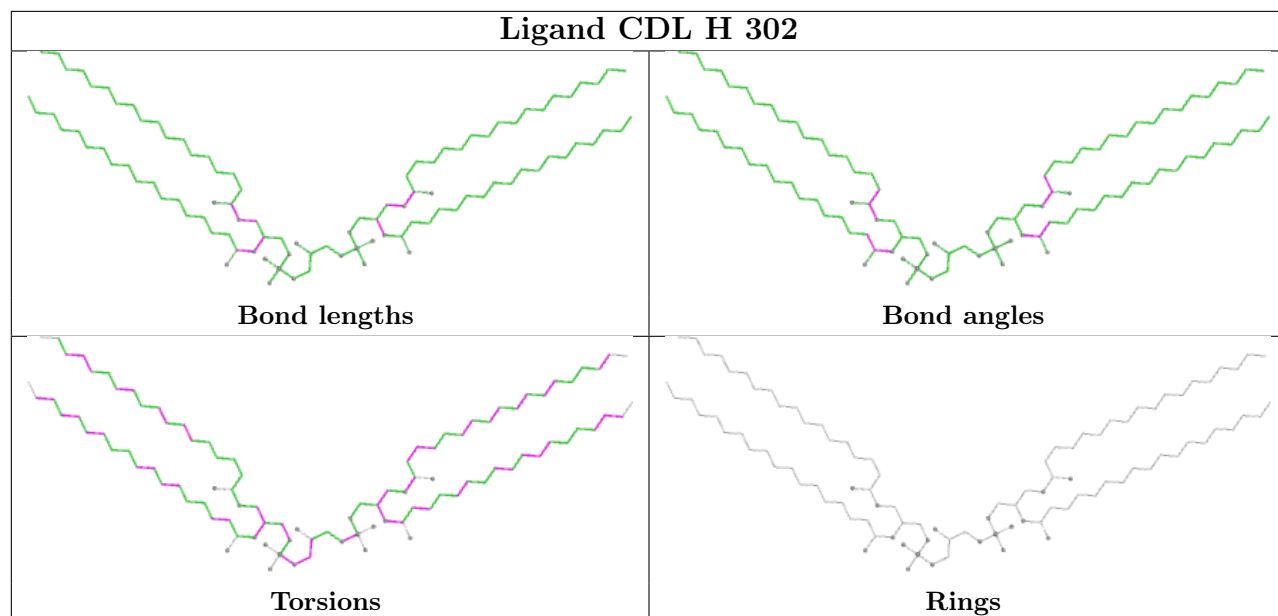


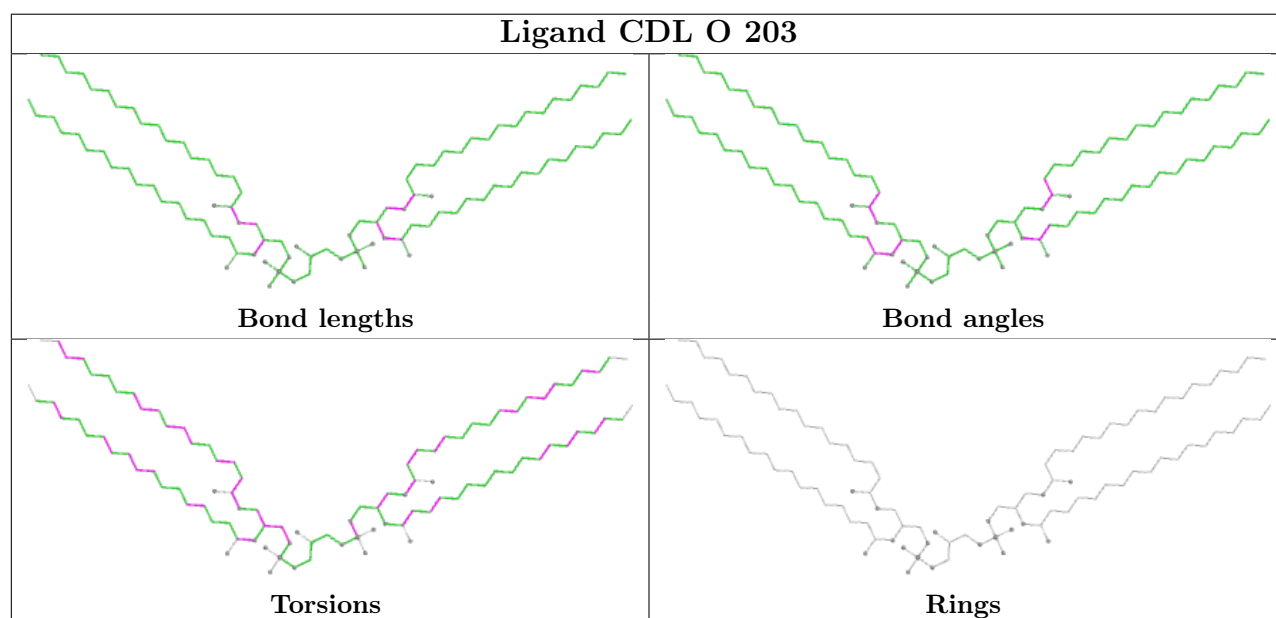
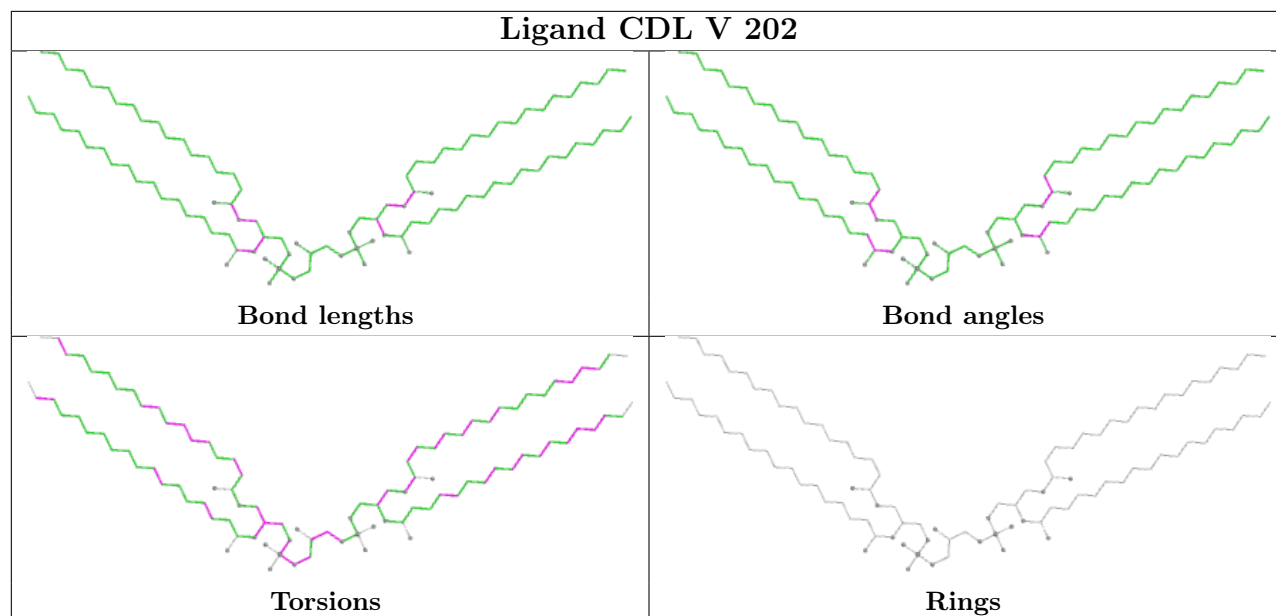


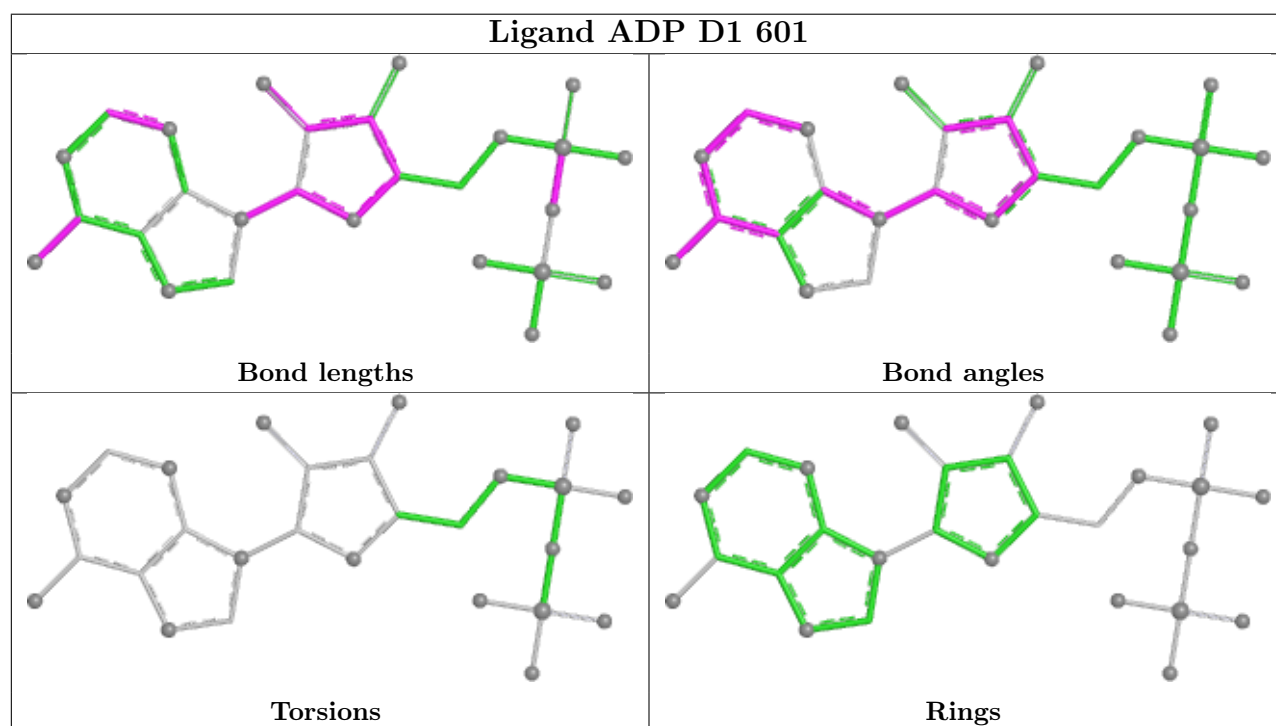
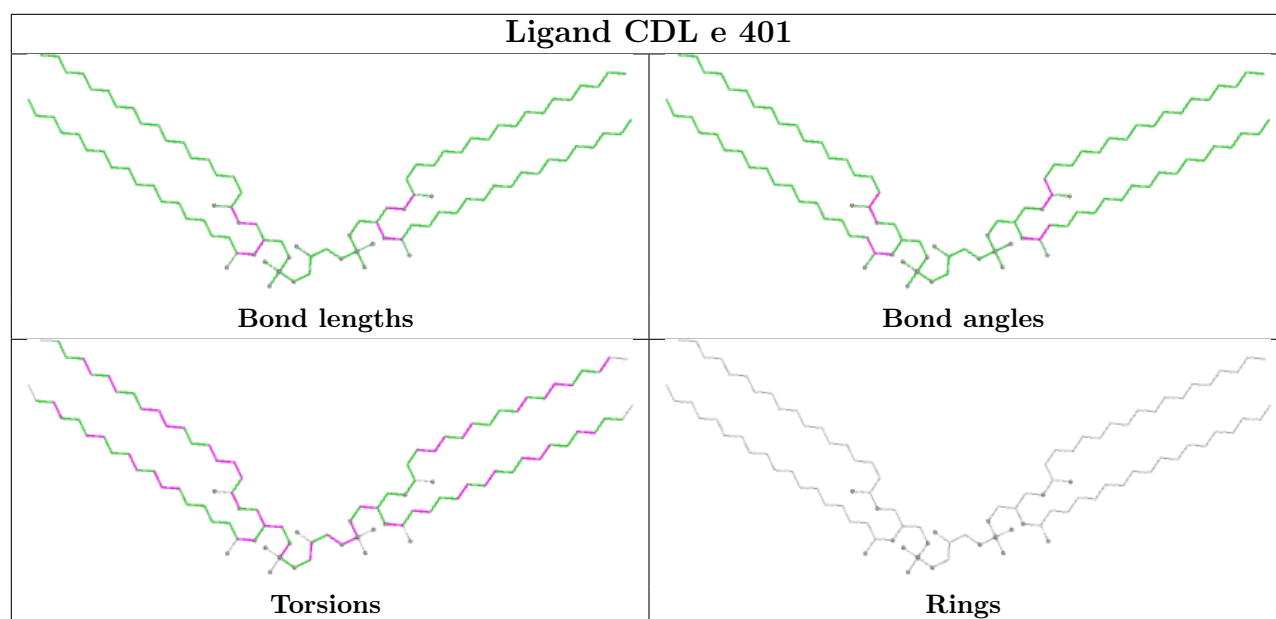


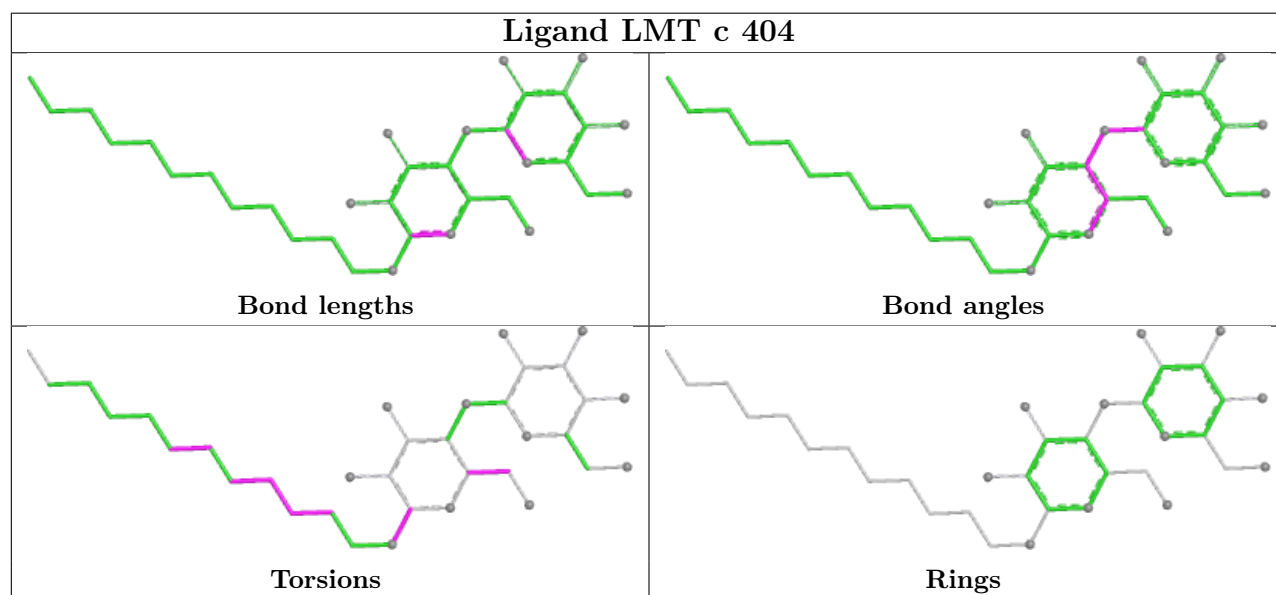
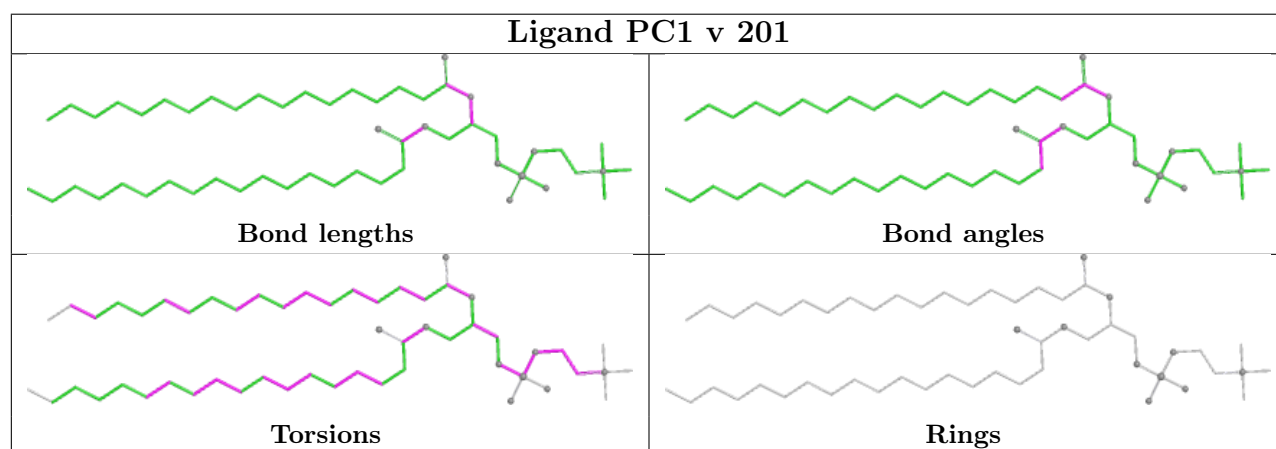
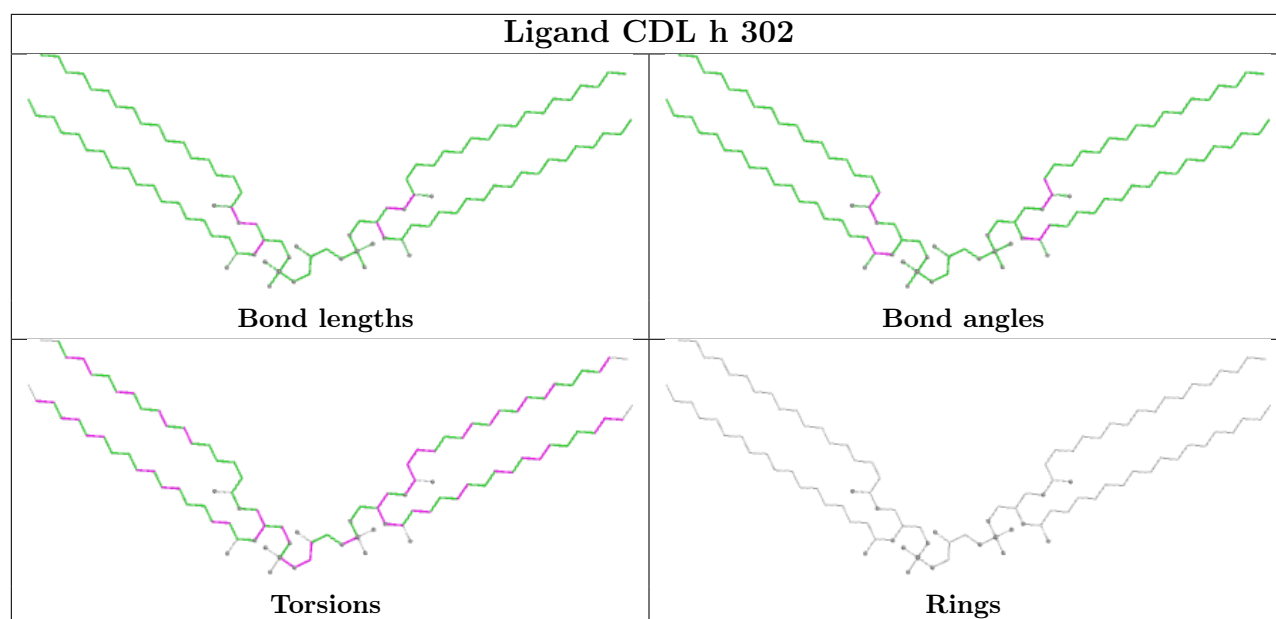


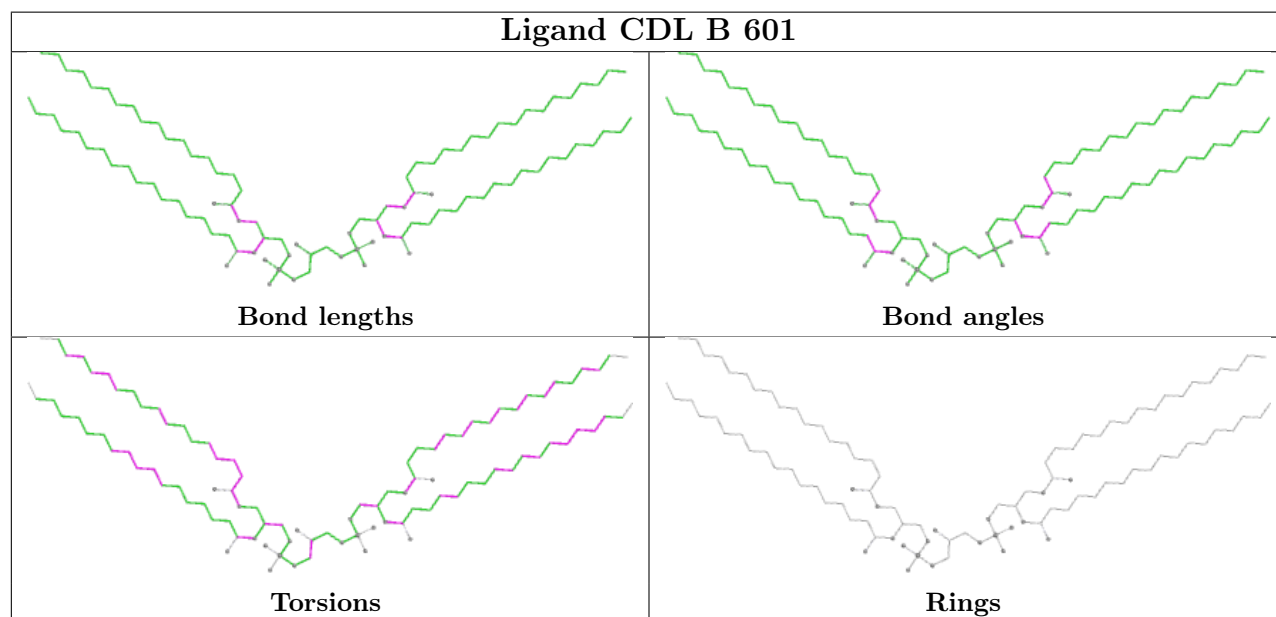
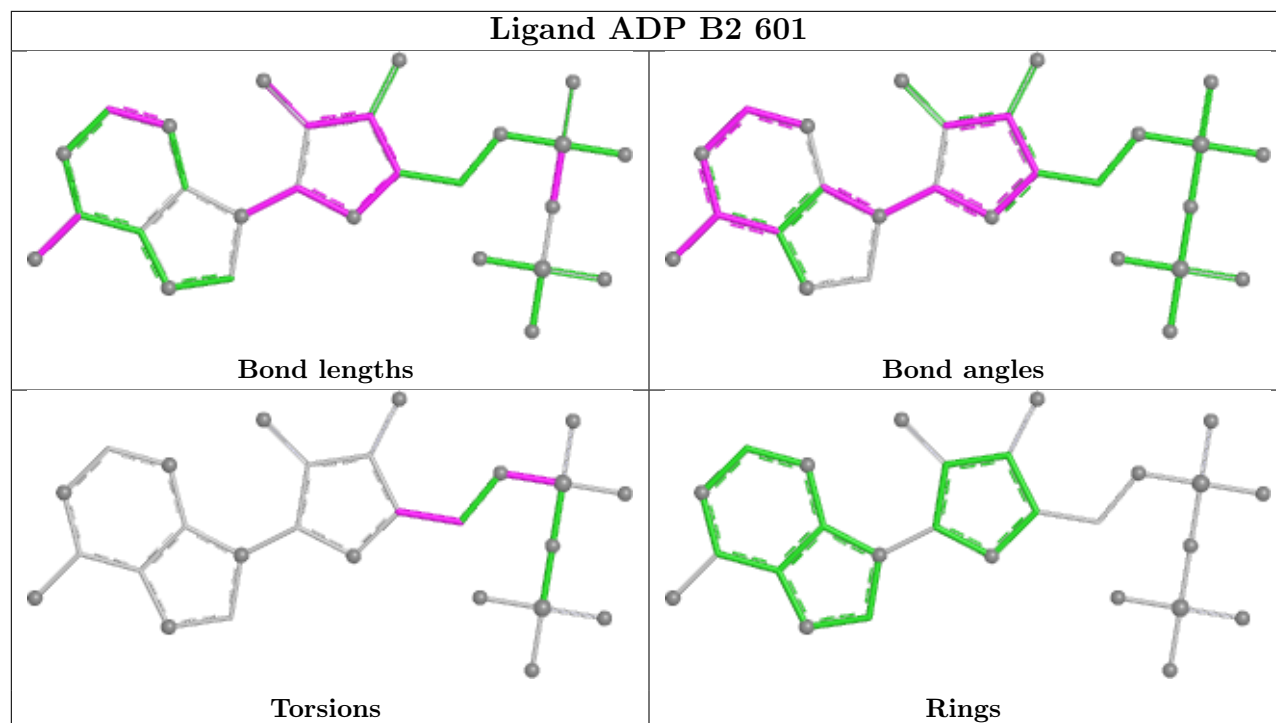


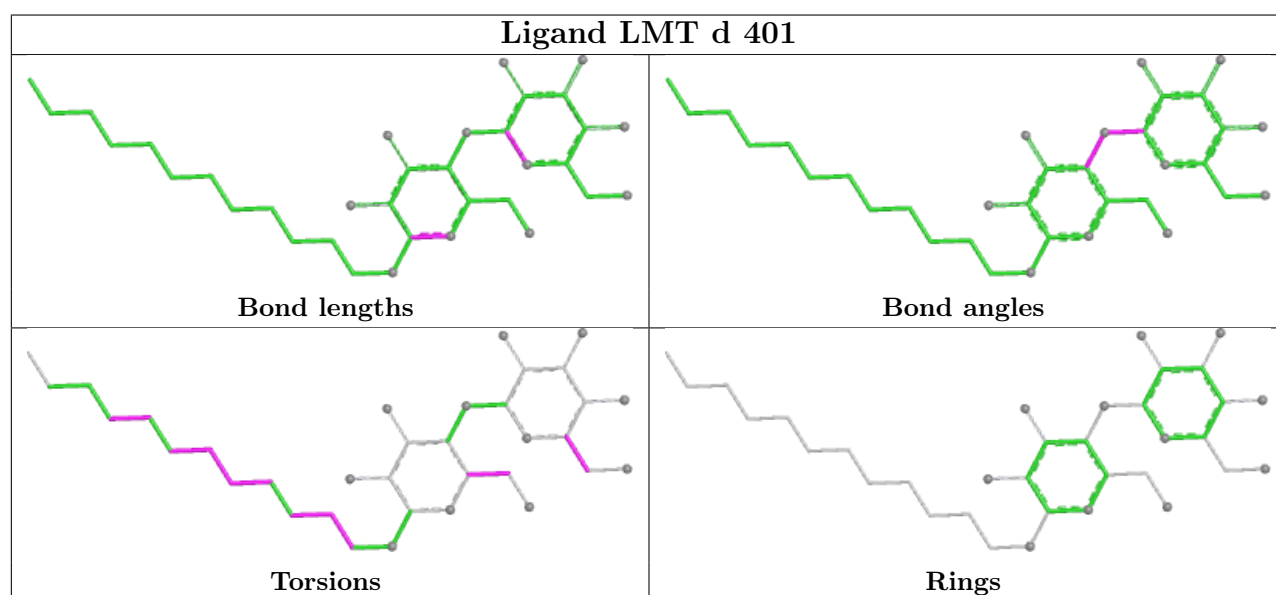
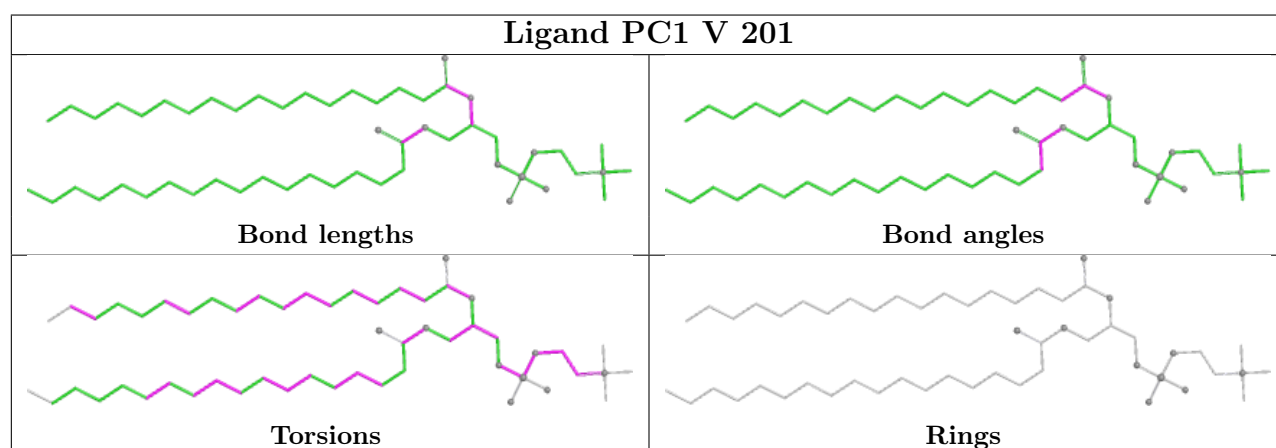
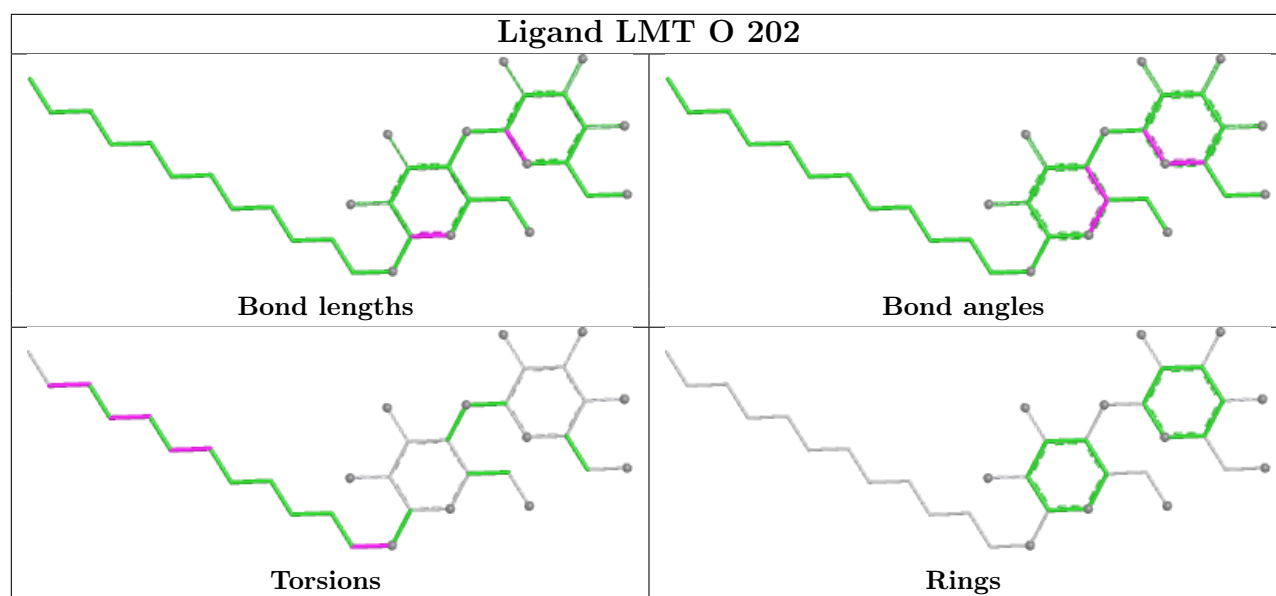


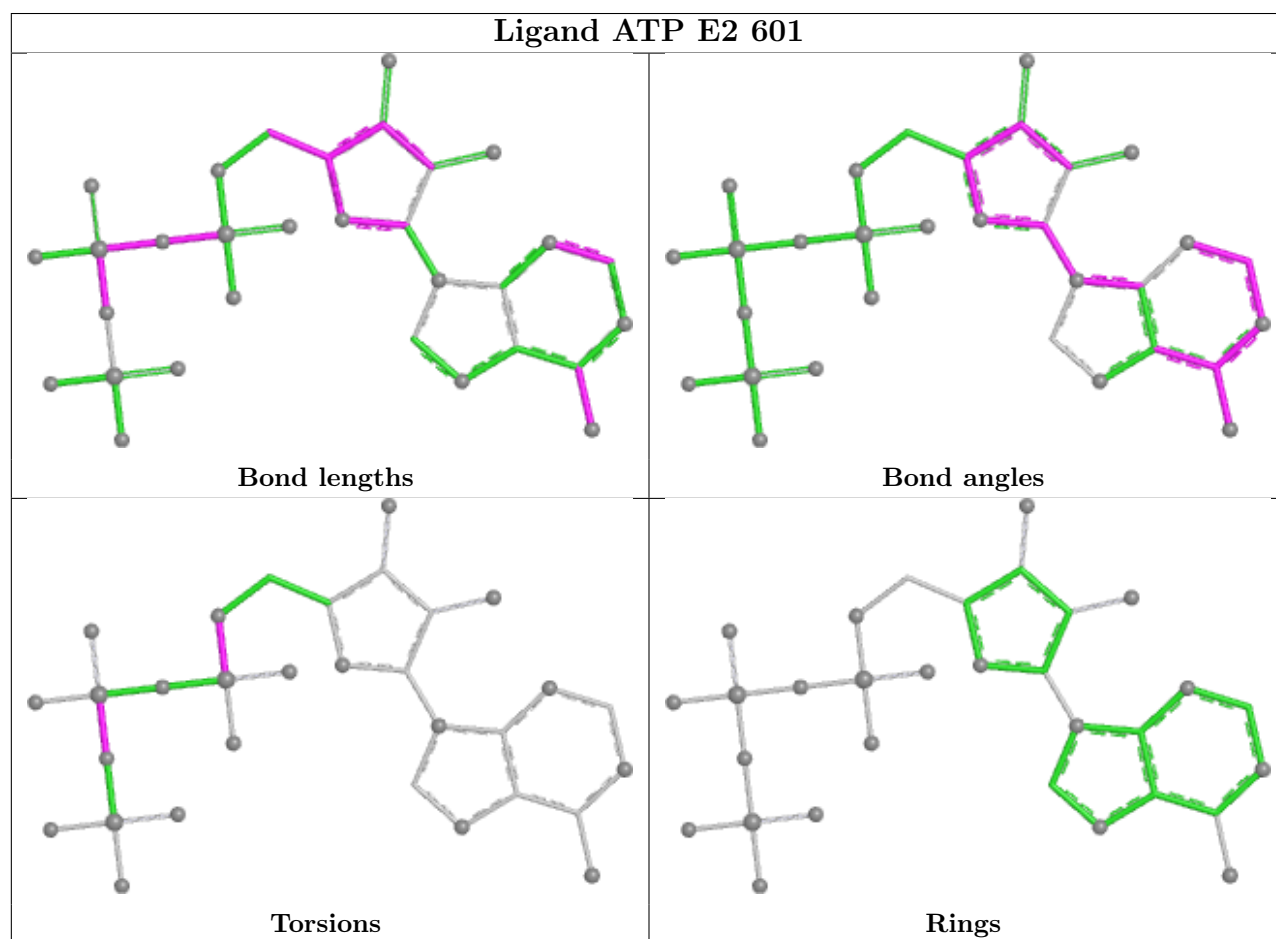
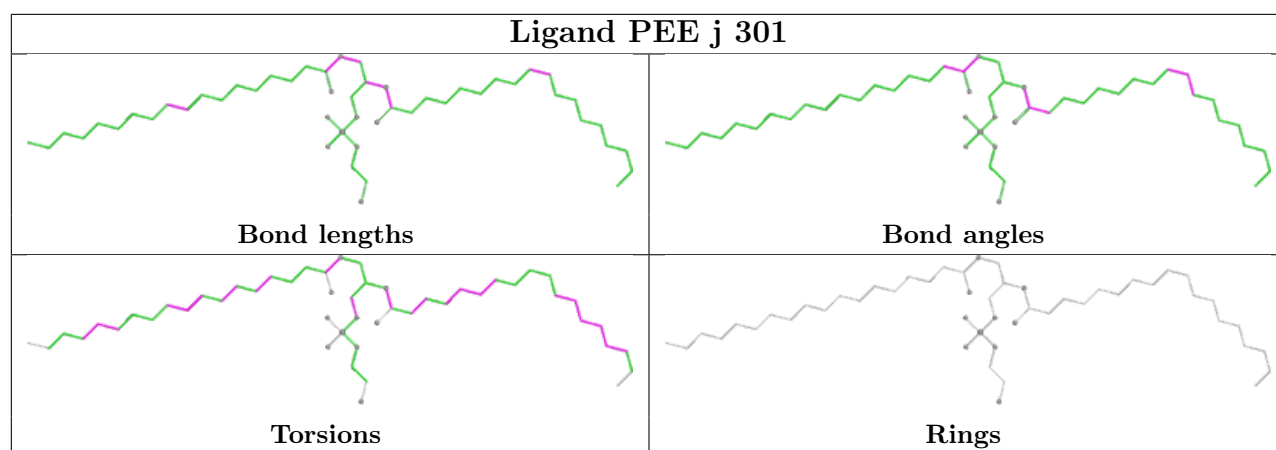


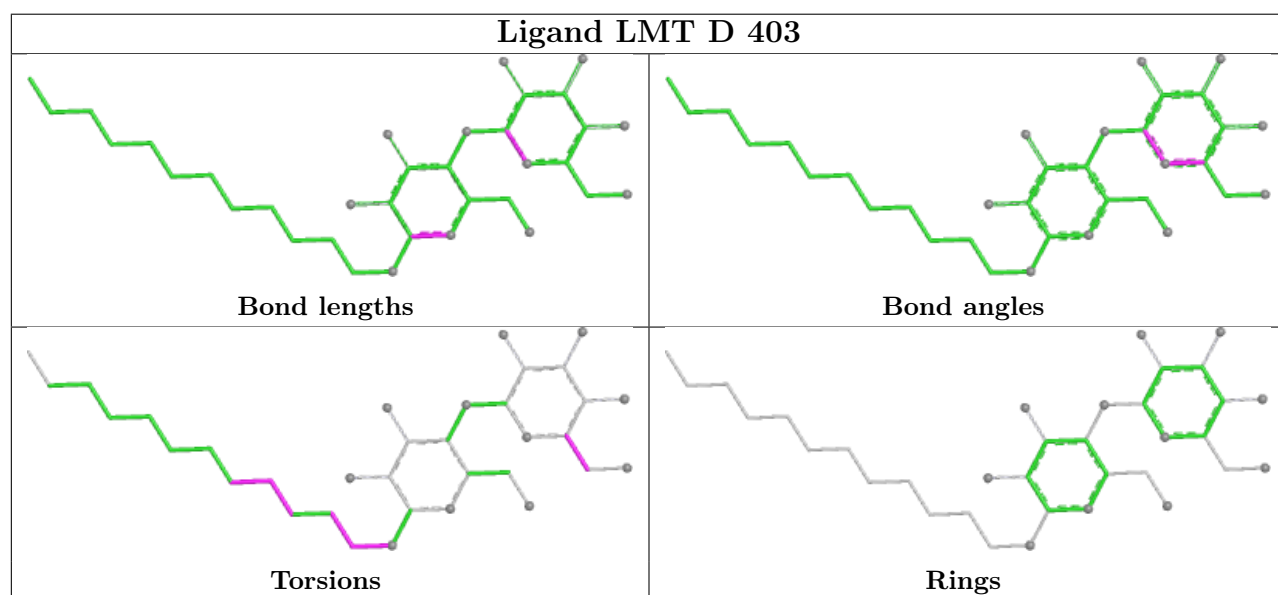
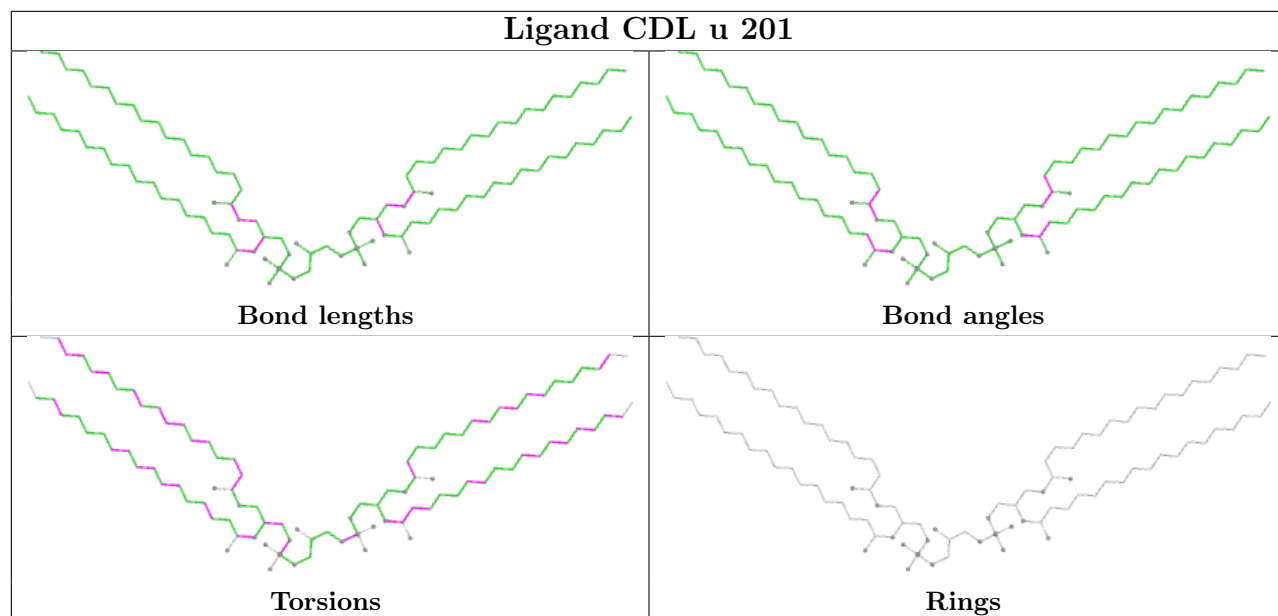


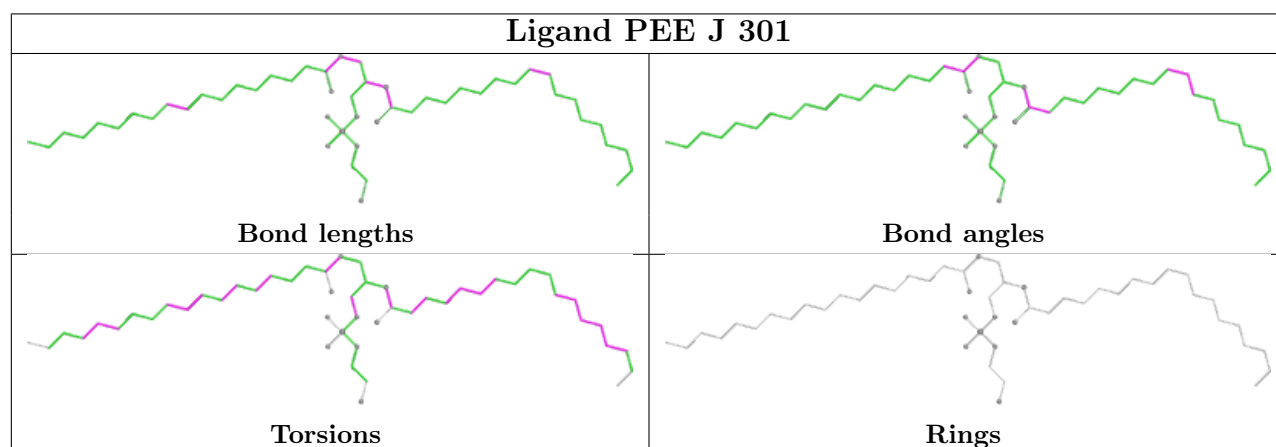
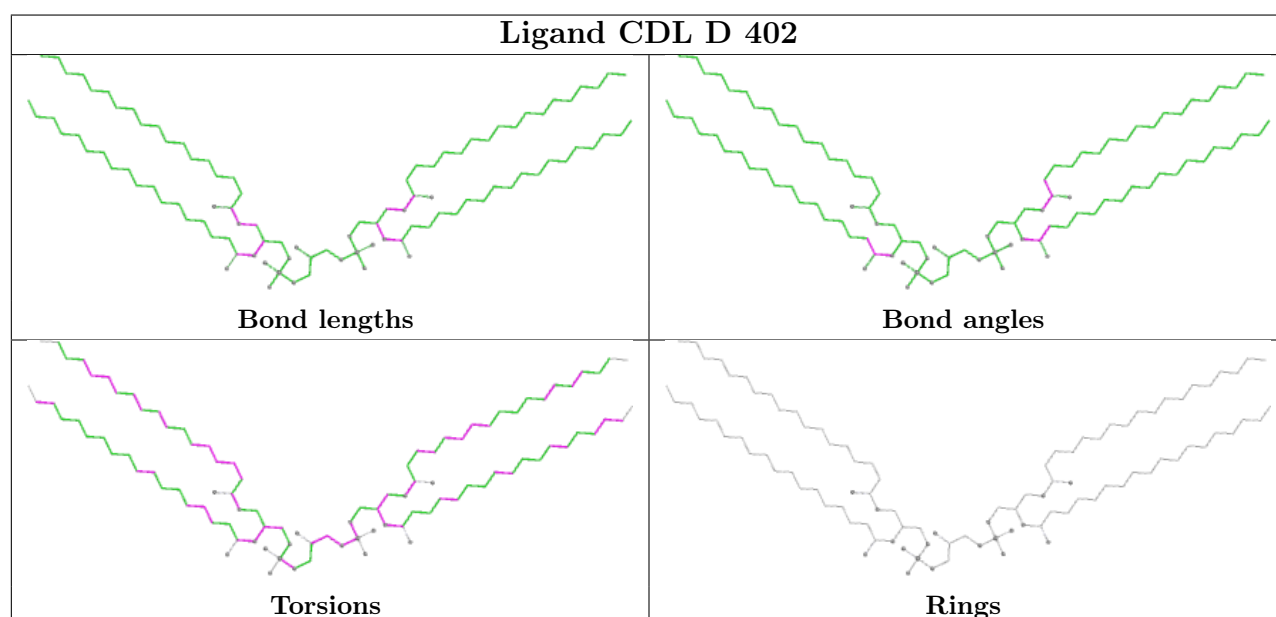
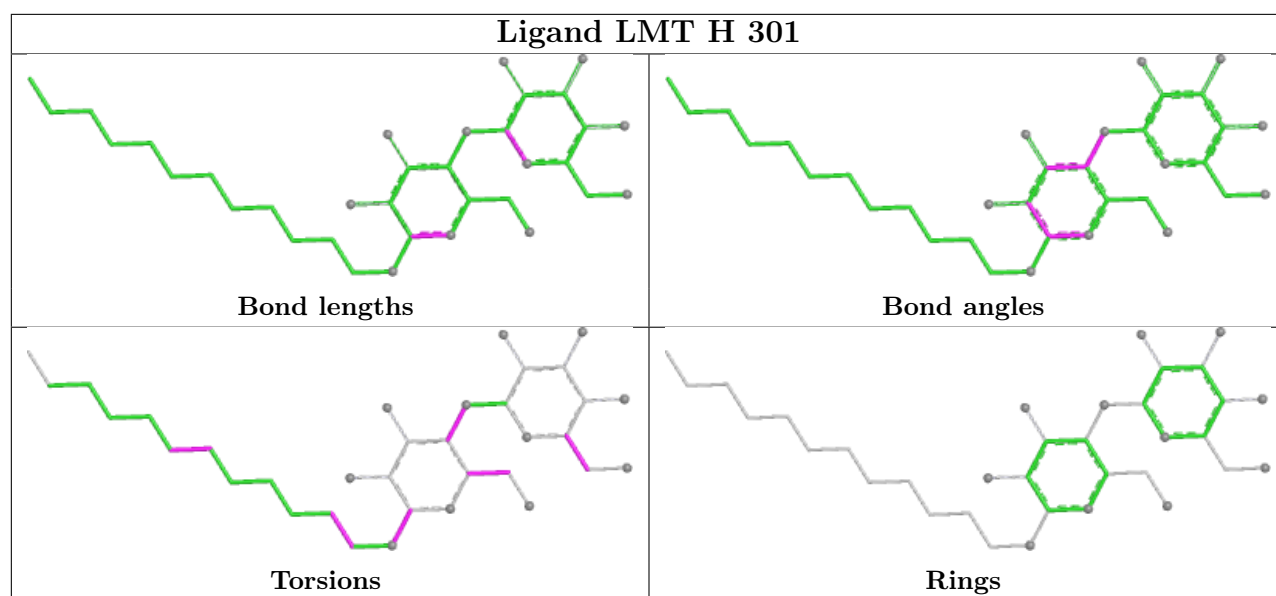


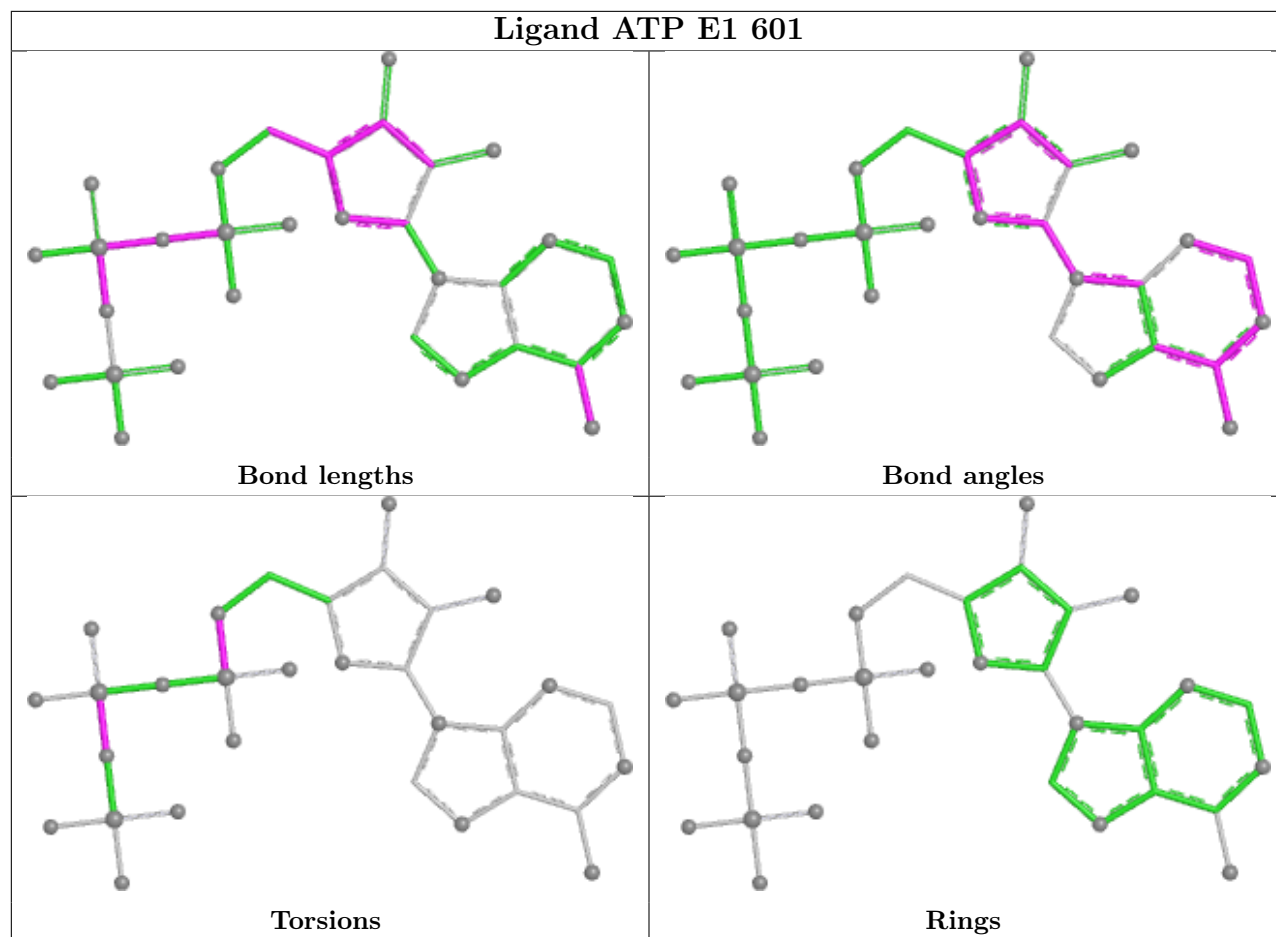


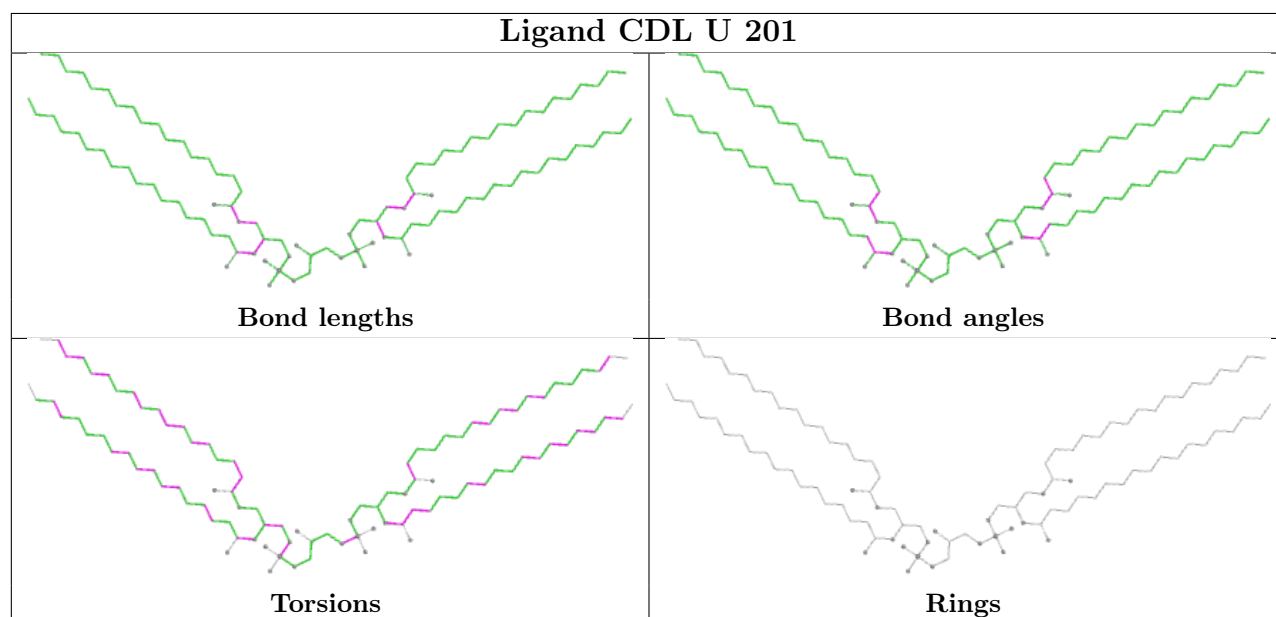
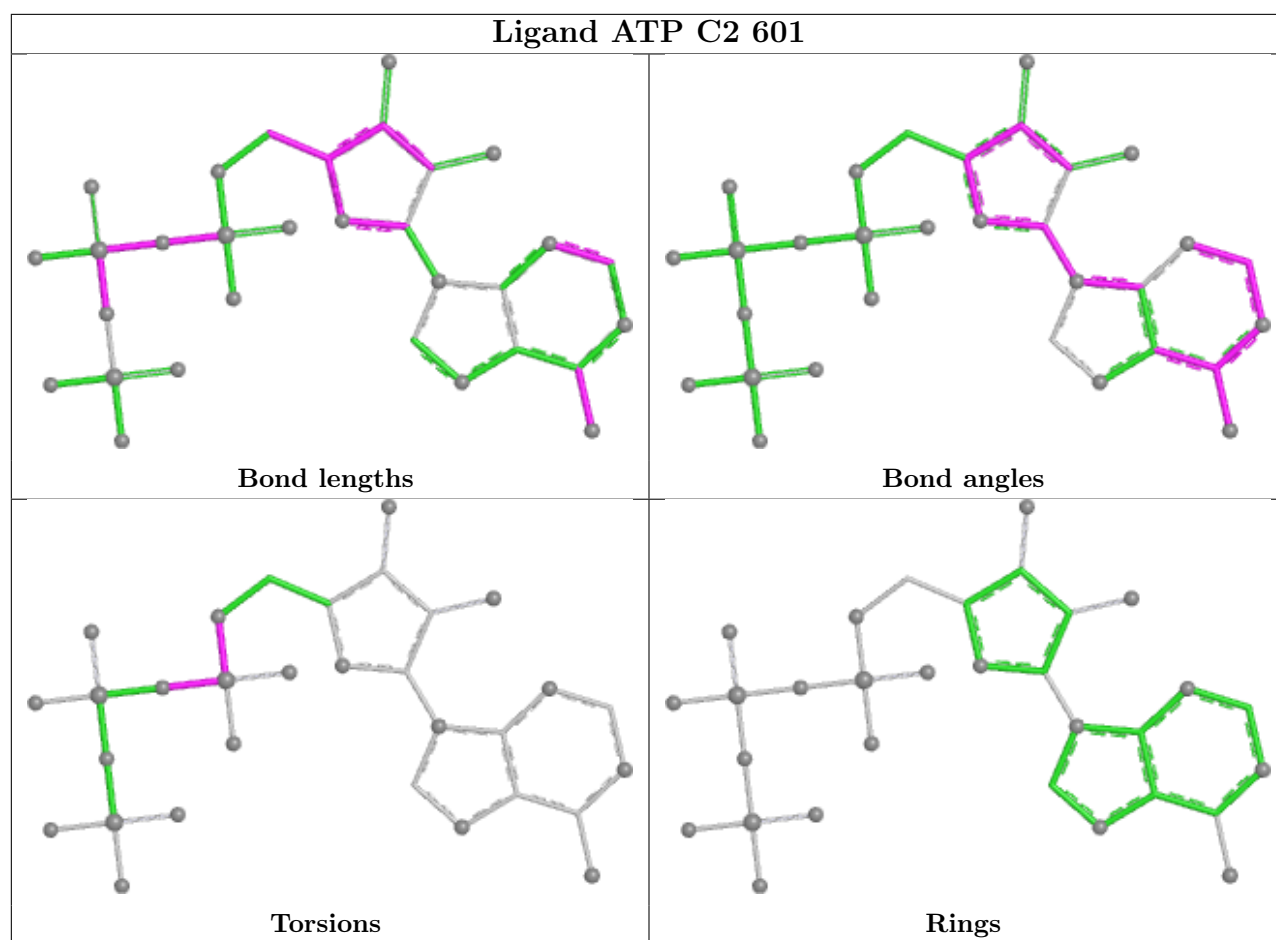


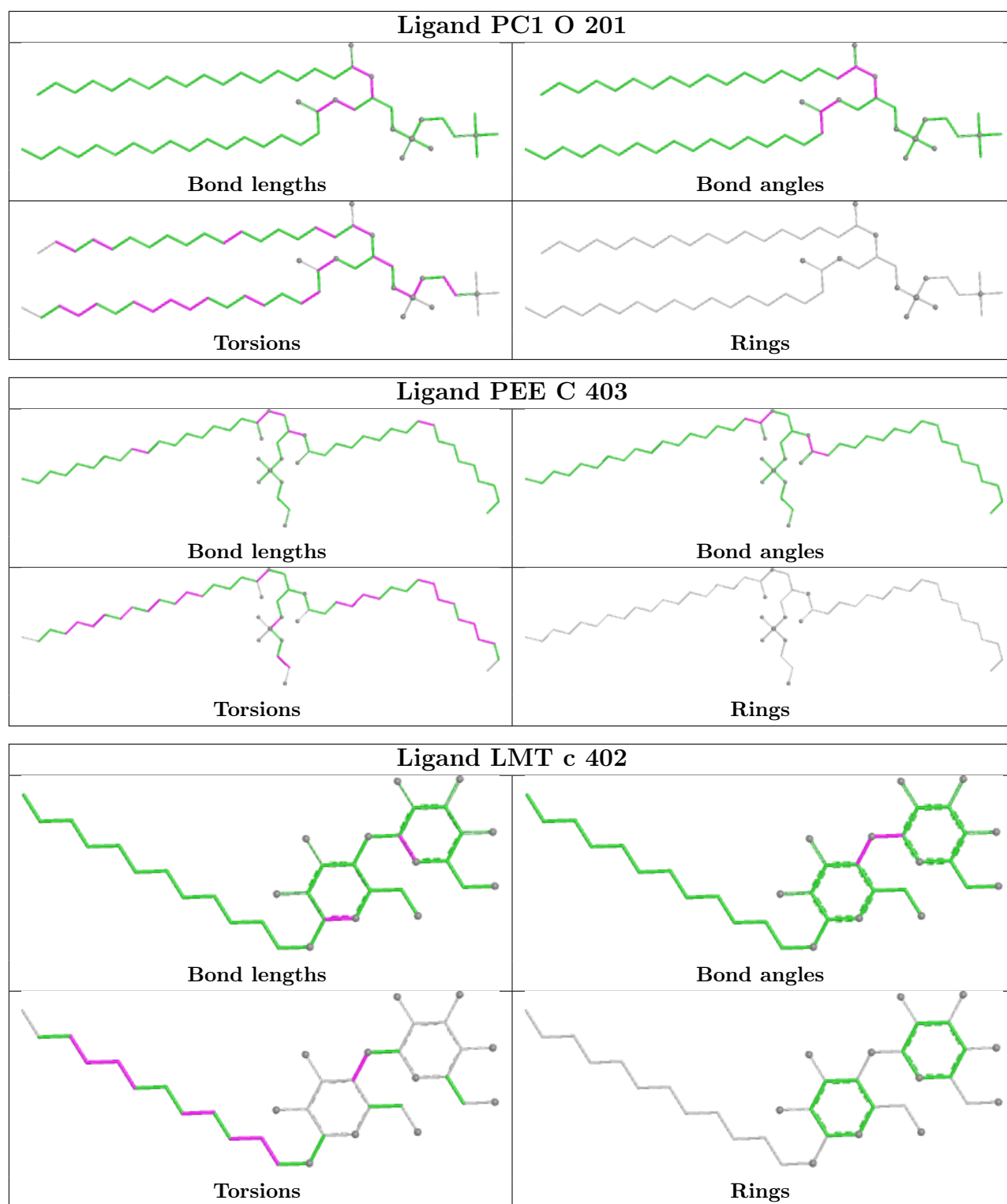


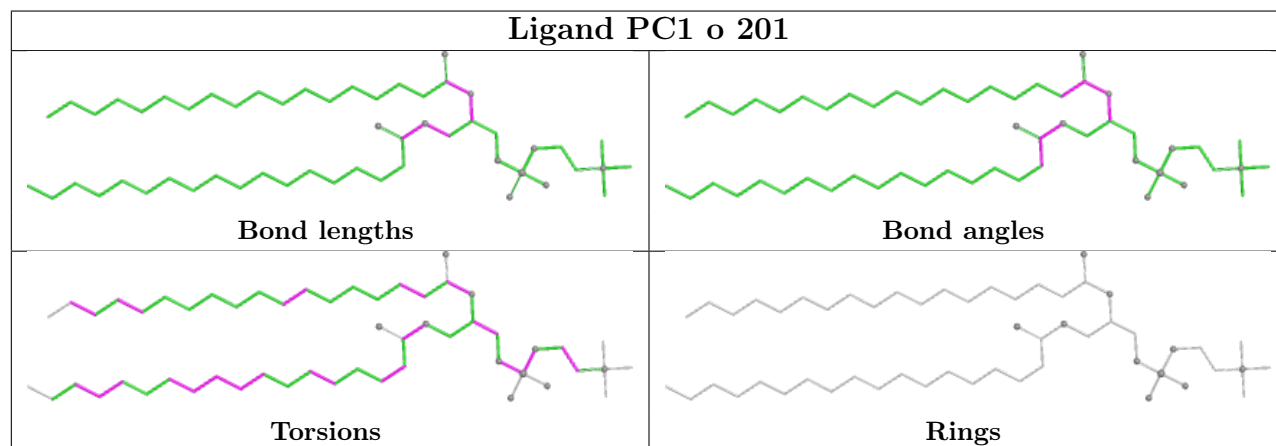
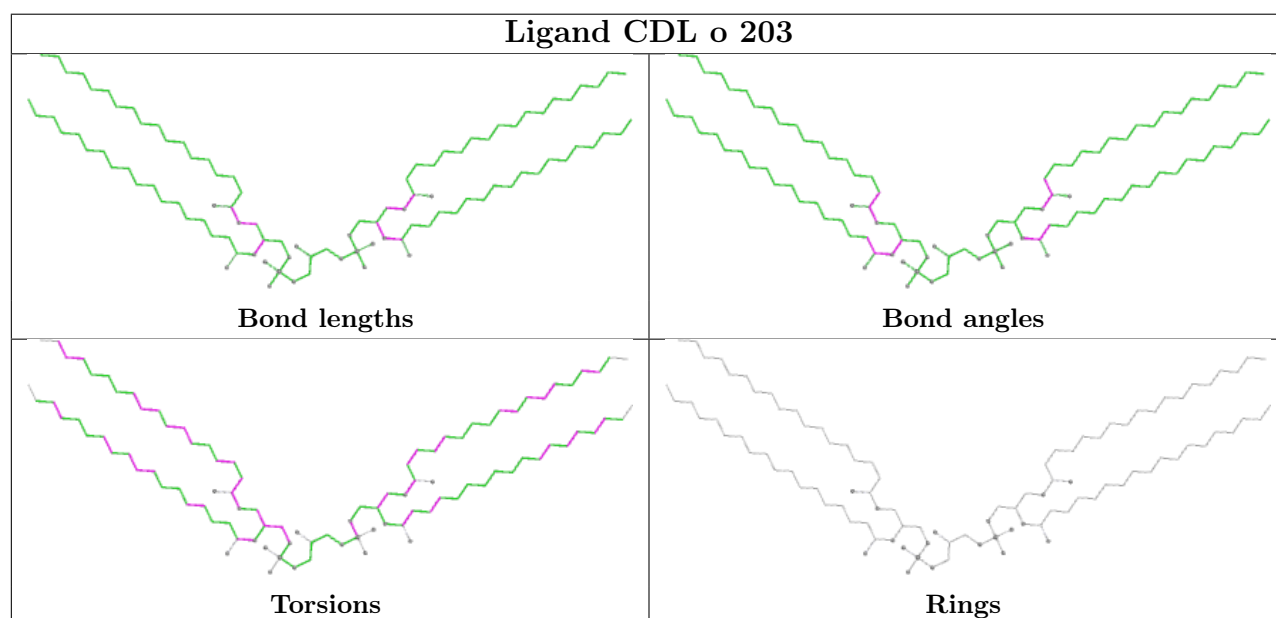
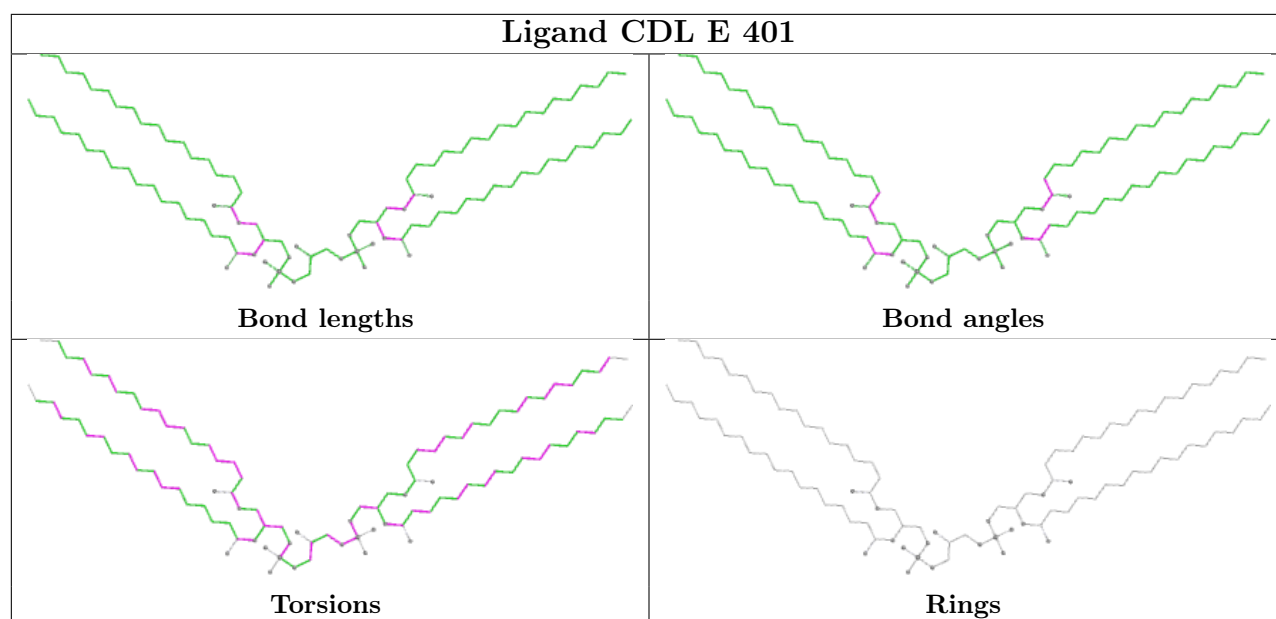


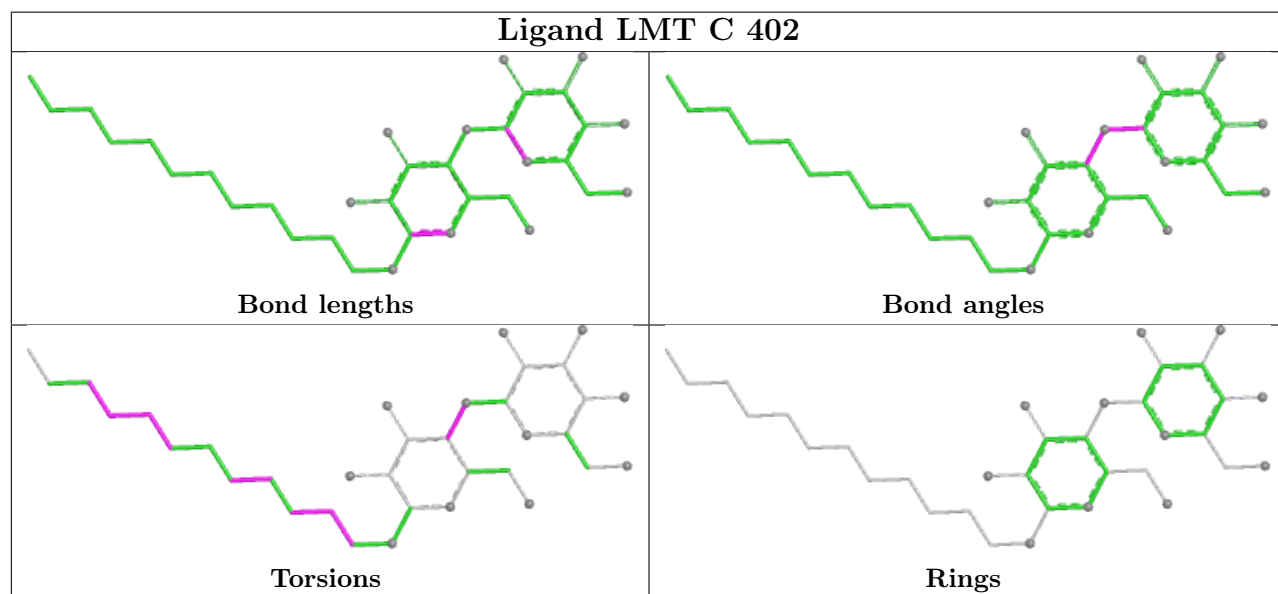
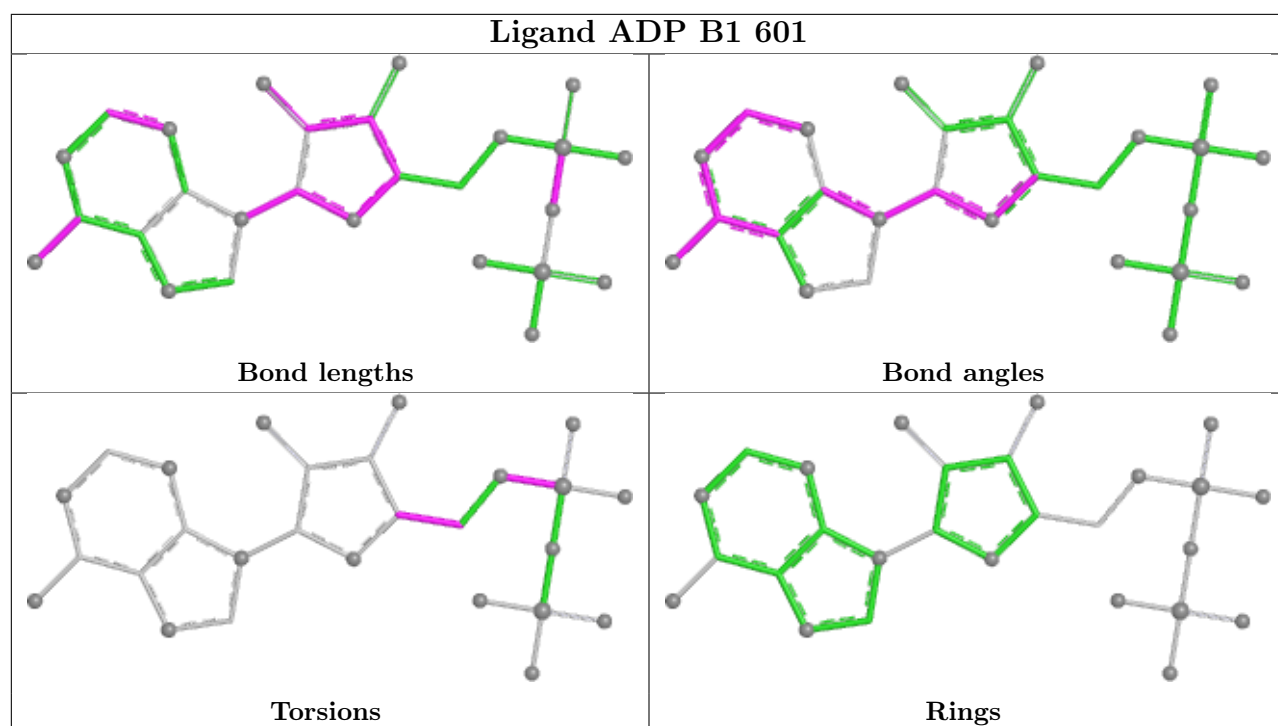


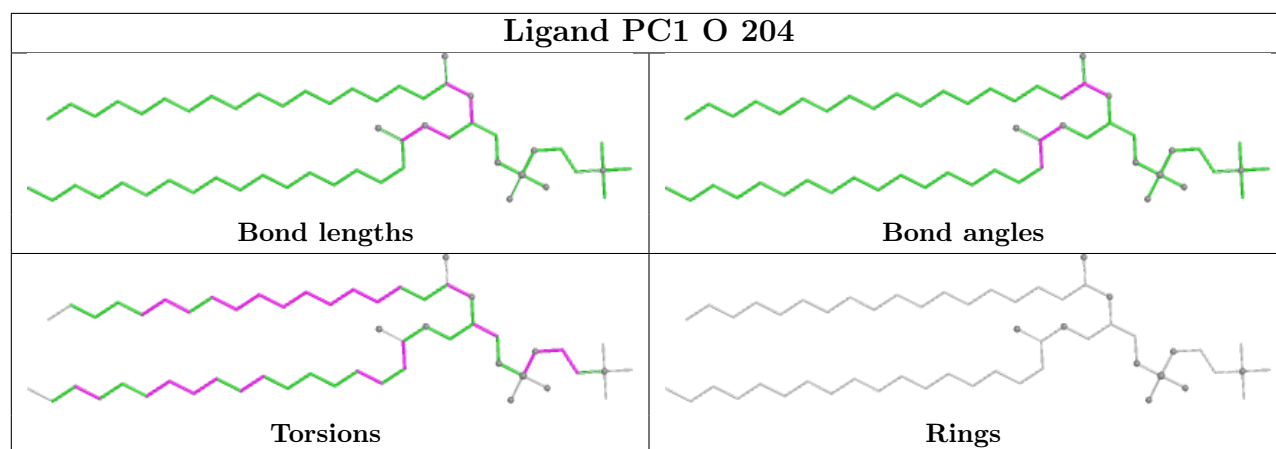
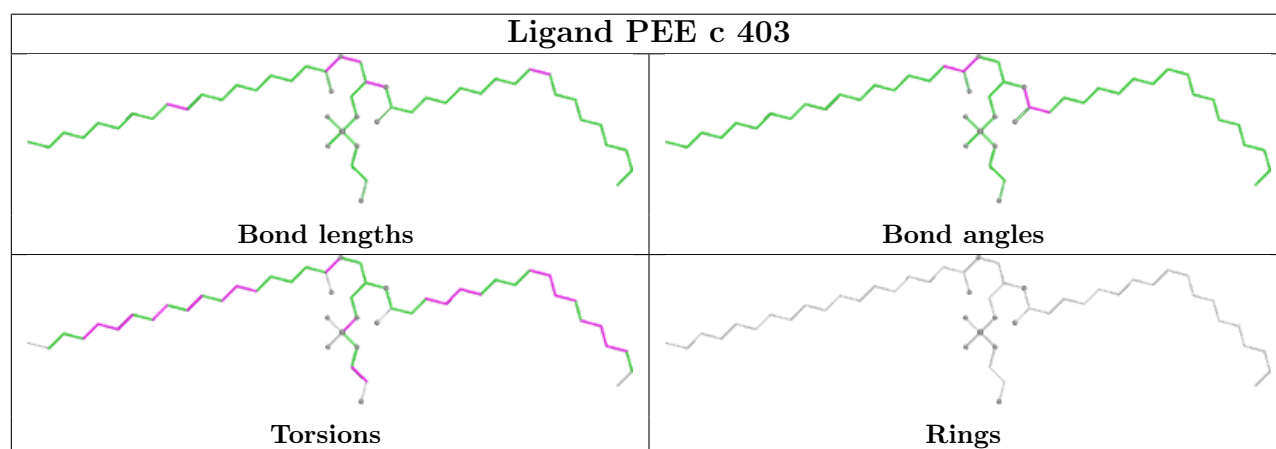
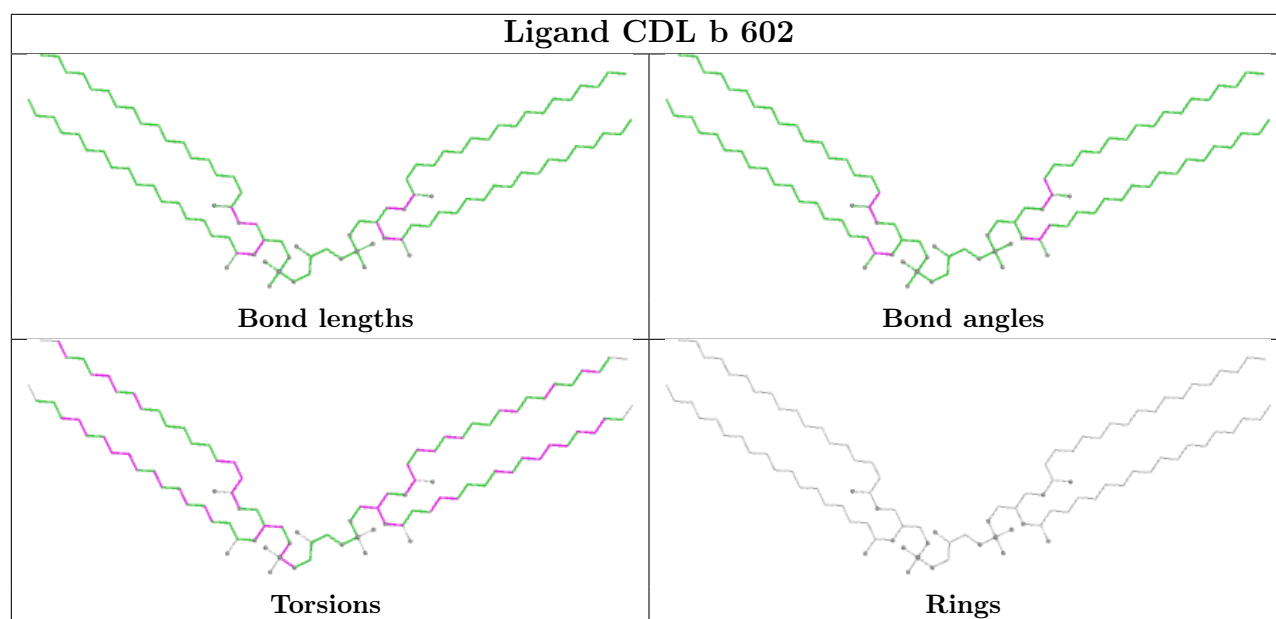


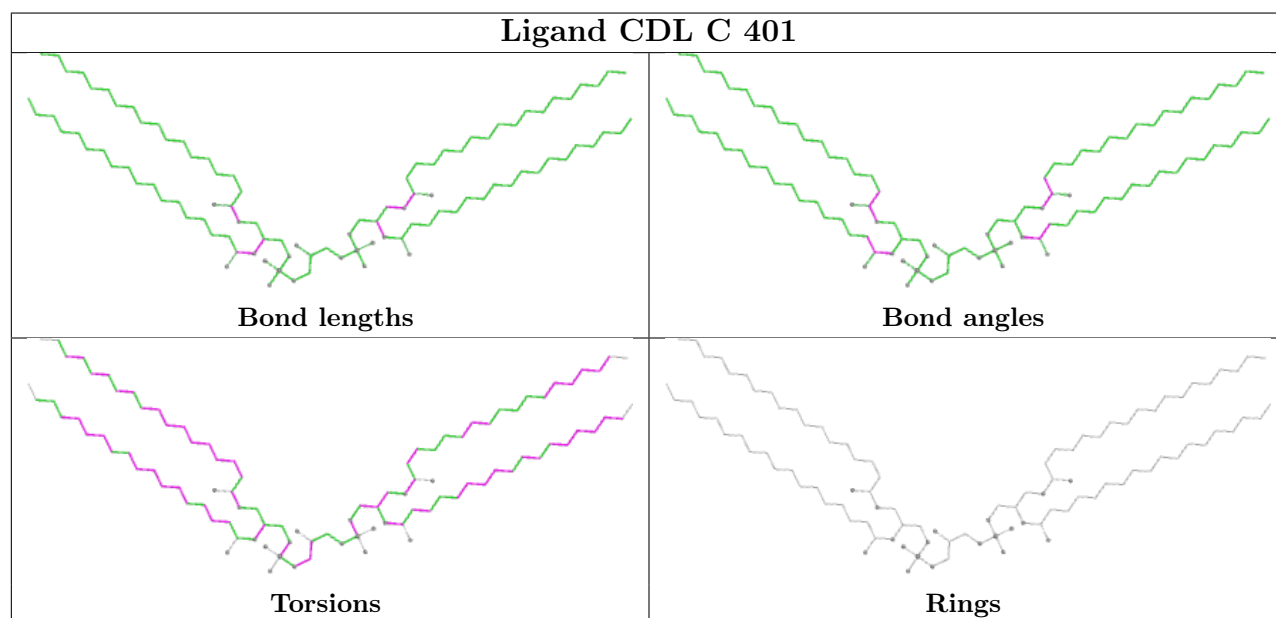
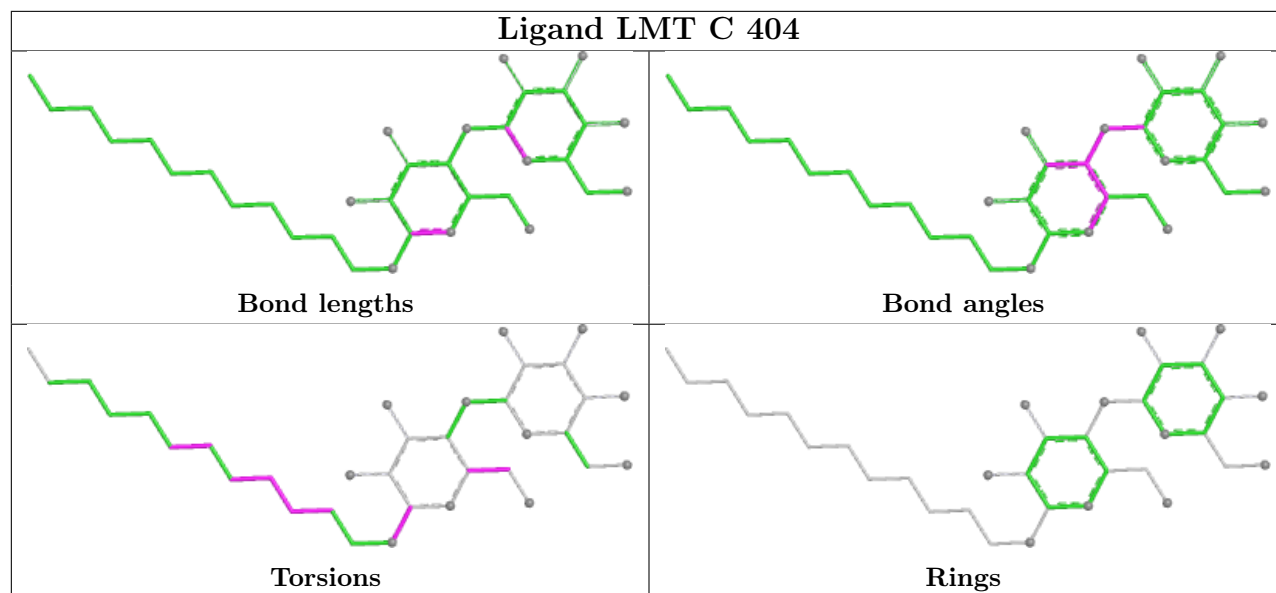


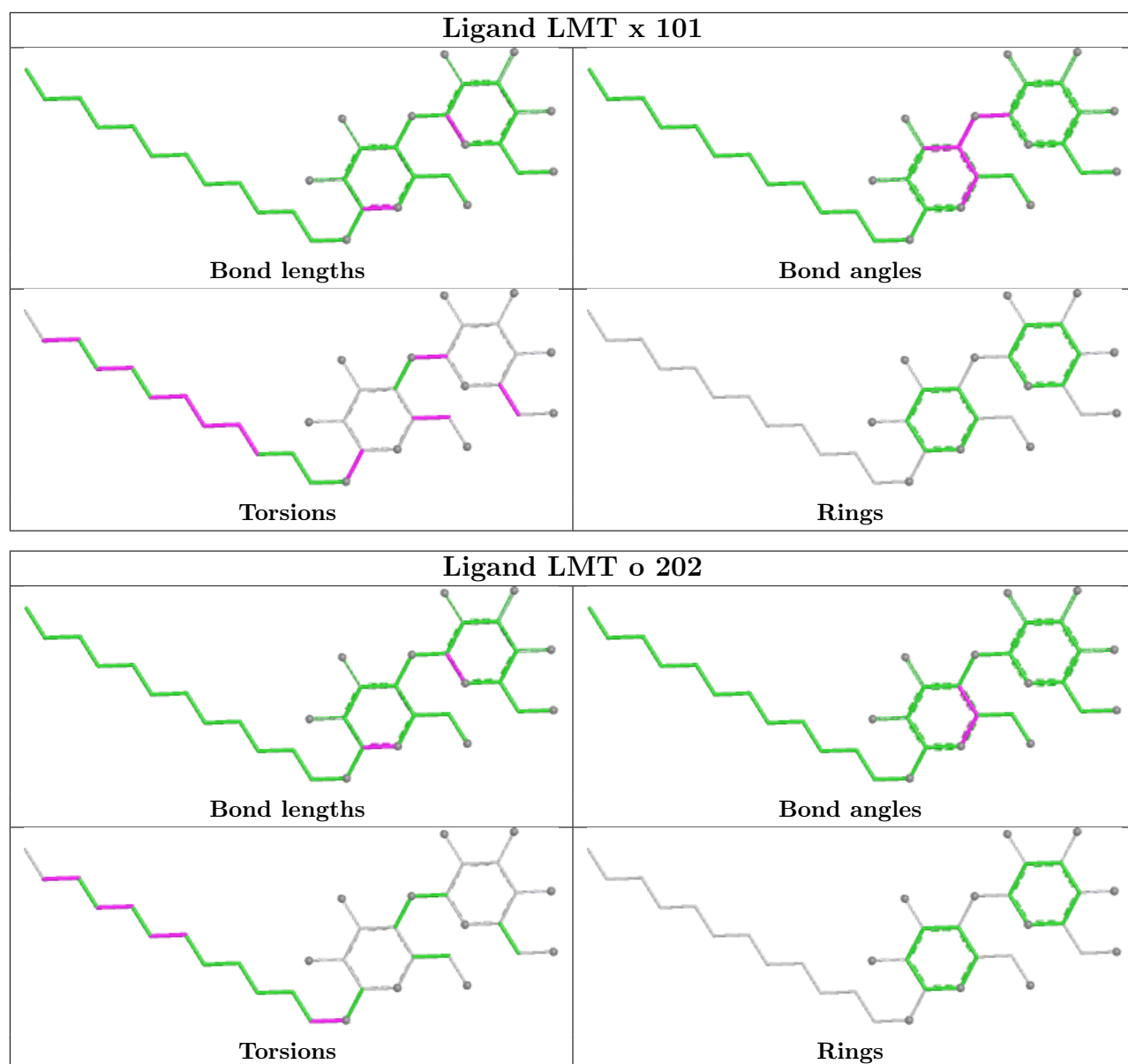


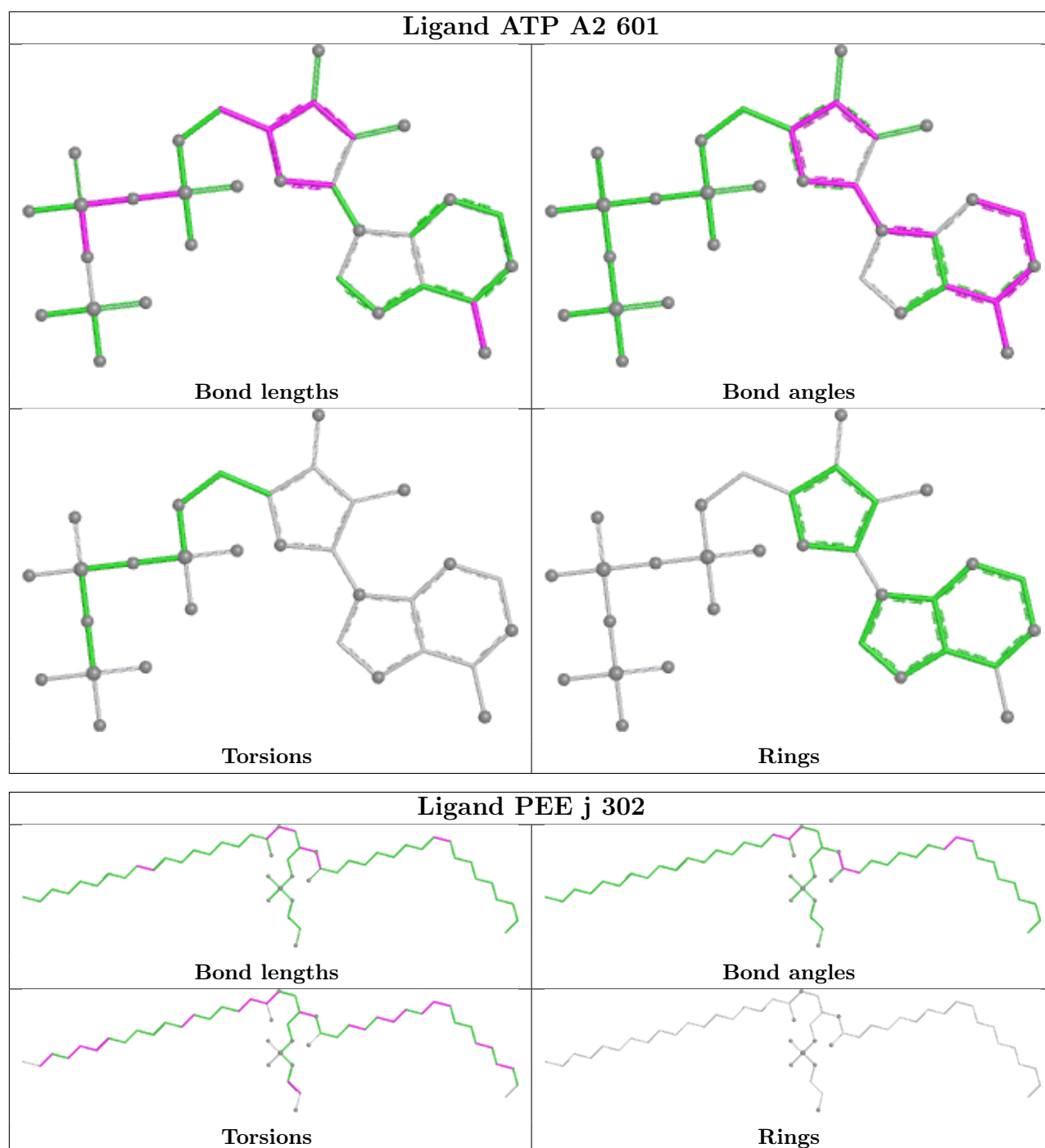












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

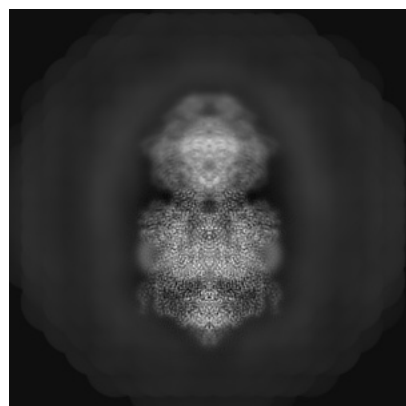
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10524. These allow visual inspection of the internal detail of the map and identification of artifacts.

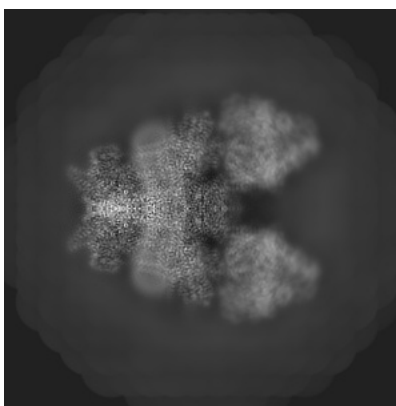
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

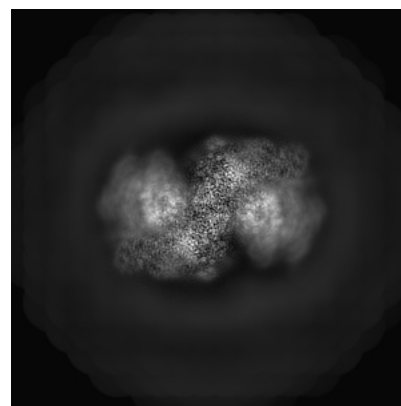
6.1.1 Primary map



X

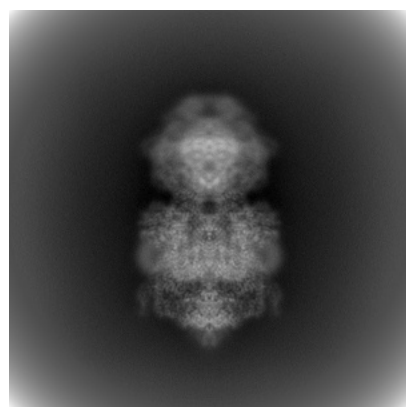


Y

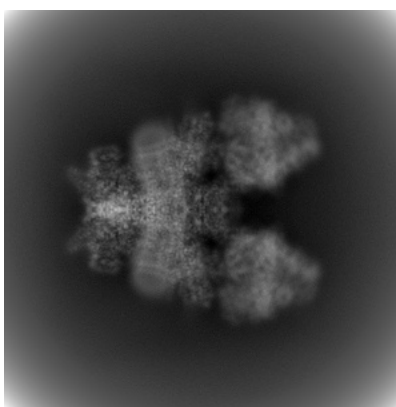


Z

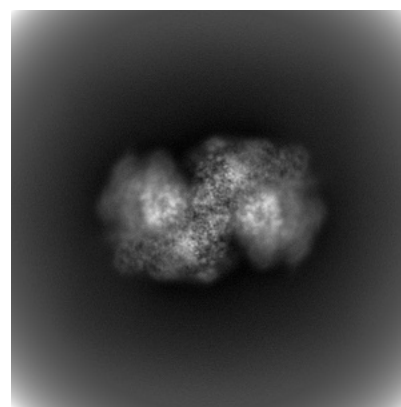
6.1.2 Raw map



X



Y

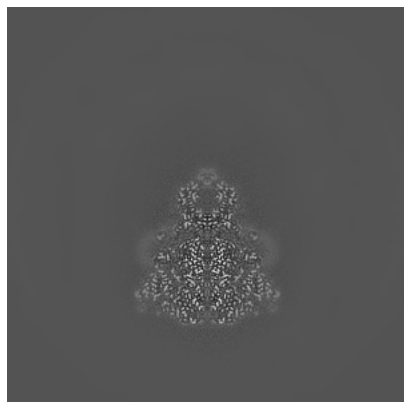


Z

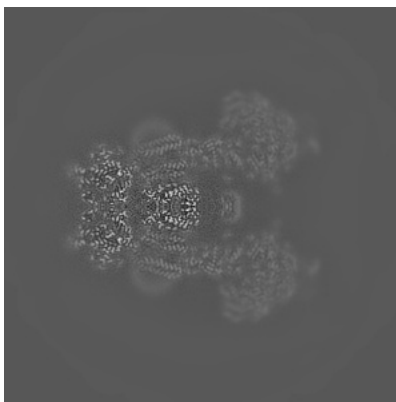
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 280

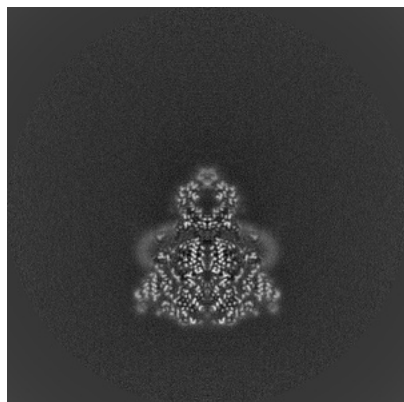


Y Index: 280

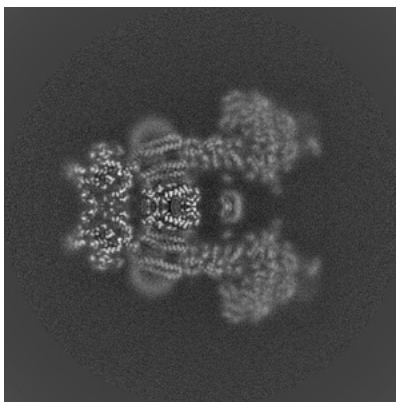


Z Index: 280

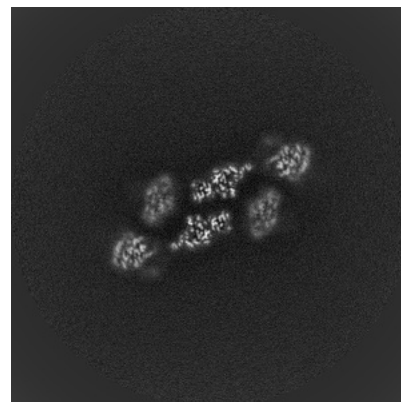
6.2.2 Raw map



X Index: 280



Y Index: 280

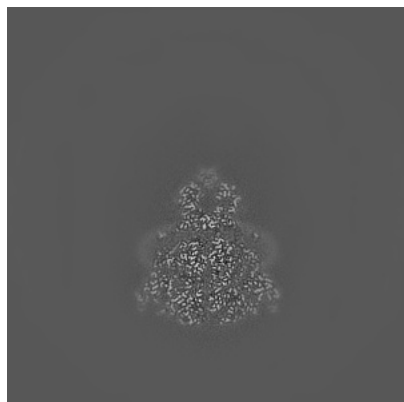


Z Index: 280

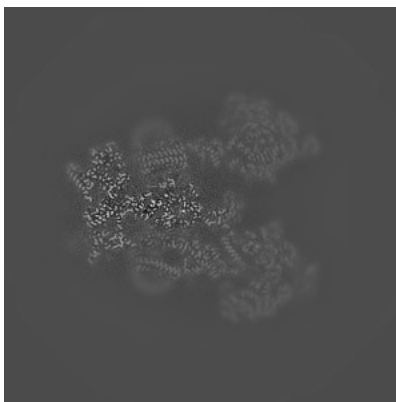
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

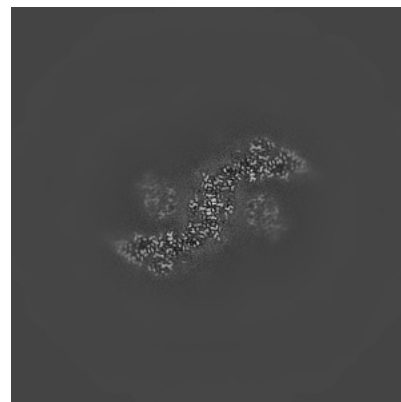
6.3.1 Primary map



X Index: 282

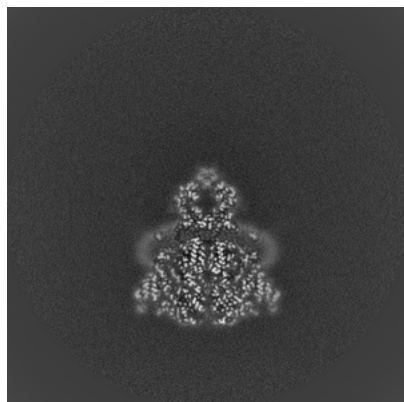


Y Index: 289

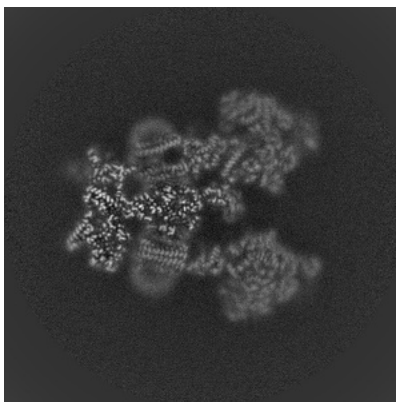


Z Index: 253

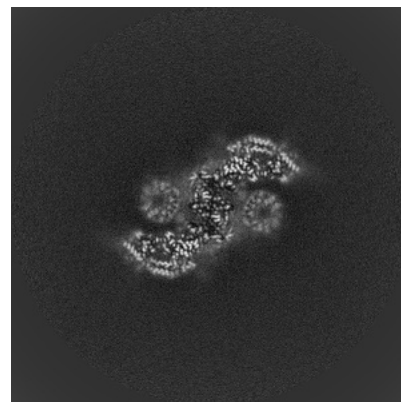
6.3.2 Raw map



X Index: 279



Y Index: 271

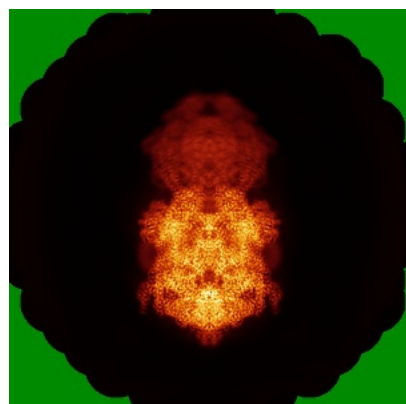


Z Index: 248

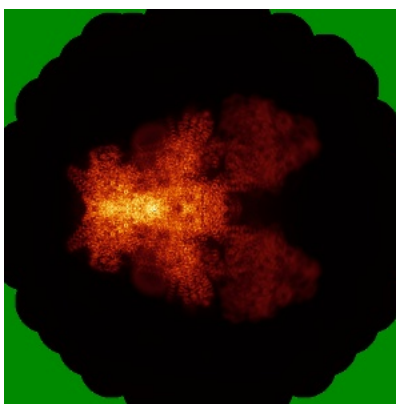
The images above show the largest variance slices of the map in three orthogonal directions.

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

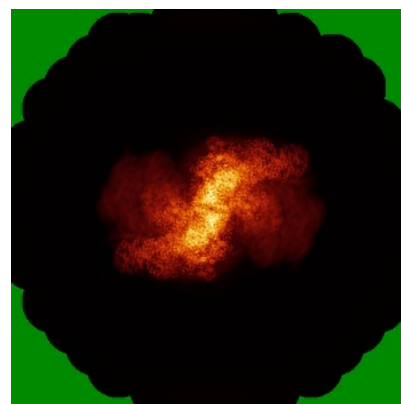
6.4.1 Primary map



X

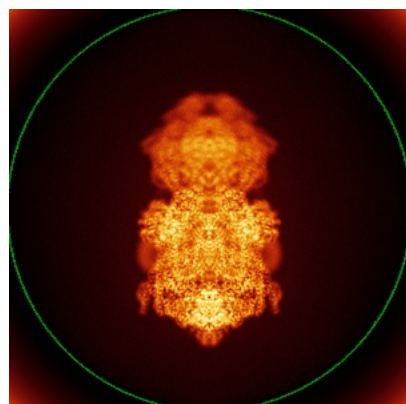


Y

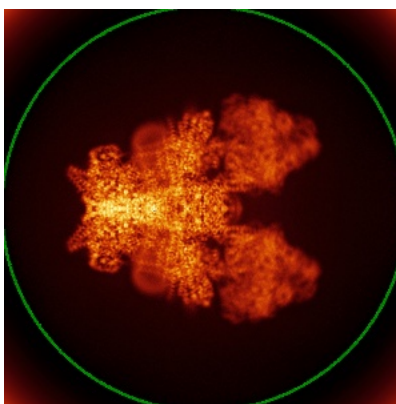


Z

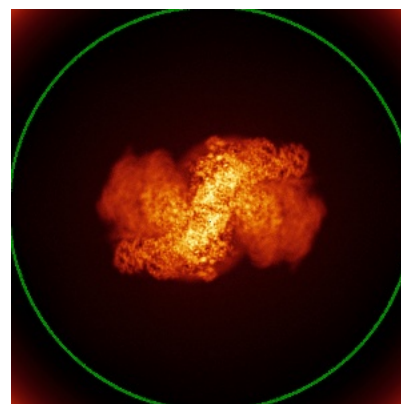
6.4.2 Raw map



X



Y



Z

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

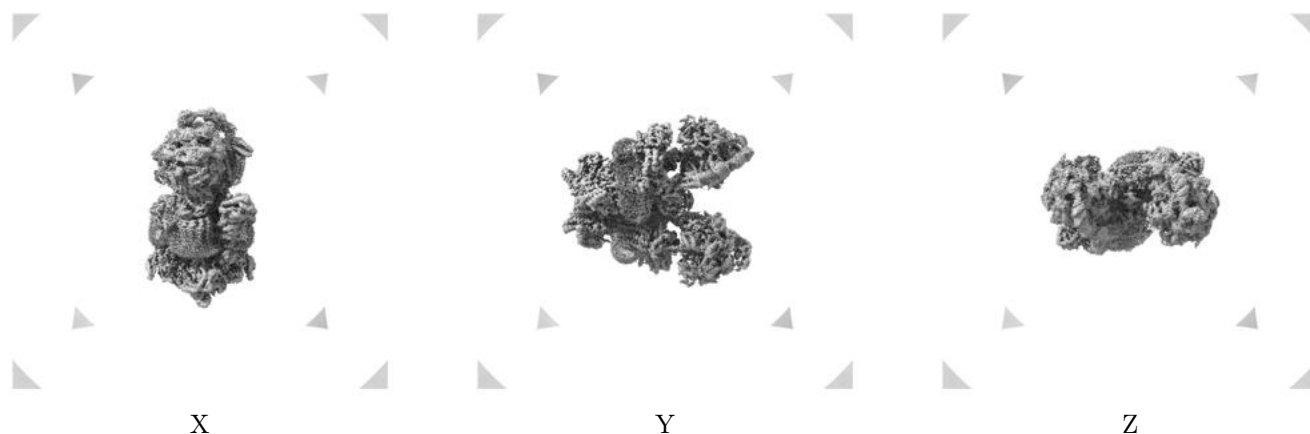
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

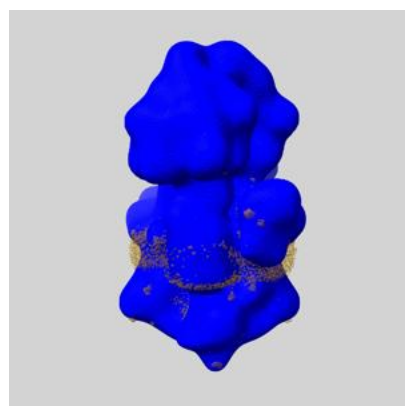
6.6 Mask visualisation [i](#)

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

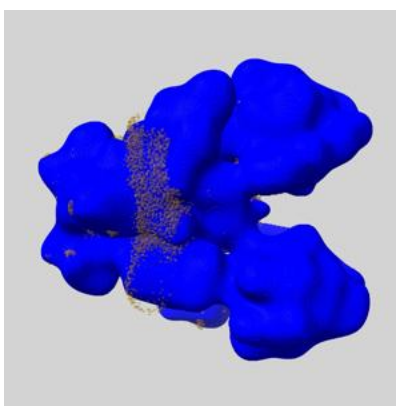
A mask typically either:

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

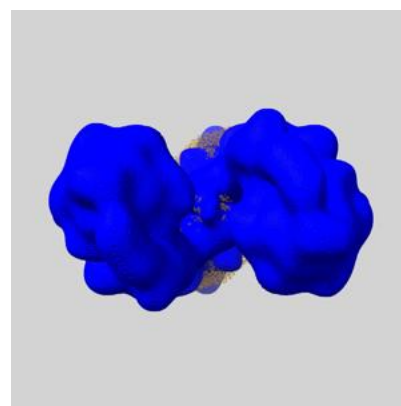
6.6.1 emd_10524_msk_1.map [i](#)



X



Y

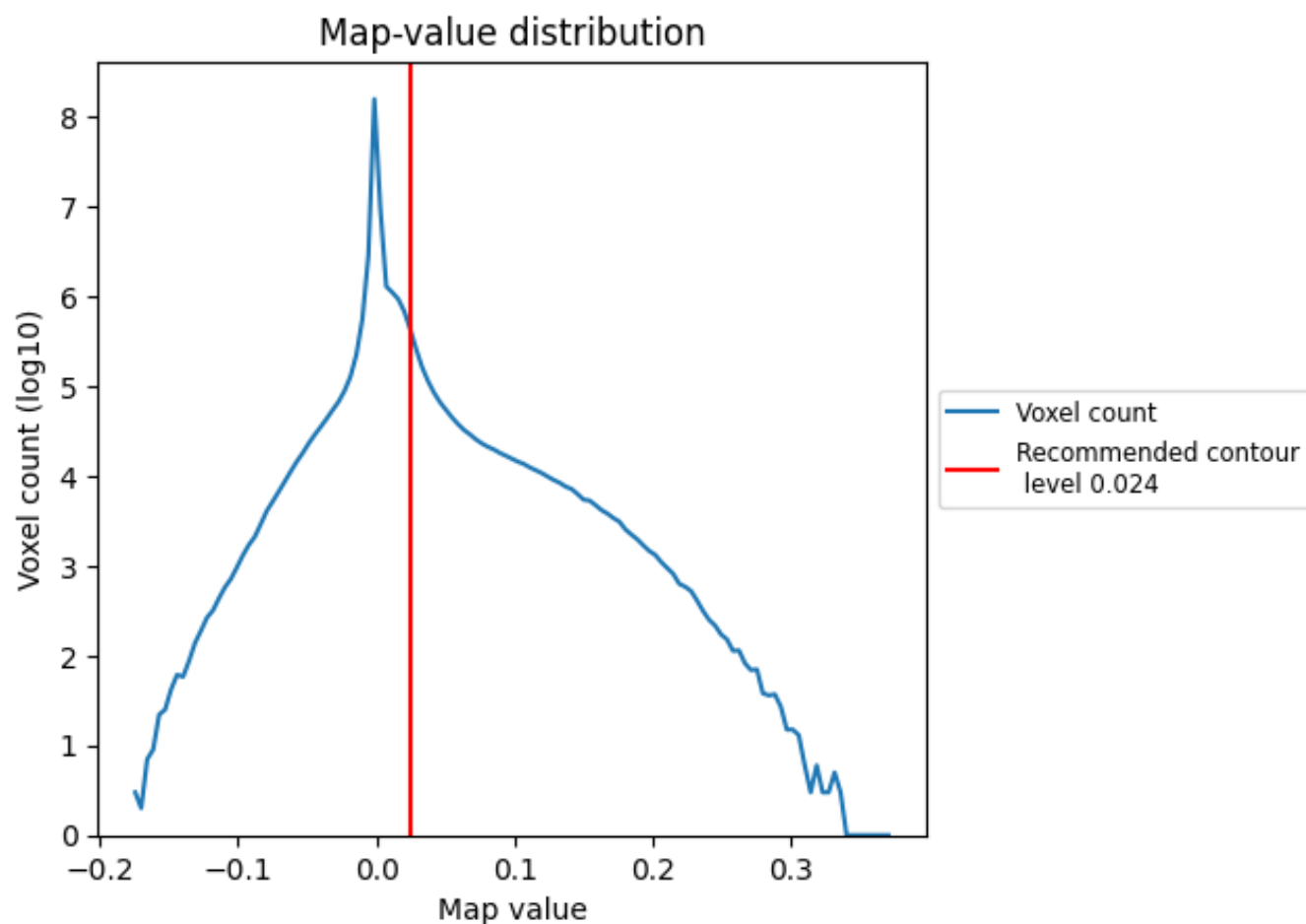


Z

7 Map analysis [i](#)

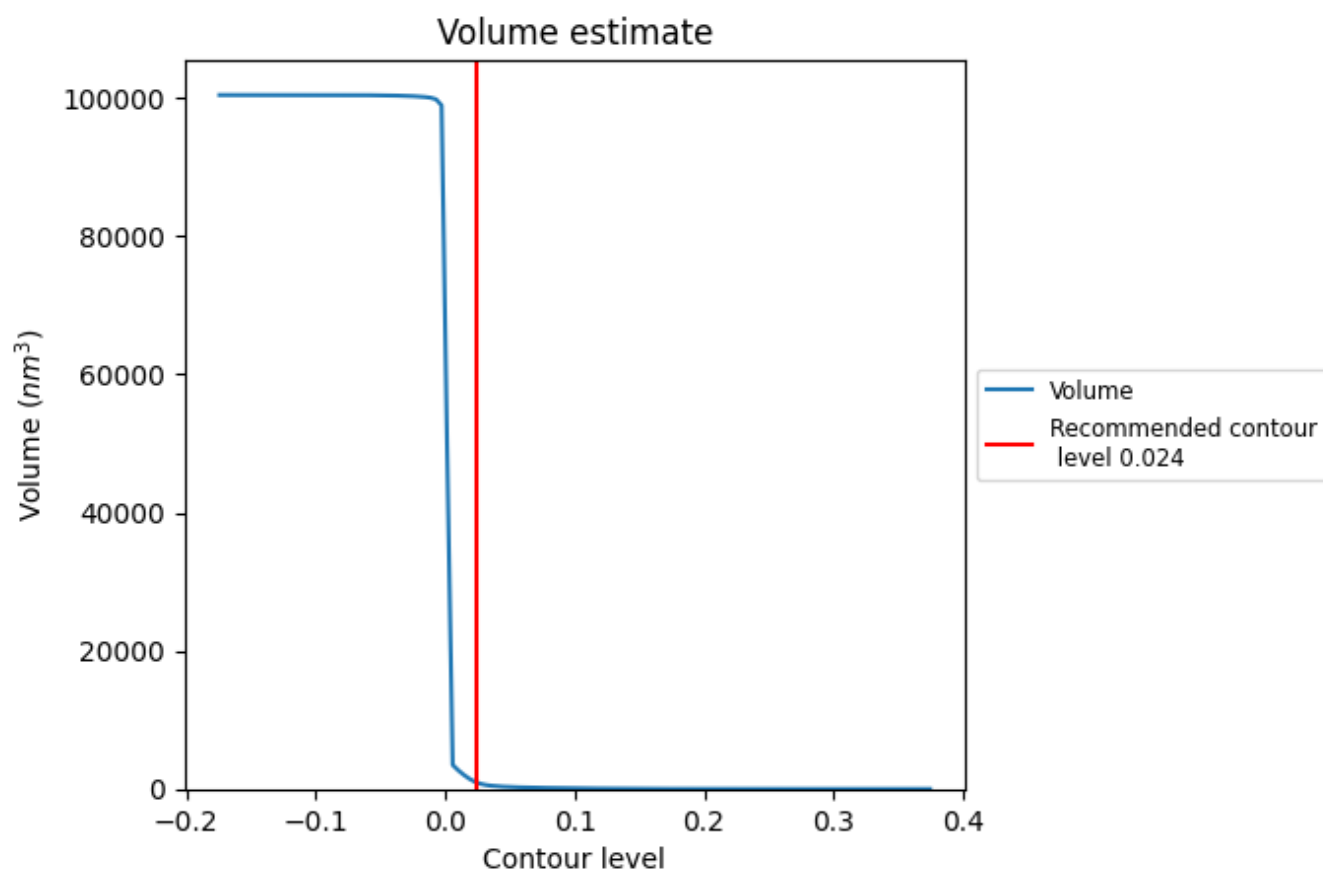
This section contains the results of statistical analysis of the map.

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.

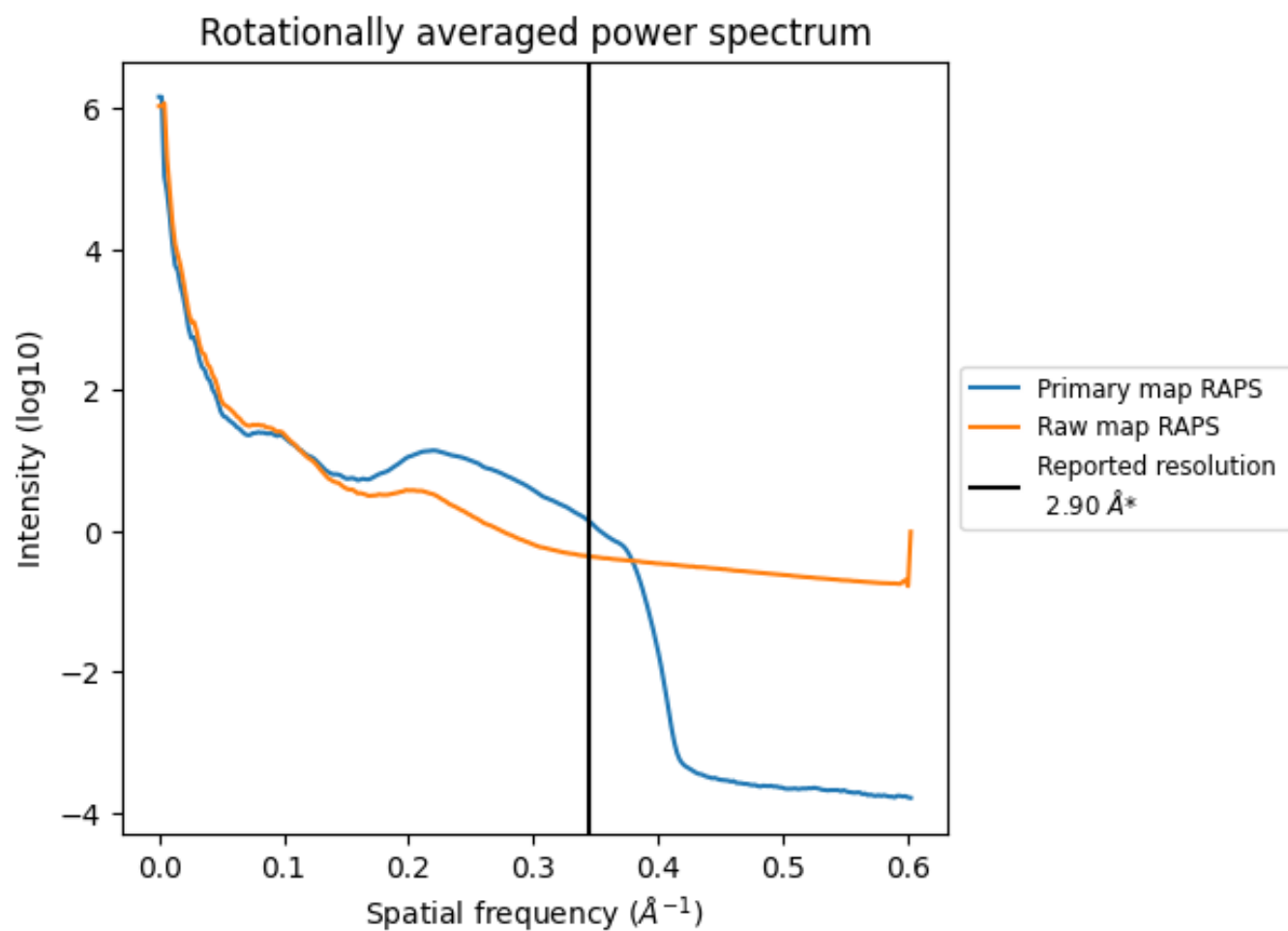
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 964 nm^3 ; this corresponds to an approximate mass of 871 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 ⓘ

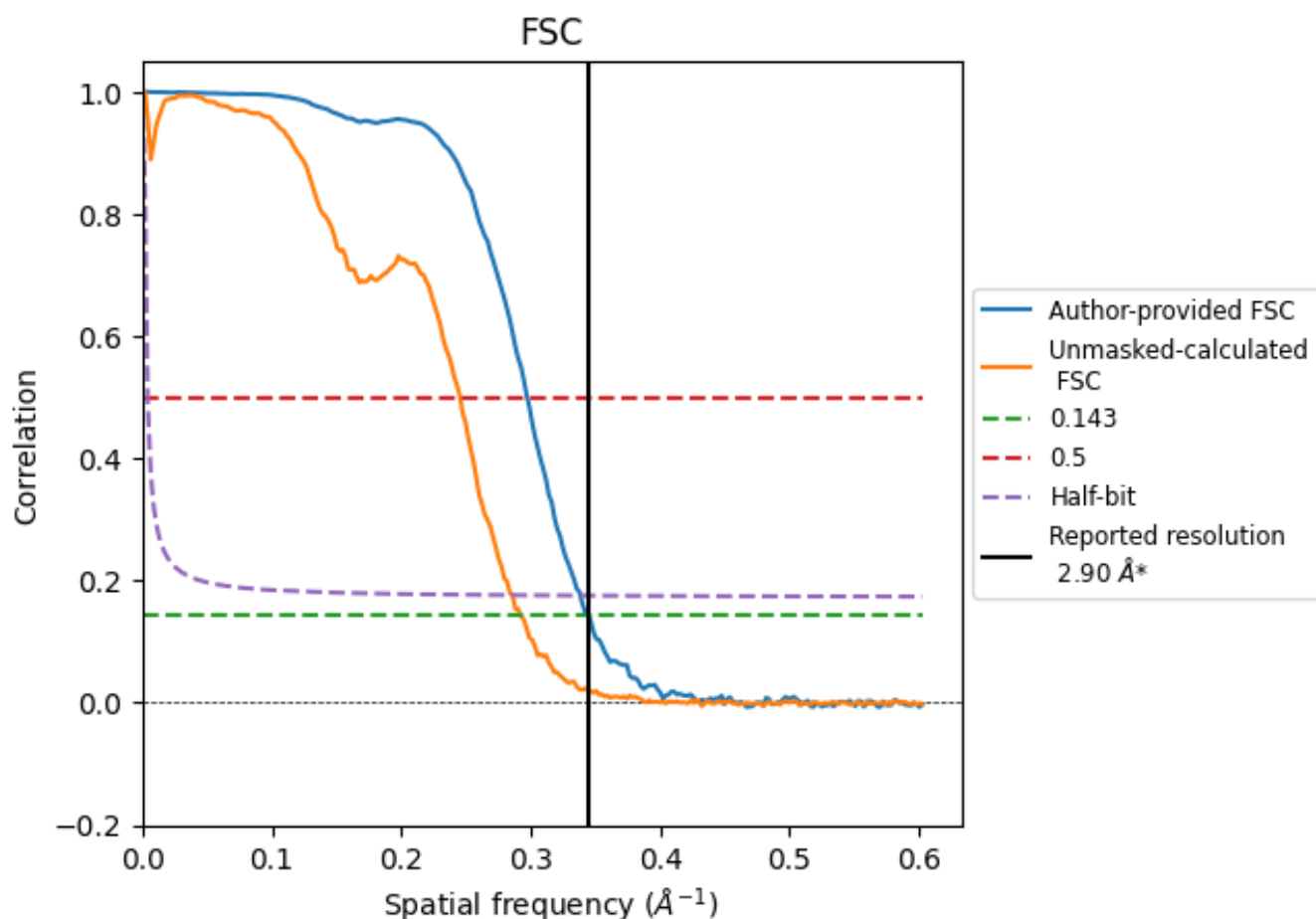


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

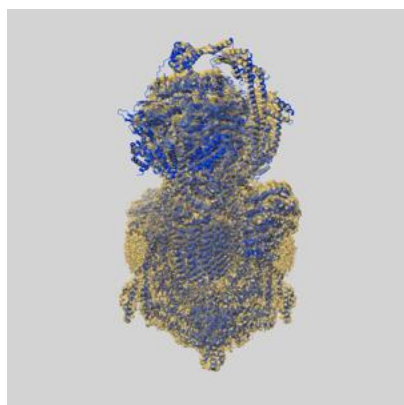
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.36	2.96
Unmasked-calculated*	3.42	4.07	3.50

*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 3.42 differs from the reported value 2.9 by more than 10 %

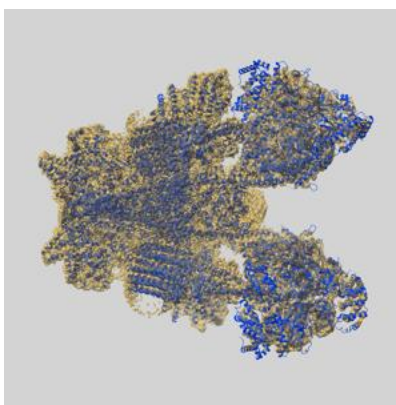
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10524 and PDB model 6TMK. Per-residue inclusion information can be found in section [3](#) on page [22](#).

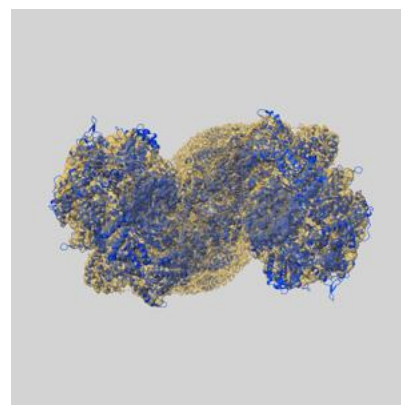
9.1 Map-model overlay [i](#)



X



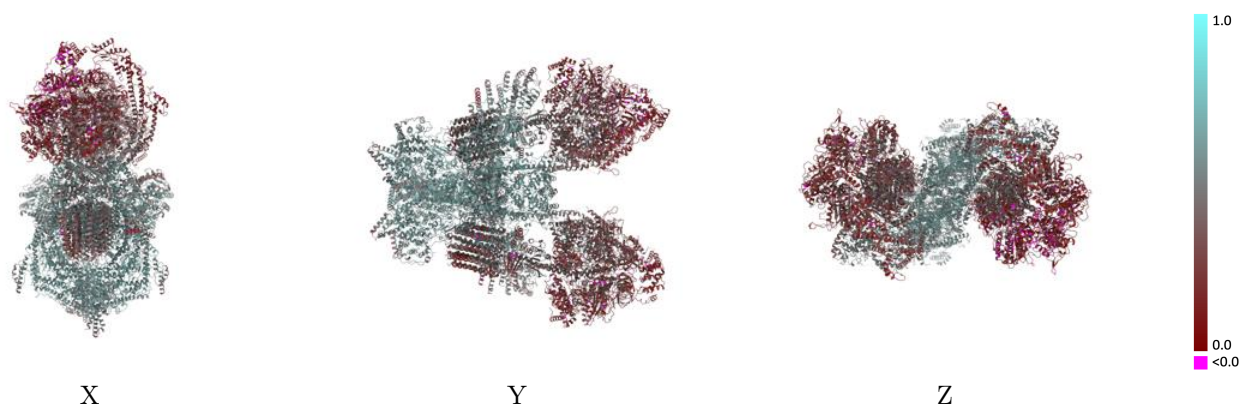
Y



Z

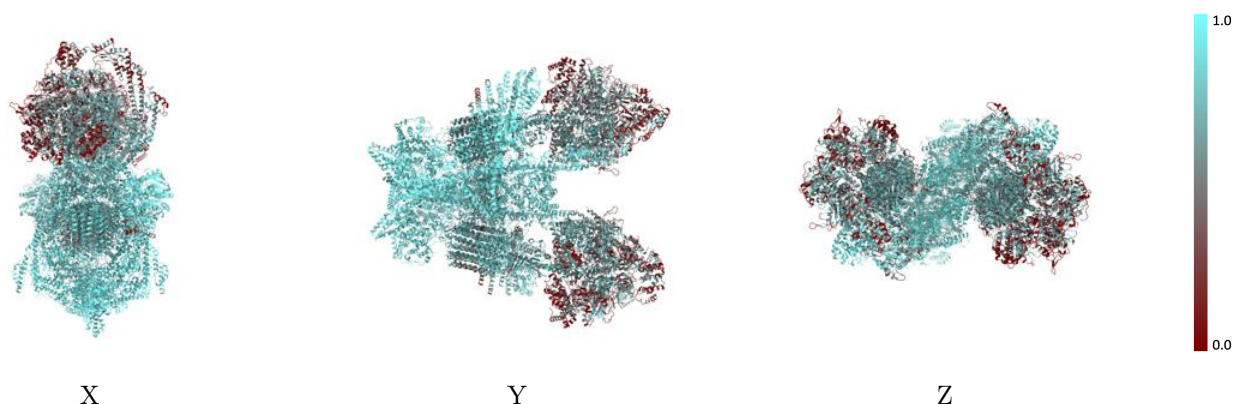
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



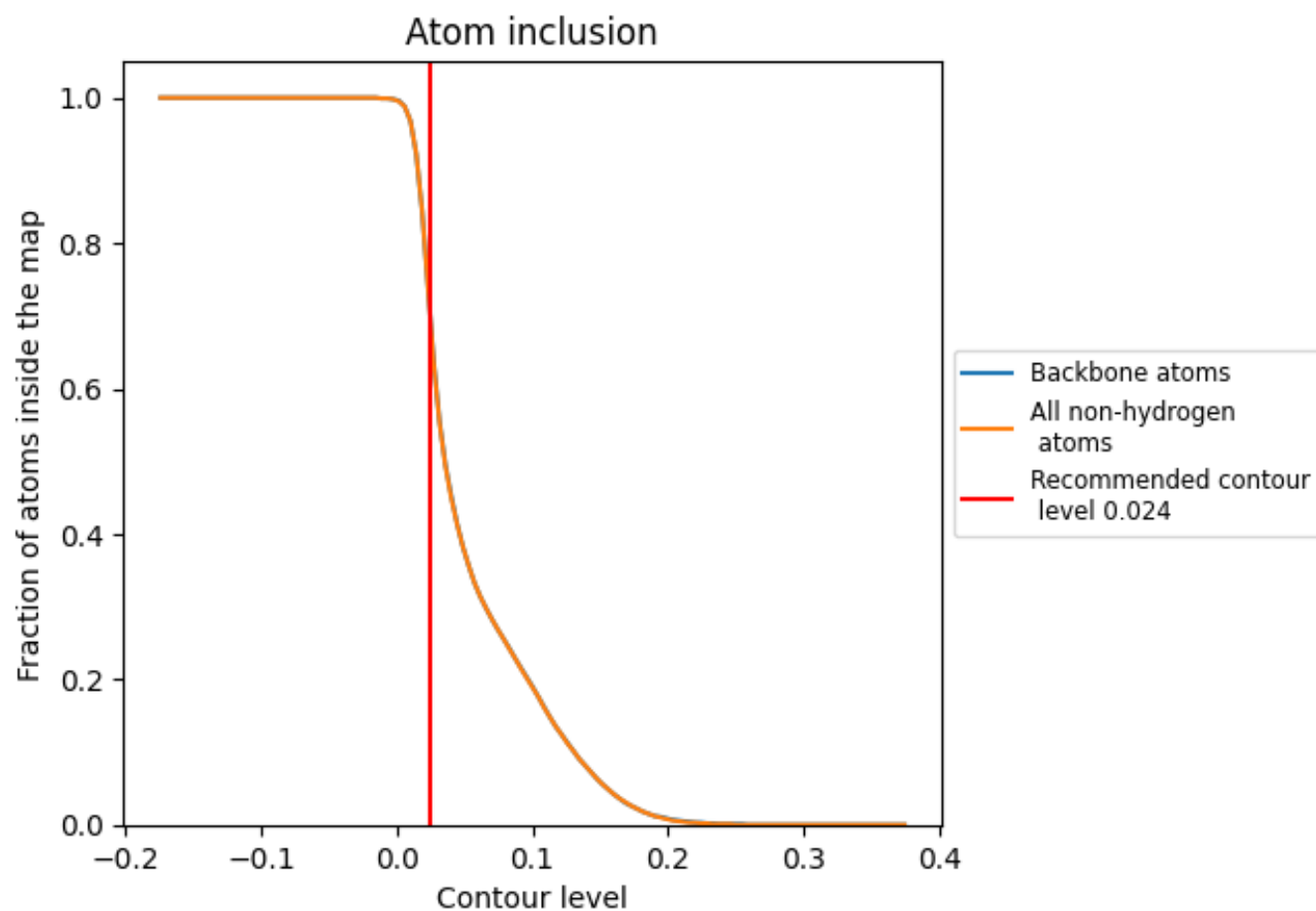
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.4280
A	 0.8470	 0.4810
A1	 0.4340	 0.2970
A2	 0.3700	 0.1910
B	 0.7260	 0.4360
B1	 0.6200	 0.3500
B2	 0.5910	 0.2850
C	 0.8440	 0.5420
C1	 0.6150	 0.3250
C2	 0.6100	 0.3240
D	 0.9320	 0.6040
D1	 0.5760	 0.3110
D2	 0.5550	 0.2820
E	 0.9330	 0.6020
E1	 0.4690	 0.2590
E2	 0.4100	 0.1970
F	 0.9180	 0.5630
F1	 0.3650	 0.2420
F2	 0.3170	 0.1800
G	 0.9400	 0.5900
G1	 0.3520	 0.1840
G2	 0.2880	 0.1440
H	 0.9410	 0.6190
H1	 0.7040	 0.3560
H2	 0.7450	 0.4120
I	 0.9050	 0.5370
I1	 0.6660	 0.3560
I2	 0.7120	 0.4010
J	 0.9650	 0.6490
J1	 0.6560	 0.3200
J2	 0.7140	 0.3860
K	 0.8900	 0.5740
K1	 0.6900	 0.3410
K2	 0.7200	 0.3920
L	 0.9450	 0.5990



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Chain	Atom inclusion	Q-score
L1	 0.7120	 0.3660
L2	 0.6760	 0.3680
M	 0.9560	 0.6260
M1	 0.7520	 0.4060
M2	 0.6840	 0.3570
N	 0.9060	 0.5500
N1	 0.7500	 0.4400
N2	 0.7300	 0.4070
O	 0.8920	 0.5760
O1	 0.8070	 0.4980
O2	 0.7790	 0.4730
P	 0.9440	 0.5960
P1	 0.8010	 0.4790
P2	 0.7890	 0.4520
Q	 0.8810	 0.4970
Q1	 0.7870	 0.4470
Q2	 0.7830	 0.4280
R	 0.8220	 0.4970
S	 0.9240	 0.5760
T	 0.9240	 0.5390
U	 0.8830	 0.5770
V	 0.9490	 0.6250
W	 0.9520	 0.6180
X	 0.9420	 0.6040
a	 0.8360	 0.4830
b	 0.7520	 0.4400
c	 0.8340	 0.5400
d	 0.9330	 0.6040
d1	 0.6060	 0.2770
d2	 0.7000	 0.4080
e	 0.9320	 0.6020
e1	 0.7470	 0.4260
e2	 0.7600	 0.4350
f	 0.9200	 0.5610
g	 0.9380	 0.5910
g1	 0.7300	 0.4080
g2	 0.7310	 0.4070
h	 0.9420	 0.6200
i	 0.9030	 0.5430
i1	 0.7200	 0.4160
i2	 0.7300	 0.4320
j	 0.9650	 0.6470

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Chain	Atom inclusion	Q-score
k	 0.8930	 0.5730
l	 0.9440	 0.5980
m	 0.9600	 0.6270
n	 0.9070	 0.5510
o	 0.8920	 0.5740
p	 0.9460	 0.5960
q	 0.8620	 0.4970
r	 0.8300	 0.5060
s	 0.9230	 0.5760
t	 0.9180	 0.5370
u	 0.8850	 0.5790
v	 0.9470	 0.6240
w	 0.9560	 0.6180
x	 0.9410	 0.6020