



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:12 AM UTC

PDB ID : 9W2V / pdb\_00009w2v  
EMDB ID : EMD-65581  
Title : Cryo-EM structure of complex I on the bovine heart submitochondrial particles, closed  
Authors : Nakano, A.; Masuya, T.; Akisada, S.; Ishikawa-Fukuda, M.; Mitsuoka, K.; Miyoshi, H.; Murai, M.; Yokoyama, K.  
Deposited on : 2025-07-28  
Resolution : 2.80 Å (reported)  
Based on initial model : 6ZPO

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

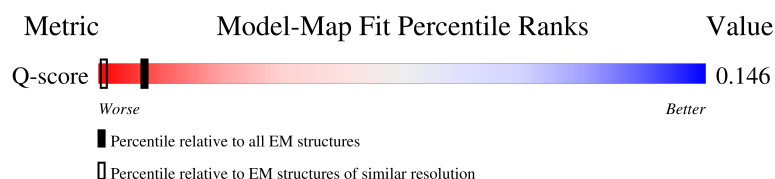
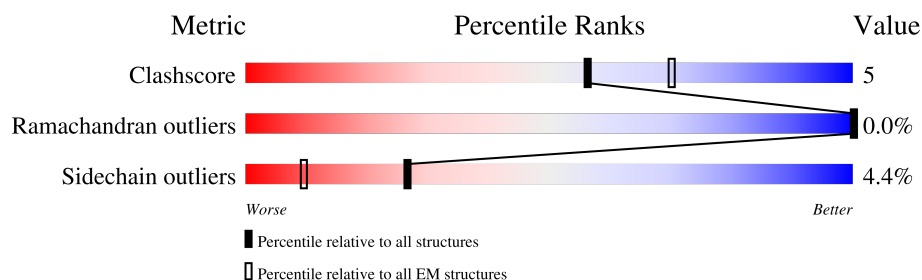


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 ( 2.30 - 3.30 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	114	<div> <div>70%</div> <div>89%</div> <div>11%</div> </div>
2	B	155	<div> <div>58%</div> <div>92%</div> <div>8%</div> </div>
3	C	209	<div> <div>58%</div> <div>89%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	430	
5	E	214	
6	F	432	
7	G	699	
8	H	318	
9	I	176	
10	J	175	
11	K	98	
12	L	605	
13	M	458	
14	N	346	
15	O	320	
16	P	342	
17	Q	129	
18	R	96	
19	S	87	
20	T	85	
21	U	86	
22	V	115	
23	W	115	
24	X	171	
25	Y	141	
26	Z	141	
27	a	70	
28	b	83	

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Mol	Chain	Length	Quality of chain
29	c	49	<div> <div>57%</div> <div>84%</div> <div>16%</div> </div>
30	d	119	<div> <div>59%</div> <div>88%</div> <div>12%</div> </div>
31	e	99	<div> <div>67%</div> <div>95%</div> <div>5%</div> </div>
32	f	57	<div> <div>72%</div> <div>82%</div> <div>18%</div> </div>
33	g	100	<div> <div>60%</div> <div>82%</div> <div>18%</div> </div>
34	h	138	<div> <div>53%</div> <div>95%</div> <div>5%</div> </div>
35	u	128	<div> <div>78%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
36	j	71	<div> <div>93%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
37	k	81	<div> <div>95%</div> <div>79%</div> <div>21%</div> </div>
38	l	156	<div> <div>86%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
39	m	128	<div> <div>80%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
40	n	172	<div> <div>80%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
41	o	122	<div> <div>79%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
42	p	173	<div> <div>65%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
43	q	145	<div> <div>57%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
44	v	113	<div> <div>32%</div> <div>80%</div> <div>5%</div> <div>15%</div> </div>
45	s	45	<div> <div>73%</div> <div>71%</div> <div>29%</div> </div>



## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 68568 atoms, of which 0 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	114	Total	C	N	O	S	0	0
			911	616	132	157	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	THR	conflict	UNP Q8WAB4

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1738	1120	298	317	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	conflict	UNP P17694



- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	2	0
			3347	2111	598	618	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	699	Total	C	N	O	S	1	0
			5366	3362	934	1030	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	1	0
			2517	1687	386	421	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	167	THR	ILE	conflict	UNP Q6EMT1

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		



- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	605	Total	C	N	O	S	0	0
			4792	3189	736	825	42		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	458	Total	C	N	O	S	0	0
			3644	2430	569	607	38		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	346	Total	C	N	O	S	0	0
			2723	1811	415	455	42		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	conflict	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	1	0
			2768	1792	489	482	5		



- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			688	444	101	138	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	9	GLU	ASP	conflict	UNP Q9CR21

- Molecule 21 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		



- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	115	Total	C	N	O	S	0	0
			976	625	181	166	4		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	139	Total	C	N	O	S	0	0
			1022	652	175	189	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	ACE	-	acetylation	UNP Q8HXG6

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	49	Total	C	N	O	S	0	0
			414	273	70	71			

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	119	Total	C	N	O	S	0	0
			988	643	171	170	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	99	Total	C	N	O	S	0	0
			829	523	158	142	6		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	100	Total	C	N	O	S	0	0
			839	539	139	157	4		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		



- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	u	128	Total	C	N	O	S	0	0
			1097	722	191	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	0	ACE	-	acetylation	UNP Q02367

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	128	Total	C	N	O	0	0
			1067	684	188	195		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.



Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	173	Total	C	N	O	S	0	0
			1453	910	268	267	8		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	96	Total	C	N	O	S	0	0
			776	490	144	139	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	0	ACE	-	acetylation	UNP Q05752

- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

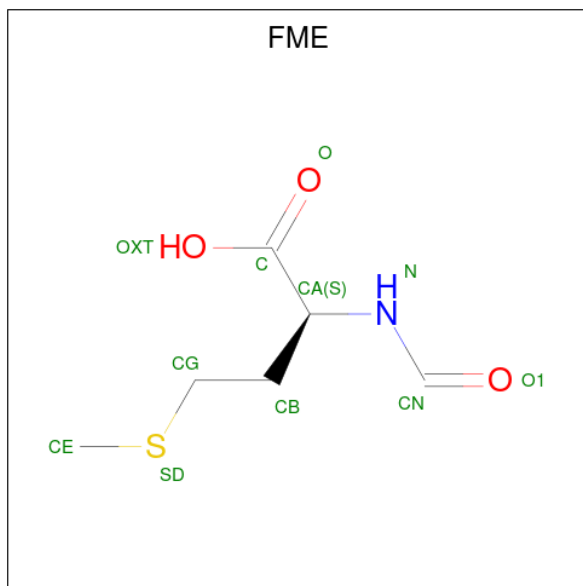
Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	45	Total	C	N	O	S	1	0
			391	244	71	75	1		



There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	57	ASP	GLU	conflict	UNP P56181

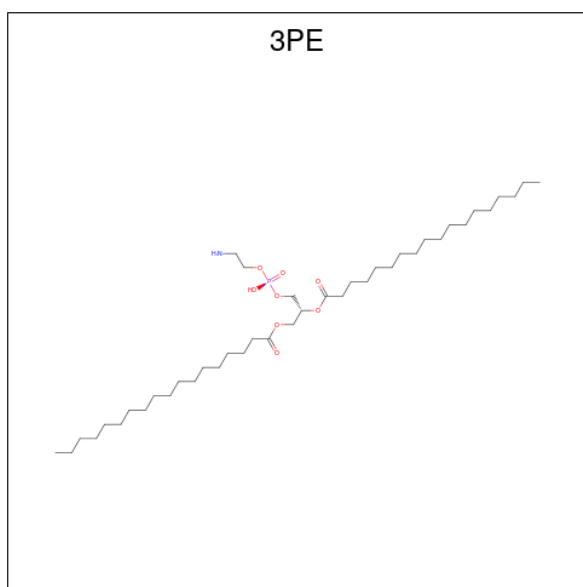
- Molecule 46 is N-FORMYLMETHIONINE (CCD ID: FME) (formula:  $C_6H_{11}NO_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	L	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	M	1	Total	C	N	O	S	0
			10	6	1	2	1	
46	N	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	K	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
47	L	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
47	N	1	Total	C	N	O	P	0
			45	35	1	8	1	
47	O	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	O	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	P	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
47	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	Y	1	Total	C	N	O	P	0
			33	23	1	8	1	

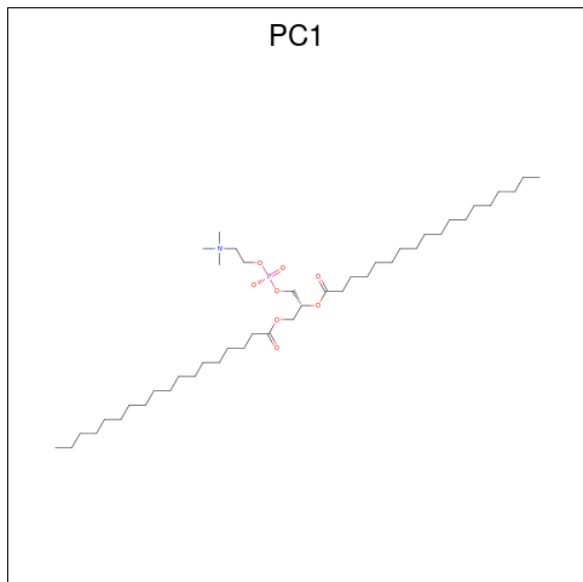
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Mol	Chain	Residues	Atoms					AltConf
47	Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
47	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	j	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 48 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
48	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
48	H	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	H	1	Total	C	N	O	P	0
			48	38	1	8	1	

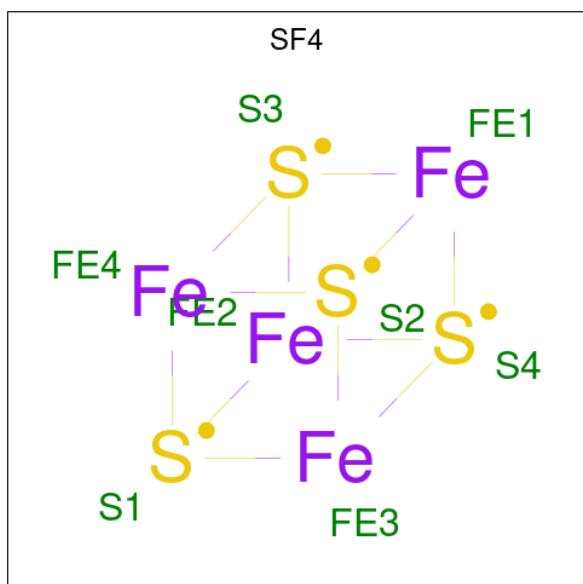
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Mol	Chain	Residues	Atoms					AltConf
48	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
48	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
48	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
48	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
48	m	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			AltConf
49	B	1	Total	Fe	S	0
			8	4	4	
49	F	1	Total	Fe	S	0
			8	4	4	
49	G	1	Total	Fe	S	0
			8	4	4	
49	G	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	

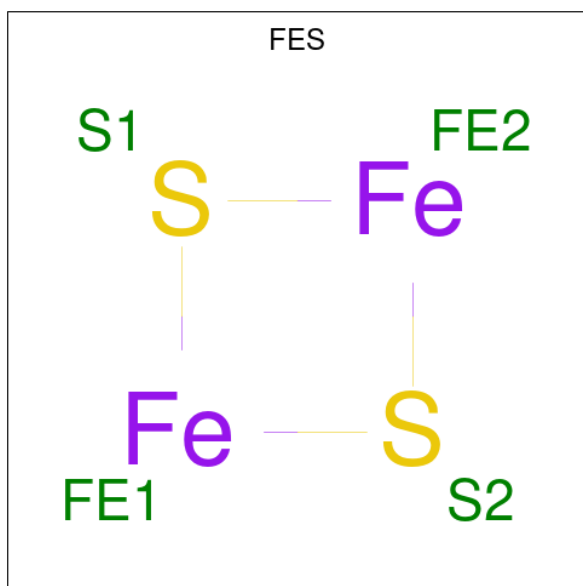
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Mol	Chain	Residues	Atoms			AltConf
49	I	1	Total	Fe	S	0
			8	4	4	

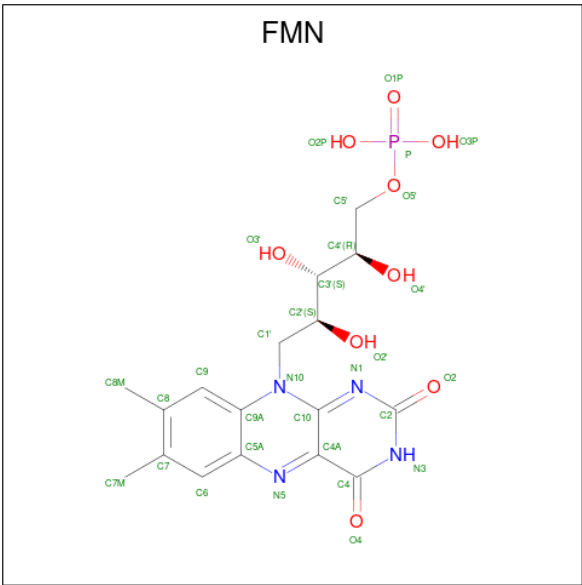
- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
50	E	1	Total	Fe	S	0
			4	2	2	
50	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 51 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



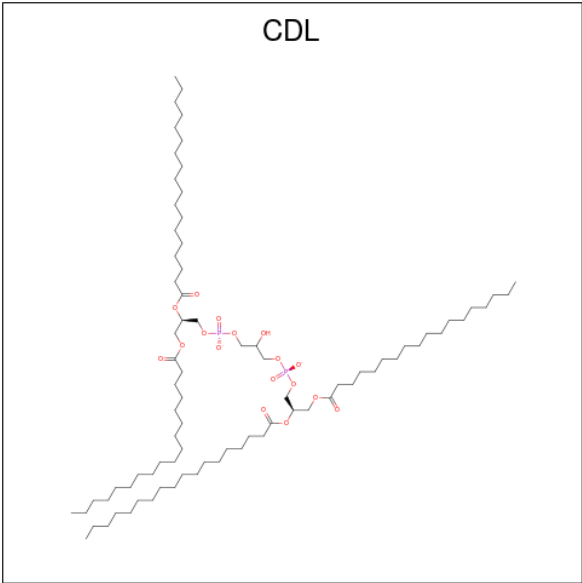


Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
52	G	1	Total	K	0
			1	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



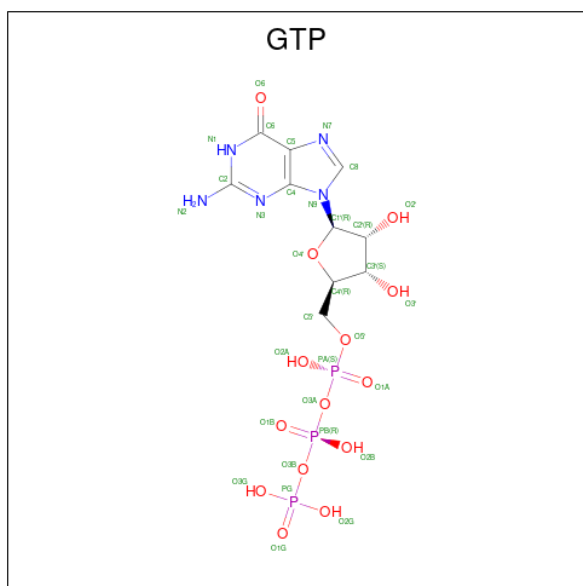


Mol	Chain	Residues	Atoms				AltConf
53	H	1	Total	C	O	P	0
			51	32	17	2	
53	L	1	Total	C	O	P	0
			76	57	17	2	
53	M	1	Total	C	O	P	0
			86	67	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			80	61	17	2	
53	v	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	O	1	Total	Mg	0
			1	1	

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

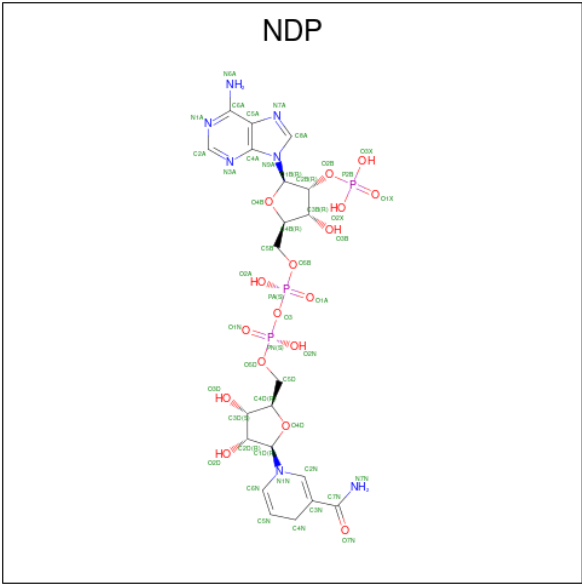


Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest")



by depositor).



Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

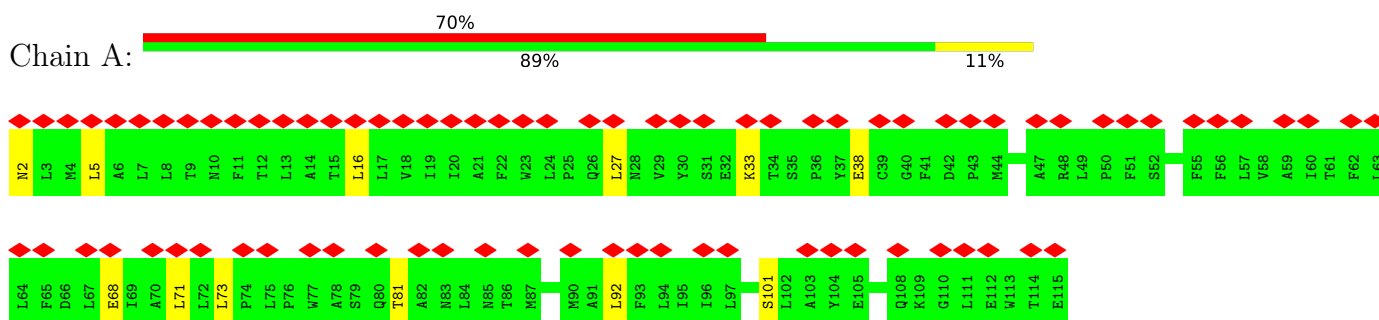
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	



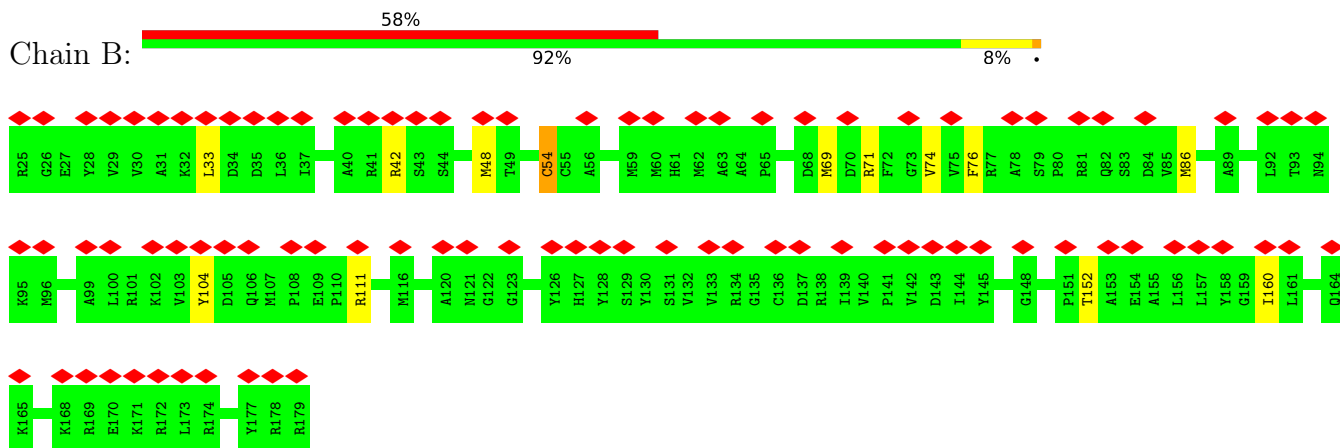
### 3 Residue-property plots

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

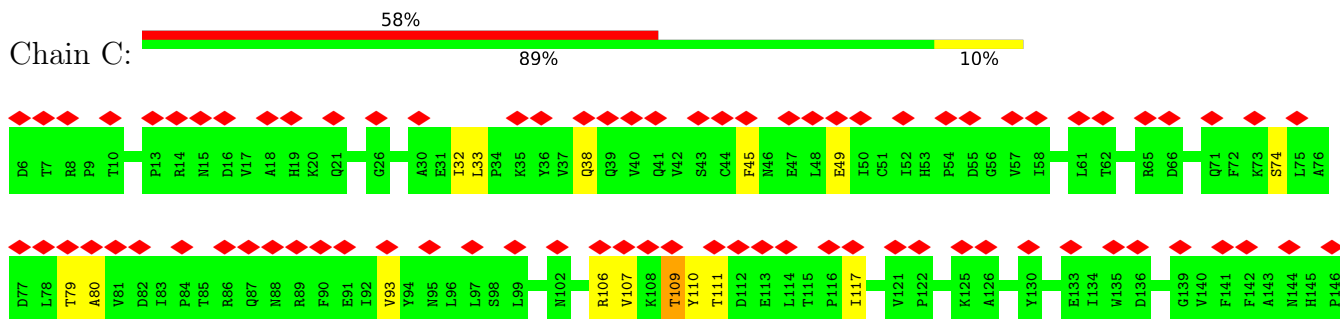
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



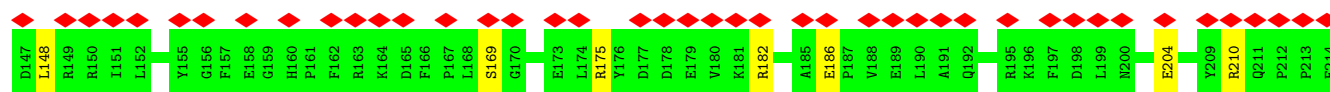
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



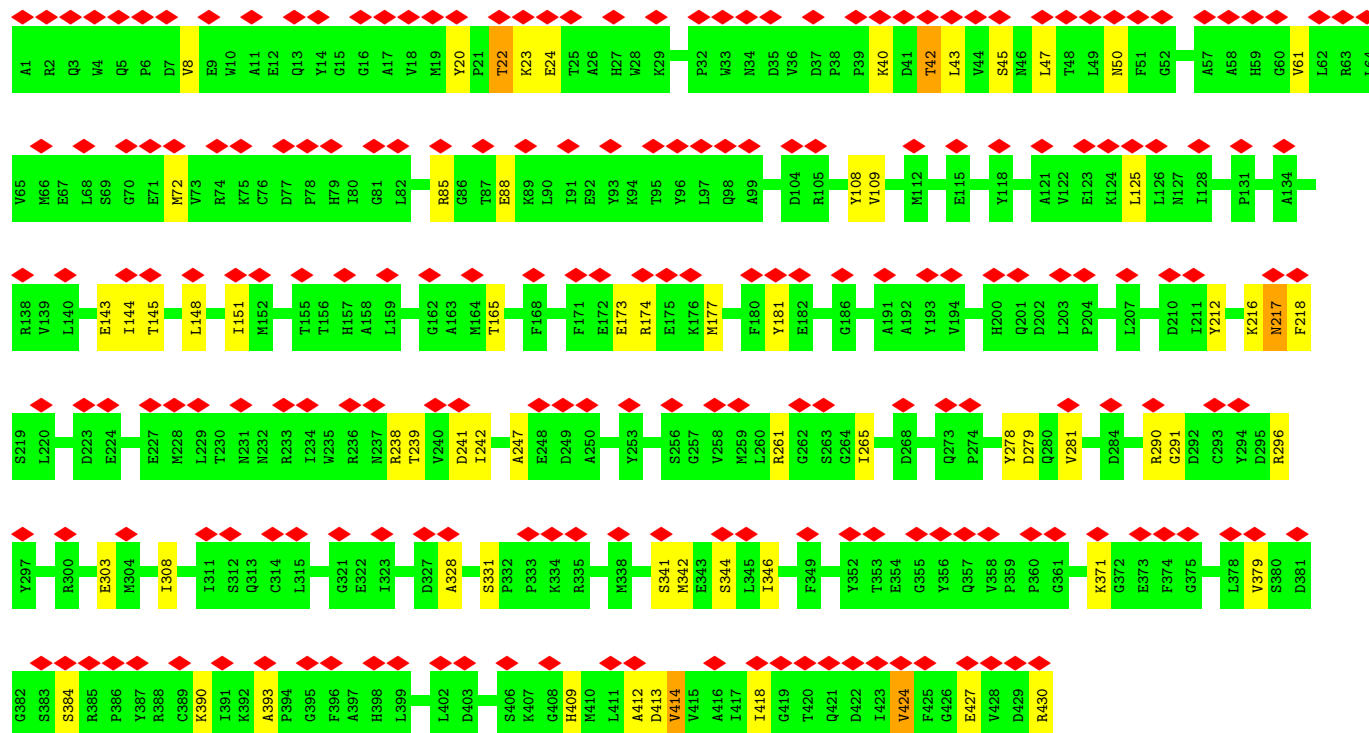
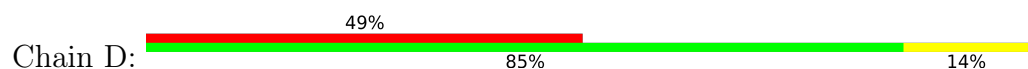
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



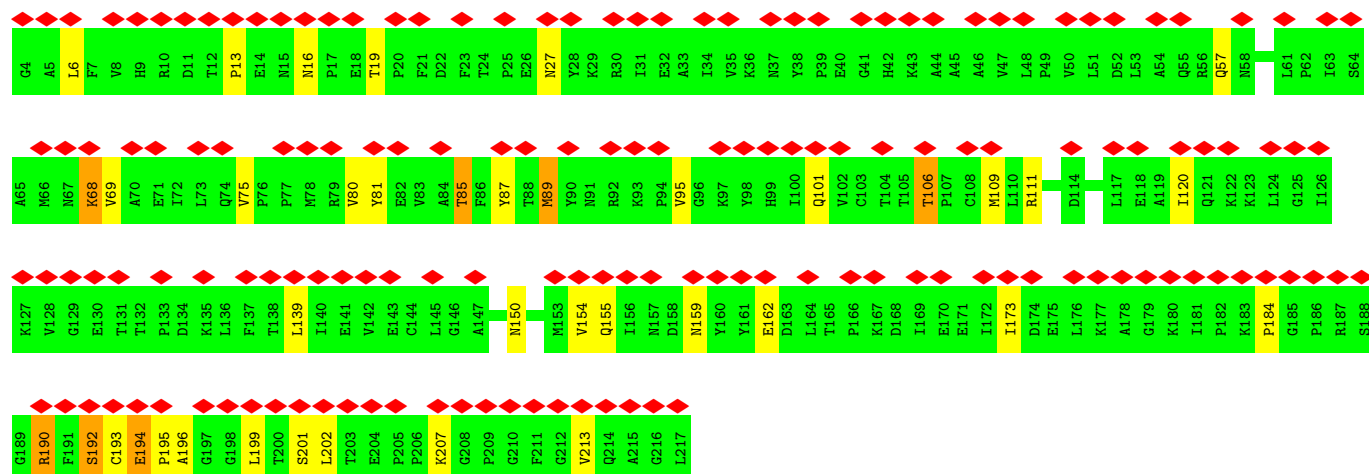
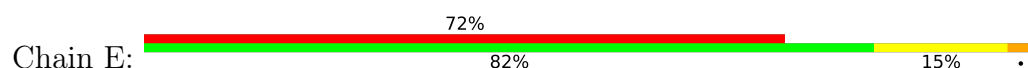




- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial




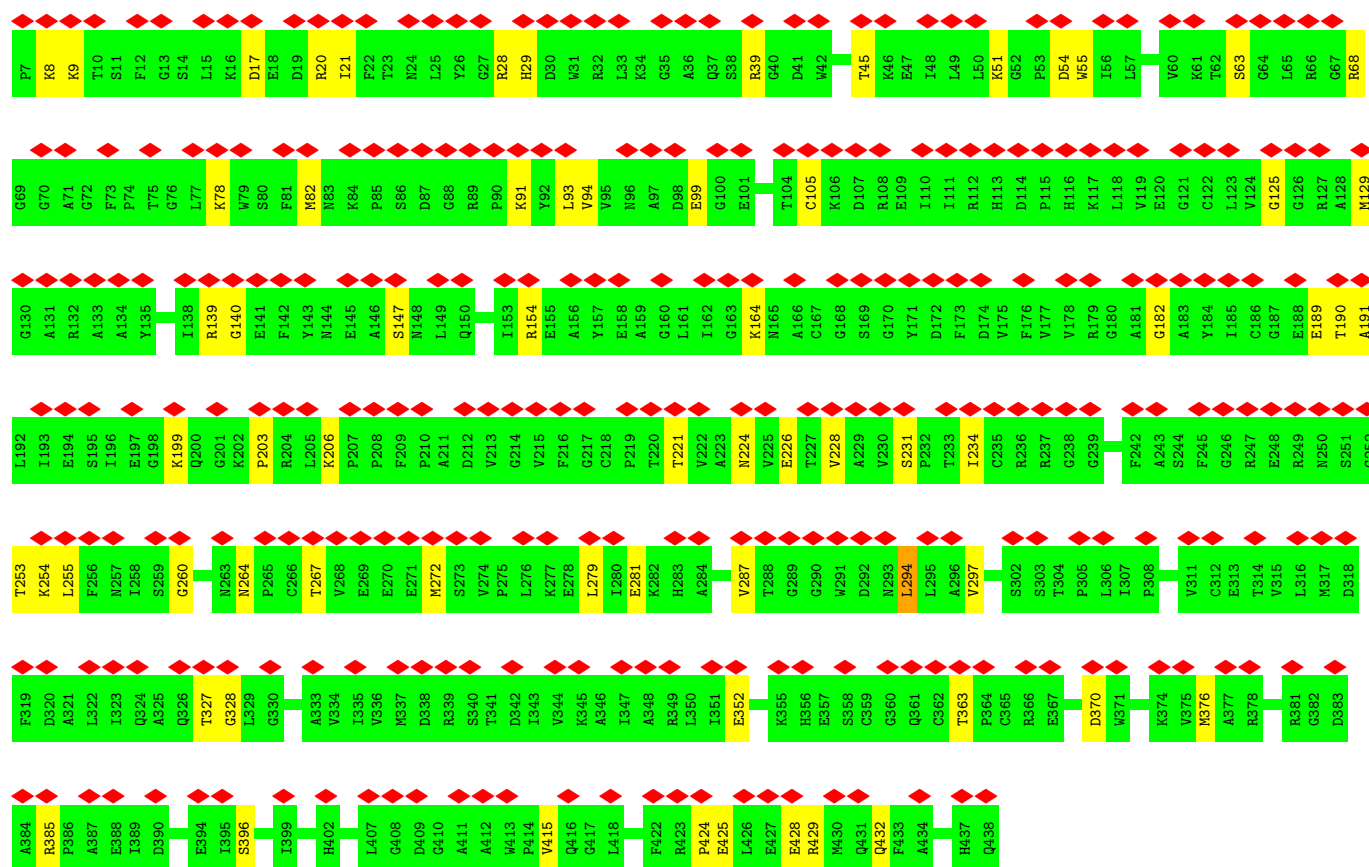
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial




- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

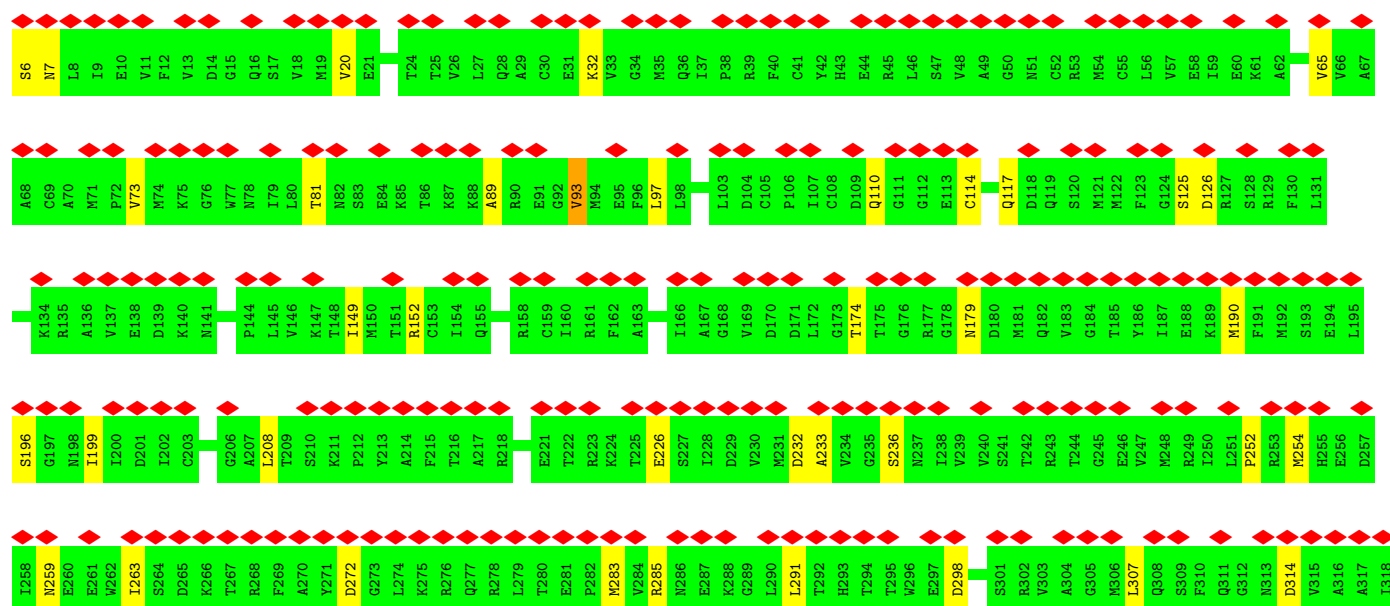


Chain F: 

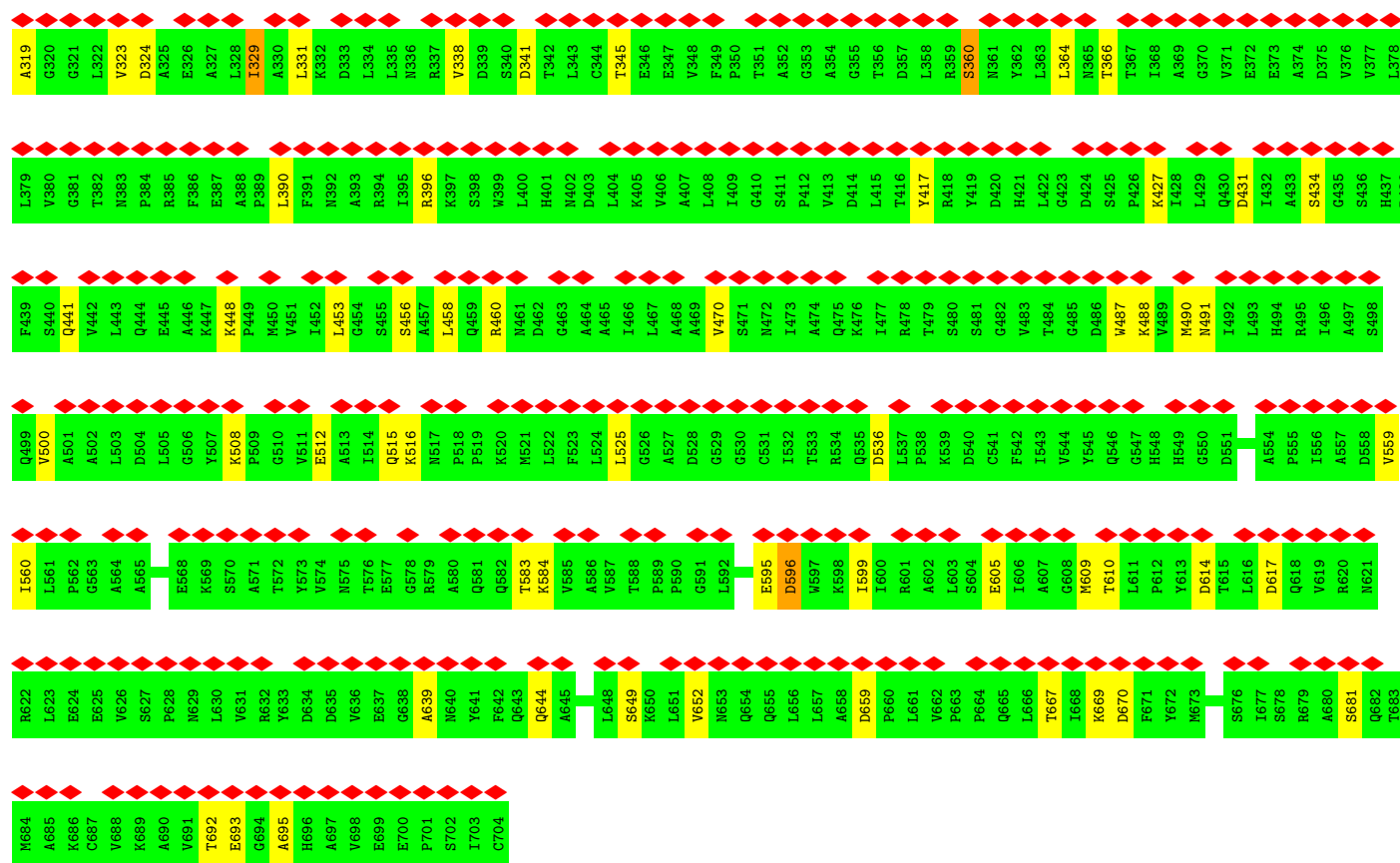


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

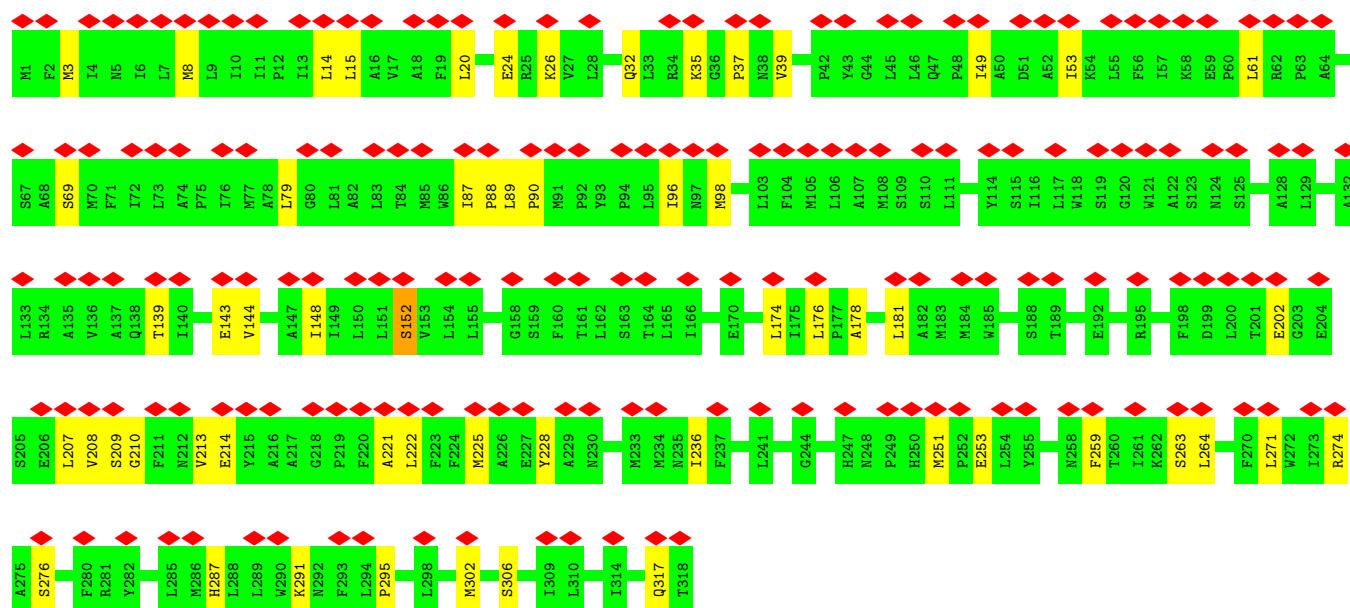
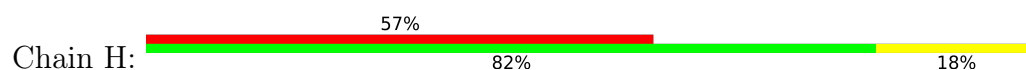
Chain G: 





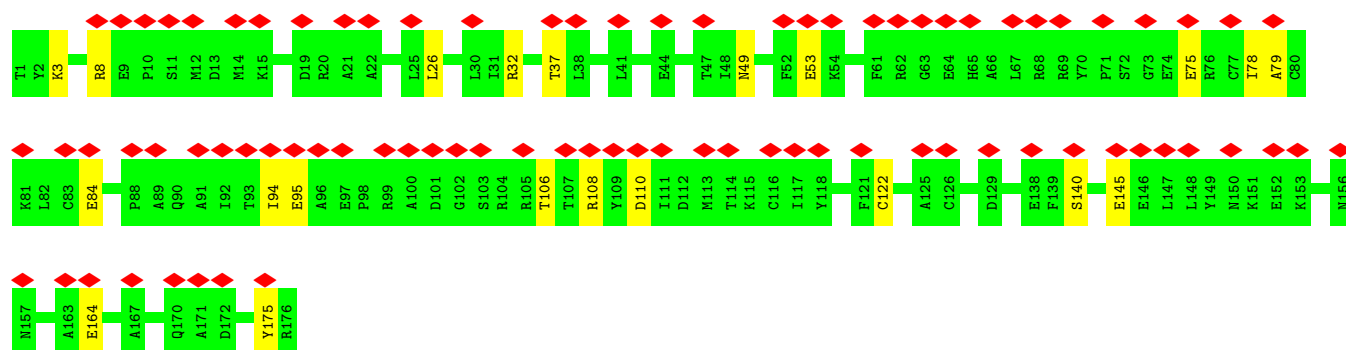
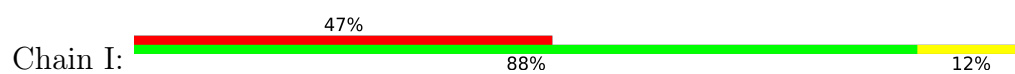


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

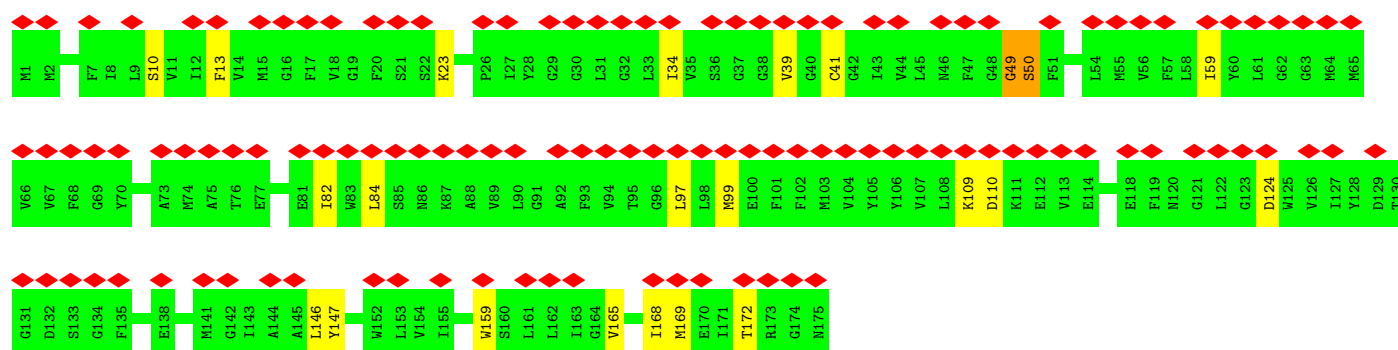
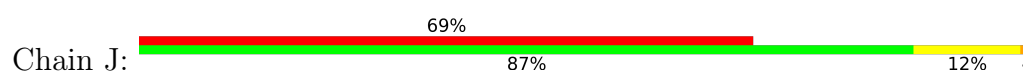


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

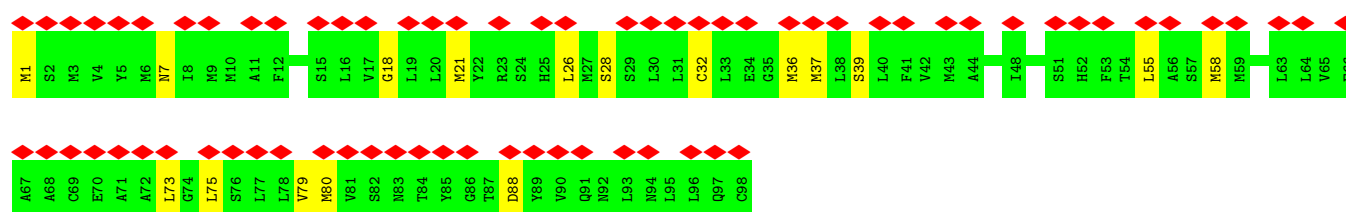
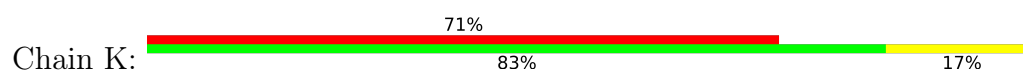




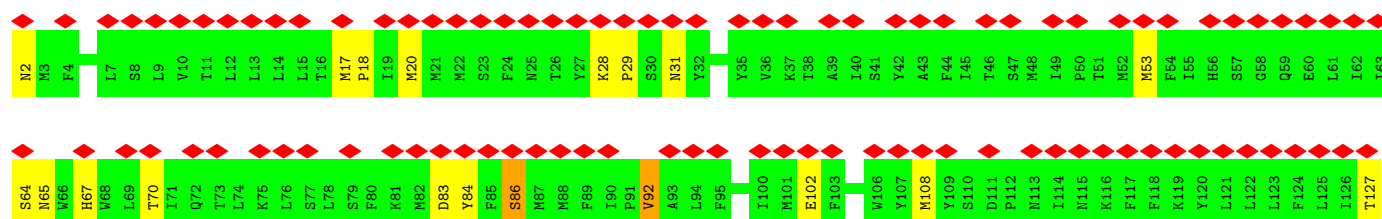
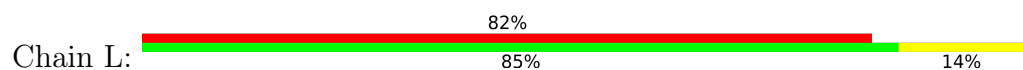
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



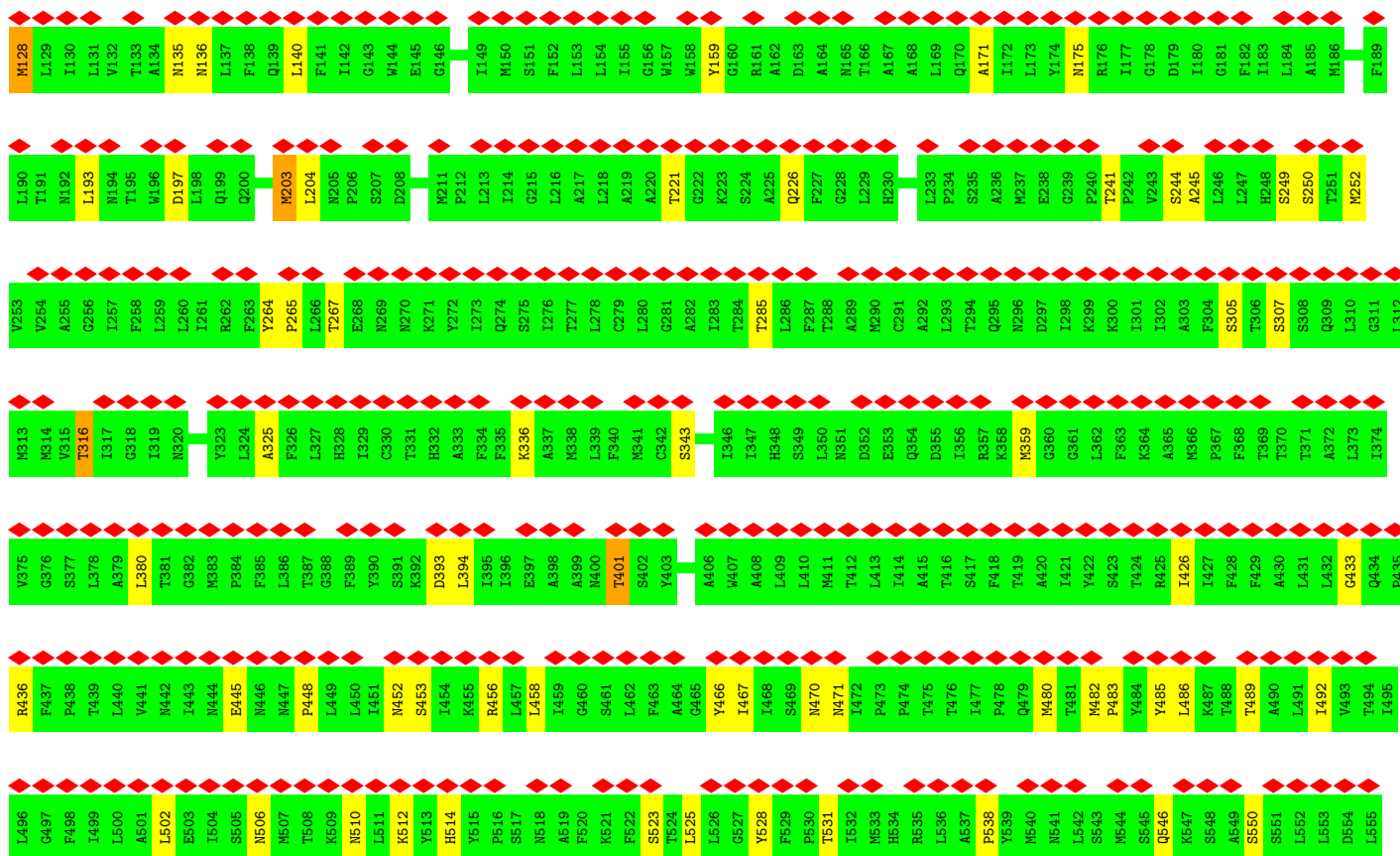
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



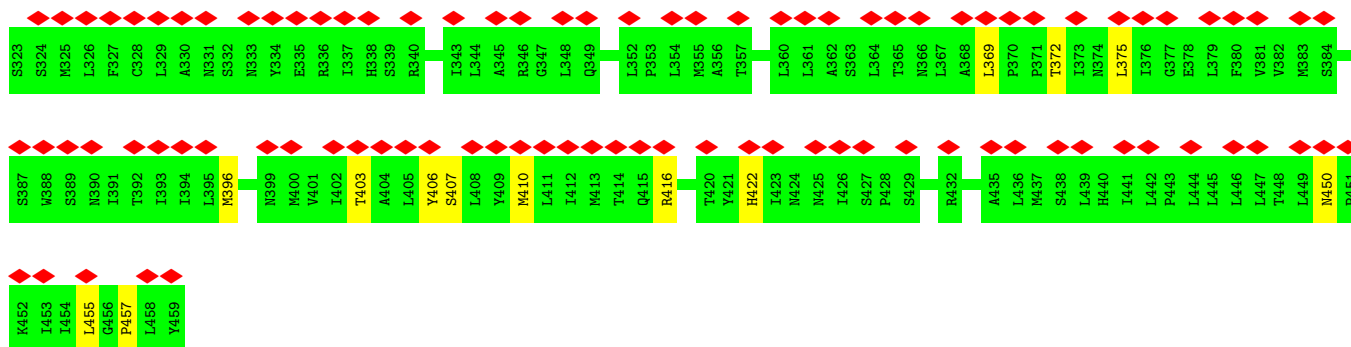
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



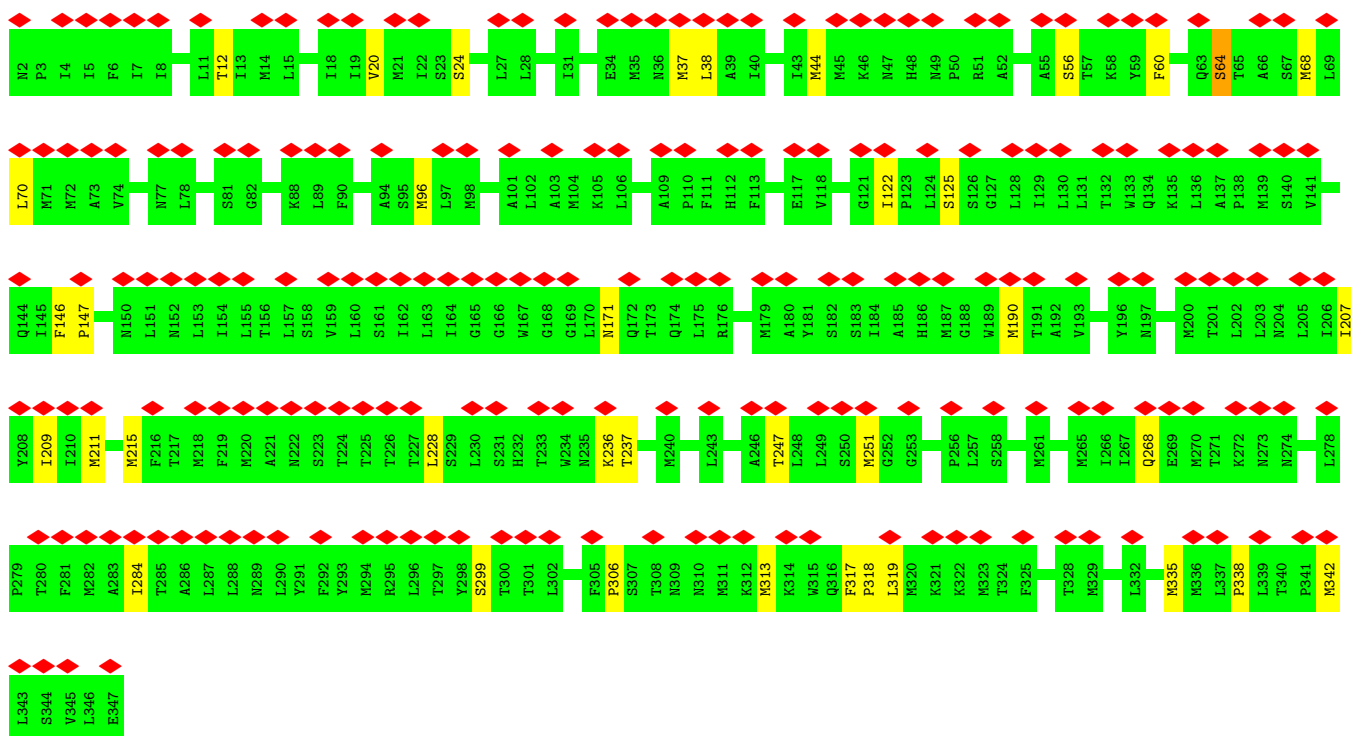
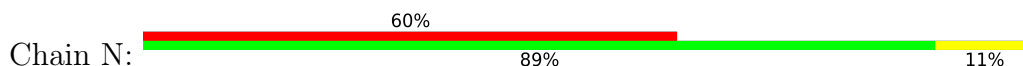




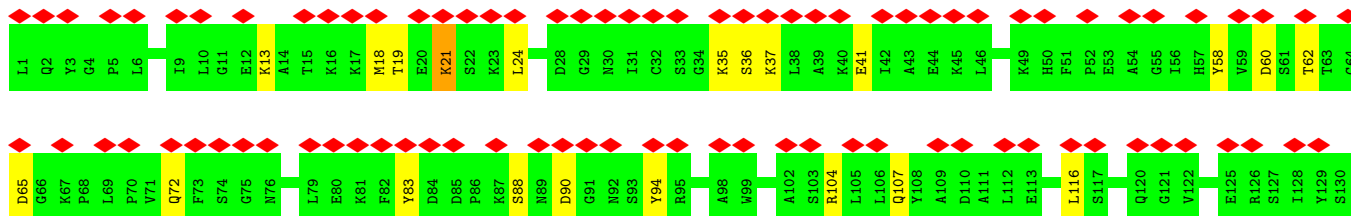
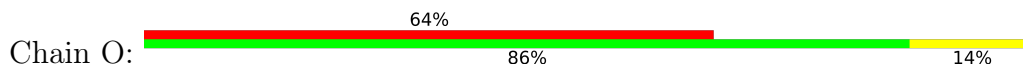




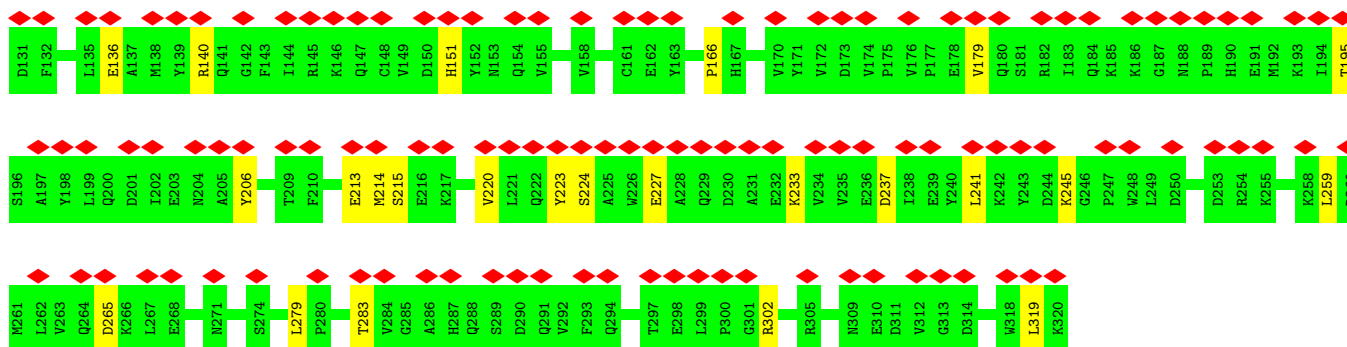
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



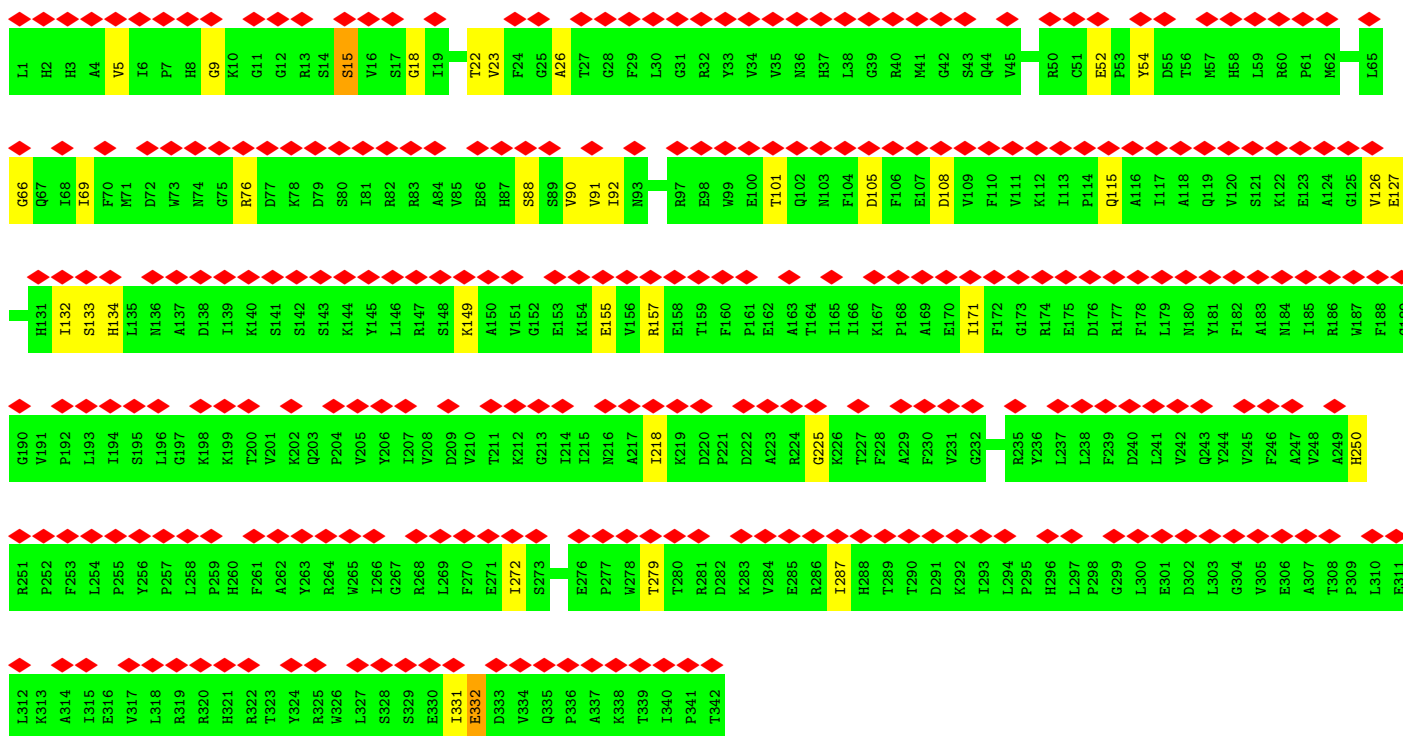
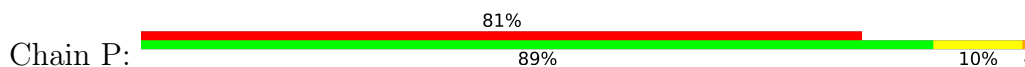
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



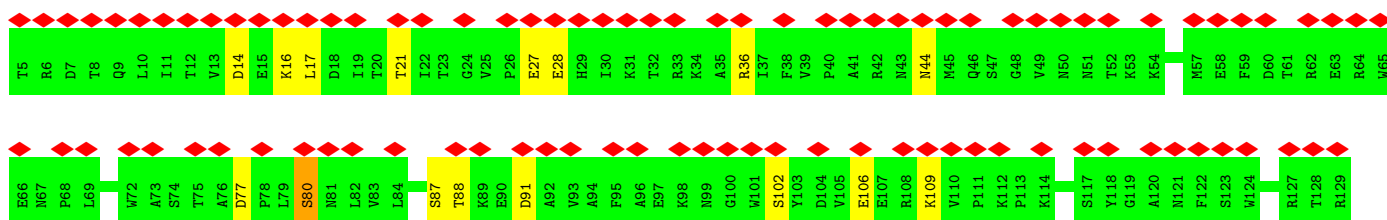
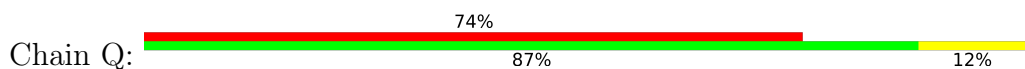




- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



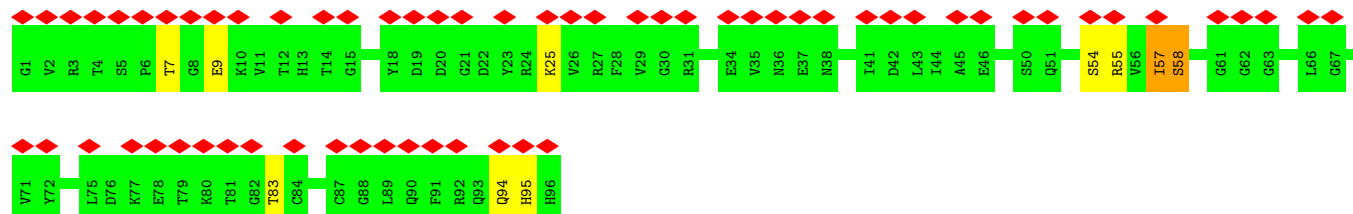
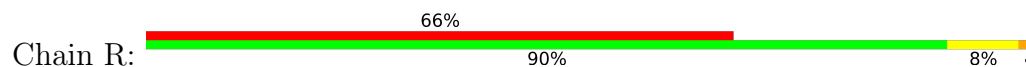
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



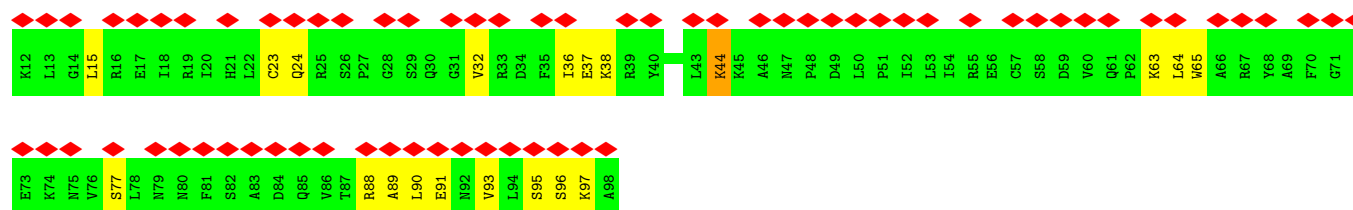
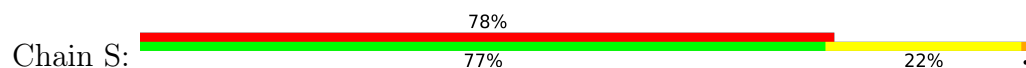




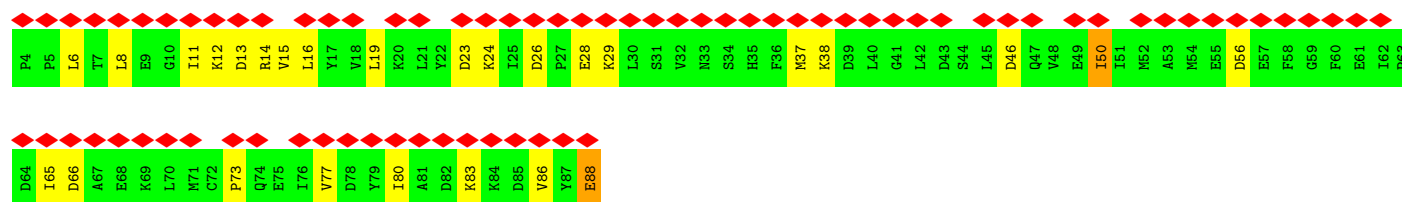
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



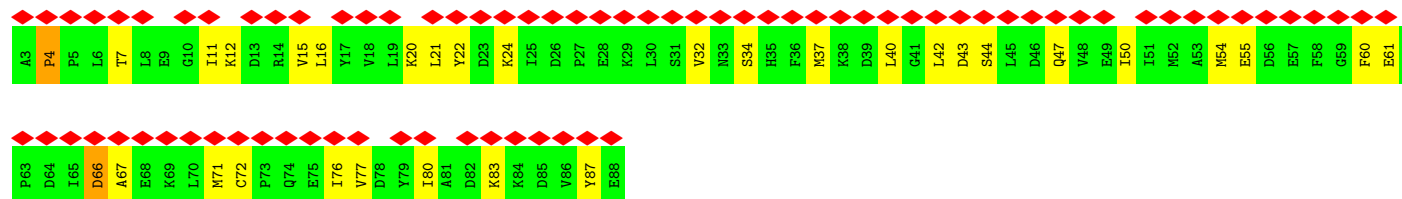
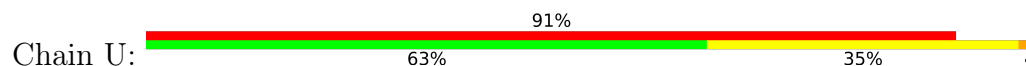
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



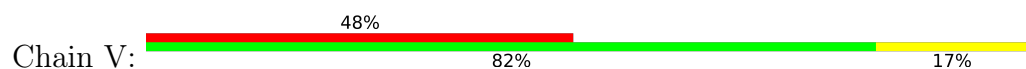
- Molecule 20: Acyl carrier protein, mitochondrial



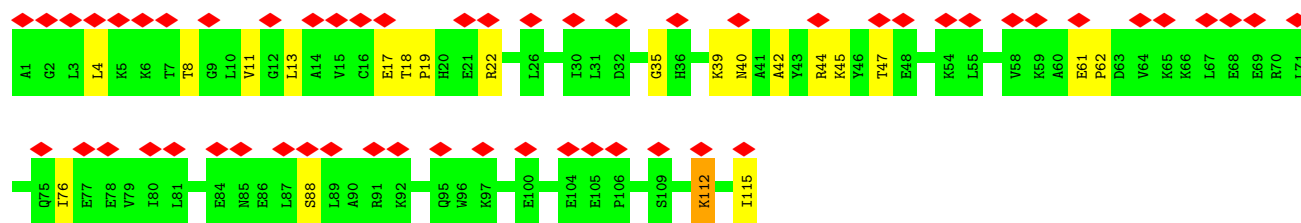
- Molecule 21: Acyl carrier protein, mitochondrial



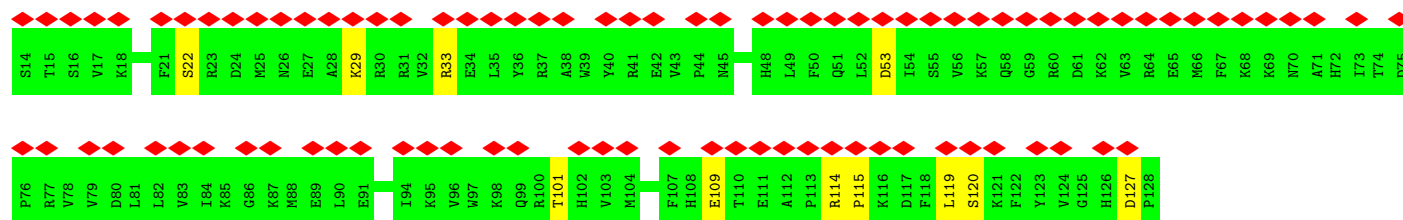
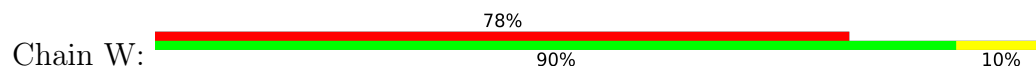
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



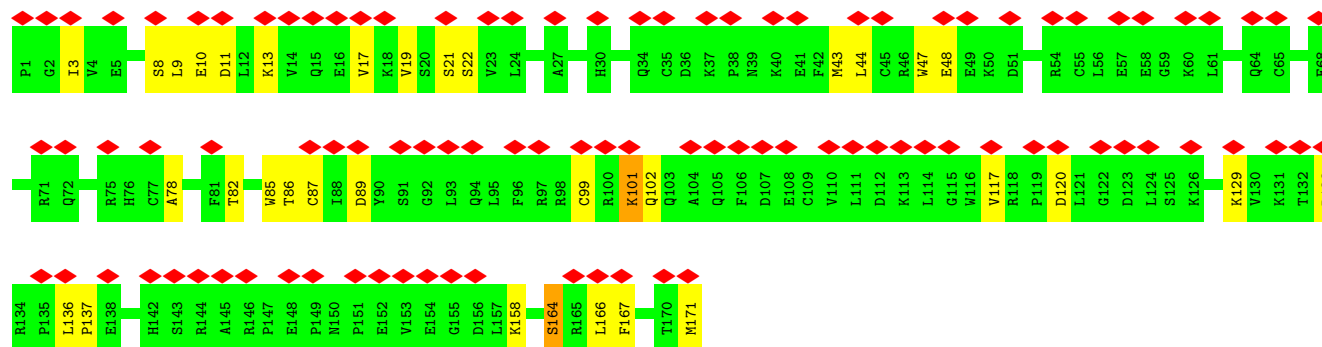
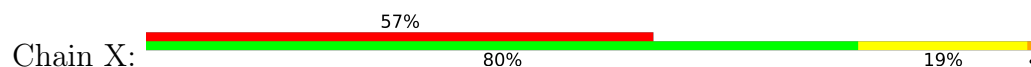




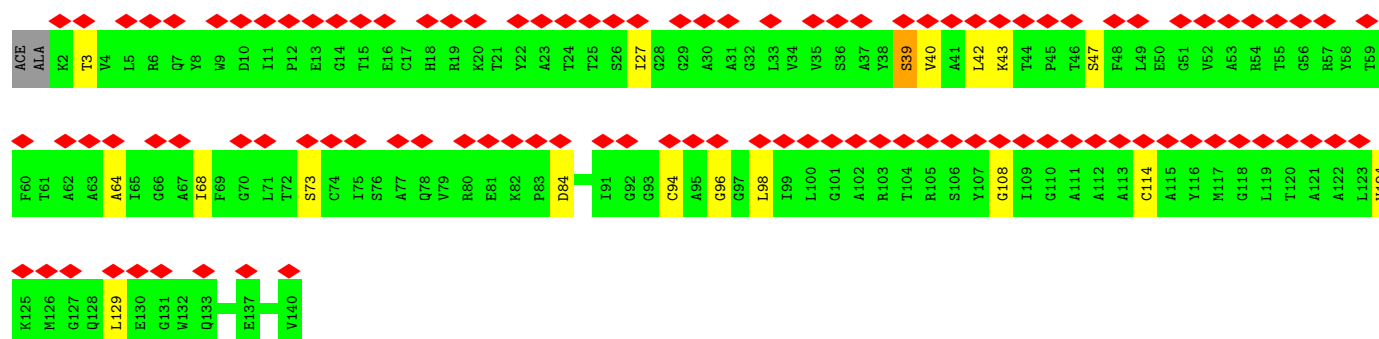
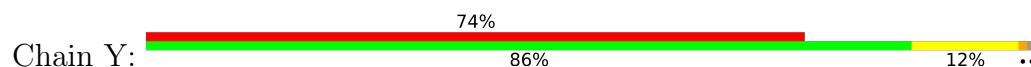
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

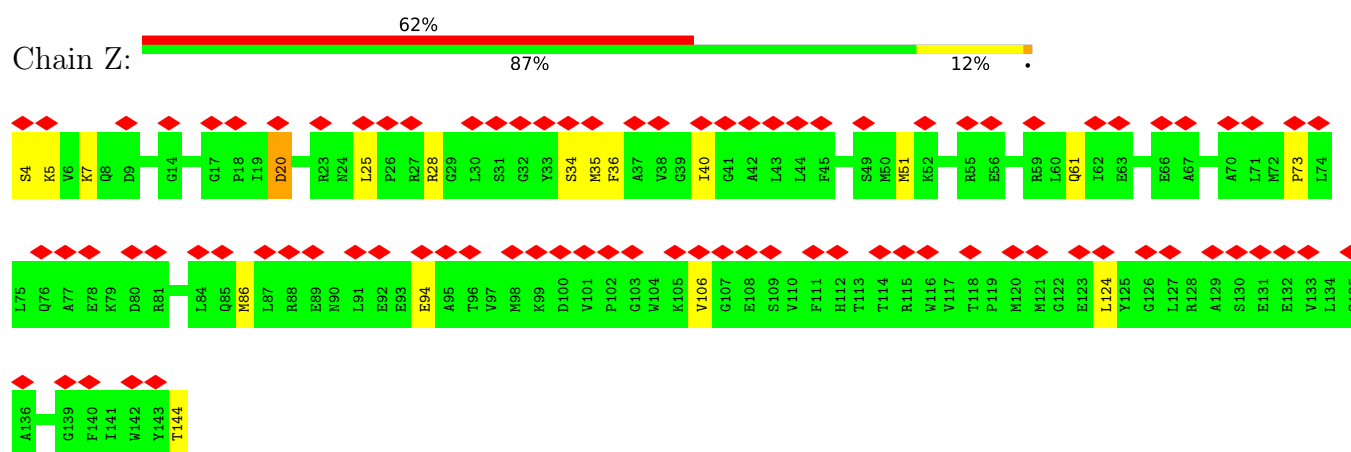


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

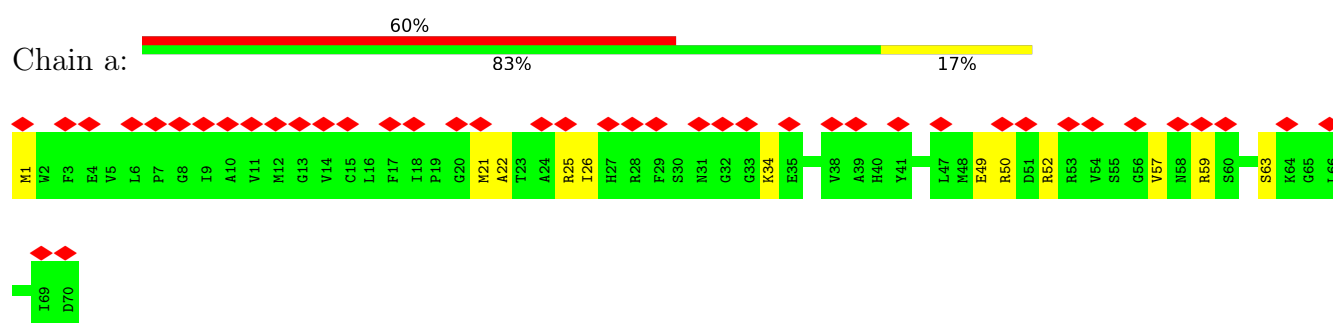


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

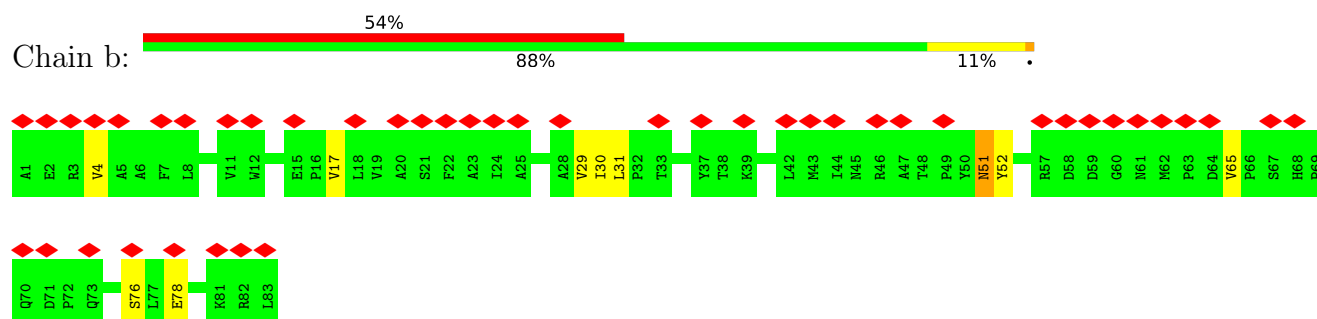




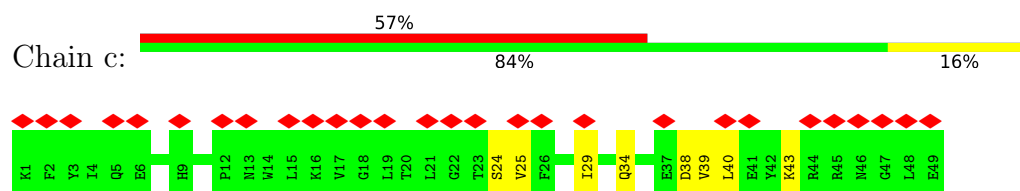
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



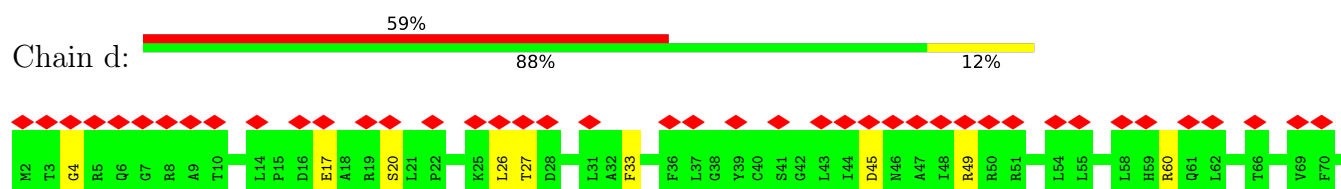
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



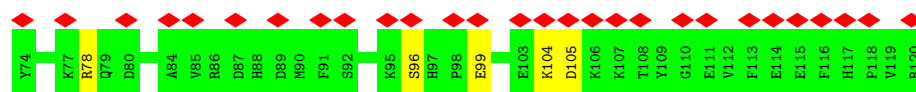
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



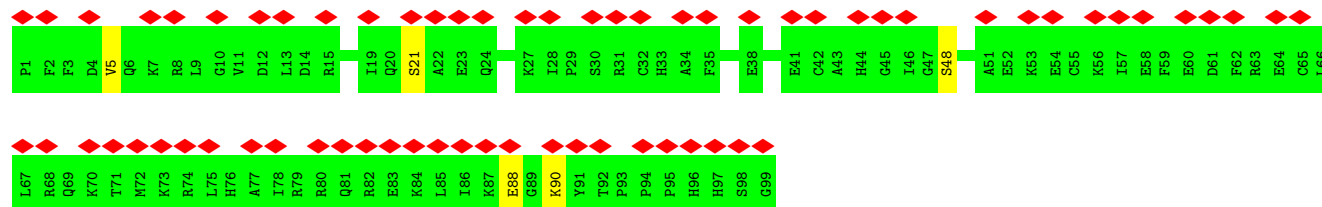
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



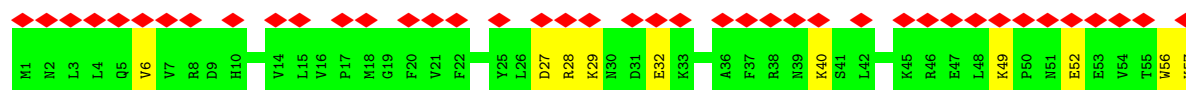
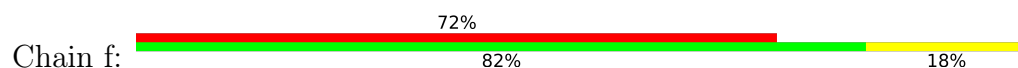




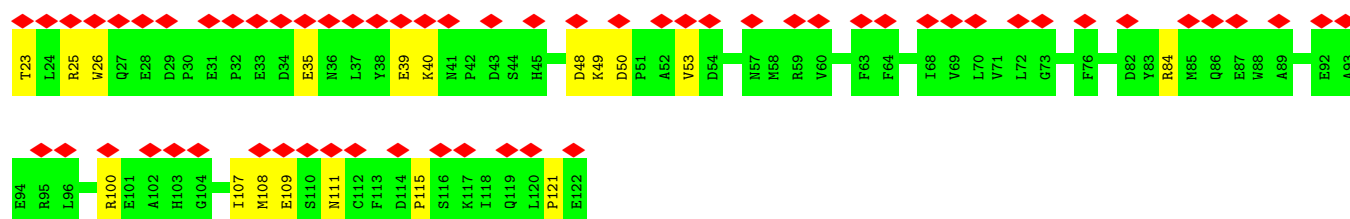
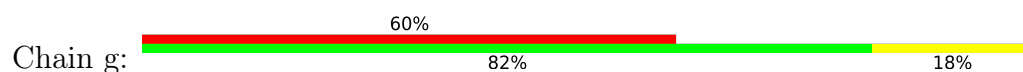
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



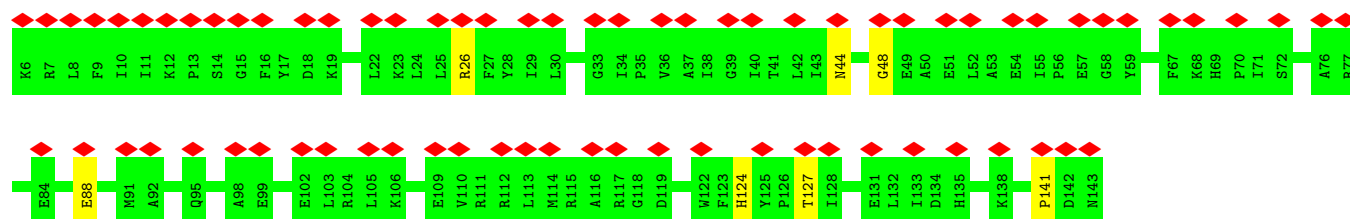
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



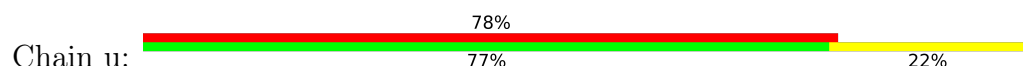
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



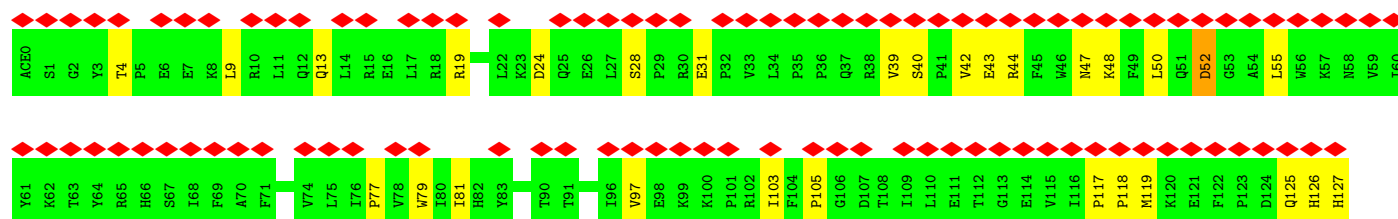
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



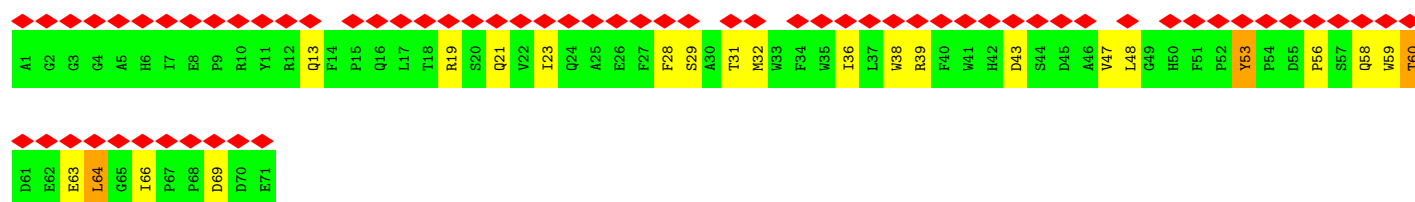
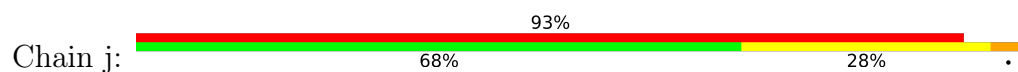
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



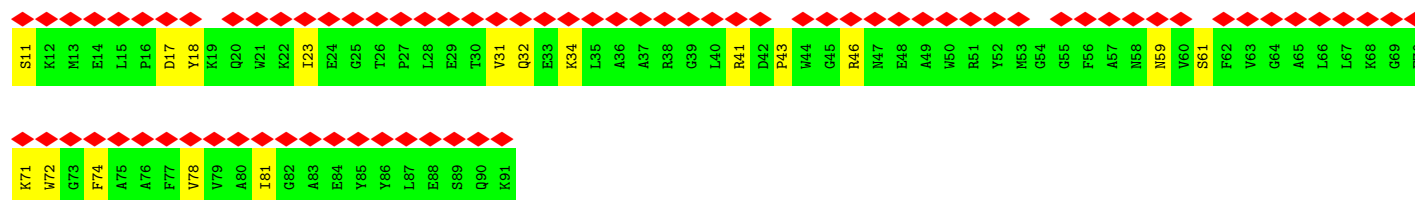
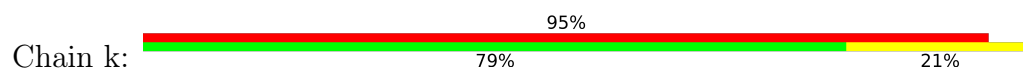




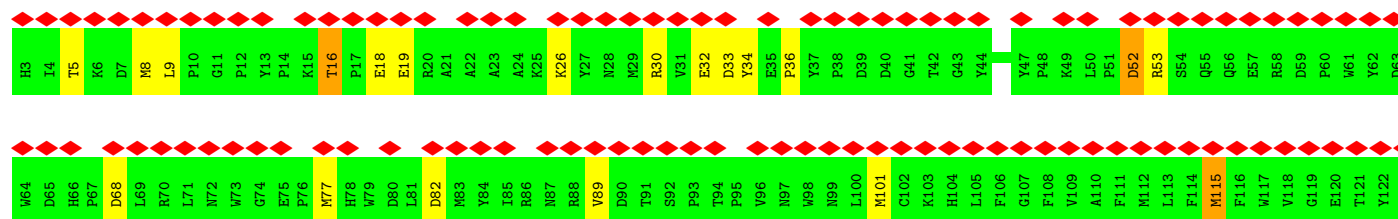
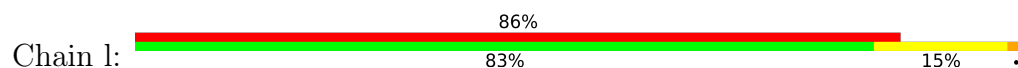
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



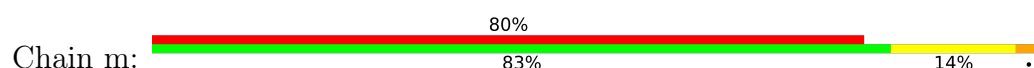
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



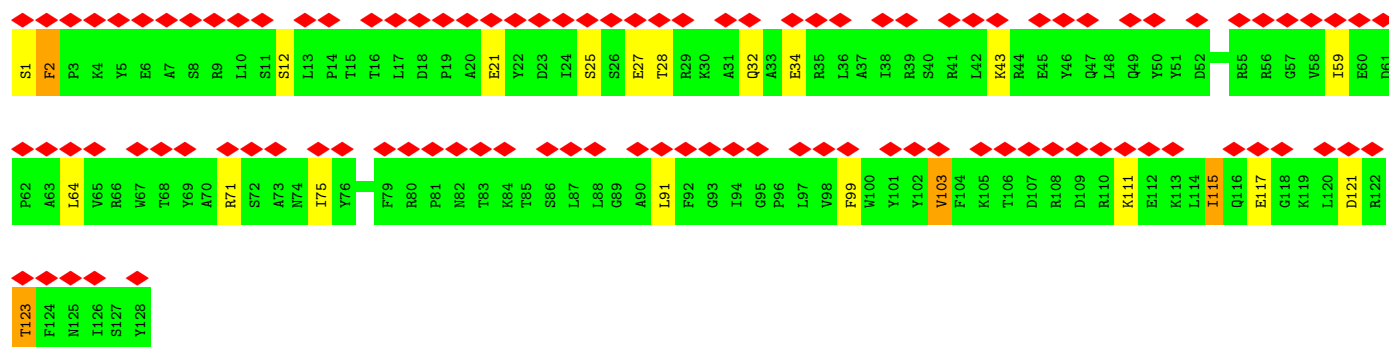
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



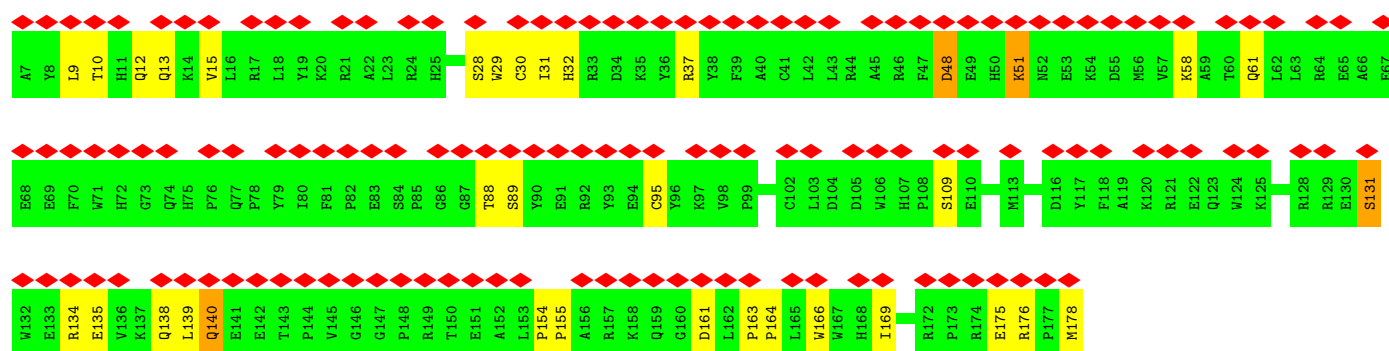
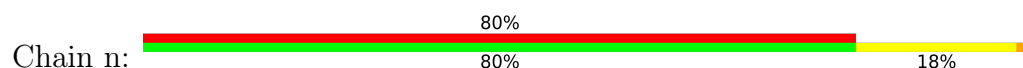
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



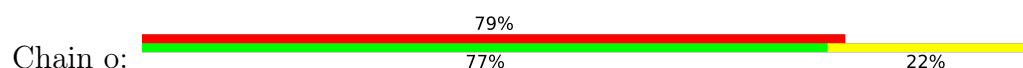




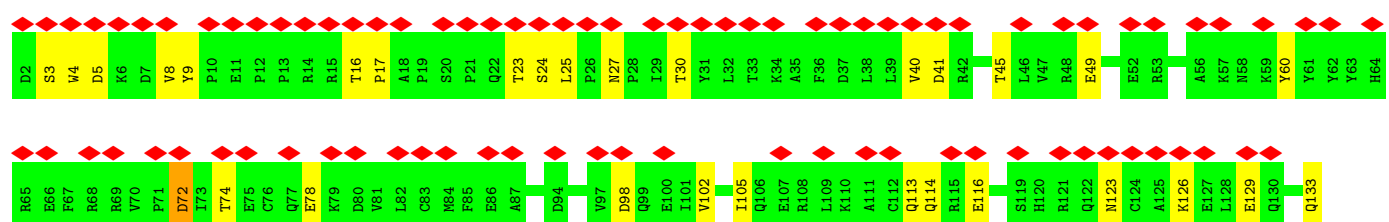
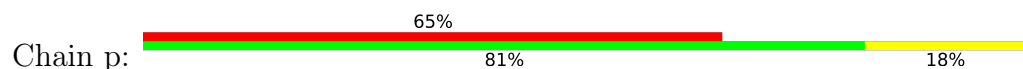
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



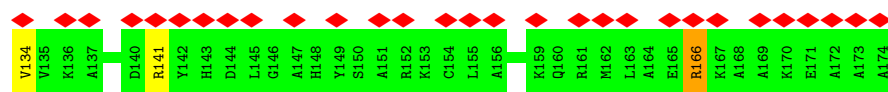
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



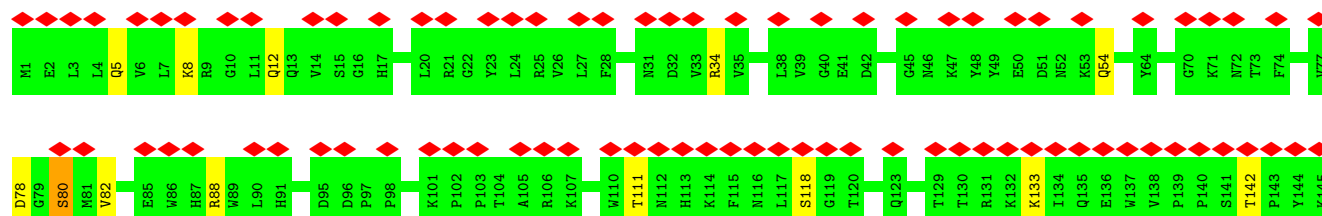
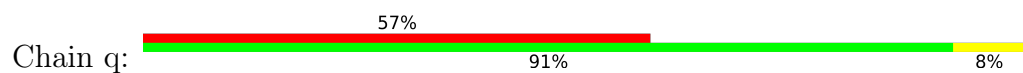
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



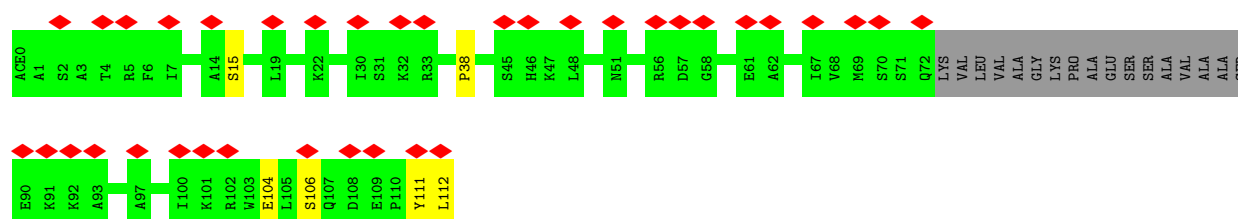
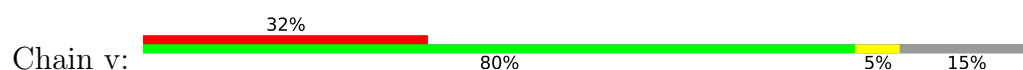




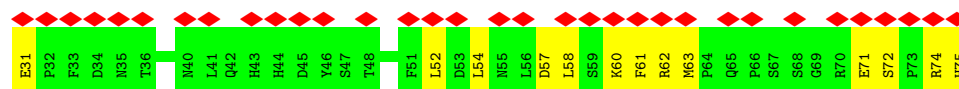
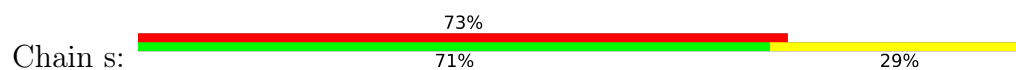
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 45: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217828	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.001	Depositor
Minimum map value	-0.584	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	654.0, 654.0, 654.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ACE, ZN, CDL, 2MR, FME, PC1, FES, K, NDP, MG, SF4, 3PE, FMN

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	A	0.14	0/936	0.35	0/1281
2	B	0.14	0/1272	0.31	0/1720
3	C	0.13	0/1789	0.32	0/2436
4	D	0.13	0/3537	0.32	0/4794
5	E	0.15	0/1699	0.39	1/2312 (0.0%)
6	F	0.13	0/3424	0.35	0/4627
7	G	0.13	0/5457	0.36	0/7397
8	H	0.16	0/2579	0.39	0/3524
9	I	0.13	0/1445	0.31	0/1956
10	J	0.19	0/1370	0.49	2/1859 (0.1%)
11	K	0.18	0/745	0.45	0/1008
12	L	0.14	0/4920	0.39	0/6694
13	M	0.12	0/3738	0.30	0/5097
14	N	0.14	0/2792	0.33	0/3800
15	O	0.14	0/2651	0.37	1/3587 (0.0%)
16	P	0.12	0/2847	0.31	0/3864
17	Q	0.11	0/1072	0.32	0/1449
18	R	0.13	0/753	0.32	0/1014
19	S	0.19	0/711	0.59	0/956
20	T	0.25	0/700	0.74	0/944
21	U	0.30	0/705	0.71	2/952 (0.2%)
22	V	0.14	0/948	0.36	0/1284
23	W	0.15	0/1000	0.37	0/1344
24	X	0.14	0/1439	0.38	0/1942
25	Y	0.21	0/1042	0.41	0/1414
26	Z	0.16	0/1181	0.37	1/1592 (0.1%)
27	a	0.19	0/584	0.47	0/786
28	b	0.18	0/672	0.46	0/923
29	c	0.24	0/427	0.52	0/579
30	d	0.16	0/1018	0.34	0/1375
31	e	0.17	0/850	0.43	0/1136
32	f	0.20	0/505	0.56	0/681



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g	0.19	0/865	0.48	0/1175
34	h	0.15	0/1188	0.34	0/1607
35	u	0.23	0/1134	0.53	0/1544
36	j	0.24	0/624	0.61	0/855
37	k	0.23	0/672	0.56	0/906
38	l	0.18	0/1369	0.49	1/1873 (0.1%)
39	m	0.21	0/1094	0.49	0/1480
40	n	0.16	0/1545	0.43	0/2092
41	o	0.23	0/1073	0.53	0/1437
42	p	0.16	0/1486	0.39	0/2004
43	q	0.11	0/1250	0.29	0/1698
44	v	0.19	0/795	0.40	0/1077
45	s	0.22	0/403	0.59	0/545
All	All	0.16	0/68306	0.40	8/92620 (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
5	E	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	4	PRO	CA-N-CD	-8.20	100.52	112.00
21	U	4	PRO	N-CD-CG	-6.69	93.17	103.20
10	J	49	GLY	CA-C-N	5.59	132.21	121.54
10	J	49	GLY	C-N-CA	5.59	132.21	121.54
5	E	202	LEU	CA-CB-CG	5.40	135.21	116.30
15	O	21	LYS	CB-CG-CD	5.33	123.56	111.30
26	Z	51	MET	CA-CB-CG	5.17	124.44	114.10
38	l	115	MET	CB-CG-SD	5.05	127.85	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	194	GLU	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	911	0	941	6	0
2	B	1241	0	1251	9	0
3	C	1738	0	1685	10	0
4	D	3459	0	3404	35	0
5	E	1659	0	1664	19	0
6	F	3347	0	3297	37	0
7	G	5366	0	5378	47	0
8	H	2517	0	2631	37	0
9	I	1414	0	1370	11	0
10	J	1345	0	1352	12	0
11	K	745	0	784	11	0
12	L	4792	0	4949	49	0
13	M	3644	0	3841	31	0
14	N	2723	0	2901	21	0
15	O	2589	0	2566	21	0
16	P	2768	0	2782	18	0
17	Q	1049	0	1045	10	0
18	R	740	0	714	4	0
19	S	700	0	719	12	0
20	T	688	0	685	19	0
21	U	693	0	689	23	0
22	V	928	0	972	12	0
23	W	976	0	991	5	0
24	X	1402	0	1379	23	0
25	Y	1022	0	1030	10	0
26	Z	1152	0	1151	12	0
27	a	569	0	568	8	0
28	b	651	0	662	5	0
29	c	414	0	415	4	0
30	d	988	0	975	10	0
31	e	829	0	829	1	0
32	f	492	0	501	6	0
33	g	839	0	790	12	0
34	h	1154	0	1168	6	0
35	u	1097	0	1108	15	0
36	j	597	0	536	16	0
37	k	653	0	639	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	1314	0	1210	22	0
39	m	1067	0	1067	14	0
40	n	1492	0	1438	22	0
41	o	1048	0	1018	22	0
42	p	1453	0	1425	21	0
43	q	1209	0	1182	4	0
44	v	776	0	782	3	0
45	s	391	0	361	9	0
46	A	10	0	10	0	0
46	L	10	0	10	0	0
46	M	10	0	10	0	0
46	N	10	0	10	0	0
47	A	47	0	71	2	0
47	H	36	0	46	1	0
47	K	44	0	62	2	0
47	L	140	0	211	0	0
47	M	50	0	77	1	0
47	N	45	0	64	0	0
47	O	99	0	155	4	0
47	P	35	0	44	0	0
47	Y	161	0	195	4	0
47	d	49	0	75	3	0
47	j	44	0	65	3	0
47	m	41	0	59	1	0
48	A	68	0	84	2	0
48	B	94	0	136	3	0
48	H	83	0	117	3	0
48	I	98	0	150	2	0
48	M	44	0	65	2	0
48	Y	35	0	44	0	0
48	d	39	0	52	6	0
48	m	46	0	66	1	0
49	B	8	0	0	0	0
49	F	8	0	0	0	0
49	G	16	0	0	0	0
49	I	16	0	0	0	0
50	E	4	0	0	0	0
50	G	4	0	0	0	0
51	F	31	0	19	2	0
52	G	1	0	0	0	0
53	H	51	0	46	1	0
53	L	76	0	99	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	M	86	0	118	8	0
53	d	65	0	77	5	0
53	h	80	0	104	3	0
53	v	61	0	66	1	0
54	O	1	0	0	0	0
55	O	32	0	12	3	0
56	P	48	0	26	0	0
57	R	1	0	0	0	0
All	All	68568	0	69290	670	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 5.

All (670) 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)
21:U:24:LYS:HG2	21:U:42:LEU:HD21	1.71	0.72
6:F:28:ARG:O	6:F:29:HIS:ND1	2.17	0.71
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.74	0.70
4:D:8:VAL:HG21	33:g:25:ARG:HH21	1.57	0.69
12:L:83:ASP:OD1	12:L:84:TYR:N	2.25	0.69
10:J:172:THR:HA	11:K:80:MET:HE2	1.74	0.69
7:G:252:PRO:HG3	7:G:263:ILE:HG12	1.76	0.68
21:U:15:VAL:HG13	21:U:54:MET:HE1	1.75	0.68
12:L:401:THR:HG21	12:L:482:MET:HG2	1.77	0.67
40:n:138:GLN:NE2	40:n:155:PRO:O	2.27	0.67
5:E:193:CYS:SG	5:E:194:GLU:N	2.69	0.66
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.29	0.65
7:G:190:MET:HE1	7:G:695:ALA:HB2	1.77	0.65
13:M:450:ASN:HB2	48:M:503:PC1:H221	1.79	0.65
16:P:5:VAL:HG13	16:P:18:GLY:HA2	1.80	0.64
41:o:16:PRO:HB2	41:o:21:MET:HE2	1.78	0.63
10:J:23:LYS:NZ	11:K:18:GLY:O	2.31	0.63
36:j:39:ARG:NH2	36:j:43:ASP:OD2	2.32	0.62
3:C:79:THR:HB	4:D:390:LYS:HE2	1.82	0.62
33:g:39:GLU:OE2	33:g:40:LYS:NZ	2.30	0.62
5:E:120:ILE:HD13	5:E:173:ILE:HD11	1.81	0.62
47:A:202:3PE:H2A1	8:H:295:PRO:HB3	1.82	0.62
6:F:82:MET:SD	6:F:221:THR:OG1	2.58	0.62
30:d:17:GLU:OE2	30:d:17:GLU:N	2.33	0.61
44:v:104:GLU:OE2	44:v:104:GLU:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.34	0.61
4:D:24:GLU:N	4:D:24:GLU:OE2	2.32	0.61
36:j:58:GLN:N	36:j:58:GLN:OE1	2.33	0.61
38:l:30:ARG:NH1	38:l:33:ASP:OD1	2.33	0.61
53:v:201:CDL:H731	53:v:201:CDL:H552	1.83	0.61
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.83	0.61
7:G:488:LYS:NZ	7:G:639:ALA:O	2.33	0.60
3:C:109:THR:OG1	3:C:110:TYR:N	2.34	0.60
20:T:65:ILE:HD12	20:T:65:ILE:H	1.66	0.60
7:G:460:ARG:NH1	7:G:659:ASP:OD1	2.34	0.60
42:p:72:ASP:N	42:p:72:ASP:OD1	2.33	0.60
13:M:422:HIS:HB2	39:m:59:ILE:HD12	1.82	0.60
12:L:171:ALA:O	12:L:175:ASN:ND2	2.35	0.60
38:l:141:GLU:OE2	38:l:141:GLU:N	2.34	0.60
24:X:11:ASP:OD1	24:X:11:ASP:N	2.35	0.60
40:n:12:GLN:OE1	40:n:12:GLN:N	2.32	0.60
40:n:140:GLN:N	40:n:140:GLN:OE1	2.34	0.60
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.84	0.59
26:Z:4:SER:OG	26:Z:5:LYS:N	2.34	0.59
7:G:617:ASP:OD1	7:G:617:ASP:N	2.35	0.59
27:a:49:GLU:OE1	27:a:52:ARG:NH2	2.35	0.59
38:l:30:ARG:NE	39:m:34:GLU:OE1	2.29	0.59
1:A:71:LEU:O	10:J:147:TYR:OH	2.20	0.59
22:V:17:GLU:N	22:V:17:GLU:OE2	2.30	0.59
24:X:87:CYS:SG	24:X:102:GLN:NE2	2.75	0.59
35:u:28:SER:HB2	35:u:31:GLU:HG3	1.83	0.59
6:F:224:ASN:ND2	51:F:502:FMN:O2	2.35	0.58
45:s:57:ASP:O	45:s:60:LYS:NZ	2.36	0.58
12:L:466:TYR:O	12:L:470:ASN:ND2	2.37	0.58
21:U:11:ILE:O	21:U:15:VAL:HG23	2.03	0.58
39:m:27:GLU:OE2	39:m:27:GLU:N	2.27	0.58
13:M:57:PHE:HB3	13:M:113:MET:HE2	1.84	0.58
22:V:8:THR:HG21	22:V:13:LEU:HD23	1.85	0.58
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.37	0.58
17:Q:16:LYS:NZ	17:Q:17:LEU:O	2.37	0.58
15:O:215:SER:O	15:O:245:LYS:NZ	2.36	0.57
33:g:50:ASP:HB3	33:g:53:VAL:HG22	1.86	0.57
15:O:104:ARG:NH2	55:O:404:GTP:O6	2.37	0.57
7:G:232:ASP:OD2	7:G:233:ALA:N	2.37	0.57
42:p:23:THR:OG1	42:p:24:SER:N	2.37	0.57
8:H:253:GLU:N	8:H:253:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:95:GLU:HG3	9:I:108:ARG:HD2	1.86	0.57
12:L:92:VAL:HG12	47:j:101:3PE:H2E1	1.86	0.57
19:S:37:GLU:HG3	19:S:38:LYS:HD3	1.85	0.57
33:g:35:GLU:OE1	33:g:35:GLU:N	2.31	0.57
6:F:99:GLU:O	6:F:139:ARG:NH1	2.38	0.57
4:D:145:THR:OG1	4:D:181:TYR:OH	2.23	0.57
20:T:28:GLU:HB2	20:T:29:LYS:NZ	2.19	0.57
48:B:203:PC1:H3C1	8:H:53:ILE:HD11	1.86	0.56
7:G:644:GLN:NE2	19:S:37:GLU:O	2.39	0.56
6:F:189:GLU:OE2	6:F:206:LYS:NZ	2.37	0.56
12:L:159:TYR:HB2	13:M:416:ARG:HG2	1.87	0.56
14:N:60:PHE:O	14:N:64:SER:OG	2.24	0.56
33:g:48:ASP:OD1	33:g:49:LYS:N	2.36	0.56
12:L:485:TYR:O	12:L:489:THR:OG1	2.22	0.56
13:M:278:ARG:NH2	38:l:82:ASP:OD1	2.37	0.56
29:c:25:VAL:O	29:c:29:ILE:HG13	2.05	0.56
43:q:5:GLN:HA	43:q:8:LYS:HB3	1.87	0.56
30:d:105:ASP:OD1	30:d:105:ASP:N	2.35	0.56
41:o:102:GLU:OE1	41:o:105:ARG:NH1	2.39	0.56
9:I:26:LEU:HD12	26:Z:35:MET:HE3	1.88	0.56
9:I:79:ALA:HB2	9:I:106:THR:HG22	1.88	0.56
48:I:204:PC1:O32	26:Z:28:ARG:NH2	2.39	0.55
25:Y:84:ASP:OD2	25:Y:84:ASP:N	2.38	0.55
13:M:369:LEU:O	13:M:372:THR:OG1	2.23	0.55
12:L:538:PRO:HB2	38:l:89:VAL:HG12	1.88	0.55
39:m:117:GLU:N	39:m:117:GLU:OE2	2.39	0.55
7:G:283:MET:HB2	7:G:560:ILE:HB	1.87	0.55
53:L:702:CDL:OA9	34:h:26:ARG:NH1	2.40	0.55
20:T:28:GLU:HB2	20:T:29:LYS:HZ2	1.70	0.55
26:Z:36:PHE:O	26:Z:40:ILE:HG12	2.07	0.55
12:L:433:GLY:O	37:k:59:ASN:ND2	2.40	0.55
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.88	0.55
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.89	0.55
4:D:371:LYS:HE3	4:D:424:VAL:HB	1.89	0.54
7:G:341:ASP:O	7:G:508:LYS:NZ	2.39	0.54
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.90	0.54
17:Q:88:THR:OG1	17:Q:91:ASP:OD1	2.24	0.54
38:l:52:ASP:OD1	38:l:52:ASP:N	2.40	0.54
3:C:182:ARG:NH2	23:W:109:GLU:OE2	2.35	0.54
7:G:226:GLU:OE1	17:Q:36:ARG:NH2	2.40	0.54
6:F:17:ASP:OD1	6:F:20:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:424:PRO:O	6:F:428:GLU:HG2	2.08	0.54
24:X:8:SER:OG	24:X:10:GLU:OE1	2.26	0.54
15:O:21:LYS:HE3	15:O:21:LYS:HA	1.88	0.54
21:U:55:GLU:HG2	21:U:61:GLU:HA	1.90	0.54
33:g:109:GLU:OE2	33:g:109:GLU:N	2.40	0.54
5:E:159:ASN:HB3	5:E:184:PRO:HB3	1.90	0.54
7:G:605:GLU:HA	7:G:610:THR:HG22	1.89	0.54
47:K:101:3PE:O22	47:K:101:3PE:N	2.41	0.54
19:S:91:GLU:O	19:S:95:SER:OG	2.21	0.54
42:p:98:ASP:OD2	42:p:141:ARG:NH1	2.40	0.54
53:M:502:CDL:H452	53:M:502:CDL:H182	1.88	0.54
24:X:120:ASP:N	24:X:120:ASP:OD1	2.38	0.54
35:u:52:ASP:OD1	35:u:52:ASP:N	2.41	0.54
12:L:17:MET:HE3	12:L:17:MET:H	1.71	0.54
2:B:42:ARG:NH2	48:B:203:PC1:O14	2.33	0.54
6:F:376:MET:HE2	6:F:376:MET:HA	1.90	0.54
41:o:24:PHE:HD2	41:o:107:LEU:HD13	1.73	0.53
4:D:42:THR:OG1	4:D:43:LEU:N	2.41	0.53
5:E:87:TYR:HD1	6:F:182:GLY:HA3	1.72	0.53
20:T:15:VAL:O	20:T:19:LEU:HD12	2.07	0.53
34:h:44:ASN:HB3	53:h:201:CDL:HB32	1.90	0.53
20:T:8:LEU:H	20:T:88:GLU:HG3	1.73	0.53
37:k:32:GLN:OE1	37:k:41:ARG:NE	2.41	0.53
14:N:335:MET:HE2	47:O:402:3PE:H2B1	1.91	0.53
28:b:29:VAL:HG12	28:b:30:ILE:HD12	1.90	0.53
9:I:145:GLU:OE2	16:P:66:GLY:N	2.42	0.53
15:O:88:SER:OG	15:O:90:ASP:OD1	2.24	0.53
21:U:22:TYR:HE1	37:k:43:PRO:HB2	1.74	0.53
7:G:324:ASP:OD1	7:G:324:ASP:N	2.37	0.53
38:l:115:MET:HE3	38:l:115:MET:HA	1.89	0.53
5:E:101:GLN:OE1	5:E:155:GLN:NE2	2.42	0.53
24:X:82:THR:HA	24:X:85:TRP:CD1	2.44	0.53
32:f:56:TRP:NE1	34:h:88:GLU:OE1	2.39	0.53
24:X:19:VAL:O	27:a:50:ARG:NH1	2.35	0.52
25:Y:27:ILE:HG23	47:Y:204:3PE:H352	1.91	0.52
36:j:66:ILE:HG12	41:o:107:LEU:HG	1.92	0.52
28:b:78:GLU:OE2	28:b:78:GLU:N	2.30	0.52
33:g:100:ARG:NH1	33:g:107:ILE:O	2.42	0.52
47:m:202:3PE:O22	47:m:202:3PE:N	2.40	0.52
30:d:104:LYS:H	30:d:104:LYS:HD3	1.74	0.52
38:l:125:TYR:OH	41:o:7:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:363:THR:HG21	7:G:97:LEU:HG	1.91	0.52
12:L:359:MET:O	12:L:436:ARG:NH2	2.42	0.52
39:m:111:LYS:O	39:m:115:ILE:HD12	2.09	0.52
7:G:331:LEU:HD22	7:G:525:LEU:HD22	1.91	0.52
2:B:48:MET:HE3	2:B:86:MET:HE2	1.90	0.52
9:I:84:GLU:HB2	9:I:94:ILE:HD12	1.91	0.52
42:p:5:ASP:HB3	42:p:8:VAL:HG22	1.92	0.52
45:s:58:LEU:HB3	45:s:62:ARG:HH21	1.74	0.52
24:X:164:SER:HB2	24:X:166:LEU:HD22	1.92	0.52
32:f:32:GLU:OE1	32:f:32:GLU:N	2.37	0.52
40:n:58:LYS:HA	40:n:61:GLN:HG3	1.91	0.52
31:e:88:GLU:OE1	31:e:90:LYS:NZ	2.42	0.52
42:p:129:GLU:OE1	42:p:133:GLN:NE2	2.43	0.52
7:G:6:SER:OG	7:G:7:ASN:OD1	2.27	0.52
22:V:35:GLY:HA2	22:V:44:ARG:HH21	1.75	0.52
24:X:129:LYS:HD3	28:b:65:VAL:HG23	1.91	0.52
32:f:49:LYS:HB2	32:f:52:GLU:HG2	1.91	0.52
2:B:71:ARG:HA	8:H:37:PRO:HA	1.91	0.52
16:P:331:ILE:HG23	16:P:332:GLU:HG3	1.92	0.52
20:T:37:MET:SD	20:T:38:LYS:NZ	2.65	0.52
36:j:32:MET:O	36:j:36:ILE:HG13	2.10	0.52
17:Q:28:GLU:OE2	17:Q:28:GLU:N	2.36	0.51
22:V:19:PRO:HB3	22:V:76:ILE:HG21	1.92	0.51
8:H:24:GLU:HG3	8:H:271:LEU:HD22	1.92	0.51
8:H:213:VAL:HG13	8:H:214:GLU:HG2	1.92	0.51
21:U:37:MET:HA	21:U:37:MET:HE3	1.92	0.51
21:U:16:LEU:O	21:U:20:LYS:HB3	2.10	0.51
29:c:34:GLN:NE2	29:c:38:ASP:OD2	2.43	0.51
26:Z:94:GLU:HG2	26:Z:106:VAL:HG13	1.92	0.51
40:n:12:GLN:HA	40:n:15:VAL:HG12	1.91	0.51
4:D:165:THR:HG23	8:H:32:GLN:HG2	1.91	0.51
11:K:73:LEU:HD22	14:N:38:LEU:HD12	1.92	0.51
38:l:30:ARG:NH2	38:l:32:GLU:OE2	2.43	0.51
4:D:409:HIS:HB3	4:D:413:ASP:HB2	1.93	0.51
7:G:512:GLU:OE1	7:G:515:GLN:NE2	2.43	0.51
12:L:31:ASN:OD1	12:L:31:ASN:N	2.39	0.51
43:q:34:ARG:NH1	43:q:54:GLN:OE1	2.36	0.51
6:F:370:ASP:OD2	7:G:179:ASN:ND2	2.44	0.51
7:G:20:VAL:HG12	7:G:32:LYS:HE2	1.92	0.51
16:P:105:ASP:OD1	16:P:105:ASP:N	2.41	0.51
35:u:79:TRP:HD1	42:p:40:VAL:HG13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:52:GLU:HG3	16:P:54:TYR:H	1.74	0.51
19:S:15:LEU:H	19:S:97:LYS:HE2	1.76	0.51
38:l:19:GLU:OE2	38:l:19:GLU:N	2.44	0.51
42:p:116:GLU:HG3	42:p:123:ASN:HB2	1.92	0.51
5:E:13:PRO:O	5:E:16:ASN:ND2	2.44	0.51
12:L:245:ALA:O	12:L:249:SER:OG	2.29	0.51
39:m:99:PHE:O	39:m:103:VAL:HG12	2.11	0.51
12:L:528:TYR:CG	38:l:101:MET:HG2	2.45	0.51
39:m:21:GLU:OE2	39:m:21:GLU:N	2.33	0.51
41:o:110:ARG:HH12	41:o:114:ARG:HE	1.58	0.51
6:F:78:LYS:NZ	51:F:502:FMN:O1P	2.39	0.50
11:K:32:CYS:O	11:K:36:MET:HG3	2.12	0.50
35:u:43:GLU:O	35:u:47:ASN:ND2	2.44	0.50
8:H:139:THR:O	8:H:143:GLU:HB2	2.10	0.50
5:E:81:TYR:O	5:E:85:THR:OG1	2.29	0.50
6:F:28:ARG:O	6:F:28:ARG:NE	2.44	0.50
16:P:9:GLY:HA3	16:P:15:SER:HB3	1.93	0.50
21:U:54:MET:HE3	21:U:76:ILE:HG21	1.91	0.50
24:X:82:THR:O	24:X:86:THR:OG1	2.24	0.50
53:d:203:CDL:H332	53:d:203:CDL:H722	1.91	0.50
12:L:2:ASN:N	12:L:2:ASN:OD1	2.44	0.50
21:U:50:ILE:O	21:U:54:MET:HG2	2.11	0.50
1:A:33:LYS:HG2	8:H:61[B]:LEU:HD11	1.93	0.50
1:A:92:LEU:HD22	8:H:302:MET:HG2	1.94	0.50
23:W:115:PRO:HB3	23:W:120:SER:HB2	1.93	0.50
39:m:1:SER:OG	39:m:2:PHE:N	2.45	0.50
4:D:393:ALA:HB1	4:D:427:GLU:HG3	1.94	0.50
17:Q:36:ARG:NE	17:Q:106:GLU:OE1	2.36	0.50
30:d:60:ARG:HG2	53:d:203:CDL:HA61	1.94	0.50
8:H:202:GLU:HA	8:H:210:GLY:HA3	1.94	0.50
13:M:27:SER:O	13:M:31:SER:OG	2.23	0.50
16:P:134:HIS:HB2	16:P:149:LYS:HD2	1.94	0.50
17:Q:27:GLU:H	17:Q:27:GLU:CD	2.20	0.50
7:G:199:ILE:HD12	7:G:208:LEU:HD13	1.93	0.49
20:T:66:ASP:OD1	20:T:66:ASP:N	2.43	0.49
21:U:47:GLN:NE2	21:U:67:ALA:O	2.42	0.49
29:c:39:VAL:O	29:c:43:LYS:HG2	2.12	0.49
2:B:69:MET:HG3	2:B:74:VAL:HB	1.94	0.49
12:L:135:ASN:ND2	12:L:197:ASP:OD1	2.45	0.49
25:Y:43:LYS:NZ	47:Y:206:3PE:O14	2.40	0.49
4:D:148:LEU:HD23	4:D:174:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:190:ARG:HG2	5:E:195:PRO:HG2	1.92	0.49
7:G:692:THR:OG1	7:G:693:GLU:OE1	2.26	0.49
10:J:10:SER:OG	11:K:7:ASN:ND2	2.41	0.49
12:L:560:ALA:O	12:L:565:THR:OG1	2.25	0.49
25:Y:124:VAL:HG22	47:Y:205:3PE:H232	1.94	0.49
34:h:48:GLY:O	42:p:60:TYR:OH	2.29	0.49
36:j:60:THR:N	36:j:63:GLU:OE2	2.46	0.49
38:l:137:ASN:O	38:l:142:ARG:NH1	2.45	0.49
39:m:121:ASP:OD1	39:m:123:THR:OG1	2.29	0.49
14:N:215:MET:HE3	14:N:251:MET:HE2	1.93	0.49
20:T:26:ASP:OD1	20:T:29:LYS:NZ	2.42	0.49
36:j:69:ASP:O	41:o:114:ARG:NH2	2.46	0.49
40:n:135:GLU:HG2	40:n:164:PRO:HA	1.95	0.49
13:M:216:LEU:HD13	13:M:291:VAL:HG22	1.93	0.49
39:m:28:THR:O	39:m:32:GLN:HG3	2.12	0.49
53:M:502:CDL:H381	53:M:502:CDL:H172	1.95	0.49
14:N:24:SER:O	14:N:24:SER:OG	2.28	0.49
25:Y:39:SER:HB2	47:Y:206:3PE:H2	1.94	0.49
15:O:83:TYR:OH	55:O:404:GTP:O2'	2.21	0.49
7:G:338:VAL:HG13	7:G:609:MET:HE1	1.95	0.49
21:U:66:ASP:OD1	21:U:66:ASP:N	2.41	0.49
40:n:175:GLU:HG2	40:n:176:ARG:HG2	1.95	0.49
12:L:502:LEU:O	12:L:506:ASN:ND2	2.46	0.49
53:M:502:CDL:H222	53:M:502:CDL:H191	1.60	0.48
15:O:35:LYS:NZ	55:O:404:GTP:O1A	2.46	0.48
22:V:40:ASN:OD1	22:V:40:ASN:N	2.39	0.48
40:n:154:PRO:HG2	40:n:164:PRO:HG2	1.94	0.48
7:G:125:SER:OG	7:G:126:ASP:N	2.45	0.48
8:H:69:SER:OG	53:H:403:CDL:OB4	2.27	0.48
24:X:136:LEU:HD12	24:X:137:PRO:HD2	1.94	0.48
12:L:65:ASN:OD1	12:L:65:ASN:N	2.42	0.48
35:u:77:PRO:O	35:u:81:ILE:HG12	2.14	0.48
22:V:17:GLU:HG2	22:V:18:THR:HG23	1.95	0.48
45:s:72:SER:HB3	45:s:75:HIS:ND1	2.28	0.48
7:G:263:ILE:HA	7:G:390:LEU:HD11	1.94	0.48
7:G:584:LYS:HE3	17:Q:36:ARG:HD2	1.94	0.48
15:O:136:GLU:O	15:O:140:ARG:HG2	2.12	0.48
40:n:131:SER:OG	40:n:135:GLU:OE2	2.31	0.48
41:o:111:LYS:NZ	41:o:115:GLU:OE2	2.46	0.48
7:G:114:CYS:HB3	7:G:117:GLN:HB2	1.96	0.48
48:d:201:PC1:H3B2	48:d:201:PC1:H351	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:LYS:HB2	5:E:68:LYS:HE2	1.56	0.48
9:I:49:ASN:O	9:I:53:GLU:N	2.44	0.48
13:M:2:LEU:N	32:f:27:ASP:OD1	2.46	0.48
33:g:121:PRO:O	42:p:166:ARG:NH2	2.40	0.48
7:G:89:ALA:O	7:G:93:VAL:HG13	2.12	0.48
45:s:52:LEU:C	45:s:54:LEU:H	2.20	0.48
4:D:143:GLU:OE2	4:D:278:TYR:OH	2.27	0.48
14:N:44:MET:HG2	14:N:122:ILE:HG21	1.95	0.48
16:P:23:VAL:HG12	16:P:92:ILE:HD12	1.96	0.48
20:T:46:ASP:O	20:T:50:ILE:HD12	2.14	0.48
37:k:17:ASP:OD1	37:k:18:TYR:N	2.46	0.48
38:l:82:ASP:OD2	39:m:71:ARG:NH1	2.40	0.48
3:C:32:ILE:HG22	3:C:33:LEU:HG	1.96	0.48
6:F:327:THR:OG1	6:F:328:GLY:N	2.46	0.48
8:H:96:ILE:HG23	26:Z:144:THR:HB	1.95	0.48
40:n:89:SER:O	40:n:89:SER:OG	2.28	0.48
7:G:6:SER:OG	7:G:7:ASN:N	2.37	0.47
12:L:193:LEU:HD22	12:L:204:LEU:HD23	1.96	0.47
4:D:22:THR:OG1	4:D:23:LYS:N	2.48	0.47
4:D:247:ALA:HB1	4:D:265:ILE:HD11	1.95	0.47
5:E:106:THR:HA	5:E:109:MET:HB3	1.97	0.47
21:U:43:ASP:N	21:U:43:ASP:OD1	2.47	0.47
25:Y:68:ILE:HD11	25:Y:96:GLY:HA2	1.95	0.47
5:E:194:GLU:HG2	6:F:267:THR:H	1.79	0.47
12:L:108:MET:HE3	12:L:108:MET:HB3	1.77	0.47
48:d:201:PC1:H242	47:d:202:3PE:H221	1.96	0.47
6:F:425:GLU:OE2	6:F:429:ARG:NH2	2.41	0.47
9:I:108:ARG:NH1	9:I:110:ASP:OD2	2.39	0.47
53:L:702:CDL:H611	53:L:702:CDL:H642	1.56	0.47
16:P:91:VAL:HG23	16:P:126:VAL:HG11	1.94	0.47
22:V:112:LYS:HE3	22:V:112:LYS:HB3	1.70	0.47
6:F:154:ARG:NH1	45:s:57:ASP:OD1	2.46	0.47
20:T:23:ASP:OD1	20:T:24:LYS:N	2.48	0.47
36:j:28:PHE:HA	36:j:31:THR:HG22	1.96	0.47
4:D:279:ASP:OD1	4:D:279:ASP:N	2.43	0.47
8:H:79:LEU:HD22	8:H:222:LEU:HG	1.97	0.47
13:M:59:ASP:O	13:M:63:THR:OG1	2.30	0.47
15:O:302:ARG:HG2	15:O:302:ARG:HH11	1.80	0.47
24:X:166:LEU:HD23	24:X:167:PHE:H	1.79	0.47
24:X:171:MET:HE2	24:X:171:MET:HB2	1.82	0.47
48:d:201:PC1:H133	48:d:201:PC1:H322	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:261:ARG:NH2	4:D:303:GLU:OE2	2.48	0.47
5:E:192:SER:OG	5:E:193:CYS:N	2.48	0.47
10:J:169:MET:HE2	10:J:169:MET:HB3	1.69	0.47
35:u:39:VAL:HG13	35:u:44:ARG:HD2	1.96	0.47
40:n:139:LEU:HG	40:n:164:PRO:HB3	1.97	0.47
16:P:23:VAL:HG23	16:P:26:ALA:HB2	1.97	0.47
40:n:10:THR:OG1	40:n:13:GLN:OE1	2.32	0.47
4:D:217:ASN:OD1	4:D:217:ASN:N	2.47	0.46
6:F:154:ARG:HA	45:s:58:LEU:HD21	1.96	0.46
7:G:360:SER:O	7:G:360:SER:OG	2.30	0.46
15:O:37:LYS:O	15:O:41:GLU:HG2	2.15	0.46
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.28	0.46
53:h:201:CDL:H591	53:h:201:CDL:H621	1.78	0.46
42:p:27:ASN:OD1	42:p:30:THR:OG1	2.26	0.46
9:I:164:GLU:HG3	43:q:88:ARG:HG3	1.97	0.46
15:O:116:LEU:HD11	15:O:259:LEU:HD23	1.97	0.46
17:Q:91:ASP:OD1	17:Q:91:ASP:N	2.48	0.46
35:u:105:PRO:HG2	35:u:119:MET:HG3	1.97	0.46
40:n:178:MET:HE3	40:n:178:MET:H	1.79	0.46
3:C:175:ARG:NH2	3:C:186:GLU:OE2	2.47	0.46
35:u:24:ASP:OD2	35:u:24:ASP:N	2.49	0.46
41:o:91:HIS:O	41:o:95:VAL:HG13	2.15	0.46
45:s:71:GLU:OE2	45:s:71:GLU:N	2.32	0.46
8:H:148:ILE:O	8:H:152:SER:OG	2.32	0.46
36:j:32:MET:HE3	36:j:36:ILE:HD11	1.97	0.46
8:H:3:MET:HE3	8:H:3:MET:HB3	1.84	0.46
11:K:75:LEU:O	11:K:79:VAL:HG23	2.16	0.46
12:L:83:ASP:N	12:L:86:SER:OG	2.38	0.46
12:L:492:ILE:HD12	12:L:492:ILE:H	1.81	0.46
15:O:279:LEU:O	15:O:283:THR:OG1	2.21	0.46
19:S:89:ALA:O	19:S:93:VAL:HG12	2.16	0.46
40:n:48:ASP:OD1	40:n:51:LYS:NZ	2.48	0.46
8:H:207:LEU:O	8:H:209:SER:N	2.48	0.46
19:S:88:ARG:NH1	19:S:88:ARG:HB2	2.31	0.46
3:C:79:THR:OG1	3:C:80:ALA:N	2.48	0.46
24:X:43:MET:HE2	26:Z:73:PRO:HA	1.97	0.46
47:d:202:3PE:H321	47:d:202:3PE:H31	1.70	0.46
12:L:17:MET:HA	12:L:20:MET:HB2	1.97	0.46
12:L:17:MET:SD	12:L:18:PRO:HD3	2.56	0.46
13:M:231:LEU:HA	13:M:235:LEU:HD12	1.97	0.46
41:o:92:LEU:O	41:o:96:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:H:404:PC1:H2C1	48:H:404:PC1:H351	1.97	0.45
15:O:213:GLU:HG3	15:O:214:MET:HE3	1.98	0.45
17:Q:77:ASP:O	17:Q:80:SER:OG	2.34	0.45
24:X:43:MET:HG3	28:b:52:TYR:CE2	2.50	0.45
2:B:69:MET:HE1	2:B:76:PHE:CD2	2.51	0.45
20:T:12:LYS:HZ1	20:T:16:LEU:HD13	1.81	0.45
30:d:4:GLY:HA3	34:h:124:HIS:HB3	1.98	0.45
35:u:125:GLN:OE1	35:u:127:HIS:NE2	2.49	0.45
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.97	0.45
7:G:669:LYS:NZ	7:G:670:ASP:OD1	2.42	0.45
33:g:108:MET:HE3	33:g:108:MET:HB2	1.84	0.45
16:P:115:GLN:HG2	16:P:155:GLU:CD	2.41	0.45
23:W:53:ASP:OD1	23:W:53:ASP:N	2.50	0.45
37:k:34:LYS:HE2	37:k:34:LYS:HB3	1.79	0.45
42:p:105:ILE:HG12	42:p:134:VAL:HG21	1.98	0.45
43:q:78:ASP:OD2	43:q:80:SER:OG	2.34	0.45
8:H:96:ILE:HG22	8:H:98:MET:HG2	1.97	0.45
10:J:159:TRP:HE1	14:N:12:THR:HG23	1.82	0.45
12:L:316:THR:HB	12:L:325:ALA:HB2	1.99	0.45
16:P:127:GLU:OE1	16:P:127:GLU:N	2.47	0.45
30:d:99:GLU:OE2	30:d:99:GLU:N	2.33	0.45
53:d:203:CDL:H721	53:d:203:CDL:H752	1.53	0.45
37:k:74:PHE:O	37:k:78:VAL:HG13	2.16	0.45
40:n:37:ARG:HA	40:n:37:ARG:HH11	1.82	0.45
12:L:606:GLU:N	12:L:606:GLU:OE2	2.50	0.45
16:P:22:THR:OG1	16:P:88:SER:OG	2.26	0.45
26:Z:86:MET:HE2	26:Z:86:MET:HB3	1.80	0.45
36:j:64:LEU:HD11	41:o:106:ARG:HH21	1.81	0.45
37:k:71:LYS:HD3	37:k:72:TRP:H	1.81	0.45
2:B:54:CYS:HB3	4:D:108:TYR:CG	2.52	0.45
13:M:108:MET:HE1	53:M:502:CDL:H192	1.79	0.45
13:M:200:MET:HE3	13:M:200:MET:HB3	1.91	0.45
22:V:18:THR:O	22:V:18:THR:OG1	2.25	0.45
25:Y:64:ALA:O	25:Y:68:ILE:HG23	2.16	0.45
4:D:173:GLU:O	4:D:177:MET:HG3	2.16	0.45
40:n:30:CYS:O	40:n:32:HIS:N	2.50	0.45
42:p:78:GLU:H	42:p:78:GLU:HG2	1.61	0.45
1:A:38:GLU:HG3	4:D:50:ASN:HB2	1.99	0.45
6:F:9:LYS:HB2	6:F:9:LYS:HE3	1.55	0.45
7:G:427:LYS:NZ	7:G:431:ASP:OD2	2.49	0.45
13:M:61:LEU:HB2	13:M:457:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:O:401:3PE:H362	47:O:401:3PE:H391	1.81	0.45
21:U:16:LEU:HD11	21:U:32:VAL:HG12	1.99	0.45
28:b:51:ASN:OD1	28:b:51:ASN:N	2.50	0.45
36:j:59:TRP:HZ3	41:o:99:LYS:HD3	1.81	0.45
40:n:9:LEU:HD23	40:n:9:LEU:HA	1.84	0.45
10:J:49:GLY:O	10:J:50:SER:HB2	2.16	0.44
13:M:125:THR:O	13:M:129:THR:OG1	2.29	0.44
6:F:54:ASP:N	6:F:54:ASP:OD1	2.50	0.44
13:M:175:ASN:HB3	13:M:178:MET:HB2	1.99	0.44
20:T:56:ASP:OD2	20:T:56:ASP:N	2.46	0.44
5:E:111:ARG:NH1	6:F:260:GLY:O	2.50	0.44
8:H:259:PHE:O	8:H:263:SER:OG	2.27	0.44
13:M:236:LEU:HD23	13:M:294:MET:HG3	1.99	0.44
47:O:401:3PE:H332	47:O:402:3PE:H232	1.99	0.44
21:U:12:LYS:HE3	21:U:12:LYS:HB3	1.74	0.44
36:j:47:VAL:HG12	36:j:48:LEU:HD22	1.99	0.44
4:D:144:ILE:HG23	4:D:177:MET:HE2	1.99	0.44
3:C:204:GLU:OE1	3:C:210:ARG:NH1	2.50	0.44
12:L:480:MET:HE1	41:o:87:ASP:HB3	1.99	0.44
19:S:23:CYS:SG	19:S:24:GLN:N	2.91	0.44
24:X:8:SER:OG	24:X:9:LEU:N	2.50	0.44
27:a:1:MET:HE3	27:a:1:MET:N	2.32	0.44
6:F:191:ALA:HB2	6:F:203:PRO:HG3	1.99	0.44
8:H:221:ALA:O	8:H:225:MET:HG3	2.17	0.44
11:K:37:MET:SD	14:N:68:MET:HE1	2.58	0.44
12:L:448:PRO:O	12:L:452:ASN:ND2	2.51	0.44
53:M:502:CDL:H192	53:M:502:CDL:H161	1.42	0.44
19:S:64:LEU:HD11	19:S:90:LEU:HD13	1.98	0.44
21:U:4:PRO:HD2	21:U:4:PRO:O	2.16	0.44
38:l:68:ASP:N	38:l:68:ASP:OD1	2.50	0.44
4:D:151:ILE:HD11	4:D:218:PHE:HZ	1.83	0.44
7:G:254:MET:HE2	7:G:254:MET:HB3	1.81	0.44
35:u:117:PRO:HA	35:u:118:PRO:HD3	1.87	0.44
38:l:16:THR:OG1	38:l:19:GLU:OE2	2.35	0.44
8:H:87:ILE:HG13	8:H:88:PRO:HD3	1.99	0.43
53:L:702:CDL:H341	53:L:702:CDL:H312	1.70	0.43
14:N:342:MET:HE1	53:d:203:CDL:H473	1.99	0.43
22:V:22:ARG:HD2	22:V:22:ARG:HA	1.83	0.43
38:l:5:THR:OG1	38:l:8:MET:SD	2.75	0.43
6:F:279:LEU:HD12	6:F:279:LEU:HA	1.91	0.43
8:H:287:HIS:O	8:H:291:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:605:HIS:HB3	14:N:96:MET:SD	2.57	0.43
16:P:157:ARG:HH12	16:P:225:GLY:HA2	1.84	0.43
20:T:12:LYS:O	20:T:12:LYS:NZ	2.40	0.43
48:A:203:PC1:H371	48:A:203:PC1:H341	1.91	0.43
6:F:199:LYS:HE3	6:F:199:LYS:HB2	1.65	0.43
7:G:236:SER:HB3	7:G:259:ASN:HD22	1.83	0.43
48:H:401:PC1:H143	48:H:401:PC1:H112	1.76	0.43
13:M:237:LYS:HD2	13:M:316:MET:HB3	1.99	0.43
47:M:504:3PE:H2D2	47:M:504:3PE:H2A1	1.88	0.43
15:O:58:TYR:CZ	15:O:107:GLN:HG3	2.53	0.43
41:o:89:CYS:HA	41:o:92:LEU:HD12	1.99	0.43
6:F:51:LYS:HG2	6:F:55:TRP:CD2	2.54	0.43
7:G:448:LYS:HB3	7:G:487:TRP:CE2	2.54	0.43
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.89	0.43
11:K:21:MET:HE2	11:K:21:MET:HB3	1.81	0.43
21:U:21:LEU:HD12	37:k:46:ARG:HH21	1.83	0.43
21:U:60:PHE:HZ	21:U:80:ILE:HG12	1.84	0.43
40:n:134:ARG:NH1	40:n:161:ASP:OD2	2.51	0.43
42:p:41:ASP:O	42:p:45:THR:OG1	2.29	0.43
3:C:49:GLU:HG2	3:C:106:ARG:HB3	2.00	0.43
7:G:272:ASP:OD1	7:G:272:ASP:N	2.46	0.43
7:G:470:VAL:HG12	7:G:490:MET:HE1	2.00	0.43
23:W:119:LEU:HD23	23:W:119:LEU:HA	1.92	0.43
27:a:22:ALA:O	27:a:26:ILE:HG13	2.19	0.43
35:u:103:ILE:HG22	42:p:17:PRO:HB3	1.99	0.43
36:j:56:PRO:HA	36:j:59:TRP:CD1	2.53	0.43
38:l:128:VAL:HG21	41:o:94:TYR:CZ	2.53	0.43
4:D:291:GLY:O	4:D:296:ARG:NH1	2.51	0.43
6:F:272:MET:HE2	6:F:272:MET:HB3	1.88	0.43
7:G:329:ILE:HD13	7:G:329:ILE:HA	1.85	0.43
8:H:8:MET:HE3	8:H:8:MET:HB3	1.87	0.43
12:L:525:LEU:HD12	12:L:528:TYR:HE1	1.83	0.43
15:O:319:LEU:HD12	15:O:319:LEU:HA	1.83	0.43
24:X:133:ASP:OD2	24:X:133:ASP:N	2.52	0.43
41:o:92:LEU:HB3	41:o:96:LYS:NZ	2.33	0.43
41:o:118:GLU:HA	41:o:121:MET:SD	2.58	0.43
7:G:441:GLN:OE1	7:G:441:GLN:N	2.44	0.43
9:I:32:ARG:NH1	48:I:204:PC1:O12	2.44	0.43
12:L:445:GLU:O	12:L:445:GLU:HG3	2.19	0.43
14:N:306:PRO:HB3	33:g:26:TRP:HZ3	1.83	0.43
15:O:18:MET:HB3	15:O:18:MET:HE3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:d:201:PC1:H2	48:d:201:PC1:H222	1.87	0.43
47:j:101:3PE:H2B2	47:j:101:3PE:H281	1.88	0.43
8:H:24:GLU:HA	8:H:271:LEU:HD13	2.00	0.43
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.84	0.43
9:I:8:ARG:NH2	44:v:111:TYR:O	2.52	0.43
35:u:9:LEU:O	35:u:13:GLN:HG3	2.19	0.43
2:B:33:LEU:HD23	2:B:33:LEU:HA	1.89	0.43
4:D:40:LYS:HE3	4:D:40:LYS:HB3	1.89	0.43
12:L:483:PRO:HG2	12:L:486:LEU:HG	2.00	0.43
13:M:104:LEU:HG	53:M:502:CDL:H241	1.78	0.43
17:Q:14:ASP:OD1	17:Q:14:ASP:N	2.49	0.43
21:U:87:TYR:HA	35:u:19:ARG:HD2	2.00	0.43
6:F:164:LYS:HG2	45:s:63:MET:HE1	1.99	0.43
12:L:393:ASP:OD1	12:L:394:LEU:HD12	2.19	0.43
27:a:21:MET:HE3	27:a:22:ALA:N	2.33	0.43
33:g:111:ASN:HD22	33:g:115:PRO:HG3	1.83	0.43
36:j:19:ARG:O	36:j:23:ILE:HD12	2.19	0.43
6:F:68:ARG:HG3	6:F:226:GLU:HB3	2.01	0.42
1:A:27:LEU:HD12	48:H:401:PC1:H133	2.00	0.42
2:B:104:TYR:O	2:B:111:ARG:NH1	2.52	0.42
10:J:165:VAL:O	10:J:168:ILE:HG13	2.18	0.42
47:O:401:3PE:H371	47:O:402:3PE:H262	2.01	0.42
37:k:78:VAL:HA	37:k:81:ILE:HG22	2.00	0.42
45:s:31:GLU:N	45:s:31:GLU:OE1	2.52	0.42
24:X:10:GLU:OE1	24:X:10:GLU:N	2.52	0.42
27:a:34:LYS:HE2	27:a:34:LYS:HB2	1.71	0.42
6:F:228:VAL:O	6:F:231:SER:OG	2.35	0.42
13:M:11:LEU:HB3	13:M:100:ILE:HD13	2.02	0.42
13:M:22:MET:O	13:M:26:ASN:ND2	2.52	0.42
13:M:196:TRP:HZ2	13:M:254:THR:HG23	1.84	0.42
14:N:146:PHE:CD1	14:N:147:PRO:HD3	2.54	0.42
14:N:317:PHE:HA	14:N:318:PRO:HD3	1.90	0.42
26:Z:124:LEU:HD12	26:Z:124:LEU:HA	1.91	0.42
41:o:92:LEU:O	41:o:95:VAL:HG22	2.20	0.42
4:D:414:VAL:O	4:D:418:ILE:HG13	2.19	0.42
7:G:285:ARG:HG2	7:G:291:LEU:HD13	2.01	0.42
16:P:272:ILE:HD12	16:P:272:ILE:H	1.84	0.42
18:R:57:ILE:HD12	18:R:58:SER:H	1.84	0.42
19:S:44:LYS:HD2	19:S:44:LYS:HA	1.75	0.42
24:X:13:LYS:HB2	24:X:13:LYS:HE2	1.76	0.42
39:m:43:LYS:HE2	39:m:43:LYS:HB2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:PHE:HB3	4:D:308:ILE:HD11	2.02	0.42
7:G:319:ALA:HB3	7:G:345:THR:HG22	2.02	0.42
47:H:402:3PE:H222	47:H:402:3PE:H251	1.77	0.42
12:L:136:ASN:OD1	12:L:136:ASN:N	2.49	0.42
20:T:12:LYS:HZ1	20:T:16:LEU:HD22	1.84	0.42
21:U:71:MET:HE3	21:U:71:MET:HA	2.01	0.42
26:Z:5:LYS:HB3	26:Z:5:LYS:HE3	1.82	0.42
27:a:57:VAL:HG23	27:a:59:ARG:HB2	2.01	0.42
36:j:38:TRP:HD1	36:j:39:ARG:HD2	1.84	0.42
6:F:428:GLU:O	6:F:432:GLN:HG3	2.20	0.42
7:G:516:LYS:HB3	7:G:516:LYS:HE2	1.93	0.42
8:H:20:LEU:HD23	8:H:228:TYR:HD2	1.84	0.42
12:L:28:LYS:HA	12:L:29:PRO:HD3	1.93	0.42
24:X:3:ILE:HD12	24:X:3:ILE:HA	1.82	0.42
25:Y:98:LEU:HD12	25:Y:98:LEU:HA	1.78	0.42
40:n:163:PRO:HA	40:n:164:PRO:HD3	1.94	0.42
41:o:93:ASP:O	41:o:97:ARG:HG3	2.18	0.42
47:A:202:3PE:H352	47:A:202:3PE:H321	1.81	0.42
8:H:89:LEU:HA	8:H:90:PRO:HD3	1.93	0.42
14:N:236:LYS:HG3	14:N:237:THR:HG23	2.02	0.42
15:O:24:LEU:HD22	15:O:166:PRO:HB3	2.02	0.42
18:R:94:GLN:OE1	18:R:95:HIS:N	2.51	0.42
36:j:66:ILE:HD11	41:o:103:ARG:O	2.20	0.42
4:D:212:TYR:CZ	4:D:216:LYS:HD2	2.55	0.42
8:H:253:GLU:OE1	27:a:25:ARG:NH2	2.53	0.42
12:L:53:MET:HE2	12:L:53:MET:HB3	1.79	0.42
15:O:224:SER:OG	15:O:227:GLU:OE1	2.24	0.42
18:R:55:ARG:H	18:R:55:ARG:HG2	1.63	0.42
20:T:73:PRO:O	20:T:77:VAL:HG23	2.20	0.42
22:V:39:LYS:O	22:V:39:LYS:NZ	2.39	0.42
23:W:29:LYS:HB3	23:W:33:ARG:NH1	2.35	0.42
9:I:175:TYR:CZ	44:v:38:PRO:HG3	2.55	0.42
10:J:146:LEU:HA	11:K:58:MET:HE3	2.01	0.42
11:K:26:LEU:N	11:K:88:ASP:OD2	2.46	0.42
12:L:336:LYS:HB2	12:L:336:LYS:HE3	1.81	0.42
12:L:510:ASN:HD22	12:L:510:ASN:HA	1.66	0.42
12:L:512:LYS:HA	12:L:512:LYS:HD3	1.79	0.42
12:L:514:HIS:HD2	40:n:29:TRP:CD2	2.37	0.42
16:P:287:ILE:HD13	16:P:287:ILE:HA	1.89	0.42
19:S:63:LYS:HG2	19:S:65:TRP:NE1	2.35	0.42
25:Y:94:CYS:HA	25:Y:114:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:6:SER:HG	7:G:7:ASN:H	1.67	0.41
10:J:13:PHE:HD2	10:J:39:VAL:HG23	1.85	0.41
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.51	0.41
48:d:201:PC1:H3D1	48:d:201:PC1:H3A1	1.95	0.41
36:j:53:TYR:HE2	41:o:98:MET:HE3	1.85	0.41
3:C:111:THR:HB	3:C:117:ILE:HD11	2.02	0.41
13:M:60:SER:OG	33:g:84:ARG:NH1	2.53	0.41
29:c:40:LEU:HD23	29:c:40:LEU:HA	1.86	0.41
38:l:77:MET:HE1	39:m:64:LEU:HD13	2.02	0.41
7:G:595:GLU:O	7:G:599:ILE:HG13	2.20	0.41
14:N:228:LEU:HD23	14:N:228:LEU:HA	1.88	0.41
18:R:9:GLU:OE1	18:R:25:LYS:NZ	2.53	0.41
20:T:13:ASP:OD2	20:T:14:ARG:N	2.53	0.41
20:T:83:LYS:HA	20:T:83:LYS:HD3	1.87	0.41
21:U:22:TYR:CE1	37:k:43:PRO:HB2	2.53	0.41
22:V:61:GLU:HA	22:V:62:PRO:HD3	1.94	0.41
32:f:28:ARG:HA	32:f:28:ARG:HD2	1.80	0.41
41:o:15:GLU:HA	41:o:16:PRO:HD3	1.92	0.41
4:D:125:LEU:HD23	4:D:125:LEU:HA	1.92	0.41
4:D:218:PHE:HD2	4:D:308:ILE:HD11	1.86	0.41
15:O:94:TYR:OH	15:O:151:HIS:ND1	2.37	0.41
21:U:7:THR:O	21:U:11:ILE:HG13	2.19	0.41
24:X:44:LEU:O	24:X:48:GLU:HB2	2.20	0.41
30:d:78:ARG:NH2	48:d:201:PC1:H31	2.36	0.41
8:H:26:LYS:HE3	8:H:26:LYS:HB3	1.78	0.41
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.93	0.41
12:L:264:TYR:CD2	12:L:265:PRO:HD3	2.55	0.41
13:M:455:LEU:HD23	13:M:455:LEU:HA	1.88	0.41
21:U:34:SER:HB3	21:U:40:LEU:HD21	2.03	0.41
26:Z:20:ASP:OD1	26:Z:20:ASP:N	2.52	0.41
30:d:45:ASP:OD1	30:d:49:ARG:NH1	2.53	0.41
35:u:48:LYS:HB3	35:u:48:LYS:HE3	1.76	0.41
38:l:9:LEU:O	38:l:26:LYS:NZ	2.43	0.41
48:A:204:PC1:H242	48:B:202:PC1:H2A1	2.02	0.41
3:C:148:LEU:HD12	3:C:148:LEU:HA	1.88	0.41
6:F:294:LEU:HD21	6:F:297:VAL:HG23	2.02	0.41
53:M:502:CDL:H541	53:M:502:CDL:H571	1.83	0.41
24:X:101:LYS:HE3	24:X:101:LYS:HB2	1.81	0.41
40:n:37:ARG:HA	40:n:37:ARG:HD2	1.81	0.41
5:E:89:MET:HE1	6:F:140:GLY:C	2.46	0.41
13:M:403:THR:HA	13:M:406:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:11:ILE:HD13	20:T:80:ILE:HG22	2.03	0.41
42:p:4:TRP:HE1	42:p:9:TYR:HB2	1.85	0.41
2:B:86:MET:HE3	2:B:86:MET:HB2	1.79	0.41
4:D:88:GLU:OE2	4:D:430:ARG:NH1	2.53	0.41
4:D:342:MET:HE3	4:D:346:ILE:HG13	2.02	0.41
6:F:8:LYS:HB3	6:F:8:LYS:HE3	1.92	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.85	0.41
38:l:18:GLU:CD	38:l:18:GLU:H	2.29	0.41
4:D:238:ARG:NH2	4:D:412:ALA:HB1	2.36	0.41
7:G:396:ARG:HG3	7:G:417:TYR:HD2	1.86	0.41
10:J:109:LYS:HG2	10:J:110:ASP:OD2	2.21	0.41
12:L:467:ILE:O	12:L:471:ASN:ND2	2.40	0.41
12:L:546:GLN:HA	12:L:550:SER:HB3	2.02	0.41
13:M:285:LEU:HD22	13:M:410:MET:HE2	2.03	0.41
53:M:502:CDL:H392	53:M:502:CDL:H422	1.62	0.41
16:P:76:ARG:NH2	16:P:108:ASP:OD2	2.51	0.41
21:U:83:LYS:HB2	21:U:83:LYS:HE3	1.79	0.41
22:V:42:ALA:HA	22:V:45:LYS:HE2	2.03	0.41
53:d:203:CDL:H351	53:d:203:CDL:H321	1.83	0.41
47:j:101:3PE:H391	47:j:101:3PE:H2D2	2.02	0.41
42:p:4:TRP:NE1	42:p:9:TYR:HB2	2.36	0.41
5:E:207:LYS:HE2	6:F:39:ARG:HG3	2.03	0.41
8:H:49:ILE:H	8:H:49:ILE:HG12	1.68	0.41
11:K:1:FME:HE3	11:K:1:FME:HB2	1.61	0.41
13:M:94:LEU:HD23	13:M:94:LEU:HA	1.88	0.41
14:N:313:MET:HE2	14:N:313:MET:HB2	1.85	0.41
24:X:47:TRP:CH2	34:h:141:PRO:HG3	2.56	0.41
26:Z:61:GLN:HE21	26:Z:61:GLN:HB3	1.67	0.41
32:f:29:LYS:HE2	32:f:29:LYS:HB2	1.79	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.92	0.40
5:E:120:ILE:HG21	5:E:139:LEU:HD13	2.03	0.40
8:H:178:ALA:HB1	8:H:181:LEU:HD12	2.02	0.40
8:H:251:MET:HE3	8:H:251:MET:HB2	1.86	0.40
12:L:203:MET:HG2	42:p:113:GLN:HG3	2.03	0.40
13:M:178:MET:HE1	13:M:182:TRP:CE2	2.56	0.40
14:N:215:MET:HE1	14:N:247:THR:HB	2.03	0.40
14:N:338:PRO:HG2	30:d:33:PHE:CZ	2.56	0.40
19:S:32:VAL:O	19:S:36:ILE:HD12	2.21	0.40
19:S:90:LEU:HD12	19:S:90:LEU:HA	1.82	0.40
53:h:201:CDL:H161	53:h:201:CDL:H131	1.73	0.40
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:99:MET:HE3	47:K:101:3PE:H3E1	2.03	0.40
20:T:6:LEU:HB3	20:T:86:VAL:HG21	2.02	0.40
37:k:23:ILE:H	37:k:23:ILE:HG22	1.64	0.40
38:l:53:ARG:HH21	39:m:12:SER:HB3	1.85	0.40
40:n:135:GLU:OE2	40:n:166:TRP:NE1	2.46	0.40
42:p:45:THR:O	42:p:49:GLU:HG2	2.21	0.40
42:p:126:LYS:O	42:p:129:GLU:HG3	2.20	0.40
4:D:72:MET:HE3	4:D:72:MET:HB3	1.90	0.40
6:F:82:MET:HE2	6:F:91:LYS:HE2	2.03	0.40
6:F:164:LYS:HD2	6:F:164:LYS:HA	1.88	0.40
13:M:208:PRO:HG3	13:M:216:LEU:HD12	2.03	0.40
13:M:403:THR:O	13:M:407:SER:OG	2.34	0.40
25:Y:108:GLY:HA3	48:m:201:PC1:H31	2.02	0.40
4:D:20:TYR:H	14:N:171:ASN:HD21	1.70	0.40
5:E:196:ALA:HB3	5:E:199:LEU:O	2.21	0.40
6:F:125:GLY:O	6:F:129:MET:HG3	2.21	0.40
14:N:190:MET:H	14:N:190:MET:HG3	1.55	0.40
24:X:78:ALA:O	24:X:82:THR:OG1	2.36	0.40
30:d:26:LEU:HD23	30:d:26:LEU:HA	1.93	0.40
47:d:202:3PE:H2C1	47:d:202:3PE:H292	1.88	0.40
35:u:97:VAL:HG23	42:p:114:GLN:HG2	2.02	0.40
38:l:34:TYR:CZ	38:l:36:PRO:HG3	2.57	0.40
7:G:596:ASP:OD1	7:G:596:ASP:N	2.55	0.40
8:H:15:LEU:HD23	8:H:15:LEU:HA	1.89	0.40
12:L:128:MET:HE3	12:L:252:MET:HA	2.04	0.40
13:M:290:SER:O	13:M:294:MET:HG2	2.21	0.40
48:M:503:PC1:H2A1	48:M:503:PC1:H2D2	1.94	0.40
15:O:233:LYS:H	15:O:233:LYS:HG2	1.68	0.40
15:O:241:LEU:HD23	15:O:241:LEU:HA	1.92	0.40
42:p:25:LEU:HD23	42:p:25:LEU:HA	1.92	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	A	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
2	B	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
3	C	207/209 (99%)	203 (98%)	4 (2%)	0	100	100
4	D	427/430 (99%)	415 (97%)	12 (3%)	0	100	100
5	E	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
6	F	432/432 (100%)	413 (96%)	19 (4%)	0	100	100
7	G	698/699 (100%)	676 (97%)	22 (3%)	0	100	100
8	H	317/318 (100%)	307 (97%)	9 (3%)	1 (0%)	36	66
9	I	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
10	J	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	21	51
11	K	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
12	L	603/605 (100%)	581 (96%)	22 (4%)	0	100	100
13	M	456/458 (100%)	453 (99%)	3 (1%)	0	100	100
14	N	344/346 (99%)	337 (98%)	7 (2%)	0	100	100
15	O	318/320 (99%)	311 (98%)	7 (2%)	0	100	100
16	P	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
17	Q	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
18	R	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	S	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
20	T	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
21	U	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
22	V	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
23	W	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
24	X	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
25	Y	137/141 (97%)	133 (97%)	4 (3%)	0	100	100
26	Z	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
27	a	68/70 (97%)	68 (100%)	0	0	100	100
28	b	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
29	c	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
30	d	117/119 (98%)	114 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	e	97/99 (98%)	97 (100%)	0	0	100	100
32	f	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
33	g	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
34	h	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
35	u	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
36	j	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
37	k	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
38	l	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
39	m	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
40	n	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	21	51
41	o	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
42	p	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
43	q	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
44	v	92/113 (81%)	87 (95%)	5 (5%)	0	100	100
45	s	44/45 (98%)	41 (93%)	3 (7%)	0	100	100
All	All	8199/8306 (99%)	7970 (97%)	226 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	50	SER
8	H	208	VAL
40	n	31	ILE

### 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	A	100/100 (100%)	94 (94%)	6 (6%)	17	47
2	B	131/131 (100%)	128 (98%)	3 (2%)	44	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	190/190 (100%)	183 (96%)	7 (4%)	30	65
4	D	370/370 (100%)	353 (95%)	17 (5%)	24	58
5	E	183/183 (100%)	168 (92%)	15 (8%)	10	33
6	F	348/346 (101%)	328 (94%)	20 (6%)	18	49
7	G	587/586 (100%)	559 (95%)	28 (5%)	23	56
8	H	275/274 (100%)	267 (97%)	8 (3%)	37	73
9	I	151/151 (100%)	145 (96%)	6 (4%)	28	63
10	J	141/141 (100%)	134 (95%)	7 (5%)	22	54
11	K	85/85 (100%)	82 (96%)	3 (4%)	32	67
12	L	533/533 (100%)	508 (95%)	25 (5%)	23	57
13	M	412/412 (100%)	396 (96%)	16 (4%)	28	64
14	N	315/315 (100%)	304 (96%)	11 (4%)	32	67
15	O	283/283 (100%)	271 (96%)	12 (4%)	26	61
16	P	297/296 (100%)	287 (97%)	10 (3%)	32	68
17	Q	116/116 (100%)	109 (94%)	7 (6%)	17	47
18	R	79/79 (100%)	74 (94%)	5 (6%)	16	45
19	S	77/77 (100%)	74 (96%)	3 (4%)	28	64
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	76
21	U	79/79 (100%)	75 (95%)	4 (5%)	21	54
22	V	101/101 (100%)	95 (94%)	6 (6%)	18	48
23	W	107/108 (99%)	103 (96%)	4 (4%)	30	65
24	X	154/154 (100%)	145 (94%)	9 (6%)	18	49
25	Y	101/101 (100%)	94 (93%)	7 (7%)	14	41
26	Z	120/120 (100%)	116 (97%)	4 (3%)	33	69
27	a	59/59 (100%)	58 (98%)	1 (2%)	53	83
28	b	71/71 (100%)	66 (93%)	5 (7%)	14	40
29	c	45/45 (100%)	44 (98%)	1 (2%)	45	78
30	d	105/105 (100%)	102 (97%)	3 (3%)	37	73
31	e	89/89 (100%)	86 (97%)	3 (3%)	32	68
32	f	54/54 (100%)	51 (94%)	3 (6%)	19	50
33	g	91/91 (100%)	90 (99%)	1 (1%)	65	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	h	121/121 (100%)	120 (99%)	1 (1%)	73	90
35	u	121/121 (100%)	114 (94%)	7 (6%)	18	49
36	j	61/61 (100%)	55 (90%)	6 (10%)	7	25
37	k	63/63 (100%)	60 (95%)	3 (5%)	23	56
38	l	140/140 (100%)	137 (98%)	3 (2%)	47	79
39	m	114/114 (100%)	107 (94%)	7 (6%)	17	46
40	n	156/156 (100%)	147 (94%)	9 (6%)	18	49
41	o	110/110 (100%)	108 (98%)	2 (2%)	51	82
42	p	155/155 (100%)	149 (96%)	6 (4%)	28	64
43	q	131/131 (100%)	124 (95%)	7 (5%)	20	52
44	v	85/96 (88%)	82 (96%)	3 (4%)	32	67
45	s	45/44 (102%)	42 (93%)	3 (7%)	15	42
All	All	7230/7236 (100%)	6911 (96%)	319 (4%)	27	59

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	LEU
1	A	16	LEU
1	A	68	GLU
1	A	81	THR
1	A	101	SER
2	B	54	CYS
2	B	152	THR
2	B	160	ILE
3	C	38	GLN
3	C	45	PHE
3	C	74	SER
3	C	93	VAL
3	C	107	VAL
3	C	109	THR
3	C	169	SER
4	D	22	THR
4	D	42	THR
4	D	45	SER
4	D	47	LEU
4	D	61	VAL

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Mol	Chain	Res	Type
4	D	109	VAL
4	D	217	ASN
4	D	239	THR
4	D	242	ILE
4	D	281	VAL
4	D	331	SER
4	D	341	SER
4	D	344	SER
4	D	379	VAL
4	D	384	SER
4	D	414	VAL
4	D	424	VAL
5	E	6	LEU
5	E	19	THR
5	E	68	LYS
5	E	69	VAL
5	E	75	VAL
5	E	80	VAL
5	E	85	THR
5	E	89	MET
5	E	95	VAL
5	E	106	THR
5	E	154	VAL
5	E	190	ARG
5	E	192	SER
5	E	201	SER
5	E	213	VAL
6	F	21	ILE
6	F	45	THR
6	F	63	SER
6	F	93	LEU
6	F	94	VAL
6	F	105	CYS
6	F	147	SER
6	F	190	THR
6	F	234	ILE
6	F	253	THR
6	F	254	LYS
6	F	255	LEU
6	F	264	ASN
6	F	281	GLU
6	F	287	VAL

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Mol	Chain	Res	Type
6	F	294	LEU
6	F	352	GLU
6	F	385	ARG
6	F	396	SER
6	F	415	VAL
7	G	65	VAL
7	G	73	VAL
7	G	81	THR
7	G	93	VAL
7	G	110	GLN
7	G	149	ILE
7	G	152	ARG
7	G	174	THR
7	G	196	SER
7	G	298	ASP
7	G	307	LEU
7	G	314	ASP
7	G	323	VAL
7	G	329	ILE
7	G	360	SER
7	G	366	THR
7	G	434	SER
7	G	456	SER
7	G	500	VAL
7	G	536	ASP
7	G	559	VAL
7	G	583	THR
7	G	596	ASP
7	G	614	ASP
7	G	649	SER
7	G	652	VAL
7	G	667	THR
7	G	681	SER
8	H	35	LYS
8	H	39	VAL
8	H	144	VAL
8	H	152	SER
8	H	176	LEU
8	H	276	SER
8	H	306	SER
8	H	317	GLN
9	I	3	LYS

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Mol	Chain	Res	Type
9	I	37	THR
9	I	75	GLU
9	I	78	ILE
9	I	122	CYS
9	I	140	SER
10	J	34	ILE
10	J	41	CYS
10	J	59	ILE
10	J	82	ILE
10	J	84	LEU
10	J	97	LEU
10	J	124	ASP
11	K	28	SER
11	K	39	SER
11	K	55	LEU
12	L	64	SER
12	L	86	SER
12	L	92	VAL
12	L	127	THR
12	L	128	MET
12	L	140	LEU
12	L	203	MET
12	L	241	THR
12	L	244	SER
12	L	250	SER
12	L	267	THR
12	L	285	THR
12	L	305	SER
12	L	307	SER
12	L	316	THR
12	L	343	SER
12	L	380	LEU
12	L	401	THR
12	L	426	ILE
12	L	453	SER
12	L	458	LEU
12	L	523	SER
12	L	531	THR
12	L	585	LYS
12	L	598	SER
13	M	15	THR
13	M	31	SER

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Mol	Chain	Res	Type
13	M	42	MET
13	M	49	SER
13	M	58	SER
13	M	75	LEU
13	M	109	THR
13	M	129	THR
13	M	234	VAL
13	M	246	ILE
13	M	247	THR
13	M	284	SER
13	M	292	SER
13	M	315	LEU
13	M	375	LEU
13	M	396	MET
14	N	20	VAL
14	N	37	MET
14	N	56	SER
14	N	64	SER
14	N	70	LEU
14	N	125	SER
14	N	209	ILE
14	N	268	GLN
14	N	284	ILE
14	N	299	SER
14	N	319	LEU
15	O	13	LYS
15	O	19	THR
15	O	36	SER
15	O	60	ASP
15	O	62	THR
15	O	65	ASP
15	O	72	GLN
15	O	179	VAL
15	O	195	THR
15	O	206	TYR
15	O	220	VAL
15	O	265	ASP
16	P	15	SER
16	P	69	ILE
16	P	90	VAL
16	P	101	THR
16	P	132	ILE

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Mol	Chain	Res	Type
16	P	133	SER
16	P	171	ILE
16	P	250	HIS
16	P	279	THR
16	P	332	GLU
17	Q	21	THR
17	Q	44	ASN
17	Q	80	SER
17	Q	87	SER
17	Q	102	SER
17	Q	109	LYS
17	Q	132	THR
18	R	7	THR
18	R	54	SER
18	R	57	ILE
18	R	58	SER
18	R	83	THR
19	S	44	LYS
19	S	77	SER
19	S	96	SER
20	T	50	ILE
20	T	88	GLU
21	U	44	SER
21	U	66	ASP
21	U	72	CYS
21	U	77	VAL
22	V	4	LEU
22	V	11	VAL
22	V	47	THR
22	V	88	SER
22	V	112	LYS
22	V	115	ILE
23	W	22	SER
23	W	101	THR
23	W	114	ARG
23	W	127	ASP
24	X	17	VAL
24	X	21	SER
24	X	22	SER
24	X	89	ASP
24	X	99	CYS
24	X	101	LYS

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Mol	Chain	Res	Type
24	X	117	VAL
24	X	158	LYS
24	X	164	SER
25	Y	3	THR
25	Y	39	SER
25	Y	40	VAL
25	Y	42	LEU
25	Y	47	SER
25	Y	73	SER
25	Y	129	LEU
26	Z	7	LYS
26	Z	20	ASP
26	Z	25	LEU
26	Z	34	SER
27	a	63	SER
28	b	4	VAL
28	b	17	VAL
28	b	31	LEU
28	b	51	ASN
28	b	76	SER
29	c	24	SER
30	d	20	SER
30	d	27	THR
30	d	96	SER
31	e	5	VAL
31	e	21	SER
31	e	48	SER
32	f	6	VAL
32	f	40	LYS
32	f	57	LYS
33	g	23	THR
34	h	127	THR
35	u	4	THR
35	u	40	SER
35	u	42	VAL
35	u	50	LEU
35	u	52	ASP
35	u	55	LEU
35	u	126	HIS
36	j	13	GLN
36	j	21	GLN
36	j	29	SER

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Mol	Chain	Res	Type
36	j	53	TYR
36	j	60	THR
36	j	64	LEU
37	k	11	SER
37	k	31	VAL
37	k	61	SER
38	l	16	THR
38	l	52	ASP
38	l	131	LYS
39	m	2	PHE
39	m	25	SER
39	m	75	ILE
39	m	91	LEU
39	m	103	VAL
39	m	115	ILE
39	m	123	THR
40	n	28	SER
40	n	48	ASP
40	n	51	LYS
40	n	88	THR
40	n	95	CYS
40	n	109	SER
40	n	131	SER
40	n	140	GLN
40	n	169	ILE
41	o	15	GLU
41	o	50	LEU
42	p	3	SER
42	p	16	THR
42	p	72	ASP
42	p	74	THR
42	p	102	VAL
42	p	166	ARG
43	q	12	GLN
43	q	80	SER
43	q	82	VAL
43	q	111	THR
43	q	118	SER
43	q	133	LYS
43	q	142	THR
44	v	15	SER
44	v	106	SER

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Mol	Chain	Res	Type
44	v	112	LEU
45	s	61	PHE
45	s	74[A]	ARG
45	s	74[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
4	D	84	HIS
4	D	114	ASN
4	D	200	HIS
5	E	121	GLN
5	E	155	GLN
6	F	200	GLN
6	F	373	ASN
6	F	421	HIS
7	G	28	GLN
7	G	119	GLN
7	G	308	GLN
7	G	459	GLN
7	G	461	ASN
8	H	97	ASN
8	H	317	GLN
11	K	91	GLN
12	L	199	GLN
12	L	351	ASN
12	L	446	ASN
12	L	452	ASN
12	L	470	ASN
12	L	506	ASN
12	L	510	ASN
12	L	579	ASN
13	M	30	HIS
13	M	304	GLN
14	N	91	ASN
14	N	120	GLN
14	N	134	GLN
14	N	171	ASN
14	N	268	GLN
14	N	273	ASN
14	N	316	GLN

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Mol	Chain	Res	Type
15	O	72	GLN
15	O	184	GLN
16	P	87	HIS
17	Q	46	GLN
17	Q	67	ASN
18	R	13	HIS
19	S	24	GLN
21	U	74	GLN
22	V	85	ASN
23	W	58	GLN
24	X	76	HIS
24	X	103	GLN
24	X	139	ASN
29	c	46	ASN
33	g	111	ASN
35	u	13	GLN
38	l	72	ASN
40	n	61	GLN
42	p	54	GLN
42	p	77	GLN
42	p	133	GLN
43	q	17	HIS
45	s	40	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
10	FME	J	1	10	8,9,10	0.96	0	8,9,11	0.88	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	FME	H	1	8	8,9,10	0.99	0	8,9,11	0.89	0
4	2MR	D	85	4	10,12,13	2.51	2 (20%)	5,13,15	0.90	0
11	FME	K	1	-	8,9,10	0.98	0	8,9,11	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FME	J	1	10	-	5/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
11	FME	K	1	-	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.38	1.44	1.33
4	D	85	2MR	CZ-NE	5.23	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	CB-CA-N-CN
10	J	1	FME	N-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	O-C-CA-CB
8	H	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 3 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
48	PC1	B	202	-	45,45,53	0.53	0	51,53,61	0.51	1 (1%)
47	3PE	L	703	-	44,44,50	0.55	0	47,49,55	0.56	1 (2%)
48	PC1	M	503	-	43,43,53	0.55	0	49,51,61	0.51	1 (2%)
47	3PE	O	401	-	47,47,50	0.53	0	50,52,55	0.55	1 (2%)
47	3PE	L	704	-	45,45,50	0.55	0	48,50,55	0.56	1 (2%)
47	3PE	Y	204	-	32,32,50	0.61	0	35,37,55	0.74	2 (5%)
47	3PE	Y	206	-	30,30,50	0.66	0	33,35,55	0.64	1 (3%)
47	3PE	K	101	-	43,43,50	0.56	0	46,48,55	0.56	1 (2%)
48	PC1	A	204	-	32,32,53	0.62	0	38,40,61	0.57	1 (2%)
48	PC1	H	401	-	34,34,53	0.60	0	40,42,61	0.55	1 (2%)
49	SF4	F	501	6	0,12,12	-	-	-	-	-
48	PC1	B	203	-	47,47,53	0.52	0	53,55,61	0.65	2 (3%)
49	SF4	I	202	9	0,12,12	-	-	-	-	-
55	GTP	O	404	54	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
47	3PE	M	504	-	49,49,50	0.52	0	52,54,55	0.54	1 (1%)
56	NDP	P	501	-	51,52,52	2.41	7 (13%)	71,80,80	1.55	15 (21%)
47	3PE	P	502	-	34,34,50	0.60	0	37,39,55	0.71	2 (5%)
48	PC1	H	404	-	47,47,53	0.52	0	53,55,61	0.49	1 (1%)
51	FMN	F	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.21	8 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	SF4	G	801	7	0,12,12	-	-	-		
47	3PE	m	202	-	40,40,50	0.58	0	43,45,55	0.57	1 (2%)
47	3PE	d	202	-	48,48,50	0.52	0	51,53,55	0.54	1 (1%)
47	3PE	H	402	-	35,35,50	0.60	0	38,40,55	0.62	1 (2%)
49	SF4	B	201	2	0,12,12	-	-	-		
53	CDL	h	201	-	79,79,99	0.34	0	85,91,111	0.22	0
53	CDL	H	403	-	50,50,99	0.43	0	56,62,111	0.29	0
47	3PE	N	401	-	44,44,50	0.55	0	47,49,55	0.55	1 (2%)
53	CDL	v	201	-	60,60,99	0.39	0	66,72,111	0.25	0
48	PC1	Y	201	-	34,34,53	0.60	0	40,42,61	0.56	1 (2%)
48	PC1	I	204	-	43,43,53	0.54	0	49,51,61	0.53	1 (2%)
47	3PE	Y	203	-	39,39,50	0.58	0	42,44,55	0.59	1 (2%)
48	PC1	m	201	-	45,45,53	0.54	0	51,53,61	0.51	1 (1%)
48	PC1	A	203	-	34,34,53	0.60	0	40,42,61	0.56	1 (2%)
48	PC1	d	201	-	38,38,53	0.57	0	44,46,61	0.56	1 (2%)
47	3PE	O	402	-	50,50,50	0.50	0	53,55,55	0.62	2 (3%)
49	SF4	G	802	7	0,12,12	-	-	-		
46	FME	L	701	-	8,9,10	0.98	0	8,9,11	0.92	0
53	CDL	M	502	-	85,85,99	0.33	0	91,97,111	0.27	0
47	3PE	A	202	-	46,46,50	0.54	0	49,51,55	0.54	1 (2%)
46	FME	M	501	-	8,9,10	0.98	0	8,9,11	0.94	0
47	3PE	j	101	-	43,43,50	0.55	0	46,48,55	0.57	1 (2%)
46	FME	N	402	-	8,9,10	1.00	0	8,9,11	0.94	0
53	CDL	d	203	-	64,64,99	0.37	0	70,76,111	0.24	0
47	3PE	Y	205	-	29,29,50	0.65	0	32,34,55	0.67	1 (3%)
48	PC1	I	201	-	53,53,53	0.49	0	59,61,61	0.50	1 (1%)
50	FES	E	301	5	0,4,4	-	-	-		
49	SF4	I	203	9	0,12,12	-	-	-		
46	FME	A	201	-	8,9,10	0.97	0	8,9,11	0.95	0
53	CDL	L	702	-	75,75,99	0.34	0	81,87,111	0.23	0
50	FES	G	803	7	0,4,4	-	-	-		
47	3PE	Y	202	-	26,26,50	0.68	0	29,31,55	0.69	1 (3%)
47	3PE	L	705	-	48,48,50	0.52	0	51,53,55	0.55	1 (1%)

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
48	PC1	B	202	-	-	27/49/49/57	-
47	3PE	L	703	-	-	22/48/48/54	-
48	PC1	M	503	-	-	19/47/47/57	-
47	3PE	O	401	-	-	28/51/51/54	-
47	3PE	L	704	-	-	26/49/49/54	-
47	3PE	Y	204	-	-	19/36/36/54	-
47	3PE	Y	206	-	-	14/34/34/54	-
47	3PE	K	101	-	-	22/47/47/54	-
48	PC1	A	204	-	-	18/36/36/57	-
48	PC1	H	401	-	-	8/38/38/57	-
49	SF4	F	501	6	-	-	0/6/5/5
48	PC1	B	203	-	-	15/51/51/57	-
55	GTP	O	404	54	-	5/22/38/38	0/3/3/3
56	NDP	P	501	-	-	10/34/77/77	0/5/5/5
47	3PE	M	504	-	-	20/53/53/54	-
49	SF4	I	202	9	-	-	0/6/5/5
47	3PE	P	502	-	-	15/38/38/54	-
48	PC1	H	404	-	-	12/51/51/57	-
51	FMN	F	502	-	-	4/18/18/18	0/3/3/3
49	SF4	G	801	7	-	-	0/6/5/5
47	3PE	m	202	-	-	14/44/44/54	-
47	3PE	d	202	-	-	21/52/52/54	-
47	3PE	H	402	-	-	8/39/39/54	-
49	SF4	B	201	2	-	-	0/6/5/5
53	CDL	h	201	-	-	59/90/90/110	-
53	CDL	H	403	-	-	38/61/61/110	-
47	3PE	N	401	-	-	21/48/48/54	-
53	CDL	v	201	-	-	33/71/71/110	-
48	PC1	Y	201	-	-	23/38/38/57	-
48	PC1	I	204	-	-	18/47/47/57	-
47	3PE	Y	203	-	-	14/43/43/54	-
48	PC1	m	201	-	-	17/49/49/57	-
48	PC1	A	203	-	-	10/38/38/57	-
48	PC1	d	201	-	-	19/42/42/57	-
47	3PE	O	402	-	-	29/54/54/54	-
49	SF4	G	802	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FME	L	701	-	-	0/7/9/11	-
53	CDL	M	502	-	-	55/96/96/110	-
47	3PE	A	202	-	-	19/50/50/54	-
46	FME	M	501	-	-	3/7/9/11	-
47	3PE	j	101	-	-	17/47/47/54	-
46	FME	N	402	-	-	4/7/9/11	-
53	CDL	d	203	-	-	42/75/75/110	-
47	3PE	Y	205	-	-	8/33/33/54	-
48	PC1	I	201	-	-	19/57/57/57	-
50	FES	E	301	5	-	-	0/1/1/1
49	SF4	I	203	9	-	-	0/6/5/5
46	FME	A	201	-	-	5/7/9/11	-
53	CDL	L	702	-	-	42/86/86/110	-
50	FES	G	803	7	-	-	0/1/1/1
47	3PE	Y	202	-	-	14/30/30/54	-
47	3PE	L	705	-	-	16/52/52/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	13.52	1.83	1.59
56	P	501	NDP	PA-O3	4.93	1.64	1.59
56	P	501	NDP	PN-O5D	4.12	1.75	1.59
51	F	502	FMN	C4A-N5	3.34	1.38	1.30
56	P	501	NDP	O2B-C2B	-3.19	1.33	1.44
51	F	502	FMN	C10-N1	2.46	1.38	1.33
56	P	501	NDP	C5A-C4A	2.45	1.43	1.39
56	P	501	NDP	C2A-N1A	2.25	1.37	1.33
55	O	404	GTP	C2-N3	2.14	1.38	1.33
56	P	501	NDP	O5D-C5D	-2.01	1.37	1.44

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	404	GTP	C5-C4-N3	-5.01	120.41	128.39
55	O	404	GTP	C2-N3-C4	4.57	120.17	112.30
56	P	501	NDP	P2B-O2B-C2B	-4.48	111.46	123.43
56	P	501	NDP	O2B-P2B-O1X	-3.61	96.48	109.33
56	P	501	NDP	O3-PA-O1A	-3.44	100.34	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	F	502	FMN	C4-N3-C2	-3.29	119.80	125.64
55	O	404	GTP	N9-C4-N3	3.26	132.48	125.95
56	P	501	NDP	PA-O5B-C5B	-3.13	103.42	121.35
56	P	501	NDP	PN-O5D-C5D	-2.88	104.85	121.35
55	O	404	GTP	C2-N1-C6	-2.87	119.91	125.11
51	F	502	FMN	O4-C4-C4A	-2.74	119.30	126.53
55	O	404	GTP	N9-C8-N7	-2.73	108.34	113.40
51	F	502	FMN	C4A-C4-N3	2.69	120.10	113.25
47	Y	204	3PE	C2-O21-C21	2.69	124.23	117.80
56	P	501	NDP	O2N-PN-O3	2.62	114.36	107.27
47	O	402	3PE	C2-O21-C21	2.60	124.03	117.80
55	O	404	GTP	C8-N7-C5	2.58	108.86	104.26
47	P	502	3PE	C2-O21-C21	2.56	123.93	117.80
56	P	501	NDP	O3X-P2B-O2X	2.54	117.34	107.80
48	I	201	PC1	O12-P-O14	2.52	124.18	112.44
48	B	203	PC1	C2-O21-C21	2.52	123.82	117.80
55	O	404	GTP	C5-C6-N1	2.49	119.60	113.25
56	P	501	NDP	O2N-PN-O1N	2.48	123.99	112.44
47	L	703	3PE	O12-P-O14	2.48	123.97	112.44
51	F	502	FMN	C4A-C10-N10	2.48	120.03	116.48
47	O	402	3PE	O12-P-O14	2.47	123.94	112.44
48	d	201	PC1	O12-P-O14	2.47	123.92	112.44
47	Y	203	3PE	O12-P-O14	2.47	123.92	112.44
47	Y	204	3PE	O12-P-O14	2.47	123.92	112.44
47	H	402	3PE	O12-P-O14	2.46	123.89	112.44
47	L	704	3PE	O12-P-O14	2.46	123.88	112.44
47	d	202	3PE	O12-P-O14	2.46	123.87	112.44
47	M	504	3PE	O12-P-O14	2.45	123.83	112.44
48	H	401	PC1	O12-P-O14	2.44	123.81	112.44
48	Y	201	PC1	O12-P-O14	2.44	123.80	112.44
47	P	502	3PE	O12-P-O14	2.44	123.79	112.44
47	A	202	3PE	O12-P-O14	2.44	123.77	112.44
47	Y	202	3PE	O12-P-O14	2.43	123.77	112.44
47	L	705	3PE	O12-P-O14	2.43	123.76	112.44
47	m	202	3PE	O12-P-O14	2.43	123.76	112.44
47	Y	205	3PE	O12-P-O14	2.43	123.75	112.44
48	I	204	PC1	O12-P-O14	2.43	123.74	112.44
48	B	203	PC1	O12-P-O14	2.43	123.74	112.44
48	M	503	PC1	O12-P-O14	2.42	123.72	112.44
48	m	201	PC1	O12-P-O14	2.42	123.71	112.44
47	O	401	3PE	O12-P-O14	2.42	123.69	112.44
48	H	404	PC1	O12-P-O14	2.42	123.68	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	K	101	3PE	O12-P-O14	2.41	123.68	112.44
47	j	101	3PE	O12-P-O14	2.41	123.68	112.44
48	A	203	PC1	O12-P-O14	2.41	123.68	112.44
48	A	204	PC1	O12-P-O14	2.41	123.66	112.44
48	B	202	PC1	O12-P-O14	2.41	123.64	112.44
47	Y	206	3PE	O12-P-O14	2.41	123.64	112.44
56	P	501	NDP	C2A-N1A-C6A	-2.40	114.78	118.73
47	N	401	3PE	O12-P-O14	2.39	123.55	112.44
55	O	404	GTP	O6-C6-C5	-2.38	120.26	126.53
56	P	501	NDP	O4B-C4B-C3B	2.35	109.81	105.15
56	P	501	NDP	O5D-PN-O1N	-2.28	99.91	108.94
56	P	501	NDP	N3A-C4A-N9A	2.26	131.02	127.17
55	O	404	GTP	C3'-C2'-C1'	2.26	105.73	101.46
51	F	502	FMN	C5A-C9A-N10	2.17	119.93	117.97
56	P	501	NDP	C5A-C4A-N3A	-2.15	123.76	126.72
51	F	502	FMN	C10-C4A-N5	-2.14	120.43	124.81
56	P	501	NDP	O3X-P2B-O2B	-2.10	97.68	105.85
56	P	501	NDP	C5B-C4B-C3B	-2.07	107.76	115.21
51	F	502	FMN	C9A-C5A-N5	-2.05	120.28	122.45
51	F	502	FMN	C4A-C10-N1	-2.03	119.62	124.59

There are no chirality outliers.

All (852) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	201	FME	O1-CN-N-CA
46	A	201	FME	CB-CA-N-CN
46	A	201	FME	N-CA-CB-CG
46	A	201	FME	C-CA-CB-CG
46	M	501	FME	N-CA-CB-CG
46	M	501	FME	C-CA-CB-CG
46	M	501	FME	O-C-CA-CB
46	N	402	FME	O1-CN-N-CA
46	N	402	FME	C-CA-CB-CG
46	N	402	FME	O-C-CA-CB
47	A	202	3PE	C1-O11-P-O13
47	A	202	3PE	C1-O11-P-O14
47	A	202	3PE	O13-C11-C12-N
47	H	402	3PE	C11-O13-P-O11
47	K	101	3PE	C1-O11-P-O12
47	K	101	3PE	C1-O11-P-O13
47	K	101	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
47	K	101	3PE	C11-O13-P-O14
47	K	101	3PE	O13-C11-C12-N
47	L	703	3PE	C11-O13-P-O14
47	L	703	3PE	C22-C21-O21-C2
47	L	704	3PE	C1-O11-P-O13
47	L	704	3PE	C1-O11-P-O14
47	L	704	3PE	C11-O13-P-O12
47	L	704	3PE	O13-C11-C12-N
47	L	705	3PE	C11-O13-P-O12
47	L	705	3PE	O13-C11-C12-N
47	M	504	3PE	C1-O11-P-O14
47	M	504	3PE	C11-O13-P-O11
47	M	504	3PE	C11-O13-P-O12
47	M	504	3PE	C11-O13-P-O14
47	M	504	3PE	O13-C11-C12-N
47	M	504	3PE	O11-C1-C2-O21
47	N	401	3PE	C1-O11-P-O12
47	N	401	3PE	C1-O11-P-O13
47	N	401	3PE	C1-O11-P-O14
47	N	401	3PE	C11-O13-P-O11
47	N	401	3PE	C11-O13-P-O12
47	O	401	3PE	C1-O11-P-O12
47	O	401	3PE	C1-O11-P-O13
47	O	401	3PE	C11-O13-P-O11
47	O	401	3PE	C11-O13-P-O12
47	O	401	3PE	O13-C11-C12-N
47	O	402	3PE	C1-O11-P-O14
47	O	402	3PE	C11-O13-P-O11
47	O	402	3PE	C11-O13-P-O12
47	O	402	3PE	C11-O13-P-O14
47	O	402	3PE	O13-C11-C12-N
47	P	502	3PE	C11-O13-P-O11
47	P	502	3PE	O13-C11-C12-N
47	Y	202	3PE	C1-O11-P-O12
47	Y	202	3PE	C1-O11-P-O13
47	Y	202	3PE	C11-O13-P-O12
47	Y	202	3PE	C11-O13-P-O14
47	Y	202	3PE	O13-C11-C12-N
47	Y	202	3PE	O22-C21-O21-C2
47	Y	203	3PE	C11-O13-P-O11
47	Y	203	3PE	C11-O13-P-O12
47	Y	203	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
47	Y	204	3PE	C1-O11-P-O12
47	Y	204	3PE	C1-O11-P-O13
47	Y	204	3PE	C11-O13-P-O11
47	Y	204	3PE	C11-O13-P-O12
47	Y	204	3PE	C11-O13-P-O14
47	Y	204	3PE	O13-C11-C12-N
47	Y	205	3PE	O13-C11-C12-N
47	Y	205	3PE	O22-C21-O21-C2
47	Y	206	3PE	C1-O11-P-O12
47	Y	206	3PE	C1-O11-P-O14
47	Y	206	3PE	C11-O13-P-O11
47	Y	206	3PE	C11-O13-P-O14
47	Y	206	3PE	O13-C11-C12-N
47	d	202	3PE	C1-O11-P-O12
47	d	202	3PE	C1-O11-P-O13
47	d	202	3PE	C11-O13-P-O14
47	d	202	3PE	O32-C31-O31-C3
47	j	101	3PE	C1-O11-P-O14
47	j	101	3PE	C11-O13-P-O14
47	j	101	3PE	O22-C21-O21-C2
47	j	101	3PE	C22-C21-O21-C2
47	m	202	3PE	C22-C21-O21-C2
48	A	203	PC1	C11-O13-P-O12
48	A	203	PC1	C11-O13-P-O14
48	A	203	PC1	C11-O13-P-O11
48	A	203	PC1	O22-C21-O21-C2
48	A	203	PC1	C22-C21-O21-C2
48	A	204	PC1	C11-O13-P-O12
48	A	204	PC1	O13-C11-C12-N
48	A	204	PC1	O11-C1-C2-O21
48	A	204	PC1	O22-C21-O21-C2
48	A	204	PC1	C22-C21-O21-C2
48	B	202	PC1	C11-O13-P-O14
48	B	202	PC1	C11-O13-P-O11
48	B	202	PC1	C1-O11-P-O12
48	B	202	PC1	C1-O11-P-O14
48	B	202	PC1	C1-O11-P-O13
48	B	203	PC1	O13-C11-C12-N
48	B	203	PC1	O22-C21-O21-C2
48	B	203	PC1	C22-C21-O21-C2
48	H	404	PC1	O11-C1-C2-O21
48	I	201	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
48	I	204	PC1	C11-O13-P-O12
48	I	204	PC1	C1-O11-P-O14
48	I	204	PC1	O21-C2-C3-O31
48	M	503	PC1	C11-O13-P-O14
48	M	503	PC1	C11-O13-P-O11
48	M	503	PC1	C1-O11-P-O12
48	M	503	PC1	C1-O11-P-O13
48	Y	201	PC1	C11-O13-P-O12
48	Y	201	PC1	C11-O13-P-O11
48	Y	201	PC1	C1-O11-P-O14
48	Y	201	PC1	C1-O11-P-O13
48	Y	201	PC1	O22-C21-O21-C2
48	d	201	PC1	C1-O11-P-O12
48	d	201	PC1	C1-O11-P-O13
48	d	201	PC1	O22-C21-O21-C2
48	m	201	PC1	C1-O11-P-O14
53	H	403	CDL	CA2-C1-CB2-OB2
53	H	403	CDL	CA2-OA2-PA1-OA3
53	H	403	CDL	CA3-OA5-PA1-OA2
53	H	403	CDL	CA3-OA5-PA1-OA4
53	H	403	CDL	CB2-OB2-PB2-OB3
53	H	403	CDL	CB2-OB2-PB2-OB4
53	H	403	CDL	CB2-OB2-PB2-OB5
53	H	403	CDL	CB3-OB5-PB2-OB2
53	H	403	CDL	CB3-OB5-PB2-OB4
53	H	403	CDL	OB7-CB5-OB6-CB4
53	H	403	CDL	C51-CB5-OB6-CB4
53	L	702	CDL	CA3-OA5-PA1-OA2
53	L	702	CDL	CA3-OA5-PA1-OA3
53	L	702	CDL	C11-CA5-OA6-CA4
53	L	702	CDL	CB3-OB5-PB2-OB2
53	L	702	CDL	CB3-OB5-PB2-OB3
53	L	702	CDL	CB3-OB5-PB2-OB4
53	M	502	CDL	CA2-OA2-PA1-OA3
53	M	502	CDL	CB2-OB2-PB2-OB4
53	M	502	CDL	CB2-OB2-PB2-OB5
53	M	502	CDL	CB3-OB5-PB2-OB2
53	M	502	CDL	CB3-OB5-PB2-OB4
53	M	502	CDL	C51-CB5-OB6-CB4
53	d	203	CDL	CA2-OA2-PA1-OA3
53	d	203	CDL	CA2-OA2-PA1-OA4
53	d	203	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
53	d	203	CDL	CA3-OA5-PA1-OA3
53	d	203	CDL	OB5-CB3-CB4-OB6
53	d	203	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CB2-OB2-PB2-OB4
53	h	201	CDL	CB2-OB2-PB2-OB5
53	h	201	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	C51-CB5-OB6-CB4
53	v	201	CDL	CA2-OA2-PA1-OA4
53	v	201	CDL	CA2-OA2-PA1-OA5
53	v	201	CDL	CA3-OA5-PA1-OA2
53	v	201	CDL	C11-CA5-OA6-CA4
53	v	201	CDL	CB3-OB5-PB2-OB2
55	O	404	GTP	C5'-O5'-PA-O3A
55	O	404	GTP	C5'-O5'-PA-O1A
47	O	402	3PE	C32-C31-O31-C3
47	L	704	3PE	O32-C31-O31-C3
47	N	401	3PE	O32-C31-O31-C3
47	O	402	3PE	O32-C31-O31-C3
47	P	502	3PE	O32-C31-O31-C3
47	Y	203	3PE	O32-C31-O31-C3
47	Y	204	3PE	O32-C31-O31-C3
47	m	202	3PE	O32-C31-O31-C3
48	M	503	PC1	O32-C31-O31-C3
47	K	101	3PE	O22-C21-O21-C2
47	L	703	3PE	O22-C21-O21-C2
47	Y	203	3PE	O22-C21-O21-C2
47	m	202	3PE	O22-C21-O21-C2
53	L	702	CDL	OA7-CA5-OA6-CA4
53	M	502	CDL	OB7-CB5-OB6-CB4
53	d	203	CDL	OB7-CB5-OB6-CB4
47	N	401	3PE	C32-C31-O31-C3
47	P	502	3PE	C32-C31-O31-C3
47	Y	203	3PE	C32-C31-O31-C3
47	Y	204	3PE	C32-C31-O31-C3
47	d	202	3PE	C32-C31-O31-C3
47	m	202	3PE	C32-C31-O31-C3
48	M	503	PC1	C32-C31-O31-C3
53	M	502	CDL	C71-CB7-OB8-CB6
53	h	201	CDL	C71-CB7-OB8-CB6
47	K	101	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
47	Y	202	3PE	C22-C21-O21-C2
47	Y	205	3PE	C22-C21-O21-C2
48	Y	201	PC1	C22-C21-O21-C2
48	d	201	PC1	C22-C21-O21-C2
53	d	203	CDL	OB9-CB7-OB8-CB6
47	L	704	3PE	C32-C31-O31-C3
48	I	204	PC1	C32-C31-O31-C3
53	M	502	CDL	OB9-CB7-OB8-CB6
53	h	201	CDL	OB9-CB7-OB8-CB6
53	v	201	CDL	OA7-CA5-OA6-CA4
53	H	403	CDL	C11-CA5-OA6-CA4
56	P	501	NDP	O4D-C4D-C5D-O5D
53	d	203	CDL	C71-CB7-OB8-CB6
48	I	204	PC1	O32-C31-O31-C3
53	M	502	CDL	C16-C17-C18-C19
53	M	502	CDL	C19-C20-C21-C22
53	M	502	CDL	C39-C40-C41-C42
47	P	502	3PE	C22-C21-O21-C2
53	H	403	CDL	OA7-CA5-OA6-CA4
53	H	403	CDL	C31-CA7-OA8-CA6
53	M	502	CDL	C31-C32-C33-C34
53	h	201	CDL	C59-C60-C61-C62
53	d	203	CDL	C37-C38-C39-C40
53	h	201	CDL	C57-C58-C59-C60
48	B	202	PC1	C11-C12-N-C15
53	d	203	CDL	C72-C73-C74-C75
53	v	201	CDL	C17-C18-C19-C20
53	L	702	CDL	C61-C62-C63-C64
53	L	702	CDL	O1-C1-CB2-OB2
53	h	201	CDL	C75-C76-C77-C78
47	L	703	3PE	C21-C22-C23-C24
47	P	502	3PE	C31-C32-C33-C34
53	H	403	CDL	OA9-CA7-OA8-CA6
47	K	101	3PE	O11-C1-C2-O21
48	Y	201	PC1	O11-C1-C2-O21
53	v	201	CDL	OB6-CB4-CB6-OB8
48	m	201	PC1	C21-C22-C23-C24
53	h	201	CDL	C13-C14-C15-C16
48	B	203	PC1	C21-C22-C23-C24
53	d	203	CDL	CB7-C71-C72-C73
55	O	404	GTP	O4'-C4'-C5'-O5'
55	O	404	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C17-C18-C19-C20
47	A	202	3PE	C31-C32-C33-C34
47	P	502	3PE	O22-C21-O21-C2
48	d	201	PC1	C11-C12-N-C13
47	O	401	3PE	C31-C32-C33-C34
48	B	202	PC1	C21-C22-C23-C24
53	L	702	CDL	CA5-C11-C12-C13
53	L	702	CDL	CB7-C71-C72-C73
47	K	101	3PE	C31-C32-C33-C34
47	d	202	3PE	C21-C22-C23-C24
48	Y	201	PC1	C21-C22-C23-C24
53	H	403	CDL	O1-C1-CA2-OA2
53	H	403	CDL	O1-C1-CB2-OB2
53	h	201	CDL	O1-C1-CB2-OB2
48	M	503	PC1	C21-C22-C23-C24
47	m	202	3PE	C31-C32-C33-C34
48	m	201	PC1	C31-C32-C33-C34
53	v	201	CDL	CB7-C71-C72-C73
47	O	402	3PE	C22-C21-O21-C2
48	H	401	PC1	C22-C21-O21-C2
53	d	203	CDL	C32-C33-C34-C35
47	Y	205	3PE	C31-C32-C33-C34
53	H	403	CDL	CB7-C71-C72-C73
47	O	402	3PE	O22-C21-O21-C2
48	H	401	PC1	O22-C21-O21-C2
53	H	403	CDL	CB2-C1-CA2-OA2
53	h	201	CDL	CA2-C1-CB2-OB2
48	A	204	PC1	C32-C31-O31-C3
53	d	203	CDL	C43-C44-C45-C46
53	h	201	CDL	C39-C40-C41-C42
46	N	402	FME	N-CA-CB-CG
48	B	202	PC1	C11-C12-N-C14
47	O	402	3PE	C31-C32-C33-C34
47	L	705	3PE	C31-C32-C33-C34
47	Y	204	3PE	C22-C21-O21-C2
53	L	702	CDL	C13-C14-C15-C16
47	Y	204	3PE	O22-C21-O21-C2
53	v	201	CDL	O1-C1-CA2-OA2
47	L	703	3PE	C25-C26-C27-C28
47	Y	203	3PE	C31-C32-C33-C34
47	L	704	3PE	C22-C21-O21-C2
47	M	504	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
48	d	201	PC1	C11-C12-N-C14
47	d	202	3PE	C35-C36-C37-C38
48	A	203	PC1	C33-C34-C35-C36
47	K	101	3PE	C32-C33-C34-C35
48	Y	201	PC1	C33-C34-C35-C36
48	d	201	PC1	C39-C3A-C3B-C3C
53	h	201	CDL	C40-C41-C42-C43
53	M	502	CDL	C34-C35-C36-C37
53	M	502	CDL	C63-C64-C65-C66
53	v	201	CDL	C51-C52-C53-C54
47	O	401	3PE	C32-C33-C34-C35
47	O	402	3PE	C37-C38-C39-C3A
48	H	404	PC1	C28-C29-C2A-C2B
47	P	502	3PE	C32-C33-C34-C35
48	B	202	PC1	C35-C36-C37-C38
53	M	502	CDL	C40-C41-C42-C43
53	M	502	CDL	C62-C63-C64-C65
53	h	201	CDL	C71-C72-C73-C74
53	M	502	CDL	C18-C19-C20-C21
53	d	203	CDL	C38-C39-C40-C41
47	Y	206	3PE	C22-C21-O21-C2
47	d	202	3PE	C22-C21-O21-C2
47	L	704	3PE	C22-C23-C24-C25
47	d	202	3PE	C36-C37-C38-C39
53	v	201	CDL	O1-C1-CB2-OB2
56	P	501	NDP	O4B-C4B-C5B-O5B
56	P	501	NDP	C3D-C4D-C5D-O5D
47	d	202	3PE	C2D-C2E-C2F-C2G
48	I	201	PC1	C36-C37-C38-C39
53	M	502	CDL	C59-C60-C61-C62
53	M	502	CDL	C15-C16-C17-C18
53	M	502	CDL	CB7-C71-C72-C73
48	A	204	PC1	O32-C31-O31-C3
47	L	703	3PE	C39-C3A-C3B-C3C
47	L	705	3PE	C32-C33-C34-C35
53	L	702	CDL	C37-C38-C39-C40
47	O	401	3PE	C1-C2-C3-O31
47	L	705	3PE	C39-C3A-C3B-C3C
47	O	401	3PE	C33-C34-C35-C36
47	O	401	3PE	C23-C24-C25-C26
47	d	202	3PE	C39-C3A-C3B-C3C
48	B	203	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
48	M	503	PC1	C26-C27-C28-C29
48	d	201	PC1	C32-C33-C34-C35
53	d	203	CDL	C73-C74-C75-C76
48	H	404	PC1	C21-C22-C23-C24
48	I	201	PC1	C29-C2A-C2B-C2C
53	H	403	CDL	C51-C52-C53-C54
53	L	702	CDL	C59-C60-C61-C62
53	M	502	CDL	C52-C53-C54-C55
53	M	502	CDL	C57-C58-C59-C60
53	h	201	CDL	C11-C12-C13-C14
47	L	703	3PE	C32-C33-C34-C35
47	L	704	3PE	C37-C38-C39-C3A
53	H	403	CDL	C31-C32-C33-C34
53	L	702	CDL	C31-C32-C33-C34
53	M	502	CDL	C44-C45-C46-C47
48	B	202	PC1	C11-C12-N-C13
53	h	201	CDL	C31-C32-C33-C34
53	M	502	CDL	C11-C12-C13-C14
47	O	402	3PE	C3E-C3F-C3G-C3H
53	M	502	CDL	C60-C61-C62-C63
48	I	201	PC1	C3E-C3F-C3G-C3H
47	L	704	3PE	O22-C21-O21-C2
47	M	504	3PE	O22-C21-O21-C2
47	Y	206	3PE	O22-C21-O21-C2
47	d	202	3PE	O22-C21-O21-C2
53	h	201	CDL	C60-C61-C62-C63
53	v	201	CDL	C16-C17-C18-C19
53	L	702	CDL	C60-C61-C62-C63
53	M	502	CDL	C55-C56-C57-C58
48	H	404	PC1	C31-C32-C33-C34
47	A	202	3PE	C2C-C2D-C2E-C2F
47	L	703	3PE	C22-C23-C24-C25
47	O	401	3PE	C22-C23-C24-C25
53	M	502	CDL	C32-C33-C34-C35
53	M	502	CDL	C58-C59-C60-C61
53	L	702	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	C11-CA5-OA6-CA4
53	d	203	CDL	C74-C75-C76-C77
53	h	201	CDL	OA7-CA5-OA6-CA4
53	L	702	CDL	C52-C53-C54-C55
47	A	202	3PE	C2B-C2C-C2D-C2E
48	I	201	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	CA7-C31-C32-C33
47	Y	204	3PE	C38-C39-C3A-C3B
53	v	201	CDL	C71-C72-C73-C74
48	d	201	PC1	C11-C12-N-C15
47	O	402	3PE	C21-C22-C23-C24
53	L	702	CDL	C54-C55-C56-C57
47	L	705	3PE	C3A-C3B-C3C-C3D
53	h	201	CDL	OB5-CB3-CB4-OB6
47	O	402	3PE	C34-C35-C36-C37
53	d	203	CDL	C75-C76-C77-C78
47	m	202	3PE	C32-C33-C34-C35
53	h	201	CDL	C34-C35-C36-C37
53	M	502	CDL	C17-C18-C19-C20
53	L	702	CDL	OB6-CB4-CB6-OB8
47	L	705	3PE	C34-C35-C36-C37
48	A	204	PC1	C32-C33-C34-C35
53	d	203	CDL	C71-C72-C73-C74
53	h	201	CDL	C52-C53-C54-C55
53	h	201	CDL	C37-C38-C39-C40
53	L	702	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	C54-C55-C56-C57
48	I	204	PC1	C31-C32-C33-C34
53	L	702	CDL	C57-C58-C59-C60
47	N	401	3PE	C24-C25-C26-C27
48	B	203	PC1	C3A-C3B-C3C-C3D
47	L	703	3PE	C38-C39-C3A-C3B
53	h	201	CDL	C38-C39-C40-C41
47	M	504	3PE	O11-C1-C2-C3
48	H	404	PC1	O11-C1-C2-C3
53	H	403	CDL	OA5-CA3-CA4-CA6
47	Y	202	3PE	C21-C22-C23-C24
47	H	402	3PE	C29-C2A-C2B-C2C
47	j	101	3PE	C37-C38-C39-C3A
53	v	201	CDL	C12-C13-C14-C15
48	H	401	PC1	C33-C34-C35-C36
53	L	702	CDL	C62-C63-C64-C65
47	H	402	3PE	C1-C2-C3-O31
47	N	401	3PE	C1-C2-C3-O31
47	Y	202	3PE	C1-C2-C3-O31
47	Y	204	3PE	C1-C2-C3-O31
47	j	101	3PE	C1-C2-C3-O31
48	B	203	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
48	I	201	PC1	C1-C2-C3-O31
48	m	201	PC1	C1-C2-C3-O31
53	H	403	CDL	CA3-CA4-CA6-OA8
53	L	702	CDL	CB3-CB4-CB6-OB8
53	M	502	CDL	CB3-CB4-CB6-OB8
53	h	201	CDL	CA3-CA4-CA6-OA8
53	h	201	CDL	CB3-CB4-CB6-OB8
53	v	201	CDL	CB3-CB4-CB6-OB8
48	B	202	PC1	C33-C34-C35-C36
47	O	401	3PE	C38-C39-C3A-C3B
47	O	401	3PE	C2B-C2C-C2D-C2E
53	M	502	CDL	C61-C62-C63-C64
53	h	201	CDL	C14-C15-C16-C17
53	L	702	CDL	C63-C64-C65-C66
53	M	502	CDL	C13-C14-C15-C16
53	d	203	CDL	C33-C34-C35-C36
53	L	702	CDL	CB5-C51-C52-C53
47	O	402	3PE	C2D-C2E-C2F-C2G
48	H	401	PC1	O11-C1-C2-O21
47	m	202	3PE	C2C-C2D-C2E-C2F
53	v	201	CDL	C72-C73-C74-C75
48	H	404	PC1	C2B-C2C-C2D-C2E
47	L	705	3PE	C27-C28-C29-C2A
48	H	401	PC1	C25-C26-C27-C28
47	L	704	3PE	C23-C24-C25-C26
47	M	504	3PE	C3E-C3F-C3G-C3H
53	M	502	CDL	C38-C39-C40-C41
53	d	203	CDL	C42-C43-C44-C45
47	N	401	3PE	C2E-C2F-C2G-C2H
47	H	402	3PE	O21-C2-C3-O31
47	j	101	3PE	O21-C2-C3-O31
53	H	403	CDL	OA6-CA4-CA6-OA8
53	d	203	CDL	C44-C45-C46-C47
47	j	101	3PE	C25-C26-C27-C28
48	B	203	PC1	C39-C3A-C3B-C3C
47	O	401	3PE	C37-C38-C39-C3A
48	I	201	PC1	C26-C27-C28-C29
53	h	201	CDL	C73-C74-C75-C76
53	H	403	CDL	C54-C55-C56-C57
53	H	403	CDL	C32-C33-C34-C35
53	L	702	CDL	C16-C17-C18-C19
53	d	203	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
53	M	502	CDL	C51-C52-C53-C54
55	O	404	GTP	PB-O3A-PA-O1A
56	P	501	NDP	PN-O3-PA-O1A
48	B	202	PC1	C34-C35-C36-C37
53	H	403	CDL	C71-C72-C73-C74
53	d	203	CDL	C77-C78-C79-C80
47	N	401	3PE	C29-C2A-C2B-C2C
47	O	401	3PE	C3A-C3B-C3C-C3D
53	L	702	CDL	C14-C15-C16-C17
48	I	201	PC1	C32-C31-O31-C3
47	N	401	3PE	C2-C1-O11-P
47	O	401	3PE	C2-C1-O11-P
47	N	401	3PE	C39-C3A-C3B-C3C
47	O	402	3PE	C2B-C2C-C2D-C2E
47	K	101	3PE	O11-C1-C2-C3
47	Y	206	3PE	O11-C1-C2-C3
48	A	204	PC1	O11-C1-C2-C3
48	Y	201	PC1	O11-C1-C2-C3
48	m	201	PC1	O11-C1-C2-C3
53	h	201	CDL	OB5-CB3-CB4-CB6
53	M	502	CDL	C24-C25-C26-C27
53	h	201	CDL	C18-C19-C20-C21
53	M	502	CDL	C33-C34-C35-C36
53	d	203	CDL	C11-C12-C13-C14
47	j	101	3PE	C24-C25-C26-C27
47	j	101	3PE	C36-C37-C38-C39
48	H	404	PC1	C22-C21-O21-C2
47	Y	205	3PE	C21-C22-C23-C24
53	v	201	CDL	CA7-C31-C32-C33
47	L	703	3PE	C1-C2-C3-O31
48	I	204	PC1	C1-C2-C3-O31
53	H	403	CDL	CB3-CB4-CB6-OB8
53	d	203	CDL	CA3-CA4-CA6-OA8
53	d	203	CDL	CB3-CB4-CB6-OB8
53	M	502	CDL	CA5-C11-C12-C13
47	L	703	3PE	C3A-C3B-C3C-C3D
47	O	402	3PE	C35-C36-C37-C38
53	h	201	CDL	C61-C62-C63-C64
47	N	401	3PE	O11-C1-C2-O21
53	d	203	CDL	OA5-CA3-CA4-OA6
48	B	202	PC1	C32-C33-C34-C35
47	Y	206	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
48	B	203	PC1	C2-C1-O11-P
48	B	202	PC1	C39-C3A-C3B-C3C
47	L	705	3PE	C3C-C3D-C3E-C3F
48	M	503	PC1	C2B-C2C-C2D-C2E
47	H	402	3PE	C28-C29-C2A-C2B
53	L	702	CDL	C12-C13-C14-C15
47	L	703	3PE	C3F-C3G-C3H-C3I
53	h	201	CDL	C36-C37-C38-C39
47	K	101	3PE	O21-C2-C3-O31
47	L	703	3PE	O21-C2-C3-O31
47	N	401	3PE	O21-C2-C3-O31
47	Y	202	3PE	O21-C2-C3-O31
47	Y	204	3PE	O21-C2-C3-O31
48	Y	201	PC1	O21-C2-C3-O31
53	M	502	CDL	OA6-CA4-CA6-OA8
53	v	201	CDL	OA6-CA4-CA6-OA8
47	L	703	3PE	C33-C34-C35-C36
48	M	503	PC1	C22-C23-C24-C25
47	K	101	3PE	C29-C2A-C2B-C2C
48	M	503	PC1	C32-C33-C34-C35
47	L	705	3PE	C21-C22-C23-C24
47	L	704	3PE	C32-C33-C34-C35
48	I	201	PC1	C2D-C2E-C2F-C2G
53	d	203	CDL	C31-C32-C33-C34
47	L	705	3PE	C38-C39-C3A-C3B
48	B	202	PC1	C3A-C3B-C3C-C3D
47	N	401	3PE	O11-C1-C2-C3
47	P	502	3PE	O11-C1-C2-C3
47	Y	204	3PE	O11-C1-C2-C3
47	d	202	3PE	O11-C1-C2-C3
48	A	203	PC1	O11-C1-C2-C3
48	H	401	PC1	O11-C1-C2-C3
53	d	203	CDL	OA5-CA3-CA4-CA6
53	d	203	CDL	OB5-CB3-CB4-CB6
47	O	402	3PE	C36-C37-C38-C39
48	H	404	PC1	C2D-C2E-C2F-C2G
48	m	201	PC1	C36-C37-C38-C39
53	h	201	CDL	C72-C73-C74-C75
53	h	201	CDL	C33-C34-C35-C36
48	I	201	PC1	O32-C31-O31-C3
53	L	702	CDL	C38-C39-C40-C41
47	O	402	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
47	P	502	3PE	C3-C2-O21-C21
53	H	403	CDL	CA3-CA4-OA6-CA5
47	j	101	3PE	C32-C33-C34-C35
47	N	401	3PE	C26-C27-C28-C29
48	I	201	PC1	C3A-C3B-C3C-C3D
53	L	702	CDL	C51-C52-C53-C54
48	I	204	PC1	C25-C26-C27-C28
47	P	502	3PE	O11-C1-C2-O21
47	Y	204	3PE	O11-C1-C2-O21
47	Y	206	3PE	O11-C1-C2-O21
47	j	101	3PE	O11-C1-C2-O21
48	m	201	PC1	O11-C1-C2-O21
53	H	403	CDL	OA5-CA3-CA4-OA6
47	A	202	3PE	C39-C3A-C3B-C3C
53	v	201	CDL	CA3-CA4-CA6-OA8
53	v	201	CDL	C11-C12-C13-C14
47	P	502	3PE	C12-C11-O13-P
48	Y	201	PC1	C31-C32-C33-C34
48	H	404	PC1	C23-C24-C25-C26
47	O	401	3PE	O21-C2-C3-O31
53	d	203	CDL	OA6-CA4-CA6-OA8
53	h	201	CDL	OA6-CA4-CA6-OA8
47	L	704	3PE	C39-C3A-C3B-C3C
53	L	702	CDL	C39-C40-C41-C42
47	m	202	3PE	C29-C2A-C2B-C2C
47	m	202	3PE	C2A-C2B-C2C-C2D
47	m	202	3PE	C2D-C2E-C2F-C2G
48	B	202	PC1	C37-C38-C39-C3A
47	K	101	3PE	C35-C36-C37-C38
53	d	203	CDL	C52-C51-CB5-OB6
48	A	203	PC1	O13-C11-C12-N
48	Y	201	PC1	O13-C11-C12-N
48	m	201	PC1	O13-C11-C12-N
48	I	204	PC1	C26-C27-C28-C29
53	d	203	CDL	C34-C35-C36-C37
53	M	502	CDL	C53-C54-C55-C56
47	M	504	3PE	C33-C34-C35-C36
47	j	101	3PE	C32-C31-O31-C3
47	H	402	3PE	C26-C27-C28-C29
53	H	403	CDL	C52-C53-C54-C55
53	h	201	CDL	C74-C75-C76-C77
51	F	502	FMN	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
47	L	704	3PE	O11-C1-C2-C3
47	O	402	3PE	O11-C1-C2-C3
47	j	101	3PE	O11-C1-C2-C3
53	M	502	CDL	C32-C31-CA7-OA8
47	A	202	3PE	C2A-C2B-C2C-C2D
48	H	404	PC1	O22-C21-O21-C2
47	A	202	3PE	C2D-C2E-C2F-C2G
53	h	201	CDL	C15-C16-C17-C18
47	L	703	3PE	C32-C31-O31-C3
47	P	502	3PE	C38-C39-C3A-C3B
47	L	704	3PE	O11-C1-C2-O21
47	d	202	3PE	O11-C1-C2-O21
48	A	203	PC1	O11-C1-C2-O21
47	H	402	3PE	C23-C24-C25-C26
48	I	204	PC1	C11-C12-N-C13
48	I	204	PC1	C11-C12-N-C14
48	B	203	PC1	C37-C38-C39-C3A
53	M	502	CDL	C41-C42-C43-C44
56	P	501	NDP	O4D-C1D-N1N-C6N
48	I	204	PC1	C27-C28-C29-C2A
47	m	202	3PE	O21-C2-C3-O31
48	B	203	PC1	O21-C2-C3-O31
48	I	201	PC1	O21-C2-C3-O31
48	m	201	PC1	O21-C2-C3-O31
53	H	403	CDL	OB6-CB4-CB6-OB8
53	d	203	CDL	OB6-CB4-CB6-OB8
53	h	201	CDL	OB6-CB4-CB6-OB8
48	m	201	PC1	C38-C39-C3A-C3B
47	m	202	3PE	C1-C2-C3-O31
48	Y	201	PC1	C1-C2-C3-O31
47	O	402	3PE	C3D-C3E-C3F-C3G
47	j	101	3PE	O32-C31-O31-C3
48	I	201	PC1	C39-C3A-C3B-C3C
47	L	703	3PE	O32-C31-O31-C3
48	H	401	PC1	C32-C33-C34-C35
47	A	202	3PE	C1-O11-P-O12
47	H	402	3PE	C1-O11-P-O14
47	K	101	3PE	C11-O13-P-O11
47	K	101	3PE	C11-O13-P-O12
47	L	704	3PE	C1-O11-P-O12
47	L	704	3PE	C11-O13-P-O11
47	L	704	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
47	L	705	3PE	C1-O11-P-O14
47	M	504	3PE	C1-O11-P-O13
47	O	401	3PE	C1-O11-P-O14
47	P	502	3PE	C11-O13-P-O14
47	Y	202	3PE	C11-O13-P-O11
47	Y	204	3PE	C1-O11-P-O14
47	Y	206	3PE	C1-O11-P-O13
47	Y	206	3PE	C11-O13-P-O12
47	d	202	3PE	C1-O11-P-O14
47	d	202	3PE	C11-O13-P-O11
48	A	204	PC1	C11-O13-P-O11
48	B	202	PC1	C11-O13-P-O12
48	I	204	PC1	C11-O13-P-O14
48	I	204	PC1	C11-O13-P-O11
48	M	503	PC1	C11-O13-P-O12
48	M	503	PC1	C1-O11-P-O14
48	Y	201	PC1	C11-O13-P-O14
48	Y	201	PC1	C1-O11-P-O12
48	d	201	PC1	C11-O13-P-O14
48	d	201	PC1	C11-O13-P-O11
48	m	201	PC1	C1-O11-P-O12
48	m	201	PC1	C1-O11-P-O13
53	H	403	CDL	CB3-OB5-PB2-OB3
53	L	702	CDL	CA3-OA5-PA1-OA4
53	M	502	CDL	CB3-OB5-PB2-OB3
53	d	203	CDL	CA2-OA2-PA1-OA5
53	d	203	CDL	CA3-OA5-PA1-OA4
53	d	203	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CA3-OA5-PA1-OA2
53	v	201	CDL	CA2-OA2-PA1-OA3
53	v	201	CDL	CA3-OA5-PA1-OA3
53	v	201	CDL	CB2-OB2-PB2-OB3
56	P	501	NDP	C5B-O5B-PA-O1A
47	Y	203	3PE	C32-C33-C34-C35
53	M	502	CDL	C14-C15-C16-C17
53	M	502	CDL	C1-CA2-OA2-PA1
53	M	502	CDL	C1-CB2-OB2-PB2
53	M	502	CDL	C37-C38-C39-C40
48	I	204	PC1	C28-C29-C2A-C2B
47	L	705	3PE	C3B-C3C-C3D-C3E
47	A	202	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
47	Y	204	3PE	C3-C2-O21-C21
53	H	403	CDL	CB3-CB4-OB6-CB5
47	d	202	3PE	C26-C27-C28-C29
48	I	204	PC1	C11-C12-N-C15
48	I	204	PC1	O11-C1-C2-C3
47	O	402	3PE	C3C-C3D-C3E-C3F
53	L	702	CDL	C15-C16-C17-C18
53	h	201	CDL	C53-C54-C55-C56
53	L	702	CDL	C71-C72-C73-C74
47	d	202	3PE	C22-C23-C24-C25
53	h	201	CDL	C1-CA2-OA2-PA1
47	A	202	3PE	O31-C31-C32-C33
53	L	702	CDL	C36-C37-C38-C39
47	O	401	3PE	C22-C21-O21-C2
56	P	501	NDP	PN-O3-PA-O2A
47	L	703	3PE	C28-C29-C2A-C2B
47	O	401	3PE	C25-C26-C27-C28
47	M	504	3PE	C34-C35-C36-C37
53	d	203	CDL	C52-C51-CB5-OB7
47	L	704	3PE	C36-C37-C38-C39
47	K	101	3PE	C32-C31-O31-C3
53	h	201	CDL	C55-C56-C57-C58
47	O	401	3PE	O22-C21-O21-C2
56	P	501	NDP	C2B-O2B-P2B-O2X
47	P	502	3PE	C35-C36-C37-C38
48	B	202	PC1	O11-C1-C2-O21
48	d	201	PC1	O11-C1-C2-O21
47	L	704	3PE	C21-C22-C23-C24
47	K	101	3PE	O32-C31-O31-C3
47	O	402	3PE	C22-C23-C24-C25
47	Y	202	3PE	C23-C24-C25-C26
47	Y	203	3PE	C2D-C2E-C2F-C2G
53	M	502	CDL	C42-C43-C44-C45
53	H	403	CDL	CA7-C31-C32-C33
47	O	402	3PE	O21-C2-C3-O31
47	O	401	3PE	C28-C29-C2A-C2B
48	B	203	PC1	C26-C27-C28-C29
48	m	201	PC1	C37-C38-C39-C3A
47	O	401	3PE	C27-C28-C29-C2A
48	B	203	PC1	C25-C26-C27-C28
47	L	704	3PE	C2-C1-O11-P
48	A	204	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
47	M	504	3PE	C28-C29-C2A-C2B
47	d	202	3PE	C29-C2A-C2B-C2C
47	A	202	3PE	C3A-C3B-C3C-C3D
53	M	502	CDL	C54-C55-C56-C57
47	Y	202	3PE	C3-C2-O21-C21
47	Y	205	3PE	C3-C2-O21-C21
53	H	403	CDL	CB6-CB4-OB6-CB5
53	h	201	CDL	CB6-CB4-OB6-CB5
48	M	503	PC1	C27-C28-C29-C2A
48	M	503	PC1	C2D-C2E-C2F-C2G
47	L	704	3PE	C28-C29-C2A-C2B
48	d	201	PC1	C3A-C3B-C3C-C3D
48	A	204	PC1	C21-C22-C23-C24
47	O	402	3PE	O11-C1-C2-O21
48	d	201	PC1	C31-C32-C33-C34
47	N	401	3PE	C33-C34-C35-C36
47	L	704	3PE	C2C-C2D-C2E-C2F
47	Y	205	3PE	C23-C24-C25-C26
47	m	202	3PE	C26-C27-C28-C29
53	L	702	CDL	C40-C41-C42-C43
53	M	502	CDL	CB5-C51-C52-C53
47	d	202	3PE	C3A-C3B-C3C-C3D
53	v	201	CDL	CA2-C1-CB2-OB2
48	B	202	PC1	C3D-C3E-C3F-C3G
47	M	504	3PE	C38-C39-C3A-C3B
48	Y	201	PC1	C25-C26-C27-C28
47	A	202	3PE	C38-C39-C3A-C3B
47	L	704	3PE	C38-C39-C3A-C3B
47	Y	206	3PE	C35-C36-C37-C38
48	m	201	PC1	C29-C2A-C2B-C2C
47	Y	203	3PE	C2-C1-O11-P
53	L	702	CDL	CA4-CA3-OA5-PA1
53	d	203	CDL	C1-CB2-OB2-PB2
47	L	705	3PE	C23-C24-C25-C26
47	m	202	3PE	C28-C29-C2A-C2B
48	m	201	PC1	C35-C36-C37-C38
47	d	202	3PE	C28-C29-C2A-C2B
48	B	202	PC1	C38-C39-C3A-C3B
47	K	101	3PE	C1-C2-C3-O31
48	B	203	PC1	C34-C35-C36-C37
53	h	201	CDL	C76-C77-C78-C79
53	v	201	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
48	I	204	PC1	O11-C1-C2-O21
47	K	101	3PE	C33-C34-C35-C36
53	v	201	CDL	C54-C55-C56-C57
47	N	401	3PE	O22-C21-O21-C2
53	L	702	CDL	CA2-C1-CB2-OB2
48	A	203	PC1	C34-C35-C36-C37
48	B	202	PC1	O11-C1-C2-C3
53	M	502	CDL	OB6-CB4-CB6-OB8
48	d	201	PC1	C21-C22-C23-C24
48	I	201	PC1	C2-C1-O11-P
47	K	101	3PE	C3A-C3B-C3C-C3D
47	M	504	3PE	C39-C3A-C3B-C3C
48	M	503	PC1	C2A-C2B-C2C-C2D
53	v	201	CDL	C73-C74-C75-C76
56	P	501	NDP	C3B-C4B-C5B-O5B
48	m	201	PC1	O21-C21-C22-C23
47	M	504	3PE	C29-C2A-C2B-C2C
51	F	502	FMN	O2'-C2'-C3'-C4'
48	I	201	PC1	O22-C21-O21-C2
48	d	201	PC1	C37-C38-C39-C3A
48	M	503	PC1	C28-C29-C2A-C2B
47	Y	202	3PE	C1-C2-O21-C21
48	A	204	PC1	C3-C2-O21-C21
53	M	502	CDL	CB6-CB4-OB6-CB5
48	B	203	PC1	C33-C34-C35-C36
48	m	201	PC1	C26-C27-C28-C29
47	L	703	3PE	C2-C1-O11-P
53	h	201	CDL	CB2-C1-CA2-OA2
53	M	502	CDL	CA3-CA4-CA6-OA8
47	N	401	3PE	C22-C23-C24-C25
47	A	202	3PE	C32-C33-C34-C35
48	A	204	PC1	C33-C34-C35-C36
48	A	204	PC1	O31-C31-C32-C33
53	M	502	CDL	C72-C71-CB7-OB8
48	B	202	PC1	C3E-C3F-C3G-C3H
48	B	202	PC1	O21-C21-C22-C23
48	H	404	PC1	C2C-C2D-C2E-C2F
47	N	401	3PE	C22-C21-O21-C2
51	F	502	FMN	O2'-C2'-C3'-O3'
47	j	101	3PE	C23-C24-C25-C26
47	O	401	3PE	C36-C37-C38-C39
47	j	101	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
48	Y	201	PC1	O31-C31-C32-C33
48	I	201	PC1	C22-C21-O21-C2
47	L	703	3PE	C27-C28-C29-C2A
48	A	204	PC1	C23-C24-C25-C26
53	h	201	CDL	C72-C71-CB7-OB8
53	v	201	CDL	C52-C51-CB5-OB6
47	Y	203	3PE	C2F-C2G-C2H-C2I
47	Y	203	3PE	C2C-C2D-C2E-C2F
48	Y	201	PC1	O21-C21-C22-C23
53	d	203	CDL	C12-C11-CA5-OA6
47	O	402	3PE	C38-C39-C3A-C3B
48	d	201	PC1	O21-C21-C22-C23
47	Y	204	3PE	O21-C21-C22-C23
47	A	202	3PE	C24-C25-C26-C27
47	O	401	3PE	O21-C21-C22-C23
48	I	201	PC1	O31-C31-C32-C33
48	M	503	PC1	C33-C34-C35-C36
48	d	201	PC1	C35-C36-C37-C38
47	L	705	3PE	O21-C21-C22-C23
48	I	201	PC1	C3C-C3D-C3E-C3F
47	L	703	3PE	O31-C31-C32-C33
48	B	202	PC1	O31-C31-C32-C33
53	H	403	CDL	C12-C11-CA5-OA6
53	h	201	CDL	C52-C51-CB5-OB6
47	Y	203	3PE	C34-C35-C36-C37
51	F	502	FMN	N10-C1'-C2'-O2'
48	M	503	PC1	C23-C24-C25-C26
48	H	401	PC1	C21-C22-C23-C24
47	Y	205	3PE	C1-C2-O21-C21
53	h	201	CDL	C32-C31-CA7-OA8
47	A	202	3PE	C29-C2A-C2B-C2C
53	L	702	CDL	C55-C56-C57-C58
47	O	401	3PE	C3C-C3D-C3E-C3F
47	A	202	3PE	C2E-C2F-C2G-C2H
46	A	201	FME	CB-CG-SD-CE
47	O	402	3PE	C39-C3A-C3B-C3C
48	B	202	PC1	C3C-C3D-C3E-C3F
48	Y	201	PC1	O22-C21-C22-C23
48	Y	201	PC1	O32-C31-O31-C3
47	O	401	3PE	O11-C1-C2-O21
48	H	404	PC1	C22-C23-C24-C25
53	v	201	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
48	Y	201	PC1	C32-C31-O31-C3
53	v	201	CDL	C31-C32-C33-C34
53	h	201	CDL	C32-C33-C34-C35
48	A	204	PC1	O32-C31-C32-C33
48	Y	201	PC1	O32-C31-C32-C33
53	v	201	CDL	C52-C51-CB5-OB7
53	v	201	CDL	C15-C16-C17-C18
47	M	504	3PE	O31-C31-C32-C33
47	L	705	3PE	O22-C21-C22-C23
47	L	703	3PE	C3D-C3E-C3F-C3G
47	A	202	3PE	C36-C37-C38-C39
48	B	202	PC1	O22-C21-C22-C23
53	d	203	CDL	C12-C11-CA5-OA7
48	B	202	PC1	O32-C31-C32-C33
47	O	402	3PE	O21-C21-C22-C23
47	Y	203	3PE	C22-C23-C24-C25
47	O	402	3PE	C1-C2-C3-O31
47	Y	204	3PE	O22-C21-C22-C23
48	I	201	PC1	O32-C31-C32-C33
53	M	502	CDL	C72-C71-CB7-OB9
53	h	201	CDL	C32-C31-CA7-OA9
53	h	201	CDL	C52-C51-CB5-OB7
47	O	401	3PE	O22-C21-C22-C23
48	d	201	PC1	O22-C21-C22-C23
53	h	201	CDL	C72-C71-CB7-OB9
56	P	501	NDP	C2D-C1D-N1N-C6N
47	M	504	3PE	C2A-C2B-C2C-C2D
53	h	201	CDL	C35-C36-C37-C38
47	L	704	3PE	C24-C25-C26-C27
47	K	101	3PE	O21-C21-C22-C23
48	A	204	PC1	O21-C21-C22-C23
53	H	403	CDL	C52-C51-CB5-OB6
47	L	703	3PE	O32-C31-C32-C33
47	Y	206	3PE	O31-C31-C32-C33
53	L	702	CDL	C32-C31-CA7-OA8
47	M	504	3PE	O32-C31-C32-C33
47	L	704	3PE	C26-C27-C28-C29

There are no ring outliers.

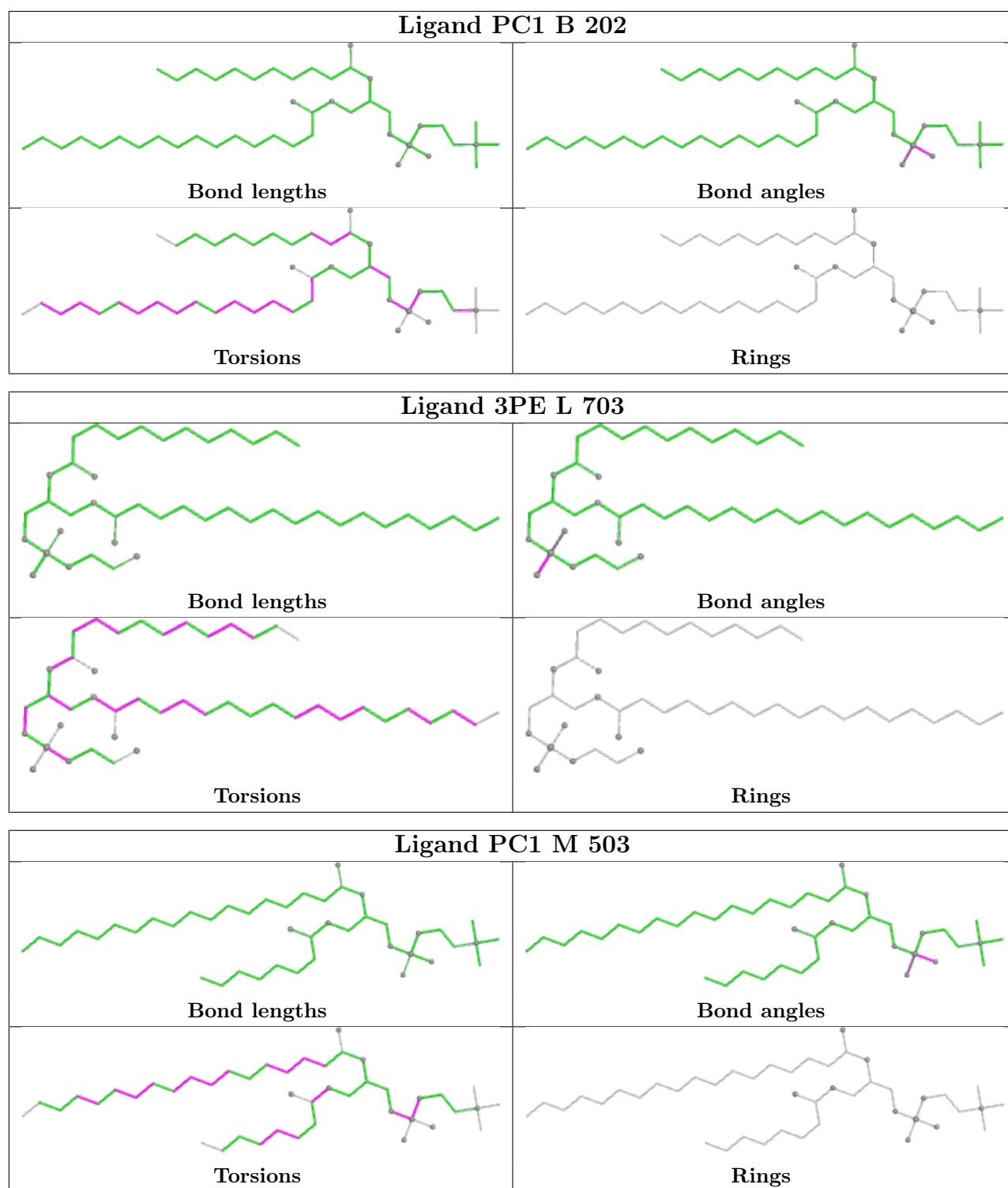
30 monomers are involved in 64 short contacts:



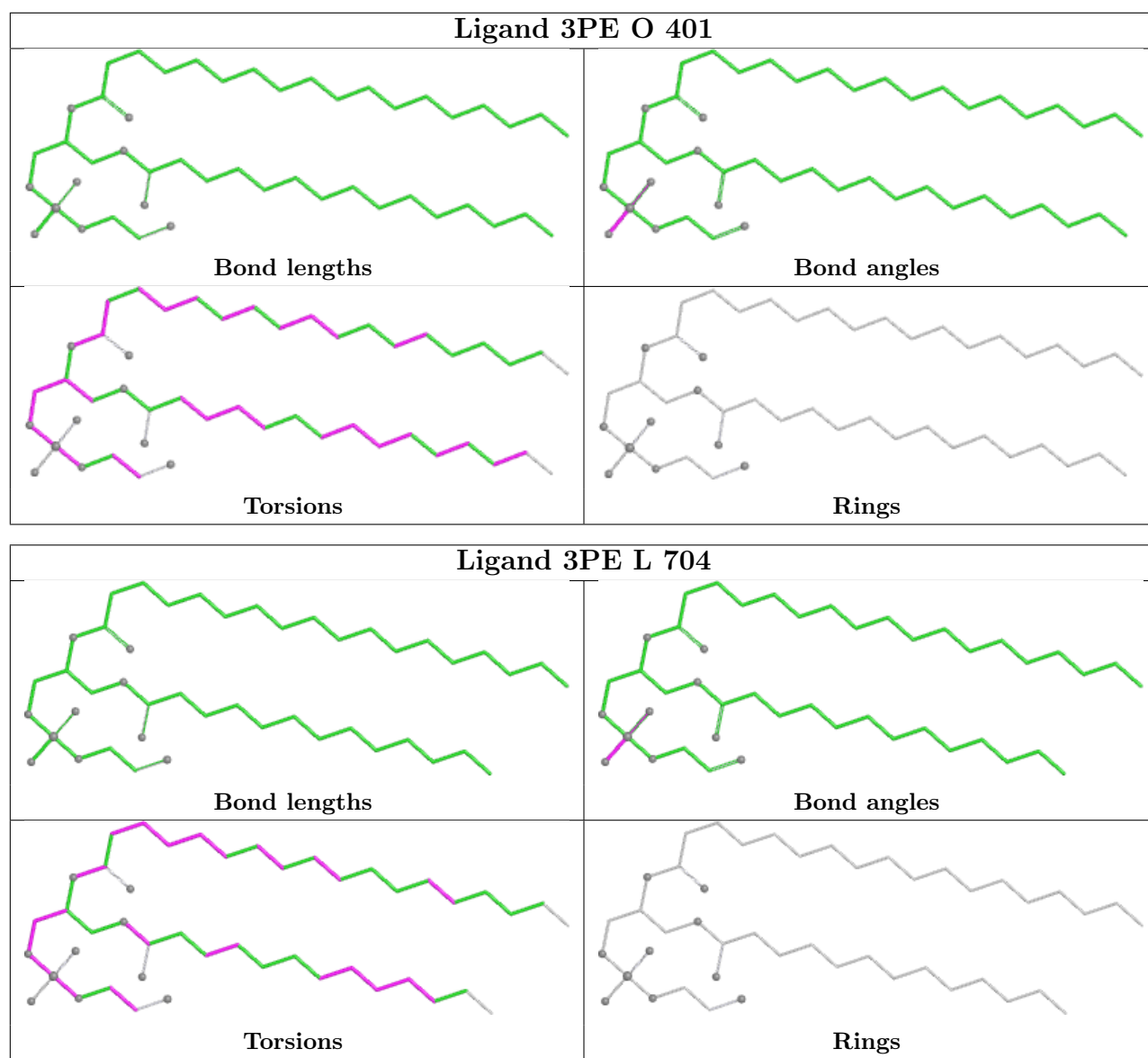
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	B	202	PC1	1	0
48	M	503	PC1	2	0
47	O	401	3PE	3	0
47	Y	204	3PE	1	0
47	Y	206	3PE	2	0
47	K	101	3PE	2	0
48	A	204	PC1	1	0
48	H	401	PC1	2	0
48	B	203	PC1	2	0
55	O	404	GTP	3	0
47	M	504	3PE	1	0
48	H	404	PC1	1	0
51	F	502	FMN	2	0
47	m	202	3PE	1	0
47	d	202	3PE	3	0
47	H	402	3PE	1	0
53	h	201	CDL	3	0
53	H	403	CDL	1	0
53	v	201	CDL	1	0
48	I	204	PC1	2	0
48	m	201	PC1	1	0
48	A	203	PC1	1	0
48	d	201	PC1	6	0
47	O	402	3PE	3	0
53	M	502	CDL	8	0
47	A	202	3PE	2	0
47	j	101	3PE	3	0
53	d	203	CDL	5	0
47	Y	205	3PE	1	0
53	L	702	CDL	3	0

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



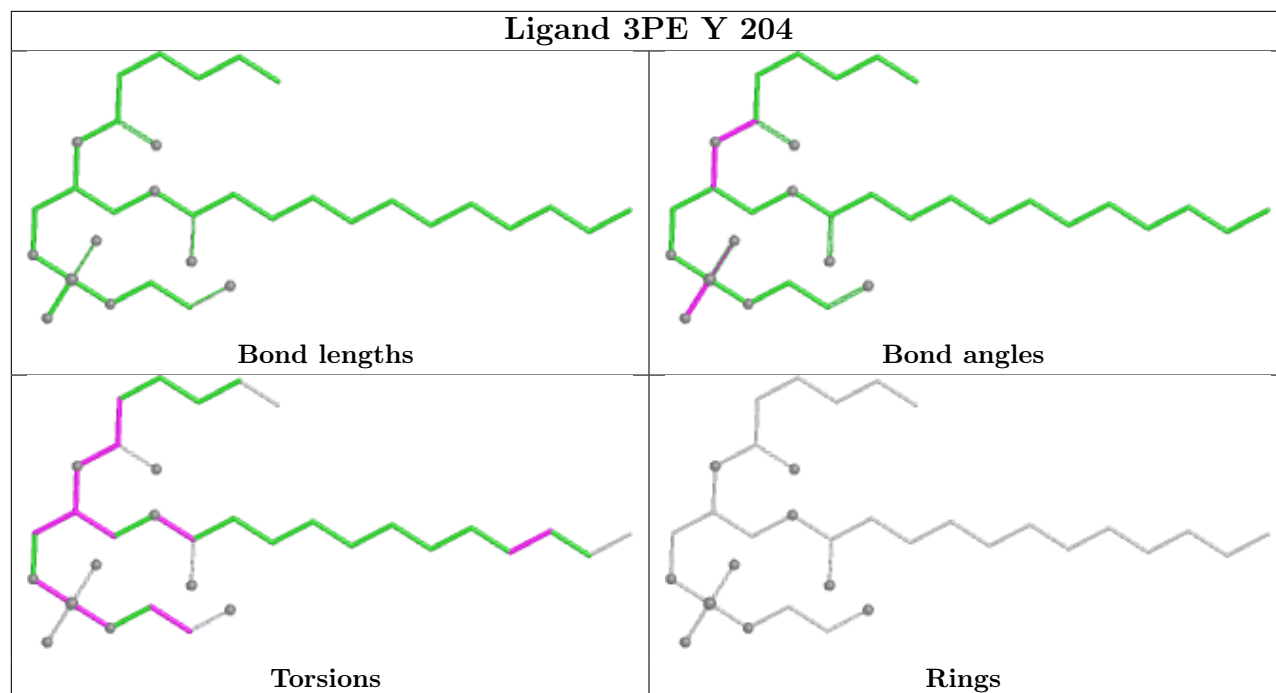




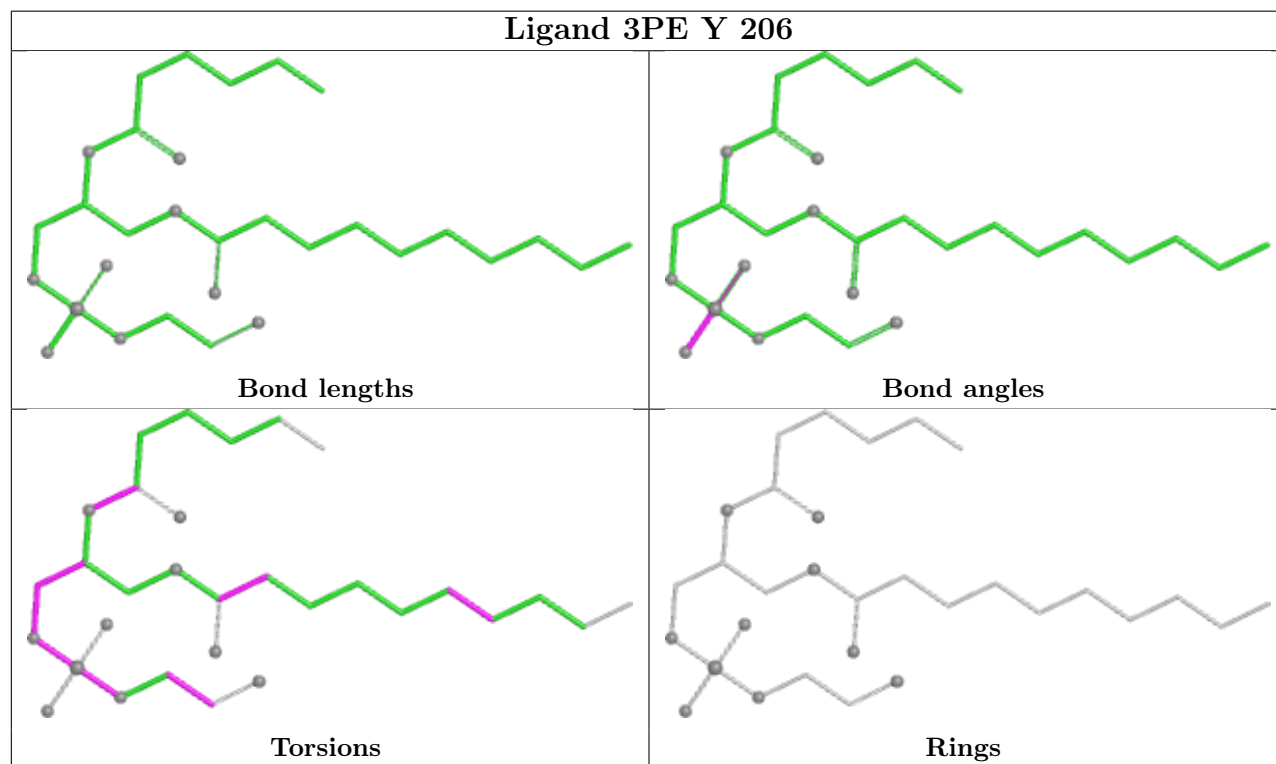




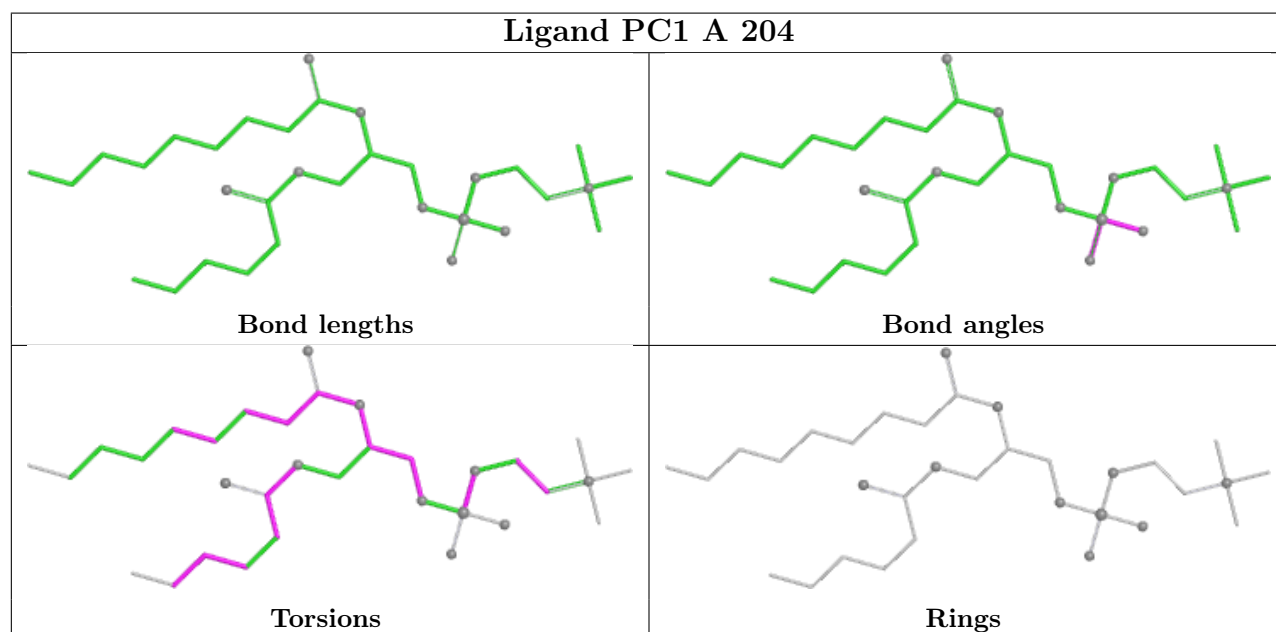
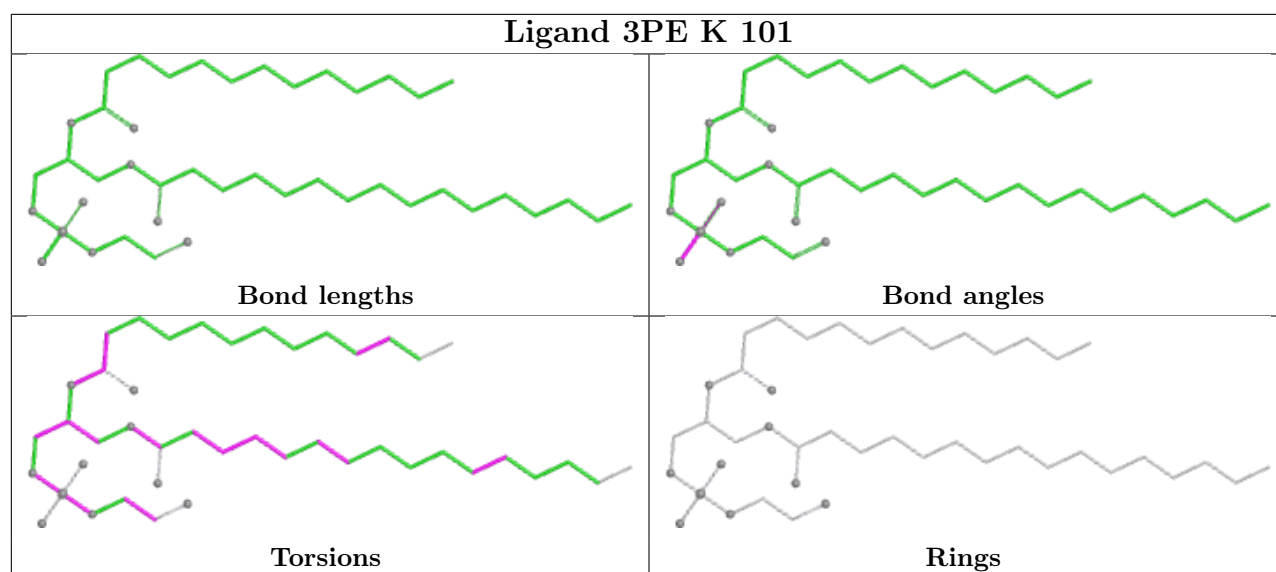
## Ligand 3PE Y 204



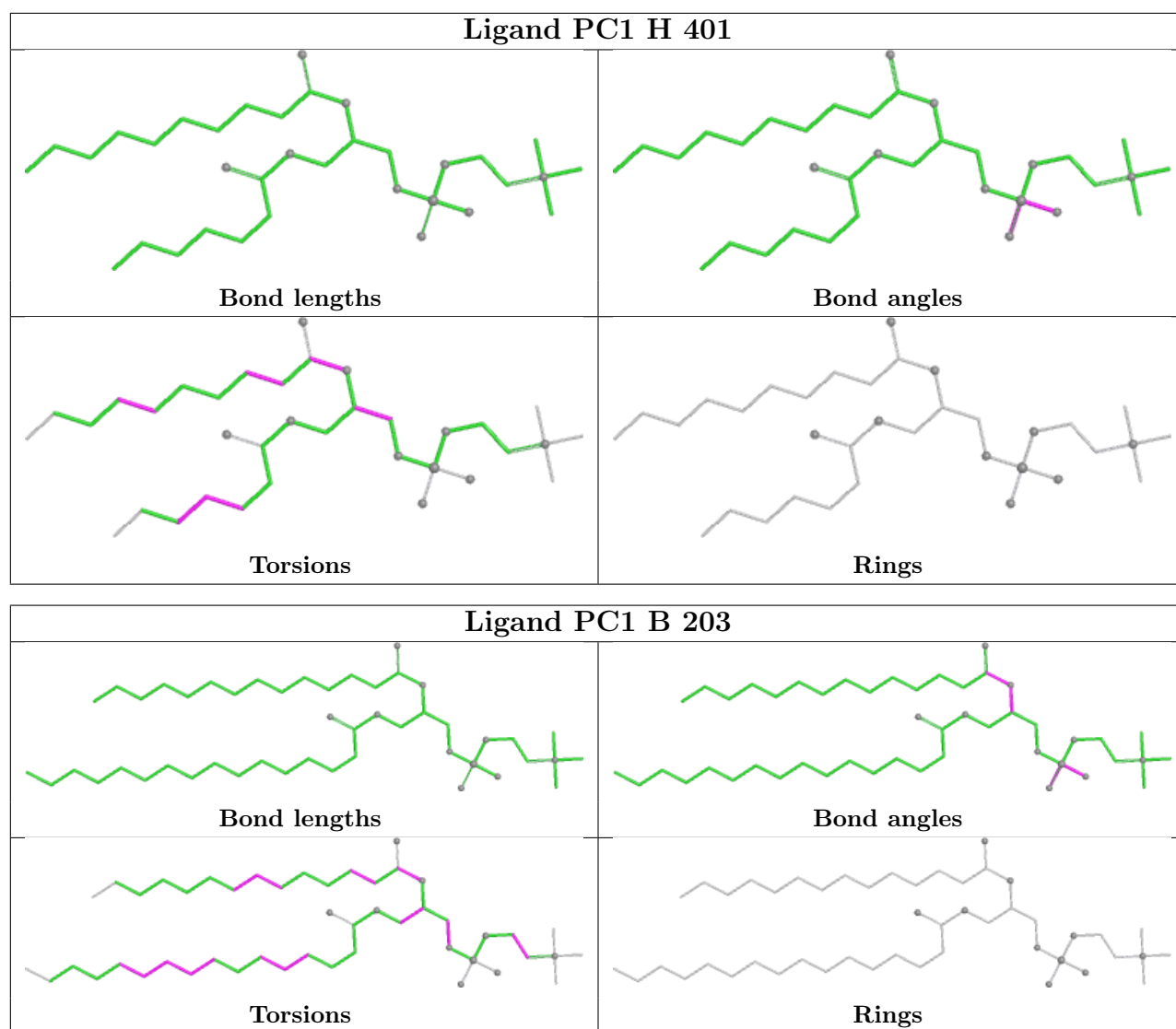
## Ligand 3PE Y 206



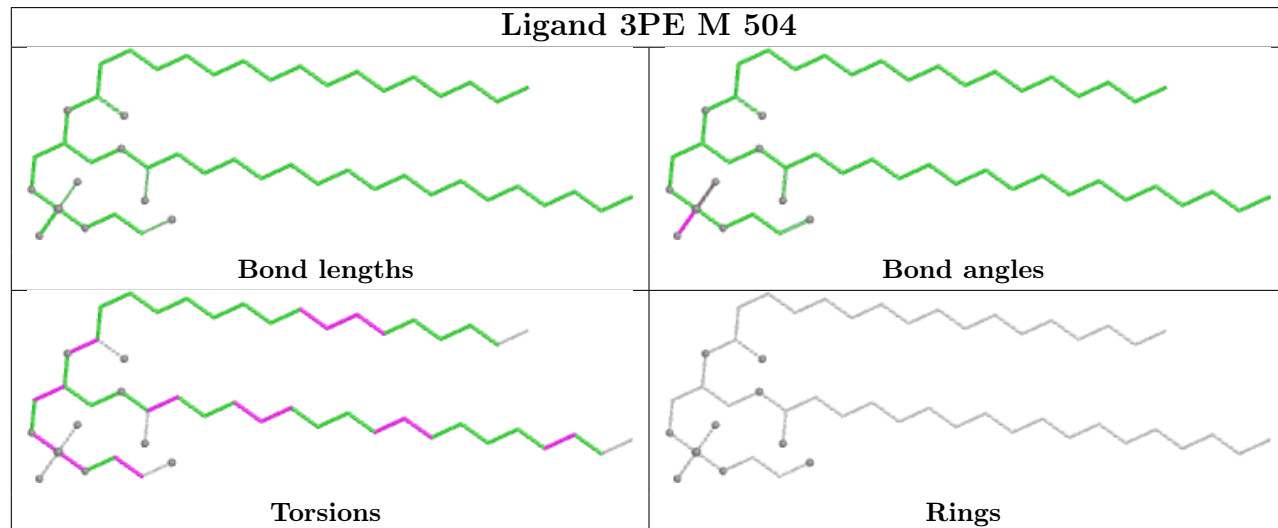
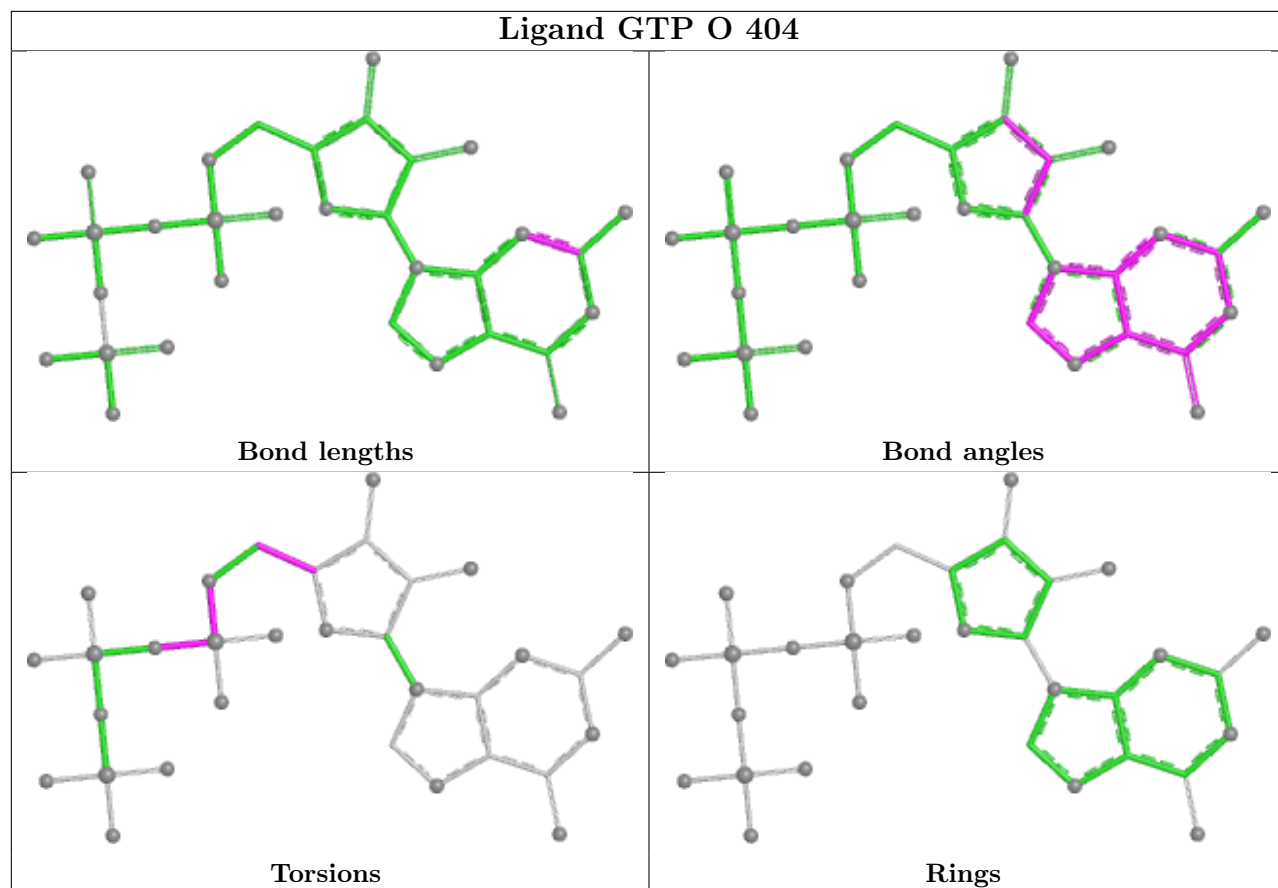




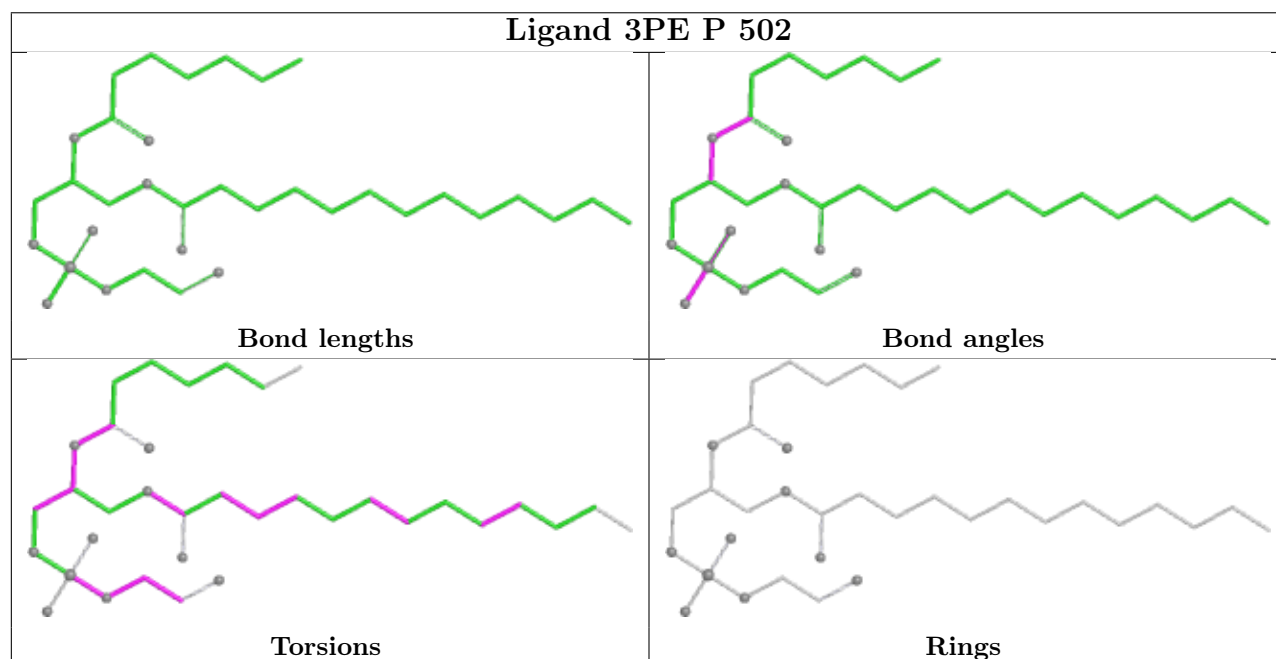
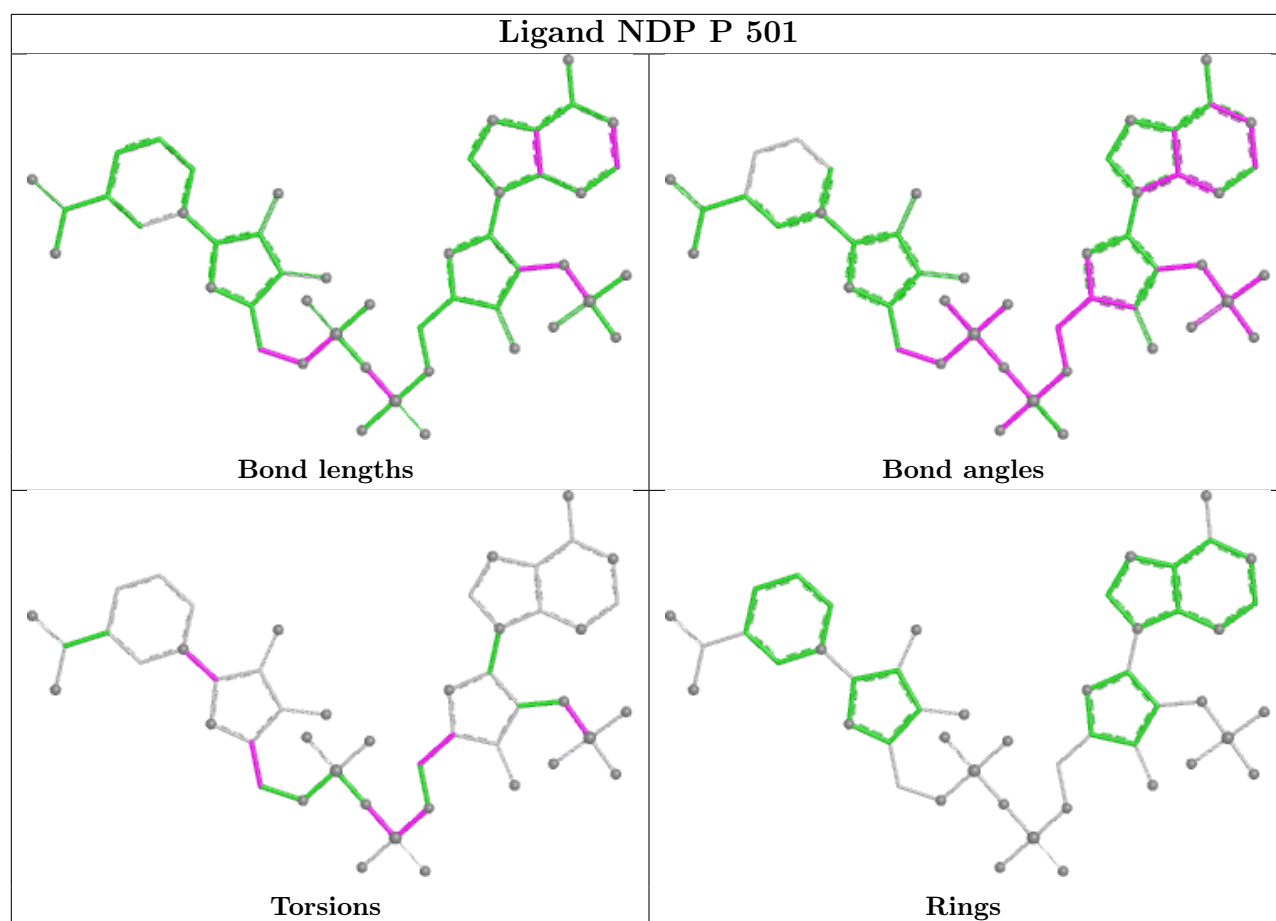




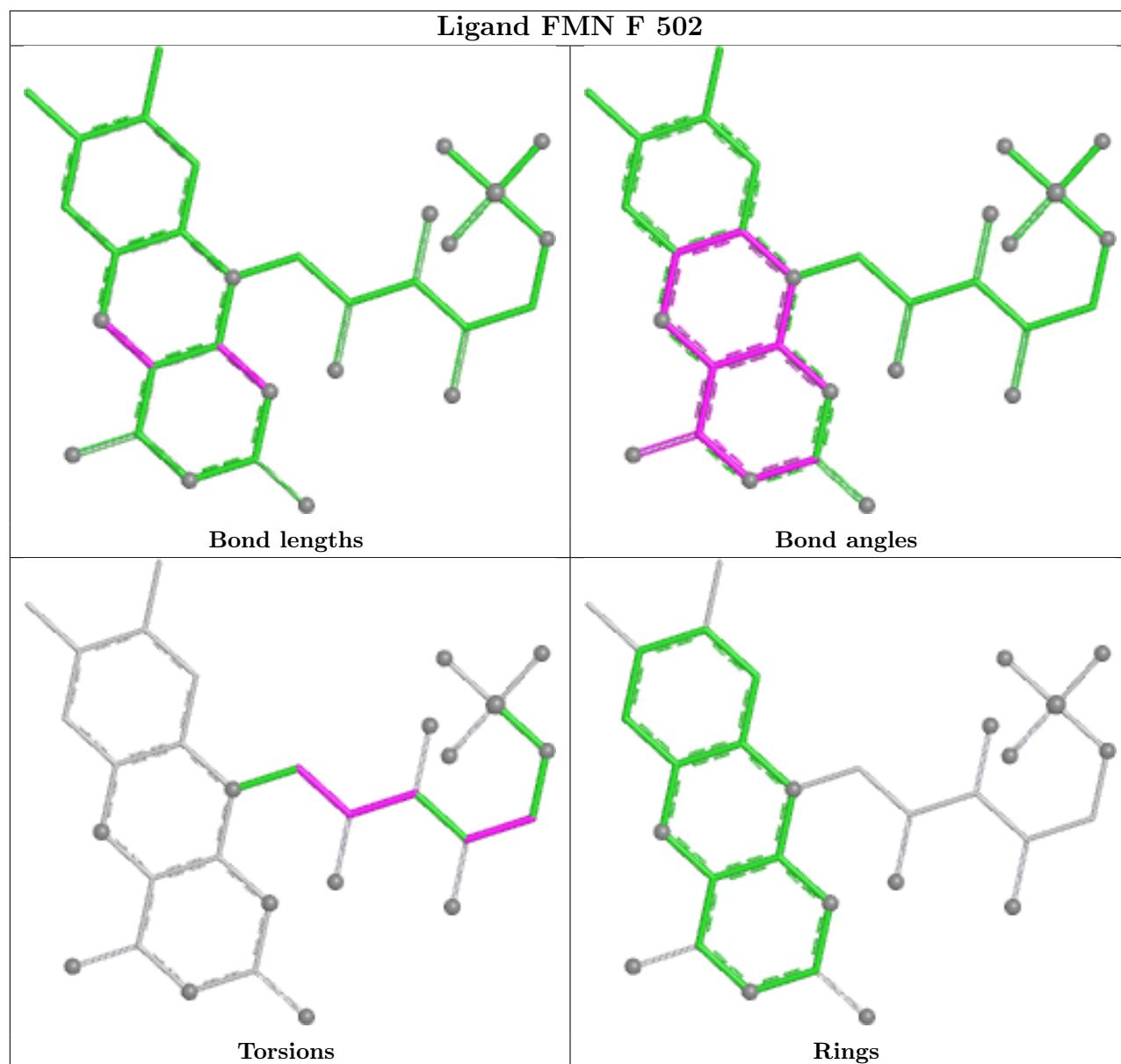
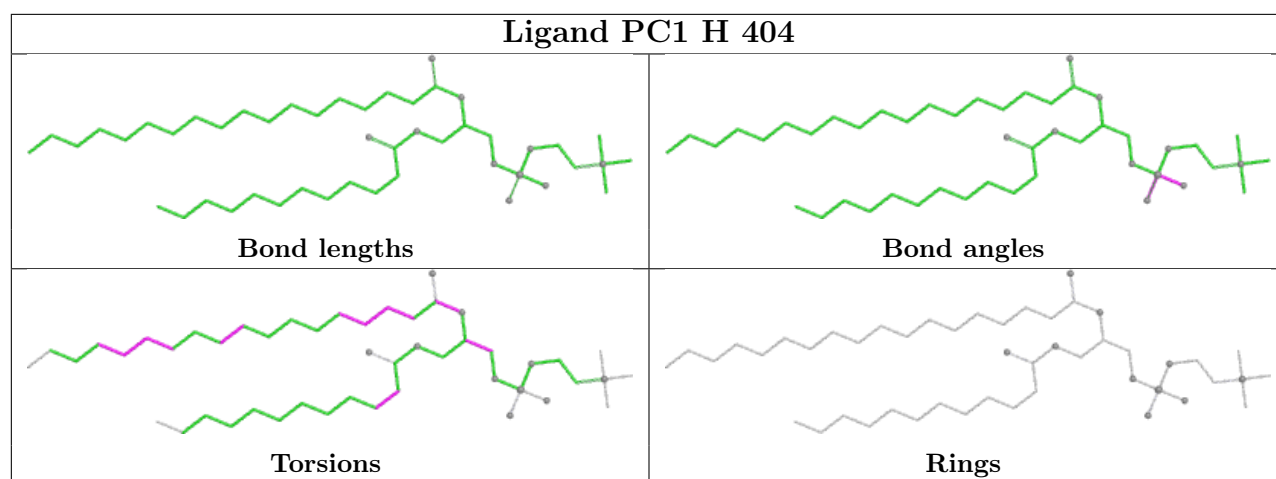




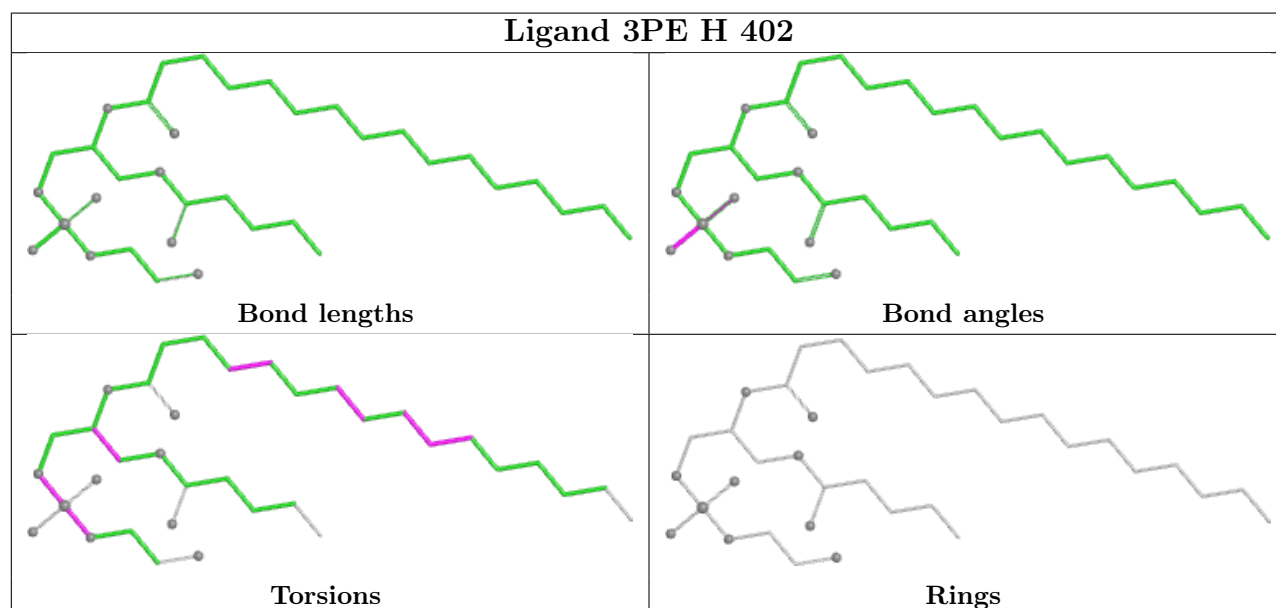
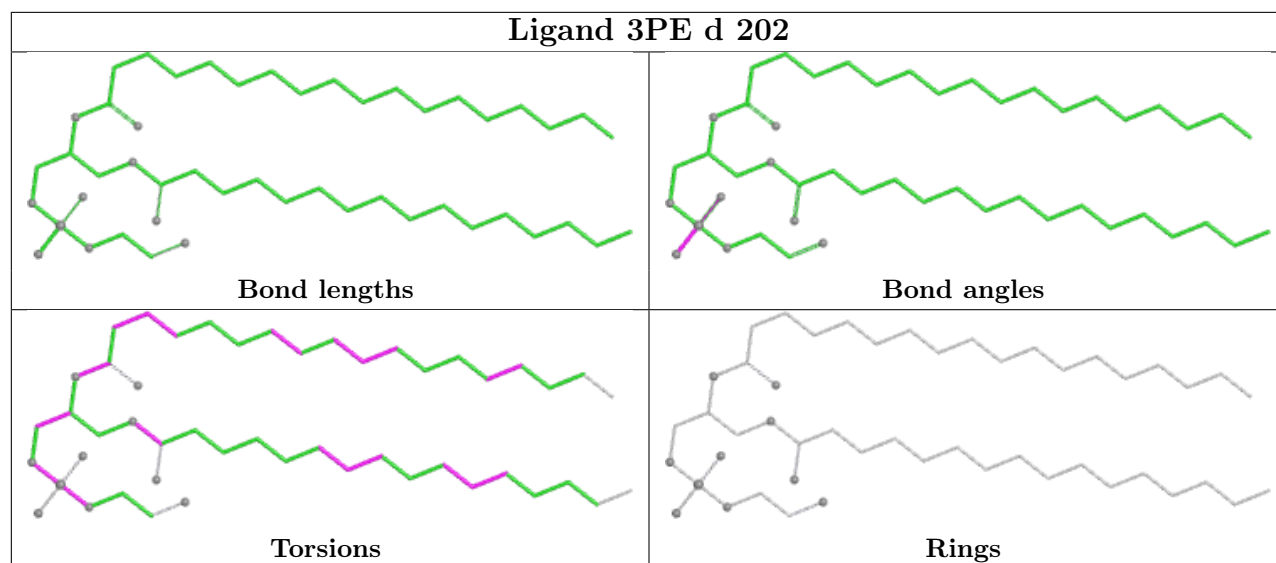
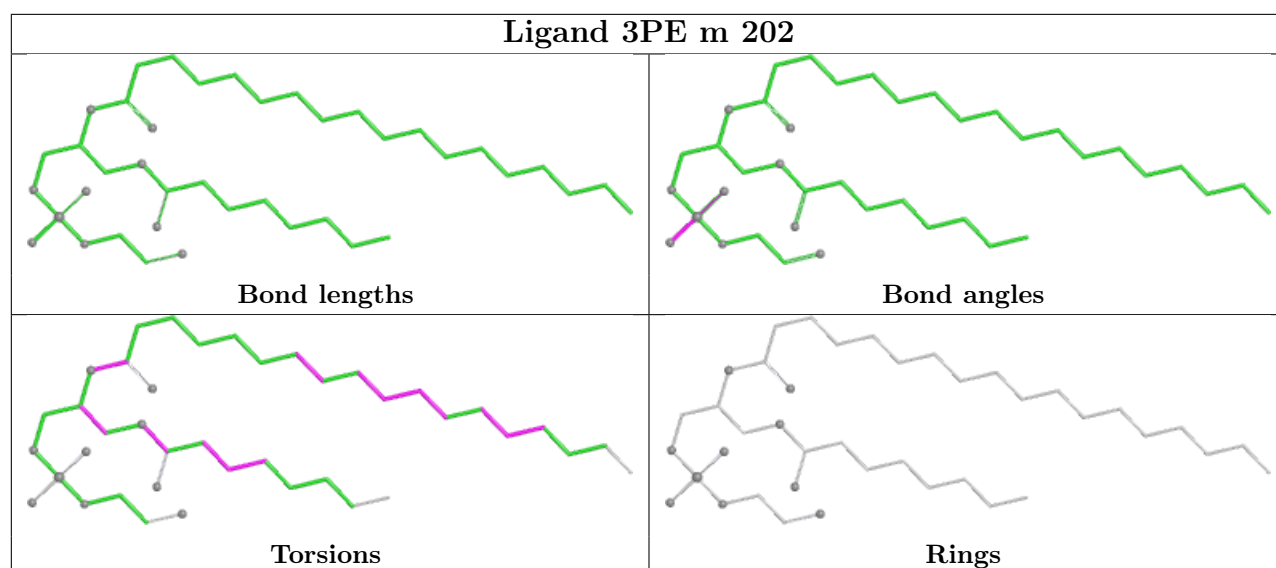




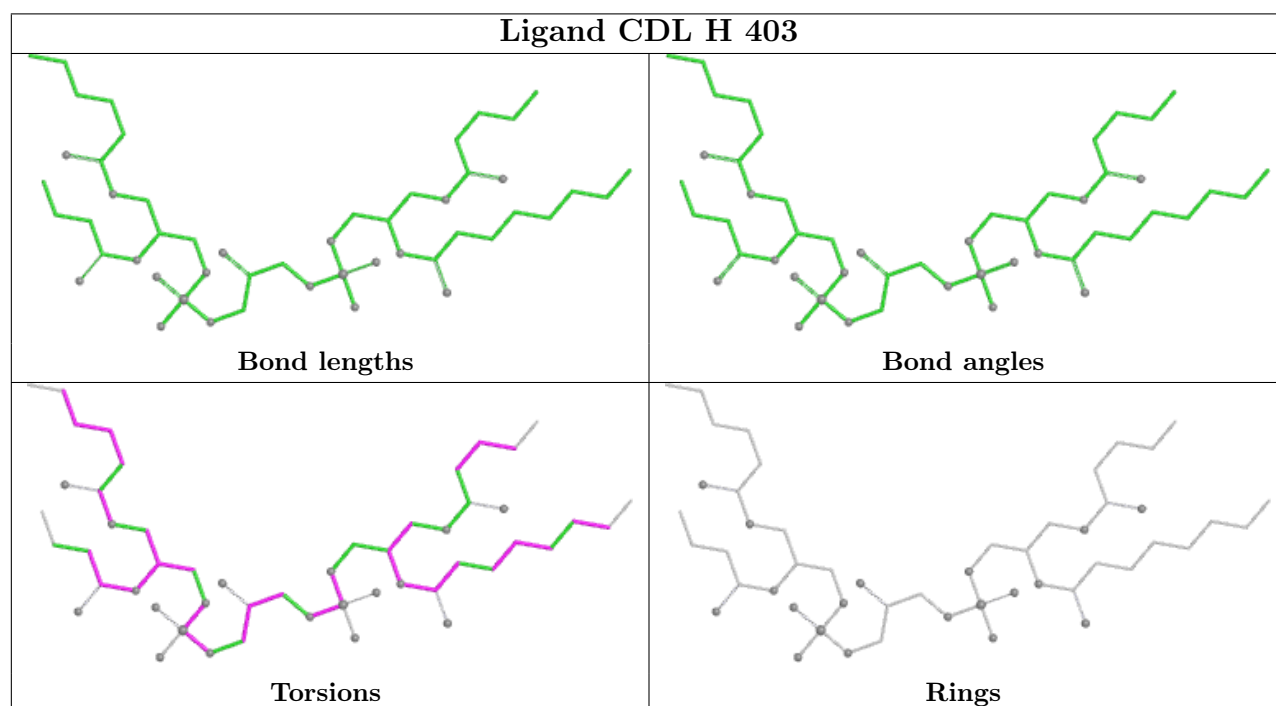
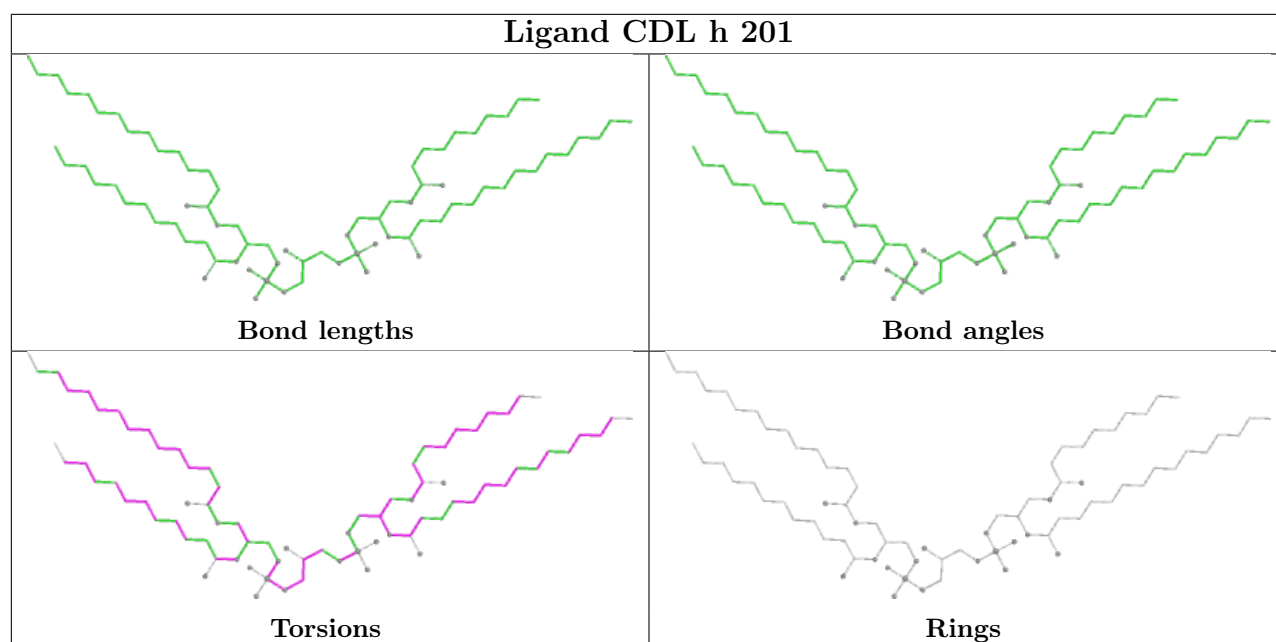




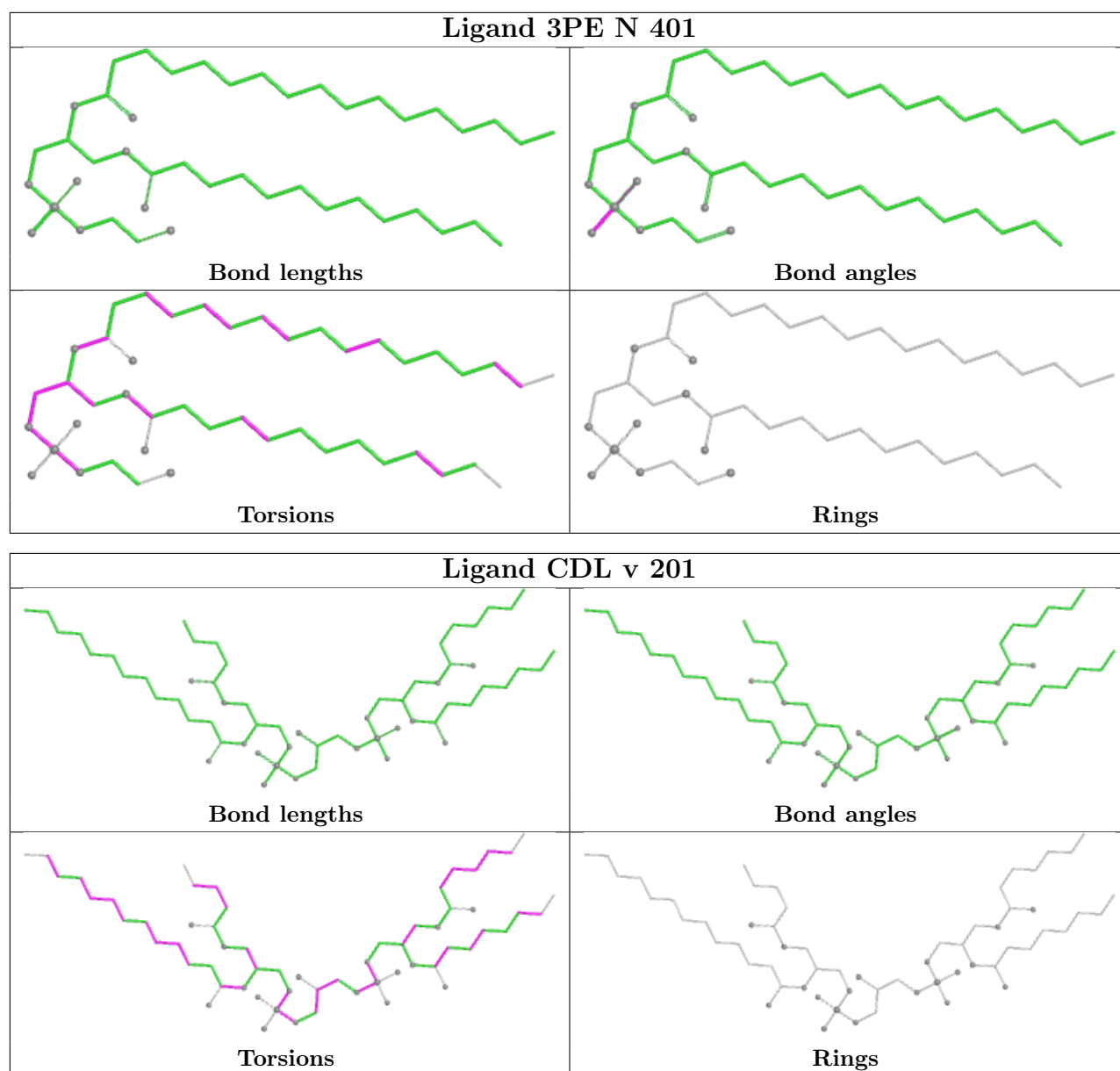




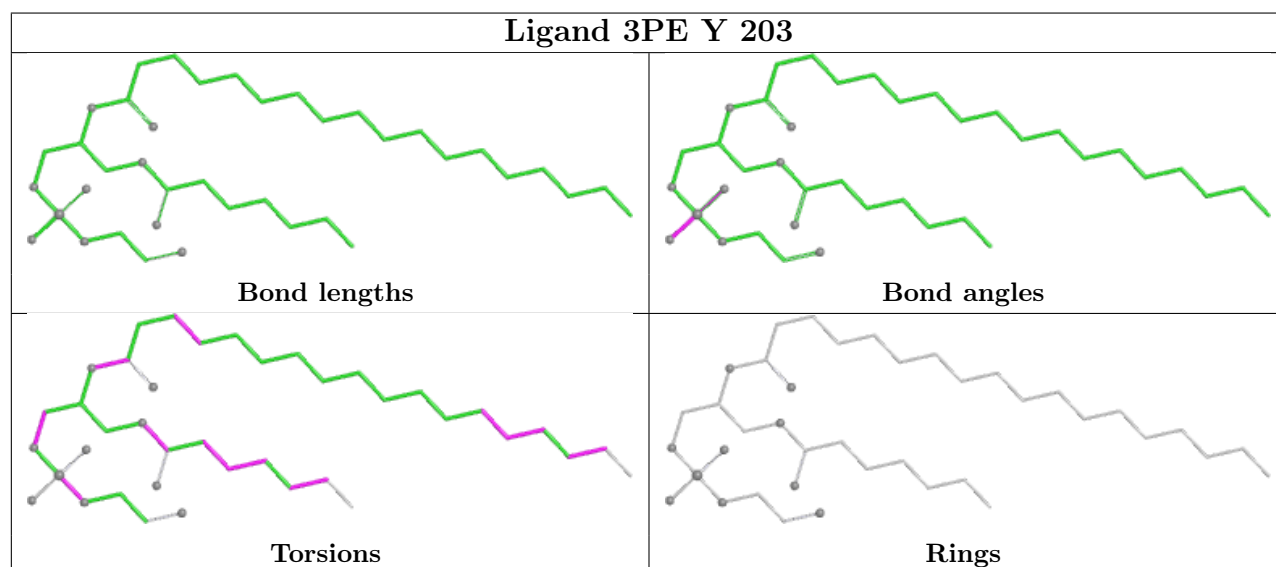
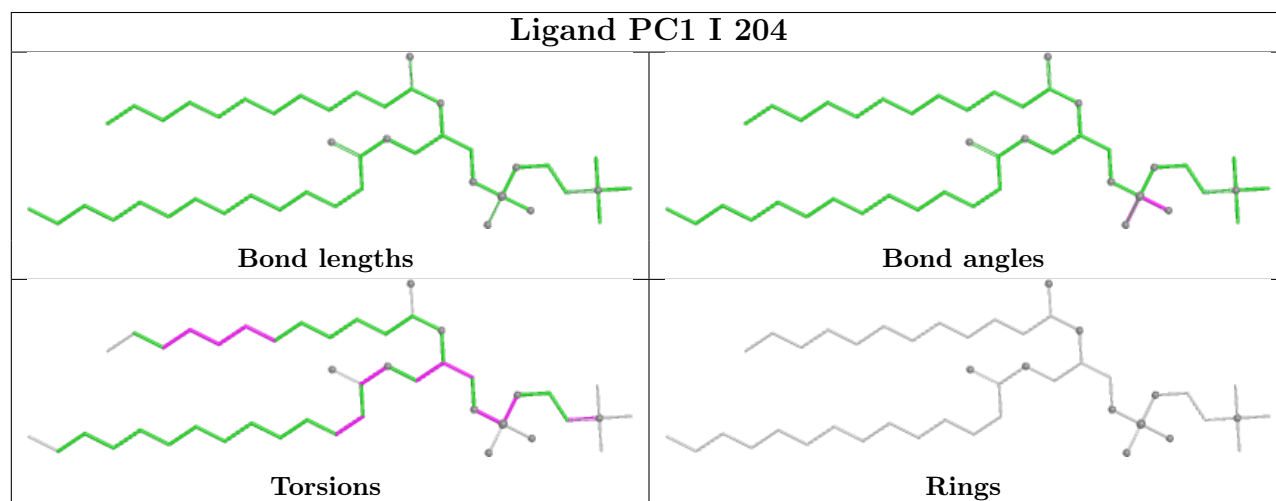
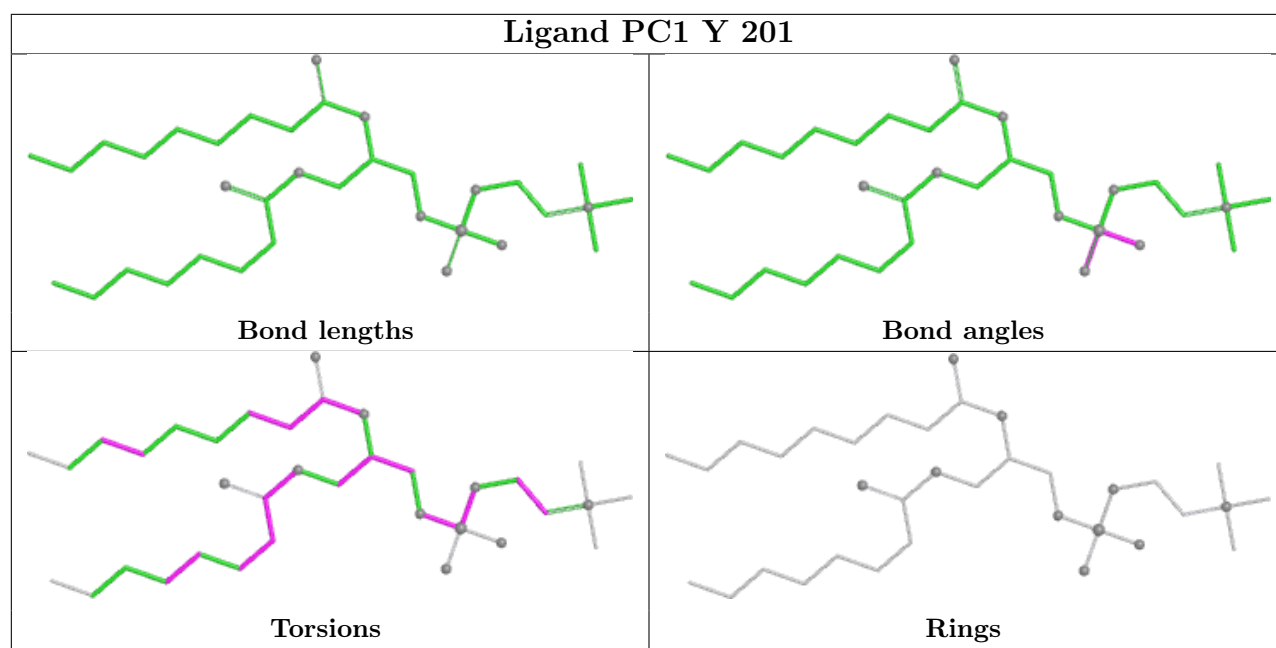




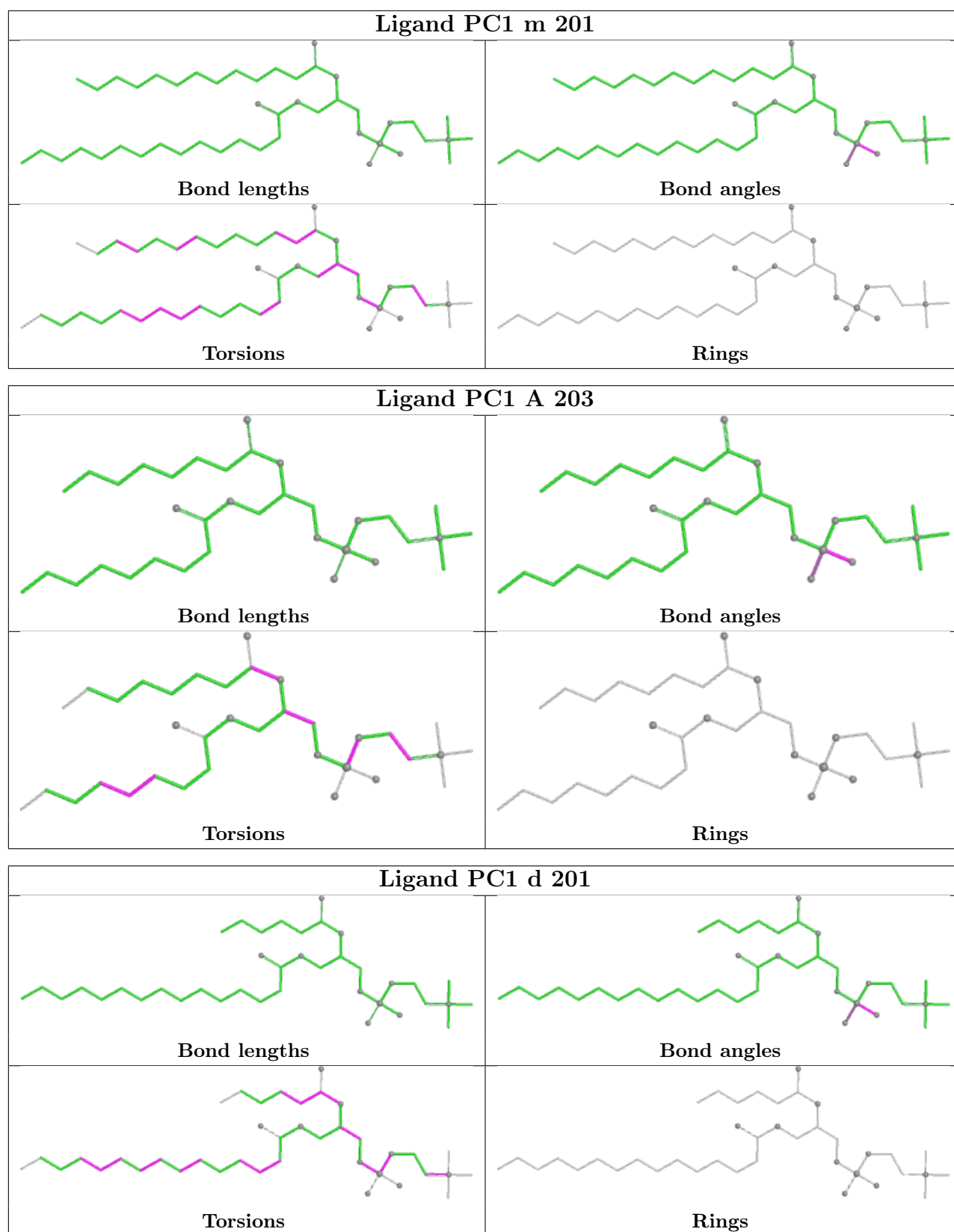




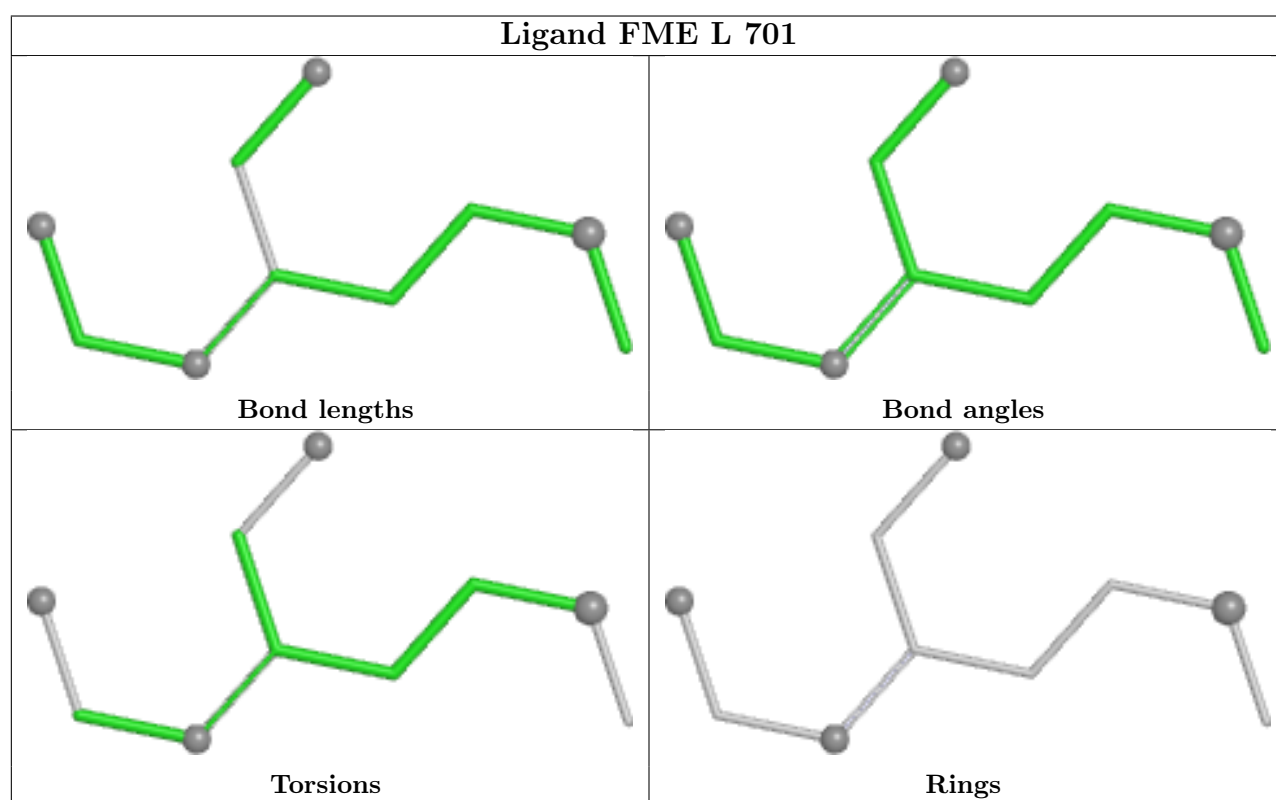
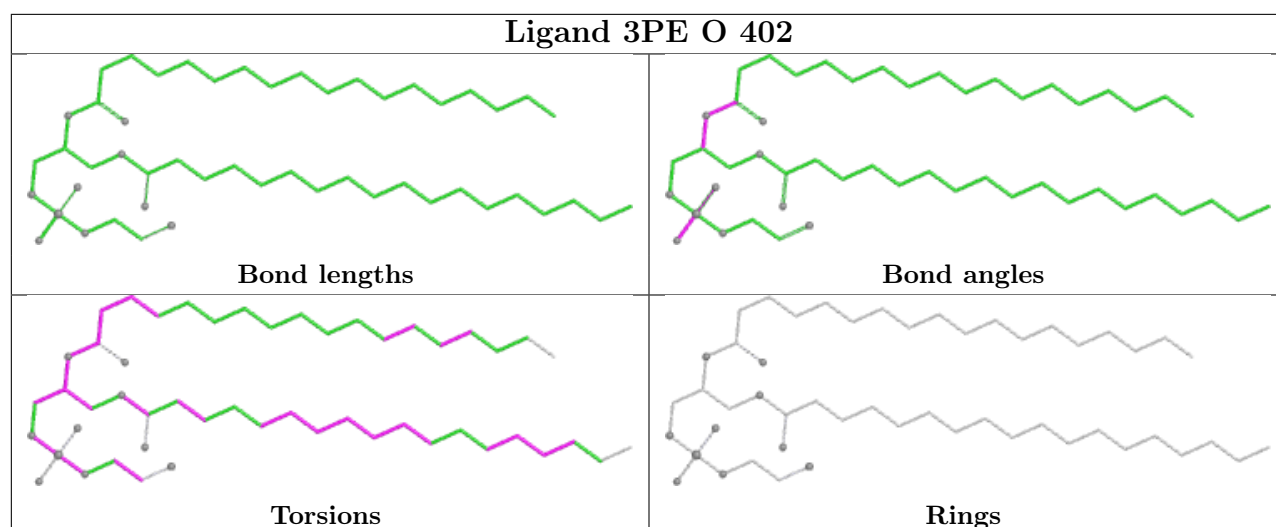




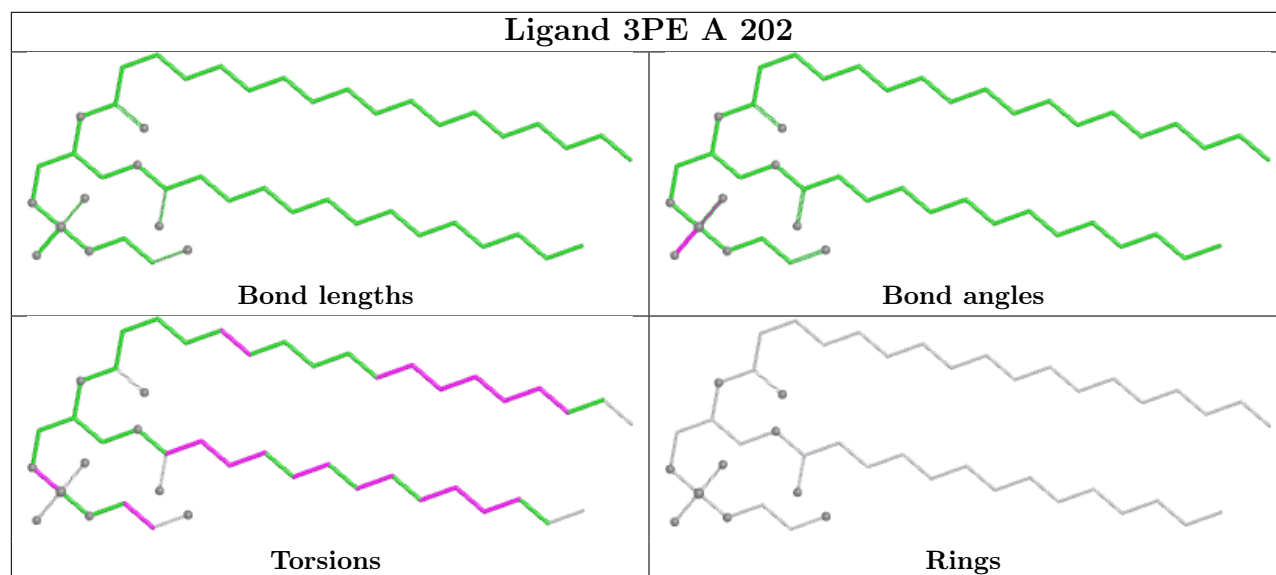
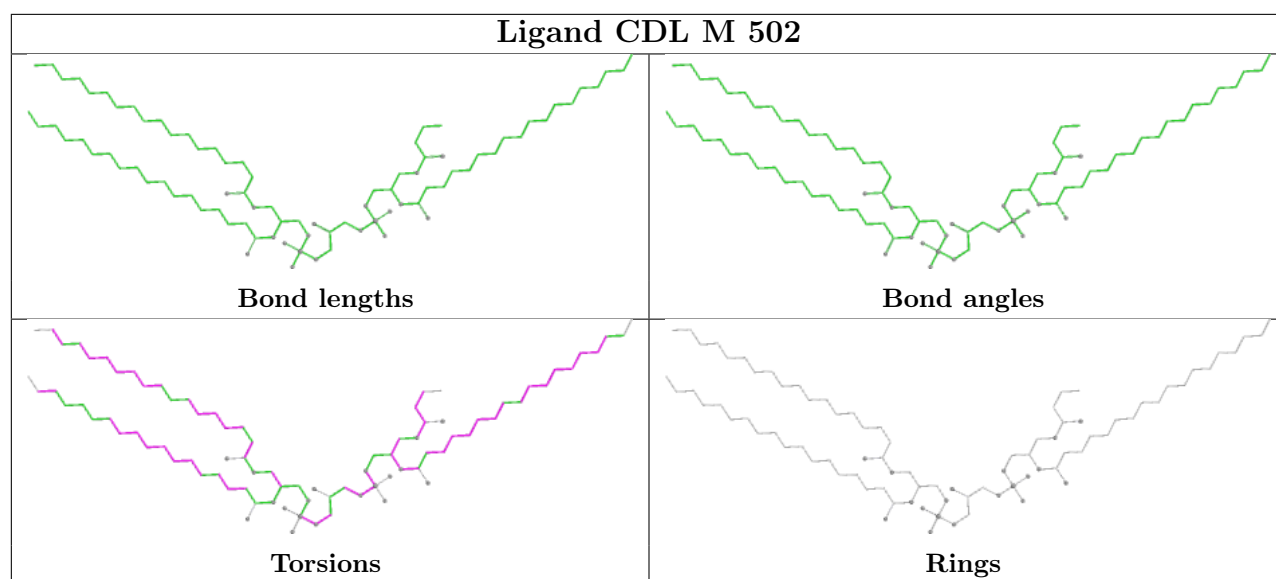




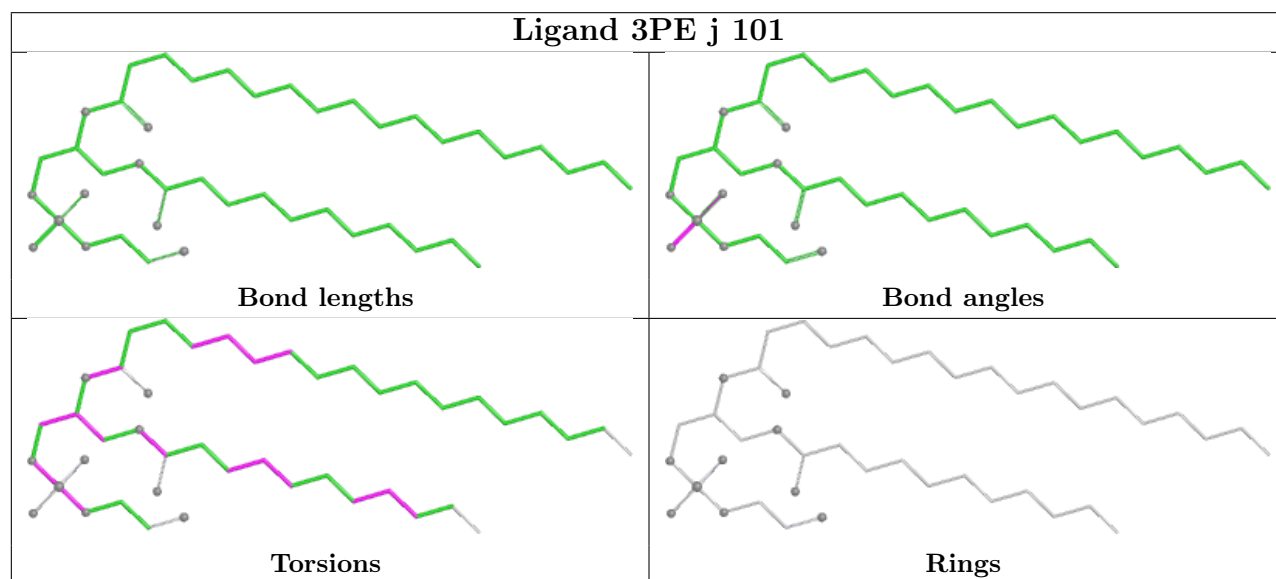
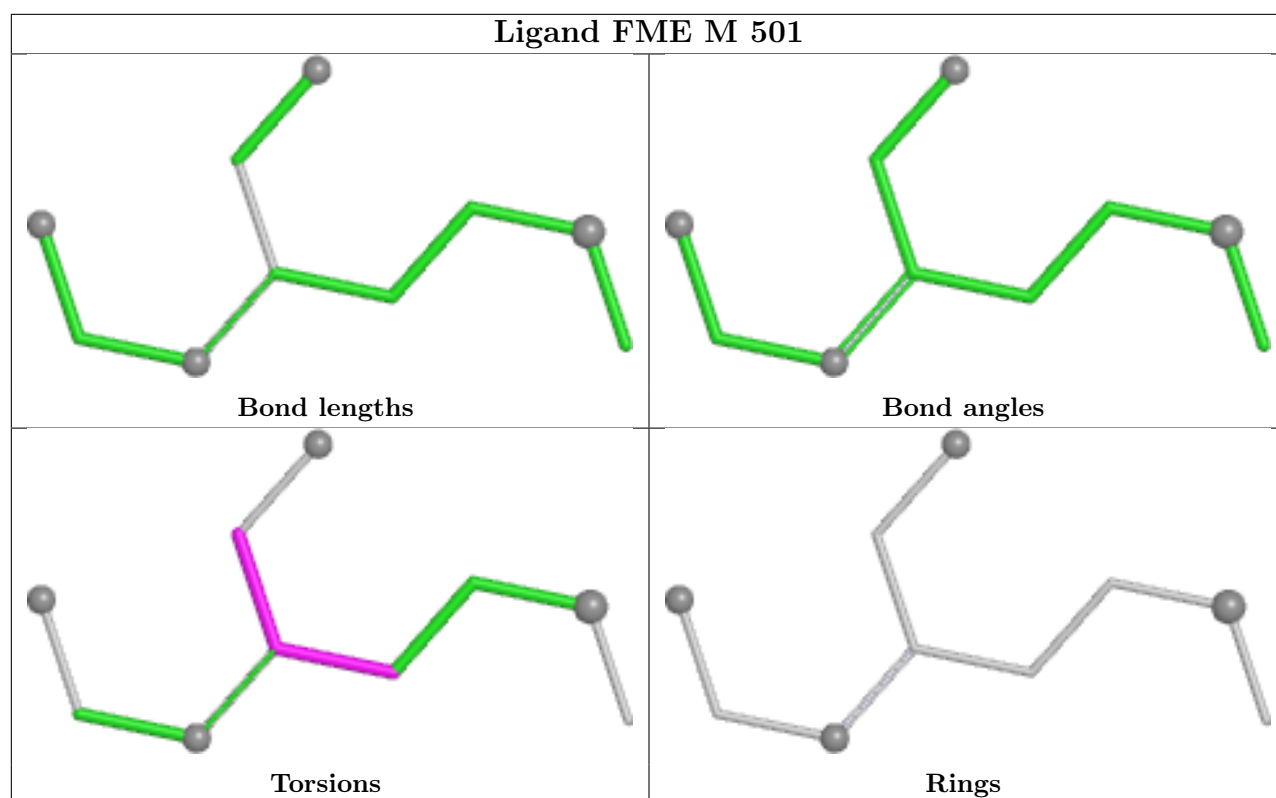




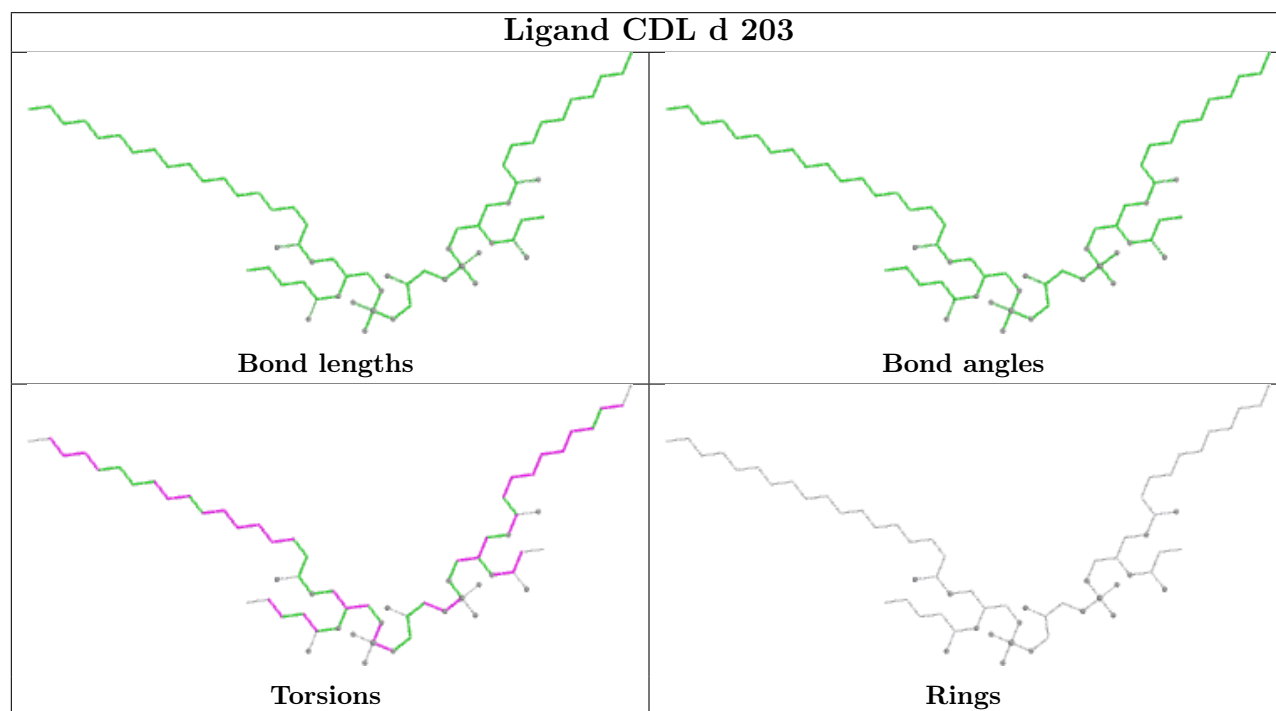
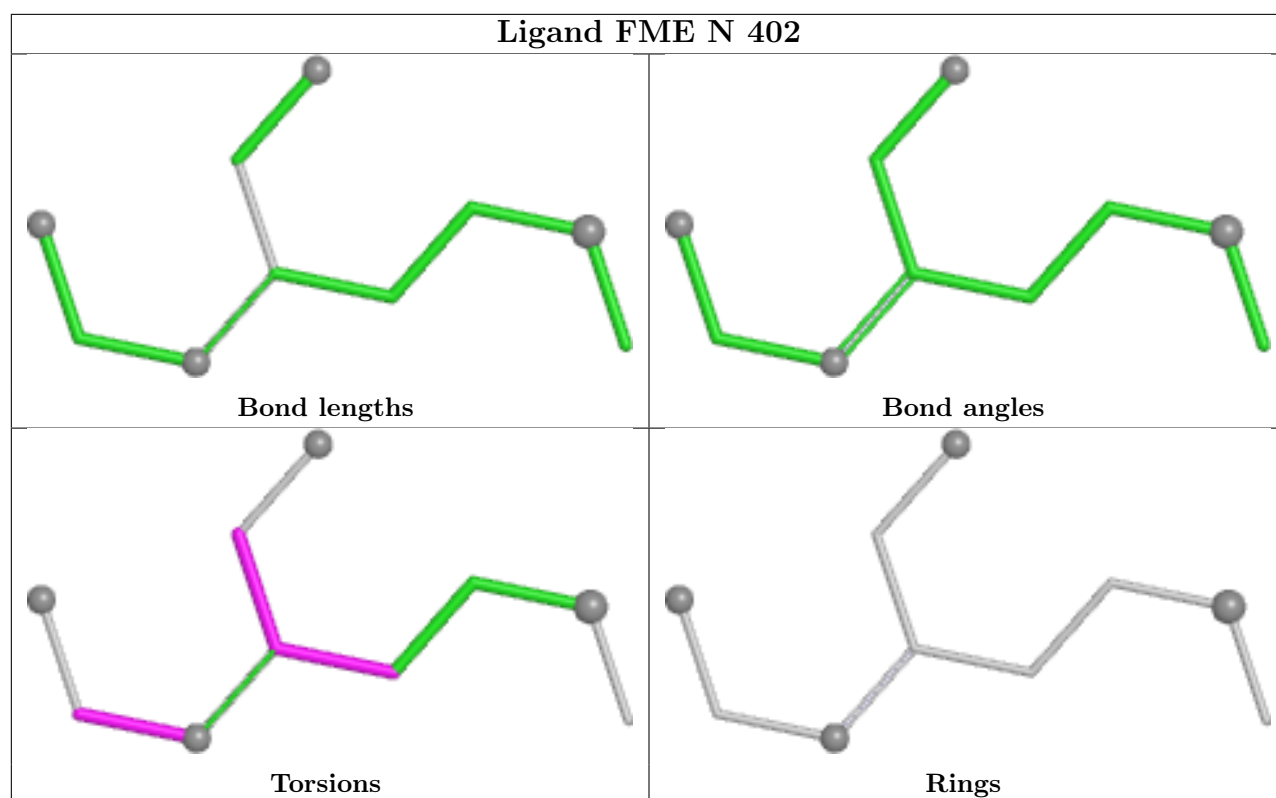




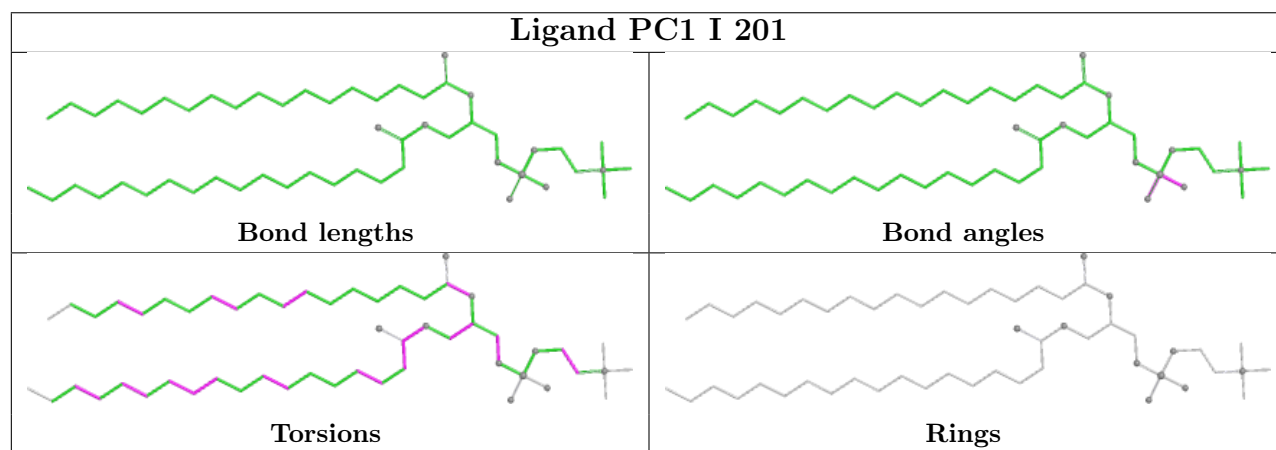
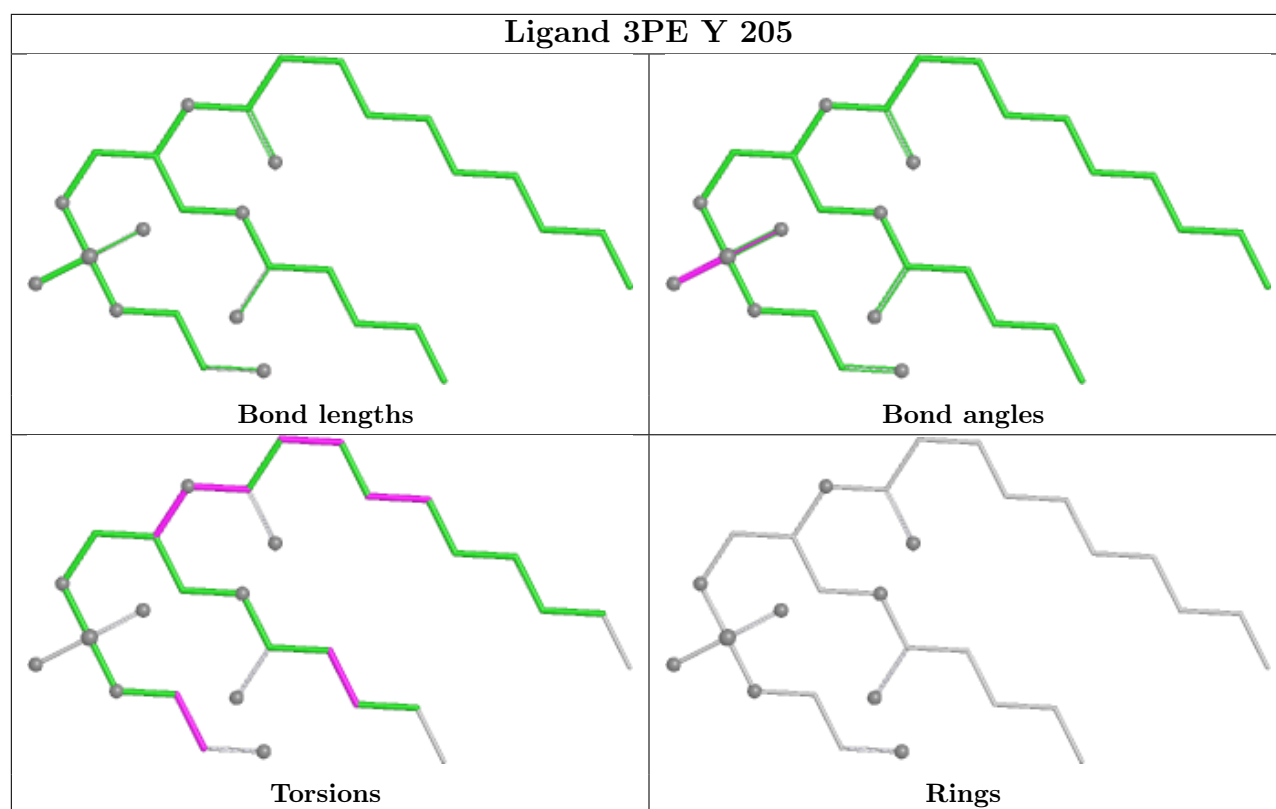




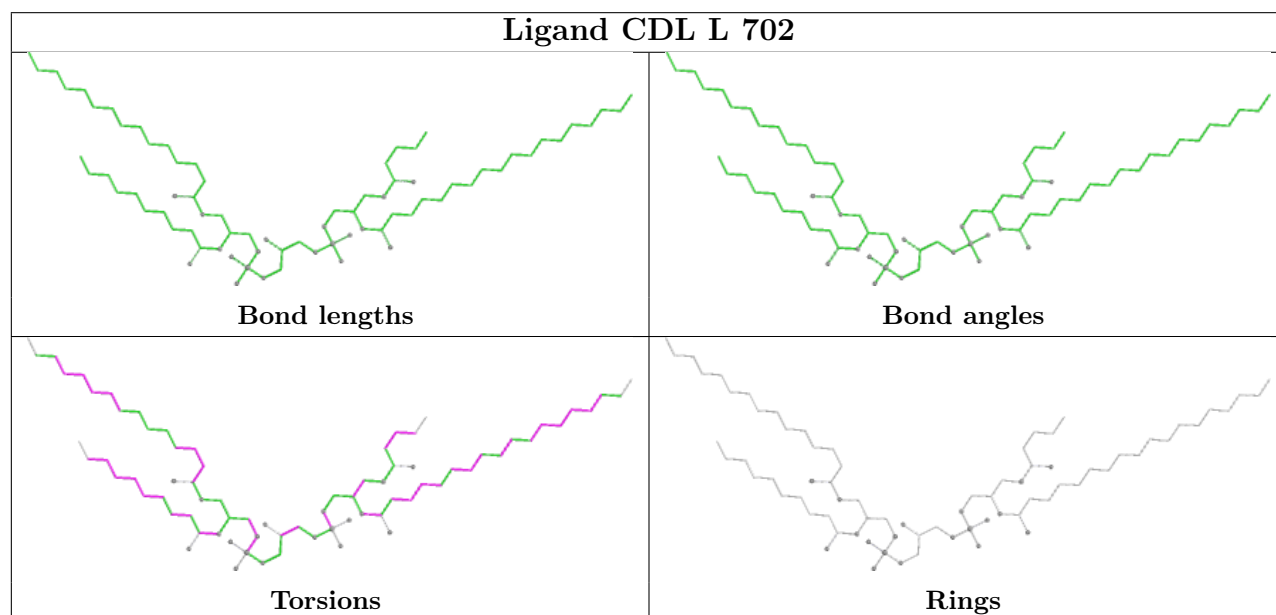
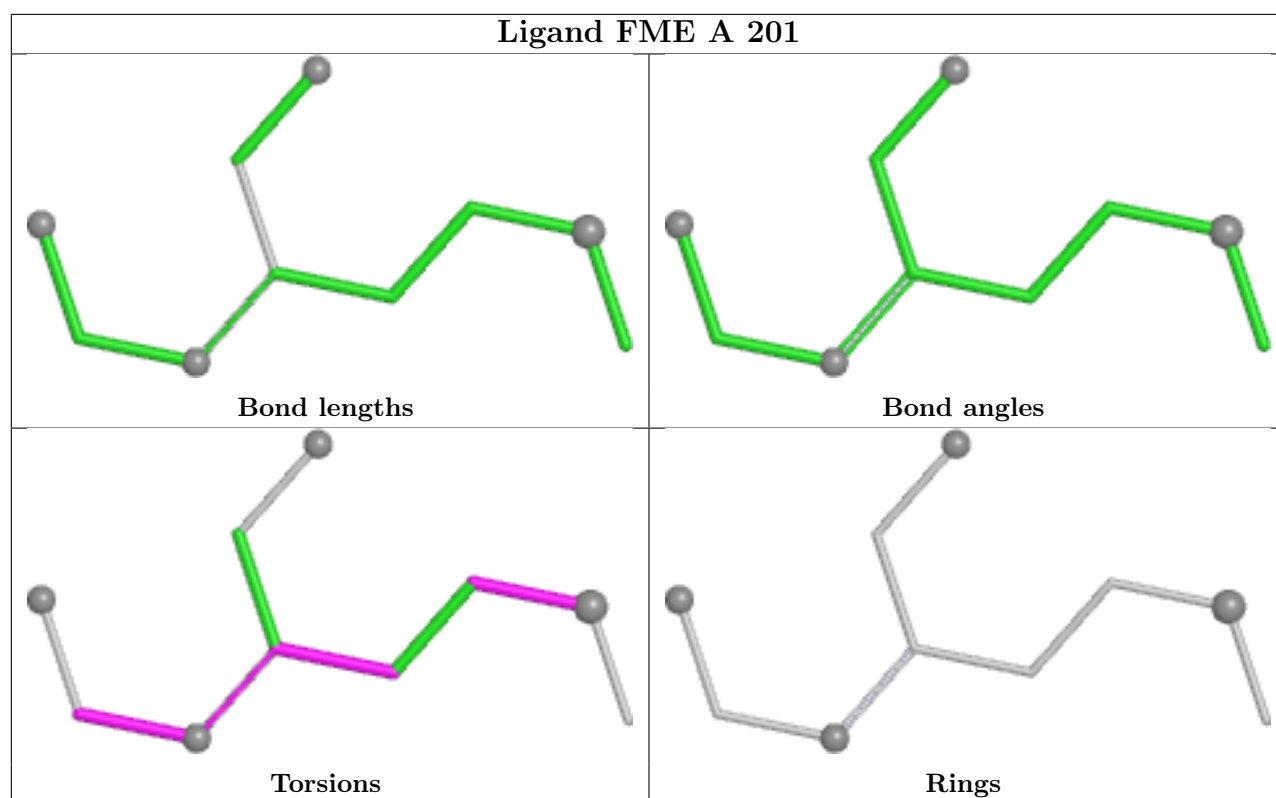




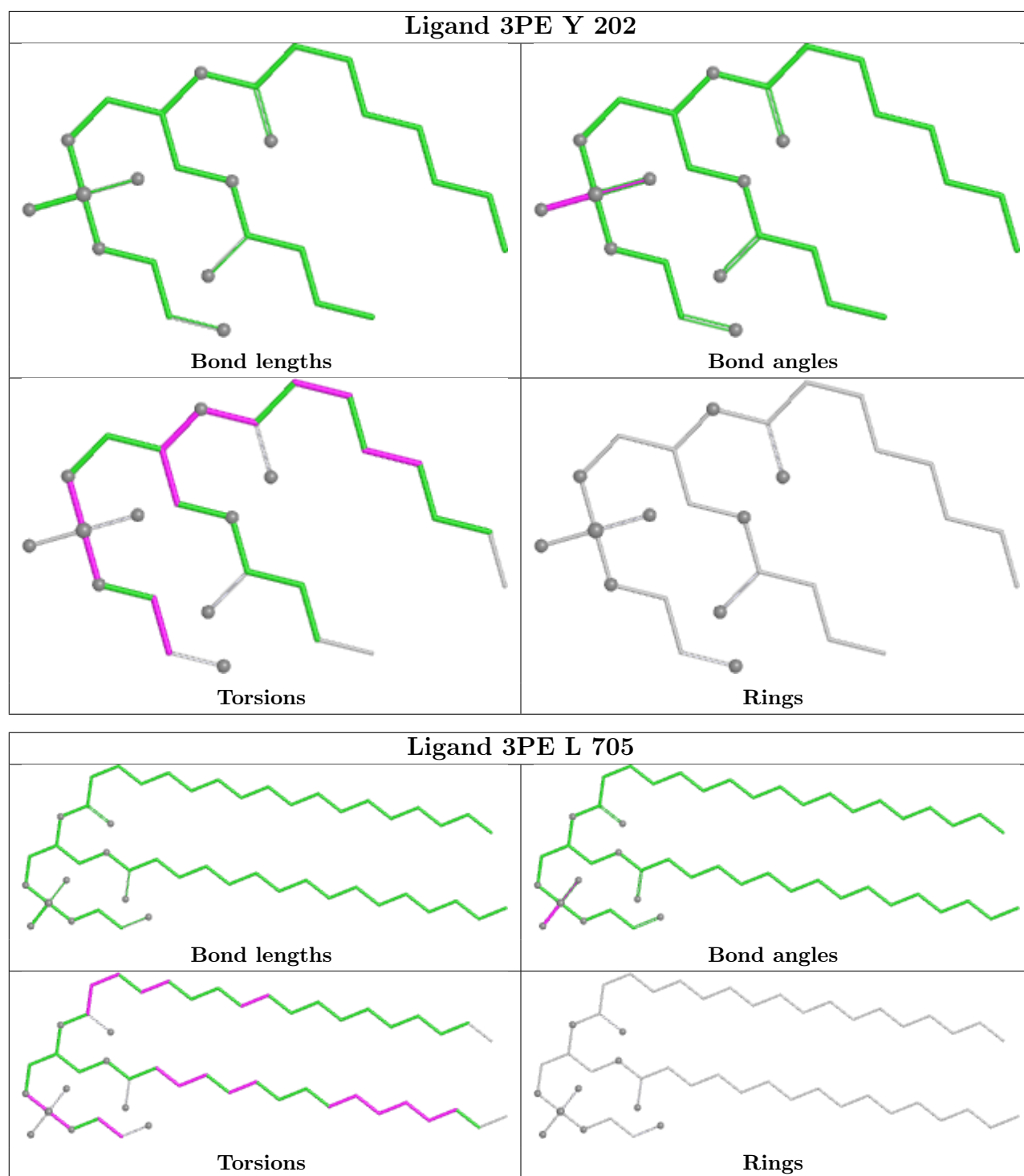












## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	1:FME	C	2:SER	N	4.74



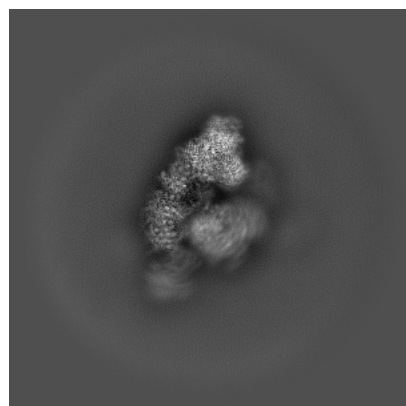
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65581. These allow visual inspection of the internal detail of the map and identification of artifacts.

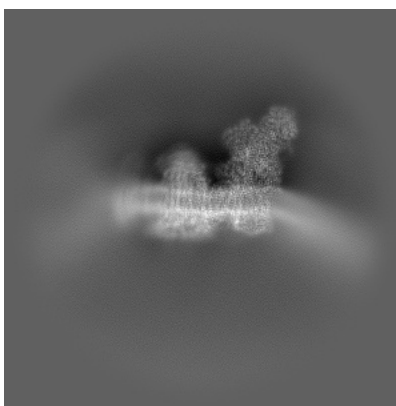
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

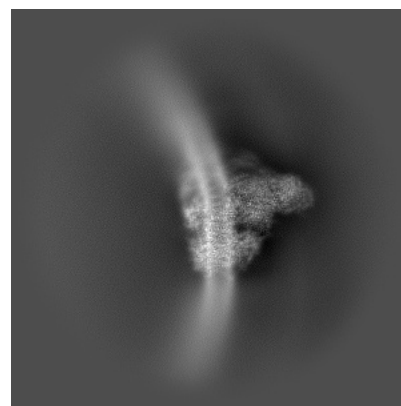
#### 6.1.1 Primary map



X

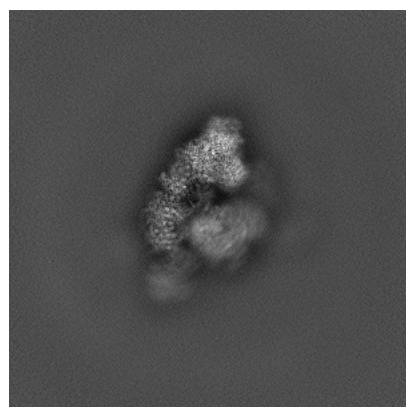


Y

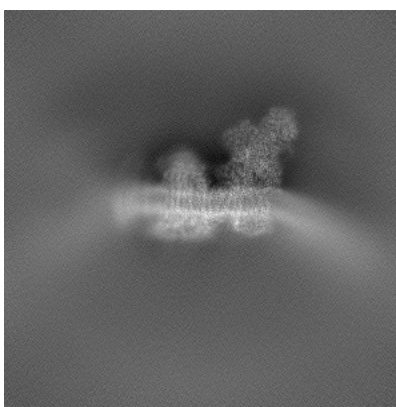


Z

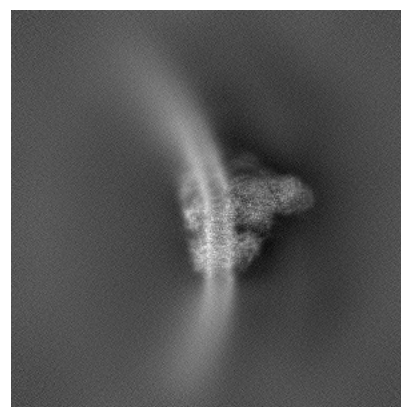
#### 6.1.2 Raw map



X



Y



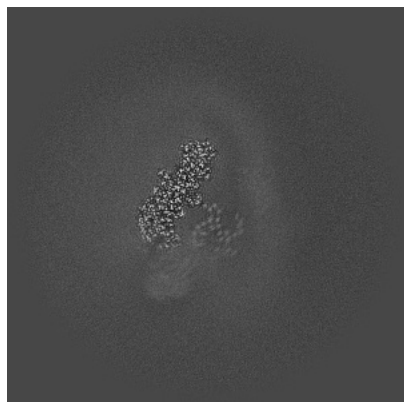
Z

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

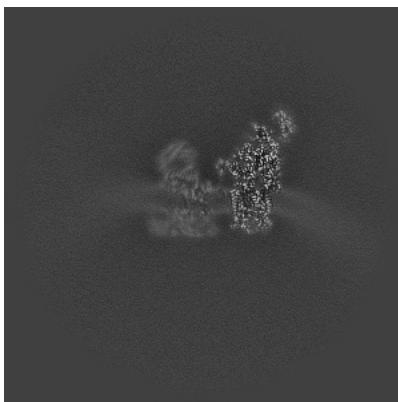


## 6.2 Central slices [i](#)

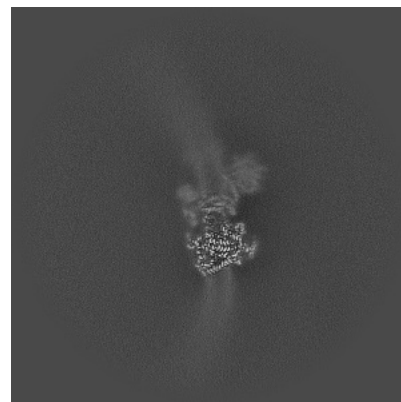
### 6.2.1 Primary map



X Index: 300

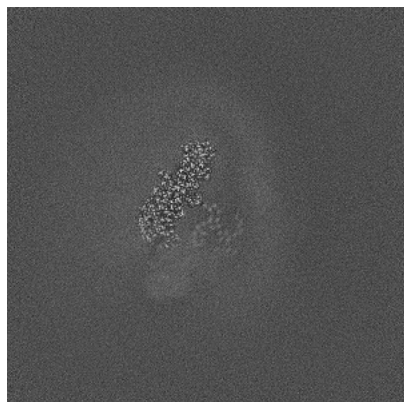


Y Index: 300

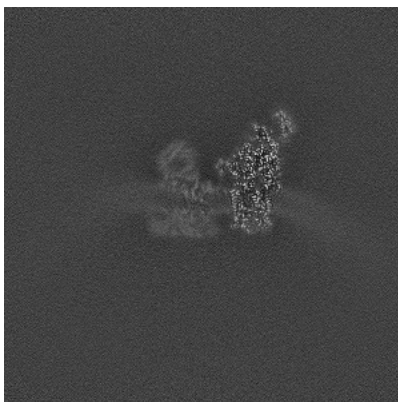


Z Index: 300

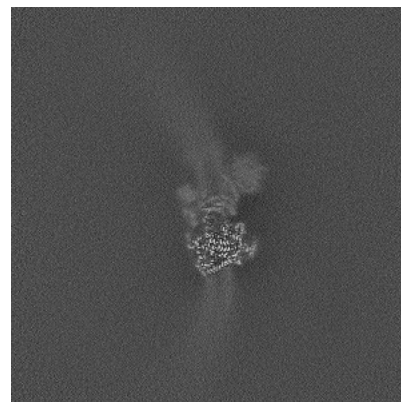
### 6.2.2 Raw map



X Index: 300



Y Index: 300



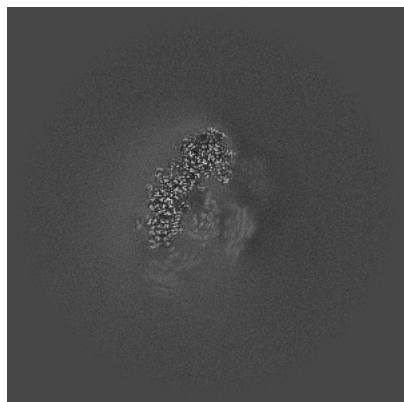
Z Index: 300

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

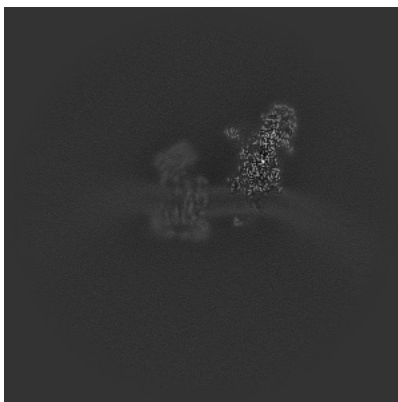


## 6.3 Largest variance slices [i](#)

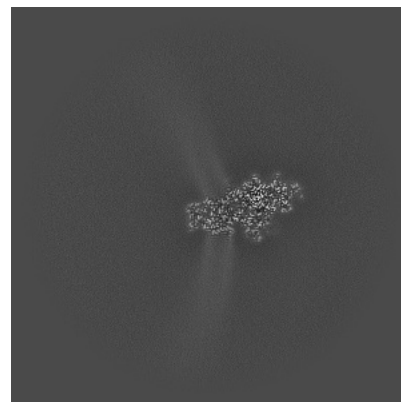
### 6.3.1 Primary map



X Index: 325

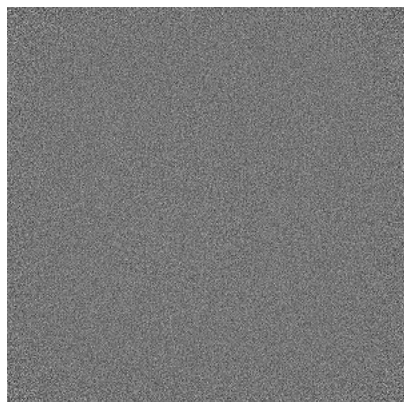


Y Index: 315

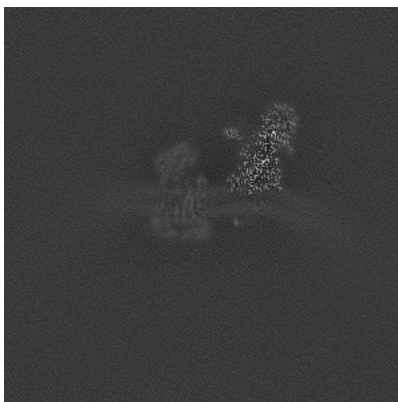


Z Index: 386

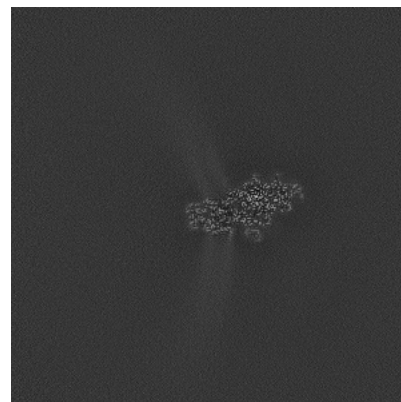
### 6.3.2 Raw map



X Index: 0



Y Index: 316



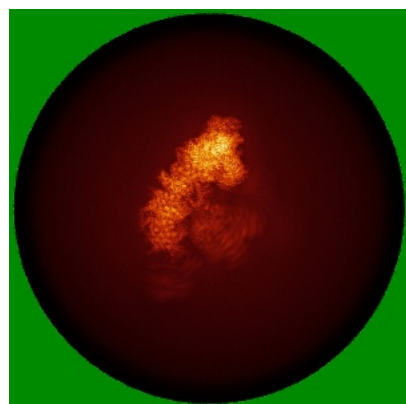
Z Index: 387

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

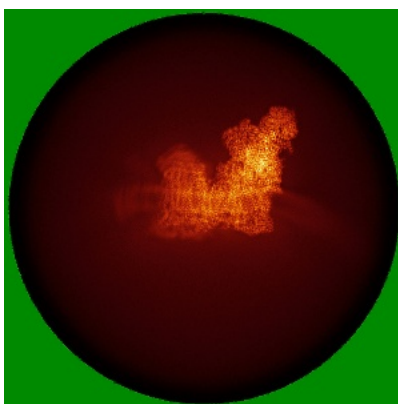


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

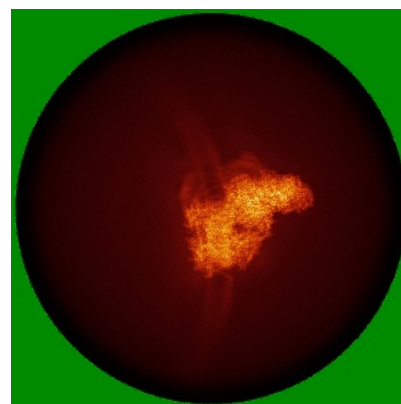
### 6.4.1 Primary map



X

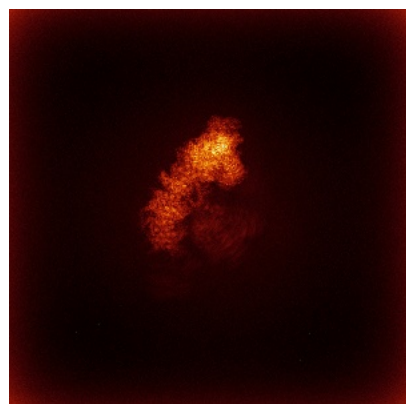


Y

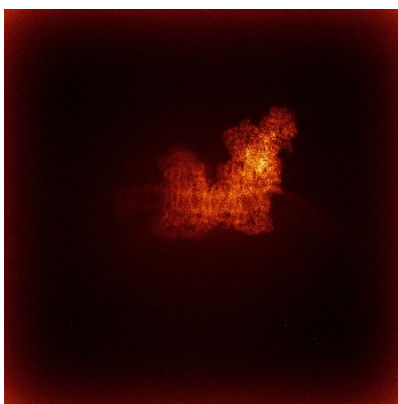


Z

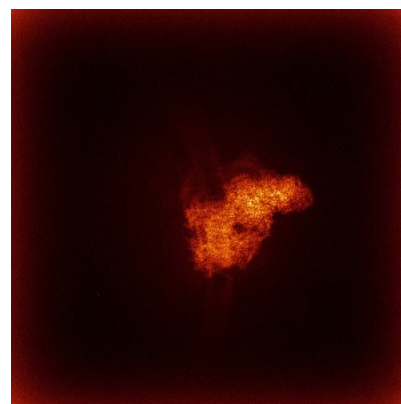
### 6.4.2 Raw map



X



Y



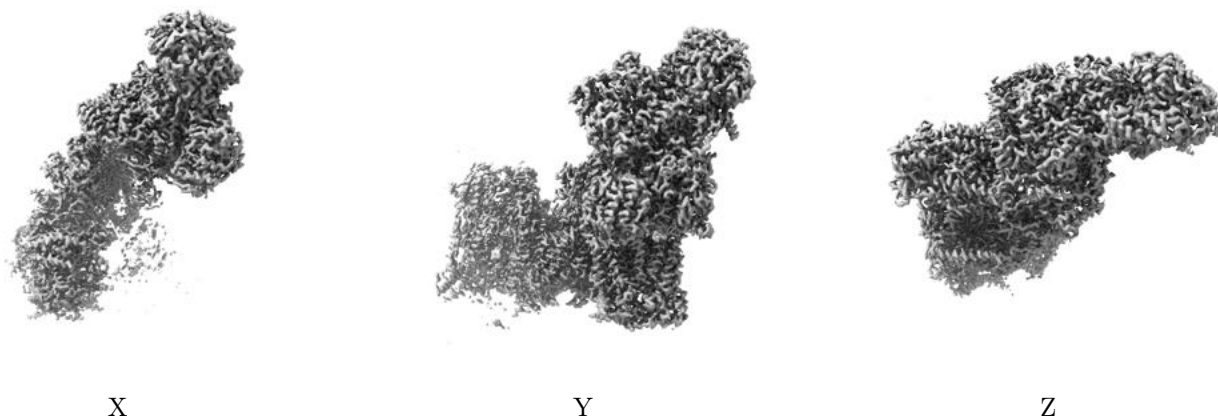
Z

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.



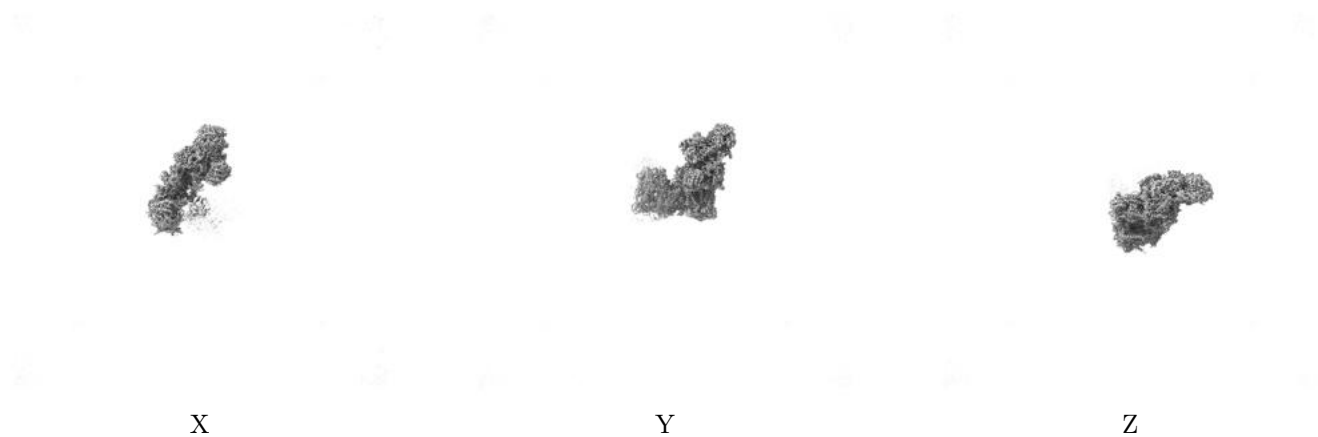
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.29. 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.



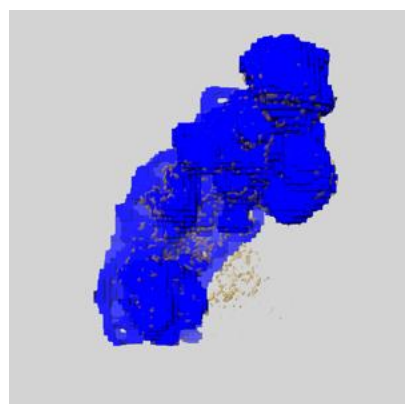
## 6.6 Mask visualisation [i](#)

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

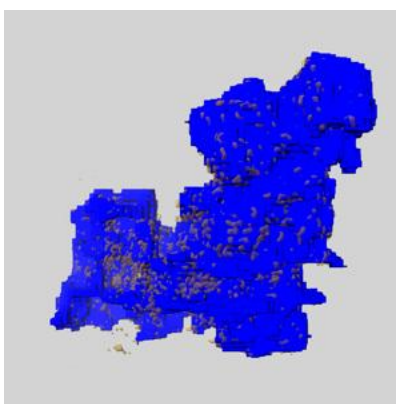
A mask typically either:

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

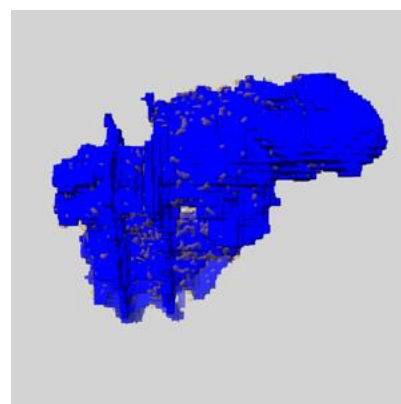
### 6.6.1 emd\_65581\_msk\_1.map [i](#)



X



Y



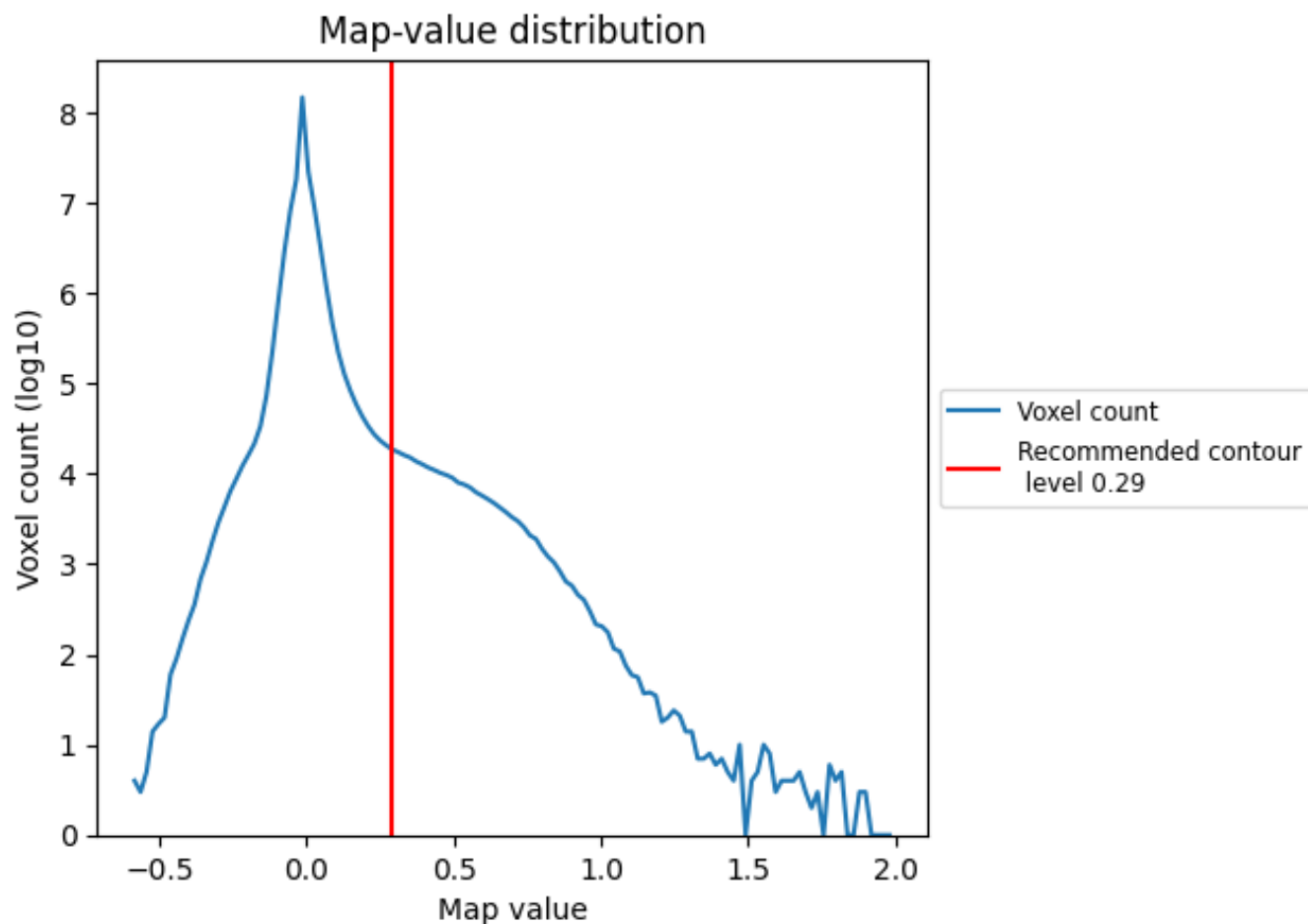
Z



## 7 Map analysis [i](#)

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

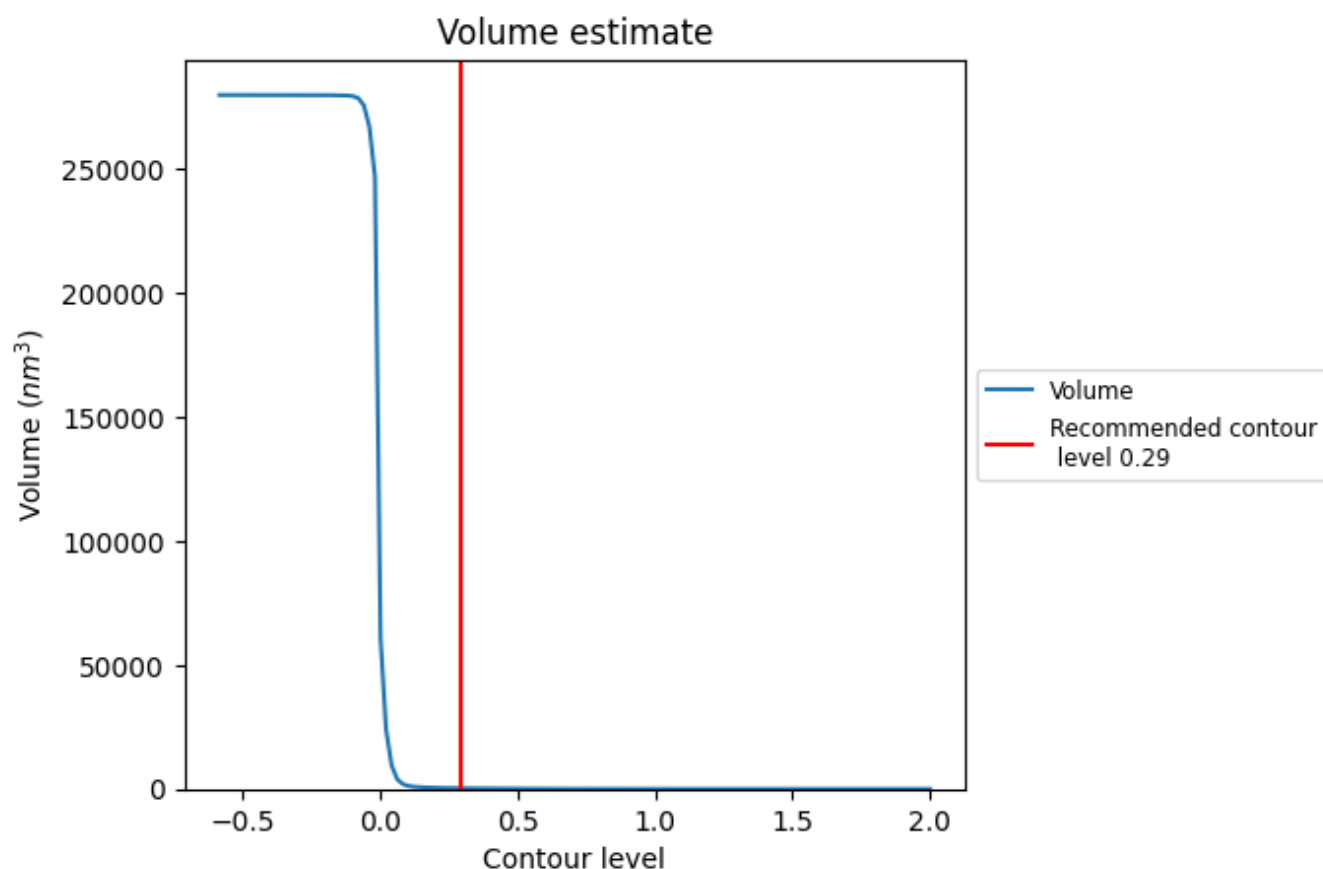
### 7.1 Map-value distribution [i](#)



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](#)

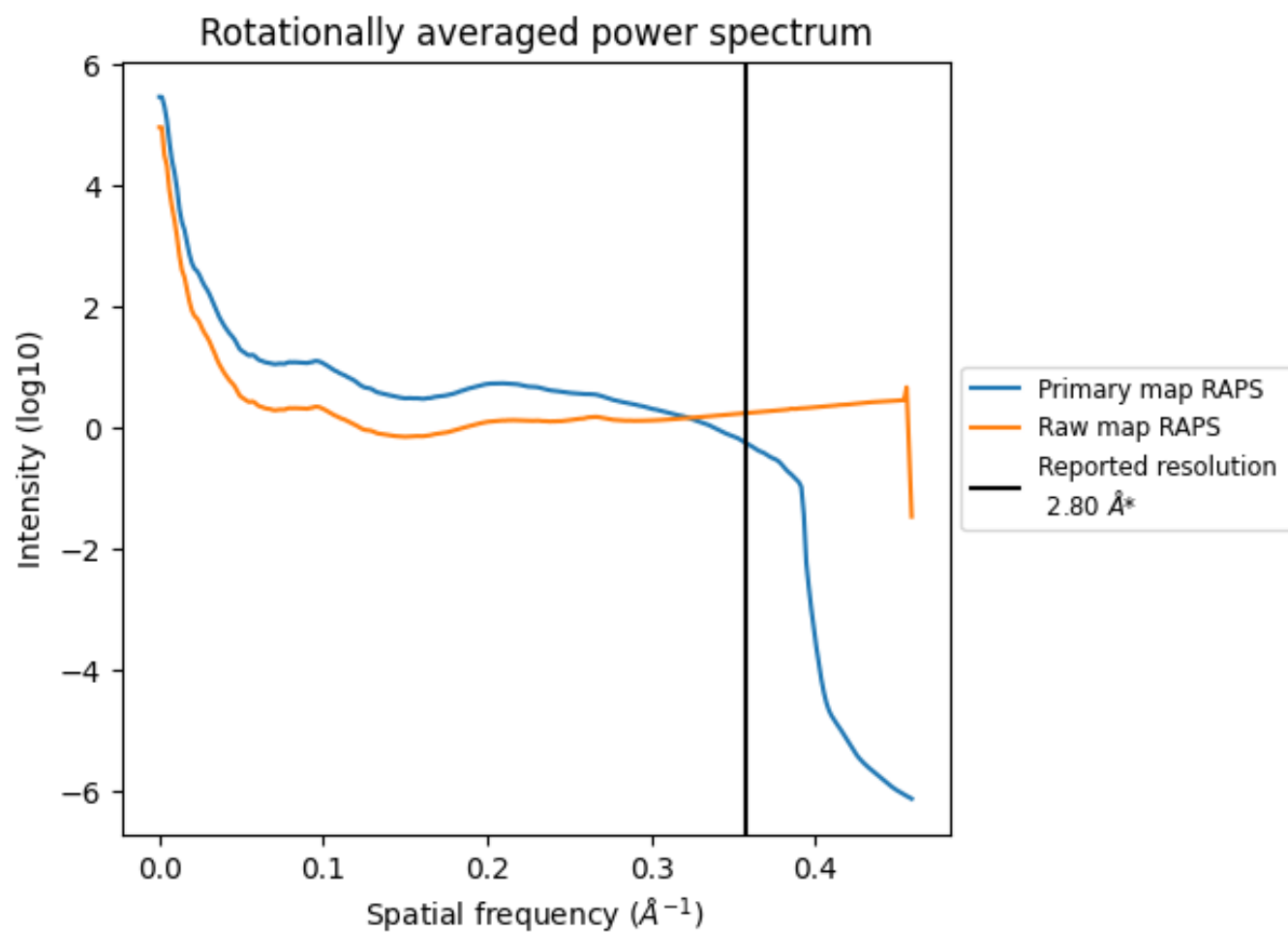


The volume at the recommended contour level is 286  $\text{nm}^3$ ; this corresponds to an approximate mass of 258 kDa.

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 ⓘ



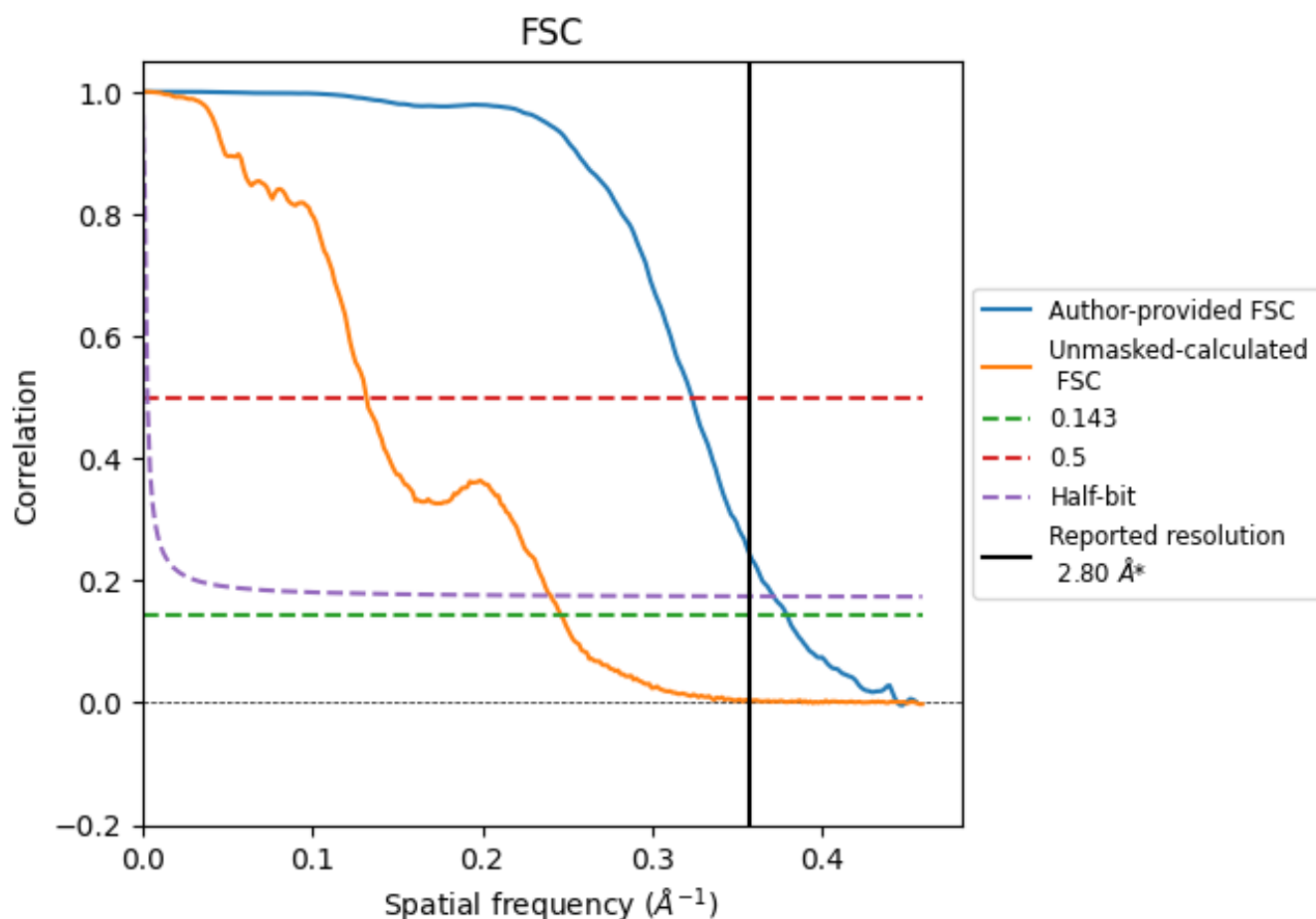
\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>



## 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 0.357  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.64	3.09	2.69
Unmasked-calculated*	4.06	7.59	4.16

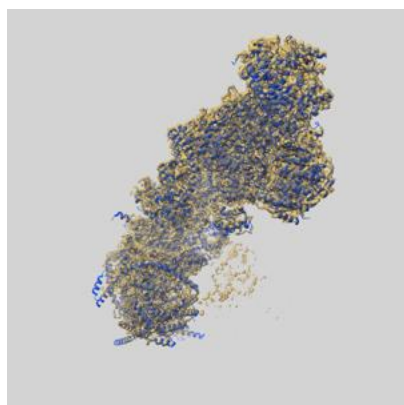
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 2.8 by more than 10 %



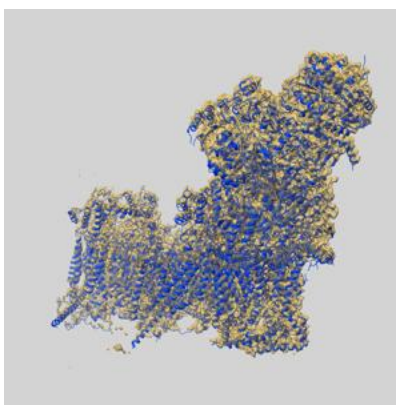
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65581 and PDB model 9W2V. Per-residue inclusion information can be found in section [3](#) on page [21](#).

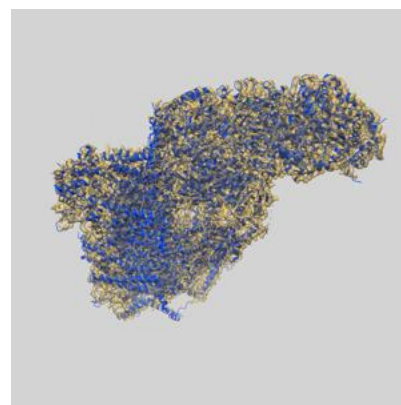
### 9.1 Map-model overlay [i](#)



X



Y

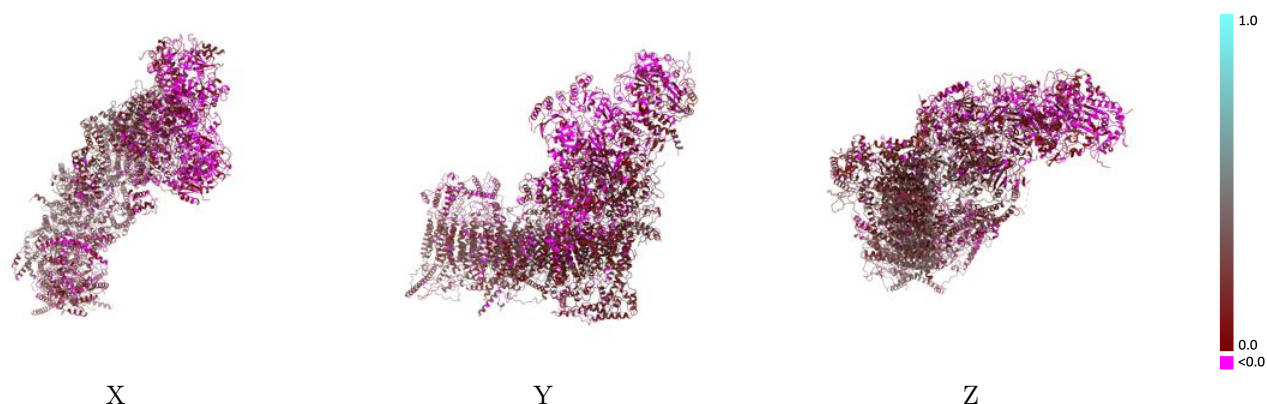


Z

The images above show the 3D surface view of the map at the recommended contour level 0.29 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.

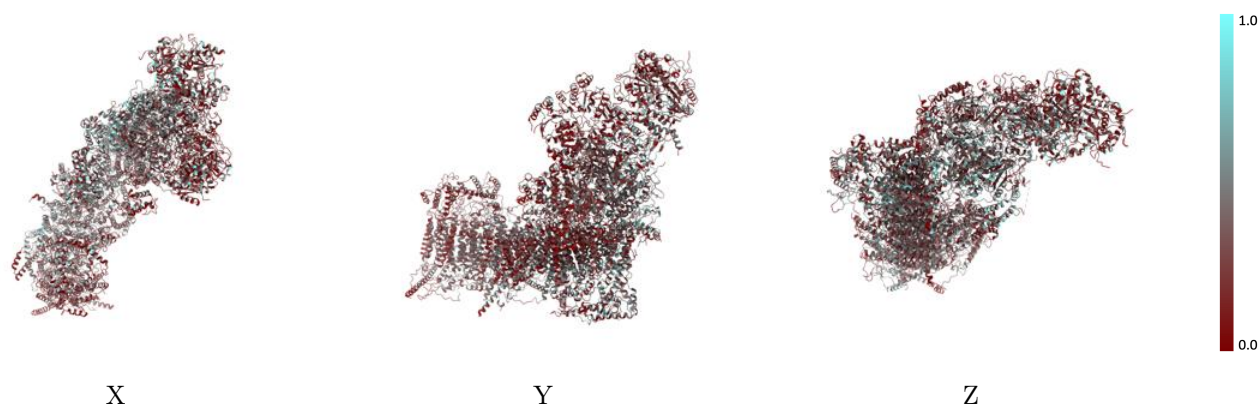


## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according 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.

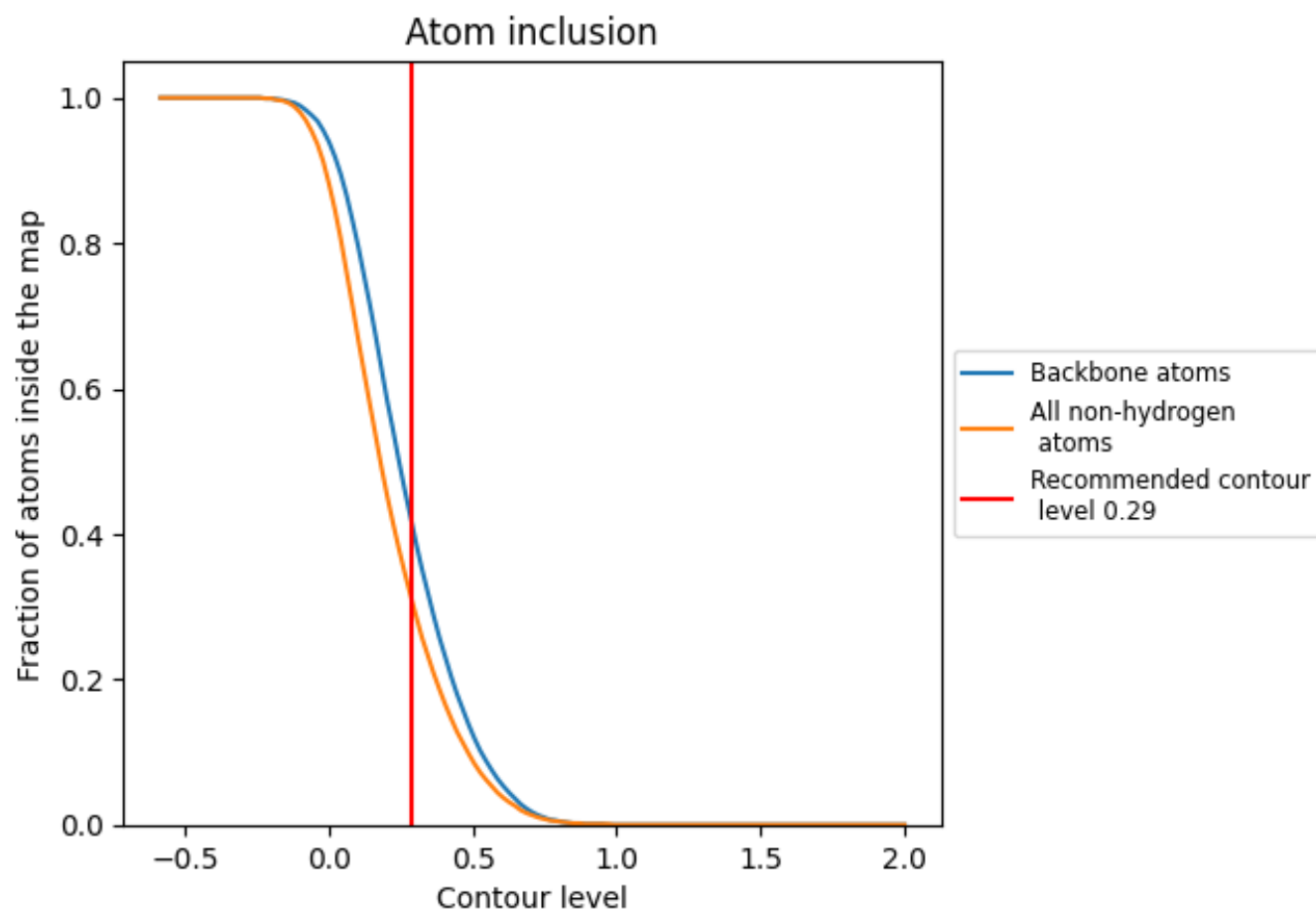
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.29).



## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 41% of all backbone atoms, 31% 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 (0.29) and Q-score for the entire model and for each chain.























Chain	Atom inclusion	Q-score
All	 0.3070	 0.1460
A	 0.3030	 0.1840
B	 0.3650	 0.1300
C	 0.3740	 0.1410
D	 0.4200	 0.1950
E	 0.2830	 0.0750
F	 0.3100	 0.0560
G	 0.2540	 -0.0000
H	 0.3720	 0.2070
I	 0.4040	 0.1730
J	 0.3030	 0.1560
K	 0.3090	 0.1640
L	 0.2500	 0.1640
M	 0.3320	 0.1720
N	 0.3780	 0.1970
O	 0.3340	 0.1860
P	 0.2310	 0.0470
Q	 0.2710	 0.0470
R	 0.3250	 0.1290
S	 0.2320	 0.0450
T	 0.1570	 0.1460
U	 0.1670	 0.0810
V	 0.4110	 0.2430
W	 0.2720	 0.0820
X	 0.3780	 0.2120
Y	 0.2160	 0.1940
Z	 0.3640	 0.2010
a	 0.3790	 0.1790
b	 0.3930	 0.3040
c	 0.3480	 0.2700
d	 0.3480	 0.2540
e	 0.3570	 0.2060
f	 0.3010	 0.2670
g	 0.3180	 0.1890
h	 0.3890	 0.2230



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
j	 0.1540	 0.1910
k	 0.0970	 0.1670
l	 0.2070	 0.1100
m	 0.1970	 0.0780
n	 0.2180	 0.0970
o	 0.2130	 0.1880
p	 0.3570	 0.2100
q	 0.3750	 0.1850
s	 0.2560	 0.0650
u	 0.2130	 0.1610
v	 0.4380	 0.2630