



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 04:02 AM UTC

PDB ID : 7B0N / pdb_00007b0n
EMDB ID : EMD-11969
Title : A 3.7-angstrom structure of Yarrowia lipolytica complex I with an R121M mutation in NUCM.
Authors : Hirst, J.; Grba, D.
Deposited on : 2020-11-20
Resolution : 3.70 Å(reported)
Based on initial model : 6YJ4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

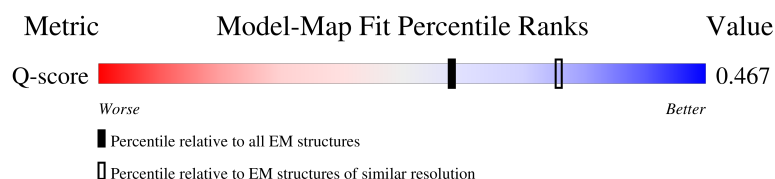
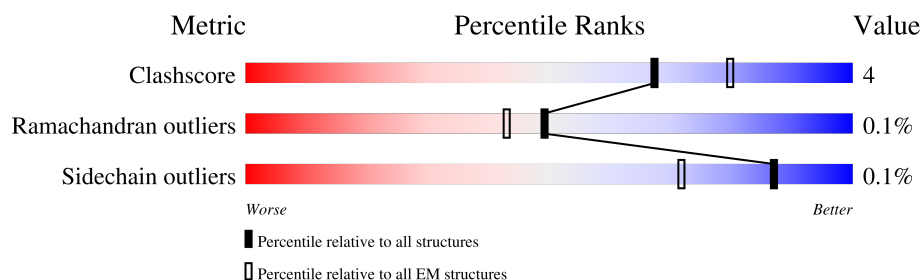
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



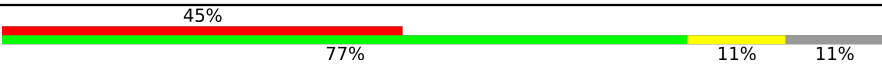
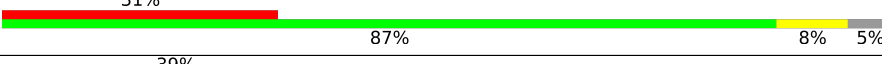
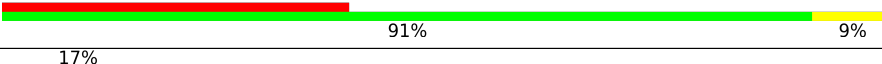
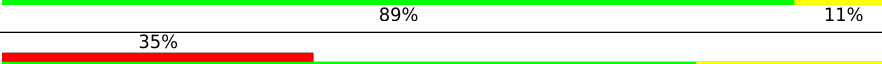
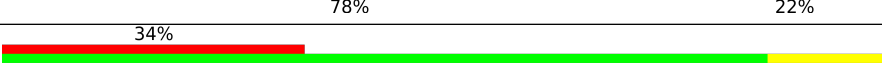
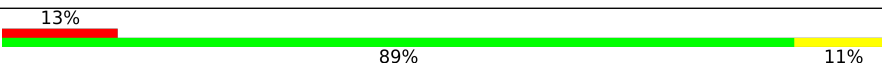
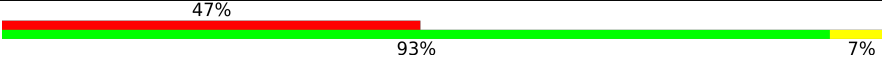
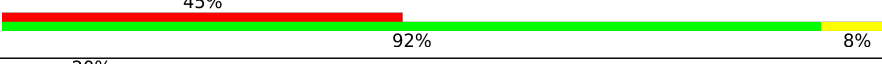
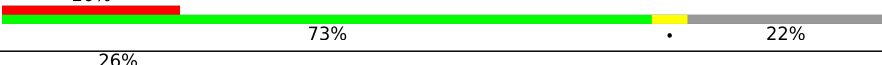
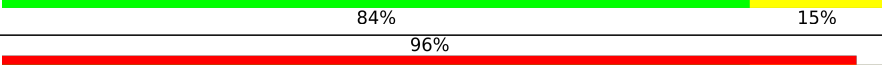
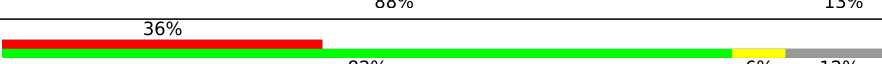
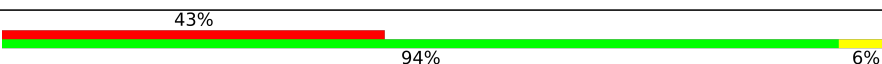
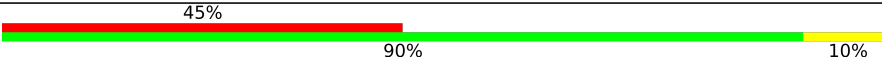
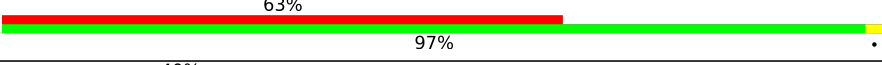
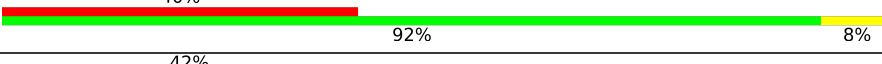
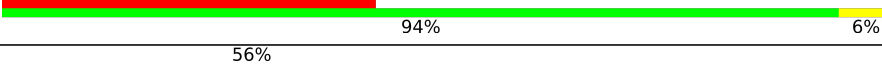
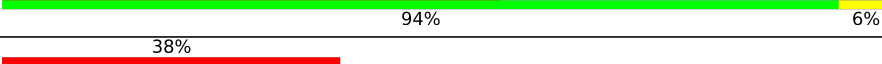
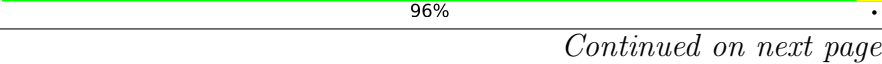
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	128	
2	B	210	
3	C	293	
4	D	466	

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Mol	Chain	Length	Quality of chain
5	E	243	
6	F	488	
7	G	728	
8	H	341	
9	I	193	
10	J	185	
11	K	89	
12	L	655	
13	M	486	
14	N	469	
15	O	169	
16	P	355	
17	Q	161	
18	R	118	
19	S	87	
20	T	81	
21	U	88	
22	V	144	
23	W	124	
24	X	172	
25	Y	180	
26	Z	122	
27	a	86	
28	b	78	
29	c	182	

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Mol	Chain	Length	Quality of chain
30	d	73	
31	e	89	
32	f	138	
33	g	249	
34	h	139	
35	i	90	
36	j	67	
37	k	60	
38	l	149	
39	m	93	
40	n	109	
41	o	99	
42	p	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	FMN	F	501	-	X	-	-
47	3PE	H	6401	X	-	-	-
47	3PE	I	501	X	-	-	-
47	3PE	M	502	X	-	-	-
47	3PE	g	301	X	-	-	-
51	EHZ	T	201	X	-	-	-
52	LMT	Y	1401	X	-	-	-
52	LMT	Y	1402	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 131131 atoms, of which 65779 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	94	Total	C	H	N	O	S	0	0
			1593	528	827	111	125	2		

- Molecule 2 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	177	Total	C	H	N	O	S	0	0
			2766	885	1373	246	249	13		

- Molecule 3 is a protein called NUGM protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	242	Total	C	H	N	O	S	0	0
			3924	1285	1925	339	371	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	282	ALA	-	expression tag	UNP Q9UUU0
C	283	ALA	-	expression tag	UNP Q9UUU0
C	284	ALA	-	expression tag	UNP Q9UUU0
C	285	ALA	-	expression tag	UNP Q9UUU0
C	286	ALA	-	expression tag	UNP Q9UUU0
C	287	ALA	-	expression tag	UNP Q9UUU0
C	288	HIS	-	expression tag	UNP Q9UUU0
C	289	HIS	-	expression tag	UNP Q9UUU0
C	290	HIS	-	expression tag	UNP Q9UUU0
C	291	HIS	-	expression tag	UNP Q9UUU0
C	292	HIS	-	expression tag	UNP Q9UUU0
C	293	HIS	-	expression tag	UNP Q9UUU0

- Molecule 4 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	437	Total	C	H	N	O	S	0	0
			6788	2181	3354	586	645	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	121	MET	ARG	engineered mutation	UNP Q9UUU1

- Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	216	Total	C	H	N	O	S	0	0
			3348	1060	1660	284	326	18		

- Molecule 6 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	460	Total	C	H	N	O	S	0	0
			7072	2248	3513	629	658	24		

- Molecule 7 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	694	Total	C	H	N	O	S	0	0
			10447	3275	5173	928	1042	29		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	341	Total	C	H	N	O	S	0	0
			5463	1828	2774	394	460	7		

- Molecule 9 is a protein called Subunit NUIM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	191	Total	C	H	N	O	S	0	0
			2997	972	1471	255	289	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	185	Total	C	H	N	O	S	0	0
			3044	990	1582	209	254	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	FME	-	initiating methionine	UNP S5U3X7

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	89	Total	C	H	N	O	S	0	0
			1446	465	753	109	116	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	655	Total	C	H	N	O	S	0	0
			10571	3485	5364	786	907	29		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	486	Total	C	H	N	O	S	0	0
			7910	2601	4053	586	655	15		

- Molecule 14 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	469	Total	C	H	N	O	S	0	0
			7780	2558	4004	550	656	12		

- Molecule 15 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	168	Total	C	H	N	O	S	0	0
			2586	845	1281	223	233	4		

- Molecule 16 is a protein called Epimerase domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	355	Total	C	H	N	O	S	0	0
			5575	1785	2763	493	524	10		

- Molecule 17 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	125	Total	C	H	N	O	S	0	0
			2031	659	994	190	186	2		

- Molecule 18 is a protein called zf-CHCC domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	118	Total	C	H	N	O	S	0	0
			1798	574	876	166	177	5		

- Molecule 19 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	86	Total	C	H	N	O	S	0	0
			1351	418	684	126	122	1		

- Molecule 20 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	81	Total	C	H	N	O		0	0
			1234	391	614	98	131			

- Molecule 21 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	88	Total	C	H	N	O	S	0	0
			1322	416	655	106	143	2		

- Molecule 22 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	126	Total	C	H	N	O	S	0	0
			2049	653	1021	173	200	2		

- Molecule 23 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	123	Total	C	H	N	O	S	0	0
			2054	667	1018	182	185	2		

- Molecule 24 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	171	Total	C	H	N	O	S	0	0
			2678	847	1333	236	252	10		

- Molecule 25 is a protein called Complex I-B14.7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	179	Total	C	H	N	O	S	0	0
			2638	842	1311	240	240	5		

- Molecule 26 is a protein called GRIM-19.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	122	Total	C	H	N	O	S	0	0
			1983	629	1000	180	169	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	86	Total	C	H	N	O	S	0	0
			1353	432	672	127	119	3		

- Molecule 28 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	78	Total	C	H	N	O	S	0	0
			1257	418	618	115	105	1		

- Molecule 29 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	182	Total	C	H	N	O	S	0	0
			2804	898	1407	241	256	2		

- Molecule 30 is a protein called subunit NEBM of protein NADH:Ubiquinone Oxidoreductase (Complex I) [*Yarrowia lipolytica*].

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	67	Total	C	H	N	O		0	0
			1042	339	532	86	85			

- Molecule 31 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	e	68	Total	C	H	N	O	S	0	0
			1082	336	536	102	102	6		

- Molecule 32 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	f	137	Total	C	H	N	O	S	0	0
			2225	730	1089	194	210	2		

- Molecule 33 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	g	198	Total	C	H	N	O	S	0	0
			3188	1019	1603	273	291	2		

- Molecule 34 is a protein called subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	h	113	Total	C	H	N	O	S	0	0
			1786	585	877	153	170	1		

- Molecule 35 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
35	i	86	Total	C	H	N	O	S	0	0
			1300	420	641	120	118	1		

- Molecule 36 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
36	j	53	Total	C	H	N	O	S	0	0
			884	299	439	77	66	3		

- Molecule 37 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
37	k	47	Total	C	H	N	O		0	0
			734	242	361	70	61			

- Molecule 38 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
38	l	125	Total	C	H	N	O	S	0	0
			2012	674	973	166	197	2		

- Molecule 39 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
39	m	92	Total	C	H	N	O		0	0
			1453	472	718	134	129			

- Molecule 40 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
40	n	108	Total	C	H	N	O	S	0	0
			1804	571	904	172	154	3		

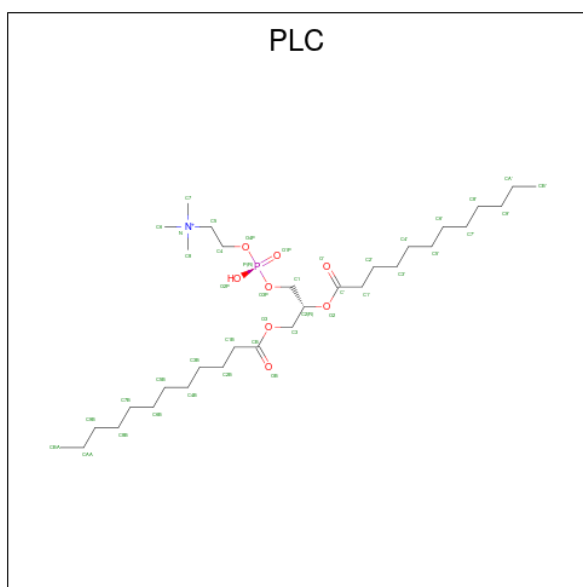
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
41	o	83	Total	C	H	N	O	S	0	0
			1366	431	685	123	119	8		

- Molecule 42 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

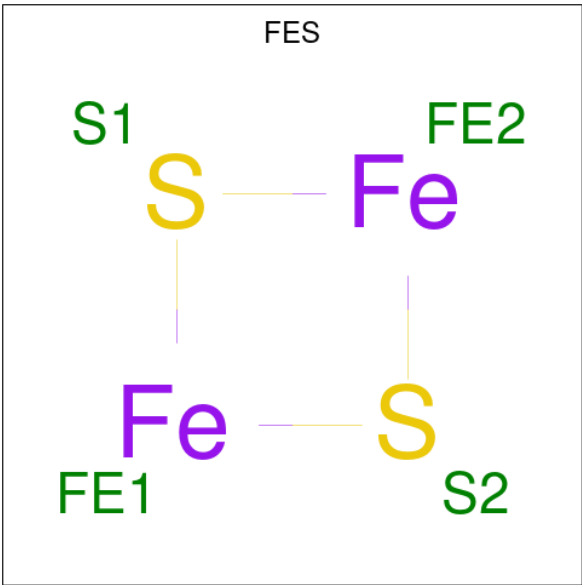
Mol	Chain	Residues	Atoms						AltConf	Trace
42	p	91	Total	C	H	N	O	S	0	0
			1492	475	726	138	150	3		

- Molecule 43 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



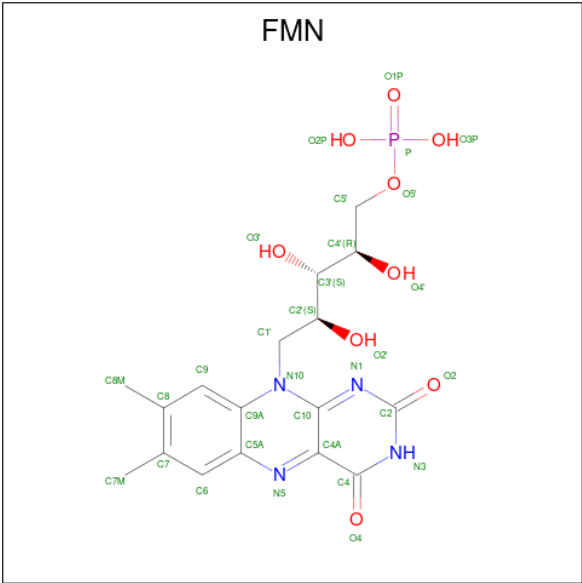
Mol	Chain	Residues	Atoms						AltConf
43	D	1	Total	C	H	N	O	P	0
			61	17	34	1	8	1	
43	H	1	Total	C	H	N	O	P	0
			64	18	36	1	8	1	
43	L	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
43	L	1	Total	C	H	N	O	P	0
			82	24	48	1	8	1	
43	N	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
43	d	1	Total	C	H	N	O	P	0
			61	17	34	1	8	1	

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



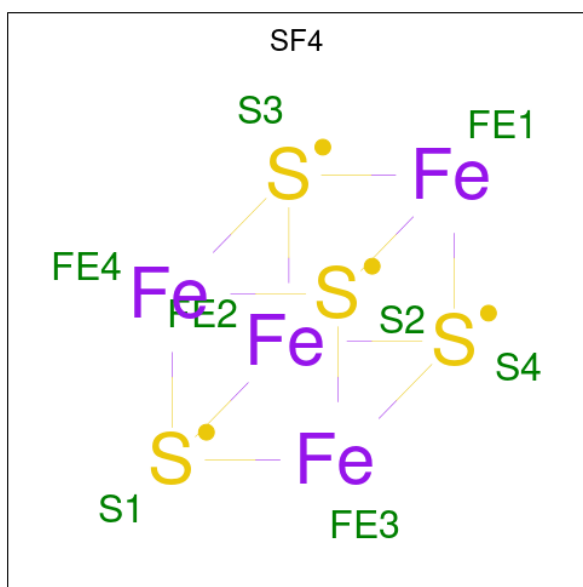
Mol	Chain	Residues	Atoms			AltConf
44	E	1	Total	Fe	S	0
			4	2	2	
44	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



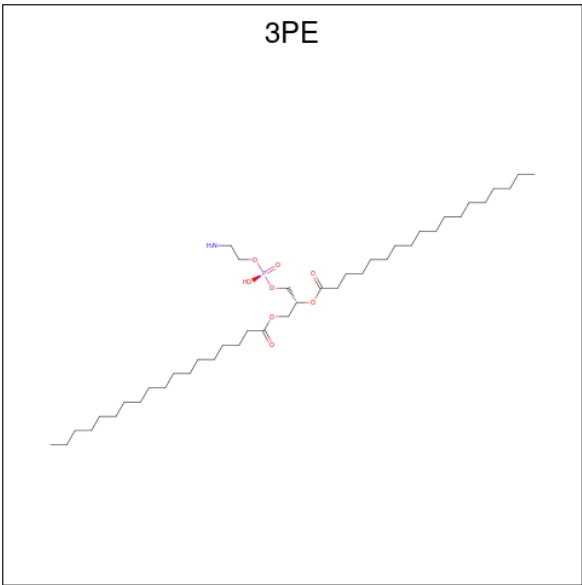
Mol	Chain	Residues	Atoms						AltConf
45	F	1	Total	C	H	N	O	P	0
			49	17	18	4	9	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



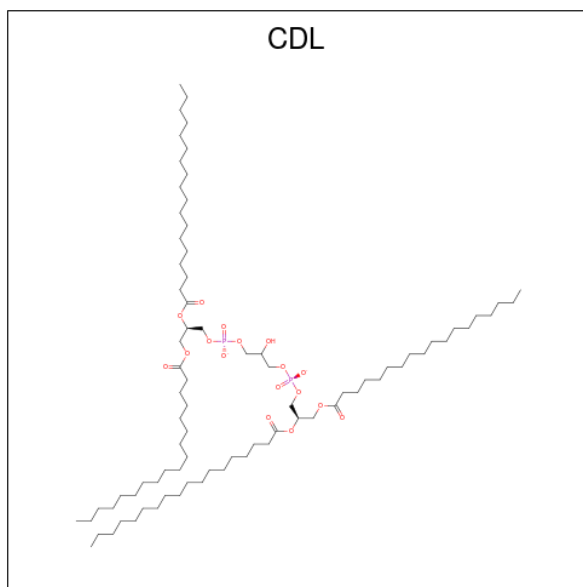
Mol	Chain	Residues	Atoms			AltConf
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



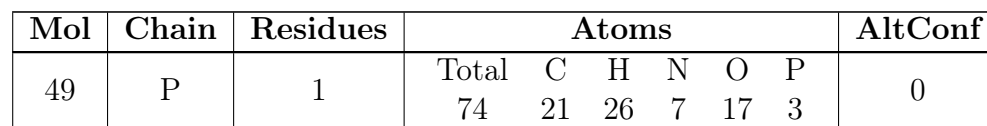
Mol	Chain	Residues	Atoms						AltConf
47	H	1	Total	C	H	N	O	P	0
			44	12	22	1	8	1	
47	H	1	Total	C	H	N	O	P	0
			118	36	72	1	8	1	
47	I	1	Total	C	H	N	O	P	0
			74	22	42	1	8	1	
47	L	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	L	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	L	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	M	1	Total	C	H	N	O	P	0
			69	20	39	1	8	1	
47	N	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	Y	1	Total	C	H	N	O	P	0
			79	23	46	1	8	1	
47	Z	1	Total	C	H	N	O	P	0
			109	33	66	1	8	1	
47	b	1	Total	C	H	N	O	P	0
			109	33	66	1	8	1	
47	d	1	Total	C	H	N	O	P	0
			52	14	28	1	8	1	
47	g	1	Total	C	H	N	O	P	0
			68	20	38	1	8	1	

- Molecule 48 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms					AltConf
48	M	1	Total	C	H	O	P	0
			205	64	122	17	2	
48	O	1	Total	C	H	O	P	0
			145	44	82	17	2	
48	Z	1	Total	C	H	O	P	0
			123	38	66	17	2	
48	a	1	Total	C	H	O	P	0
			108	33	56	17	2	
48	b	1	Total	C	H	O	P	0
			100	29	52	17	2	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

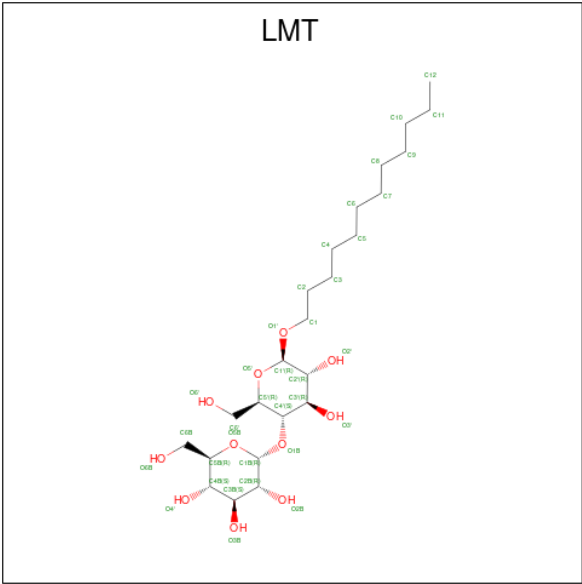


- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 50 | R | 1 | Total Zn
1 1 | 0 |

- # EHZ
-
- The chemical structure of EHZ (Ergosterol) is shown. It features a long hydrocarbon side chain (C18 to C28) attached to a steroid nucleus. The side chain is saturated and ends in a methyl group (C28). The steroid nucleus is composed of four fused rings (A, B, C, D) and a hydroxyl group (OH) at C3. A phosphate group (PO4) is attached to the side chain at C28 via an ester linkage. The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms (O), with one oxygen atom (O1) being part of the ester linkage and the other three (O2, O3, O4) being terminal. The structure is labeled with atom numbers (C1 to C28, O1 to O4, P1) and includes a legend for the atoms: C (Carbon), O (Oxygen), P (Phosphorus), and H (Hydrogen).

Mol	Chain	Residues	Atoms							AltConf
51	T	1	Total	C	H	N	O	P	S	0
			75	22	40	2	9	1	1	
51	U	1	Total	C	H	N	O	P	S	0
			77	23	41	2	9	1	1	

- Molecule 52 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

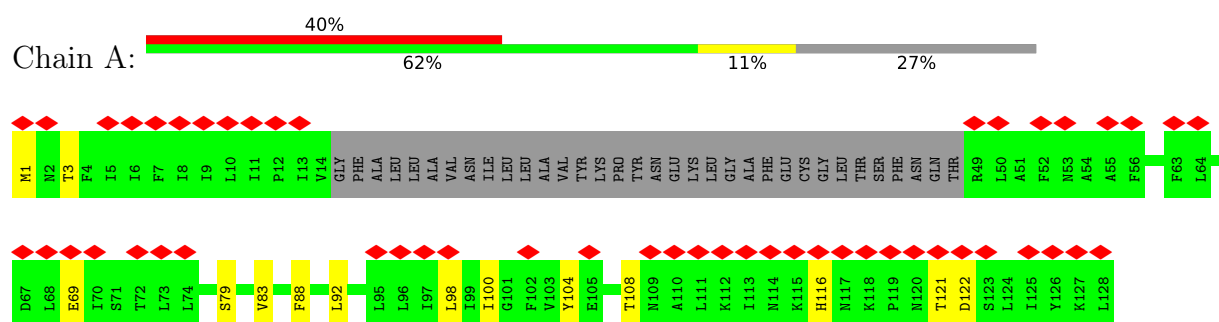


Mol	Chain	Residues	Atoms				AltConf
52	Y	1	Total	C	H	O	0
			81	24	46	11	
52	Y	1	Total	C	H	O	0
			81	24	46	11	

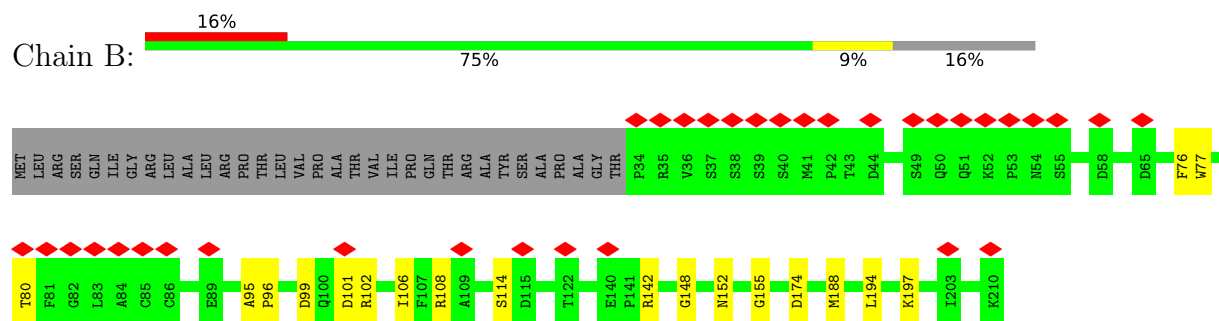
3 Residue-property plots [i](#)

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

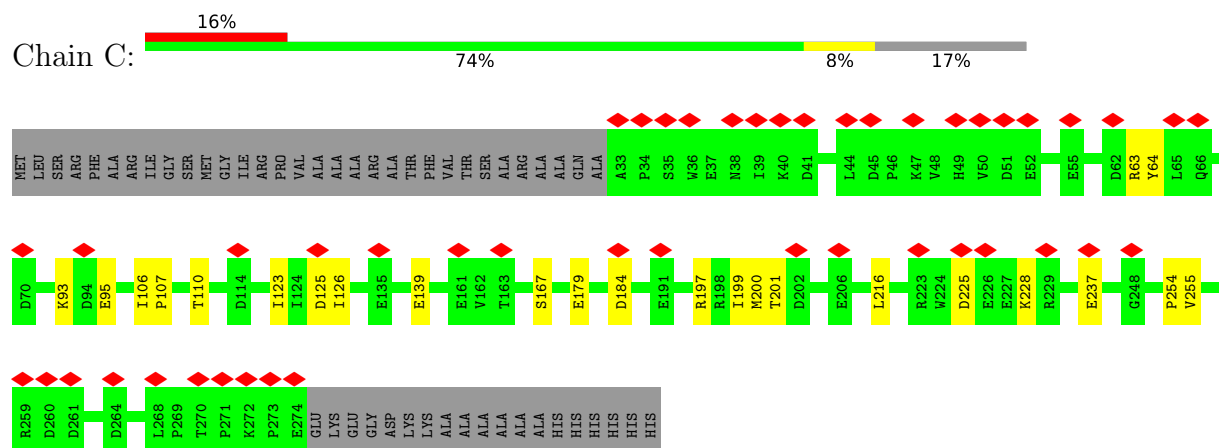
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



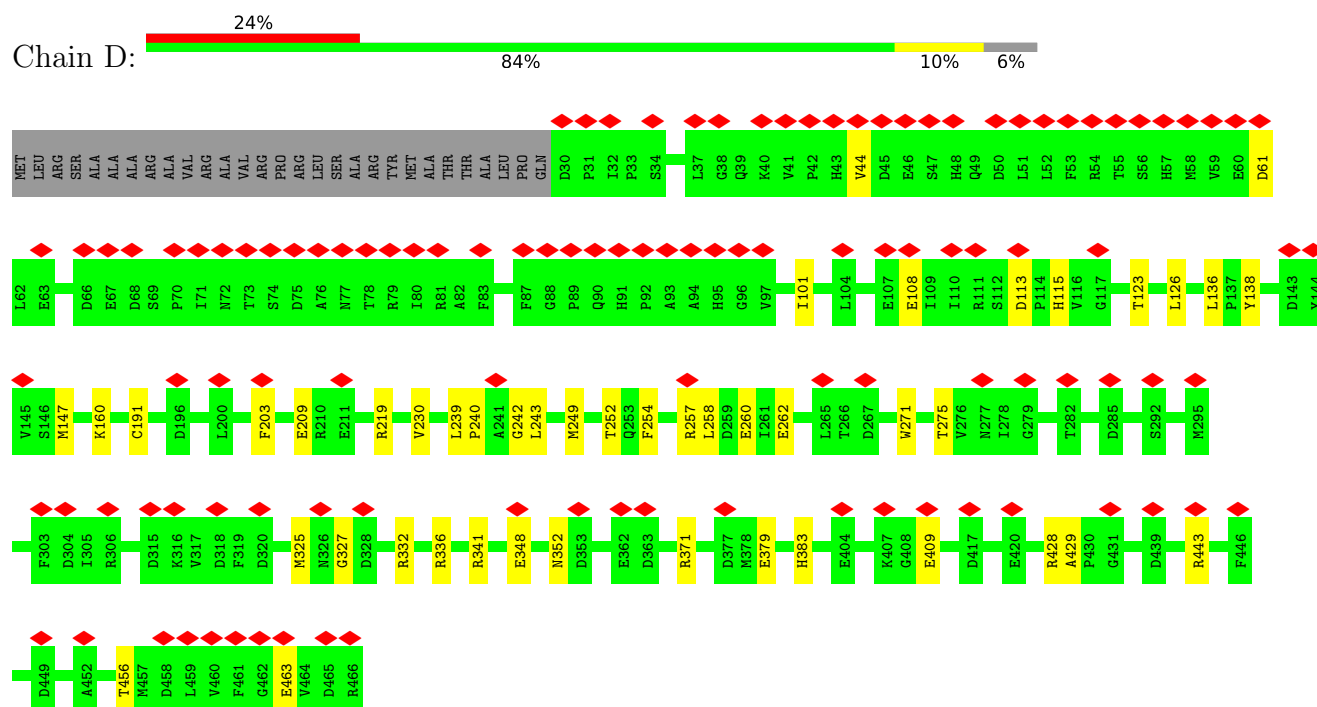
• Molecule 2: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)



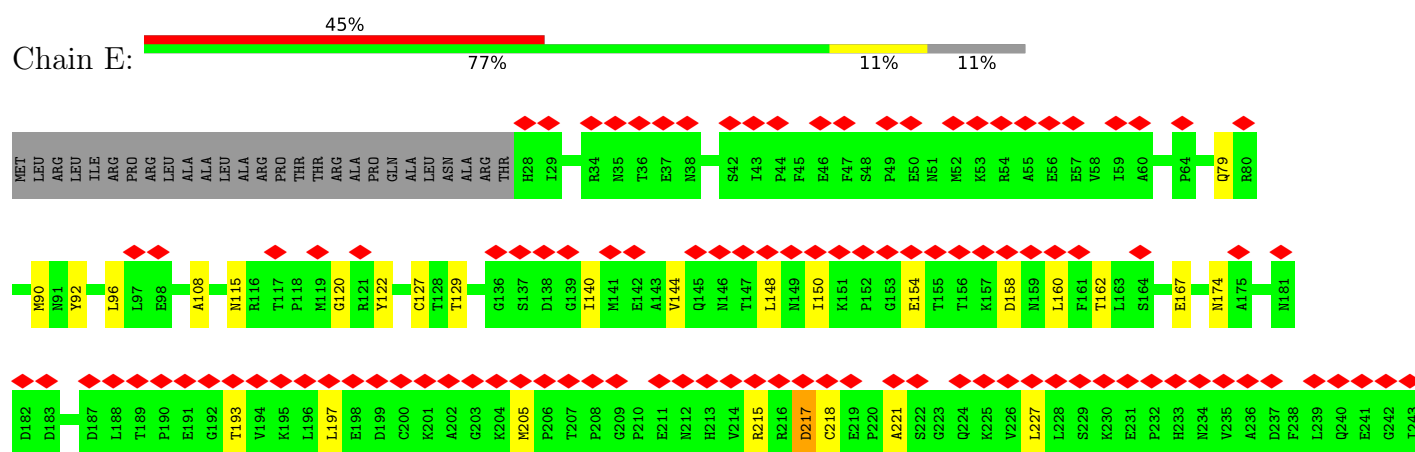
• Molecule 3: NUGM protein



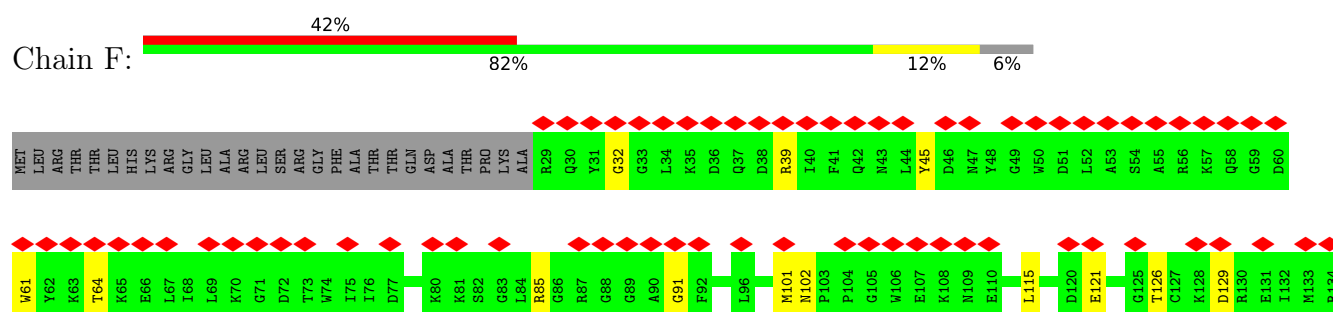
- Molecule 4: NUCM protein

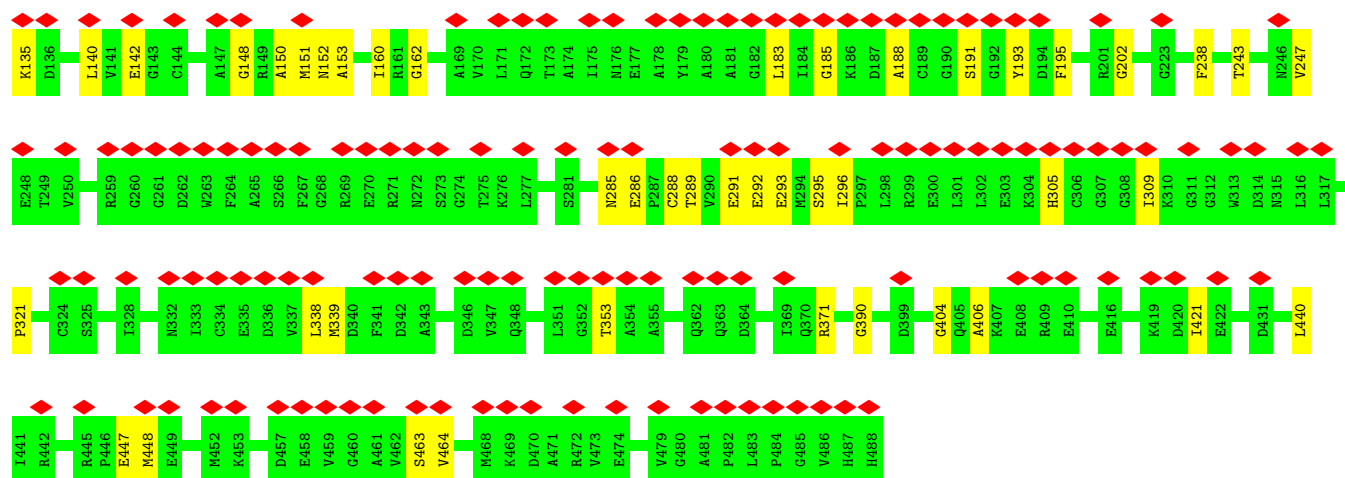


- Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

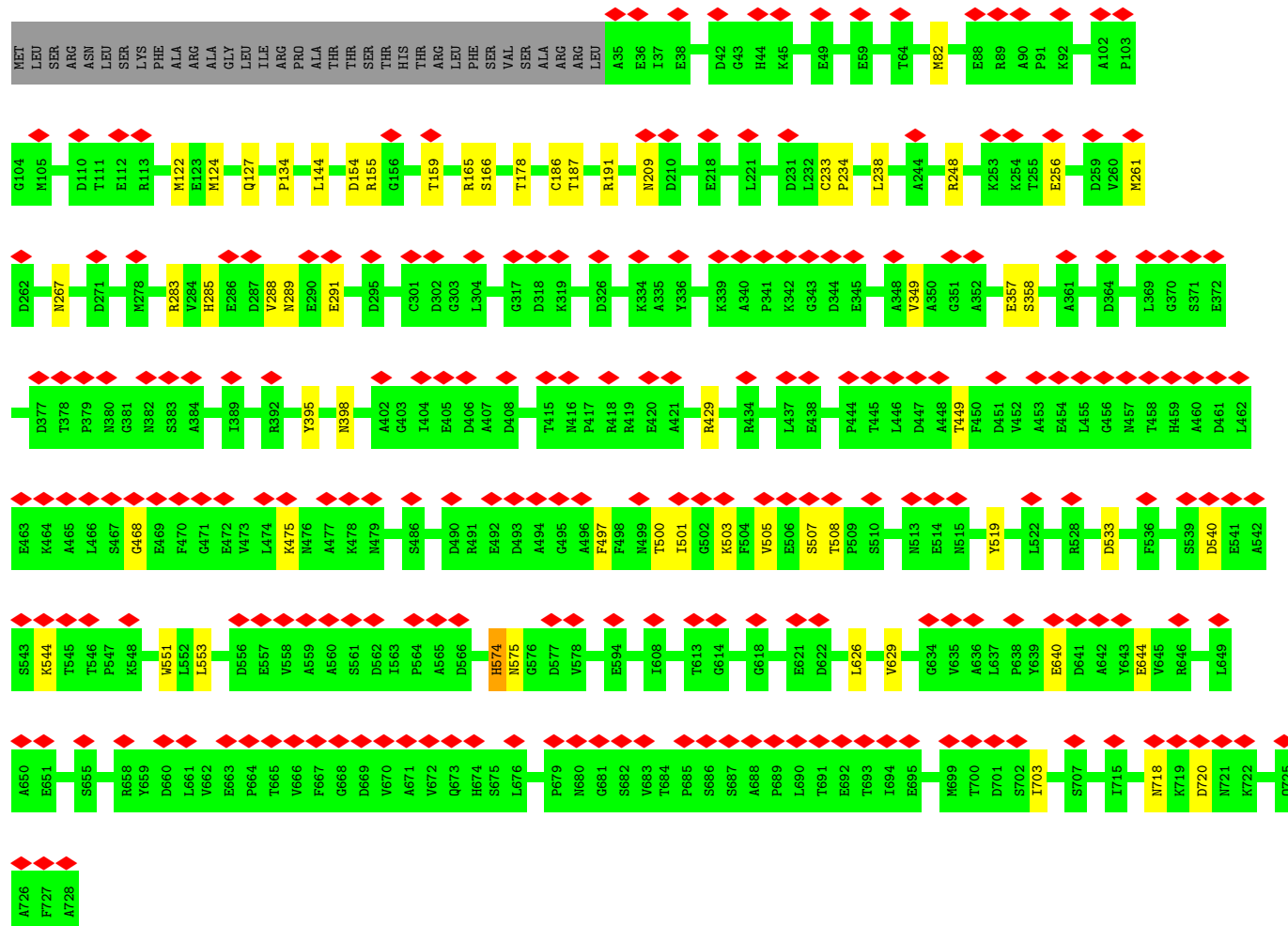
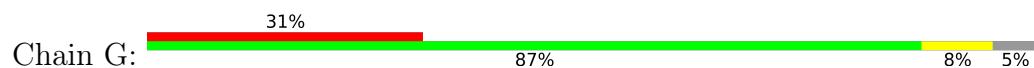


- Molecule 6: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)

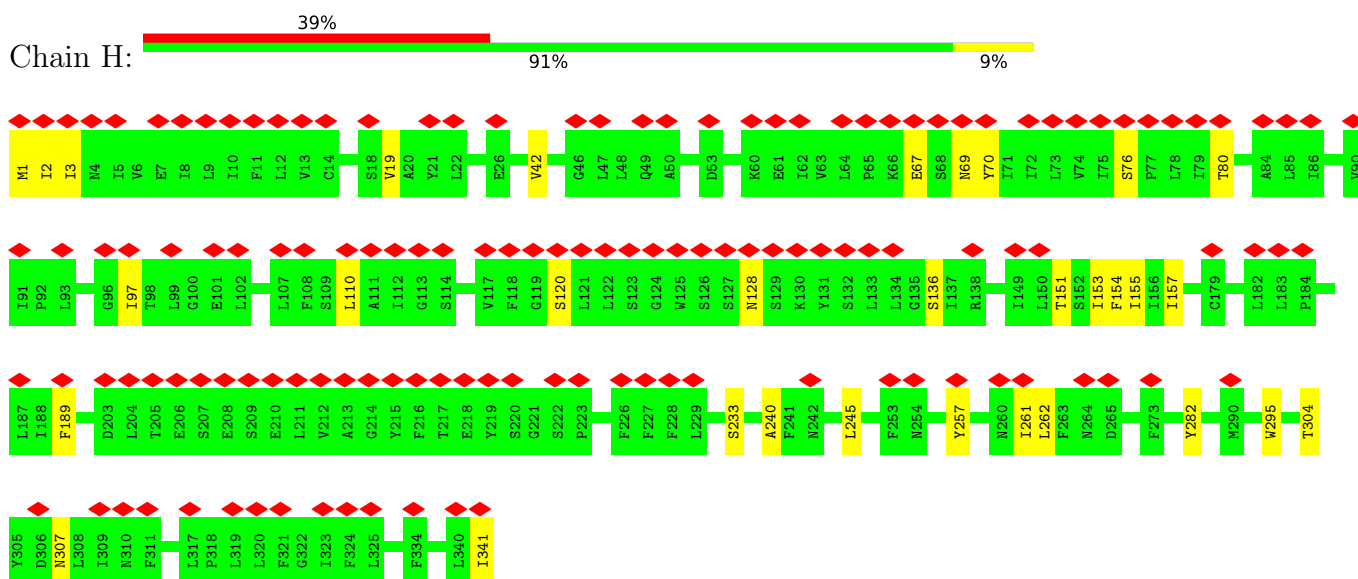




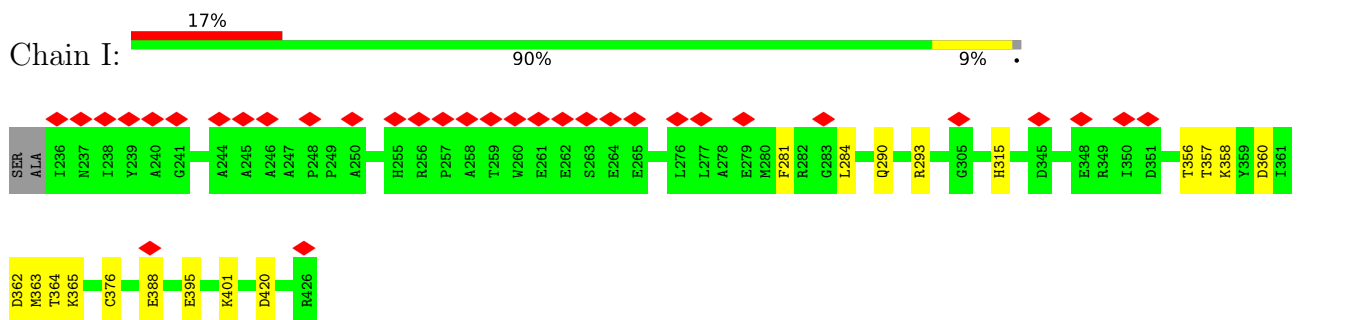
• Molecule 7: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)



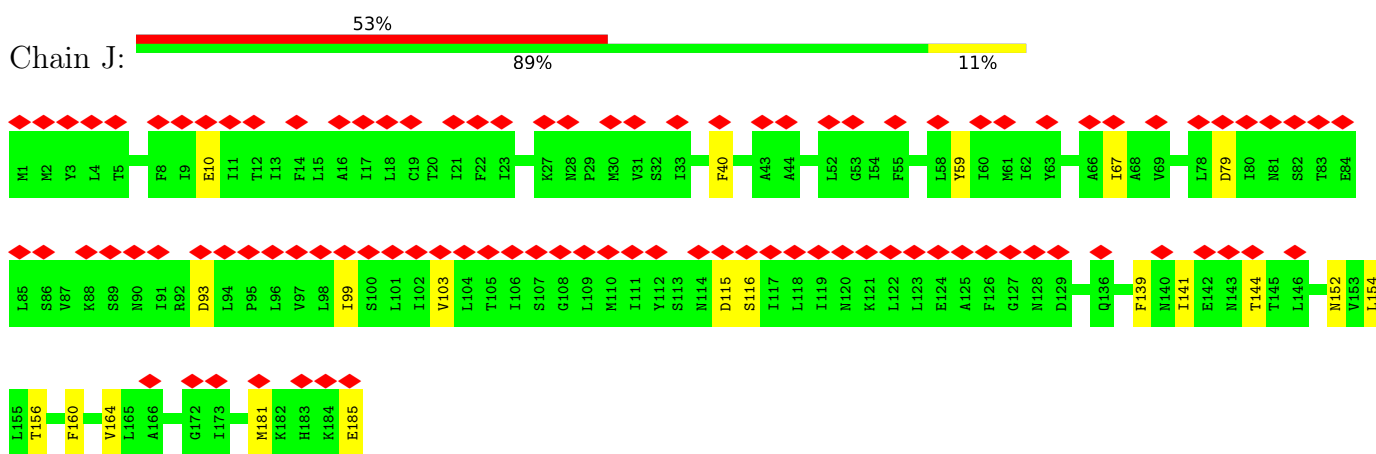
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



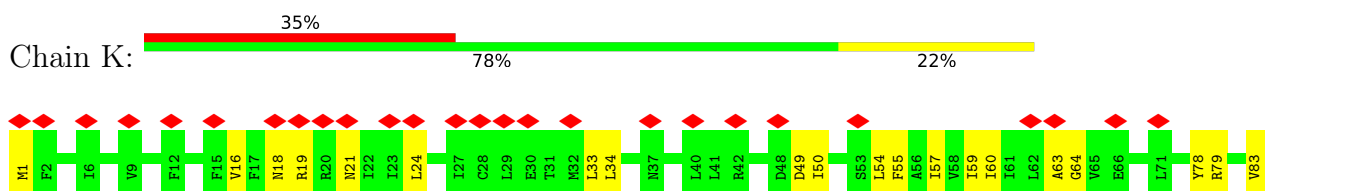
- Molecule 9: Subunit NUIM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

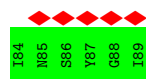


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

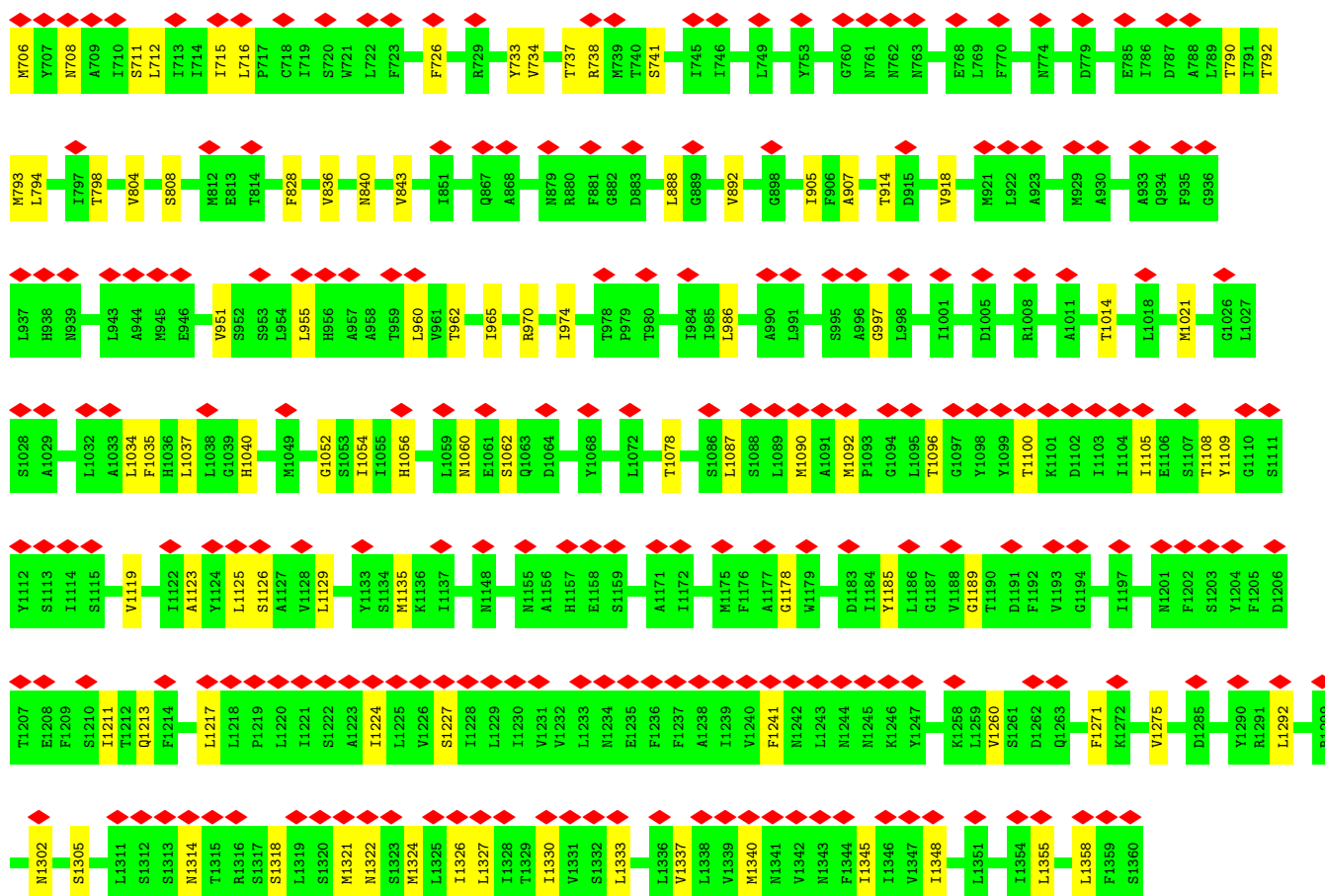
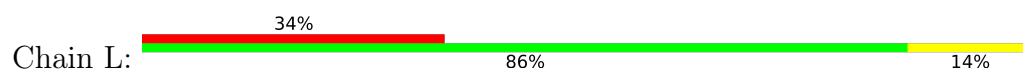


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

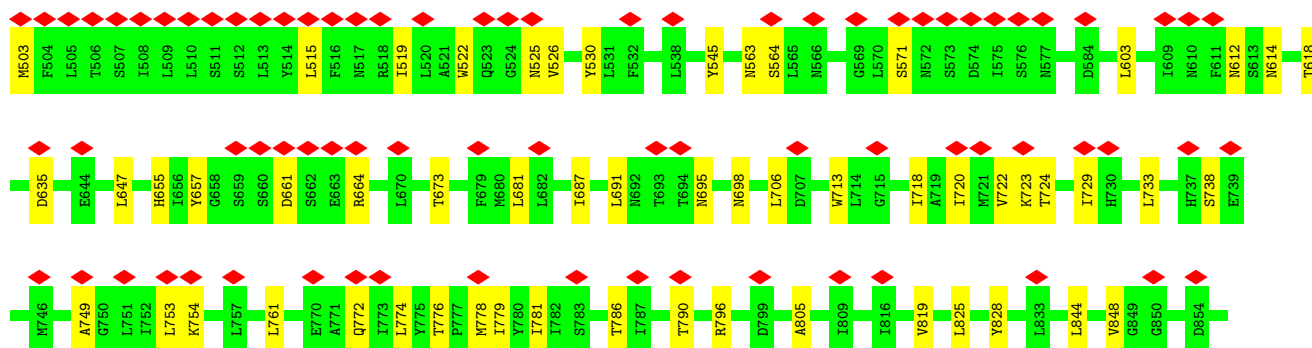
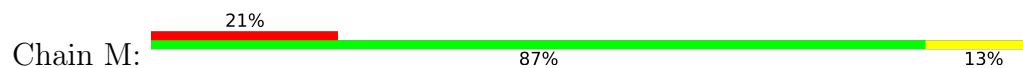


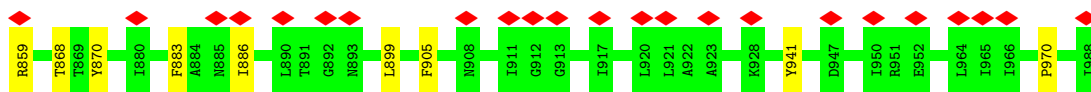


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

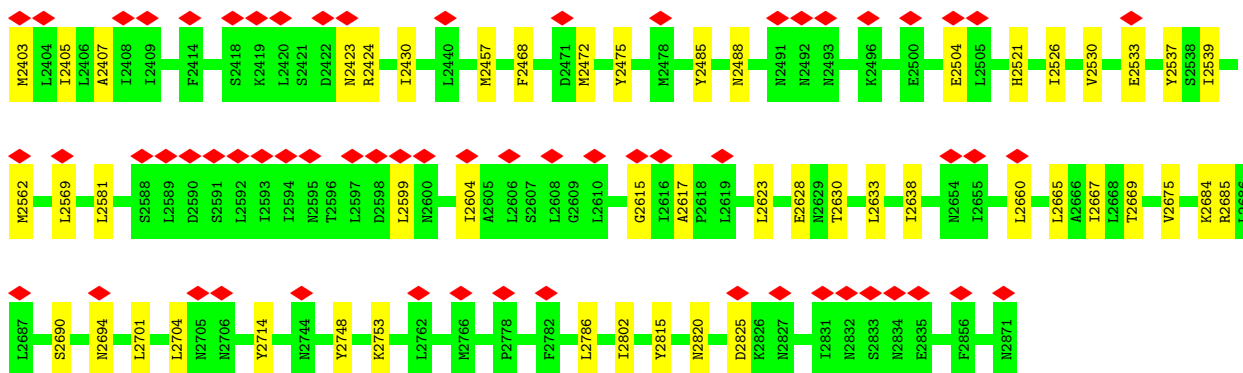
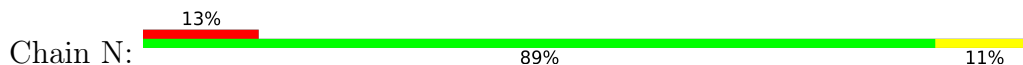


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

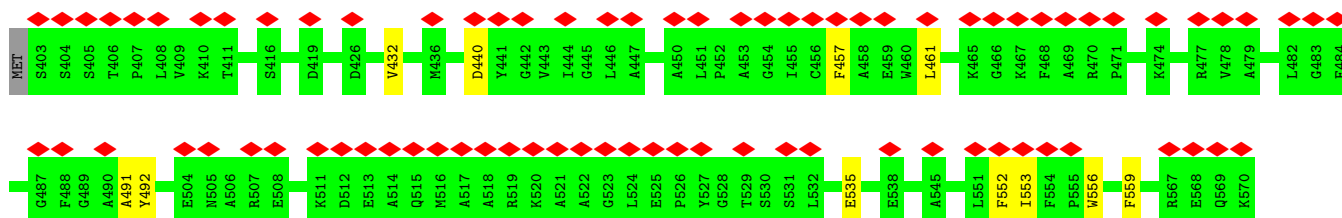
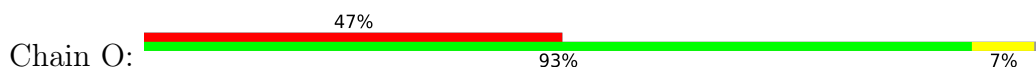




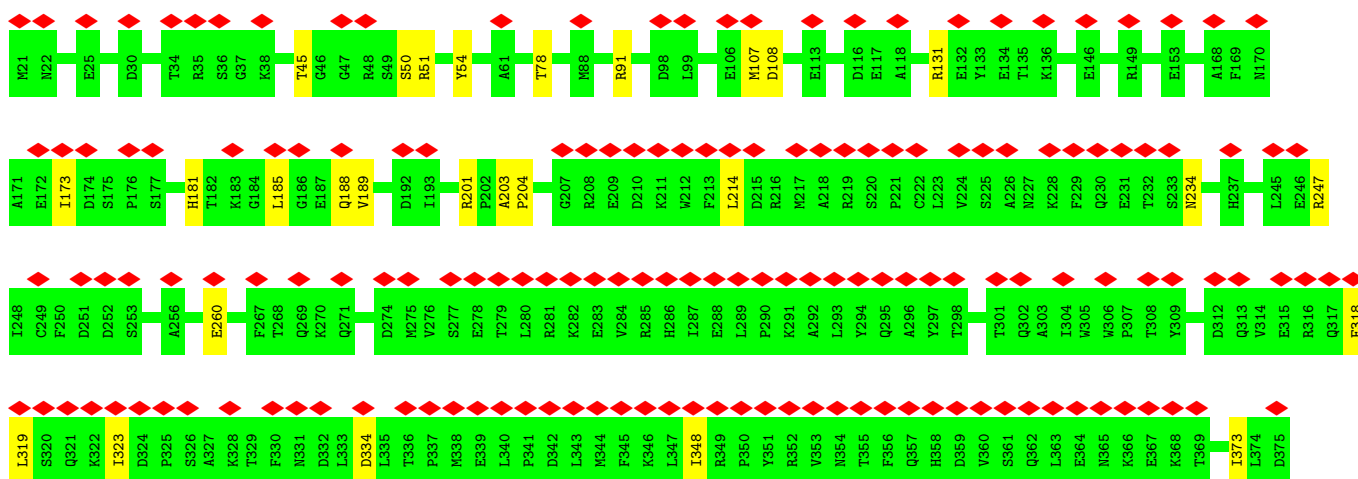
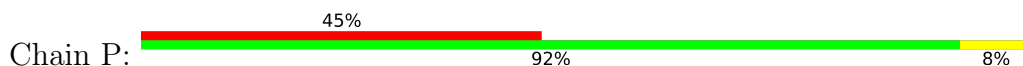
• Molecule 14: NADH dehydrogenase subunit 2



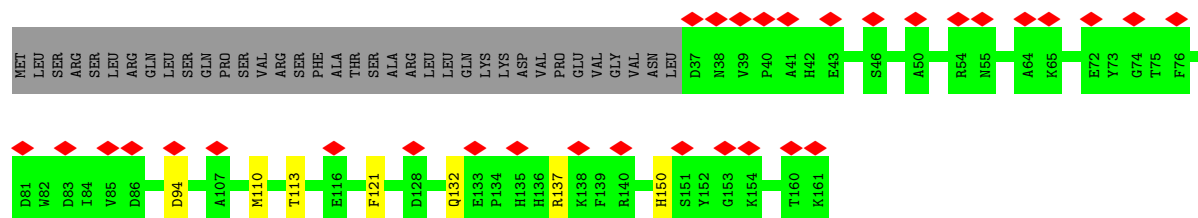
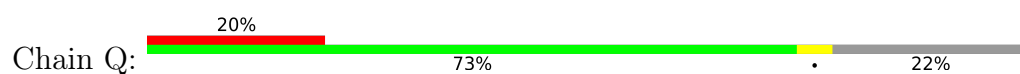
• Molecule 15: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)



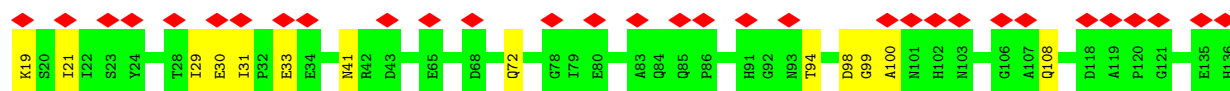
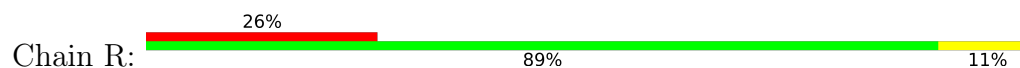
• Molecule 16: Epimerase domain-containing protein



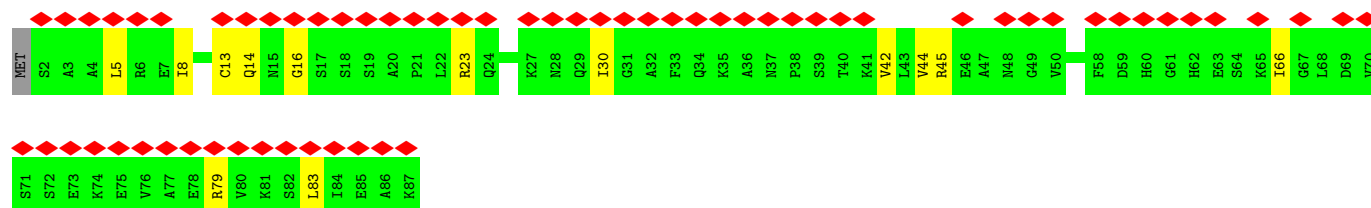
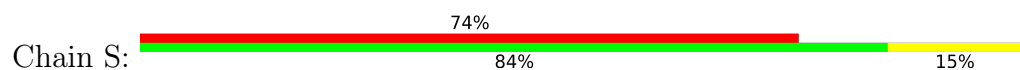
• Molecule 17: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)



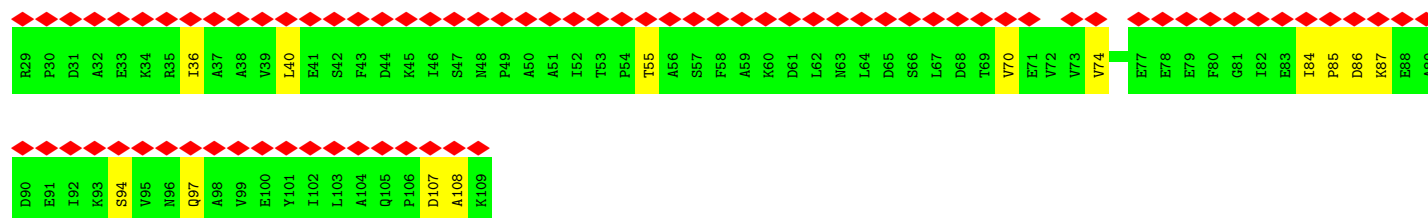
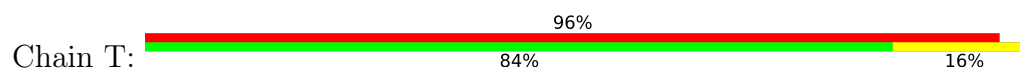
- Molecule 18: zf-CHCC domain-containing protein



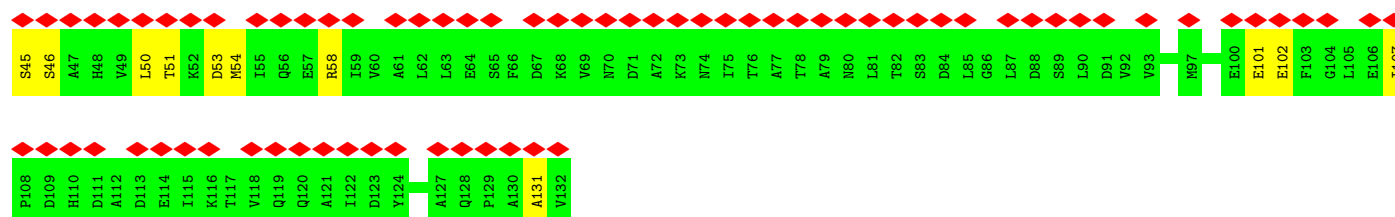
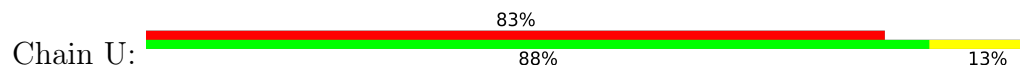
- Molecule 19: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)



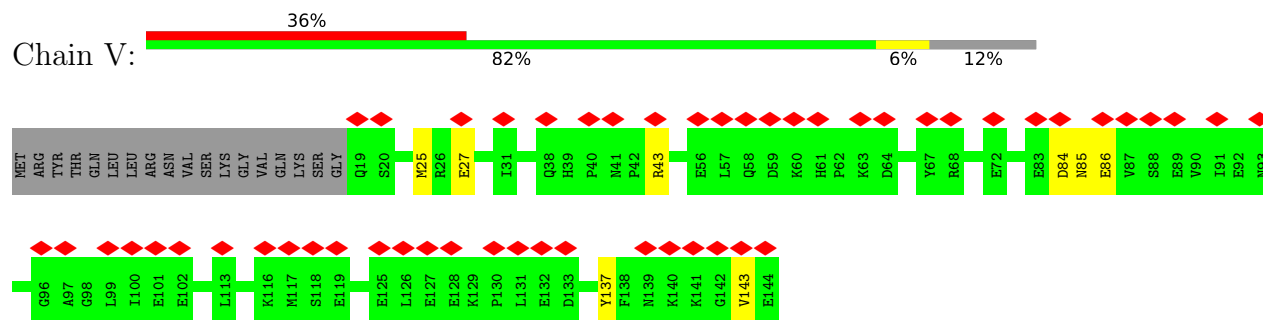
- Molecule 20: Acyl carrier protein



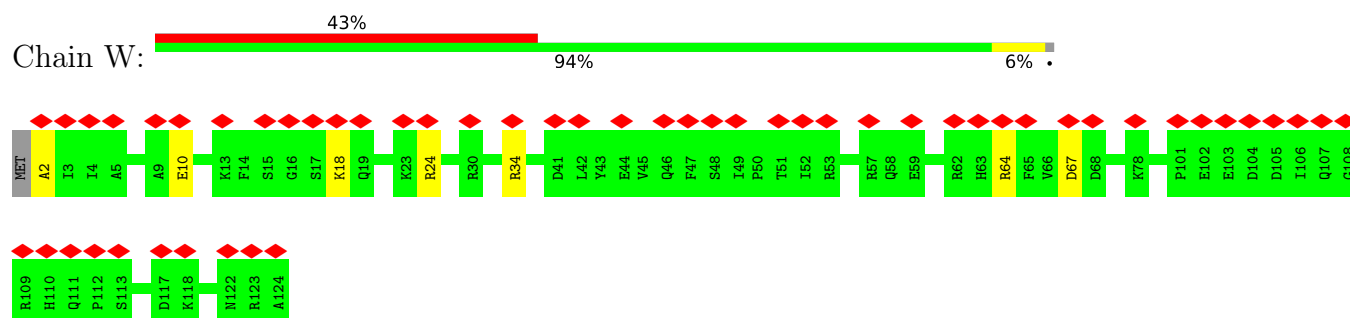
- Molecule 21: Acyl carrier protein



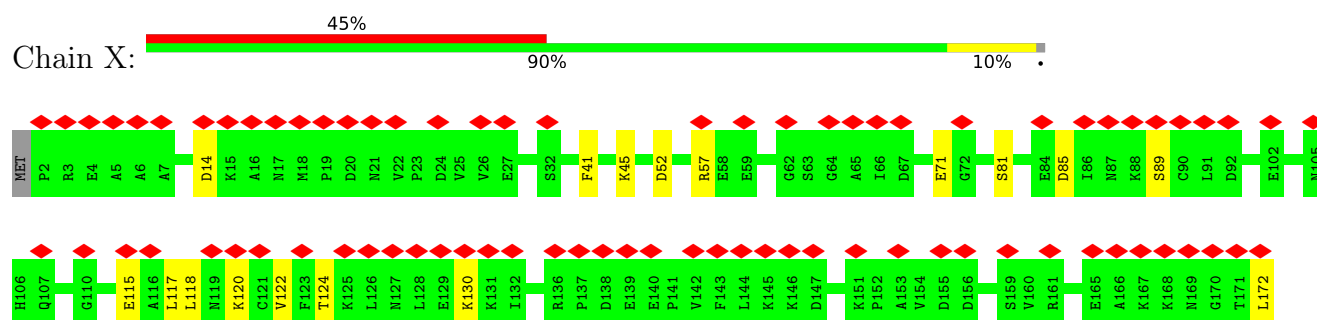
- Molecule 22: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



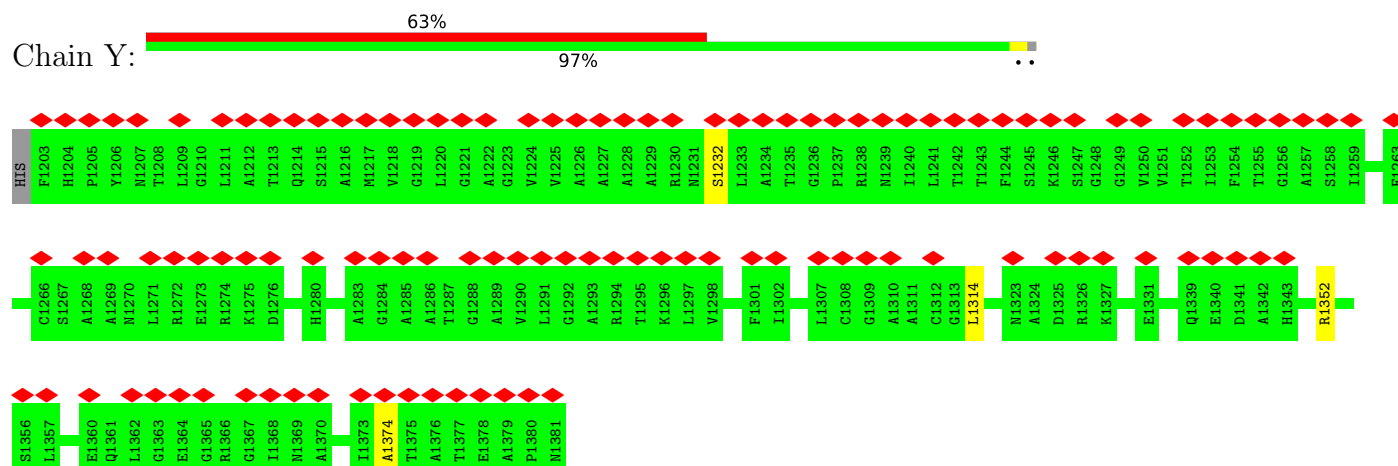
- Molecule 23: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



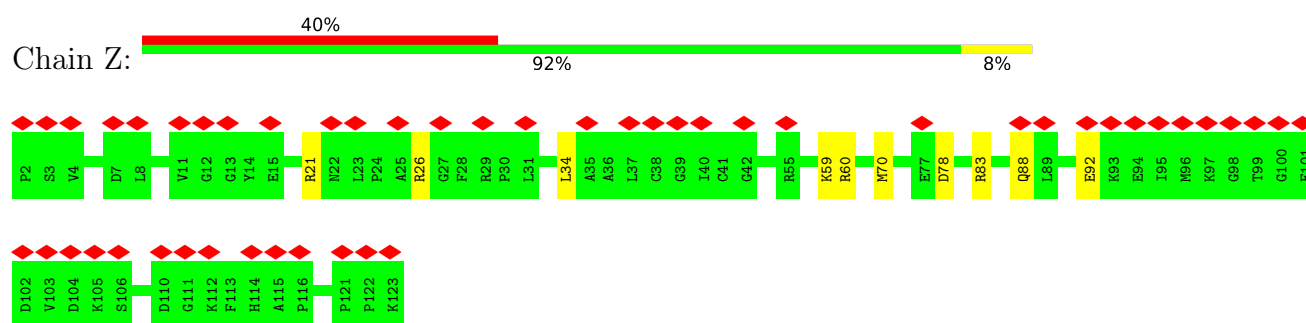
- Molecule 24: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



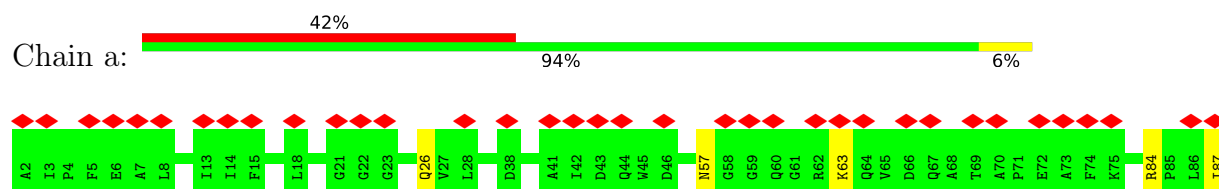
- Molecule 25: Complex I-B14.7



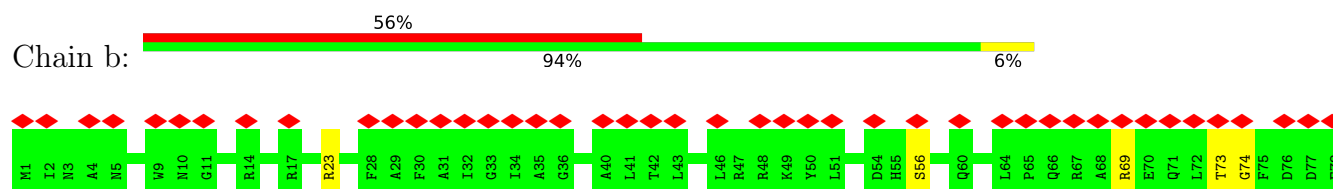
- Molecule 26: GRIM-19



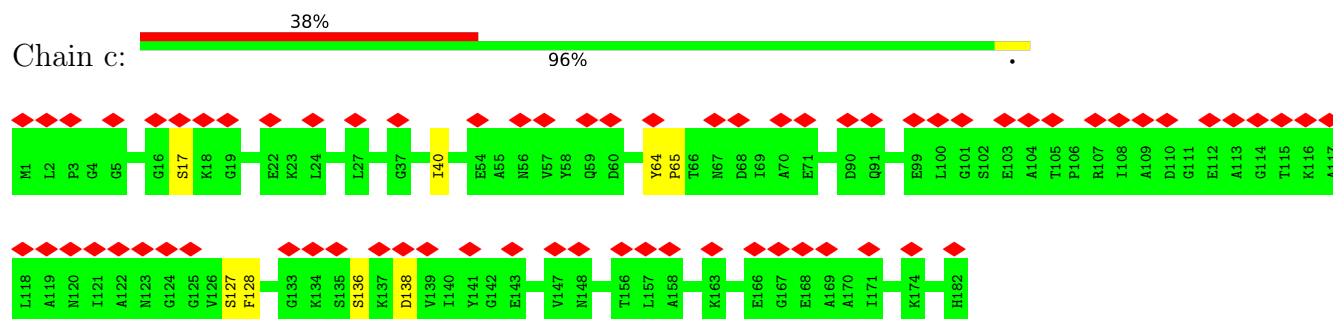
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



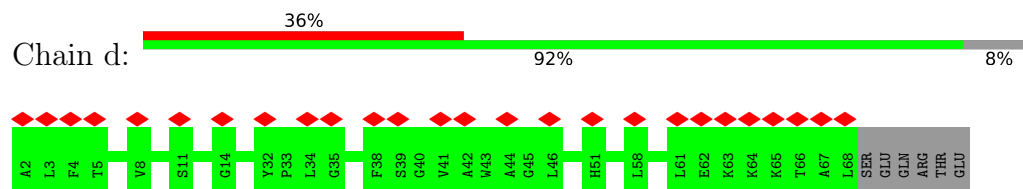
- Molecule 28: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 29: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

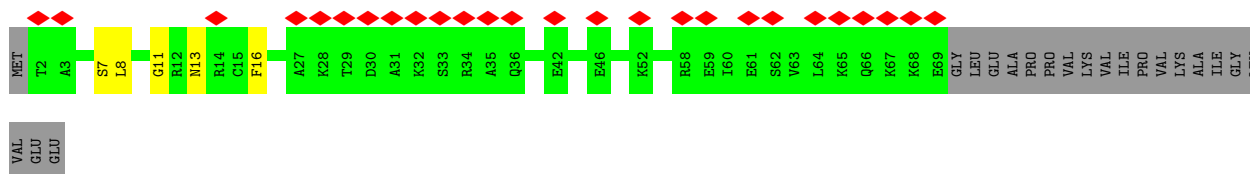


- Molecule 30: subunit NEBM of protein NADH:Ubiquinone Oxidoreductase (Complex I) [Yarrowia lipolytica]

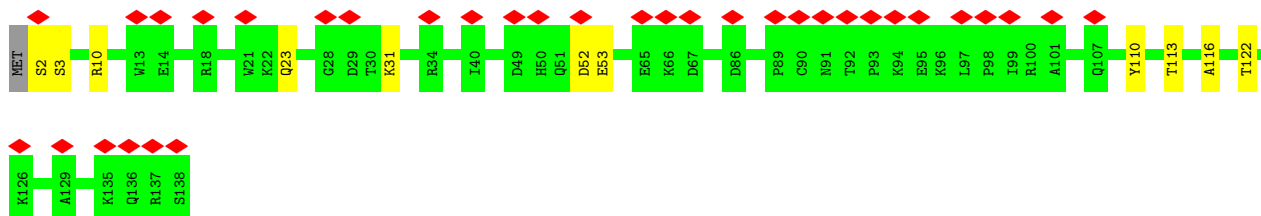
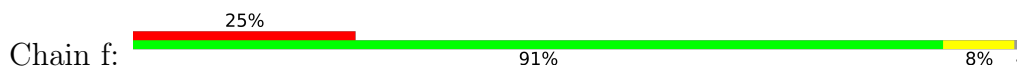


- Molecule 31: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

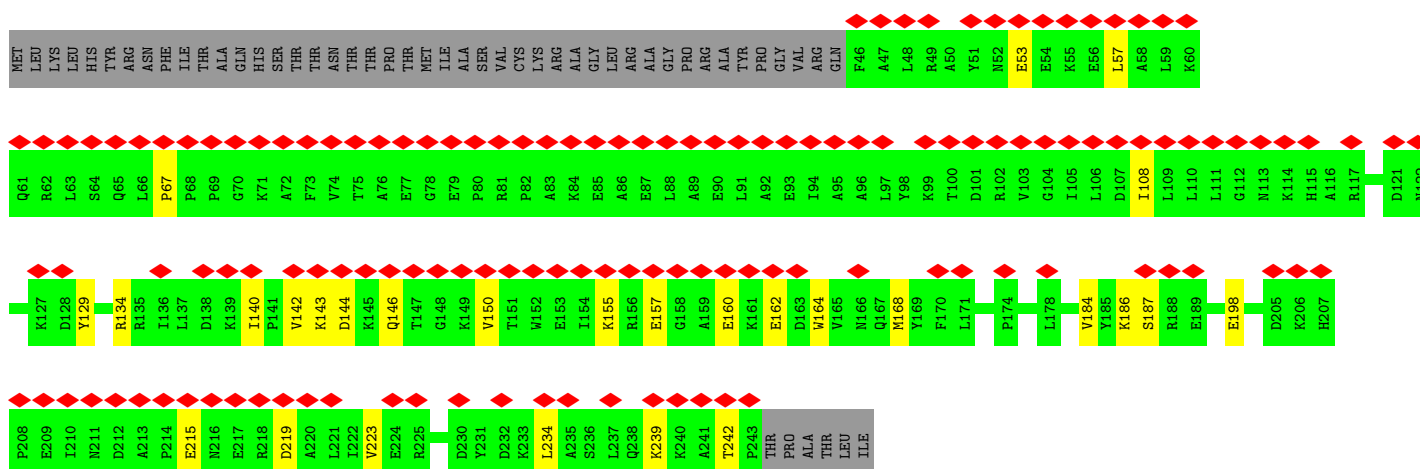




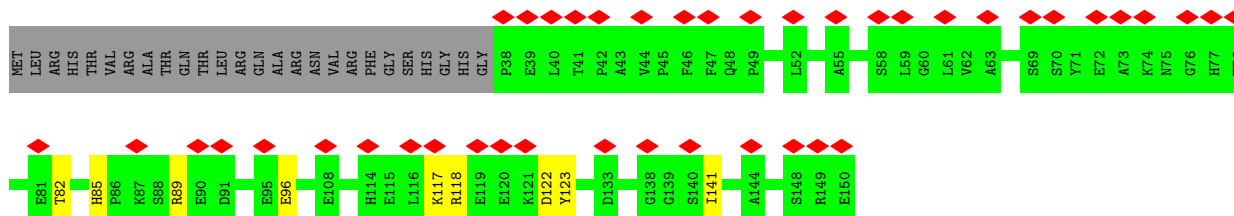
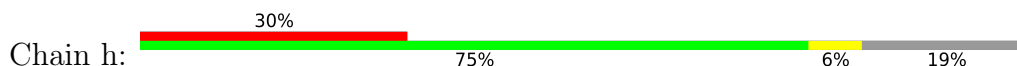
- Molecule 32: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)



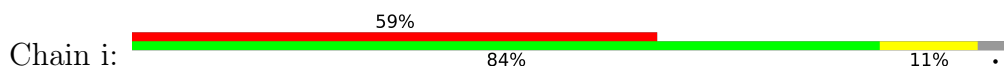
- Molecule 33: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

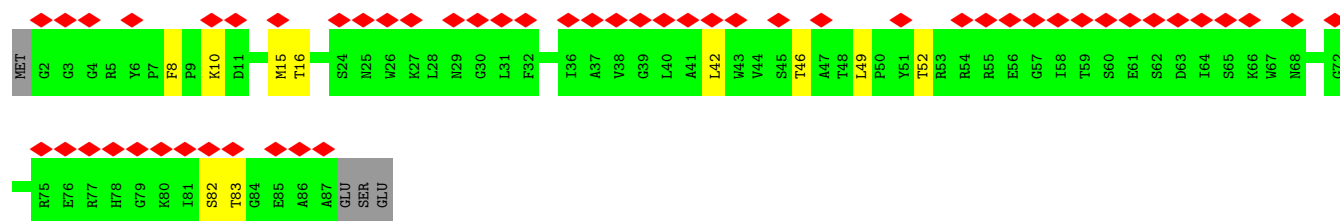


- Molecule 34: subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

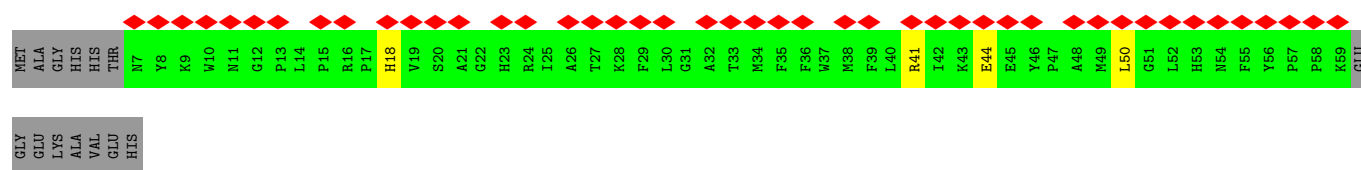


- Molecule 35: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

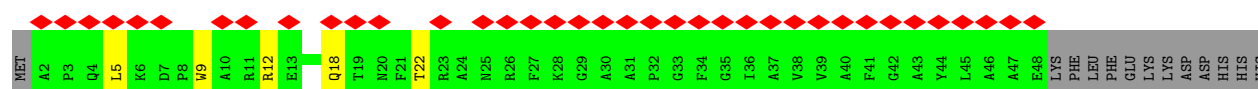




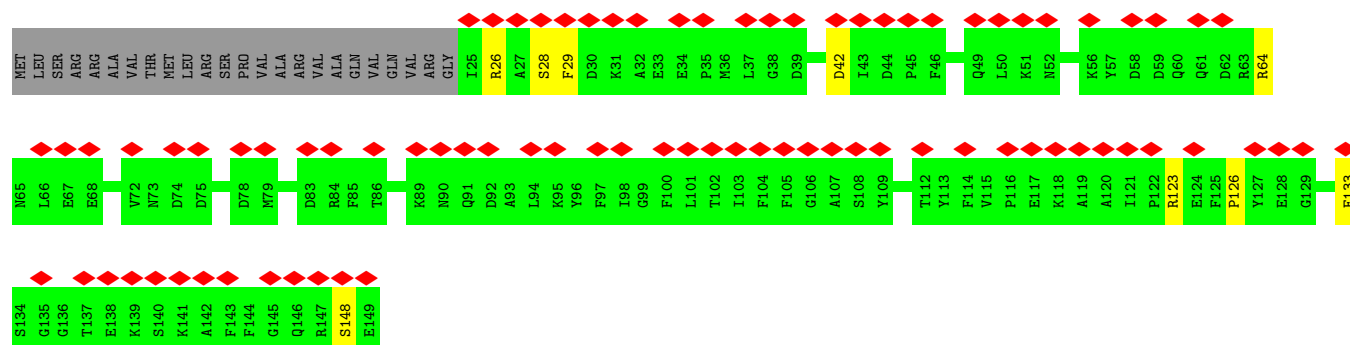
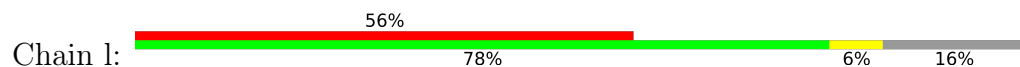
- Molecule 36: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)



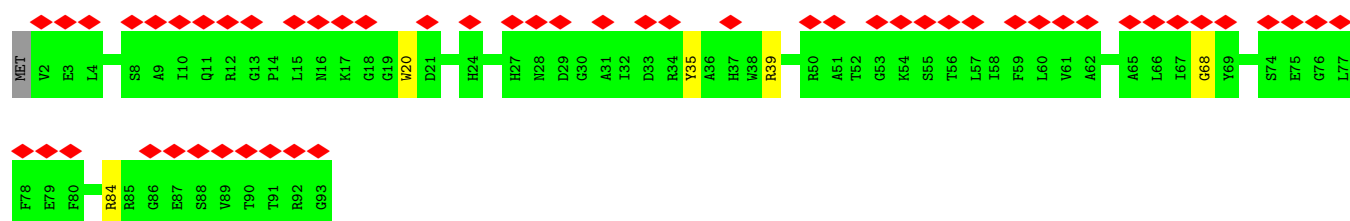
- Molecule 37: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 38: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 39: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Chain p: 

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, FES, FMN, SF4, EHZ, CDL, LMT, FME, PLC, ZN, NDP

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	0.72	0/773	0.77	0/1054
2	B	0.86	0/1432	0.68	0/1948
3	C	0.84	0/2062	0.59	0/2813
4	D	0.82	0/3513	0.64	0/4763
5	E	0.63	0/1725	0.59	0/2343
6	F	0.67	0/3638	0.59	0/4910
7	G	0.79	1/5368 (0.0%)	0.65	5/7285 (0.1%)
8	H	0.69	0/2751	0.62	0/3758
9	I	0.99	0/1564	0.63	0/2121
10	J	0.62	0/1477	0.56	0/2015
11	K	0.72	0/692	0.58	0/937
12	L	0.68	0/5327	0.56	0/7273
13	M	0.79	0/3941	0.56	0/5382
14	N	0.84	0/3846	0.56	0/5242
15	O	0.66	0/1344	0.53	0/1822
16	P	0.65	0/2873	0.58	0/3894
17	Q	0.76	0/1067	0.56	0/1442
18	R	0.74	0/946	0.56	0/1283
19	S	0.59	0/677	0.56	0/907
20	T	0.42	0/628	0.64	0/854
21	U	0.47	0/673	0.51	0/916
22	V	0.61	0/1049	0.57	0/1420
23	W	0.66	0/1061	0.53	0/1427
24	X	0.62	0/1374	0.59	0/1856
25	Y	0.58	0/1359	0.55	0/1851
26	Z	0.72	0/1007	0.63	0/1357
27	a	0.62	0/697	0.63	0/940
28	b	0.62	0/665	0.61	0/909
29	c	0.67	0/1438	0.62	2/1965 (0.1%)
30	d	0.65	0/523	0.47	0/707
31	e	0.62	0/555	0.56	0/740
32	f	0.76	0/1174	0.55	0/1597

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.53	0/1614	0.59	0/2182
34	h	0.61	0/937	0.55	0/1270
35	i	0.60	0/679	0.59	0/924
36	j	0.54	0/465	0.53	0/630
37	k	0.53	0/385	0.64	0/522
38	l	0.57	0/1073	0.53	0/1451
39	m	0.61	0/756	0.52	0/1021
40	n	0.58	0/926	0.62	0/1253
41	o	0.51	0/695	0.57	0/930
42	p	0.71	0/782	0.55	0/1051
All	All	0.71	1/65531 (0.0%)	0.59	7/88965 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	574	HIS	CG-ND1	-7.39	1.30	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	233	CYS	CA-C-N	7.52	127.04	118.85
7	G	233	CYS	C-N-CA	7.52	127.04	118.85
7	G	233	CYS	O-C-N	6.93	127.47	121.30
29	c	40	ILE	CA-C-N	6.43	124.29	120.24
29	c	40	ILE	C-N-CA	6.43	124.29	120.24
7	G	468	GLY	N-CA-C	5.20	114.94	110.21
7	G	234	PRO	N-CA-C	-5.18	106.46	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	766	827	826	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1393	1373	1373	12	0
3	C	1999	1925	1925	16	0
4	D	3434	3354	3354	34	0
5	E	1688	1660	1660	22	0
6	F	3559	3513	3513	35	0
7	G	5274	5173	5173	38	0
8	H	2689	2774	2774	23	0
9	I	1526	1471	1471	15	0
10	J	1462	1582	1582	19	0
11	K	693	753	753	18	0
12	L	5207	5364	5364	70	0
13	M	3857	4053	4053	47	0
14	N	3776	4004	4004	36	0
15	O	1305	1281	1281	8	0
16	P	2812	2763	2763	19	0
17	Q	1037	994	994	6	0
18	R	922	876	876	9	0
19	S	667	684	684	7	0
20	T	620	614	614	7	0
21	U	667	655	655	8	0
22	V	1028	1021	1021	5	0
23	W	1036	1018	1018	5	0
24	X	1345	1333	1333	11	0
25	Y	1327	1311	1310	4	0
26	Z	983	1000	1000	11	0
27	a	681	672	671	4	0
28	b	639	618	620	4	0
29	c	1397	1407	1407	4	0
30	d	510	532	532	0	0
31	e	546	536	536	3	0
32	f	1136	1089	1089	7	0
33	g	1585	1603	1603	21	0
34	h	909	877	877	6	0
35	i	659	641	641	6	0
36	j	445	439	439	3	0
37	k	373	361	361	4	0
38	l	1039	973	973	5	0
39	m	735	718	718	5	0
40	n	900	904	904	7	0
41	o	681	685	685	6	0
42	p	766	726	726	10	0
43	D	27	34	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	H	28	36	27	0	0
43	L	76	112	106	5	0
43	N	42	64	64	0	0
43	d	27	34	28	0	0
44	E	4	0	0	1	0
44	G	4	0	0	0	0
45	F	31	18	18	1	0
46	F	8	0	0	0	0
46	G	16	0	0	0	0
46	I	16	0	0	1	0
47	H	68	94	87	1	0
47	I	32	42	38	0	0
47	L	153	246	246	3	0
47	M	30	39	34	0	0
47	N	51	82	82	3	0
47	Y	33	46	40	1	0
47	Z	43	66	60	0	0
47	b	43	66	63	2	0
47	d	24	28	22	0	0
47	g	30	38	34	0	0
48	M	83	122	113	0	0
48	O	63	82	73	2	0
48	Z	57	66	58	1	0
48	a	52	56	48	1	0
48	b	48	52	40	1	0
49	P	48	26	26	2	0
50	R	1	0	0	0	0
51	T	35	40	0	3	0
51	U	36	41	0	0	0
52	Y	70	92	92	0	0
All	All	65352	65779	65583	500	0

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

All (500) 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)
14:N:2539:ILE:HD11	14:N:2638:ILE:HG22	1.44	0.97
3:C:216:LEU:HD11	4:D:126:LEU:HD23	1.58	0.84
43:L:701:PLC:O2P	35:i:16:THR:OG1	1.97	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:T:201:EHZ:N2	51:T:201:EHZ:O3	2.12	0.81
16:P:131:ARG:NH2	49:P:401:NDP:O2X	2.15	0.80
16:P:247:ARG:NH1	16:P:334:ASP:O	2.16	0.79
26:Z:60:ARG:NH2	28:b:56:SER:O	2.17	0.78
7:G:540:ASP:OD2	7:G:544:LYS:NZ	2.17	0.77
10:J:152:ASN:O	10:J:156:THR:OG1	2.02	0.76
5:E:129:THR:OG1	44:E:301:FES:S2	2.44	0.76
5:E:127:CYS:SG	5:E:129:THR:OG1	2.45	0.75
35:i:8:PHE:O	35:i:10:LYS:NZ	2.19	0.75
21:U:107:ILE:O	40:n:20:ARG:NH2	2.20	0.74
4:D:336:ARG:NH2	4:D:456:THR:O	2.20	0.74
24:X:85:ASP:O	24:X:89:SER:OG	2.04	0.74
21:U:51:THR:OG1	21:U:53:ASP:OD1	2.04	0.74
16:P:173:ILE:O	16:P:181:HIS:ND1	2.20	0.74
7:G:154:ASP:OD2	7:G:155:ARG:NH2	2.21	0.73
12:L:1324:MET:SD	25:Y:1232:SER:OG	2.45	0.73
33:g:184:VAL:O	33:g:187:SER:OG	2.07	0.73
24:X:115:GLU:OE2	24:X:130:LYS:NZ	2.20	0.73
4:D:61:ASP:OD1	14:N:2685:ARG:NE	2.22	0.73
4:D:327:GLY:O	4:D:332:ARG:NH2	2.22	0.72
3:C:197:ARG:NH2	4:D:113:ASP:OD1	2.23	0.72
16:P:201:ARG:NE	16:P:260:GLU:OE2	2.21	0.72
12:L:986:LEU:HD21	12:L:1119:VAL:HG21	1.71	0.71
13:M:749:ALA:O	13:M:754:LYS:NZ	2.23	0.71
7:G:124:MET:SD	7:G:127:GLN:NE2	2.64	0.71
24:X:45:LYS:NZ	24:X:81:SER:OG	2.24	0.70
4:D:325:MET:SD	4:D:325:MET:N	2.65	0.70
5:E:174:ASN:OD1	5:E:215:ARG:NH1	2.24	0.70
13:M:796:ARG:O	39:m:39:ARG:NH2	2.25	0.69
4:D:257:ARG:NH2	4:D:260:GLU:OE1	2.25	0.69
8:H:157:ILE:HD11	8:H:245:LEU:HD22	1.75	0.69
22:V:84:ASP:OD1	22:V:85:ASN:ND2	2.26	0.68
3:C:139:GLU:OE2	22:V:137:TYR:OH	2.11	0.68
3:C:225:ASP:OD2	3:C:228:LYS:NZ	2.26	0.68
29:c:136:SER:OG	29:c:138:ASP:OD2	2.10	0.68
28:b:23:ARG:NE	47:b:402:3PE:O12	2.24	0.68
13:M:545:TYR:O	33:g:186:LYS:NZ	2.28	0.67
7:G:267:ASN:OD1	7:G:283:ARG:NH1	2.28	0.67
13:M:713:TRP:HZ2	13:M:779:ILE:HD11	1.58	0.67
2:B:102:ARG:HH22	2:B:188:MET:HE1	1.59	0.66
36:j:41:ARG:NH2	36:j:44:GLU:OE1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:718:ASN:ND2	7:G:720:ASP:OD2	2.29	0.66
13:M:530:TYR:OH	13:M:618:THR:HG22	1.96	0.65
6:F:39:ARG:NH1	6:F:291:GLU:O	2.29	0.65
12:L:1224:ILE:O	12:L:1227:SER:OG	2.15	0.65
12:L:1090:MET:HE1	12:L:1135:MET:HE2	1.79	0.64
14:N:2753:LYS:NZ	14:N:2825:ASP:O	2.30	0.64
12:L:737:THR:O	12:L:741:SER:OG	2.09	0.64
4:D:429:ALA:HB1	4:D:463:GLU:HG2	1.79	0.64
10:J:10:GLU:OE2	27:a:84:ARG:NH2	2.30	0.63
9:I:357:THR:O	32:f:122:THR:OG1	2.14	0.63
1:A:100:ILE:HD11	47:b:402:3PE:H2I2	1.80	0.63
12:L:733:TYR:O	12:L:737:THR:HG23	1.98	0.63
4:D:209:GLU:N	4:D:209:GLU:OE1	2.31	0.63
43:L:702:PLC:H63	40:n:29:TRP:O	1.98	0.62
43:L:701:PLC:H81	13:M:868:THR:HG22	1.82	0.62
13:M:772:GLN:O	13:M:776:THR:OG1	2.16	0.62
6:F:292:GLU:OE2	6:F:305:HIS:NE2	2.32	0.62
6:F:321:PRO:HB2	6:F:339:MET:HE1	1.82	0.62
18:R:19:LYS:N	18:R:33:GLU:OE1	2.32	0.62
10:J:144:THR:HG21	34:h:141:ILE:HG21	1.81	0.62
12:L:888:LEU:O	12:L:892:VAL:HG23	2.00	0.62
19:S:66:ILE:HG12	19:S:83:LEU:HD22	1.81	0.62
5:E:215:ARG:HE	5:E:221:ALA:HB2	1.65	0.61
4:D:271:TRP:O	4:D:275:THR:OG1	2.13	0.61
7:G:503:LYS:O	7:G:507:SER:OG	2.09	0.61
24:X:117:LEU:HD23	24:X:172:LEU:HD11	1.82	0.61
12:L:1087:LEU:HD22	12:L:1092:MET:HG3	1.82	0.61
7:G:574:HIS:HE1	7:G:703:ILE:HG12	1.66	0.61
9:I:420:ASP:OD1	18:R:108:GLN:NE2	2.34	0.61
51:T:201:EHZ:O2	51:T:201:EHZ:O1	2.17	0.61
8:H:120:SER:O	8:H:136:SER:OG	2.18	0.61
18:R:19:LYS:N	18:R:31:ILE:O	2.35	0.60
1:A:108:THR:O	10:J:181:MET:HE1	2.02	0.60
9:I:356:THR:OG1	9:I:401:LYS:NZ	2.35	0.60
11:K:33:LEU:HD13	11:K:63:ALA:HB2	1.84	0.60
12:L:792:THR:OG1	12:L:1185:TYR:OH	2.13	0.60
6:F:447:GLU:OE1	6:F:447:GLU:N	2.34	0.60
7:G:395:TYR:OH	7:G:533:ASP:OD1	2.11	0.60
38:l:26:ARG:NH2	38:l:42:ASP:O	2.35	0.60
2:B:99:ASP:OD2	2:B:101:ASP:N	2.35	0.60
6:F:295:SER:O	6:F:338:LEU:HD22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:165:ARG:NH2	7:G:209:ASN:O	2.35	0.59
6:F:85:ARG:NE	6:F:91:GLY:O	2.34	0.59
7:G:357:GLU:N	7:G:357:GLU:OE1	2.34	0.59
9:I:388:GLU:OE1	9:I:388:GLU:N	2.36	0.59
41:o:61:ASP:OD2	41:o:64:ARG:NH2	2.36	0.59
31:e:7:SER:OG	31:e:8:LEU:N	2.36	0.58
12:L:1105:ILE:O	12:L:1108:THR:OG1	2.20	0.58
13:M:870:TYR:OH	40:n:97:ARG:O	2.16	0.58
32:f:10:ARG:NH1	32:f:52:ASP:OD2	2.34	0.58
34:h:96:GLU:OE2	42:p:24:ARG:NH2	2.37	0.58
4:D:409:GLU:O	4:D:428:ARG:NH1	2.35	0.58
12:L:1241:PHE:O	43:L:702:PLC:H62	2.03	0.58
42:p:38:LEU:HD21	42:p:78:ARG:HA	1.84	0.58
3:C:95:GLU:OE2	4:D:160:LYS:NZ	2.26	0.58
8:H:151:THR:O	8:H:154:PHE:N	2.37	0.58
6:F:64:THR:OG1	6:F:142:GLU:OE1	2.22	0.58
13:M:733:LEU:HD23	13:M:805:ALA:HB1	1.85	0.57
4:D:371:ARG:NH2	9:I:376:CYS:O	2.37	0.57
6:F:188:ALA:O	6:F:191:SER:OG	2.20	0.57
12:L:1345:ILE:HA	12:L:1348:ILE:HD12	1.85	0.57
12:L:905:ILE:CG2	12:L:974:ILE:HD11	2.35	0.57
12:L:1052:GLY:O	12:L:1056:HIS:ND1	2.35	0.57
31:e:7:SER:N	31:e:11:GLY:O	2.37	0.57
12:L:892:VAL:HG22	13:M:905:PHE:CE2	2.39	0.57
13:M:563:ASN:OD1	13:M:564:SER:N	2.37	0.57
13:M:941:TYR:OH	38:l:64:ARG:NH2	2.38	0.57
38:l:28:SER:OG	38:l:29:PHE:N	2.37	0.57
5:E:218:CYS:SG	6:F:135:LYS:NZ	2.78	0.57
18:R:98:ASP:O	18:R:100:ALA:N	2.37	0.57
5:E:144:VAL:HG22	5:E:197:LEU:HD11	1.86	0.57
23:W:18:LYS:NZ	23:W:67:ASP:O	2.22	0.57
38:l:133:GLU:OE2	38:l:133:GLU:N	2.38	0.57
33:g:144:ASP:OD2	33:g:146:GLN:NE2	2.38	0.57
34:h:122:ASP:OD1	34:h:123:TYR:N	2.37	0.57
13:M:661:ASP:OD2	13:M:664:ARG:NH2	2.36	0.56
14:N:2468:PHE:CE2	14:N:2472:MET:HE2	2.39	0.56
33:g:219:ASP:O	33:g:223:VAL:HG23	2.04	0.56
10:J:59:TYR:HE1	11:K:60:ILE:HD11	1.70	0.56
12:L:1217:LEU:HD21	36:j:50:LEU:HA	1.87	0.56
14:N:2405:ILE:HD11	48:O:601:CDL:H672	1.87	0.56
10:J:141:ILE:HD11	26:Z:70:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:2468:PHE:CD2	14:N:2472:MET:HE2	2.40	0.56
8:H:67:GLU:O	8:H:128:ASN:ND2	2.38	0.56
11:K:21:ASN:OD1	11:K:24:LEU:HD13	2.06	0.56
33:g:215:GLU:N	33:g:215:GLU:OE1	2.39	0.56
13:M:695:ASN:ND2	13:M:698:ASN:OD1	2.38	0.56
51:T:201:EHZ:O9	23:W:64:ARG:NH2	2.38	0.56
15:O:535:GLU:N	15:O:535:GLU:OE1	2.39	0.55
6:F:238:PHE:O	17:Q:150:HIS:ND1	2.37	0.55
14:N:2630:THR:O	14:N:2684:LYS:NZ	2.39	0.55
21:U:45:SER:OG	21:U:46:SER:N	2.37	0.55
12:L:711:SER:O	12:L:715:ILE:HG22	2.05	0.55
1:A:116:HIS:N	4:D:108:GLU:OE2	2.37	0.55
43:L:701:PLC:H12	43:L:701:PLC:H82	1.89	0.55
11:K:55:PHE:CE2	11:K:59:ILE:HD11	2.41	0.55
8:H:69:ASN:OD1	8:H:70:TYR:N	2.40	0.55
22:V:43:ARG:NH1	22:V:86:GLU:OE1	2.40	0.55
17:Q:110:MET:HE1	17:Q:121:PHE:CE2	2.42	0.54
21:U:53:ASP:OD1	21:U:54:MET:N	2.39	0.54
7:G:134:PRO:O	7:G:248:ARG:NH1	2.40	0.54
12:L:1087:LEU:HD23	12:L:1090:MET:HE3	1.88	0.54
16:P:54:TYR:HB2	16:P:78:THR:HG23	1.89	0.54
5:E:120:GLY:N	5:E:162:THR:OG1	2.40	0.54
24:X:120:LYS:O	24:X:124:THR:HG23	2.07	0.54
13:M:778:MET:HA	13:M:781:ILE:HD12	1.90	0.54
12:L:1355:LEU:HD11	47:L:705:3PE:H2E1	1.90	0.54
4:D:348:GLU:O	4:D:352:ASN:ND2	2.41	0.54
7:G:501:ILE:O	7:G:505:VAL:HG23	2.08	0.54
41:o:17:LYS:NZ	42:p:54:GLU:O	2.41	0.54
7:G:551:TRP:HH2	7:G:629:VAL:HG11	1.73	0.54
14:N:2533:GLU:OE1	14:N:2537:TYR:OH	2.21	0.54
48:a:101:CDL:OB4	29:c:17:SER:OG	2.12	0.54
4:D:249:MET:O	4:D:252:THR:HG22	2.07	0.53
13:M:828:TYR:OH	13:M:970:PRO:O	2.27	0.53
35:i:42:LEU:O	35:i:46:THR:HG23	2.08	0.53
12:L:1189:GLY:O	41:o:37:ARG:NH2	2.41	0.53
13:M:781:ILE:HD11	39:m:68:GLY:HA2	1.91	0.53
7:G:551:TRP:CH2	7:G:629:VAL:HG11	2.43	0.53
13:M:655:HIS:NE2	14:N:2820:ASN:OD1	2.40	0.53
32:f:23:GLN:OE1	32:f:31:LYS:N	2.41	0.53
8:H:157:ILE:CD1	8:H:245:LEU:HD22	2.38	0.53
23:W:10:GLU:OE2	23:W:24:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:o:11:GLU:N	41:o:11:GLU:OE1	2.40	0.53
7:G:574:HIS:ND1	7:G:575:ASN:OD1	2.41	0.53
7:G:429:ARG:NH1	7:G:449:THR:O	2.41	0.53
13:M:614:ASN:O	13:M:618:THR:HG23	2.09	0.53
13:M:825:LEU:HD22	13:M:899:LEU:HD22	1.90	0.53
33:g:142:VAL:C	33:g:150:VAL:HG23	2.34	0.53
14:N:2690:SER:OG	14:N:2815:TYR:OH	2.12	0.52
6:F:101:MET:SD	6:F:243:THR:OG1	2.66	0.52
14:N:2665:LEU:O	14:N:2669:THR:HG23	2.10	0.52
12:L:790:THR:OG1	12:L:970:ARG:NH1	2.41	0.52
13:M:722:VAL:HG22	13:M:729:ILE:HG21	1.92	0.52
29:c:127:SER:OG	29:c:128:PHE:N	2.42	0.52
10:J:185:GLU:N	10:J:185:GLU:OE1	2.42	0.52
14:N:2457:MET:HE1	15:O:556:TRP:CG	2.44	0.52
19:S:5:LEU:HD21	19:S:8:ILE:HD11	1.90	0.52
11:K:18:ASN:ND2	11:K:21:ASN:O	2.43	0.52
12:L:708:ASN:O	12:L:712:LEU:HD23	2.09	0.52
11:K:79:ARG:HG2	16:P:373:ILE:HD12	1.92	0.51
13:M:738:SER:O	13:M:859:ARG:NH2	2.42	0.51
14:N:2407:ALA:HB1	14:N:2430:ILE:HD11	1.92	0.51
12:L:1125:LEU:O	12:L:1129:LEU:HD13	2.09	0.51
14:N:2521:HIS:CE1	15:O:553:ILE:HD11	2.45	0.51
7:G:166:SER:HB2	18:R:94:THR:HG22	1.92	0.51
11:K:79:ARG:CG	16:P:373:ILE:HD12	2.39	0.51
19:S:30:ILE:HD11	19:S:42:VAL:HG11	1.91	0.51
33:g:157:GLU:OE1	33:g:157:GLU:N	2.44	0.51
5:E:227:LEU:HD12	6:F:45:TYR:CD2	2.46	0.51
12:L:793:MET:HE1	12:L:1037:LEU:HD13	1.92	0.51
4:D:239:LEU:HD22	4:D:243:LEU:HD23	1.93	0.51
5:E:90:MET:HE2	5:E:108:ALA:CB	2.41	0.51
6:F:61:TRP:CD2	6:F:183:LEU:HD13	2.46	0.51
7:G:187:THR:O	7:G:191:ARG:NE	2.43	0.51
12:L:1326:ILE:HG22	12:L:1330:ILE:HD12	1.93	0.50
33:g:239:LYS:NZ	42:p:14:ASP:OD1	2.31	0.50
3:C:167:SER:OG	3:C:179:GLU:OE1	2.29	0.50
22:V:84:ASP:OD1	22:V:85:ASN:N	2.44	0.50
4:D:262:GLU:OE1	26:Z:21:ARG:NH1	2.44	0.50
33:g:53:GLU:OE1	33:g:57:LEU:HD22	2.11	0.50
6:F:162:GLY:N	6:F:202:GLY:O	2.44	0.50
7:G:256:GLU:OE1	17:Q:132:GLN:NE2	2.38	0.50
12:L:1333:LEU:O	12:L:1337:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:151:THR:HG22	8:H:155:ILE:CD1	2.41	0.50
12:L:792:THR:HG21	12:L:1034:LEU:CD2	2.42	0.50
1:A:69:GLU:OE1	1:A:98:LEU:HD22	2.12	0.50
1:A:79:SER:O	1:A:83:VAL:HG22	2.12	0.50
3:C:184:ASP:OD1	3:C:201:THR:OG1	2.26	0.50
20:T:94:SER:N	20:T:97:GLN:OE1	2.44	0.50
31:e:13:ASN:OD1	31:e:16:PHE:N	2.44	0.50
11:K:78:TYR:HD2	16:P:373:ILE:HD11	1.76	0.50
16:P:181:HIS:NE2	16:P:185:LEU:HD11	2.27	0.50
2:B:80:THR:HG23	2:B:108:ARG:O	2.12	0.50
12:L:1326:ILE:HD11	14:N:2562:MET:CE	2.42	0.49
6:F:153:ALA:O	6:F:193:TYR:OH	2.15	0.49
7:G:358:SER:OG	7:G:553:LEU:HD21	2.13	0.49
14:N:2701:LEU:HA	14:N:2704:LEU:HD13	1.93	0.49
26:Z:88:GLN:NE2	26:Z:92:GLU:OE2	2.45	0.49
35:i:82:SER:OG	35:i:83:THR:N	2.45	0.49
2:B:142:ARG:O	16:P:91:ARG:NH2	2.41	0.49
4:D:379:GLU:O	4:D:383:HIS:ND1	2.45	0.49
25:Y:1374:ALA:HB2	33:g:234:LEU:HD23	1.94	0.49
5:E:215:ARG:NE	5:E:221:ALA:HB2	2.28	0.49
9:I:290:GLN:OE1	9:I:293:ARG:NH1	2.45	0.49
16:P:234:ASN:HD22	16:P:323:ILE:HD11	1.78	0.49
39:m:35:TYR:OH	39:m:39:ARG:NH1	2.46	0.49
6:F:285:ASN:ND2	6:F:309:ILE:O	2.46	0.49
12:L:792:THR:HG1	12:L:1185:TYR:HH	1.42	0.49
33:g:140:ILE:HD11	33:g:155:LYS:O	2.12	0.49
3:C:106:ILE:O	3:C:110:THR:HG23	2.13	0.49
4:D:219:ARG:HD2	4:D:243:LEU:HD13	1.94	0.49
2:B:102:ARG:NH2	2:B:188:MET:HE1	2.27	0.49
12:L:1087:LEU:HD22	12:L:1092:MET:CG	2.43	0.49
13:M:612:ASN:O	13:M:657:TYR:OH	2.29	0.49
14:N:2526:ILE:O	14:N:2530:VAL:HG23	2.12	0.49
39:m:84:ARG:NH1	42:p:72:ASP:OD1	2.42	0.49
4:D:136:LEU:HD21	4:D:230:VAL:O	2.13	0.49
5:E:221:ALA:HB3	6:F:286:GLU:OE1	2.13	0.49
12:L:1096:THR:O	12:L:1100:THR:HG23	2.12	0.49
13:M:635:ASP:OD1	13:M:635:ASP:N	2.45	0.49
32:f:2:SER:O	32:f:3:SER:OG	2.26	0.49
14:N:2617:ALA:H	14:N:2669:THR:HG22	1.77	0.48
26:Z:26:ARG:NH1	48:Z:201:CDL:OA3	2.45	0.48
33:g:239:LYS:O	33:g:242:THR:OG1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:41:PHE:CE1	24:X:122:VAL:HG21	2.48	0.48
12:L:1337:VAL:HG11	47:N:2402:3PE:C21	2.42	0.48
13:M:522:TRP:CD2	33:g:108:ILE:HG22	2.48	0.48
13:M:563:ASN:ND2	13:M:571:SER:OG	2.47	0.48
13:M:687:ILE:HG23	13:M:691:LEU:HD12	1.95	0.48
12:L:914:THR:O	12:L:918:VAL:HG23	2.12	0.48
12:L:997:GLY:C	12:L:1129:LEU:HD23	2.39	0.48
13:M:883:PHE:CD1	13:M:886:ILE:HD11	2.49	0.48
21:U:102:GLU:OE2	37:k:12:ARG:NH2	2.47	0.48
5:E:92:TYR:CE2	5:E:96:LEU:HD11	2.48	0.48
12:L:1035:PHE:CD2	12:L:1100:THR:HG22	2.48	0.48
12:L:1358:LEU:HD21	47:L:705:3PE:H31	1.95	0.48
2:B:174:ASP:OD1	2:B:197:LYS:NZ	2.45	0.48
12:L:892:VAL:HG22	13:M:905:PHE:CZ	2.49	0.48
12:L:962:THR:HB	12:L:1037:LEU:HD11	1.96	0.48
4:D:239:LEU:HD22	4:D:243:LEU:CD2	2.43	0.48
5:E:150:ILE:HD11	5:E:154:GLU:HB3	1.95	0.48
5:E:158:ASP:OD2	5:E:160:LEU:HD22	2.13	0.48
10:J:40:PHE:HD1	11:K:34:LEU:HD22	1.79	0.48
12:L:1213:GLN:HG2	12:L:1217:LEU:HD12	1.95	0.48
20:T:36:ILE:O	20:T:40:LEU:HD23	2.14	0.48
5:E:140:ILE:HG23	5:E:193:THR:HG21	1.95	0.47
12:L:1326:ILE:HD11	14:N:2562:MET:HE1	1.96	0.47
10:J:139:PHE:HA	26:Z:70:MET:HE2	1.96	0.47
4:D:262:GLU:OE2	4:D:341:ARG:NH1	2.44	0.47
7:G:398:ASN:ND2	7:G:519:TYR:O	2.47	0.47
12:L:737:THR:OG1	12:L:738:ARG:NH1	2.45	0.47
6:F:115:LEU:HD13	6:F:151:MET:CE	2.44	0.47
12:L:1322:ASN:HB3	14:N:2562:MET:HE2	1.95	0.47
19:S:44:VAL:O	19:S:45:ARG:NH2	2.47	0.47
39:m:20:TRP:CG	40:n:106:LEU:HD13	2.49	0.47
12:L:792:THR:HG21	12:L:1034:LEU:HD21	1.96	0.47
14:N:2628:GLU:OE1	14:N:2685:ARG:NH2	2.46	0.47
18:R:72:GLN:NE2	32:f:116:ALA:O	2.47	0.47
33:g:198:GLU:OE1	42:p:6:ARG:NE	2.47	0.47
1:A:69:GLU:CD	1:A:98:LEU:HD22	2.40	0.47
6:F:160:ILE:O	6:F:202:GLY:N	2.46	0.47
9:I:315:HIS:ND1	9:I:363:MET:HE1	2.30	0.47
10:J:10:GLU:OE2	27:a:87:ILE:HD11	2.14	0.47
13:M:883:PHE:HD1	13:M:886:ILE:HD11	1.78	0.47
21:U:101:GLU:OE1	40:n:33:ARG:NH1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:32:GLY:HA2	6:F:296:ILE:HD12	1.96	0.47
10:J:79:ASP:OD1	11:K:83:VAL:HG23	2.14	0.47
13:M:733:LEU:CD2	13:M:805:ALA:HB1	2.44	0.47
16:P:214:LEU:HD13	16:P:348:ILE:HD11	1.96	0.47
10:J:160:PHE:O	10:J:164:VAL:HG23	2.15	0.47
8:H:257:TYR:CZ	8:H:261:ILE:HD11	2.50	0.47
14:N:2694:ASN:OD1	14:N:2714:TYR:OH	2.32	0.47
18:R:30:GLU:O	18:R:31:ILE:HD13	2.15	0.47
38:l:123:ARG:NH2	41:o:24:ASP:OD2	2.48	0.47
12:L:1337:VAL:HG13	12:L:1340:MET:HE2	1.98	0.46
6:F:126:THR:OG1	6:F:353:THR:OG1	2.24	0.46
9:I:281:PHE:HA	9:I:284:LEU:HD12	1.98	0.46
11:K:16:VAL:HG11	12:L:1327:LEU:HD22	1.96	0.46
12:L:1109:TYR:CD2	12:L:1211:ILE:HD12	2.50	0.46
20:T:86:ASP:OD2	20:T:87:LYS:N	2.49	0.46
32:f:53:GLU:N	32:f:53:GLU:OE1	2.49	0.46
1:A:83:VAL:HG23	1:A:83:VAL:O	2.14	0.46
6:F:140:LEU:HD13	6:F:247:VAL:HG13	1.96	0.46
14:N:2475:TYR:OH	15:O:552:PHE:O	2.31	0.46
3:C:107:PRO:O	3:C:110:THR:OG1	2.27	0.46
4:D:219:ARG:HG2	4:D:240:PRO:HG3	1.97	0.46
8:H:151:THR:HG22	8:H:155:ILE:HD11	1.98	0.46
12:L:840:ASN:OD1	12:L:843:VAL:HG23	2.15	0.46
12:L:1305:SER:OG	14:N:2675:VAL:O	2.30	0.46
13:M:761:LEU:HD21	13:M:819:VAL:HG23	1.97	0.46
7:G:261:MET:HE1	7:G:703:ILE:HB	1.97	0.46
10:J:154:LEU:HD13	11:K:54:LEU:HD11	1.97	0.46
24:X:14:ASP:O	26:Z:83:ARG:NH1	2.47	0.46
33:g:67:PRO:O	33:g:129:TYR:OH	2.28	0.46
6:F:121:GLU:OE2	6:F:129:ASP:N	2.46	0.46
9:I:395:GLU:N	9:I:395:GLU:OE1	2.49	0.46
12:L:804:VAL:O	12:L:808:SER:OG	2.21	0.46
17:Q:113:THR:HG22	22:V:143:VAL:HG11	1.98	0.46
19:S:16:GLY:O	19:S:23:ARG:NH2	2.49	0.46
5:E:174:ASN:ND2	5:E:217:ASP:O	2.48	0.45
10:J:115:ASP:OD1	10:J:116:SER:N	2.49	0.45
13:M:525:ASN:OD1	13:M:526:VAL:N	2.47	0.45
12:L:794:LEU:O	12:L:798:THR:OG1	2.24	0.45
7:G:154:ASP:OD1	7:G:154:ASP:N	2.49	0.45
2:B:77:TRP:NE1	2:B:106:ILE:HD12	2.31	0.45
7:G:626:LEU:HA	7:G:629:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:715:ILE:HG23	12:L:716:LEU:HD12	1.99	0.45
6:F:463:SER:OG	6:F:464:VAL:N	2.49	0.45
12:L:1054:ILE:HG13	12:L:1078:THR:HG21	1.98	0.45
15:O:432:VAL:HG11	15:O:492:TYR:CD1	2.51	0.45
13:M:786:THR:O	13:M:790:THR:OG1	2.31	0.45
15:O:440:ASP:HB3	15:O:491:ALA:HB1	1.99	0.45
10:J:99:ILE:O	10:J:103:VAL:HG23	2.17	0.45
33:g:143:LYS:N	33:g:150:VAL:HG23	2.32	0.45
3:C:63:ARG:NH2	3:C:64:TYR:OH	2.50	0.45
8:H:19:VAL:HG21	8:H:233:SER:OG	2.16	0.45
8:H:295:TRP:CH2	9:I:284:LEU:HD13	2.52	0.45
14:N:2485:TYR:OH	14:N:2633:LEU:O	2.30	0.45
14:N:2569:LEU:HB2	47:N:2402:3PE:H3I1	1.98	0.45
16:P:51:ARG:NE	17:Q:94:ASP:OD2	2.47	0.45
24:X:118:LEU:O	24:X:122:VAL:HG22	2.17	0.45
5:E:227:LEU:HD12	6:F:45:TYR:HD2	1.80	0.45
10:J:67:ILE:HD11	11:K:64:GLY:HA2	1.99	0.45
12:L:726:PHE:HA	35:i:15:MET:HE2	1.98	0.45
16:P:107:MET:SD	16:P:108:ASP:N	2.90	0.45
5:E:122:TYR:CE1	5:E:205:MET:HE1	2.52	0.44
47:H:6403:3PE:H2I2	26:Z:34:LEU:HD13	1.98	0.44
7:G:475:LYS:HG2	7:G:508:THR:HG23	1.98	0.44
7:G:82:MET:HE1	7:G:122:MET:CG	2.47	0.44
12:L:1292:LEU:HD11	47:Y:1403:3PE:H351	1.99	0.44
6:F:404:GLY:O	6:F:406:ALA:N	2.51	0.44
7:G:122:MET:HE1	7:G:144:LEU:HD12	1.99	0.44
8:H:341:ILE:HD12	26:Z:59:LYS:NZ	2.32	0.44
21:U:50:LEU:HD12	21:U:131:ALA:HB3	1.98	0.44
8:H:304:THR:OG1	8:H:307:ASN:OD1	2.27	0.44
13:M:718:ILE:O	13:M:722:VAL:HG23	2.18	0.44
14:N:2615:GLY:CA	14:N:2623:LEU:HD12	2.47	0.44
36:j:18:HIS:ND1	36:j:18:HIS:O	2.50	0.44
3:C:125:ASP:OD1	3:C:126:ILE:N	2.50	0.44
6:F:440:LEU:HD21	6:F:448:MET:HE3	1.99	0.44
7:G:159:THR:HG22	7:G:159:THR:O	2.18	0.44
12:L:1096:THR:HG22	12:L:1178:GLY:H	1.83	0.44
33:g:142:VAL:HG13	33:g:142:VAL:O	2.18	0.44
8:H:110:LEU:HD11	8:H:151:THR:HG23	2.00	0.44
14:N:2423:ASN:OD1	14:N:2424:ARG:N	2.51	0.44
19:S:13:CYS:SG	19:S:14:GLN:N	2.91	0.44
20:T:70:VAL:O	20:T:74:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1340:MET:SD	14:N:2660:LEU:HD23	2.58	0.43
13:M:522:TRP:CG	33:g:108:ILE:HG22	2.53	0.43
13:M:603:LEU:HD22	33:g:168:MET:HE2	2.00	0.43
6:F:32:GLY:N	6:F:293:GLU:OE2	2.50	0.43
6:F:148:GLY:O	6:F:152:ASN:N	2.51	0.43
6:F:185:GLY:N	6:F:195:PHE:O	2.43	0.43
14:N:2604:ILE:HG21	47:N:2402:3PE:O32	2.18	0.43
20:T:55:THR:HG22	20:T:55:THR:O	2.18	0.43
8:H:295:TRP:CZ3	9:I:284:LEU:HD13	2.53	0.43
12:L:965:ILE:HG21	12:L:1021:MET:HE2	1.99	0.43
13:M:515:LEU:HD11	13:M:519:ILE:HD11	2.00	0.43
24:X:57:ARG:NH1	26:Z:78:ASP:OD2	2.51	0.43
3:C:255:VAL:HG23	3:C:255:VAL:O	2.18	0.43
7:G:497:PHE:O	7:G:500:THR:N	2.52	0.43
13:M:720:ILE:O	13:M:724:THR:OG1	2.29	0.43
10:J:40:PHE:CD1	11:K:34:LEU:HD22	2.54	0.43
12:L:793:MET:HB3	12:L:836:VAL:HG11	2.01	0.43
13:M:844:LEU:O	13:M:848:VAL:HG22	2.19	0.43
4:D:44:VAL:HG21	14:N:2748:TYR:CZ	2.54	0.43
13:M:706:LEU:HD11	13:M:774:LEU:HD12	2.00	0.43
13:M:733:LEU:HD11	13:M:753:LEU:HD21	2.00	0.43
15:O:559:PHE:O	48:O:601:CDL:O1	2.25	0.43
40:n:64:ASP:OD1	40:n:67:ARG:NH1	2.48	0.43
7:G:497:PHE:O	7:G:501:ILE:HD12	2.19	0.43
11:K:57:ILE:HA	11:K:60:ILE:HD12	2.00	0.43
14:N:2581:LEU:HD11	14:N:2599:LEU:HD11	2.01	0.43
18:R:21:ILE:O	18:R:29:ILE:N	2.51	0.43
7:G:178:THR:HG22	7:G:238:LEU:HD23	2.01	0.43
7:G:285:HIS:CE1	7:G:288:VAL:HG23	2.53	0.43
8:H:76:SER:O	8:H:80:THR:OG1	2.34	0.43
12:L:905:ILE:HG22	12:L:974:ILE:HD11	2.01	0.43
12:L:1271:PHE:O	12:L:1275:VAL:HG23	2.18	0.43
24:X:71:GLU:OE1	24:X:71:GLU:N	2.45	0.43
32:f:110:TYR:O	32:f:113:THR:OG1	2.28	0.43
1:A:104:TYR:OH	14:N:2504:GLU:OE1	2.37	0.43
2:B:77:TRP:O	2:B:114:SER:OG	2.33	0.42
13:M:673:THR:HG23	13:M:723:LYS:HD3	2.00	0.42
14:N:2802:ILE:HD13	25:Y:1314:LEU:HD21	2.00	0.42
42:p:89:ASP:OD1	42:p:91:SER:OG	2.37	0.42
5:E:167:GLU:OE1	6:F:371:ARG:NH1	2.47	0.42
24:X:52:ASP:OD1	28:b:69:ARG:NE	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:1352:ARG:NH2	42:p:13:ASP:OD1	2.52	0.42
2:B:148:GLY:O	2:B:152:ASN:ND2	2.52	0.42
10:J:141:ILE:HD11	26:Z:70:MET:CE	2.49	0.42
35:i:49:LEU:O	35:i:52:THR:OG1	2.34	0.42
4:D:123:THR:HG23	4:D:138:TYR:CD2	2.55	0.42
5:E:90:MET:HE2	5:E:108:ALA:HB3	2.00	0.42
6:F:390:GLY:HA3	6:F:421:ILE:HD11	2.01	0.42
16:P:318:PHE:C	16:P:319:LEU:HD12	2.44	0.42
20:T:84:ILE:O	23:W:34:ARG:NH2	2.51	0.42
3:C:237:GLU:OE1	16:P:45:THR:OG1	2.29	0.42
8:H:240:ALA:HB1	8:H:282:TYR:OH	2.20	0.42
12:L:734:VAL:O	12:L:737:THR:OG1	2.32	0.42
13:M:825:LEU:HD22	13:M:899:LEU:CD2	2.49	0.42
4:D:191:CYS:HB3	4:D:203:PHE:HA	2.02	0.42
5:E:79:GLN:OE1	5:E:115:ASN:N	2.47	0.42
8:H:97:ILE:HD12	27:a:26:GLN:HA	2.01	0.42
8:H:261:ILE:HG22	8:H:262:LEU:HD23	2.01	0.42
8:H:153:ILE:HG21	8:H:189:PHE:HD1	1.85	0.42
11:K:33:LEU:HD13	11:K:63:ALA:CB	2.48	0.42
16:P:188:GLN:NE2	16:P:189:VAL:HG13	2.35	0.42
34:h:117:LYS:O	34:h:118:ARG:HG2	2.19	0.42
16:P:203:ALA:HB1	16:P:204:PRO:HD2	2.02	0.42
4:D:443:ARG:NH2	23:W:2:ALA:O	2.45	0.42
7:G:291:GLU:OE2	17:Q:137:ARG:NE	2.48	0.42
1:A:121:THR:C	1:A:122:ASP:O	2.60	0.41
3:C:123:ILE:HG23	3:C:123:ILE:O	2.19	0.41
4:D:219:ARG:NH1	4:D:242:GLY:O	2.53	0.41
7:G:82:MET:HE1	7:G:122:MET:HG2	2.01	0.41
7:G:186:CYS:C	7:G:187:THR:HG1	2.17	0.41
33:g:162:GLU:OE1	33:g:164:TRP:NE1	2.42	0.41
8:H:42:VAL:HG12	8:H:42:VAL:O	2.19	0.41
9:I:358:LYS:NZ	9:I:360:ASP:OD2	2.44	0.41
48:b:401:CDL:OA4	48:b:401:CDL:O1	2.34	0.41
3:C:93:LYS:NZ	4:D:160:LYS:O	2.51	0.41
12:L:986:LEU:C	12:L:986:LEU:HD23	2.45	0.41
12:L:1014:THR:HG23	12:L:1040:HIS:CE1	2.56	0.41
13:M:681:LEU:HD11	14:N:2786:LEU:HD13	2.02	0.41
1:A:88:PHE:CE1	1:A:92:LEU:HD11	2.56	0.41
33:g:134:ARG:NE	33:g:160:GLU:OE2	2.54	0.41
8:H:2:ILE:HG23	8:H:3:ILE:N	2.35	0.41
11:K:49:ASP:OD2	11:K:50:ILE:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:L:705:3PE:H2F1	14:N:2667:ILE:HG21	2.03	0.41
6:F:102:ASN:ND2	6:F:150:ALA:O	2.52	0.41
12:L:907:ALA:HB2	42:p:52:TYR:CD1	2.56	0.41
7:G:289:ASN:OD1	7:G:289:ASN:N	2.54	0.41
12:L:828:PHE:HE2	12:L:960:LEU:HD12	1.86	0.41
49:P:401:NDP:H51N	49:P:401:NDP:H2N	2.02	0.41
4:D:101:ILE:HD12	4:D:115:HIS:CD2	2.55	0.41
28:b:73:THR:OG1	28:b:74:GLY:N	2.53	0.41
3:C:199:ILE:HG23	3:C:200:MET:HG2	2.02	0.41
4:D:147:MET:SD	4:D:147:MET:N	2.94	0.41
7:G:349:VAL:O	7:G:553:LEU:N	2.44	0.41
7:G:640:GLU:N	7:G:644:GLU:OE1	2.49	0.41
12:L:1060:ASN:O	12:L:1062:SER:N	2.53	0.41
12:L:1123:ALA:O	12:L:1126:SER:OG	2.25	0.41
13:M:647:LEU:HD21	13:M:673:THR:HG21	2.01	0.41
37:k:5:LEU:HD23	40:n:41:VAL:CG1	2.51	0.41
9:I:362:ASP:OD1	9:I:364:THR:OG1	2.25	0.41
12:L:1314:ASN:O	12:L:1321:MET:HE1	2.21	0.41
34:h:82:THR:O	34:h:85:HIS:NE2	2.53	0.41
34:h:89:ARG:NH2	42:p:28:GLU:OE1	2.49	0.41
2:B:95:ALA:HB1	2:B:96:PRO:CD	2.51	0.40
2:B:155:GLY:HA2	9:I:365:LYS:HA	2.03	0.40
6:F:288:CYS:SG	6:F:289:THR:N	2.94	0.40
12:L:1318:SER:O	12:L:1322:ASN:ND2	2.51	0.40
16:P:50:SER:O	16:P:51:ARG:NH1	2.44	0.40
18:R:41:ASN:OD1	18:R:41:ASN:N	2.54	0.40
45:F:501:FMN:H9	45:F:501:FMN:H1'1	1.96	0.40
8:H:151:THR:O	8:H:155:ILE:HD12	2.21	0.40
10:J:93:ASP:OD1	11:K:19:ARG:NH2	2.53	0.40
13:M:722:VAL:HG22	13:M:729:ILE:HD13	2.02	0.40
19:S:66:ILE:CD1	19:S:79:ARG:HG2	2.51	0.40
29:c:64:TYR:HB3	29:c:65:PRO:HD3	2.03	0.40
41:o:55:GLU:O	41:o:59:VAL:HG23	2.21	0.40
2:B:76:PHE:CZ	2:B:194:LEU:HD23	2.56	0.40
20:T:107:ASP:OD1	20:T:108:ALA:N	2.54	0.40
27:a:57:ASN:ND2	27:a:63:LYS:O	2.51	0.40
37:k:18:GLN:O	37:k:22:THR:HG23	2.22	0.40
4:D:126:LEU:HD13	4:D:138:TYR:OH	2.21	0.40
5:E:148:LEU:HB2	5:E:150:ILE:HG22	2.02	0.40
12:L:951:VAL:HG13	12:L:955:LEU:HD22	2.02	0.40
15:O:457:PHE:CE2	15:O:461:LEU:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:58:ARG:NH2	21:U:102:GLU:OE1	2.48	0.40
4:D:254:PHE:CZ	4:D:258:LEU:HD21	2.56	0.40
6:F:440:LEU:CD2	6:F:448:MET:HE3	2.51	0.40
9:I:315:HIS:NE2	46:I:503:SF4:S2	2.95	0.40
37:k:9:TRP:O	37:k:12:ARG:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	90/128 (70%)	85 (94%)	5 (6%)	0	100	100
2	B	175/210 (83%)	168 (96%)	7 (4%)	0	100	100
3	C	240/293 (82%)	221 (92%)	18 (8%)	1 (0%)	30	60
4	D	435/466 (93%)	410 (94%)	25 (6%)	0	100	100
5	E	214/243 (88%)	199 (93%)	14 (6%)	1 (0%)	24	56
6	F	458/488 (94%)	425 (93%)	33 (7%)	0	100	100
7	G	692/728 (95%)	639 (92%)	53 (8%)	0	100	100
8	H	339/341 (99%)	321 (95%)	18 (5%)	0	100	100
9	I	189/193 (98%)	181 (96%)	8 (4%)	0	100	100
10	J	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
11	K	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
12	L	653/655 (100%)	616 (94%)	36 (6%)	1 (0%)	43	72
13	M	484/486 (100%)	464 (96%)	20 (4%)	0	100	100
14	N	467/469 (100%)	452 (97%)	15 (3%)	0	100	100
15	O	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
16	P	353/355 (99%)	337 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	123/161 (76%)	118 (96%)	5 (4%)	0	100	100
18	R	116/118 (98%)	106 (91%)	9 (8%)	1 (1%)	14	45
19	S	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
20	T	79/81 (98%)	73 (92%)	5 (6%)	1 (1%)	9	38
21	U	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
22	V	124/144 (86%)	119 (96%)	5 (4%)	0	100	100
23	W	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
24	X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
25	Y	177/180 (98%)	171 (97%)	6 (3%)	0	100	100
26	Z	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
27	a	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
28	b	76/78 (97%)	67 (88%)	9 (12%)	0	100	100
29	c	180/182 (99%)	166 (92%)	14 (8%)	0	100	100
30	d	65/73 (89%)	65 (100%)	0	0	100	100
31	e	66/89 (74%)	65 (98%)	1 (2%)	0	100	100
32	f	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
33	g	196/249 (79%)	187 (95%)	9 (5%)	0	100	100
34	h	111/139 (80%)	106 (96%)	5 (4%)	0	100	100
35	i	84/90 (93%)	82 (98%)	2 (2%)	0	100	100
36	j	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
37	k	45/60 (75%)	41 (91%)	4 (9%)	0	100	100
38	l	123/149 (83%)	112 (91%)	9 (7%)	2 (2%)	7	35
39	m	90/93 (97%)	84 (93%)	6 (7%)	0	100	100
40	n	106/109 (97%)	99 (93%)	6 (6%)	1 (1%)	14	45
41	o	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
42	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
All	All	8006/8568 (93%)	7557 (94%)	441 (6%)	8 (0%)	49	78

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	1260	VAL
5	E	217	ASP

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Mol	Chain	Res	Type
38	l	148	SER
40	n	90	TYR
3	C	254	PRO
18	R	99	GLY
20	T	85	PRO
38	l	126	PRO

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	86/113 (76%)	85 (99%)	1 (1%)	63	72
2	B	152/180 (84%)	152 (100%)	0	100	100
3	C	218/251 (87%)	218 (100%)	0	100	100
4	D	367/394 (93%)	367 (100%)	0	100	100
5	E	191/212 (90%)	191 (100%)	0	100	100
6	F	367/389 (94%)	367 (100%)	0	100	100
7	G	566/595 (95%)	566 (100%)	0	100	100
8	H	293/301 (97%)	293 (100%)	0	100	100
9	I	157/158 (99%)	157 (100%)	0	100	100
10	J	166/166 (100%)	166 (100%)	0	100	100
11	K	76/76 (100%)	76 (100%)	0	100	100
12	L	579/579 (100%)	578 (100%)	1 (0%)	87	86
13	M	433/433 (100%)	433 (100%)	0	100	100
14	N	432/432 (100%)	431 (100%)	1 (0%)	87	86
15	O	132/133 (99%)	132 (100%)	0	100	100
16	P	299/311 (96%)	299 (100%)	0	100	100
17	Q	107/140 (76%)	107 (100%)	0	100	100
18	R	98/98 (100%)	98 (100%)	0	100	100
19	S	72/73 (99%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	68/68 (100%)	68 (100%)	0	100	100
21	U	75/75 (100%)	75 (100%)	0	100	100
22	V	113/129 (88%)	111 (98%)	2 (2%)	51	67
23	W	109/110 (99%)	109 (100%)	0	100	100
24	X	147/148 (99%)	147 (100%)	0	100	100
25	Y	130/131 (99%)	130 (100%)	0	100	100
26	Z	101/101 (100%)	101 (100%)	0	100	100
27	a	68/68 (100%)	68 (100%)	0	100	100
28	b	65/65 (100%)	65 (100%)	0	100	100
29	c	148/148 (100%)	148 (100%)	0	100	100
30	d	52/58 (90%)	52 (100%)	0	100	100
31	e	59/76 (78%)	59 (100%)	0	100	100
32	f	122/123 (99%)	122 (100%)	0	100	100
33	g	161/211 (76%)	161 (100%)	0	100	100
34	h	98/119 (82%)	98 (100%)	0	100	100
35	i	64/68 (94%)	64 (100%)	0	100	100
36	j	45/55 (82%)	45 (100%)	0	100	100
37	k	32/45 (71%)	32 (100%)	0	100	100
38	l	109/129 (84%)	109 (100%)	0	100	100
39	m	72/73 (99%)	72 (100%)	0	100	100
40	n	99/100 (99%)	99 (100%)	0	100	100
41	o	70/76 (92%)	70 (100%)	0	100	100
42	p	84/85 (99%)	84 (100%)	0	100	100
All	All	6882/7295 (94%)	6877 (100%)	5 (0%)	87	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
12	L	1302	ASN
14	N	2488	ASN
22	V	25	MET
22	V	27	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	73	GLN
3	C	208	HIS
4	D	57	HIS
4	D	72	ASN
4	D	193	HIS
4	D	237	GLN
7	G	127	GLN
7	G	285	HIS
7	G	425	ASN
10	J	128	ASN
12	L	761	ASN
12	L	934	GLN
12	L	1148	ASN
13	M	908	ASN
14	N	2452	GLN
14	N	2582	ASN
14	N	2705	ASN
14	N	2706	ASN
15	O	546	HIS
16	P	103	ASN
16	P	121	HIS
16	P	234	ASN
16	P	365	ASN
17	Q	136	HIS
18	R	50	GLN
23	W	58	GLN
31	e	24	HIS
31	e	40	ASN
31	e	50	HIS
32	f	50	HIS
33	g	65	GLN
33	g	211	ASN
34	h	125	HIS
35	i	68	ASN
36	j	11	ASN
38	l	65	ASN
38	l	146	GLN
40	n	21	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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
11	FME	K	1	11	8,9,10	1.06	1 (12%)	8,9,11	1.19	1 (12%)
13	FME	M	503	13	8,9,10	0.89	0	8,9,11	1.16	1 (12%)
10	FME	J	1	10	8,9,10	1.00	0	8,9,11	0.89	0
14	FME	N	2403	14	8,9,10	1.46	1 (12%)	8,9,11	0.49	0
12	FME	L	706	12	8,9,10	1.03	1 (12%)	8,9,11	1.16	1 (12%)
1	FME	A	1	1	8,9,10	1.11	1 (12%)	8,9,11	1.11	1 (12%)
8	FME	H	1	8	8,9,10	1.20	1 (12%)	8,9,11	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	K	1	11	-	2/7/9/11	-
13	FME	M	503	13	-	0/7/9/11	-
10	FME	J	1	10	-	2/7/9/11	-
14	FME	N	2403	14	-	2/7/9/11	-
12	FME	L	706	12	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
8	FME	H	1	8	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	2403	FME	CA-N	-3.76	1.41	1.46
8	H	1	FME	CA-N	-2.52	1.42	1.46
11	K	1	FME	CA-N	-2.28	1.43	1.46
1	A	1	FME	CA-N	-2.27	1.43	1.46
12	L	706	FME	CN-N	2.10	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	2.69	114.70	109.50
11	K	1	FME	C-CA-N	2.29	113.92	109.50
13	M	503	FME	C-CA-N	2.10	113.55	109.50
12	L	706	FME	CB-CA-N	2.09	114.32	110.52

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O-C-CA-CB
8	H	1	FME	O1-CN-N-CA
10	J	1	FME	N-CA-CB-CG
11	K	1	FME	N-CA-CB-CG
12	L	706	FME	N-CA-CB-CG
14	N	2403	FME	CB-CG-SD-CE
10	J	1	FME	C-CA-CB-CG
1	A	1	FME	N-CA-CB-CG
12	L	706	FME	CB-CG-SD-CE
14	N	2403	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 1 is monoatomic - leaving 37 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	CDL	O	601	-	62,62,99	1.20	7 (11%)	68,74,111	1.23	7 (10%)
47	3PE	L	704	-	50,50,50	0.88	4 (8%)	53,55,55	1.10	3 (5%)
52	LMT	Y	1401	-	36,36,36	0.92	2 (5%)	47,47,47	1.13	2 (4%)
43	PLC	L	701	-	41,41,41	1.32	6 (14%)	47,49,49	1.16	4 (8%)
47	3PE	Z	202	-	42,42,50	0.98	4 (9%)	45,47,55	1.05	3 (6%)
43	PLC	d	501	-	26,26,41	1.49	5 (19%)	32,34,49	1.33	6 (18%)
49	NDP	P	401	-	51,52,52	2.57	10 (19%)	71,80,80	1.60	18 (25%)
46	SF4	I	502	9	0,12,12	-	-	-	-	-
47	3PE	d	502	-	23,23,50	1.34	4 (17%)	26,28,55	1.29	3 (11%)
47	3PE	H	6403	-	45,45,50	1.21	3 (6%)	48,50,55	1.12	3 (6%)
46	SF4	I	503	9	0,12,12	-	-	-	-	-
47	3PE	L	705	-	50,50,50	0.91	4 (8%)	53,55,55	1.31	3 (5%)
48	CDL	Z	201	-	56,56,99	1.22	8 (14%)	62,68,111	1.24	8 (12%)
43	PLC	N	2401	-	41,41,41	1.13	5 (12%)	47,49,49	1.10	3 (6%)
47	3PE	b	402	-	42,42,50	1.24	6 (14%)	45,47,55	1.13	3 (6%)
43	PLC	H	6402	-	26,26,41	1.50	5 (19%)	30,32,49	1.89	4 (13%)
47	3PE	H	6401	-	21,21,50	1.31	2 (9%)	24,26,55	1.21	2 (8%)
45	FMN	F	501	-	33,33,33	3.19	13 (39%)	48,50,50	2.60	20 (41%)
48	CDL	a	101	-	51,51,99	1.28	9 (17%)	57,63,111	1.48	6 (10%)
46	SF4	G	802	7	0,12,12	-	-	-	-	-
47	3PE	N	2402	-	50,50,50	0.91	4 (8%)	53,55,55	1.10	2 (3%)
51	EHZ	U	201	21	33,35,37	2.03	8 (24%)	41,45,47	1.43	5 (12%)
46	SF4	G	801	7	0,12,12	-	-	-	-	-
43	PLC	D	501	-	26,26,41	1.51	7 (26%)	32,34,49	1.14	3 (9%)
47	3PE	I	501	-	31,31,50	1.16	4 (12%)	34,36,55	1.23	3 (8%)
51	EHZ	T	201	20	32,34,37	2.07	9 (28%)	40,44,47	1.56	9 (22%)
47	3PE	g	301	-	29,29,50	1.23	3 (10%)	32,34,55	1.33	5 (15%)
46	SF4	F	502	6	0,12,12	-	-	-	-	-
47	3PE	Y	1403	-	32,32,50	1.18	5 (15%)	35,37,55	1.13	3 (8%)
44	FES	E	301	5	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	PLC	L	702	-	33,33,41	1.38	3 (9%)	39,41,49	1.13	3 (7%)
47	3PE	M	502	-	29,29,50	1.22	4 (13%)	32,34,55	1.24	4 (12%)
48	CDL	b	401	-	47,47,99	1.35	7 (14%)	53,59,111	1.36	7 (13%)
48	CDL	M	501	-	82,82,99	1.37	9 (10%)	88,94,111	1.13	5 (5%)
47	3PE	L	703	-	50,50,50	0.87	4 (8%)	53,55,55	1.02	2 (3%)
52	LMT	Y	1402	-	36,36,36	0.88	0	47,47,47	1.19	6 (12%)
44	FES	G	803	7	0,4,4	-	-	-	-	-

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	CDL	O	601	-	-	27/73/73/110	-
47	3PE	L	704	-	-	19/54/54/54	-
52	LMT	Y	1401	-	4/4/10/10	10/21/61/61	0/2/2/2
43	PLC	L	701	-	-	23/45/45/45	-
47	3PE	Z	202	-	-	12/46/46/54	-
43	PLC	d	501	-	-	9/30/30/45	-
49	NDP	P	401	-	-	10/34/77/77	0/5/5/5
46	SF4	I	502	9	-	-	0/6/5/5
47	3PE	d	502	-	-	14/27/27/54	-
47	3PE	H	6403	-	-	18/49/49/54	-
47	3PE	L	705	-	-	23/54/54/54	-
48	CDL	Z	201	-	-	37/67/67/110	-
46	SF4	I	503	9	-	-	0/6/5/5
43	PLC	N	2401	-	-	16/45/45/45	-
47	3PE	b	402	-	-	15/46/46/54	-
43	PLC	H	6402	-	-	12/30/30/45	-
47	3PE	H	6401	-	1/1/4/4	12/24/24/54	-
45	FMN	F	501	-	-	13/18/18/18	0/3/3/3
48	CDL	a	101	-	-	20/62/62/110	-
46	SF4	G	802	7	-	-	0/6/5/5
47	3PE	N	2402	-	-	24/54/54/54	-
51	EHZ	U	201	21	-	9/43/43/45	-
46	SF4	G	801	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PLC	D	501	-	-	10/30/30/45	-
47	3PE	I	501	-	1/1/4/4	20/35/35/54	-
51	EHZ	T	201	20	1/1/9/9	14/42/42/45	-
47	3PE	g	301	-	1/1/4/4	8/33/33/54	-
46	SF4	F	502	6	-	-	0/6/5/5
47	3PE	Y	1403	-	-	14/36/36/54	-
44	FES	E	301	5	-	-	0/1/1/1
43	PLC	L	702	-	-	18/37/37/45	-
47	3PE	M	502	-	1/1/4/4	18/33/33/54	-
48	CDL	b	401	-	-	19/58/58/110	-
48	CDL	M	501	-	-	43/93/93/110	-
47	3PE	L	703	-	-	23/54/54/54	-
52	LMT	Y	1402	-	4/4/10/10	12/21/61/61	0/2/2/2
44	FES	G	803	7	-	-	0/1/1/1

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	401	NDP	P2B-O2B	15.26	1.86	1.59
45	F	501	FMN	O3'-C3'	-9.73	1.18	1.43
45	F	501	FMN	O4-C4	8.27	1.39	1.23
45	F	501	FMN	O2-C2	7.74	1.39	1.24
51	T	201	EHZ	C15-N2	5.96	1.47	1.33
51	U	201	EHZ	C15-N2	5.95	1.47	1.33
51	T	201	EHZ	C12-N1	5.90	1.47	1.33
51	U	201	EHZ	C12-N1	5.64	1.46	1.33
45	F	501	FMN	C4A-C4	4.67	1.61	1.44
49	P	401	NDP	PN-O5D	4.50	1.77	1.59
51	U	201	EHZ	P1-OP3	-3.85	1.40	1.54
47	H	6403	3PE	O31-C31	3.71	1.44	1.33
48	M	501	CDL	OA6-CA5	3.55	1.44	1.34
51	T	201	EHZ	P1-OP3	-3.53	1.41	1.54
43	L	702	PLC	O3-CB	3.39	1.43	1.33
47	b	402	3PE	O21-C2	-3.35	1.38	1.46
45	F	501	FMN	C5A-N5	3.32	1.45	1.39
48	O	601	CDL	OB6-CB4	-3.28	1.38	1.46
43	L	702	PLC	O2-C'	3.25	1.43	1.34
51	U	201	EHZ	O4-C15	-3.25	1.17	1.23
47	b	402	3PE	O31-C31	3.19	1.42	1.33
43	L	701	PLC	O3-CB	3.13	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	M	502	3PE	O21-C2	-3.08	1.39	1.46
47	H	6403	3PE	O21-C2	-3.07	1.39	1.46
45	F	501	FMN	C6-C5A	-3.04	1.35	1.40
48	M	501	CDL	OB8-CB7	3.03	1.42	1.33
47	H	6403	3PE	O21-C21	3.02	1.42	1.34
47	g	301	3PE	O21-C2	-3.02	1.39	1.46
47	b	402	3PE	O21-C21	3.02	1.42	1.34
51	T	201	EHZ	P1-O9	-3.00	1.41	1.50
48	b	401	CDL	OA6-CA4	-2.98	1.39	1.46
43	d	501	PLC	O2-C2	-2.98	1.39	1.46
48	M	501	CDL	OB6-CB4	-2.96	1.39	1.46
48	M	501	CDL	OB6-CB5	2.93	1.42	1.34
48	M	501	CDL	OA8-CA7	2.92	1.41	1.33
43	H	6402	PLC	O3-CB	2.92	1.41	1.33
49	P	401	NDP	O2B-C2B	-2.90	1.34	1.44
51	T	201	EHZ	C9-S1	2.90	1.83	1.76
45	F	501	FMN	C2-N3	-2.89	1.32	1.39
48	a	101	CDL	OB6-CB4	-2.89	1.39	1.46
51	T	201	EHZ	O4-C15	-2.85	1.17	1.23
48	O	601	CDL	OB8-CB6	-2.85	1.38	1.45
47	d	502	3PE	O31-C31	2.84	1.41	1.33
51	U	201	EHZ	C9-S1	2.82	1.82	1.76
43	L	701	PLC	O2-C2	-2.79	1.40	1.46
51	U	201	EHZ	P1-O9	-2.78	1.41	1.50
47	I	501	3PE	O21-C2	-2.77	1.40	1.46
48	Z	201	CDL	OA6-CA4	-2.75	1.40	1.46
47	I	501	3PE	O31-C3	-2.74	1.39	1.45
43	H	6402	PLC	O2-C2	-2.72	1.40	1.46
43	D	501	PLC	O2-C2	-2.71	1.40	1.46
43	H	6402	PLC	O2-C'	2.70	1.41	1.34
47	L	703	3PE	O21-C2	-2.70	1.40	1.46
45	F	501	FMN	C10-N10	-2.70	1.31	1.37
47	L	705	3PE	O21-C21	2.69	1.41	1.34
47	L	704	3PE	O21-C2	-2.66	1.40	1.46
52	Y	1401	LMT	O5B-C5B	-2.64	1.37	1.44
48	b	401	CDL	OB6-CB4	-2.64	1.40	1.46
48	O	601	CDL	OA6-CA4	-2.63	1.40	1.46
47	Y	1403	3PE	O21-C21	2.62	1.41	1.34
47	N	2402	3PE	O31-C31	2.59	1.40	1.33
45	F	501	FMN	P-O3P	-2.57	1.45	1.54
45	F	501	FMN	P-O2P	-2.56	1.45	1.54
43	L	701	PLC	O2-C'	2.56	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	g	301	3PE	O31-C3	-2.54	1.39	1.45
47	H	6401	3PE	O21-C2	-2.52	1.40	1.46
52	Y	1401	LMT	O1'-C1'	-2.52	1.36	1.40
47	L	705	3PE	O21-C2	-2.51	1.40	1.46
47	Y	1403	3PE	O21-C2	-2.50	1.40	1.46
48	O	601	CDL	OA8-CA7	2.49	1.40	1.33
47	Z	202	3PE	O31-C31	2.48	1.40	1.33
48	Z	201	CDL	OB8-CB7	2.48	1.40	1.33
51	T	201	EHZ	O3-C12	-2.46	1.18	1.23
47	N	2402	3PE	O21-C21	2.46	1.41	1.34
43	N	2401	PLC	O2-C'	2.44	1.41	1.34
48	Z	201	CDL	OA8-CA7	2.44	1.40	1.33
47	L	704	3PE	O31-C3	-2.43	1.39	1.45
51	U	201	EHZ	O3-C12	-2.43	1.18	1.23
48	b	401	CDL	OA8-CA6	-2.42	1.39	1.45
47	Y	1403	3PE	O31-C31	2.42	1.40	1.33
48	Z	201	CDL	OB6-CB5	2.42	1.41	1.34
43	N	2401	PLC	O2-C2	-2.41	1.40	1.46
48	a	101	CDL	OB8-CB6	-2.41	1.39	1.45
47	M	502	3PE	O31-C31	2.40	1.40	1.33
43	D	501	PLC	O3-CB	2.40	1.40	1.33
49	P	401	NDP	C4N-C3N	-2.39	1.45	1.50
48	b	401	CDL	OB8-CB7	2.38	1.40	1.33
47	L	704	3PE	O31-C31	2.38	1.40	1.33
48	b	401	CDL	OB8-CB6	-2.38	1.39	1.45
48	a	101	CDL	OA8-CA7	2.37	1.40	1.33
43	H	6402	PLC	C6-N	2.37	1.53	1.46
48	a	101	CDL	OA8-CA6	-2.36	1.39	1.45
48	b	401	CDL	OA8-CA7	2.35	1.40	1.33
48	Z	201	CDL	OB6-CB4	-2.35	1.41	1.46
47	Y	1403	3PE	O31-C3	-2.34	1.39	1.45
48	a	101	CDL	OA6-CA5	2.33	1.40	1.34
43	d	501	PLC	O3-CB	2.33	1.40	1.33
47	M	502	3PE	O31-C3	-2.32	1.40	1.45
43	d	501	PLC	O3-C3	-2.32	1.40	1.45
47	L	705	3PE	O31-C31	2.31	1.40	1.33
43	N	2401	PLC	O3-CB	2.29	1.40	1.33
47	b	402	3PE	P-O11	2.28	1.68	1.59
47	L	703	3PE	O31-C31	2.27	1.40	1.33
49	P	401	NDP	O4B-C4B	-2.27	1.40	1.45
43	L	701	PLC	P-O2P	-2.26	1.44	1.55
43	D	501	PLC	C7-N	-2.25	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	501	PLC	C6-N	-2.25	1.43	1.50
43	D	501	PLC	C8-N	-2.25	1.43	1.50
45	F	501	FMN	C9A-C5A	2.24	1.44	1.41
49	P	401	NDP	PA-O3	2.23	1.61	1.59
43	D	501	PLC	C5-N	-2.23	1.44	1.51
43	L	701	PLC	O3-C3	-2.23	1.40	1.45
43	D	501	PLC	O2-C'	2.23	1.40	1.34
43	N	2401	PLC	O3-C3	-2.22	1.40	1.45
47	g	301	3PE	O31-C31	2.21	1.39	1.33
47	b	402	3PE	O31-C3	-2.21	1.40	1.45
47	L	703	3PE	O31-C3	-2.21	1.40	1.45
47	H	6401	3PE	O21-C21	2.20	1.40	1.34
47	d	502	3PE	O21-C2	-2.20	1.41	1.46
48	a	101	CDL	OA6-CA4	-2.20	1.41	1.46
45	F	501	FMN	C4A-N5	2.20	1.35	1.30
47	d	502	3PE	O21-C21	2.18	1.40	1.34
48	Z	201	CDL	OA8-CA6	-2.17	1.40	1.45
49	P	401	NDP	PN-O3	-2.17	1.57	1.59
48	O	601	CDL	PB2-OB4	-2.17	1.45	1.55
48	M	501	CDL	PB2-OB4	-2.16	1.45	1.55
47	L	704	3PE	O21-C21	2.16	1.40	1.34
47	b	402	3PE	P-O12	-2.15	1.45	1.55
48	a	101	CDL	OB8-CB7	2.15	1.39	1.33
47	L	705	3PE	O31-C3	-2.14	1.40	1.45
48	a	101	CDL	PA1-OA4	-2.14	1.45	1.55
47	L	703	3PE	O21-C21	2.14	1.40	1.34
47	I	501	3PE	O31-C31	2.13	1.39	1.33
49	P	401	NDP	O5D-C5D	-2.13	1.36	1.44
43	H	6402	PLC	C7-N	2.13	1.52	1.46
48	O	601	CDL	OB8-CB7	2.12	1.39	1.33
43	N	2401	PLC	P-O2P	-2.12	1.45	1.55
47	Z	202	3PE	O21-C21	2.12	1.40	1.34
48	M	501	CDL	OA6-CA4	-2.11	1.41	1.46
48	Z	201	CDL	OB8-CB6	-2.11	1.40	1.45
45	F	501	FMN	O4'-C4'	-2.11	1.38	1.43
47	Z	202	3PE	O31-C3	-2.09	1.40	1.45
48	O	601	CDL	OA6-CA5	2.08	1.40	1.34
47	Z	202	3PE	O21-C2	-2.08	1.41	1.46
51	T	201	EHZ	C13-C12	2.08	1.55	1.51
43	L	702	PLC	O2-C2	-2.07	1.41	1.46
48	M	501	CDL	PA1-OA4	-2.07	1.45	1.55
49	P	401	NDP	O3D-C3D	-2.07	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	L	701	PLC	P-O3P	2.07	1.67	1.59
48	M	501	CDL	PB2-OB5	2.06	1.67	1.59
51	T	201	EHZ	O2-C9	-2.06	1.17	1.21
48	a	101	CDL	PB2-OB4	-2.06	1.45	1.55
48	b	401	CDL	OA6-CA5	2.06	1.40	1.34
47	N	2402	3PE	O21-C2	-2.05	1.41	1.46
43	d	501	PLC	P-O2P	-2.05	1.45	1.55
47	Y	1403	3PE	P-O12	-2.04	1.45	1.55
47	N	2402	3PE	O31-C3	-2.03	1.40	1.45
43	D	501	PLC	O3-C3	-2.02	1.40	1.45
47	M	502	3PE	O21-C21	2.02	1.40	1.34
51	U	201	EHZ	O2-C9	-2.02	1.17	1.21
49	P	401	NDP	O2D-C2D	-2.02	1.38	1.43
48	Z	201	CDL	PA1-OA4	-2.02	1.46	1.55
47	I	501	3PE	O21-C21	2.01	1.39	1.34
47	d	502	3PE	P-O12	-2.00	1.46	1.55

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	F	501	FMN	C9-C9A-N10	8.02	132.64	121.85
43	H	6402	PLC	C7-N-C6	-7.14	91.43	109.72
47	L	705	3PE	O21-C21-C22	6.84	126.27	111.48
45	F	501	FMN	C9A-N10-C10	5.89	129.72	120.75
45	F	501	FMN	C10-N1-C2	5.80	129.40	116.85
48	a	101	CDL	OA6-CA5-C11	5.14	122.59	111.48
45	F	501	FMN	C5A-C9A-N10	-4.73	113.69	117.97
43	H	6402	PLC	O2-C'-C1'	4.69	121.63	111.48
48	a	101	CDL	OB6-CB5-C51	4.59	121.42	111.48
43	N	2401	PLC	O2-C'-C1'	4.54	121.30	111.48
48	b	401	CDL	OA6-CA5-C11	4.52	121.26	111.48
47	L	703	3PE	O21-C21-C22	4.41	121.03	111.48
48	Z	201	CDL	OB6-CB5-C51	4.31	120.81	111.48
51	T	201	EHZ	C8-C9-S1	4.23	118.90	113.56
43	d	501	PLC	O2-C'-C1'	4.23	120.64	111.48
47	N	2402	3PE	O21-C21-C22	4.21	120.59	111.48
48	O	601	CDL	OA6-CA5-C11	4.21	120.59	111.48
51	U	201	EHZ	C8-C9-S1	4.18	118.84	113.56
47	I	501	3PE	O21-C21-C22	4.05	120.25	111.48
43	D	501	PLC	O2-C'-C1'	3.99	120.12	111.48
43	L	701	PLC	O2-C'-C1'	3.91	119.95	111.48
47	g	301	3PE	O21-C21-C22	3.83	119.76	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	b	402	3PE	O21-C21-C22	3.82	119.74	111.48
48	M	501	CDL	OA6-CA5-C11	3.78	119.66	111.48
47	H	6401	3PE	O21-C21-C22	3.75	119.59	111.48
47	Y	1403	3PE	O21-C21-C22	3.69	119.47	111.48
47	Z	202	3PE	O21-C21-C22	3.67	119.41	111.48
47	L	704	3PE	O21-C21-C22	3.66	119.39	111.48
48	Z	201	CDL	OA6-CA5-C11	3.65	119.38	111.48
47	N	2402	3PE	O31-C31-C32	3.62	122.86	111.83
45	F	501	FMN	C9-C9A-C5A	-3.60	113.66	120.03
51	T	201	EHZ	O5-C16-C17	3.58	118.48	110.18
45	F	501	FMN	C4-C4A-C10	-3.51	110.91	116.93
47	M	502	3PE	O21-C21-C22	3.50	119.06	111.48
48	b	401	CDL	OB6-CB5-C51	3.49	119.04	111.48
52	Y	1401	LMT	O5B-C5B-C4B	-3.43	103.52	109.70
47	d	502	3PE	O21-C21-C22	3.39	118.82	111.48
43	L	702	PLC	O3-CB-C1B	3.39	122.17	111.83
49	P	401	NDP	PN-O5D-C5D	-3.39	101.95	121.35
45	F	501	FMN	O5'-P-O1P	3.38	115.57	106.44
49	P	401	NDP	P2B-O2B-C2B	-3.36	114.45	123.43
45	F	501	FMN	C6-C5A-C9A	3.32	123.62	119.05
47	L	704	3PE	C3-C2-C1	-3.30	104.10	111.78
48	M	501	CDL	OB6-CB5-C51	3.29	118.61	111.48
49	P	401	NDP	O2B-P2B-O1X	-3.28	97.64	109.33
49	P	401	NDP	C2A-N1A-C6A	-3.27	113.36	118.73
45	F	501	FMN	O2P-P-O5'	3.21	115.05	106.67
48	O	601	CDL	OB6-CB5-C51	3.17	118.35	111.48
47	L	705	3PE	O21-C21-O22	-3.07	116.53	123.70
43	L	702	PLC	O2-C'-C1'	3.06	118.09	111.48
45	F	501	FMN	O3P-P-O5'	3.05	114.62	106.67
47	L	705	3PE	O31-C31-C32	3.05	121.12	111.83
49	P	401	NDP	PA-O5B-C5B	-3.04	103.93	121.35
49	P	401	NDP	O7N-C7N-N7N	-2.98	116.21	122.89
52	Y	1402	LMT	C1B-O1B-C4'	-2.96	110.97	117.98
52	Y	1402	LMT	C1'-C2'-C3'	2.96	116.23	110.01
52	Y	1402	LMT	C1-O1'-C1'	2.92	118.67	113.68
48	O	601	CDL	OB8-CB7-C71	2.89	120.66	111.83
47	d	502	3PE	O31-C31-C32	2.86	120.56	111.83
48	M	501	CDL	OA8-CA7-C31	2.85	120.53	111.83
48	a	101	CDL	OA4-PA1-OA3	-2.85	99.18	112.44
49	P	401	NDP	N3A-C4A-N9A	2.84	131.99	127.17
51	U	201	EHZ	C10-S1-C9	2.80	110.11	101.84
49	P	401	NDP	O2N-PN-O3	2.79	114.82	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	Y	1402	LMT	C2'-C3'-C4'	2.79	116.00	109.68
48	M	501	CDL	OB4-PB2-OB3	-2.79	99.48	112.44
43	H	6402	PLC	O3-CB-C1B	2.78	119.60	111.15
47	H	6403	3PE	O21-C21-C22	2.77	117.48	111.48
45	F	501	FMN	C1'-N10-C9A	-2.77	115.25	120.63
45	F	501	FMN	C4'-C3'-C2'	-2.77	108.96	113.57
49	P	401	NDP	O3-PA-O1A	-2.77	102.37	110.70
48	b	401	CDL	OA8-CA7-C31	2.76	119.53	111.15
47	g	301	3PE	O12-P-O14	-2.75	99.64	112.44
47	M	502	3PE	O31-C31-C32	2.74	120.19	111.83
47	Y	1403	3PE	O12-P-O14	-2.73	99.73	112.44
52	Y	1401	LMT	O1B-C1B-O5B	-2.71	103.56	110.69
45	F	501	FMN	C4-C4A-N5	2.71	121.95	118.21
49	P	401	NDP	O4B-C4B-C3B	2.70	110.52	105.15
51	T	201	EHZ	C13-C12-N1	2.70	121.25	116.34
47	H	6403	3PE	O31-C31-C32	2.69	120.05	111.83
47	L	703	3PE	O31-C31-C32	2.68	120.00	111.83
48	Z	201	CDL	OB8-CB7-C71	2.68	120.00	111.83
48	a	101	CDL	OA8-CA7-C31	2.65	119.92	111.83
48	Z	201	CDL	OB4-PB2-OB3	-2.65	100.12	112.44
43	L	701	PLC	O3-CB-C1B	2.63	119.85	111.83
43	N	2401	PLC	O2P-P-O1P	-2.61	100.32	112.44
51	T	201	EHZ	O5-C16-C15	2.60	120.25	109.38
51	U	201	EHZ	C14-N2-C15	-2.59	117.89	122.55
49	P	401	NDP	C5A-C4A-N3A	-2.58	123.16	126.72
47	d	502	3PE	O12-P-O14	-2.57	100.49	112.44
48	M	501	CDL	OA4-PA1-OA3	-2.56	100.54	112.44
47	b	402	3PE	O31-C31-C32	2.54	119.59	111.83
43	d	501	PLC	C2-O2-C'	-2.54	111.72	117.80
48	Z	201	CDL	CA4-OA6-CA5	-2.54	111.72	117.80
47	H	6401	3PE	O12-P-O14	-2.53	100.69	112.44
49	P	401	NDP	C5A-C6A-N1A	2.53	123.93	117.51
51	T	201	EHZ	C10-S1-C9	2.52	109.28	101.84
47	Y	1403	3PE	C3-C2-C1	-2.51	105.93	111.78
48	b	401	CDL	CA4-OA6-CA5	-2.51	111.79	117.80
45	F	501	FMN	N3-C2-N1	-2.50	114.18	119.50
48	Z	201	CDL	OA8-CA7-C31	2.48	119.39	111.83
47	g	301	3PE	O21-C21-O22	-2.47	117.93	123.70
47	I	501	3PE	O31-C31-C32	2.46	119.34	111.83
43	H	6402	PLC	O2P-P-O1P	-2.46	101.02	112.44
43	d	501	PLC	O3-CB-C1B	2.45	119.30	111.83
45	F	501	FMN	O2'-C2'-C3'	-2.44	103.55	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g	301	3PE	O31-C31-C32	2.44	119.26	111.83
47	H	6403	3PE	O12-P-O14	-2.43	101.13	112.44
51	U	201	EHZ	O2-C9-C8	-2.43	119.92	123.74
48	b	401	CDL	OB4-PB2-OB3	-2.42	101.17	112.44
45	F	501	FMN	O3P-P-O1P	-2.42	101.41	110.83
48	a	101	CDL	OB4-PB2-OB3	-2.41	101.21	112.44
49	P	401	NDP	O3X-P2B-O2X	2.41	116.85	107.80
48	O	601	CDL	CB4-OB6-CB5	-2.41	112.03	117.80
48	O	601	CDL	OB4-PB2-OB3	-2.38	101.36	112.44
43	D	501	PLC	O2P-P-O1P	-2.38	101.36	112.44
47	M	502	3PE	O12-P-O14	-2.36	101.47	112.44
45	F	501	FMN	C9A-C5A-N5	-2.36	119.95	122.45
47	L	704	3PE	O31-C31-C32	2.34	118.98	111.83
43	D	501	PLC	O3-CB-C1B	2.34	118.24	111.15
48	Z	201	CDL	OA4-PA1-OA3	-2.32	101.66	112.44
45	F	501	FMN	O2-C2-N3	2.31	123.02	118.58
48	b	401	CDL	OB8-CB7-C71	2.31	118.88	111.83
47	b	402	3PE	O12-P-O14	-2.30	101.75	112.44
47	g	301	3PE	C2-O21-C21	-2.29	112.31	117.80
47	Z	202	3PE	O12-P-O14	-2.28	101.83	112.44
48	a	101	CDL	OB8-CB7-C71	2.28	118.78	111.83
48	O	601	CDL	OA4-PA1-OA3	-2.28	101.85	112.44
43	d	501	PLC	O2P-P-O1P	-2.27	101.88	112.44
51	U	201	EHZ	OP3-P1-O6	2.27	112.58	106.67
43	L	701	PLC	C2-O2-C'	-2.26	112.39	117.80
45	F	501	FMN	O3'-C3'-C2'	2.26	114.06	108.93
49	P	401	NDP	C5B-C4B-C3B	-2.26	107.09	115.21
47	M	502	3PE	C2-O21-C21	-2.25	112.40	117.80
49	P	401	NDP	O3-PN-O1N	-2.23	103.99	110.70
47	Z	202	3PE	O31-C31-C32	2.20	118.56	111.83
49	P	401	NDP	O3X-P2B-O2B	-2.20	97.28	105.85
51	T	201	EHZ	O6-P1-O9	2.20	112.38	106.44
51	T	201	EHZ	O2-C9-C8	-2.19	120.29	123.74
43	d	501	PLC	C8-N-C6	-2.18	103.24	108.98
47	I	501	3PE	O12-P-O14	-2.18	102.30	112.44
43	L	701	PLC	O2P-P-O1P	-2.18	102.30	112.44
48	O	601	CDL	OA8-CA7-C31	2.17	118.45	111.83
48	b	401	CDL	OA4-PA1-OA3	-2.17	102.35	112.44
43	d	501	PLC	O2-C'-O'	-2.17	118.64	123.70
49	P	401	NDP	O2N-PN-O1N	2.16	122.50	112.44
43	N	2401	PLC	O3-CB-C1B	2.15	118.39	111.83
45	F	501	FMN	C1'-C2'-C3'	2.13	115.43	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	T	201	EHZ	O3-C12-N1	-2.12	118.87	123.03
52	Y	1402	LMT	C6'-C5'-C4'	-2.12	107.42	113.38
52	Y	1402	LMT	C1'-O5'-C5'	-2.10	109.61	113.72
48	Z	201	CDL	OB6-CB5-OB7	-2.06	118.88	123.70
51	T	201	EHZ	C19-C17-C16	2.05	112.26	108.77
43	L	702	PLC	O3-CB-OB	-2.03	118.55	123.63
49	P	401	NDP	C5A-C6A-N6A	-2.02	118.28	123.29

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
47	H	6401	3PE	C2
47	I	501	3PE	C2
47	M	502	3PE	C2
47	g	301	3PE	C2
51	T	201	EHZ	C16
52	Y	1401	LMT	C2B
52	Y	1401	LMT	C4B
52	Y	1401	LMT	C1'
52	Y	1401	LMT	C5B
52	Y	1402	LMT	C2B
52	Y	1402	LMT	C4B
52	Y	1402	LMT	C1'
52	Y	1402	LMT	C5B

All (522) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	D	501	PLC	C1-O3P-P-O2P
43	D	501	PLC	C1-O3P-P-O4P
43	H	6402	PLC	O3P-C1-C2-O2
43	H	6402	PLC	C4-O4P-P-O1P
43	H	6402	PLC	C4-O4P-P-O2P
43	H	6402	PLC	C4-O4P-P-O3P
43	L	701	PLC	O4P-C4-C5-N
43	L	701	PLC	C1'-C'-O2-C2
43	L	701	PLC	O'-C'-O2-C2
43	L	701	PLC	C1-O3P-P-O1P
43	L	701	PLC	C1-O3P-P-O2P
43	L	702	PLC	C1'-C'-O2-C2
43	L	702	PLC	C1-O3P-P-O1P
43	L	702	PLC	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
43	L	702	PLC	C1-O3P-P-O4P
43	L	702	PLC	C4-O4P-P-O1P
43	L	702	PLC	C4-O4P-P-O3P
43	N	2401	PLC	C1'-C'-O2-C2
43	N	2401	PLC	O'-C'-O2-C2
43	d	501	PLC	O4P-C4-C5-N
45	F	501	FMN	N10-C1'-C2'-O2'
45	F	501	FMN	N10-C1'-C2'-C3'
45	F	501	FMN	C1'-C2'-C3'-O3'
45	F	501	FMN	C1'-C2'-C3'-C4'
45	F	501	FMN	O2'-C2'-C3'-O3'
45	F	501	FMN	O2'-C2'-C3'-C4'
45	F	501	FMN	C3'-C4'-C5'-O5'
45	F	501	FMN	O4'-C4'-C5'-O5'
45	F	501	FMN	C5'-O5'-P-O2P
45	F	501	FMN	C5'-O5'-P-O3P
47	H	6401	3PE	C1-O11-P-O14
47	H	6401	3PE	C11-O13-P-O11
47	H	6401	3PE	C11-O13-P-O12
47	H	6401	3PE	C11-O13-P-O14
47	H	6401	3PE	C22-C21-O21-C2
47	H	6403	3PE	C1-O11-P-O12
47	H	6403	3PE	C1-O11-P-O13
47	H	6403	3PE	C1-O11-P-O14
47	H	6403	3PE	C11-O13-P-O11
47	H	6403	3PE	C11-O13-P-O12
47	H	6403	3PE	C11-O13-P-O14
47	I	501	3PE	C1-O11-P-O12
47	I	501	3PE	C11-O13-P-O11
47	I	501	3PE	C11-O13-P-O12
47	I	501	3PE	C11-O13-P-O14
47	I	501	3PE	O13-C11-C12-N
47	L	703	3PE	C1-O11-P-O12
47	L	703	3PE	C1-O11-P-O13
47	L	703	3PE	C11-O13-P-O11
47	L	703	3PE	C11-O13-P-O12
47	L	703	3PE	C11-O13-P-O14
47	L	703	3PE	O13-C11-C12-N
47	L	704	3PE	C11-O13-P-O11
47	L	704	3PE	C11-O13-P-O12
47	L	704	3PE	C11-O13-P-O14
47	L	705	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
47	L	705	3PE	C1-O11-P-O13
47	L	705	3PE	O13-C11-C12-N
47	L	705	3PE	O22-C21-O21-C2
47	L	705	3PE	C22-C21-O21-C2
47	M	502	3PE	C1-O11-P-O12
47	M	502	3PE	C1-O11-P-O13
47	M	502	3PE	C1-O11-P-O14
47	M	502	3PE	C11-O13-P-O11
47	M	502	3PE	C11-O13-P-O12
47	M	502	3PE	C11-O13-P-O14
47	M	502	3PE	C12-C11-O13-P
47	M	502	3PE	O13-C11-C12-N
47	M	502	3PE	C22-C21-O21-C2
47	N	2402	3PE	C22-C21-O21-C2
47	Y	1403	3PE	O13-C11-C12-N
47	Z	202	3PE	C1-O11-P-O14
47	d	502	3PE	C11-O13-P-O11
47	d	502	3PE	C11-O13-P-O12
47	d	502	3PE	C11-O13-P-O14
47	g	301	3PE	O13-C11-C12-N
47	g	301	3PE	C22-C21-O21-C2
48	M	501	CDL	CA2-C1-CB2-OB2
48	M	501	CDL	OA6-CA4-CA6-OA8
48	M	501	CDL	CB2-OB2-PB2-OB3
48	M	501	CDL	CB2-OB2-PB2-OB4
48	M	501	CDL	CB2-OB2-PB2-OB5
48	M	501	CDL	CB3-OB5-PB2-OB2
48	M	501	CDL	CB3-OB5-PB2-OB3
48	M	501	CDL	CB3-OB5-PB2-OB4
48	M	501	CDL	OB6-CB4-CB6-OB8
48	O	601	CDL	CB2-C1-CA2-OA2
48	O	601	CDL	CA3-OA5-PA1-OA2
48	O	601	CDL	CA3-OA5-PA1-OA3
48	O	601	CDL	CB3-OB5-PB2-OB2
48	O	601	CDL	CB3-OB5-PB2-OB4
48	O	601	CDL	OB5-CB3-CB4-OB6
48	Z	201	CDL	CA2-OA2-PA1-OA3
48	Z	201	CDL	CA2-OA2-PA1-OA4
48	Z	201	CDL	CA2-OA2-PA1-OA5
48	Z	201	CDL	CA3-OA5-PA1-OA2
48	Z	201	CDL	CA3-OA5-PA1-OA3
48	Z	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
48	Z	201	CDL	CB2-OB2-PB2-OB5
48	Z	201	CDL	CB3-OB5-PB2-OB2
48	Z	201	CDL	CB3-OB5-PB2-OB3
48	Z	201	CDL	CB3-OB5-PB2-OB4
48	a	101	CDL	CA3-OA5-PA1-OA2
48	a	101	CDL	CA3-OA5-PA1-OA4
48	a	101	CDL	C11-CA5-OA6-CA4
48	a	101	CDL	CB2-OB2-PB2-OB3
48	b	401	CDL	CA3-OA5-PA1-OA2
48	b	401	CDL	CA3-OA5-PA1-OA3
48	b	401	CDL	OA7-CA5-OA6-CA4
48	b	401	CDL	C11-CA5-OA6-CA4
49	P	401	NDP	C5D-O5D-PN-O3
51	T	201	EHZ	C6-C7-C8-C9
51	T	201	EHZ	C11-C10-S1-C9
51	T	201	EHZ	C12-C13-C14-N2
51	T	201	EHZ	O5-C16-C17-C18
51	T	201	EHZ	O5-C16-C17-C19
51	T	201	EHZ	O5-C16-C17-C20
51	T	201	EHZ	C20-O6-P1-O7
51	T	201	EHZ	C20-O6-P1-OP3
51	U	201	EHZ	C11-C10-S1-C9
52	Y	1401	LMT	C2'-C1'-O1'-C1
52	Y	1401	LMT	O5'-C1'-O1'-C1
43	H	6402	PLC	OB-CB-O3-C3
43	N	2401	PLC	OB-CB-O3-C3
47	I	501	3PE	O32-C31-O31-C3
43	N	2401	PLC	C1B-CB-O3-C3
43	d	501	PLC	OB-CB-O3-C3
43	L	702	PLC	O'-C'-O2-C2
47	M	502	3PE	O22-C21-O21-C2
47	N	2402	3PE	O22-C21-O21-C2
47	g	301	3PE	O22-C21-O21-C2
48	Z	201	CDL	OA7-CA5-OA6-CA4
48	a	101	CDL	OA7-CA5-OA6-CA4
43	H	6402	PLC	C1B-CB-O3-C3
47	I	501	3PE	C32-C31-O31-C3
43	d	501	PLC	C1B-CB-O3-C3
47	L	703	3PE	C32-C31-O31-C3
48	O	601	CDL	C71-CB7-OB8-CB6
43	L	701	PLC	OB-CB-O3-C3
47	H	6401	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
48	M	501	CDL	O1-C1-CB2-OB2
48	O	601	CDL	O1-C1-CA2-OA2
43	L	701	PLC	C1B-CB-O3-C3
47	L	704	3PE	C32-C31-O31-C3
48	O	601	CDL	C51-CB5-OB6-CB4
47	L	703	3PE	O32-C31-O31-C3
48	O	601	CDL	OB9-CB7-OB8-CB6
47	L	704	3PE	O32-C31-O31-C3
48	O	601	CDL	OB7-CB5-OB6-CB4
43	L	702	PLC	C1B-CB-O3-C3
47	b	402	3PE	C32-C31-O31-C3
48	Z	201	CDL	C71-CB7-OB8-CB6
48	a	101	CDL	O1-C1-CB2-OB2
47	b	402	3PE	O32-C31-O31-C3
43	D	501	PLC	C'-C1'-C2'-C3'
51	T	201	EHZ	C5-C6-C7-O1
43	D	501	PLC	O2-C2-C3-O3
47	M	502	3PE	C32-C31-O31-C3
52	Y	1401	LMT	O5'-C5'-C6'-O6'
43	L	702	PLC	CB-C1B-C2B-C3B
47	I	501	3PE	C21-C22-C23-C24
47	b	402	3PE	C31-C32-C33-C34
48	Z	201	CDL	OB9-CB7-OB8-CB6
48	a	101	CDL	CB7-C71-C72-C73
52	Y	1402	LMT	O5'-C1'-O1'-C1
47	N	2402	3PE	C32-C31-O31-C3
47	g	301	3PE	C32-C31-O31-C3
47	H	6403	3PE	C31-C32-C33-C34
43	L	702	PLC	OB-CB-O3-C3
48	b	401	CDL	C71-CB7-OB8-CB6
43	d	501	PLC	C1'-C'-O2-C2
47	M	502	3PE	O32-C31-O31-C3
43	L	701	PLC	C'-C1'-C2'-C3'
49	P	401	NDP	O4B-C4B-C5B-O5B
49	P	401	NDP	C3B-C4B-C5B-O5B
47	N	2402	3PE	C21-C22-C23-C24
47	d	502	3PE	C22-C21-O21-C2
43	d	501	PLC	O'-C'-O2-C2
47	d	502	3PE	O22-C21-O21-C2
52	Y	1402	LMT	C2'-C1'-O1'-C1
47	g	301	3PE	O32-C31-O31-C3
48	b	401	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
47	H	6403	3PE	C22-C21-O21-C2
47	g	301	3PE	C21-C22-C23-C24
47	N	2402	3PE	C38-C39-C3A-C3B
47	L	705	3PE	C31-C32-C33-C34
47	N	2402	3PE	O32-C31-O31-C3
43	N	2401	PLC	C4B-C5B-C6B-C7B
47	N	2402	3PE	C2B-C2C-C2D-C2E
48	M	501	CDL	C53-C54-C55-C56
43	N	2401	PLC	C3'-C4'-C5'-C6'
48	M	501	CDL	C17-C18-C19-C20
47	I	501	3PE	C33-C34-C35-C36
47	L	704	3PE	C38-C39-C3A-C3B
47	N	2402	3PE	C25-C26-C27-C28
47	b	402	3PE	C29-C2A-C2B-C2C
43	N	2401	PLC	C6'-C7'-C8'-C9'
51	U	201	EHZ	C2-C1-C21-C22
52	Y	1402	LMT	C3-C4-C5-C6
48	O	601	CDL	CB7-C71-C72-C73
49	P	401	NDP	O4D-C4D-C5D-O5D
47	L	704	3PE	C35-C36-C37-C38
47	Z	202	3PE	C29-C2A-C2B-C2C
48	b	401	CDL	CB3-CB4-CB6-OB8
43	L	702	PLC	C1'-C2'-C3'-C4'
48	O	601	CDL	C60-C61-C62-C63
47	I	501	3PE	C31-C32-C33-C34
48	Z	201	CDL	CB5-C51-C52-C53
47	H	6403	3PE	C32-C33-C34-C35
47	L	703	3PE	C2C-C2D-C2E-C2F
47	Y	1403	3PE	C34-C35-C36-C37
48	O	601	CDL	C56-C57-C58-C59
47	Y	1403	3PE	C26-C27-C28-C29
48	M	501	CDL	C51-C52-C53-C54
43	L	701	PLC	C4'-C5'-C6'-C7'
47	L	703	3PE	C3C-C3D-C3E-C3F
47	N	2402	3PE	C22-C23-C24-C25
47	H	6403	3PE	C2C-C2D-C2E-C2F
47	L	705	3PE	C28-C29-C2A-C2B
43	N	2401	PLC	C5B-C6B-C7B-C8B
47	L	704	3PE	C37-C38-C39-C3A
48	a	101	CDL	C32-C33-C34-C35
48	M	501	CDL	C20-C21-C22-C23
48	M	501	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
48	M	501	CDL	C14-C15-C16-C17
48	O	601	CDL	C55-C56-C57-C58
47	L	704	3PE	C32-C33-C34-C35
47	L	705	3PE	C2B-C2C-C2D-C2E
47	b	402	3PE	C24-C25-C26-C27
48	M	501	CDL	C18-C19-C20-C21
43	H	6402	PLC	C2'-C3'-C4'-C5'
43	H	6402	PLC	C1'-C'-O2-C2
47	I	501	3PE	C22-C21-O21-C2
48	a	101	CDL	C51-CB5-OB6-CB4
52	Y	1402	LMT	C7-C8-C9-C10
47	H	6403	3PE	O22-C21-O21-C2
47	H	6403	3PE	C27-C28-C29-C2A
47	L	704	3PE	C3B-C3C-C3D-C3E
47	N	2402	3PE	C36-C37-C38-C39
47	Y	1403	3PE	C23-C24-C25-C26
47	Y	1403	3PE	C25-C26-C27-C28
47	L	703	3PE	C38-C39-C3A-C3B
48	O	601	CDL	C62-C63-C64-C65
47	M	502	3PE	C32-C33-C34-C35
48	M	501	CDL	C35-C36-C37-C38
47	I	501	3PE	O22-C21-O21-C2
47	M	502	3PE	C35-C36-C37-C38
47	L	705	3PE	C3D-C3E-C3F-C3G
43	H	6402	PLC	O3P-C1-C2-C3
48	O	601	CDL	OB5-CB3-CB4-CB6
48	a	101	CDL	OB5-CB3-CB4-CB6
51	U	201	EHZ	C5-C6-C7-C8
48	M	501	CDL	C79-C80-C81-C82
52	Y	1401	LMT	C4'-C5'-C6'-O6'
47	L	703	3PE	C37-C38-C39-C3A
47	b	402	3PE	C34-C35-C36-C37
47	L	703	3PE	C2E-C2F-C2G-C2H
43	L	701	PLC	C6'-C7'-C8'-C9'
47	H	6403	3PE	C23-C24-C25-C26
48	O	601	CDL	CB5-C51-C52-C53
43	D	501	PLC	C1-C2-C3-O3
47	H	6401	3PE	C1-C2-C3-O31
47	L	703	3PE	C1-C2-C3-O31
47	L	705	3PE	C1-C2-C3-O31
48	M	501	CDL	CA3-CA4-CA6-OA8
43	N	2401	PLC	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
52	Y	1402	LMT	C4-C5-C6-C7
52	Y	1401	LMT	C2-C3-C4-C5
47	Y	1403	3PE	C32-C31-O31-C3
43	N	2401	PLC	C7B-C8B-C9B-CAA
47	Y	1403	3PE	C32-C33-C34-C35
47	b	402	3PE	C2D-C2E-C2F-C2G
43	H	6402	PLC	O'-C'-O2-C2
45	F	501	FMN	C5'-O5'-P-O1P
47	N	2402	3PE	C3A-C3B-C3C-C3D
48	M	501	CDL	C74-C75-C76-C77
47	N	2402	3PE	C32-C33-C34-C35
48	Z	201	CDL	C52-C53-C54-C55
47	N	2402	3PE	C28-C29-C2A-C2B
51	U	201	EHZ	C5-C6-C7-O1
47	d	502	3PE	C32-C31-O31-C3
48	b	401	CDL	C11-C12-C13-C14
47	L	705	3PE	C29-C2A-C2B-C2C
52	Y	1402	LMT	C2-C3-C4-C5
43	L	702	PLC	C5B-C6B-C7B-C8B
47	N	2402	3PE	C2F-C2G-C2H-C2I
48	M	501	CDL	C71-C72-C73-C74
51	U	201	EHZ	C1-C2-C3-C4
48	O	601	CDL	C59-C60-C61-C62
47	I	501	3PE	C25-C26-C27-C28
48	Z	201	CDL	C31-CA7-OA8-CA6
48	a	101	CDL	C71-CB7-OB8-CB6
47	N	2402	3PE	C3E-C3F-C3G-C3H
48	M	501	CDL	CA5-C11-C12-C13
51	T	201	EHZ	O4-C15-C16-C17
47	Y	1403	3PE	O32-C31-O31-C3
47	N	2402	3PE	C3F-C3G-C3H-C3I
48	a	101	CDL	OB7-CB5-OB6-CB4
47	b	402	3PE	C33-C34-C35-C36
48	M	501	CDL	C1-CB2-OB2-PB2
52	Y	1402	LMT	C5-C6-C7-C8
49	P	401	NDP	O4D-C1D-N1N-C6N
43	L	701	PLC	O3P-C1-C2-C3
47	Z	202	3PE	C3A-C3B-C3C-C3D
48	O	601	CDL	C64-C65-C66-C67
47	g	301	3PE	C23-C24-C25-C26
47	M	502	3PE	C38-C39-C3A-C3B
48	M	501	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
43	d	501	PLC	C'-C1'-C2'-C3'
47	I	501	3PE	C1-C2-C3-O31
47	M	502	3PE	C1-C2-C3-O31
47	Y	1403	3PE	C1-C2-C3-O31
48	Z	201	CDL	CA3-CA4-CA6-OA8
47	L	705	3PE	C33-C34-C35-C36
43	L	701	PLC	O3P-C1-C2-O2
48	b	401	CDL	C51-CB5-OB6-CB4
48	b	401	CDL	C1-CA2-OA2-PA1
47	L	704	3PE	C3E-C3F-C3G-C3H
51	T	201	EHZ	O1-C7-C8-C9
47	M	502	3PE	O21-C2-C3-O31
48	Z	201	CDL	OB6-CB4-CB6-OB8
47	b	402	3PE	C36-C37-C38-C39
47	N	2402	3PE	C34-C35-C36-C37
49	P	401	NDP	PA-O3-PN-O5D
47	d	502	3PE	O32-C31-O31-C3
47	H	6403	3PE	C39-C3A-C3B-C3C
43	H	6402	PLC	C'-C1'-C2'-C3'
48	Z	201	CDL	C15-C16-C17-C18
48	O	601	CDL	CA2-C1-CB2-OB2
52	Y	1401	LMT	C4-C5-C6-C7
52	Y	1401	LMT	C5-C6-C7-C8
43	d	501	PLC	O3P-C1-C2-C3
47	Z	202	3PE	O11-C1-C2-C3
47	d	502	3PE	C22-C23-C24-C25
43	L	701	PLC	C7'-C8'-C9'-CA'
48	Z	201	CDL	OA9-CA7-OA8-CA6
47	H	6403	3PE	C2B-C2C-C2D-C2E
47	L	705	3PE	C27-C28-C29-C2A
48	a	101	CDL	OB9-CB7-OB8-CB6
47	L	704	3PE	C33-C34-C35-C36
51	U	201	EHZ	C2-C3-C4-C5
47	N	2402	3PE	C2D-C2E-C2F-C2G
43	N	2401	PLC	O3P-C1-C2-O2
47	L	704	3PE	C23-C24-C25-C26
48	M	501	CDL	CB3-CB4-CB6-OB8
43	L	702	PLC	C5-C4-O4P-P
47	L	704	3PE	C3D-C3E-C3F-C3G
47	H	6401	3PE	O21-C2-C3-O31
47	L	703	3PE	O21-C2-C3-O31
48	b	401	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
48	O	601	CDL	C51-C52-C53-C54
47	I	501	3PE	C24-C25-C26-C27
48	a	101	CDL	CA4-CA3-OA5-PA1
43	D	501	PLC	O4P-C4-C5-N
43	L	702	PLC	O4P-C4-C5-N
43	N	2401	PLC	O4P-C4-C5-N
47	H	6403	3PE	C35-C36-C37-C38
47	L	705	3PE	C35-C36-C37-C38
51	T	201	EHZ	C2-C3-C4-C5
47	L	703	3PE	C33-C34-C35-C36
48	O	601	CDL	C53-C54-C55-C56
43	N	2401	PLC	O3P-C1-C2-C3
51	U	201	EHZ	C18-C17-C20-O6
49	P	401	NDP	C3D-C4D-C5D-O5D
47	L	704	3PE	C3F-C3G-C3H-C3I
47	H	6401	3PE	C22-C23-C24-C25
43	d	501	PLC	O3P-C1-C2-O2
48	a	101	CDL	OB5-CB3-CB4-OB6
48	b	401	CDL	OA5-CA3-CA4-OA6
43	L	701	PLC	C8'-C9'-CA'-CB'
43	L	701	PLC	C2B-C3B-C4B-C5B
47	I	501	3PE	O21-C2-C3-O31
47	L	705	3PE	O21-C2-C3-O31
47	Y	1403	3PE	O21-C2-C3-O31
48	b	401	CDL	OB6-CB4-CB6-OB8
47	H	6403	3PE	C33-C34-C35-C36
48	M	501	CDL	C55-C56-C57-C58
48	Z	201	CDL	CB3-CB4-CB6-OB8
43	D	501	PLC	C1-O3P-P-O1P
43	L	701	PLC	C1-O3P-P-O4P
43	L	702	PLC	C4-O4P-P-O2P
43	N	2401	PLC	C1-O3P-P-O1P
47	H	6401	3PE	C1-O11-P-O13
47	H	6401	3PE	O13-C11-C12-N
47	I	501	3PE	C1-O11-P-O13
47	I	501	3PE	C1-O11-P-O14
47	L	703	3PE	C1-O11-P-O14
47	Y	1403	3PE	C1-O11-P-O13
47	Y	1403	3PE	C1-O11-P-O14
47	Y	1403	3PE	C11-O13-P-O12
47	d	502	3PE	C1-O11-P-O13
47	d	502	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
47	d	502	3PE	O13-C11-C12-N
48	M	501	CDL	CA3-OA5-PA1-OA2
48	M	501	CDL	CA3-OA5-PA1-OA3
48	O	601	CDL	CA3-OA5-PA1-OA4
48	O	601	CDL	CB3-OB5-PB2-OB3
48	Z	201	CDL	CA3-OA5-PA1-OA4
48	a	101	CDL	CA2-OA2-PA1-OA3
48	a	101	CDL	CA3-OA5-PA1-OA3
48	b	401	CDL	CB3-OB5-PB2-OB3
49	P	401	NDP	C5B-O5B-PA-O1A
48	M	501	CDL	C1-CA2-OA2-PA1
48	M	501	CDL	CA4-CA3-OA5-PA1
47	b	402	3PE	C2E-C2F-C2G-C2H
47	L	703	3PE	C2A-C2B-C2C-C2D
43	L	702	PLC	C1-C2-O2-C'
47	Z	202	3PE	C3-C2-O21-C21
48	a	101	CDL	CA3-CA4-OA6-CA5
47	N	2402	3PE	C39-C3A-C3B-C3C
47	L	705	3PE	C2F-C2G-C2H-C2I
52	Y	1401	LMT	C9-C10-C11-C12
43	D	501	PLC	O3P-C1-C2-C3
51	T	201	EHZ	C5-C6-C7-C8
48	a	101	CDL	CA2-C1-CB2-OB2
43	D	501	PLC	O3P-C1-C2-O2
47	Z	202	3PE	O11-C1-C2-O21
47	Z	202	3PE	C33-C34-C35-C36
43	L	702	PLC	C2B-C1B-CB-O3
48	Z	201	CDL	OA6-CA4-CA6-OA8
48	b	401	CDL	C31-CA7-OA8-CA6
52	Y	1402	LMT	C6-C7-C8-C9
47	L	705	3PE	O31-C31-C32-C33
48	b	401	CDL	OA9-CA7-OA8-CA6
47	b	402	3PE	C2A-C2B-C2C-C2D
47	Z	202	3PE	C31-C32-C33-C34
47	N	2402	3PE	C26-C27-C28-C29
47	L	704	3PE	O11-C1-C2-O21
48	Z	201	CDL	OB5-CB3-CB4-OB6
48	b	401	CDL	OB5-CB3-CB4-OB6
48	M	501	CDL	C11-C12-C13-C14
51	T	201	EHZ	N2-C15-C16-C17
47	L	704	3PE	C34-C35-C36-C37
43	N	2401	PLC	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
43	L	702	PLC	C3B-C4B-C5B-C6B
48	M	501	CDL	C34-C35-C36-C37
48	O	601	CDL	O1-C1-CB2-OB2
47	L	705	3PE	C34-C35-C36-C37
47	d	502	3PE	C3-C2-O21-C21
47	L	705	3PE	C32-C33-C34-C35
47	Y	1403	3PE	C21-C22-C23-C24
47	b	402	3PE	C2C-C2D-C2E-C2F
52	Y	1401	LMT	C3-C4-C5-C6
47	H	6401	3PE	O11-C1-C2-C3
47	L	703	3PE	C24-C25-C26-C27
43	N	2401	PLC	C1'-C2'-C3'-C4'
47	Z	202	3PE	O21-C2-C3-O31
49	P	401	NDP	C2N-C3N-C7N-N7N
47	H	6403	3PE	C34-C35-C36-C37
43	L	701	PLC	C6B-C7B-C8B-C9B
48	M	501	CDL	C39-C40-C41-C42
48	M	501	CDL	C21-C22-C23-C24
48	M	501	CDL	OA7-CA5-OA6-CA4
48	M	501	CDL	C12-C13-C14-C15
49	P	401	NDP	PA-O3-PN-O1N
47	L	705	3PE	C2C-C2D-C2E-C2F
47	b	402	3PE	C28-C29-C2A-C2B
48	M	501	CDL	C22-C23-C24-C25
47	g	301	3PE	C26-C27-C28-C29
47	I	501	3PE	O11-C1-C2-O21
48	b	401	CDL	C72-C73-C74-C75
43	d	501	PLC	O2-C'-C1'-C2'
48	O	601	CDL	C12-C13-C14-C15
47	I	501	3PE	O11-C1-C2-C3
47	L	704	3PE	O11-C1-C2-C3
48	Z	201	CDL	OB5-CB3-CB4-CB6
48	b	401	CDL	OA5-CA3-CA4-CA6
48	Z	201	CDL	CA7-C31-C32-C33
48	Z	201	CDL	C12-C13-C14-C15
48	M	501	CDL	OB9-CB7-OB8-CB6
45	F	501	FMN	C2'-C3'-C4'-C5'
43	L	701	PLC	C5B-C6B-C7B-C8B
47	N	2402	3PE	C1-C2-O21-C21
43	L	701	PLC	C4B-C5B-C6B-C7B
48	Z	201	CDL	C32-C31-CA7-OA8
52	Y	1402	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
48	Z	201	CDL	C14-C15-C16-C17
48	M	501	CDL	C19-C20-C21-C22
47	L	703	3PE	O31-C31-C32-C33
48	a	101	CDL	C34-C35-C36-C37
47	Z	202	3PE	O31-C31-C32-C33
43	L	701	PLC	C7B-C8B-C9B-CAA
48	M	501	CDL	C52-C51-CB5-OB6
48	M	501	CDL	C11-CA5-OA6-CA4
43	L	701	PLC	O2-C'-C1'-C2'
51	U	201	EHZ	C21-C1-C2-C3
48	Z	201	CDL	C12-C11-CA5-OA6
45	F	501	FMN	O3'-C3'-C4'-C5'
47	d	502	3PE	O31-C31-C32-C33
47	L	705	3PE	O21-C21-C22-C23
52	Y	1402	LMT	O5B-C1B-O1B-C4'
48	Z	201	CDL	C72-C71-CB7-OB8
43	L	701	PLC	C3B-C4B-C5B-C6B
51	U	201	EHZ	C19-C17-C20-O6
48	Z	201	CDL	C11-C12-C13-C14
52	Y	1402	LMT	C11-C10-C9-C8
43	H	6402	PLC	C2B-C1B-CB-O3
47	L	703	3PE	O21-C21-C22-C23
48	Z	201	CDL	C13-C14-C15-C16
47	N	2402	3PE	C2-C1-O11-P
52	Y	1402	LMT	C9-C10-C11-C12
47	L	703	3PE	O32-C31-C32-C33
47	Z	202	3PE	O32-C31-C32-C33
47	Z	202	3PE	C26-C27-C28-C29
48	Z	201	CDL	CB7-C71-C72-C73
43	L	701	PLC	O'-C'-C1'-C2'
47	L	704	3PE	C21-C22-C23-C24
48	Z	201	CDL	C32-C31-CA7-OA9
48	Z	201	CDL	C72-C71-CB7-OB9
48	M	501	CDL	C52-C51-CB5-OB7
48	Z	201	CDL	C12-C11-CA5-OA7
47	b	402	3PE	O31-C31-C32-C33
43	D	501	PLC	C4-C5-N-C8
47	L	705	3PE	C2-C3-O31-C31
47	L	705	3PE	O22-C21-C22-C23
47	b	402	3PE	C2B-C2C-C2D-C2E
47	N	2402	3PE	C23-C24-C25-C26
52	Y	1401	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

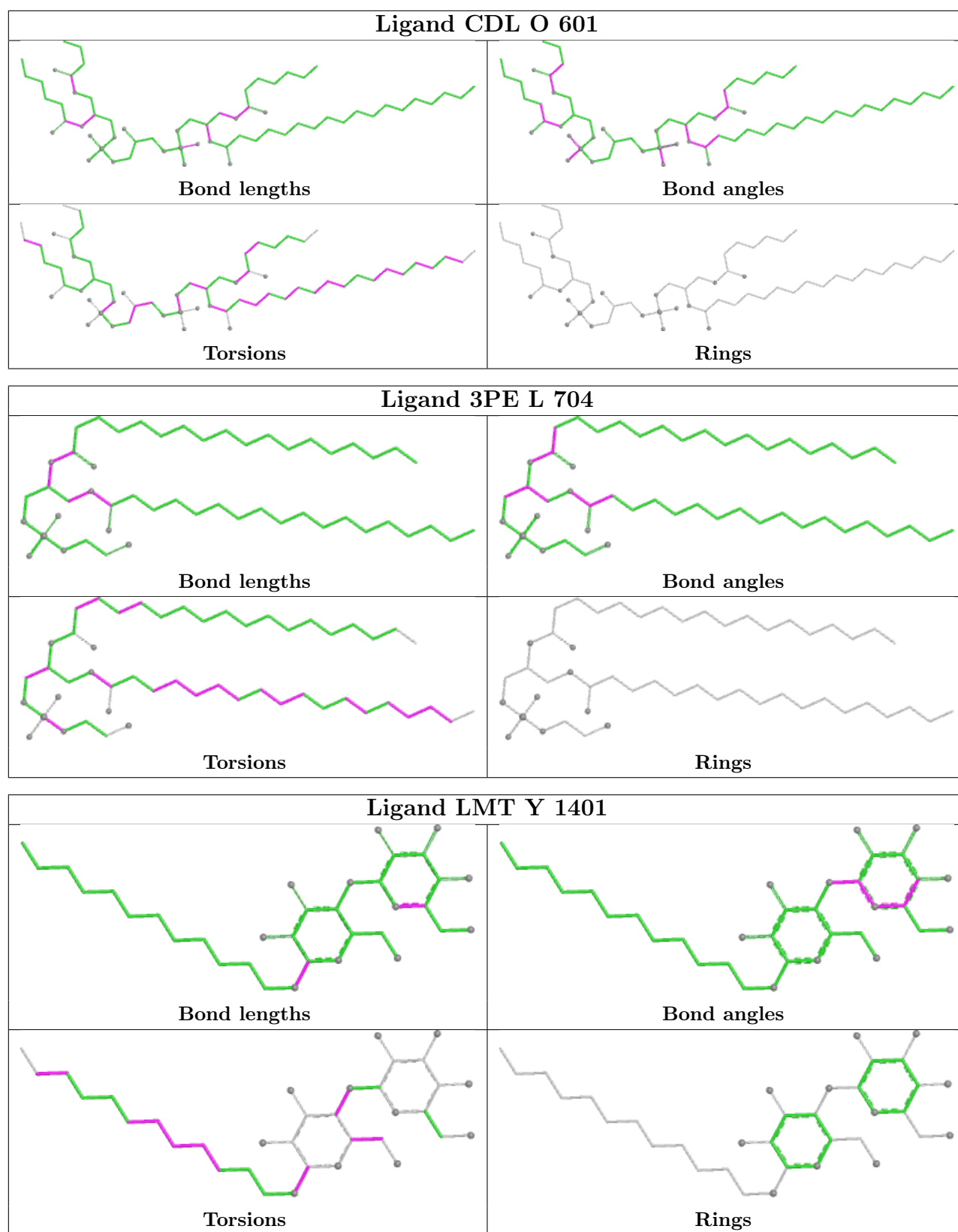
Mol	Chain	Res	Type	Atoms
47	L	703	3PE	O22-C21-C22-C23
47	M	502	3PE	C33-C34-C35-C36
47	d	502	3PE	O32-C31-C32-C33
47	N	2402	3PE	C27-C28-C29-C2A

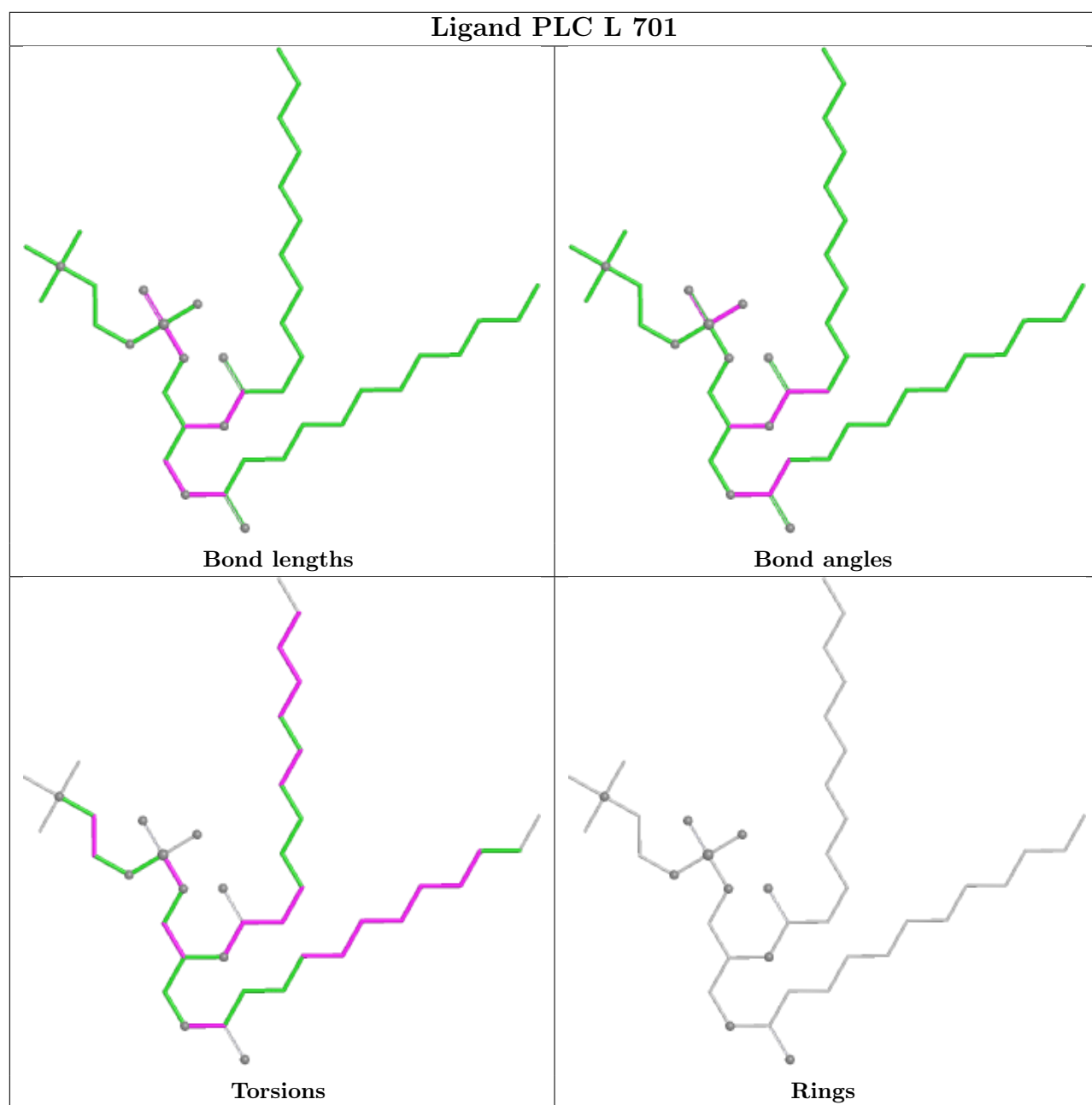
There are no ring outliers.

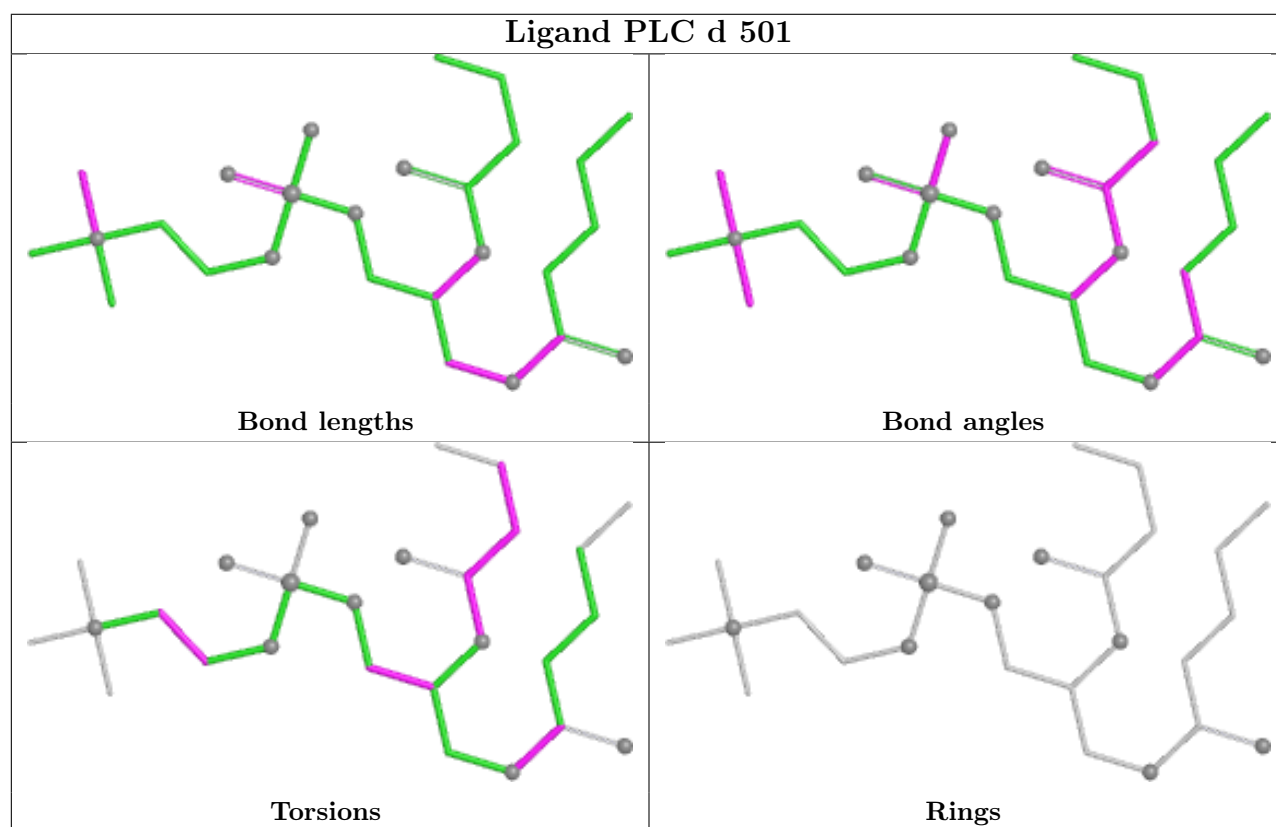
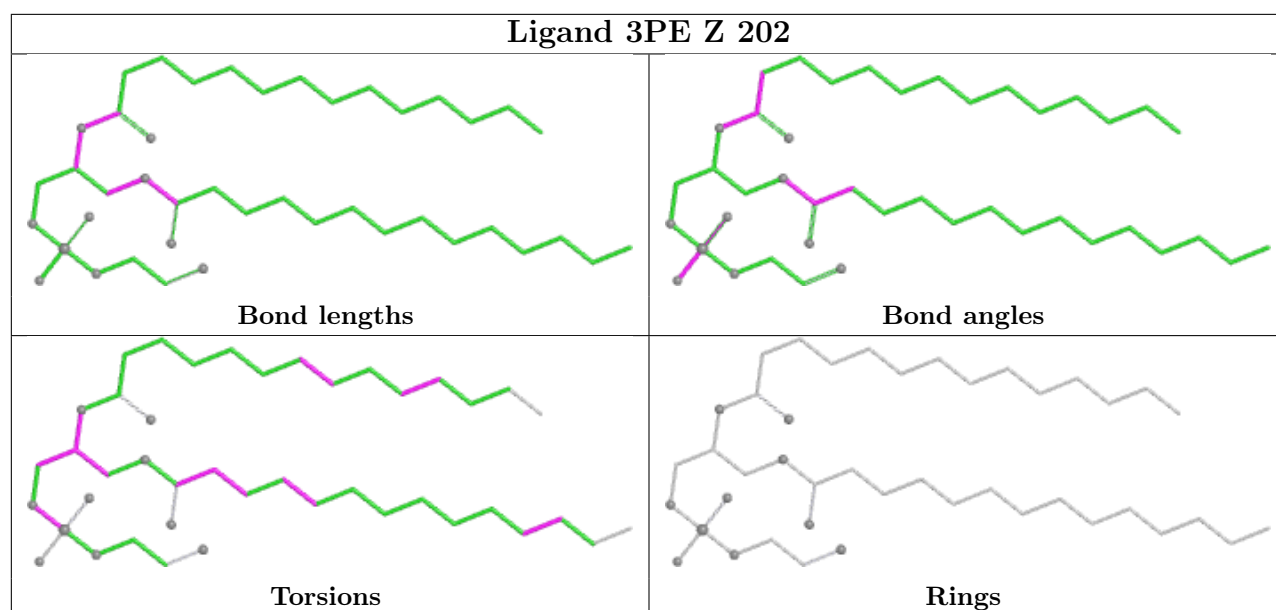
16 monomers are involved in 28 short contacts:

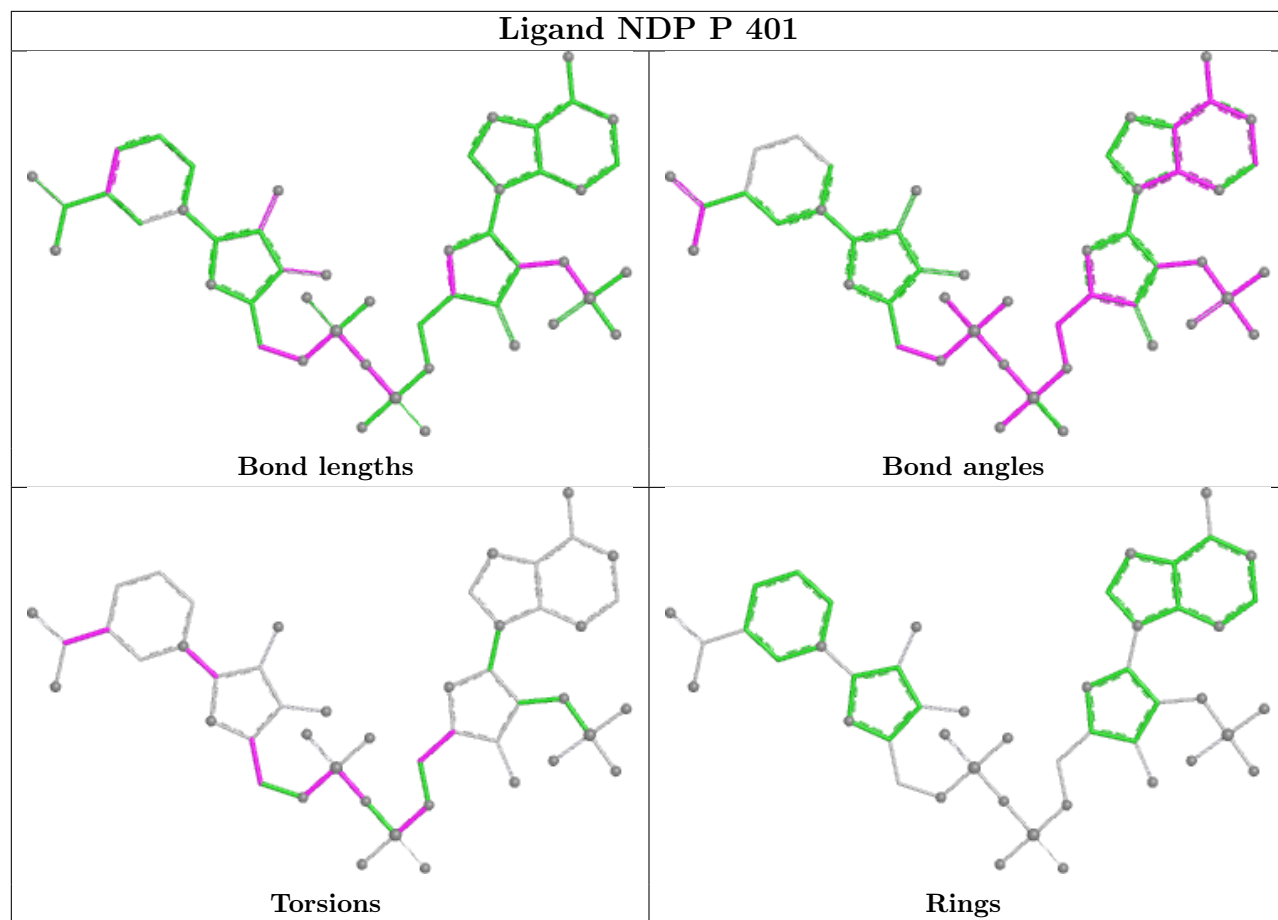
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	O	601	CDL	2	0
43	L	701	PLC	3	0
49	P	401	NDP	2	0
47	H	6403	3PE	1	0
46	I	503	SF4	1	0
47	L	705	3PE	3	0
48	Z	201	CDL	1	0
47	b	402	3PE	2	0
45	F	501	FMN	1	0
48	a	101	CDL	1	0
47	N	2402	3PE	3	0
51	T	201	EHZ	3	0
47	Y	1403	3PE	1	0
44	E	301	FES	1	0
43	L	702	PLC	2	0
48	b	401	CDL	1	0

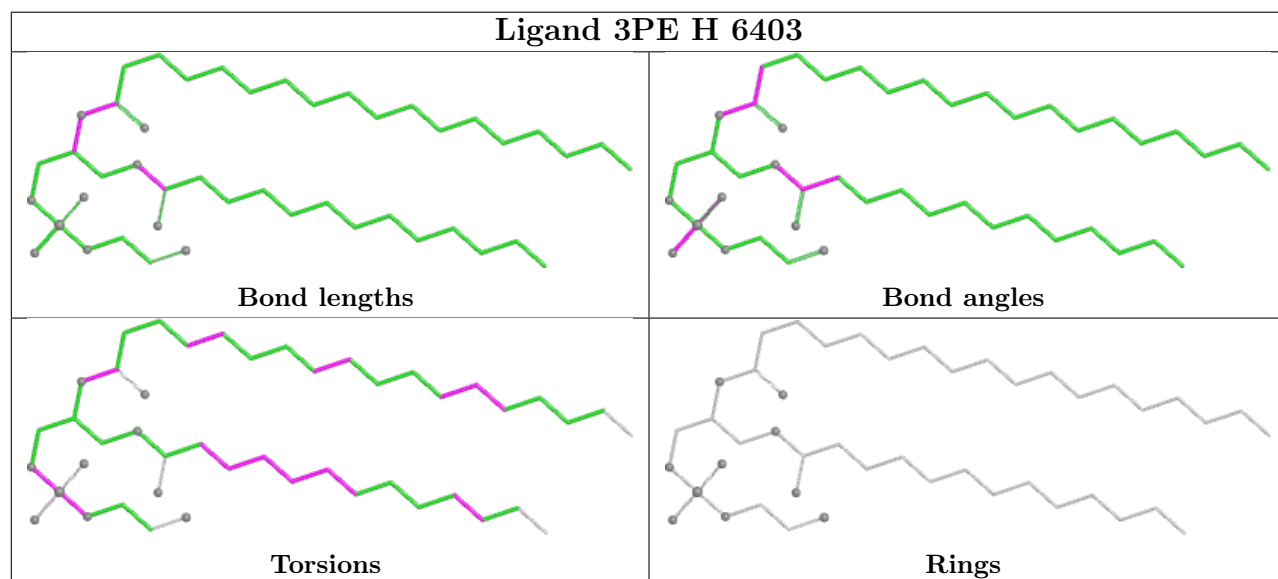
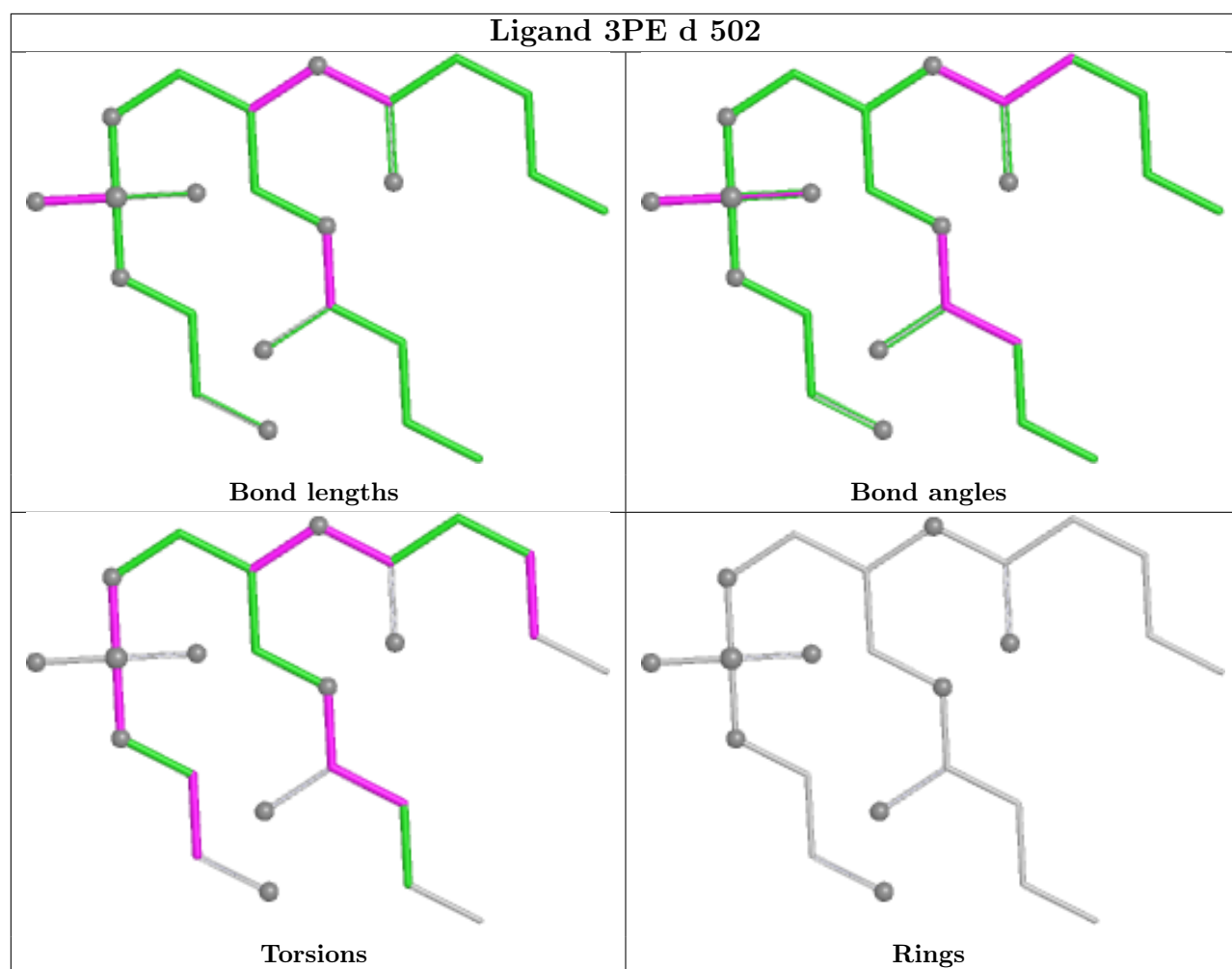
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

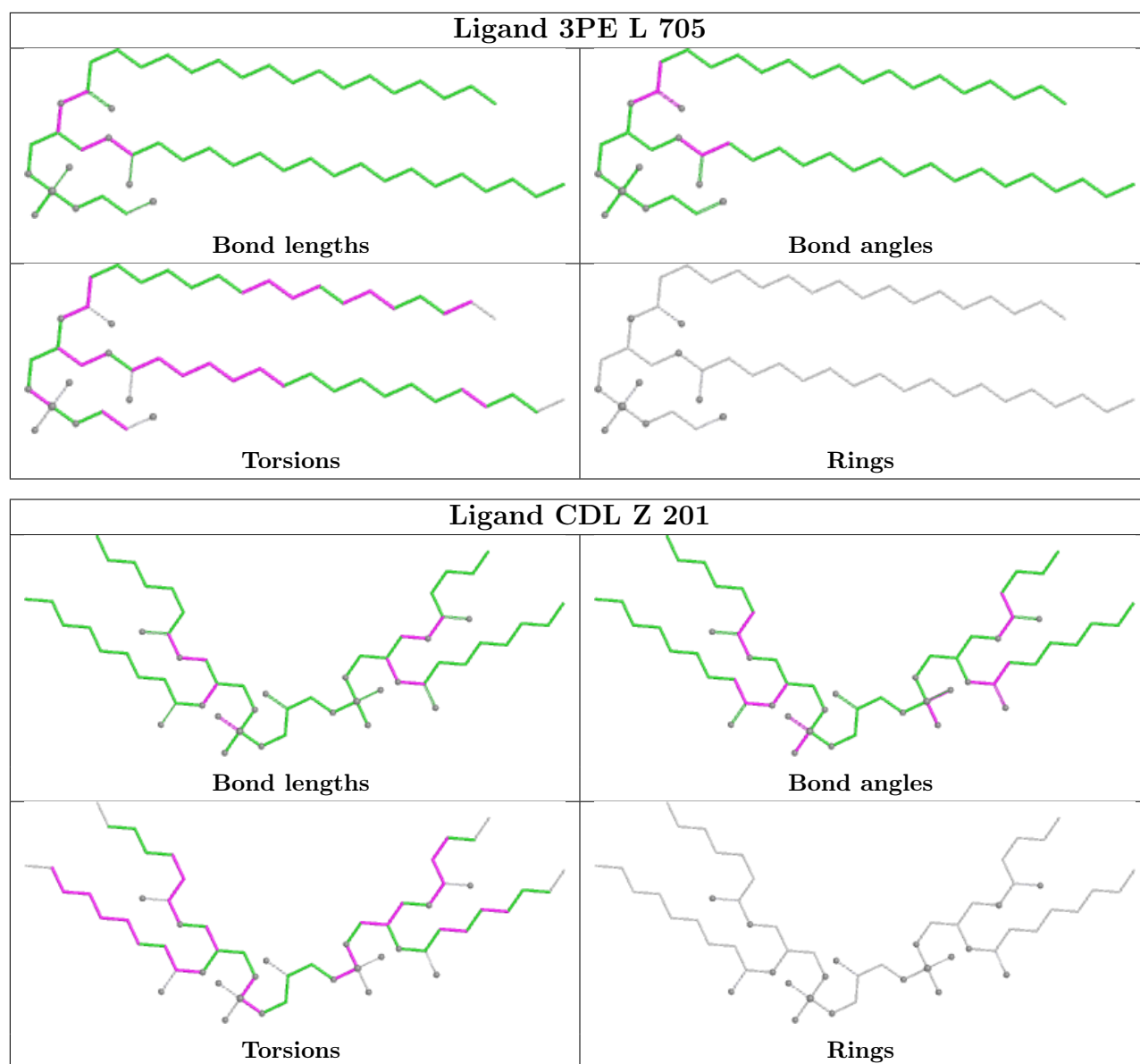


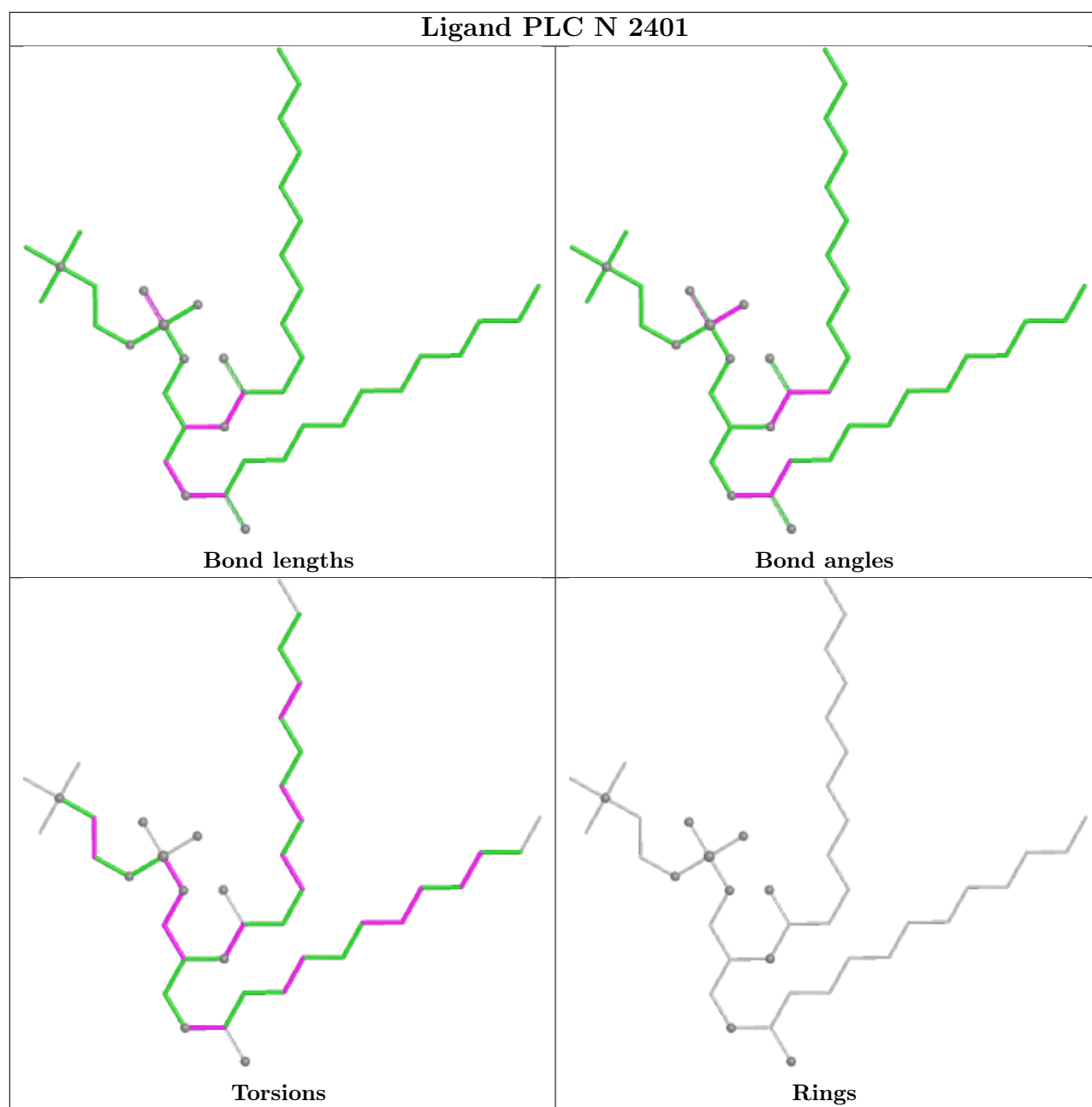


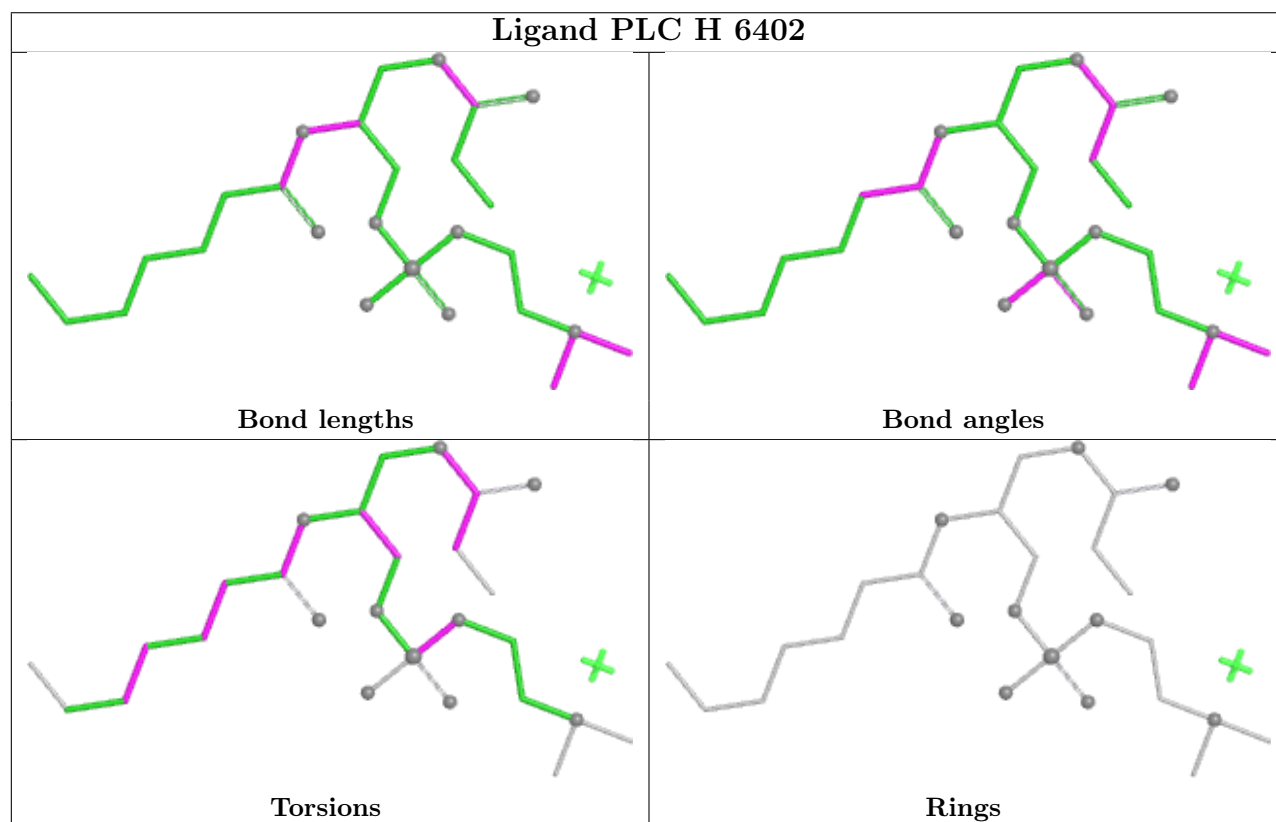
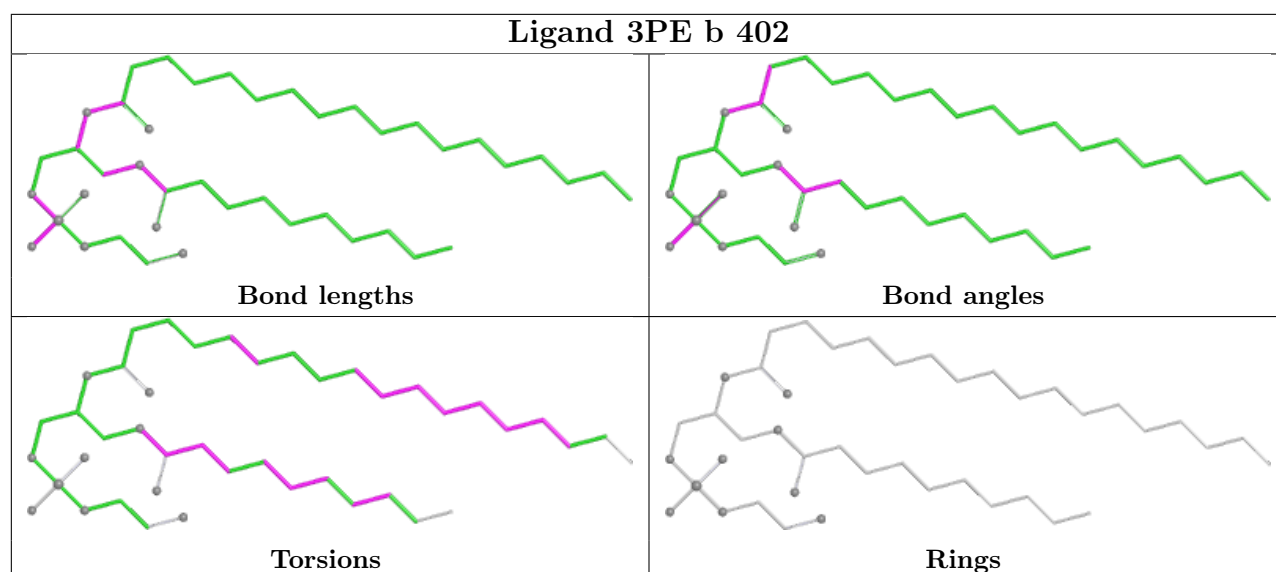


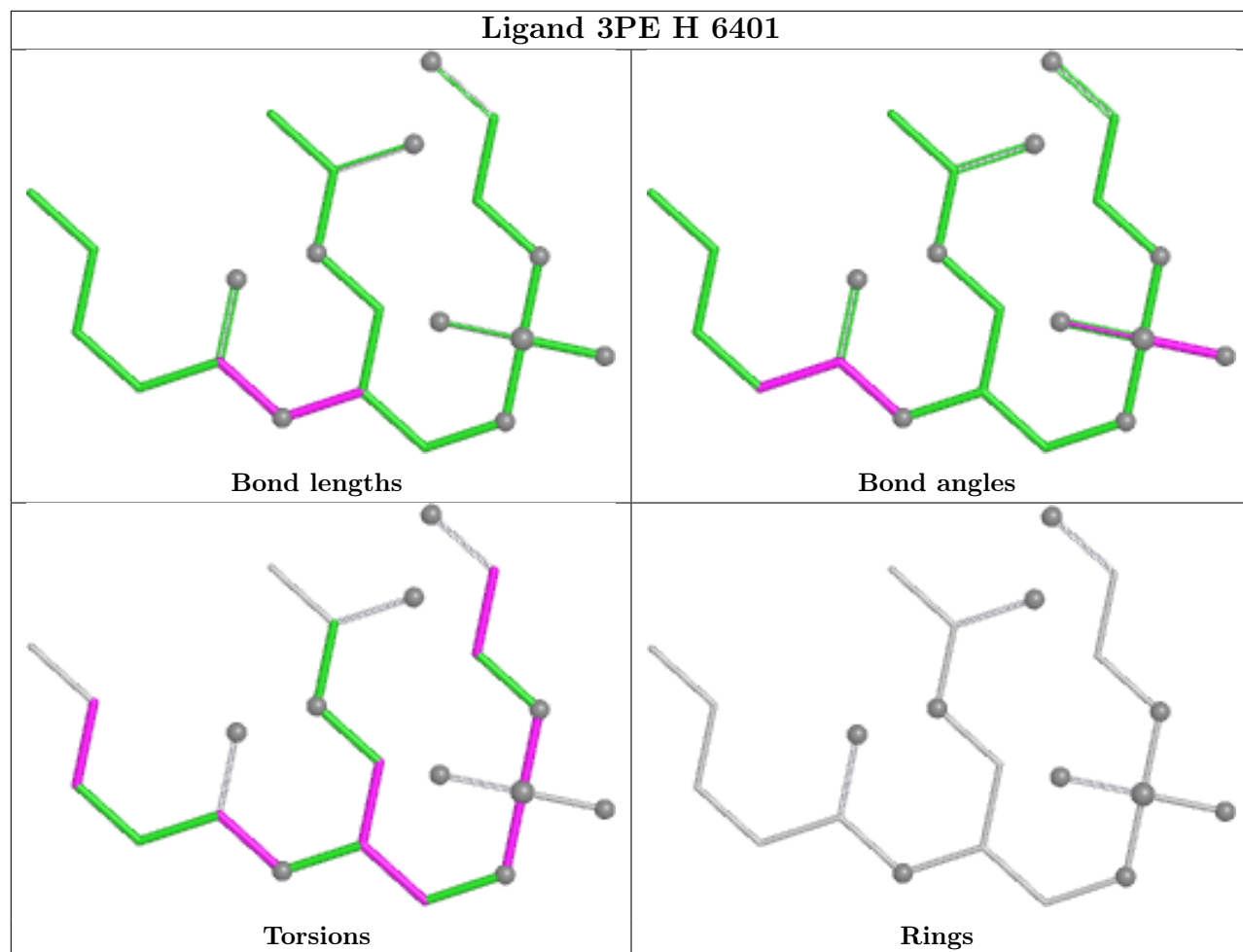


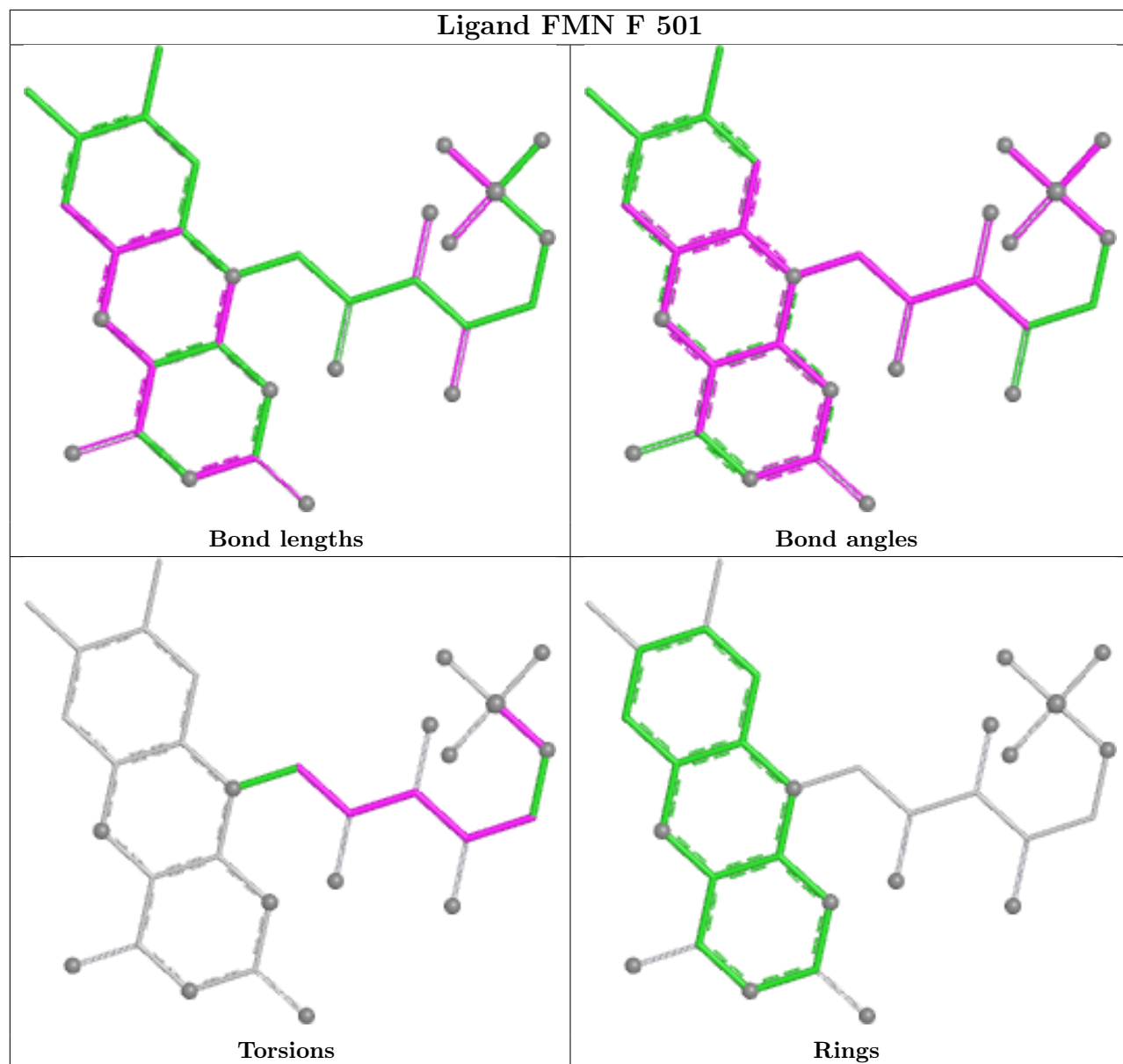


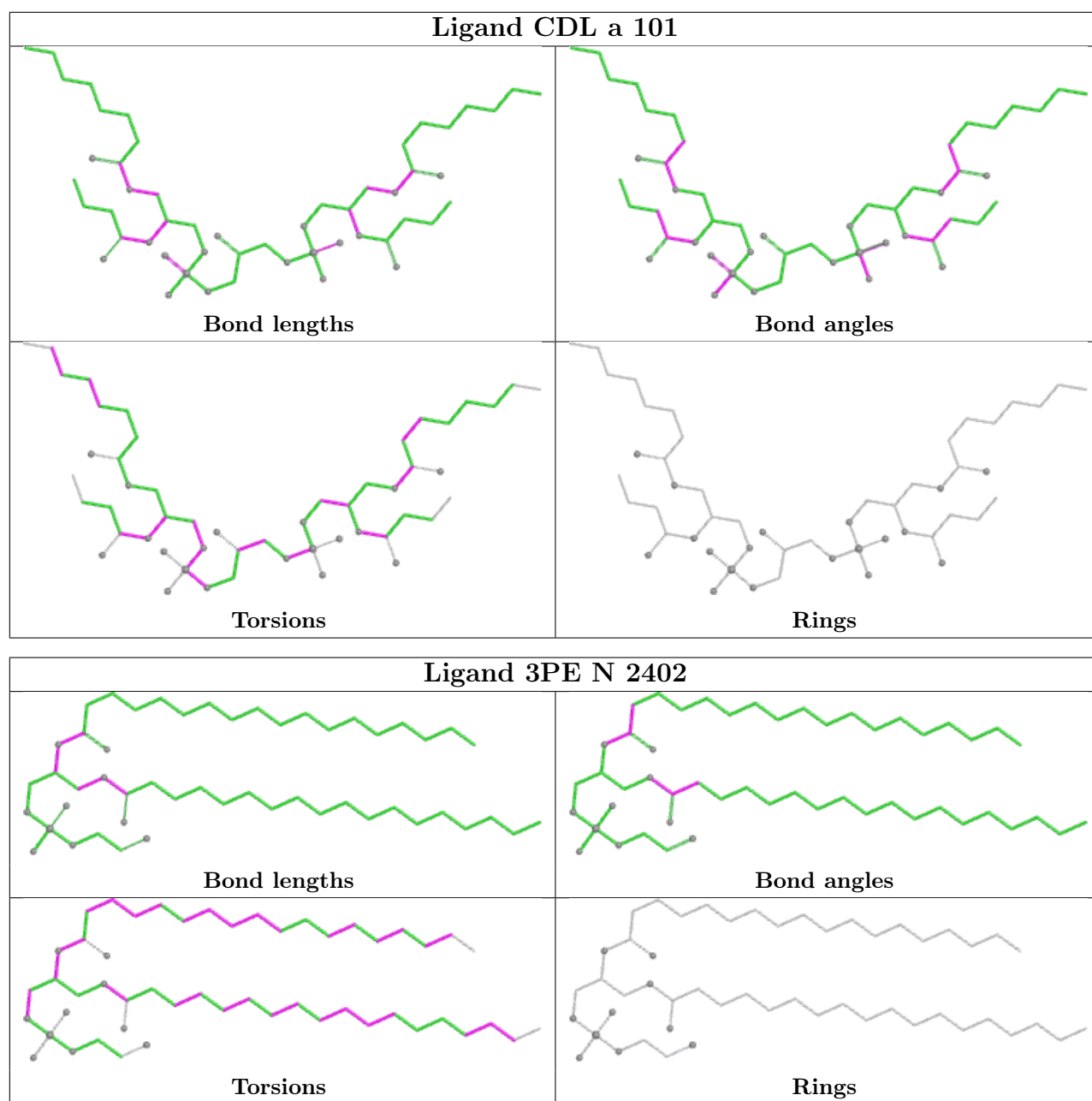


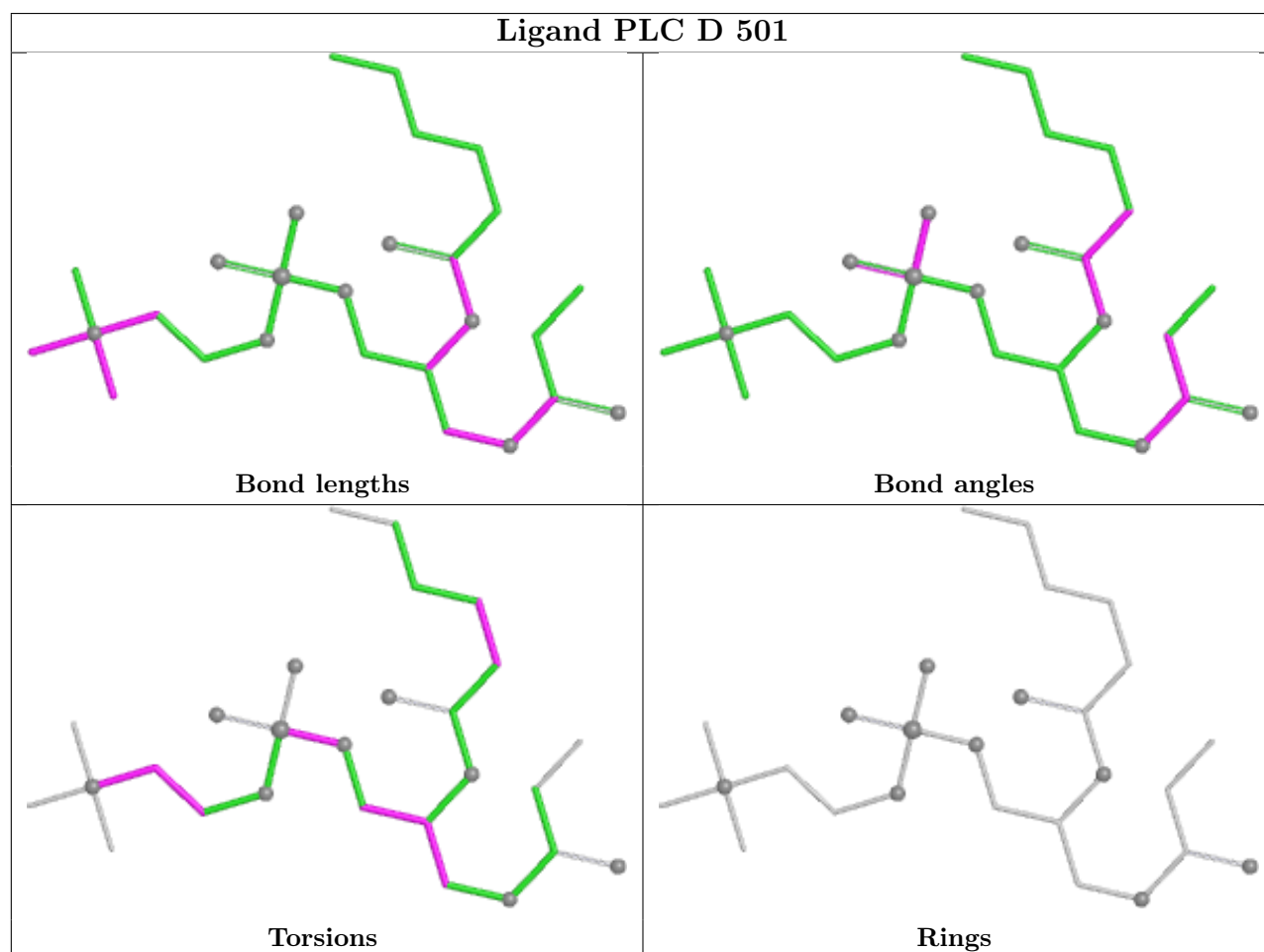
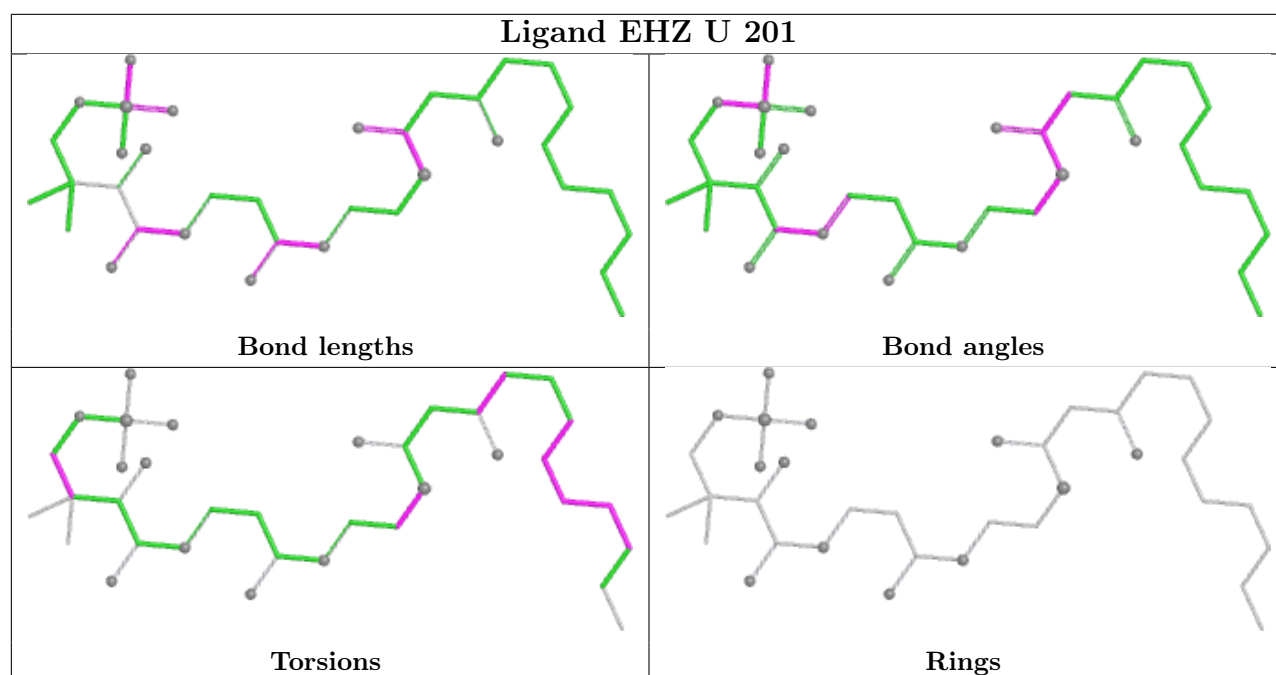


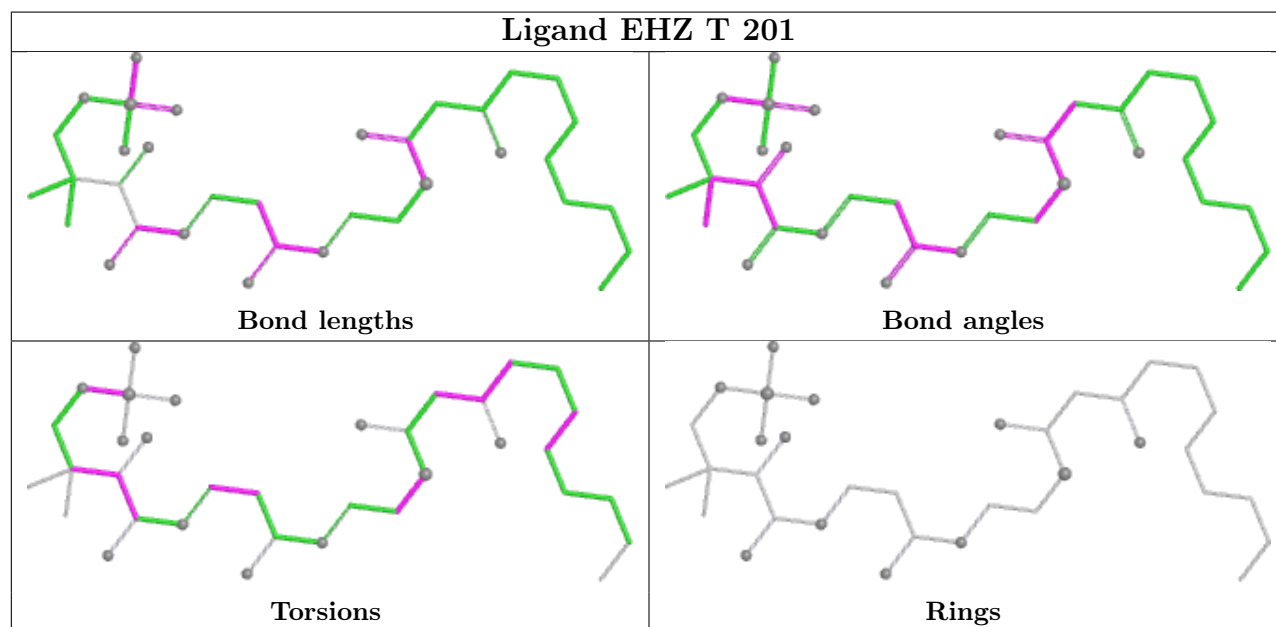
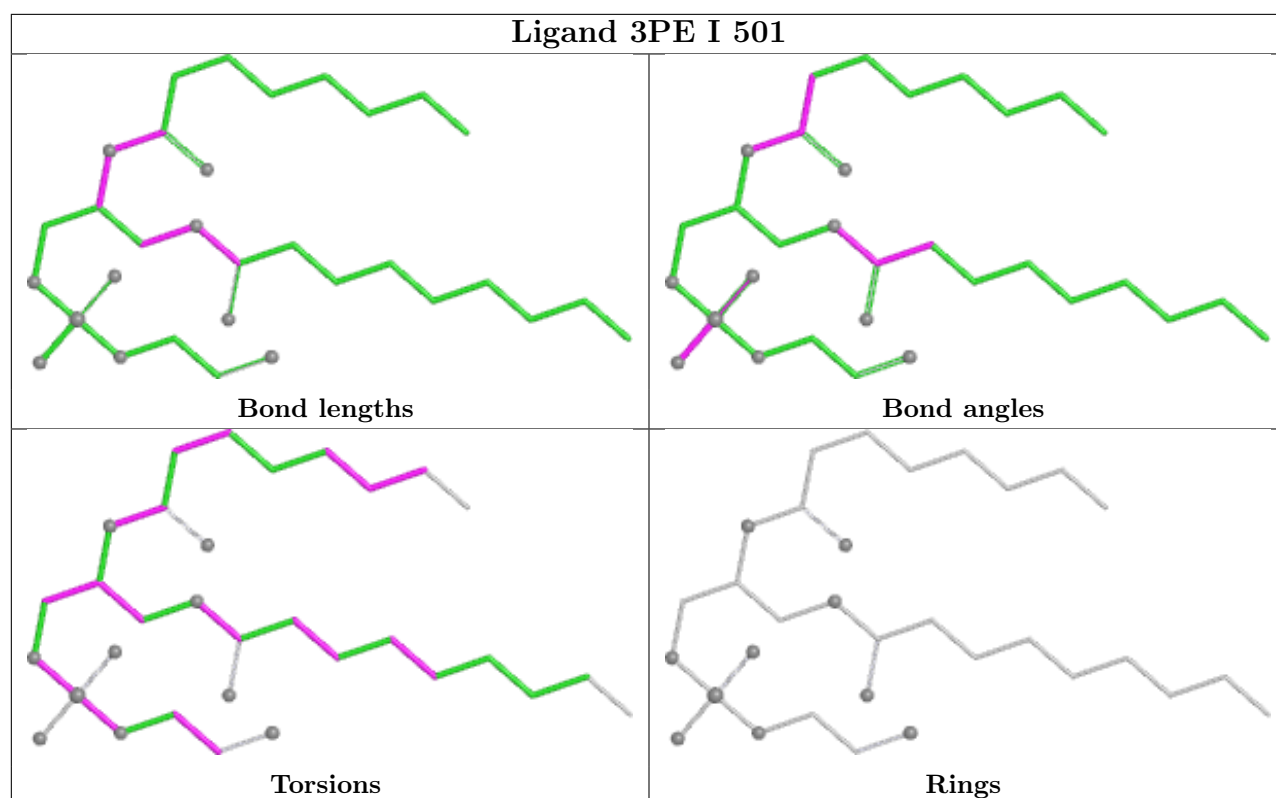


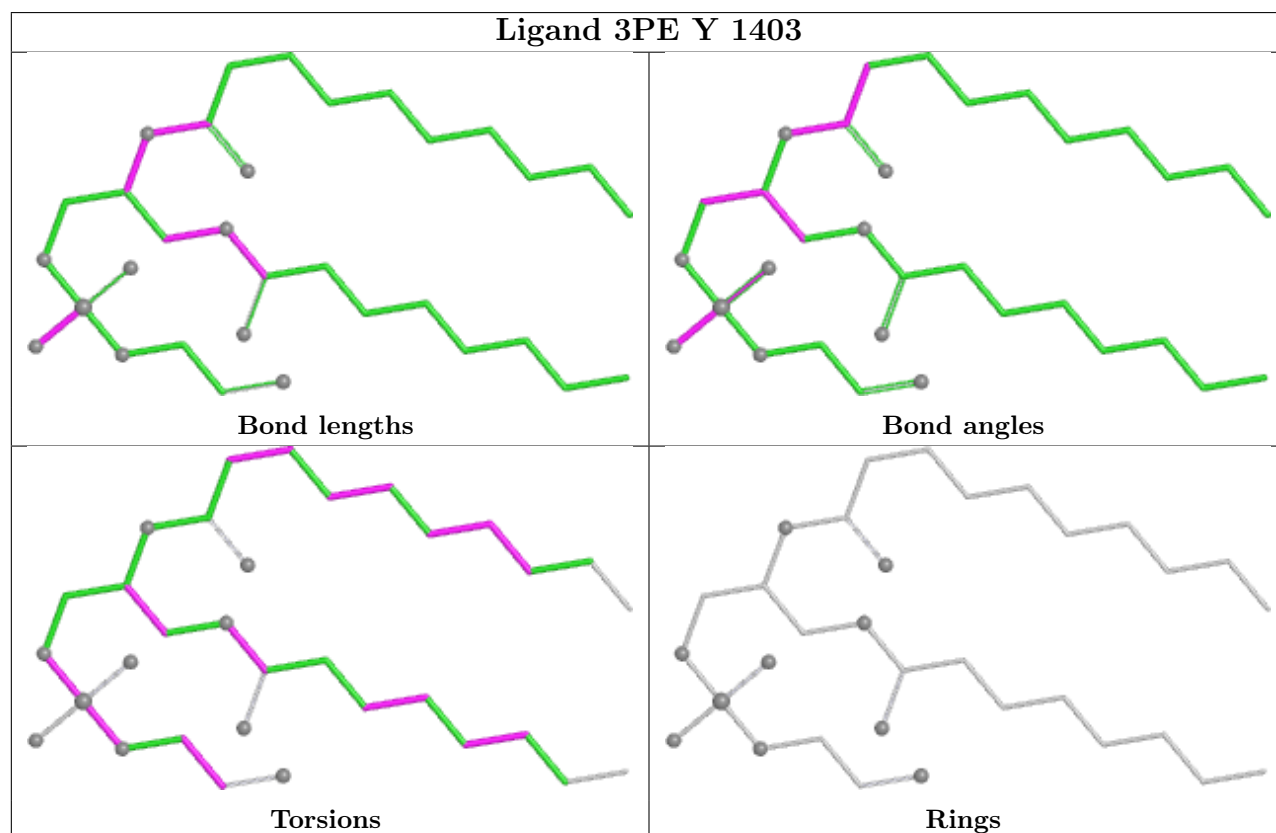
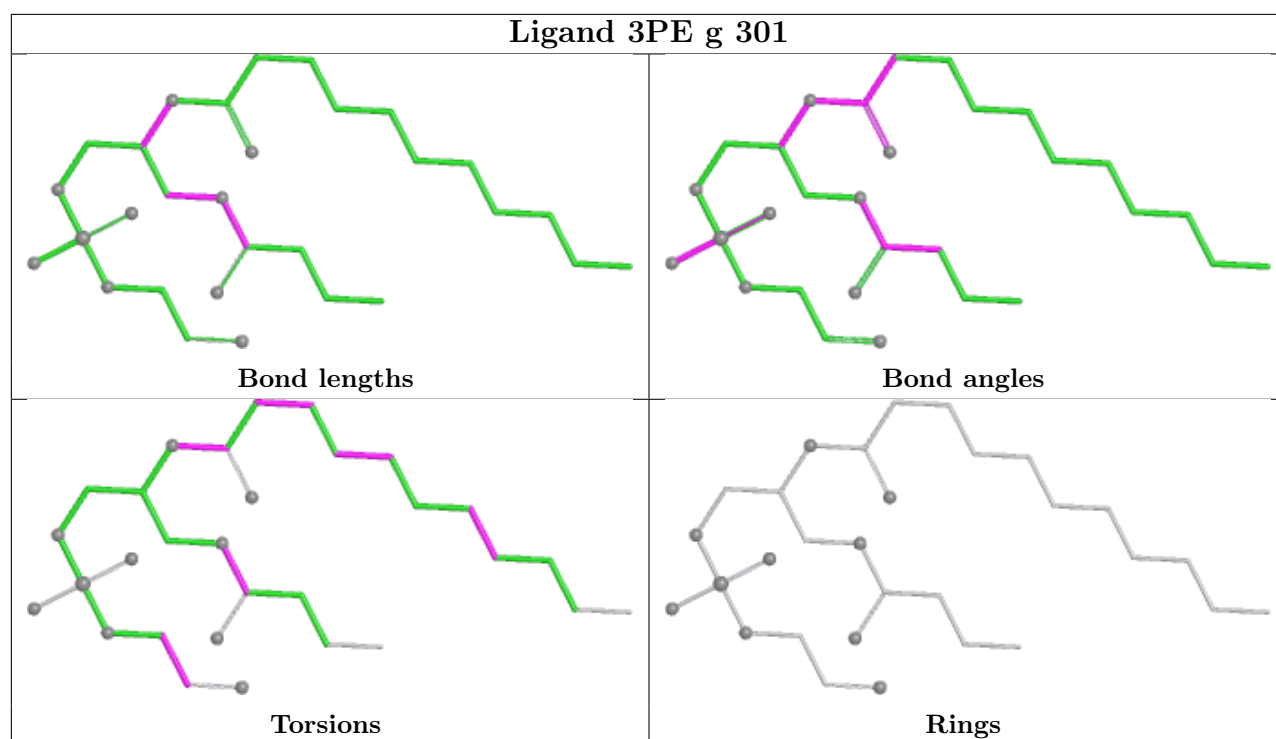




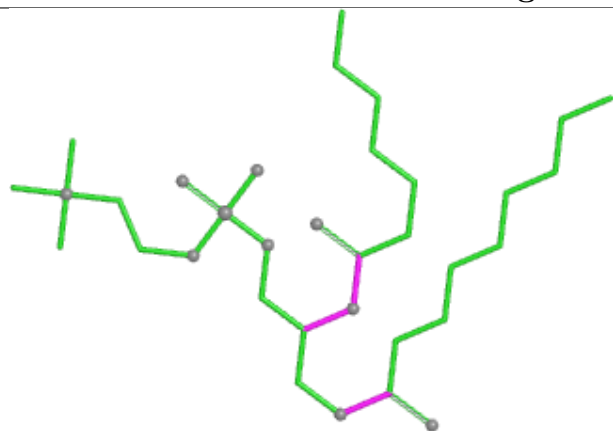




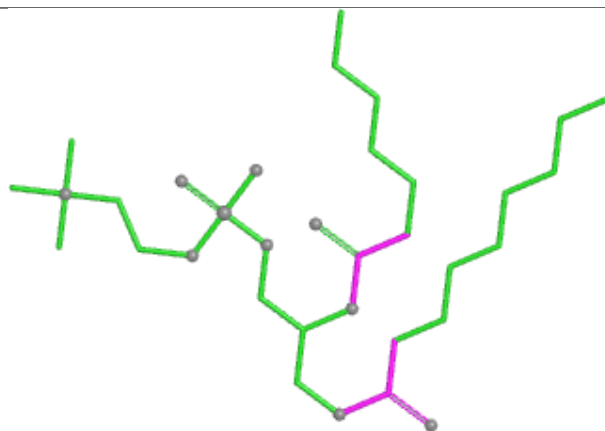




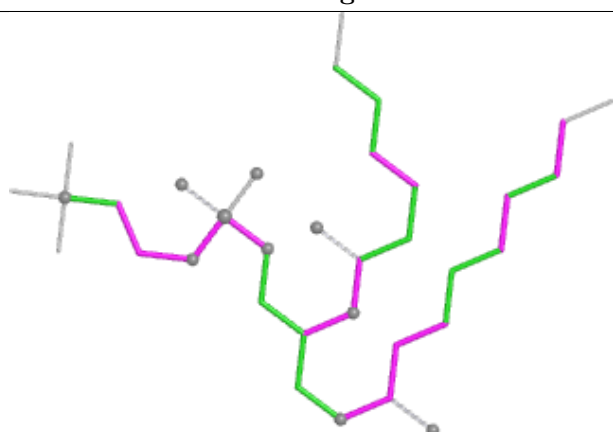
Ligand PLC L 702



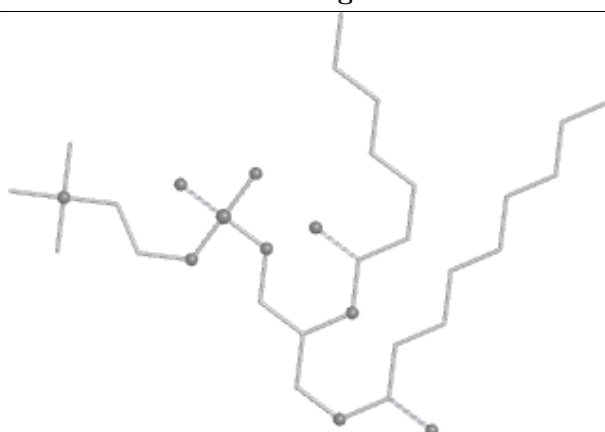
Bond lengths



Bond angles

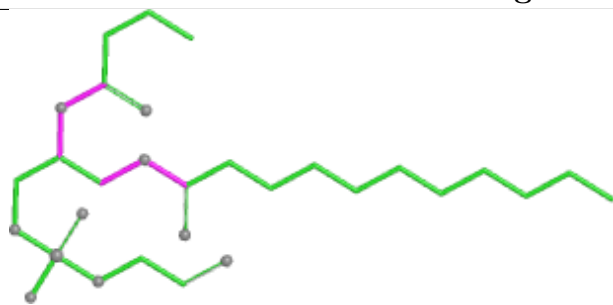


Torsions

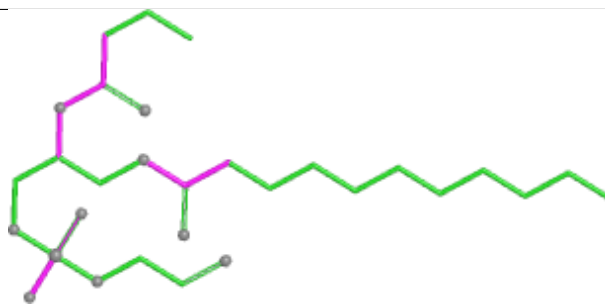


Rings

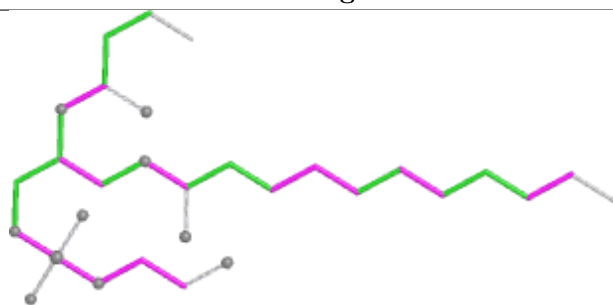
Ligand 3PE M 502



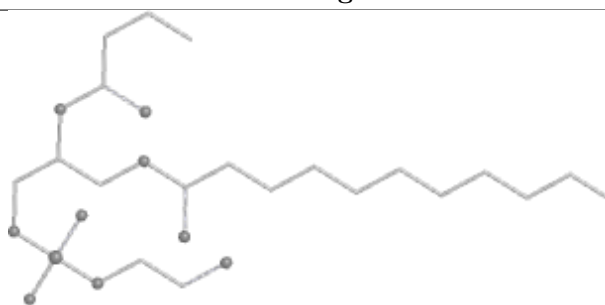
Bond lengths



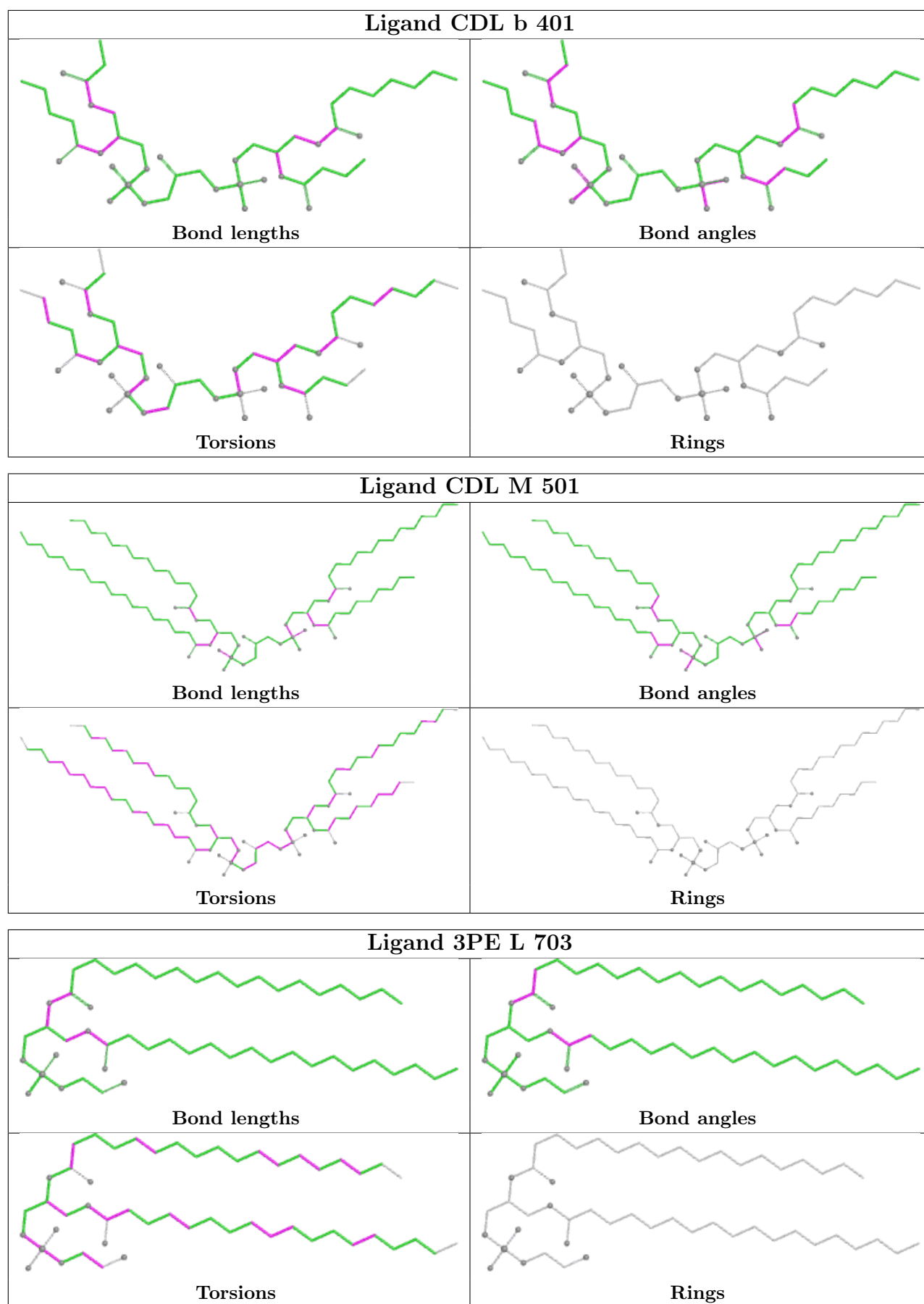
Bond angles

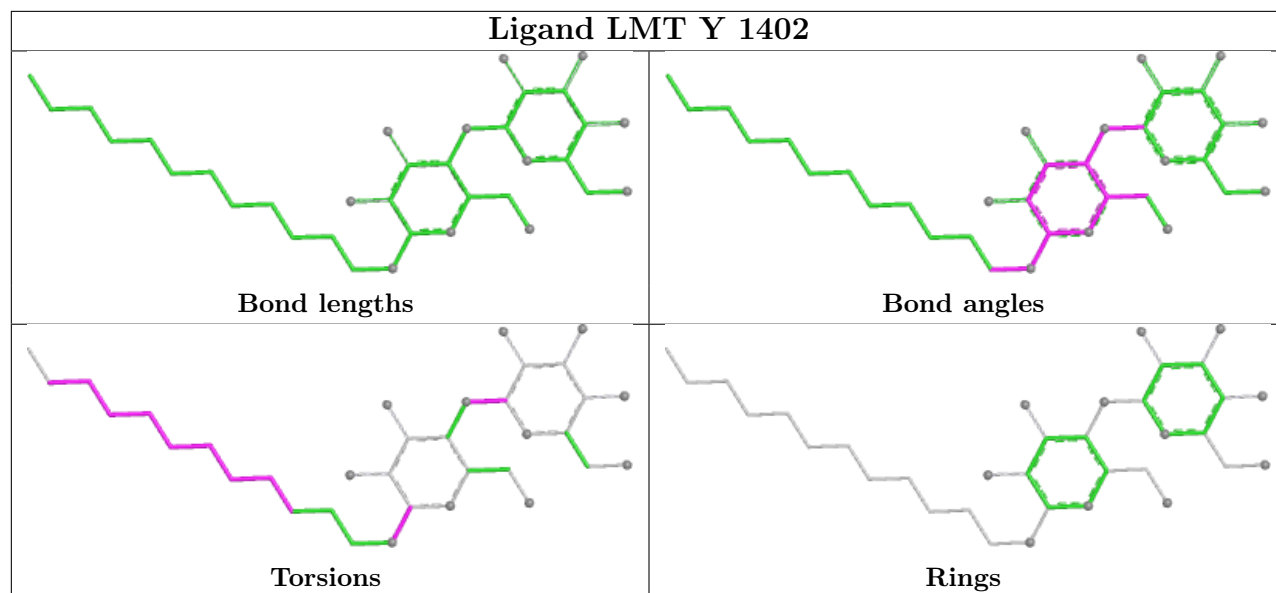


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

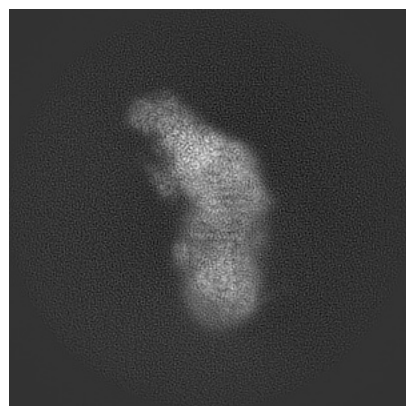
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11969. These allow visual inspection of the internal detail of the map and identification of artifacts.

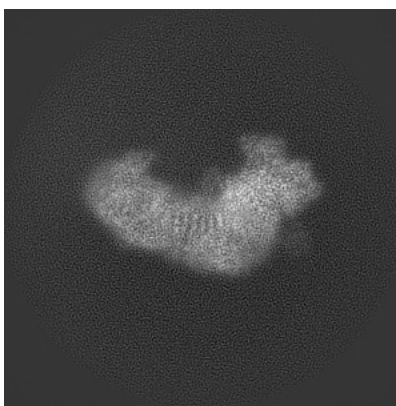
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

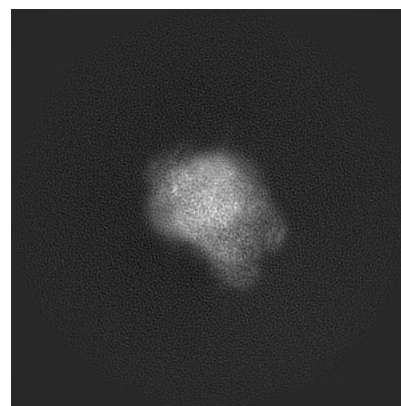
6.1.1 Primary map



X

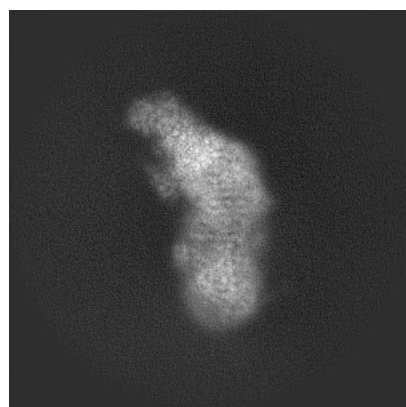


Y

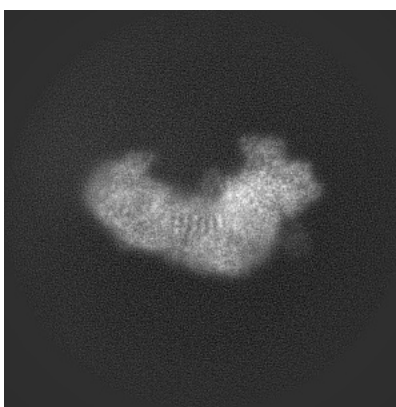


Z

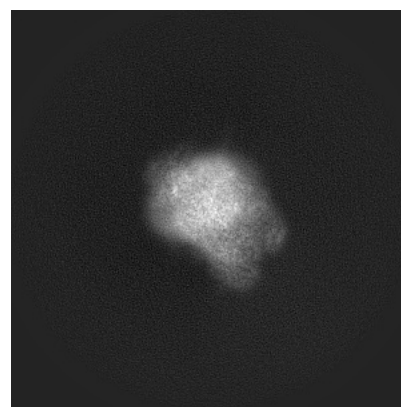
6.1.2 Raw map



X



Y

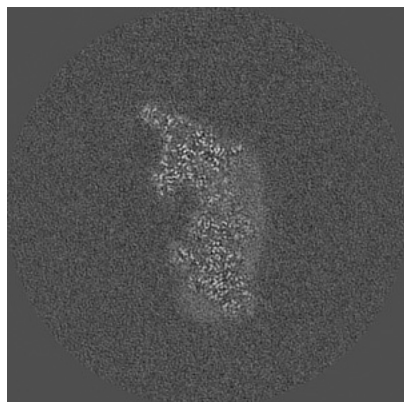


Z

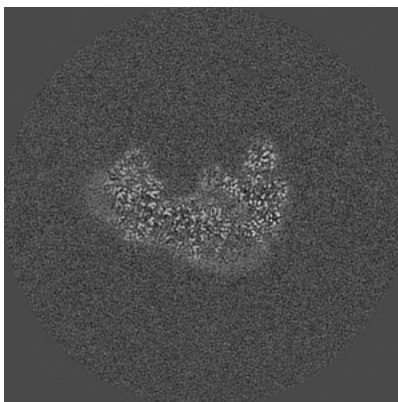
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

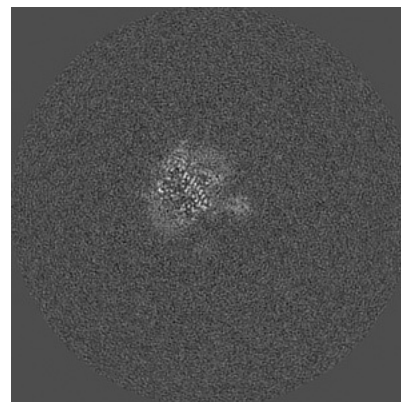
6.2.1 Primary map



X Index: 225

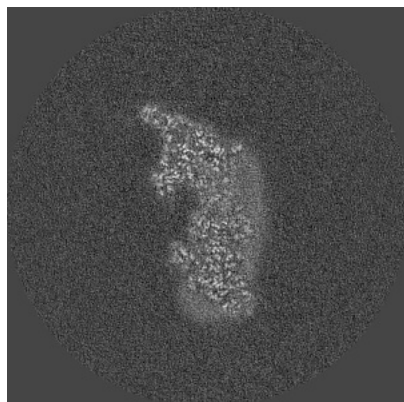


Y Index: 225

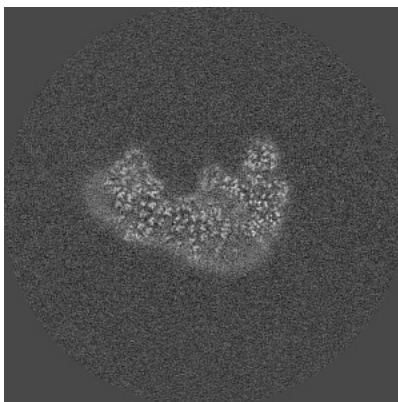


Z Index: 225

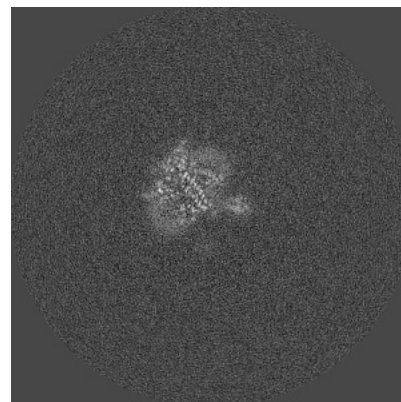
6.2.2 Raw map



X Index: 225



Y Index: 225

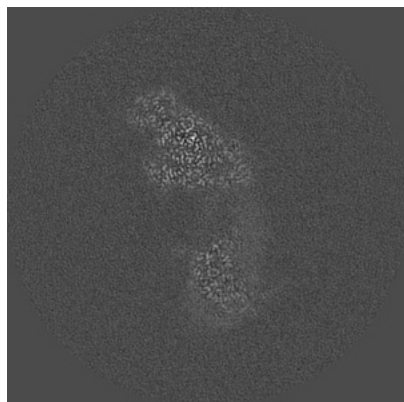


Z Index: 225

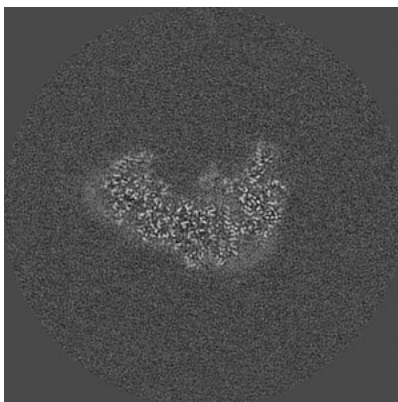
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

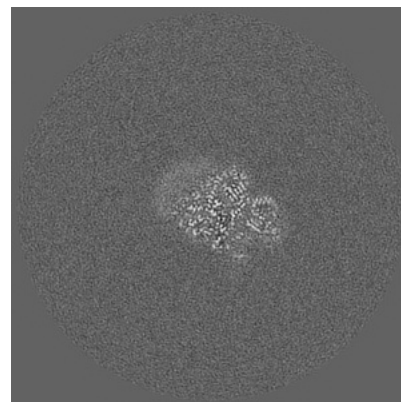
6.3.1 Primary map



X Index: 241

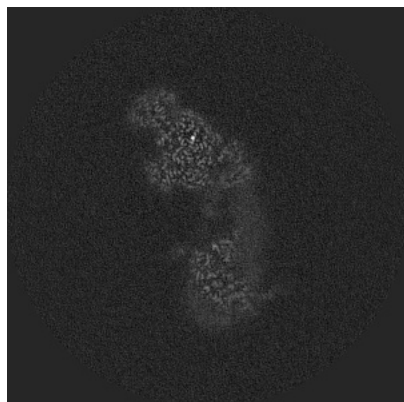


Y Index: 231

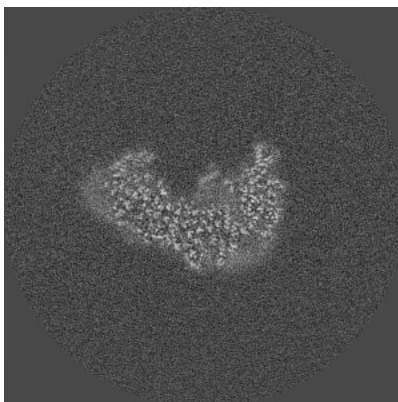


Z Index: 286

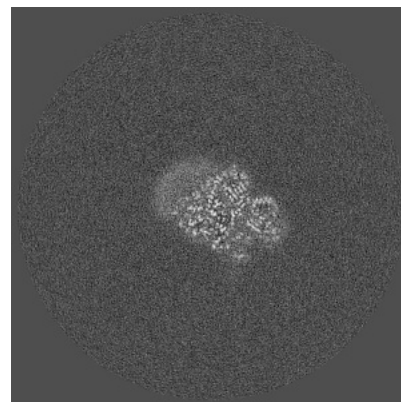
6.3.2 Raw map



X Index: 240



Y Index: 232

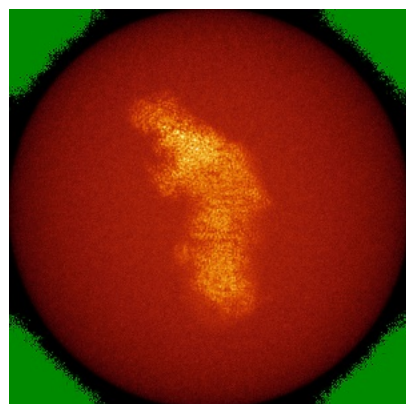


Z Index: 286

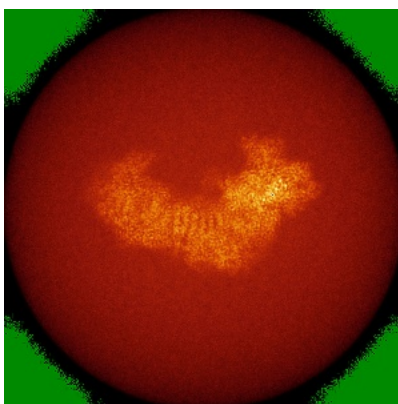
The images above show the largest variance slices of the map in three orthogonal directions.

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

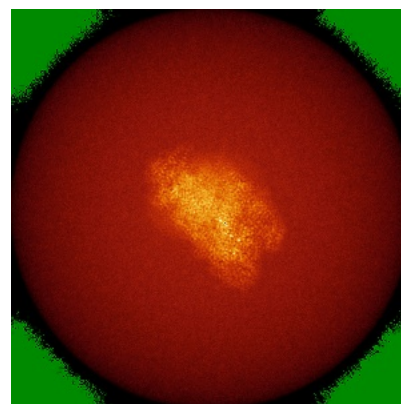
6.4.1 Primary map



X

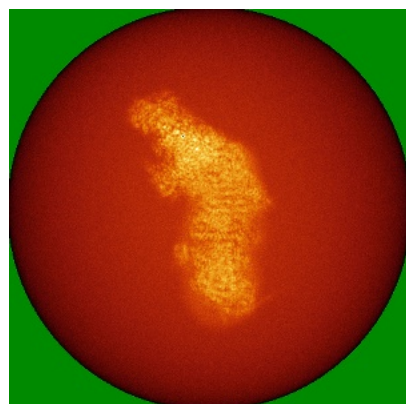


Y

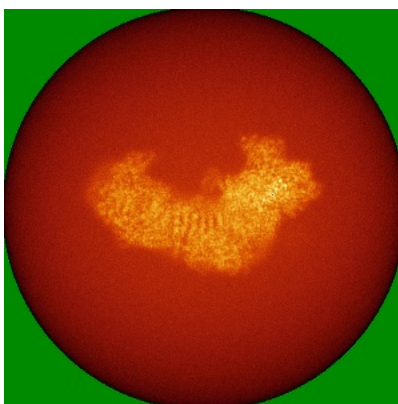


Z

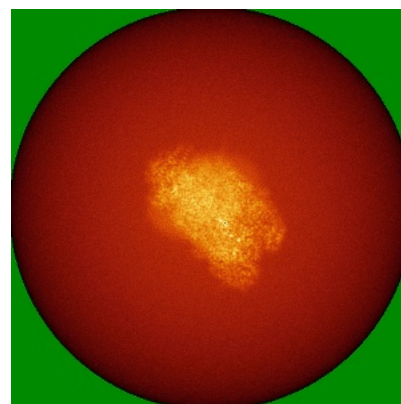
6.4.2 Raw map



X



Y

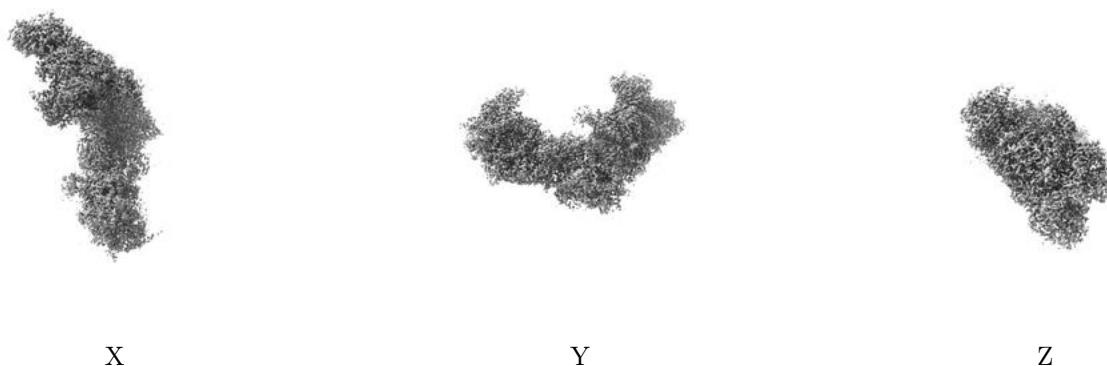


Z

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

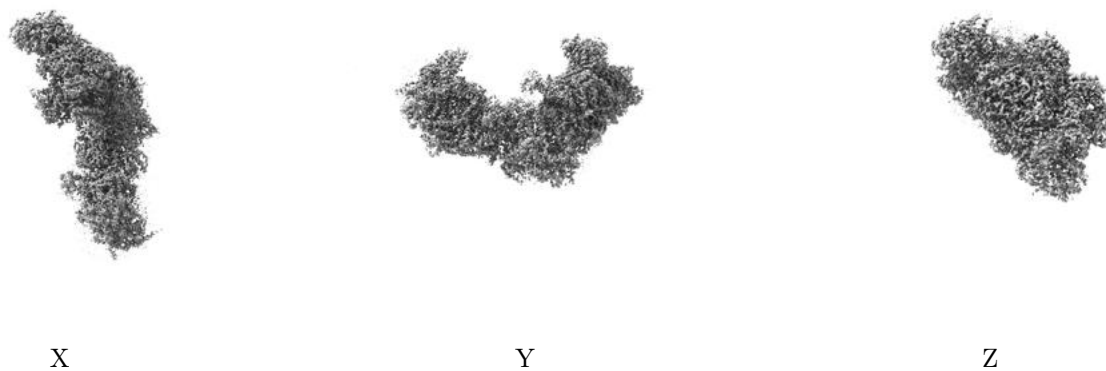
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

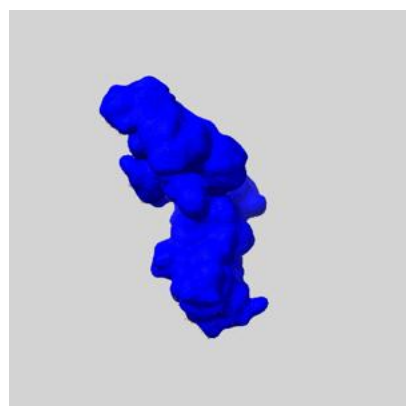
6.6 Mask visualisation [i](#)

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

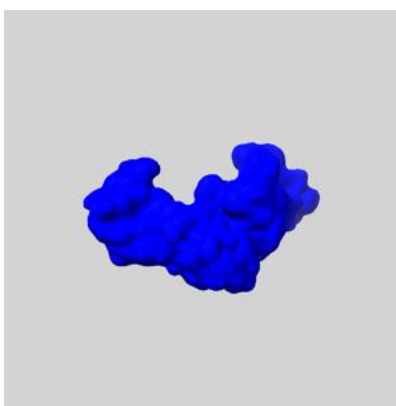
A mask typically either:

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

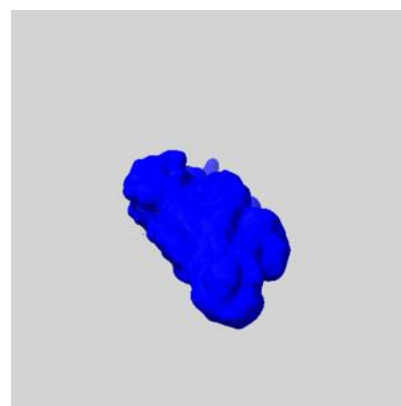
6.6.1 emd_11969_msk_1.map [i](#)



X



Y

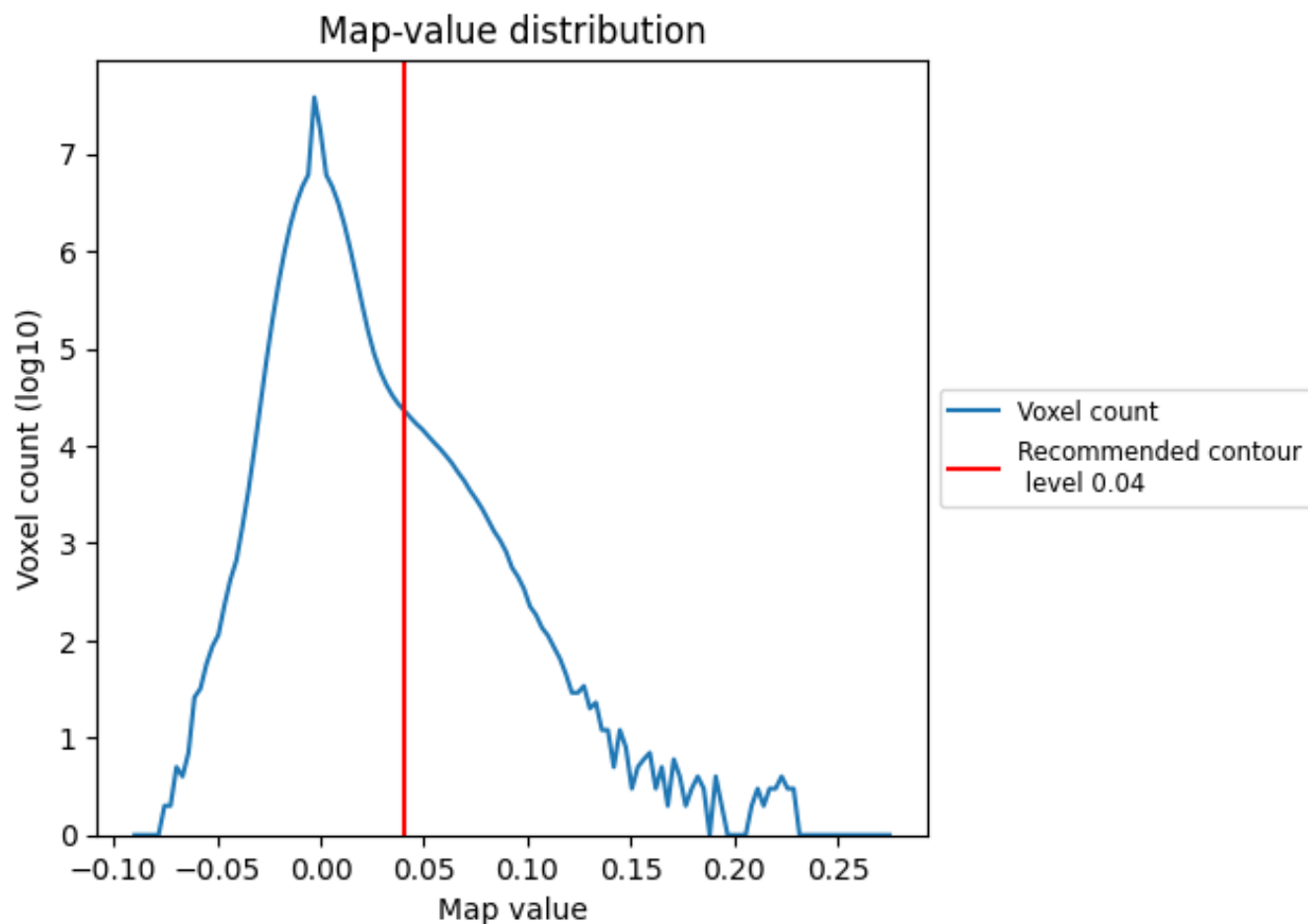


Z

7 Map analysis [i](#)

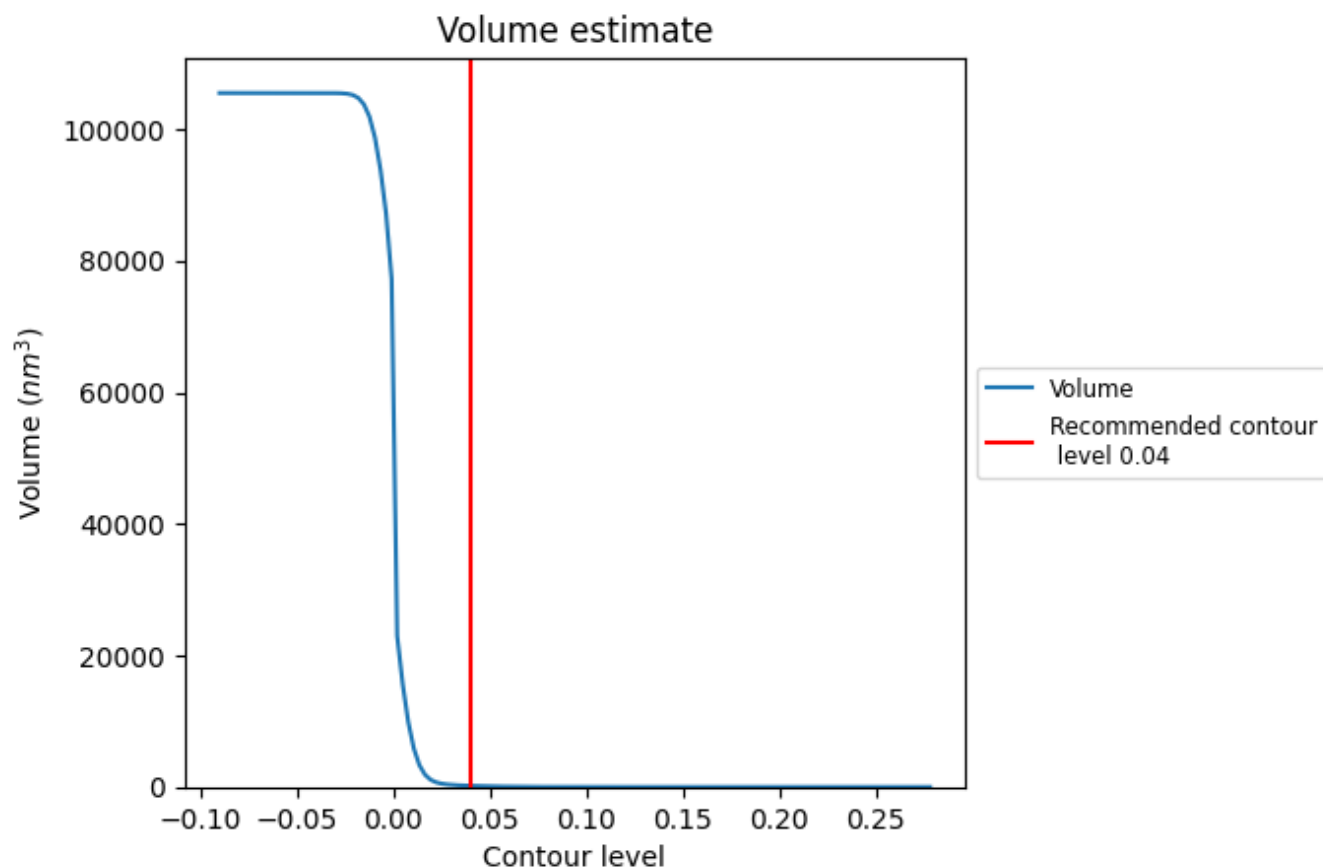
This section contains the results of statistical analysis of the map.

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.

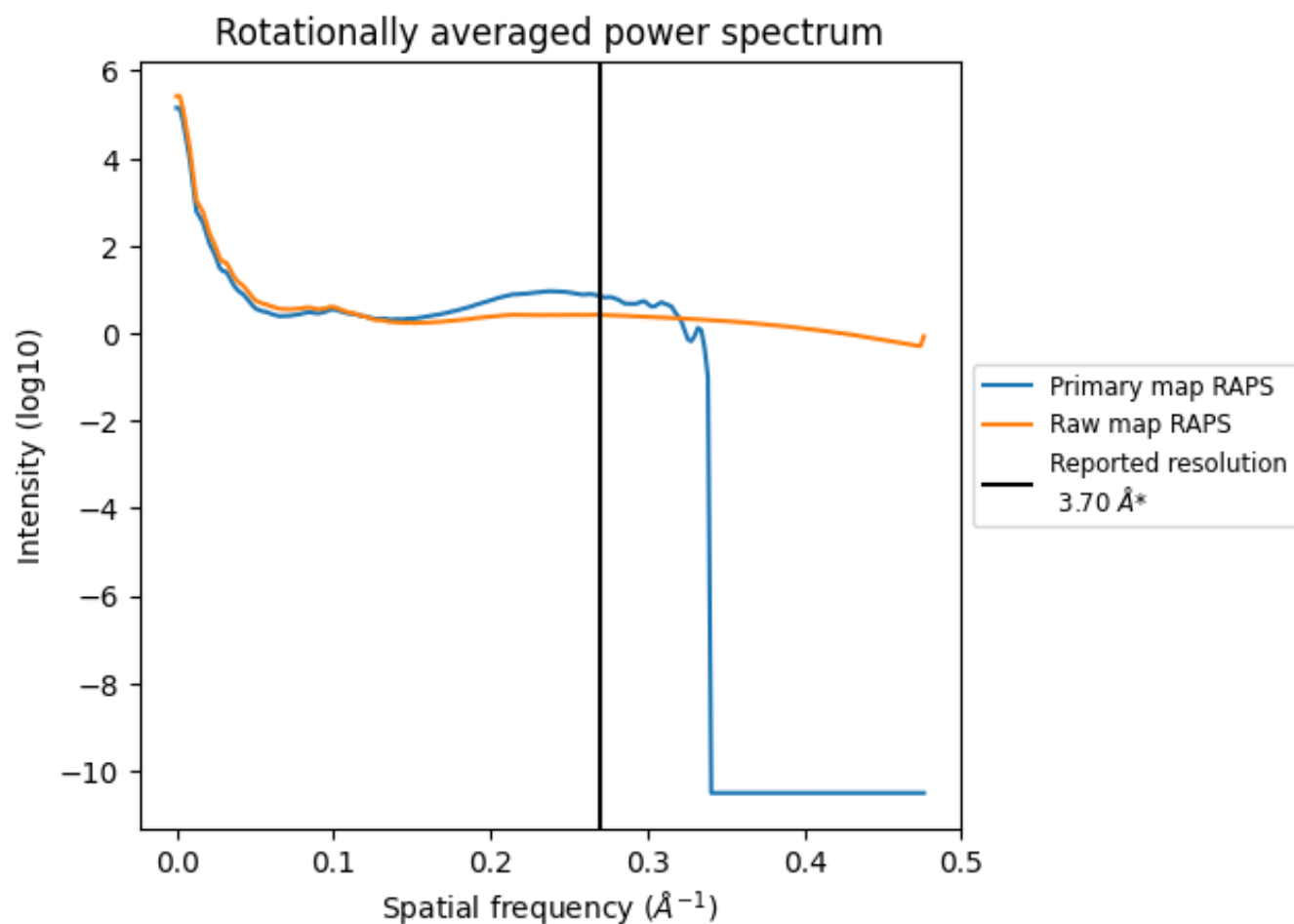
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm³; this corresponds to an approximate mass of 159 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

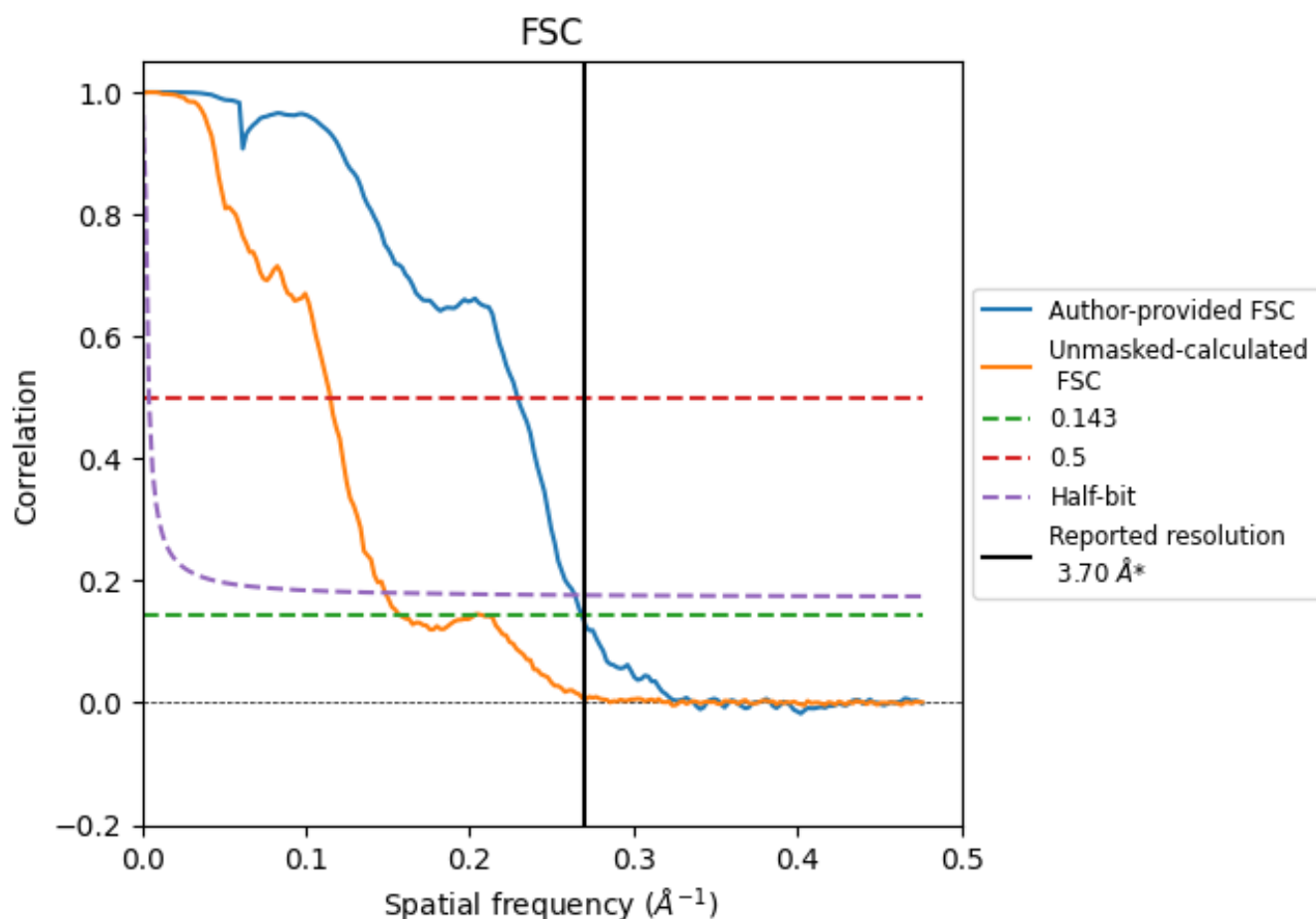


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

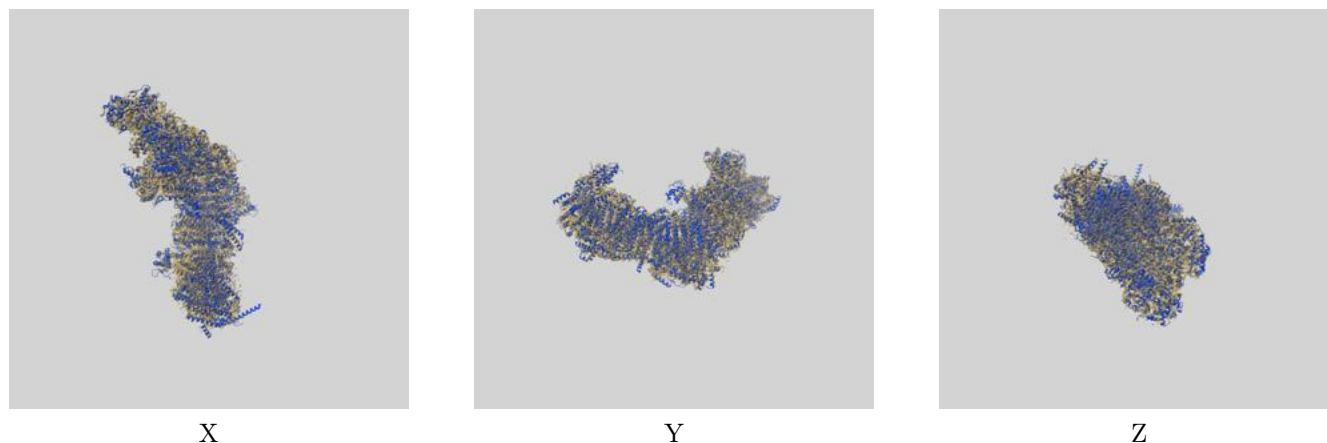
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.36	3.79
Unmasked-calculated*	6.35	8.71	6.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.35 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

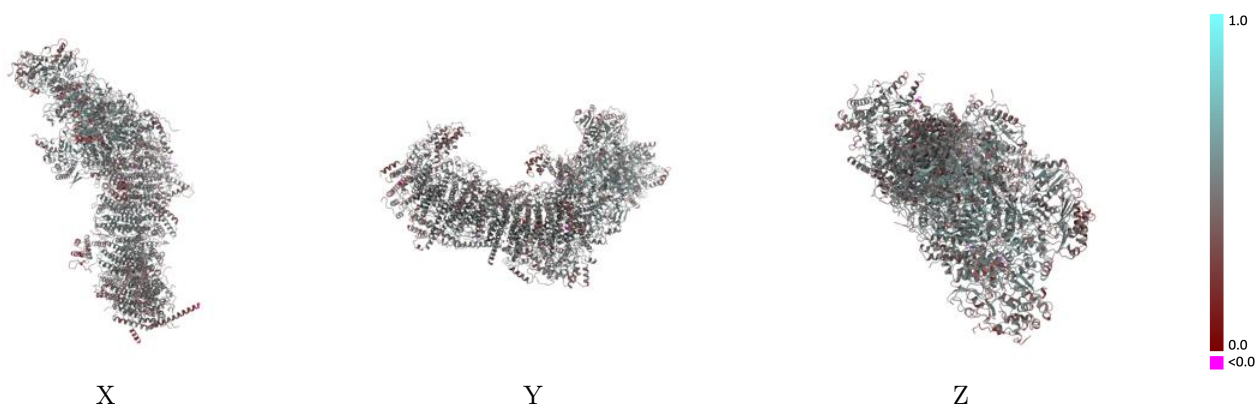
This section contains information regarding the fit between EMDB map EMD-11969 and PDB model 7B0N. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



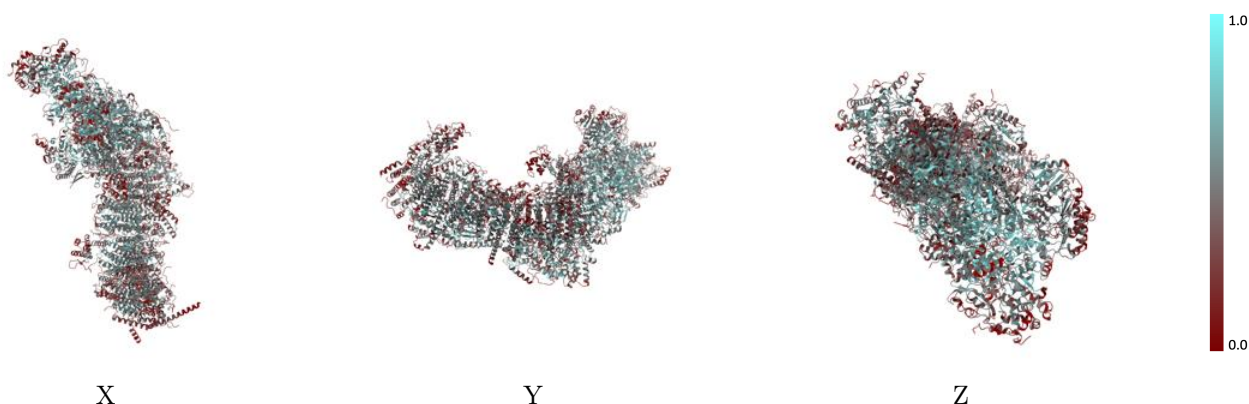
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



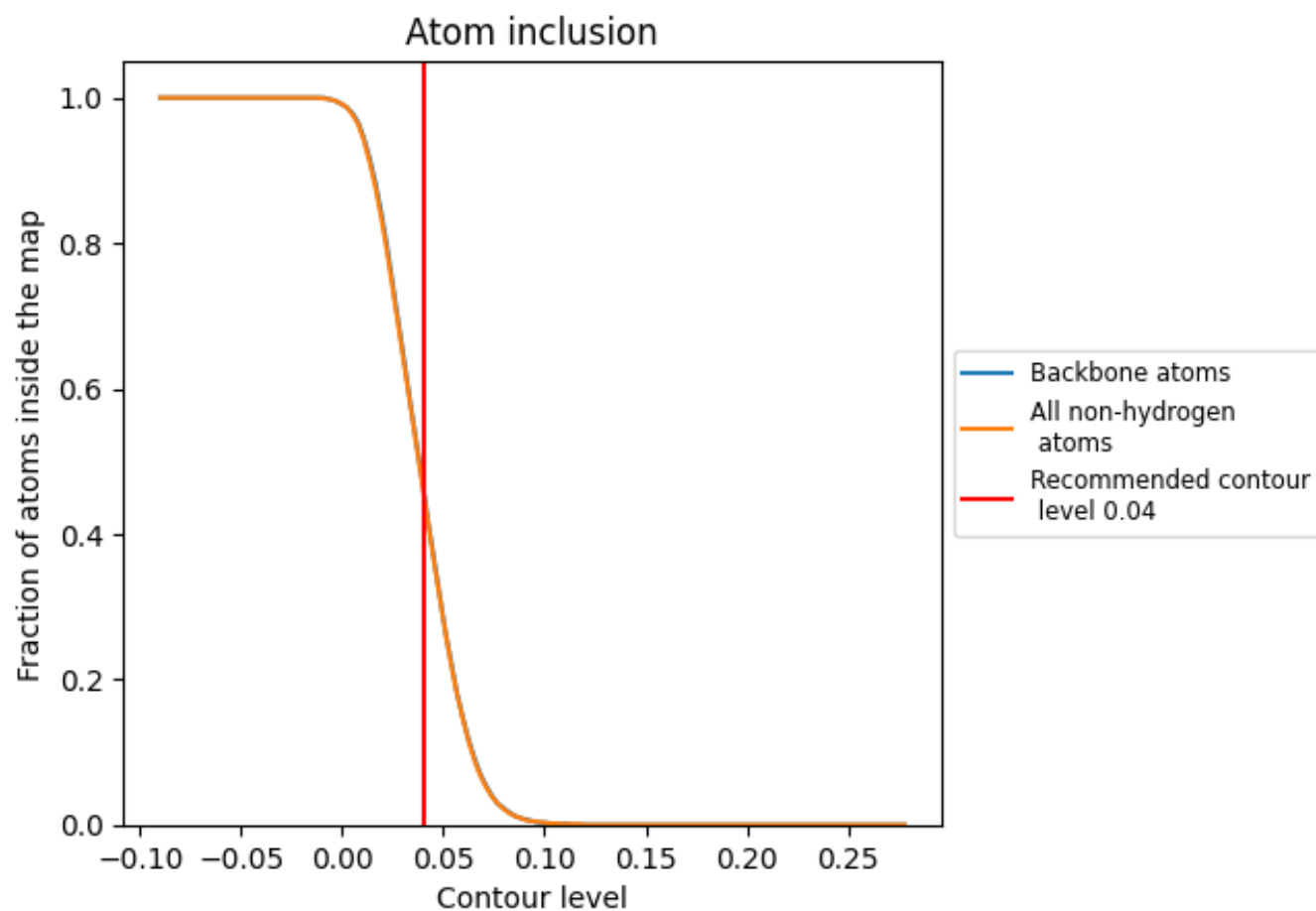
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 46% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4600	 0.4670
A	 0.3680	 0.4450
B	 0.5880	 0.5110
C	 0.5970	 0.5190
D	 0.5490	 0.4970
E	 0.4060	 0.4400
F	 0.4410	 0.4530
G	 0.5200	 0.4860
H	 0.4430	 0.4580
I	 0.6290	 0.5180
J	 0.3720	 0.4470
K	 0.4600	 0.4680
L	 0.4680	 0.4730
M	 0.5430	 0.4950
N	 0.5780	 0.5130
O	 0.4170	 0.4500
P	 0.4430	 0.4580
Q	 0.5520	 0.5010
R	 0.5480	 0.5010
S	 0.3110	 0.3990
T	 0.0880	 0.3100
U	 0.1940	 0.3840
V	 0.4310	 0.4720
W	 0.4530	 0.4540
X	 0.4270	 0.4400
Y	 0.3190	 0.4390
Z	 0.4450	 0.4680
a	 0.4270	 0.4650
b	 0.3600	 0.4570
c	 0.4790	 0.4840
d	 0.4180	 0.4600
e	 0.4570	 0.4530
f	 0.5470	 0.4960
g	 0.2850	 0.3810
h	 0.4510	 0.4660



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Chain	Atom inclusion	Q-score
i	 0.3770	 0.4280
j	 0.2400	 0.3850
k	 0.2810	 0.3820
l	 0.3390	 0.4380
m	 0.3860	 0.4420
n	 0.3780	 0.4180
o	 0.2760	 0.3770
p	 0.5310	 0.4730