



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:48 PM UTC

PDB ID : 6ZTQ / pdb_00006ztq
EMDB ID : EMD-11424
Title : Cryo-EM structure of respiratory complex I from *Mus musculus* inhibited by piericidin A at 3.0 Å
Authors : Bridges, H.R.; Blaza, J.N.; Agip, A.N.A.; Hirst, J.
Deposited on : 2020-07-20
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

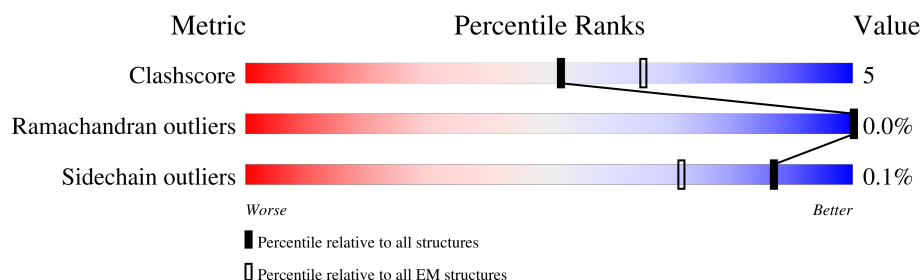
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	115	84% 81%19%
2	B	224	59% 58%12%30%
3	C	263	72% 67%11%21%
4	D	463	80% 79%14%7%
5	E	248	76% 69%17%15%
6	F	464	84% 76%16%8%
7	G	727	83% 82%13%5%
8	H	318	81% 78%22%

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Mol	Chain	Length	Quality of chain
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	151	

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Mol	Chain	Length	Quality of chain
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 67072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			933	633	133	160	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	796	223	214	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3464	2215	595	630	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1648	1048	277	312	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	428	Total	C	N	O	S	0	0
			3300	2080	589	609	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5296	3321	919	1015	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1300	874	185	226	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2696	1791	416	452	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1015	642	179	190	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	94	Total	C	N	O	S	0	0
			738	458	135	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			611	392	90	124	5		
20	U	86	Total	C	N	O	S	0	0
			692	446	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total	C	N	O	S	0	0
			927	604	154	166	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	68	Total	C	N	O	S	0	0
			556	360	99	93	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	94	Total	C	N	O	S	0	0
			787	515	134	135	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	62	Total	C	N	O	S	0	0
			537	355	88	93	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	75	Total	C	N	O	S	0	0
			609	404	103	100	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	154	Total	C	N	O	S	0	0
			1294	834	215	234	11		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	126	Total	C	N	O		0	0
			1050	676	189	185			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	111	Total	C	N	O	S	0	0
			957	605	176	168	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	169	Total	C	N	O	S	0	0
			1433	901	257	267	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1203	773	213	212	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	100	Total	C	N	O	S	0	0
			802	507	149	143	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

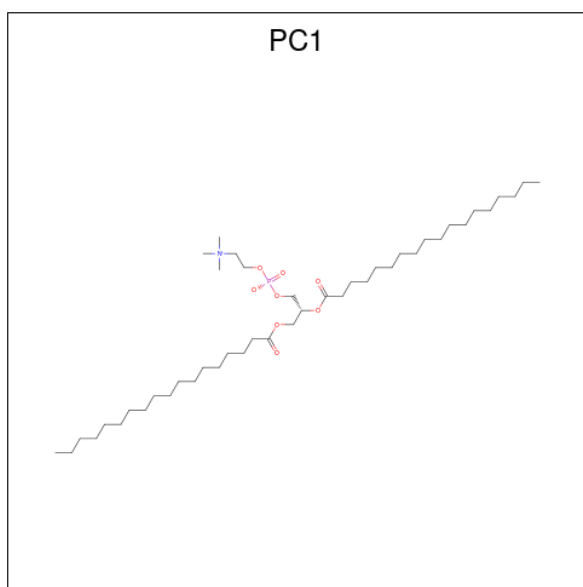
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	41	Total	C	N	O	0	0
			344	215	61	68		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



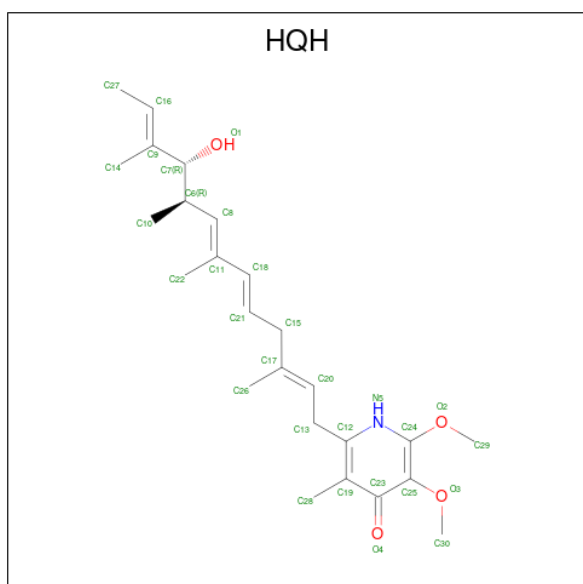
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



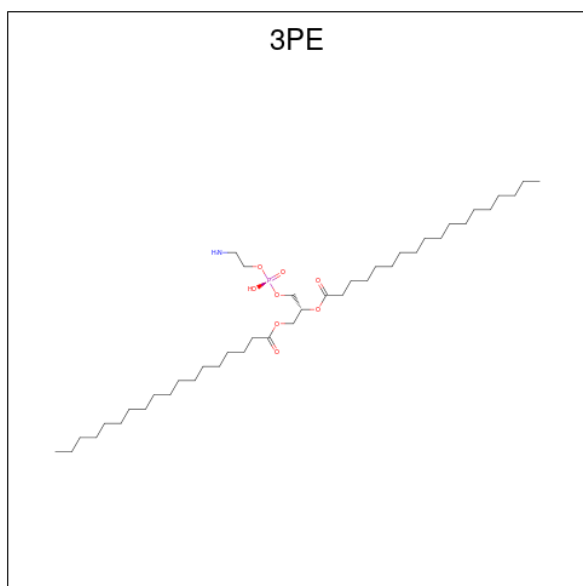
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	J	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	Z	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 47 is Piericidin A (CCD ID: HQH) (formula: $C_{25}H_{37}NO_4$) (labeled as "Ligand of Interest" by depositor).



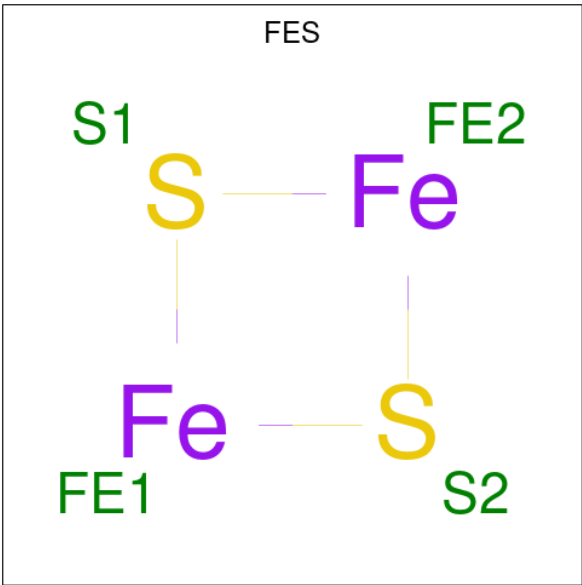
Mol	Chain	Residues	Atoms				AltConf
47	D	1	Total	C	N	O	0
			30	25	1	4	

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



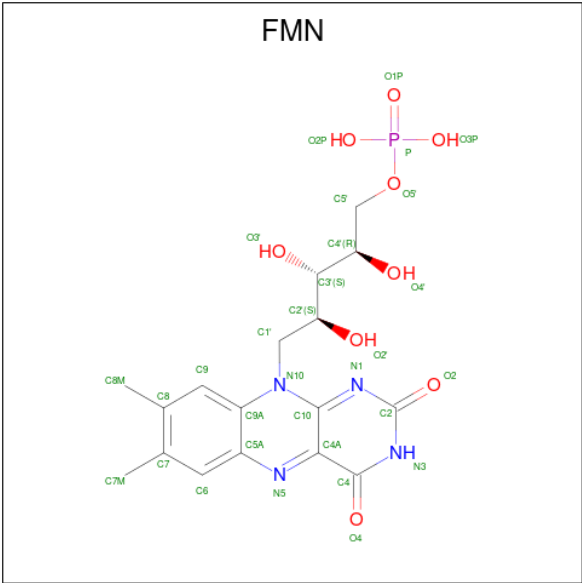
Mol	Chain	Residues	Atoms					AltConf
48	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
48	K	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
48	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	h	1	Total	C	N	O	P	0
			37	27	1	8	1	
48	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	l	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



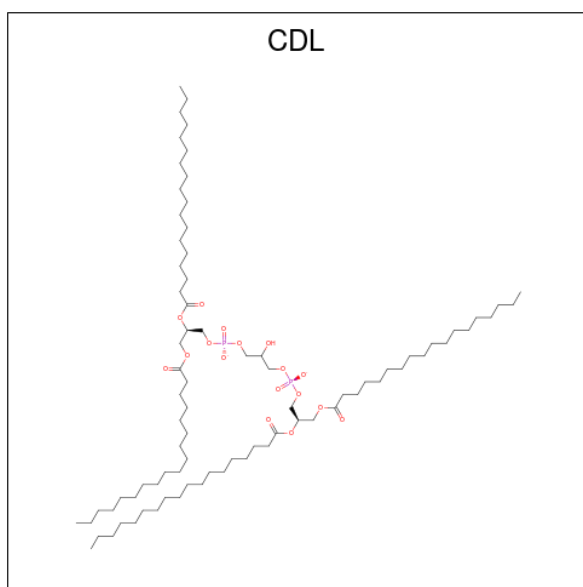
Mol	Chain	Residues	Atoms			AltConf
49	E	1	Total	Fe	S	0
			4	2	2	
49	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



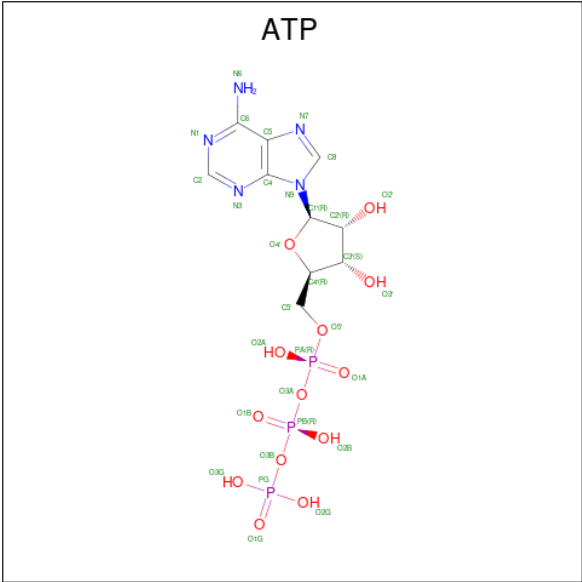
Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



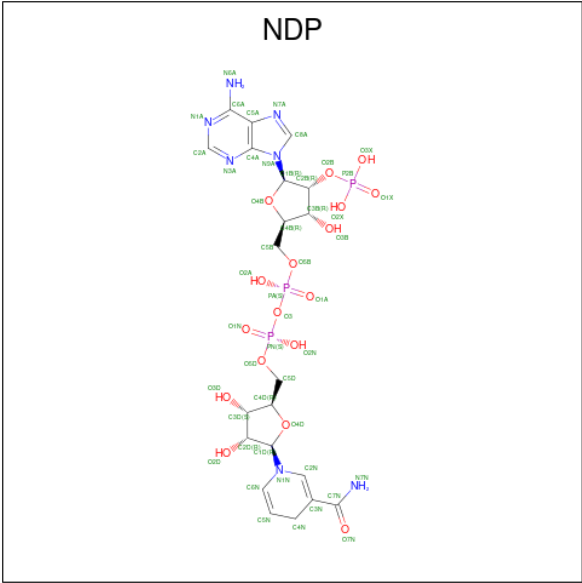
Mol	Chain	Residues	Atoms				AltConf
51	L	1	Total	C	O	P	0
			74	55	17	2	
51	N	1	Total	C	O	P	0
			59	41	16	2	
51	N	1	Total	C	O	P	0
			65	46	17	2	
51	d	1	Total	C	O	P	0
			67	48	17	2	
51	d	1	Total	C	O	P	0
			63	44	17	2	
51	h	1	Total	C	O	P	0
			70	51	17	2	
51	q	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 52 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
52	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

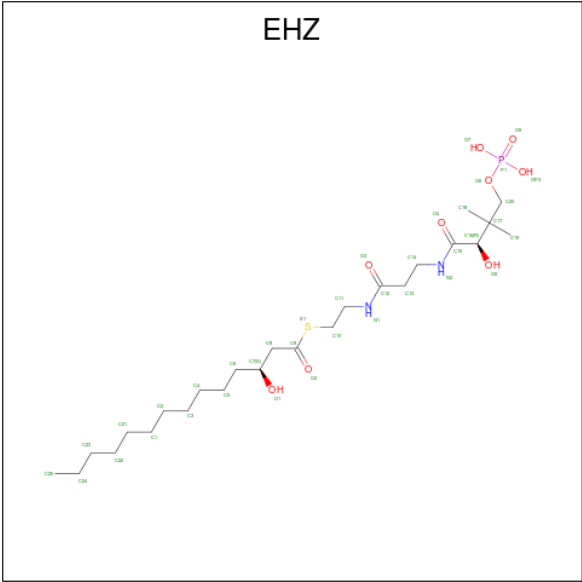


Mol	Chain	Residues	Atoms					AltConf
53	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

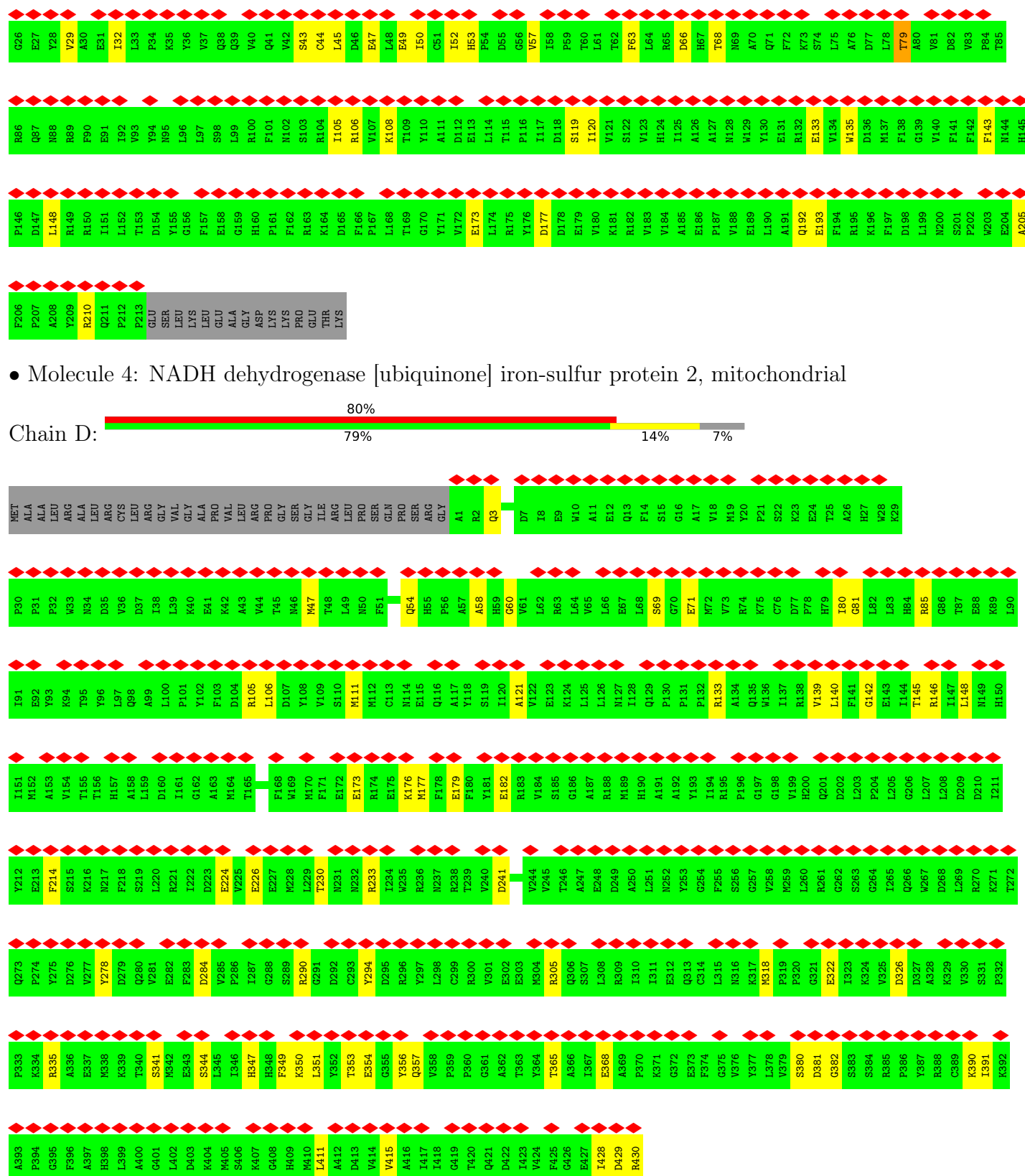
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

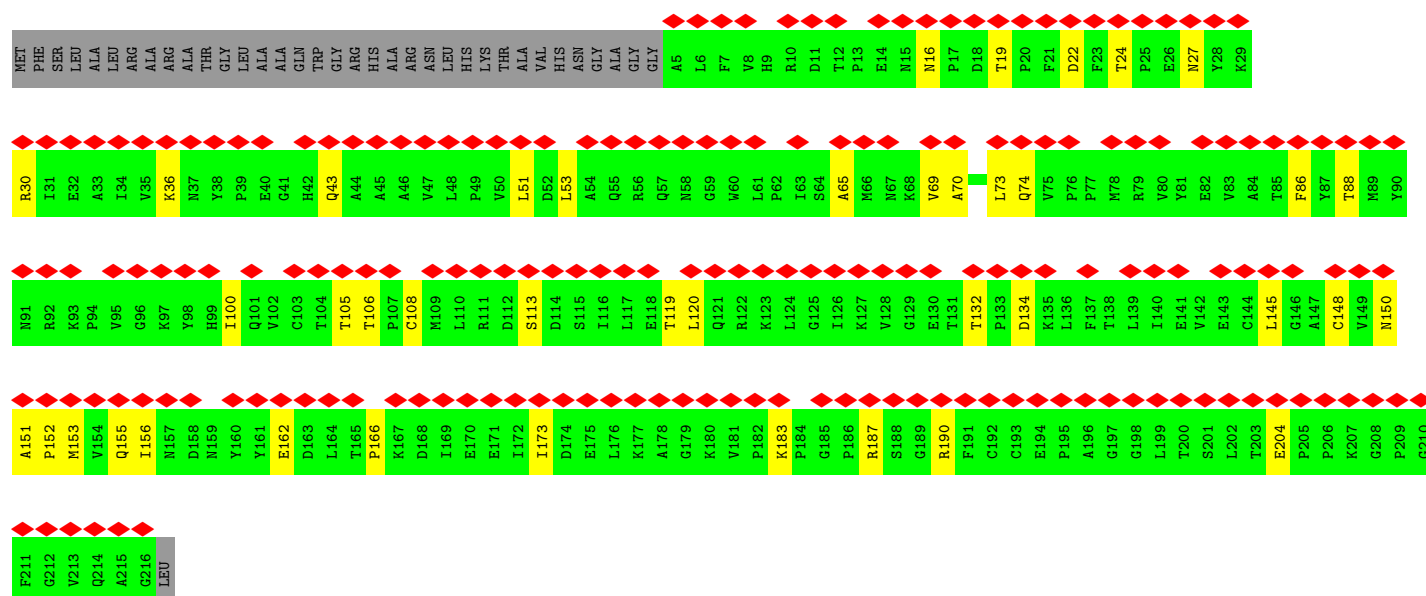
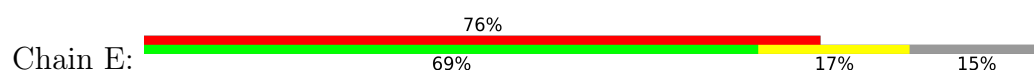
Mol	Chain	Residues	Atoms		AltConf
54	R	1	Total	Zn	0
			1	1	

- Molecule 55 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

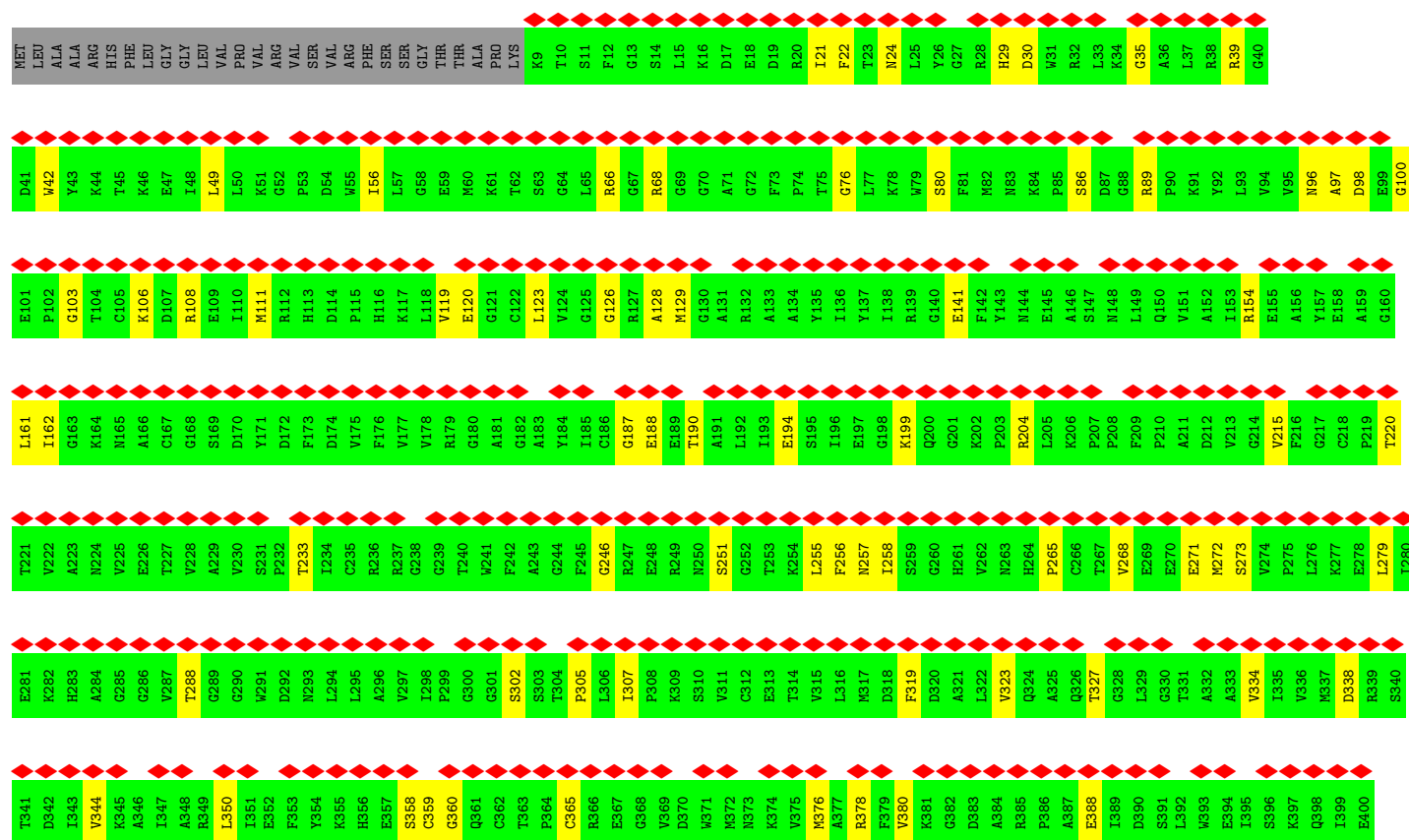
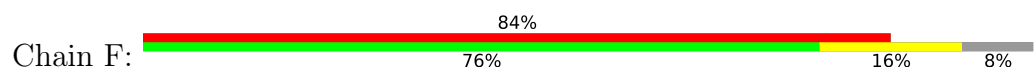


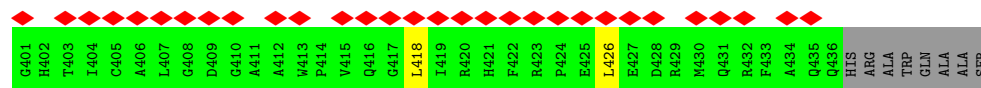
Mol	Chain	Residues	Atoms						AltConf
55	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
55	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	



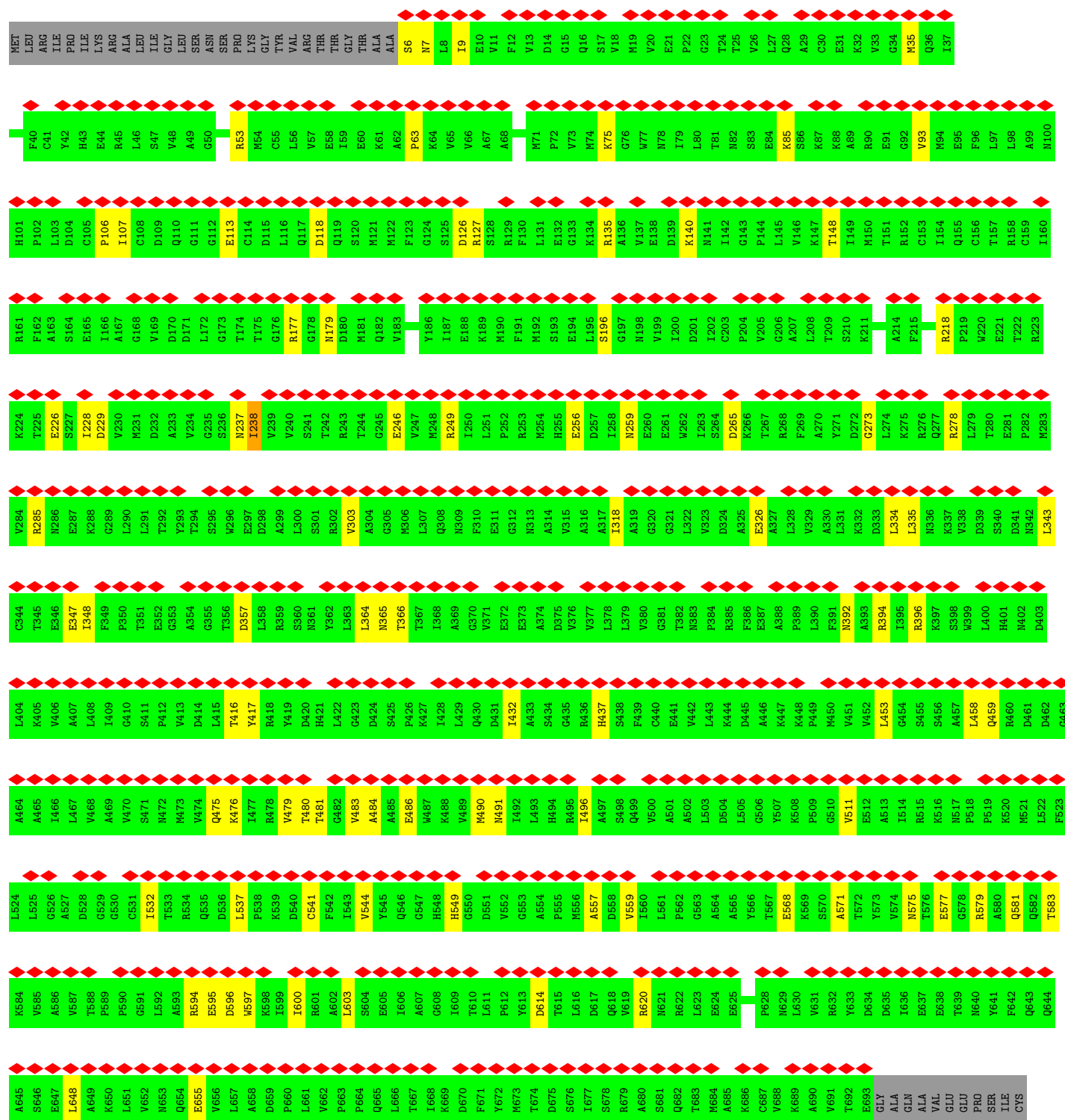
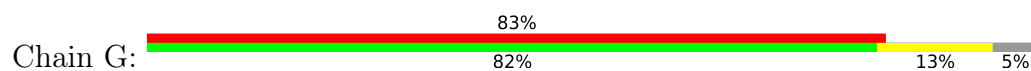


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

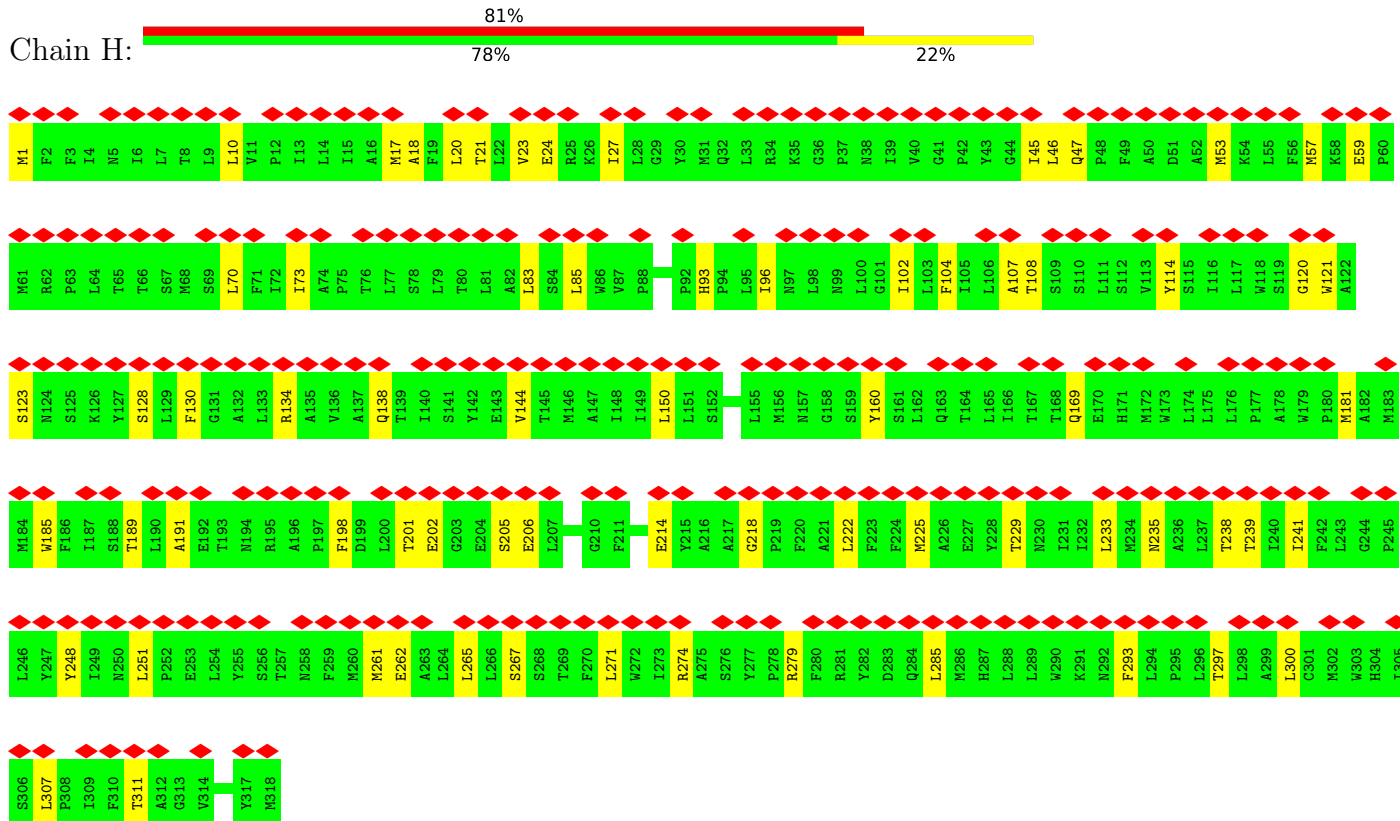




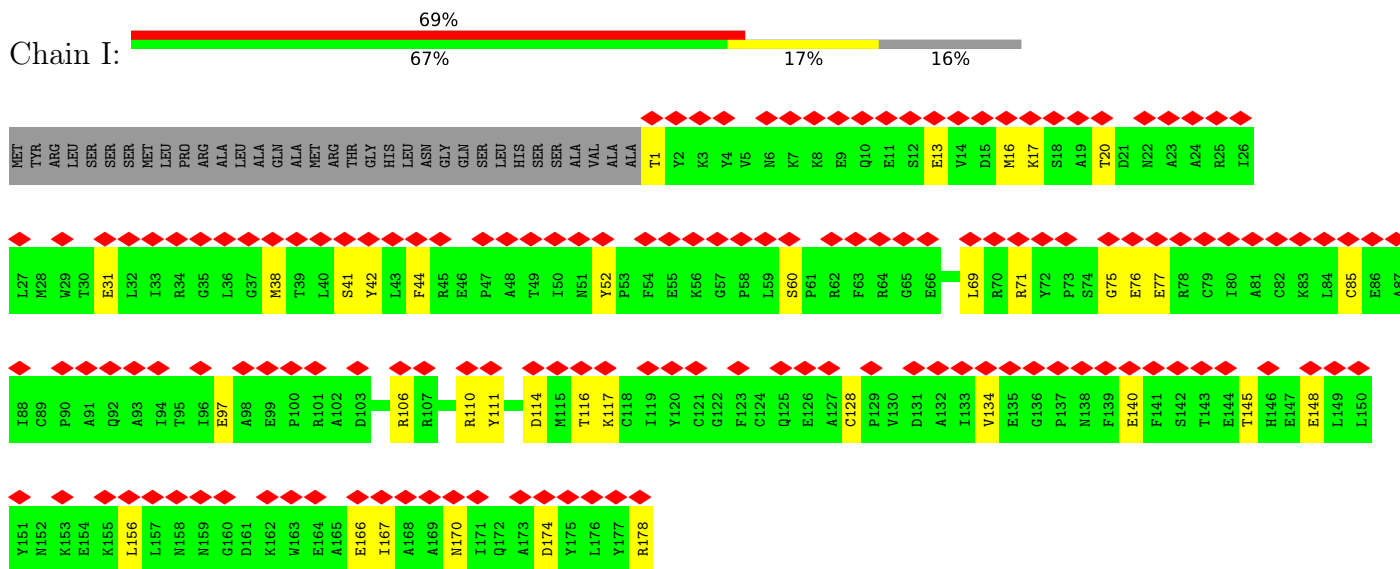
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



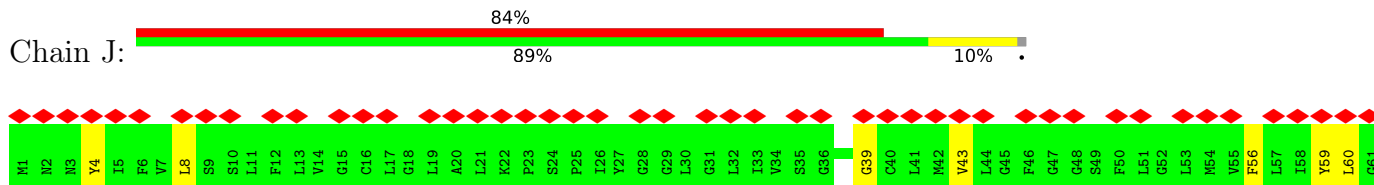
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

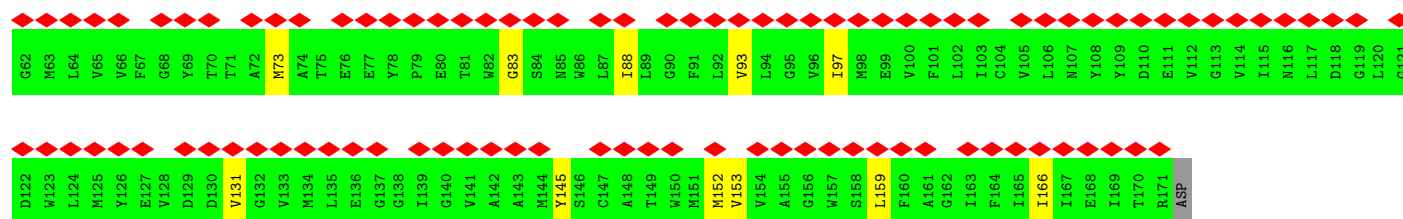


- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

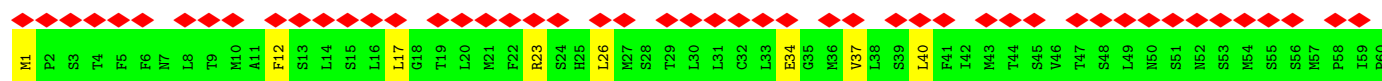
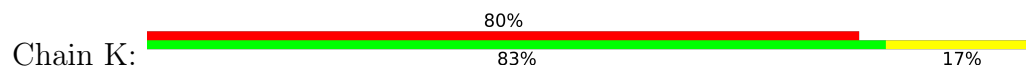


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

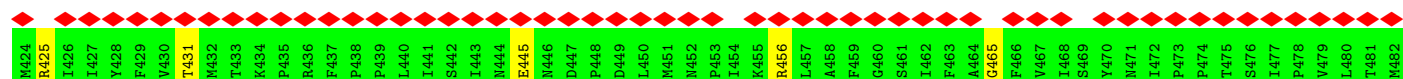
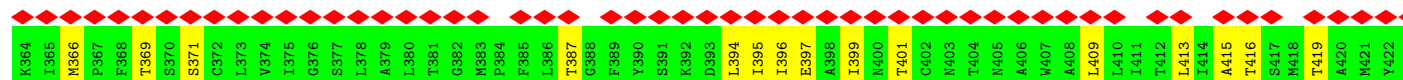
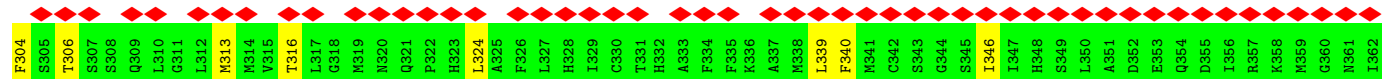
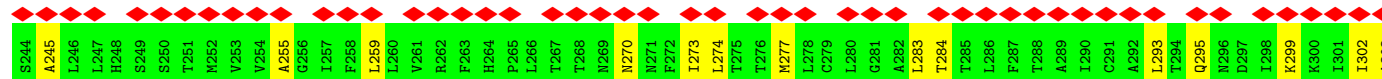
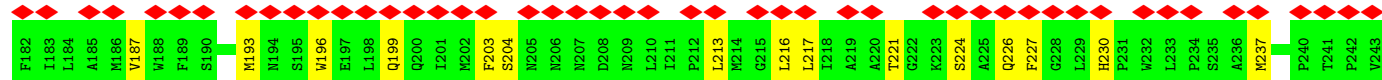
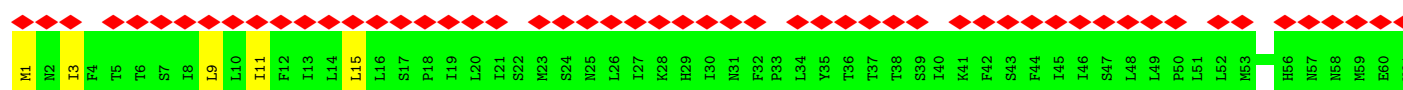
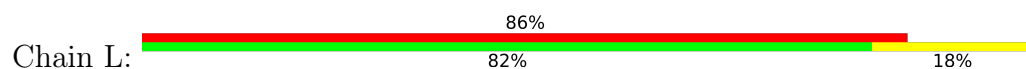


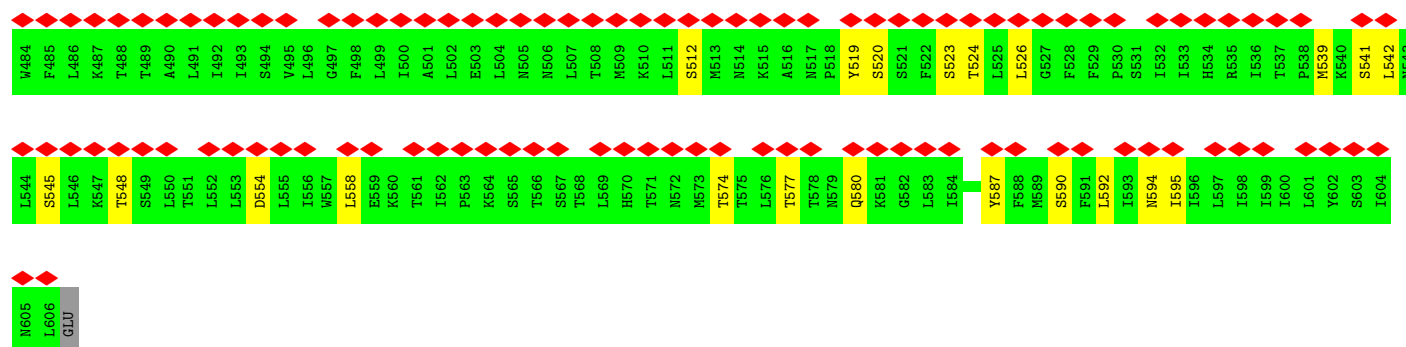


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

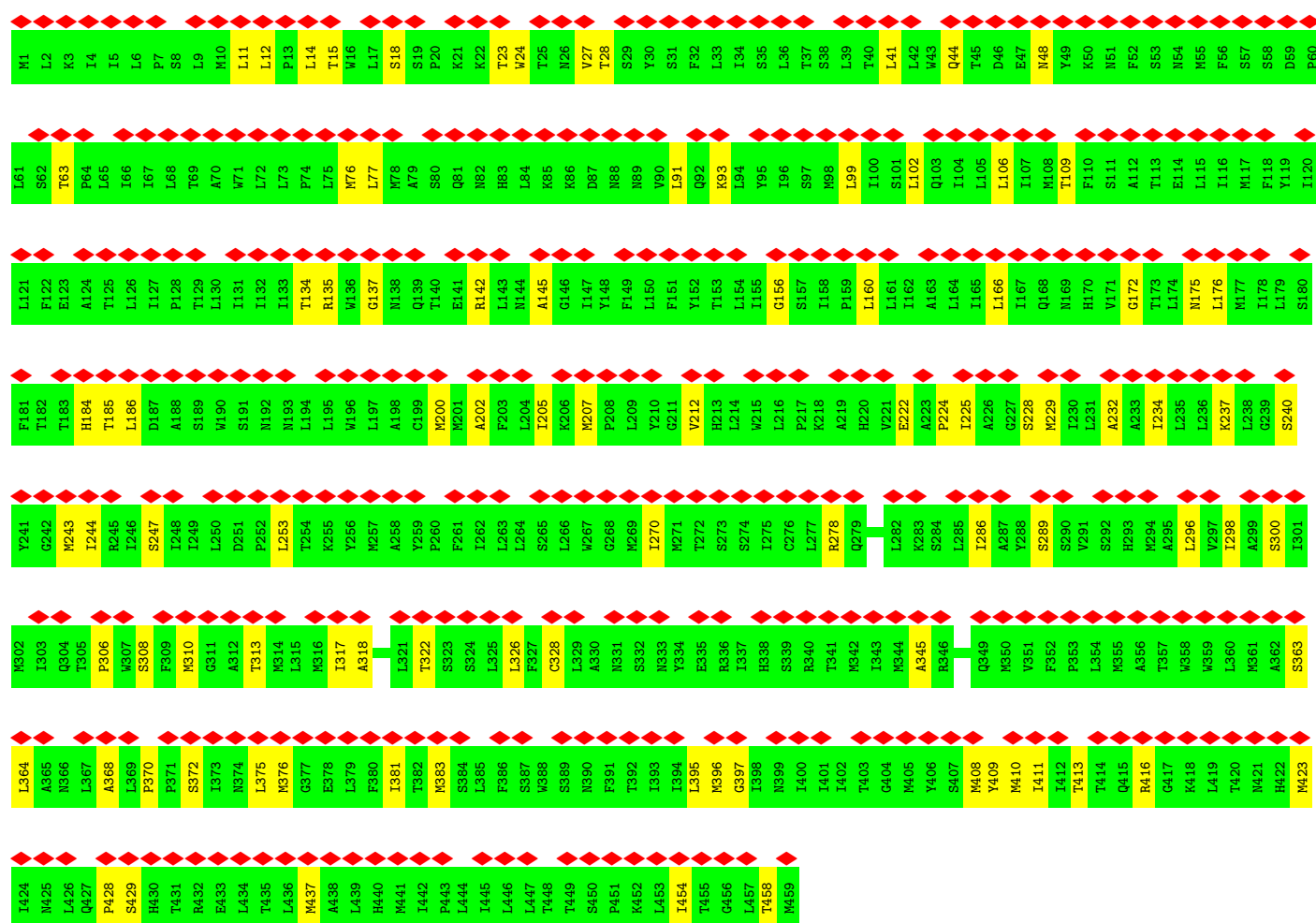
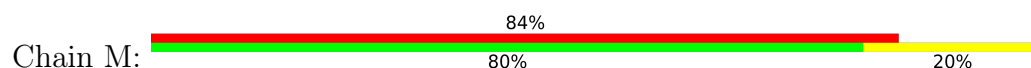


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

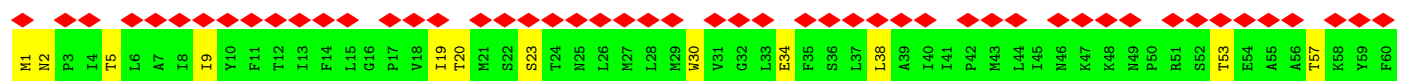
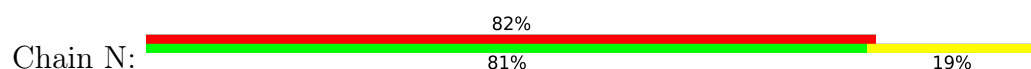


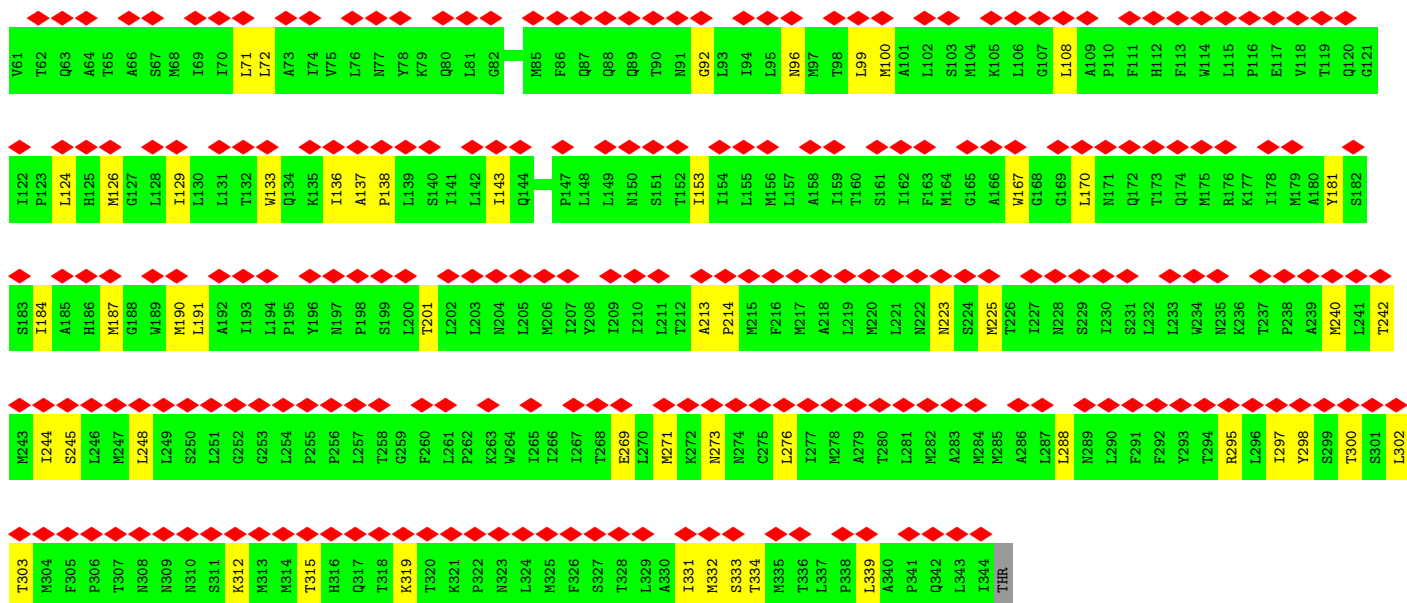


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

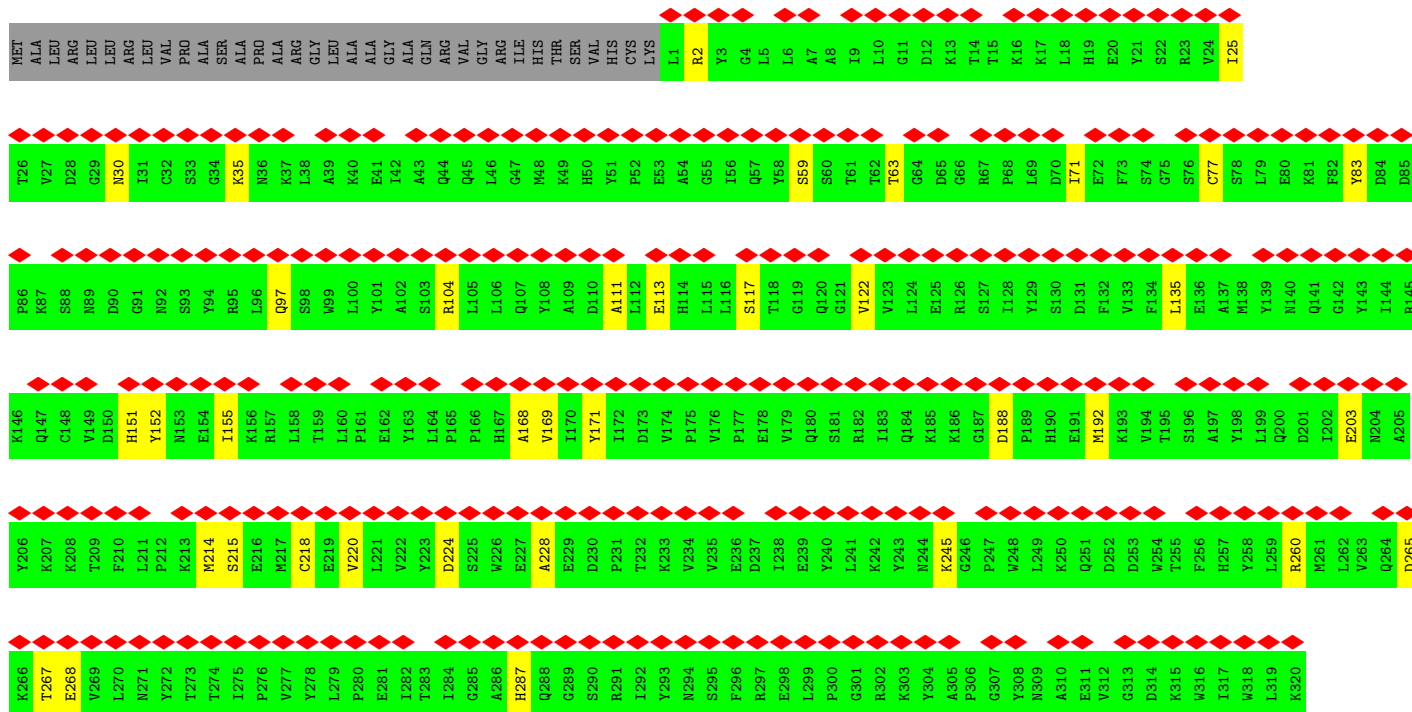
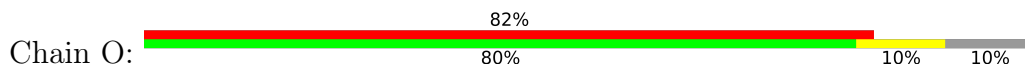


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

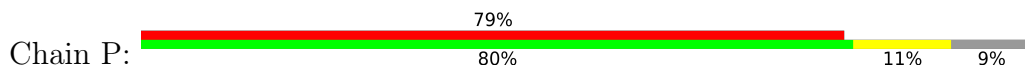


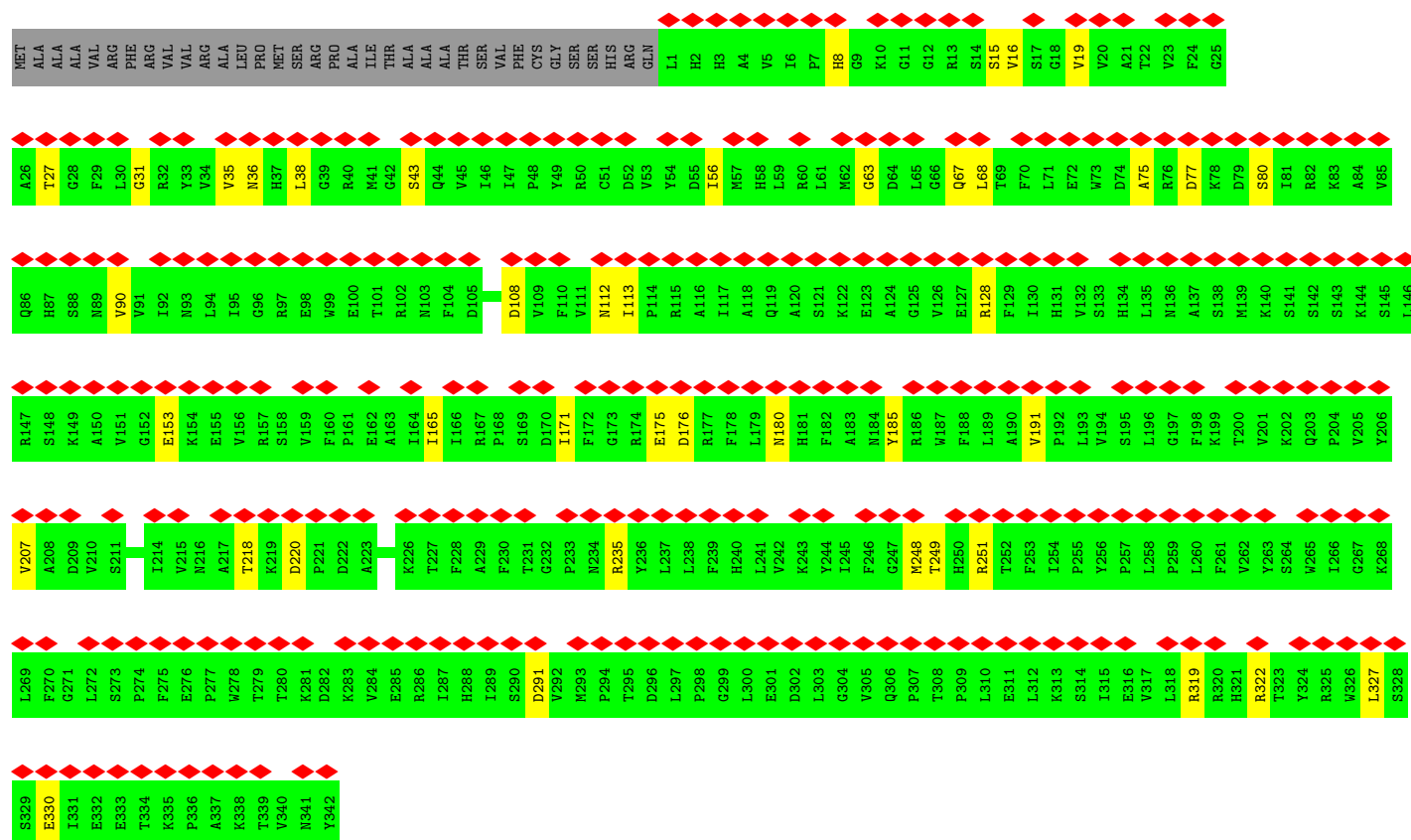


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

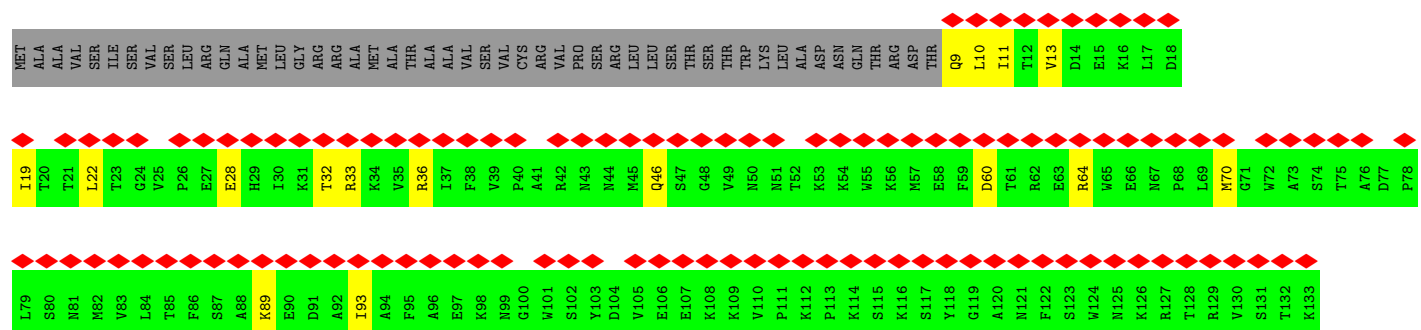


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

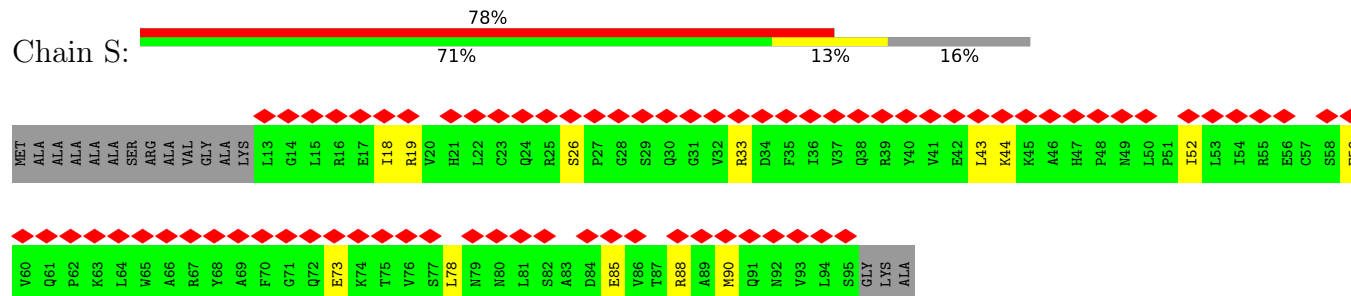




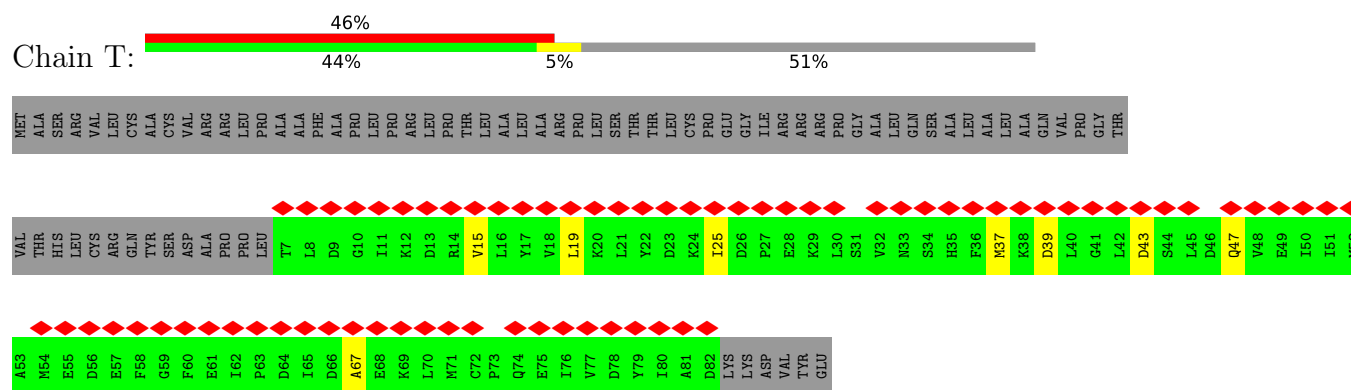
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



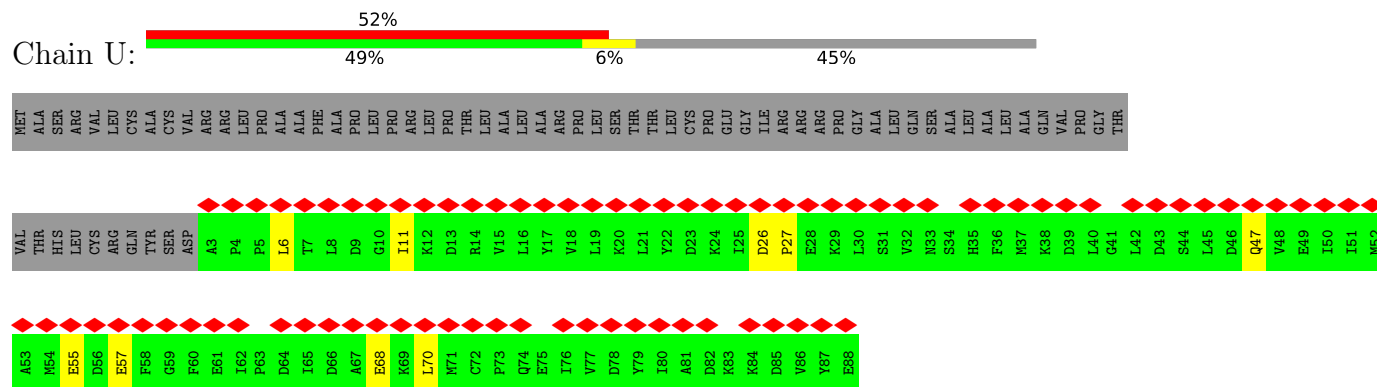
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 20: Acyl carrier protein, mitochondrial



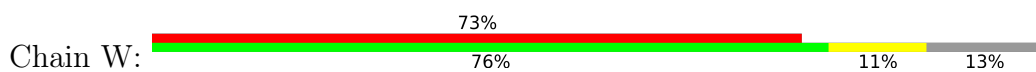
- Molecule 20: Acyl carrier protein, mitochondrial



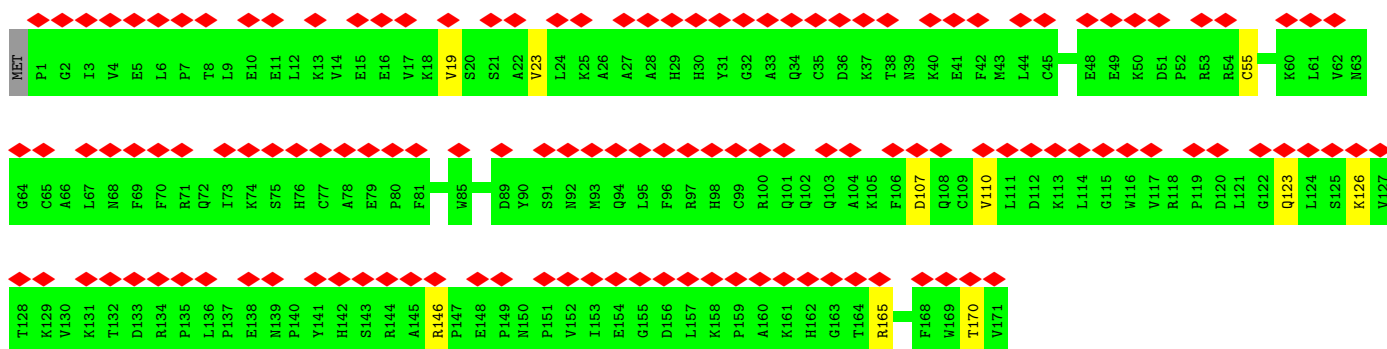
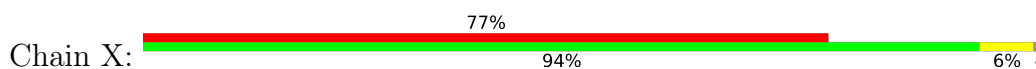
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



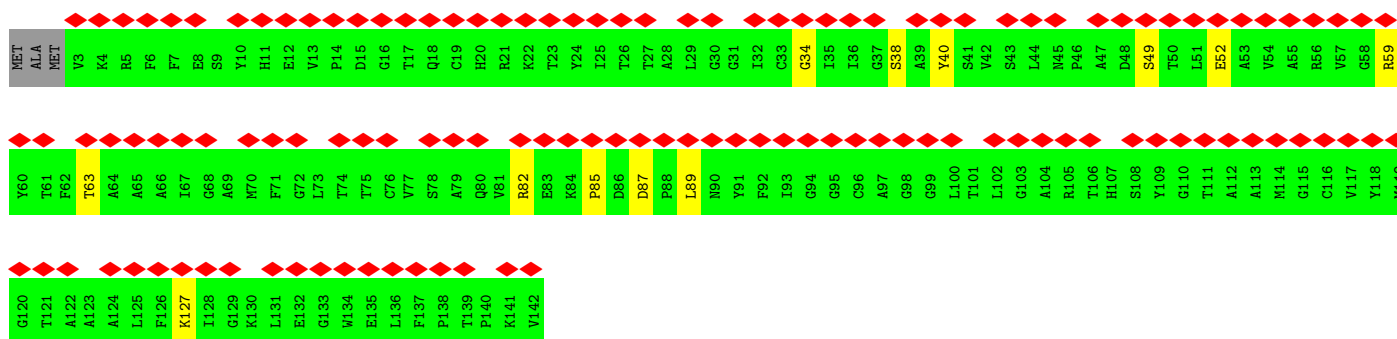
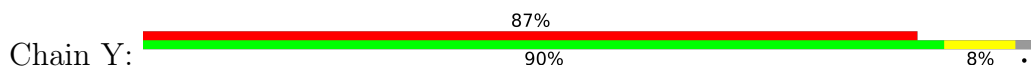
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



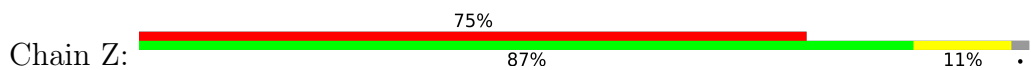
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

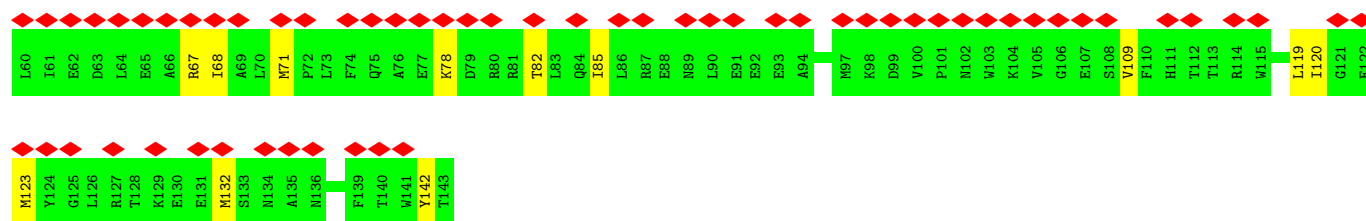


• Molecule 24: MCG5603

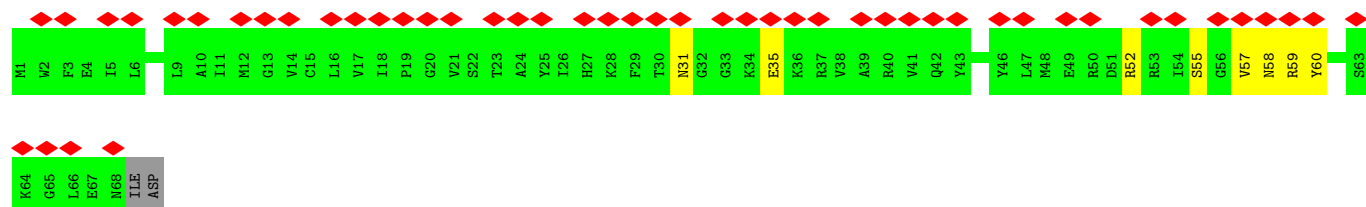
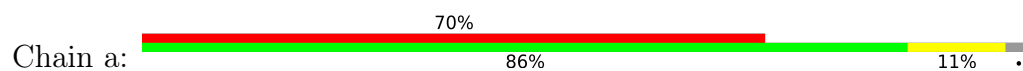


• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

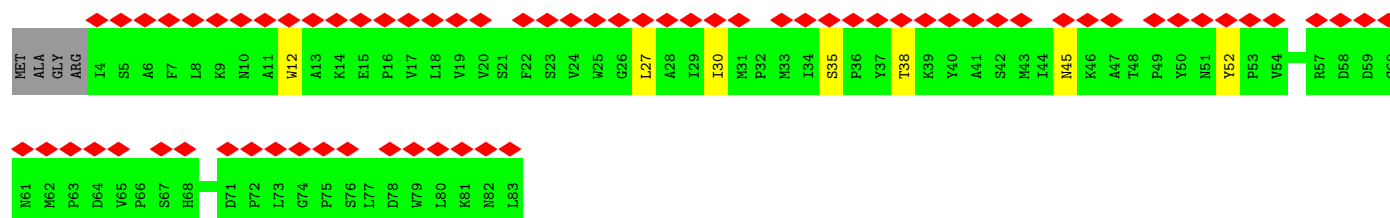
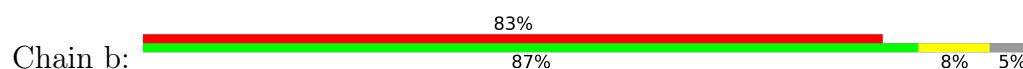




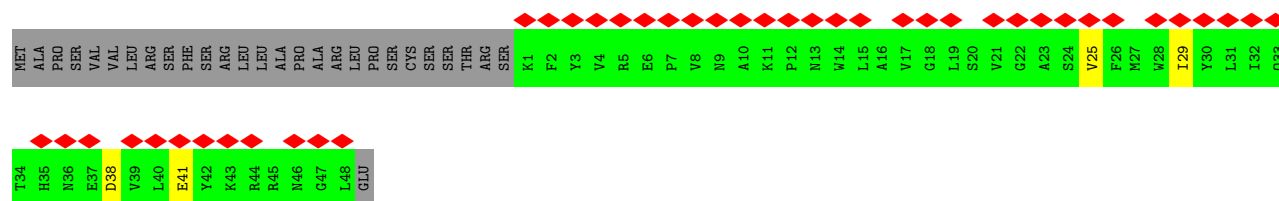
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



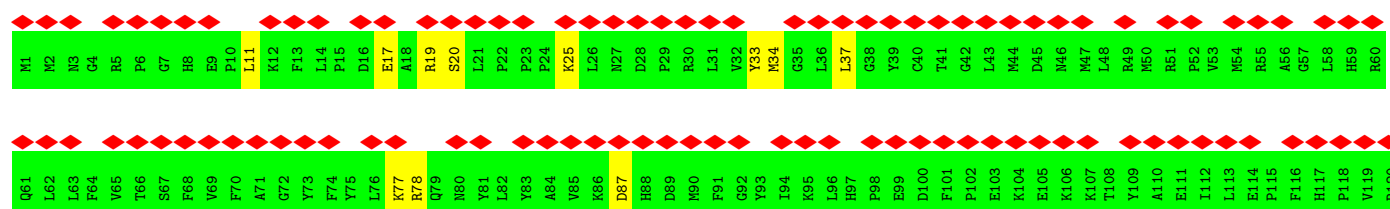
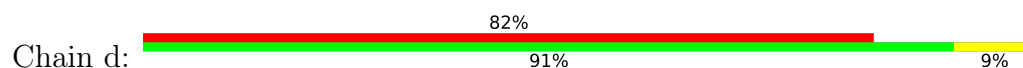
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

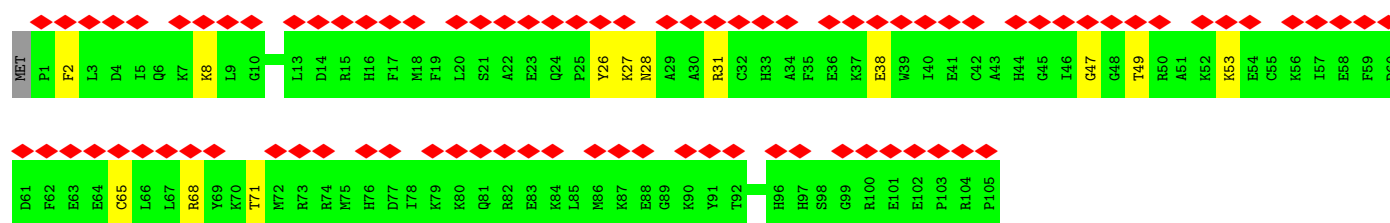


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



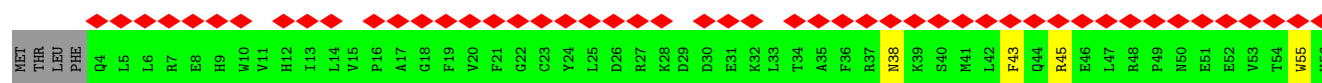
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 



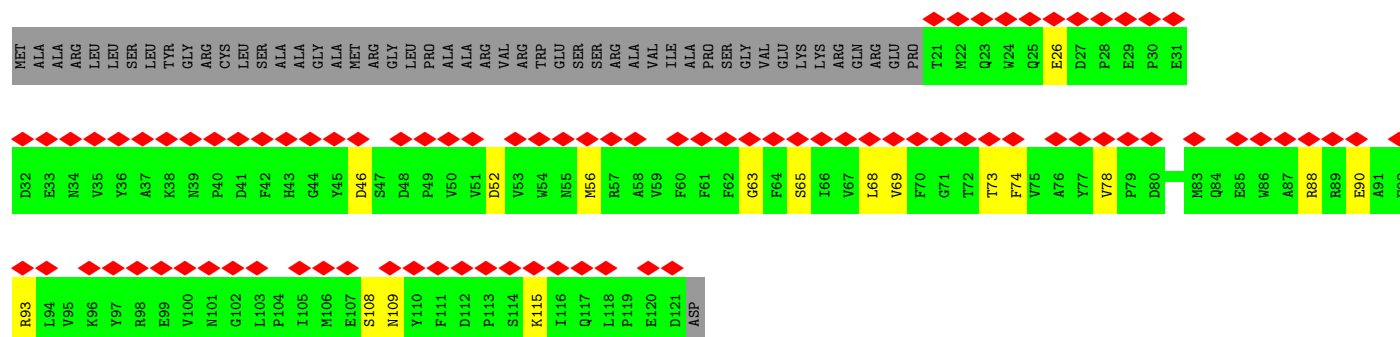
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 



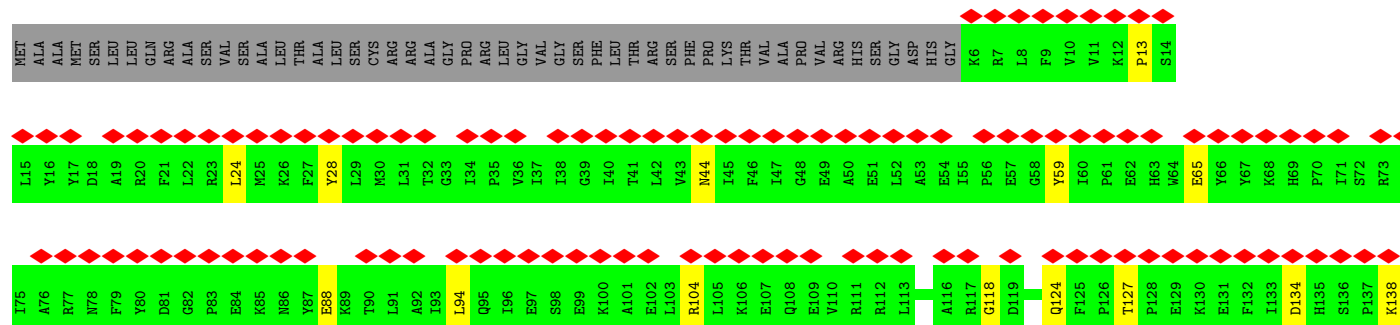
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

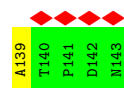
Chain g: 



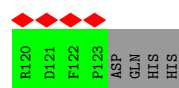
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 

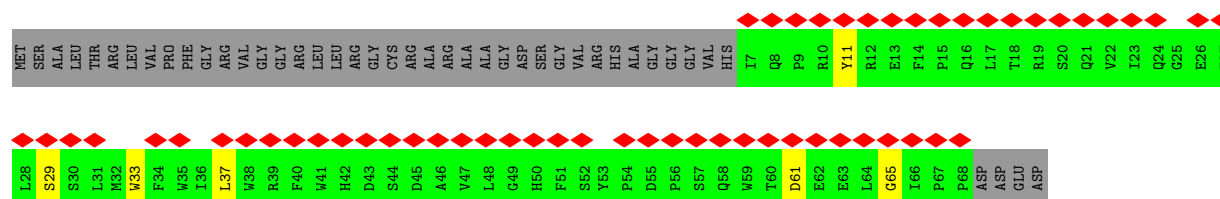




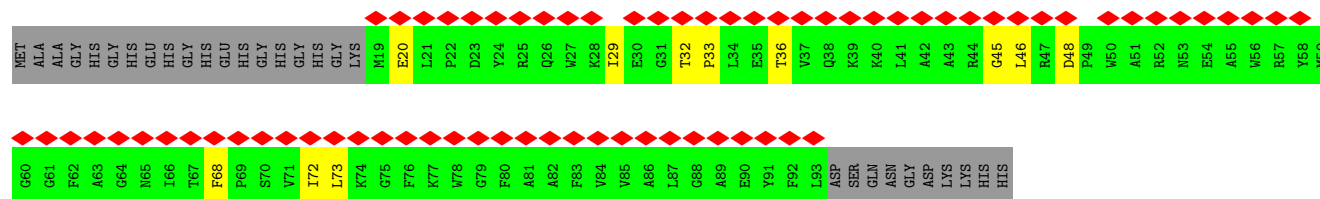
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

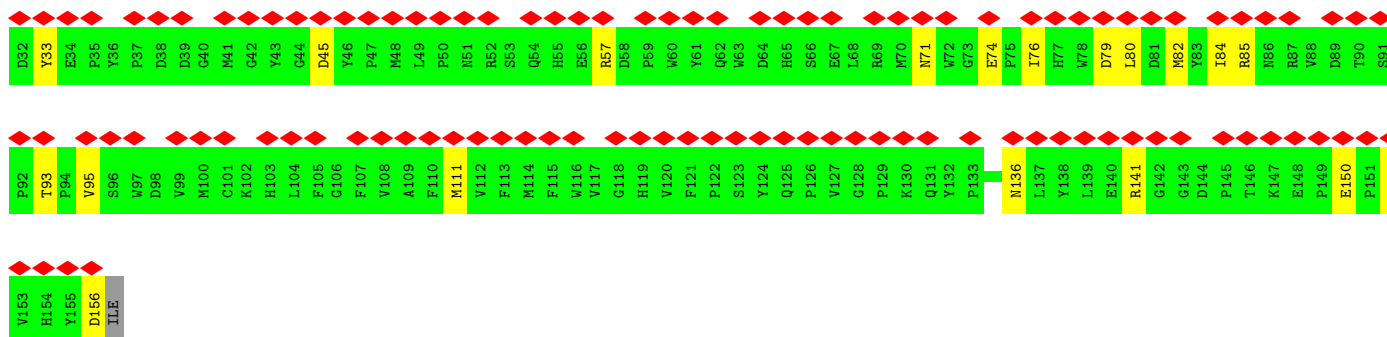


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

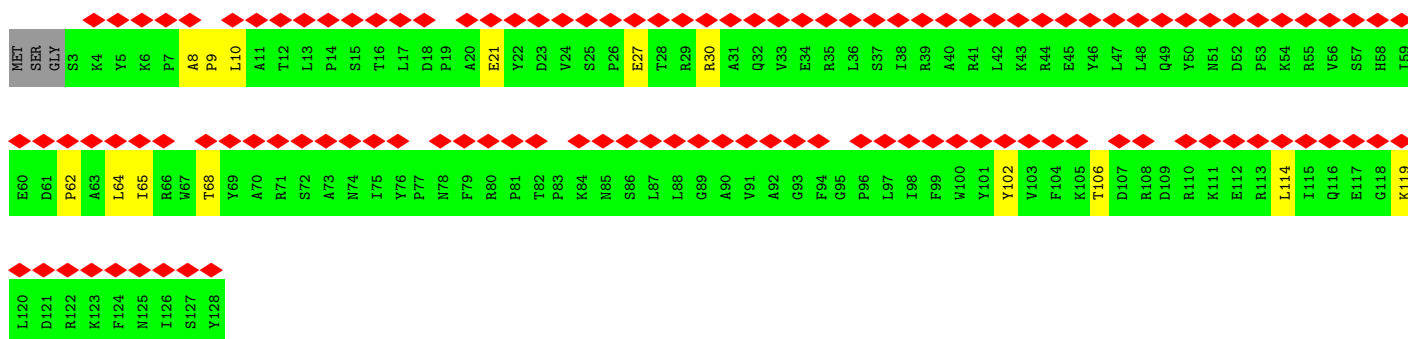
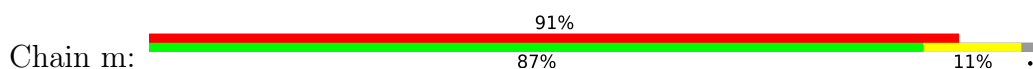


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

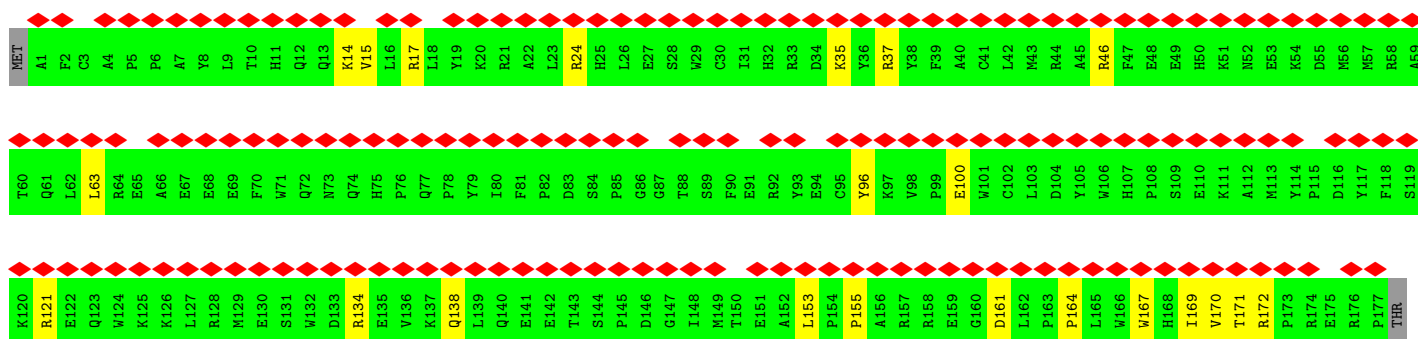
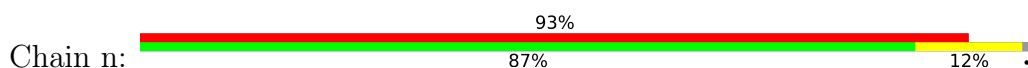




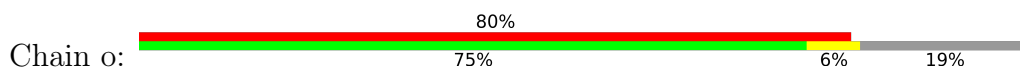
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

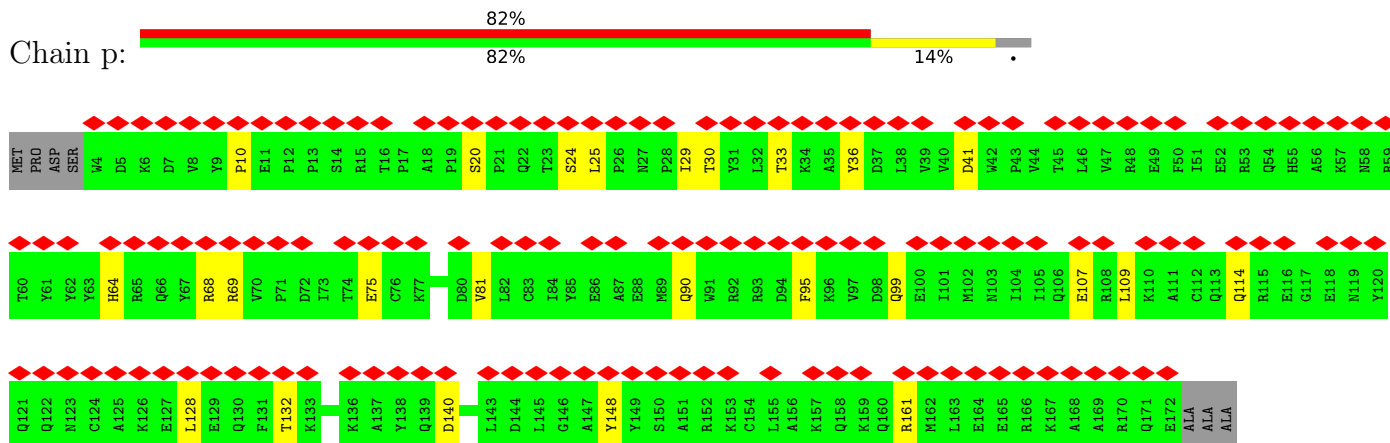


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

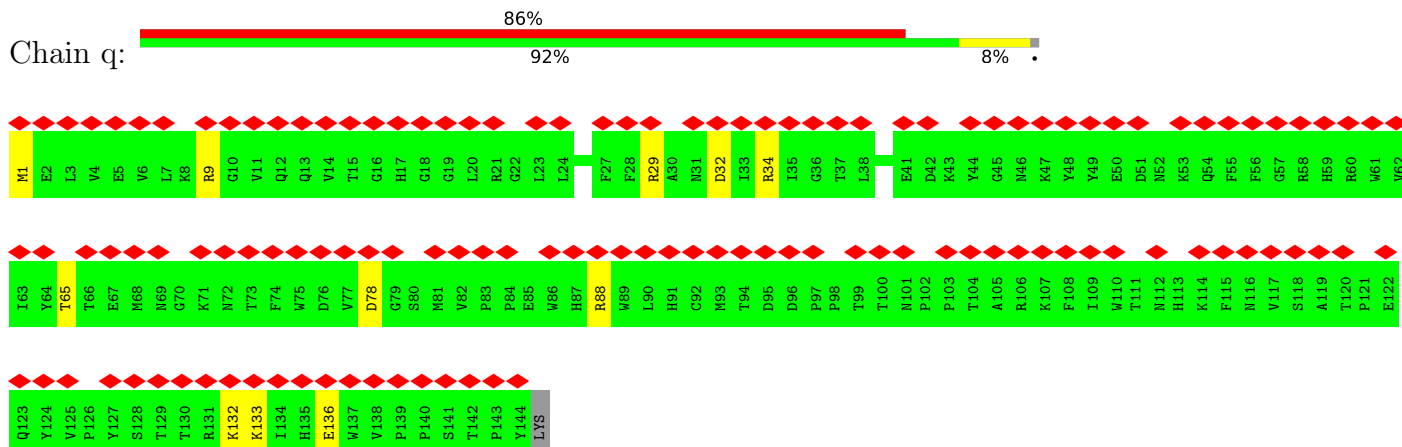


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LEU

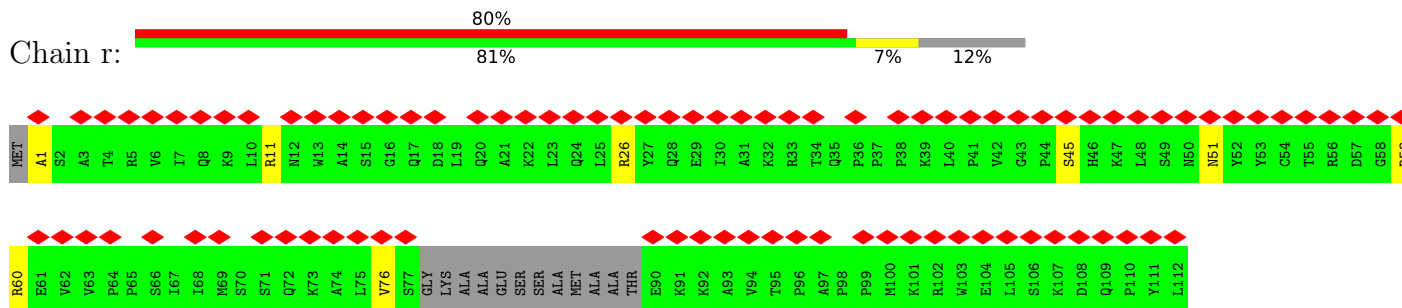
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



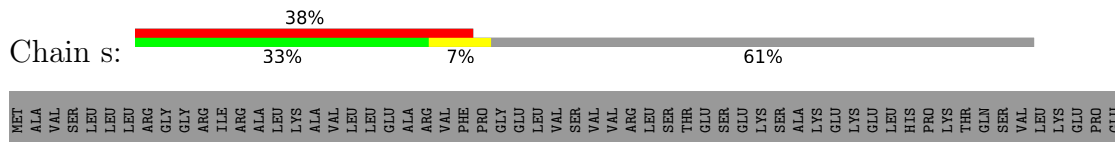
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27193	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.065	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0245	Depositor
Map size ($\text{\AA}$)	474.30002, 474.30002, 474.30002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HQT, SF4, FME, NDP, AYA, CDL, EHZ, FES, AME, FMN, SAC, 3PE, ZN, ATP, 2MR, PC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/949	0.52	0/1297
2	B	0.51	0/1278	0.58	0/1730
3	C	0.45	0/1771	0.50	0/2412
4	D	0.47	0/3540	0.51	0/4795
5	E	0.30	0/1688	0.46	0/2300
6	F	0.34	0/3374	0.49	0/4557
7	G	0.38	0/5383	0.49	0/7293
8	H	0.45	0/2607	0.56	0/3564
9	I	0.50	0/1461	0.51	0/1974
10	J	0.37	0/1322	0.47	0/1799
11	K	0.42	0/738	0.46	0/1002
12	L	0.38	0/4913	0.51	0/6686
13	M	0.43	0/3709	0.51	0/5052
14	N	0.44	0/2748	0.54	0/3741
15	O	0.37	0/2674	0.44	0/3626
16	P	0.38	0/2823	0.50	0/3828
17	Q	0.40	0/1038	0.45	0/1401
18	R	0.37	0/751	0.44	0/1011
19	S	0.30	0/678	0.45	0/915
20	T	0.28	0/620	0.45	0/836
20	U	0.30	0/704	0.40	0/951
21	V	0.36	0/949	0.46	0/1286
22	W	0.36	0/993	0.48	0/1335
23	X	0.34	0/1434	0.48	0/1937
24	Y	0.30	0/1061	0.42	0/1439
25	Z	0.36	0/1198	0.50	0/1616
26	a	0.39	0/569	0.50	0/766
27	b	0.33	0/651	0.43	0/895
28	c	0.30	0/409	0.40	0/555
29	d	0.36	0/1028	0.44	0/1387
30	e	0.33	0/900	0.50	0/1199
31	f	0.29	0/468	0.45	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.34	0/878	0.49	0/1196
33	h	0.37	0/1197	0.47	0/1621
34	i	0.35	0/804	0.52	0/1094
35	j	0.28	0/561	0.41	0/768
36	k	0.27	0/629	0.39	0/851
37	l	0.34	0/1348	0.46	0/1840
38	m	0.34	0/1079	0.49	0/1463
39	n	0.32	0/1589	0.47	0/2152
40	o	0.27	0/982	0.51	0/1320
41	p	0.32	0/1466	0.45	0/1981
42	q	0.38	0/1234	0.44	0/1681
43	r	0.38	0/812	0.55	1/1098 (0.1%)
44	s	0.29	0/353	0.40	0/479
All	All	0.38	0/67361	0.49	1/91359 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	r	76	VAL	CG1-CB-CG2	5.13	122.09	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	933	0	969	23	0
2	B	1247	0	1255	20	0
3	C	1721	0	1680	24	0
4	D	3464	0	3416	49	0
5	E	1648	0	1639	29	0
6	F	3300	0	3258	49	0
7	G	5296	0	5322	59	0
8	H	2540	0	2626	51	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1431	0	1383	29	0
10	J	1300	0	1315	16	0
11	K	737	0	768	16	0
12	L	4800	0	4985	82	0
13	M	3632	0	3853	74	0
14	N	2696	0	2895	48	0
15	O	2607	0	2566	24	0
16	P	2748	0	2768	26	0
17	Q	1015	0	1016	13	0
18	R	738	0	717	8	0
19	S	667	0	685	10	0
20	T	611	0	602	7	0
20	U	692	0	686	6	0
21	V	927	0	968	5	0
22	W	970	0	991	12	0
23	X	1396	0	1379	7	0
24	Y	1037	0	1024	7	0
25	Z	1167	0	1166	13	0
26	a	556	0	568	6	0
27	b	628	0	628	6	0
28	c	398	0	401	3	0
29	d	996	0	1001	10	0
30	e	877	0	871	11	0
31	f	456	0	452	3	0
32	g	850	0	783	13	0
33	h	1162	0	1163	11	0
34	i	787	0	797	12	0
35	j	537	0	495	4	0
36	k	609	0	603	8	0
37	l	1294	0	1186	15	0
38	m	1050	0	1061	10	0
39	n	1534	0	1466	16	0
40	o	957	0	937	5	0
41	p	1433	0	1399	21	0
42	q	1203	0	1158	8	0
43	r	802	0	836	5	0
44	s	344	0	324	6	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	B	78	0	107	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	J	42	0	58	2	0
46	Z	45	0	64	0	0
47	D	30	0	0	0	0
48	D	51	0	82	1	0
48	H	44	0	65	0	0
48	K	33	0	40	0	0
48	L	49	0	75	0	0
48	M	42	0	61	0	0
48	Y	41	0	56	0	0
48	h	37	0	48	0	0
48	i	42	0	61	1	0
48	l	49	0	75	0	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	1	0
51	L	74	0	92	0	0
51	N	124	0	145	1	0
51	d	130	0	151	4	0
51	h	70	0	87	3	0
51	q	57	0	58	1	0
52	O	31	0	12	4	0
53	P	48	0	26	1	0
54	R	1	0	0	0	0
55	T	37	0	0	0	0
55	U	37	0	0	1	0
All	All	67072	0	67443	722	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (722) 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:170:LEU:HD12	14:N:288:LEU:HD21	1.52	0.92
1:A:37:TYR:OH	4:D:54:GLN:OE1	1.98	0.81
4:D:146:ARG:NH1	4:D:368:GLU:O	2.14	0.80
3:C:43:SER:OG	3:C:45:LEU:O	2.01	0.79
4:D:326:ASP:OD1	7:G:127:ARG:NH2	2.16	0.78
4:D:341:SER:OG	4:D:344:SER:OG	2.02	0.78
1:A:73:LEU:O	8:H:160:TYR:OH	2.01	0.78
2:B:91:ARG:NH1	8:H:214:GLU:OE1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:307:LEU:O	8:H:311:THR:OG1	2.03	0.77
14:N:271:MET:HE3	14:N:276:LEU:HD13	1.67	0.76
7:G:594:ARG:NH1	22:W:124:PHE:O	2.18	0.76
25:Z:57:ARG:NH1	27:b:45:ASN:OD1	2.19	0.76
42:q:29:ARG:NH2	42:q:65:THR:O	2.18	0.76
24:Y:49:SER:OG	24:Y:52:GLU:OE1	2.02	0.76
15:O:35:LYS:NZ	52:O:401:ATP:O1G	2.19	0.76
4:D:335:ARG:NH2	9:I:128:CYS:O	2.19	0.75
12:L:363:THR:OG1	12:L:431:THR:O	2.03	0.75
3:C:210:ARG:NH1	7:G:35:MET:SD	2.60	0.75
2:B:52:ARG:NH1	46:B:202:PC1:O12	2.19	0.75
4:D:226:GLU:O	4:D:230:THR:OG1	2.03	0.75
2:B:35:ARG:NH2	2:B:37:GLU:OE1	2.20	0.75
34:i:10:ARG:NH1	39:n:164:PRO:O	2.20	0.75
18:R:81:THR:OG1	18:R:91:PHE:O	2.05	0.74
32:g:65:SER:OG	33:h:28:TYR:O	2.04	0.74
6:F:86:SER:OG	6:F:89:ARG:O	2.05	0.74
12:L:227:PHE:O	12:L:230:HIS:ND1	2.20	0.74
12:L:594:ASN:OD1	24:Y:40:TYR:OH	2.05	0.74
12:L:217:LEU:O	12:L:221:THR:OG1	2.04	0.74
6:F:188:GLU:OE1	6:F:190:THR:OG1	2.06	0.74
19:S:26:SER:O	19:S:33:ARG:NH2	2.21	0.74
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.05	0.74
7:G:140:LYS:O	7:G:148:THR:OG1	2.06	0.73
9:I:71:ARG:NH1	9:I:75:GLY:O	2.21	0.73
39:n:134:ARG:NE	39:n:161:ASP:OD1	2.21	0.73
12:L:156:GLY:O	13:M:416:ARG:NH1	2.22	0.73
12:L:295:GLN:O	12:L:425:ARG:NH1	2.21	0.73
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.05	0.72
37:l:33:TYR:OH	37:l:45:ASP:O	2.06	0.72
6:F:246:GLY:N	6:F:271:GLU:OE2	2.21	0.72
4:D:182:GLU:OE2	9:I:60:SER:N	2.23	0.72
12:L:416:THR:O	12:L:419:THR:OG1	2.08	0.72
5:E:24:THR:OG1	5:E:27:ASN:OD1	2.08	0.72
12:L:512:SER:O	39:n:35:LYS:NZ	2.23	0.72
7:G:196:SER:OG	7:G:265:ASP:OD2	2.08	0.72
21:V:5:LYS:NZ	21:V:68:GLU:OE2	2.22	0.72
1:A:71:LEU:O	10:J:145:TYR:OH	2.07	0.72
9:I:85:CYS:SG	9:I:111:TYR:OH	2.47	0.71
12:L:62:MET:SD	12:L:199:GLN:NE2	2.63	0.71
12:L:79:SER:OG	12:L:136:ASN:OD1	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:313:MET:O	12:L:316:THR:OG1	2.07	0.71
6:F:194:GLU:OE2	6:F:204:ARG:NH1	2.24	0.71
34:i:94:TYR:OH	41:p:10:PRO:O	2.08	0.71
13:M:14:LEU:O	13:M:18:SER:OG	2.08	0.71
13:M:207:MET:SD	13:M:240:SER:OG	2.45	0.71
37:l:57:ARG:NH1	37:l:74:GLU:OE2	2.24	0.70
12:L:216:LEU:HD22	12:L:259:LEU:HD21	1.73	0.70
7:G:237:ASN:O	7:G:259:ASN:ND2	2.24	0.70
8:H:205:SER:OG	8:H:279:ARG:NH2	2.25	0.70
29:d:25:LYS:NZ	51:d:201:CDL:OA3	2.25	0.70
34:i:89:MET:O	34:i:95:THR:OG1	2.08	0.69
16:P:77:ASP:O	16:P:80:SER:OG	2.09	0.69
16:P:235:ARG:NH2	16:P:291:ASP:O	2.25	0.69
6:F:76:GLY:O	6:F:80:SER:OG	2.04	0.69
12:L:577:THR:O	12:L:580:GLN:NE2	2.25	0.69
12:L:303:ALA:O	12:L:306:THR:OG1	2.10	0.69
13:M:15:THR:O	13:M:93:LYS:NZ	2.25	0.69
6:F:358:SER:OG	6:F:365:CYS:SG	2.45	0.69
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.74	0.69
9:I:170:ASN:OD1	42:q:88:ARG:NH1	2.26	0.69
16:P:38:LEU:O	16:P:43:SER:OG	2.10	0.69
8:H:18:ALA:O	8:H:21:THR:OG1	2.10	0.68
4:D:350:LYS:NZ	7:G:118:ASP:OD1	2.26	0.68
12:L:369:THR:OG1	12:L:445:GLU:OE2	2.08	0.68
18:R:12:THR:OG1	18:R:14:THR:O	2.11	0.68
15:O:59:SER:O	15:O:63:THR:OG1	2.04	0.68
6:F:68:ARG:NH2	6:F:251:SER:O	2.28	0.67
7:G:365:ASN:N	7:G:491:ASN:OD1	2.27	0.67
7:G:392:ASN:OD1	7:G:417:TYR:OH	2.08	0.67
22:W:48:THR:HG21	22:W:95:THR:HG22	1.74	0.67
7:G:577:GLU:OE1	7:G:579:ARG:NH1	2.28	0.67
6:F:126:GLY:O	6:F:129:MET:O	2.13	0.66
7:G:396:ARG:NH1	7:G:416:THR:O	2.29	0.66
6:F:66:ARG:O	6:F:68:ARG:NH1	2.28	0.66
34:i:10:ARG:HE	34:i:14:LEU:HD11	1.60	0.66
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.77	0.66
33:h:44:ASN:OD1	51:h:201:CDL:O1	2.11	0.66
2:B:144:ARG:NH1	3:C:173:GLU:OE2	2.28	0.66
42:q:32:ASP:OD2	42:q:34:ARG:NH1	2.28	0.66
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.28	0.65
42:q:9:ARG:NH2	51:q:201:CDL:O1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:149:ILE:HD12	13:M:364:LEU:HD21	1.79	0.65
13:M:44:GLN:NE2	13:M:48:ASN:O	2.30	0.65
27:b:35:SER:OG	27:b:38:THR:OG1	2.15	0.65
7:G:285:ARG:NH1	7:G:557:ALA:O	2.30	0.64
35:j:61:ASP:O	35:j:65:GLY:N	2.30	0.64
39:n:138:GLN:NE2	39:n:155:PRO:O	2.30	0.64
3:C:50:ILE:HD12	3:C:105:ILE:HD11	1.78	0.64
13:M:368:ALA:HB1	13:M:375:LEU:HD12	1.78	0.64
4:D:81:GLY:N	4:D:429:ASP:OD2	2.31	0.64
14:N:126:MET:HE2	14:N:129:ILE:HD13	1.80	0.64
4:D:3:GLN:NE2	13:M:135:ARG:O	2.29	0.64
7:G:357:ASP:OD2	19:S:44:LYS:NZ	2.30	0.64
18:R:23:TYR:O	18:R:26:VAL:HG23	1.96	0.64
34:i:88:HIS:O	34:i:92:LYS:NZ	2.22	0.64
15:O:117:SER:OG	15:O:260:ARG:NH1	2.31	0.63
19:S:43:LEU:HD11	19:S:90:MET:HE2	1.80	0.63
41:p:30:THR:O	41:p:33:THR:OG1	2.12	0.63
5:E:150:ASN:OD1	5:E:190:ARG:NH1	2.31	0.63
2:B:53:SER:O	8:H:47:GLN:NE2	2.32	0.63
6:F:288:THR:OG1	6:F:338:ASP:OD1	2.16	0.63
13:M:106:LEU:HD13	13:M:234:ILE:CD1	2.29	0.63
12:L:520:SER:O	12:L:524:THR:OG1	2.10	0.63
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.31	0.63
13:M:160:LEU:HD12	13:M:202:ALA:HB3	1.80	0.63
15:O:30:ASN:ND2	15:O:203:GLU:OE1	2.32	0.63
5:E:120:LEU:HD13	5:E:173:ILE:HD11	1.80	0.62
12:L:363:THR:OG1	12:L:431:THR:HG22	1.99	0.62
50:F:501:FMN:N1	50:F:501:FMN:O3'	2.24	0.62
23:X:165:ARG:NH2	29:d:87:ASP:OD1	2.32	0.62
29:d:17:GLU:O	29:d:20:SER:OG	2.17	0.62
26:a:31:ASN:OD1	26:a:60:TYR:OH	2.07	0.62
4:D:284:ASP:OD1	9:I:1:THR:OG1	2.16	0.62
15:O:25:ILE:CD1	15:O:168:ALA:HB3	2.30	0.62
3:C:177:ASP:OD1	16:P:36:ASN:ND2	2.32	0.62
41:p:29:ILE:O	41:p:33:THR:HG23	2.00	0.62
3:C:57:VAL:CG1	3:C:120:ILE:HD11	2.30	0.62
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.33	0.62
4:D:322:GLU:N	4:D:322:GLU:OE1	2.33	0.61
16:P:8:HIS:O	16:P:15:SER:OG	2.17	0.61
4:D:177:MET:HE3	4:D:214:PHE:CZ	2.35	0.61
10:J:73:MET:HE1	11:K:79:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:74:PHE:O	32:g:78:VAL:HG23	2.00	0.61
9:I:38:MET:O	9:I:41:SER:OG	2.16	0.61
13:M:278:ARG:NH2	37:l:79:ASP:OD1	2.34	0.61
13:M:106:LEU:O	13:M:109:THR:OG1	2.19	0.61
16:P:175:GLU:N	16:P:175:GLU:OE1	2.33	0.61
40:o:82:GLU:N	40:o:82:GLU:OE1	2.34	0.61
4:D:226:GLU:OE1	4:D:305:ARG:NH2	2.33	0.61
1:A:79:ILE:O	27:b:45:ASN:ND2	2.33	0.60
7:G:135:ARG:NH2	7:G:179:ASN:O	2.34	0.60
13:M:207:MET:HE2	13:M:243:MET:CE	2.31	0.60
7:G:595:GLU:OE1	7:G:597:TRP:NE1	2.33	0.60
34:i:1:SAC:OAC	34:i:1:SAC:CB	2.49	0.60
9:I:76:GLU:OE2	9:I:77:GLU:N	2.34	0.60
4:D:341:SER:HG	4:D:344:SER:HG	1.43	0.60
5:E:86:PHE:O	7:G:177:ARG:NH1	2.34	0.60
9:I:71:ARG:NH2	18:R:38:ASN:O	2.33	0.60
16:P:248:MET:SD	16:P:322:ARG:NH1	2.74	0.60
9:I:114:ASP:OD1	9:I:116:THR:OG1	2.18	0.60
13:M:24:TRP:O	13:M:28:THR:OG1	2.10	0.60
12:L:304:PHE:CZ	12:L:526:LEU:HD11	2.36	0.60
3:C:68:THR:OG1	21:V:86:GLU:OE1	2.08	0.60
5:E:162:GLU:OE2	6:F:108:ARG:NH2	2.35	0.60
7:G:63:PRO:O	7:G:85:LYS:NZ	2.34	0.60
14:N:339:LEU:HD13	51:d:202:CDL:H831	1.83	0.60
14:N:312:LYS:O	14:N:315:THR:OG1	2.16	0.60
6:F:194:GLU:OE1	6:F:199:LYS:NZ	2.32	0.60
41:p:24:SER:O	41:p:25:LEU:HD23	2.02	0.59
12:L:316:THR:HG21	12:L:395:ILE:HD12	1.84	0.59
24:Y:82:ARG:NH2	24:Y:87:ASP:OD2	2.35	0.59
7:G:366:THR:OG1	7:G:491:ASN:ND2	2.35	0.59
8:H:202:GLU:N	8:H:202:GLU:OE1	2.35	0.59
17:Q:10:LEU:O	22:W:25:ARG:NH2	2.34	0.59
36:k:29:ILE:O	36:k:32:THR:OG1	2.16	0.59
1:A:1:FME:O	1:A:5:THR:OG1	2.17	0.59
14:N:298:TYR:HD1	14:N:302:LEU:HD12	1.68	0.59
12:L:86:SER:O	12:L:90:THR:OG1	2.19	0.59
13:M:12:LEU:O	13:M:15:THR:OG1	2.17	0.59
14:N:332:MET:HE1	29:d:34:MET:HE1	1.84	0.59
36:k:72:ILE:HG23	36:k:73:LEU:HD12	1.85	0.59
13:M:229:MET:HE2	13:M:328:CYS:SG	2.43	0.58
5:E:100:ILE:HG12	5:E:156:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:20:THR:HG21	14:N:137:ALA:HB1	1.84	0.58
6:F:126:GLY:O	6:F:129:MET:C	2.45	0.58
13:M:134:THR:OG1	14:N:302:LEU:HD13	2.04	0.58
14:N:223:ASN:ND2	15:O:268:GLU:OE1	2.36	0.58
3:C:119:SER:OG	3:C:143:PHE:O	2.20	0.58
5:E:119:THR:HG21	5:E:166:PRO:HB3	1.85	0.58
13:M:205:ILE:CD1	13:M:212:VAL:HG21	2.34	0.58
16:P:75:ALA:HB1	16:P:113:ILE:HD12	1.86	0.58
13:M:106:LEU:HD13	13:M:234:ILE:HD12	1.84	0.58
14:N:269:GLU:O	14:N:273:ASN:ND2	2.36	0.58
3:C:133:GLU:OE2	4:D:430:ARG:NH2	2.37	0.58
37:l:93:THR:OG1	37:l:95:VAL:O	2.16	0.58
7:G:348:ILE:N	7:G:459:GLN:OE1	2.37	0.58
8:H:293:PHE:O	8:H:297:THR:OG1	2.14	0.58
16:P:90:VAL:HG21	16:P:218:THR:OG1	2.03	0.58
3:C:192:GLN:OE1	9:I:117:LYS:NZ	2.37	0.58
7:G:364:LEU:HD23	7:G:491:ASN:HB3	1.85	0.58
5:E:16:ASN:OD1	5:E:19:THR:N	2.37	0.57
8:H:120:GLY:O	8:H:128:SER:OG	2.21	0.57
15:O:83:TYR:OH	52:O:401:ATP:O2'	2.10	0.57
7:G:544:VAL:HG23	7:G:559:VAL:HG13	1.85	0.57
7:G:318:ILE:HD13	7:G:532:ILE:HD13	1.87	0.57
12:L:139:GLN:HA	12:L:142:ILE:HD12	1.87	0.57
13:M:172:GLY:O	33:h:104:ARG:NH1	2.35	0.57
24:Y:85:PRO:O	24:Y:127:LYS:NZ	2.37	0.57
12:L:346:ILE:HA	12:L:366:MET:HE1	1.86	0.57
13:M:232:ALA:O	13:M:237:LYS:NZ	2.38	0.57
8:H:239:THR:OG1	8:H:262:GLU:OE1	2.23	0.57
9:I:44:PHE:O	43:r:11:ARG:NH2	2.38	0.57
5:E:36:LYS:O	44:s:59:GLN:NE2	2.37	0.56
9:I:52:TYR:OH	9:I:140:GLU:OE2	2.21	0.56
12:L:387:THR:HG22	12:L:465:GLY:H	1.70	0.56
3:C:63:PHE:HA	21:V:89:LEU:HD11	1.87	0.56
4:D:173:GLU:OE2	4:D:176:LYS:NZ	2.38	0.56
15:O:287:HIS:ND1	32:g:26:GLU:OE2	2.26	0.56
40:o:36:ARG:NH1	40:o:93:ASP:OD1	2.39	0.56
7:G:118:ASP:OD2	17:Q:46:GLN:NE2	2.38	0.56
12:L:539:MET:SD	38:m:10:LEU:HD21	2.46	0.56
2:B:124:VAL:HG22	2:B:154:ILE:CG2	2.35	0.56
3:C:79:THR:HG22	4:D:390:LYS:HD3	1.87	0.56
19:S:19:ARG:NH2	19:S:73:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:170:VAL:O	39:n:171:THR:OG1	2.23	0.56
13:M:166:LEU:HB2	14:N:271:MET:HE1	1.87	0.56
4:D:142:GLY:O	4:D:145:THR:OG1	2.23	0.56
4:D:224:GLU:OE1	9:I:42:TYR:OH	2.16	0.56
8:H:248:TYR:O	8:H:251:LEU:N	2.39	0.56
4:D:233:ARG:NH1	48:D:502:3PE:O21	2.40	0.55
9:I:166:GLU:OE1	9:I:170:ASN:ND2	2.39	0.55
7:G:303:VAL:HG11	7:G:603:LEU:HD11	1.87	0.55
16:P:15:SER:OG	16:P:16:VAL:N	2.39	0.55
13:M:318:ALA:O	13:M:322:THR:HG22	2.07	0.55
41:p:20:SER:O	41:p:20:SER:OG	2.24	0.55
30:e:31:ARG:NH2	30:e:65:CYS:O	2.40	0.55
41:p:69:ARG:NH1	41:p:90:GLN:OE1	2.40	0.55
4:D:111:MET:SD	4:D:111:MET:N	2.79	0.55
7:G:6:SER:OG	7:G:7:ASN:N	2.40	0.55
7:G:475:GLN:O	7:G:479:VAL:HG23	2.07	0.55
6:F:307:ILE:CD1	6:F:327:THR:HG21	2.36	0.55
13:M:363:SER:CB	13:M:411:ILE:HD11	2.37	0.55
20:T:47:GLN:NE2	20:T:67:ALA:O	2.40	0.54
8:H:169:GLN:NE2	8:H:241:ILE:O	2.40	0.54
15:O:104:ARG:NH2	52:O:401:ATP:N7	2.56	0.54
39:n:167:TRP:O	39:n:171:THR:OG1	2.25	0.54
13:M:345:ALA:HB2	13:M:423:MET:HE1	1.89	0.54
20:U:68:GLU:OE2	39:n:17:ARG:NH2	2.40	0.54
36:k:68:PHE:O	36:k:72:ILE:HG22	2.08	0.54
37:l:150:GLU:N	37:l:150:GLU:OE1	2.40	0.54
15:O:169:VAL:CG2	15:O:220:VAL:HG12	2.38	0.54
6:F:344:VAL:HG23	6:F:380:VAL:HG22	1.89	0.54
38:m:62:PRO:HA	38:m:65:ILE:HD12	1.90	0.54
28:c:41:GLU:OE1	29:d:19:ARG:NE	2.37	0.54
29:d:11:LEU:O	30:e:8:LYS:NZ	2.40	0.54
13:M:326:LEU:HD22	13:M:410:MET:CE	2.37	0.54
16:P:31:GLY:O	16:P:35:VAL:HG23	2.07	0.54
7:G:278:ARG:NH2	7:G:568:GLU:OE1	2.42	0.53
9:I:110:ARG:NH2	17:Q:70:MET:O	2.41	0.53
3:C:66:ASP:HB2	21:V:89:LEU:HD12	1.88	0.53
7:G:476:LYS:O	7:G:480:THR:HG23	2.08	0.53
32:g:90:GLU:OE1	41:p:64:HIS:NE2	2.39	0.53
33:h:118:GLY:O	33:h:124:GLN:NE2	2.41	0.53
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.91	0.53
14:N:298:TYR:O	14:N:303:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:LEU:HD12	5:E:153:MET:HE2	1.90	0.53
7:G:614:ASP:N	7:G:614:ASP:OD1	2.42	0.53
13:M:205:ILE:HD13	13:M:212:VAL:HG21	1.90	0.53
8:H:225:MET:O	8:H:229:THR:OG1	2.14	0.53
6:F:272:MET:O	6:F:273:SER:OG	2.24	0.53
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.41	0.53
15:O:215:SER:O	15:O:245:LYS:NZ	2.23	0.53
12:L:397:GLU:O	12:L:401:THR:OG1	2.18	0.53
3:C:47:GLU:OE1	3:C:106:ARG:NH2	2.43	0.52
4:D:139:VAL:HG23	4:D:278:TYR:CZ	2.45	0.52
15:O:171:TYR:OH	15:O:203:GLU:OE2	2.26	0.52
6:F:359:CYS:SG	6:F:360:GLY:N	2.83	0.52
12:L:3:ILE:HD13	41:p:33:THR:HG22	1.90	0.52
13:M:186:LEU:HD23	13:M:253:LEU:HD11	1.92	0.52
14:N:319:LYS:HE2	15:O:267:THR:HG21	1.91	0.52
17:Q:22:LEU:HD21	22:W:83:LEU:HD13	1.92	0.52
20:T:19:LEU:O	20:T:25:ILE:HD11	2.09	0.52
6:F:307:ILE:HD13	6:F:327:THR:HG21	1.91	0.52
7:G:326:GLU:OE2	7:G:620:ARG:NE	2.40	0.52
8:H:134:ARG:NH1	8:H:206:GLU:OE1	2.42	0.52
12:L:541:SER:O	12:L:545:SER:OG	2.17	0.52
13:M:300:SER:O	13:M:308:SER:OG	2.27	0.52
15:O:111:ALA:HB1	15:O:122:VAL:HG11	1.91	0.52
2:B:46:LEU:HD21	8:H:53:MET:HE1	1.92	0.52
6:F:21:ILE:HD11	6:F:233:THR:CG2	2.39	0.52
13:M:137:GLY:O	13:M:142:ARG:NH1	2.43	0.52
43:r:45:SER:O	43:r:51:ASN:ND2	2.43	0.52
13:M:310:MET:O	13:M:313:THR:OG1	2.24	0.52
12:L:9:LEU:HD23	48:i:201:3PE:H2B1	1.92	0.52
7:G:655:GLU:N	7:G:655:GLU:OE1	2.40	0.52
12:L:574:THR:HG23	14:N:167:TRP:O	2.10	0.52
22:W:40:ALA:HB1	22:W:92:LEU:HD21	1.91	0.52
26:a:52:ARG:NH2	26:a:58:ASN:OD1	2.43	0.52
4:D:179:GLU:OE1	43:r:26:ARG:NH2	2.42	0.52
9:I:97:GLU:OE1	42:q:133:LYS:NZ	2.37	0.52
15:O:188:ASP:H	15:O:192:MET:HE3	1.75	0.52
16:P:128:ARG:NH1	16:P:220:ASP:O	2.43	0.52
24:Y:59:ARG:O	24:Y:63:THR:OG1	2.19	0.52
37:l:136:ASN:OD1	37:l:141:ARG:NH1	2.42	0.52
1:A:33:LYS:NZ	8:H:59:GLU:OE2	2.17	0.51
1:A:67:LEU:HD11	11:K:68:ALA:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:258:ILE:HD11	6:F:279:LEU:HD21	1.92	0.51
31:f:55:TRP:NE1	33:h:88:GLU:OE1	2.40	0.51
8:H:20:LEU:O	8:H:20:LEU:HD23	2.10	0.51
8:H:96:ILE:HD13	25:Z:142:TYR:OH	2.10	0.51
8:H:104:PHE:O	8:H:108:THR:OG1	2.20	0.51
13:M:184:HIS:ND1	13:M:185:THR:O	2.42	0.51
5:E:132:THR:OG1	5:E:134:ASP:OD1	2.28	0.51
8:H:10:LEU:HD22	8:H:83:LEU:HG	1.93	0.51
14:N:297:ILE:HD12	14:N:300:THR:CG2	2.40	0.51
51:h:201:CDL:O1	51:h:201:CDL:OA3	2.27	0.51
12:L:149:ILE:HD12	13:M:364:LEU:CD2	2.40	0.51
12:L:193:MET:HE3	12:L:204:SER:HB2	1.92	0.51
30:e:26:TYR:O	30:e:28:ASN:N	2.41	0.51
8:H:17:MET:HE2	8:H:225:MET:HB2	1.93	0.51
12:L:324:LEU:HD11	12:L:394:LEU:HB2	1.91	0.51
37:l:71:ASN:N	37:l:74:GLU:OE1	2.43	0.51
9:I:76:GLU:HB2	18:R:44:ILE:HD13	1.92	0.51
11:K:97:GLN:N	11:K:97:GLN:OE1	2.42	0.51
26:a:55:SER:OG	26:a:57:VAL:O	2.08	0.51
13:M:225:ILE:O	13:M:228:SER:N	2.42	0.51
12:L:131:LEU:HD12	12:L:140:LEU:HG	1.93	0.50
13:M:27:VAL:HG13	13:M:77:LEU:HD21	1.93	0.50
15:O:224:ASP:O	15:O:228:ALA:N	2.42	0.50
20:U:47:GLN:NE2	20:U:70:LEU:O	2.42	0.50
38:m:21:GLU:O	39:n:14:LYS:NZ	2.25	0.50
14:N:92:GLY:O	14:N:96:ASN:ND2	2.44	0.50
2:B:141:SER:O	2:B:142:VAL:HG23	2.10	0.50
11:K:12:PHE:CE2	14:N:72:LEU:HD22	2.46	0.50
32:g:115:LYS:NZ	41:p:75:GLU:OE2	2.43	0.50
38:m:8:ALA:HB3	38:m:10:LEU:O	2.12	0.50
40:o:17:ASP:OD1	40:o:19:GLU:N	2.42	0.50
16:P:185:TYR:HD2	16:P:191:VAL:HG23	1.77	0.50
13:M:326:LEU:HD22	13:M:410:MET:HE1	1.93	0.50
32:g:69:VAL:O	32:g:73:THR:HG23	2.12	0.50
40:o:102:GLU:OE2	40:o:105:ARG:NH2	2.45	0.50
3:C:49:GLU:OE2	3:C:108:LYS:NZ	2.32	0.50
11:K:37:VAL:HG21	11:K:67:ALA:HB1	1.93	0.50
29:d:78:ARG:NH1	51:d:202:CDL:OA9	2.45	0.50
1:A:54:LYS:NZ	4:D:69:SER:O	2.39	0.50
6:F:42:TRP:N	6:F:120:GLU:OE1	2.40	0.50
7:G:481:THR:O	7:G:483:VAL:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:26:SER:OG	19:S:59:GLU:OE1	2.29	0.50
25:Z:109:VAL:HG21	30:e:71:THR:CG2	2.42	0.50
13:M:76:MET:SD	13:M:99:LEU:HD22	2.51	0.49
14:N:108:LEU:HD22	14:N:191:LEU:HD22	1.93	0.49
1:A:68:GLU:HG2	10:J:159:LEU:HD13	1.93	0.49
2:B:58:MET:HE1	2:B:113:VAL:CG1	2.42	0.49
14:N:108:LEU:CD2	14:N:191:LEU:HD22	2.42	0.49
12:L:76:LEU:HD11	12:L:196:TRP:HZ3	1.78	0.49
2:B:114:TYR:O	2:B:121:ARG:NH2	2.46	0.49
5:E:108:CYS:O	5:E:113:SER:OG	2.20	0.49
9:I:145:THR:OG1	9:I:148:GLU:OE2	2.29	0.49
4:D:347:HIS:O	4:D:351:LEU:HD23	2.12	0.49
7:G:273:GLY:O	7:G:549:HIS:NE2	2.39	0.49
15:O:214:MET:O	15:O:218:CYS:N	2.46	0.49
20:U:26:ASP:HB2	20:U:27:PRO:HD2	1.95	0.49
12:L:595:ILE:HA	14:N:100:MET:HE1	1.93	0.49
42:q:78:ASP:N	42:q:78:ASP:OD1	2.45	0.49
4:D:148:LEU:HD12	4:D:177:MET:SD	2.52	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
9:I:16:MET:O	9:I:20:THR:HG23	2.12	0.49
16:P:108:ASP:OD1	16:P:112:ASN:ND2	2.46	0.49
5:E:100:ILE:HG21	5:E:120:LEU:HD21	1.94	0.49
5:E:70:ALA:O	5:E:74:GLN:N	2.46	0.49
12:L:415:ALA:O	12:L:419:THR:HG23	2.12	0.49
19:S:85:GLU:OE1	19:S:88:ARG:NH1	2.44	0.49
29:d:33:TYR:O	29:d:37:LEU:HD23	2.13	0.49
5:E:190:ARG:NH2	6:F:265:PRO:O	2.46	0.48
5:E:204:GLU:N	5:E:204:GLU:OE1	2.45	0.48
41:p:95:PHE:O	41:p:99:GLN:NE2	2.45	0.48
2:B:124:VAL:HG22	2:B:154:ILE:HG22	1.94	0.48
3:C:44:CYS:SG	3:C:45:LEU:N	2.85	0.48
7:G:347:GLU:OE2	7:G:496:ILE:HG21	2.12	0.48
8:H:235:ASN:O	8:H:239:THR:HG22	2.12	0.48
11:K:75:LEU:O	11:K:79:VAL:HG23	2.12	0.48
30:e:27:LYS:O	33:h:139:ALA:N	2.46	0.48
8:H:114:TYR:OH	10:J:60:LEU:O	2.29	0.48
11:K:17:LEU:HD12	12:L:592:LEU:HD11	1.94	0.48
31:f:43:PHE:O	41:p:68:ARG:NH2	2.46	0.48
7:G:648:LEU:HD21	19:S:44:LYS:HG2	1.93	0.48
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.96	0.48
37:l:76:ILE:HG23	37:l:80:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:128:LEU:O	41:p:132:THR:HG23	2.12	0.48
4:D:380:SER:OG	4:D:381:ASP:N	2.46	0.48
4:D:349:PHE:O	4:D:353:THR:HG22	2.14	0.48
6:F:305:PRO:HG2	6:F:327:THR:HG22	1.96	0.48
12:L:293:LEU:O	12:L:523:SER:OG	2.31	0.48
14:N:124:LEU:CD2	14:N:225:MET:HE2	2.43	0.48
33:h:59:TYR:OH	33:h:65:GLU:OE2	2.28	0.48
12:L:3:ILE:CD1	41:p:33:THR:HG22	2.43	0.48
12:L:71:MET:HE2	13:M:310:MET:CE	2.44	0.48
20:U:55:GLU:OE1	39:n:24:ARG:NH2	2.43	0.48
32:g:56:MET:CE	33:h:24:LEU:HD13	2.43	0.48
36:k:45:GLY:C	36:k:46:LEU:HD12	2.38	0.48
2:B:107:ALA:HB1	2:B:149:ILE:HD13	1.95	0.48
8:H:93:HIS:NE2	26:a:35:GLU:OE2	2.45	0.48
13:M:212:VAL:O	13:M:212:VAL:HG23	2.14	0.48
16:P:171:ILE:CG2	16:P:207:VAL:HG22	2.44	0.48
16:P:319:ARG:NH1	16:P:327:LEU:O	2.46	0.48
1:A:48:ARG:NH1	8:H:121:TRP:O	2.45	0.48
1:A:68:GLU:HG3	1:A:98:LEU:HD13	1.96	0.48
3:C:135:TRP:CE2	22:W:90:MET:HE1	2.49	0.48
6:F:141:GLU:OE1	6:F:141:GLU:N	2.47	0.48
8:H:85:LEU:HD13	8:H:233:LEU:CD2	2.43	0.48
15:O:135:LEU:HD22	15:O:152:TYR:CD2	2.48	0.48
24:Y:82:ARG:HH12	24:Y:89:LEU:HD23	1.79	0.48
15:O:97:GLN:NE2	52:O:401:ATP:N1	2.61	0.48
12:L:187:VAL:HG22	13:M:383:MET:HG3	1.96	0.47
12:L:519:TYR:O	12:L:520:SER:OG	2.29	0.47
16:P:67:GLN:O	16:P:68:LEU:HD22	2.14	0.47
14:N:19:ILE:O	14:N:23:SER:OG	2.11	0.47
1:A:90:MET:HE1	10:J:153:VAL:HG12	1.96	0.47
2:B:76:ARG:NH1	4:D:179:GLU:OE2	2.47	0.47
25:Z:68:ILE:HD12	27:b:52:TYR:HA	1.95	0.47
1:A:64:LEU:HD11	10:J:166:ILE:CD1	2.43	0.47
12:L:409:LEU:O	12:L:413:LEU:HD23	2.14	0.47
17:Q:89:LYS:O	17:Q:93:ILE:HD12	2.14	0.47
2:B:137:HIS:O	2:B:144:ARG:NE	2.46	0.47
5:E:53:LEU:HD13	44:s:46:LEU:HD13	1.95	0.47
6:F:42:TRP:CD2	6:F:161:LEU:HD13	2.49	0.47
12:L:71:MET:HE2	13:M:310:MET:HE3	1.95	0.47
20:T:43:ASP:OD1	22:W:66:ARG:NH2	2.48	0.47
4:D:106:LEU:HD11	4:D:391:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:23:VAL:HG12	8:H:27:ILE:HD12	1.97	0.47
10:J:83:GLY:N	46:J:201:PC1:O32	2.45	0.47
39:n:100:GLU:OE2	39:n:121:ARG:NH2	2.48	0.47
6:F:215:VAL:HG12	6:F:220:THR:HG21	1.95	0.47
7:G:113:GLU:OE2	7:G:249:ARG:NH1	2.47	0.47
7:G:334:LEU:HD13	7:G:600:ILE:HG23	1.97	0.47
8:H:102:ILE:HB	8:H:150:LEU:HD21	1.97	0.47
8:H:107:ALA:HB1	10:J:56:PHE:CD2	2.50	0.47
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.96	0.47
13:M:286:ILE:O	13:M:289:SER:OG	2.28	0.47
13:M:428:PRO:O	13:M:429:SER:OG	2.30	0.47
14:N:170:LEU:O	14:N:295:ARG:NH2	2.48	0.47
16:P:330:GLU:N	16:P:330:GLU:OE1	2.48	0.47
36:k:33:PRO:O	36:k:36:THR:OG1	2.30	0.47
13:M:11:LEU:O	13:M:15:THR:HG23	2.15	0.47
13:M:106:LEU:HD13	13:M:234:ILE:HD11	1.97	0.47
19:S:52:ILE:CD1	19:S:90:MET:HE1	2.45	0.47
39:n:15:VAL:HG22	39:n:63:LEU:HD13	1.96	0.47
51:h:201:CDL:OB4	34:i:88:HIS:NE2	2.47	0.47
6:F:256:PHE:N	6:F:268:VAL:O	2.46	0.47
7:G:365:ASN:ND2	7:G:490:MET:O	2.47	0.47
12:L:217:LEU:HD21	12:L:273:ILE:HG23	1.97	0.47
14:N:298:TYR:CD1	14:N:302:LEU:HD12	2.47	0.47
25:Z:67:ARG:HG2	25:Z:71:MET:HE3	1.96	0.47
1:A:69:ILE:HD11	8:H:144:VAL:HA	1.97	0.46
1:A:71:LEU:HD22	10:J:152:MET:HE1	1.96	0.46
12:L:71:MET:HE1	13:M:376:MET:CE	2.45	0.46
12:L:273:ILE:HG22	12:L:277:MET:SD	2.56	0.46
38:m:64:LEU:O	38:m:68:THR:HG23	2.15	0.46
5:E:151:ALA:HB3	5:E:152:PRO:HD3	1.97	0.46
7:G:486:GLU:OE1	7:G:486:GLU:N	2.48	0.46
14:N:181:TYR:HA	14:N:184:ILE:HD12	1.97	0.46
13:M:408:MET:HE2	13:M:411:ILE:HD12	1.98	0.46
18:R:2:VAL:HG12	18:R:2:VAL:O	2.16	0.46
5:E:105:THR:HG22	5:E:106:THR:H	1.81	0.46
11:K:26:LEU:HD23	11:K:78:LEU:HD13	1.97	0.46
4:D:80:ILE:HD12	4:D:428:ILE:HG22	1.96	0.46
5:E:22:ASP:OD2	5:E:22:ASP:N	2.48	0.46
5:E:155:GLN:O	5:E:156:ILE:HD13	2.15	0.46
6:F:56:ILE:HG21	6:F:128:ALA:HB2	1.98	0.46
7:G:226:GLU:OE1	17:Q:36:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:5:THR:HG22	14:N:9:ILE:HD12	1.98	0.46
23:X:19:VAL:HG22	23:X:23:VAL:HG11	1.97	0.46
25:Z:3:SER:OG	25:Z:4:LYS:N	2.48	0.46
13:M:363:SER:HB2	13:M:411:ILE:HD11	1.98	0.46
25:Z:85:ILE:HG21	25:Z:123:MET:HG3	1.98	0.46
28:c:38:ASP:OD2	29:d:77:LYS:NZ	2.45	0.46
4:D:47:MET:HE1	8:H:130:PHE:HE1	1.79	0.46
13:M:23:THR:O	13:M:27:VAL:HG12	2.15	0.46
19:S:78:LEU:O	19:S:78:LEU:HD12	2.16	0.46
2:B:79:MET:HE1	2:B:86:PHE:CE2	2.50	0.46
6:F:106:LYS:HB2	6:F:255:LEU:HD13	1.97	0.46
12:L:199:GLN:NE2	41:p:114:GLN:OE1	2.48	0.46
6:F:119:VAL:CG1	6:F:162:ILE:HD11	2.46	0.46
7:G:106:PRO:O	7:G:218:ARG:NH1	2.49	0.46
7:G:596:ASP:O	7:G:600:ILE:HD12	2.16	0.46
12:L:152:PHE:CD1	12:L:168:ALA:HB1	2.50	0.46
14:N:242:THR:HG23	51:N:401:CDL:H351	1.98	0.46
25:Z:109:VAL:HG21	30:e:71:THR:HG22	1.98	0.46
25:Z:78:LYS:O	25:Z:82:THR:HG23	2.16	0.45
3:C:29:VAL:HA	3:C:32:ILE:HG22	1.96	0.45
5:E:88:THR:HG23	7:G:177:ARG:HH12	1.81	0.45
13:M:207:MET:HE3	13:M:298:ILE:HG13	1.98	0.45
13:M:328:CYS:HB3	13:M:437:MET:HE1	1.98	0.45
14:N:240:MET:SD	14:N:244:ILE:HD11	2.56	0.45
13:M:102:LEU:O	13:M:106:LEU:HD12	2.17	0.45
15:O:2:ARG:NH1	15:O:265:ASP:OD1	2.49	0.45
11:K:40:LEU:HD13	14:N:71:LEU:HD23	1.98	0.45
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.99	0.45
12:L:226:GLN:O	12:L:230:HIS:N	2.50	0.45
22:W:47:ASN:O	22:W:51:LEU:HD23	2.17	0.45
3:C:148:LEU:O	3:C:148:LEU:HD23	2.17	0.45
5:E:155:GLN:C	5:E:156:ILE:HD13	2.42	0.45
10:J:4:TYR:O	10:J:8:LEU:HD23	2.16	0.45
12:L:324:LEU:HD11	12:L:394:LEU:HD12	1.98	0.45
14:N:143:ILE:HG21	30:e:2:PHE:HE1	1.82	0.45
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.98	0.45
12:L:371:SER:OG	35:j:29:SER:OG	2.22	0.45
13:M:156:GLY:O	13:M:202:ALA:HB2	2.16	0.45
34:i:31:GLU:O	34:i:33:VAL:N	2.48	0.45
13:M:363:SER:OG	13:M:411:ILE:HD11	2.17	0.45
14:N:213:ALA:HB3	14:N:214:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:153:GLU:HG3	16:P:165:ILE:HD13	1.98	0.45
10:J:88:ILE:HD11	11:K:23:ARG:NH1	2.32	0.45
6:F:29:HIS:NE2	44:s:29:THR:OG1	2.50	0.45
8:H:201:THR:OG1	8:H:202:GLU:OE1	2.35	0.45
12:L:76:LEU:HD11	12:L:196:TRP:CZ3	2.51	0.45
14:N:30:TRP:CZ2	14:N:71:LEU:HD22	2.52	0.45
1:A:66:ASP:HA	1:A:69:ILE:HD12	1.99	0.44
13:M:244:ILE:O	41:p:148:TYR:OH	2.27	0.44
16:P:19:VAL:HG12	16:P:19:VAL:O	2.17	0.44
26:a:57:VAL:O	26:a:59:ARG:N	2.50	0.44
4:D:233:ARG:NE	9:I:31:GLU:OE2	2.41	0.44
34:i:82:HIS:ND1	41:p:36:TYR:OH	2.37	0.44
5:E:148:CYS:SG	6:F:103:GLY:N	2.88	0.44
12:L:131:LEU:HD21	12:L:255:ALA:HB1	2.00	0.44
20:T:15:VAL:O	20:T:19:LEU:HD23	2.17	0.44
38:m:27:GLU:OE2	38:m:30:ARG:NH1	2.51	0.44
4:D:230:THR:O	4:D:294:TYR:OH	2.21	0.44
5:E:43:GLN:NE2	5:E:73:LEU:O	2.43	0.44
6:F:24:ASN:ND2	6:F:30:ASP:O	2.50	0.44
6:F:35:GLY:O	6:F:39:ARG:NH1	2.50	0.44
12:L:542:LEU:HD23	37:l:82:MET:HB3	2.00	0.44
6:F:154:ARG:HA	44:s:52:LEU:HD21	1.99	0.44
16:P:15:SER:HG	16:P:16:VAL:H	1.64	0.44
32:g:108:SER:O	32:g:108:SER:OG	2.24	0.44
1:A:90:MET:HE2	10:J:152:MET:HG3	1.99	0.44
5:E:65:ALA:O	5:E:69:VAL:HG23	2.17	0.44
13:M:270:ILE:HD12	13:M:395:LEU:HD22	1.99	0.44
34:i:1:SAC:OAC	34:i:1:SAC:HB2	2.18	0.44
2:B:159:CYS:SG	4:D:105:ARG:NH2	2.86	0.44
8:H:185:TRP:CD1	8:H:238:THR:HG22	2.53	0.44
38:m:102:TYR:O	38:m:106:THR:HG23	2.18	0.44
7:G:335:LEU:HD12	7:G:343:LEU:HD21	1.99	0.44
10:J:59:TYR:OH	11:K:34:GLU:O	2.33	0.44
14:N:190:MET:HB3	14:N:201:THR:HG23	2.00	0.44
25:Z:119:LEU:HD13	30:e:68:ARG:NH2	2.33	0.44
7:G:53:ARG:O	7:G:93:VAL:HG21	2.18	0.43
20:T:39:ASP:OD1	20:T:39:ASP:N	2.48	0.43
30:e:49:THR:O	30:e:53:LYS:NZ	2.49	0.43
4:D:356:TYR:O	43:r:59:ARG:NH1	2.51	0.43
13:M:317:ILE:HG21	13:M:454:ILE:HD11	1.99	0.43
14:N:133:TRP:HA	14:N:136:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:20:GLU:N	36:k:20:GLU:OE1	2.51	0.43
38:m:114:LEU:HD22	38:m:119:LYS:CE	2.48	0.43
4:D:133:ARG:NH1	25:Z:7:GLN:O	2.51	0.43
7:G:256:GLU:O	7:G:394:ARG:NH1	2.51	0.43
24:Y:34:GLY:O	24:Y:38:SER:OG	2.32	0.43
33:h:134:ASP:O	33:h:138:LYS:NZ	2.49	0.43
6:F:418:LEU:CD2	6:F:426:LEU:HD11	2.49	0.43
9:I:69:LEU:HG	9:I:156:LEU:HD23	1.99	0.43
12:L:141:PHE:HE2	13:M:375:LEU:HD11	1.83	0.43
16:P:27:THR:HG22	16:P:56:ILE:CD1	2.48	0.43
19:S:18:ILE:HD13	19:S:90:MET:HE3	2.00	0.43
22:W:83:LEU:HA	22:W:86:ILE:HD12	2.00	0.43
6:F:376:MET:O	6:F:380:VAL:HG23	2.18	0.43
15:O:169:VAL:HG22	15:O:220:VAL:HG12	1.99	0.43
17:Q:13:VAL:O	22:W:17:THR:N	2.52	0.43
2:B:40:VAL:HG13	2:B:183:LEU:HB3	2.00	0.43
7:G:453:LEU:HD21	7:G:458:LEU:HD21	2.00	0.43
13:M:306:PRO:HA	13:M:458:THR:HG21	2.00	0.43
16:P:249:THR:HG22	16:P:251:ARG:HG2	2.01	0.43
31:f:38:ASN:ND2	31:f:45:ARG:O	2.44	0.43
32:g:88:ARG:NH2	41:p:107:GLU:OE1	2.50	0.43
4:D:381:ASP:OD1	4:D:382:GLY:N	2.49	0.43
13:M:207:MET:SD	13:M:240:SER:N	2.92	0.43
14:N:34:GLU:O	14:N:38:LEU:HD23	2.19	0.43
14:N:288:LEU:HD23	14:N:288:LEU:O	2.19	0.43
20:T:19:LEU:C	20:T:25:ILE:HD11	2.43	0.43
25:Z:120:ILE:O	25:Z:132:MET:HE1	2.19	0.43
34:i:86:LYS:NZ	41:p:41:ASP:OD1	2.46	0.43
3:C:52:ILE:HG22	3:C:53:HIS:O	2.18	0.43
12:L:396:ILE:HA	12:L:399:ILE:HG22	2.01	0.43
12:L:542:LEU:HD23	37:l:82:MET:CB	2.48	0.43
4:D:140:LEU:HD13	4:D:318:MET:HE1	2.01	0.43
6:F:378:ARG:NH1	6:F:388:GLU:OE1	2.46	0.43
7:G:228:ILE:HG21	7:G:581:GLN:HB3	2.00	0.43
11:K:71:ALA:O	11:K:75:LEU:HD13	2.18	0.43
13:M:175:ASN:OD1	13:M:176:LEU:N	2.51	0.43
14:N:245:SER:OG	14:N:297:ILE:HD11	2.19	0.43
1:A:60:ILE:CG2	11:K:72:ALA:HB1	2.49	0.43
3:C:148:LEU:O	22:W:90:MET:HE2	2.19	0.43
6:F:96:ASN:ND2	6:F:187:GLY:O	2.45	0.43
6:F:97:ALA:CB	6:F:111:MET:HE3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:258:ILE:HD11	6:F:279:LEU:CD2	2.49	0.43
12:L:180:ILE:HD12	13:M:397:GLY:HA2	2.01	0.43
12:L:302:ILE:HD12	12:L:339:LEU:HD23	2.00	0.43
12:L:554:ASP:OD1	12:L:558:LEU:HD12	2.19	0.43
13:M:370:PRO:O	13:M:372:SER:N	2.52	0.43
12:L:180:ILE:HD12	13:M:397:GLY:CA	2.49	0.42
12:L:283:LEU:HD13	37:l:111:MET:HG2	2.01	0.42
17:Q:11:ILE:N	22:W:19:VAL:O	2.49	0.42
4:D:58:ALA:O	4:D:60:GLY:N	2.52	0.42
18:R:14:THR:O	18:R:14:THR:OG1	2.37	0.42
1:A:17:LEU:HD22	8:H:222:LEU:HD21	2.00	0.42
4:D:177:MET:HE3	4:D:214:PHE:HZ	1.80	0.42
17:Q:33:ARG:NH1	17:Q:60:ASP:OD1	2.47	0.42
20:U:6:LEU:CD1	20:U:11:ILE:HD11	2.49	0.42
23:X:107:ASP:HA	23:X:110:VAL:HG12	2.01	0.42
30:e:47:GLY:N	33:h:124:GLN:OE1	2.52	0.42
37:l:156:ASP:O	40:o:33:ARG:NH2	2.52	0.42
2:B:59:THR:O	4:D:54:GLN:NE2	2.53	0.42
5:E:51:LEU:HD12	5:E:69:VAL:HG21	2.02	0.42
7:G:511:VAL:CG2	7:G:532:ILE:HD11	2.49	0.42
8:H:138:GLN:NE2	8:H:191:ALA:O	2.49	0.42
9:I:17:LYS:O	9:I:20:THR:OG1	2.28	0.42
12:L:270:ASN:O	12:L:274:LEU:HD13	2.20	0.42
13:M:296:LEU:HD22	13:M:396:MET:HE1	2.00	0.42
23:X:123:GLN:OE1	23:X:126:LYS:NZ	2.22	0.42
2:B:46:LEU:CD2	8:H:53:MET:HE1	2.49	0.42
12:L:224:SER:O	12:L:224:SER:OG	2.31	0.42
26:a:52:ARG:O	26:a:55:SER:OG	2.37	0.42
42:q:132:LYS:NZ	42:q:136:GLU:OE1	2.30	0.42
1:A:15:LEU:O	1:A:19:LEU:HD23	2.20	0.42
7:G:483:VAL:HG23	7:G:484:ALA:N	2.35	0.42
7:G:571:ALA:N	7:G:583:THR:OG1	2.52	0.42
14:N:108:LEU:HD11	14:N:187:MET:HB3	2.02	0.42
14:N:333:SER:O	14:N:334:THR:OG1	2.26	0.42
55:U:201:EHZ:O1	39:n:46:ARG:HB3	2.20	0.42
36:k:72:ILE:HG23	36:k:73:LEU:CD1	2.49	0.42
7:G:9:ILE:HG23	7:G:75:LYS:HE3	2.00	0.42
8:H:123:SER:O	8:H:123:SER:OG	2.37	0.42
32:g:46:ASP:N	32:g:52:ASP:OD1	2.50	0.42
39:n:169:ILE:O	39:n:172:ARG:NH1	2.49	0.42
5:E:30:ARG:NH2	44:s:47:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:246:GLU:OE2	42:q:133:LYS:NZ	2.37	0.42
8:H:123:SER:OG	8:H:128:SER:OG	2.37	0.42
9:I:134:VAL:HG21	9:I:167:ILE:HG21	2.02	0.42
37:l:3:MET:SD	38:m:65:ILE:HG21	2.59	0.42
6:F:319:PHE:O	6:F:323:VAL:HG23	2.20	0.42
8:H:45:ILE:O	8:H:46:LEU:HD12	2.20	0.42
12:L:213:LEU:O	12:L:217:LEU:HD23	2.20	0.42
23:X:19:VAL:HG22	23:X:23:VAL:CG1	2.50	0.42
35:j:33:TRP:O	35:j:37:LEU:HD23	2.19	0.42
6:F:22:PHE:CD2	6:F:255:LEU:HD21	2.55	0.42
8:H:70:LEU:HA	8:H:73:ILE:HG22	2.02	0.42
8:H:235:ASN:OD1	8:H:267:SER:OG	2.15	0.42
10:J:131:VAL:HG11	25:Z:71:MET:HE1	2.02	0.42
12:L:237:MET:O	12:L:299:LYS:NZ	2.51	0.42
14:N:53:THR:O	14:N:57:THR:HG23	2.19	0.42
16:P:63:GLY:HA3	16:P:68:LEU:HD23	2.02	0.42
33:h:94:LEU:HD22	41:p:81:VAL:HG11	2.02	0.42
1:A:87:MET:SD	1:A:88:MET:N	2.93	0.41
11:K:61:ILE:H	11:K:61:ILE:HD12	1.85	0.41
12:L:245:ALA:HB2	12:L:340:PHE:CB	2.50	0.41
13:M:200:MET:HE1	13:M:247:SER:OG	2.20	0.41
23:X:146:ARG:NH2	30:e:38:GLU:OE2	2.52	0.41
12:L:111:ASP:OD1	39:n:96:TYR:OH	2.31	0.41
14:N:297:ILE:HA	14:N:300:THR:HG22	2.02	0.41
15:O:113:GLU:O	15:O:117:SER:OG	2.26	0.41
27:b:27:LEU:HA	27:b:30:ILE:HG22	2.01	0.41
7:G:126:ASP:OD2	7:G:127:ARG:NH1	2.53	0.41
7:G:575:ASN:OD1	7:G:579:ARG:N	2.53	0.41
9:I:174:ASP:OD2	9:I:178:ARG:NH2	2.45	0.41
12:L:83:ASP:OD2	12:L:83:ASP:N	2.51	0.41
12:L:587:TYR:O	12:L:590:SER:OG	2.32	0.41
7:G:229:ASP:HB2	7:G:238:ILE:HD12	2.03	0.41
12:L:99:SER:OG	12:L:456:ARG:NH1	2.54	0.41
2:B:47:ILE:HG22	8:H:57:MET:CE	2.51	0.41
8:H:85:LEU:HD13	8:H:233:LEU:HD22	2.02	0.41
8:H:198:PHE:CD1	8:H:285:LEU:HD13	2.55	0.41
13:M:296:LEU:HB3	13:M:381:ILE:HD12	2.03	0.41
14:N:331:ILE:HG22	29:d:37:LEU:HD12	2.01	0.41
38:m:8:ALA:HB1	38:m:9:PRO:HD2	2.02	0.41
3:C:205:ALA:O	43:r:60:ARG:NH2	2.53	0.41
4:D:224:GLU:HG2	9:I:38:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:183:LYS:O	5:E:187:ARG:NH2	2.50	0.41
9:I:13:GLU:OE1	9:I:13:GLU:N	2.53	0.41
10:J:39:GLY:O	10:J:43:VAL:HG23	2.20	0.41
11:K:12:PHE:HE1	11:K:40:LEU:HD11	1.86	0.41
14:N:248:LEU:HD12	14:N:297:ILE:HD13	2.03	0.41
15:O:71:ILE:HD11	15:O:77:CYS:O	2.21	0.41
18:R:60:ASP:OD1	18:R:60:ASP:N	2.54	0.41
36:k:48:ASP:OD1	39:n:37:ARG:NE	2.49	0.41
44:s:50:LEU:O	44:s:53:SER:OG	2.38	0.41
6:F:97:ALA:HB2	6:F:111:MET:HE3	2.02	0.41
7:G:432:ILE:HD13	7:G:437:HIS:HB3	2.01	0.41
8:H:261:MET:O	8:H:265:LEU:HD23	2.20	0.41
10:J:93:VAL:HG12	10:J:97:ILE:HD12	2.02	0.41
13:M:207:MET:HE2	13:M:243:MET:HE2	2.01	0.41
17:Q:9:GLN:C	17:Q:10:LEU:HD22	2.45	0.41
1:A:64:LEU:HA	1:A:67:LEU:HD12	2.03	0.41
6:F:215:VAL:HG12	6:F:220:THR:CG2	2.51	0.41
7:G:107:ILE:O	9:I:106:ARG:NH1	2.54	0.41
7:G:537:LEU:HD23	7:G:541:CYS:SG	2.61	0.41
12:L:149:ILE:CD1	13:M:364:LEU:HD11	2.51	0.41
12:L:203:PHE:CE2	41:p:109:LEU:HD21	2.55	0.41
12:L:548:THR:HG22	12:L:548:THR:O	2.21	0.41
13:M:145:ALA:HB2	13:M:222:GLU:OE1	2.20	0.41
13:M:205:ILE:HD12	13:M:212:VAL:HG21	2.03	0.41
14:N:99:LEU:HD23	14:N:153:ILE:CD1	2.51	0.41
14:N:129:ILE:HD12	14:N:129:ILE:H	1.86	0.41
15:O:151:HIS:CE1	15:O:155:ILE:HD11	2.56	0.41
28:c:25:VAL:HG12	28:c:29:ILE:HD12	2.03	0.41
37:l:150:GLU:O	37:l:152:VAL:N	2.52	0.41
3:C:68:THR:HG21	21:V:54:LYS:HE3	2.02	0.41
8:H:85:LEU:HD21	8:H:108:THR:HB	2.03	0.41
41:p:140:ASP:O	41:p:161:ARG:NH1	2.54	0.41
4:D:71:GLU:OE2	8:H:134:ARG:NH2	2.47	0.40
6:F:49:LEU:HD21	6:F:123:LEU:HD23	2.02	0.40
6:F:257:ASN:O	6:F:334:VAL:N	2.54	0.40
13:M:91:LEU:HD21	13:M:135:ARG:NH2	2.36	0.40
23:X:170:THR:OG1	51:d:201:CDL:OB4	2.38	0.40
32:g:109:ASN:OD1	32:g:109:ASN:N	2.54	0.40
34:i:10:ARG:NH2	39:n:153:LEU:O	2.54	0.40
3:C:193:GLU:OE1	17:Q:64:ARG:NE	2.50	0.40
9:I:20:THR:HG22	27:b:12:TRP:HE1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:J:201:PC1:H153	16:P:251:ARG:HH22	1.87	0.40
12:L:226:GLN:HA	12:L:284:THR:HG21	2.03	0.40
13:M:41:LEU:HG	13:M:63:THR:HG23	2.03	0.40
32:g:63:GLY:O	32:g:68:LEU:HD23	2.20	0.40
4:D:121:ALA:HA	4:D:365:THR:HG21	2.02	0.40
8:H:181:MET:HE3	8:H:300:LEU:HG	2.02	0.40
12:L:11:ILE:O	12:L:15:LEU:HD23	2.21	0.40
13:M:409:TYR:O	13:M:413:THR:HG22	2.22	0.40
53:P:501:NDP:H2N	53:P:501:NDP:O5D	2.21	0.40
20:T:37:MET:HE1	20:T:43:ASP:HA	2.03	0.40
37:l:84:ILE:HG22	37:l:85:ARG:H	1.86	0.40
6:F:98:ASP:O	6:F:100:GLY:N	2.55	0.40
14:N:2:ASN:OD1	14:N:2:ASN:N	2.55	0.40
17:Q:19:ILE:HG22	17:Q:19:ILE:O	2.22	0.40
32:g:90:GLU:OE2	32:g:93:ARG:NH2	2.54	0.40
4:D:411:LEU:O	4:D:415:VAL:HG23	2.22	0.40
12:L:245:ALA:HB2	12:L:340:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
2	B	154/224 (69%)	141 (92%)	13 (8%)	0	100	100
3	C	205/263 (78%)	191 (93%)	14 (7%)	0	100	100
4	D	427/463 (92%)	399 (93%)	28 (7%)	0	100	100
5	E	210/248 (85%)	194 (92%)	16 (8%)	0	100	100
6	F	426/464 (92%)	383 (90%)	43 (10%)	0	100	100
7	G	686/727 (94%)	633 (92%)	53 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	316/318 (99%)	291 (92%)	24 (8%)	1 (0%)	36	70
9	I	176/212 (83%)	166 (94%)	10 (6%)	0	100	100
10	J	169/172 (98%)	153 (90%)	16 (10%)	0	100	100
11	K	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
12	L	604/607 (100%)	555 (92%)	49 (8%)	0	100	100
13	M	457/459 (100%)	434 (95%)	22 (5%)	1 (0%)	43	76
14	N	342/345 (99%)	320 (94%)	22 (6%)	0	100	100
15	O	318/355 (90%)	283 (89%)	35 (11%)	0	100	100
16	P	340/377 (90%)	303 (89%)	37 (11%)	0	100	100
17	Q	123/175 (70%)	114 (93%)	9 (7%)	0	100	100
18	R	92/116 (79%)	86 (94%)	6 (6%)	0	100	100
19	S	81/99 (82%)	73 (90%)	8 (10%)	0	100	100
20	T	74/156 (47%)	63 (85%)	11 (15%)	0	100	100
20	U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	V	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
24	Y	138/143 (96%)	132 (96%)	6 (4%)	0	100	100
25	Z	139/144 (96%)	129 (93%)	10 (7%)	0	100	100
26	a	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
27	b	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
30	e	103/106 (97%)	93 (90%)	10 (10%)	0	100	100
31	f	51/57 (90%)	45 (88%)	6 (12%)	0	100	100
32	g	99/151 (66%)	89 (90%)	10 (10%)	0	100	100
33	h	136/189 (72%)	123 (90%)	12 (9%)	1 (1%)	18	53
34	i	90/128 (70%)	85 (94%)	5 (6%)	0	100	100
35	j	60/105 (57%)	54 (90%)	6 (10%)	0	100	100
36	k	73/104 (70%)	69 (94%)	4 (6%)	0	100	100
37	l	152/186 (82%)	135 (89%)	17 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	124/129 (96%)	115 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
40	o	109/137 (80%)	101 (93%)	8 (7%)	0	100	100
41	p	167/176 (95%)	155 (93%)	12 (7%)	0	100	100
42	q	142/145 (98%)	128 (90%)	14 (10%)	0	100	100
43	r	96/113 (85%)	82 (85%)	14 (15%)	0	100	100
44	s	39/104 (38%)	35 (90%)	4 (10%)	0	100	100
All	All	8087/9214 (88%)	7445 (92%)	639 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	h	13	PRO
13	M	224	PRO
8	H	218	GLY

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	103/103 (100%)	103 (100%)	0	100	100
2	B	132/185 (71%)	131 (99%)	1 (1%)	73	86
3	C	189/227 (83%)	188 (100%)	1 (0%)	81	89
4	D	370/394 (94%)	370 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	580/610 (95%)	579 (100%)	1 (0%)	87	92
8	H	279/279 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	136/137 (99%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	548 (100%)	0	100	100
13	M	414/414 (100%)	414 (100%)	0	100	100
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	299/325 (92%)	299 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	79/96 (82%)	79 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	152 (99%)	1 (1%)	76	86
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	122/123 (99%)	122 (100%)	0	100	100
26	a	58/60 (97%)	58 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	42/67 (63%)	42 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	49/53 (92%)	49 (100%)	0	100	100
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	123/162 (76%)	122 (99%)	1 (1%)	73	86
34	i	88/119 (74%)	88 (100%)	0	100	100
35	j	58/87 (67%)	58 (100%)	0	100	100
36	k	58/78 (74%)	58 (100%)	0	100	100
37	l	139/161 (86%)	139 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	162/164 (99%)	162 (100%)	0	100	100
40	o	104/121 (86%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	129/130 (99%)	129 (100%)	0	100	100
43	r	89/96 (93%)	89 (100%)	0	100	100
44	s	40/95 (42%)	40 (100%)	0	100	100
All	All	7176/7947 (90%)	7171 (100%)	5 (0%)	87	93

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

Mol	Chain	Res	Type
2	B	64	CYS
3	C	79	THR
7	G	238	ILE
23	X	55	CYS
33	h	127	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	21	GLN
3	C	69	ASN
4	D	116	GLN
4	D	252	ASN
4	D	409	HIS
6	F	165	ASN
6	F	283	HIS
6	F	293	ASN
7	G	517	ASN
7	G	582	GLN
8	H	97	ASN
8	H	99	ASN
8	H	169	GLN
9	I	67	HIS
10	J	107	ASN
12	L	269	ASN
12	L	270	ASN
12	L	452	ASN
13	M	26	ASN
13	M	54	ASN
13	M	338	HIS
13	M	374	ASN

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Mol	Chain	Res	Type
14	N	91	ASN
14	N	125	HIS
14	N	317	GLN
14	N	342	GLN
17	Q	99	ASN
18	R	13	HIS
23	X	30	HIS
26	a	42	GLN
28	c	33	GLN
29	d	8	HIS
29	d	117	HIS
30	e	96	HIS
32	g	25	GLN
32	g	55	ASN
35	j	42	HIS
36	k	65	ASN
39	n	25	HIS
39	n	77	GLN
40	o	109	GLN
41	p	139	GLN
42	q	116	ASN
44	s	34	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 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
43	AYA	r	1	43	6,7,8	1.86	1 (16%)	6,8,10	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	SAC	i	1	34	7,8,9	0.63	0	7,9,11	1.16	1 (14%)
42	AME	q	1	42	9,10,11	1.53	1 (11%)	9,11,13	1.25	1 (11%)
10	FME	J	1	10	8,9,10	0.97	0	8,9,11	0.97	0
13	FME	M	1	13	8,9,10	1.00	0	8,9,11	1.01	0
11	FME	K	1	11	8,9,10	1.06	1 (12%)	8,9,11	1.42	1 (12%)
14	FME	N	1	14	8,9,10	0.95	0	8,9,11	1.38	1 (12%)
12	FME	L	1	12	8,9,10	1.06	1 (12%)	8,9,11	0.90	1 (12%)
4	2MR	D	85	4	10,12,13	2.49	3 (30%)	5,13,15	2.90	2 (40%)
8	FME	H	1	8	8,9,10	0.93	0	8,9,11	1.85	3 (37%)
1	FME	A	1	1	8,9,10	1.02	0	8,9,11	0.90	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
43	AYA	r	1	43	-	1/5/6/8	-
34	SAC	i	1	34	-	3/7/8/10	-
42	AME	q	1	42	-	0/9/10/12	-
10	FME	J	1	10	-	1/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
14	FME	N	1	14	-	2/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
4	2MR	D	85	4	-	2/10/13/15	-
8	FME	H	1	8	-	5/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.03	1.45	1.34
4	D	85	2MR	CZ-NH2	4.68	1.43	1.33
42	q	1	AME	CT1-N	3.46	1.45	1.34
43	r	1	AYA	CT-N	3.21	1.44	1.34
4	D	85	2MR	CQ1-NH1	-2.68	1.41	1.46
11	K	1	FME	CA-N	-2.08	1.43	1.46
12	L	1	FME	CA-N	-2.08	1.43	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	CD-NE-CZ	4.43	131.69	123.36
4	D	85	2MR	NE-CZ-NH2	-4.43	115.42	119.48
8	H	1	FME	CA-N-CN	3.93	128.87	122.82
11	K	1	FME	C-CA-N	3.37	116.01	109.50
14	N	1	FME	C-CA-N	3.32	115.91	109.50
34	i	1	SAC	O-C-CA	-3.01	117.02	124.77
8	H	1	FME	C-CA-N	2.36	114.06	109.50
8	H	1	FME	CB-CA-N	2.28	114.67	110.52
42	q	1	AME	O-C-CA	-2.16	119.22	124.77
12	L	1	FME	CG-CB-CA	2.01	119.01	112.87

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CA-N-CN
14	N	1	FME	CB-CA-N-CN
34	i	1	SAC	CB-CA-N-C1A
43	r	1	AYA	O-C-CA-CB
4	D	85	2MR	NE-CD-CG-CB
11	K	1	FME	CA-CB-CG-SD
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
12	L	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
13	M	1	FME	CB-CG-SD-CE
4	D	85	2MR	CA-CB-CG-CD
8	H	1	FME	CA-CB-CG-SD
8	H	1	FME	N-CA-CB-CG
34	i	1	SAC	C2A-C1A-N-CA
1	A	1	FME	C-CA-CB-CG
34	i	1	SAC	OAC-C1A-N-CA
12	L	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	i	1	SAC	2	0
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 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	3PE	K	201	-	32,32,50	1.08	4 (12%)	35,37,55	1.12	2 (5%)
55	EHZ	U	201	20	31,36,37	1.62	4 (12%)	36,44,47	2.37	12 (33%)
52	ATP	O	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.83	9 (18%)
51	CDL	q	201	-	56,56,99	1.15	8 (14%)	62,68,111	1.10	4 (6%)
47	HQH	D	501	-	28,30,30	0.92	1 (3%)	27,40,40	1.19	2 (7%)
48	3PE	Y	401	-	40,40,50	0.98	4 (10%)	43,45,55	1.07	2 (4%)
51	CDL	L	701	-	73,73,99	1.03	8 (10%)	79,85,111	1.13	5 (6%)
48	3PE	l	701	-	48,48,50	0.90	3 (6%)	51,53,55	1.15	3 (5%)
45	SF4	I	201	9	0,12,12	-	-	-	-	-
51	CDL	d	202	-	62,62,99	1.10	8 (12%)	68,74,111	1.14	5 (7%)
51	CDL	d	201	-	66,66,99	1.07	8 (12%)	72,78,111	1.11	4 (5%)
51	CDL	N	402	-	64,64,99	1.09	8 (12%)	70,76,111	1.07	4 (5%)
55	EHZ	T	201	20	31,36,37	1.60	5 (16%)	36,44,47	1.61	6 (16%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
46	PC1	J	201	-	41,41,53	1.06	4 (9%)	47,49,61	1.02	2 (4%)
46	PC1	B	203	-	42,42,53	1.09	4 (9%)	48,50,61	0.96	2 (4%)
50	FMN	F	501	-	33,33,33	1.13	2 (6%)	48,50,50	1.44	9 (18%)
45	SF4	G	801	7	0,12,12	-	-	-	-	-
45	SF4	F	502	6	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	3PE	L	702	-	48,48,50	0.87	4 (8%)	51,53,55	1.06	2 (3%)
48	3PE	D	502	-	50,50,50	0.89	4 (8%)	53,55,55	1.15	4 (7%)
46	PC1	Z	201	-	44,44,53	1.06	4 (9%)	50,52,61	1.07	2 (4%)
51	CDL	h	201	-	69,69,99	1.03	8 (11%)	75,81,111	1.07	4 (5%)
45	SF4	I	202	9	0,12,12	-	-	-	-	-
48	3PE	H	401	-	43,43,50	0.93	4 (9%)	46,48,55	1.17	2 (4%)
45	SF4	G	802	7	0,12,12	-	-	-	-	-
53	NDP	P	501	-	51,52,52	2.30	7 (13%)	71,80,80	1.52	14 (19%)
48	3PE	h	202	-	36,36,50	1.03	3 (8%)	39,41,55	1.02	2 (5%)
48	3PE	i	201	-	41,41,50	0.97	4 (9%)	44,46,55	1.08	2 (4%)
45	SF4	B	201	2	0,12,12	-	-	-	-	-
48	3PE	M	501	-	41,41,50	0.96	3 (7%)	44,46,55	1.09	2 (4%)
46	PC1	B	202	-	34,34,53	1.19	4 (11%)	40,42,61	1.05	2 (5%)
51	CDL	N	401	-	58,58,99	1.03	6 (10%)	63,69,111	1.01	3 (4%)
49	FES	E	301	5	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	3PE	K	201	-	-	19/36/36/54	-
55	EHZ	U	201	20	-	14/42/44/45	-
52	ATP	O	401	-	-	5/22/38/38	0/3/3/3
51	CDL	q	201	-	-	26/67/67/110	-
47	HQH	D	501	-	-	10/27/29/29	0/1/1/1
48	3PE	Y	401	-	-	23/44/44/54	-
51	CDL	L	701	-	-	29/84/84/110	-
48	3PE	l	701	-	-	18/52/52/54	-
45	SF4	I	201	9	-	-	0/6/5/5
51	CDL	d	202	-	-	28/73/73/110	-
51	CDL	d	201	-	-	32/77/77/110	-
51	CDL	N	402	-	-	35/75/75/110	-
55	EHZ	T	201	20	-	15/42/44/45	-
49	FES	G	803	7	-	-	0/1/1/1
46	PC1	J	201	-	-	19/45/45/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	B	203	-	-	17/46/46/57	-
50	FMN	F	501	-	-	5/18/18/18	0/3/3/3
45	SF4	G	801	7	-	-	0/6/5/5
45	SF4	F	502	6	-	-	0/6/5/5
48	3PE	L	702	-	-	22/52/52/54	-
48	3PE	D	502	-	-	22/54/54/54	-
46	PC1	Z	201	-	-	18/48/48/57	-
51	CDL	h	201	-	-	29/80/80/110	-
45	SF4	I	202	9	-	-	0/6/5/5
48	3PE	H	401	-	-	19/47/47/54	-
45	SF4	G	802	7	-	-	0/6/5/5
53	NDP	P	501	-	-	6/34/77/77	0/5/5/5
48	3PE	h	202	-	-	17/40/40/54	-
48	3PE	i	201	-	-	17/45/45/54	-
45	SF4	B	201	2	-	-	0/6/5/5
48	3PE	M	501	-	-	19/45/45/54	-
46	PC1	B	202	-	-	11/38/38/57	-
51	CDL	N	401	-	-	30/67/67/110	-
49	FES	E	301	5	-	-	0/1/1/1

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	P	501	NDP	P2B-O2B	12.93	1.82	1.59
55	U	201	EHZ	C15-N2	5.51	1.46	1.33
55	T	201	EHZ	C15-N2	5.27	1.46	1.33
55	T	201	EHZ	C12-N1	4.96	1.45	1.33
55	U	201	EHZ	C12-N1	4.79	1.44	1.33
52	O	401	ATP	C5-C4	4.19	1.46	1.39
53	P	501	NDP	PN-O5D	4.16	1.75	1.59
53	P	501	NDP	PA-O3	3.88	1.63	1.59
53	P	501	NDP	O2B-C2B	-3.42	1.32	1.44
47	D	501	HQH	C12-C19	3.08	1.41	1.37
48	l	701	3PE	O21-C2	-2.89	1.39	1.46
51	L	701	CDL	OB6-CB4	-2.86	1.39	1.46
48	M	501	3PE	O21-C2	-2.86	1.39	1.46
50	F	501	FMN	C4A-N5	2.85	1.36	1.30
46	B	203	PC1	O21-C2	-2.84	1.39	1.46
48	h	202	3PE	O21-C2	-2.81	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	L	702	3PE	O21-C2	-2.80	1.40	1.46
51	N	402	CDL	OA6-CA4	-2.80	1.40	1.46
48	D	502	3PE	O31-C3	-2.76	1.39	1.45
48	i	201	3PE	O21-C2	-2.72	1.40	1.46
55	U	201	EHZ	O4-C15	-2.69	1.18	1.23
51	h	201	CDL	OB6-CB4	-2.65	1.40	1.46
46	B	202	PC1	O21-C2	-2.64	1.40	1.46
51	N	402	CDL	OB6-CB4	-2.64	1.40	1.46
51	h	201	CDL	OA6-CA4	-2.64	1.40	1.46
51	q	201	CDL	OB6-CB4	-2.63	1.40	1.46
48	D	502	3PE	O21-C2	-2.63	1.40	1.46
48	K	201	3PE	O21-C2	-2.62	1.40	1.46
48	M	501	3PE	O31-C3	-2.60	1.39	1.45
48	H	401	3PE	O31-C3	-2.57	1.39	1.45
55	U	201	EHZ	O3-C12	-2.57	1.18	1.23
51	d	201	CDL	OA6-CA4	-2.55	1.40	1.46
48	i	201	3PE	O31-C31	2.55	1.40	1.33
51	d	202	CDL	OB6-CB4	-2.54	1.40	1.46
51	N	401	CDL	OB8-CB7	2.53	1.40	1.33
46	Z	201	PC1	O21-C21	2.52	1.41	1.34
48	K	201	3PE	O31-C3	-2.50	1.39	1.45
51	d	202	CDL	OA6-CA4	-2.50	1.40	1.46
48	Y	401	3PE	O21-C2	-2.50	1.40	1.46
51	q	201	CDL	OA8-CA6	-2.49	1.39	1.45
51	d	201	CDL	OB8-CB7	2.47	1.40	1.33
46	J	201	PC1	O21-C2	-2.47	1.40	1.46
48	l	701	3PE	O31-C3	-2.47	1.39	1.45
55	T	201	EHZ	O4-C15	-2.47	1.18	1.23
52	O	401	ATP	C5-N7	-2.47	1.34	1.39
51	q	201	CDL	OB8-CB7	2.46	1.40	1.33
51	d	201	CDL	OB6-CB4	-2.46	1.40	1.46
48	h	202	3PE	O31-C31	2.46	1.40	1.33
51	L	701	CDL	OA8-CA7	2.45	1.40	1.33
46	B	203	PC1	O31-C31	2.45	1.40	1.33
51	N	401	CDL	OA8-CA7	2.44	1.40	1.33
51	N	402	CDL	OB8-CB7	2.43	1.40	1.33
51	L	701	CDL	OA6-CA4	-2.43	1.40	1.46
46	Z	201	PC1	O31-C31	2.42	1.40	1.33
51	N	402	CDL	OA8-CA7	2.42	1.40	1.33
51	q	201	CDL	OA6-CA4	-2.42	1.40	1.46
55	T	201	EHZ	C9-S1	2.41	1.81	1.76
51	N	401	CDL	OB6-CB4	-2.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	d	202	CDL	OB8-CB7	2.40	1.40	1.33
51	d	202	CDL	OA8-CA7	2.39	1.40	1.33
48	Y	401	3PE	O31-C31	2.39	1.40	1.33
46	J	201	PC1	O31-C31	2.38	1.40	1.33
53	P	501	NDP	O4B-C4B	-2.38	1.39	1.45
51	h	201	CDL	OB8-CB7	2.38	1.40	1.33
46	B	202	PC1	O31-C31	2.37	1.40	1.33
48	H	401	3PE	O31-C31	2.37	1.40	1.33
51	L	701	CDL	OB8-CB7	2.36	1.40	1.33
48	D	502	3PE	O21-C21	2.35	1.40	1.34
51	h	201	CDL	OA8-CA7	2.34	1.40	1.33
51	d	201	CDL	OA8-CA7	2.34	1.40	1.33
48	Y	401	3PE	O31-C3	-2.34	1.39	1.45
53	P	501	NDP	C2B-C1B	2.32	1.58	1.53
51	d	201	CDL	OA8-CA6	-2.31	1.40	1.45
46	J	201	PC1	O21-C21	2.31	1.40	1.34
51	d	202	CDL	OB6-CB5	2.29	1.40	1.34
51	q	201	CDL	OA8-CA7	2.29	1.40	1.33
51	L	701	CDL	OB8-CB6	-2.29	1.40	1.45
48	Y	401	3PE	O21-C21	2.29	1.40	1.34
48	H	401	3PE	O21-C21	2.28	1.40	1.34
48	K	201	3PE	O31-C31	2.28	1.40	1.33
55	T	201	EHZ	O3-C12	-2.27	1.18	1.23
48	L	702	3PE	O31-C31	2.26	1.40	1.33
51	h	201	CDL	OB8-CB6	-2.26	1.40	1.45
51	N	402	CDL	OB6-CB5	2.26	1.40	1.34
46	Z	201	PC1	O31-C3	-2.26	1.40	1.45
46	J	201	PC1	O31-C3	-2.24	1.40	1.45
51	L	701	CDL	OA8-CA6	-2.24	1.40	1.45
51	q	201	CDL	OB6-CB5	2.24	1.40	1.34
46	Z	201	PC1	O21-C2	-2.24	1.41	1.46
51	d	202	CDL	OA8-CA6	-2.24	1.40	1.45
51	N	402	CDL	OA8-CA6	-2.23	1.40	1.45
51	q	201	CDL	OB8-CB6	-2.23	1.40	1.45
51	d	202	CDL	OB8-CB6	-2.23	1.40	1.45
52	O	401	ATP	C5-C6	2.23	1.47	1.41
48	H	401	3PE	O21-C2	-2.22	1.41	1.46
46	B	202	PC1	O21-C21	2.22	1.40	1.34
48	L	702	3PE	O31-C3	-2.22	1.40	1.45
51	d	201	CDL	OB8-CB6	-2.22	1.40	1.45
51	q	201	CDL	OA6-CA5	2.21	1.40	1.34
50	F	501	FMN	C10-N1	2.21	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	i	201	3PE	O21-C21	2.21	1.40	1.34
51	N	401	CDL	OB6-CB5	2.20	1.40	1.34
48	h	202	3PE	O31-C3	-2.20	1.40	1.45
51	N	401	CDL	OA8-CA6	-2.20	1.40	1.45
46	B	202	PC1	O31-C3	-2.19	1.40	1.45
51	d	202	CDL	OA6-CA5	2.19	1.40	1.34
48	K	201	3PE	O21-C21	2.19	1.40	1.34
48	l	701	3PE	O31-C31	2.17	1.39	1.33
51	N	402	CDL	OB8-CB6	-2.17	1.40	1.45
51	h	201	CDL	OB6-CB5	2.17	1.40	1.34
51	N	401	CDL	OB8-CB6	-2.16	1.40	1.45
51	h	201	CDL	OA6-CA5	2.15	1.40	1.34
52	O	401	ATP	C4-N9	-2.13	1.33	1.37
51	d	201	CDL	OA6-CA5	2.13	1.40	1.34
51	h	201	CDL	OA8-CA6	-2.13	1.40	1.45
51	d	201	CDL	OB6-CB5	2.12	1.40	1.34
48	i	201	3PE	O31-C3	-2.11	1.40	1.45
46	B	203	PC1	O21-C21	2.10	1.40	1.34
51	L	701	CDL	OA6-CA5	2.09	1.40	1.34
51	N	402	CDL	OA6-CA5	2.09	1.40	1.34
48	M	501	3PE	O31-C31	2.08	1.39	1.33
46	B	203	PC1	O31-C3	-2.07	1.40	1.45
52	O	401	ATP	C8-N7	2.06	1.35	1.31
48	L	702	3PE	O21-C21	2.03	1.40	1.34
53	P	501	NDP	O5D-C5D	-2.02	1.37	1.44
48	D	502	3PE	O31-C31	2.01	1.39	1.33
51	L	701	CDL	OB6-CB5	2.01	1.39	1.34

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	U	201	EHZ	C16-C15-N2	6.37	128.58	116.48
55	T	201	EHZ	C8-C9-S1	5.80	120.88	113.56
52	O	401	ATP	C5-C4-N3	-5.52	119.12	126.72
48	l	701	3PE	O21-C21-C22	5.00	122.30	111.48
52	O	401	ATP	N3-C4-N9	4.94	135.56	127.17
55	U	201	EHZ	O4-C15-N2	-4.75	112.93	122.98
53	P	501	NDP	P2B-O2B-C2B	-4.74	110.79	123.43
48	i	201	3PE	O21-C21-C22	4.50	121.22	111.48
46	Z	201	PC1	O21-C21-C22	4.38	120.95	111.48
48	H	401	3PE	O21-C21-C22	4.16	120.49	111.48
50	F	501	FMN	C4-N3-C2	-4.12	118.32	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	d	201	CDL	OB6-CB5-C51	4.12	120.39	111.48
51	N	402	CDL	OA6-CA5-C11	4.11	120.37	111.48
46	B	202	PC1	O21-C21-C22	4.11	120.37	111.48
48	D	502	3PE	O21-C21-C22	4.07	120.28	111.48
48	Y	401	3PE	O21-C21-C22	4.06	120.26	111.48
46	J	201	PC1	O21-C21-C22	4.00	120.14	111.48
55	U	201	EHZ	C11-N1-C12	-3.97	115.44	122.82
48	K	201	3PE	O21-C21-C22	3.92	119.97	111.48
51	h	201	CDL	OA6-CA5-C11	3.90	119.92	111.48
55	U	201	EHZ	C13-C12-N1	3.89	123.43	116.34
55	U	201	EHZ	C14-N2-C15	3.87	129.50	122.55
52	O	401	ATP	N3-C2-N1	-3.85	122.75	128.58
51	h	201	CDL	OB6-CB5-C51	3.83	119.77	111.48
51	d	201	CDL	OA6-CA5-C11	3.82	119.75	111.48
55	U	201	EHZ	C14-C13-C12	-3.76	106.12	112.39
52	O	401	ATP	C2-N3-C4	3.75	120.99	111.83
51	N	401	CDL	OB6-CB5-C51	3.75	119.58	111.48
51	L	701	CDL	OB6-CB5-C51	3.72	119.53	111.48
51	d	202	CDL	OB6-CB5-C51	3.68	119.44	111.48
51	d	202	CDL	OA6-CA5-C11	3.67	119.41	111.48
48	h	202	3PE	O21-C21-C22	3.65	119.37	111.48
51	L	701	CDL	OA6-CA5-C11	3.64	119.35	111.48
55	U	201	EHZ	C8-C9-S1	3.63	118.15	113.56
55	U	201	EHZ	C10-S1-C9	3.63	112.58	101.84
48	M	501	3PE	O21-C21-C22	3.62	119.31	111.48
52	O	401	ATP	C4-N9-C8	3.61	109.53	105.74
53	P	501	NDP	O2B-P2B-O1X	-3.57	96.62	109.33
48	L	702	3PE	O21-C21-C22	3.53	119.12	111.48
51	q	201	CDL	OA6-CA5-C11	3.50	119.06	111.48
50	F	501	FMN	C4A-C10-N10	3.42	121.38	116.48
46	B	203	PC1	O21-C21-C22	3.42	118.87	111.48
53	P	501	NDP	O3-PA-O1A	-3.40	100.48	110.70
51	q	201	CDL	OB6-CB5-C51	3.37	118.78	111.48
55	U	201	EHZ	C19-C17-C16	3.35	114.48	108.77
48	H	401	3PE	O31-C31-C32	3.22	121.64	111.83
51	N	402	CDL	OB6-CB5-C51	3.19	118.39	111.48
47	D	501	HQH	O3-C25-C23	3.11	127.13	116.64
50	F	501	FMN	C4A-C4-N3	3.06	121.04	113.25
51	L	701	CDL	OB8-CB7-C71	2.94	120.80	111.83
51	d	202	CDL	OA8-CA7-C31	2.92	120.73	111.83
50	F	501	FMN	O4-C4-C4A	-2.91	118.84	126.53
51	N	401	CDL	OB8-CB7-C71	2.87	120.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	J	201	PC1	O31-C31-C32	2.83	120.47	111.83
51	q	201	CDL	OA8-CA7-C31	2.83	120.47	111.83
51	d	201	CDL	OA8-CA7-C31	2.83	120.45	111.83
51	L	701	CDL	OA8-CA7-C31	2.82	120.45	111.83
48	h	202	3PE	O31-C31-C32	2.82	120.44	111.83
53	P	501	NDP	PA-O5B-C5B	-2.80	105.30	121.35
51	N	402	CDL	OA8-CA7-C31	2.79	120.33	111.83
52	O	401	ATP	C4-C5-N7	-2.77	107.42	110.58
51	d	201	CDL	OB8-CB7-C71	2.75	120.22	111.83
51	h	201	CDL	OB8-CB7-C71	2.73	120.17	111.83
46	Z	201	PC1	O31-C31-C32	2.73	120.16	111.83
53	P	501	NDP	C2A-N1A-C6A	-2.67	114.34	118.73
48	Y	401	3PE	O31-C31-C32	2.67	119.98	111.83
51	N	401	CDL	OA8-CA7-C31	2.66	119.95	111.83
50	F	501	FMN	C4A-C10-N1	-2.65	118.09	124.59
47	D	501	HQH	C21-C18-C11	2.65	129.90	125.89
53	P	501	NDP	N3A-C4A-N9A	2.63	131.65	127.17
53	P	501	NDP	O4B-C4B-C3B	2.63	110.37	105.15
51	d	202	CDL	OB8-CB7-C71	2.62	119.83	111.83
46	B	202	PC1	O31-C31-C32	2.62	119.82	111.83
48	l	701	3PE	O31-C31-C32	2.61	119.79	111.83
55	T	201	EHZ	O2-C9-C8	-2.59	119.67	123.74
48	M	501	3PE	O31-C31-C32	2.58	119.71	111.83
48	L	702	3PE	O31-C31-C32	2.58	119.69	111.83
55	T	201	EHZ	O2-C9-S1	-2.54	119.45	122.68
51	d	202	CDL	CA6-CA4-CA3	-2.53	105.88	111.78
53	P	501	NDP	O3X-P2B-O2X	2.53	117.30	107.80
46	B	203	PC1	O31-C31-C32	2.52	119.52	111.83
48	l	701	3PE	O21-C21-O22	-2.52	117.81	123.70
51	q	201	CDL	OB8-CB7-C71	2.51	119.48	111.83
51	N	402	CDL	OB8-CB7-C71	2.50	119.47	111.83
48	K	201	3PE	O31-C31-C32	2.50	119.47	111.83
48	D	502	3PE	O31-C31-C32	2.49	119.43	111.83
53	P	501	NDP	O2N-PN-O3	2.49	114.00	107.27
53	P	501	NDP	PN-O5D-C5D	-2.45	107.32	121.35
55	U	201	EHZ	O3-C12-N1	-2.43	118.27	123.03
51	h	201	CDL	OA8-CA7-C31	2.40	119.14	111.83
52	O	401	ATP	N9-C8-N7	-2.36	110.58	113.94
52	O	401	ATP	C5-N7-C8	2.36	107.15	103.45
53	P	501	NDP	C5A-C4A-N3A	-2.35	123.48	126.72
53	P	501	NDP	O2N-PN-O1N	2.34	123.31	112.44
55	T	201	EHZ	C10-S1-C9	2.27	108.54	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	D	502	3PE	C3-C2-C1	-2.25	106.53	111.78
48	i	201	3PE	O31-C31-C32	2.18	118.48	111.83
53	P	501	NDP	O5D-PN-O1N	-2.14	100.45	108.94
50	F	501	FMN	C10-C4A-N5	-2.09	120.53	124.81
55	T	201	EHZ	C16-C15-N2	2.09	120.45	116.48
53	P	501	NDP	O7N-C7N-N7N	-2.05	118.29	122.89
55	U	201	EHZ	O3-C12-C13	-2.05	118.30	122.02
50	F	501	FMN	C1'-N10-C9A	2.04	124.59	120.63
51	L	701	CDL	CB4-OB6-CB5	-2.03	112.93	117.80
55	U	201	EHZ	C7-C8-C9	-2.03	109.32	113.86
50	F	501	FMN	C10-N1-C2	2.02	121.21	116.85
48	D	502	3PE	C3-O31-C31	-2.01	109.75	117.12
52	O	401	ATP	C2-N1-C6	2.01	122.03	118.73
50	F	501	FMN	C4-C4A-C10	2.01	120.38	116.93
55	T	201	EHZ	C11-N1-C12	-2.00	119.10	122.82

There are no chirality outliers.

All (505) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C11-O13-P-O11
46	B	203	PC1	C1-O11-P-O14
46	B	203	PC1	O13-C11-C12-N
46	J	201	PC1	O13-C11-C12-N
46	Z	201	PC1	C1-O11-P-O13
46	Z	201	PC1	O13-C11-C12-N
47	D	501	HQH	C11-C18-C21-C15
47	D	501	HQH	C22-C11-C18-C21
47	D	501	HQH	C8-C11-C18-C21
47	D	501	HQH	C19-C12-C13-C20
48	H	401	3PE	C1-O11-P-O14
48	H	401	3PE	C11-O13-P-O11
48	H	401	3PE	C11-O13-P-O14
48	K	201	3PE	C1-O11-P-O13
48	K	201	3PE	C1-O11-P-O14
48	K	201	3PE	C11-O13-P-O11
48	K	201	3PE	C11-O13-P-O12
48	K	201	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
48	K	201	3PE	O13-C11-C12-N
48	L	702	3PE	C1-O11-P-O12
48	L	702	3PE	C1-O11-P-O14
48	L	702	3PE	C11-O13-P-O11
48	L	702	3PE	C11-O13-P-O14
48	L	702	3PE	O13-C11-C12-N
48	M	501	3PE	C11-O13-P-O11
48	M	501	3PE	C11-O13-P-O14
48	M	501	3PE	O13-C11-C12-N
48	Y	401	3PE	C1-O11-P-O13
48	Y	401	3PE	C1-O11-P-O14
48	Y	401	3PE	C11-O13-P-O11
48	Y	401	3PE	C11-O13-P-O12
48	Y	401	3PE	C11-O13-P-O14
48	Y	401	3PE	O13-C11-C12-N
48	h	202	3PE	C1-O11-P-O12
48	h	202	3PE	C1-O11-P-O13
48	h	202	3PE	C1-O11-P-O14
48	h	202	3PE	C11-O13-P-O11
48	h	202	3PE	C11-O13-P-O12
48	h	202	3PE	C11-O13-P-O14
48	h	202	3PE	O13-C11-C12-N
48	h	202	3PE	O22-C21-O21-C2
48	i	201	3PE	O13-C11-C12-N
48	i	201	3PE	C22-C21-O21-C2
48	l	701	3PE	C1-O11-P-O14
48	l	701	3PE	O13-C11-C12-N
48	l	701	3PE	C22-C21-O21-C2
50	F	501	FMN	N10-C1'-C2'-O2'
50	F	501	FMN	N10-C1'-C2'-C3'
50	F	501	FMN	C5'-O5'-P-O1P
50	F	501	FMN	C5'-O5'-P-O2P
50	F	501	FMN	C5'-O5'-P-O3P
51	L	701	CDL	OB7-CB5-OB6-CB4
51	L	701	CDL	C51-CB5-OB6-CB4
51	N	401	CDL	CB2-C1-CA2-OA2
51	N	401	CDL	CB2-OB2-PB2-OB3
51	N	401	CDL	CB2-OB2-PB2-OB4
51	N	401	CDL	CB2-OB2-PB2-OB5
51	N	401	CDL	C51-CB5-OB6-CB4
51	N	402	CDL	C1-CA2-OA2-PA1
51	N	402	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	N	402	CDL	C11-CA5-OA6-CA4
51	N	402	CDL	CB2-OB2-PB2-OB4
51	N	402	CDL	CB2-OB2-PB2-OB5
51	d	201	CDL	CA2-C1-CB2-OB2
51	d	201	CDL	CA3-OA5-PA1-OA2
51	d	201	CDL	CA3-OA5-PA1-OA3
51	d	201	CDL	CB2-OB2-PB2-OB5
51	d	201	CDL	C51-CB5-OB6-CB4
51	d	202	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	O1-C1-CB2-OB2
51	h	201	CDL	CA2-C1-CB2-OB2
51	h	201	CDL	CA2-OA2-PA1-OA4
51	h	201	CDL	CA2-OA2-PA1-OA5
51	h	201	CDL	CA3-OA5-PA1-OA2
51	h	201	CDL	CA3-OA5-PA1-OA3
51	h	201	CDL	CA3-OA5-PA1-OA4
51	h	201	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	CB2-OB2-PB2-OB5
51	q	201	CDL	CA2-OA2-PA1-OA3
51	q	201	CDL	OB6-CB4-CB6-OB8
52	O	401	ATP	C5'-O5'-PA-O3A
53	P	501	NDP	O4D-C4D-C5D-O5D
53	P	501	NDP	O4D-C1D-N1N-C6N
55	T	201	EHZ	C6-C7-C8-C9
55	T	201	EHZ	C16-C17-C20-O6
55	U	201	EHZ	O1-C7-C8-C9
55	U	201	EHZ	C6-C7-C8-C9
55	U	201	EHZ	C11-C10-S1-C9
55	U	201	EHZ	C16-C15-N2-C14
46	J	201	PC1	O32-C31-O31-C3
48	D	502	3PE	O32-C31-O31-C3
48	H	401	3PE	O32-C31-O31-C3
51	N	402	CDL	OA9-CA7-OA8-CA6
46	J	201	PC1	C32-C31-O31-C3
48	H	401	3PE	C32-C31-O31-C3
51	d	201	CDL	C71-CB7-OB8-CB6
51	q	201	CDL	C31-CA7-OA8-CA6
48	L	702	3PE	O32-C31-O31-C3
48	h	202	3PE	O32-C31-O31-C3
51	d	201	CDL	OA9-CA7-OA8-CA6
51	d	201	CDL	OB9-CB7-OB8-CB6
51	d	202	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
51	d	202	CDL	OB9-CB7-OB8-CB6
51	h	201	CDL	OB9-CB7-OB8-CB6
51	q	201	CDL	OA9-CA7-OA8-CA6
48	M	501	3PE	O22-C21-O21-C2
48	i	201	3PE	O22-C21-O21-C2
48	l	701	3PE	O22-C21-O21-C2
51	N	401	CDL	OB7-CB5-OB6-CB4
51	N	402	CDL	OA7-CA5-OA6-CA4
51	d	201	CDL	OB7-CB5-OB6-CB4
48	D	502	3PE	C32-C31-O31-C3
48	L	702	3PE	C32-C31-O31-C3
51	N	402	CDL	C31-CA7-OA8-CA6
51	d	202	CDL	C31-CA7-OA8-CA6
51	d	202	CDL	C71-CB7-OB8-CB6
51	h	201	CDL	C71-CB7-OB8-CB6
48	M	501	3PE	C22-C21-O21-C2
48	h	202	3PE	C22-C21-O21-C2
48	K	201	3PE	C32-C31-O31-C3
48	h	202	3PE	C32-C31-O31-C3
51	d	201	CDL	C31-CA7-OA8-CA6
51	N	401	CDL	O1-C1-CA2-OA2
51	d	201	CDL	O1-C1-CB2-OB2
51	q	201	CDL	O1-C1-CB2-OB2
48	Y	401	3PE	C32-C31-O31-C3
48	l	701	3PE	C32-C31-O31-C3
51	N	402	CDL	C71-CB7-OB8-CB6
48	K	201	3PE	O32-C31-O31-C3
48	l	701	3PE	O32-C31-O31-C3
55	U	201	EHZ	O4-C15-N2-C14
46	B	202	PC1	C22-C21-O21-C2
48	L	702	3PE	C22-C21-O21-C2
51	h	201	CDL	C11-CA5-OA6-CA4
51	L	701	CDL	C71-CB7-OB8-CB6
51	N	402	CDL	OB9-CB7-OB8-CB6
48	Y	401	3PE	O32-C31-O31-C3
51	L	701	CDL	OB9-CB7-OB8-CB6
51	h	201	CDL	OA7-CA5-OA6-CA4
51	d	202	CDL	CB2-C1-CA2-OA2
46	B	203	PC1	C32-C31-O31-C3
51	N	401	CDL	C31-CA7-OA8-CA6
51	q	201	CDL	C71-CB7-OB8-CB6
48	h	202	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
51	L	701	CDL	O1-C1-CA2-OA2
46	B	203	PC1	O32-C31-O31-C3
48	H	401	3PE	C22-C21-O21-C2
51	N	402	CDL	CA7-C31-C32-C33
46	B	202	PC1	O22-C21-O21-C2
48	L	702	3PE	O22-C21-O21-C2
48	l	701	3PE	C21-C22-C23-C24
51	d	201	CDL	CA5-C11-C12-C13
51	N	401	CDL	OA9-CA7-OA8-CA6
51	q	201	CDL	OB9-CB7-OB8-CB6
46	J	201	PC1	C21-C22-C23-C24
51	d	201	CDL	CB5-C51-C52-C53
51	N	401	CDL	OA5-CA3-CA4-OA6
48	i	201	3PE	C21-C22-C23-C24
51	N	401	CDL	C71-CB7-OB8-CB6
51	d	202	CDL	CA7-C31-C32-C33
51	h	201	CDL	CB7-C71-C72-C73
48	H	401	3PE	O22-C21-O21-C2
51	L	701	CDL	CB2-C1-CA2-OA2
51	N	401	CDL	OA5-CA3-CA4-CA6
51	q	201	CDL	CA2-C1-CB2-OB2
48	M	501	3PE	C32-C31-O31-C3
51	d	202	CDL	O1-C1-CA2-OA2
46	B	202	PC1	C2-C1-O11-P
55	T	201	EHZ	C5-C6-C7-O1
48	h	202	3PE	C34-C35-C36-C37
51	L	701	CDL	C11-CA5-OA6-CA4
51	N	401	CDL	OB9-CB7-OB8-CB6
48	M	501	3PE	C36-C37-C38-C39
47	D	501	HQH	C24-C25-O3-C30
48	h	202	3PE	C25-C26-C27-C28
51	N	401	CDL	C31-C32-C33-C34
46	J	201	PC1	C27-C28-C29-C2A
48	D	502	3PE	C28-C29-C2A-C2B
48	H	401	3PE	C34-C35-C36-C37
48	Y	401	3PE	C33-C34-C35-C36
51	L	701	CDL	OA7-CA5-OA6-CA4
51	d	201	CDL	C31-C32-C33-C34
51	q	201	CDL	C31-C32-C33-C34
48	i	201	3PE	C22-C23-C24-C25
51	h	201	CDL	C18-C19-C20-C21
46	B	203	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
53	P	501	NDP	C3D-C4D-C5D-O5D
51	L	701	CDL	C52-C53-C54-C55
48	M	501	3PE	O32-C31-O31-C3
51	N	402	CDL	C79-C80-C81-C82
48	l	701	3PE	C22-C23-C24-C25
51	q	201	CDL	C15-C16-C17-C18
51	N	402	CDL	C83-C84-C85-C86
51	L	701	CDL	CB3-CB4-CB6-OB8
48	l	701	3PE	C39-C3A-C3B-C3C
46	B	202	PC1	C21-C22-C23-C24
48	D	502	3PE	C21-C22-C23-C24
48	K	201	3PE	C31-C32-C33-C34
51	d	202	CDL	CA5-C11-C12-C13
48	M	501	3PE	C22-C23-C24-C25
46	Z	201	PC1	C29-C2A-C2B-C2C
48	M	501	3PE	C3D-C3E-C3F-C3G
51	d	202	CDL	C11-CA5-OA6-CA4
51	N	402	CDL	C52-C53-C54-C55
46	Z	201	PC1	C2C-C2D-C2E-C2F
51	h	201	CDL	C51-C52-C53-C54
46	B	203	PC1	C22-C23-C24-C25
46	B	203	PC1	C3B-C3C-C3D-C3E
51	h	201	CDL	CA5-C11-C12-C13
51	d	201	CDL	C59-C60-C61-C62
48	L	702	3PE	C32-C33-C34-C35
48	l	701	3PE	C3B-C3C-C3D-C3E
48	D	502	3PE	C22-C21-O21-C2
48	Y	401	3PE	C22-C21-O21-C2
51	q	201	CDL	C51-CB5-OB6-CB4
46	B	203	PC1	O22-C21-O21-C2
48	D	502	3PE	O22-C21-O21-C2
46	B	203	PC1	C35-C36-C37-C38
51	L	701	CDL	C74-C75-C76-C77
48	Y	401	3PE	C37-C38-C39-C3A
46	J	201	PC1	C24-C25-C26-C27
48	D	502	3PE	O11-C1-C2-O21
51	L	701	CDL	OA5-CA3-CA4-OA6
51	d	201	CDL	C11-CA5-OA6-CA4
48	l	701	3PE	C32-C33-C34-C35
51	N	401	CDL	C54-C55-C56-C57
48	H	401	3PE	C39-C3A-C3B-C3C
48	L	702	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
55	U	201	EHZ	C2-C3-C4-C5
51	h	201	CDL	CB5-C51-C52-C53
46	J	201	PC1	O21-C2-C3-O31
48	Y	401	3PE	O21-C2-C3-O31
51	L	701	CDL	OB6-CB4-CB6-OB8
51	L	701	CDL	C78-C79-C80-C81
51	d	201	CDL	C56-C57-C58-C59
51	h	201	CDL	C1-CA2-OA2-PA1
51	L	701	CDL	C36-C37-C38-C39
48	Y	401	3PE	O22-C21-O21-C2
51	N	402	CDL	CA2-C1-CB2-OB2
51	N	402	CDL	O1-C1-CA2-OA2
48	K	201	3PE	C23-C24-C25-C26
46	Z	201	PC1	C27-C28-C29-C2A
48	K	201	3PE	O11-C1-C2-C3
51	L	701	CDL	OA5-CA3-CA4-CA6
51	d	202	CDL	OA7-CA5-OA6-CA4
51	q	201	CDL	OB7-CB5-OB6-CB4
46	B	203	PC1	C1-C2-C3-O31
46	Z	201	PC1	C1-C2-C3-O31
48	M	501	3PE	C1-C2-C3-O31
48	h	202	3PE	C1-C2-C3-O31
51	d	201	CDL	CB3-CB4-CB6-OB8
51	d	202	CDL	CB3-CB4-CB6-OB8
51	h	201	CDL	CA3-CA4-CA6-OA8
51	N	402	CDL	O1-C1-CB2-OB2
55	U	201	EHZ	C3-C4-C5-C6
51	N	401	CDL	CB4-CB3-OB5-PB2
48	D	502	3PE	C3C-C3D-C3E-C3F
48	L	702	3PE	C34-C35-C36-C37
51	L	701	CDL	CA6-CA4-OA6-CA5
51	d	202	CDL	C76-C77-C78-C79
55	T	201	EHZ	C21-C1-C2-C3
51	d	201	CDL	C34-C35-C36-C37
48	i	201	3PE	C24-C25-C26-C27
51	L	701	CDL	C76-C77-C78-C79
48	l	701	3PE	C2E-C2F-C2G-C2H
46	B	203	PC1	C3F-C3G-C3H-C3I
48	D	502	3PE	C37-C38-C39-C3A
48	D	502	3PE	C2B-C2C-C2D-C2E
48	M	501	3PE	C3A-C3B-C3C-C3D
48	l	701	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
46	Z	201	PC1	O21-C2-C3-O31
51	N	402	CDL	C76-C77-C78-C79
46	J	201	PC1	C39-C3A-C3B-C3C
48	D	502	3PE	C32-C33-C34-C35
53	P	501	NDP	PN-O3-PA-O1A
51	d	202	CDL	C33-C34-C35-C36
46	J	201	PC1	C34-C35-C36-C37
46	J	201	PC1	C32-C33-C34-C35
48	L	702	3PE	C3F-C3G-C3H-C3I
47	D	501	HQH	O1-C7-C9-C16
48	Y	401	3PE	C23-C24-C25-C26
46	Z	201	PC1	C25-C26-C27-C28
48	K	201	3PE	C33-C34-C35-C36
48	L	702	3PE	C2B-C2C-C2D-C2E
51	L	701	CDL	CA7-C31-C32-C33
48	D	502	3PE	O11-C1-C2-C3
51	N	402	CDL	OA5-CA3-CA4-CA6
51	L	701	CDL	C57-C58-C59-C60
51	N	402	CDL	CB5-C51-C52-C53
51	L	701	CDL	C33-C34-C35-C36
51	N	402	CDL	C54-C55-C56-C57
46	J	201	PC1	C1-C2-C3-O31
48	Y	401	3PE	C1-C2-C3-O31
48	i	201	3PE	C1-C2-C3-O31
51	N	402	CDL	CB3-CB4-CB6-OB8
48	H	401	3PE	C36-C37-C38-C39
51	N	401	CDL	C71-C72-C73-C74
51	d	201	CDL	OA7-CA5-OA6-CA4
51	L	701	CDL	C1-CA2-OA2-PA1
51	d	202	CDL	C73-C74-C75-C76
55	T	201	EHZ	O1-C7-C8-C9
55	T	201	EHZ	O2-C9-S1-C10
48	Y	401	3PE	C35-C36-C37-C38
46	B	203	PC1	O21-C2-C3-O31
48	h	202	3PE	C31-C32-C33-C34
48	i	201	3PE	C31-C32-C33-C34
55	T	201	EHZ	C8-C9-S1-C10
51	h	201	CDL	C74-C75-C76-C77
51	q	201	CDL	C71-C72-C73-C74
48	l	701	3PE	O11-C1-C2-C3
51	q	201	CDL	OA5-CA3-CA4-CA6
51	N	402	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
48	H	401	3PE	C3-C2-O21-C21
51	N	401	CDL	CB6-CB4-OB6-CB5
51	N	402	CDL	CA5-C11-C12-C13
51	d	202	CDL	CA6-CA4-OA6-CA5
55	U	201	EHZ	C4-C5-C6-C7
48	l	701	3PE	O11-C1-C2-O21
51	q	201	CDL	OA5-CA3-CA4-OA6
51	L	701	CDL	C14-C15-C16-C17
51	d	202	CDL	C79-C80-C81-C82
46	B	202	PC1	C12-C11-O13-P
48	K	201	3PE	C12-C11-O13-P
48	L	702	3PE	C12-C11-O13-P
55	U	201	EHZ	C15-C16-C17-C19
51	q	201	CDL	C17-C18-C19-C20
48	i	201	3PE	O21-C2-C3-O31
51	d	201	CDL	OB6-CB4-CB6-OB8
51	h	201	CDL	OA6-CA4-CA6-OA8
47	D	501	HQH	C6-C7-C9-C14
51	L	701	CDL	C35-C36-C37-C38
51	d	201	CDL	C13-C14-C15-C16
51	L	701	CDL	C31-C32-C33-C34
46	B	202	PC1	O13-C11-C12-N
46	Z	201	PC1	C37-C38-C39-C3A
51	L	701	CDL	C11-C12-C13-C14
48	H	401	3PE	C26-C27-C28-C29
47	D	501	HQH	C6-C7-C9-C16
48	D	502	3PE	C35-C36-C37-C38
48	Y	401	3PE	C25-C26-C27-C28
55	U	201	EHZ	C1-C2-C3-C4
48	H	401	3PE	O11-C1-C2-C3
55	T	201	EHZ	C18-C17-C20-O6
55	T	201	EHZ	C19-C17-C20-O6
55	U	201	EHZ	C15-C16-C17-C20
51	N	401	CDL	C56-C57-C58-C59
48	L	702	3PE	C24-C25-C26-C27
48	i	201	3PE	C27-C28-C29-C2A
48	Y	401	3PE	C39-C3A-C3B-C3C
51	N	402	CDL	OA5-CA3-CA4-OA6
48	i	201	3PE	C34-C35-C36-C37
48	h	202	3PE	O21-C2-C3-O31
51	N	402	CDL	OB6-CB4-CB6-OB8
51	N	401	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
48	H	401	3PE	C24-C25-C26-C27
48	l	701	3PE	C29-C2A-C2B-C2C
51	q	201	CDL	CB3-CB4-CB6-OB8
51	d	201	CDL	C12-C13-C14-C15
51	q	201	CDL	CB7-C71-C72-C73
51	q	201	CDL	C52-C53-C54-C55
46	B	203	PC1	C37-C38-C39-C3A
46	B	202	PC1	C1-O11-P-O13
48	D	502	3PE	C1-O11-P-O12
48	D	502	3PE	C1-O11-P-O13
48	D	502	3PE	O13-C11-C12-N
48	H	401	3PE	C1-O11-P-O13
48	H	401	3PE	C11-O13-P-O12
48	K	201	3PE	C1-O11-P-O12
48	L	702	3PE	C1-O11-P-O13
48	L	702	3PE	C11-O13-P-O12
48	M	501	3PE	C1-O11-P-O12
48	M	501	3PE	C1-O11-P-O13
48	M	501	3PE	C1-O11-P-O14
48	M	501	3PE	C11-O13-P-O12
48	Y	401	3PE	C1-O11-P-O12
48	l	701	3PE	C1-O11-P-O13
51	N	401	CDL	CA3-OA5-PA1-OA3
51	N	401	CDL	CB3-OB5-PB2-OB2
51	N	401	CDL	CB3-OB5-PB2-OB3
51	N	401	CDL	CB3-OB5-PB2-OB4
51	N	402	CDL	CA2-OA2-PA1-OA3
51	N	402	CDL	CA3-OA5-PA1-OA2
51	N	402	CDL	CA3-OA5-PA1-OA4
51	N	402	CDL	CB2-OB2-PB2-OB3
51	d	201	CDL	CA3-OA5-PA1-OA4
51	d	201	CDL	CB2-OB2-PB2-OB3
51	d	202	CDL	CA2-OA2-PA1-OA3
51	q	201	CDL	CA2-OA2-PA1-OA4
51	q	201	CDL	CA2-OA2-PA1-OA5
51	q	201	CDL	CB3-OB5-PB2-OB2
51	q	201	CDL	CB3-OB5-PB2-OB4
52	O	401	ATP	C5'-O5'-PA-O1A
48	i	201	3PE	C2B-C2C-C2D-C2E
48	D	502	3PE	C25-C26-C27-C28
51	d	201	CDL	CB3-CB4-OB6-CB5
51	h	201	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
51	q	201	CDL	CA6-CA4-OA6-CA5
46	Z	201	PC1	C22-C23-C24-C25
55	T	201	EHZ	C5-C6-C7-C8
48	M	501	3PE	C33-C34-C35-C36
51	d	202	CDL	CA2-C1-CB2-OB2
48	K	201	3PE	O11-C1-C2-O21
46	Z	201	PC1	C36-C37-C38-C39
51	d	202	CDL	CA4-CA3-OA5-PA1
48	L	702	3PE	C25-C26-C27-C28
48	M	501	3PE	O21-C2-C3-O31
51	d	202	CDL	OB6-CB4-CB6-OB8
51	d	201	CDL	C71-C72-C73-C74
51	N	402	CDL	C74-C75-C76-C77
51	N	401	CDL	C72-C71-CB7-OB8
47	D	501	HQH	O1-C7-C9-C14
52	O	401	ATP	PB-O3A-PA-O2A
48	H	401	3PE	C38-C39-C3A-C3B
55	T	201	EHZ	C7-C8-C9-O2
51	N	401	CDL	C75-C76-C77-C78
51	d	201	CDL	CA7-C31-C32-C33
51	d	201	CDL	C54-C55-C56-C57
48	i	201	3PE	C2A-C2B-C2C-C2D
48	D	502	3PE	C2D-C2E-C2F-C2G
51	L	701	CDL	C73-C74-C75-C76
46	J	201	PC1	O11-C1-C2-O21
46	Z	201	PC1	O11-C1-C2-C3
51	h	201	CDL	C32-C33-C34-C35
48	l	701	3PE	C2A-C2B-C2C-C2D
46	J	201	PC1	C36-C37-C38-C39
47	D	501	HQH	C23-C25-O3-C30
48	Y	401	3PE	C21-C22-C23-C24
46	J	201	PC1	C37-C38-C39-C3A
51	d	201	CDL	CA6-CA4-OA6-CA5
48	i	201	3PE	C36-C37-C38-C39
51	h	201	CDL	C24-C25-C26-C27
48	i	201	3PE	O11-C1-C2-O21
48	i	201	3PE	C2-C1-O11-P
51	d	202	CDL	C1-CA2-OA2-PA1
51	h	201	CDL	C1-CB2-OB2-PB2
46	J	201	PC1	C38-C39-C3A-C3B
55	T	201	EHZ	C21-C22-C23-C24
51	d	202	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
46	Z	201	PC1	C11-C12-N-C14
51	N	401	CDL	O1-C1-CB2-OB2
52	O	401	ATP	PG-O3B-PB-O1B
53	P	501	NDP	O4B-C4B-C5B-O5B
51	N	402	CDL	C82-C83-C84-C85
46	J	201	PC1	C28-C29-C2A-C2B
48	H	401	3PE	O11-C1-C2-O21
48	Y	401	3PE	C26-C27-C28-C29
46	Z	201	PC1	O21-C21-C22-C23
46	J	201	PC1	O11-C1-C2-C3
48	L	702	3PE	C21-C22-C23-C24
51	d	201	CDL	C11-C12-C13-C14
48	L	702	3PE	C36-C37-C38-C39
48	D	502	3PE	O31-C31-C32-C33
51	h	201	CDL	CB3-CB4-OB6-CB5
48	K	201	3PE	C25-C26-C27-C28
48	i	201	3PE	C32-C33-C34-C35
48	D	502	3PE	C3E-C3F-C3G-C3H
52	O	401	ATP	O4'-C4'-C5'-O5'
51	N	401	CDL	C51-C52-C53-C54
55	U	201	EHZ	C15-C16-C17-C18
46	B	203	PC1	C32-C33-C34-C35
55	T	201	EHZ	C1-C2-C3-C4
48	M	501	3PE	C32-C33-C34-C35
48	K	201	3PE	O21-C21-C22-C23
55	T	201	EHZ	C4-C5-C6-C7
51	N	402	CDL	C32-C31-CA7-OA8
51	q	201	CDL	C12-C13-C14-C15
53	P	501	NDP	PN-O3-PA-O2A
48	D	502	3PE	C22-C23-C24-C25
46	Z	201	PC1	C11-C12-N-C13
46	Z	201	PC1	C11-C12-N-C15
51	d	202	CDL	C12-C11-CA5-OA6
46	J	201	PC1	C3A-C3B-C3C-C3D
46	J	201	PC1	C23-C24-C25-C26
55	T	201	EHZ	C2-C1-C21-C22
51	d	202	CDL	C71-C72-C73-C74
55	U	201	EHZ	C18-C17-C20-O6
55	U	201	EHZ	C19-C17-C20-O6
51	N	402	CDL	C75-C76-C77-C78
48	D	502	3PE	C24-C25-C26-C27
48	L	702	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	Y	401	3PE	O21-C21-C22-C23
51	N	402	CDL	C32-C31-CA7-OA9
51	d	202	CDL	C12-C11-CA5-OA7
51	d	202	CDL	C32-C31-CA7-OA8
51	d	202	CDL	O1-C1-CB2-OB2
46	Z	201	PC1	C32-C33-C34-C35
51	h	201	CDL	OB7-CB5-OB6-CB4
51	q	201	CDL	OA7-CA5-OA6-CA4
48	K	201	3PE	O22-C21-C22-C23
51	L	701	CDL	C53-C54-C55-C56
46	B	202	PC1	C35-C36-C37-C38
48	H	401	3PE	O21-C21-C22-C23
51	N	401	CDL	C74-C75-C76-C77
46	B	203	PC1	C23-C24-C25-C26
48	K	201	3PE	C27-C28-C29-C2A
48	Y	401	3PE	O22-C21-C22-C23
51	N	401	CDL	C52-C51-CB5-OB6
51	d	201	CDL	C64-C65-C66-C67
51	h	201	CDL	C51-CB5-OB6-CB4
46	Z	201	PC1	C34-C35-C36-C37
51	L	701	CDL	C72-C71-CB7-OB8

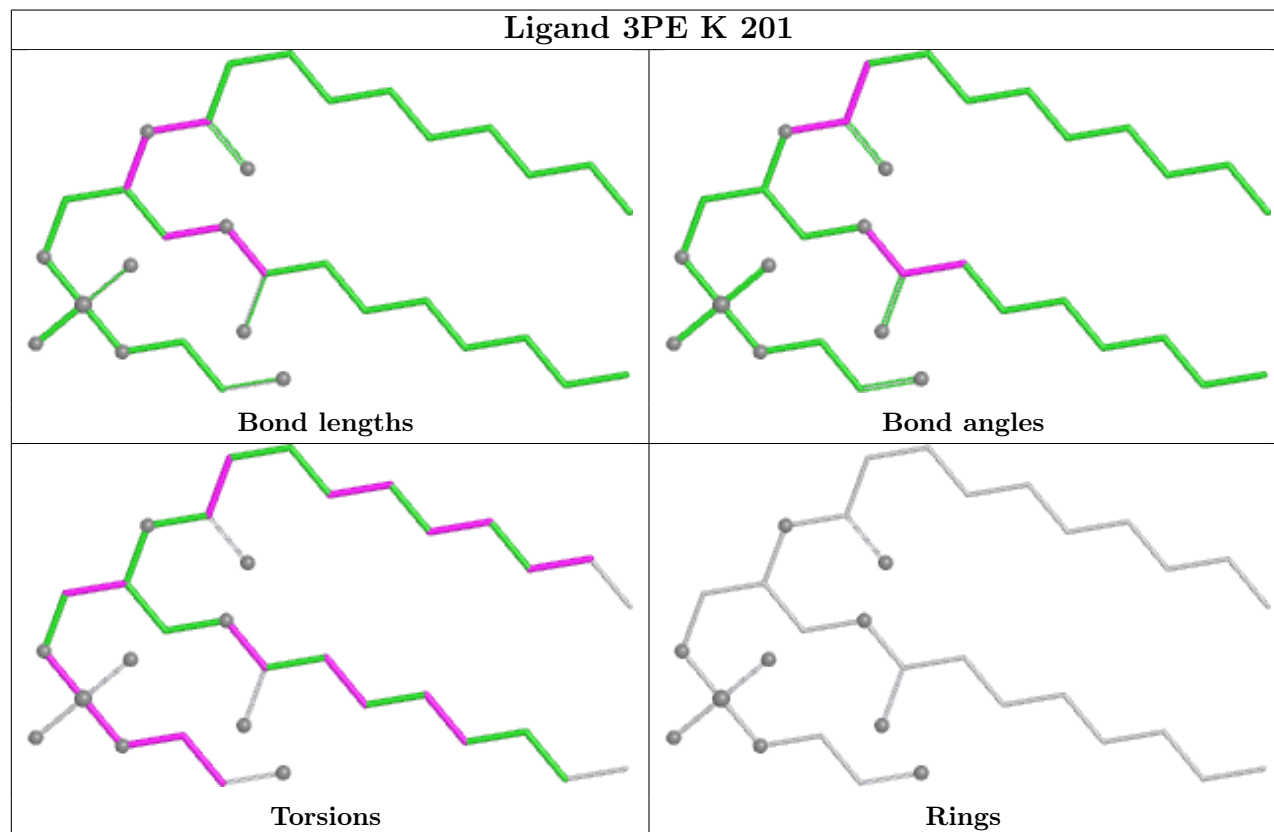
There are no ring outliers.

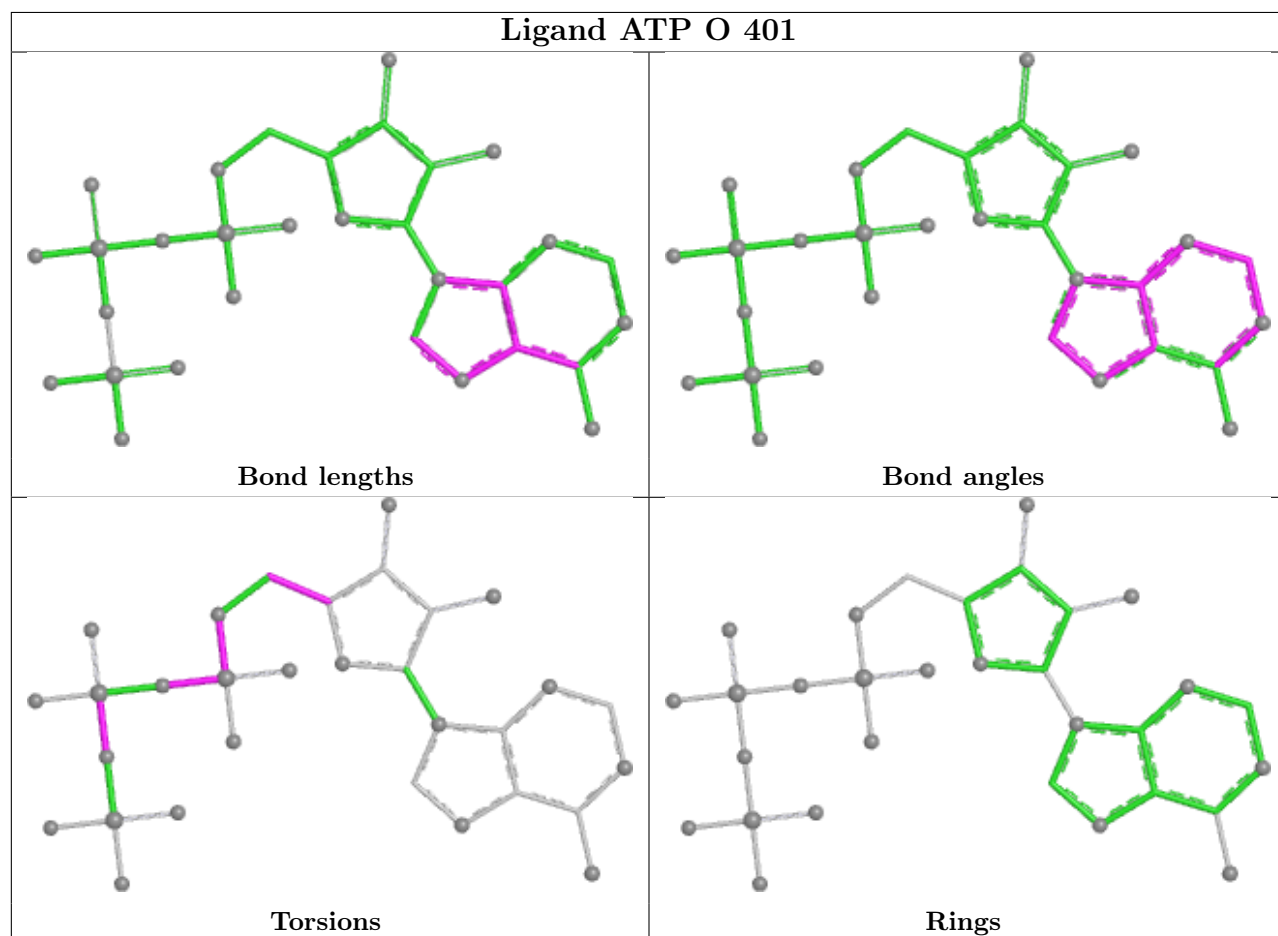
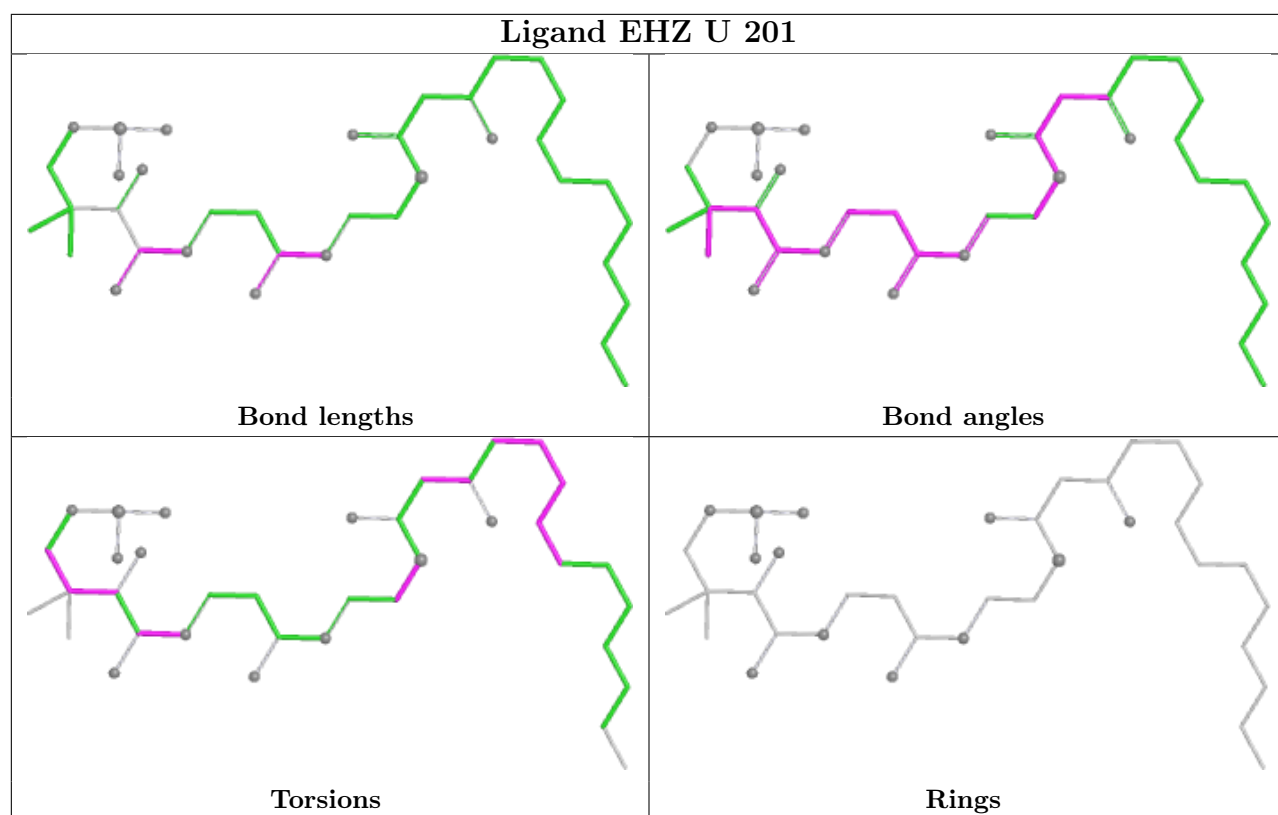
13 monomers are involved in 21 short contacts:

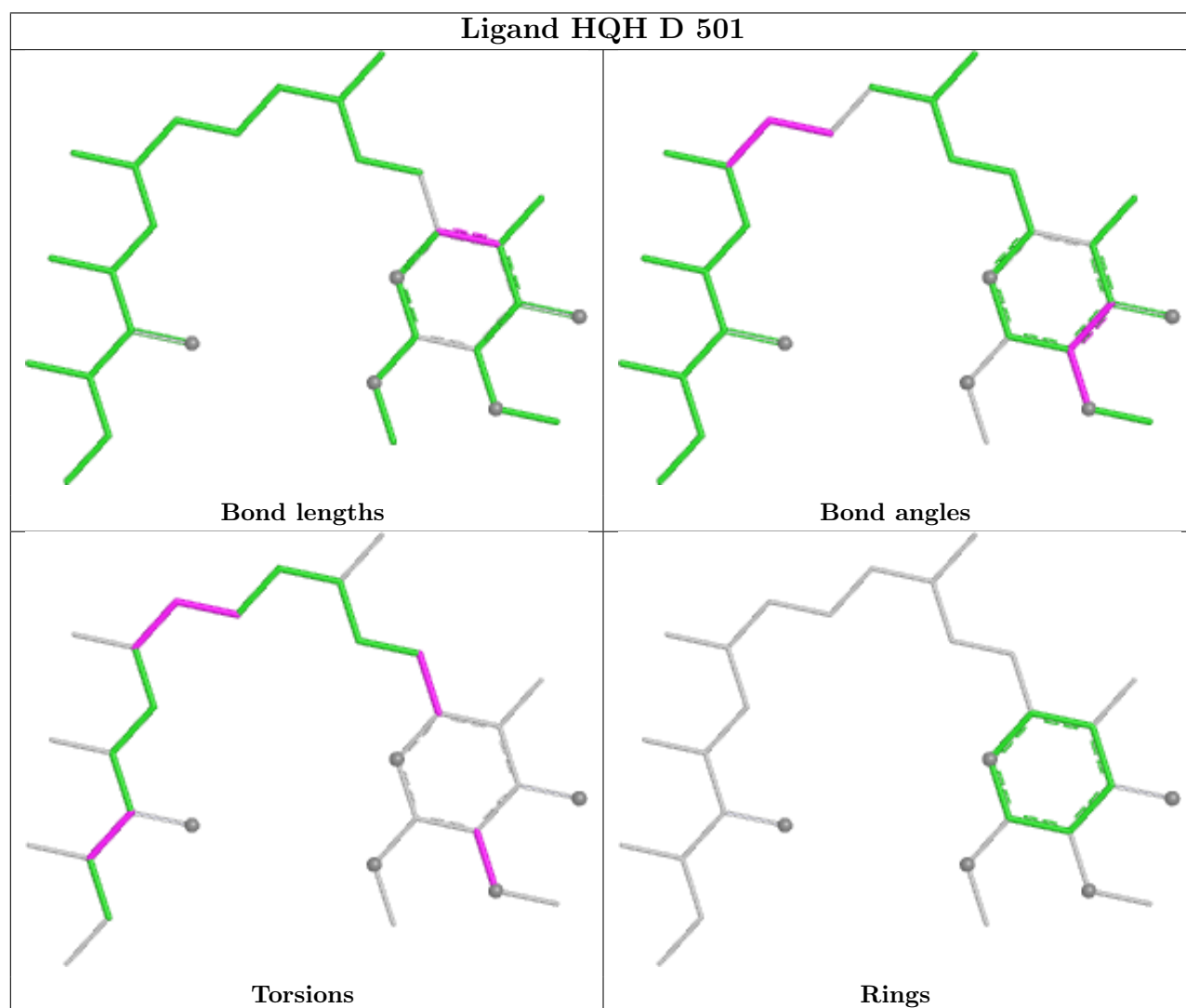
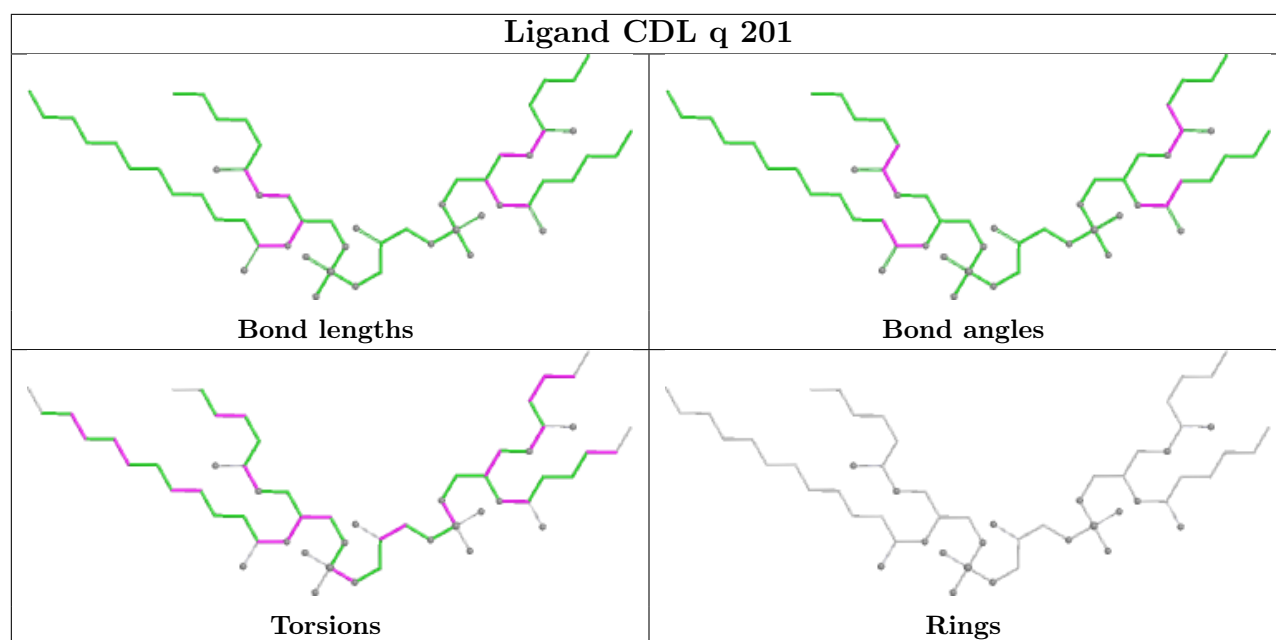
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	U	201	EHZ	1	0
52	O	401	ATP	4	0
51	q	201	CDL	1	0
51	d	202	CDL	2	0
51	d	201	CDL	2	0
46	J	201	PC1	2	0
50	F	501	FMN	1	0
48	D	502	3PE	1	0
51	h	201	CDL	3	0
53	P	501	NDP	1	0
48	i	201	3PE	1	0
46	B	202	PC1	1	0
51	N	401	CDL	1	0

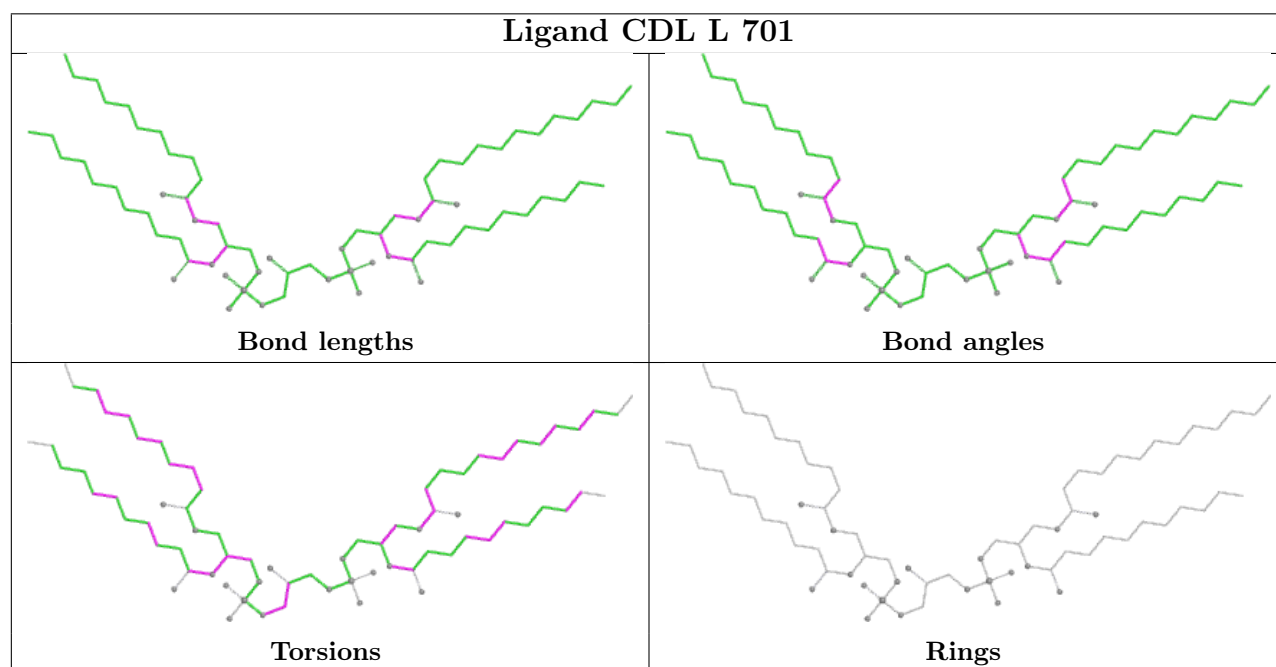
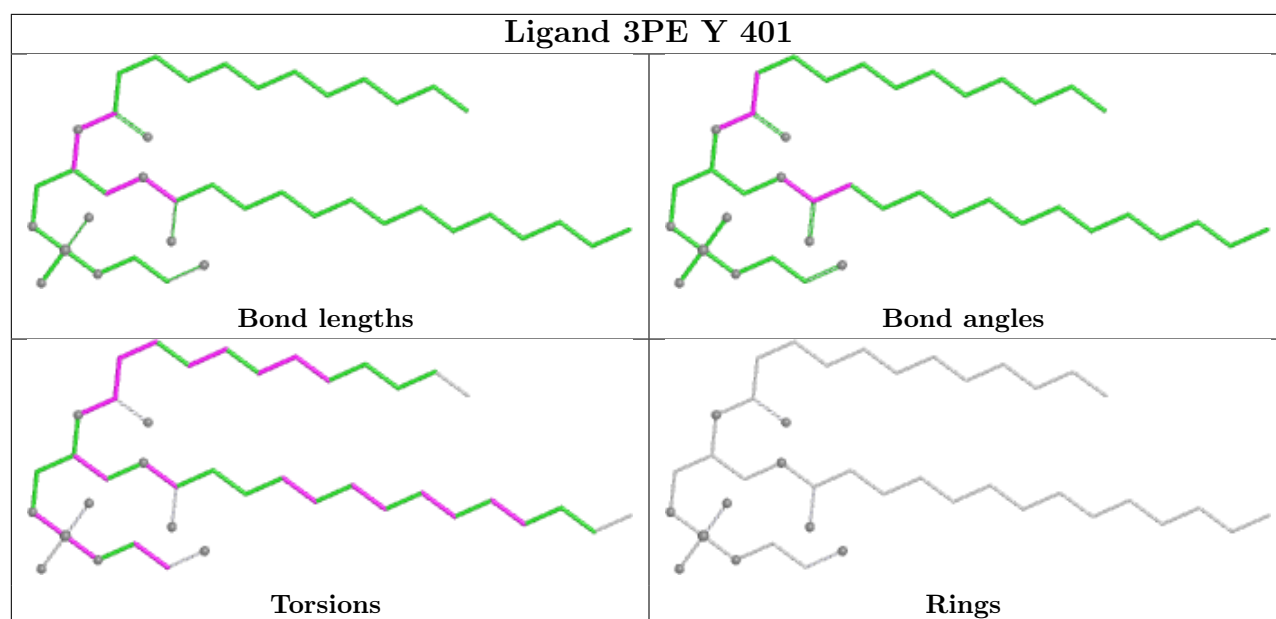
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

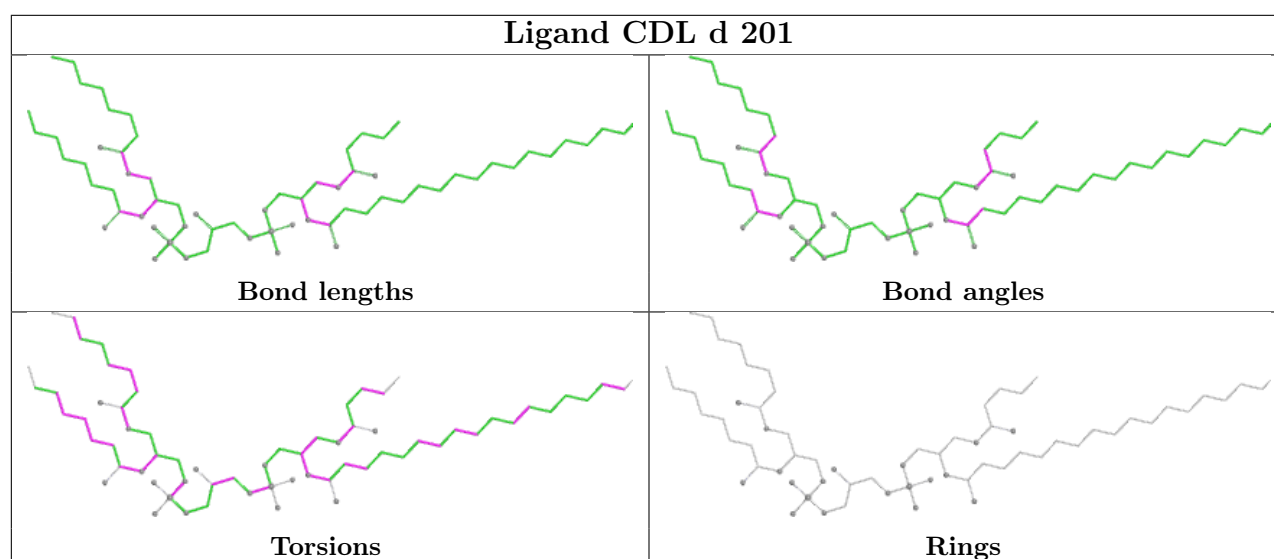
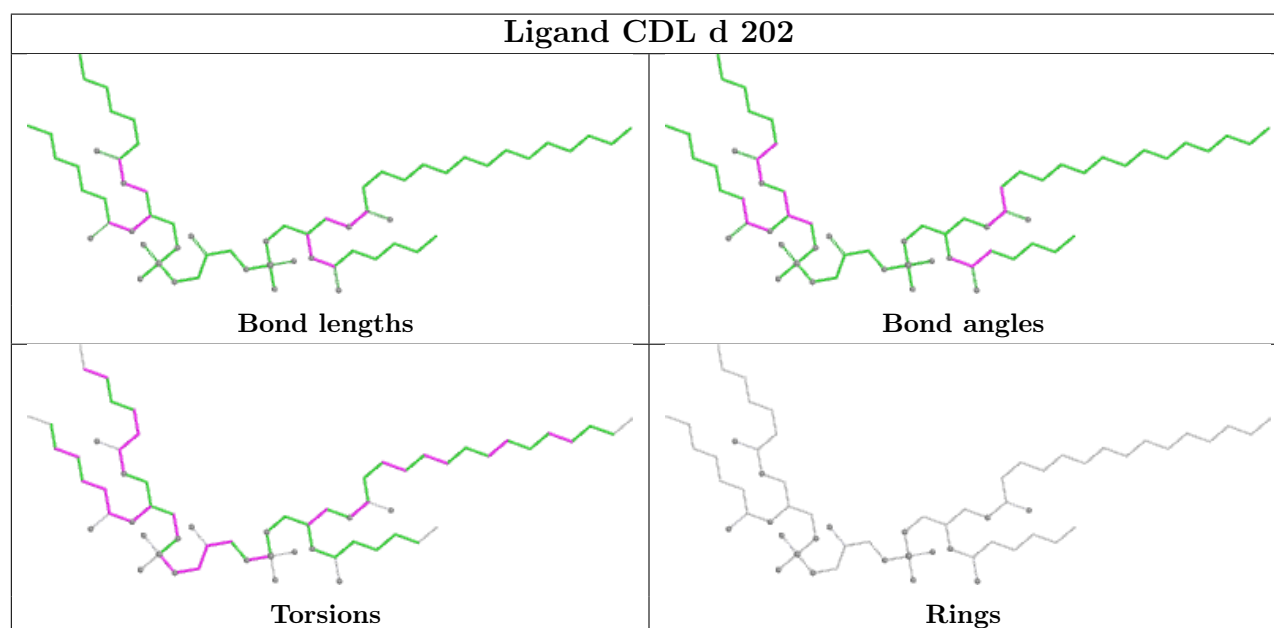
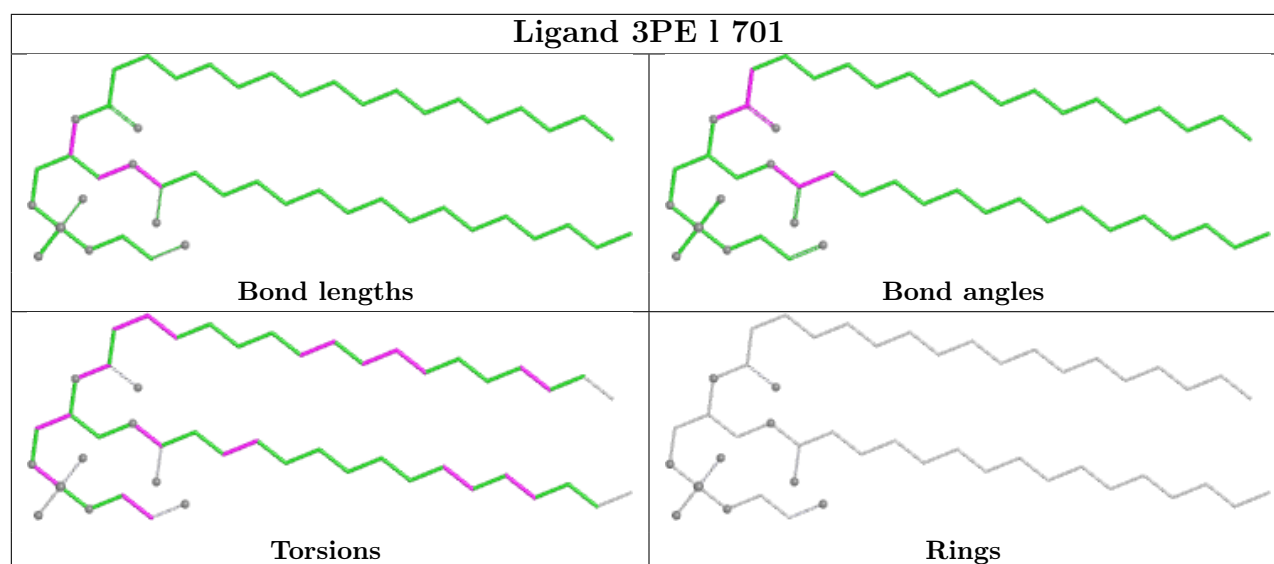
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

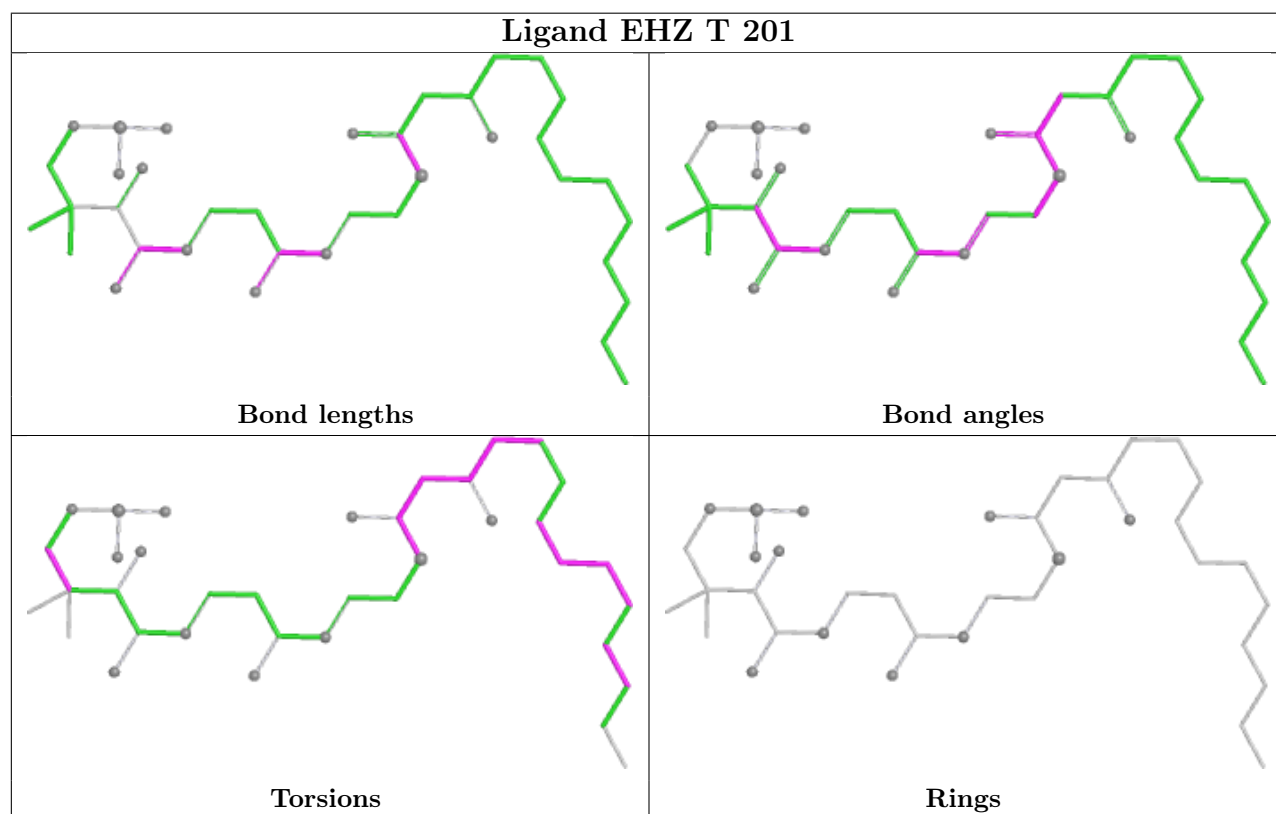
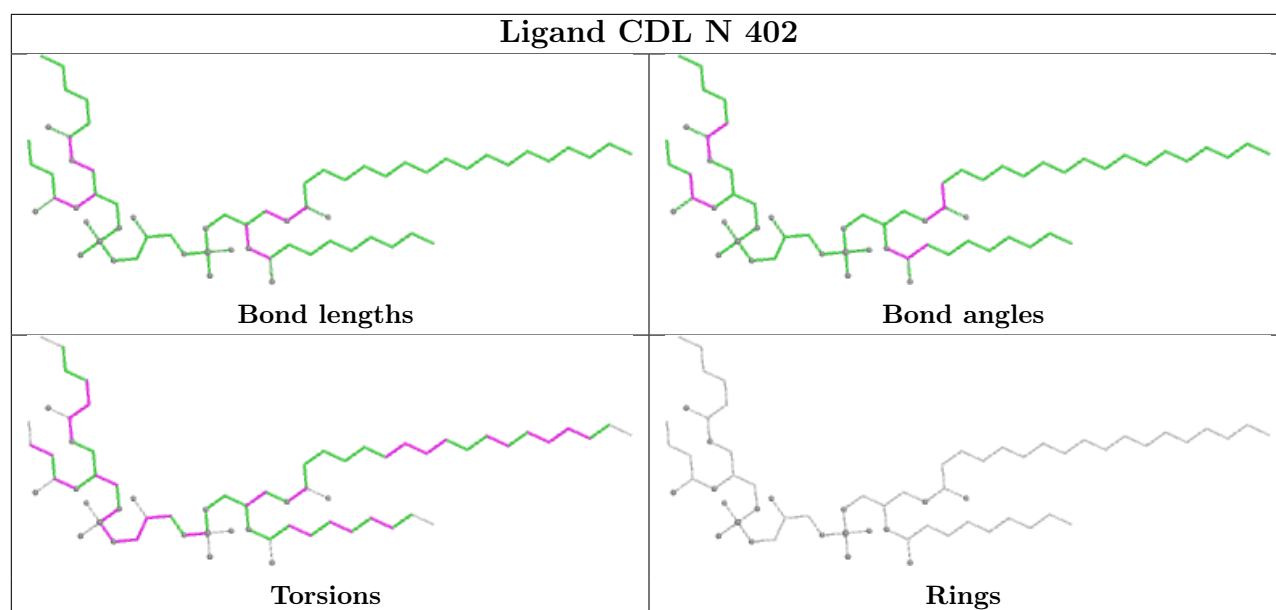


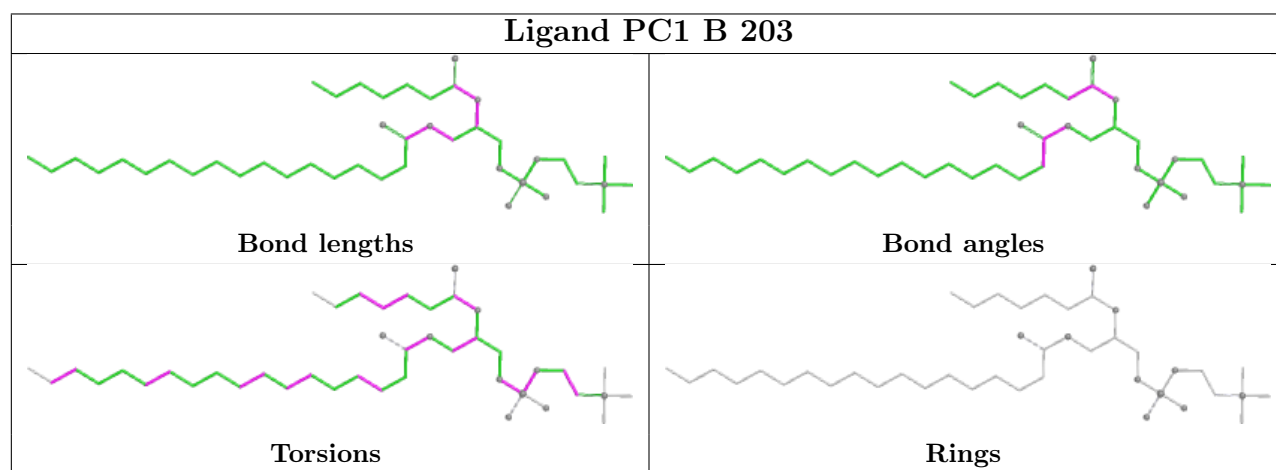
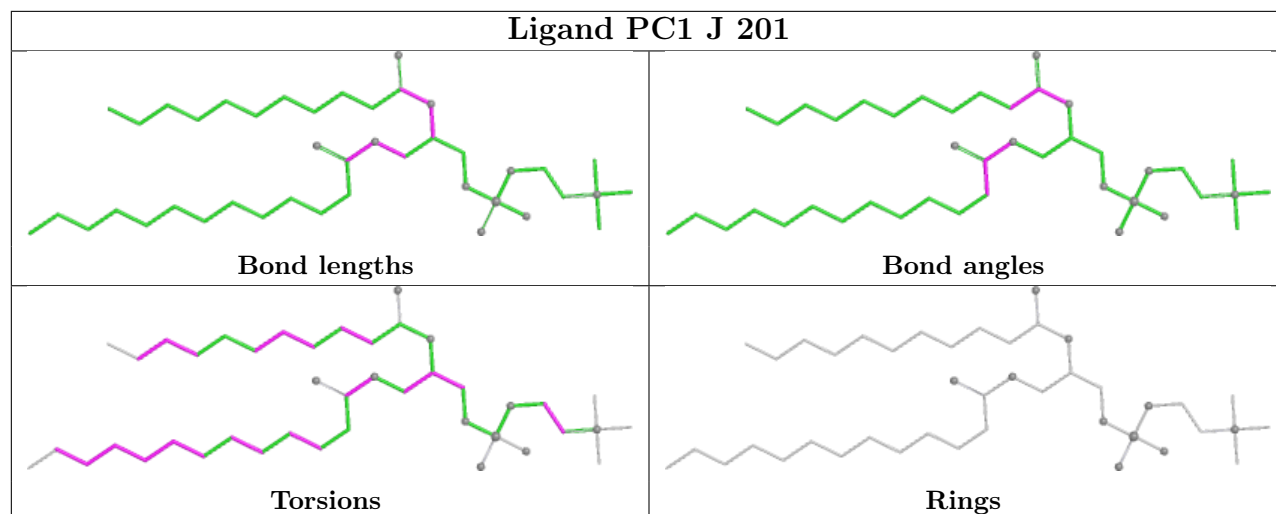


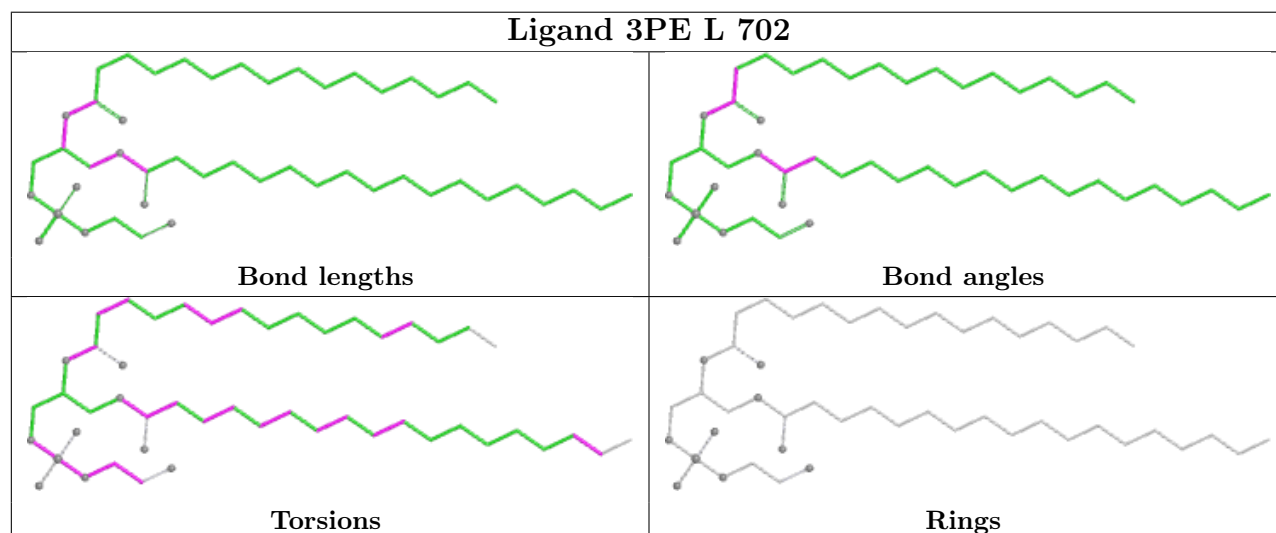
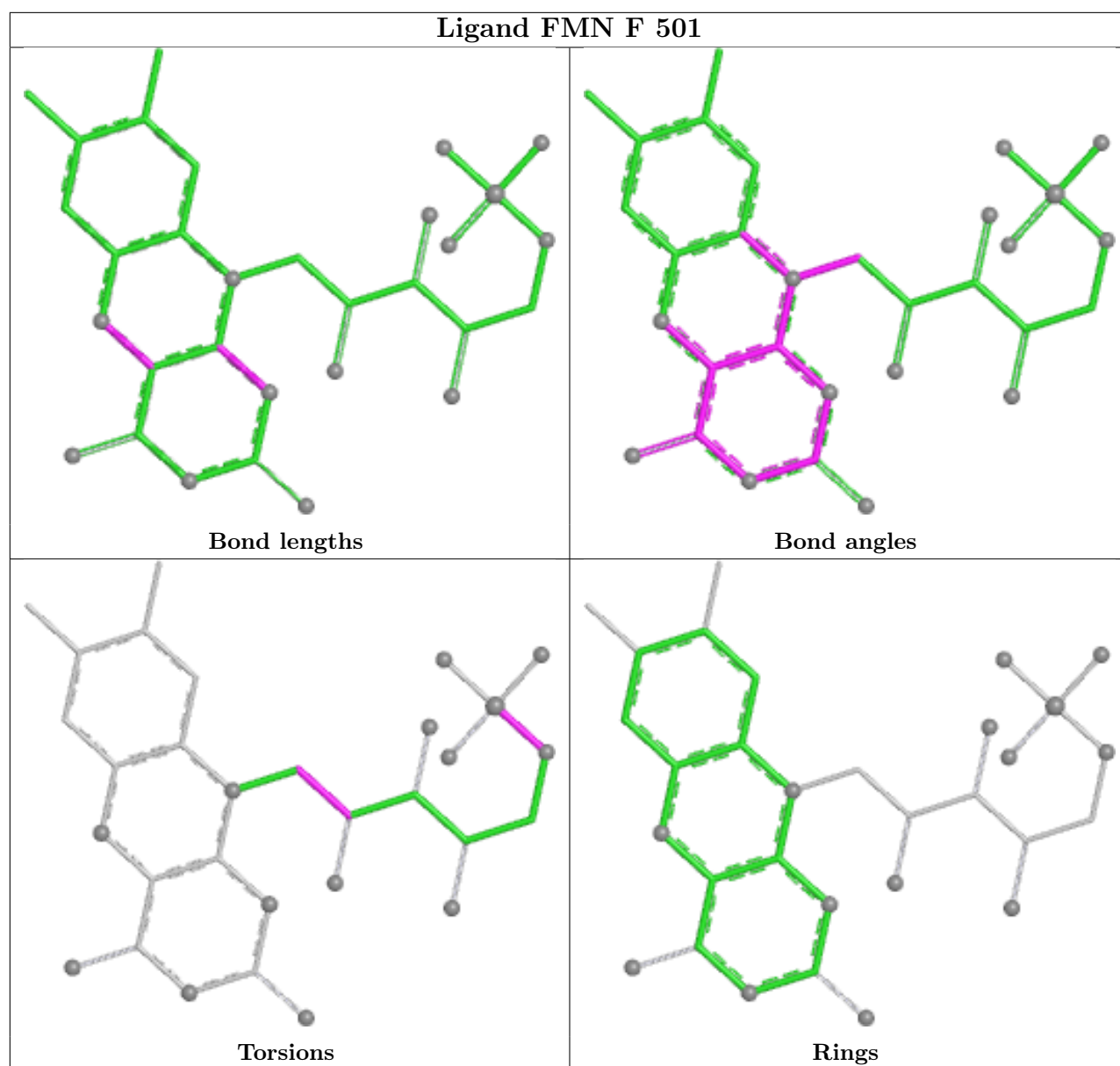


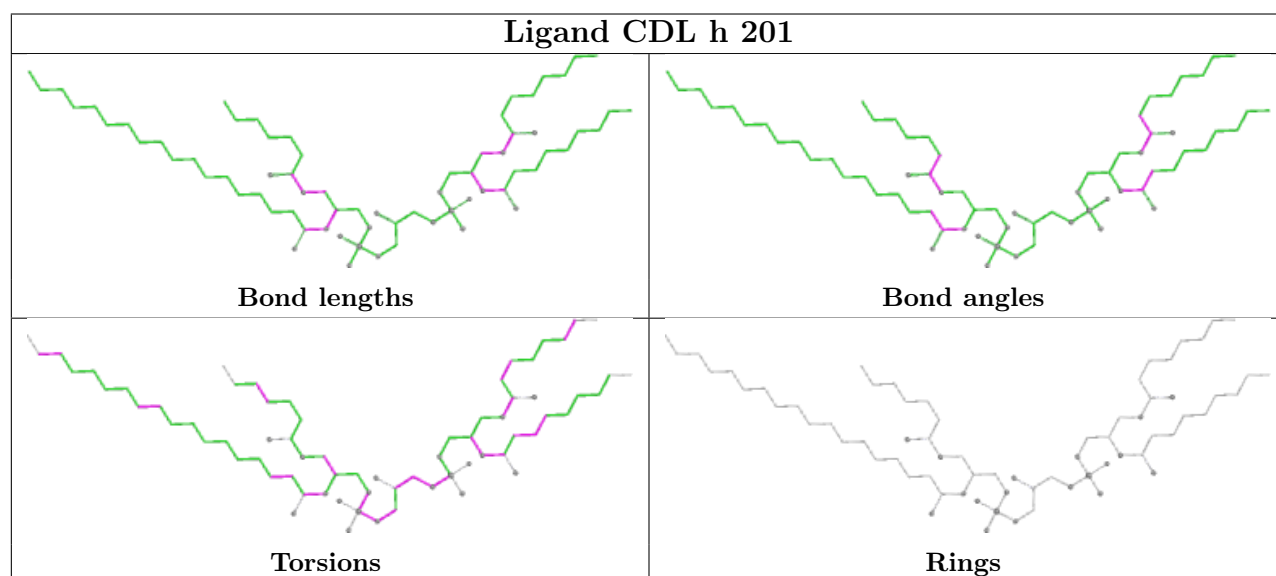
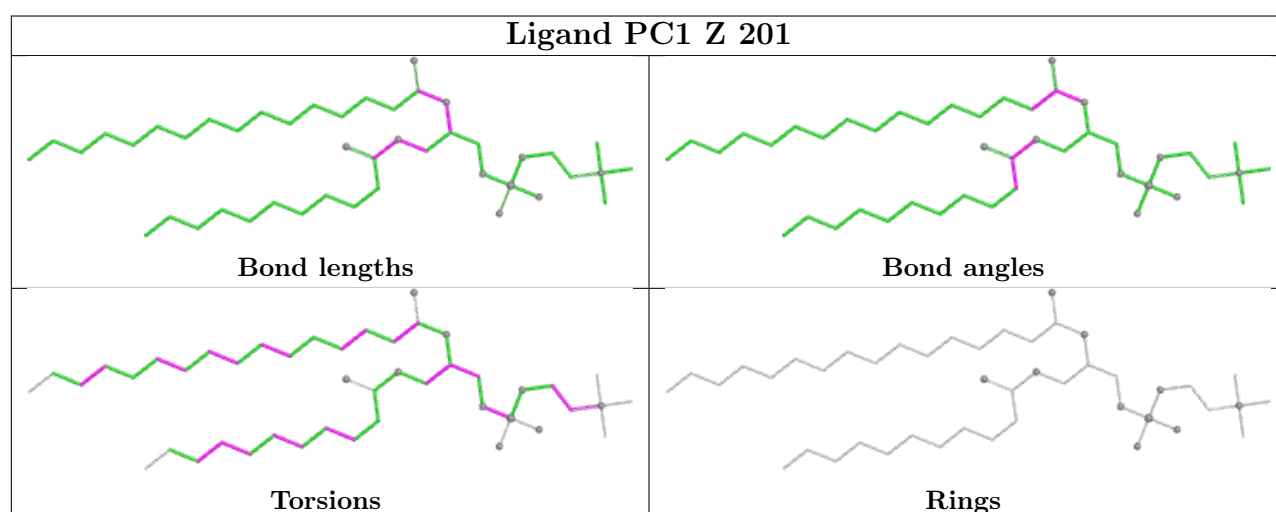
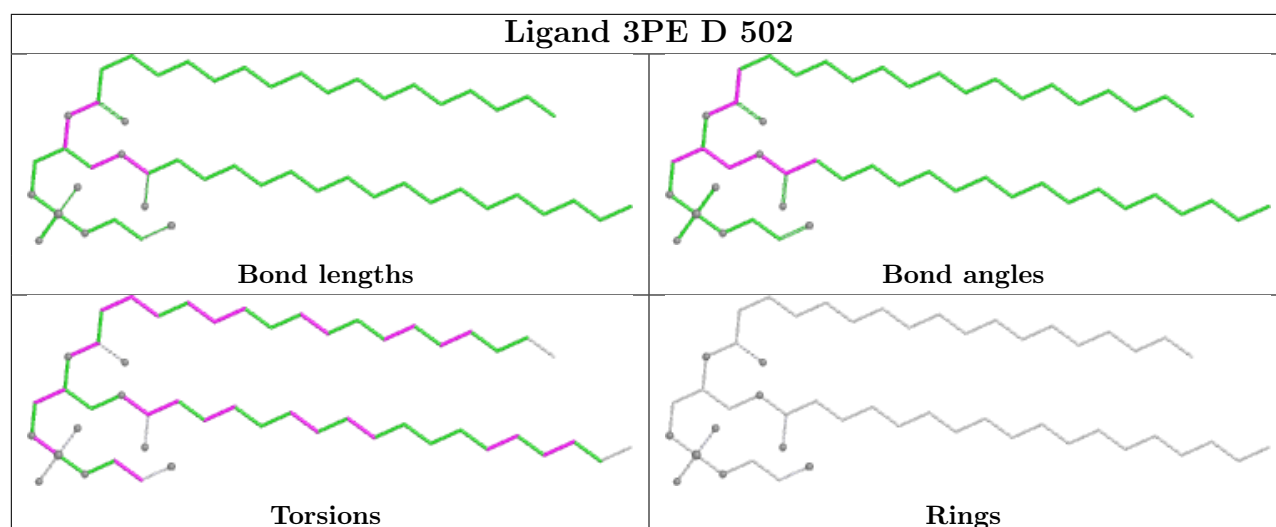


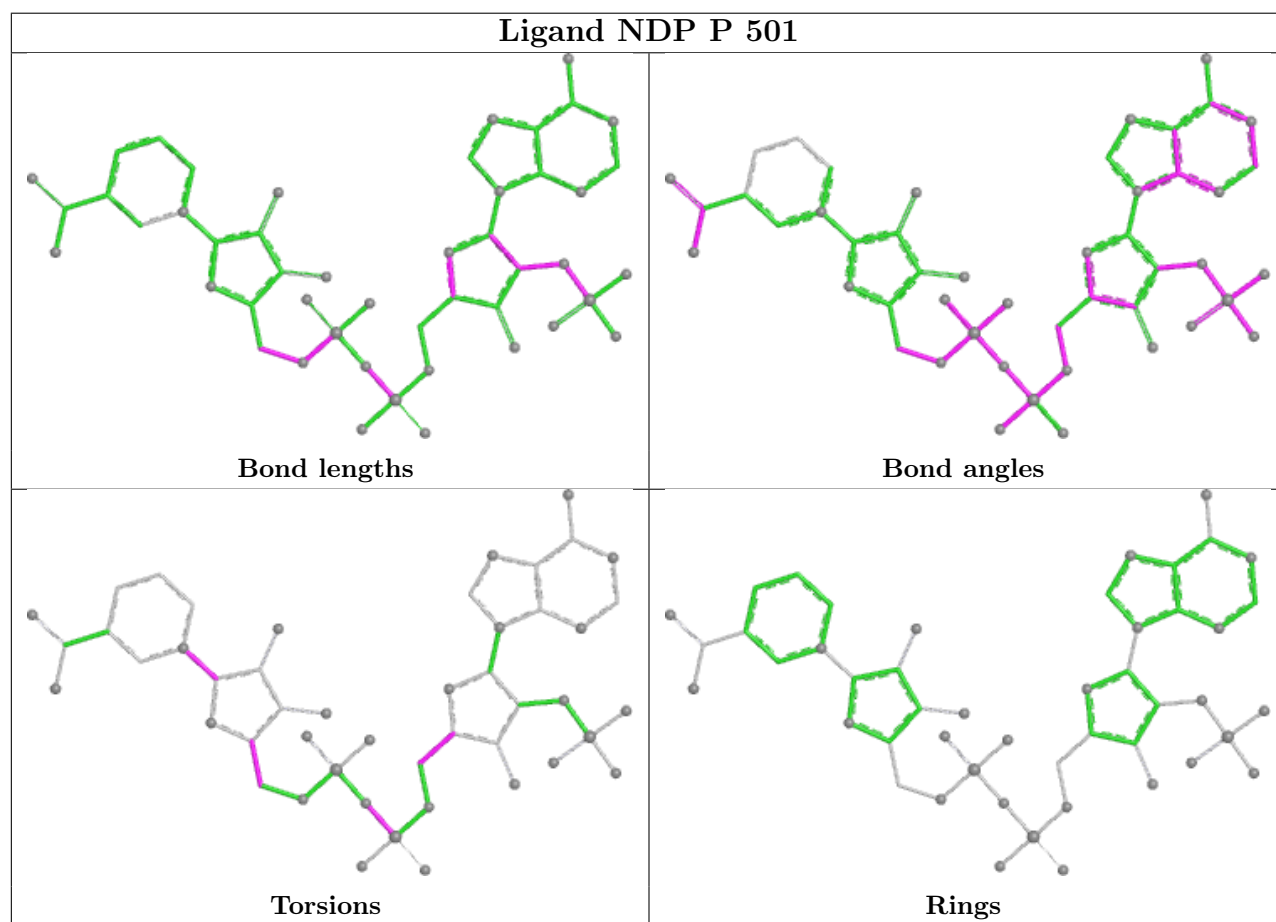
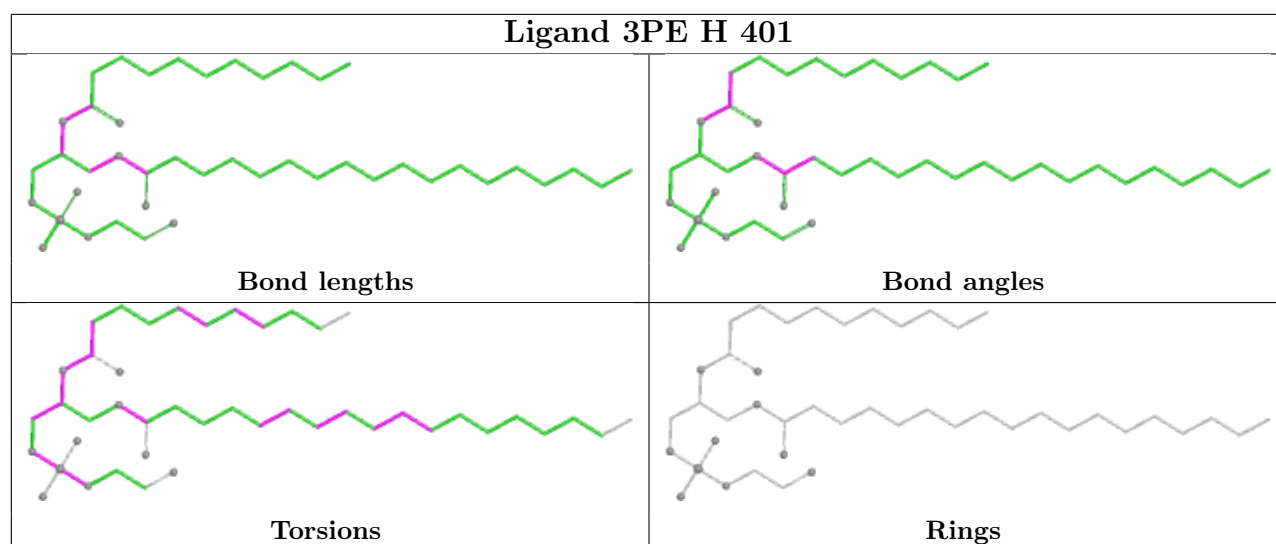


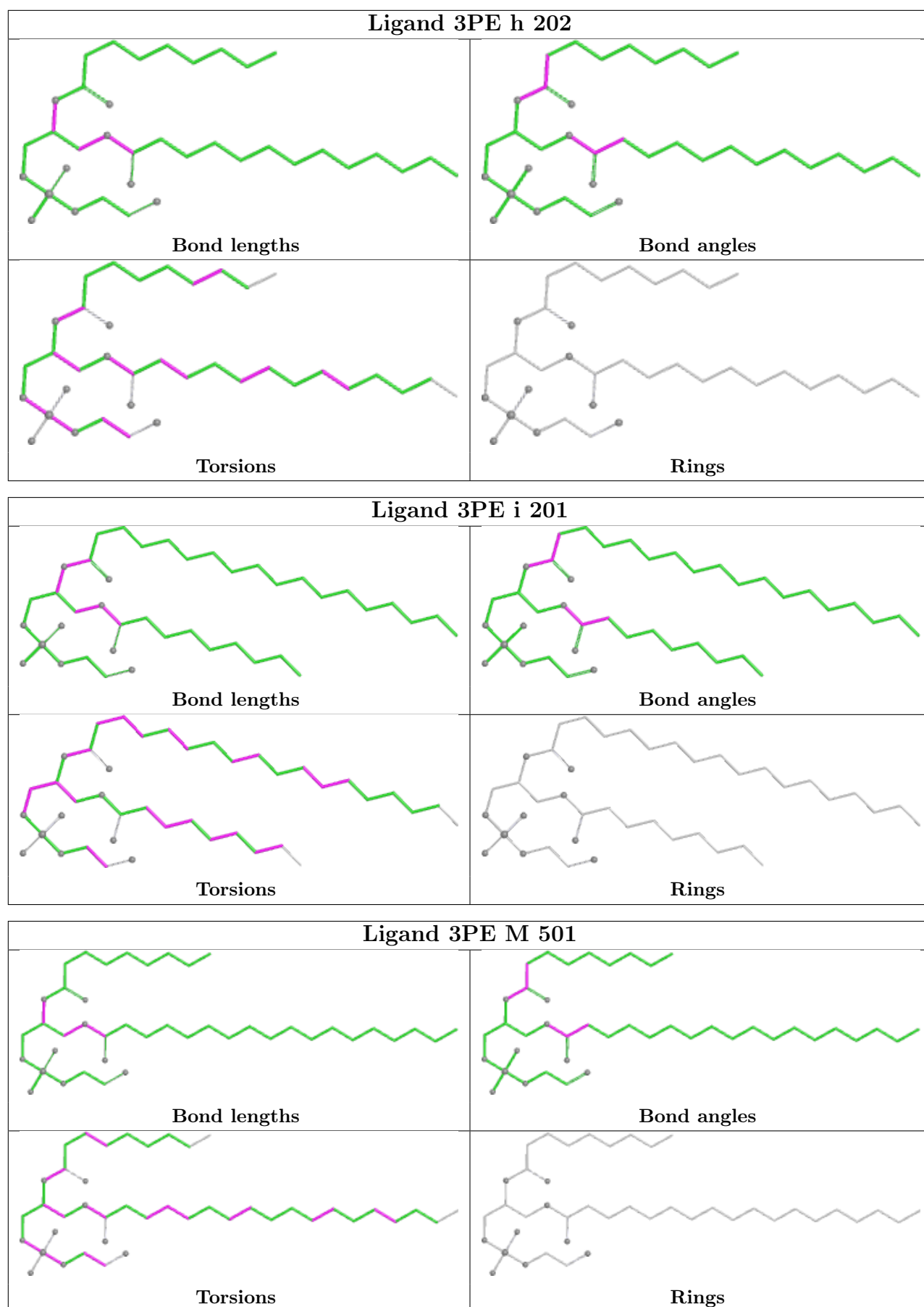


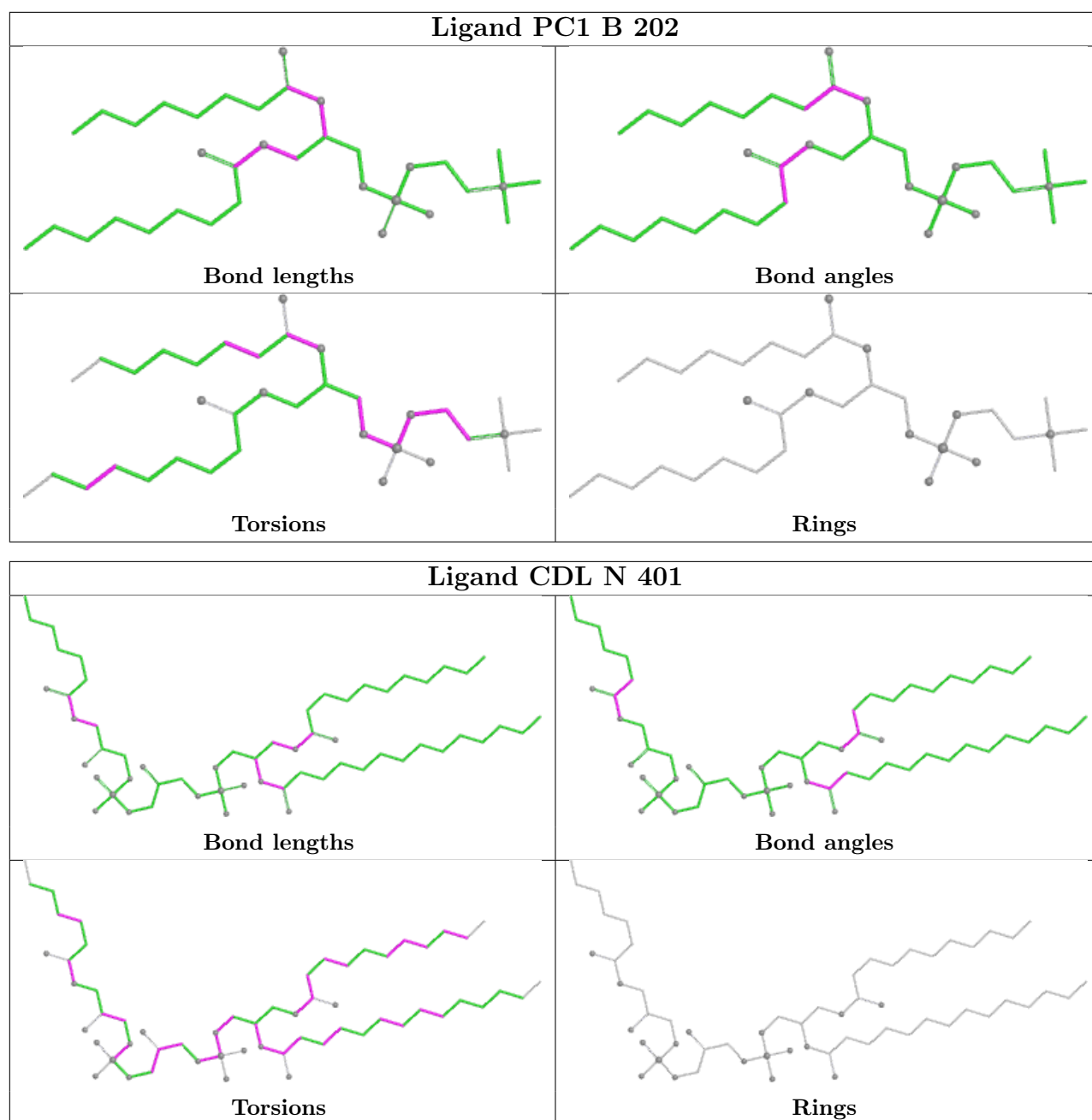












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

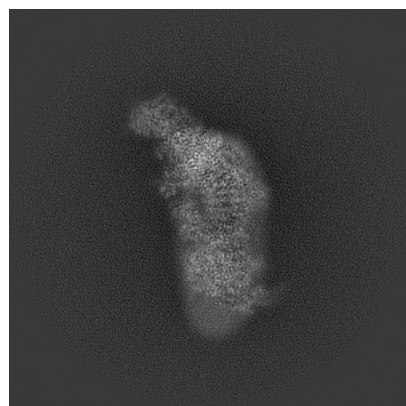
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11424. These allow visual inspection of the internal detail of the map and identification of artifacts.

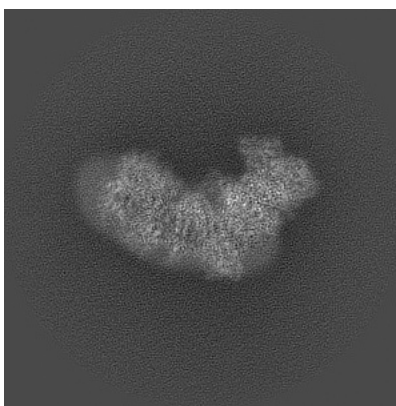
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

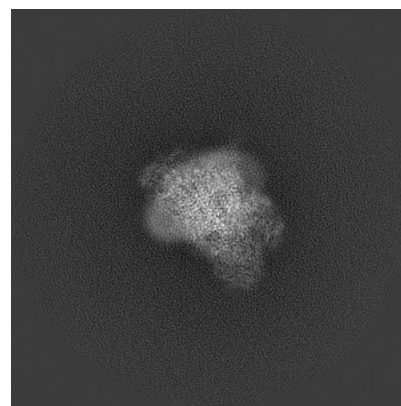
6.1.1 Primary map



X

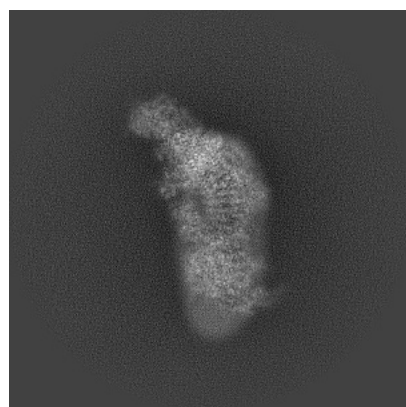


Y

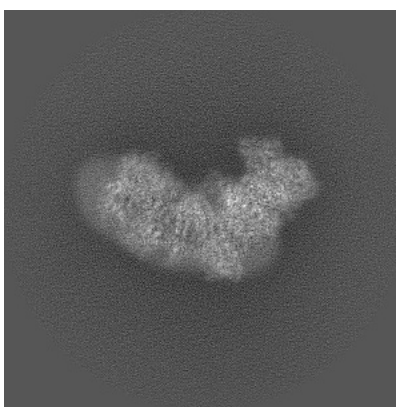


Z

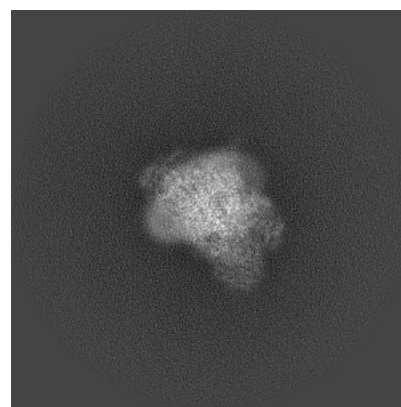
6.1.2 Raw map



X



Y

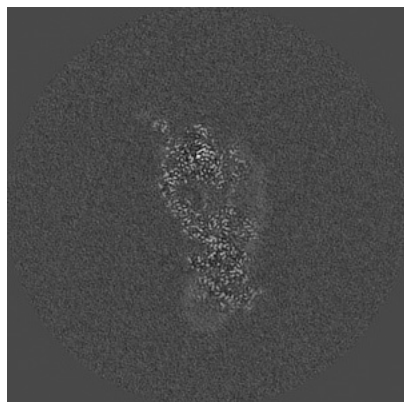


Z

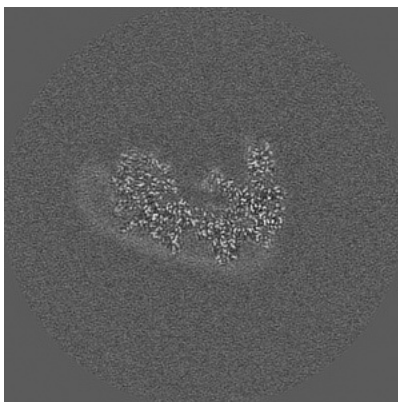
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

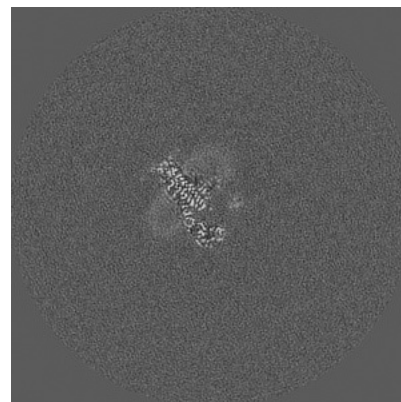
6.2.1 Primary map



X Index: 225

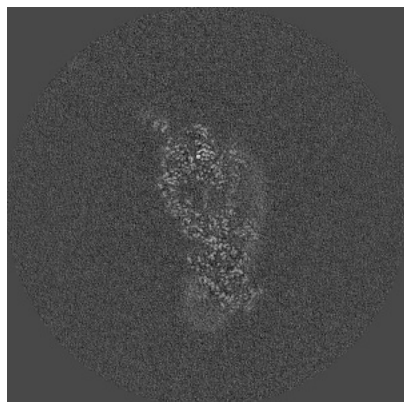


Y Index: 225

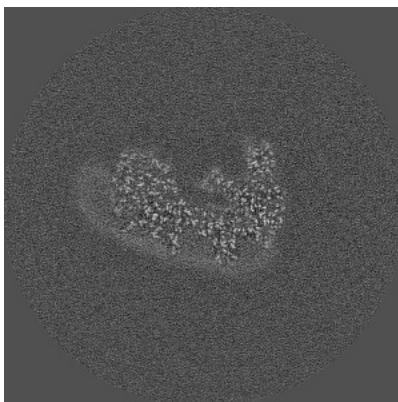


Z Index: 225

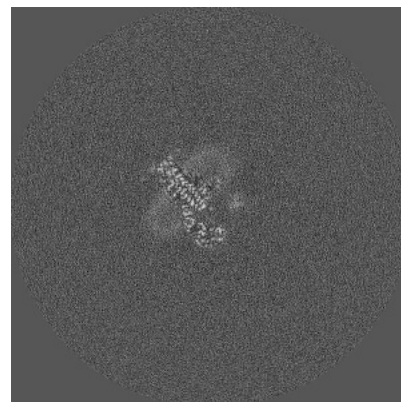
6.2.2 Raw map



X Index: 225



Y Index: 225

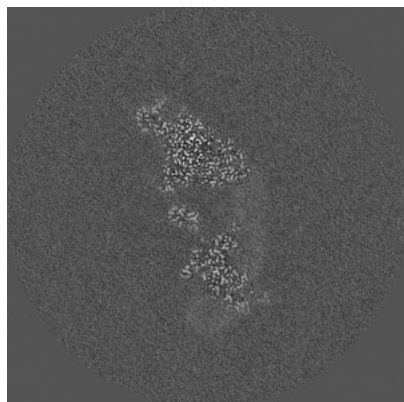


Z Index: 225

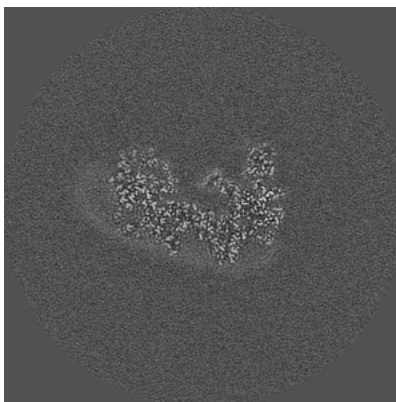
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

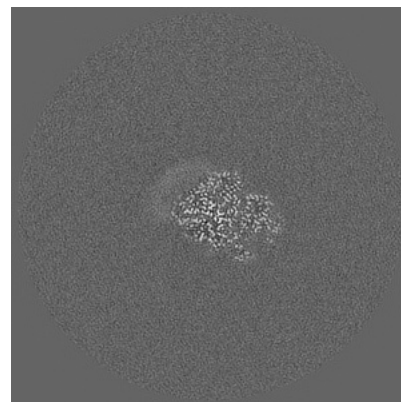
6.3.1 Primary map



X Index: 238

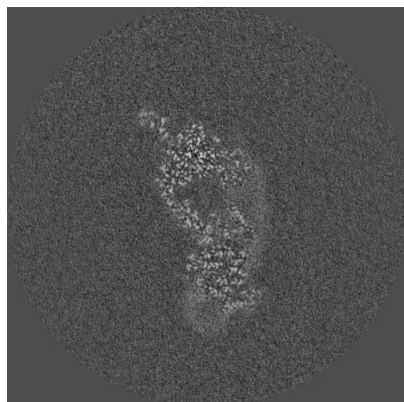


Y Index: 227

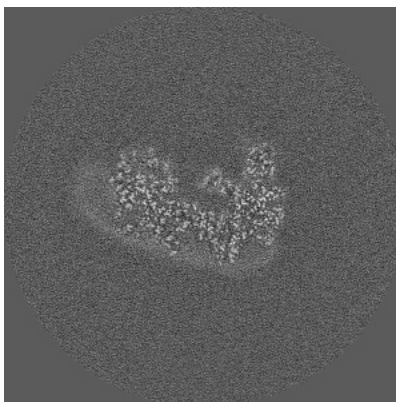


Z Index: 287

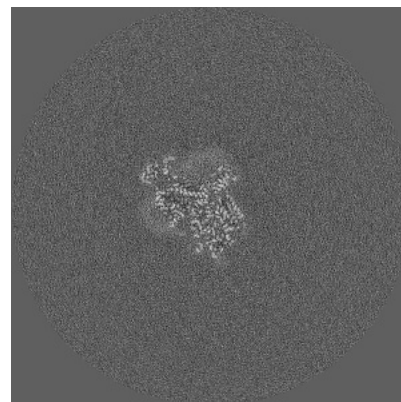
6.3.2 Raw map



X Index: 229



Y Index: 227

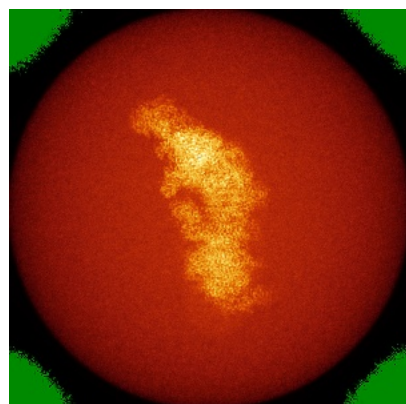


Z Index: 255

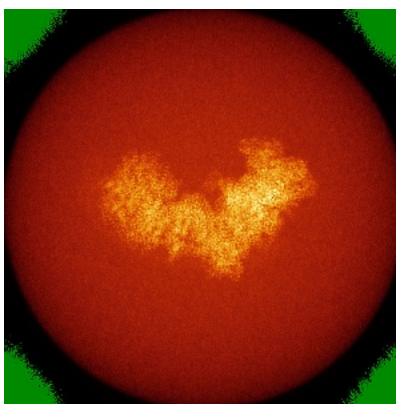
The images above show the largest variance slices of the map in three orthogonal directions.

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

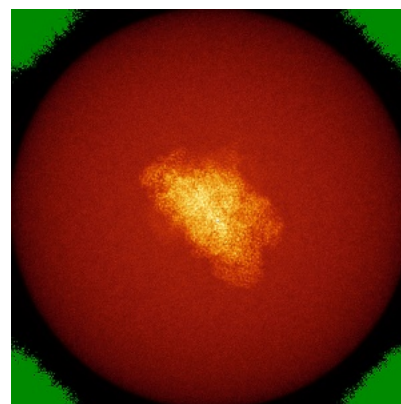
6.4.1 Primary map



X

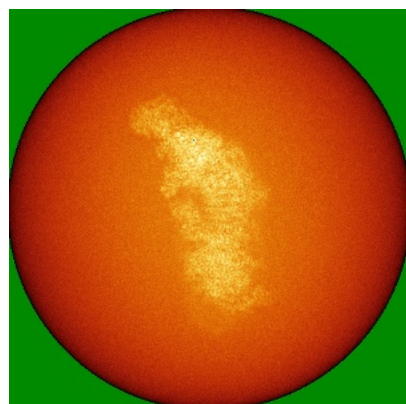


Y

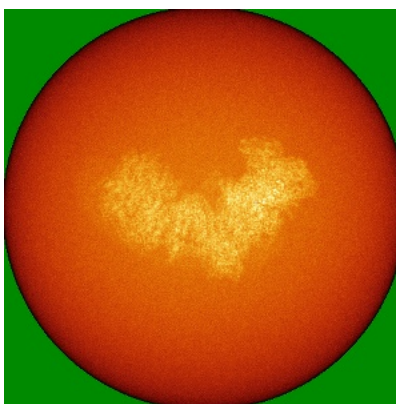


Z

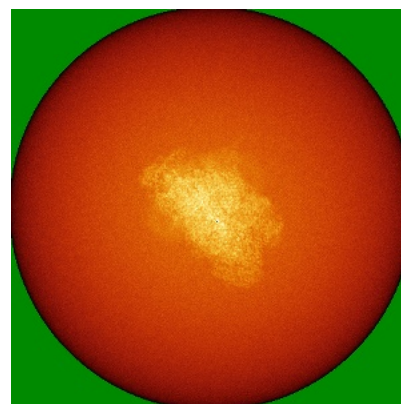
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

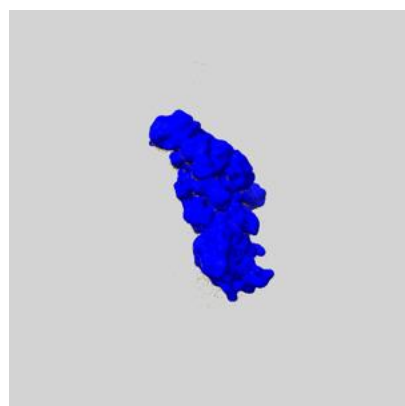
6.6 Mask visualisation [i](#)

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

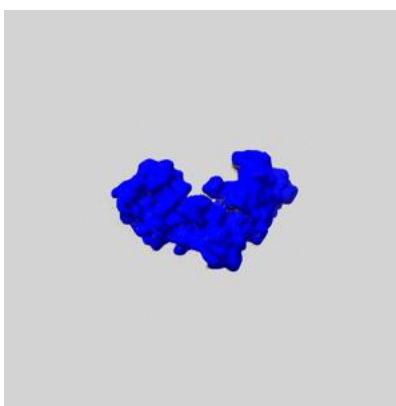
A mask typically either:

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

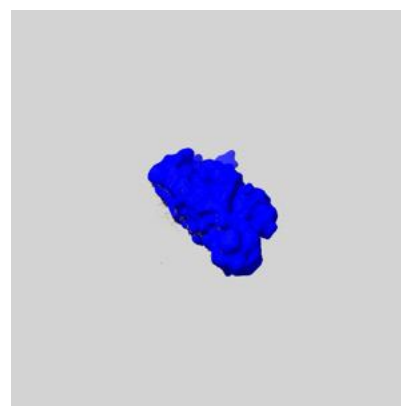
6.6.1 emd_11377_msk_1.map [i](#)



X



Y

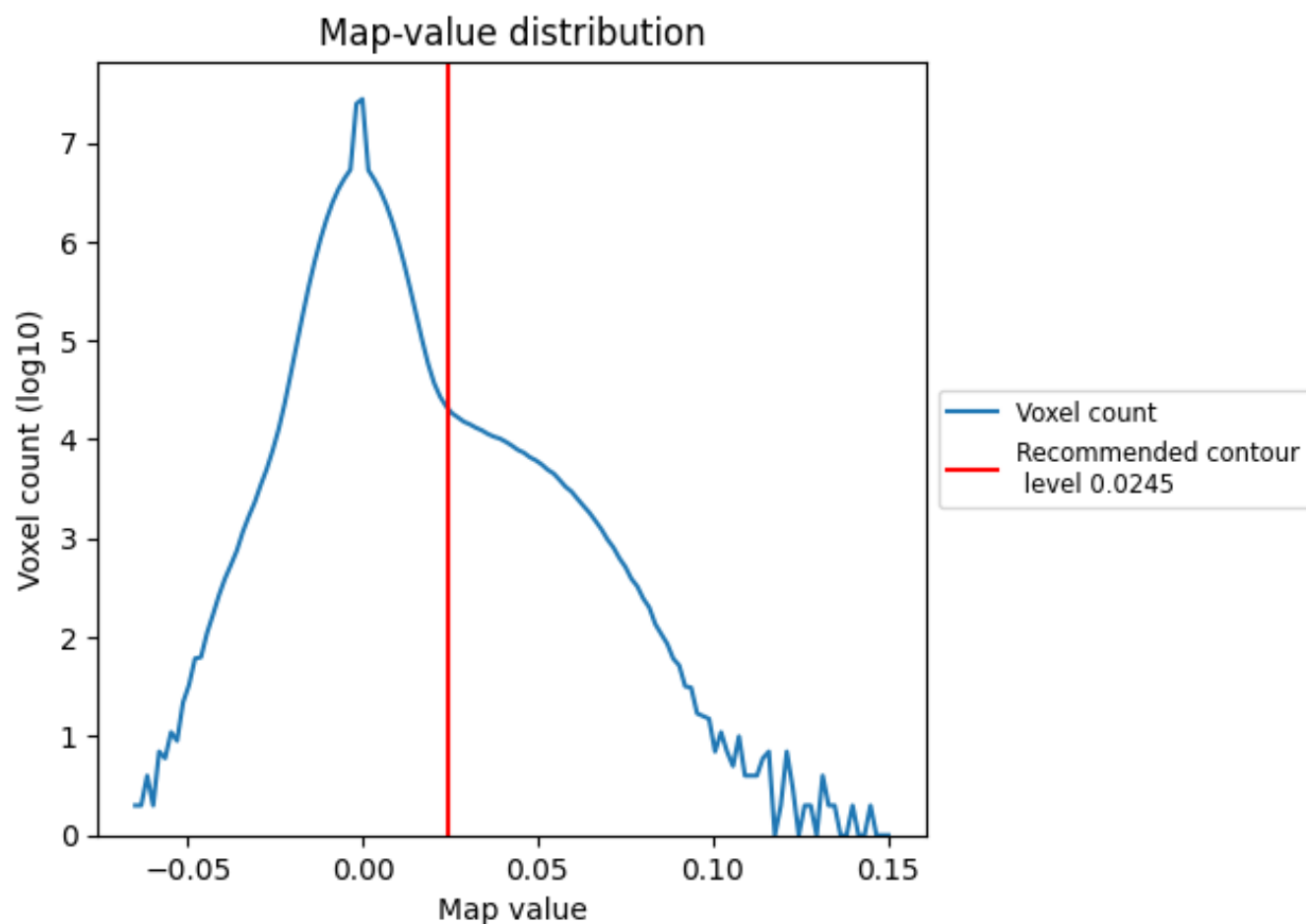


Z

7 Map analysis [i](#)

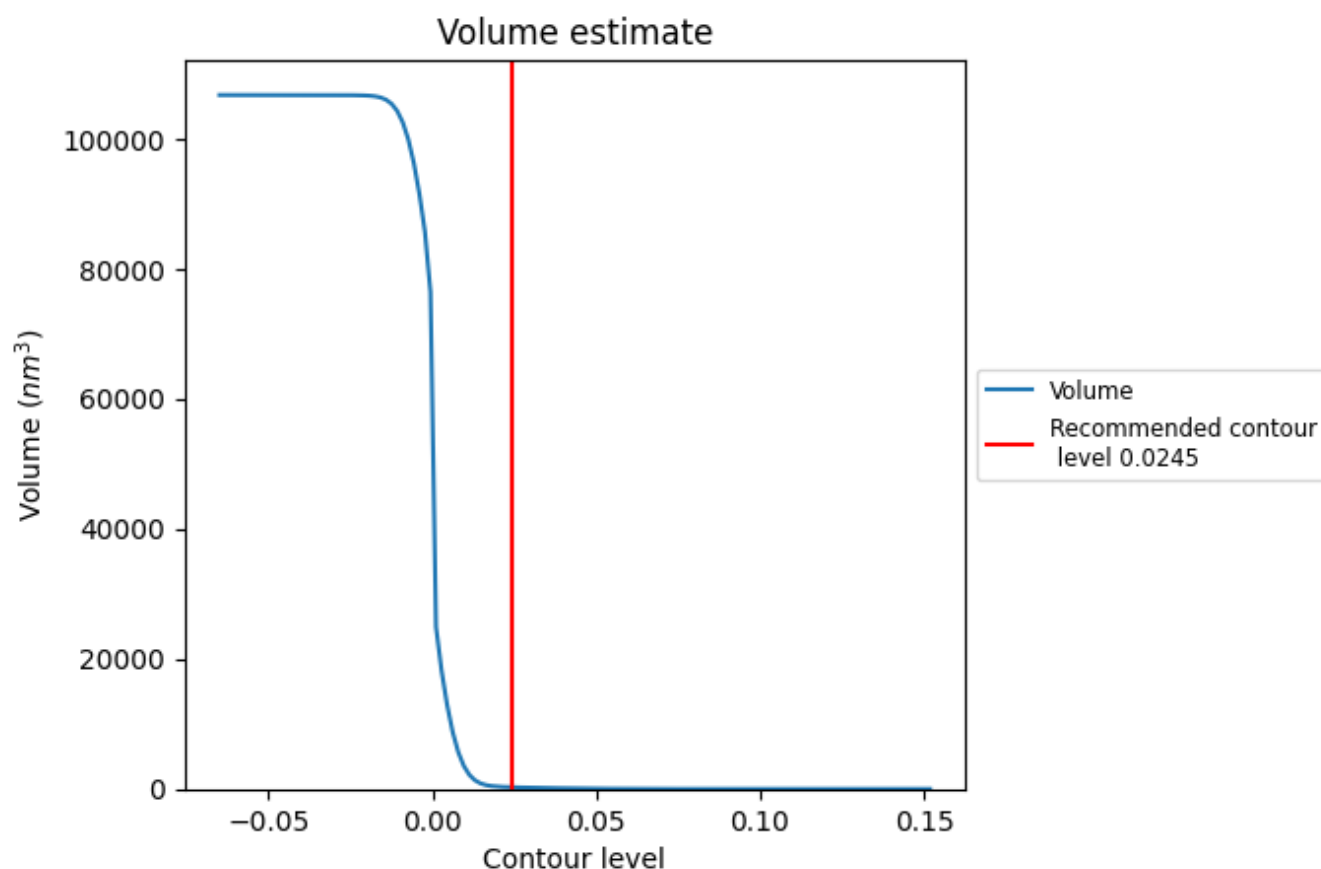
This section contains the results of statistical analysis of the map.

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.

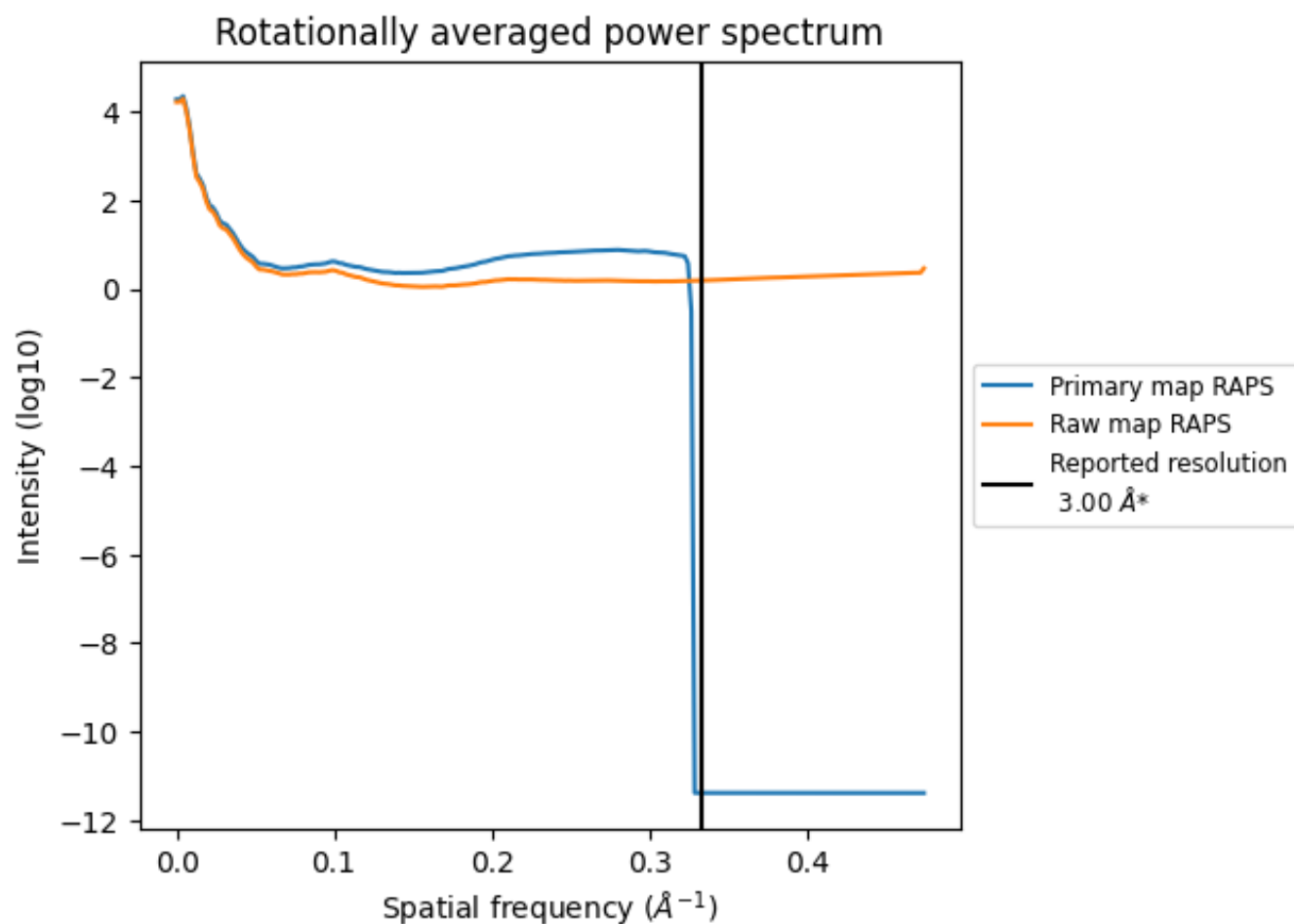
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 258 nm^3 ; this corresponds to an approximate mass of 233 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 ⓘ

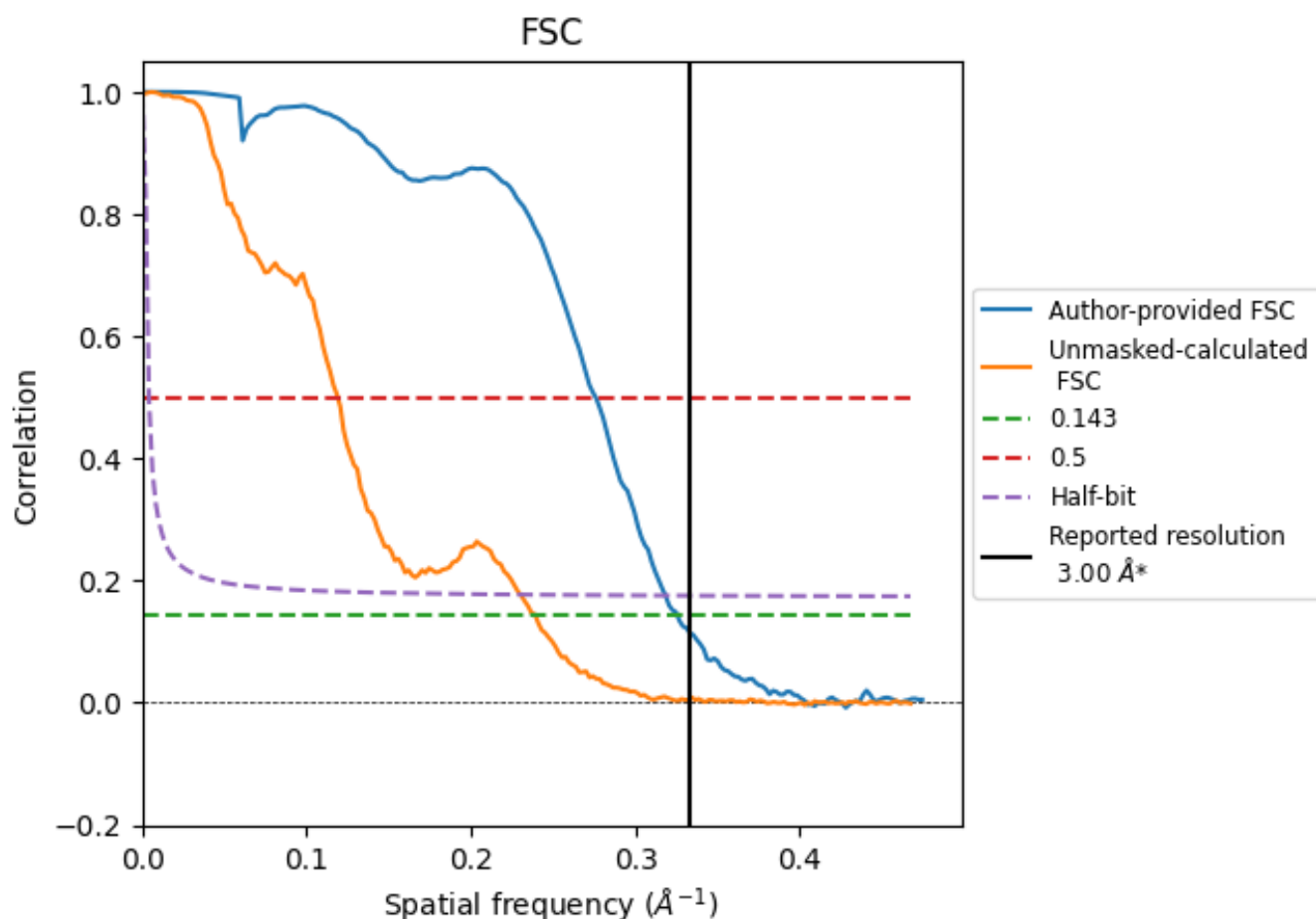


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

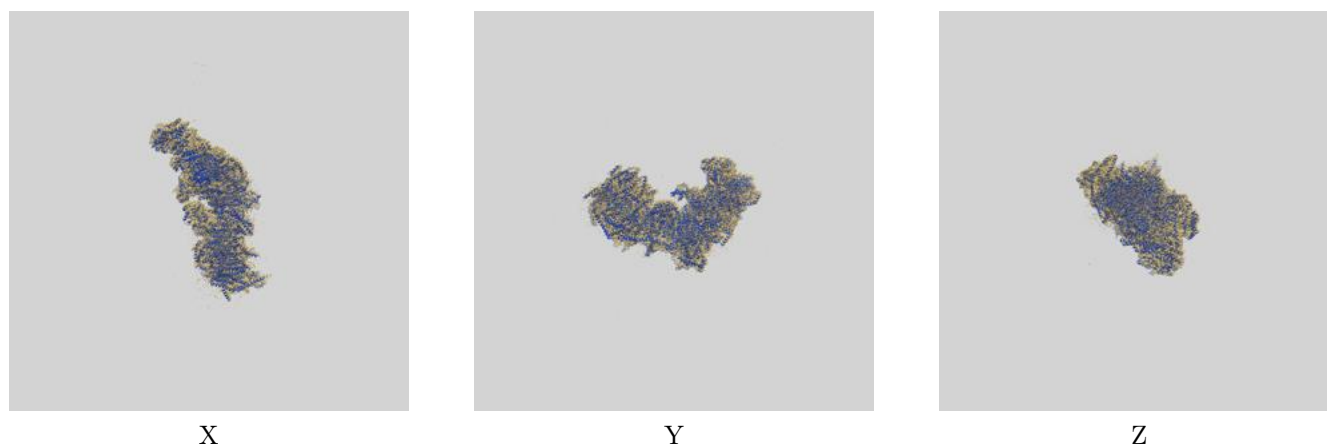
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.07	3.63	3.14
Unmasked-calculated*	4.18	8.41	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

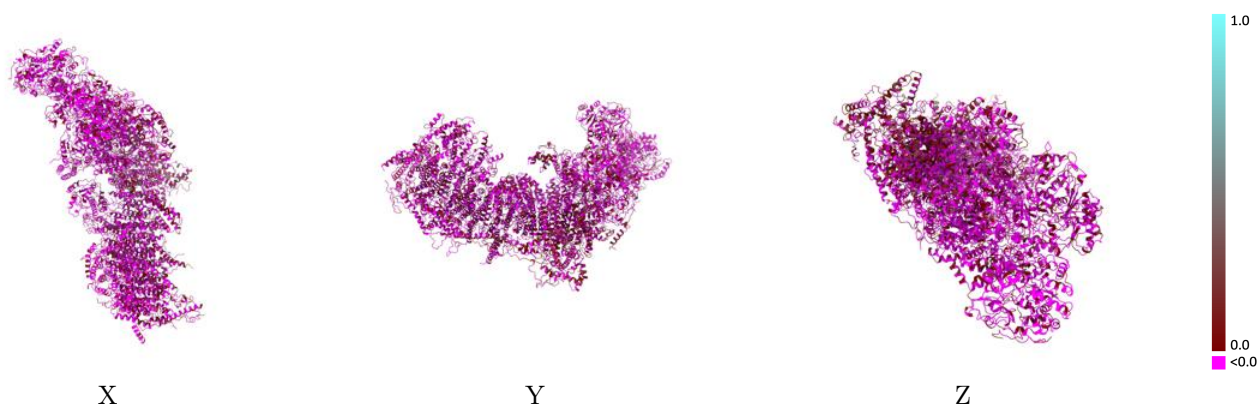
This section contains information regarding the fit between EMDB map EMD-11424 and PDB model 6ZTQ. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



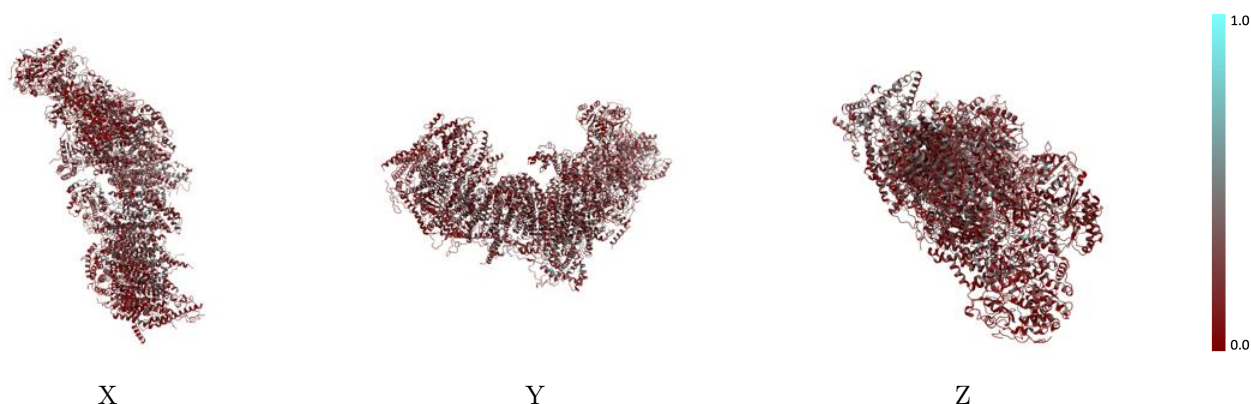
The images above show the 3D surface view of the map at the recommended contour level 0.0245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



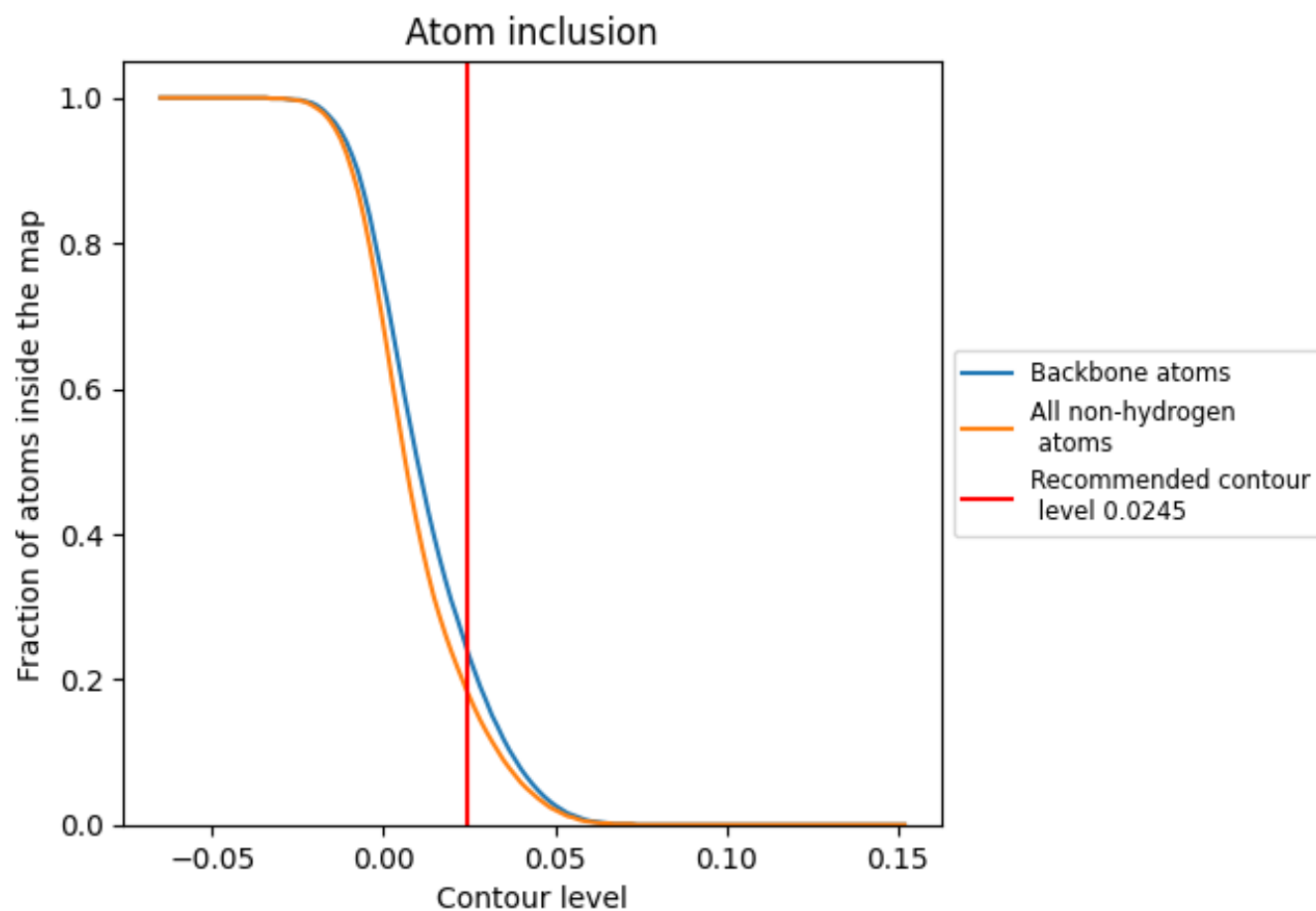
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0245).

9.4 Atom inclusion [i](#)



At the recommended contour level, 24% of all backbone atoms, 18% 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 (0.0245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1820	-0.0400
A	0.2130	-0.0190
B	0.2100	-0.0460
C	0.1760	-0.1060
D	0.2050	-0.0550
E	0.1690	-0.0500
F	0.1380	-0.0830
G	0.1670	-0.0680
H	0.2250	-0.0120
I	0.2130	-0.0840
J	0.2000	0.0200
K	0.2290	-0.0100
L	0.1770	-0.0490
M	0.2090	-0.0510
N	0.2090	-0.0460
O	0.1550	-0.0700
P	0.1980	-0.0230
Q	0.1520	-0.0960
R	0.2100	-0.0050
S	0.1250	-0.0310
T	0.1180	0.0430
U	0.1180	-0.0450
V	0.1660	-0.0590
W	0.1780	-0.0410
X	0.2520	0.0650
Y	0.1680	-0.0490
Z	0.2490	0.0260
a	0.2660	0.0350
b	0.1910	-0.0050
c	0.1470	-0.0240
d	0.2000	0.0030
e	0.2330	0.0430
f	0.1420	-0.0500
g	0.1880	-0.0350
h	0.1760	-0.0460



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Chain	Atom inclusion	Q-score
i	 0.1170	 -0.0490
j	 0.1260	 0.0210
k	 0.0930	 -0.0500
l	 0.1490	 -0.0630
m	 0.1660	 -0.0290
n	 0.1410	 -0.0580
o	 0.1310	 0.0080
p	 0.1840	 -0.0130
q	 0.2010	 -0.0050
r	 0.1650	 -0.0600
s	 0.1130	 -0.1100