



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2025 – 10:20 am BST

PDB ID : 6ZR2 / pdb\_00006zr2  
EMDB ID : EMD-11377  
Title : Cryo-EM structure of respiratory complex I in the active state from *Mus musculus* at 3.1 Å  
Authors : Bridges, H.R.; Blaza, J.N.; Agip, A.N.A.; Hirst, J.  
Deposited on : 2020-07-10  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

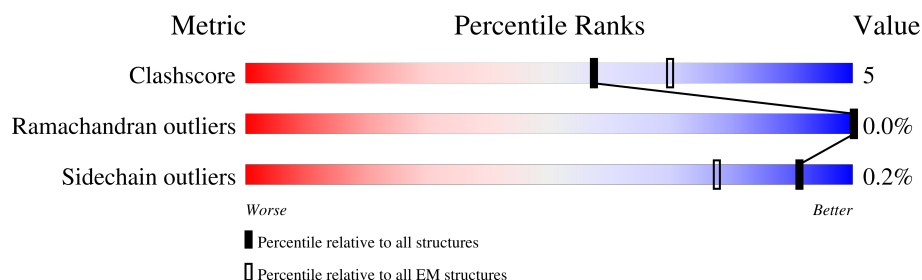
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	115	<div> <div>83%</div> <div>78% 21% .</div> </div>
2	B	224	<div> <div>58%</div> <div>60% 10% 30%</div> </div>
3	C	263	<div> <div>70%</div> <div>66% 13% 21%</div> </div>
4	D	463	<div> <div>80%</div> <div>77% 16% 7%</div> </div>
5	E	248	<div> <div>79%</div> <div>73% 12% 15%</div> </div>
6	F	464	<div> <div>84%</div> <div>80% 13% 8%</div> </div>
7	G	727	<div> <div>85%</div> <div>83% 11% 5%</div> </div>
8	H	318	<div> <div>82%</div> <div>84% 16%</div> </div>

Continued on next page...

Continued from previous page...

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	

Continued on next page...

*Continued from previous page...*

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 54 unique types of molecules in this entry. The entry contains 67042 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		

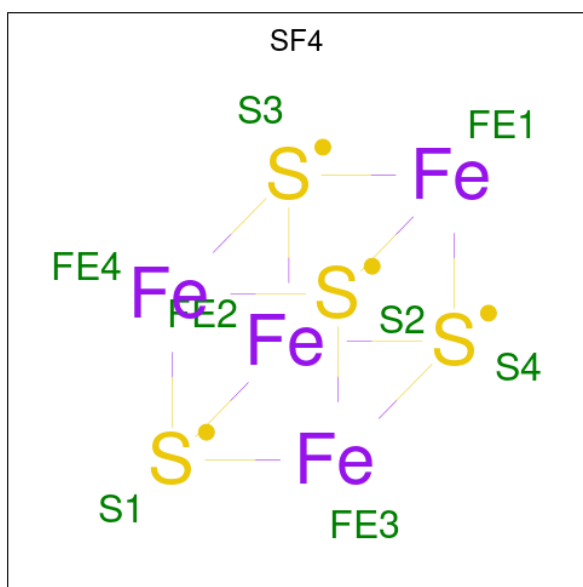
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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.

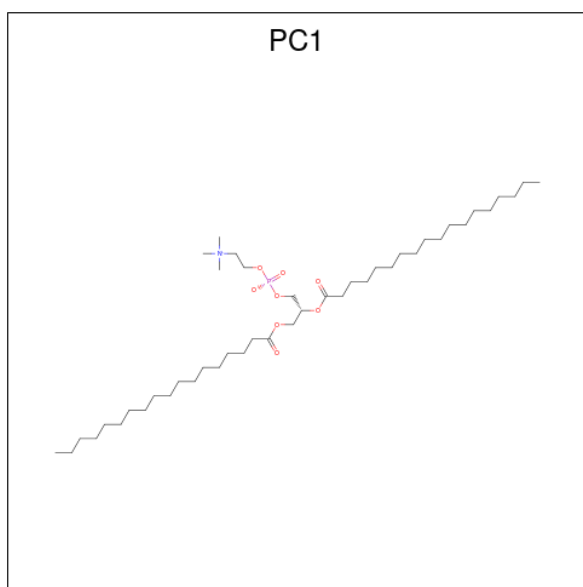
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	41	Total	C	N	O	0	0
			344	215	61	68		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



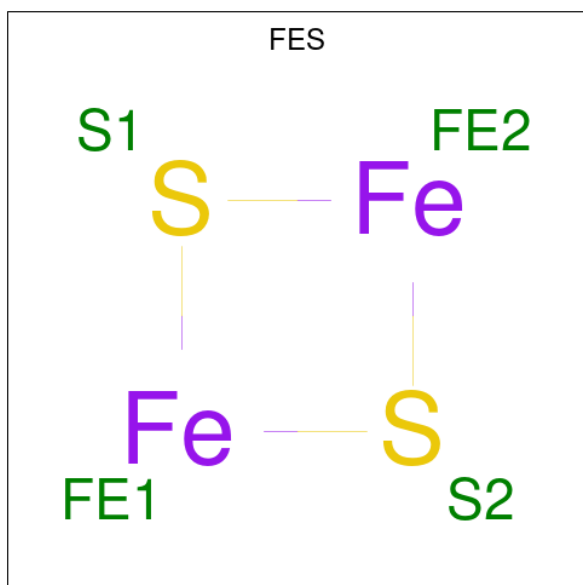
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

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



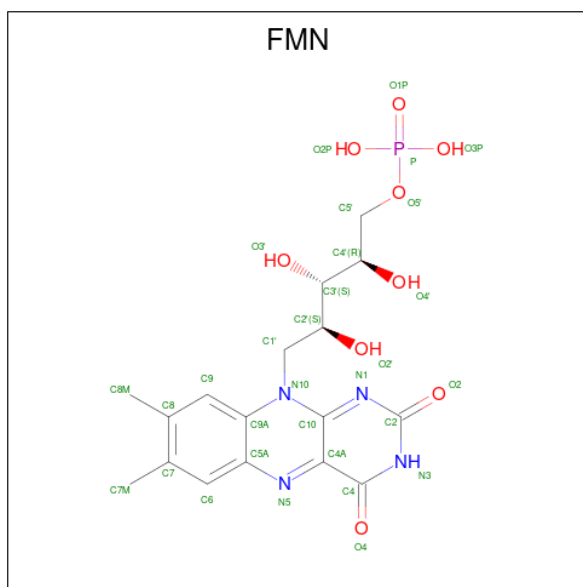
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	I	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



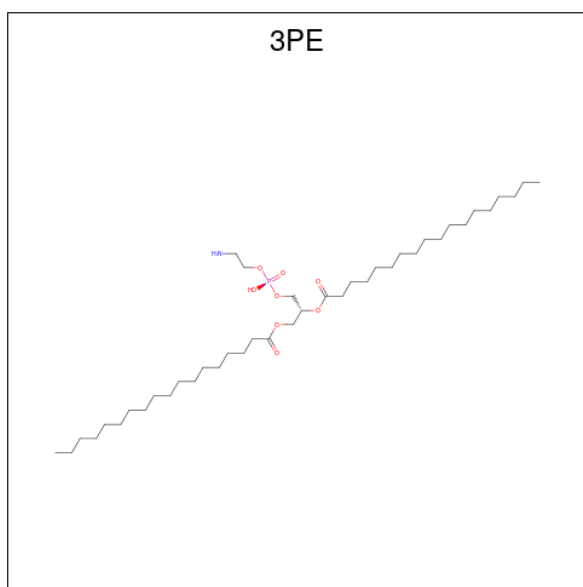
Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



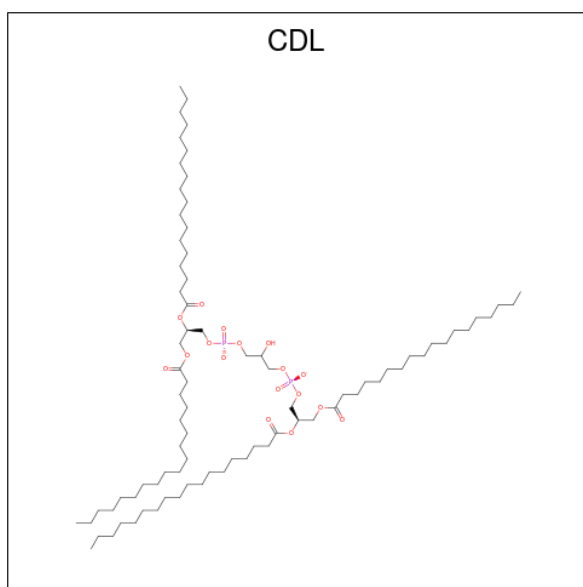
Mol	Chain	Residues	Atoms					AltConf
48	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



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

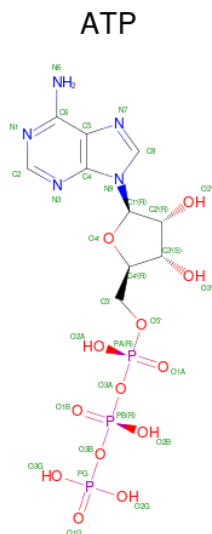
- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

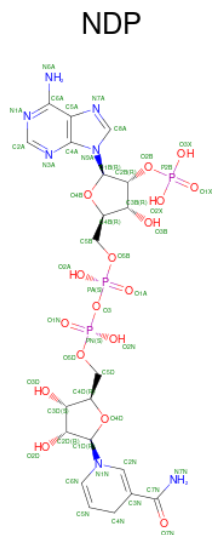
- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





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

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$ ).

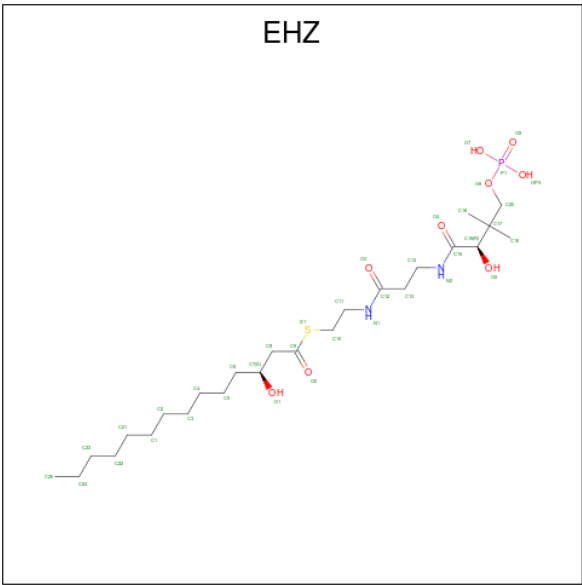


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 54 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: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).

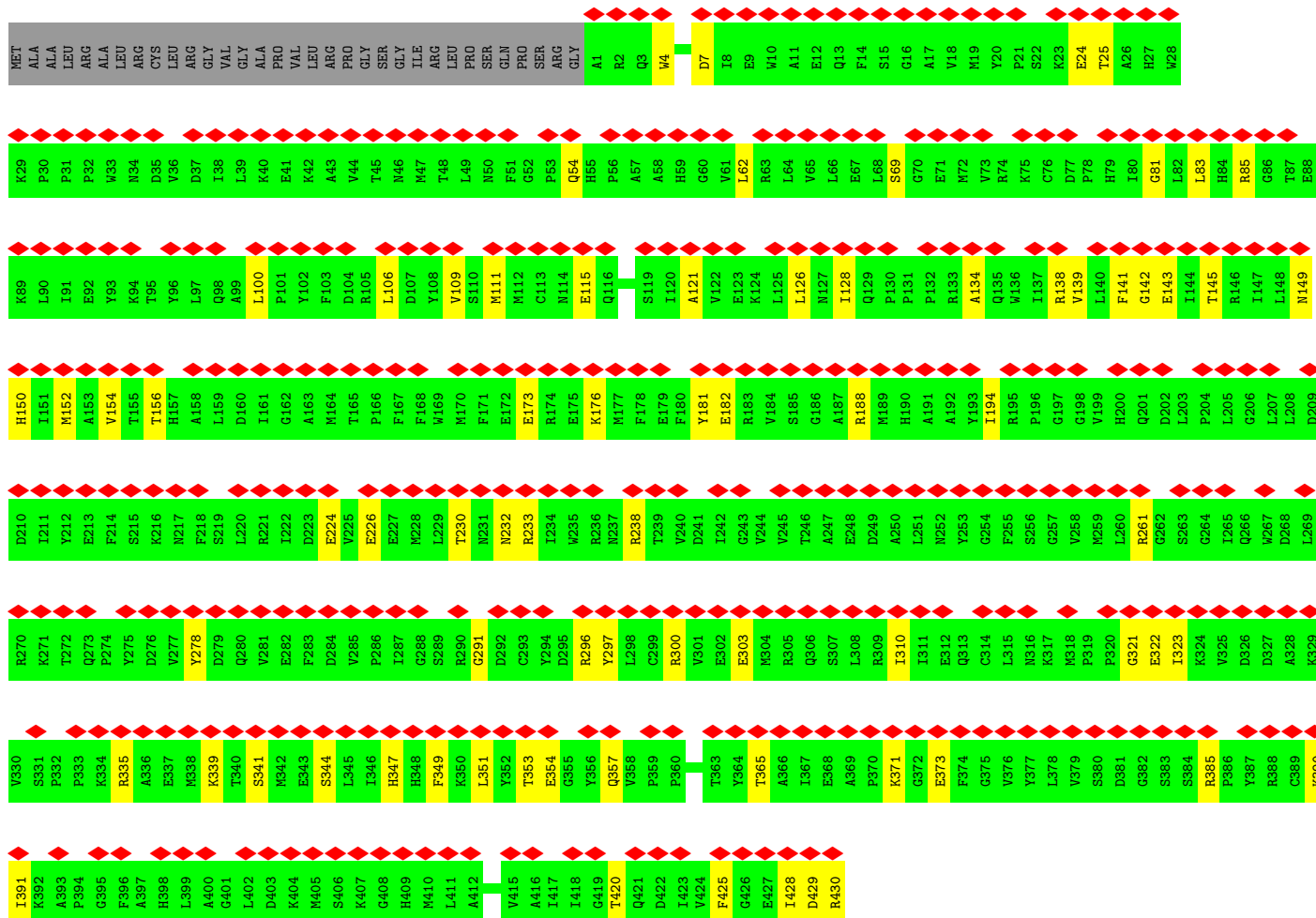
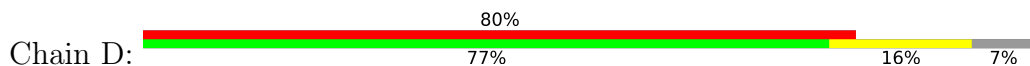


Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

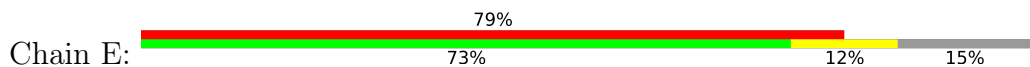


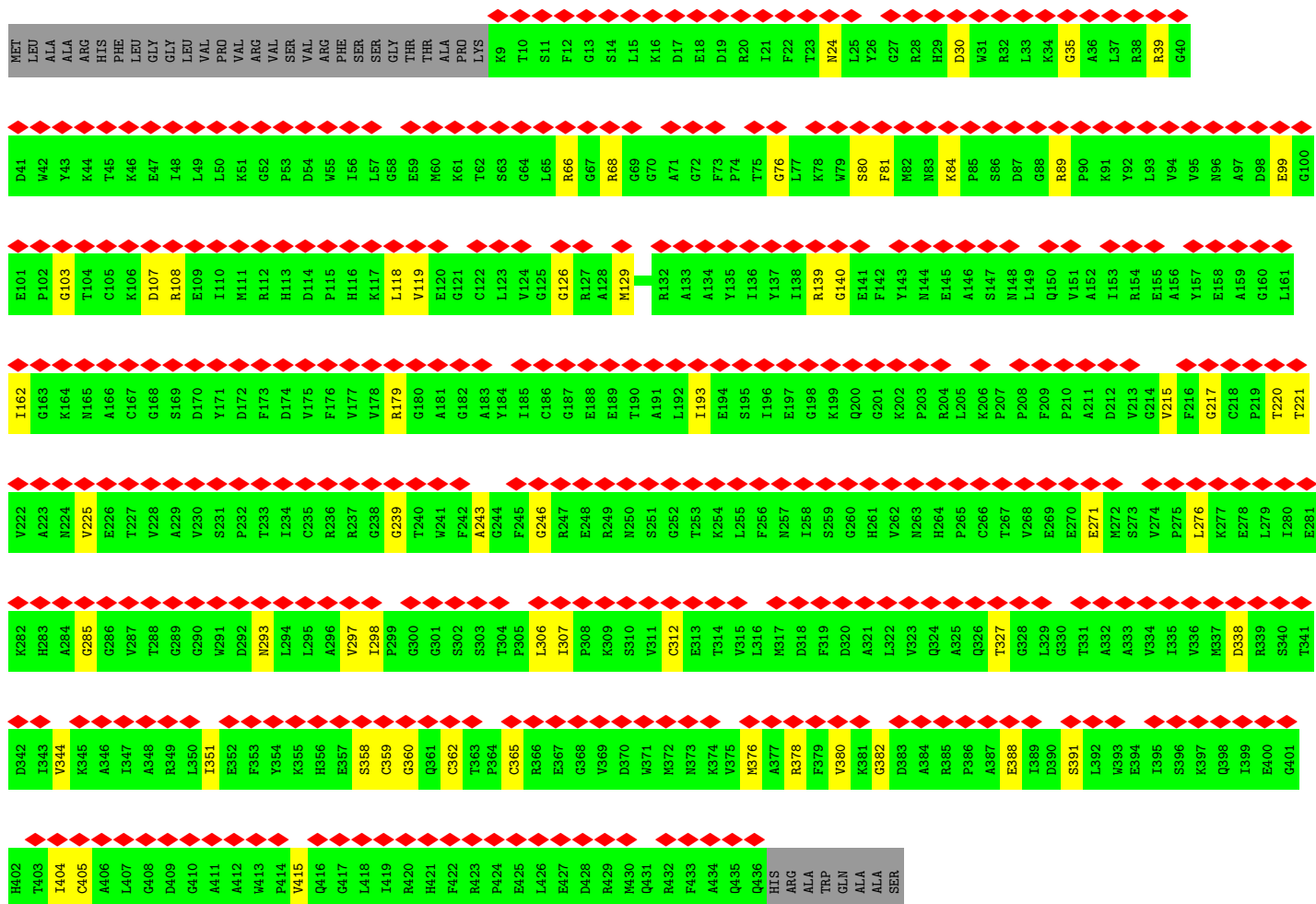


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

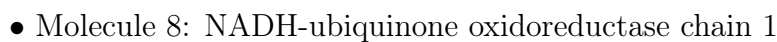


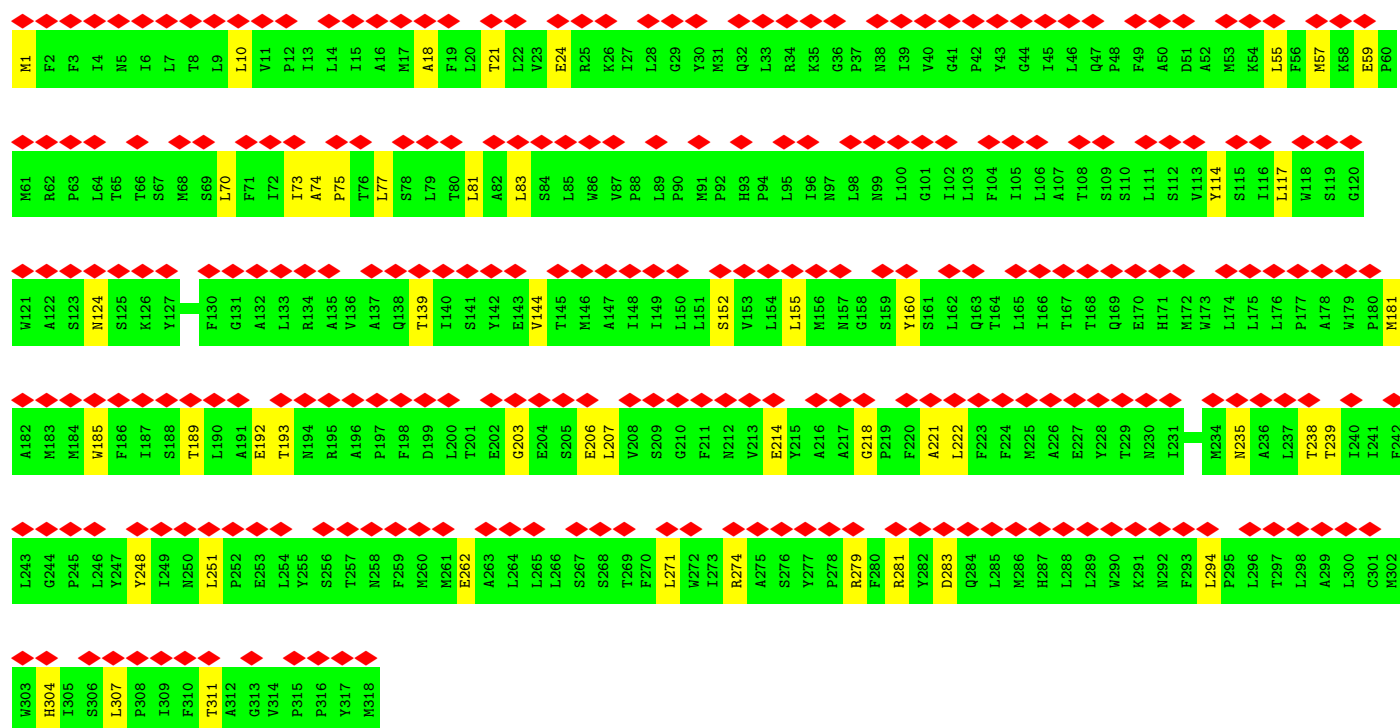
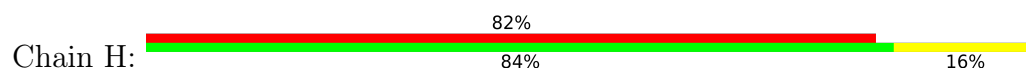
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





- Chain G:

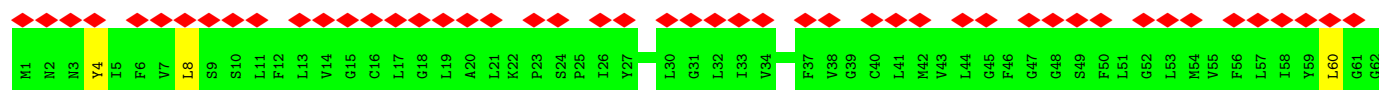
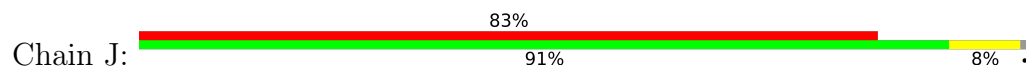


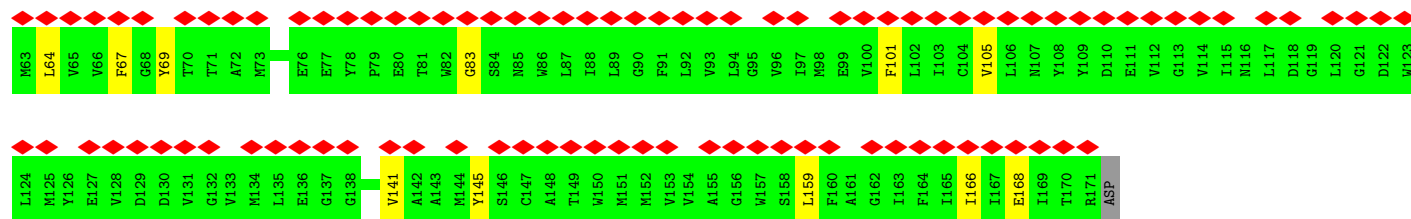


- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

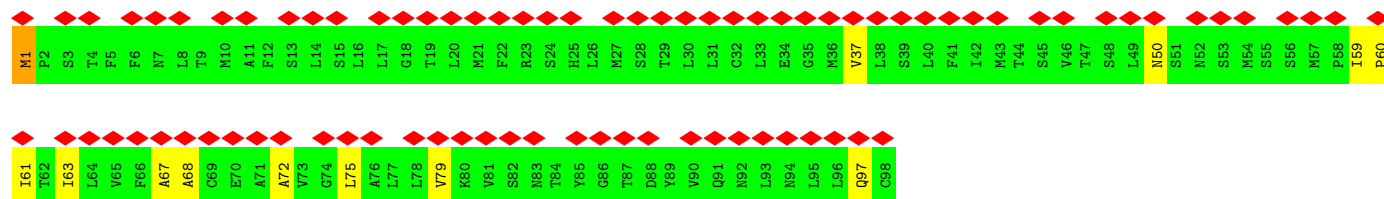
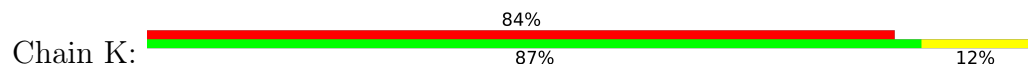


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

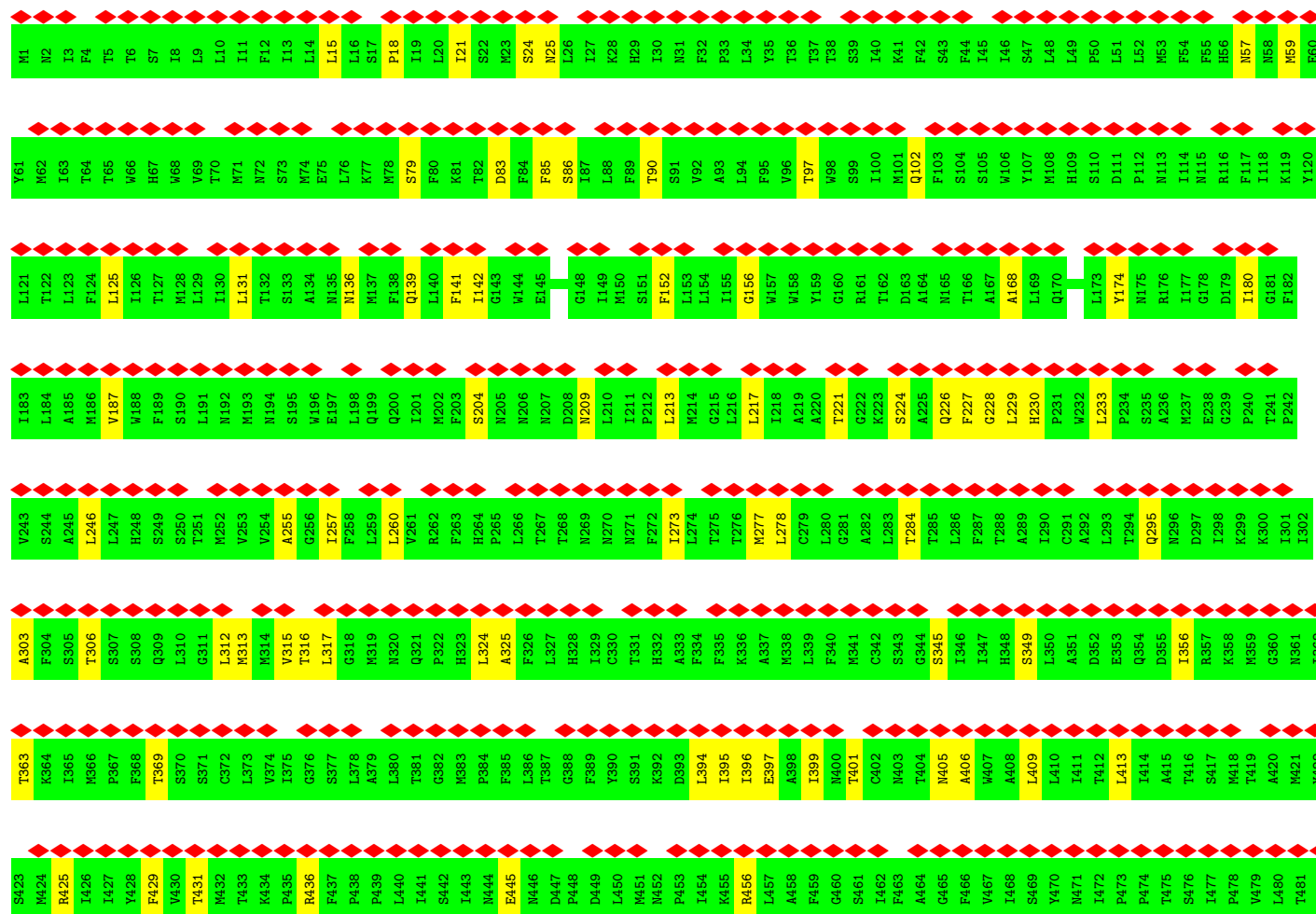
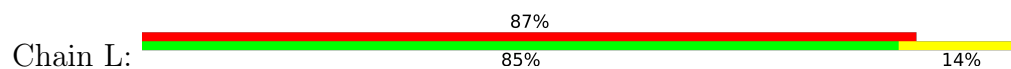




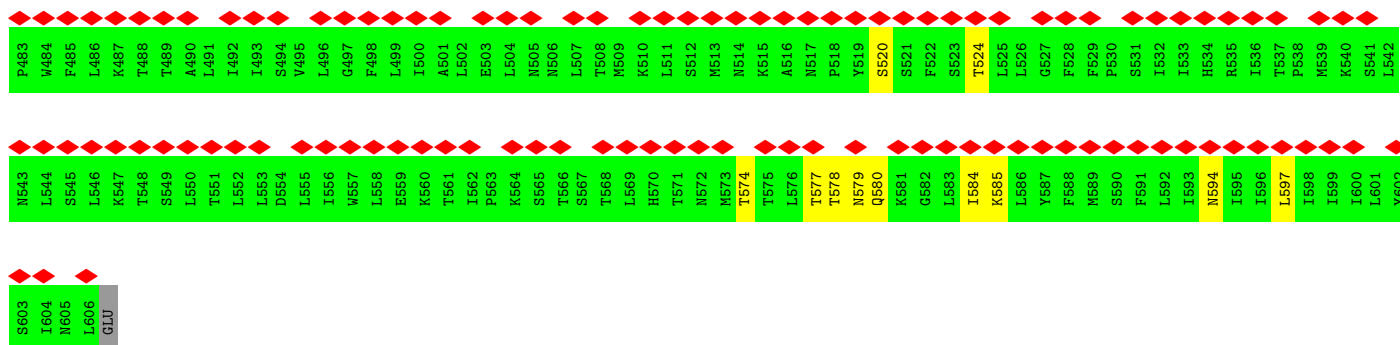
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



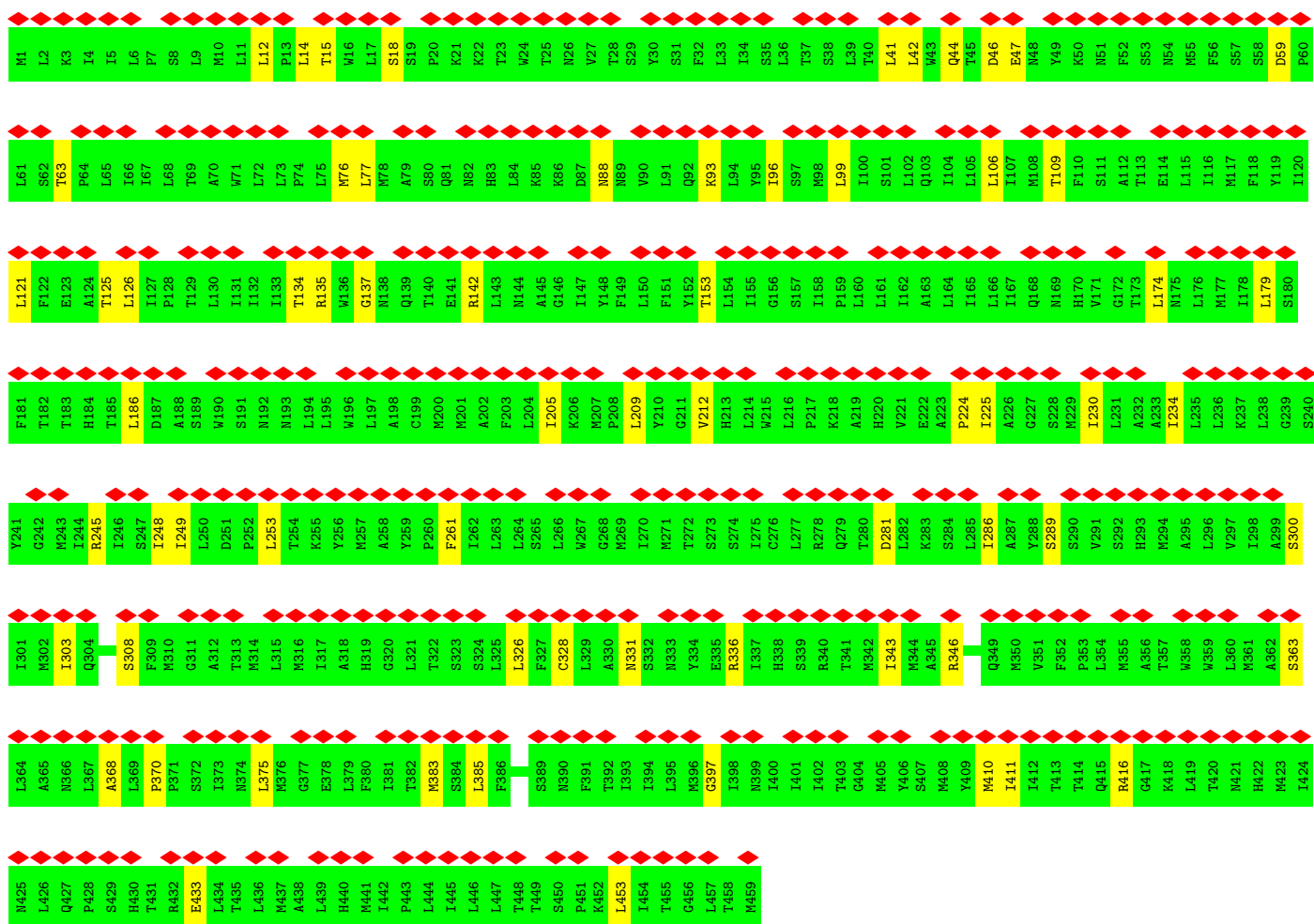
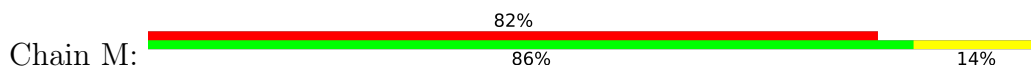
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



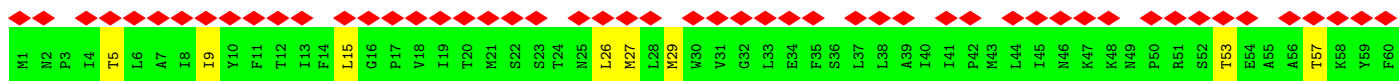
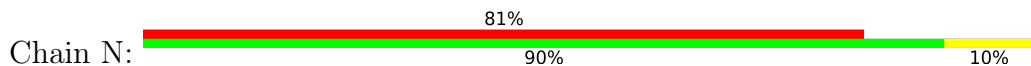


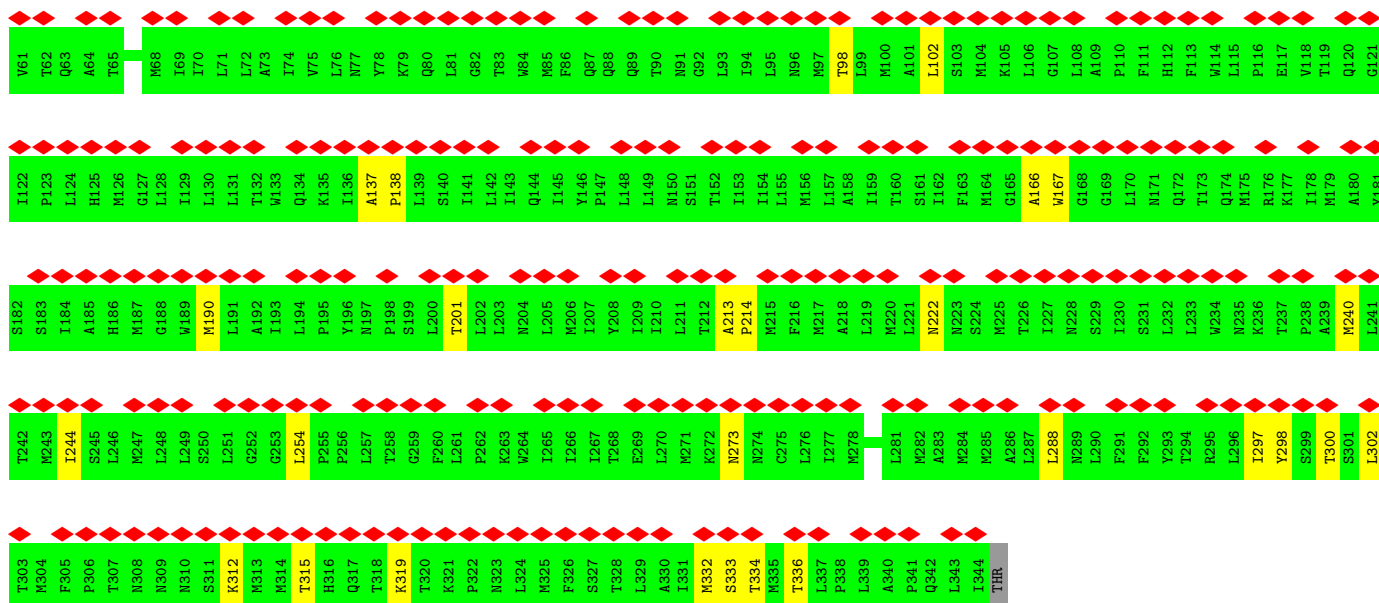


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

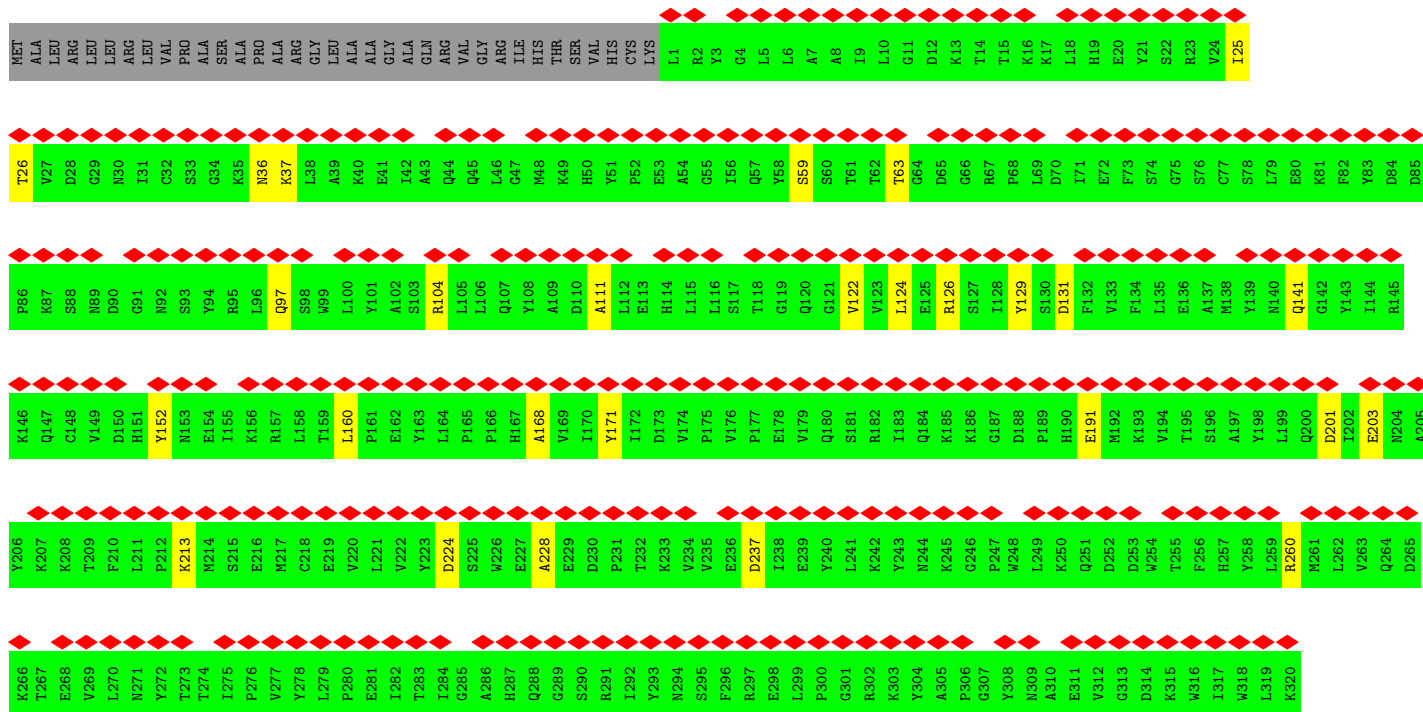
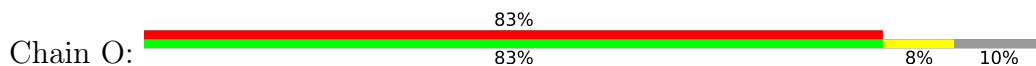


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

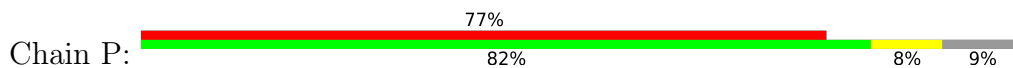




- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial




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



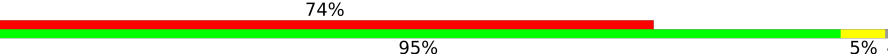


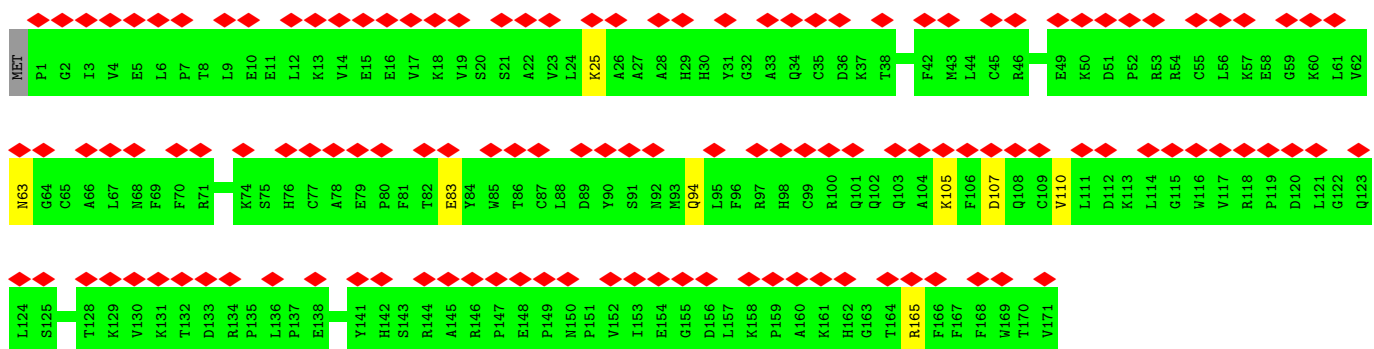


Chain W: 




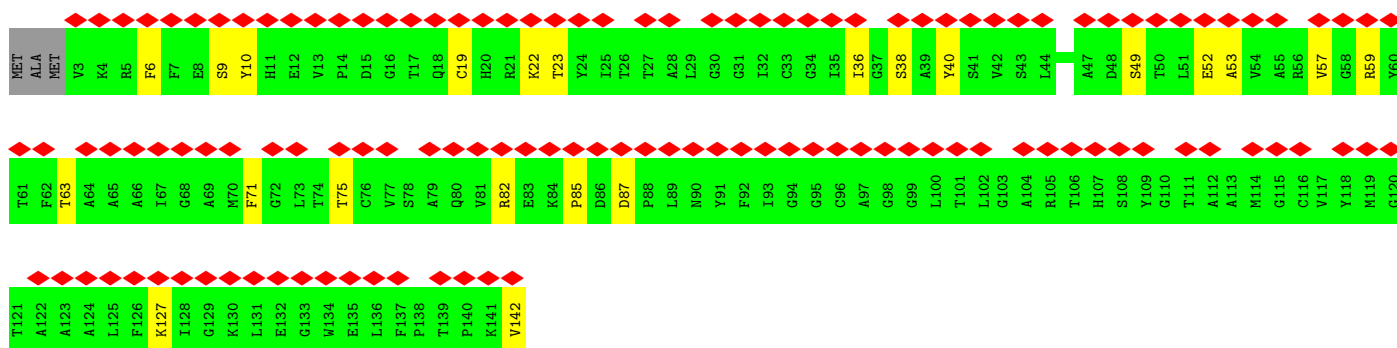
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X: 

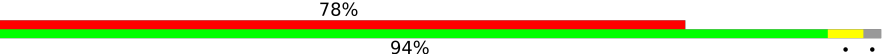


- Molecule 24: MCG5603

Chain Y: 



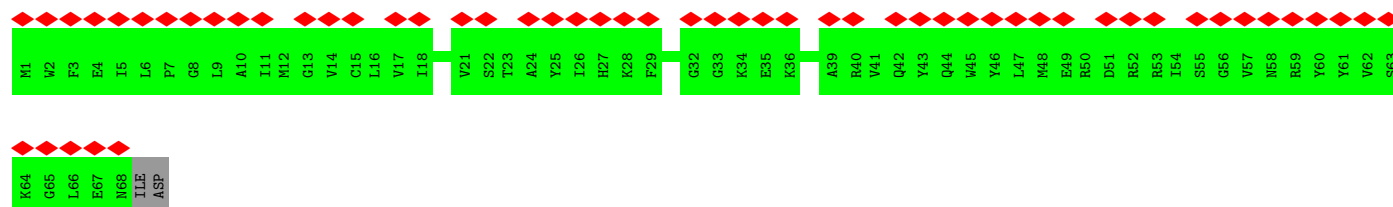
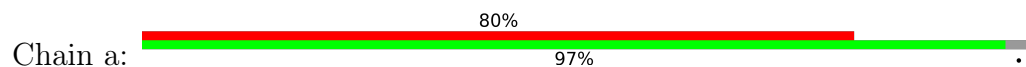
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z: 

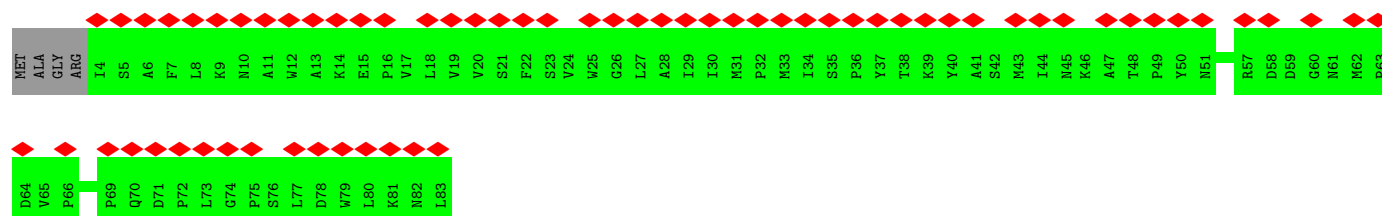
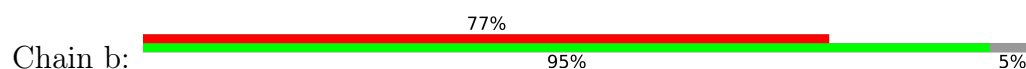




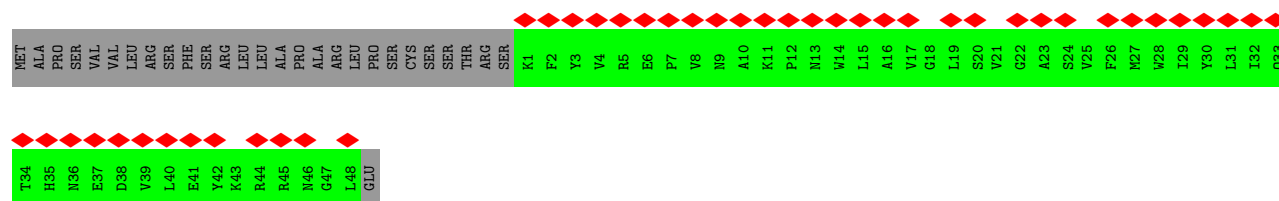
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



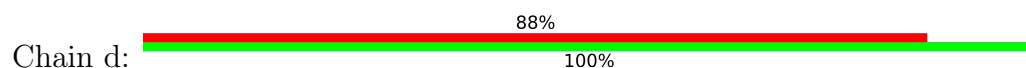
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



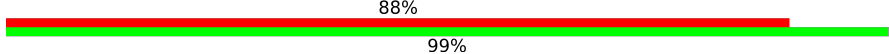
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

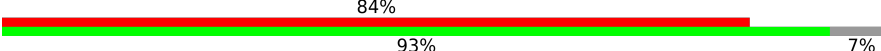


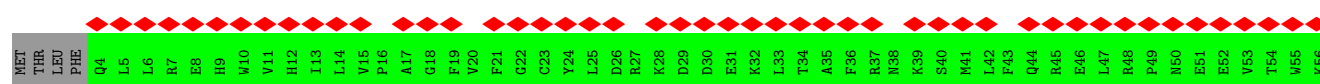
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 



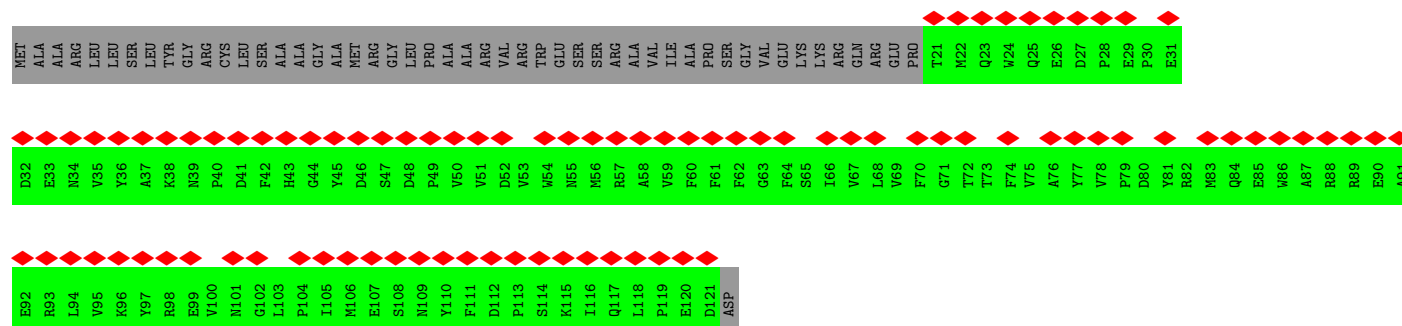
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 




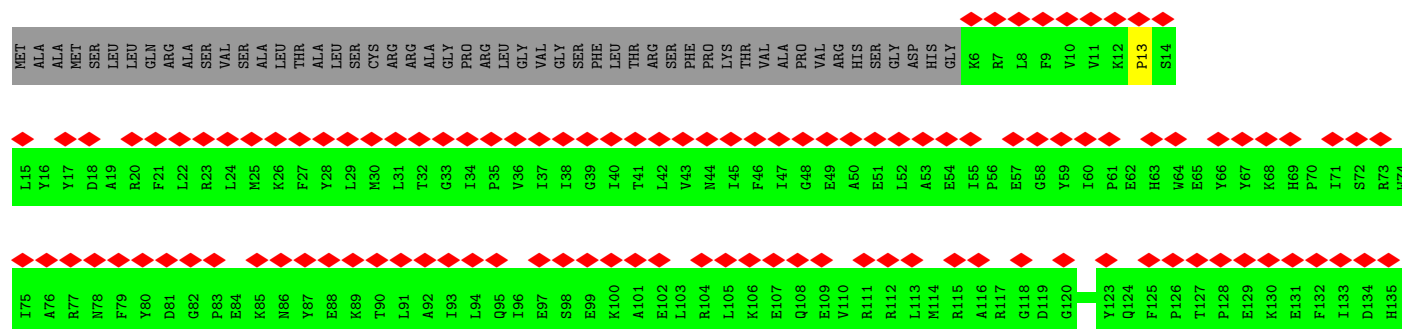
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

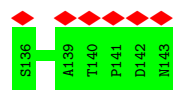
Chain g: 



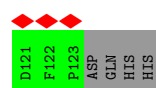
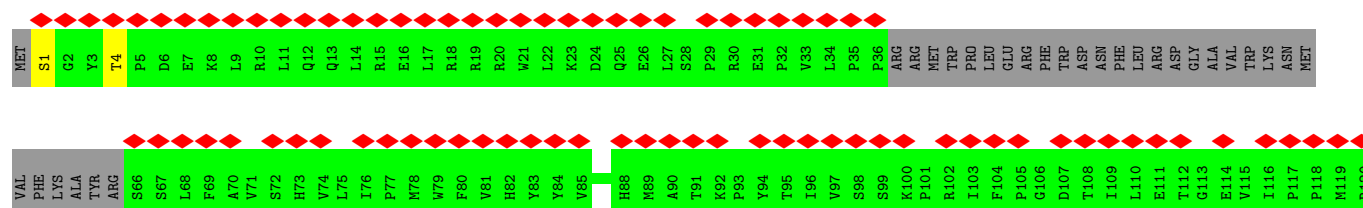
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 

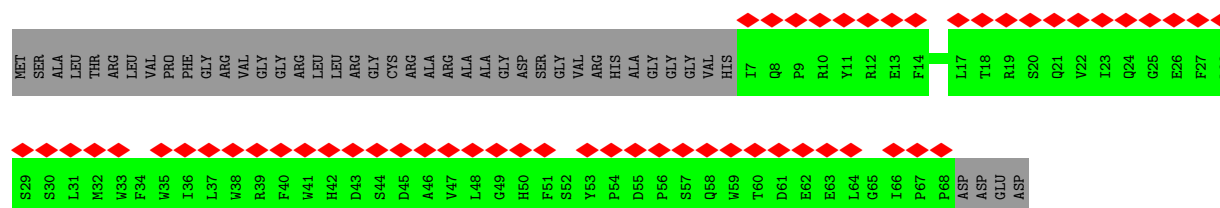




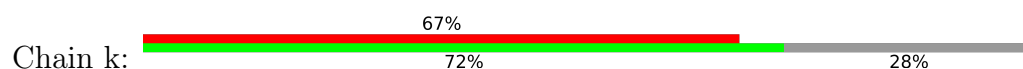
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



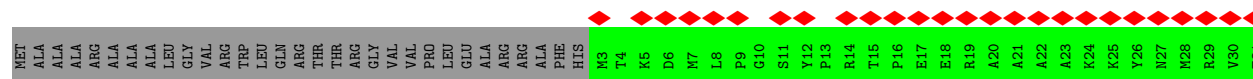
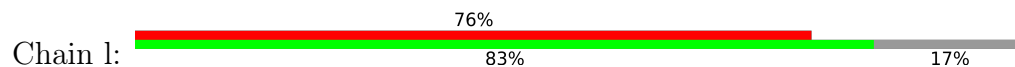
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



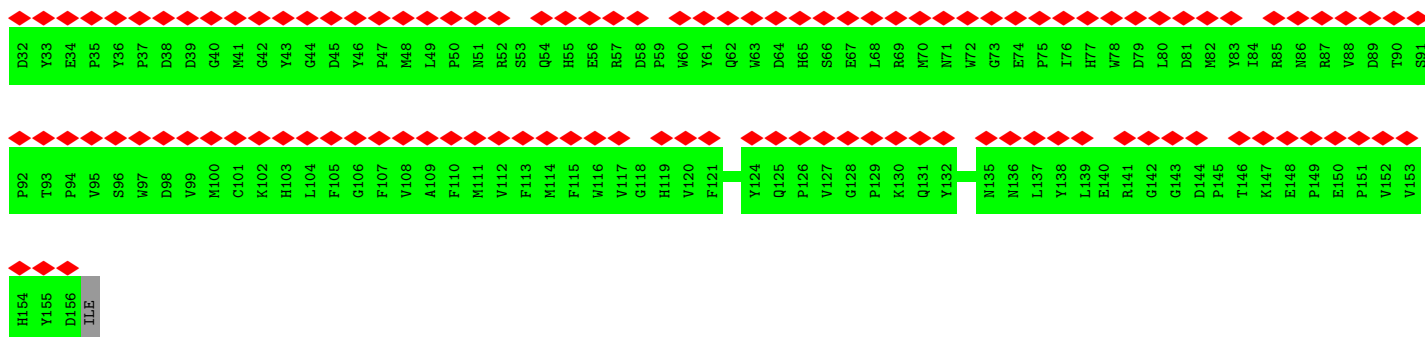
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



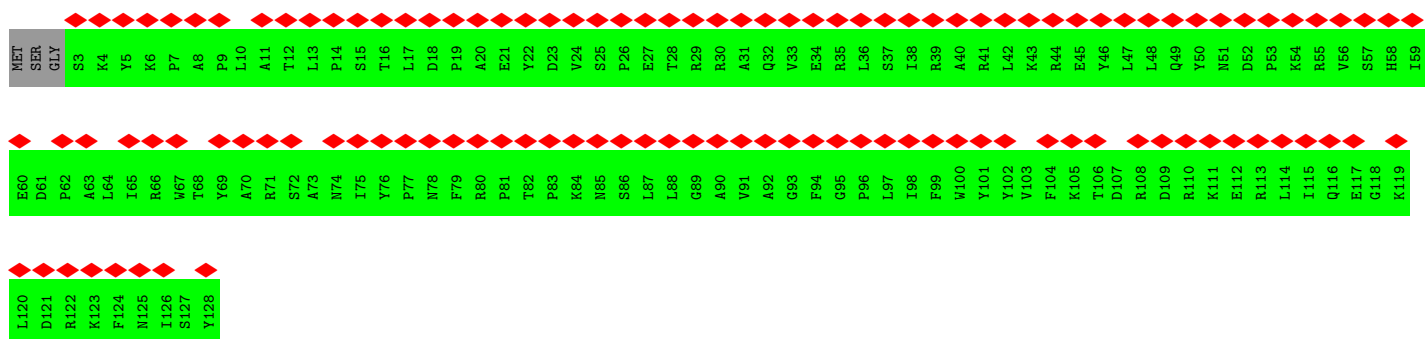
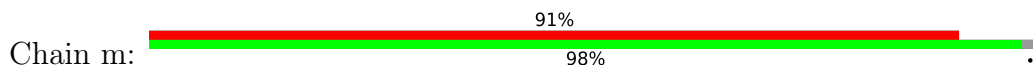
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



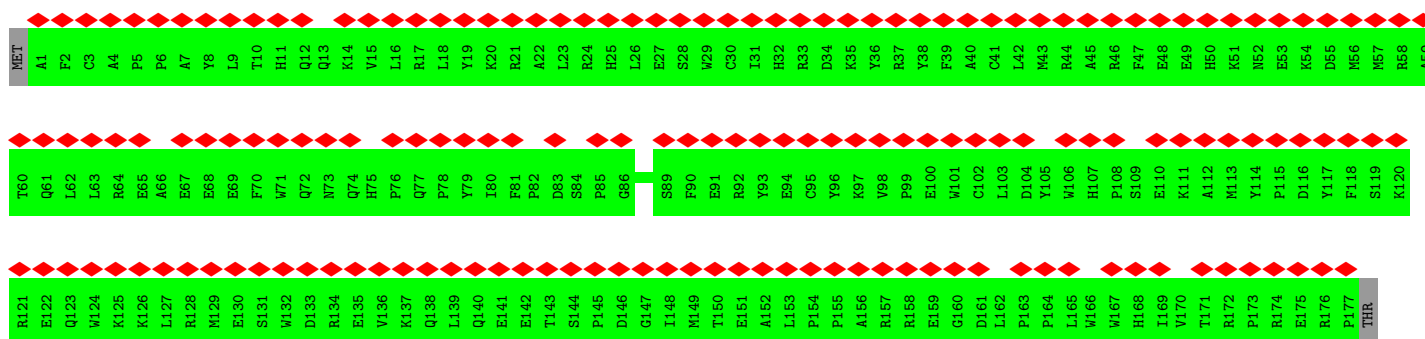




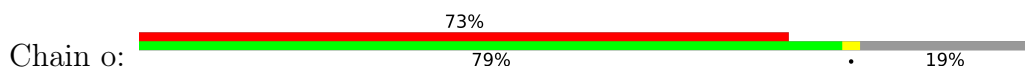
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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

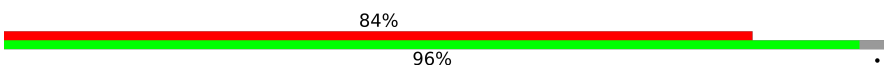


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



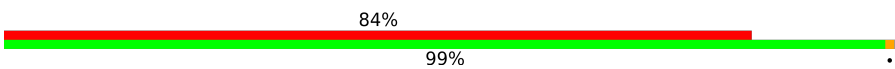
ARG  
VAL  
ALA  
GLN  
GLY  
GLN  
GLY  
GLY  
GLY  
VAL  
VAL  
PRO  
GLU  
VAL  
ALA  
LEU

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

Chain p: 


MET PRO ASP SER W4 D5 D6 D7 D8 D9 D10 D11 D12 D13 D14 D15 D16 D17 D18 D19 D20 D21 D22 D23 D24 D25 D26 D27 D28 D29 D30 D31 D32 D33 D34 D35 D36 D37 D38 D39 D40 D41 D42 D43 D44 D45 D46 D47 D48 D49 D50 D51 D52 D53 D54 D55 D56 D57 D58 D59  
T60 Y61 Y62 Y63 Y64 Y65 Y66 Y67 Y68 Y69 Y70 Y71 Y72 Y73 Y74 Y75 Y76 Y77 Y78 Y79 Y80 Y81 Y82 Y83 Y84 Y85 Y86 Y87 Y88 Y89 Y90 Y91 Y92 Y93 Y94 Y95 Y96 Y97 Y98 Y99  
Y120 Q121 Q122 Q123 Q124 Q125 Q126 Q127 Q128 Q129 Q130 Q131 Q132 Q133 K136 A137 Y138 Q139 D140 R141 Y142 L143 D144 L145 G146 A147 Y148 Y149 S150 A151 R152 K153 C154 L155 A156 K157 Y158 Q159 Q160 R161 M162 L163 E164 E165 R166 K167 A168 A169 R170 Q171 E172 ALA ALA ALA

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

Chain q: 

M1 E2 L3 V4 V5 V6 V7 V8 V9 V10 V11 V12 V13 V14 V15 V16 V17 V18 V19 V20 V21 V22 V23 V24 V25 V26 V27 V28 V29 V30 V31 V32 V33 V34 V35 V36 V37 V38 V39 V40 V41 V42 V43 V44 V45 V46 V47 V48 V49 V50 V51 V52 V53 V54 V55 V56 V57 V58 V59 V60  
W61 V62 I63 Y64 T65 T66 E67 M68 M69 M70 K71 N72 T73 F74 V75 W76 V77 G78 G79 S80 M81 P84 E85 W86 H87 W88 W89 L90 H91 C92 M93 T94 D95 D96 P97 P98 T99 T100 N101 P102 P103 K104 A105 A106 K107 F108 I109 T110 T111 N112 H113 K114 F115 N116 V117 P121 E122 Q123  
Y124 V125 P126 Y127 S128 T129 T130 R131 K132 K133 I134 H135 E136 V137 V138 P139 P140 S141 T142 P143 Y144 LYS

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

Chain r: 

MET A1 S2 A3 T4 R5 V6 V7 V8 V9 V10 V11 V12 V13 V14 V15 V16 V17 V18 V19 V20 V21 V22 V23 V24 V25 V26 V27 V28 V29 V30 V31 V32 V33 V34 V35 V36 V37 V38 V39 V40 V41 V42 V43 V44 V45 V46 V47 V48 V49 V50 V51 V52 V53 V54 V55 V56 V57 V58 V59  
R60 E61 V62 V63 V64 V65 V66 V67 V68 V69 V70 V71 V72 V73 V74 V75 V76 V77 GLY LYS ALA ALA ALA GLY GLY SER SER SER MET VAL VAL ARG LEU THR E90 K91 K92 A93 V94 T95 P96 A97 P98 P99 M100 K101 R102 V103 W104 L105 S106 D107 D108 Q109 Y110 Y111 L112

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

Chain s: 

MET ALA VAL SER LEU LEU LEU ARG GLY GLY ARG ARG ARG ARG LEU LYS ALA VAL LEU LEU LEU LEU ARG VAL PHE PRO GLY GLY LEU VAL SER SER VAL VAL ARG LEU THR E90 K91 K92 A93 V94 T95 P96 A97 P98 P99 M100 K101 R102 V103 W104 L105 S106 D107 D108 Q109 Y110 Y111 L112

PRO	
THR	
D28	
T29	
T30	
T31	
Y32	
X33	
N34	
L35	
Q36	
H37	
H38	
D39	
Y40	
M41	
T42	
Y43	
T44	
F45	
L46	
D47	
L48	
M49	
L50	
D51	
L52	
S53	
X54	
F55	
R56	
L57	
P58	
Q59	
P60	
S61	
S62	
G63	
R64	
E65	
S66	
P67	
R68	
HIS	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20370	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)	1500	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0241	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.32	0/949	0.57	0/1297
2	B	0.38	0/1278	0.59	0/1730
3	C	0.35	0/1771	0.60	0/2412
4	D	0.36	0/3540	0.57	0/4795
5	E	0.32	0/1688	0.58	0/2300
6	F	0.30	0/3374	0.59	0/4557
7	G	0.32	0/5383	0.58	0/7293
8	H	0.35	0/2607	0.57	0/3564
9	I	0.37	0/1461	0.60	0/1974
10	J	0.36	0/1322	0.53	0/1799
11	K	0.31	0/738	0.50	0/1002
12	L	0.31	0/4913	0.53	0/6686
13	M	0.31	0/3709	0.55	0/5052
14	N	0.31	0/2748	0.57	3/3741 (0.1%)
15	O	0.32	0/2674	0.53	0/3626
16	P	0.31	0/2823	0.57	0/3828
17	Q	0.31	0/1038	0.54	0/1401
18	R	0.32	0/751	0.54	0/1011
19	S	0.30	0/678	0.61	0/915
20	T	0.29	0/620	0.49	0/836
20	U	0.29	0/704	0.46	0/951
21	V	0.30	0/949	0.50	0/1286
22	W	0.30	0/993	0.56	0/1335
23	X	0.31	0/1434	0.57	0/1937
24	Y	0.30	0/1061	0.55	0/1439
25	Z	0.32	0/1198	0.59	0/1616
26	a	0.33	0/569	0.56	0/766
27	b	0.30	0/651	0.49	0/895
28	c	0.30	0/409	0.51	0/555
29	d	0.33	0/1028	0.56	0/1387
30	e	0.30	0/900	0.59	0/1199
31	f	0.30	0/468	0.56	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	g	0.32	0/878	0.52	0/1196
33	h	0.32	0/1197	0.56	0/1621
34	i	0.31	0/804	0.57	0/1094
35	j	0.28	0/561	0.51	0/768
36	k	0.29	0/629	0.50	0/851
37	l	0.33	0/1348	0.54	0/1840
38	m	0.31	0/1079	0.59	0/1463
39	n	0.32	0/1589	0.57	0/2152
40	o	0.34	0/982	0.61	0/1320
41	p	0.32	0/1466	0.58	0/1981
42	q	0.33	0/1234	0.55	0/1681
43	r	0.32	0/812	0.65	1/1098 (0.1%)
44	s	0.30	0/353	0.53	0/479
All	All	0.32	0/67361	0.56	4/91359 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
42	q	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	r	76	VAL	CG1-CB-CG2	6.78	121.75	110.90
14	N	254	LEU	CB-CG-CD2	6.44	121.95	111.00
14	N	15	LEU	CB-CG-CD2	5.52	120.39	111.00
14	N	15	LEU	CB-CG-CD1	5.25	119.93	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	q	1	AME	Mainchain

## 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	17	0
3	C	1721	0	1680	30	0
4	D	3464	0	3416	55	0
5	E	1648	0	1639	21	0
6	F	3300	0	3258	37	0
7	G	5296	0	5322	51	0
8	H	2540	0	2626	33	0
9	I	1431	0	1383	25	0
10	J	1300	0	1315	14	0
11	K	737	0	768	12	0
12	L	4800	0	4985	63	0
13	M	3632	0	3853	46	0
14	N	2696	0	2895	21	0
15	O	2607	0	2566	14	0
16	P	2748	0	2768	23	0
17	Q	1015	0	1016	19	0
18	R	738	0	717	9	0
19	S	667	0	685	4	0
20	T	611	0	602	7	0
20	U	692	0	686	3	0
21	V	927	0	968	12	0
22	W	970	0	991	11	0
23	X	1396	0	1379	4	0
24	Y	1037	0	1024	13	0
25	Z	1167	0	1166	5	0
26	a	556	0	568	0	0
27	b	628	0	628	0	0
28	c	398	0	401	0	0
29	d	996	0	1001	0	0
30	e	877	0	871	0	0
31	f	456	0	452	0	0
32	g	850	0	783	0	0
33	h	1162	0	1163	0	0
34	i	787	0	797	0	0
35	j	537	0	495	0	0
36	k	609	0	603	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1294	0	1186	0	0
38	m	1050	0	1061	0	0
39	n	1534	0	1466	0	0
40	o	957	0	937	0	0
41	p	1433	0	1399	0	0
42	q	1203	0	1158	0	0
43	r	802	0	836	0	0
44	s	344	0	324	0	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	1	0
45	I	16	0	0	0	0
46	B	78	0	107	1	0
46	H	42	0	58	1	0
46	I	45	0	64	0	0
47	E	4	0	0	1	0
47	G	4	0	0	0	0
48	F	31	0	19	1	0
49	H	44	0	65	1	0
49	I	51	0	82	0	0
49	K	33	0	40	1	0
49	L	140	0	211	0	0
49	M	79	0	109	0	0
49	Y	41	0	56	0	0
50	L	74	0	92	0	0
50	N	124	0	145	1	0
50	d	130	0	151	0	0
50	h	70	0	87	0	0
50	q	57	0	58	0	0
51	O	31	0	12	2	0
52	P	48	0	26	1	0
53	R	1	0	0	0	0
54	T	37	0	0	0	0
54	U	37	0	0	1	0
All	All	67042	0	67443	481	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 (481) 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)
7:G:594:ARG:NH1	22:W:124:PHE:O	2.16	0.79
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.65	0.79
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.16	0.78
12:L:577:THR:O	12:L:580:GLN:NE2	2.16	0.77
12:L:313:MET:O	12:L:316:THR:OG1	2.02	0.76
4:D:335:ARG:NH2	9:I:128:CYS:O	2.20	0.75
1:A:37:TYR:OH	4:D:54:GLN:OE1	2.05	0.75
8:H:307:LEU:O	8:H:311:THR:OG1	2.02	0.74
15:O:104:ARG:NH1	15:O:126:ARG:O	2.20	0.74
2:B:52:ARG:NH1	46:B:202:PC1:O12	2.19	0.74
12:L:429:PHE:O	12:L:436:ARG:NH1	2.21	0.74
2:B:91:ARG:NH1	8:H:214:GLU:OE1	2.21	0.73
12:L:594:ASN:OD1	24:Y:40:TYR:OH	2.05	0.73
5:E:105:THR:OG1	47:E:301:FES:S2	2.45	0.73
9:I:174:ASP:OD2	9:I:178:ARG:NH2	2.22	0.73
5:E:162:GLU:OE2	6:F:108:ARG:NH2	2.21	0.73
6:F:358:SER:OG	6:F:365:CYS:SG	2.44	0.73
13:M:137:GLY:O	13:M:142:ARG:NH1	2.22	0.73
17:Q:33:ARG:NH1	17:Q:60:ASP:O	2.20	0.73
1:A:73:LEU:O	8:H:160:TYR:OH	2.07	0.73
8:H:18:ALA:O	8:H:21:THR:OG1	2.05	0.73
16:P:8:HIS:O	16:P:15:SER:OG	2.07	0.72
16:P:235:ARG:NH2	16:P:291:ASP:O	2.22	0.72
13:M:106:LEU:HD13	13:M:234:ILE:HD12	1.71	0.72
16:P:180:ASN:OD1	16:P:320:ARG:NH1	2.23	0.72
18:R:81:THR:OG1	18:R:91:PHE:O	2.06	0.72
24:Y:10:TYR:O	24:Y:22:LYS:NZ	2.22	0.72
24:Y:85:PRO:O	24:Y:127:LYS:NZ	2.22	0.71
3:C:192:GLN:OE1	9:I:117:LYS:NZ	2.22	0.71
12:L:295:GLN:O	12:L:425:ARG:NH1	2.23	0.71
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.73	0.71
23:X:83:GLU:OE1	23:X:105:LYS:NZ	2.23	0.70
3:C:197:PHE:O	4:D:385:ARG:NH2	2.23	0.70
6:F:378:ARG:NH1	6:F:388:GLU:OE1	2.24	0.70
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.06	0.70
18:R:12:THR:OG1	18:R:14:THR:O	2.09	0.70
3:C:43:SER:OG	3:C:45:LEU:O	2.10	0.70
1:A:33:LYS:NZ	8:H:59:GLU:OE2	2.18	0.69
6:F:246:GLY:N	6:F:271:GLU:OE2	2.25	0.69
7:G:544:VAL:HG23	7:G:559:VAL:HG13	1.75	0.69
12:L:102:GLN:OE1	12:L:456:ARG:NH2	2.25	0.69
13:M:300:SER:OG	13:M:308:SER:OG	2.05	0.69

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:620:ARG:NH1	7:G:633:TYR:OH	2.26	0.69
12:L:369:THR:OG1	12:L:445:GLU:OE2	2.05	0.69
14:N:222:ASN:OD1	14:N:319:LYS:NZ	2.25	0.69
4:D:4:TRP:O	13:M:142:ARG:NH2	2.26	0.69
7:G:303:VAL:HG11	7:G:603:LEU:HD11	1.75	0.69
23:X:25:LYS:NZ	23:X:94:GLN:O	2.24	0.69
13:M:205:ILE:HD13	13:M:212:VAL:HG21	1.74	0.68
4:D:106:LEU:HD11	4:D:391:ILE:HD13	1.74	0.68
12:L:303:ALA:O	12:L:306:THR:OG1	2.10	0.68
1:A:71:LEU:O	10:J:145:TYR:OH	2.12	0.68
6:F:24:ASN:ND2	6:F:30:ASP:O	2.27	0.68
16:P:235:ARG:NH1	16:P:293:MET:SD	2.66	0.68
22:W:32:ARG:NH2	22:W:36:GLU:OE2	2.26	0.67
6:F:81:PHE:O	6:F:84:LYS:NZ	2.26	0.67
17:Q:13:VAL:O	22:W:17:THR:N	2.27	0.67
24:Y:49:SER:OG	24:Y:52:GLU:OE1	2.10	0.67
1:A:33:LYS:O	2:B:91:ARG:NH2	2.27	0.67
6:F:126:GLY:O	6:F:129:MET:O	2.12	0.67
2:B:37:GLU:OE2	2:B:188:ARG:NH2	2.28	0.67
9:I:38:MET:O	9:I:41:SER:OG	2.12	0.66
16:P:77:ASP:O	16:P:80:SER:OG	2.13	0.66
2:B:35:ARG:NH2	2:B:37:GLU:OE1	2.28	0.66
6:F:99:GLU:O	6:F:139:ARG:NH2	2.29	0.66
12:L:363:THR:OG1	12:L:431:THR:O	2.08	0.66
54:U:201:EHZ:C19	54:U:201:EHZ:O4	2.43	0.66
3:C:49:GLU:OE1	3:C:106:ARG:NH1	2.28	0.65
4:D:233:ARG:NH2	9:I:25:ARG:O	2.29	0.65
7:G:199:VAL:HG12	7:G:208:LEU:HD11	1.78	0.65
3:C:66:ASP:HB2	21:V:89:LEU:HD12	1.77	0.65
4:D:428:ILE:O	4:D:430:ARG:NH1	2.30	0.65
3:C:68:THR:OG1	21:V:86:GLU:OE1	2.11	0.64
4:D:182:GLU:OE2	9:I:60:SER:N	2.30	0.64
11:K:1:FME:SD	11:K:50:ASN:ND2	2.70	0.64
12:L:79:SER:OG	12:L:136:ASN:OD1	2.14	0.64
12:L:356:ILE:O	12:L:436:ARG:NH1	2.31	0.64
5:E:132:THR:OG1	5:E:134:ASP:OD1	2.11	0.64
9:I:158:ASN:ND2	18:R:36:ASN:OD1	2.31	0.64
12:L:86:SER:O	12:L:90:THR:OG1	2.14	0.64
13:M:106:LEU:O	13:M:109:THR:OG1	2.15	0.64
16:P:248:MET:SD	16:P:322:ARG:NH1	2.71	0.64
12:L:227:PHE:O	12:L:230:HIS:ND1	2.22	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:GLU:OE2	4:D:176:LYS:NZ	2.31	0.63
7:G:113:GLU:OE2	7:G:249:ARG:NH1	2.31	0.63
7:G:140:LYS:O	7:G:148:THR:OG1	2.16	0.62
12:L:131:LEU:HD21	12:L:255:ALA:HB1	1.82	0.62
4:D:238:ARG:NH2	8:H:206:GLU:OE2	2.32	0.62
3:C:86:ARG:NH1	3:C:91:GLU:OE1	2.32	0.61
4:D:138:ARG:HG2	4:D:194:ILE:HD12	1.82	0.61
5:E:100:ILE:HG21	5:E:120:LEU:HD21	1.82	0.61
8:H:239:THR:OG1	8:H:262:GLU:OE1	2.19	0.61
6:F:66:ARG:O	6:F:68:ARG:NH1	2.34	0.61
9:I:66:GLU:O	9:I:136:GLY:N	2.33	0.61
17:Q:10:LEU:O	22:W:25:ARG:NH2	2.34	0.61
4:D:341:SER:OG	4:D:344:SER:OG	2.17	0.61
13:M:14:LEU:O	13:M:18:SER:OG	2.10	0.61
16:P:90:VAL:HG21	16:P:218:THR:OG1	2.00	0.61
3:C:31:GLU:OE2	21:V:46:TYR:OH	2.13	0.61
14:N:332:MET:O	14:N:336:THR:OG1	2.10	0.61
19:S:26:SER:O	19:S:33:ARG:NH2	2.34	0.61
5:E:119:THR:HG21	5:E:166:PRO:HB3	1.82	0.61
7:G:367:THR:OG1	7:G:370:GLY:N	2.34	0.61
12:L:97:THR:HG23	12:L:246:LEU:HD11	1.82	0.61
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.33	0.61
14:N:312:LYS:O	14:N:315:THR:OG1	2.12	0.60
7:G:261:GLU:OE2	17:Q:42:ARG:NH2	2.35	0.60
16:P:153:GLU:HG3	16:P:165:ILE:HD13	1.84	0.60
2:B:81:ARG:NH2	9:I:50:ILE:O	2.35	0.60
6:F:307:ILE:HD11	6:F:327:THR:HG21	1.84	0.60
13:M:76:MET:SD	13:M:99:LEU:HD22	2.41	0.60
13:M:363:SER:HB2	13:M:411:ILE:HD11	1.83	0.60
7:G:577:GLU:OE1	7:G:579:ARG:NH1	2.35	0.60
1:A:1:FME:O	1:A:5:THR:OG1	2.17	0.59
15:O:59:SER:O	15:O:63:THR:OG1	2.14	0.59
4:D:141:PHE:O	4:D:145:THR:HG23	2.02	0.59
15:O:191:GLU:OE2	51:O:401:ATP:O3'	2.16	0.59
5:E:24:THR:OG1	5:E:27:ASN:OD1	2.14	0.59
17:Q:11:ILE:N	22:W:19:VAL:O	2.36	0.59
16:P:212:LYS:O	16:P:216:ASN:ND2	2.34	0.58
3:C:79:THR:HG22	4:D:390:LYS:HD2	1.85	0.58
12:L:316:THR:CG2	12:L:395:ILE:HD12	2.33	0.58
13:M:106:LEU:HD13	13:M:234:ILE:CD1	2.34	0.58
6:F:129:MET:SD	6:F:221:THR:OG1	2.49	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:47:GLN:NE2	20:U:67:ALA:O	2.35	0.58
11:K:37:VAL:HG21	11:K:67:ALA:HB1	1.85	0.58
16:P:175:GLU:N	16:P:175:GLU:OE1	2.36	0.58
12:L:141:PHE:HE2	13:M:375:LEU:HD11	1.68	0.58
7:G:200:ILE:HD13	7:G:210:SER:HB3	1.86	0.58
15:O:111:ALA:HB1	15:O:122:VAL:HG11	1.86	0.58
4:D:261:ARG:NH1	4:D:303:GLU:OE2	2.37	0.58
12:L:187:VAL:HG22	13:M:383:MET:HG3	1.85	0.58
7:G:591:GLY:HA2	16:P:6:ILE:HG21	1.86	0.58
1:A:68:GLU:HG2	10:J:159:LEU:HD13	1.85	0.57
7:G:252:PRO:O	17:Q:44:ASN:ND2	2.37	0.57
12:L:226:GLN:HA	12:L:284:THR:HG21	1.86	0.57
12:L:316:THR:HG21	12:L:395:ILE:HD12	1.86	0.57
12:L:397:GLU:O	12:L:401:THR:OG1	2.14	0.57
13:M:134:THR:OG1	14:N:302:LEU:HD13	2.04	0.57
4:D:226:GLU:O	4:D:230:THR:OG1	2.13	0.57
48:F:501:FMN:N1	48:F:501:FMN:O3'	2.25	0.57
7:G:350:PRO:HG2	7:G:467:LEU:HD12	1.85	0.57
1:A:17:LEU:HD22	8:H:222:LEU:HD21	1.86	0.57
10:J:69:TYR:CE2	11:K:75:LEU:HD23	2.39	0.57
4:D:138:ARG:CG	4:D:194:ILE:HD12	2.35	0.57
2:B:48:ASN:ND2	2:B:180:GLU:OE1	2.37	0.57
3:C:63:PHE:HA	21:V:89:LEU:HD11	1.87	0.57
6:F:35:GLY:O	6:F:39:ARG:NH1	2.38	0.56
6:F:276:LEU:HD21	6:F:297:VAL:HG11	1.87	0.56
13:M:336:ARG:NH2	13:M:433:GLU:OE2	2.36	0.56
2:B:107:ALA:HB1	2:B:149:ILE:HD13	1.84	0.56
5:E:16:ASN:OD1	5:E:19:THR:OG1	2.16	0.56
13:M:42:LEU:HD22	13:M:453:LEU:HD22	1.87	0.56
13:M:230:ILE:HD12	13:M:234:ILE:HD11	1.86	0.56
13:M:343:ILE:O	13:M:346:ARG:NH1	2.38	0.56
13:M:363:SER:CB	13:M:411:ILE:HD11	2.34	0.56
13:M:121:LEU:O	13:M:125:THR:HG23	2.05	0.56
9:I:166:GLU:OE2	9:I:170:ASN:ND2	2.38	0.56
7:G:366:THR:OG1	7:G:491:ASN:ND2	2.37	0.56
7:G:396:ARG:NH1	7:G:416:THR:O	2.38	0.56
3:C:210:ARG:NH1	7:G:35:MET:SD	2.79	0.56
15:O:36:ASN:OD1	15:O:37:LYS:N	2.38	0.56
4:D:111:MET:SD	4:D:111:MET:N	2.79	0.55
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.40	0.55
4:D:81:GLY:N	4:D:429:ASP:OD2	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:257:ILE:HG13	12:L:317:LEU:HD11	1.88	0.55
6:F:376:MET:O	6:F:380:VAL:HG23	2.06	0.55
9:I:15:ASP:OD1	9:I:15:ASP:N	2.40	0.55
14:N:333:SER:O	14:N:334:THR:OG1	2.25	0.55
13:M:12:LEU:O	13:M:15:THR:OG1	2.18	0.54
14:N:240:MET:SD	14:N:244:ILE:HD11	2.46	0.54
21:V:34:LEU:HD22	21:V:44:ARG:HA	1.88	0.54
6:F:118:LEU:HD12	6:F:225:VAL:HG13	1.89	0.54
6:F:126:GLY:O	6:F:129:MET:C	2.45	0.54
12:L:345:SER:O	12:L:349:SER:OG	2.15	0.54
4:D:139:VAL:HG23	4:D:278:TYR:CZ	2.42	0.54
4:D:224:GLU:OE1	9:I:42:TYR:OH	2.11	0.54
24:Y:19:CYS:O	24:Y:23:THR:OG1	2.14	0.54
2:B:144:ARG:NH1	3:C:173:GLU:OE2	2.41	0.54
8:H:248:TYR:O	8:H:251:LEU:N	2.40	0.54
49:K:201:3PE:O14	12:L:585:LYS:NZ	2.33	0.54
14:N:5:THR:HG22	14:N:9:ILE:HD12	1.90	0.54
6:F:359:CYS:SG	6:F:360:GLY:N	2.80	0.54
9:I:13:GLU:OE1	9:I:13:GLU:N	2.40	0.54
12:L:324:LEU:CD2	12:L:395:ILE:HD13	2.37	0.54
5:E:151:ALA:HB3	5:E:152:PRO:HD3	1.90	0.54
12:L:180:ILE:HD12	13:M:397:GLY:HA2	1.89	0.54
4:D:142:GLY:O	4:D:145:THR:OG1	2.22	0.54
5:E:70:ALA:HB1	5:E:75:VAL:O	2.08	0.54
2:B:68:GLU:OE1	4:D:188:ARG:NH1	2.42	0.53
4:D:300:ARG:NH2	4:D:420:THR:O	2.40	0.53
8:H:281:ARG:NE	8:H:283:ASP:OD1	2.41	0.53
14:N:190:MET:HB3	14:N:201:THR:HG23	1.91	0.53
14:N:298:TYR:CD1	14:N:302:LEU:HD12	2.44	0.53
17:Q:33:ARG:NH2	17:Q:77:ASP:OD2	2.40	0.53
11:K:97:GLN:N	11:K:97:GLN:OE1	2.40	0.53
21:V:5:LYS:NZ	21:V:68:GLU:OE2	2.42	0.53
10:J:69:TYR:HE2	11:K:75:LEU:HD23	1.73	0.53
4:D:238:ARG:NH1	8:H:279:ARG:O	2.42	0.52
6:F:119:VAL:CG1	6:F:162:ILE:HD11	2.40	0.52
12:L:315:VAL:HG11	12:L:399:ILE:HD12	1.90	0.52
20:T:39:ASP:OD1	20:T:40:LEU:N	2.42	0.52
15:O:25:ILE:CD1	15:O:168:ALA:HB3	2.39	0.52
5:E:120:LEU:HD13	5:E:173:ILE:HD11	1.91	0.52
20:T:19:LEU:O	20:T:25:ILE:HD11	2.10	0.52
7:G:575:ASN:OD1	7:G:579:ARG:N	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:203:GLY:O	8:H:207:LEU:N	2.43	0.52
6:F:76:GLY:O	6:F:80:SER:OG	2.12	0.52
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.91	0.51
15:O:224:ASP:O	15:O:228:ALA:N	2.39	0.51
13:M:209:LEU:HD11	13:M:261:PHE:HD1	1.76	0.51
20:U:66:ASP:OD2	20:U:79:TYR:OH	2.25	0.51
6:F:344:VAL:HG23	6:F:380:VAL:HG22	1.91	0.51
13:M:326:LEU:HD22	13:M:410:MET:HE1	1.91	0.51
7:G:28:GLN:NE2	17:Q:114:LYS:O	2.43	0.51
4:D:347:HIS:O	4:D:351:LEU:HD23	2.10	0.51
7:G:53:ARG:O	7:G:93:VAL:HG21	2.10	0.51
8:H:235:ASN:O	8:H:238:THR:OG1	2.28	0.51
13:M:225:ILE:HD12	13:M:331:ASN:CB	2.41	0.51
3:C:177:ASP:OD1	16:P:36:ASN:ND2	2.44	0.50
8:H:117:LEU:HD21	10:J:67:PHE:CG	2.46	0.50
11:K:75:LEU:O	11:K:79:VAL:HG23	2.11	0.50
3:C:86:ARG:NH2	21:V:112:LYS:O	2.44	0.50
4:D:150:HIS:NE2	4:D:303:GLU:OE1	2.43	0.50
12:L:15:LEU:HD11	12:L:125:LEU:HD23	1.94	0.50
13:M:248:ILE:HG23	13:M:249:ILE:HG23	1.93	0.50
14:N:166:ALA:HB1	14:N:288:LEU:HD22	1.94	0.50
24:Y:38:SER:HB3	24:Y:57:VAL:HG22	1.92	0.50
6:F:404:ILE:HD11	7:G:50:GLY:O	2.12	0.50
13:M:88:ASN:ND2	50:N:401:CDL:OA4	2.43	0.50
12:L:180:ILE:HD12	13:M:397:GLY:CA	2.42	0.50
13:M:303:ILE:HD11	13:M:385:LEU:HD23	1.94	0.50
16:P:231:THR:HG21	16:P:294:PRO:HB3	1.93	0.50
7:G:462:ASP:OD1	7:G:462:ASP:N	2.43	0.50
13:M:368:ALA:HB1	13:M:375:LEU:HD12	1.93	0.50
21:V:21:GLU:O	21:V:24:THR:OG1	2.18	0.50
7:G:571:ALA:N	7:G:583:THR:OG1	2.45	0.49
4:D:121:ALA:HB2	4:D:365:THR:OG1	2.13	0.49
6:F:378:ARG:O	6:F:382:GLY:N	2.41	0.49
24:Y:71:PHE:O	24:Y:75:THR:HG23	2.12	0.49
3:C:69:ASN:OD1	21:V:50:ILE:HD11	2.11	0.49
4:D:62:LEU:HD13	4:D:425:PHE:CZ	2.47	0.49
7:G:278:ARG:NH2	7:G:568:GLU:OE1	2.45	0.49
9:I:29:TRP:HB3	9:I:32:LEU:HD12	1.93	0.49
14:N:213:ALA:HB3	14:N:214:PRO:HD3	1.95	0.49
4:D:322:GLU:OE1	4:D:322:GLU:N	2.44	0.49
12:L:139:GLN:HA	12:L:142:ILE:HD12	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:82:ARG:NH2	24:Y:87:ASP:OD2	2.46	0.49
3:C:50:ILE:HD12	3:C:105:ILE:HD11	1.95	0.49
9:I:116:THR:HG21	9:I:146:HIS:CD2	2.47	0.49
10:J:101:PHE:O	10:J:105:VAL:HG23	2.13	0.49
4:D:25:THR:HG21	12:L:579:ASN:ND2	2.28	0.49
7:G:89:ALA:O	7:G:93:VAL:HG23	2.13	0.49
4:D:232:ASN:OD1	4:D:233:ARG:N	2.46	0.49
8:H:114:TYR:OH	10:J:60:LEU:O	2.31	0.49
7:G:6:SER:OG	7:G:7:ASN:N	2.46	0.48
7:G:174:THR:HG22	7:G:183:VAL:HG22	1.95	0.48
20:T:71:MET:N	20:T:75:GLU:OE1	2.44	0.48
4:D:100:LEU:HD11	4:D:115:GLU:HB2	1.95	0.48
7:G:153:CYS:SG	7:G:154:ILE:N	2.86	0.48
7:G:537:LEU:HD23	7:G:541:CYS:SG	2.54	0.48
9:I:76:GLU:HB2	18:R:44:ILE:HD13	1.95	0.48
4:D:134:ALA:HB2	4:D:323:ILE:O	2.13	0.48
1:A:69:ILE:HD11	8:H:144:VAL:HA	1.96	0.48
6:F:89:ARG:NH1	6:F:217:GLY:O	2.46	0.48
5:E:13:PRO:O	5:E:16:ASN:ND2	2.46	0.48
7:G:152:ARG:O	7:G:205:VAL:HG11	2.14	0.48
16:P:185:TYR:HH	16:P:263:TYR:HH	1.62	0.48
8:H:192:GLU:O	8:H:193:THR:OG1	2.23	0.48
5:E:148:CYS:SG	6:F:103:GLY:N	2.87	0.48
7:G:273:GLY:O	7:G:549:HIS:NE2	2.44	0.48
9:I:69:LEU:HG	9:I:156:LEU:HD23	1.94	0.48
6:F:307:ILE:CD1	6:F:327:THR:HG21	2.43	0.48
3:C:132:ARG:HB2	3:C:151:ILE:HD11	1.96	0.48
1:A:66:ASP:HA	1:A:69:ILE:HD12	1.96	0.47
5:E:131:THR:HG22	5:E:138:THR:HG22	1.95	0.47
3:C:73:LYS:NZ	21:V:82:GLN:OE1	2.25	0.47
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.94	0.47
12:L:213:LEU:O	12:L:217:LEU:HD23	2.14	0.47
13:M:77:LEU:HD11	13:M:96:ILE:HD12	1.95	0.47
1:A:15:LEU:O	1:A:19:LEU:HD23	2.14	0.47
3:C:193:GLU:OE2	7:G:223:ARG:NH2	2.47	0.47
9:I:116:THR:HG21	9:I:146:HIS:NE2	2.30	0.47
16:P:31:GLY:O	16:P:35:VAL:HG23	2.14	0.47
22:W:83:LEU:HA	22:W:86:ILE:HD12	1.96	0.47
3:C:47:GLU:OE1	3:C:106:ARG:NH2	2.45	0.47
7:G:378:LEU:HD21	7:G:409:ILE:HD12	1.95	0.47
8:H:55:LEU:HD13	8:H:221:ALA:HB2	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:44:GLN:NE2	13:M:46:ASP:OD1	2.48	0.47
3:C:195:ARG:NH1	9:I:94:ILE:O	2.43	0.47
4:D:349:PHE:O	4:D:353:THR:HG22	2.15	0.47
7:G:318:ILE:HD13	7:G:532:ILE:HD13	1.97	0.47
9:I:59:LEU:HD12	9:I:63:PHE:CD1	2.49	0.47
12:L:597:LEU:HD21	24:Y:36:ILE:HD12	1.97	0.47
1:A:83:LYS:O	1:A:84:THR:OG1	2.29	0.47
13:M:77:LEU:CD1	13:M:96:ILE:HD12	2.44	0.47
15:O:171:TYR:OH	15:O:203:GLU:OE2	2.31	0.47
12:L:396:ILE:HA	12:L:399:ILE:HG22	1.97	0.46
3:C:195:ARG:NH2	9:I:92:GLN:O	2.48	0.46
6:F:119:VAL:HG11	6:F:162:ILE:HD11	1.98	0.46
3:C:79:THR:HG22	4:D:390:LYS:CD	2.44	0.46
19:S:81:LEU:HD12	19:S:85:GLU:HB3	1.96	0.46
6:F:140:GLY:O	6:F:179:ARG:NH2	2.49	0.46
9:I:84:LEU:CD1	9:I:127:ALA:HB1	2.46	0.46
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.97	0.46
1:A:54:LYS:NZ	4:D:69:SER:O	2.34	0.46
5:E:67:ASN:OD1	5:E:81:TYR:OH	2.14	0.46
13:M:370:PRO:HA	13:M:375:LEU:HD13	1.98	0.46
1:A:102:LEU:HD11	8:H:294:LEU:HD23	1.97	0.46
1:A:64:LEU:HD11	10:J:166:ILE:CD1	2.46	0.46
12:L:316:THR:OG1	12:L:325:ALA:HB2	2.15	0.46
7:G:415:LEU:O	7:G:416:THR:OG1	2.25	0.46
1:A:67:LEU:HD11	11:K:68:ALA:CB	2.41	0.45
4:D:24:GLU:N	4:D:24:GLU:OE2	2.49	0.45
8:H:139:THR:HB	10:J:64:LEU:HD21	1.97	0.45
6:F:99:GLU:OE1	6:F:107:ASP:N	2.48	0.45
9:I:16:MET:O	9:I:20:THR:HG23	2.16	0.45
11:K:60:PRO:HA	11:K:63:ILE:HD12	1.99	0.45
4:D:109:VAL:HG23	4:D:149:ASN:OD1	2.17	0.45
5:E:172:ILE:HD11	5:E:187:ARG:HE	1.81	0.45
18:R:2:VAL:HG12	18:R:2:VAL:O	2.16	0.45
3:C:50:ILE:CD1	3:C:105:ILE:HD11	2.46	0.45
12:L:24:SER:OG	12:L:25:ASN:N	2.50	0.45
17:Q:25:VAL:HG21	17:Q:30:ILE:HD11	1.99	0.45
12:L:18:PRO:HA	12:L:21:ILE:HG22	1.98	0.45
4:D:339:LYS:NZ	18:R:65:ALA:O	2.49	0.45
6:F:293:ASN:ND2	6:F:338:ASP:O	2.50	0.45
7:G:205:VAL:HG13	45:G:801:SF4:S2	2.56	0.45
8:H:70:LEU:HA	8:H:73:ILE:HG22	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:185:TRP:O	8:H:189:THR:HG23	2.16	0.45
20:T:47:GLN:NE2	20:T:67:ALA:O	2.49	0.45
12:L:278:LEU:HD12	12:L:315:VAL:HG13	1.98	0.45
16:P:231:THR:HG21	16:P:294:PRO:CB	2.47	0.45
25:Z:85:ILE:HG21	25:Z:123:MET:HG3	1.99	0.45
4:D:126:LEU:HB3	4:D:128:ILE:HD12	1.99	0.45
7:G:531:CYS:HB2	7:G:532:ILE:HD12	1.98	0.45
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.48	0.45
2:B:62:LEU:O	4:D:83:LEU:HD11	2.17	0.44
3:C:119:SER:OG	3:C:144:ASN:OD1	2.35	0.44
7:G:460:ARG:NH1	7:G:466:ILE:HD11	2.32	0.44
13:M:59:ASP:OD2	13:M:245:ARG:NH2	2.49	0.44
3:C:114:LEU:HD12	17:Q:17:LEU:HD11	1.98	0.44
5:E:27:ASN:HD22	5:E:53:LEU:HD11	1.83	0.44
7:G:103:LEU:HD23	18:R:69:PRO:HB3	1.99	0.44
8:H:152:SER:OG	8:H:181:MET:SD	2.71	0.44
16:P:149:LYS:NZ	52:P:501:NDP:O2D	2.29	0.44
19:S:56:GLU:N	19:S:56:GLU:OE1	2.50	0.44
22:W:41:TRP:O	22:W:45:VAL:HG23	2.17	0.44
3:C:171:TYR:CE2	17:Q:25:VAL:HG12	2.52	0.44
3:C:29:VAL:HA	3:C:32:ILE:HG22	2.00	0.44
15:O:131:ASP:OD2	15:O:152:TYR:OH	2.26	0.44
1:A:60:ILE:CG2	11:K:72:ALA:HB1	2.48	0.44
2:B:141:SER:O	2:B:142:VAL:HG23	2.18	0.44
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.43	0.44
9:I:110:ARG:NH2	17:Q:70:MET:O	2.50	0.44
13:M:15:THR:O	13:M:93:LYS:NZ	2.42	0.44
15:O:237:ASP:OD1	21:V:29:LYS:NZ	2.50	0.44
3:C:14:ARG:NH2	3:C:44:CYS:SG	2.91	0.44
10:J:4:TYR:O	10:J:8:LEU:HD23	2.17	0.44
12:L:233:LEU:CD2	12:L:303:ALA:HB1	2.48	0.44
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.99	0.44
7:G:321:GLY:O	7:G:498:SER:OG	2.29	0.43
12:L:174:TYR:HD1	12:L:229:LEU:HD22	1.83	0.43
12:L:228:GLY:O	12:L:229:LEU:HD23	2.17	0.43
25:Z:100:VAL:HG21	25:Z:103:TRP:HB2	1.99	0.43
4:D:152:MET:O	4:D:156:THR:OG1	2.33	0.43
17:Q:10:LEU:O	17:Q:11:ILE:HD13	2.17	0.43
1:A:68:GLU:HG3	1:A:98:LEU:HD13	2.01	0.43
12:L:260:LEU:HB3	12:L:317:LEU:HD13	1.99	0.43
13:M:326:LEU:HD22	13:M:410:MET:CE	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:129:TYR:CE2	15:O:160:LEU:HD11	2.53	0.43
17:Q:132:THR:OG1	17:Q:133:LYS:N	2.51	0.43
2:B:58:MET:SD	4:D:54:GLN:NE2	2.91	0.43
7:G:483:VAL:HG23	7:G:484:ALA:H	1.83	0.43
16:P:19:VAL:HG12	16:P:19:VAL:O	2.19	0.43
18:R:49:VAL:HG11	18:R:92:LYS:HE2	1.99	0.43
2:B:47:ILE:HG22	8:H:57:MET:CE	2.48	0.43
2:B:162:THR:HG23	4:D:188:ARG:HD2	2.01	0.43
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.01	0.43
8:H:10:LEU:HD22	8:H:83:LEU:HD21	2.00	0.43
14:N:98:THR:O	14:N:102:LEU:HD23	2.19	0.43
14:N:273:ASN:OD1	24:Y:142:VAL:N	2.47	0.43
16:P:325:ARG:O	16:P:325:ARG:NH1	2.51	0.43
19:S:78:LEU:O	19:S:78:LEU:HD12	2.19	0.43
6:F:298:ILE:CG1	6:F:306:LEU:HD23	2.49	0.43
8:H:74:ALA:HB3	8:H:75:PRO:HD3	2.01	0.43
9:I:77:GLU:OE2	9:I:153:LYS:NZ	2.25	0.43
7:G:348:ILE:N	7:G:459:GLN:OE1	2.45	0.43
12:L:152:PHE:CD1	12:L:168:ALA:HB1	2.54	0.43
14:N:53:THR:O	14:N:57:THR:HG23	2.18	0.43
5:E:165:THR:OG1	5:E:168:ASP:OD2	2.29	0.43
12:L:574:THR:O	12:L:578:THR:HG22	2.19	0.43
20:T:73:PRO:HA	20:T:76:ILE:HD12	2.01	0.43
22:W:75:VAL:HG21	22:W:80:VAL:HG11	2.00	0.43
12:L:204:SER:OG	12:L:209:ASN:OD1	2.37	0.43
17:Q:19:ILE:HG22	17:Q:19:ILE:O	2.19	0.43
2:B:40:VAL:HG13	2:B:183:LEU:HB3	2.01	0.43
6:F:215:VAL:HG12	6:F:220:THR:CG2	2.49	0.43
15:O:26:THR:HG22	15:O:124:LEU:HB2	2.01	0.43
2:B:47:ILE:HG22	8:H:57:MET:HE1	2.01	0.42
3:C:104:ARG:NH2	4:D:373:GLU:OE2	2.49	0.42
4:D:143:GLU:OE2	4:D:310:ILE:HG21	2.19	0.42
13:M:41:LEU:HG	13:M:63:THR:HG23	2.01	0.42
6:F:239:GLY:O	6:F:243:ALA:N	2.48	0.42
8:H:77:LEU:HD11	8:H:81:LEU:HD11	2.01	0.42
12:L:156:GLY:O	13:M:416:ARG:NH1	2.52	0.42
18:R:23:TYR:O	18:R:26:VAL:HG23	2.19	0.42
15:O:97:GLN:NE2	51:O:401:ATP:N1	2.65	0.42
1:A:56:PHE:O	10:J:69:TYR:OH	2.36	0.42
12:L:409:LEU:O	12:L:413:LEU:HD23	2.19	0.42
7:G:296:TRP:HZ3	7:G:561:LEU:HD22	1.85	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD22	8:H:83:LEU:CD2	2.50	0.42
12:L:273:ILE:HG22	12:L:277:MET:SD	2.59	0.42
13:M:47:GLU:OE1	13:M:47:GLU:N	2.45	0.42
7:G:232:ASP:OD1	7:G:232:ASP:N	2.53	0.42
4:D:291:GLY:O	4:D:296:ARG:NH1	2.52	0.42
5:E:144:CYS:O	6:F:139:ARG:NH1	2.53	0.42
7:G:588:THR:HG21	17:Q:63:GLU:HA	2.02	0.42
24:Y:59:ARG:O	24:Y:63:THR:OG1	2.28	0.42
7:G:324:ASP:HB2	7:G:571:ALA:HB1	2.01	0.42
16:P:15:SER:OG	16:P:16:VAL:N	2.51	0.42
7:G:229:ASP:HB2	7:G:238:ILE:HD12	2.01	0.42
17:Q:11:ILE:HD13	22:W:25:ARG:NH2	2.35	0.42
22:W:116:ARG:NH2	22:W:130:PRO:O	2.53	0.42
23:X:107:ASP:HA	23:X:110:VAL:HG12	2.01	0.42
24:Y:6:PHE:O	24:Y:9:SER:OG	2.38	0.42
12:L:224:SER:O	12:L:224:SER:OG	2.32	0.41
12:L:405:ASN:OD1	12:L:406:ALA:N	2.50	0.41
13:M:186:LEU:HD23	13:M:253:LEU:HD11	2.01	0.41
20:U:11:ILE:O	20:U:15:VAL:HG23	2.20	0.41
4:D:62:LEU:HD13	4:D:425:PHE:CE1	2.54	0.41
4:D:321:GLY:O	25:Z:7:GLN:NE2	2.52	0.41
8:H:155:LEU:HD23	8:H:304:HIS:O	2.20	0.41
11:K:59:ILE:HD12	14:N:27:MET:HG2	2.00	0.41
12:L:324:LEU:HD23	12:L:395:ILE:HD13	2.01	0.41
12:L:520:SER:O	12:L:524:THR:OG1	2.22	0.41
16:P:248:MET:O	16:P:322:ARG:NE	2.48	0.41
21:V:33:ILE:CD1	21:V:87:LEU:HD11	2.50	0.41
24:Y:53:ALA:O	24:Y:57:VAL:HG23	2.20	0.41
4:D:154:VAL:HG13	4:D:297:TYR:HE1	1.84	0.41
12:L:141:PHE:CE2	13:M:375:LEU:HD11	2.52	0.41
20:T:19:LEU:HD12	20:T:25:ILE:HD13	2.01	0.41
5:E:172:ILE:HD11	5:E:187:ARG:NE	2.35	0.41
16:P:231:THR:HG21	16:P:294:PRO:HG3	2.02	0.41
5:E:70:ALA:O	5:E:74:GLN:N	2.53	0.41
10:J:168:GLU:HG3	14:N:5:THR:HG21	2.02	0.41
13:M:174:LEU:HA	13:M:179:LEU:HD11	2.03	0.41
14:N:297:ILE:HA	14:N:300:THR:HG22	2.02	0.41
22:W:37:LEU:HD23	22:W:41:TRP:HD1	1.86	0.41
12:L:574:THR:HG23	14:N:167:TRP:O	2.20	0.41
13:M:286:ILE:O	13:M:289:SER:OG	2.34	0.41
16:P:24:PHE:HB3	16:P:95:ILE:HD11	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:THR:HG22	4:D:181:TYR:OH	2.20	0.41
46:H:402:PC1:O32	10:J:83:GLY:N	2.49	0.41
10:J:141:VAL:HG13	11:K:61:ILE:HD13	2.02	0.41
12:L:83:ASP:OD1	12:L:85:PHE:N	2.49	0.41
12:L:363:THR:OG1	12:L:431:THR:HG22	2.20	0.41
12:L:152:PHE:HD1	12:L:168:ALA:HB1	1.85	0.41
12:L:312:LEU:HG	12:L:395:ILE:HG21	2.02	0.41
12:L:584:ILE:HD12	12:L:584:ILE:H	1.86	0.41
25:Z:100:VAL:HG21	25:Z:103:TRP:CB	2.51	0.41
1:A:47:ALA:HB3	8:H:124:ASN:OD1	2.21	0.41
1:A:58:VAL:HA	1:A:61:THR:HG22	2.03	0.41
13:M:135:ARG:O	13:M:135:ARG:NH1	2.46	0.41
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.52	0.41
6:F:307:ILE:HG21	6:F:312:CYS:HB3	2.03	0.41
7:G:338:VAL:O	7:G:338:VAL:HG12	2.21	0.41
14:N:26:LEU:HD23	14:N:29:MET:SD	2.60	0.41
14:N:297:ILE:HD12	14:N:300:THR:CG2	2.51	0.41
1:A:3:LEU:HD23	49:H:401:3PE:H232	2.03	0.40
5:E:172:ILE:O	5:E:176:LEU:HD23	2.21	0.40
7:G:327:ALA:HB2	7:G:596:ASP:HB2	2.03	0.40
7:G:317:ALA:CB	7:G:331:LEU:HD21	2.51	0.40
12:L:324:LEU:HD11	12:L:394:LEU:HB2	2.02	0.40
13:M:225:ILE:HD11	13:M:328:CYS:HA	2.04	0.40
7:G:364:LEU:HD23	7:G:491:ASN:HB3	2.04	0.40
4:D:7:ASP:N	4:D:7:ASP:OD1	2.54	0.40
6:F:351:ILE:HD11	6:F:415:VAL:CG2	2.52	0.40
6:F:388:GLU:O	6:F:391:SER:OG	2.29	0.40
12:L:57:ASN:ND2	12:L:59:MET:SD	2.95	0.40
20:T:51:ILE:HD12	20:T:70:LEU:HD12	2.04	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%)	104 (92%)	9 (8%)	0	100	100
2	B	154/224 (69%)	145 (94%)	9 (6%)	0	100	100
3	C	205/263 (78%)	192 (94%)	13 (6%)	0	100	100
4	D	427/463 (92%)	393 (92%)	34 (8%)	0	100	100
5	E	210/248 (85%)	190 (90%)	20 (10%)	0	100	100
6	F	426/464 (92%)	387 (91%)	38 (9%)	1 (0%)	44	74
7	G	686/727 (94%)	642 (94%)	44 (6%)	0	100	100
8	H	316/318 (99%)	296 (94%)	19 (6%)	1 (0%)	37	68
9	I	176/212 (83%)	164 (93%)	12 (7%)	0	100	100
10	J	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	552 (91%)	52 (9%)	0	100	100
13	M	457/459 (100%)	433 (95%)	23 (5%)	1 (0%)	44	74
14	N	342/345 (99%)	320 (94%)	22 (6%)	0	100	100
15	O	318/355 (90%)	297 (93%)	21 (7%)	0	100	100
16	P	340/377 (90%)	310 (91%)	30 (9%)	0	100	100
17	Q	123/175 (70%)	119 (97%)	4 (3%)	0	100	100
18	R	92/116 (79%)	85 (92%)	7 (8%)	0	100	100
19	S	81/99 (82%)	74 (91%)	7 (9%)	0	100	100
20	T	74/156 (47%)	68 (92%)	6 (8%)	0	100	100
20	U	84/156 (54%)	80 (95%)	4 (5%)	0	100	100
21	V	112/116 (97%)	107 (96%)	5 (4%)	0	100	100
22	W	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
24	Y	138/143 (96%)	132 (96%)	6 (4%)	0	100	100
25	Z	139/144 (96%)	133 (96%)	6 (4%)	0	100	100
26	a	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
27	b	78/84 (93%)	71 (91%)	7 (9%)	0	100	100
28	c	46/76 (60%)	44 (96%)	2 (4%)	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%)	47 (92%)	4 (8%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	99/151 (66%)	90 (91%)	9 (9%)	0	100	100
33	h	136/189 (72%)	127 (93%)	8 (6%)	1 (1%)	19	51
34	i	90/128 (70%)	85 (94%)	5 (6%)	0	100	100
35	j	60/105 (57%)	57 (95%)	3 (5%)	0	100	100
36	k	73/104 (70%)	70 (96%)	3 (4%)	0	100	100
37	l	152/186 (82%)	137 (90%)	15 (10%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
40	o	109/137 (80%)	104 (95%)	5 (5%)	0	100	100
41	p	167/176 (95%)	154 (92%)	13 (8%)	0	100	100
42	q	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
43	r	96/113 (85%)	87 (91%)	9 (9%)	0	100	100
44	s	39/104 (38%)	36 (92%)	3 (8%)	0	100	100
All	All	8087/9214 (88%)	7527 (93%)	556 (7%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	h	13	PRO
13	M	224	PRO
8	H	218	GLY
6	F	285	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%)	130 (98%)	2 (2%)	60	80
3	C	189/227 (83%)	189 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	341 (99%)	2 (1%)	84	91
7	G	580/610 (95%)	579 (100%)	1 (0%)	92	96
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
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%)	413 (100%)	1 (0%)	92	96
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	282 (99%)	2 (1%)	81	90
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%)	73 (99%)	1 (1%)	62	81
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%)	81	90
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%)	123 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	i	88/119 (74%)	87 (99%)	1 (1%)	70	84
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%)	101 (97%)	3 (3%)	37	65
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%)	7162 (100%)	14 (0%)	91	96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	CYS
2	B	135	TYR
6	F	362	CYS
6	F	405	CYS
7	G	669	LYS
13	M	281	ASP
15	O	213	LYS
15	O	260	ARG
19	S	39	ARG
23	X	165	ARG
34	i	4	THR
40	o	79	CYS
40	o	110	ARG
40	o	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	48	ASN
2	B	172	GLN
4	D	116	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	D	190	HIS
4	D	237	ASN
4	D	252	ASN
4	D	313	GLN
5	E	99	HIS
6	F	200	GLN
6	F	293	ASN
7	G	51	ASN
7	G	365	ASN
7	G	475	GLN
8	H	169	GLN
9	I	158	ASN
13	M	390	ASN
14	N	235	ASN
15	O	200	GLN
15	O	251	GLN
16	P	93	ASN
16	P	131	HIS
16	P	136	ASN
17	Q	46	GLN
20	T	47	GLN
30	e	28	ASN
37	l	135	ASN
39	n	61	GLN
41	p	99	GLN
41	p	139	GLN
43	r	51	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	$\# Z  > 2$
12	FME	L	1	12	8,9,10	1.00	0	7,9,11	0.61	0
4	2MR	D	85	4	10,12,13	2.45	3 (30%)	5,13,15	2.17	2 (40%)
13	FME	M	1	13	8,9,10	0.95	0	7,9,11	1.03	0
42	AME	q	1	42	9,10,11	1.47	1 (11%)	9,11,13	1.49	2 (22%)
1	FME	A	1	1	8,9,10	0.96	0	7,9,11	1.08	1 (14%)
11	FME	K	1	11	8,9,10	1.00	0	7,9,11	1.38	1 (14%)
8	FME	H	1	8	8,9,10	0.91	0	7,9,11	1.45	2 (28%)
43	AYA	r	1	43	6,7,8	1.77	1 (16%)	5,8,10	1.06	0
10	FME	J	1	10	8,9,10	0.99	0	7,9,11	0.82	0
34	SAC	i	1	34	7,8,9	0.55	0	8,9,11	1.04	1 (12%)
14	FME	N	1	14	8,9,10	0.93	0	7,9,11	1.08	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
12	FME	L	1	12	-	2/7/9/11	-
4	2MR	D	85	4	-	2/10/13/15	-
13	FME	M	1	13	-	1/7/9/11	-
42	AME	q	1	42	-	2/9/10/12	-
1	FME	A	1	1	-	3/7/9/11	-
11	FME	K	1	11	-	5/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
10	FME	J	1	10	-	0/7/9/11	-
34	SAC	i	1	34	-	1/7/8/10	-
14	FME	N	1	14	-	2/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.34	1.45	1.34
4	D	85	2MR	CZ-NH2	4.68	1.43	1.33
42	q	1	AME	CT1-N	3.40	1.46	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	r	1	AYA	CT-N	3.19	1.45	1.34
4	D	85	2MR	CQ1-NH1	-2.15	1.42	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	CD-NE-CZ	3.43	129.83	123.41
4	D	85	2MR	NE-CZ-NH2	-3.10	116.64	119.48
8	H	1	FME	CA-N-CN	3.04	127.50	122.82
11	K	1	FME	C-CA-N	2.76	114.72	109.73
34	i	1	SAC	O-C-CA	-2.64	117.87	124.78
42	q	1	AME	O-C-CA	-2.59	118.00	124.78
42	q	1	AME	CE-SD-CG	2.51	109.02	100.40
1	A	1	FME	C-CA-N	2.30	113.89	109.73
8	H	1	FME	C-CA-N	2.05	113.42	109.73

There are no chirality outliers.

All (22) 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	N-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	O-C-CA-CB
13	M	1	FME	O-C-CA-CB
14	N	1	FME	CA-CB-CG-SD
34	i	1	SAC	CB-CA-N-C1A
42	q	1	AME	O-C-CA-CB
4	D	85	2MR	NE-CD-CG-CB
11	K	1	FME	CB-CG-SD-CE
8	H	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
12	L	1	FME	CB-CG-SD-CE
4	D	85	2MR	CA-CB-CG-CD
1	A	1	FME	C-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
42	q	1	AME	CA-CB-CG-SD
11	K	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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
52	NDP	P	501	-	45,52,52	2.27	5 (11%)	53,80,80	1.66	9 (16%)
50	CDL	d	201	-	66,66,99	1.06	8 (12%)	72,78,111	1.10	4 (5%)
49	3PE	Y	401	-	40,40,50	0.96	4 (10%)	43,45,55	1.07	2 (4%)
46	PC1	I	202	-	44,44,53	1.03	4 (9%)	50,52,61	1.00	2 (4%)
48	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.35	9 (18%)
47	FES	G	803	7	0,4,4	-	-	-	-	-
46	PC1	B	202	-	34,34,53	1.16	4 (11%)	40,42,61	1.10	2 (5%)
46	PC1	H	402	-	41,41,53	1.06	4 (9%)	47,49,61	0.98	2 (4%)
54	EHZ	U	201	20	29,36,37	1.76	5 (17%)	35,44,47	1.78	6 (17%)
50	CDL	q	201	-	56,56,99	1.14	8 (14%)	62,68,111	1.14	4 (6%)
45	SF4	G	801	7	0,12,12	-	-	-	-	-
49	3PE	M	501	-	41,41,50	0.94	4 (9%)	44,46,55	1.05	2 (4%)
45	SF4	I	203	9	0,12,12	-	-	-	-	-
49	3PE	M	502	-	36,36,50	1.02	4 (11%)	39,41,55	1.02	2 (5%)
51	ATP	O	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.72	5 (16%)
49	3PE	L	701	-	48,48,50	0.90	3 (6%)	51,53,55	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	SF4	I	204	9	0,12,12	-	-	-		
45	SF4	F	502	6	0,12,12	-	-	-		
50	CDL	d	202	-	62,62,99	1.09	8 (12%)	68,74,111	1.14	5 (7%)
45	SF4	G	802	7	0,12,12	-	-	-		
50	CDL	N	402	-	64,64,99	1.08	8 (12%)	70,76,111	1.09	4 (5%)
49	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
45	SF4	B	201	2	0,12,12	-	-	-		
49	3PE	K	201	-	32,32,50	1.06	4 (12%)	35,37,55	1.17	2 (5%)
50	CDL	N	401	-	58,58,99	1.02	6 (10%)	63,69,111	1.05	3 (4%)
50	CDL	h	201	-	69,69,99	1.03	8 (11%)	75,81,111	1.09	4 (5%)
47	FES	E	301	5	0,4,4	-	-	-		
49	3PE	L	703	-	41,41,50	0.94	4 (9%)	44,46,55	1.05	2 (4%)
50	CDL	L	702	-	73,73,99	1.01	7 (9%)	79,85,111	1.10	5 (6%)
49	3PE	H	401	-	43,43,50	0.92	3 (6%)	46,48,55	1.10	2 (4%)
54	EHZ	T	201	20	29,36,37	1.72	5 (17%)	35,44,47	1.42	4 (11%)
46	PC1	B	203	-	42,42,53	1.06	3 (7%)	48,50,61	0.95	2 (4%)
49	3PE	L	704	-	48,48,50	0.87	4 (8%)	51,53,55	1.06	2 (3%)

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
52	NDP	P	501	-	-	11/30/77/77	0/5/5/5
50	CDL	d	201	-	-	31/77/77/110	-
49	3PE	Y	401	-	-	24/44/44/54	-
46	PC1	I	202	-	-	17/48/48/57	-
48	FMN	F	501	-	-	5/18/18/18	0/3/3/3
47	FES	G	803	7	-	-	0/1/1/1
46	PC1	B	202	-	-	15/38/38/57	-
46	PC1	H	402	-	-	17/45/45/57	-
54	EHZ	U	201	20	-	6/42/44/45	-
50	CDL	q	201	-	-	25/67/67/110	-
45	SF4	G	801	7	-	-	0/6/5/5
49	3PE	M	501	-	-	19/45/45/54	-
49	3PE	M	502	-	-	20/40/40/54	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	I	203	9	-	-	0/6/5/5
51	ATP	O	401	-	-	3/18/38/38	0/3/3/3
49	3PE	L	701	-	-	20/52/52/54	-
45	SF4	I	204	9	-	-	0/6/5/5
45	SF4	F	502	6	-	-	0/6/5/5
50	CDL	d	202	-	-	30/73/73/110	-
50	CDL	N	402	-	-	33/75/75/110	-
45	SF4	G	802	7	-	-	0/6/5/5
50	CDL	N	401	-	-	27/67/67/110	-
49	3PE	I	201	-	-	20/54/54/54	-
49	3PE	K	201	-	-	14/36/36/54	-
50	CDL	h	201	-	-	39/80/80/110	-
45	SF4	B	201	2	-	-	0/6/5/5
47	FES	E	301	5	-	-	0/1/1/1
49	3PE	L	703	-	-	19/45/45/54	-
50	CDL	L	702	-	-	39/84/84/110	-
49	3PE	H	401	-	-	16/47/47/54	-
54	EHZ	T	201	20	-	9/42/44/45	-
46	PC1	B	203	-	-	25/46/46/57	-
49	3PE	L	704	-	-	24/52/52/54	-

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.34	1.82	1.59
54	U	201	EHZ	C15-N2	6.02	1.46	1.33
54	T	201	EHZ	C15-N2	5.57	1.45	1.33
54	U	201	EHZ	C12-N1	5.30	1.45	1.33
54	T	201	EHZ	C12-N1	5.28	1.45	1.33
52	P	501	NDP	PN-O5D	4.13	1.76	1.59
48	F	501	FMN	C4A-N5	3.38	1.37	1.30
52	P	501	NDP	O2B-C2B	-3.17	1.32	1.44
50	L	702	CDL	OA8-CA7	2.65	1.41	1.33
50	h	201	CDL	OA6-CA4	-2.63	1.40	1.46
49	L	701	3PE	O21-C2	-2.63	1.40	1.46
50	L	702	CDL	OB6-CB4	-2.60	1.40	1.46
49	L	703	3PE	O21-C2	-2.57	1.40	1.46
46	B	203	PC1	O21-C2	-2.54	1.40	1.46
46	H	402	PC1	O31-C31	2.54	1.40	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	B	203	PC1	O31-C31	2.52	1.40	1.33
50	N	402	CDL	OA6-CA4	-2.52	1.40	1.46
50	N	401	CDL	OB8-CB7	2.52	1.40	1.33
50	d	201	CDL	OA6-CA4	-2.51	1.40	1.46
49	L	704	3PE	O21-C2	-2.51	1.40	1.46
50	h	201	CDL	OB8-CB7	2.50	1.40	1.33
49	M	502	3PE	O21-C2	-2.48	1.40	1.46
50	d	202	CDL	OA8-CA7	2.48	1.40	1.33
49	Y	401	3PE	O21-C2	-2.48	1.40	1.46
50	d	202	CDL	OB6-CB4	-2.48	1.40	1.46
50	h	201	CDL	OB6-CB4	-2.47	1.40	1.46
46	I	202	PC1	O31-C31	2.47	1.40	1.33
49	M	502	3PE	O31-C31	2.47	1.40	1.33
54	U	201	EHZ	C9-S1	2.47	1.82	1.76
46	B	202	PC1	O21-C2	-2.47	1.40	1.46
48	F	501	FMN	C10-N1	2.47	1.38	1.33
50	q	201	CDL	OB6-CB4	-2.47	1.40	1.46
49	K	201	3PE	O31-C31	2.46	1.40	1.33
50	d	201	CDL	OB8-CB7	2.45	1.40	1.33
49	I	201	3PE	O21-C2	-2.45	1.40	1.46
46	B	202	PC1	O31-C31	2.44	1.40	1.33
50	d	202	CDL	OB8-CB7	2.43	1.40	1.33
50	N	402	CDL	OA8-CA7	2.42	1.40	1.33
49	K	201	3PE	O21-C2	-2.42	1.40	1.46
50	q	201	CDL	OB8-CB7	2.41	1.40	1.33
49	L	704	3PE	O31-C31	2.41	1.40	1.33
50	L	702	CDL	OB8-CB7	2.41	1.40	1.33
46	I	202	PC1	O21-C2	-2.39	1.40	1.46
54	T	201	EHZ	C9-S1	2.39	1.81	1.76
49	M	501	3PE	O21-C2	-2.39	1.40	1.46
49	L	701	3PE	O31-C3	-2.37	1.39	1.45
50	d	201	CDL	OA8-CA7	2.37	1.40	1.33
50	q	201	CDL	OA6-CA5	2.37	1.41	1.34
49	H	401	3PE	O31-C31	2.36	1.40	1.33
46	I	202	PC1	O21-C21	2.36	1.41	1.34
50	h	201	CDL	OA8-CA7	2.36	1.40	1.33
54	U	201	EHZ	O4-C15	-2.36	1.18	1.23
50	N	402	CDL	OB8-CB7	2.35	1.40	1.33
50	N	402	CDL	OB6-CB4	-2.35	1.40	1.46
50	q	201	CDL	OA8-CA7	2.35	1.40	1.33
49	L	703	3PE	O31-C31	2.34	1.40	1.33
49	M	501	3PE	O31-C31	2.32	1.40	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	I	201	3PE	O31-C3	-2.31	1.39	1.45
46	H	402	PC1	O21-C2	-2.31	1.40	1.46
50	N	402	CDL	OB6-CB5	2.30	1.40	1.34
50	N	401	CDL	OA8-CA7	2.29	1.40	1.33
54	T	201	EHZ	O4-C15	-2.29	1.18	1.23
50	N	401	CDL	OB6-CB5	2.29	1.40	1.34
49	L	701	3PE	O31-C31	2.29	1.40	1.33
49	H	401	3PE	O21-C21	2.28	1.40	1.34
49	I	201	3PE	O21-C21	2.28	1.40	1.34
50	d	201	CDL	OB6-CB4	-2.28	1.40	1.46
46	H	402	PC1	O21-C21	2.28	1.40	1.34
50	q	201	CDL	OB6-CB5	2.27	1.40	1.34
49	Y	401	3PE	O31-C3	-2.27	1.40	1.45
49	I	201	3PE	O31-C31	2.27	1.40	1.33
50	N	401	CDL	OA8-CA6	-2.26	1.40	1.45
49	Y	401	3PE	O31-C31	2.25	1.39	1.33
49	L	703	3PE	O31-C3	-2.25	1.40	1.45
50	d	201	CDL	OB8-CB6	-2.24	1.40	1.45
49	K	201	3PE	O21-C21	2.24	1.40	1.34
49	M	501	3PE	O21-C21	2.23	1.40	1.34
46	B	202	PC1	O21-C21	2.23	1.40	1.34
50	d	202	CDL	OA6-CA4	-2.22	1.41	1.46
49	H	401	3PE	O31-C3	-2.22	1.40	1.45
51	O	401	ATP	C5-C4	2.22	1.46	1.40
50	d	202	CDL	OA6-CA5	2.21	1.40	1.34
54	T	201	EHZ	O3-C12	-2.21	1.18	1.23
50	q	201	CDL	OA8-CA6	-2.21	1.40	1.45
50	d	201	CDL	OA8-CA6	-2.20	1.40	1.45
46	I	202	PC1	O31-C3	-2.19	1.40	1.45
50	d	202	CDL	OB6-CB5	2.18	1.40	1.34
46	B	202	PC1	O31-C3	-2.18	1.40	1.45
49	M	501	3PE	O31-C3	-2.17	1.40	1.45
50	L	702	CDL	OB8-CB6	-2.17	1.40	1.45
50	d	202	CDL	OB8-CB6	-2.17	1.40	1.45
50	q	201	CDL	OB8-CB6	-2.16	1.40	1.45
50	d	201	CDL	OB6-CB5	2.15	1.40	1.34
50	h	201	CDL	OB6-CB5	2.14	1.40	1.34
50	L	702	CDL	OA6-CA4	-2.13	1.41	1.46
52	P	501	NDP	O4B-C4B	-2.13	1.40	1.45
49	K	201	3PE	O31-C3	-2.12	1.40	1.45
50	N	402	CDL	OA6-CA5	2.12	1.40	1.34
50	N	402	CDL	OB8-CB6	-2.12	1.40	1.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	U	201	EHZ	O3-C12	-2.12	1.19	1.23
49	M	502	3PE	O21-C21	2.12	1.40	1.34
50	h	201	CDL	OA8-CA6	-2.10	1.40	1.45
50	L	702	CDL	OA6-CA5	2.10	1.40	1.34
49	L	704	3PE	O31-C3	-2.10	1.40	1.45
46	B	203	PC1	O21-C21	2.09	1.40	1.34
50	d	201	CDL	OA6-CA5	2.09	1.40	1.34
50	N	402	CDL	OA8-CA6	-2.09	1.40	1.45
49	Y	401	3PE	O21-C21	2.09	1.40	1.34
49	L	704	3PE	O21-C21	2.08	1.40	1.34
49	M	502	3PE	O31-C3	-2.08	1.40	1.45
52	P	501	NDP	C2A-N1A	2.06	1.37	1.33
50	N	401	CDL	OB8-CB6	-2.06	1.40	1.45
50	L	702	CDL	OB6-CB5	2.06	1.40	1.34
50	h	201	CDL	OA6-CA5	2.05	1.40	1.34
50	N	401	CDL	OB6-CB4	-2.05	1.41	1.46
49	L	703	3PE	O21-C21	2.05	1.40	1.34
50	q	201	CDL	OA6-CA4	-2.04	1.41	1.46
50	d	202	CDL	OA8-CA6	-2.04	1.40	1.45
46	H	402	PC1	O31-C3	-2.02	1.40	1.45
50	h	201	CDL	OB8-CB6	-2.01	1.40	1.45

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	P	501	NDP	PN-O3-PA	-7.20	108.11	132.83
54	U	201	EHZ	C16-C15-N2	5.68	127.88	116.58
54	T	201	EHZ	C8-C9-S1	5.48	120.41	113.63
54	U	201	EHZ	C8-C9-S1	4.81	119.58	113.63
49	L	701	3PE	O21-C21-C22	4.74	121.72	111.50
50	N	402	CDL	OA6-CA5-C11	4.28	120.73	111.50
51	O	401	ATP	PA-O3A-PB	-4.25	118.24	132.83
51	O	401	ATP	PB-O3B-PG	-4.22	118.33	132.83
49	I	201	3PE	O21-C21-C22	4.22	120.59	111.50
46	B	202	PC1	O21-C21-C22	4.21	120.57	111.50
50	d	201	CDL	OB6-CB5-C51	4.10	120.34	111.50
49	M	501	3PE	O21-C21-C22	4.05	120.22	111.50
49	L	703	3PE	O21-C21-C22	4.04	120.22	111.50
49	Y	401	3PE	O21-C21-C22	4.03	120.19	111.50
50	L	702	CDL	OB6-CB5-C51	4.02	120.17	111.50
49	H	401	3PE	O21-C21-C22	3.99	120.11	111.50
49	K	201	3PE	O21-C21-C22	3.97	120.06	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	N	401	CDL	OB6-CB5-C51	3.93	119.98	111.50
50	d	202	CDL	OB6-CB5-C51	3.89	119.89	111.50
50	h	201	CDL	OA6-CA5-C11	3.85	119.79	111.50
50	d	202	CDL	OA6-CA5-C11	3.80	119.69	111.50
46	H	402	PC1	O21-C21-C22	3.75	119.59	111.50
50	q	201	CDL	OB6-CB5-C51	3.72	119.52	111.50
49	M	502	3PE	O21-C21-C22	3.69	119.46	111.50
49	L	704	3PE	O21-C21-C22	3.68	119.43	111.50
50	h	201	CDL	OB6-CB5-C51	3.68	119.43	111.50
51	O	401	ATP	N3-C2-N1	-3.66	122.96	128.68
46	I	202	PC1	O21-C21-C22	3.64	119.34	111.50
50	q	201	CDL	OA6-CA5-C11	3.62	119.31	111.50
50	d	201	CDL	OA6-CA5-C11	3.57	119.19	111.50
46	B	203	PC1	O21-C21-C22	3.56	119.18	111.50
50	L	702	CDL	OA6-CA5-C11	3.55	119.15	111.50
48	F	501	FMN	C4-N3-C2	-3.41	119.33	125.64
50	N	402	CDL	OB6-CB5-C51	3.40	118.83	111.50
54	U	201	EHZ	O4-C15-N2	-3.25	116.03	122.99
52	P	501	NDP	O2B-P2B-O1X	-3.16	97.20	109.39
49	H	401	3PE	O31-C31-C32	3.06	121.51	111.91
50	d	202	CDL	OA8-CA7-C31	3.06	121.50	111.91
48	F	501	FMN	C4A-C10-N10	3.00	120.86	116.48
54	U	201	EHZ	C14-N2-C15	2.98	127.90	122.59
46	H	402	PC1	O31-C31-C32	2.91	121.05	111.91
50	d	201	CDL	OB8-CB7-C71	2.90	121.02	111.91
49	K	201	3PE	O31-C31-C32	2.89	120.99	111.91
50	N	401	CDL	OB8-CB7-C71	2.87	120.92	111.91
51	O	401	ATP	C3'-C2'-C1'	2.85	105.27	100.98
50	h	201	CDL	OB8-CB7-C71	2.84	120.81	111.91
52	P	501	NDP	PA-O5B-C5B	-2.83	105.09	121.68
49	M	502	3PE	O31-C31-C32	2.81	120.71	111.91
48	F	501	FMN	C4A-C10-N1	-2.79	118.26	124.73
48	F	501	FMN	C4A-C4-N3	2.79	120.26	113.19
50	d	201	CDL	OA8-CA7-C31	2.78	120.64	111.91
50	N	402	CDL	OA8-CA7-C31	2.73	120.48	111.91
50	N	401	CDL	OA8-CA7-C31	2.66	120.26	111.91
48	F	501	FMN	O4-C4-C4A	-2.66	119.54	126.60
46	B	202	PC1	O31-C31-C32	2.66	120.25	111.91
50	L	702	CDL	OB8-CB7-C71	2.65	120.22	111.91
54	U	201	EHZ	C10-S1-C9	2.64	110.09	101.87
52	P	501	NDP	PN-O5D-C5D	-2.63	106.24	121.68
49	I	201	3PE	O31-C31-C32	2.62	120.12	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	I	202	PC1	O31-C31-C32	2.60	120.07	111.91
49	Y	401	3PE	O31-C31-C32	2.59	120.04	111.91
50	d	202	CDL	OB8-CB7-C71	2.58	120.00	111.91
50	q	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
52	P	501	NDP	O3X-P2B-O2X	2.57	117.46	107.64
49	L	704	3PE	O31-C31-C32	2.56	119.94	111.91
50	q	201	CDL	OA8-CA7-C31	2.56	119.93	111.91
54	T	201	EHZ	C19-C17-C16	2.56	113.25	108.82
49	L	701	3PE	O21-C21-O22	-2.53	117.58	123.70
46	B	203	PC1	O31-C31-C32	2.52	119.81	111.91
50	L	702	CDL	OA8-CA7-C31	2.48	119.69	111.91
50	N	402	CDL	OB8-CB7-C71	2.46	119.63	111.91
52	P	501	NDP	C2A-N1A-C6A	-2.44	114.57	118.75
50	h	201	CDL	OA8-CA7-C31	2.43	119.54	111.91
49	L	703	3PE	O31-C31-C32	2.36	119.31	111.91
54	U	201	EHZ	C13-C12-N1	2.35	120.38	116.42
48	F	501	FMN	C4-C4A-C10	2.33	120.70	116.79
51	O	401	ATP	C4-C5-N7	-2.31	106.99	109.40
48	F	501	FMN	C1'-N10-C9A	2.29	124.32	120.51
49	L	701	3PE	O31-C31-C32	2.27	119.02	111.91
52	P	501	NDP	O2N-PN-O1N	2.26	123.39	112.24
49	M	501	3PE	O31-C31-C32	2.25	118.96	111.91
54	T	201	EHZ	O2-C9-S1	-2.25	119.69	122.61
50	L	702	CDL	OA6-CA4-CA6	2.18	116.30	108.40
54	T	201	EHZ	C10-S1-C9	2.18	108.65	101.87
52	P	501	NDP	O4B-C4B-C3B	2.15	109.37	105.11
48	F	501	FMN	C10-C4A-N5	-2.05	120.50	124.86
50	d	202	CDL	CA6-CA4-CA3	-2.04	106.96	111.79
52	P	501	NDP	O5D-PN-O1N	-2.02	101.16	109.07
48	F	501	FMN	C10-N1-C2	2.01	120.92	116.90

There are no chirality outliers.

All (508) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C2-C1-O11-P
46	B	203	PC1	O13-C11-C12-N
46	H	402	PC1	O32-C31-O31-C3
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C5'-O5'-P-O1P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
48	F	501	FMN	C5'-O5'-P-O2P
49	H	401	3PE	C1-O11-P-O14
49	I	201	3PE	C1-O11-P-O12
49	I	201	3PE	C1-O11-P-O13
49	I	201	3PE	C1-O11-P-O14
49	K	201	3PE	C11-O13-P-O11
49	K	201	3PE	C11-O13-P-O12
49	K	201	3PE	C11-O13-P-O14
49	K	201	3PE	O13-C11-C12-N
49	L	701	3PE	C1-O11-P-O12
49	L	701	3PE	C1-O11-P-O13
49	L	701	3PE	C1-O11-P-O14
49	L	703	3PE	C11-O13-P-O12
49	L	703	3PE	C11-O13-P-O14
49	L	703	3PE	O13-C11-C12-N
49	L	703	3PE	C22-C21-O21-C2
49	L	704	3PE	C1-O11-P-O12
49	L	704	3PE	O13-C11-C12-N
49	M	501	3PE	C1-O11-P-O14
49	M	501	3PE	C11-O13-P-O12
49	M	501	3PE	C11-O13-P-O14
49	M	501	3PE	O13-C11-C12-N
49	M	502	3PE	C1-O11-P-O12
49	M	502	3PE	C1-O11-P-O14
49	M	502	3PE	O13-C11-C12-N
49	M	502	3PE	O22-C21-O21-C2
49	Y	401	3PE	C1-O11-P-O12
49	Y	401	3PE	C1-O11-P-O14
49	Y	401	3PE	C11-O13-P-O11
49	Y	401	3PE	C11-O13-P-O12
49	Y	401	3PE	C11-O13-P-O14
49	Y	401	3PE	O13-C11-C12-N
50	L	702	CDL	C11-CA5-OA6-CA4
50	L	702	CDL	CB2-OB2-PB2-OB3
50	L	702	CDL	CB2-OB2-PB2-OB5
50	L	702	CDL	CB3-OB5-PB2-OB3
50	L	702	CDL	CB3-OB5-PB2-OB4
50	L	702	CDL	C51-CB5-OB6-CB4
50	N	401	CDL	CA2-OA2-PA1-OA5
50	N	401	CDL	C51-CB5-OB6-CB4
50	N	402	CDL	CB2-OB2-PB2-OB3
50	N	402	CDL	CB2-OB2-PB2-OB4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
50	N	402	CDL	CB3-OB5-PB2-OB3
50	d	201	CDL	O1-C1-CB2-OB2
50	d	201	CDL	C51-CB5-OB6-CB4
50	d	202	CDL	CB2-OB2-PB2-OB3
50	h	201	CDL	CA2-C1-CB2-OB2
50	h	201	CDL	CA2-OA2-PA1-OA5
50	h	201	CDL	CA3-OA5-PA1-OA3
50	h	201	CDL	CA3-OA5-PA1-OA4
50	h	201	CDL	CB2-OB2-PB2-OB4
50	q	201	CDL	O1-C1-CB2-OB2
50	q	201	CDL	CA3-OA5-PA1-OA3
51	O	401	ATP	C5'-O5'-PA-O3A
52	P	501	NDP	C5B-O5B-PA-O1A
52	P	501	NDP	C5B-O5B-PA-O3
52	P	501	NDP	C2B-O2B-P2B-O3X
54	T	201	EHZ	C6-C7-C8-C9
54	T	201	EHZ	S1-C10-C11-N1
54	T	201	EHZ	C11-C10-S1-C9
54	U	201	EHZ	C16-C15-N2-C14
49	M	502	3PE	O32-C31-O31-C3
50	d	202	CDL	OB9-CB7-OB8-CB6
50	q	201	CDL	OA9-CA7-OA8-CA6
50	d	202	CDL	C71-CB7-OB8-CB6
50	q	201	CDL	C31-CA7-OA8-CA6
49	H	401	3PE	O32-C31-O31-C3
49	I	201	3PE	O32-C31-O31-C3
49	K	201	3PE	O32-C31-O31-C3
49	L	701	3PE	O32-C31-O31-C3
50	N	402	CDL	OA9-CA7-OA8-CA6
50	N	402	CDL	OB9-CB7-OB8-CB6
50	d	201	CDL	OA9-CA7-OA8-CA6
50	d	201	CDL	OB9-CB7-OB8-CB6
50	d	202	CDL	OA9-CA7-OA8-CA6
50	h	201	CDL	OB9-CB7-OB8-CB6
46	B	203	PC1	O22-C21-O21-C2
49	H	401	3PE	O22-C21-O21-C2
49	M	501	3PE	O22-C21-O21-C2
50	L	702	CDL	OA7-CA5-OA6-CA4
50	L	702	CDL	OB7-CB5-OB6-CB4
50	d	201	CDL	OB7-CB5-OB6-CB4
46	H	402	PC1	C32-C31-O31-C3
49	K	201	3PE	C32-C31-O31-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
49	M	502	3PE	C32-C31-O31-C3
50	d	201	CDL	C71-CB7-OB8-CB6
50	d	202	CDL	C31-CA7-OA8-CA6
50	h	201	CDL	C71-CB7-OB8-CB6
46	B	203	PC1	C22-C21-O21-C2
49	H	401	3PE	C22-C21-O21-C2
49	M	501	3PE	C22-C21-O21-C2
49	M	502	3PE	C22-C21-O21-C2
49	H	401	3PE	C32-C31-O31-C3
49	I	201	3PE	C32-C31-O31-C3
49	L	701	3PE	C32-C31-O31-C3
49	L	704	3PE	C32-C31-O31-C3
50	N	402	CDL	C31-CA7-OA8-CA6
50	N	402	CDL	C71-CB7-OB8-CB6
50	d	201	CDL	C31-CA7-OA8-CA6
49	L	703	3PE	O22-C21-O21-C2
50	N	401	CDL	OB7-CB5-OB6-CB4
49	L	704	3PE	O32-C31-O31-C3
50	h	201	CDL	O1-C1-CB2-OB2
54	U	201	EHZ	O4-C15-N2-C14
49	I	201	3PE	C22-C21-O21-C2
49	L	701	3PE	C22-C21-O21-C2
49	L	704	3PE	C22-C21-O21-C2
50	d	202	CDL	C11-CA5-OA6-CA4
52	P	501	NDP	O4B-C4B-C5B-O5B
50	N	401	CDL	C31-CA7-OA8-CA6
50	N	402	CDL	C1-CA2-OA2-PA1
50	N	401	CDL	OA9-CA7-OA8-CA6
50	N	402	CDL	C11-CA5-OA6-CA4
50	N	401	CDL	CB2-C1-CA2-OA2
50	N	401	CDL	OA5-CA3-CA4-CA6
49	I	201	3PE	O22-C21-O21-C2
49	L	701	3PE	O22-C21-O21-C2
49	L	704	3PE	O22-C21-O21-C2
46	B	203	PC1	C32-C31-O31-C3
49	Y	401	3PE	C32-C31-O31-C3
50	N	401	CDL	C71-CB7-OB8-CB6
50	N	401	CDL	OA5-CA3-CA4-OA6
46	H	402	PC1	C21-C22-C23-C24
46	B	203	PC1	O32-C31-O31-C3
49	Y	401	3PE	O32-C31-O31-C3
50	N	401	CDL	OB9-CB7-OB8-CB6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
50	q	201	CDL	C71-CB7-OB8-CB6
50	d	202	CDL	CA5-C11-C12-C13
50	q	201	CDL	CB7-C71-C72-C73
50	d	201	CDL	CA5-C11-C12-C13
52	P	501	NDP	O4D-C4D-C5D-O5D
50	N	402	CDL	OA7-CA5-OA6-CA4
50	d	202	CDL	OA7-CA5-OA6-CA4
50	d	202	CDL	C78-C79-C80-C81
50	L	702	CDL	O1-C1-CA2-OA2
50	N	401	CDL	O1-C1-CA2-OA2
50	d	202	CDL	O1-C1-CA2-OA2
50	h	201	CDL	C11-CA5-OA6-CA4
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O13
46	B	203	PC1	C11-O13-P-O11
46	B	203	PC1	C1-O11-P-O13
46	I	202	PC1	C1-O11-P-O13
49	L	703	3PE	C11-O13-P-O11
49	L	704	3PE	C1-O11-P-O13
49	M	501	3PE	C11-O13-P-O11
49	Y	401	3PE	C1-O11-P-O13
50	L	702	CDL	CB3-OB5-PB2-OB2
50	N	401	CDL	CB2-OB2-PB2-OB5
50	N	402	CDL	CB2-OB2-PB2-OB5
50	d	201	CDL	CB2-OB2-PB2-OB5
50	h	201	CDL	CA3-OA5-PA1-OA2
50	h	201	CDL	CB2-OB2-PB2-OB5
50	h	201	CDL	CA5-C11-C12-C13
50	L	702	CDL	CB2-C1-CA2-OA2
50	d	201	CDL	CA2-C1-CB2-OB2
50	d	202	CDL	CB2-C1-CA2-OA2
50	q	201	CDL	CA2-C1-CB2-OB2
50	h	201	CDL	OA7-CA5-OA6-CA4
50	L	702	CDL	C31-C32-C33-C34
46	B	202	PC1	C22-C21-O21-C2
49	H	401	3PE	C34-C35-C36-C37
49	L	703	3PE	C22-C23-C24-C25
49	Y	401	3PE	C33-C34-C35-C36
50	h	201	CDL	C18-C19-C20-C21
50	q	201	CDL	OB9-CB7-OB8-CB6
49	I	201	3PE	C35-C36-C37-C38
49	H	401	3PE	C3-C2-O21-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
50	L	702	CDL	CA6-CA4-OA6-CA5
46	B	202	PC1	O22-C21-O21-C2
49	M	501	3PE	C36-C37-C38-C39
50	N	402	CDL	C52-C53-C54-C55
49	L	703	3PE	C2D-C2E-C2F-C2G
50	L	702	CDL	C73-C74-C75-C76
50	N	402	CDL	C79-C80-C81-C82
50	q	201	CDL	C31-C32-C33-C34
49	L	703	3PE	C24-C25-C26-C27
46	H	402	PC1	C32-C33-C34-C35
49	K	201	3PE	C31-C32-C33-C34
46	B	203	PC1	C3D-C3E-C3F-C3G
49	I	201	3PE	C25-C26-C27-C28
49	L	701	3PE	C2E-C2F-C2G-C2H
49	Y	401	3PE	C37-C38-C39-C3A
50	L	702	CDL	C52-C53-C54-C55
50	q	201	CDL	C15-C16-C17-C18
49	I	201	3PE	C32-C33-C34-C35
49	I	201	3PE	C2B-C2C-C2D-C2E
49	M	501	3PE	C3D-C3E-C3F-C3G
50	h	201	CDL	CB7-C71-C72-C73
50	N	402	CDL	C83-C84-C85-C86
46	B	202	PC1	C32-C31-O31-C3
52	P	501	NDP	O4D-C1D-N1N-C6N
46	I	202	PC1	C29-C2A-C2B-C2C
50	L	702	CDL	C14-C15-C16-C17
49	K	201	3PE	C33-C34-C35-C36
49	M	501	3PE	C33-C34-C35-C36
49	M	502	3PE	C23-C24-C25-C26
49	Y	401	3PE	C35-C36-C37-C38
49	Y	401	3PE	C22-C21-O21-C2
50	q	201	CDL	C51-CB5-OB6-CB4
50	L	702	CDL	C36-C37-C38-C39
49	L	701	3PE	C27-C28-C29-C2A
49	L	704	3PE	C2B-C2C-C2D-C2E
49	M	502	3PE	C25-C26-C27-C28
50	d	201	CDL	C59-C60-C61-C62
49	Y	401	3PE	O22-C21-O21-C2
50	q	201	CDL	OB7-CB5-OB6-CB4
50	d	202	CDL	C80-C81-C82-C83
50	h	201	CDL	C1-CB2-OB2-PB2
50	L	702	CDL	CB5-C51-C52-C53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	O32-C31-O31-C3
49	I	201	3PE	C37-C38-C39-C3A
50	d	201	CDL	OA7-CA5-OA6-CA4
50	d	202	CDL	OB7-CB5-OB6-CB4
49	L	704	3PE	C32-C33-C34-C35
49	I	201	3PE	C21-C22-C23-C24
49	L	701	3PE	C39-C3A-C3B-C3C
50	d	201	CDL	C11-CA5-OA6-CA4
50	d	202	CDL	C51-CB5-OB6-CB4
50	N	401	CDL	C54-C55-C56-C57
46	H	402	PC1	O21-C2-C3-O31
50	q	201	CDL	OB6-CB4-CB6-OB8
46	B	203	PC1	C3B-C3C-C3D-C3E
46	B	203	PC1	C35-C36-C37-C38
46	H	402	PC1	C26-C27-C28-C29
46	H	402	PC1	C39-C3A-C3B-C3C
50	N	402	CDL	C81-C82-C83-C84
50	d	201	CDL	C56-C57-C58-C59
50	N	402	CDL	CB3-OB5-PB2-OB2
50	L	702	CDL	C1-CA2-OA2-PA1
50	L	702	CDL	C71-CB7-OB8-CB6
50	N	401	CDL	OB5-CB3-CB4-CB6
49	L	704	3PE	C3C-C3D-C3E-C3F
50	L	702	CDL	C78-C79-C80-C81
50	L	702	CDL	C34-C35-C36-C37
50	h	201	CDL	C32-C33-C34-C35
46	B	202	PC1	C1-C2-C3-O31
50	N	402	CDL	C76-C77-C78-C79
50	d	202	CDL	CB3-CB4-CB6-OB8
50	q	201	CDL	CB3-CB4-CB6-OB8
46	I	202	PC1	C36-C37-C38-C39
49	Y	401	3PE	C26-C27-C28-C29
49	L	704	3PE	C34-C35-C36-C37
50	N	402	CDL	C74-C75-C76-C77
50	N	402	CDL	CA7-C31-C32-C33
49	L	701	3PE	C23-C24-C25-C26
52	P	501	NDP	C3B-C4B-C5B-O5B
54	U	201	EHZ	C5-C6-C7-O1
49	L	703	3PE	C21-C22-C23-C24
50	d	201	CDL	C34-C35-C36-C37
49	L	701	3PE	C21-C22-C23-C24
50	h	201	CDL	CB5-C51-C52-C53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
46	I	202	PC1	C24-C25-C26-C27
50	d	201	CDL	C71-C72-C73-C74
49	L	701	3PE	C2B-C2C-C2D-C2E
49	M	501	3PE	C32-C31-O31-C3
50	L	702	CDL	OA5-CA3-CA4-OA6
50	L	702	CDL	OB9-CB7-OB8-CB6
49	L	703	3PE	C36-C37-C38-C39
50	d	201	CDL	OB6-CB4-CB6-OB8
50	d	202	CDL	C76-C77-C78-C79
46	B	202	PC1	C21-C22-C23-C24
49	H	401	3PE	C38-C39-C3A-C3B
49	M	501	3PE	O32-C31-O31-C3
54	U	201	EHZ	C5-C6-C7-C8
50	N	402	CDL	C82-C83-C84-C85
46	B	203	PC1	C3F-C3G-C3H-C3I
50	N	401	CDL	C75-C76-C77-C78
49	Y	401	3PE	C23-C24-C25-C26
50	L	702	CDL	C54-C55-C56-C57
49	K	201	3PE	O11-C1-C2-C3
50	L	702	CDL	OA5-CA3-CA4-CA6
50	d	201	CDL	C12-C13-C14-C15
50	L	702	CDL	CB7-C71-C72-C73
50	N	402	CDL	O1-C1-CA2-OA2
49	L	701	3PE	C32-C33-C34-C35
50	h	201	CDL	C14-C15-C16-C17
54	T	201	EHZ	C21-C22-C23-C24
50	N	401	CDL	C31-C32-C33-C34
46	B	203	PC1	C32-C33-C34-C35
46	B	203	PC1	C1-C2-C3-O31
46	H	402	PC1	C1-C2-C3-O31
49	M	502	3PE	C1-C2-C3-O31
50	h	201	CDL	CA3-CA4-CA6-OA8
50	q	201	CDL	C52-C53-C54-C55
49	L	703	3PE	C33-C34-C35-C36
49	M	501	3PE	C1-O11-P-O13
49	M	502	3PE	C1-O11-P-O13
50	q	201	CDL	CA3-OA5-PA1-OA2
49	L	703	3PE	C27-C28-C29-C2A
50	d	202	CDL	C32-C33-C34-C35
49	M	502	3PE	O11-C1-C2-O21
49	Y	401	3PE	C25-C26-C27-C28
49	L	703	3PE	C32-C33-C34-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
50	d	201	CDL	C31-C32-C33-C34
46	B	202	PC1	O21-C2-C3-O31
46	B	203	PC1	O21-C2-C3-O31
50	d	202	CDL	OB6-CB4-CB6-OB8
50	h	201	CDL	OB6-CB4-CB6-OB8
49	M	502	3PE	C34-C35-C36-C37
50	d	202	CDL	C1-CA2-OA2-PA1
50	d	201	CDL	C64-C65-C66-C67
49	L	701	3PE	C36-C37-C38-C39
54	U	201	EHZ	O2-C9-S1-C10
50	h	201	CDL	C51-CB5-OB6-CB4
49	L	701	3PE	C38-C39-C3A-C3B
49	H	401	3PE	C24-C25-C26-C27
46	I	202	PC1	O11-C1-C2-C3
49	H	401	3PE	O11-C1-C2-C3
50	N	402	CDL	OA5-CA3-CA4-CA6
50	N	402	CDL	OB5-CB3-CB4-CB6
49	L	704	3PE	C36-C37-C38-C39
48	F	501	FMN	C5'-O5'-P-O3P
49	I	201	3PE	C24-C25-C26-C27
50	d	201	CDL	CB3-CB4-OB6-CB5
50	d	202	CDL	CA6-CA4-OA6-CA5
49	M	501	3PE	C1-C2-C3-O31
50	N	402	CDL	CB3-CB4-CB6-OB8
46	B	203	PC1	O11-C1-C2-O21
49	K	201	3PE	O11-C1-C2-O21
54	T	201	EHZ	C3-C4-C5-C6
49	M	501	3PE	O21-C2-C3-O31
46	H	402	PC1	C37-C38-C39-C3A
50	h	201	CDL	OB7-CB5-OB6-CB4
50	d	201	CDL	C11-C12-C13-C14
52	P	501	NDP	C3D-C4D-C5D-O5D
52	P	501	NDP	PN-O3-PA-O2A
49	L	704	3PE	C24-C25-C26-C27
46	B	202	PC1	C1-O11-P-O12
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C1-O11-P-O12
46	B	203	PC1	C1-O11-P-O14
46	I	202	PC1	C1-O11-P-O12
49	L	704	3PE	C1-O11-P-O14
50	N	401	CDL	CA2-OA2-PA1-OA4
50	N	401	CDL	CB2-OB2-PB2-OB4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
50	N	402	CDL	CA3-OA5-PA1-OA4
50	N	402	CDL	CB3-OB5-PB2-OB4
50	d	201	CDL	CB2-OB2-PB2-OB3
50	d	201	CDL	CB3-OB5-PB2-OB3
50	h	201	CDL	CB2-OB2-PB2-OB3
51	O	401	ATP	C5'-O5'-PA-O1A
52	P	501	NDP	C5B-O5B-PA-O2A
46	B	203	PC1	C21-C22-C23-C24
46	H	402	PC1	C24-C25-C26-C27
49	M	502	3PE	O11-C1-C2-C3
49	K	201	3PE	C12-C11-O13-P
49	L	703	3PE	C12-C11-O13-P
46	I	202	PC1	C22-C23-C24-C25
49	I	201	3PE	C3C-C3D-C3E-C3F
46	H	402	PC1	O11-C1-C2-O21
50	N	401	CDL	OB5-CB3-CB4-OB6
50	N	402	CDL	OA5-CA3-CA4-OA6
50	q	201	CDL	OA5-CA3-CA4-OA6
50	N	401	CDL	C71-C72-C73-C74
49	Y	401	3PE	C21-C22-C23-C24
46	B	202	PC1	O13-C11-C12-N
46	H	402	PC1	O13-C11-C12-N
50	h	201	CDL	CB3-CB4-CB6-OB8
50	N	402	CDL	OB6-CB4-CB6-OB8
50	h	201	CDL	OA6-CA4-CA6-OA8
46	B	203	PC1	C37-C38-C39-C3A
49	M	501	3PE	C3A-C3B-C3C-C3D
50	d	202	CDL	CB7-C71-C72-C73
46	I	202	PC1	O21-C21-C22-C23
49	L	704	3PE	C38-C39-C3A-C3B
54	U	201	EHZ	C3-C4-C5-C6
49	L	704	3PE	C3F-C3G-C3H-C3I
50	q	201	CDL	C12-C13-C14-C15
49	M	502	3PE	C36-C37-C38-C39
50	h	201	CDL	C51-C52-C53-C54
46	I	202	PC1	C34-C35-C36-C37
50	L	702	CDL	C57-C58-C59-C60
50	N	401	CDL	CB6-CB4-OB6-CB5
46	I	202	PC1	O11-C1-C2-O21
49	H	401	3PE	O11-C1-C2-O21
50	L	702	CDL	C35-C36-C37-C38
49	M	502	3PE	O21-C2-C3-O31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
46	H	402	PC1	C1-O11-P-O13
49	L	701	3PE	C11-O13-P-O11
50	L	702	CDL	CA3-OA5-PA1-OA2
50	d	202	CDL	CB3-OB5-PB2-OB2
50	q	201	CDL	CB2-OB2-PB2-OB5
49	I	201	3PE	C2F-C2G-C2H-C2I
49	M	502	3PE	C39-C3A-C3B-C3C
49	I	201	3PE	C2E-C2F-C2G-C2H
50	N	401	CDL	C56-C57-C58-C59
50	d	202	CDL	C73-C74-C75-C76
54	T	201	EHZ	C1-C2-C3-C4
50	L	702	CDL	C79-C80-C81-C82
50	d	201	CDL	C60-C61-C62-C63
49	M	502	3PE	C31-C32-C33-C34
49	K	201	3PE	C2-C1-O11-P
50	N	401	CDL	CB4-CB3-OB5-PB2
49	K	201	3PE	C27-C28-C29-C2A
50	h	201	CDL	C31-CA7-OA8-CA6
49	M	502	3PE	C35-C36-C37-C38
49	L	701	3PE	C22-C23-C24-C25
49	L	701	3PE	O21-C21-C22-C23
54	T	201	EHZ	C10-C11-N1-C12
50	N	402	CDL	C72-C73-C74-C75
50	d	201	CDL	CB3-CB4-CB6-OB8
49	M	501	3PE	C3B-C3C-C3D-C3E
46	B	203	PC1	C39-C3A-C3B-C3C
50	q	201	CDL	CA6-CA4-OA6-CA5
46	I	202	PC1	C32-C31-O31-C3
46	I	202	PC1	C11-C12-N-C14
50	q	201	CDL	CB3-OB5-PB2-OB2
50	N	401	CDL	CB7-C71-C72-C73
49	L	704	3PE	C29-C2A-C2B-C2C
51	O	401	ATP	O4'-C4'-C5'-O5'
46	B	202	PC1	C22-C23-C24-C25
50	L	702	CDL	C12-C13-C14-C15
49	H	401	3PE	C31-C32-C33-C34
50	L	702	CDL	C74-C75-C76-C77
46	B	203	PC1	C22-C23-C24-C25
49	L	701	3PE	C33-C34-C35-C36
46	I	202	PC1	O32-C31-O31-C3
50	h	201	CDL	OA9-CA7-OA8-CA6
50	d	202	CDL	C31-C32-C33-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
50	d	202	CDL	CA7-C31-C32-C33
49	L	704	3PE	O11-C1-C2-O21
50	N	402	CDL	OB5-CB3-CB4-OB6
46	I	202	PC1	C11-C12-N-C13
46	B	202	PC1	C36-C37-C38-C39
49	M	501	3PE	C23-C24-C25-C26
46	H	402	PC1	O11-C1-C2-C3
49	L	704	3PE	O11-C1-C2-C3
50	h	201	CDL	C24-C25-C26-C27
50	h	201	CDL	C11-C12-C13-C14
49	Y	401	3PE	O21-C2-C3-O31
50	q	201	CDL	OA7-CA5-OA6-CA4
49	L	704	3PE	O31-C31-C32-C33
49	L	704	3PE	C25-C26-C27-C28
50	L	702	CDL	C51-C52-C53-C54
50	d	202	CDL	C33-C34-C35-C36
50	d	202	CDL	CB2-OB2-PB2-OB5
54	T	201	EHZ	C18-C17-C20-O6
46	I	202	PC1	C2B-C2C-C2D-C2E
50	h	201	CDL	CB6-CB4-OB6-CB5
50	d	201	CDL	CA7-C31-C32-C33
50	N	402	CDL	CB7-C71-C72-C73
49	H	401	3PE	O21-C21-C22-C23
49	H	401	3PE	C3B-C3C-C3D-C3E
49	L	704	3PE	C26-C27-C28-C29
49	L	703	3PE	C2A-C2B-C2C-C2D
50	N	402	CDL	C32-C31-CA7-OA8
50	N	401	CDL	C52-C51-CB5-OB6
54	T	201	EHZ	O1-C7-C8-C9
50	h	201	CDL	C72-C71-CB7-OB8
46	B	203	PC1	O11-C1-C2-C3
50	q	201	CDL	C17-C18-C19-C20
50	h	201	CDL	C12-C11-CA5-OA6
46	H	402	PC1	C28-C29-C2A-C2B
46	I	202	PC1	C11-C12-N-C15
50	d	201	CDL	C53-C54-C55-C56
50	N	401	CDL	C72-C71-CB7-OB8
49	Y	401	3PE	C3B-C3C-C3D-C3E
52	P	501	NDP	PN-O3-PA-O1A
49	K	201	3PE	C25-C26-C27-C28
49	H	401	3PE	C37-C38-C39-C3A
49	L	704	3PE	O32-C31-C32-C33

*Continued on next page...*

*Continued from previous page...*

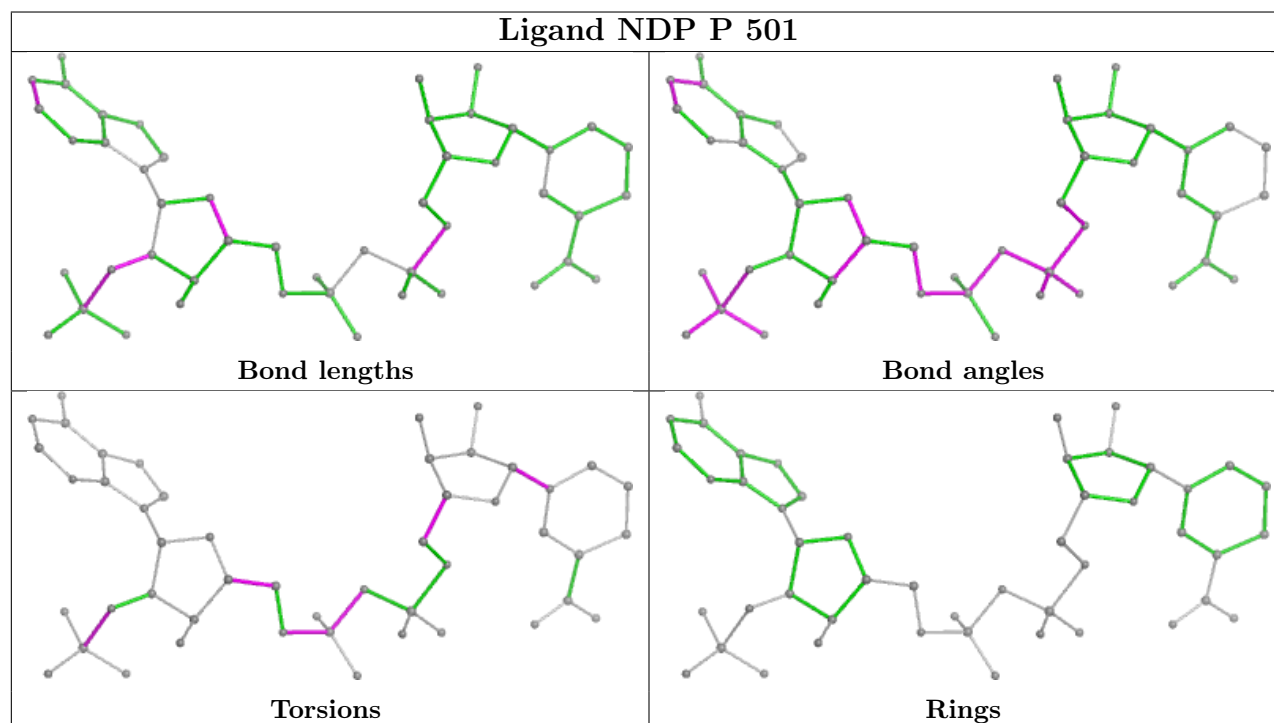
Mol	Chain	Res	Type	Atoms
50	N	402	CDL	C32-C31-CA7-OA9
49	L	703	3PE	C28-C29-C2A-C2B
46	B	203	PC1	C23-C24-C25-C26
50	N	401	CDL	C52-C51-CB5-OB7
49	L	703	3PE	C34-C35-C36-C37
46	B	203	PC1	C11-O13-P-O12
46	I	202	PC1	C11-O13-P-O14
49	I	201	3PE	C11-O13-P-O14
49	M	502	3PE	C11-O13-P-O14
50	d	201	CDL	CA3-OA5-PA1-OA4
50	d	202	CDL	CB3-OB5-PB2-OB3
50	q	201	CDL	C11-CA5-OA6-CA4
49	Y	401	3PE	C27-C28-C29-C2A
49	Y	401	3PE	O21-C21-C22-C23
50	q	201	CDL	OA5-CA3-CA4-CA6
50	h	201	CDL	C12-C11-CA5-OA7
50	h	201	CDL	C72-C71-CB7-OB9
49	L	704	3PE	C23-C24-C25-C26
49	Y	401	3PE	O31-C31-C32-C33
50	h	201	CDL	CB3-CB4-OB6-CB5
49	H	401	3PE	O22-C21-C22-C23
50	L	702	CDL	C52-C51-CB5-OB6
50	L	702	CDL	C72-C71-CB7-OB8
49	I	201	3PE	C22-C23-C24-C25
46	H	402	PC1	C27-C28-C29-C2A
46	H	402	PC1	O21-C21-C22-C23
50	d	202	CDL	C32-C31-CA7-OA8
49	L	703	3PE	O21-C21-C22-C23
50	d	201	CDL	C54-C55-C56-C57
50	d	202	CDL	C32-C31-CA7-OA9
50	d	201	CDL	C32-C33-C34-C35
50	h	201	CDL	C23-C24-C25-C26
49	M	501	3PE	O31-C31-C32-C33
49	Y	401	3PE	O22-C21-C22-C23
50	L	702	CDL	C37-C38-C39-C40
50	L	702	CDL	C52-C51-CB5-OB7
50	L	702	CDL	C72-C71-CB7-OB9
49	I	201	3PE	C23-C24-C25-C26
50	h	201	CDL	C32-C31-CA7-OA8

There are no ring outliers.

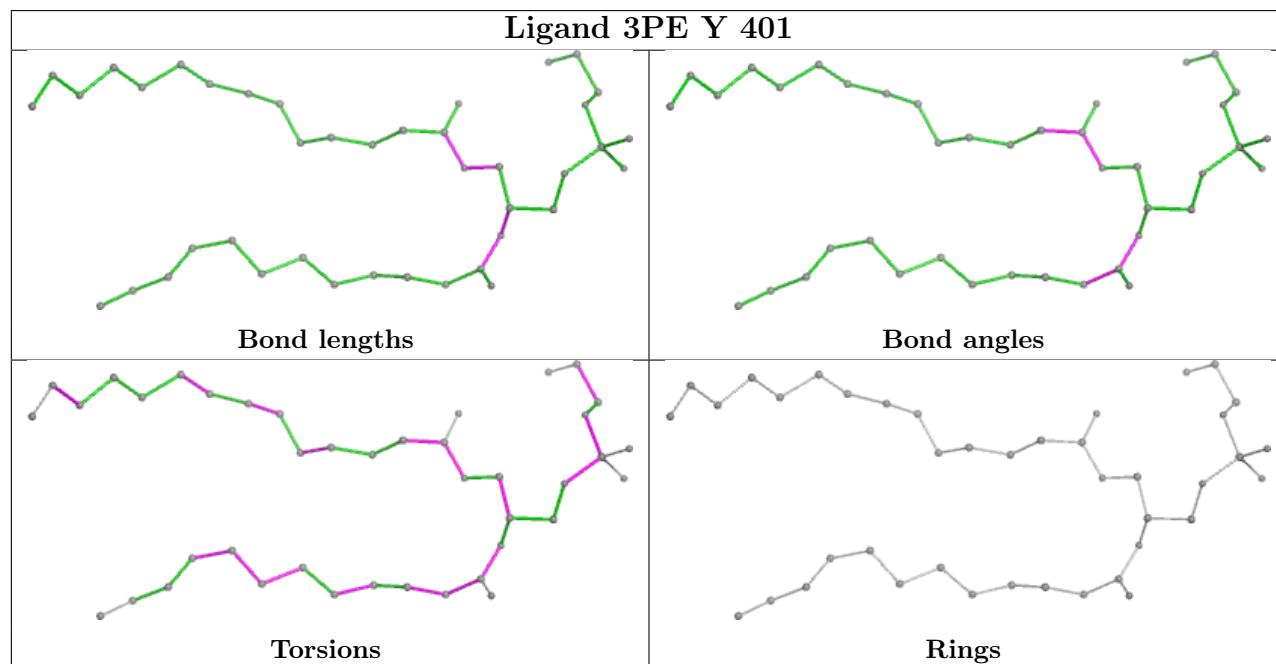
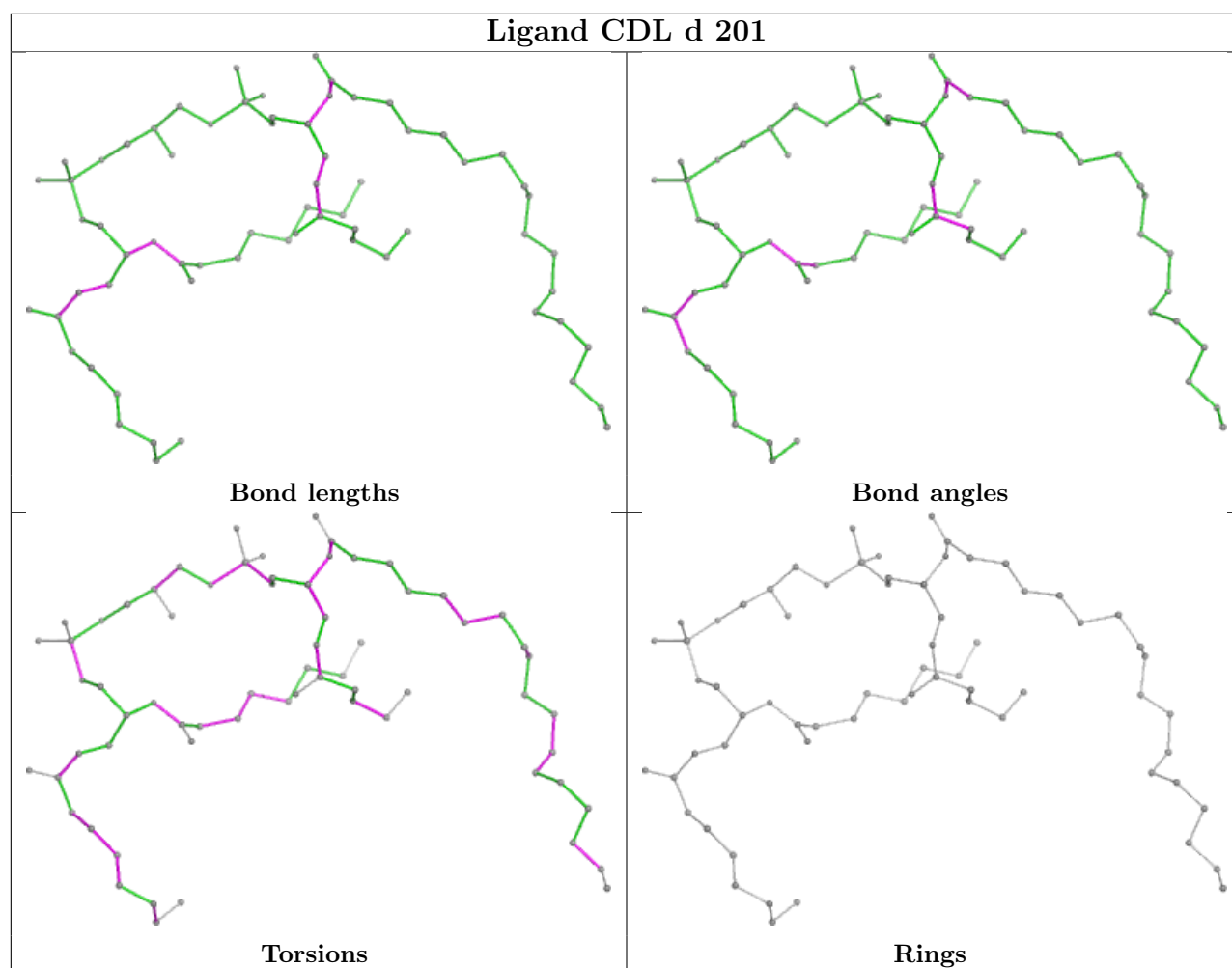
11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	P	501	NDP	1	0
48	F	501	FMN	1	0
46	B	202	PC1	1	0
46	H	402	PC1	1	0
54	U	201	EHZ	1	0
45	G	801	SF4	1	0
51	O	401	ATP	2	0
49	K	201	3PE	1	0
50	N	401	CDL	1	0
47	E	301	FES	1	0
49	H	401	3PE	1	0

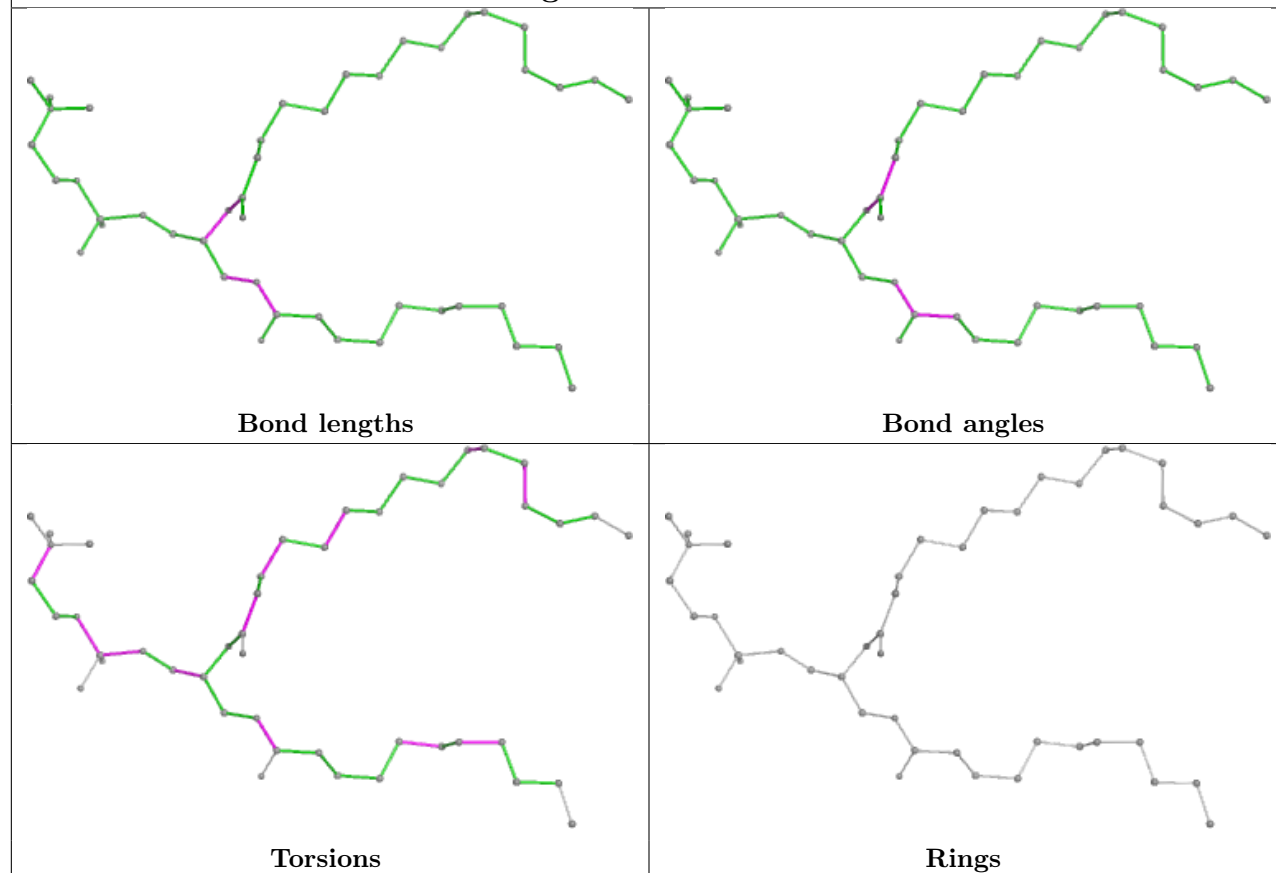
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



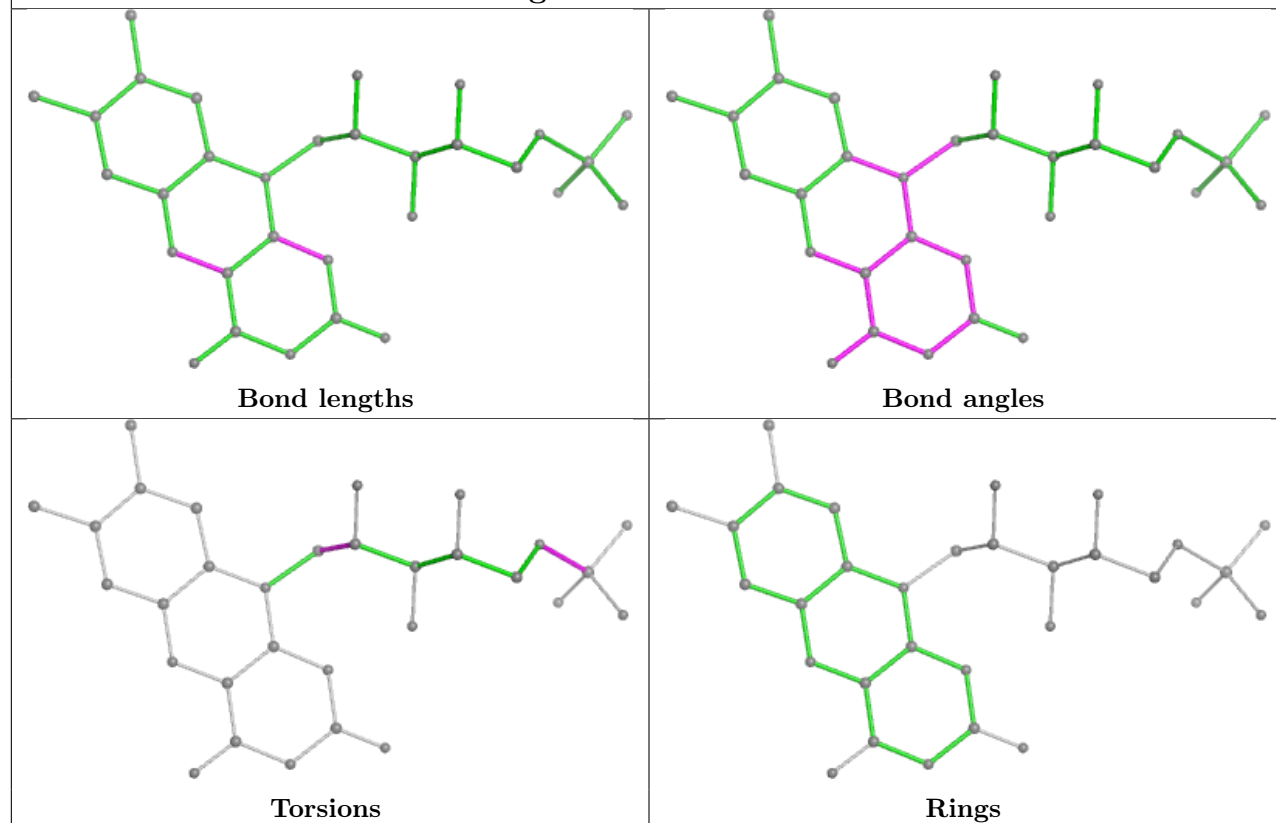


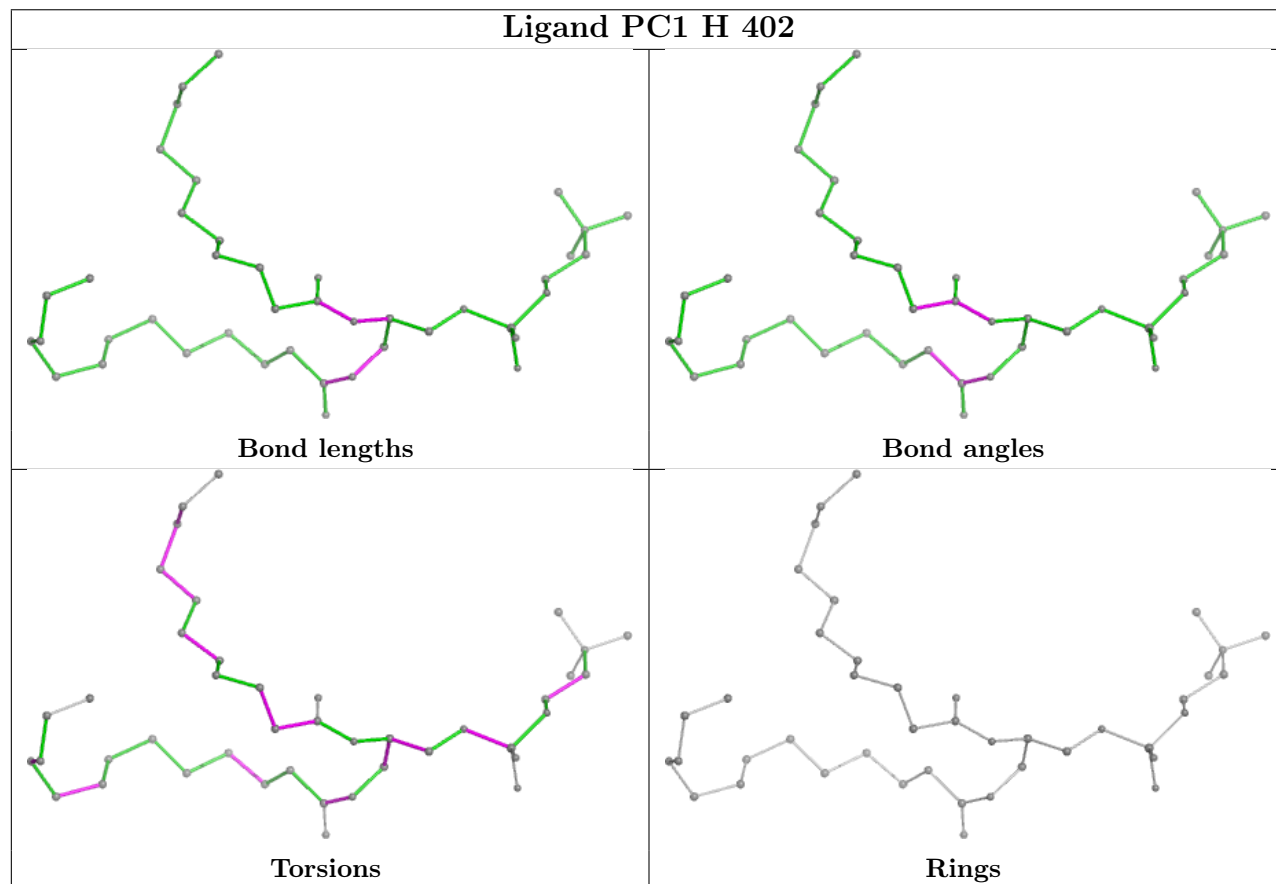
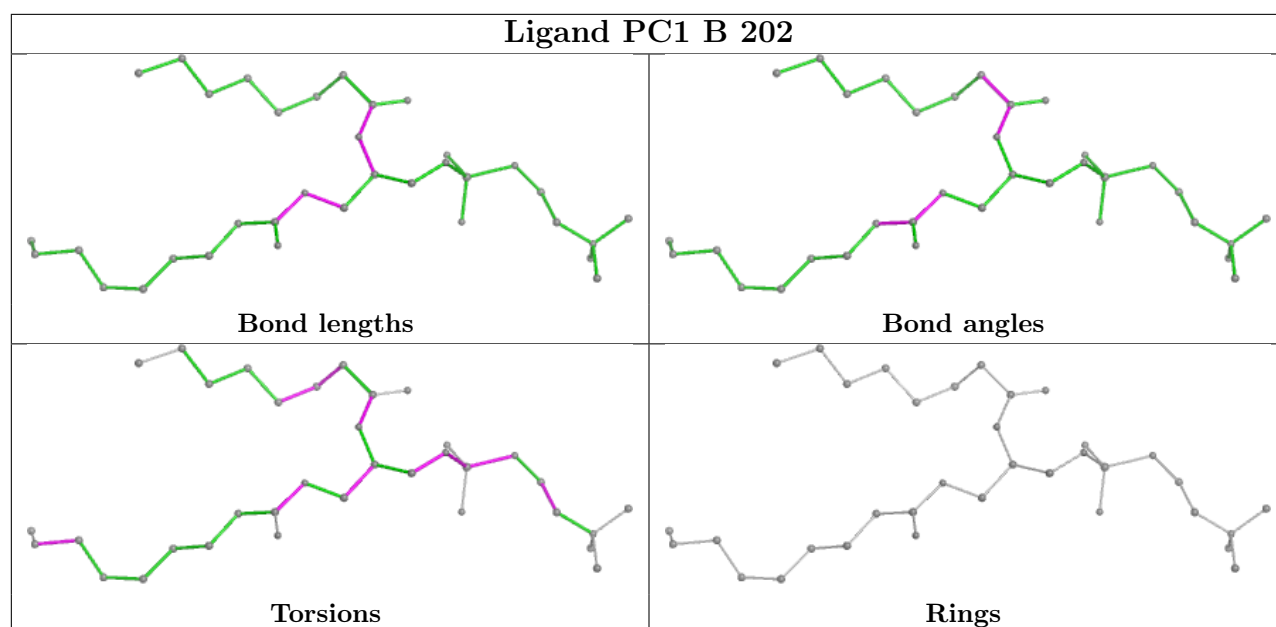


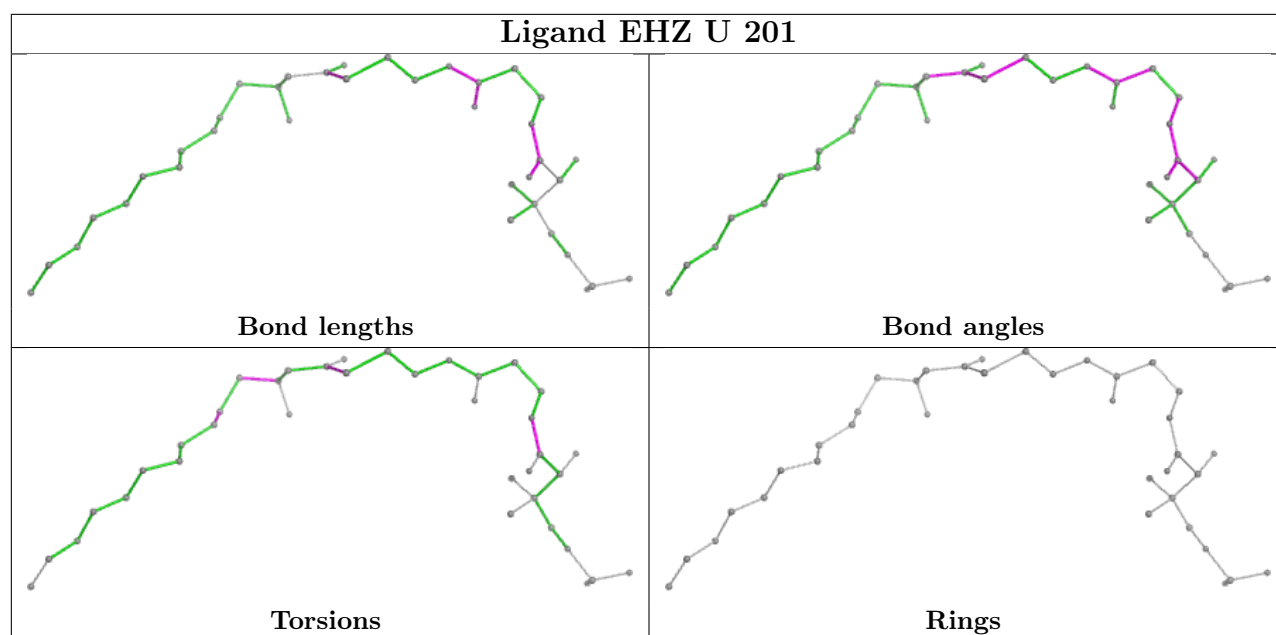
## Ligand PC1 I 202

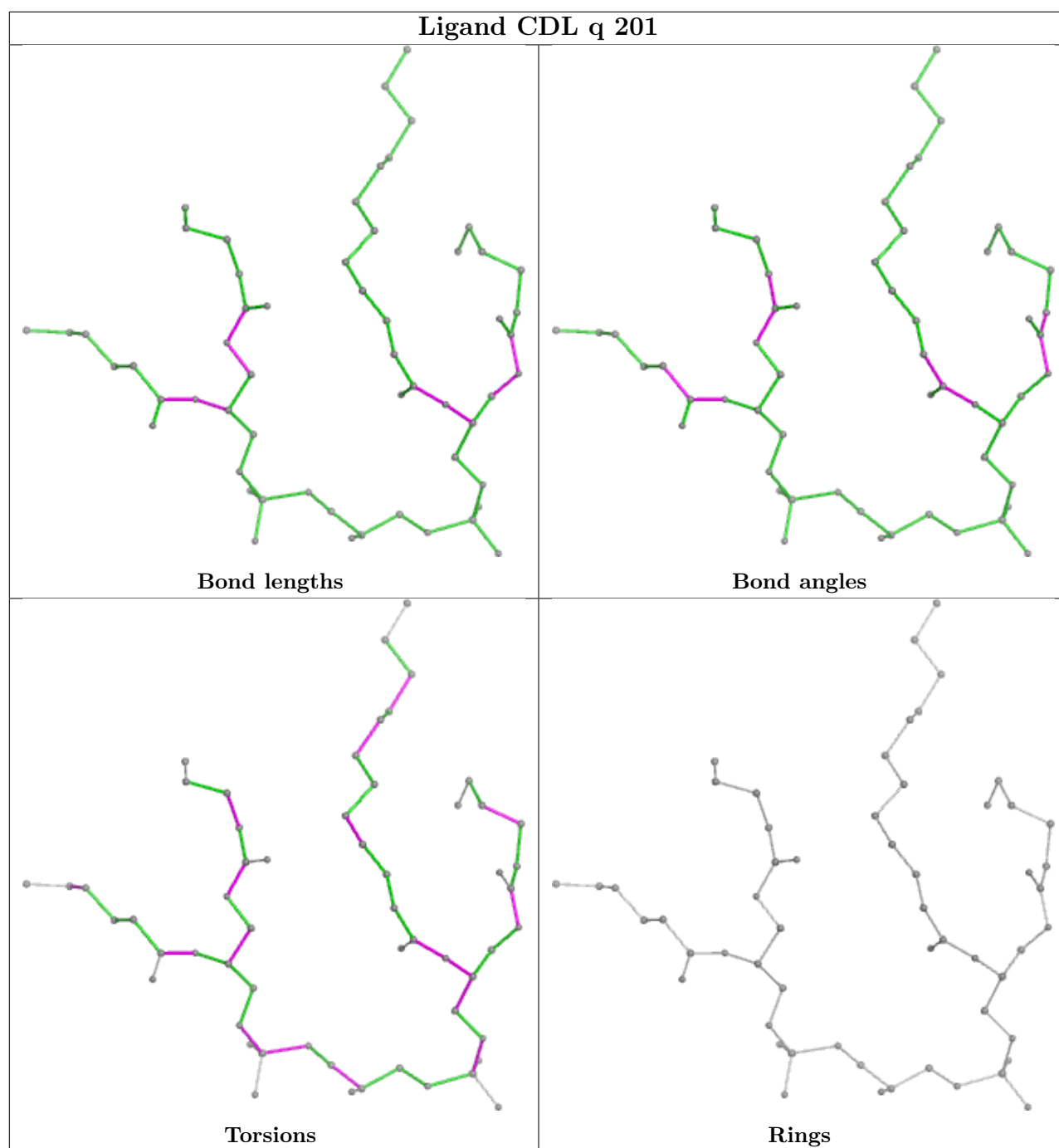


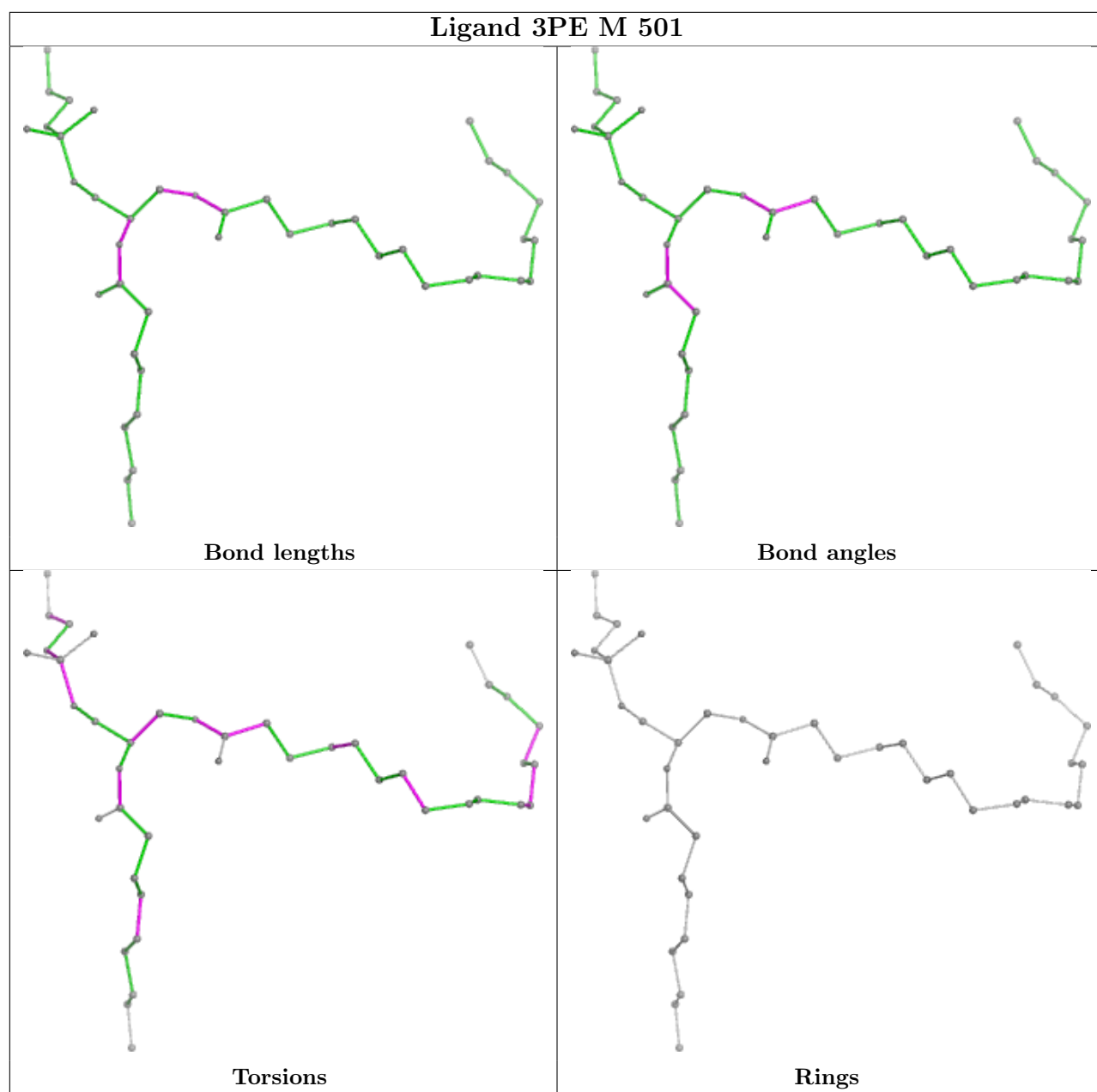
## Ligand FMN F 501

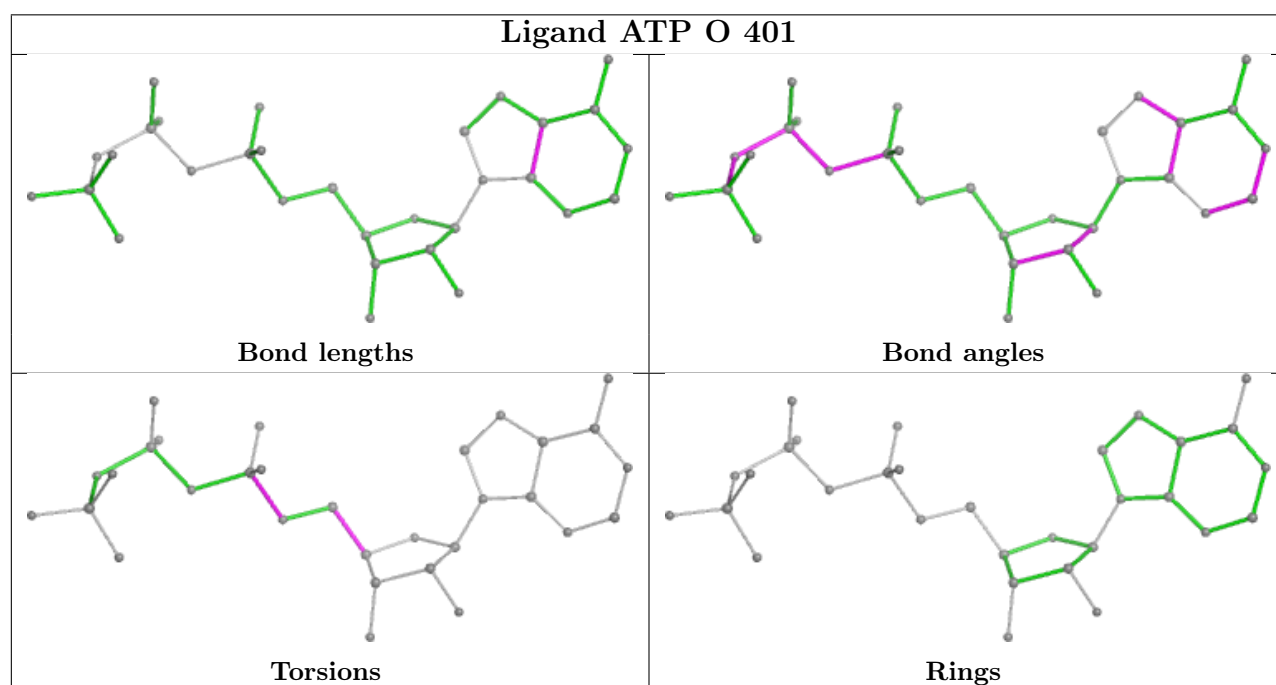
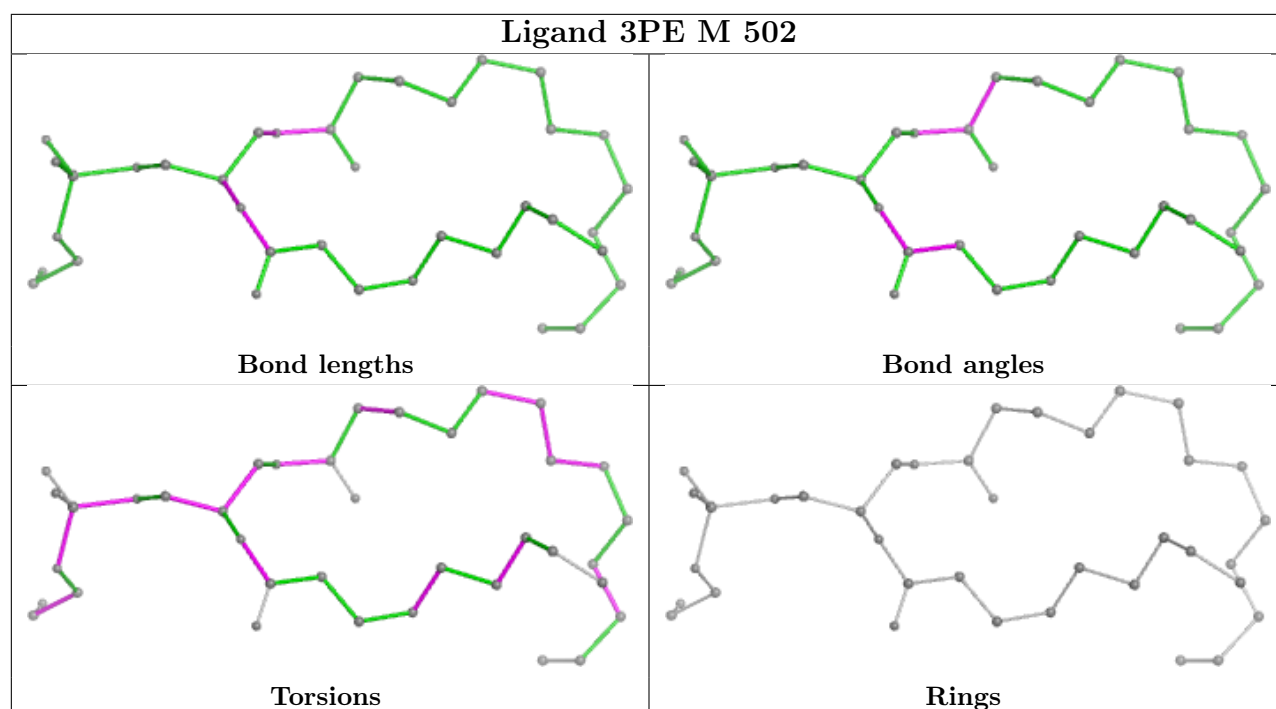


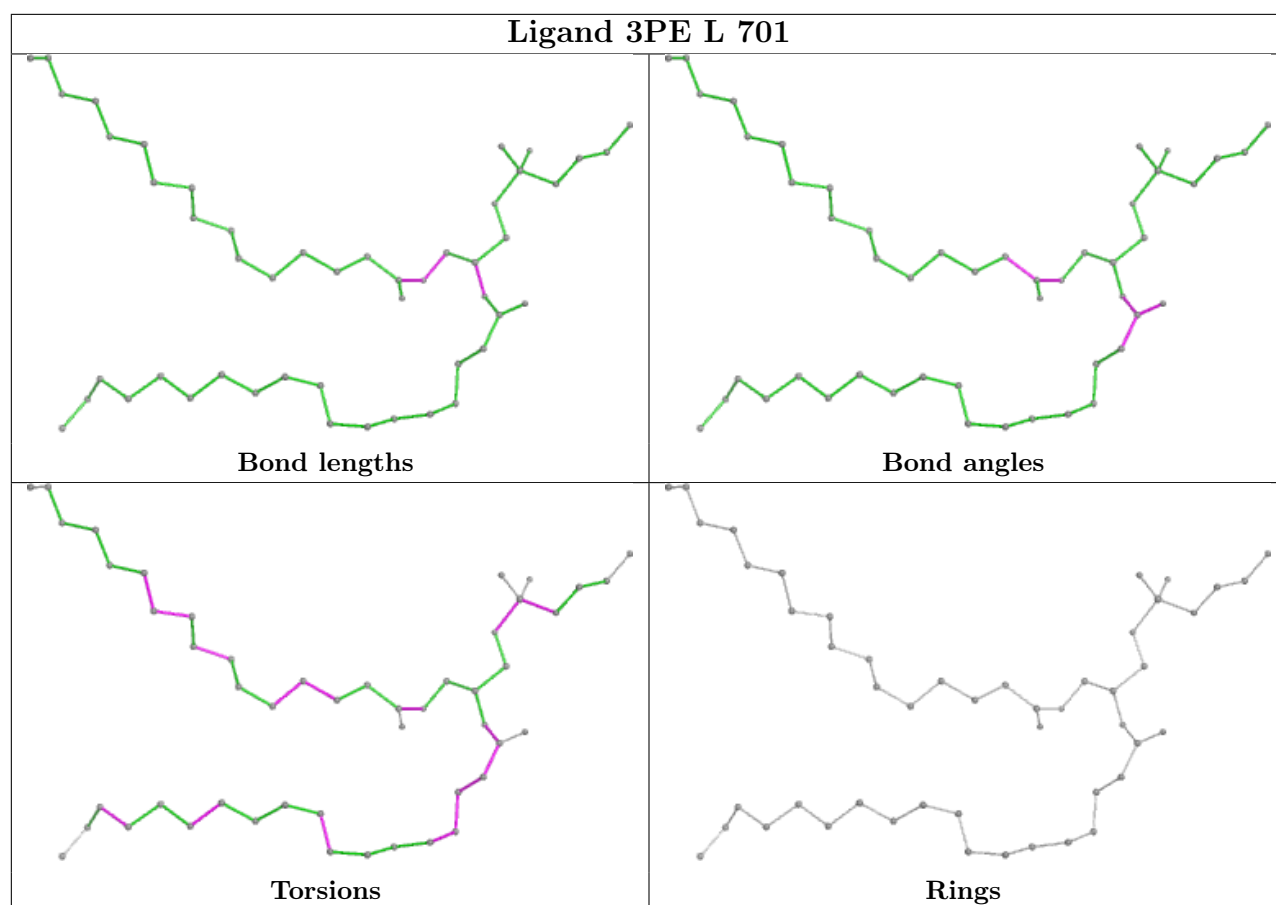




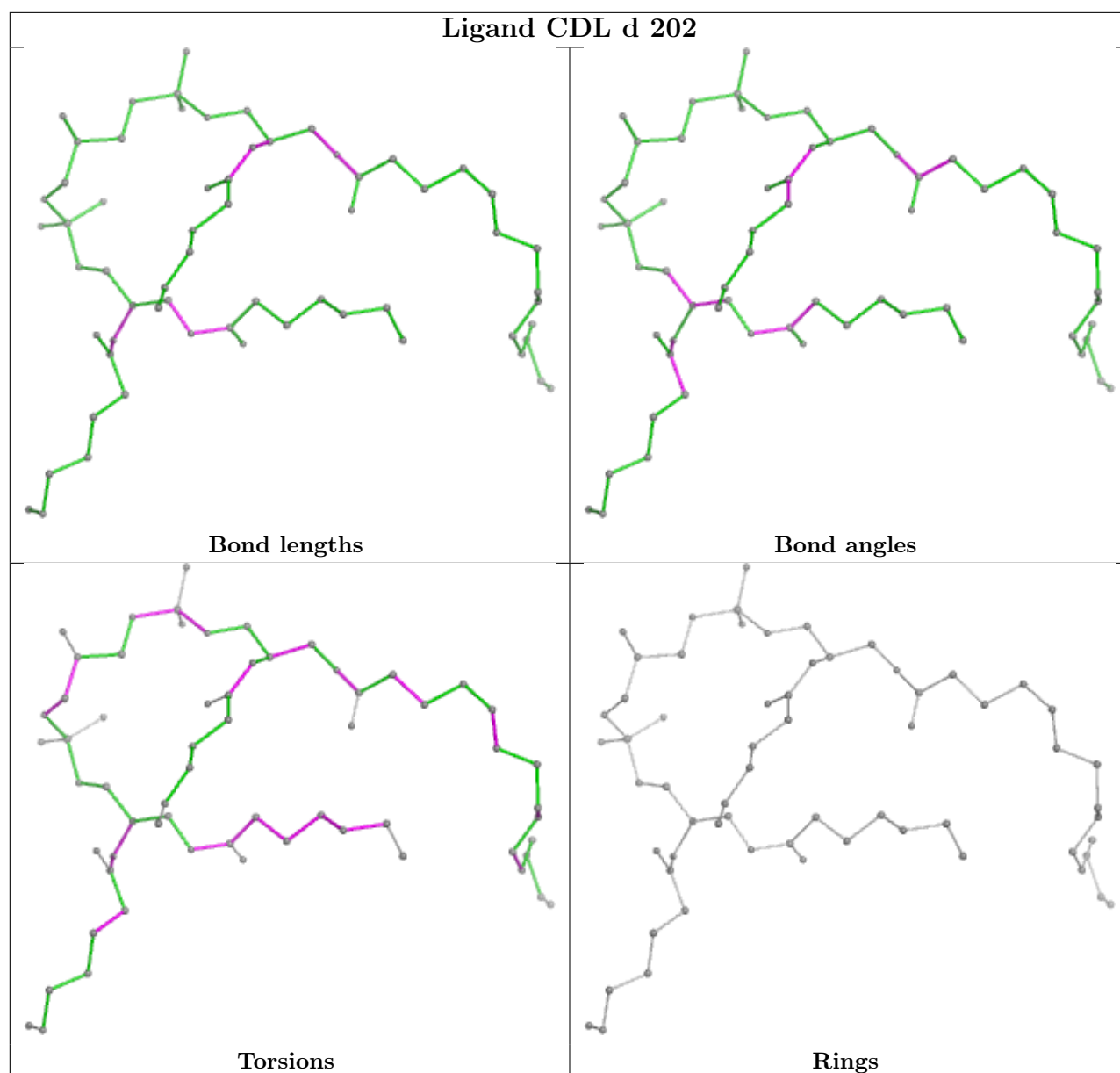


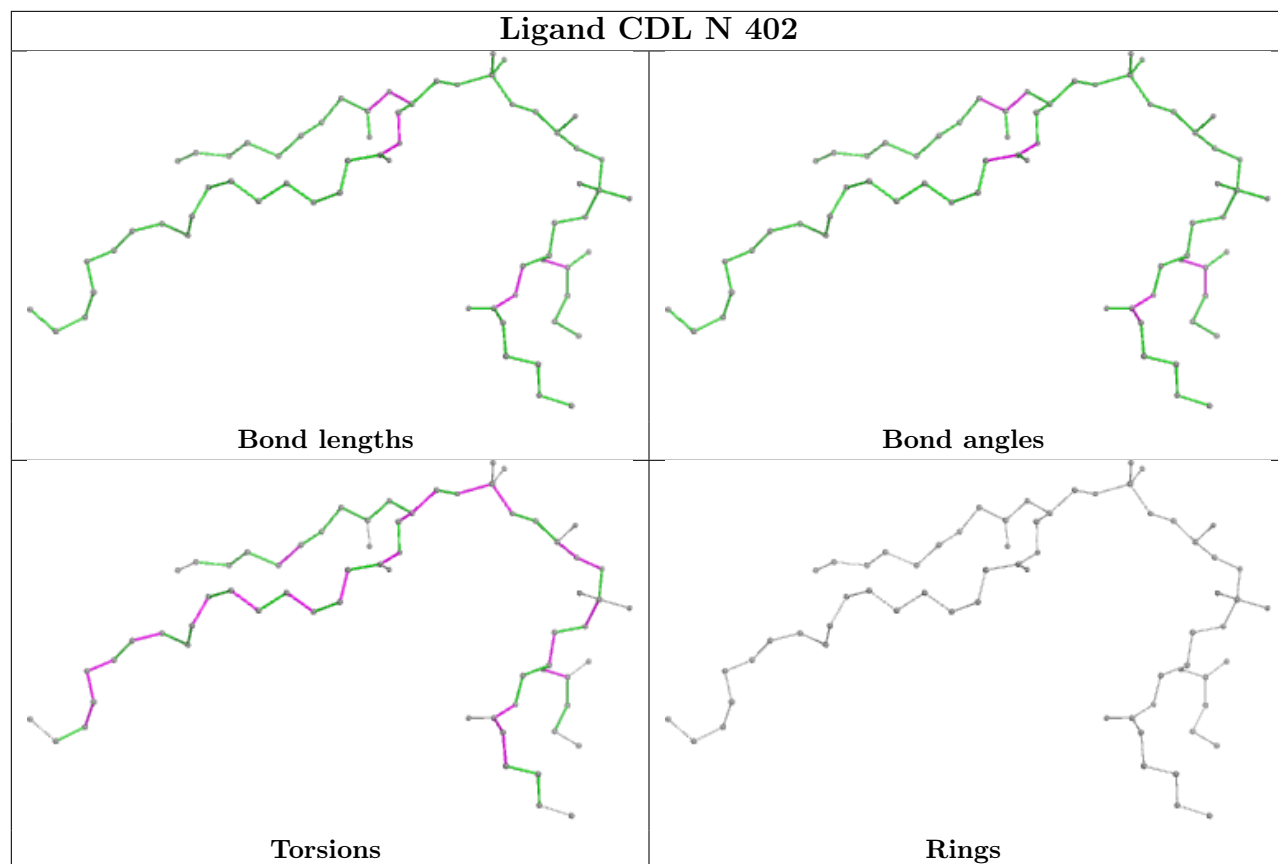


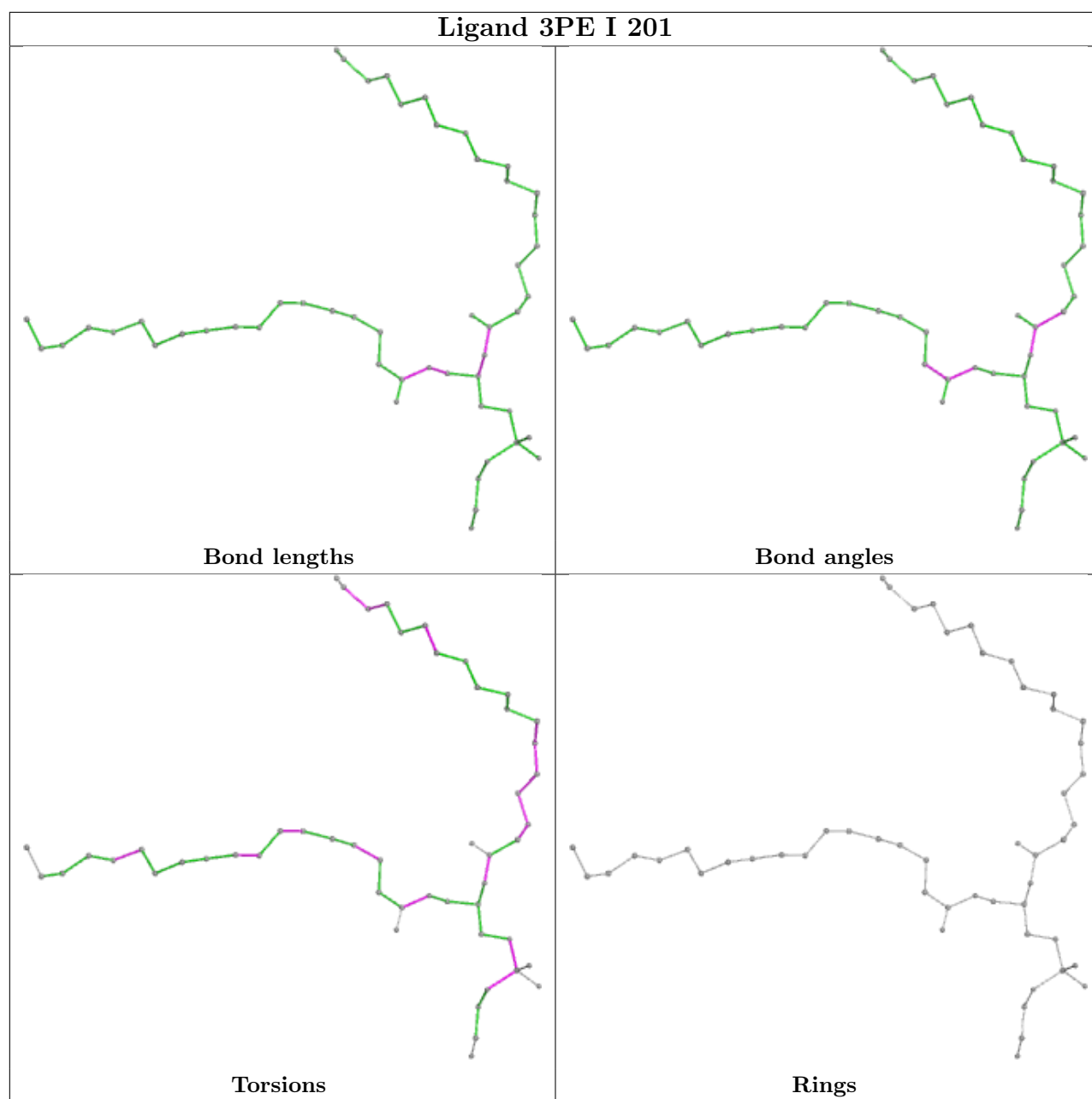


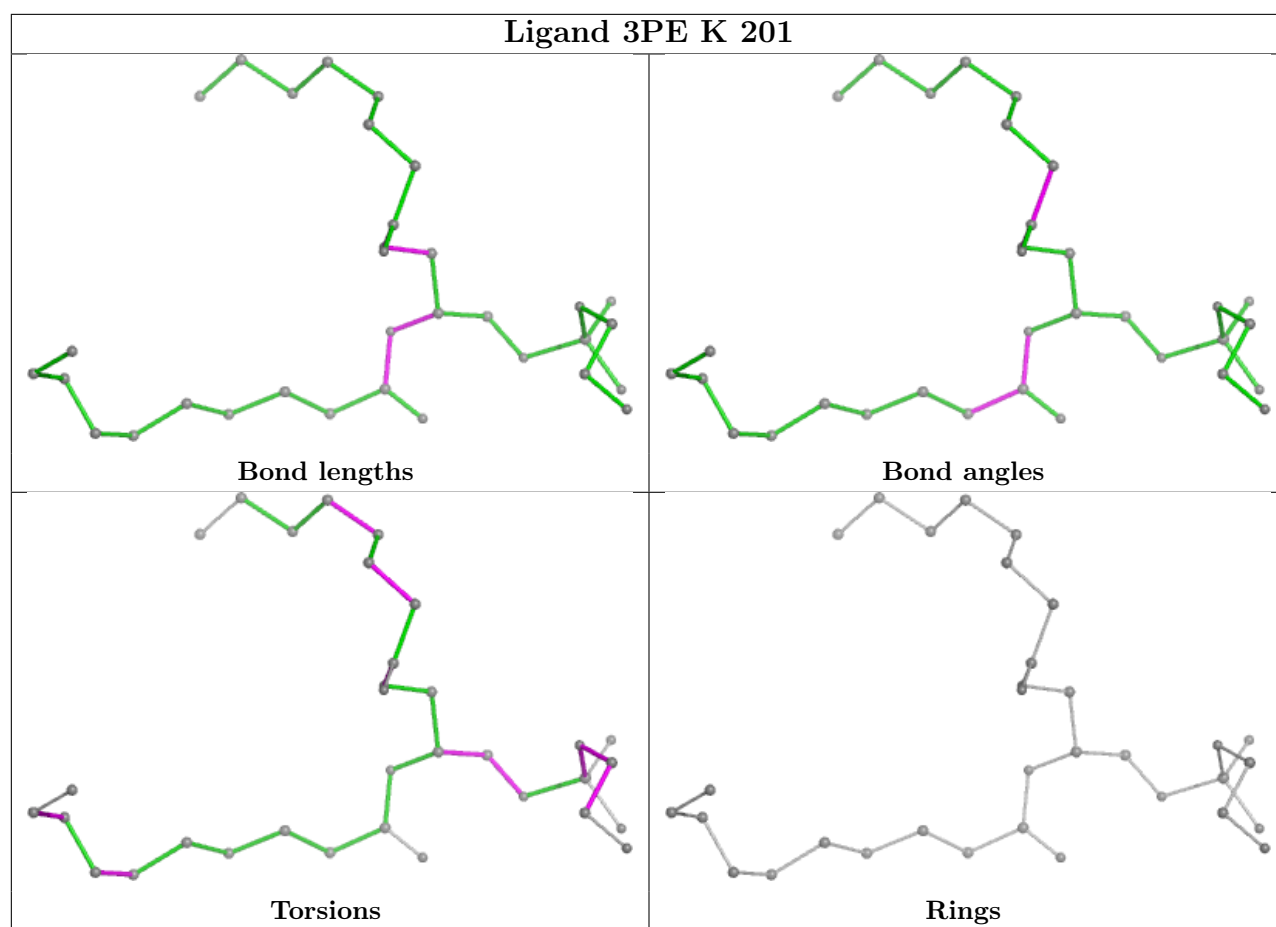


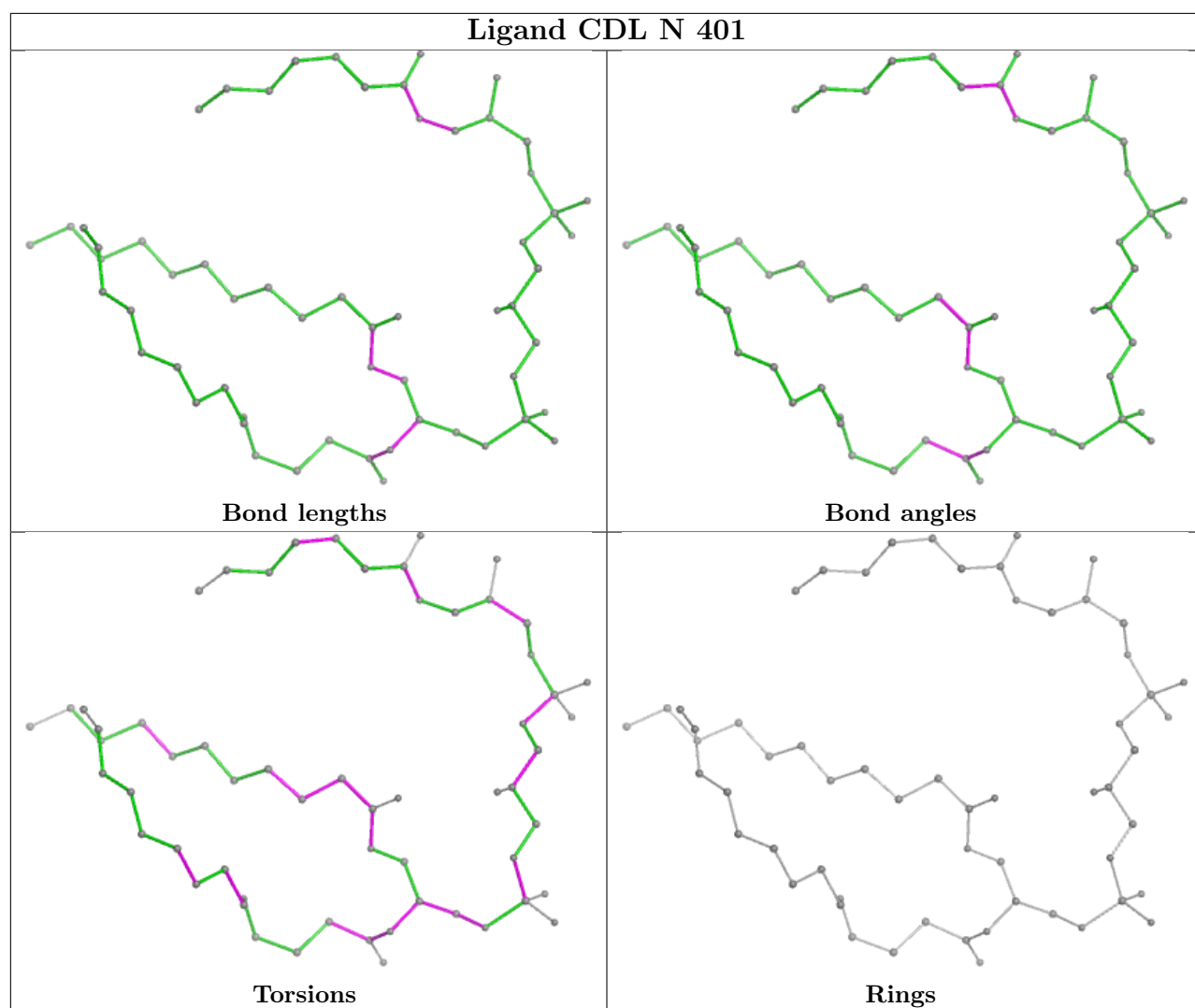


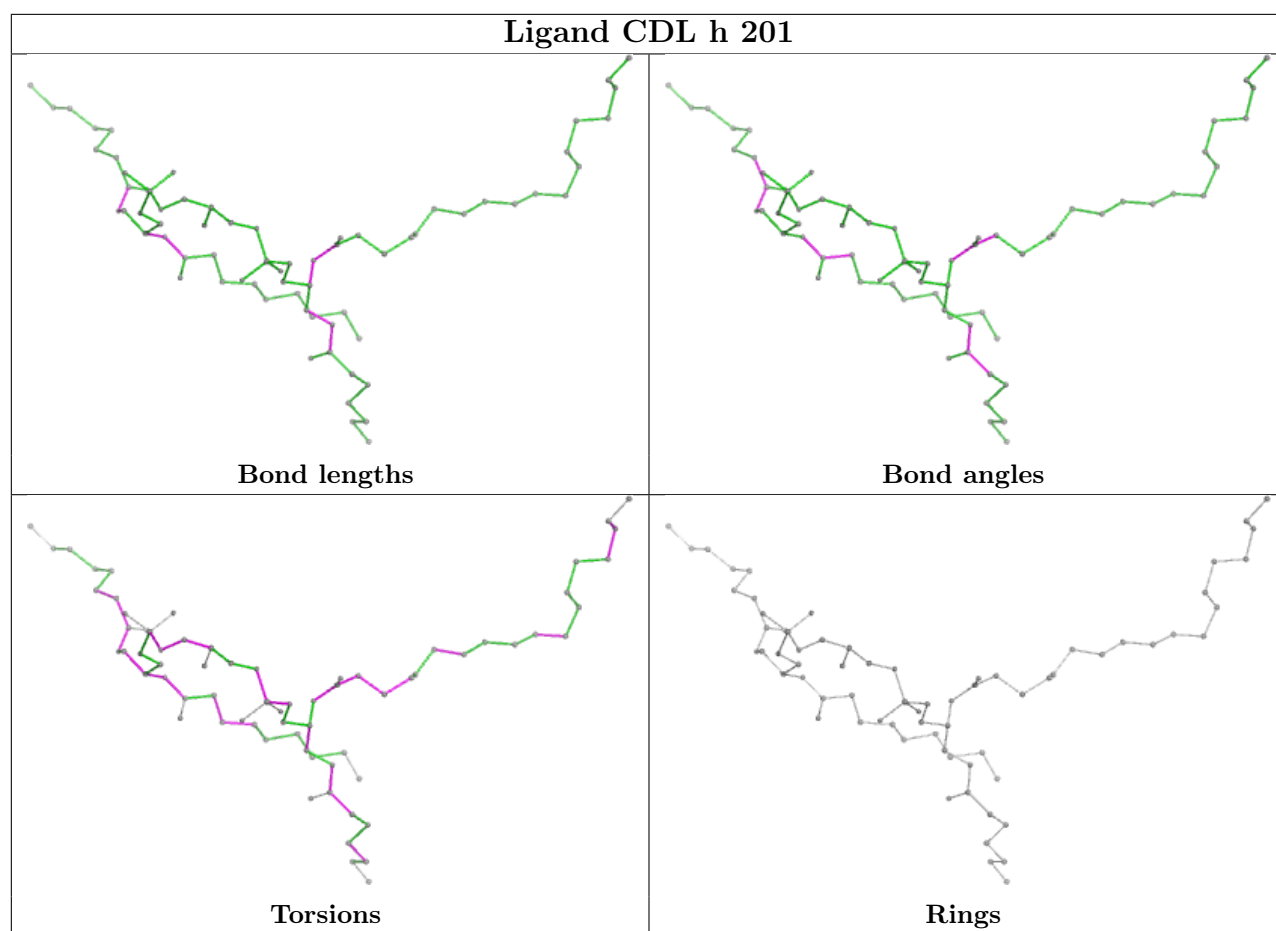


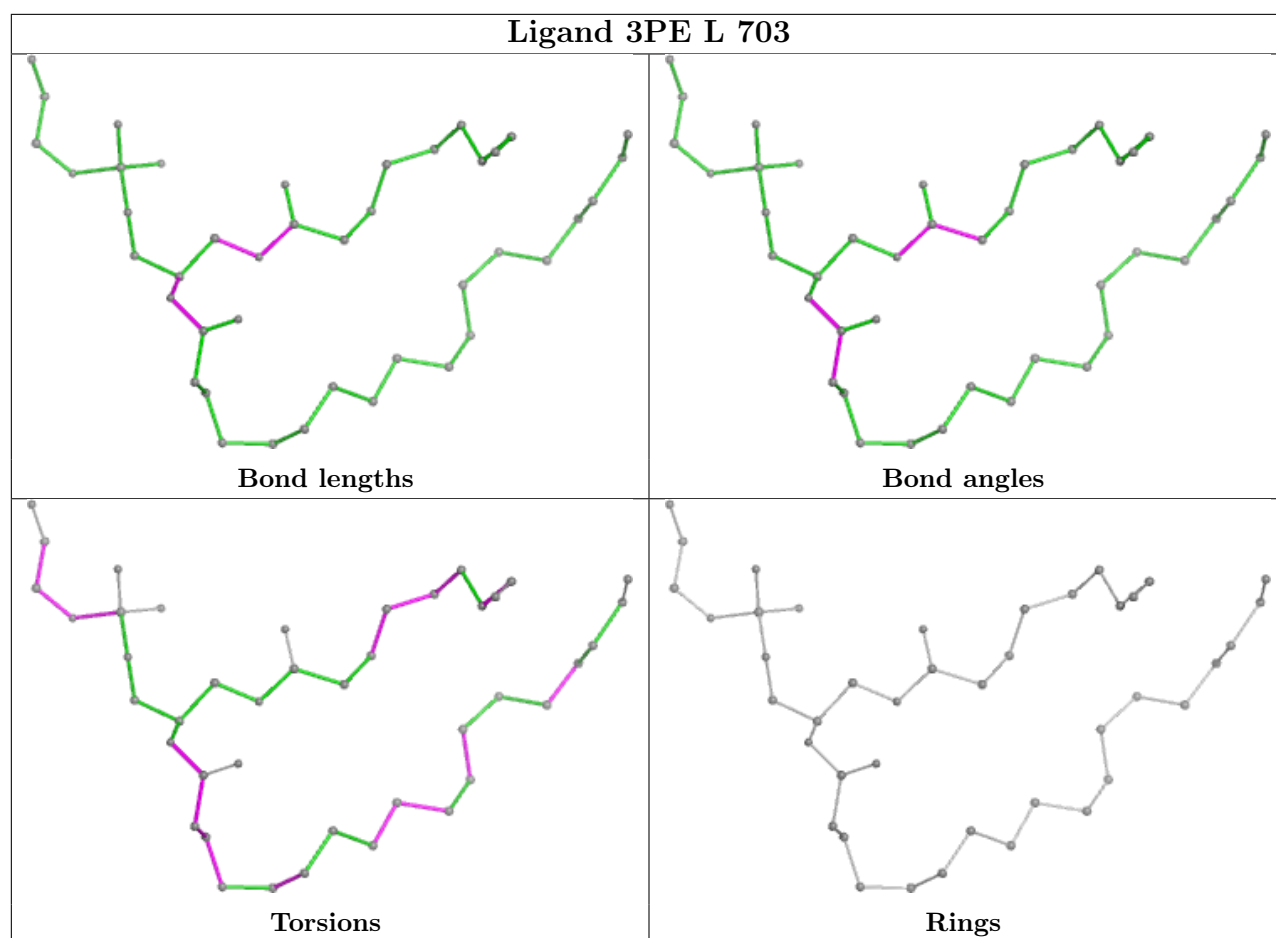


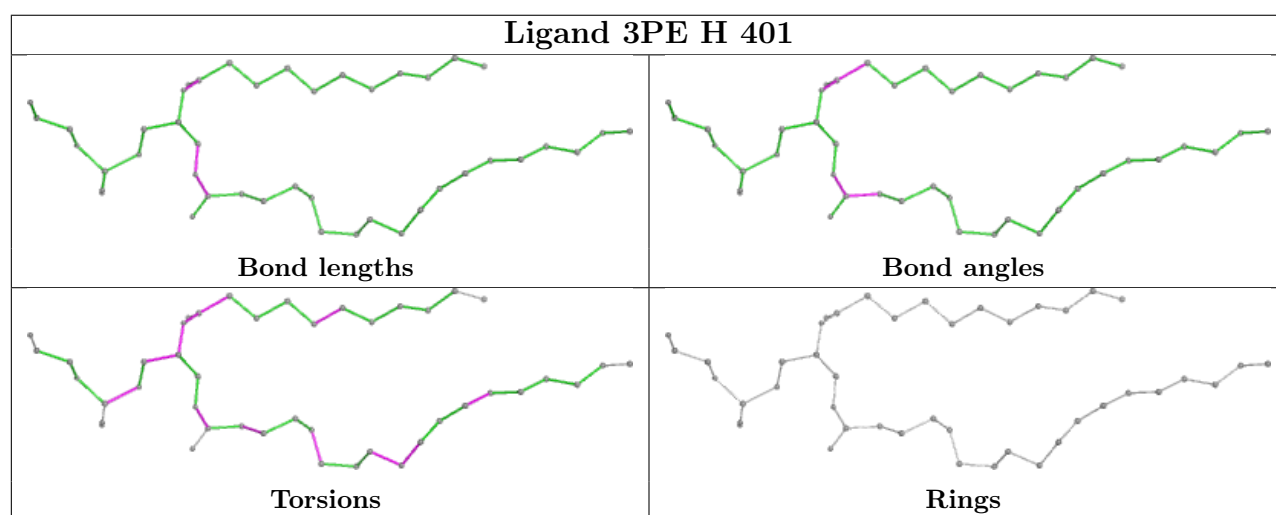
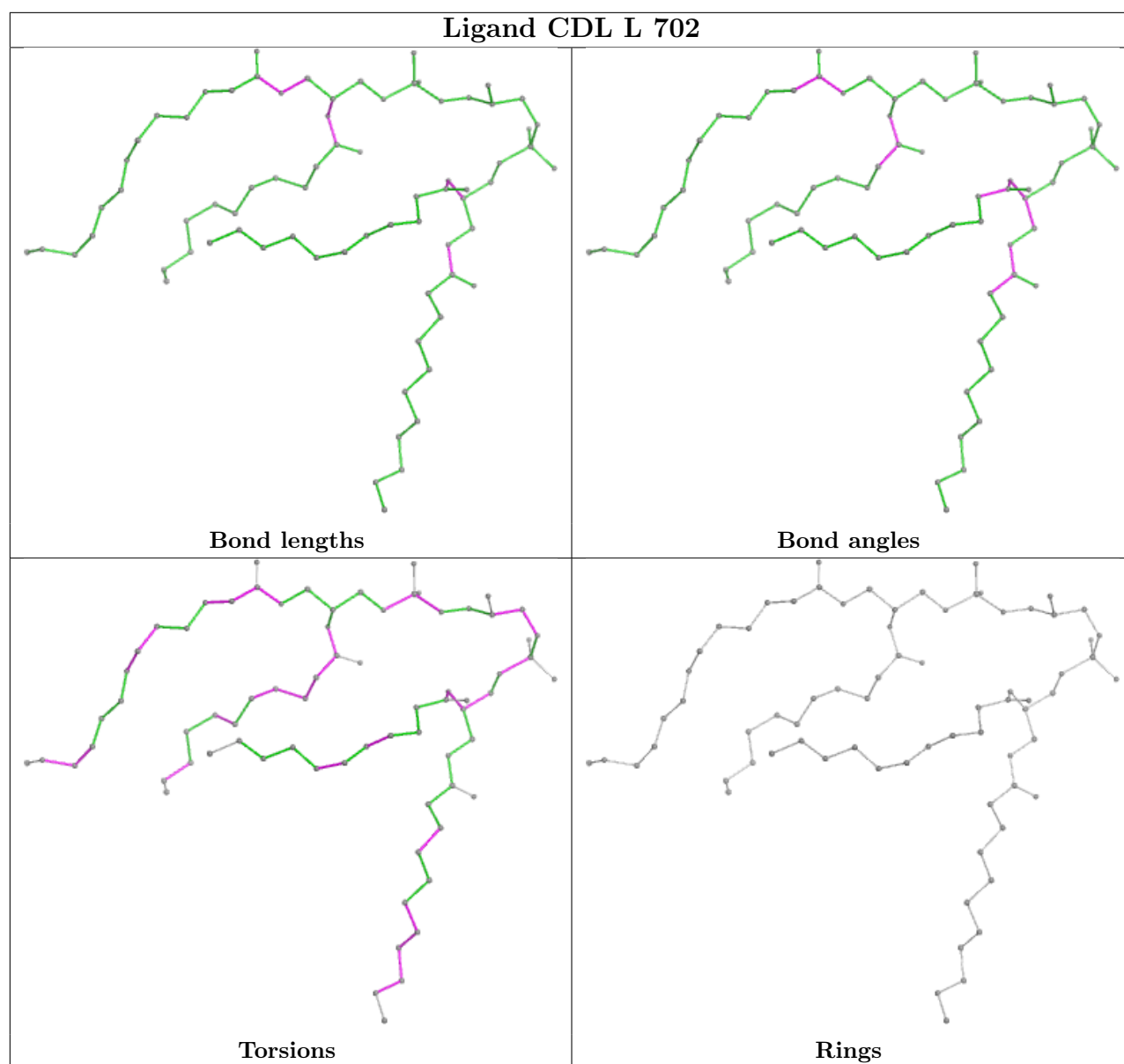




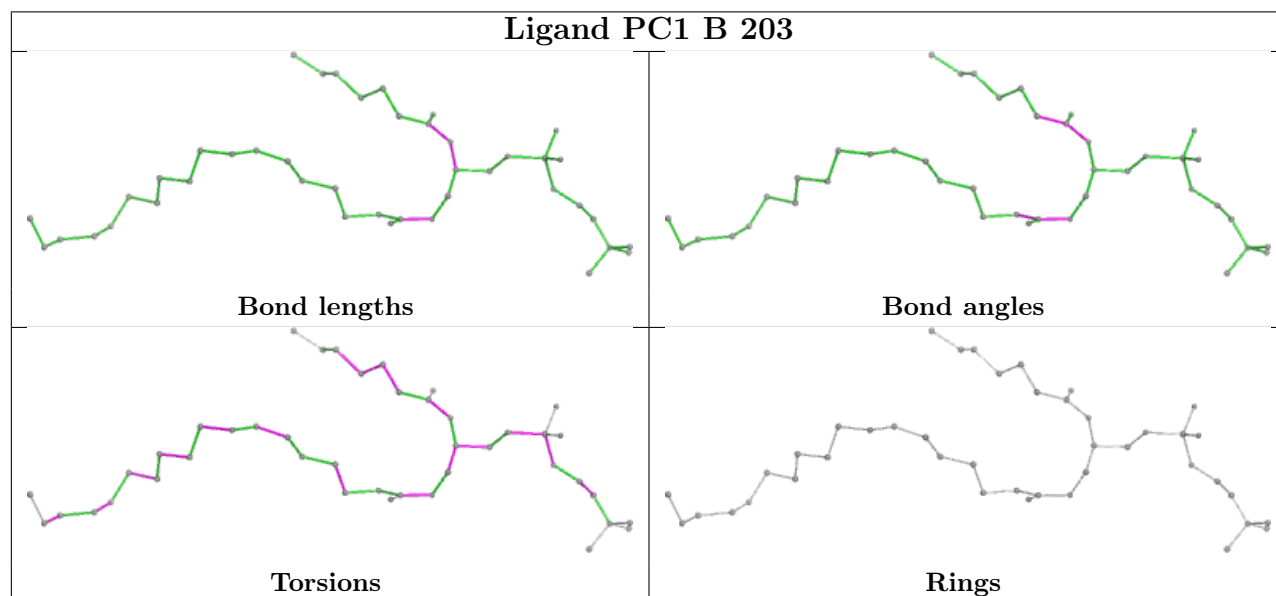
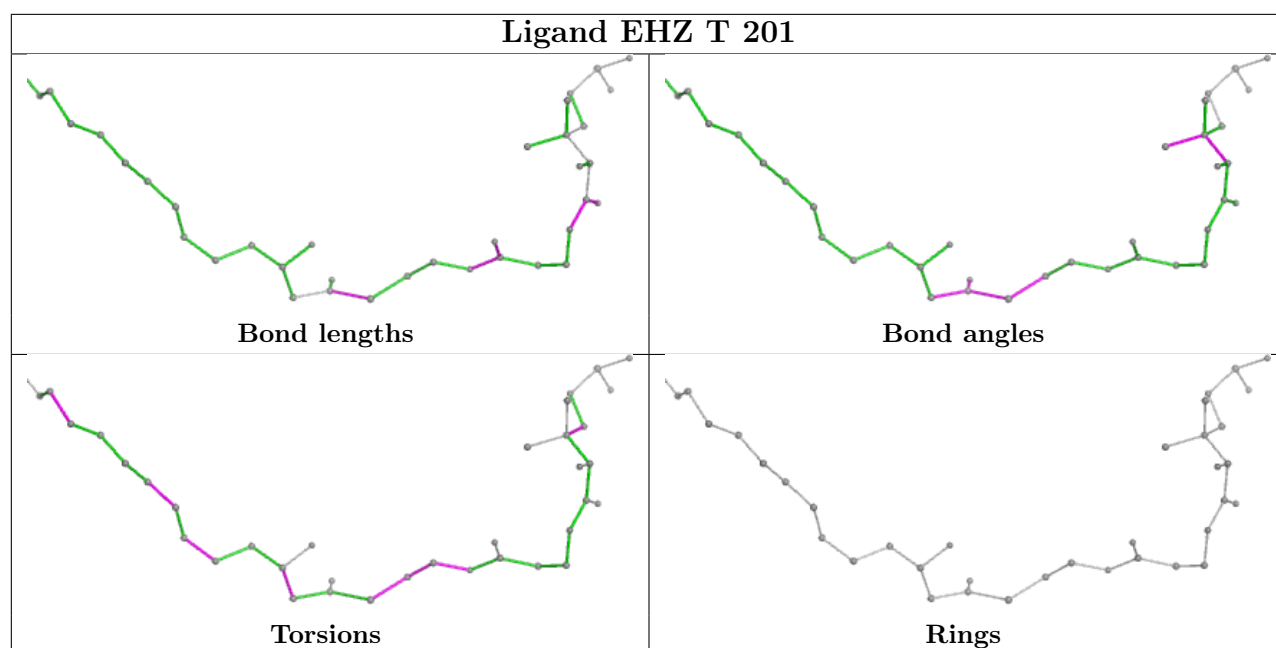


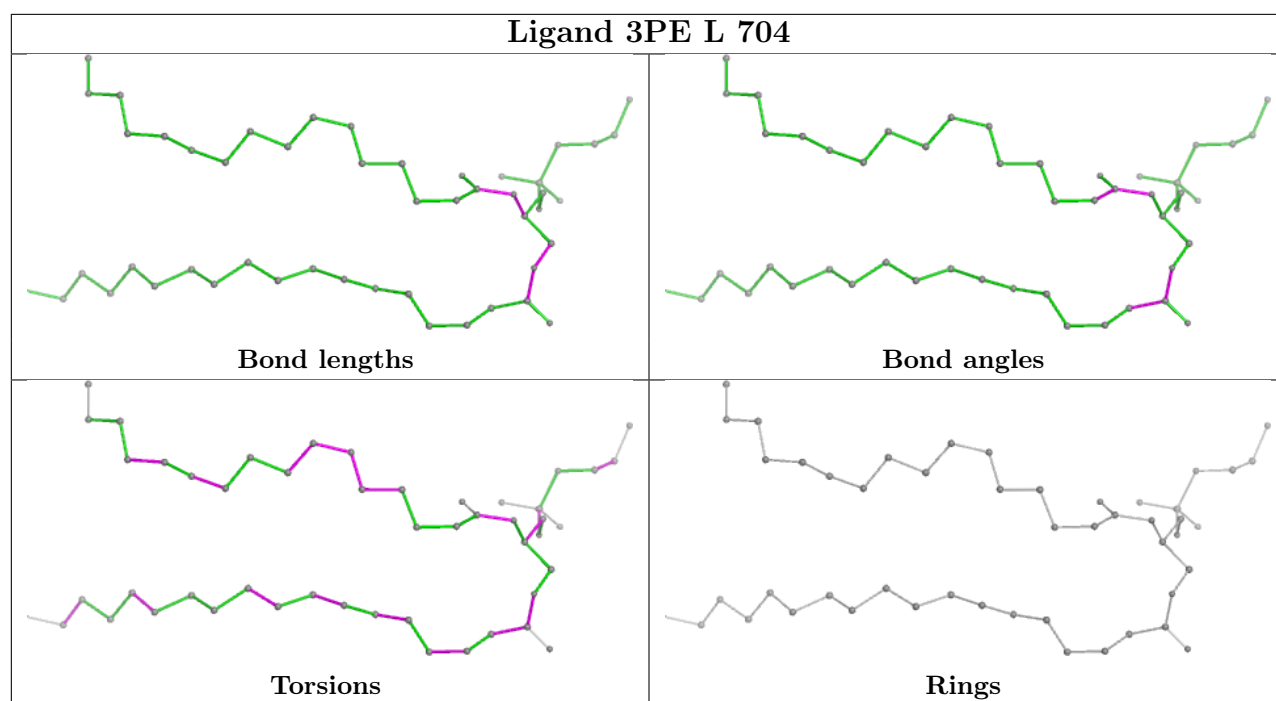












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

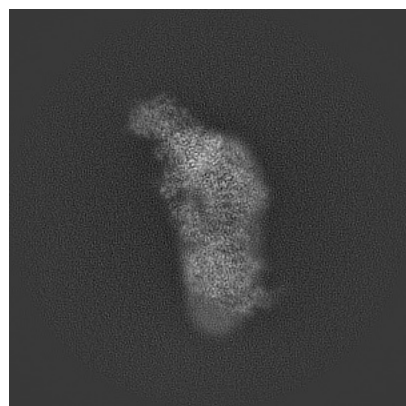
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11377. These allow visual inspection of the internal detail of the map and identification of artifacts.

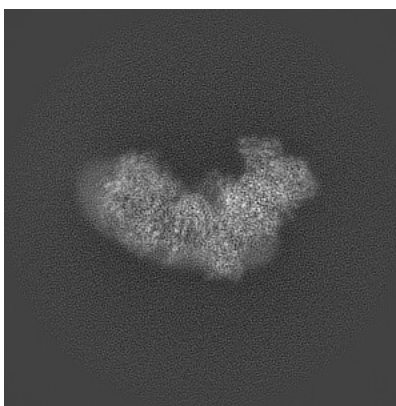
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

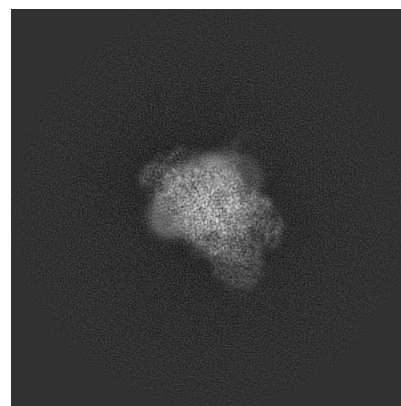
#### 6.1.1 Primary map



X

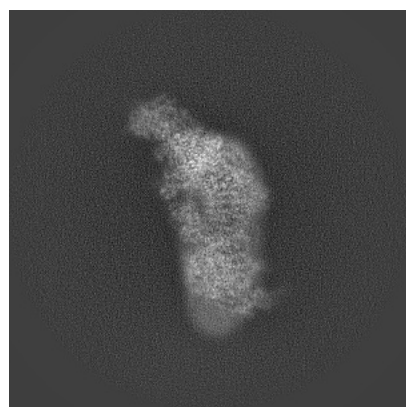


Y

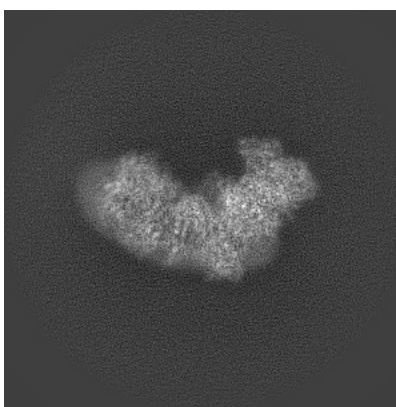


Z

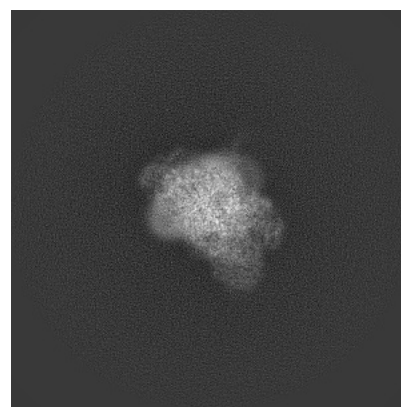
#### 6.1.2 Raw map



X



Y

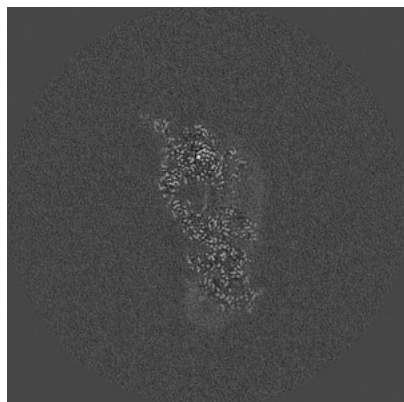


Z

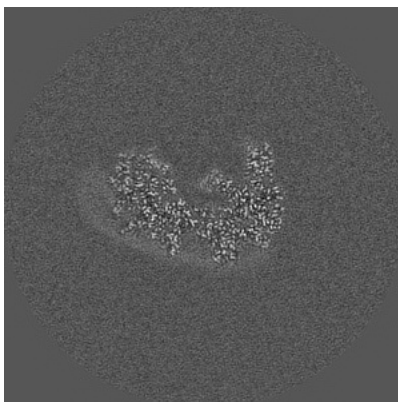
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

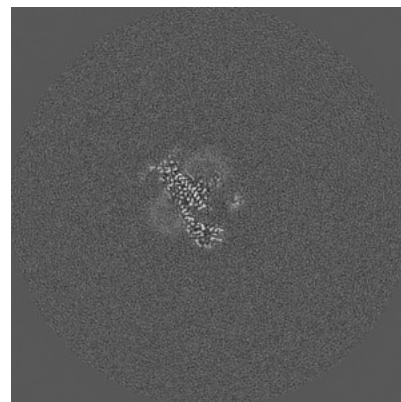
### 6.2.1 Primary map



X Index: 225

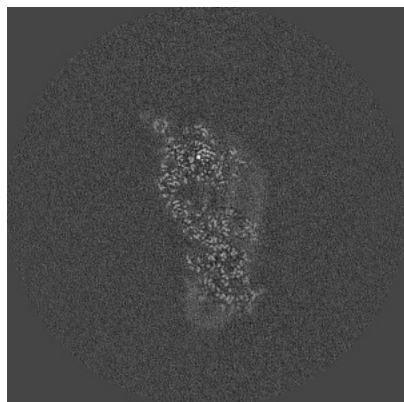


Y Index: 225

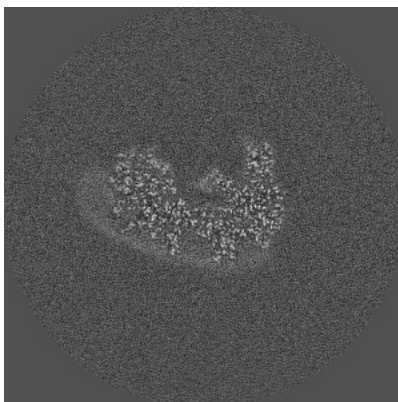


Z Index: 225

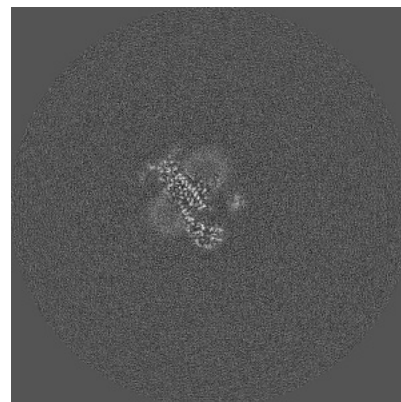
### 6.2.2 Raw map



X Index: 225



Y Index: 225

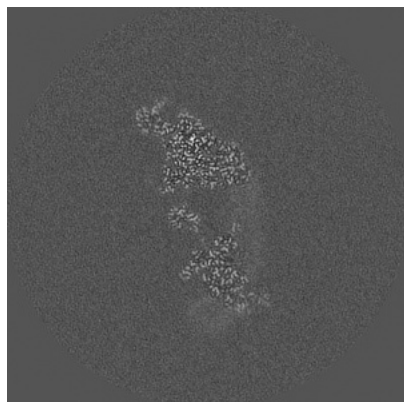


Z Index: 225

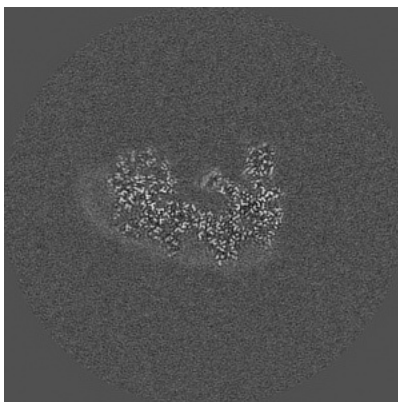
The images above show central slices of the map in three orthogonal directions.

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

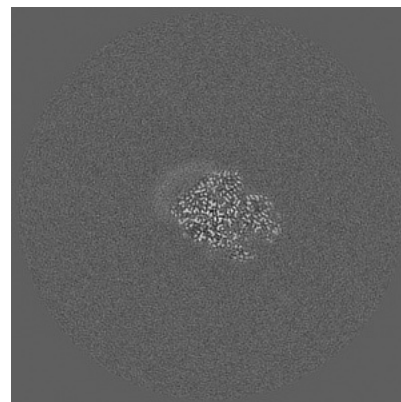
### 6.3.1 Primary map



X Index: 237

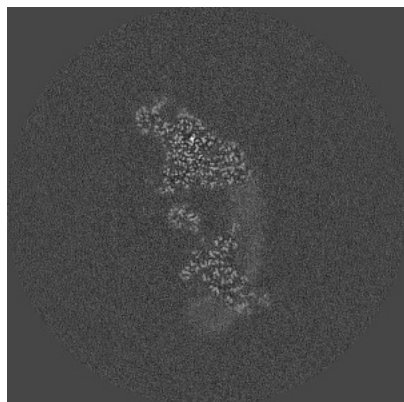


Y Index: 227

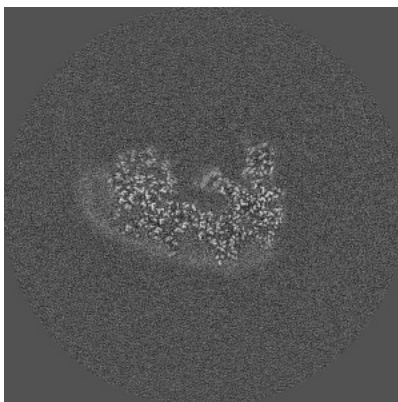


Z Index: 286

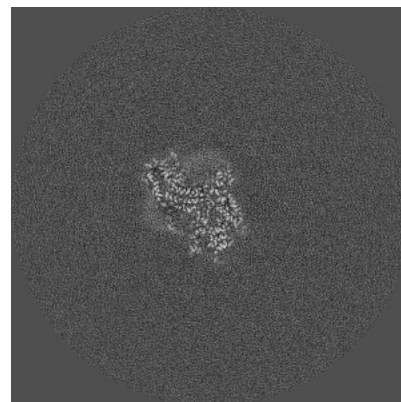
### 6.3.2 Raw map



X Index: 237



Y Index: 227



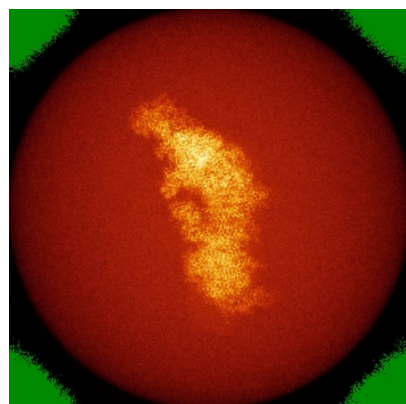
Z Index: 252

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

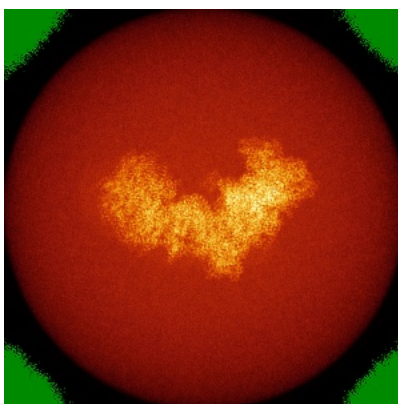


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

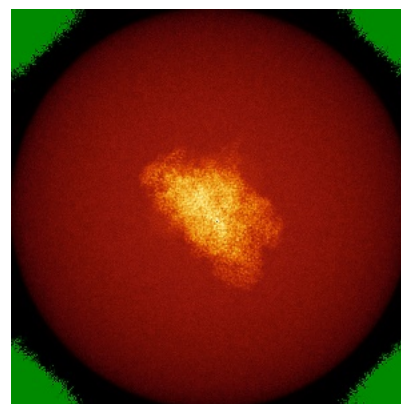
### 6.4.1 Primary map



X

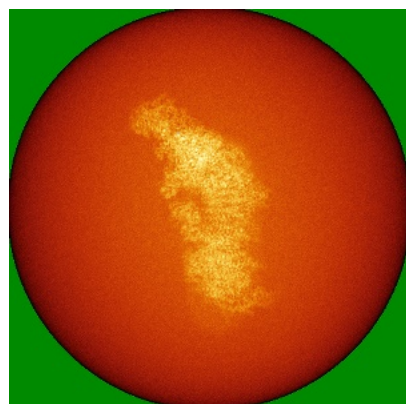


Y

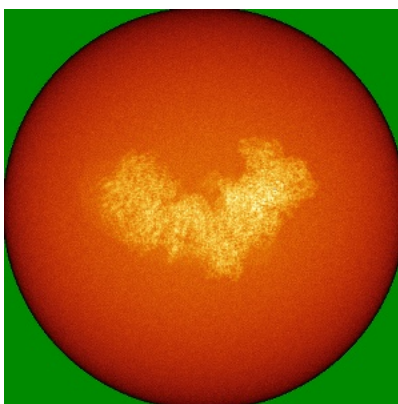


Z

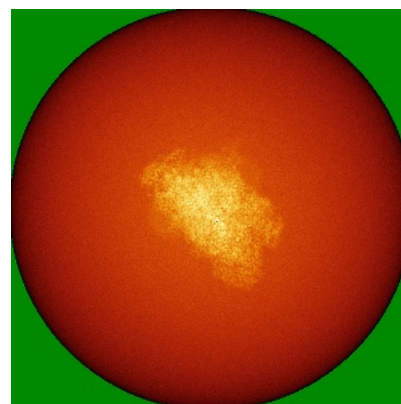
### 6.4.2 Raw map



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 0.0241. 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.

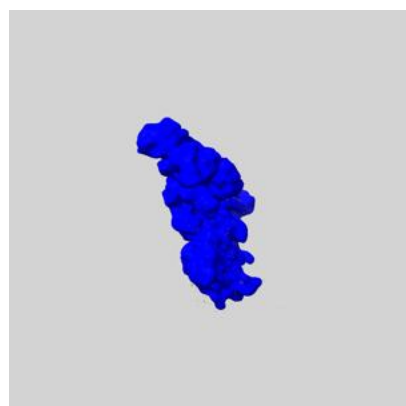
## 6.6 Mask visualisation [i](#)

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

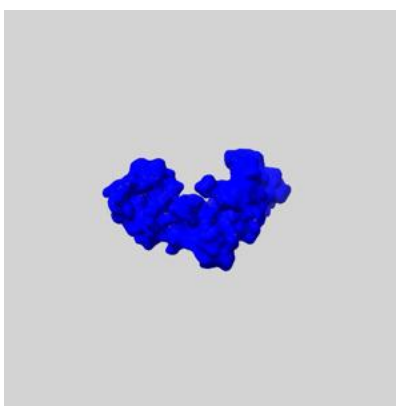
A mask typically either:

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

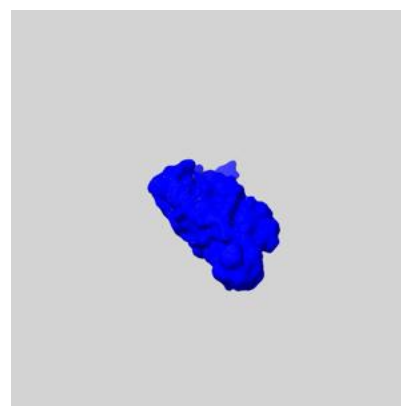
### 6.6.1 emd\_11424\_msk\_1.map [i](#)



X



Y



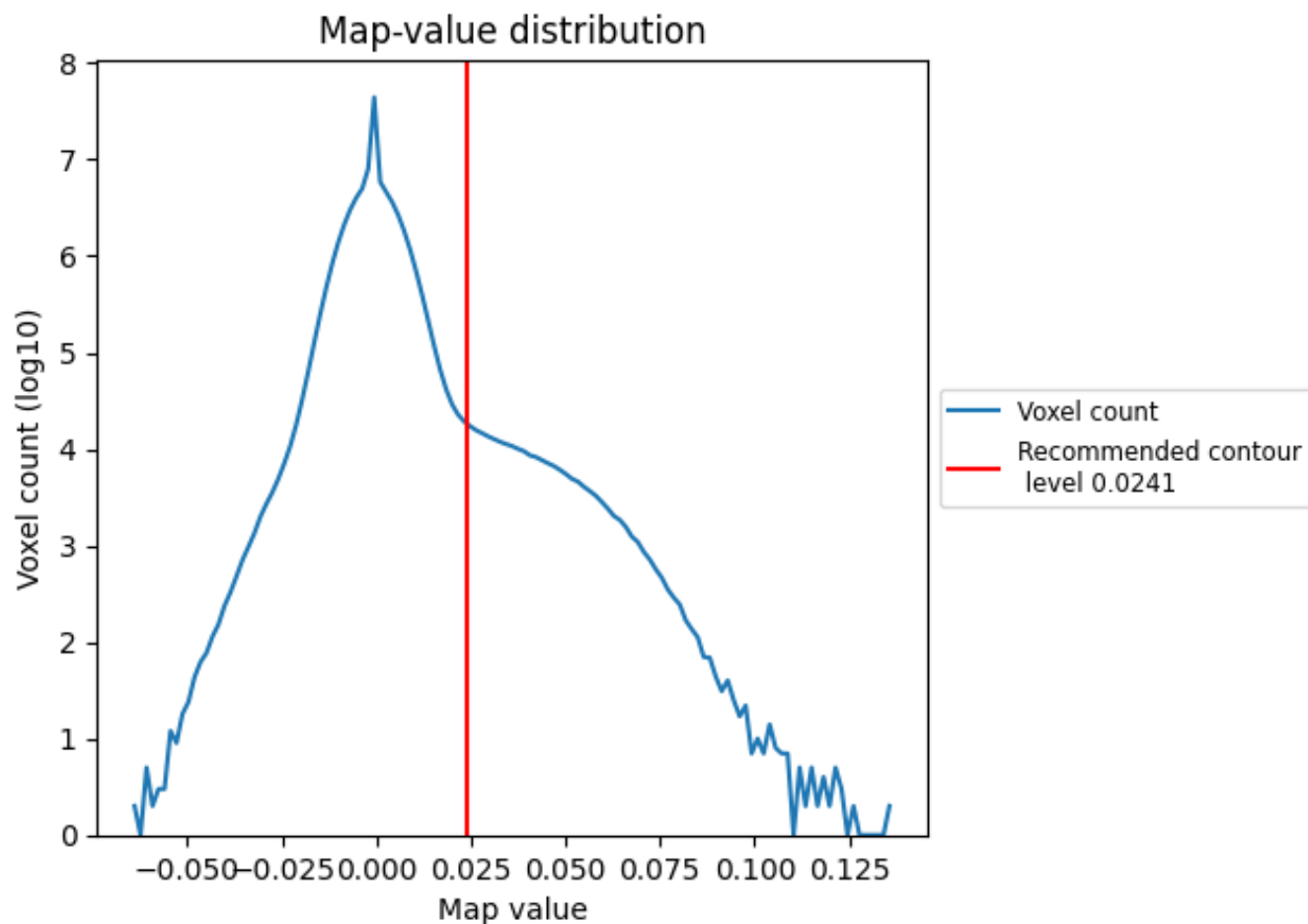
Z



## 7 Map analysis [i](#)

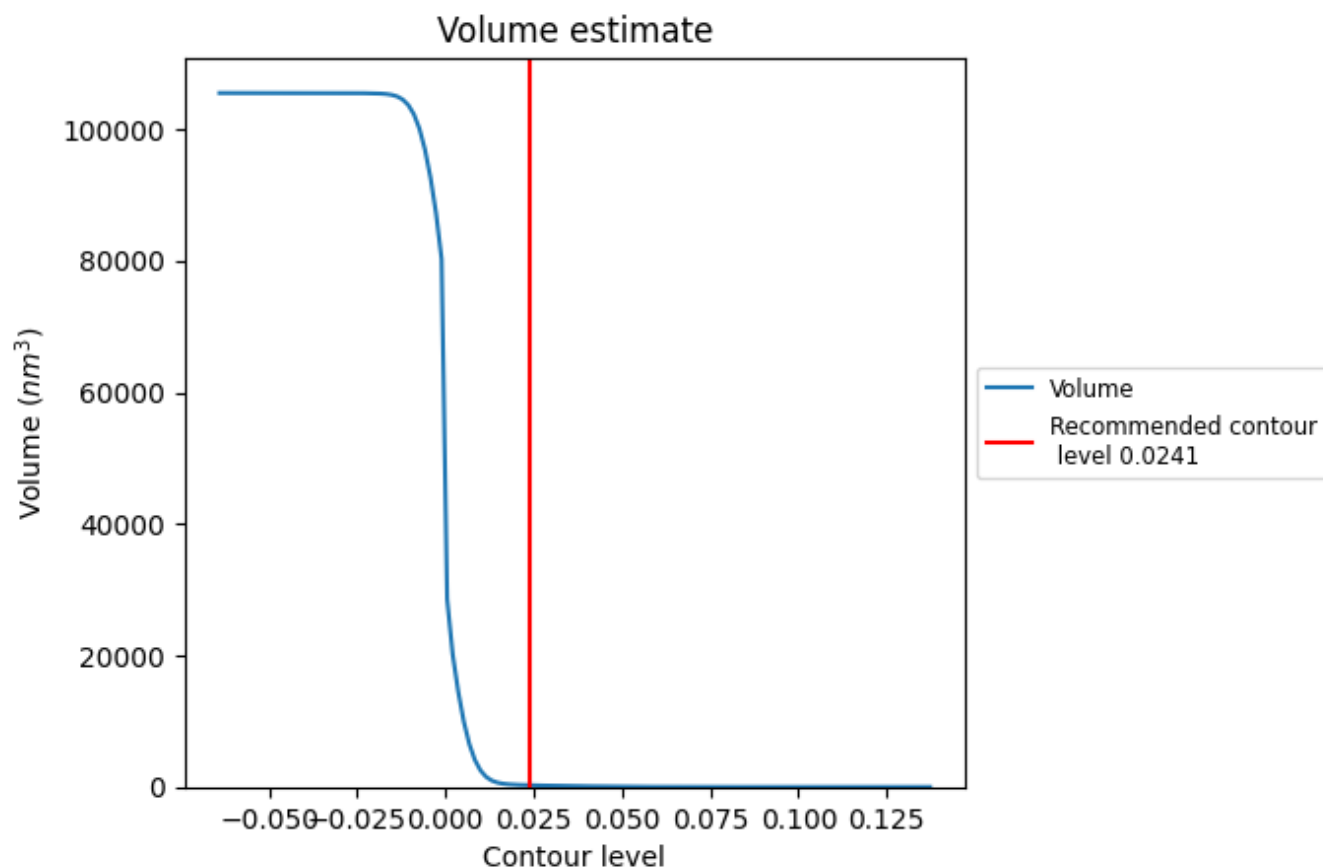
This section contains the results of statistical analysis of the map.

### 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.

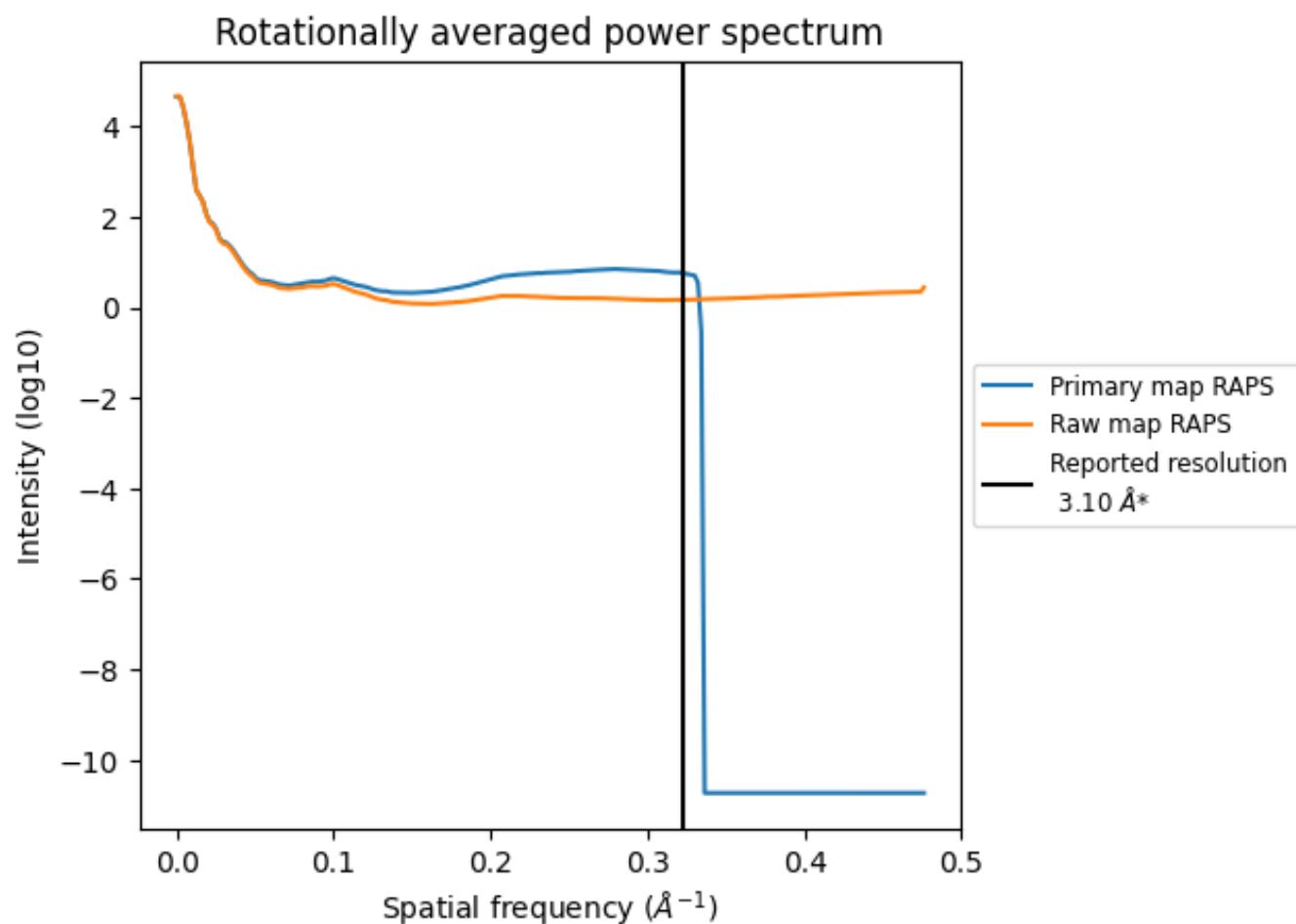
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 258  $\text{nm}^3$ ; 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 ⓘ

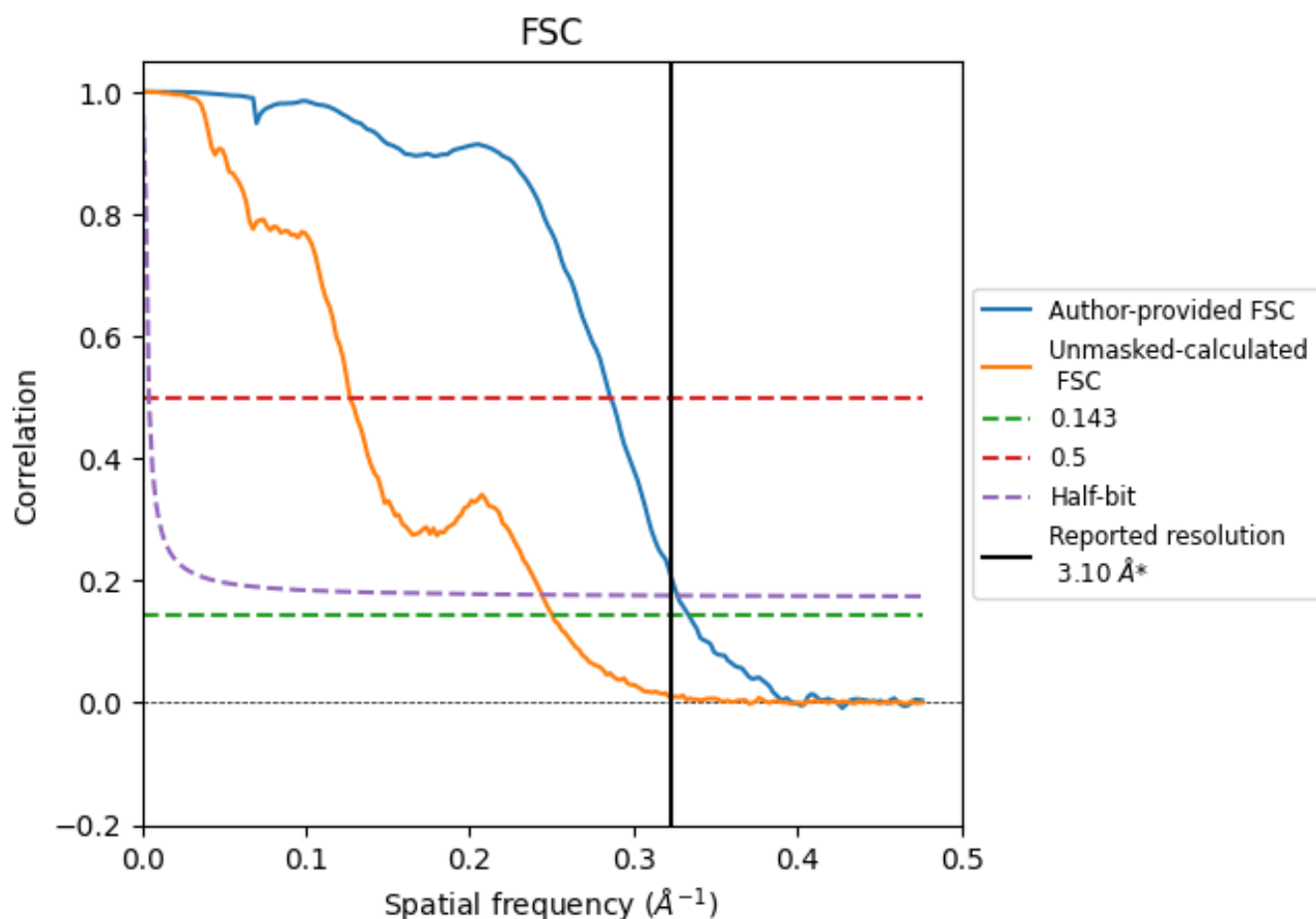


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

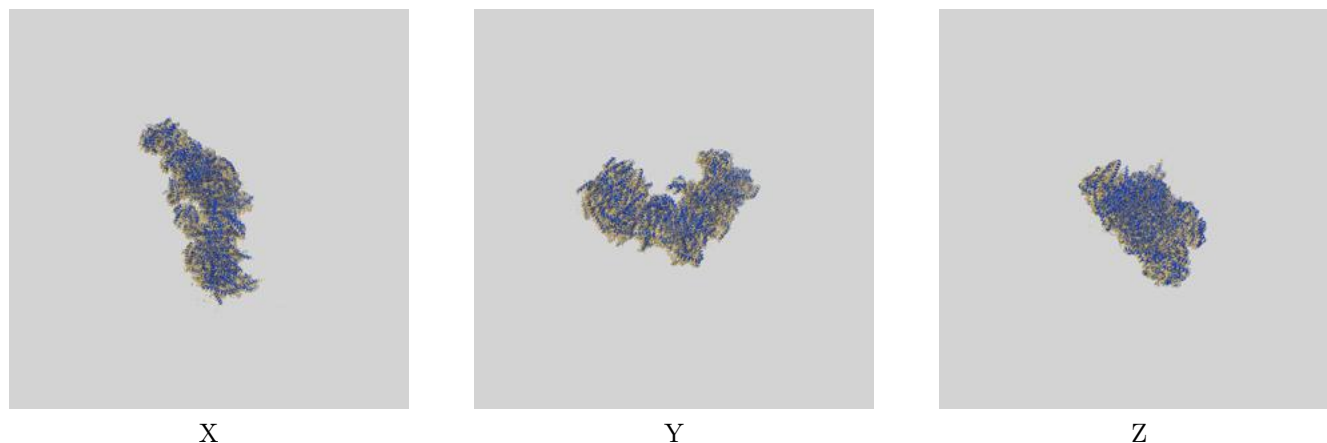
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.00	3.50	3.06
Unmasked-calculated*	3.99	7.89	4.10

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.1 by more than 10 %

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

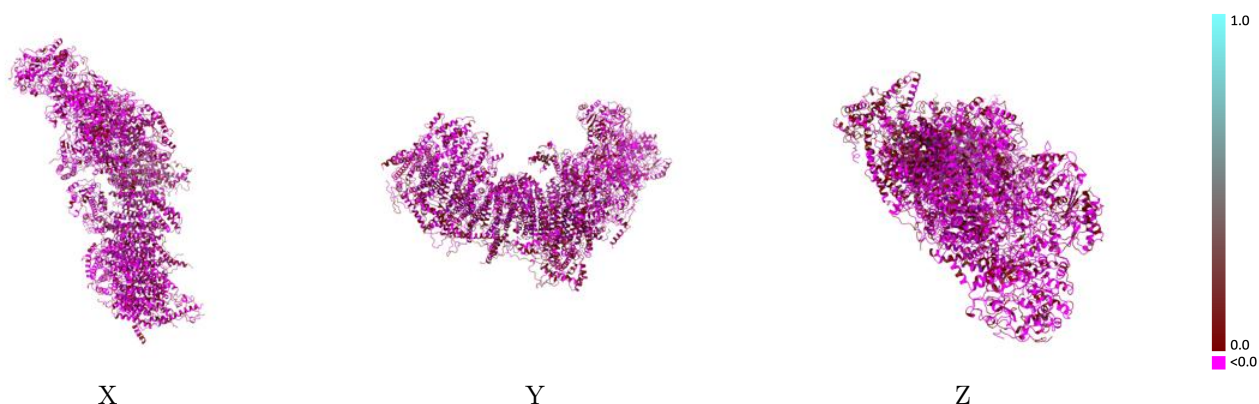
This section contains information regarding the fit between EMDB map EMD-11377 and PDB model 6ZR2. Per-residue inclusion information can be found in section [3](#) on page [19](#).

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



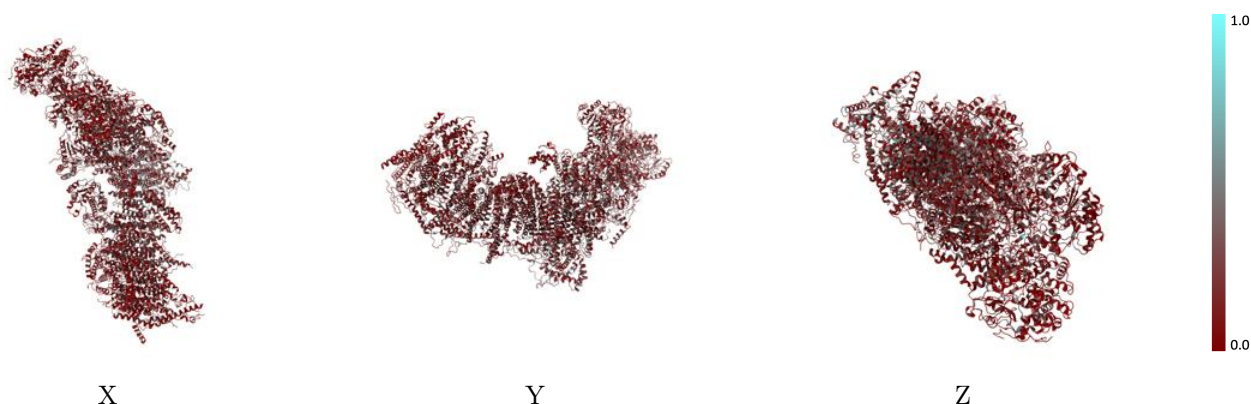
The images above show the 3D surface view of the map at the recommended contour level 0.0241 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



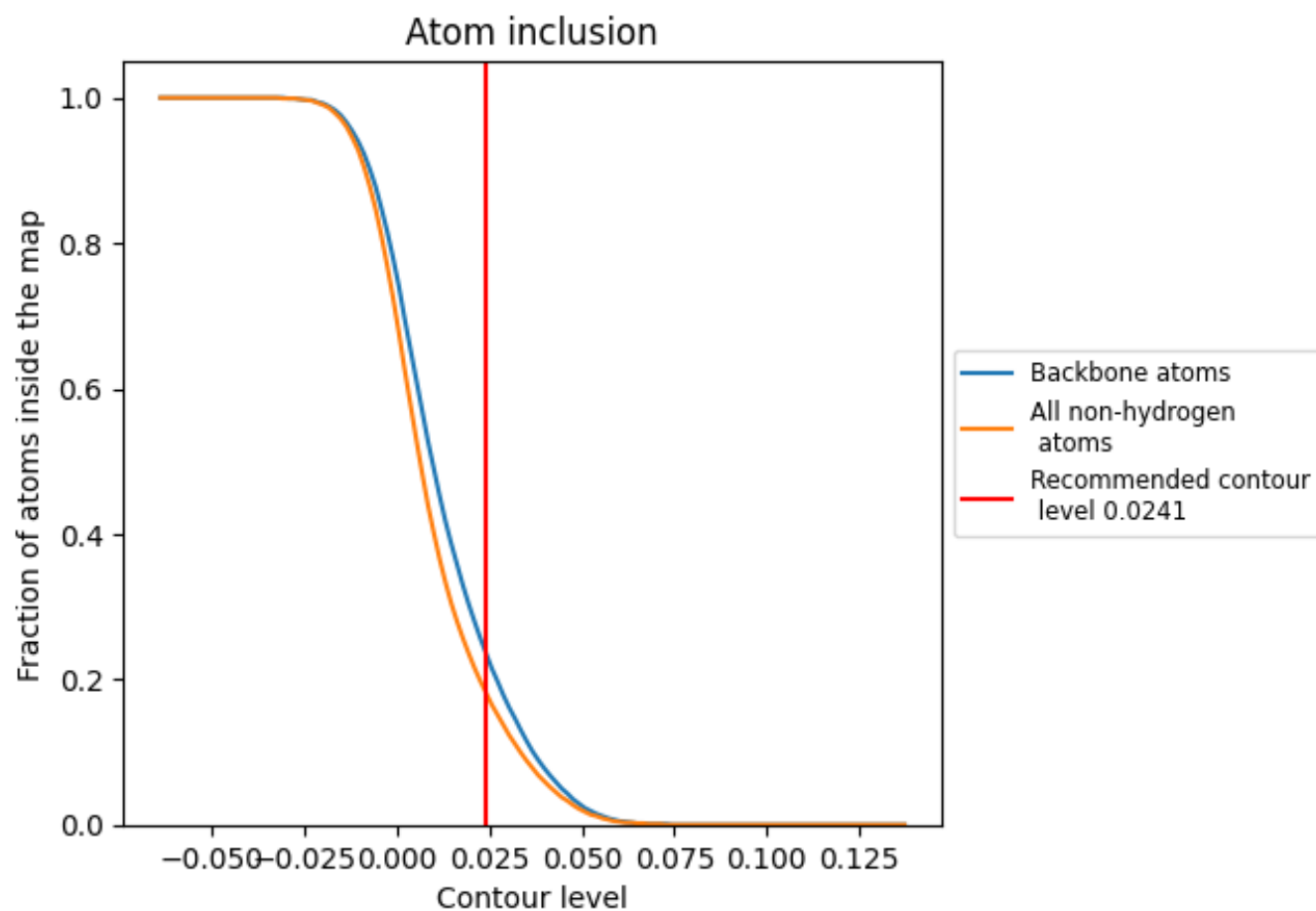
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0241).

## 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 (0.0241) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1810	 -0.0390
A	 0.2170	 -0.0230
B	 0.1930	 -0.0530
C	 0.1670	 -0.1110
D	 0.2080	 -0.0570
E	 0.1400	 -0.0220
F	 0.1380	 -0.0870
G	 0.1660	 -0.0590
H	 0.2290	 -0.0110
I	 0.1990	 -0.0750
J	 0.2090	 0.0100
K	 0.2290	 -0.0110
L	 0.1670	 -0.0580
M	 0.2000	 -0.0540
N	 0.2130	 -0.0310
O	 0.1730	 -0.0650
P	 0.2010	 -0.0230
Q	 0.1250	 -0.1150
R	 0.1890	 -0.0290
S	 0.1190	 -0.0080
T	 0.1030	 0.0470
U	 0.1290	 -0.0600
V	 0.1620	 -0.0770
W	 0.1900	 -0.0260
X	 0.2710	 0.0960
Y	 0.1600	 -0.0390
Z	 0.2430	 0.0250
a	 0.2460	 0.0480
b	 0.2210	 0.0190
c	 0.1650	 0.0160
d	 0.1930	 0.0020
e	 0.2020	 0.0240
f	 0.1720	 -0.0150
g	 0.1890	 -0.0010
h	 0.1930	 -0.0440



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.1490	 -0.0430
j	 0.1360	 0.0100
k	 0.1200	 -0.0600
l	 0.1490	 -0.0520
m	 0.1560	 -0.0650
n	 0.1410	 -0.0590
o	 0.1210	 -0.0170
p	 0.1940	 -0.0070
q	 0.1880	 -0.0330
r	 0.1830	 -0.0320
s	 0.0870	 -0.0710