Full wwPDB EM Validation Report

Apr 2, 2025 – 01:49 am BST

PDB ID	:	6G2J / pdb_00006g2j
EMDB ID	:	EMD-4345
Title	:	Mouse mitochondrial complex I in the active state
Authors	:	Agip, A.N.A.; Blaza, J.N.; Bridges, H.R.; Viscomi, C.; Rawson, S.; Muench, S.P.; Hirst, J.
Deposited on	:	2018-03-23
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

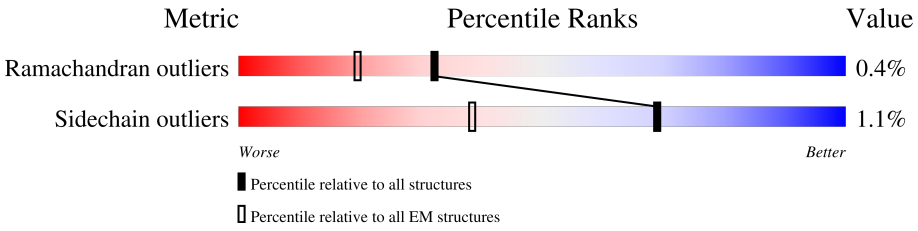
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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)
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 >=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 <=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	17% 97%
2	B	224	7% 67% 31%
3	C	263	13% 75% 22%
4	D	463	11% 91% 7%
5	E	248	37% 84% 15%
6	F	428	33% 99%
7	G	727	24% 93% 5%
8	H	318	11% 98%
9	I	212	8% 83% 16%

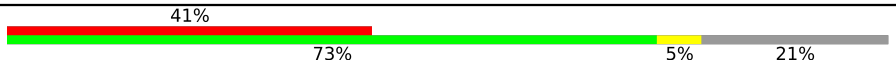
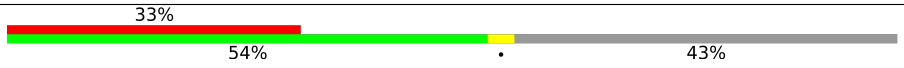
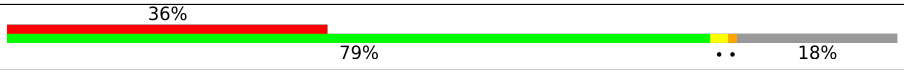
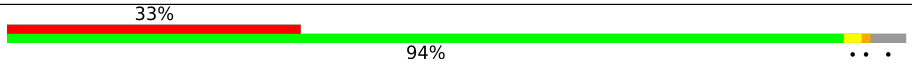
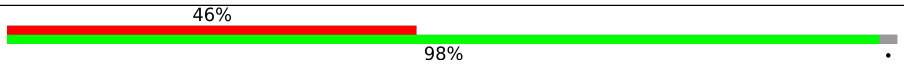
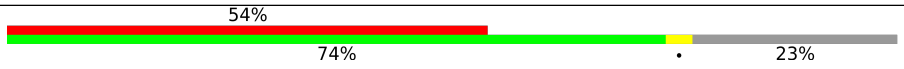
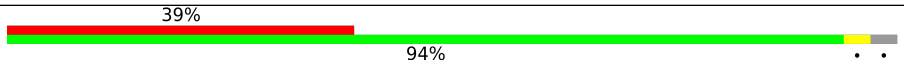
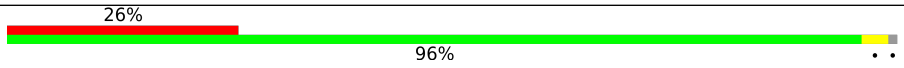
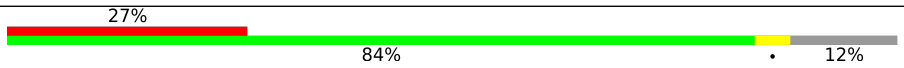
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	172	30% 98%
11	K	98	11% 98%
12	L	607	26% 98%
13	M	459	11% 98%
14	N	345	9% 97%
15	O	355	26% 88% 10%
16	P	377	26% 88% 9%
17	Q	175	20% 69% 29%
18	R	116	16% 81% 18%
19	S	99	44% 83% 16%
20	T	156	43% 48% 52%
20	U	156	33% 56% 44%
21	V	116	29% 94%
22	W	131	32% 85% 13%
23	X	172	28% 97%
24	Y	143	40% 96%
25	Z	144	29% 92%
26	a	67	19% 93% 7%
27	b	84	39% 94% 5%
28	c	76	37% 59% 38%
29	d	120	33% 98%
30	e	106	25% 95%
31	f	57	42% 84% 11%
32	g	151	26% 64% 33%
33	h	189	22% 72% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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 66810 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
			Total	C	N	O	S		
1	A	115	933	633	133	160	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	793	222	212	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1712	1105	294	310	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3452	2207	593	628	24	0	0

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

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

- 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
			3301	2080	590	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
			1408	885	243	268	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	95	Total	C	N	O	S	0	0
			748	464	138	143	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	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	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	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	119	Total	C	N	O	S	0	0
			985	645	167	164	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			870	550	161	151	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			433	278	78	75	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	137	Total	C	N	O	S	0	0
			1154	758	192	201	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	101	Total	C	N	O	S	0	0
			820	534	141	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	60	Total	C	N	O	S	0	0
			525	345	88	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	72	Total	C	N	O	S	0	0
			582	384	100	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	152	Total	C	N	O	S	0	0
			1274	821	213	229	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	124	Total	C	N	O	0	0
			1035	667	186	182		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	176	Total	C	N	O	S	0	0
			1527	976	274	266	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	105	Total	C	N	O	S	0	0
			898	565	167	158	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1438	903	258	269	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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	1	AME	MET	conflict	UNP Q7TMF3

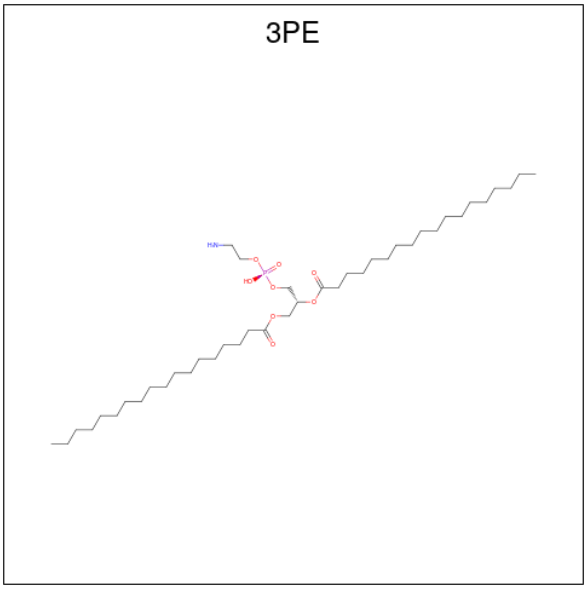
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	99	Total	C	N	O	S	0	0
			796	504	148	141	3		

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

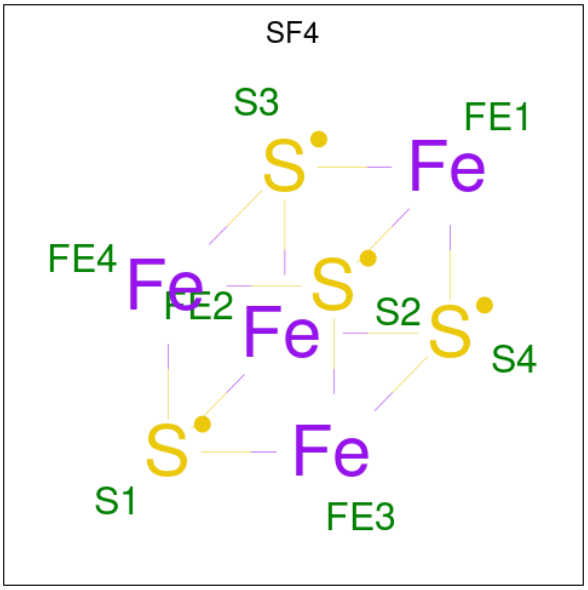
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	40	Total	C	N	O	0	0
			336	211	60	65		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



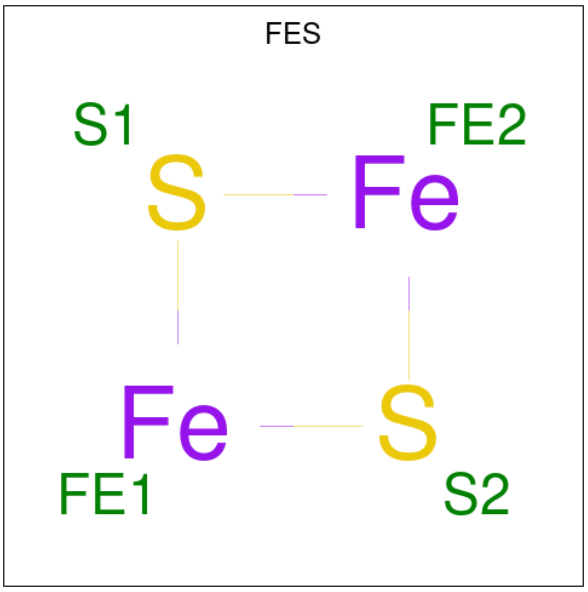
Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total C N O P 41 31 1 8 1	0
45	H	1	Total C N O P 51 41 1 8 1	0
45	H	1	Total C N O P 51 41 1 8 1	0
45	L	1	Total C N O P 51 41 1 8 1	0
45	L	1	Total C N O P 42 32 1 8 1	0
45	M	1	Total C N O P 51 41 1 8 1	0
45	M	1	Total C O P 42 33 8 1	0
45	M	1	Total C N O P 51 41 1 8 1	0
45	M	1	Total C N O P 51 41 1 8 1	0
45	M	1	Total C N O P 51 41 1 8 1	0
45	M	1	Total C N O P 31 21 1 8 1	0
45	N	1	Total C N O P 51 41 1 8 1	0

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



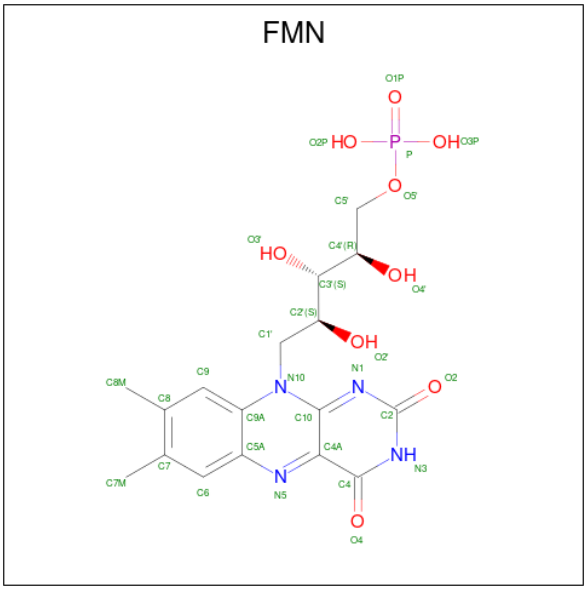
Mol	Chain	Residues	Atoms	AltConf
46	B	1	Total Fe S 8 4 4	0
46	F	1	Total Fe S 8 4 4	0
46	G	1	Total Fe S 8 4 4	0
46	G	1	Total Fe S 8 4 4	0
46	I	1	Total Fe S 8 4 4	0
46	I	1	Total Fe S 8 4 4	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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	

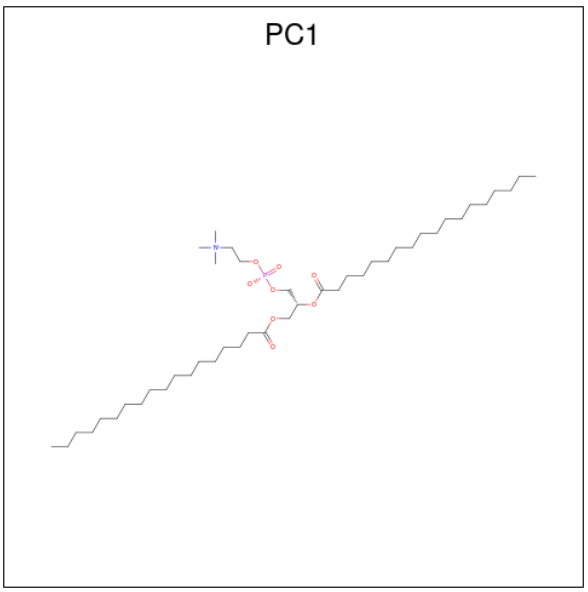
- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

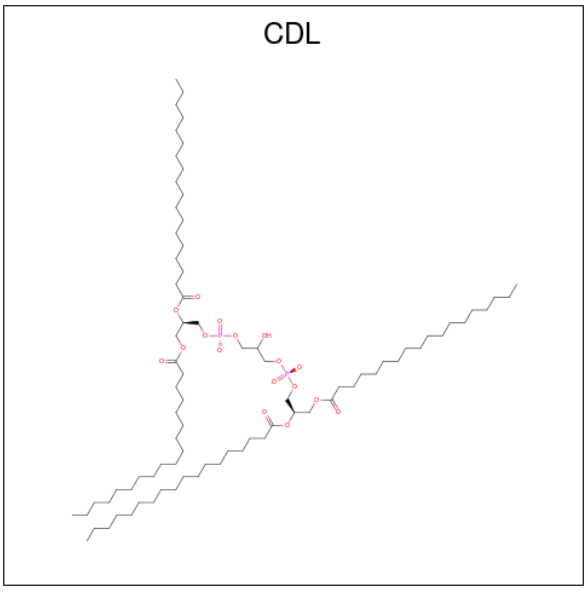
- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula: $C_{44}H_{88}NO_8P$).



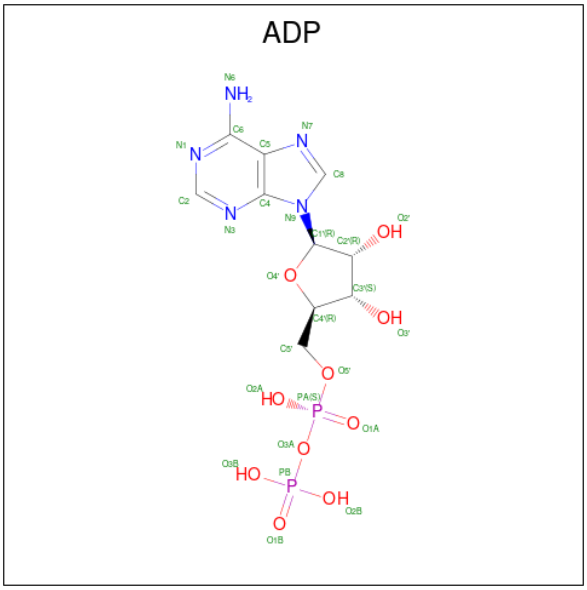
Mol	Chain	Residues	Atoms					AltConf
49	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
49	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
49	H	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	P	1	Total	C	N	O	P	0
			43	33	1	8	1	

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



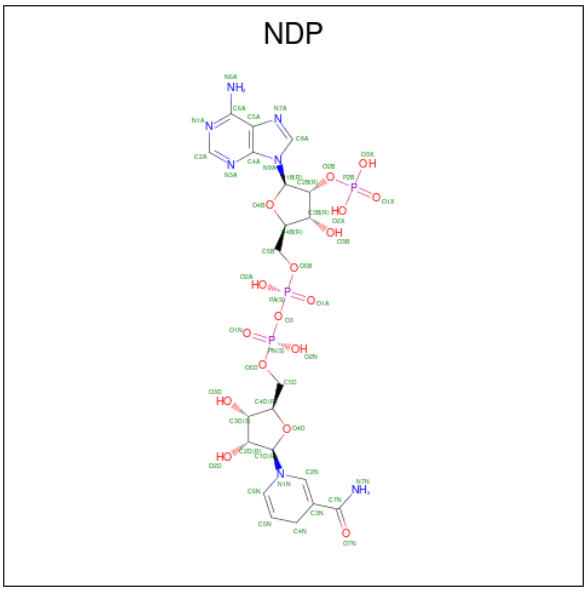
Mol	Chain	Residues	Atoms				AltConf
50	H	1	Total	C	O	P	0
			57	38	17	2	
50	L	1	Total	C	O	P	0
			78	59	17	2	
50	L	1	Total	C	O	P	0
			70	51	17	2	
50	M	1	Total	C	O	P	0
			67	48	17	2	

- Molecule 51 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
51	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

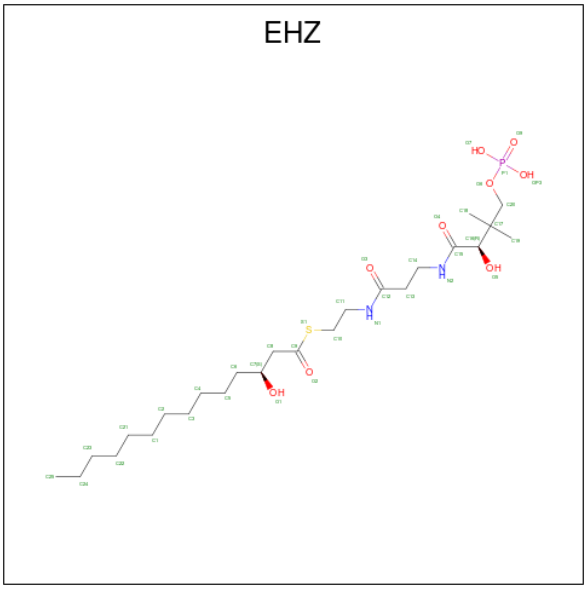


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- 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: $C_{25}H_{49}N_2O_9PS$).

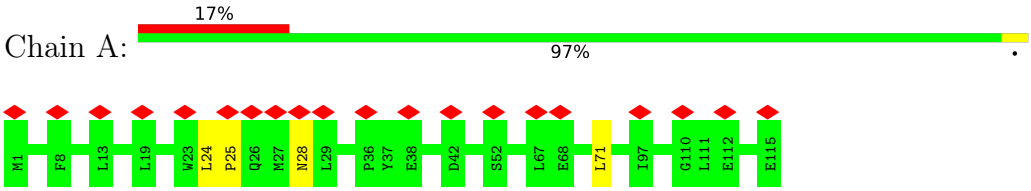


Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			34	22	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

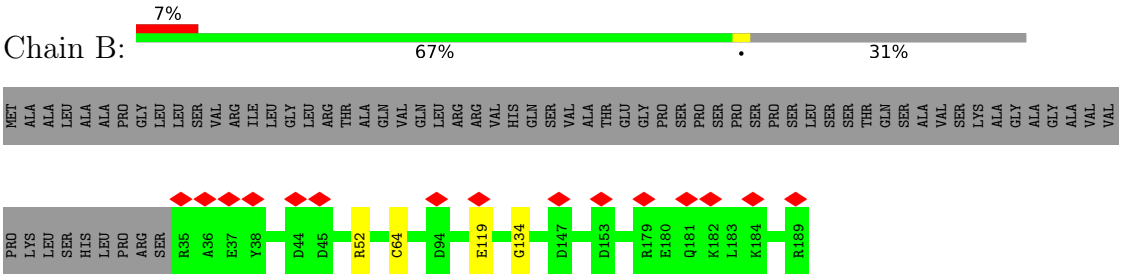
3 Residue-property plots (i)

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

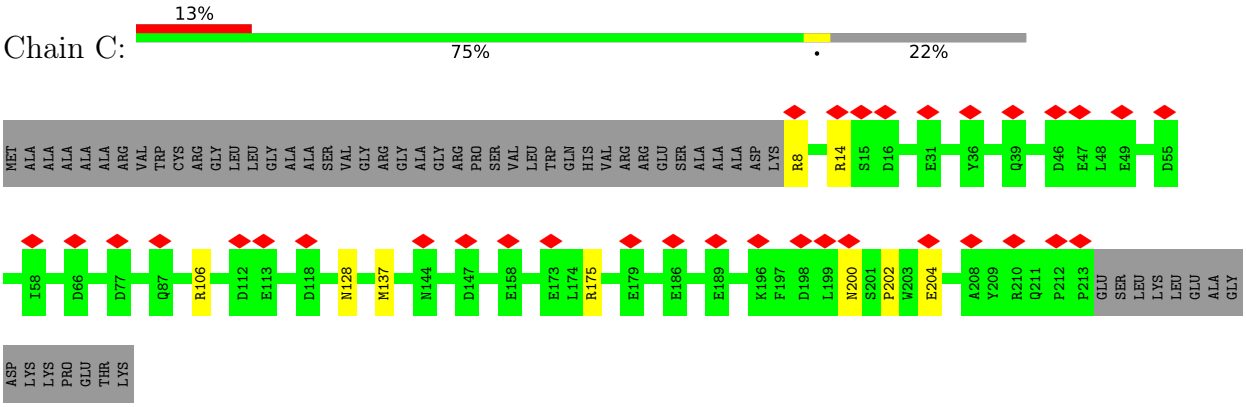
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



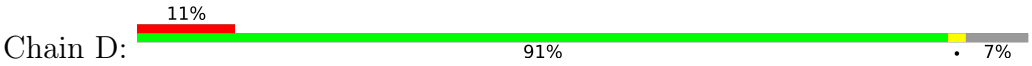
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

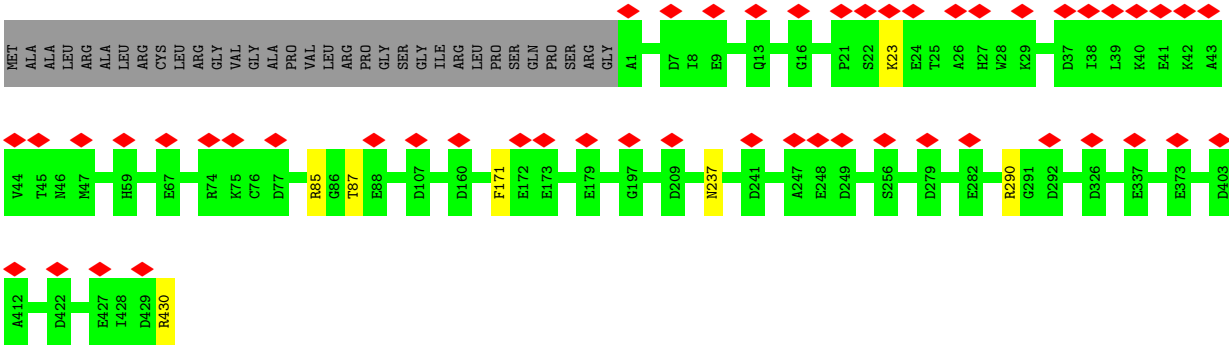


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

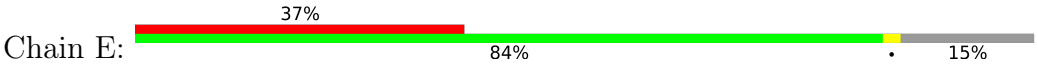


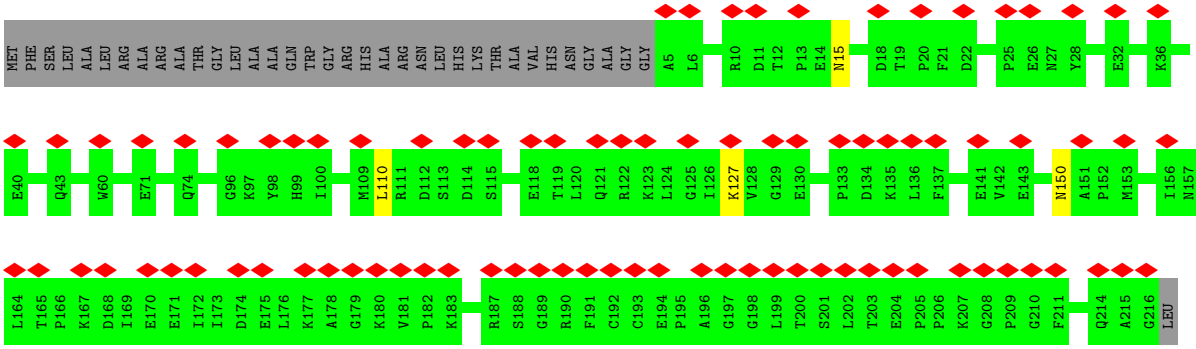
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



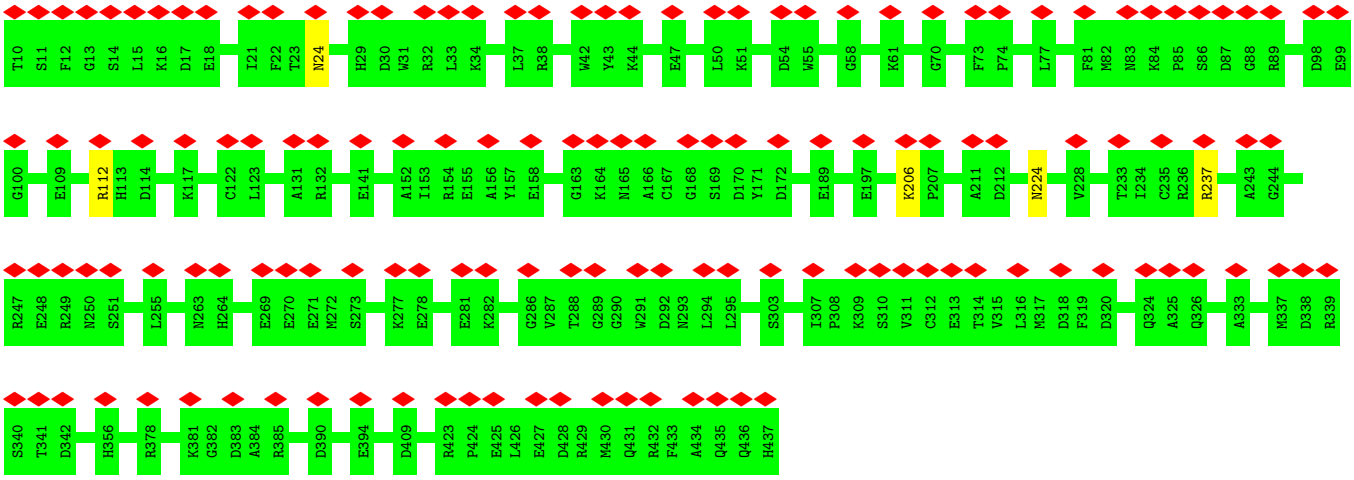


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

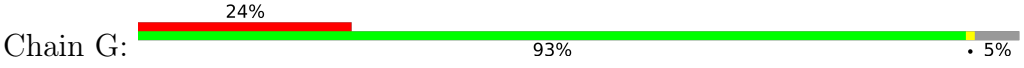


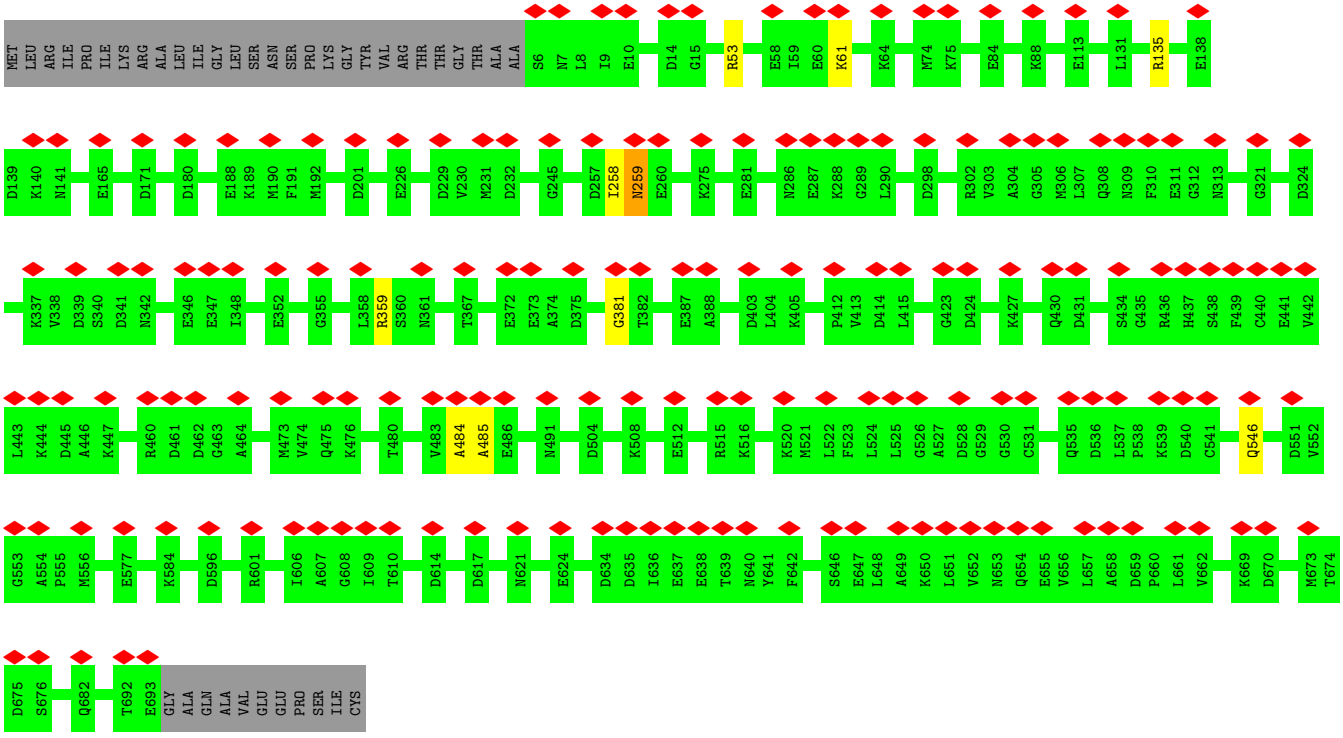


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

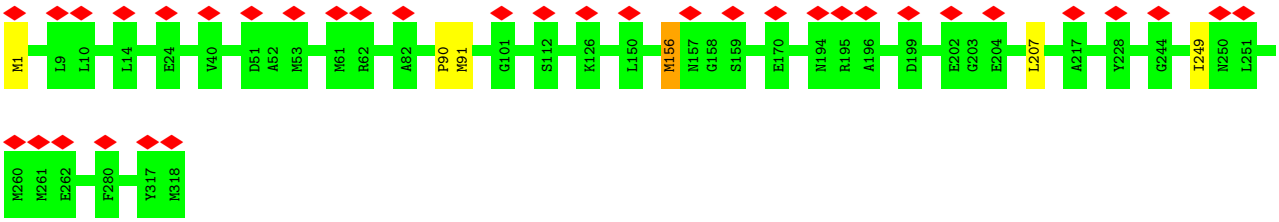


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

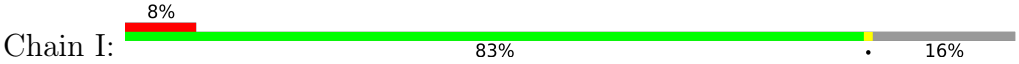


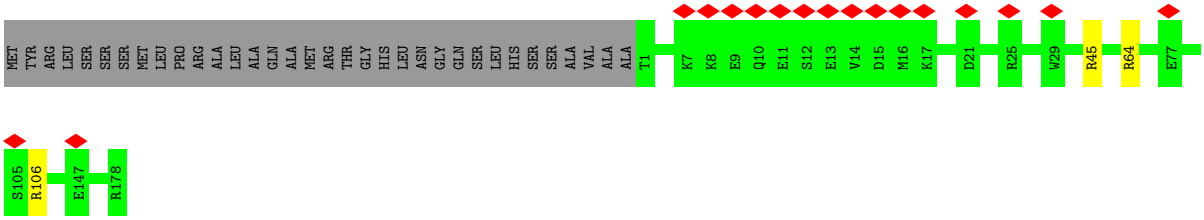


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

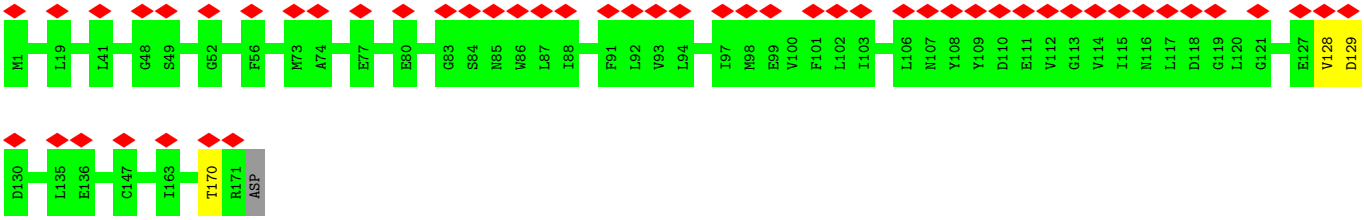


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

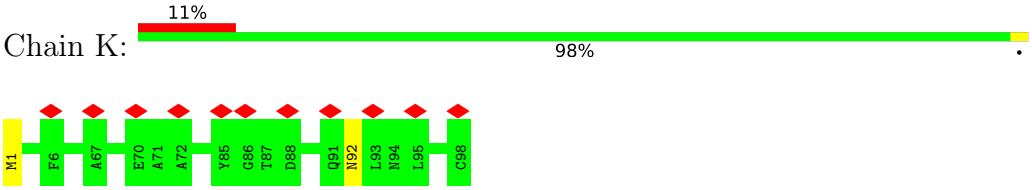




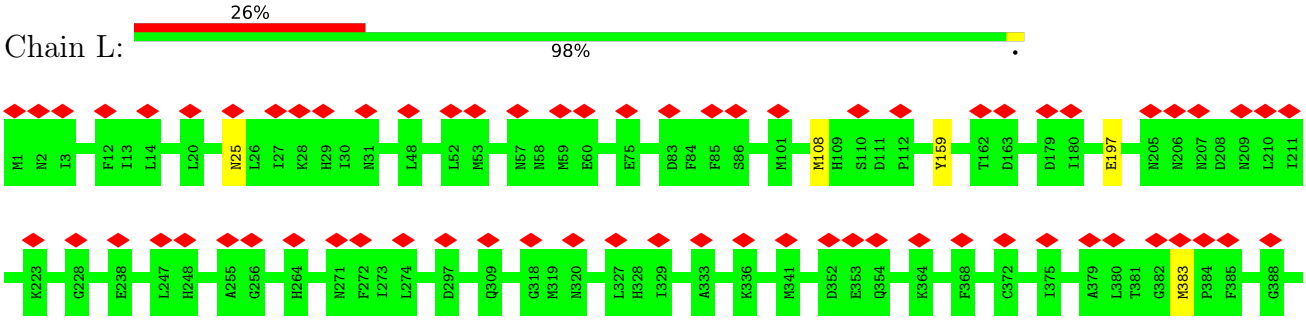
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



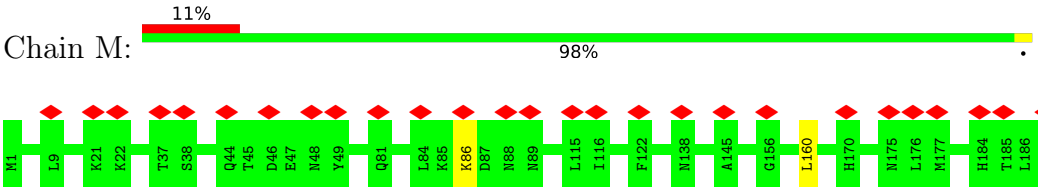
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

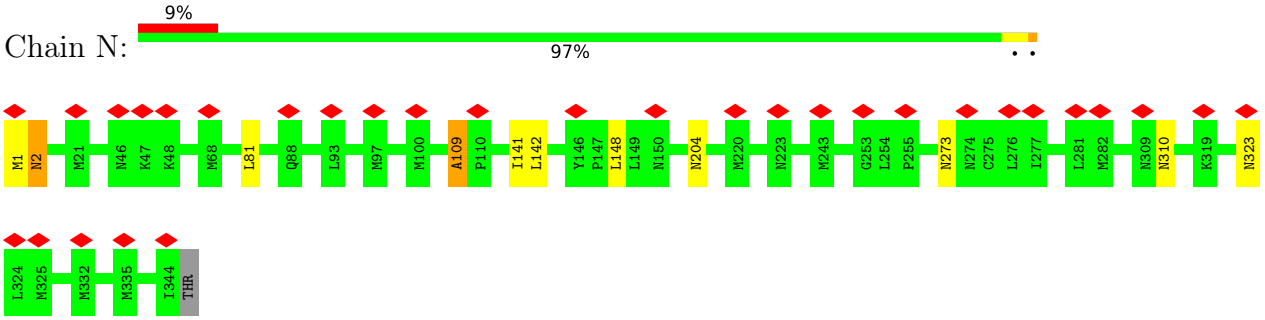


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



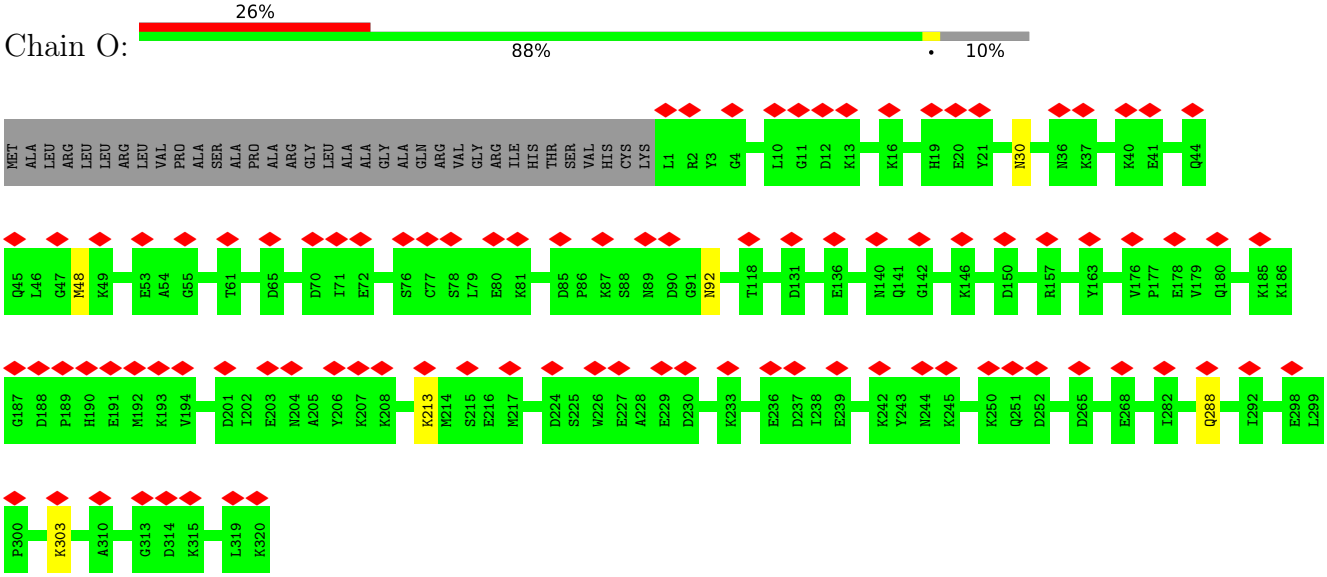
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



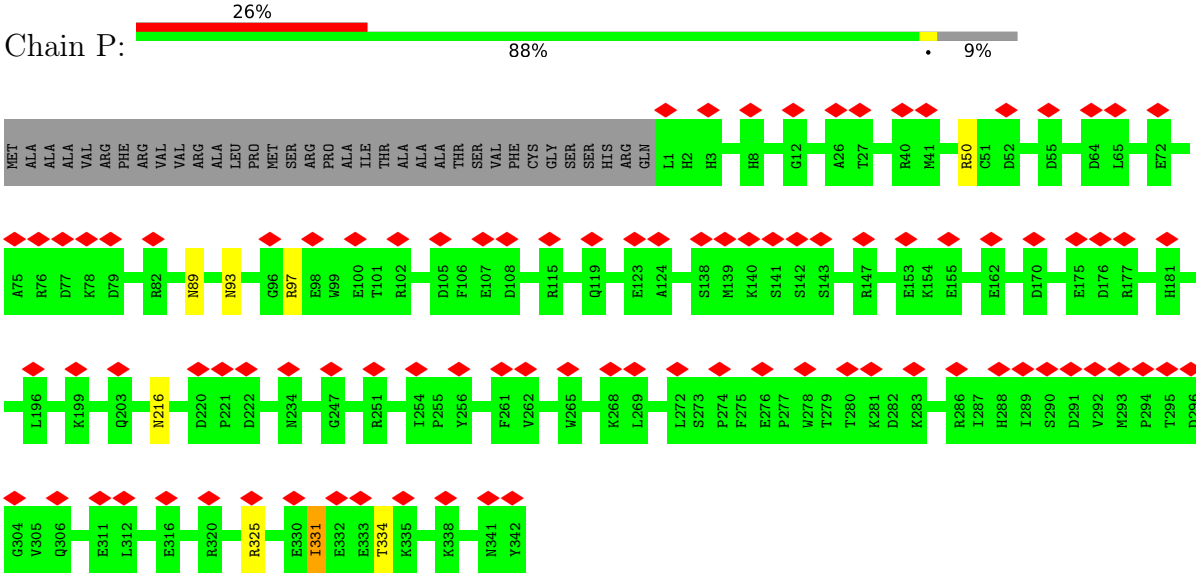
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



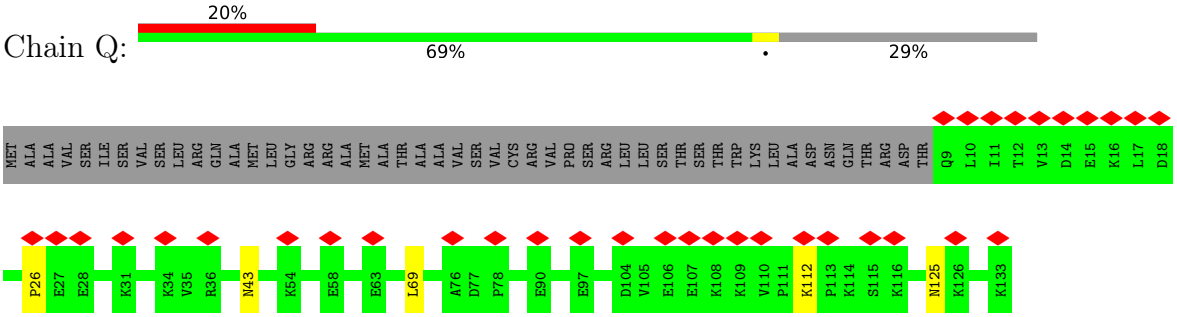
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



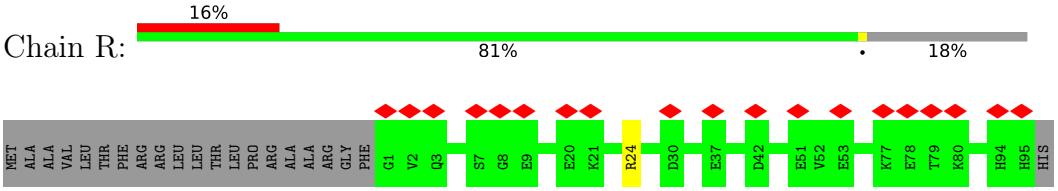
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



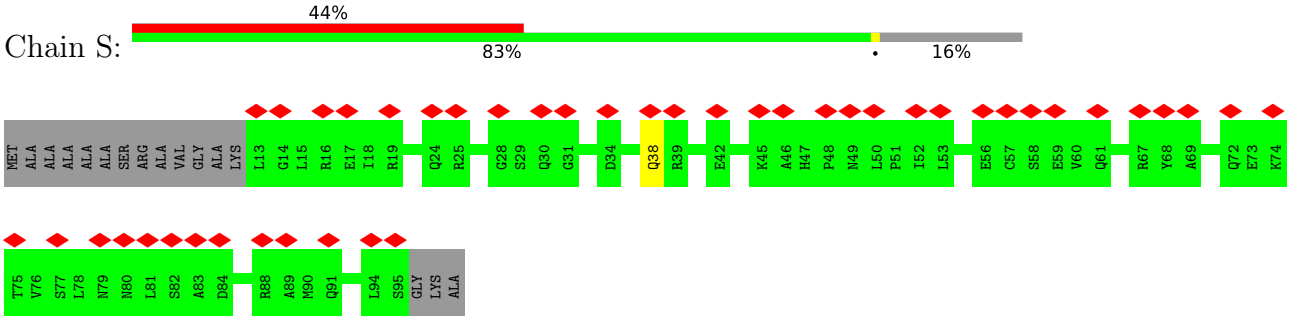
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



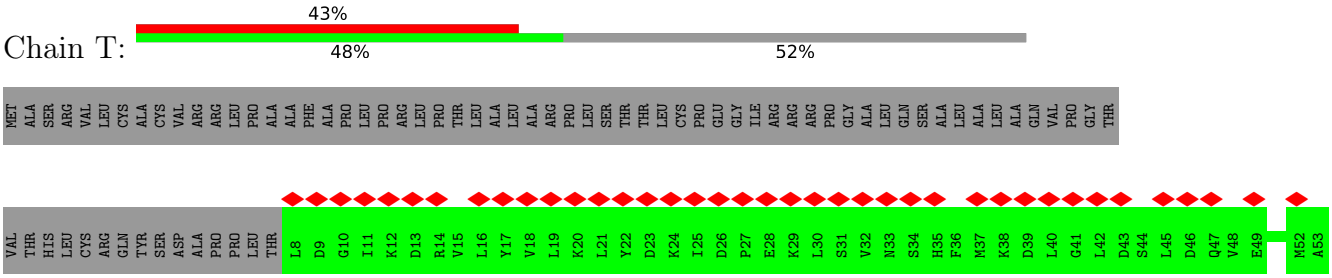
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



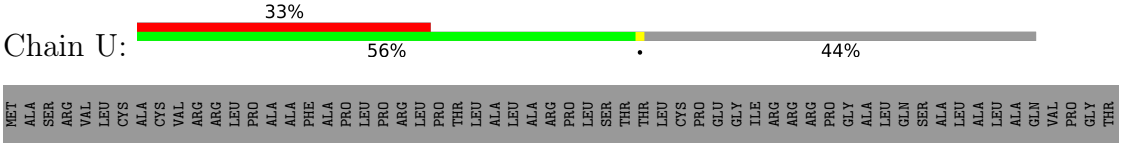
• Molecule 20: Acyl carrier protein, mitochondrial

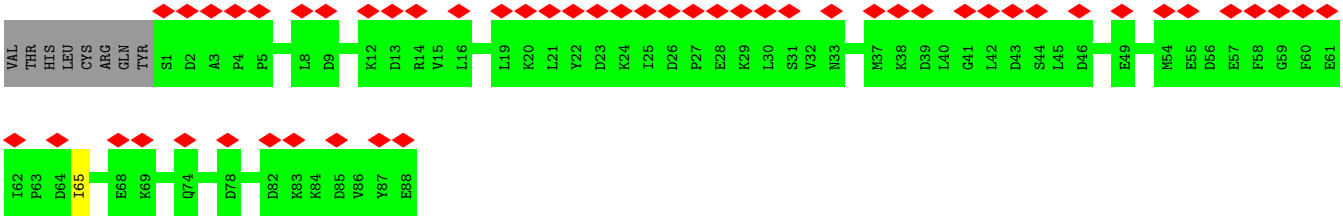
Chain T:



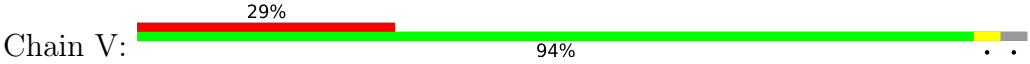
• Molecule 20: Acyl carrier protein, mitochondrial

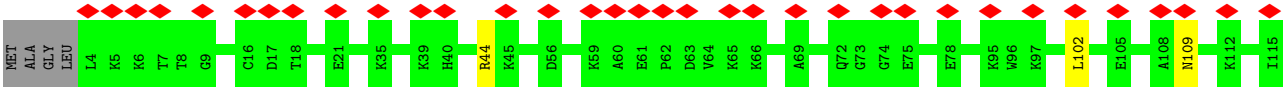
Chain U:



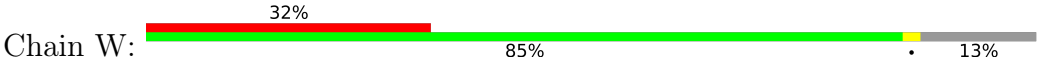


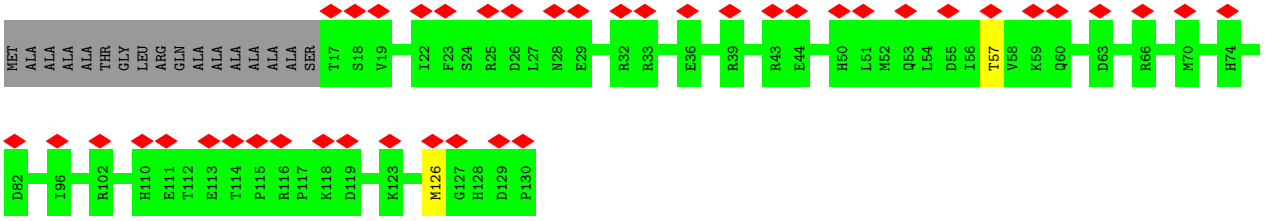
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



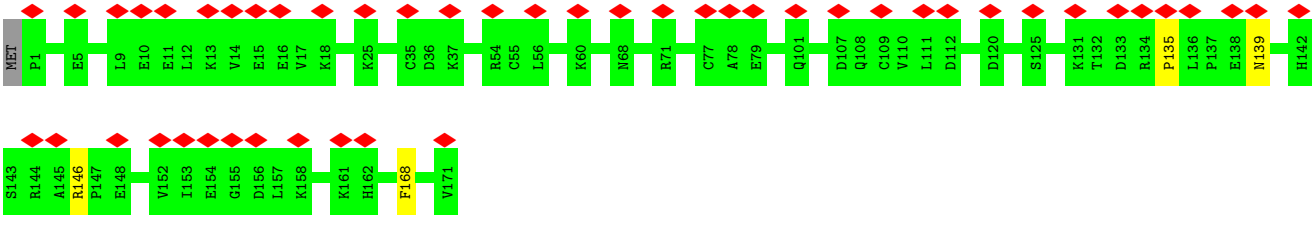


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

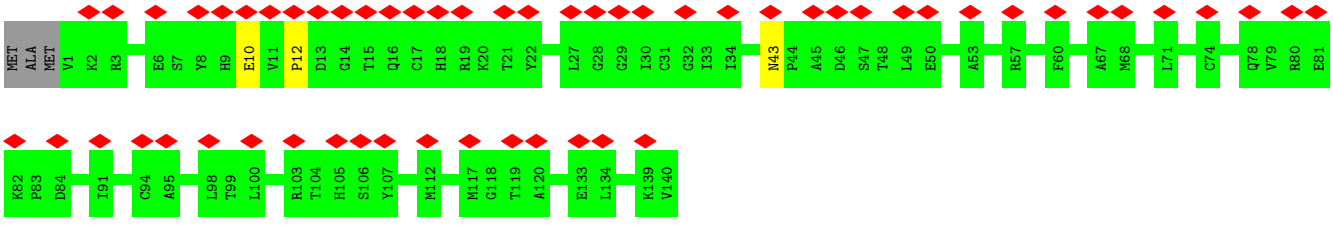




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

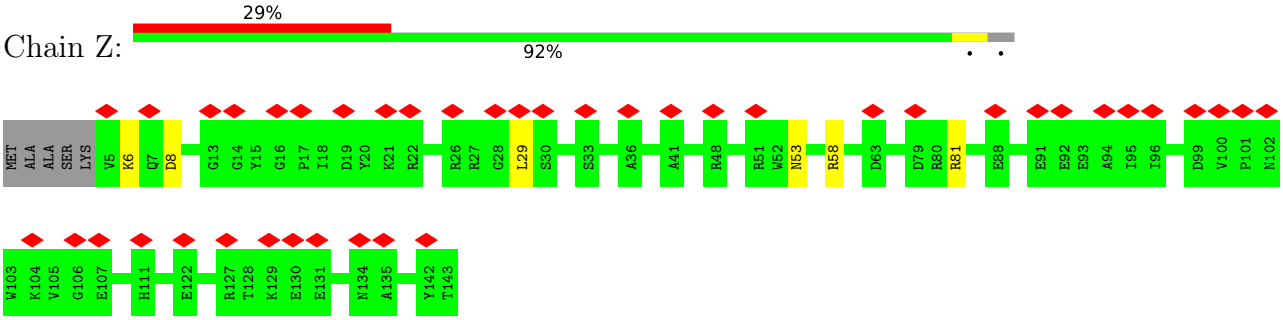


• Molecule 24: MCG5603



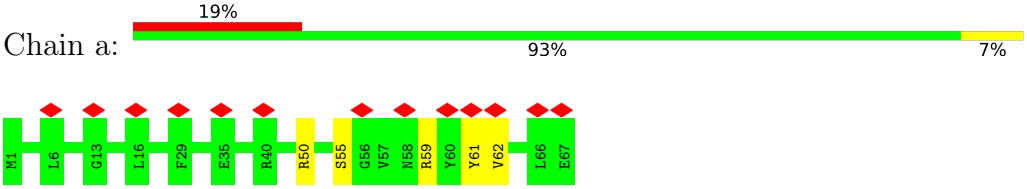
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



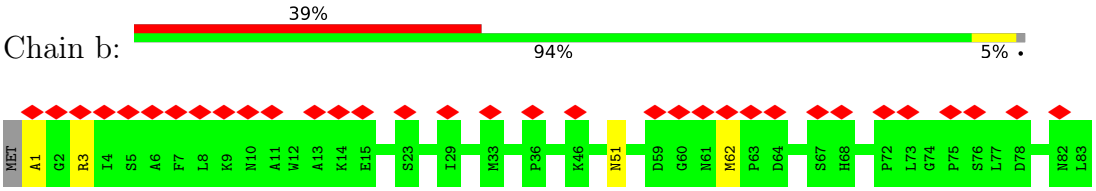
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



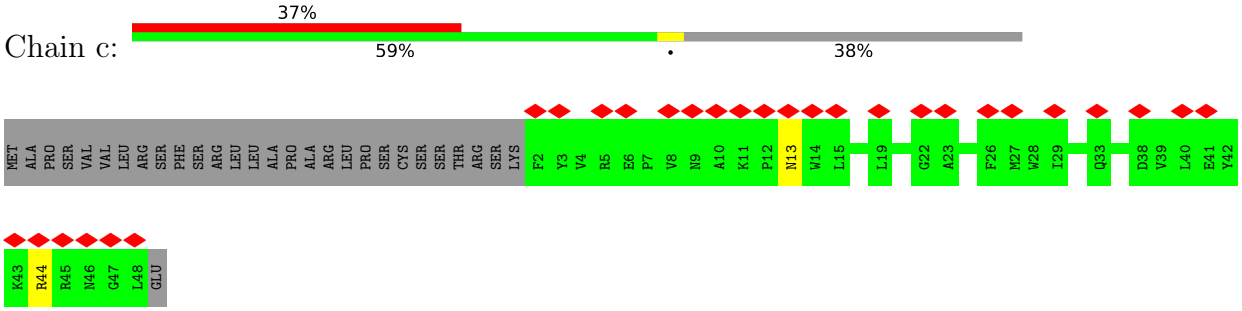
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:



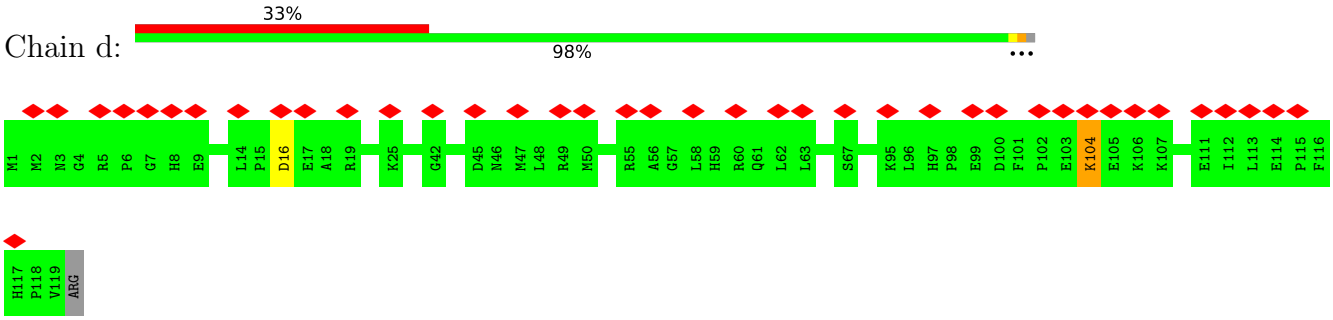
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



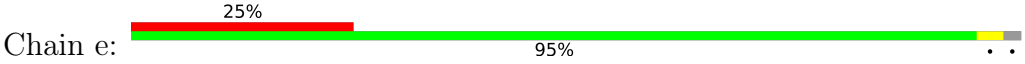
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



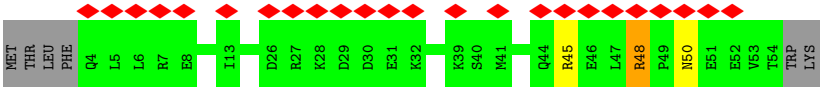
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



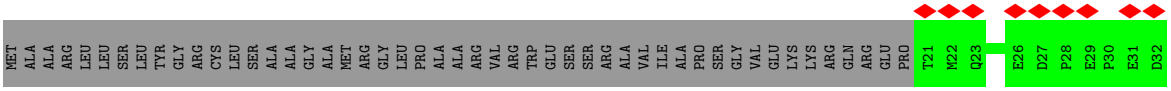
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

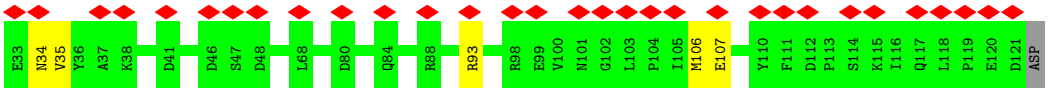
Chain f:



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

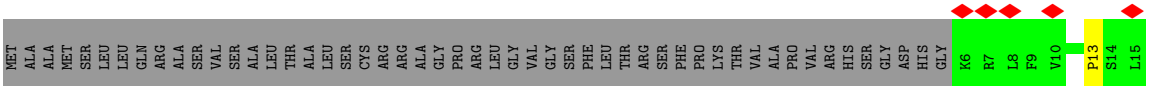
Chain g:

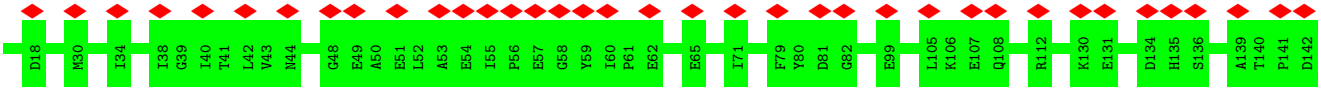




• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

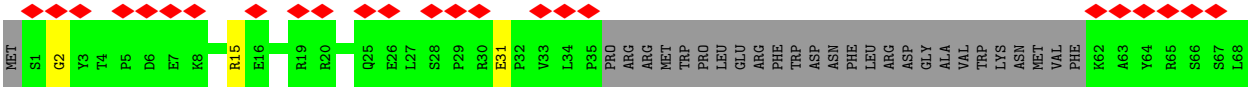
Chain h:

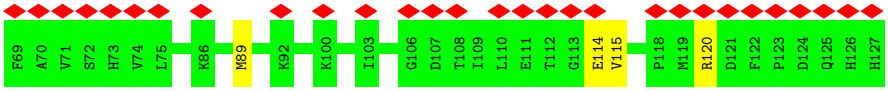




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

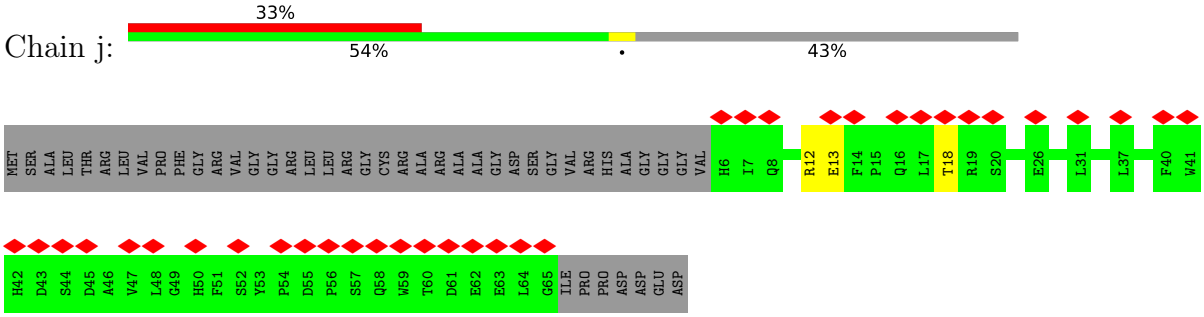
Chain i:





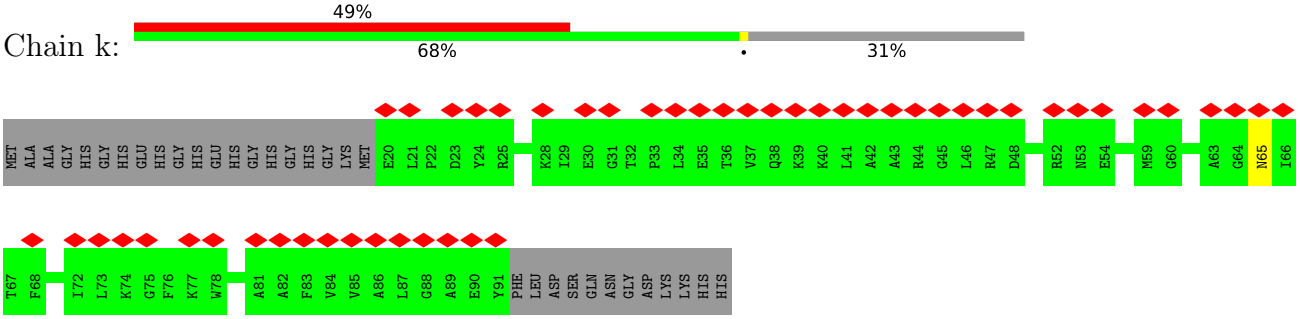
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



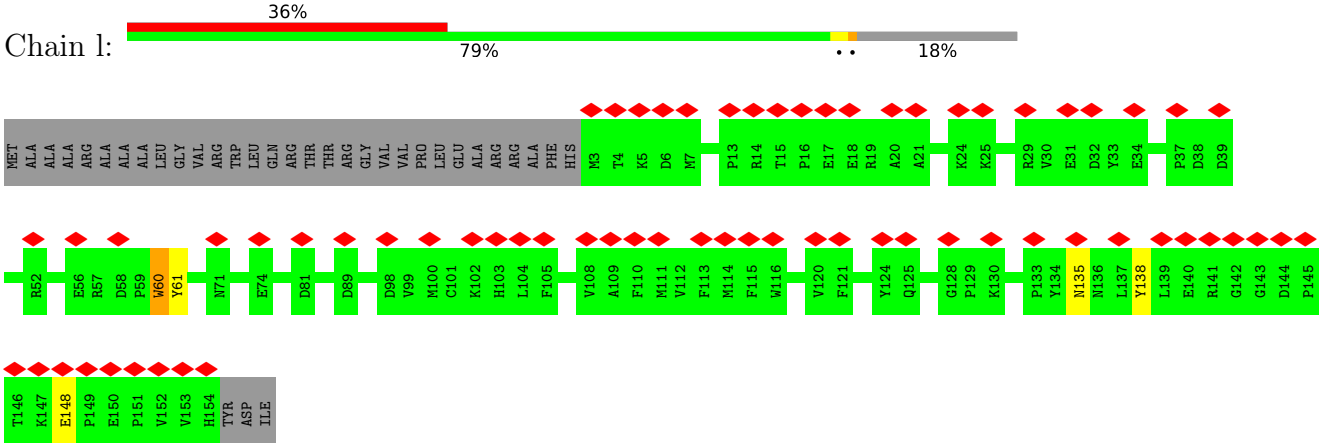
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



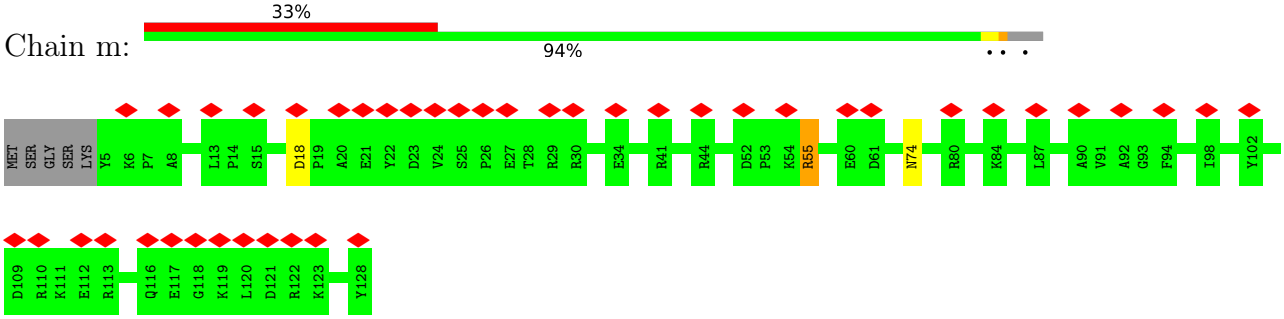
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



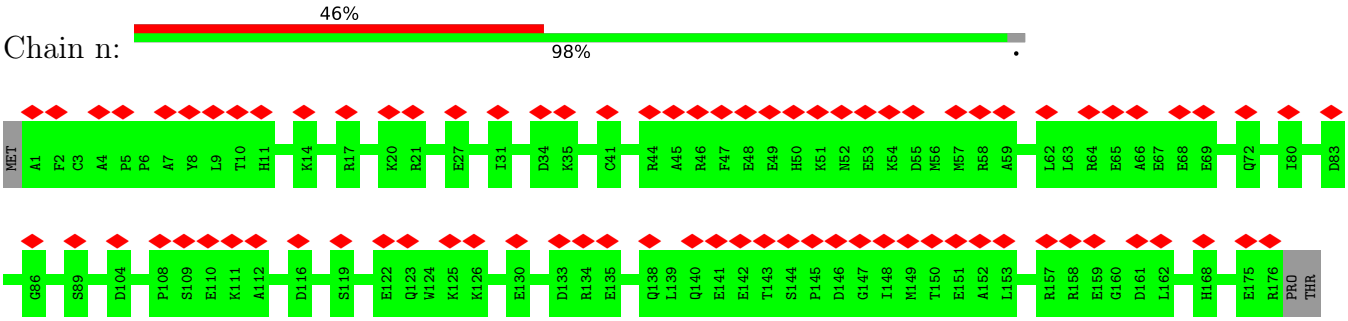
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



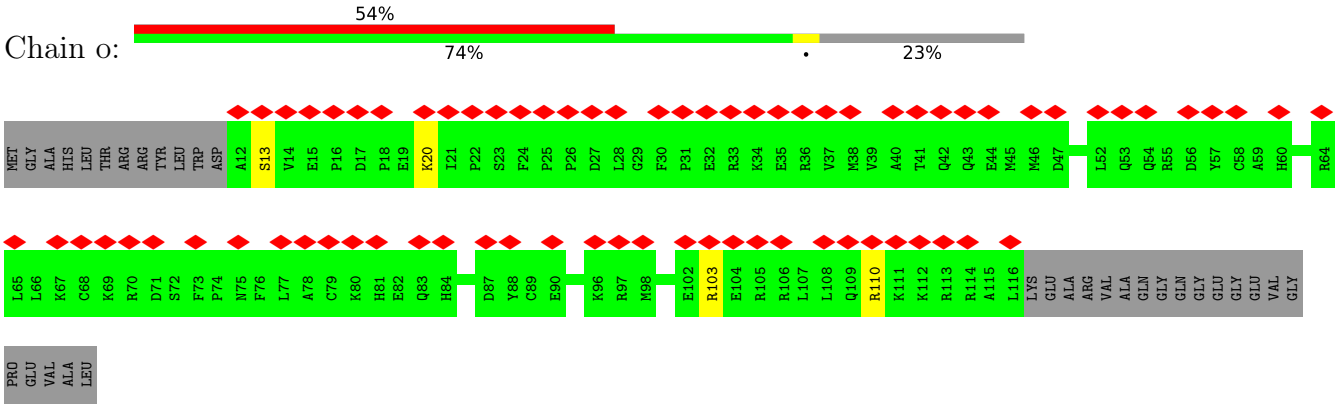
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



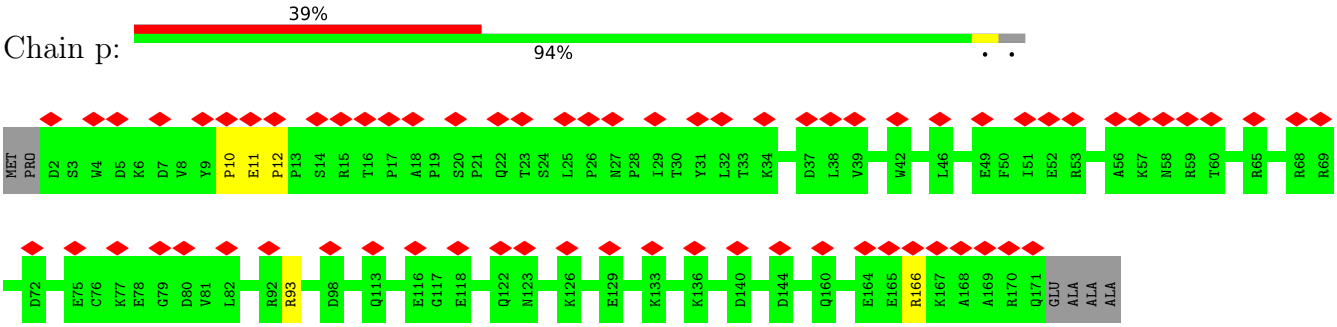
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



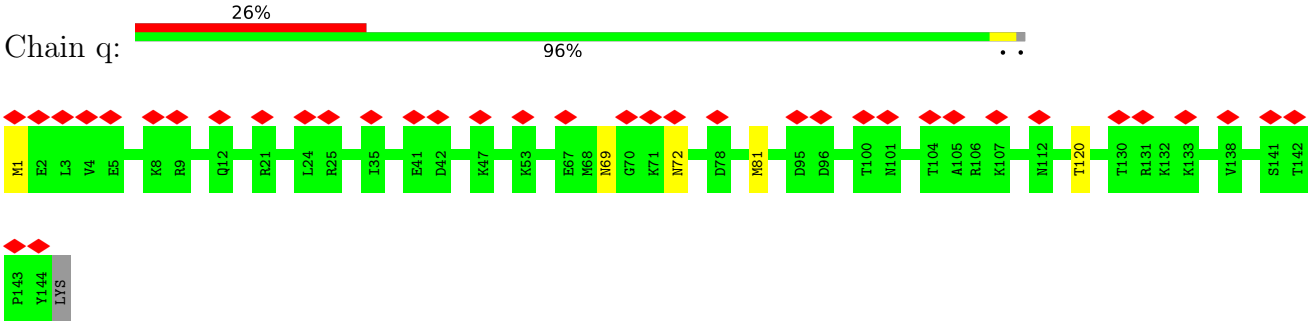
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:



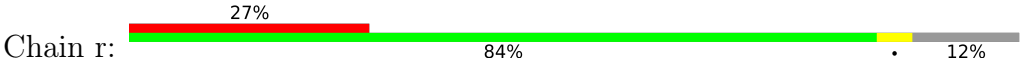
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

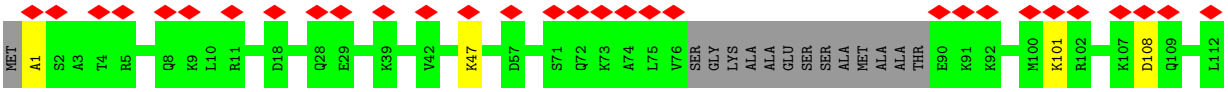
Chain q:



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

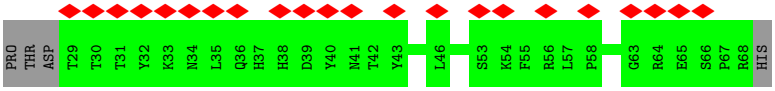
Chain r:





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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
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 ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.450	Depositor
Minimum map value	-0.156	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.075	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: SF4, AME, 3PE, 2MR, PC1, EHZ, FMN, FES, AYA, ADP, ZN, SAC, NDP, FME, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/949	0.71	2/1297 (0.2%)
2	B	0.52	0/1272	0.72	0/1722
3	C	0.46	0/1762	0.69	1/2401 (0.0%)
4	D	0.46	0/3528	0.64	0/4782
5	E	0.39	0/1688	0.63	1/2300 (0.0%)
6	F	0.39	0/3376	0.63	0/4561
7	G	0.39	0/5383	0.64	1/7293 (0.0%)
8	H	0.42	0/2607	0.64	0/3564
9	I	0.52	0/1438	0.77	1/1946 (0.1%)
10	J	0.41	0/1322	0.61	0/1799
11	K	0.39	0/738	0.65	0/1002
12	L	0.39	0/4913	0.62	0/6686
13	M	0.39	0/3709	0.64	2/5052 (0.0%)
14	N	0.40	0/2748	0.65	3/3741 (0.1%)
15	O	0.40	0/2674	0.61	0/3626
16	P	0.38	0/2823	0.66	0/3828
17	Q	0.39	0/1038	0.64	0/1401
18	R	0.40	0/762	0.63	1/1026 (0.1%)
19	S	0.34	0/678	0.65	0/915
20	T	0.30	0/613	0.51	0/826
20	U	0.38	0/718	0.55	0/970
21	V	0.35	0/937	0.66	1/1270 (0.1%)
22	W	0.38	0/993	0.68	0/1335
23	X	0.37	0/1434	0.61	0/1937
24	Y	0.35	0/1061	0.61	0/1439
25	Z	0.39	0/1183	0.67	1/1597 (0.1%)
26	a	0.39	0/561	0.64	0/755
27	b	0.39	0/666	0.60	0/914
28	c	0.34	0/400	0.55	0/544
29	d	0.40	0/1017	0.67	0/1373
30	e	0.36	0/892	0.65	0/1187
31	f	0.36	0/443	0.65	0/596

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	g	0.38	0/878	0.60	0/1196
33	h	0.39	0/1189	0.60	0/1610
34	i	0.36	0/836	0.63	1/1138 (0.1%)
35	j	0.36	0/548	0.67	0/748
36	k	0.35	0/601	0.61	0/814
37	l	0.40	0/1327	0.62	0/1811
38	m	0.38	0/1064	0.71	1/1444 (0.1%)
39	n	0.39	0/1581	0.64	0/2140
40	o	0.35	0/919	0.63	0/1232
41	p	0.39	0/1471	0.64	1/1988 (0.1%)
42	q	0.45	0/1234	0.68	0/1681
43	r	0.38	0/806	0.71	1/1090 (0.1%)
44	s	0.32	0/345	0.56	0/468
All	All	0.40	0/67125	0.64	18/91045 (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
2	B	0	2
3	C	0	1
4	D	0	2
5	E	0	1
6	F	0	1
7	G	0	5
8	H	0	5
10	J	0	2
12	L	0	7
13	M	0	1
14	N	0	2
16	P	0	3
17	Q	0	1
20	U	0	1
22	W	0	1
23	X	0	1
25	Z	0	1
26	a	0	2
29	d	0	2
30	e	0	1
31	f	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
32	g	0	2
34	i	0	3
35	j	0	2
37	l	0	3
38	m	0	1
40	o	0	2
41	p	0	3
42	q	0	1
All	All	0	60

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	LEU	CA-CB-CG	7.87	133.40	115.30
38	m	18	ASP	CB-CG-OD1	7.04	124.64	118.30
21	V	102	LEU	CB-CG-CD2	6.87	122.67	111.00
43	r	108	ASP	CB-CG-OD1	6.40	124.06	118.30
14	N	148	LEU	CA-CB-CG	5.75	128.53	115.30
13	M	434	LEU	CA-CB-CG	5.74	128.51	115.30
14	N	81	LEU	CA-CB-CG	5.69	128.40	115.30
7	G	53	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	71	LEU	CA-CB-CG	5.53	128.02	115.30
41	p	93	ARG	NE-CZ-NH1	5.29	122.94	120.30
3	C	106	ARG	NE-CZ-NH1	5.28	122.94	120.30
13	M	160	LEU	CA-CB-CG	5.17	127.19	115.30
9	I	45	ARG	NE-CZ-NH2	-5.11	117.75	120.30
18	R	24	ARG	NE-CZ-NH1	5.06	122.83	120.30
34	i	15	ARG	NE-CZ-NH1	5.06	122.83	120.30
5	E	110	LEU	CA-CB-CG	5.03	126.87	115.30
25	Z	58	ARG	NE-CZ-NH1	5.02	122.81	120.30
14	N	142	LEU	CA-CB-CG	5.01	126.84	115.30

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	119	GLU	Peptide
2	B	134	GLY	Peptide
3	C	8	ARG	Peptide
4	D	171	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	D	87	THR	Peptide
5	E	150	ASN	Peptide
6	F	206	LYS	Peptide
7	G	258	ILE	Peptide
7	G	259	ASN	Peptide
7	G	484	ALA	Peptide
7	G	485	ALA	Peptide
7	G	61	LYS	Peptide
8	H	156	MET	Peptide
8	H	207	LEU	Peptide
8	H	249	ILE	Peptide
8	H	90	PRO	Peptide
8	H	91	MET	Peptide
10	J	129	ASP	Peptide
10	J	170	THR	Mainchain
12	L	108	MET	Peptide
12	L	159	TYR	Peptide
12	L	197	GLU	Peptide
12	L	383	MET	Peptide
12	L	434	LYS	Peptide
12	L	520	SER	Peptide
12	L	598	ILE	Mainchain
13	M	369	LEU	Peptide
14	N	109	ALA	Peptide
14	N	141	ILE	Peptide
16	P	331	ILE	Peptide
16	P	334	THR	Peptide
16	P	97	ARG	Peptide
17	Q	69	LEU	Peptide
20	U	65	ILE	Peptide
22	W	57	THR	Peptide
23	X	146	ARG	Peptide
25	Z	29	LEU	Peptide
26	a	55	SER	Peptide
26	a	61	TYR	Peptide
29	d	104	LYS	Peptide
29	d	16	ASP	Peptide
30	e	46	ILE	Peptide
31	f	48	ARG	Peptide
32	g	106	MET	Peptide
32	g	35	VAL	Peptide
34	i	114	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
34	i	120	ARG	Peptide
34	i	31	GLU	Peptide
35	j	12	ARG	Peptide
35	j	18	THR	Peptide
37	l	135	ASN	Peptide
37	l	148	GLU	Peptide
37	l	60	TRP	Peptide
38	m	55	ARG	Peptide
40	o	13	SER	Peptide
40	o	20	LYS	Peptide
41	p	10	PRO	Peptide
41	p	11	GLU	Peptide
41	p	12	PRO	Peptide
42	q	120	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	113/115 (98%)	90 (80%)	22 (20%)	1 (1%)	14 44
2	B	153/224 (68%)	134 (88%)	19 (12%)	0	100 100
3	C	204/263 (78%)	172 (84%)	30 (15%)	2 (1%)	13 42
4	D	427/463 (92%)	372 (87%)	55 (13%)	0	100 100
5	E	210/248 (85%)	169 (80%)	40 (19%)	1 (0%)	25 56
6	F	426/428 (100%)	360 (84%)	66 (16%)	0	100 100
7	G	686/727 (94%)	593 (86%)	90 (13%)	3 (0%)	30 61
8	H	316/318 (99%)	272 (86%)	44 (14%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	176/212 (83%)	145 (82%)	31 (18%)	0	100	100
10	J	169/172 (98%)	148 (88%)	20 (12%)	1 (1%)	22	53
11	K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
12	L	604/607 (100%)	508 (84%)	96 (16%)	0	100	100
13	M	457/459 (100%)	413 (90%)	43 (9%)	1 (0%)	44	71
14	N	342/345 (99%)	309 (90%)	31 (9%)	2 (1%)	22	53
15	O	318/355 (90%)	273 (86%)	44 (14%)	1 (0%)	37	66
16	P	340/377 (90%)	280 (82%)	59 (17%)	1 (0%)	37	66
17	Q	123/175 (70%)	109 (89%)	13 (11%)	1 (1%)	16	46
18	R	93/116 (80%)	80 (86%)	13 (14%)	0	100	100
19	S	81/99 (82%)	69 (85%)	12 (15%)	0	100	100
20	T	73/156 (47%)	66 (90%)	7 (10%)	0	100	100
20	U	86/156 (55%)	69 (80%)	17 (20%)	0	100	100
21	V	110/116 (95%)	92 (84%)	18 (16%)	0	100	100
22	W	112/131 (86%)	101 (90%)	11 (10%)	0	100	100
23	X	169/172 (98%)	140 (83%)	27 (16%)	2 (1%)	11	38
24	Y	138/143 (96%)	120 (87%)	16 (12%)	2 (1%)	9	34
25	Z	137/144 (95%)	114 (83%)	22 (16%)	1 (1%)	19	50
26	a	65/67 (97%)	55 (85%)	9 (14%)	1 (2%)	8	33
27	b	81/84 (96%)	63 (78%)	18 (22%)	0	100	100
28	c	45/76 (59%)	42 (93%)	3 (7%)	0	100	100
29	d	117/120 (98%)	98 (84%)	19 (16%)	0	100	100
30	e	102/106 (96%)	84 (82%)	17 (17%)	1 (1%)	13	42
31	f	49/57 (86%)	37 (76%)	11 (22%)	1 (2%)	6	28
32	g	99/151 (66%)	76 (77%)	22 (22%)	1 (1%)	13	42
33	h	135/189 (71%)	113 (84%)	21 (16%)	1 (1%)	19	50
34	i	97/128 (76%)	76 (78%)	19 (20%)	2 (2%)	5	27
35	j	58/105 (55%)	41 (71%)	16 (28%)	1 (2%)	7	31
36	k	70/104 (67%)	54 (77%)	16 (23%)	0	100	100
37	l	150/186 (81%)	112 (75%)	35 (23%)	3 (2%)	6	28
38	m	122/129 (95%)	102 (84%)	20 (16%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	n	174/179 (97%)	149 (86%)	25 (14%)	0	100 100
40	o	103/137 (75%)	85 (82%)	18 (18%)	0	100 100
41	p	168/176 (96%)	142 (84%)	26 (16%)	0	100 100
42	q	142/145 (98%)	108 (76%)	32 (22%)	2 (1%)	9 34
43	r	95/113 (84%)	77 (81%)	18 (19%)	0	100 100
44	s	38/104 (36%)	32 (84%)	6 (16%)	0	100 100
All	All	8069/9175 (88%)	6833 (85%)	1204 (15%)	32 (0%)	32 61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	g	107	GLU
35	j	13	GLU
37	l	61	TYR
7	G	259	ASN
15	O	303	LYS
24	Y	10	GLU
26	a	62	VAL
37	l	60	TRP
34	i	2	GLY
37	l	138	TYR
7	G	359	ARG
14	N	2	ASN
16	P	331	ILE
23	X	168	PHE
30	e	88	GLU
31	f	48	ARG
33	h	13	PRO
42	q	69	ASN
42	q	81	MET
3	C	204	GLU
13	M	224	PRO
24	Y	12	PRO
25	Z	8	ASP
1	A	25	PRO
5	E	127	LYS
14	N	109	ALA
34	i	115	VAL
7	G	381	GLY
3	C	202	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	26	PRO
23	X	135	PRO
10	J	128	VAL

5.3.2 Protein sidechains (i)

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%)	102 (99%)	1 (1%)	73	84
2	B	131/185 (71%)	129 (98%)	2 (2%)	60	77
3	C	188/227 (83%)	183 (97%)	5 (3%)	40	65
4	D	367/394 (93%)	363 (99%)	4 (1%)	70	82
5	E	183/206 (89%)	182 (100%)	1 (0%)	86	91
6	F	343/343 (100%)	339 (99%)	4 (1%)	67	80
7	G	580/610 (95%)	578 (100%)	2 (0%)	91	94
8	H	279/279 (100%)	278 (100%)	1 (0%)	89	93
9	I	145/178 (82%)	143 (99%)	2 (1%)	62	78
10	J	136/137 (99%)	136 (100%)	0	100	100
11	K	87/87 (100%)	86 (99%)	1 (1%)	70	82
12	L	548/549 (100%)	543 (99%)	5 (1%)	75	85
13	M	414/414 (100%)	411 (99%)	3 (1%)	81	88
14	N	306/307 (100%)	301 (98%)	5 (2%)	58	76
15	O	284/309 (92%)	279 (98%)	5 (2%)	54	74
16	P	299/325 (92%)	293 (98%)	6 (2%)	50	71
17	Q	112/153 (73%)	109 (97%)	3 (3%)	40	65
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	74/80 (92%)	73 (99%)	1 (1%)	62	78
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	V	100/102 (98%)	98 (98%)	2 (2%)	50 71
22	W	108/114 (95%)	107 (99%)	1 (1%)	75 85
23	X	153/154 (99%)	152 (99%)	1 (1%)	81 88
24	Y	105/107 (98%)	104 (99%)	1 (1%)	73 84
25	Z	120/123 (98%)	117 (98%)	3 (2%)	42 67
26	a	57/57 (100%)	55 (96%)	2 (4%)	31 58
27	b	72/73 (99%)	69 (96%)	3 (4%)	25 53
28	c	41/67 (61%)	39 (95%)	2 (5%)	21 49
29	d	106/107 (99%)	105 (99%)	1 (1%)	75 85
30	e	92/94 (98%)	91 (99%)	1 (1%)	70 82
31	f	47/53 (89%)	45 (96%)	2 (4%)	25 53
32	g	92/129 (71%)	90 (98%)	2 (2%)	47 69
33	h	122/162 (75%)	122 (100%)	0	100 100
34	i	87/119 (73%)	86 (99%)	1 (1%)	70 82
35	j	56/87 (64%)	56 (100%)	0	100 100
36	k	55/78 (70%)	54 (98%)	1 (2%)	54 74
37	l	137/161 (85%)	137 (100%)	0	100 100
38	m	110/114 (96%)	108 (98%)	2 (2%)	54 74
39	n	161/164 (98%)	161 (100%)	0	100 100
40	o	98/121 (81%)	96 (98%)	2 (2%)	50 71
41	p	155/158 (98%)	154 (99%)	1 (1%)	84 90
42	q	129/130 (99%)	128 (99%)	1 (1%)	79 87
43	r	88/96 (92%)	86 (98%)	2 (2%)	45 68
44	s	39/95 (41%)	39 (100%)	0	100 100
All	All	7139/7917 (90%)	7057 (99%)	82 (1%)	69 82

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
2	B	52	ARG
2	B	64	CYS
3	C	14	ARG
3	C	128	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	137	MET
3	C	175	ARG
3	C	200	ASN
4	D	23	LYS
4	D	237	ASN
4	D	290	ARG
4	D	430	ARG
5	E	15	ASN
6	F	24	ASN
6	F	112	ARG
6	F	224	ASN
6	F	237	ARG
7	G	135	ARG
7	G	546	GLN
8	H	156	MET
9	I	64	ARG
9	I	106	ARG
11	K	92	ASN
12	L	25	ASN
12	L	425	ARG
12	L	436	ARG
12	L	444	ASN
12	L	572	ASN
13	M	86	LYS
13	M	331	ASN
13	M	366	ASN
14	N	2	ASN
14	N	204	ASN
14	N	273	ASN
14	N	310	ASN
14	N	323	ASN
15	O	30	ASN
15	O	48	MET
15	O	92	ASN
15	O	213	LYS
15	O	288	GLN
16	P	50	ARG
16	P	89	ASN
16	P	93	ASN
16	P	186	ARG
16	P	216	ASN
16	P	325	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	43	ASN
17	Q	112	LYS
17	Q	125	ASN
19	S	38	GLN
21	V	44	ARG
21	V	109	ASN
22	W	126	MET
23	X	139	ASN
24	Y	43	ASN
25	Z	6	LYS
25	Z	53	ASN
25	Z	81	ARG
26	a	50	ARG
26	a	59	ARG
27	b	3	ARG
27	b	51	ASN
27	b	62	MET
28	c	13	ASN
28	c	44	ARG
29	d	104	LYS
30	e	73	ARG
31	f	45	ARG
31	f	50	ASN
32	g	34	ASN
32	g	93	ARG
34	i	89	MET
36	k	65	ASN
38	m	55	ARG
38	m	74	ASN
40	o	103	ARG
40	o	110	ARG
41	p	166	ARG
42	q	72	ASN
43	r	47	LYS
43	r	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
2	B	48	ASN
2	B	92	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	200	ASN
4	D	54	GLN
4	D	79	HIS
4	D	84	HIS
4	D	232	ASN
4	D	409	HIS
5	E	15	ASN
5	E	27	ASN
5	E	121	GLN
6	F	165	ASN
6	F	263	ASN
7	G	36	GLN
7	G	51	ASN
8	H	235	ASN
9	I	92	GLN
9	I	138	ASN
11	K	83	ASN
12	L	25	ASN
12	L	67	HIS
12	L	135	ASN
12	L	320	ASN
12	L	444	ASN
13	M	48	ASN
13	M	51	ASN
13	M	88	ASN
13	M	139	GLN
13	M	366	ASN
14	N	2	ASN
14	N	63	GLN
14	N	91	ASN
14	N	144	GLN
14	N	317	GLN
14	N	323	ASN
14	N	342	GLN
15	O	30	ASN
15	O	294	ASN
16	P	37	HIS
16	P	136	ASN
21	V	109	ASN
23	X	123	GLN
23	X	139	ASN
24	Y	18	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Y	88	ASN
26	a	42	GLN
27	b	45	ASN
28	c	13	ASN
30	e	97	HIS
31	f	50	ASN
32	g	34	ASN
33	h	44	ASN
33	h	95	GLN
36	k	65	ASN
37	l	103	HIS
40	o	54	GLN
42	q	17	HIS
42	q	31	ASN
42	q	72	ASN
42	q	113	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.97	0	7,9,11	0.83	0
42	AME	q	1	42	9,10,11	1.76	2 (22%)	9,11,13	2.00	4 (44%)
8	FME	H	1	8	8,9,10	0.94	0	7,9,11	1.31	1 (14%)
13	FME	M	1	13	8,9,10	0.97	0	7,9,11	0.76	0
11	FME	K	1	11	8,9,10	1.06	0	7,9,11	1.39	1 (14%)
27	AYA	b	1	27	6,7,8	1.24	1 (16%)	5,8,10	1.16	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	AYA	r	1	43	6,7,8	1.22	1 (16%)	5,8,10	1.25	1 (20%)
4	2MR	D	85	4	10,12,13	2.53	3 (30%)	5,13,15	1.68	1 (20%)
10	FME	J	1	10	8,9,10	0.91	0	7,9,11	0.63	0
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	0.71	0
14	FME	N	1	14	8,9,10	0.94	0	7,9,11	1.32	1 (14%)
34	SAC	i	1	34	7,8,9	1.03	0	8,9,11	0.93	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
1	FME	A	1	1	-	3/7/9/11	-
42	AME	q	1	42	-	4/9/10/12	-
8	FME	H	1	8	-	4/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	5/7/9/11	-
27	AYA	b	1	27	-	1/4/6/8	-
43	AYA	r	1	43	-	0/4/6/8	-
4	2MR	D	85	4	-	3/10/13/15	-
10	FME	J	1	10	-	2/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
34	SAC	i	1	34	-	2/7/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.58	1.46	1.34
4	D	85	2MR	CZ-NH2	4.92	1.44	1.33
42	q	1	AME	CT1-N	3.89	1.47	1.34
43	r	1	AYA	CA-N	-2.42	1.44	1.46
27	b	1	AYA	CA-N	-2.30	1.44	1.46
42	q	1	AME	OT-CT1	-2.04	1.18	1.23
4	D	85	2MR	CQ1-NH1	-2.02	1.42	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	85	2MR	CD-NE-CZ	3.51	129.97	123.41
42	q	1	AME	CE-SD-CG	3.47	112.33	100.40
42	q	1	AME	CT2-CT1-N	3.08	121.31	116.10
8	H	1	FME	C-CA-N	3.04	115.21	109.73
14	N	1	FME	C-CA-N	2.70	114.60	109.73
43	r	1	AYA	CB-CA-N	2.51	112.40	109.61
11	K	1	FME	CG-CB-CA	2.37	119.54	112.95
42	q	1	AME	O-C-CA	-2.33	118.68	124.78
27	b	1	AYA	CB-CA-N	2.25	112.11	109.61
42	q	1	AME	C-CA-N	2.08	113.48	109.73

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	CA-CB-CG-SD
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	O-C-CA-CB
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
34	i	1	SAC	C-CA-CB-OG
4	D	85	2MR	NE-CD-CG-CB
42	q	1	AME	CT2-CT1-N-CA
42	q	1	AME	OT-CT1-N-CA
42	q	1	AME	CA-CB-CG-SD
1	A	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
34	i	1	SAC	N-CA-CB-OG
42	q	1	AME	CB-CG-SD-CE
4	D	85	2MR	CA-CB-CG-CD
14	N	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
27	b	1	AYA	C-CA-N-CT
8	H	1	FME	CB-CG-SD-CE
4	D	85	2MR	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
12	L	1	FME	N-CA-CB-CG
12	L	1	FME	CB-CG-SD-CE
10	J	1	FME	CA-CB-CG-SD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	K	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
51	ADP	O	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
45	3PE	M	501	-	50,50,50	0.87	4 (8%)	53,55,55	0.98	2 (3%)
45	3PE	M	505	-	50,50,50	0.86	3 (6%)	53,55,55	1.01	3 (5%)
45	3PE	H	401	-	50,50,50	0.85	4 (8%)	53,55,55	0.98	2 (3%)
54	EHZ	T	201	20	26,33,37	1.80	5 (19%)	32,41,47	1.34	2 (6%)
46	SF4	I	202	9	0,12,12	-	-	-		
50	CDL	H	405	-	56,56,99	1.13	7 (12%)	62,68,111	1.11	4 (6%)
46	SF4	G	802	7	0,12,12	-	-	-		
49	PC1	P	401	-	42,42,53	1.06	4 (9%)	48,50,61	1.03	2 (4%)
47	FES	G	803	7	0,4,4	-	-	-		
50	CDL	L	702	-	77,77,99	0.99	6 (7%)	83,89,111	1.12	4 (4%)
54	EHZ	U	201	20	27,34,37	1.79	6 (22%)	33,42,47	1.18	3 (9%)
50	CDL	M	507	-	66,66,99	1.05	8 (12%)	72,78,111	1.22	5 (6%)
50	CDL	L	703	-	69,69,99	1.02	8 (11%)	75,81,111	1.08	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	NDP	P	501	-	45,52,52	2.28	8 (17%)	53,80,80	1.57	9 (16%)
46	SF4	B	201	2	0,12,12	-	-	-		
45	3PE	N	401	-	50,50,50	0.89	4 (8%)	53,55,55	1.09	2 (3%)
46	SF4	G	801	7	0,12,12	-	-	-		
45	3PE	L	701	-	50,50,50	0.85	4 (8%)	53,55,55	1.01	2 (3%)
49	PC1	H	404	-	46,46,53	1.02	4 (8%)	52,54,61	1.02	2 (3%)
47	FES	E	301	5	0,4,4	-	-	-		
49	PC1	H	402	-	41,41,53	1.07	3 (7%)	47,49,61	0.92	2 (4%)
45	3PE	L	704	-	41,41,50	0.95	4 (9%)	44,46,55	1.01	2 (4%)
49	PC1	H	406	-	34,34,53	1.17	4 (11%)	40,42,61	1.09	2 (5%)
45	3PE	M	506	-	30,30,50	1.10	4 (13%)	33,35,55	1.13	2 (6%)
48	FMN	F	501	-	33,33,33	1.12	2 (6%)	48,50,50	1.42	8 (16%)
45	3PE	H	403	-	50,50,50	0.87	3 (6%)	53,55,55	1.10	2 (3%)
46	SF4	I	201	9	0,12,12	-	-	-		
45	3PE	M	504	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
46	SF4	F	502	6	0,12,12	-	-	-		
45	3PE	M	502	-	41,41,50	1.04	4 (9%)	45,46,55	1.20	3 (6%)
45	3PE	A	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.06	2 (4%)
45	3PE	M	503	-	50,50,50	0.87	3 (6%)	53,55,55	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
51	ADP	O	401	-	-	5/12/32/32	0/3/3/3
45	3PE	M	501	-	-	29/54/54/54	-
45	3PE	M	505	-	-	25/54/54/54	-
45	3PE	H	401	-	-	27/54/54/54	-
54	EHZ	T	201	20	-	7/39/41/45	-
46	SF4	I	202	9	-	-	0/6/5/5
50	CDL	H	405	-	-	39/67/67/110	-
46	SF4	G	802	7	-	-	0/6/5/5
49	PC1	P	401	-	-	27/46/46/57	-
47	FES	G	803	7	-	-	0/1/1/1
50	CDL	L	702	-	-	43/88/88/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	EHZ	U	201	20	-	16/40/42/45	-
50	CDL	M	507	-	-	32/77/77/110	-
52	NDP	P	501	-	-	4/30/77/77	0/5/5/5
46	SF4	F	502	6	-	-	0/6/5/5
46	SF4	B	201	2	-	-	0/6/5/5
45	3PE	N	401	-	-	25/54/54/54	-
46	SF4	G	801	7	-	-	0/6/5/5
45	3PE	L	701	-	-	20/54/54/54	-
45	3PE	M	503	-	-	21/54/54/54	-
47	FES	E	301	5	-	-	0/1/1/1
49	PC1	H	402	-	-	26/45/45/57	-
45	3PE	L	704	-	-	18/45/45/54	-
49	PC1	H	406	-	-	19/38/38/57	-
45	3PE	M	506	-	-	16/34/34/54	-
48	FMN	F	501	-	-	7/18/18/18	0/3/3/3
45	3PE	H	403	-	-	26/54/54/54	-
46	SF4	I	201	9	-	-	0/6/5/5
45	3PE	M	504	-	-	23/54/54/54	-
50	CDL	L	703	-	-	39/80/80/110	-
45	3PE	M	502	-	-	17/43/43/54	-
45	3PE	A	201	-	-	19/44/44/54	-
49	PC1	H	404	-	-	21/50/50/57	-

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.21	1.82	1.59
54	U	201	EHZ	C15-N2	5.53	1.45	1.33
54	T	201	EHZ	C15-N2	5.51	1.45	1.33
54	U	201	EHZ	C12-N1	5.32	1.45	1.33
54	T	201	EHZ	C12-N1	5.31	1.45	1.33
52	P	501	NDP	PN-O5D	3.55	1.73	1.59
48	F	501	FMN	C4A-N5	3.23	1.37	1.30
52	P	501	NDP	O2B-C2B	-3.16	1.32	1.44
45	M	502	3PE	O31-C31	2.85	1.41	1.33
45	M	505	3PE	O21-C2	-2.77	1.39	1.46
45	M	502	3PE	P-O13	2.69	1.65	1.54
45	M	503	3PE	O21-C2	-2.66	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	H	405	CDL	OB6-CB4	-2.60	1.40	1.46
45	H	403	3PE	O21-C2	-2.60	1.40	1.46
45	M	505	3PE	O31-C3	-2.56	1.39	1.45
52	P	501	NDP	O3B-C3B	-2.55	1.37	1.43
49	H	404	PC1	O31-C31	2.55	1.40	1.33
50	L	702	CDL	OA6-CA4	-2.54	1.40	1.46
45	N	401	3PE	O21-C2	-2.53	1.40	1.46
48	F	501	FMN	C10-N1	2.53	1.38	1.33
50	M	507	CDL	OA8-CA7	2.52	1.40	1.33
49	H	402	PC1	O31-C31	2.52	1.40	1.33
45	L	704	3PE	O21-C2	-2.51	1.40	1.46
54	U	201	EHZ	C9-S1	2.50	1.82	1.76
54	T	201	EHZ	C9-S1	2.50	1.82	1.76
45	M	502	3PE	O21-C2	-2.49	1.40	1.46
50	L	702	CDL	OA8-CA7	2.48	1.40	1.33
50	L	702	CDL	OB8-CB7	2.48	1.40	1.33
50	L	703	CDL	OA6-CA4	-2.48	1.40	1.46
50	H	405	CDL	OA8-CA7	2.48	1.40	1.33
45	M	503	3PE	O31-C31	2.48	1.40	1.33
50	H	405	CDL	OA6-CA4	-2.48	1.40	1.46
45	M	501	3PE	O21-C2	-2.46	1.40	1.46
52	P	501	NDP	O4B-C4B	-2.45	1.39	1.45
50	L	702	CDL	OB6-CB4	-2.45	1.40	1.46
49	H	404	PC1	O21-C2	-2.45	1.40	1.46
52	P	501	NDP	O5D-C5D	-2.45	1.35	1.44
49	H	406	PC1	O21-C2	-2.44	1.40	1.46
50	H	405	CDL	OB8-CB7	2.44	1.40	1.33
49	H	402	PC1	O21-C2	-2.43	1.40	1.46
45	L	701	3PE	O21-C2	-2.41	1.40	1.46
50	M	507	CDL	OB8-CB7	2.40	1.40	1.33
45	A	201	3PE	O21-C21	2.40	1.41	1.34
45	L	704	3PE	O31-C31	2.38	1.40	1.33
45	M	502	3PE	O21-C21	2.38	1.41	1.34
45	H	403	3PE	O31-C3	-2.37	1.39	1.45
45	N	401	3PE	O31-C3	-2.36	1.39	1.45
49	P	401	PC1	O21-C21	2.35	1.40	1.34
45	M	504	3PE	O21-C2	-2.35	1.40	1.46
45	A	201	3PE	O31-C31	2.35	1.40	1.33
50	M	507	CDL	OB6-CB5	2.34	1.40	1.34
49	H	406	PC1	O31-C31	2.34	1.40	1.33
45	M	506	3PE	O31-C31	2.34	1.40	1.33
45	M	504	3PE	O31-C31	2.34	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	O	401	ADP	C5-C4	2.33	1.47	1.40
45	M	506	3PE	O21-C2	-2.32	1.40	1.46
49	P	401	PC1	O31-C31	2.32	1.40	1.33
45	M	501	3PE	O31-C31	2.32	1.40	1.33
45	A	201	3PE	O31-C3	-2.32	1.39	1.45
50	L	703	CDL	OB8-CB7	2.32	1.40	1.33
50	L	703	CDL	OB8-CB6	-2.30	1.39	1.45
49	H	406	PC1	O31-C3	-2.30	1.39	1.45
45	H	401	3PE	O31-C3	-2.29	1.39	1.45
45	N	401	3PE	O31-C31	2.29	1.40	1.33
45	A	201	3PE	O21-C2	-2.29	1.40	1.46
50	L	703	CDL	OA8-CA7	2.28	1.40	1.33
54	U	201	EHZ	O4-C15	-2.28	1.18	1.23
49	H	404	PC1	O21-C21	2.27	1.40	1.34
45	H	401	3PE	O21-C2	-2.27	1.40	1.46
45	M	506	3PE	O21-C21	2.27	1.40	1.34
45	M	506	3PE	O31-C3	-2.26	1.40	1.45
45	H	403	3PE	O31-C31	2.26	1.39	1.33
50	L	703	CDL	OB6-CB5	2.25	1.40	1.34
54	T	201	EHZ	O4-C15	-2.25	1.18	1.23
54	U	201	EHZ	O3-C12	-2.25	1.18	1.23
45	M	501	3PE	O21-C21	2.24	1.40	1.34
45	M	504	3PE	O21-C21	2.23	1.40	1.34
49	P	401	PC1	O31-C3	-2.23	1.40	1.45
45	M	501	3PE	O31-C3	-2.22	1.40	1.45
49	H	406	PC1	O21-C21	2.21	1.40	1.34
45	H	401	3PE	O31-C31	2.21	1.39	1.33
50	M	507	CDL	OB8-CB6	-2.20	1.40	1.45
45	L	701	3PE	O31-C31	2.20	1.39	1.33
50	M	507	CDL	OA6-CA4	-2.19	1.41	1.46
54	T	201	EHZ	O3-C12	-2.17	1.18	1.23
49	H	402	PC1	O21-C21	2.17	1.40	1.34
50	L	702	CDL	OB6-CB5	2.17	1.40	1.34
50	L	703	CDL	OA8-CA6	-2.16	1.40	1.45
50	M	507	CDL	OB6-CB4	-2.16	1.41	1.46
45	L	704	3PE	O31-C3	-2.14	1.40	1.45
50	M	507	CDL	OA6-CA5	2.14	1.40	1.34
50	L	703	CDL	OA6-CA5	2.12	1.40	1.34
50	H	405	CDL	OA6-CA5	2.11	1.40	1.34
45	N	401	3PE	O21-C21	2.11	1.40	1.34
45	L	701	3PE	O31-C3	-2.10	1.40	1.45
54	U	201	EHZ	O6-C20	-2.09	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	503	3PE	O31-C3	-2.09	1.40	1.45
45	L	701	3PE	O21-C21	2.08	1.40	1.34
50	H	405	CDL	OB8-CB6	-2.08	1.40	1.45
52	P	501	NDP	O2D-C2D	-2.08	1.38	1.43
45	M	504	3PE	O31-C3	-2.08	1.40	1.45
45	M	505	3PE	O31-C31	2.07	1.39	1.33
50	L	702	CDL	OA6-CA5	2.07	1.40	1.34
45	H	401	3PE	O21-C21	2.05	1.40	1.34
50	L	703	CDL	OB6-CB4	-2.05	1.41	1.46
45	L	704	3PE	O21-C21	2.05	1.40	1.34
49	H	404	PC1	O31-C3	-2.04	1.40	1.45
52	P	501	NDP	PA-O5B	2.02	1.67	1.59
50	H	405	CDL	OB6-CB5	2.01	1.40	1.34
50	M	507	CDL	OA8-CA6	-2.01	1.40	1.45
49	P	401	PC1	O21-C2	-2.00	1.41	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	PN-O3-PA	-5.92	112.52	132.83
54	T	201	EHZ	C8-C9-S1	5.04	119.86	113.63
45	M	502	3PE	O31-C31-C32	4.61	126.36	111.91
50	M	507	CDL	OB6-CB5-C51	4.60	121.42	111.50
45	M	504	3PE	O21-C21-C22	4.53	121.26	111.50
49	H	404	PC1	O21-C21-C22	4.49	121.17	111.50
45	N	401	3PE	O21-C21-C22	4.43	121.05	111.50
45	H	403	3PE	O21-C21-C22	4.38	120.95	111.50
50	L	702	CDL	OB6-CB5-C51	4.34	120.85	111.50
50	L	702	CDL	OA6-CA5-C11	4.32	120.82	111.50
49	H	406	PC1	O21-C21-C22	4.32	120.81	111.50
54	U	201	EHZ	C8-C9-S1	4.23	118.86	113.63
45	M	503	3PE	O21-C21-C22	4.16	120.47	111.50
45	M	506	3PE	O21-C21-C22	3.96	120.05	111.50
45	M	501	3PE	O21-C21-C22	3.93	119.97	111.50
45	A	201	3PE	O21-C21-C22	3.91	119.93	111.50
49	P	401	PC1	O21-C21-C22	3.91	119.92	111.50
50	H	405	CDL	OB6-CB5-C51	3.86	119.81	111.50
50	H	405	CDL	OA6-CA5-C11	3.84	119.78	111.50
50	L	703	CDL	OB6-CB5-C51	3.83	119.75	111.50
49	H	402	PC1	O21-C21-C22	3.82	119.73	111.50
45	H	401	3PE	O21-C21-C22	3.79	119.68	111.50
50	L	703	CDL	OA6-CA5-C11	3.73	119.54	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	O	401	ADP	N3-C2-N1	-3.70	122.90	128.68
45	L	704	3PE	O21-C21-C22	3.67	119.42	111.50
48	F	501	FMN	C4-N3-C2	-3.59	119.00	125.64
45	L	701	3PE	O21-C21-C22	3.42	118.87	111.50
50	M	507	CDL	OA8-CA7-C31	3.40	122.59	111.91
45	M	505	3PE	O21-C21-C22	3.39	118.82	111.50
50	M	507	CDL	OA6-CA5-C11	3.34	118.70	111.50
52	P	501	NDP	O2B-P2B-O1X	-3.32	96.56	109.39
45	M	505	3PE	C2-O21-C21	-3.12	110.11	117.79
51	O	401	ADP	PA-O3A-PB	-3.09	122.22	132.83
49	H	404	PC1	O31-C31-C32	2.98	121.26	111.91
48	F	501	FMN	O4-C4-C4A	-2.97	118.71	126.60
45	M	502	3PE	O31-C31-O32	-2.97	116.09	123.59
50	L	702	CDL	OA8-CA7-C31	2.96	121.21	111.91
48	F	501	FMN	C4A-C10-N1	-2.87	118.06	124.73
48	F	501	FMN	C4A-C4-N3	2.84	120.39	113.19
50	L	702	CDL	OB8-CB7-C71	2.81	120.72	111.91
51	O	401	ADP	C4-C5-N7	-2.79	106.49	109.40
49	H	406	PC1	O31-C31-C32	2.79	120.65	111.91
48	F	501	FMN	C4A-C10-N10	2.76	120.52	116.48
45	N	401	3PE	O31-C31-C32	2.70	120.40	111.91
45	M	504	3PE	O31-C31-C32	2.70	120.39	111.91
50	H	405	CDL	OA8-CA7-C31	2.69	120.34	111.91
50	M	507	CDL	OB8-CB7-C71	2.68	120.33	111.91
51	O	401	ADP	O4'-C1'-C2'	-2.68	103.01	106.93
45	M	503	3PE	O31-C31-C32	2.65	120.24	111.91
45	M	502	3PE	O21-C21-C22	2.65	117.20	111.50
52	P	501	NDP	O5D-PN-O1N	-2.64	98.75	109.07
45	L	701	3PE	O31-C31-C32	2.63	120.17	111.91
50	L	703	CDL	OA8-CA7-C31	2.59	120.03	111.91
45	M	506	3PE	O31-C31-C32	2.59	120.03	111.91
50	H	405	CDL	OB8-CB7-C71	2.57	119.99	111.91
45	A	201	3PE	O31-C31-C32	2.56	119.95	111.91
45	L	704	3PE	O31-C31-C32	2.55	119.92	111.91
52	P	501	NDP	C2A-N1A-C6A	-2.53	114.43	118.75
48	F	501	FMN	C4-C4A-C10	2.52	121.03	116.79
52	P	501	NDP	O3X-P2B-O2X	2.52	117.26	107.64
50	L	703	CDL	OB8-CB7-C71	2.49	119.72	111.91
45	M	501	3PE	O31-C31-C32	2.49	119.71	111.91
54	U	201	EHZ	C19-C17-C16	2.47	113.11	108.82
45	H	403	3PE	O31-C31-C32	2.43	119.55	111.91
49	P	401	PC1	O31-C31-C32	2.40	119.45	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	H	401	3PE	O31-C31-C32	2.40	119.44	111.91
45	M	505	3PE	O31-C31-C32	2.38	119.39	111.91
54	T	201	EHZ	C10-S1-C9	2.33	109.12	101.87
52	P	501	NDP	PN-O5D-C5D	-2.29	108.24	121.68
52	P	501	NDP	O2N-PN-O1N	2.25	123.39	112.24
48	F	501	FMN	C1'-N10-C9A	2.25	124.27	120.51
52	P	501	NDP	C5B-C4B-C3B	-2.25	106.75	115.18
52	P	501	NDP	PA-O5B-C5B	-2.21	108.71	121.68
49	H	402	PC1	O31-C31-C32	2.18	118.74	111.91
50	M	507	CDL	OA6-CA4-CA6	2.11	116.04	108.40
48	F	501	FMN	C10-N1-C2	2.01	120.93	116.90
54	U	201	EHZ	C10-S1-C9	2.00	108.11	101.87

There are no chirality outliers.

All (551) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O14
45	H	401	3PE	O13-C11-C12-N
45	H	401	3PE	C22-C21-O21-C2
45	H	403	3PE	C1-O11-P-O12
45	H	403	3PE	C1-O11-P-O13
45	H	403	3PE	C1-O11-P-O14
45	H	403	3PE	C11-O13-P-O12
45	H	403	3PE	C11-O13-P-O14
45	L	701	3PE	C1-O11-P-O14
45	L	704	3PE	C1-O11-P-O12
45	L	704	3PE	C1-O11-P-O14
45	L	704	3PE	O13-C11-C12-N
45	M	501	3PE	C1-O11-P-O12
45	M	501	3PE	O13-C11-C12-N
45	M	501	3PE	O22-C21-O21-C2
45	M	502	3PE	O32-C31-O31-C3
45	M	502	3PE	C32-C31-O31-C3
45	M	503	3PE	C11-O13-P-O11
45	M	503	3PE	C11-O13-P-O12
45	M	503	3PE	C11-O13-P-O14
45	M	503	3PE	O13-C11-C12-N
45	M	503	3PE	C22-C21-O21-C2
45	M	504	3PE	C11-O13-P-O11
45	M	504	3PE	C11-O13-P-O14
45	M	504	3PE	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	504	3PE	C22-C21-O21-C2
45	M	505	3PE	O13-C11-C12-N
45	M	505	3PE	C22-C21-O21-C2
45	M	506	3PE	O13-C11-C12-N
45	M	506	3PE	C22-C21-O21-C2
45	N	401	3PE	C1-O11-P-O12
45	N	401	3PE	C1-O11-P-O13
45	N	401	3PE	C1-O11-P-O14
45	N	401	3PE	C11-O13-P-O11
45	N	401	3PE	O13-C11-C12-N
45	N	401	3PE	O21-C2-C3-O31
45	N	401	3PE	C22-C21-O21-C2
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C3'-C4'-C5'-O5'
48	F	501	FMN	O4'-C4'-C5'-O5'
48	F	501	FMN	C5'-O5'-P-O2P
49	H	402	PC1	C1-O11-P-O14
49	H	402	PC1	O13-C11-C12-N
49	H	404	PC1	C11-O13-P-O14
49	H	404	PC1	C1-O11-P-O14
49	H	406	PC1	C11-O13-P-O14
49	H	406	PC1	C1-O11-P-O12
49	H	406	PC1	C1-O11-P-O14
49	H	406	PC1	O13-C11-C12-N
49	H	406	PC1	O22-C21-O21-C2
49	P	401	PC1	C11-O13-P-O12
49	P	401	PC1	C1-O11-P-O12
49	P	401	PC1	C1-O11-P-O13
49	P	401	PC1	O13-C11-C12-N
49	P	401	PC1	C3-C2-O21-C21
49	P	401	PC1	C22-C21-O21-C2
50	H	405	CDL	CA3-OA5-PA1-OA2
50	H	405	CDL	CA3-OA5-PA1-OA3
50	H	405	CDL	C11-CA5-OA6-CA4
50	H	405	CDL	C1-CB2-OB2-PB2
50	L	702	CDL	CA2-C1-CB2-OB2
50	L	702	CDL	CA3-OA5-PA1-OA3
50	L	702	CDL	OA7-CA5-OA6-CA4
50	L	702	CDL	OB7-CB5-OB6-CB4
50	L	703	CDL	CB2-C1-CA2-OA2
50	L	703	CDL	CA2-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	L	703	CDL	CA2-OA2-PA1-OA3
50	L	703	CDL	CA2-OA2-PA1-OA4
50	L	703	CDL	CA3-OA5-PA1-OA3
50	L	703	CDL	CA3-OA5-PA1-OA4
50	M	507	CDL	CA3-OA5-PA1-OA3
50	M	507	CDL	CA3-OA5-PA1-OA4
50	M	507	CDL	OA5-CA3-CA4-OA6
50	M	507	CDL	OA7-CA5-OA6-CA4
50	M	507	CDL	C11-CA5-OA6-CA4
50	M	507	CDL	CB2-OB2-PB2-OB4
50	M	507	CDL	C51-CB5-OB6-CB4
52	P	501	NDP	C2N-C3N-C7N-N7N
54	T	201	EHZ	O1-C7-C8-C9
54	T	201	EHZ	C11-C10-S1-C9
54	T	201	EHZ	C12-C13-C14-N2
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	C15-C16-C17-C18
54	U	201	EHZ	C15-C16-C17-C19
54	U	201	EHZ	C15-C16-C17-C20
54	U	201	EHZ	O5-C16-C17-C18
54	U	201	EHZ	O5-C16-C17-C19
54	U	201	EHZ	O5-C16-C17-C20
54	U	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
45	H	401	3PE	C32-C31-O31-C3
45	H	401	3PE	O32-C31-O31-C3
45	M	505	3PE	O32-C31-O31-C3
49	H	406	PC1	O32-C31-O31-C3
50	H	405	CDL	OA9-CA7-OA8-CA6
50	H	405	CDL	OB9-CB7-OB8-CB6
50	L	702	CDL	OA9-CA7-OA8-CA6
50	L	703	CDL	OB9-CB7-OB8-CB6
45	H	401	3PE	O22-C21-O21-C2
45	M	505	3PE	O22-C21-O21-C2
45	M	506	3PE	O22-C21-O21-C2
45	N	401	3PE	O22-C21-O21-C2
50	H	405	CDL	OA7-CA5-OA6-CA4
50	M	507	CDL	OB7-CB5-OB6-CB4
49	H	406	PC1	C32-C31-O31-C3
50	H	405	CDL	C31-CA7-OA8-CA6
45	M	501	3PE	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	H	406	PC1	C22-C21-O21-C2
50	L	702	CDL	C11-CA5-OA6-CA4
50	L	702	CDL	C51-CB5-OB6-CB4
45	M	505	3PE	C32-C31-O31-C3
50	H	405	CDL	C71-CB7-OB8-CB6
50	L	702	CDL	C31-CA7-OA8-CA6
50	L	703	CDL	C71-CB7-OB8-CB6
45	M	503	3PE	O22-C21-O21-C2
45	M	504	3PE	O22-C21-O21-C2
49	P	401	PC1	O22-C21-O21-C2
50	L	702	CDL	O1-C1-CB2-OB2
50	L	703	CDL	O1-C1-CA2-OA2
50	L	703	CDL	O1-C1-CB2-OB2
45	A	201	3PE	C32-C31-O31-C3
50	M	507	CDL	C71-CB7-OB8-CB6
45	N	401	3PE	O32-C31-O31-C3
50	H	405	CDL	C51-CB5-OB6-CB4
45	N	401	3PE	C32-C31-O31-C3
45	A	201	3PE	O32-C31-O31-C3
50	M	507	CDL	OB9-CB7-OB8-CB6
50	M	507	CDL	CB2-C1-CA2-OA2
45	L	704	3PE	O32-C31-O31-C3
45	L	704	3PE	C32-C31-O31-C3
45	M	501	3PE	C32-C31-O31-C3
45	M	506	3PE	C32-C31-O31-C3
50	M	507	CDL	O1-C1-CA2-OA2
45	M	501	3PE	O32-C31-O31-C3
50	H	405	CDL	OB7-CB5-OB6-CB4
49	H	402	PC1	C22-C21-O21-C2
45	H	401	3PE	C31-C32-C33-C34
45	L	701	3PE	C21-C22-C23-C24
49	H	402	PC1	C31-C32-C33-C34
50	L	702	CDL	CA7-C31-C32-C33
52	P	501	NDP	C3D-C4D-C5D-O5D
45	A	201	3PE	C31-C32-C33-C34
45	M	506	3PE	C31-C32-C33-C34
45	M	506	3PE	C21-C22-C23-C24
50	H	405	CDL	CA4-CA6-OA8-CA7
45	M	506	3PE	O32-C31-O31-C3
45	H	401	3PE	C11-O13-P-O11
45	H	403	3PE	C11-O13-P-O11
45	L	701	3PE	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	L	704	3PE	C1-O11-P-O13
45	M	501	3PE	C1-O11-P-O13
45	M	506	3PE	C1-O11-P-O13
49	H	402	PC1	C1-O11-P-O13
49	H	406	PC1	C1-O11-P-O13
49	P	401	PC1	C11-O13-P-O11
50	L	702	CDL	CA2-OA2-PA1-OA5
50	L	702	CDL	CB2-OB2-PB2-OB5
50	L	703	CDL	CA2-OA2-PA1-OA5
50	L	703	CDL	CA3-OA5-PA1-OA2
50	M	507	CDL	CA3-OA5-PA1-OA2
50	M	507	CDL	CB2-OB2-PB2-OB5
49	H	402	PC1	O22-C21-O21-C2
45	M	504	3PE	C32-C31-O31-C3
45	L	701	3PE	C22-C21-O21-C2
45	H	401	3PE	C38-C39-C3A-C3B
45	L	701	3PE	C35-C36-C37-C38
45	M	501	3PE	C3E-C3F-C3G-C3H
45	M	502	3PE	C28-C29-C2A-C2B
45	M	503	3PE	C3E-C3F-C3G-C3H
45	M	504	3PE	C37-C38-C39-C3A
45	M	503	3PE	C35-C36-C37-C38
45	M	504	3PE	C34-C35-C36-C37
50	L	702	CDL	C56-C57-C58-C59
50	M	507	CDL	C54-C55-C56-C57
50	M	507	CDL	CA6-CA4-OA6-CA5
45	L	701	3PE	O22-C21-O21-C2
50	L	702	CDL	CB5-C51-C52-C53
45	A	201	3PE	C2B-C2C-C2D-C2E
45	M	501	3PE	C38-C39-C3A-C3B
49	H	404	PC1	C24-C25-C26-C27
50	L	702	CDL	C74-C75-C76-C77
45	M	505	3PE	C2C-C2D-C2E-C2F
45	M	506	3PE	C34-C35-C36-C37
49	H	404	PC1	C27-C28-C29-C2A
49	P	401	PC1	C37-C38-C39-C3A
50	L	703	CDL	C19-C20-C21-C22
50	M	507	CDL	C51-C52-C53-C54
50	H	405	CDL	CA5-C11-C12-C13
45	L	701	3PE	C32-C31-O31-C3
45	H	401	3PE	C2B-C2C-C2D-C2E
49	H	404	PC1	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	H	404	PC1	C35-C36-C37-C38
45	H	403	3PE	C25-C26-C27-C28
45	M	503	3PE	C2B-C2C-C2D-C2E
49	H	402	PC1	C35-C36-C37-C38
50	H	405	CDL	CB7-C71-C72-C73
45	H	401	3PE	C3E-C3F-C3G-C3H
45	M	501	3PE	C24-C25-C26-C27
45	M	502	3PE	C22-C23-C24-C25
45	M	503	3PE	C24-C25-C26-C27
45	N	401	3PE	C3C-C3D-C3E-C3F
45	H	403	3PE	C22-C21-O21-C2
49	H	402	PC1	C21-C22-C23-C24
49	P	401	PC1	C31-C32-C33-C34
45	M	501	3PE	C28-C29-C2A-C2B
45	N	401	3PE	C28-C29-C2A-C2B
49	H	402	PC1	C26-C27-C28-C29
49	H	404	PC1	C22-C23-C24-C25
50	L	702	CDL	C77-C78-C79-C80
49	H	406	PC1	C23-C24-C25-C26
45	M	504	3PE	C27-C28-C29-C2A
49	H	404	PC1	C29-C2A-C2B-C2C
50	L	703	CDL	C11-C12-C13-C14
50	L	702	CDL	C51-C52-C53-C54
54	T	201	EHZ	S1-C10-C11-N1
45	H	401	3PE	C36-C37-C38-C39
45	M	505	3PE	C25-C26-C27-C28
45	N	401	3PE	C2C-C2D-C2E-C2F
45	M	501	3PE	C22-C23-C24-C25
45	M	505	3PE	C29-C2A-C2B-C2C
50	L	703	CDL	C22-C23-C24-C25
50	M	507	CDL	C57-C58-C59-C60
50	H	405	CDL	CB5-C51-C52-C53
45	M	501	3PE	C2D-C2E-C2F-C2G
45	H	401	3PE	C37-C38-C39-C3A
50	L	702	CDL	C34-C35-C36-C37
50	L	702	CDL	C54-C55-C56-C57
45	A	201	3PE	C33-C34-C35-C36
45	M	504	3PE	O32-C31-O31-C3
45	L	704	3PE	C2D-C2E-C2F-C2G
45	M	505	3PE	C37-C38-C39-C3A
45	M	501	3PE	C2-C1-O11-P
45	L	701	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	N	401	3PE	C2E-C2F-C2G-C2H
50	L	703	CDL	C14-C15-C16-C17
54	U	201	EHZ	C3-C4-C5-C6
50	M	507	CDL	C31-CA7-OA8-CA6
45	M	505	3PE	C3A-C3B-C3C-C3D
45	M	504	3PE	C3C-C3D-C3E-C3F
45	M	502	3PE	C38-C39-C3A-C3B
45	H	403	3PE	O22-C21-O21-C2
50	L	702	CDL	CB7-C71-C72-C73
45	M	503	3PE	C32-C31-O31-C3
50	L	702	CDL	C72-C73-C74-C75
45	M	505	3PE	C24-C25-C26-C27
49	H	402	PC1	C24-C25-C26-C27
45	H	401	3PE	C2C-C2D-C2E-C2F
45	M	501	3PE	C39-C3A-C3B-C3C
49	P	401	PC1	C33-C34-C35-C36
45	H	403	3PE	C22-C23-C24-C25
45	H	403	3PE	C28-C29-C2A-C2B
50	M	507	CDL	C33-C34-C35-C36
52	P	501	NDP	O4D-C4D-C5D-O5D
49	H	404	PC1	C36-C37-C38-C39
45	M	505	3PE	C34-C35-C36-C37
50	H	405	CDL	C14-C15-C16-C17
50	M	507	CDL	OA9-CA7-OA8-CA6
50	H	405	CDL	CB2-OB2-PB2-OB5
50	L	703	CDL	CB3-OB5-PB2-OB2
45	H	401	3PE	C23-C24-C25-C26
49	H	406	PC1	C2-C1-O11-P
45	A	201	3PE	C27-C28-C29-C2A
49	H	404	PC1	O11-C1-C2-C3
50	M	507	CDL	OA5-CA3-CA4-CA6
45	N	401	3PE	C34-C35-C36-C37
49	H	402	PC1	C36-C37-C38-C39
45	M	504	3PE	C2-C3-O31-C31
45	H	403	3PE	C32-C33-C34-C35
45	N	401	3PE	C36-C37-C38-C39
45	L	701	3PE	C2C-C2D-C2E-C2F
45	L	701	3PE	C32-C33-C34-C35
45	M	504	3PE	C1-C2-C3-O31
49	H	402	PC1	C3A-C3B-C3C-C3D
50	H	405	CDL	CA3-CA4-CA6-OA8
50	H	405	CDL	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	L	702	CDL	CB3-CB4-CB6-OB8
45	A	201	3PE	C35-C36-C37-C38
45	M	503	3PE	O32-C31-O31-C3
45	M	501	3PE	C2F-C2G-C2H-C2I
45	M	503	3PE	C38-C39-C3A-C3B
49	H	404	PC1	C32-C33-C34-C35
50	H	405	CDL	C18-C19-C20-C21
50	L	703	CDL	C55-C56-C57-C58
49	H	406	PC1	C31-C32-C33-C34
45	L	701	3PE	C2B-C2C-C2D-C2E
48	F	501	FMN	C5'-O5'-P-O1P
45	A	201	3PE	C2F-C2G-C2H-C2I
45	M	503	3PE	C2E-C2F-C2G-C2H
45	N	401	3PE	C37-C38-C39-C3A
45	N	401	3PE	C2F-C2G-C2H-C2I
50	M	507	CDL	C12-C13-C14-C15
50	H	405	CDL	O1-C1-CB2-OB2
45	N	401	3PE	C3F-C3G-C3H-C3I
50	L	702	CDL	C31-C32-C33-C34
49	H	402	PC1	C25-C26-C27-C28
45	L	701	3PE	C3A-C3B-C3C-C3D
50	L	702	CDL	C11-C12-C13-C14
54	U	201	EHZ	C1-C2-C3-C4
45	M	505	3PE	C3F-C3G-C3H-C3I
49	H	402	PC1	C28-C29-C2A-C2B
45	H	401	3PE	C2F-C2G-C2H-C2I
49	H	402	PC1	C23-C24-C25-C26
50	M	507	CDL	C31-C32-C33-C34
45	L	704	3PE	O11-C1-C2-C3
45	H	401	3PE	C25-C26-C27-C28
45	H	403	3PE	C27-C28-C29-C2A
45	M	505	3PE	C32-C33-C34-C35
49	P	401	PC1	C3C-C3D-C3E-C3F
50	L	703	CDL	C31-CA7-OA8-CA6
45	L	701	3PE	C2-C1-O11-P
50	L	703	CDL	C1-CA2-OA2-PA1
50	M	507	CDL	C61-C62-C63-C64
45	H	403	3PE	C2C-C2D-C2E-C2F
49	H	404	PC1	C38-C39-C3A-C3B
49	P	401	PC1	C34-C35-C36-C37
45	M	503	3PE	C39-C3A-C3B-C3C
45	N	401	3PE	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	H	406	PC1	C33-C34-C35-C36
45	A	201	3PE	C1-O11-P-O13
49	H	402	PC1	C11-O13-P-O11
49	H	404	PC1	C11-O13-P-O11
49	H	406	PC1	C11-O13-P-O11
50	L	702	CDL	CA3-OA5-PA1-OA2
45	L	704	3PE	O11-C1-C2-O21
49	H	404	PC1	O11-C1-C2-O21
50	H	405	CDL	OA5-CA3-CA4-OA6
50	L	702	CDL	OB5-CB3-CB4-OB6
45	M	505	3PE	C27-C28-C29-C2A
49	P	401	PC1	C3F-C3G-C3H-C3I
45	A	201	3PE	C21-C22-C23-C24
45	M	503	3PE	C28-C29-C2A-C2B
49	P	401	PC1	C39-C3A-C3B-C3C
45	L	704	3PE	C34-C35-C36-C37
45	N	401	3PE	C2A-C2B-C2C-C2D
45	M	505	3PE	O21-C2-C3-O31
50	H	405	CDL	OB6-CB4-CB6-OB8
45	L	701	3PE	C3D-C3E-C3F-C3G
45	M	502	3PE	C26-C27-C28-C29
45	M	502	3PE	C2-C1-O11-P
50	L	703	CDL	CA4-CA3-OA5-PA1
45	M	502	3PE	C2A-C2B-C2C-C2D
51	O	401	ADP	PB-O3A-PA-O5'
45	M	502	3PE	O11-C1-C2-C3
49	P	401	PC1	O11-C1-C2-C3
45	M	504	3PE	C24-C25-C26-C27
45	M	503	3PE	C26-C27-C28-C29
45	L	704	3PE	C36-C37-C38-C39
48	F	501	FMN	C5'-O5'-P-O3P
50	M	507	CDL	CB3-CB4-OB6-CB5
45	M	505	3PE	C1-C2-C3-O31
50	L	703	CDL	CA3-CA4-CA6-OA8
50	M	507	CDL	CB3-CB4-CB6-OB8
45	M	506	3PE	O11-C1-C2-O21
45	M	501	3PE	C32-C33-C34-C35
50	L	703	CDL	OA9-CA7-OA8-CA6
45	A	201	3PE	O21-C2-C3-O31
49	H	406	PC1	O21-C2-C3-O31
50	H	405	CDL	OA6-CA4-CA6-OA8
50	L	702	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	504	3PE	C31-C32-C33-C34
51	O	401	ADP	C5'-O5'-PA-O3A
45	M	503	3PE	C33-C34-C35-C36
50	L	703	CDL	C11-CA5-OA6-CA4
45	A	201	3PE	C22-C23-C24-C25
50	M	507	CDL	C62-C63-C64-C65
50	L	703	CDL	OA7-CA5-OA6-CA4
45	M	502	3PE	C24-C25-C26-C27
45	M	503	3PE	C37-C38-C39-C3A
50	L	703	CDL	C71-C72-C73-C74
54	U	201	EHZ	C5-C6-C7-O1
49	H	406	PC1	C36-C37-C38-C39
49	P	401	PC1	C21-C22-C23-C24
45	M	501	3PE	C11-O13-P-O11
49	H	404	PC1	C1-O11-P-O13
45	M	503	3PE	C3C-C3D-C3E-C3F
50	L	702	CDL	CA4-CA3-OA5-PA1
45	H	401	3PE	C11-O13-P-O12
45	L	701	3PE	C1-O11-P-O12
45	L	701	3PE	C11-O13-P-O12
45	M	501	3PE	C11-O13-P-O12
45	M	504	3PE	C11-O13-P-O12
45	M	506	3PE	C1-O11-P-O14
49	H	404	PC1	C1-O11-P-O12
49	P	401	PC1	C11-O13-P-O14
49	P	401	PC1	C1-O11-P-O14
50	H	405	CDL	CB2-OB2-PB2-OB3
50	H	405	CDL	CB2-OB2-PB2-OB4
50	L	702	CDL	CA2-OA2-PA1-OA3
50	L	702	CDL	CA3-OA5-PA1-OA4
50	L	702	CDL	CB2-OB2-PB2-OB3
50	L	703	CDL	CB2-OB2-PB2-OB3
50	L	703	CDL	CB3-OB5-PB2-OB4
50	M	507	CDL	CB2-OB2-PB2-OB3
54	T	201	EHZ	C6-C7-C8-C9
50	L	703	CDL	CA7-C31-C32-C33
45	M	501	3PE	O11-C1-C2-C3
45	M	506	3PE	O11-C1-C2-C3
45	M	503	3PE	C12-C11-O13-P
45	N	401	3PE	C12-C11-O13-P
45	H	403	3PE	C2A-C2B-C2C-C2D
45	L	704	3PE	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	H	403	3PE	C3E-C3F-C3G-C3H
45	H	401	3PE	C24-C25-C26-C27
49	H	404	PC1	C2E-C2F-C2G-C2H
45	M	506	3PE	C23-C24-C25-C26
54	U	201	EHZ	C2-C1-C21-C22
49	P	401	PC1	C11-C12-N-C14
45	N	401	3PE	C1-C2-C3-O31
49	H	406	PC1	C1-C2-C3-O31
50	H	405	CDL	CB3-CB4-CB6-OB8
45	M	504	3PE	O21-C2-C3-O31
45	M	502	3PE	C31-C32-C33-C34
45	M	505	3PE	C2F-C2G-C2H-C2I
45	H	403	3PE	C34-C35-C36-C37
45	H	403	3PE	C3C-C3D-C3E-C3F
45	M	505	3PE	C26-C27-C28-C29
50	L	702	CDL	C12-C13-C14-C15
52	P	501	NDP	O4D-C1D-N1N-C6N
50	L	703	CDL	C16-C17-C18-C19
50	L	702	CDL	C19-C20-C21-C22
45	M	502	3PE	C37-C38-C39-C3A
50	L	702	CDL	C15-C16-C17-C18
45	H	401	3PE	C3-C2-O21-C21
45	L	701	3PE	C3-C2-O21-C21
49	P	401	PC1	C3D-C3E-C3F-C3G
45	M	504	3PE	C29-C2A-C2B-C2C
45	M	502	3PE	O11-C1-C2-O21
45	A	201	3PE	C11-O13-P-O11
45	L	704	3PE	C11-O13-P-O11
50	L	703	CDL	C72-C73-C74-C75
45	A	201	3PE	C1-C2-C3-O31
50	L	702	CDL	CA3-CA4-CA6-OA8
50	H	405	CDL	C11-C12-C13-C14
45	M	502	3PE	C35-C36-C37-C38
45	A	201	3PE	C2-C1-O11-P
45	H	401	3PE	C2-C1-O11-P
45	H	403	3PE	C29-C2A-C2B-C2C
45	M	504	3PE	C25-C26-C27-C28
45	H	401	3PE	C28-C29-C2A-C2B
45	H	401	3PE	C2E-C2F-C2G-C2H
45	H	401	3PE	C2D-C2E-C2F-C2G
49	P	401	PC1	C11-C12-N-C15
50	L	703	CDL	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	M	507	CDL	C60-C61-C62-C63
45	M	502	3PE	C2B-C2C-C2D-C2E
50	L	702	CDL	C16-C17-C18-C19
50	L	703	CDL	OA6-CA4-CA6-OA8
49	P	401	PC1	C23-C24-C25-C26
50	L	702	CDL	C52-C53-C54-C55
50	H	405	CDL	C12-C13-C14-C15
45	L	701	3PE	C39-C3A-C3B-C3C
45	L	704	3PE	C1-C2-C3-O31
49	H	402	PC1	C1-C2-C3-O31
54	U	201	EHZ	C18-C17-C20-O6
45	M	502	3PE	C33-C34-C35-C36
45	M	504	3PE	C28-C29-C2A-C2B
54	U	201	EHZ	C4-C5-C6-C7
50	L	703	CDL	CA3-CA4-OA6-CA5
50	L	703	CDL	CB3-CB4-OB6-CB5
49	P	401	PC1	C11-C12-N-C13
49	H	402	PC1	C33-C34-C35-C36
45	M	501	3PE	O11-C1-C2-O21
49	H	404	PC1	O21-C21-C22-C23
45	M	505	3PE	O11-C1-C2-C3
50	L	702	CDL	OB5-CB3-CB4-CB6
45	M	504	3PE	C2F-C2G-C2H-C2I
45	M	505	3PE	C2E-C2F-C2G-C2H
54	U	201	EHZ	C11-C10-S1-C9
45	L	701	3PE	O21-C2-C3-O31
50	H	405	CDL	CB2-C1-CA2-OA2
45	H	403	3PE	C2F-C2G-C2H-C2I
49	P	401	PC1	C24-C25-C26-C27
49	H	402	PC1	O32-C31-O31-C3
45	M	505	3PE	C39-C3A-C3B-C3C
50	H	405	CDL	OB5-CB3-CB4-OB6
50	M	507	CDL	OB5-CB3-CB4-OB6
50	H	405	CDL	OA5-CA3-CA4-CA6
45	H	403	3PE	C24-C25-C26-C27
45	H	403	3PE	C36-C37-C38-C39
49	H	404	PC1	C2F-C2G-C2H-C2I
45	M	501	3PE	O31-C31-C32-C33
45	N	401	3PE	O21-C21-C22-C23
45	L	704	3PE	C2C-C2D-C2E-C2F
49	H	404	PC1	O31-C31-C32-C33
45	L	704	3PE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	505	3PE	C35-C36-C37-C38
49	H	402	PC1	C3-C2-O21-C21
45	M	501	3PE	C3C-C3D-C3E-C3F
49	P	401	PC1	C3E-C3F-C3G-C3H
50	L	703	CDL	C72-C71-CB7-OB8
45	H	401	3PE	O31-C31-C32-C33
49	H	402	PC1	C34-C35-C36-C37
45	N	401	3PE	C39-C3A-C3B-C3C
50	H	405	CDL	O1-C1-CA2-OA2
50	L	702	CDL	C12-C11-CA5-OA6
50	H	405	CDL	C32-C33-C34-C35
45	A	201	3PE	C28-C29-C2A-C2B
45	M	501	3PE	O21-C21-C22-C23
50	H	405	CDL	C52-C51-CB5-OB6
50	L	703	CDL	C51-C52-C53-C54
45	M	501	3PE	C3B-C3C-C3D-C3E
49	H	402	PC1	O31-C31-C32-C33
50	L	702	CDL	C53-C54-C55-C56
45	A	201	3PE	O21-C21-C22-C23
49	H	402	PC1	C32-C31-O31-C3
45	H	403	3PE	C3A-C3B-C3C-C3D
50	L	703	CDL	C72-C71-CB7-OB9
45	M	501	3PE	C3A-C3B-C3C-C3D
45	M	501	3PE	O32-C31-C32-C33
49	H	404	PC1	O32-C31-C32-C33
50	L	702	CDL	C12-C11-CA5-OA7
54	U	201	EHZ	C2-C3-C4-C5
50	L	702	CDL	C52-C51-CB5-OB6
45	L	704	3PE	O22-C21-O21-C2
45	M	504	3PE	C3B-C3C-C3D-C3E
49	H	402	PC1	C11-O13-P-O12
50	M	507	CDL	CA2-OA2-PA1-OA3
51	O	401	ADP	C5'-O5'-PA-O1A
51	O	401	ADP	C5'-O5'-PA-O2A
51	O	401	ADP	O4'-C4'-C5'-O5'
50	H	405	CDL	C52-C51-CB5-OB7
45	M	504	3PE	O31-C31-C32-C33
45	H	403	3PE	O13-C11-C12-N
45	L	701	3PE	O13-C11-C12-N
45	M	505	3PE	C22-C23-C24-C25
45	M	501	3PE	C34-C35-C36-C37
45	H	401	3PE	C12-C11-O13-P

Continued on next page...

Continued from previous page...

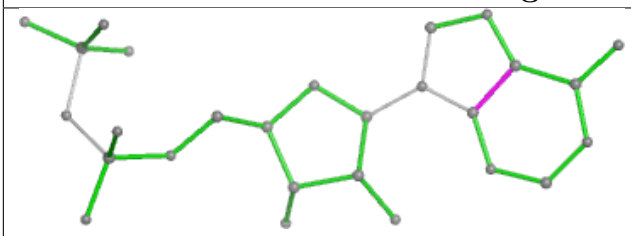
Mol	Chain	Res	Type	Atoms
45	H	403	3PE	C12-C11-O13-P
45	M	506	3PE	C12-C11-O13-P
49	H	402	PC1	C1-C2-O21-C21
50	H	405	CDL	CA3-CA4-OA6-CA5
50	L	703	CDL	CA6-CA4-OA6-CA5
45	L	704	3PE	C31-C32-C33-C34
45	H	401	3PE	O32-C31-C32-C33
49	H	406	PC1	O31-C31-C32-C33
45	M	502	3PE	O31-C31-C32-C33
49	P	401	PC1	O31-C31-C32-C33
49	H	402	PC1	O32-C31-C32-C33
45	H	403	3PE	C2B-C2C-C2D-C2E
50	H	405	CDL	C12-C11-CA5-OA6
45	M	501	3PE	O22-C21-C22-C23
45	A	201	3PE	O22-C21-C22-C23
45	M	506	3PE	O31-C31-C32-C33
49	H	406	PC1	O32-C31-C32-C33
50	H	405	CDL	C12-C11-CA5-OA7
50	L	702	CDL	C52-C51-CB5-OB7
45	H	401	3PE	C32-C33-C34-C35
45	M	505	3PE	O21-C21-C22-C23
45	M	506	3PE	O32-C31-C32-C33

There are no ring outliers.

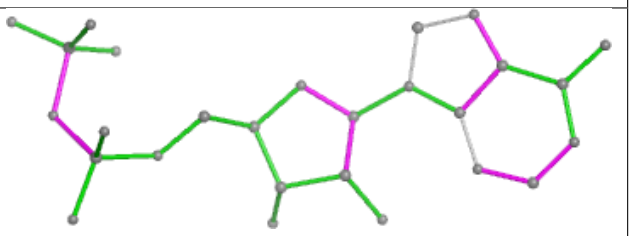
No monomer is involved in short contacts.

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 then 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.

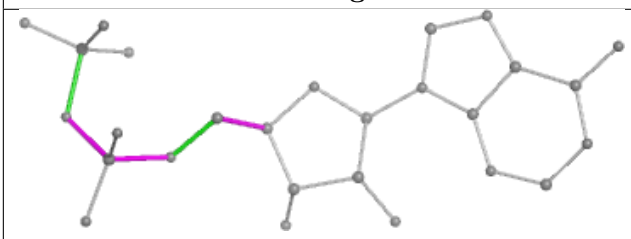
Ligand ADP O 401



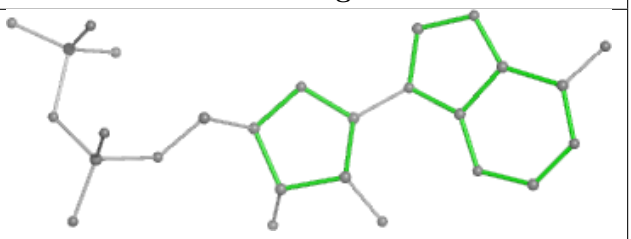
Bond lengths



Bond angles

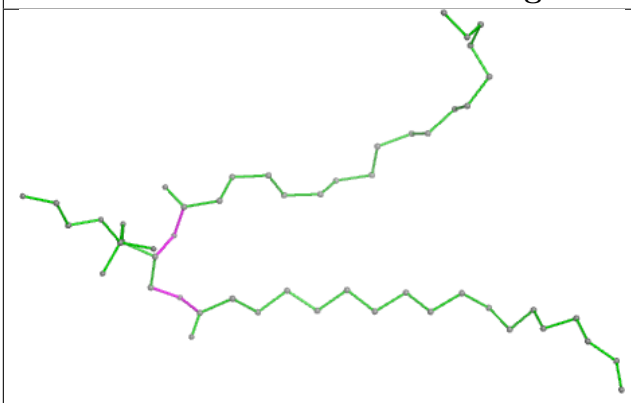


Torsions

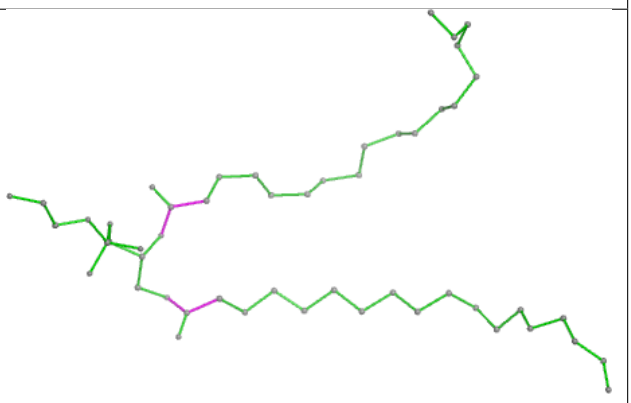


Rings

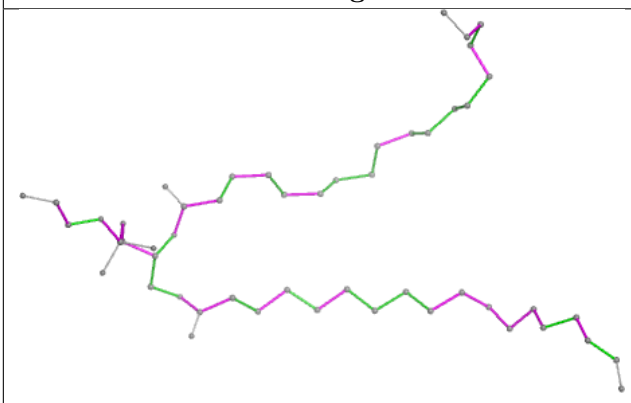
Ligand 3PE M 501



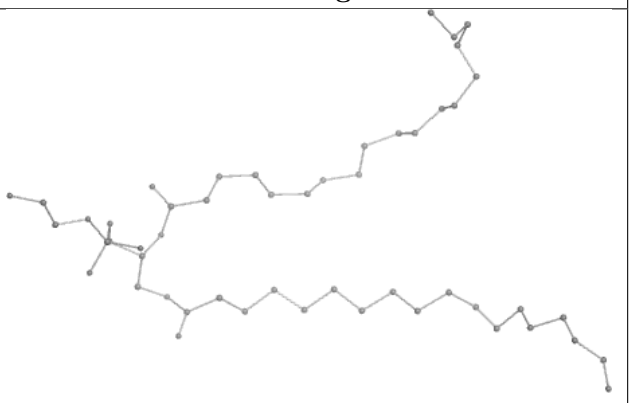
Bond lengths



Bond angles

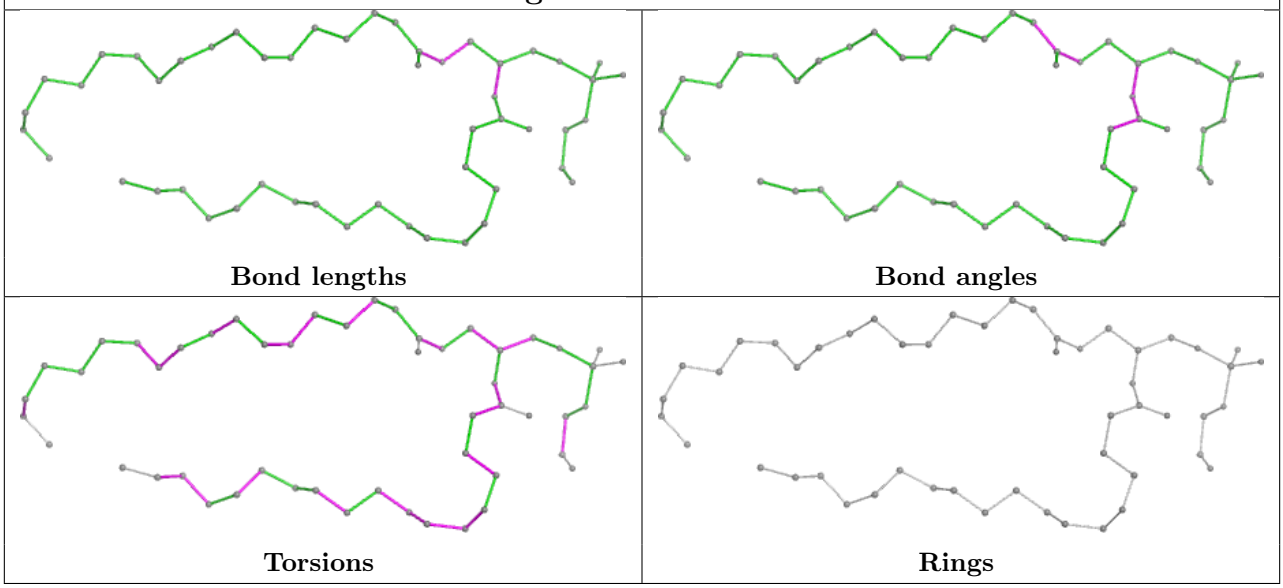


Torsions

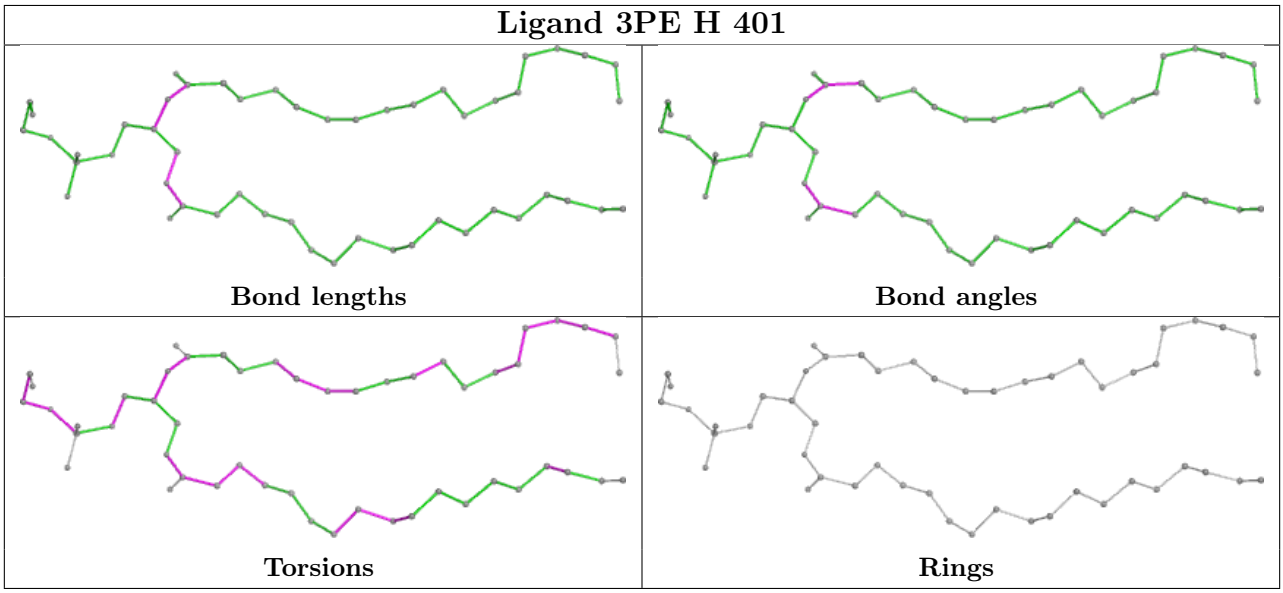


Rings

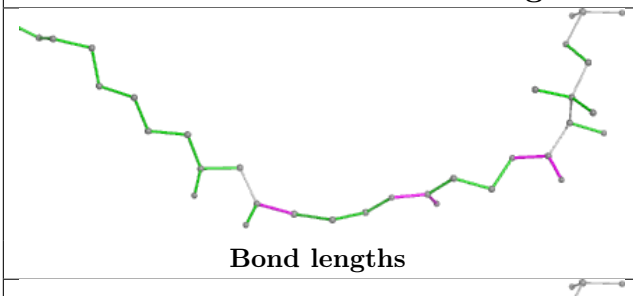
Ligand 3PE M 505



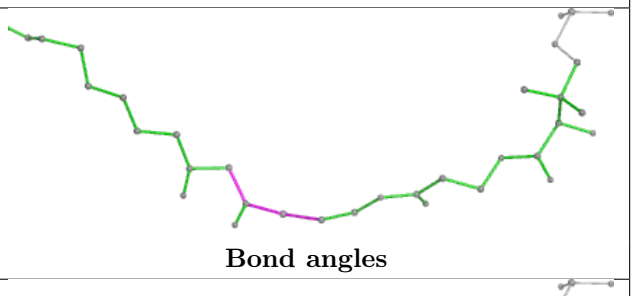
Ligand 3PE H 401



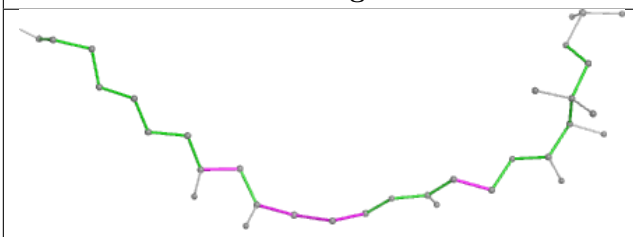
Ligand EHZ T 201



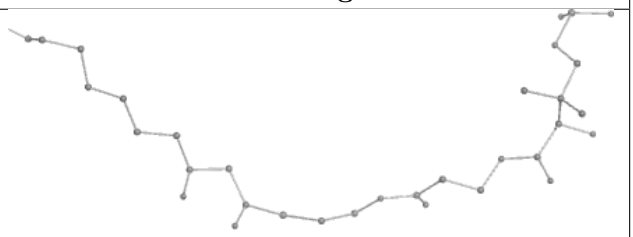
Bond lengths



Bond angles

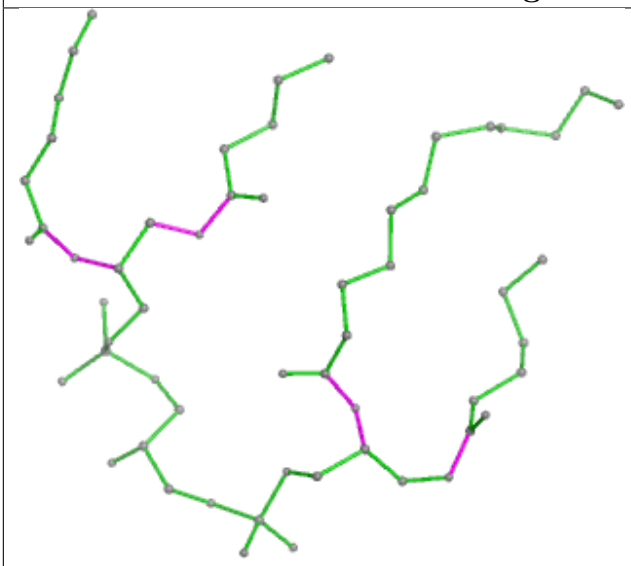


Torsions

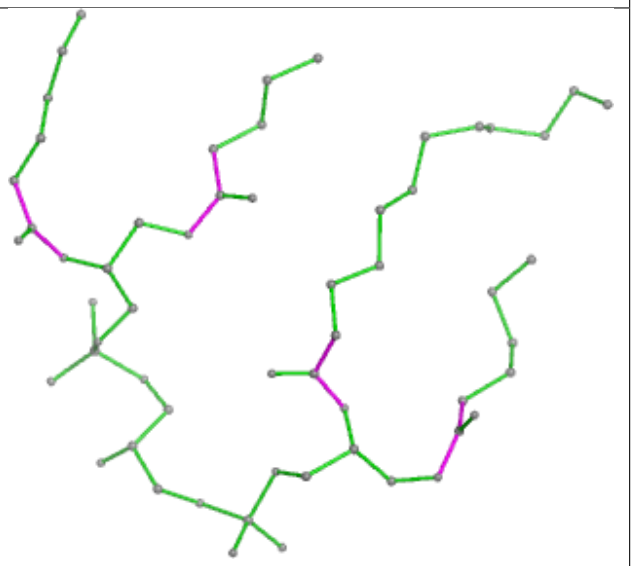


Rings

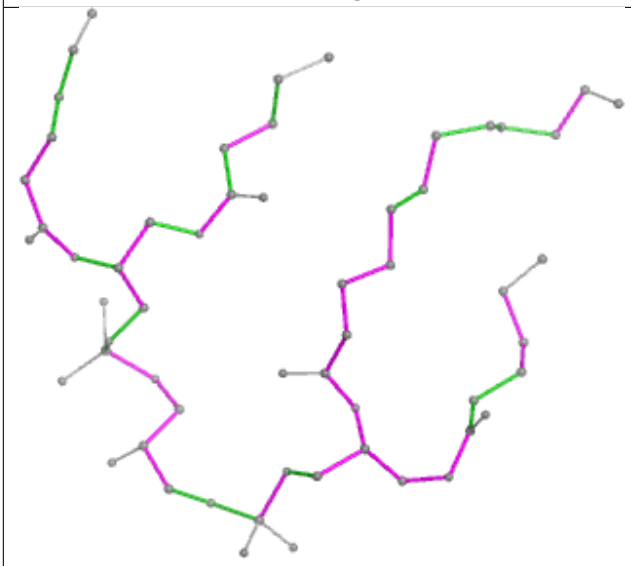
Ligand CDL H 405



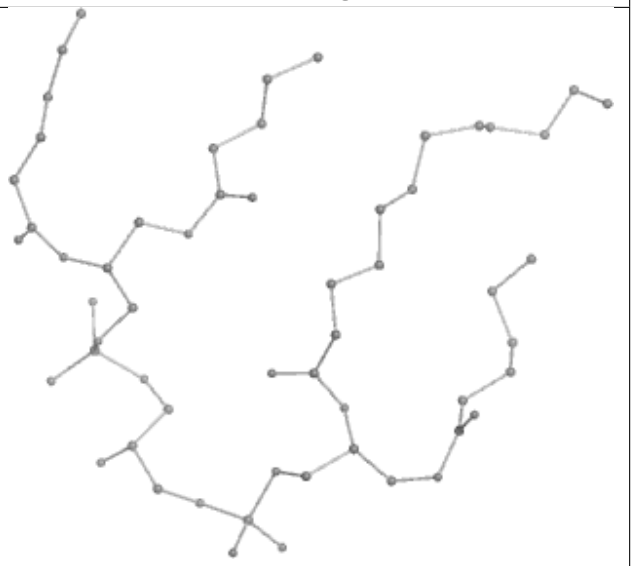
Bond lengths



Bond angles

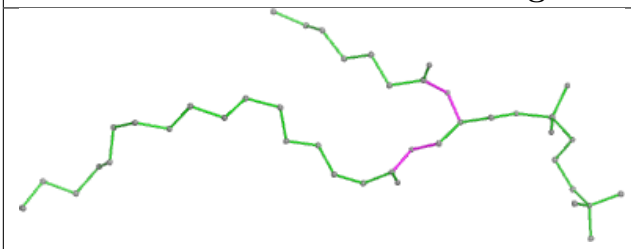


Torsions

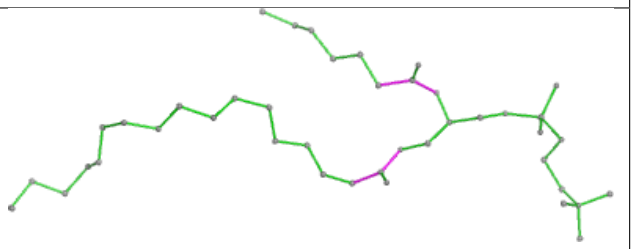


Rings

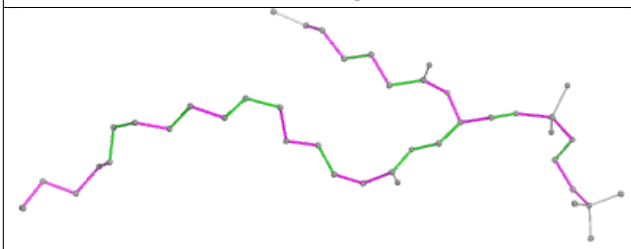
Ligand PC1 P 401



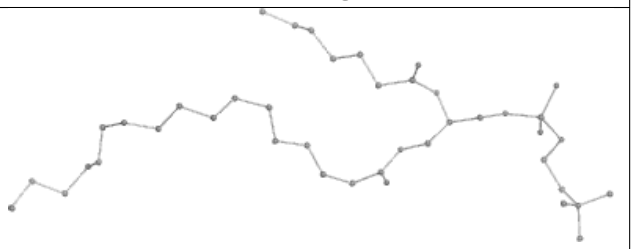
Bond lengths



Bond angles



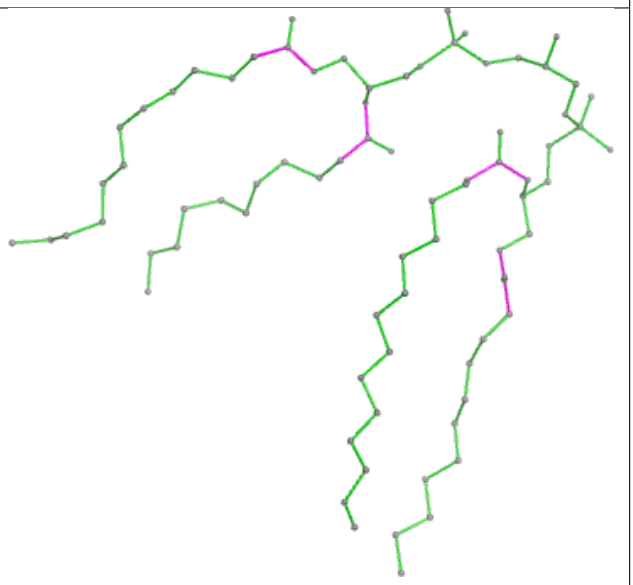
Torsions



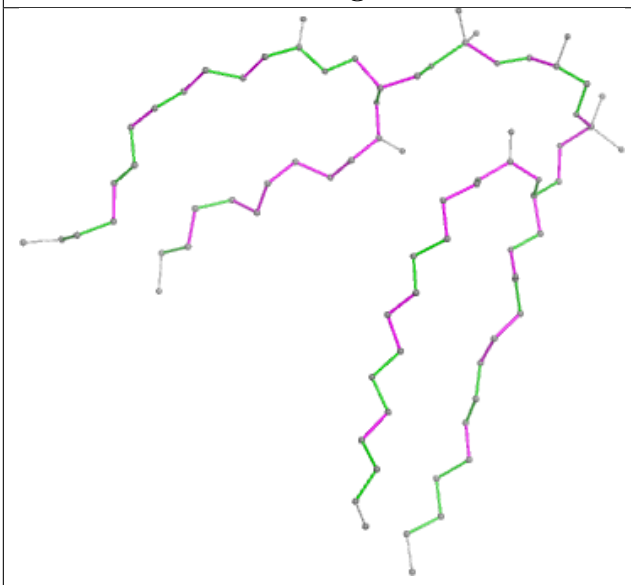
Rings

Ligand CDL L 702

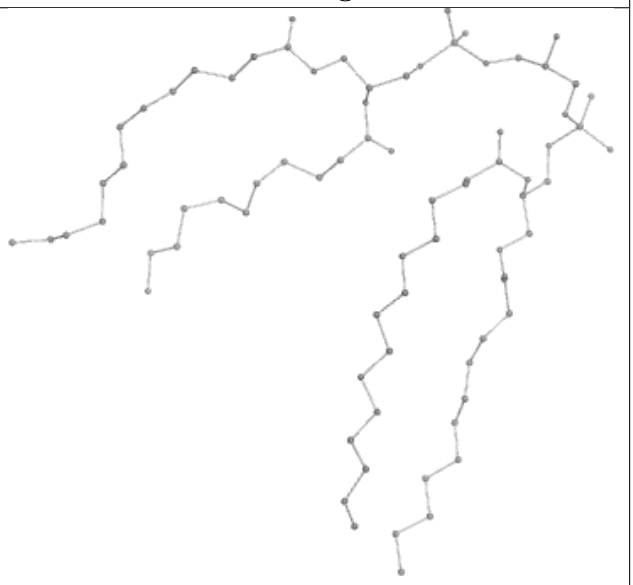
Bond lengths



Bond angles

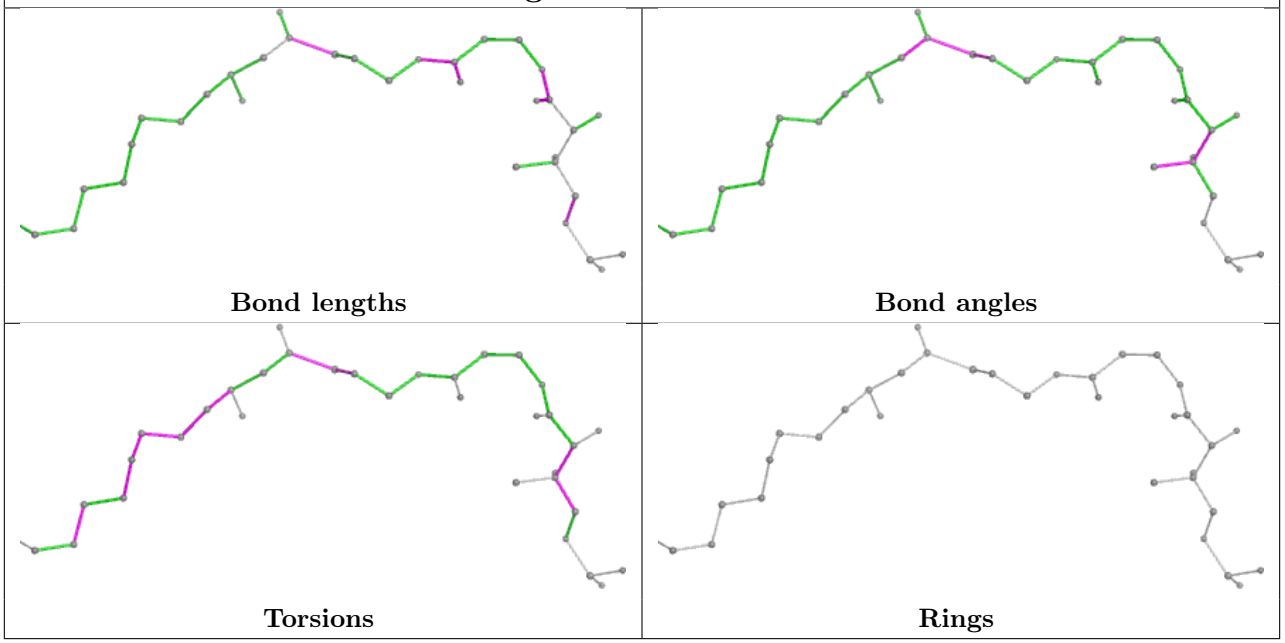


Torsions

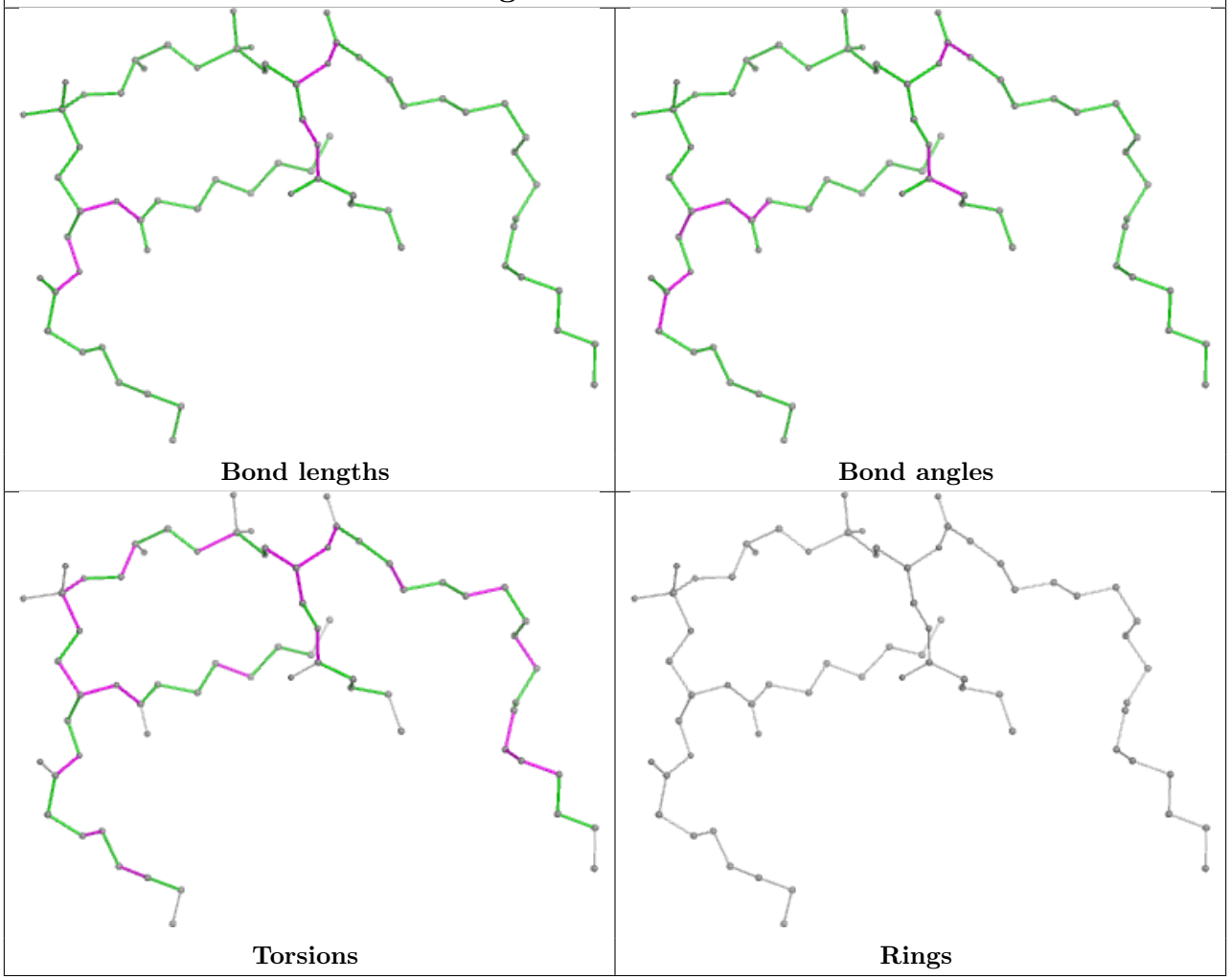


Rings

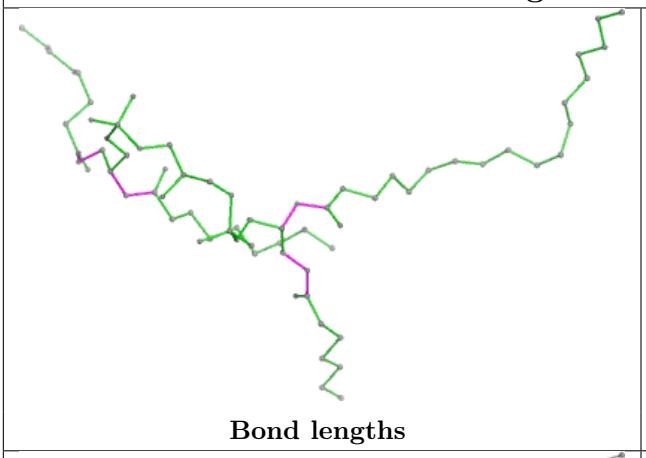
Ligand EHZ U 201



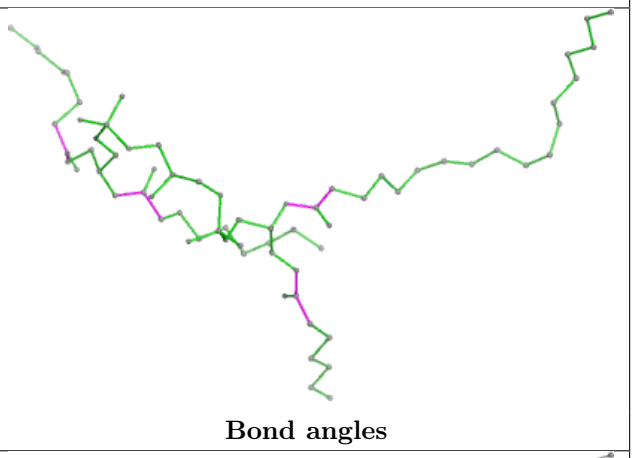
Ligand CDL M 507



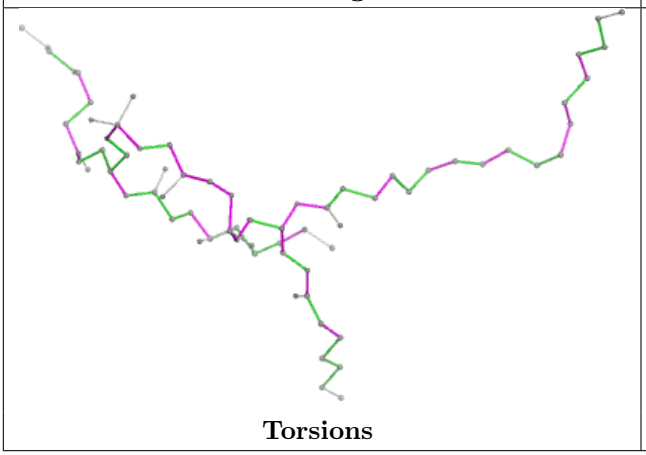
Ligand CDL L 703



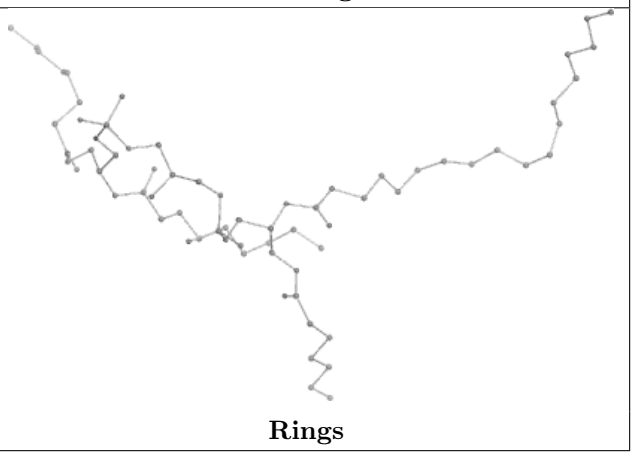
Bond lengths



Bond angles

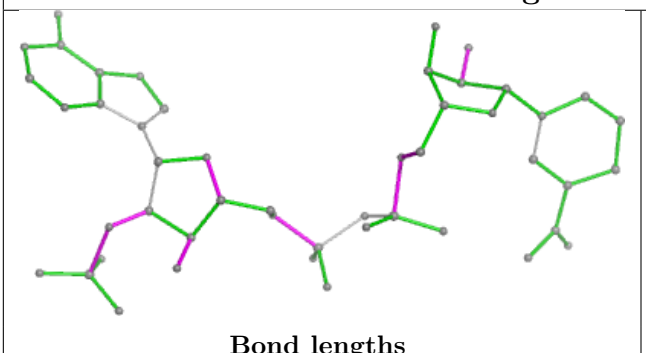


Torsions

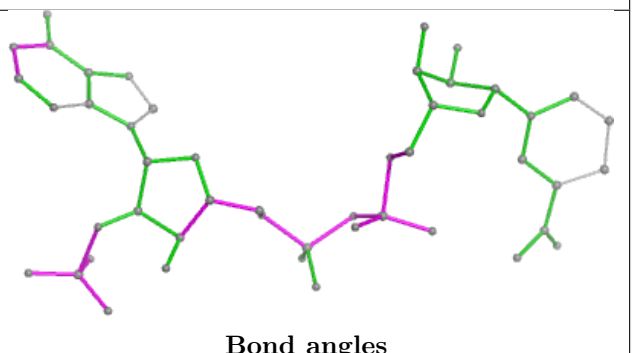


Rings

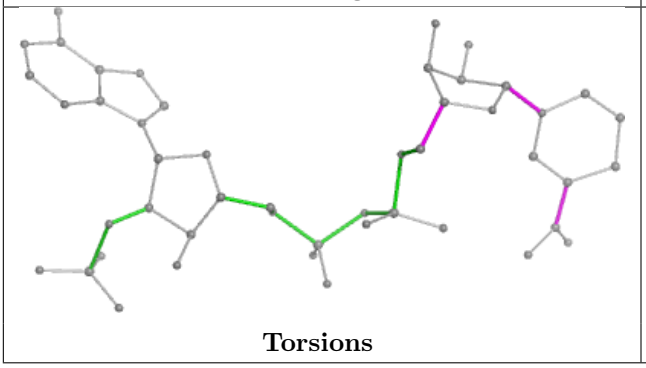
Ligand NDP P 501



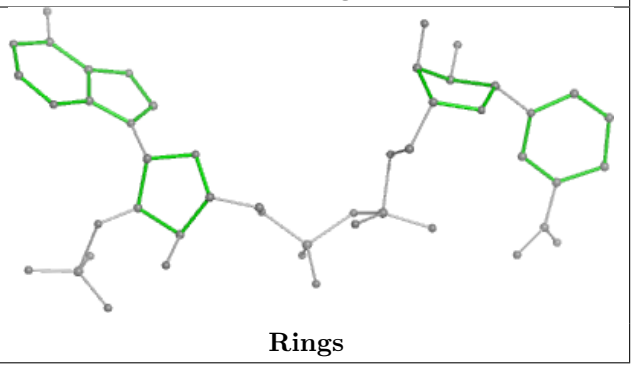
Bond lengths



Bond angles

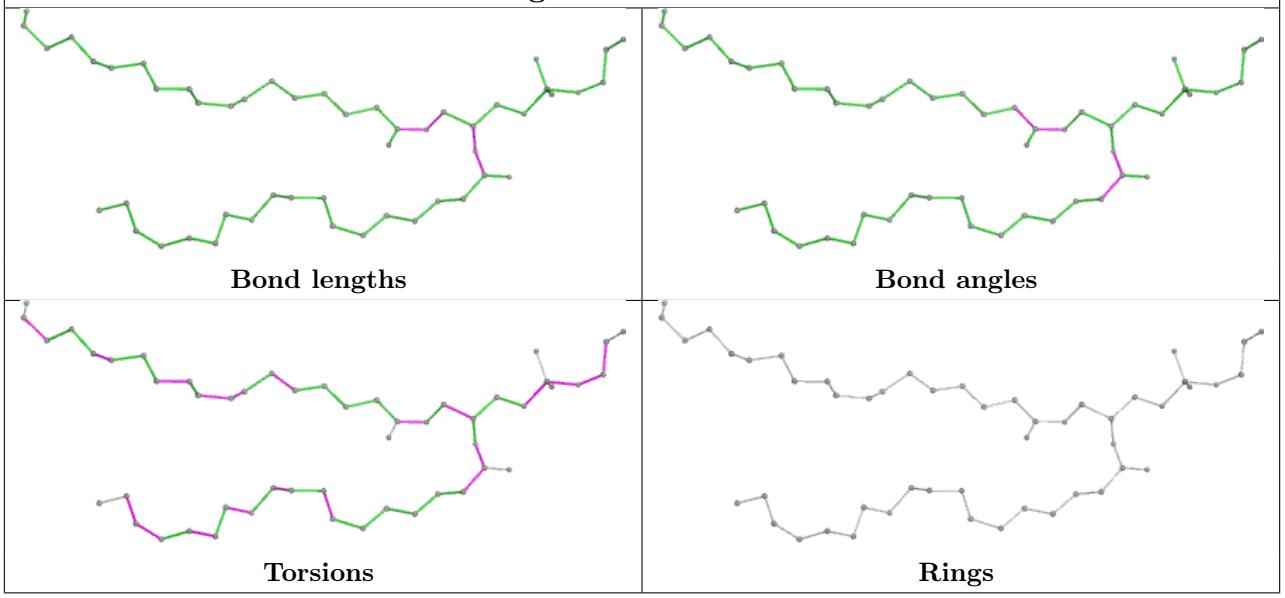


Torsions

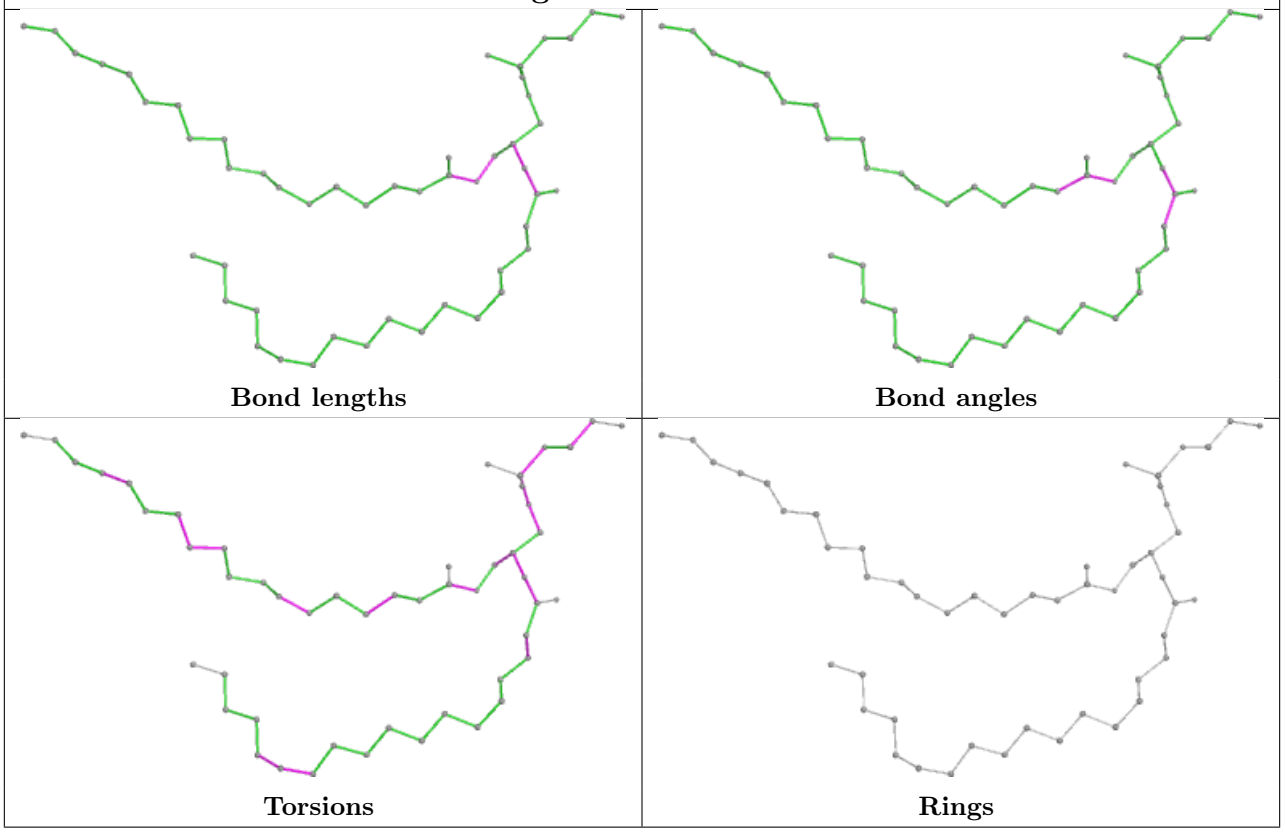


Rings

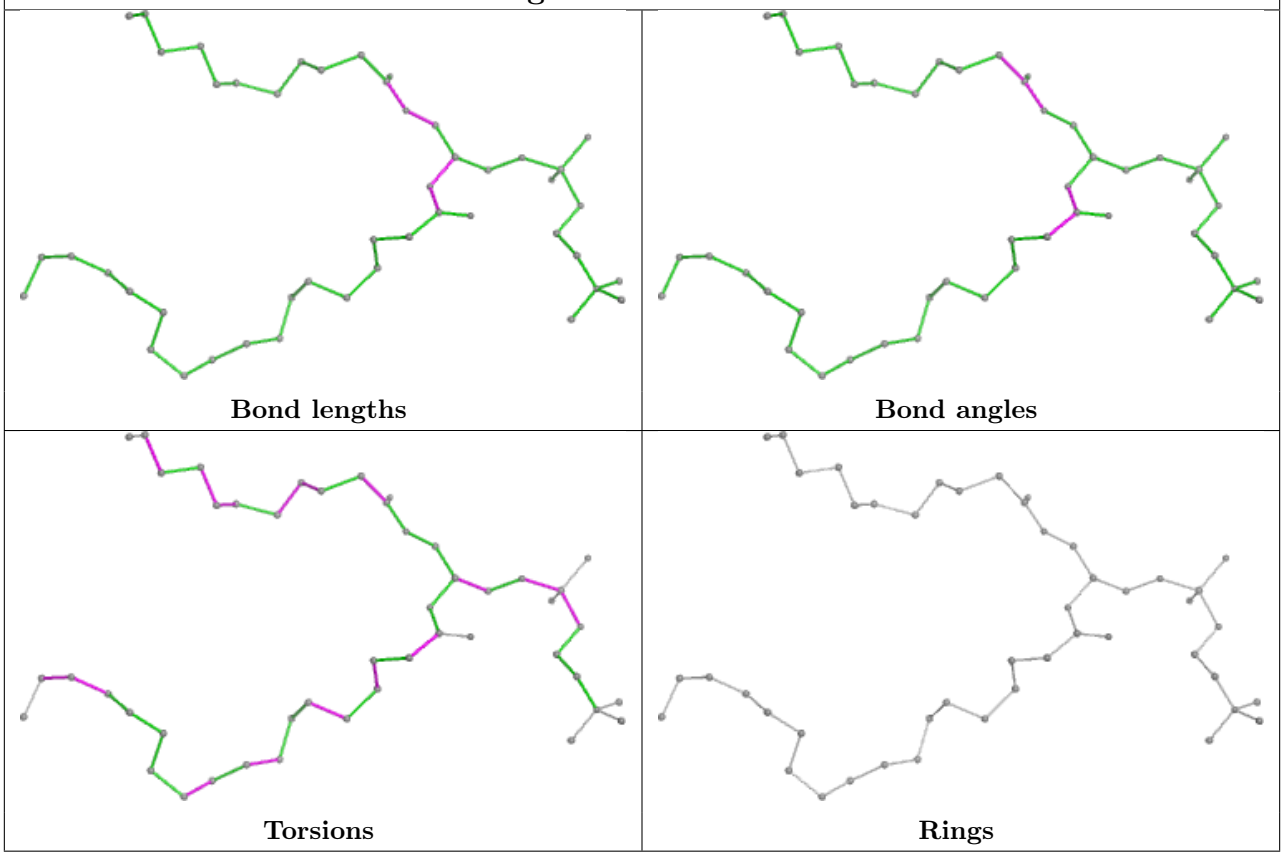
Ligand 3PE N 401



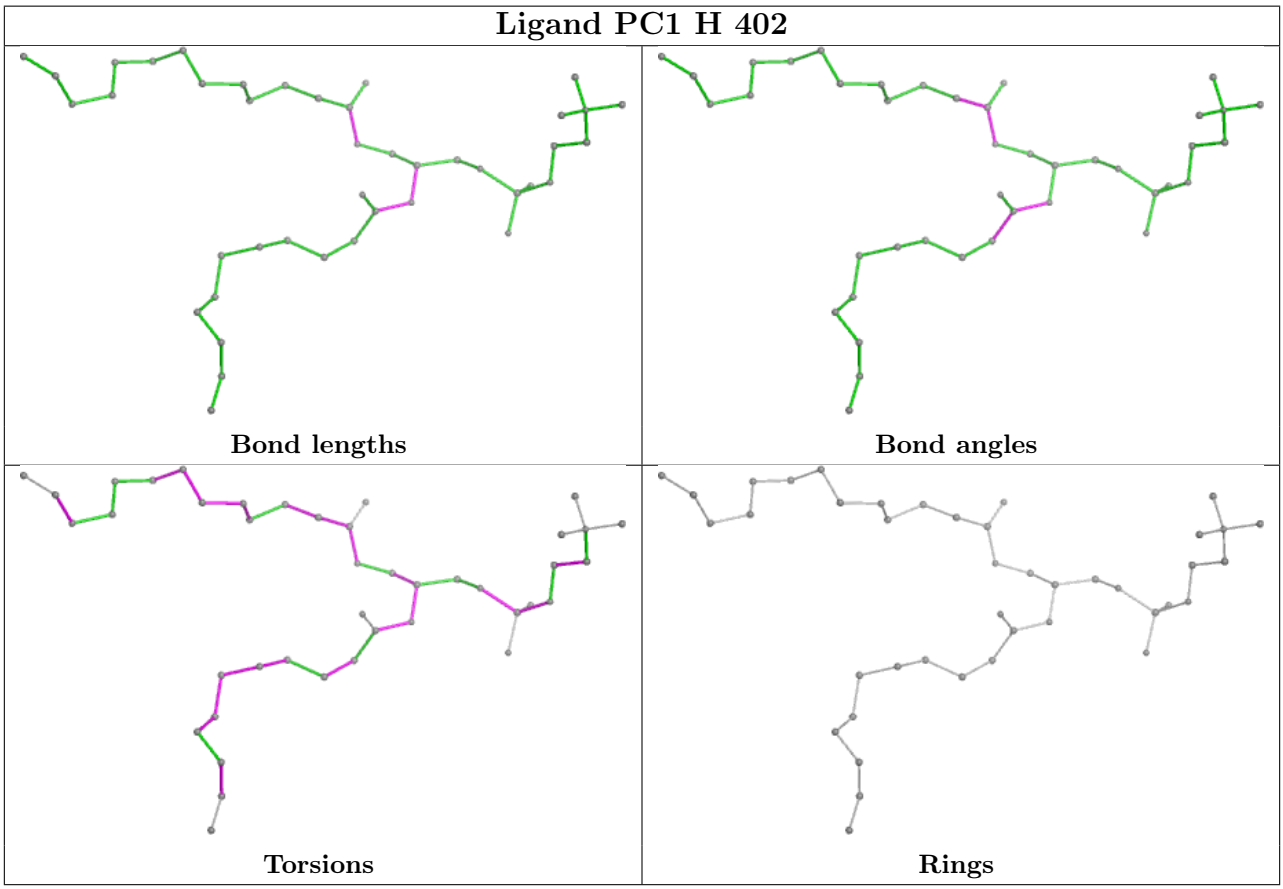
Ligand 3PE L 701



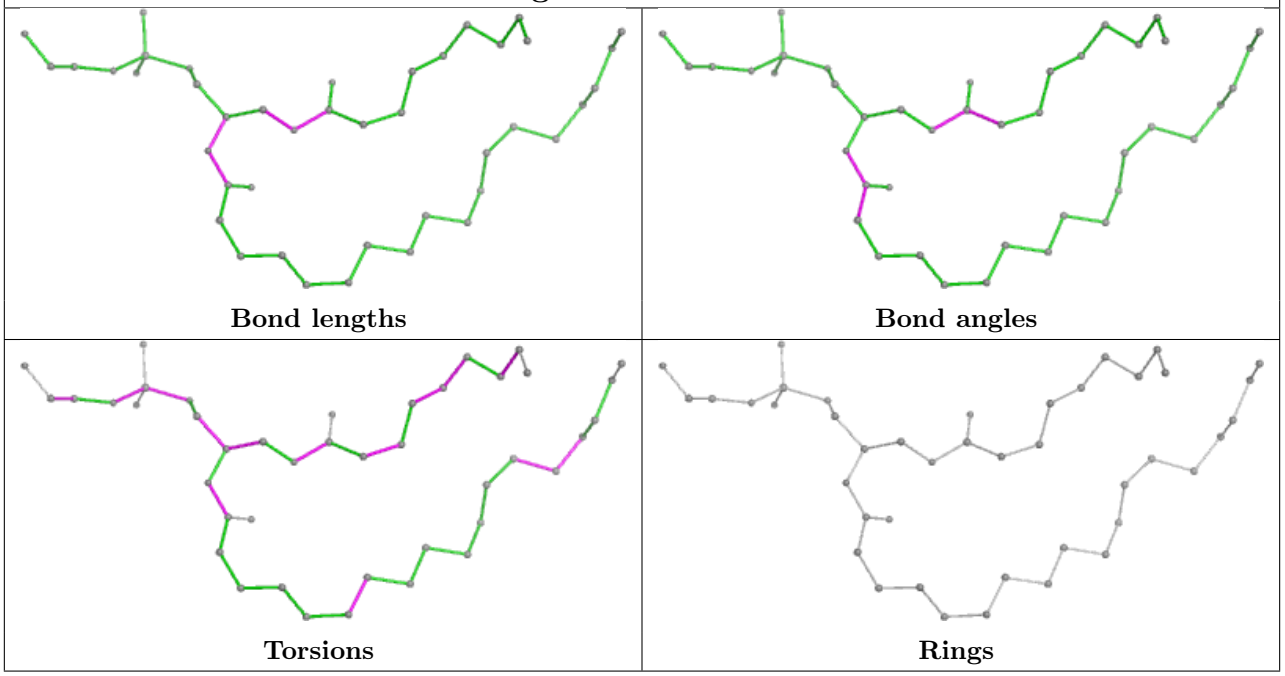
Ligand PC1 H 404



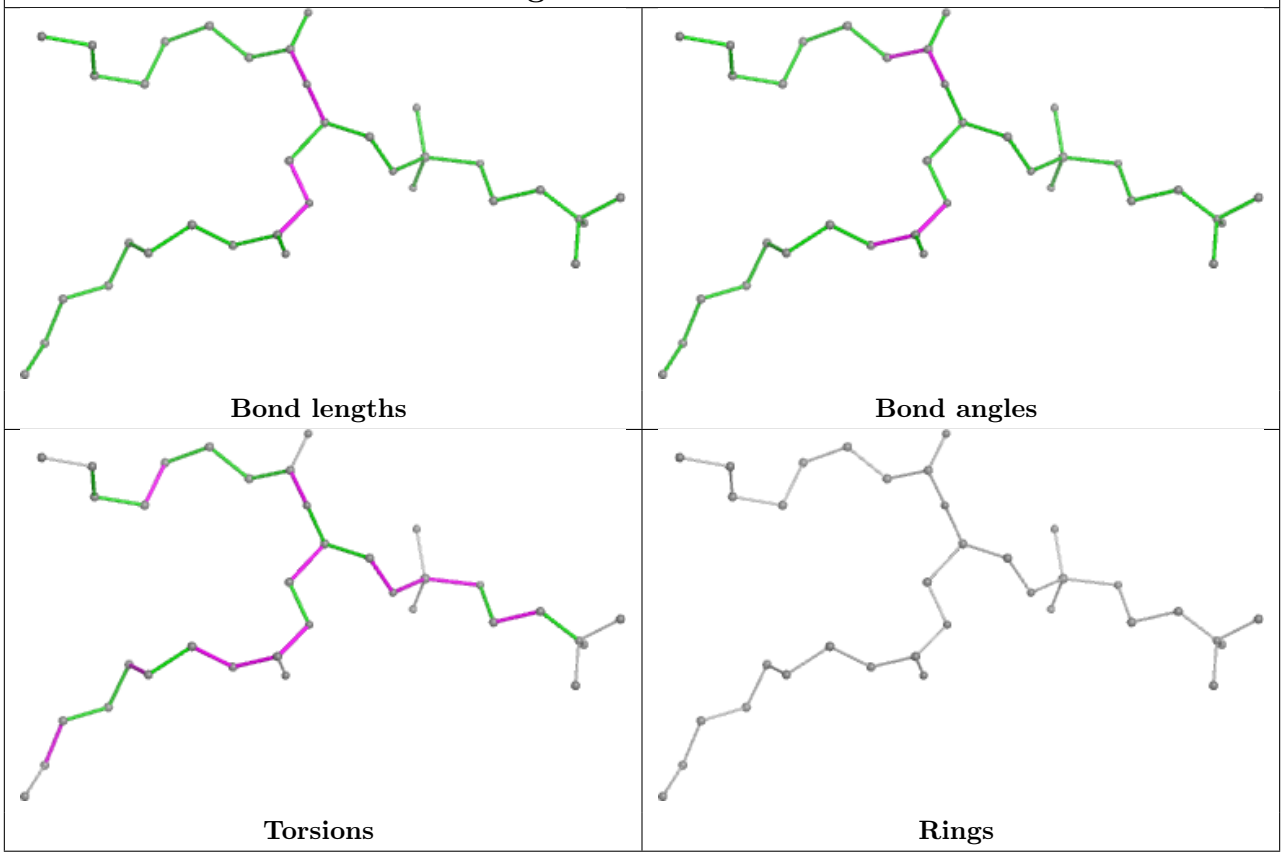
Ligand PC1 H 402



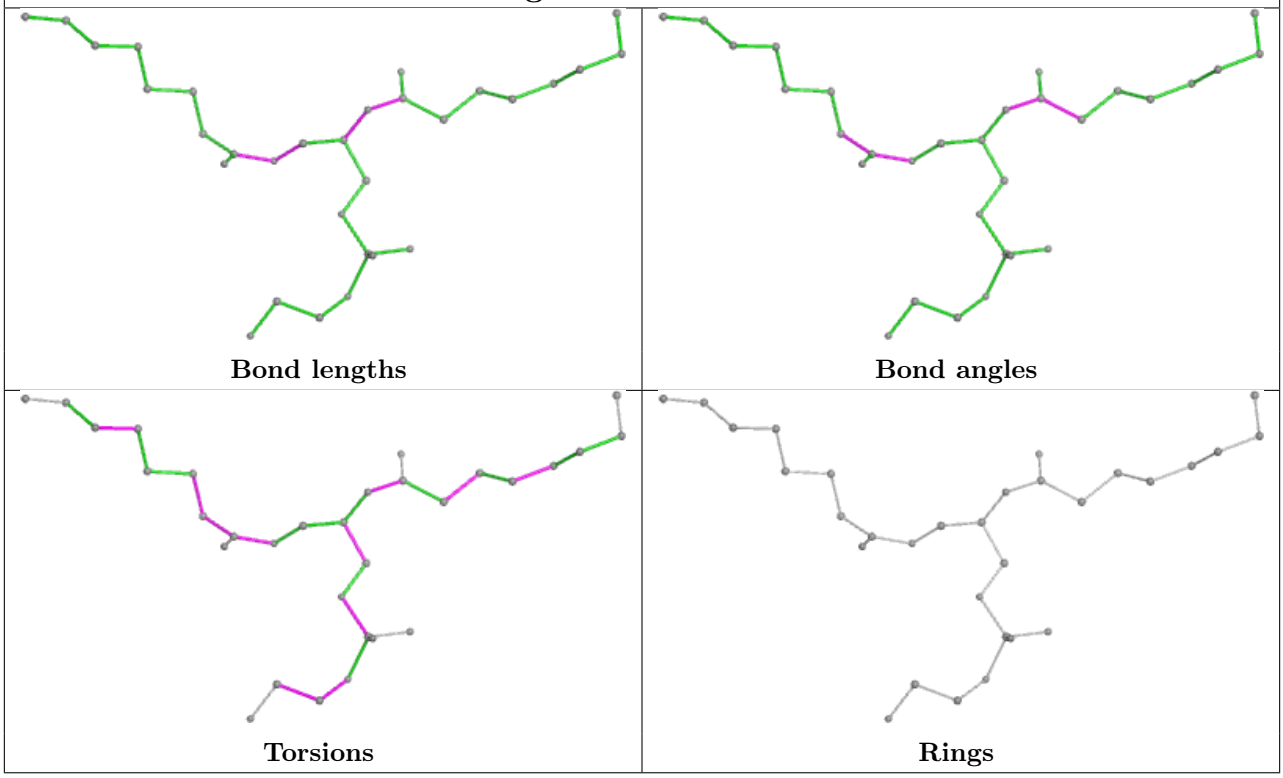
Ligand 3PE L 704



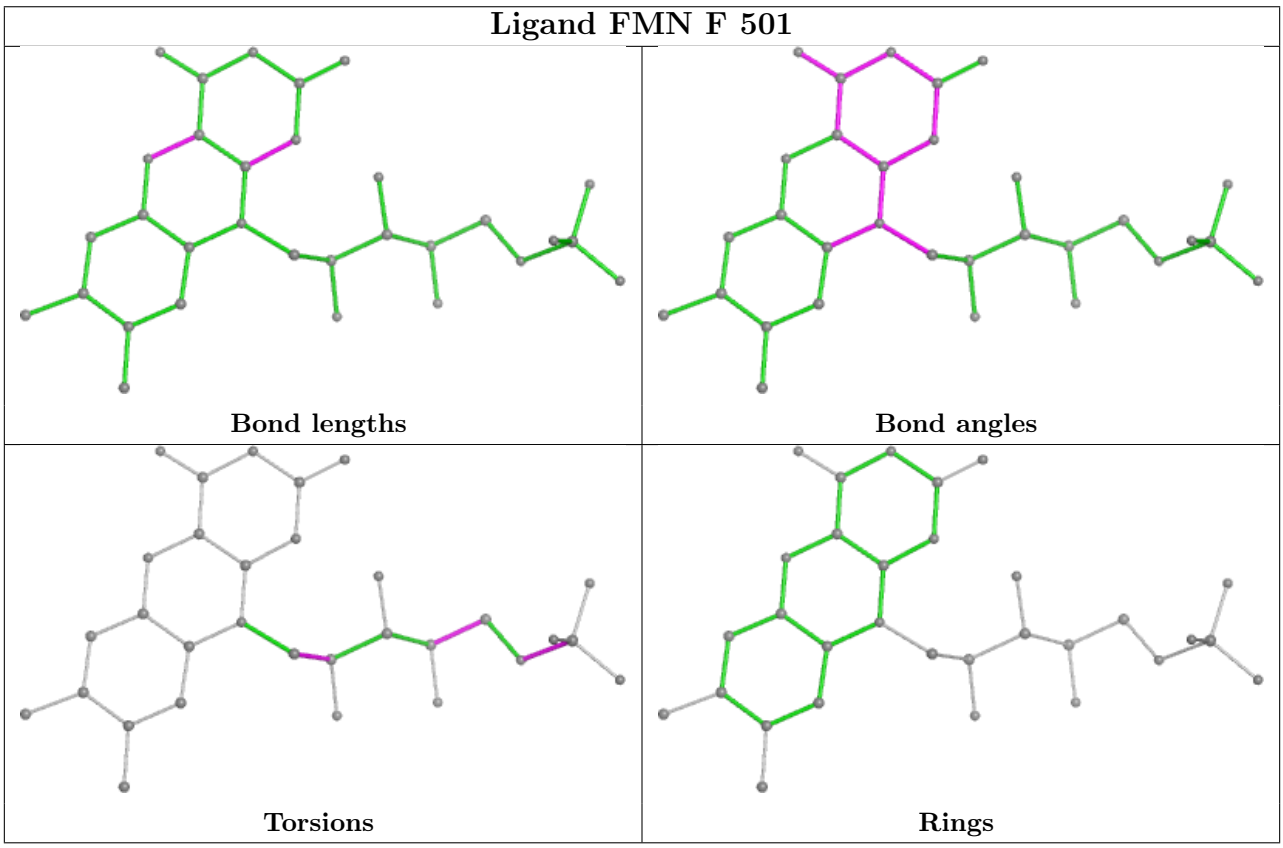
Ligand PC1 H 406



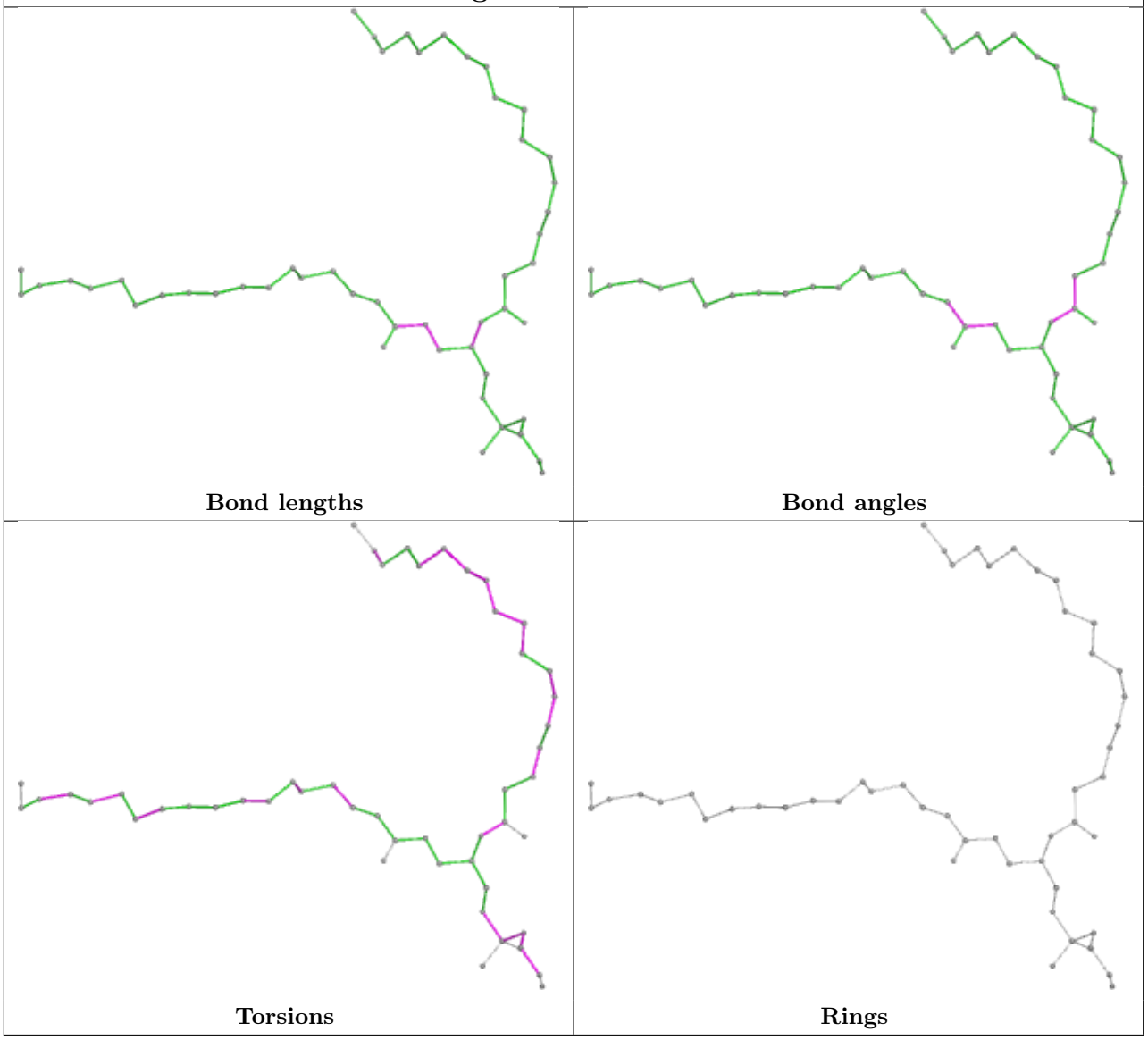
Ligand 3PE M 506



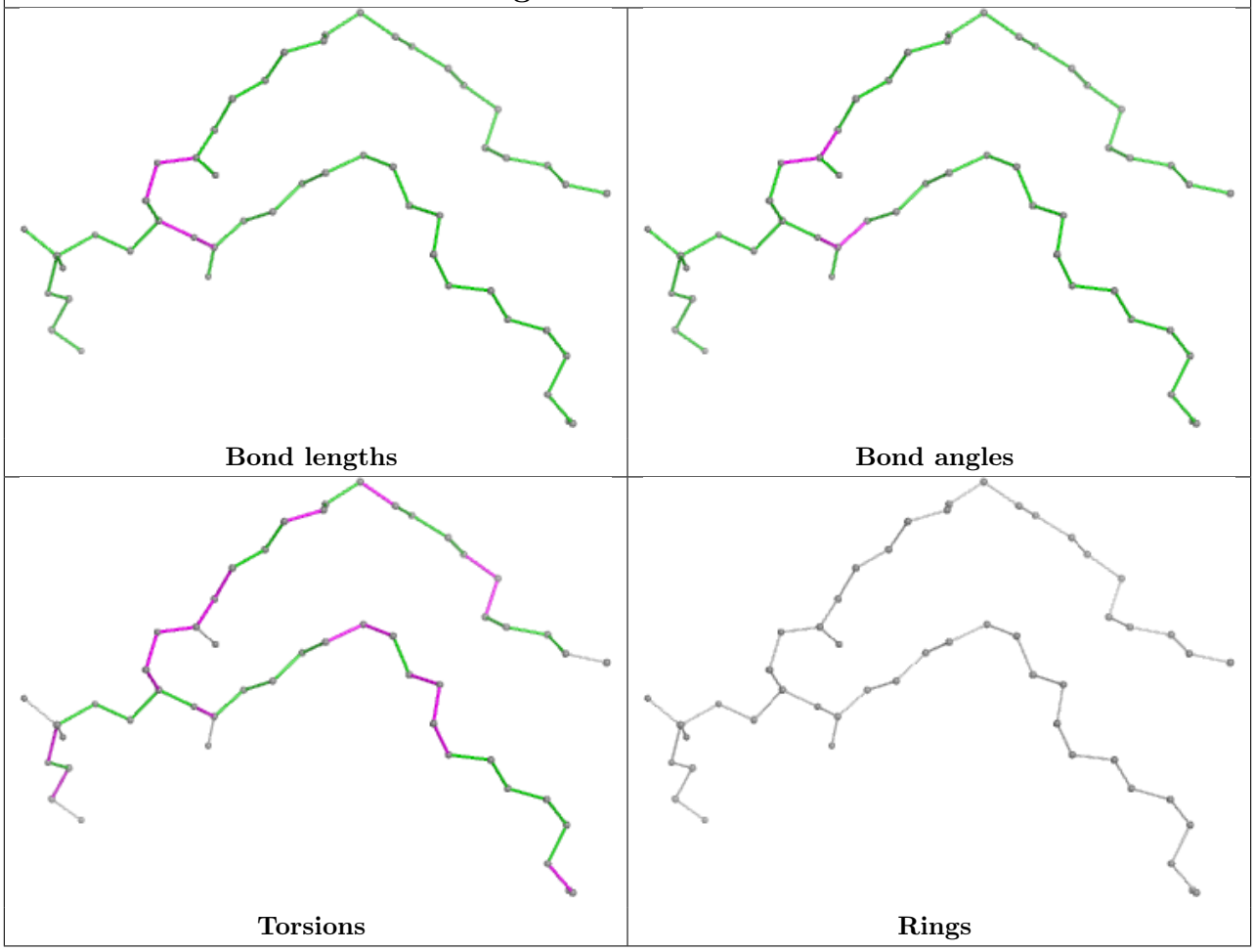
Ligand FMN F 501



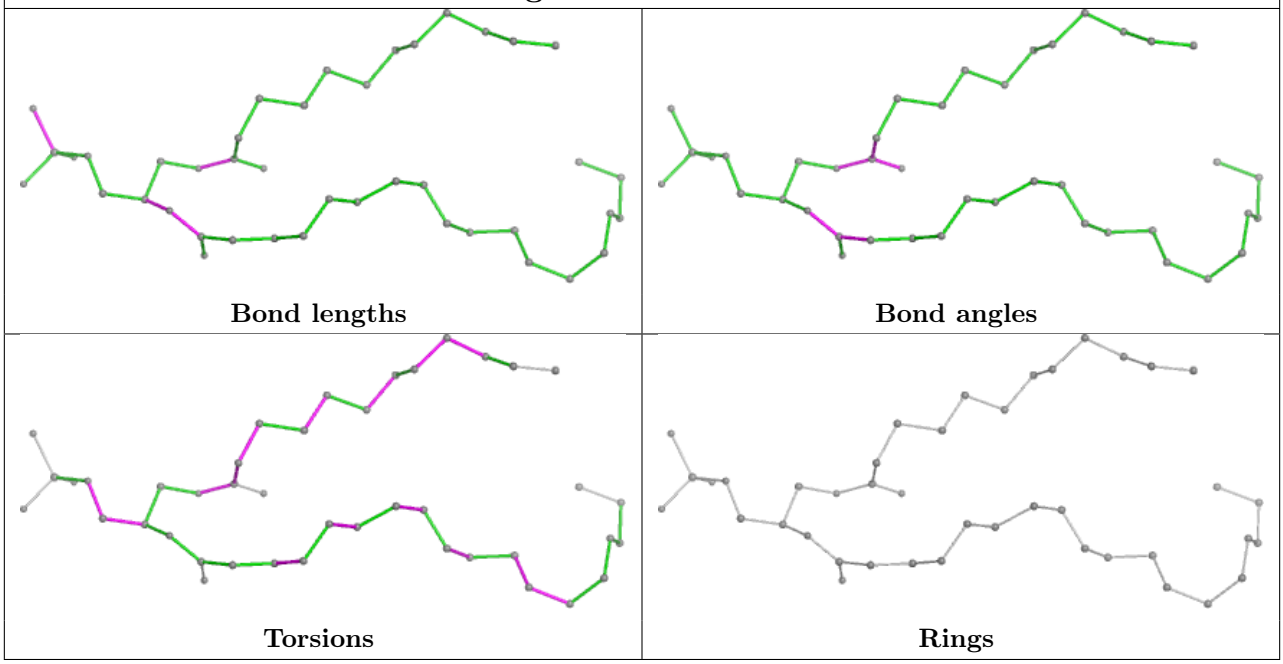
Ligand 3PE H 403



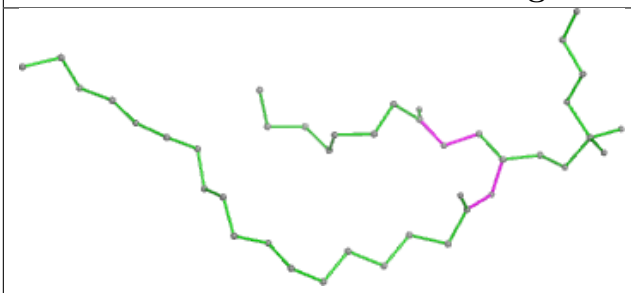
Ligand 3PE M 504



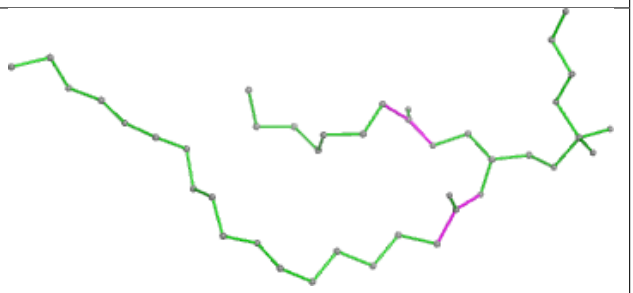
Ligand 3PE M 502



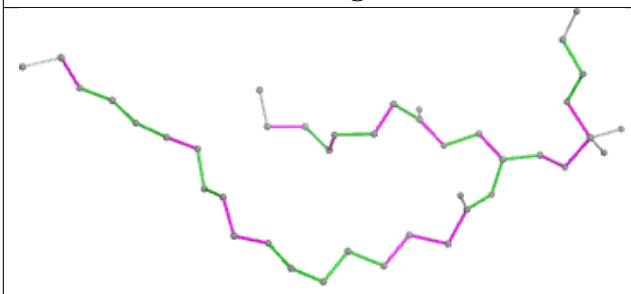
Ligand 3PE A 201



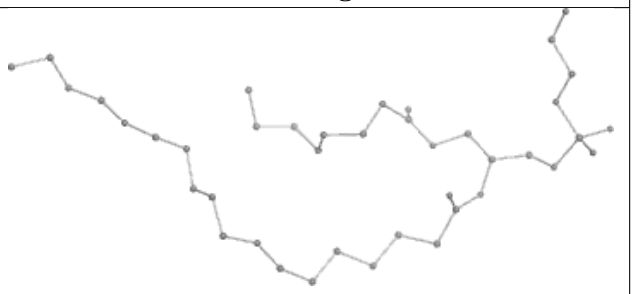
Bond lengths



Bond angles

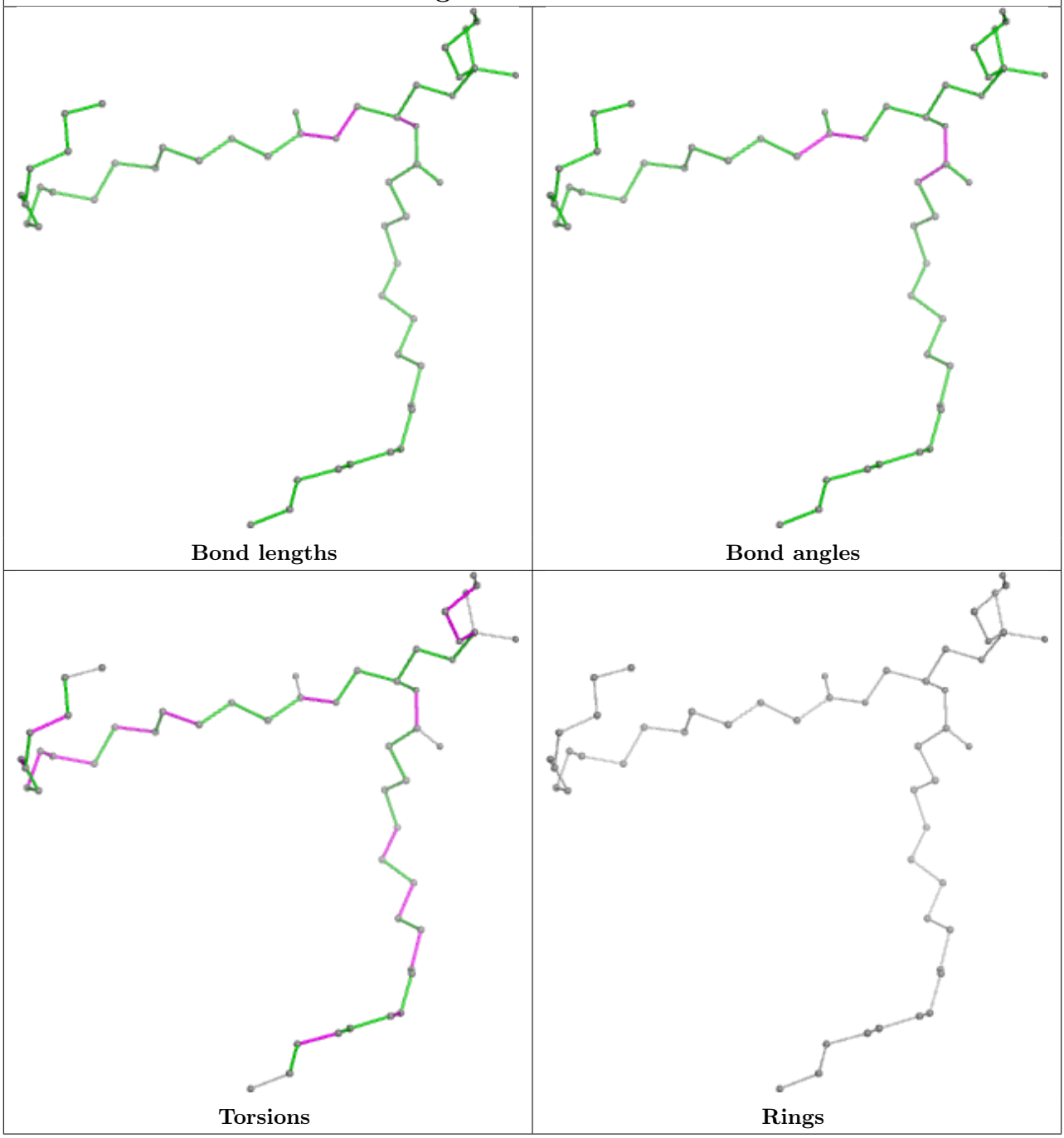


Torsions



Rings

Ligand 3PE M 503



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.

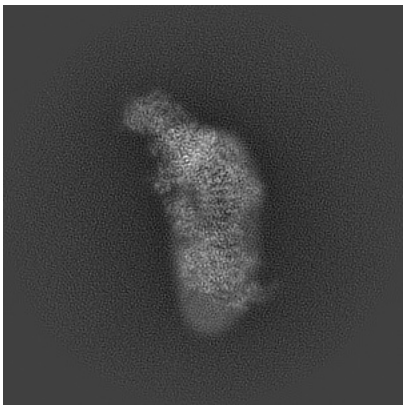
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4345. These allow visual inspection of the internal detail of the map and identification of artifacts.

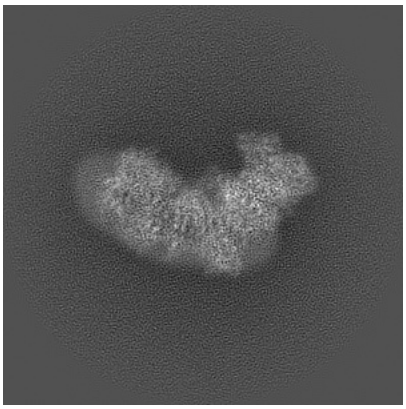
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

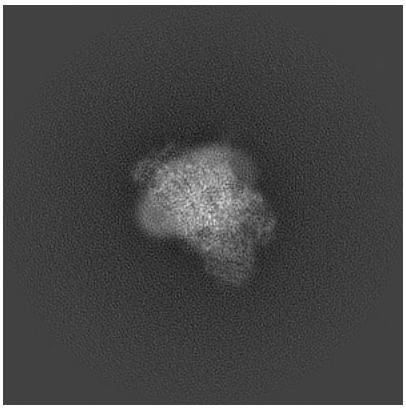
6.1.1 Primary map



X

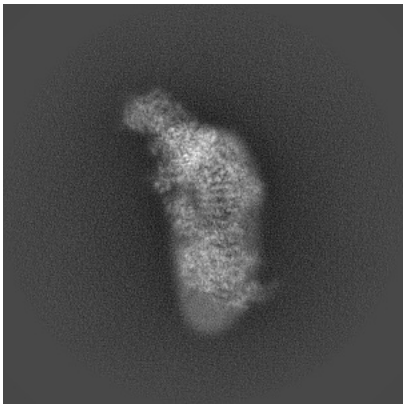


Y

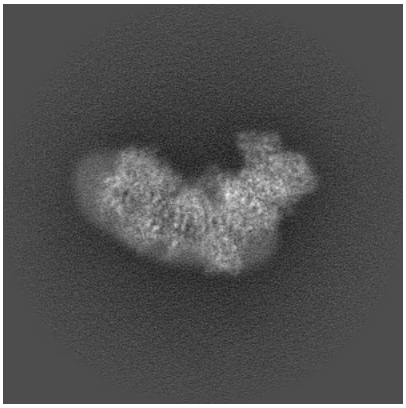


Z

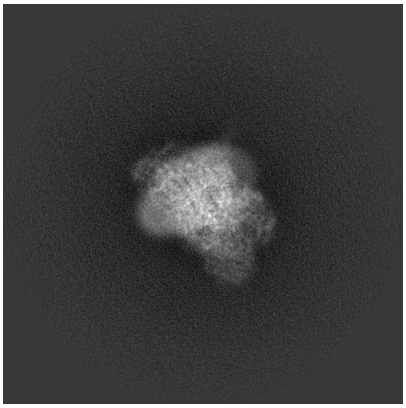
6.1.2 Raw map



X



Y

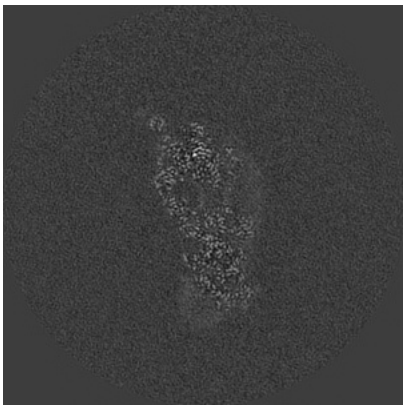


Z

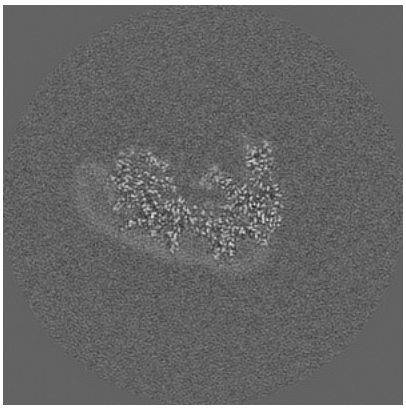
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

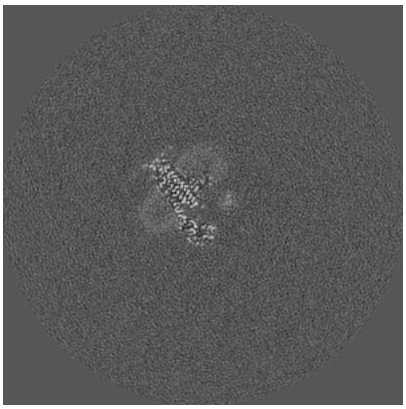
6.2.1 Primary map



X Index: 225

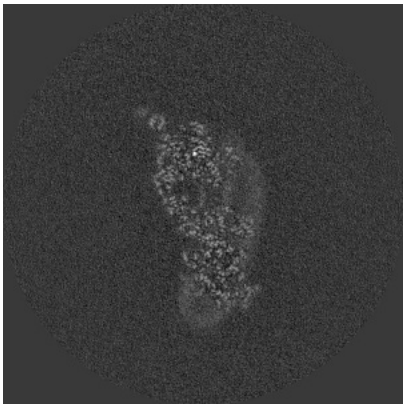


Y Index: 225

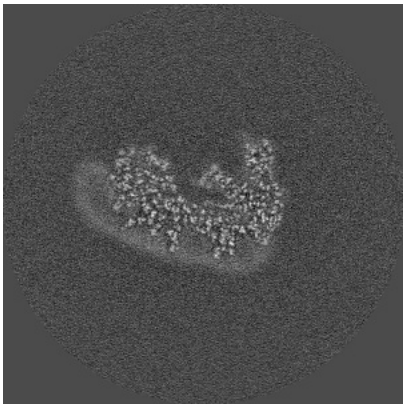


Z Index: 225

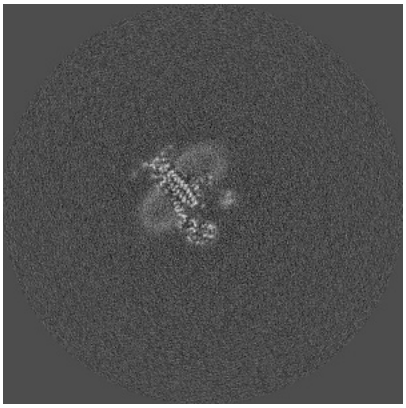
6.2.2 Raw map



X Index: 225



Y Index: 225

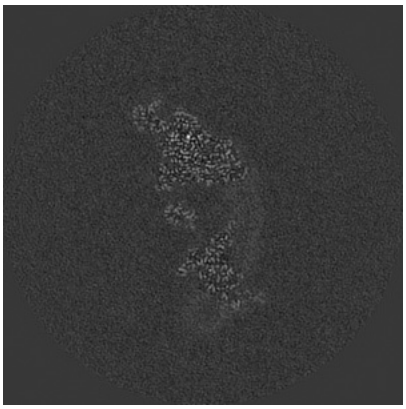


Z Index: 225

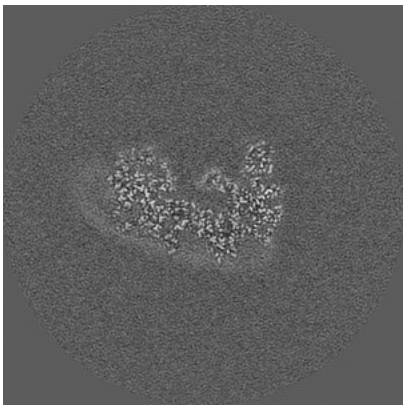
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

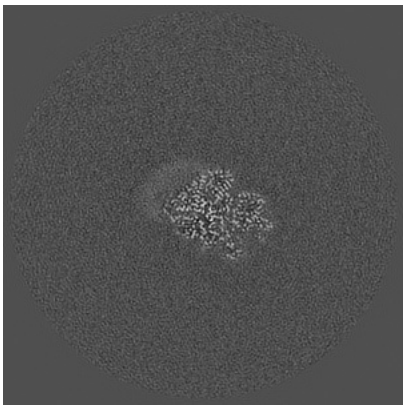
6.3.1 Primary map



X Index: 237

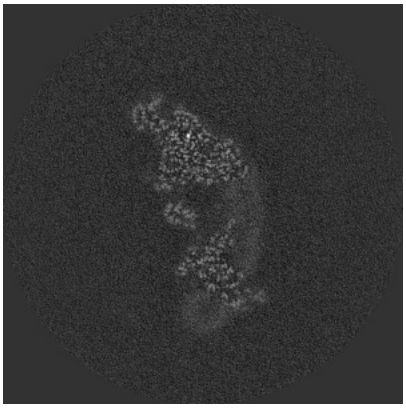


Y Index: 227

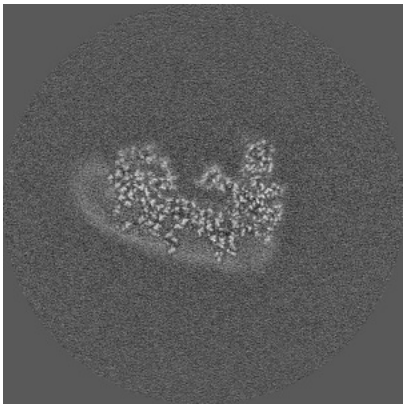


Z Index: 287

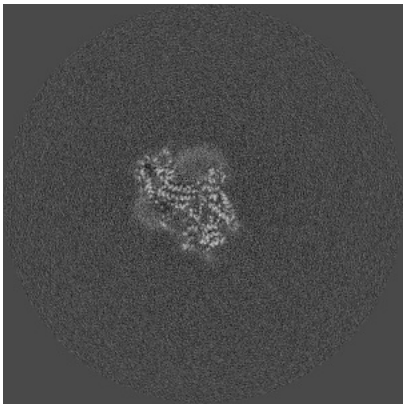
6.3.2 Raw map



X Index: 237



Y Index: 227

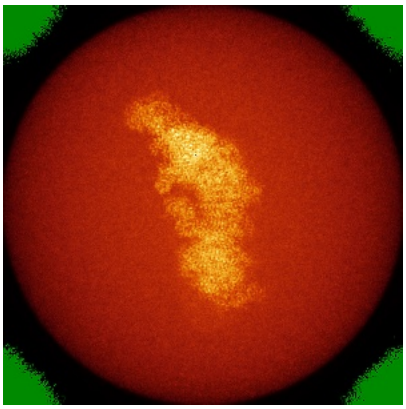


Z Index: 252

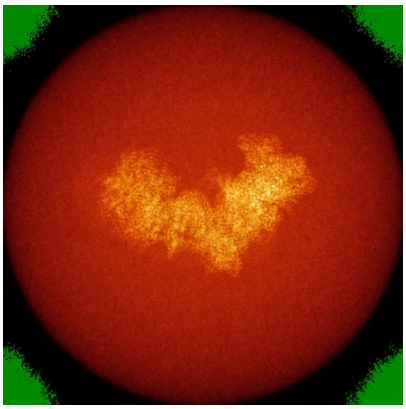
The images above show the largest variance slices of the map in three orthogonal directions.

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

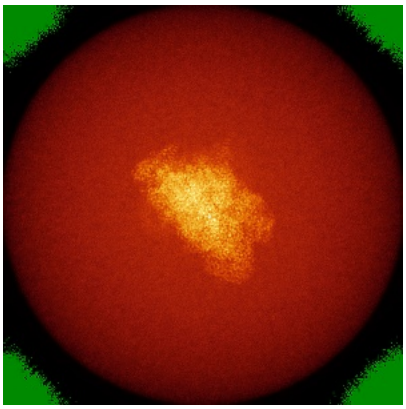
6.4.1 Primary map



X

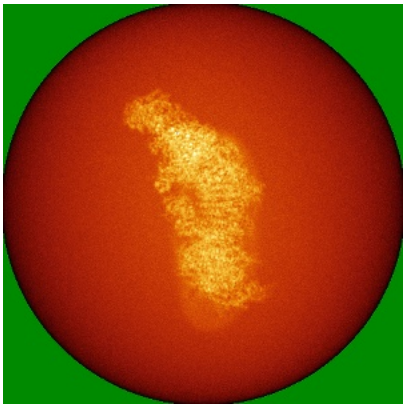


Y

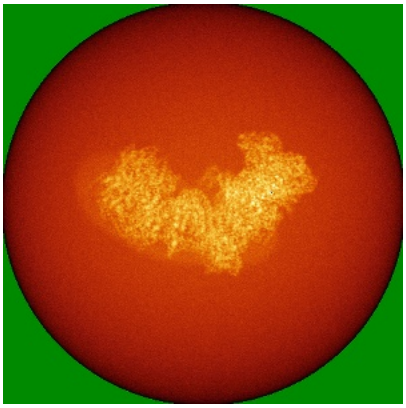


Z

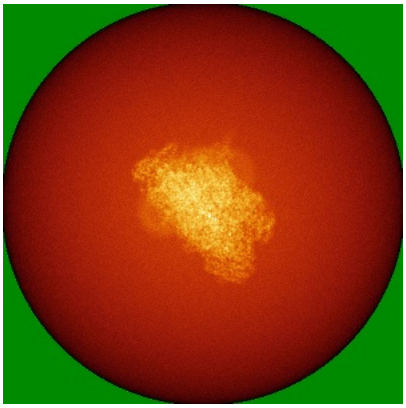
6.4.2 Raw map



X



Y

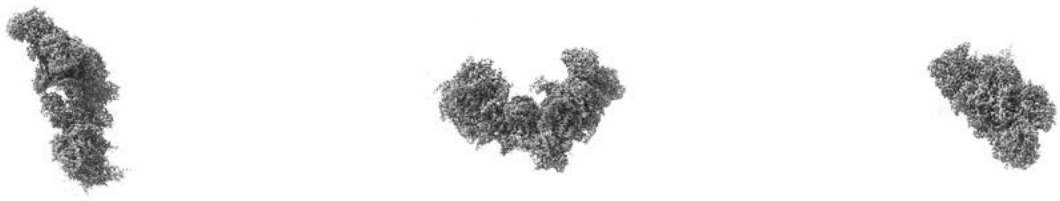


Z

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 0.075. 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.

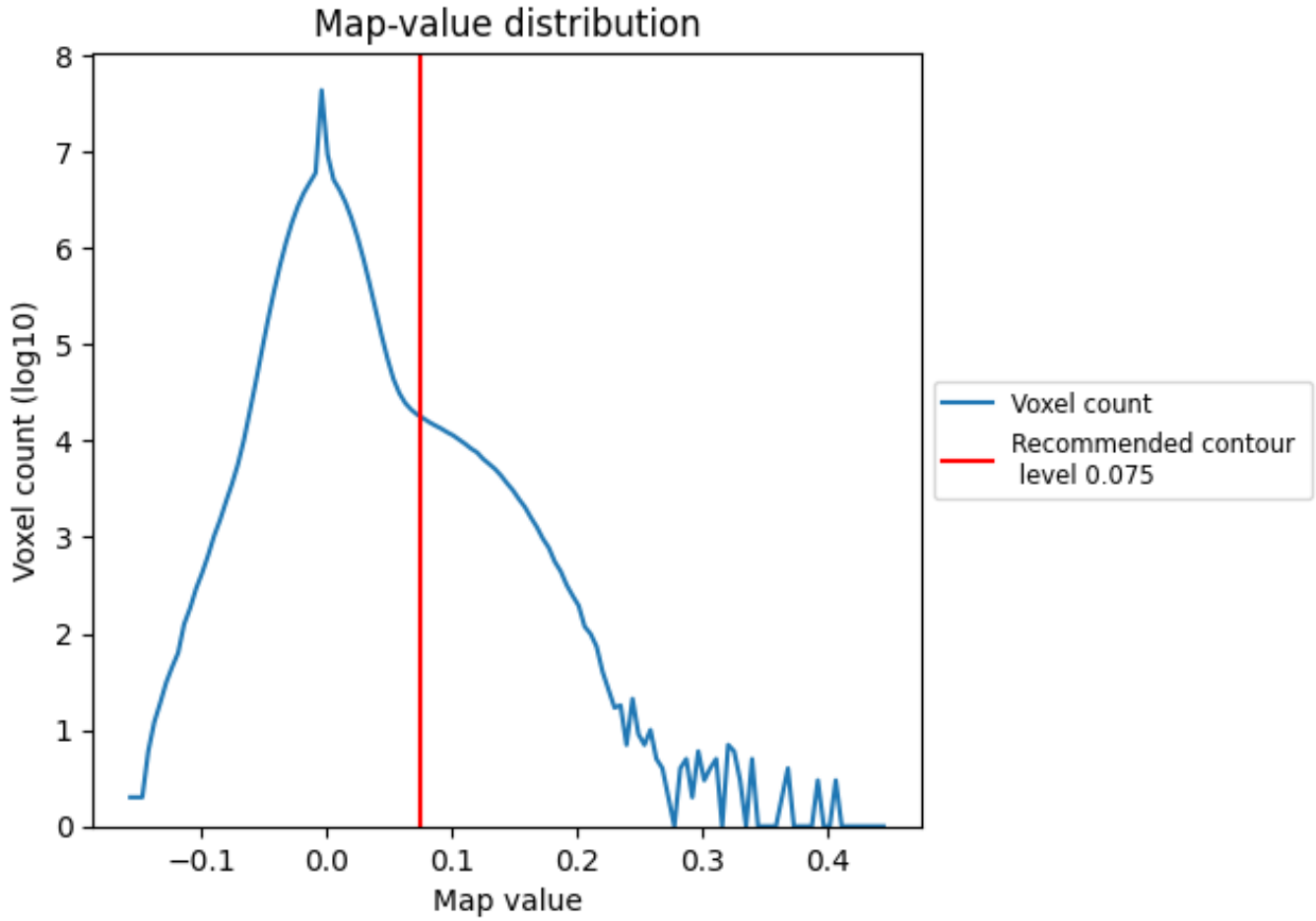
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

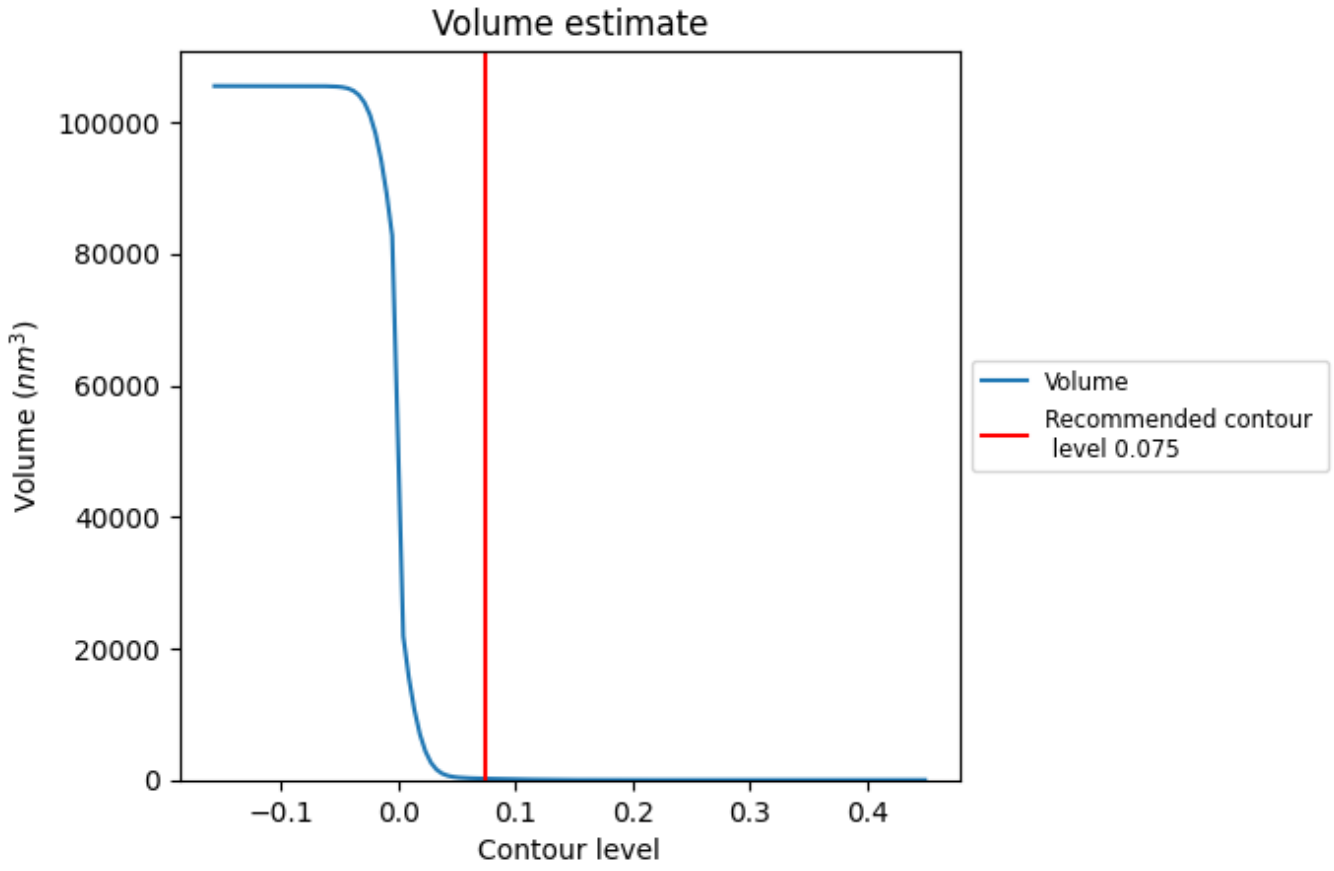
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

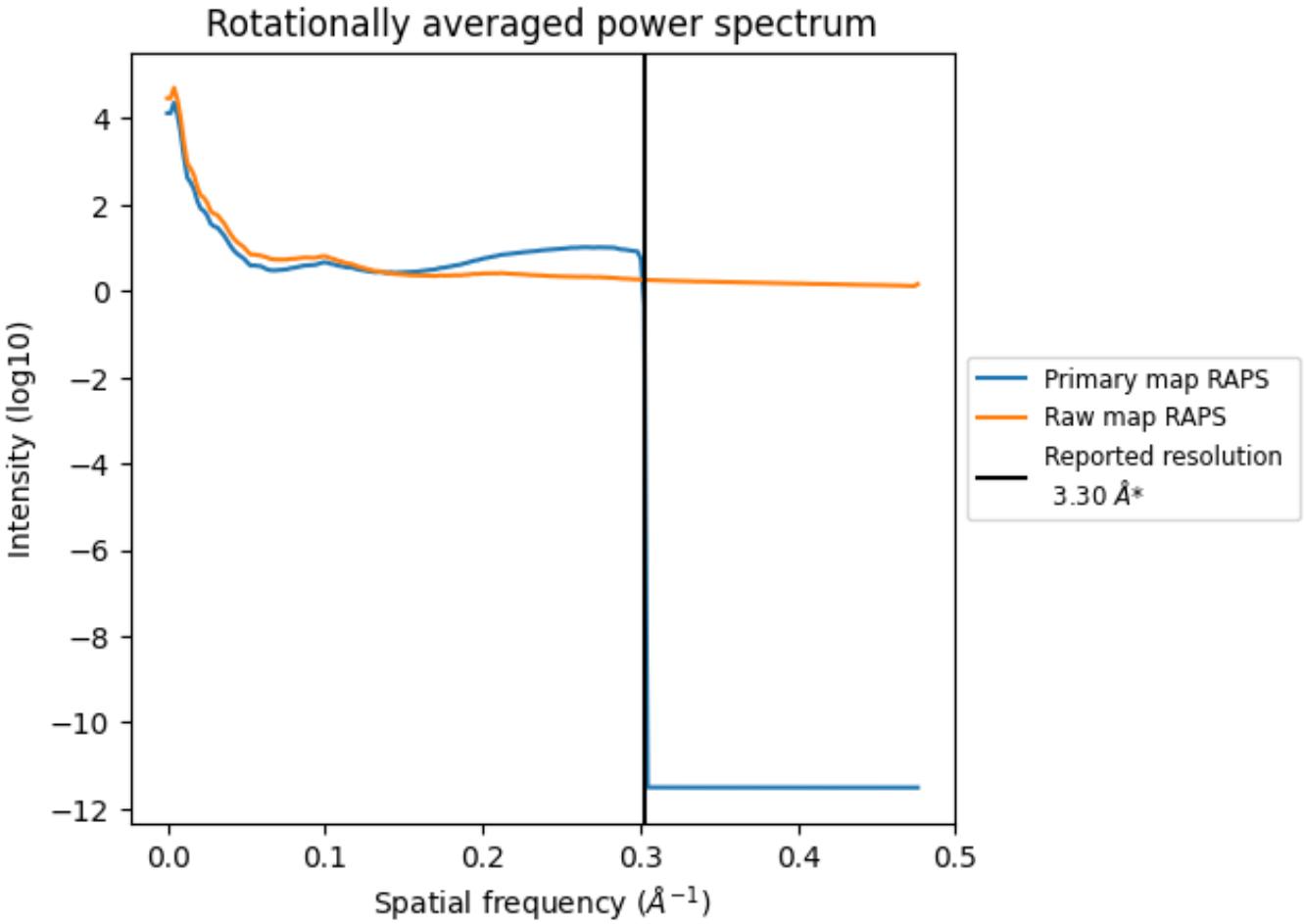
7.2 Volume estimate



The volume at the recommended contour level is 195 nm^3; this corresponds to an approximate mass of 176 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 (i)

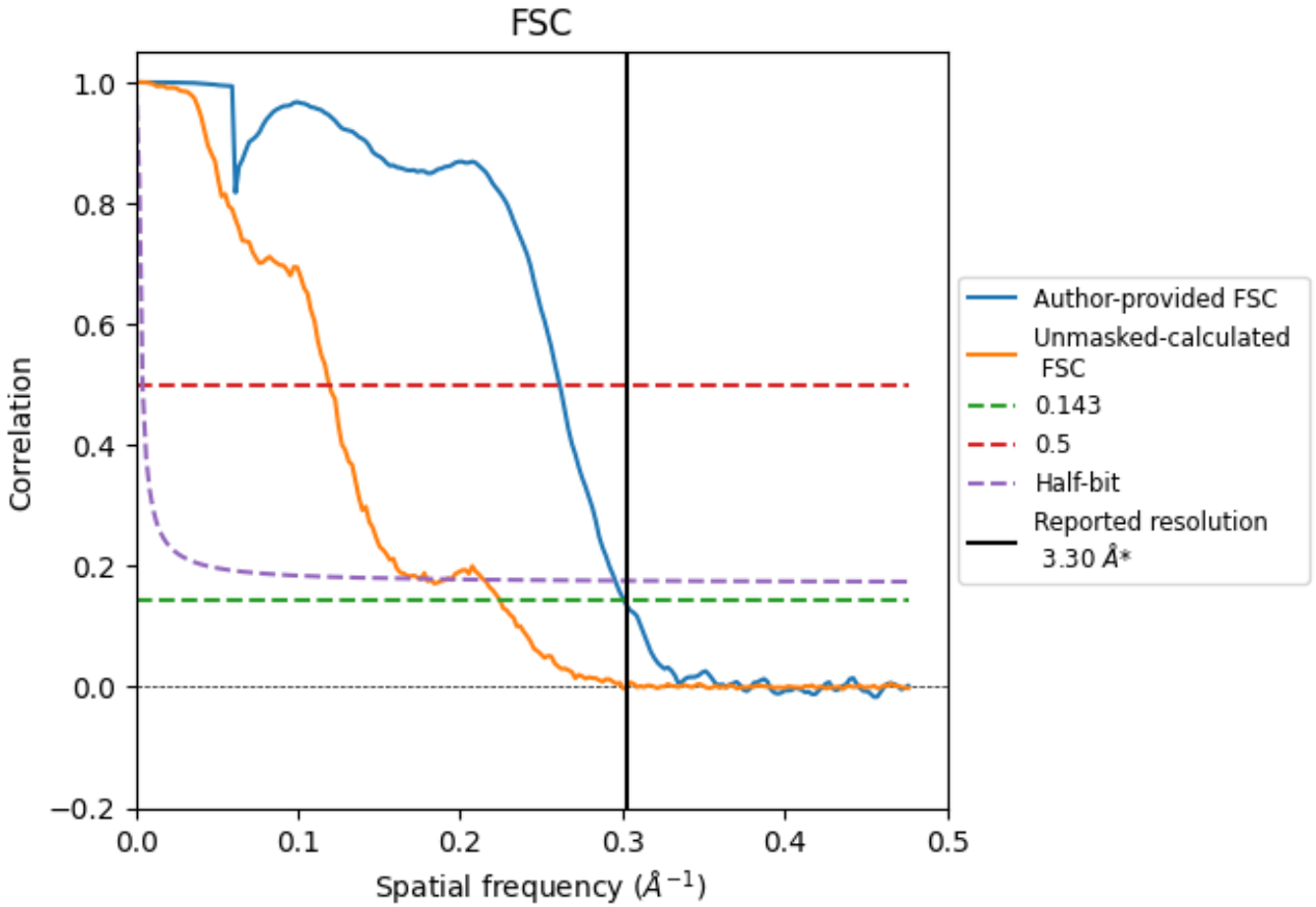


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

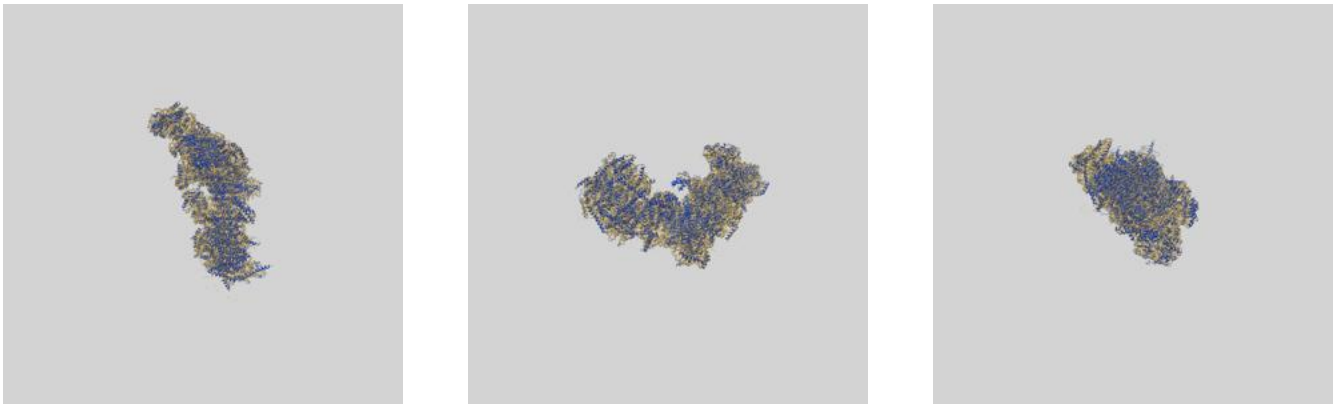
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.83	3.38
Unmasked-calculated*	4.45	8.39	5.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.45 differs from the reported value 3.3 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4345 and PDB model 6G2J. Per-residue inclusion information can be found in section 3 on page 19.

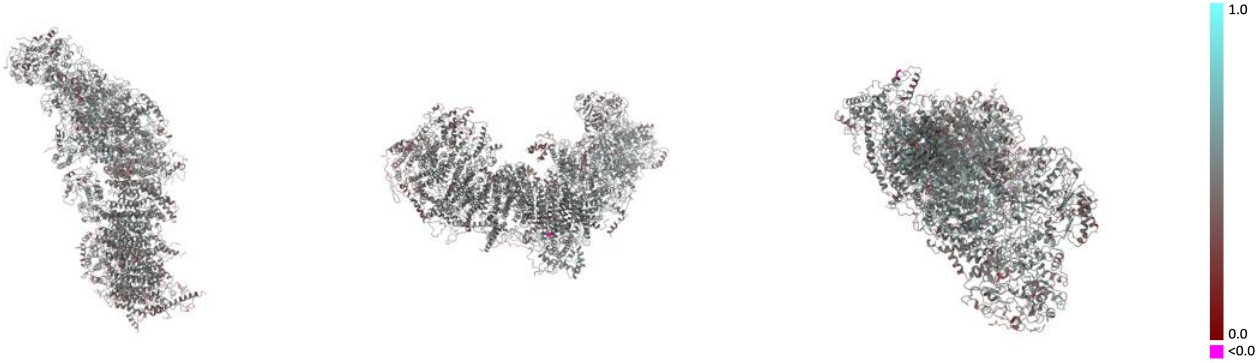
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.075 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.

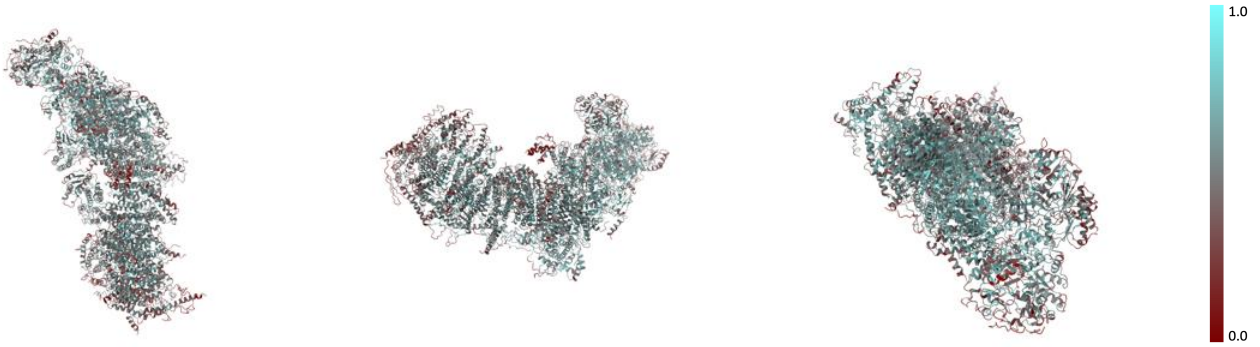
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

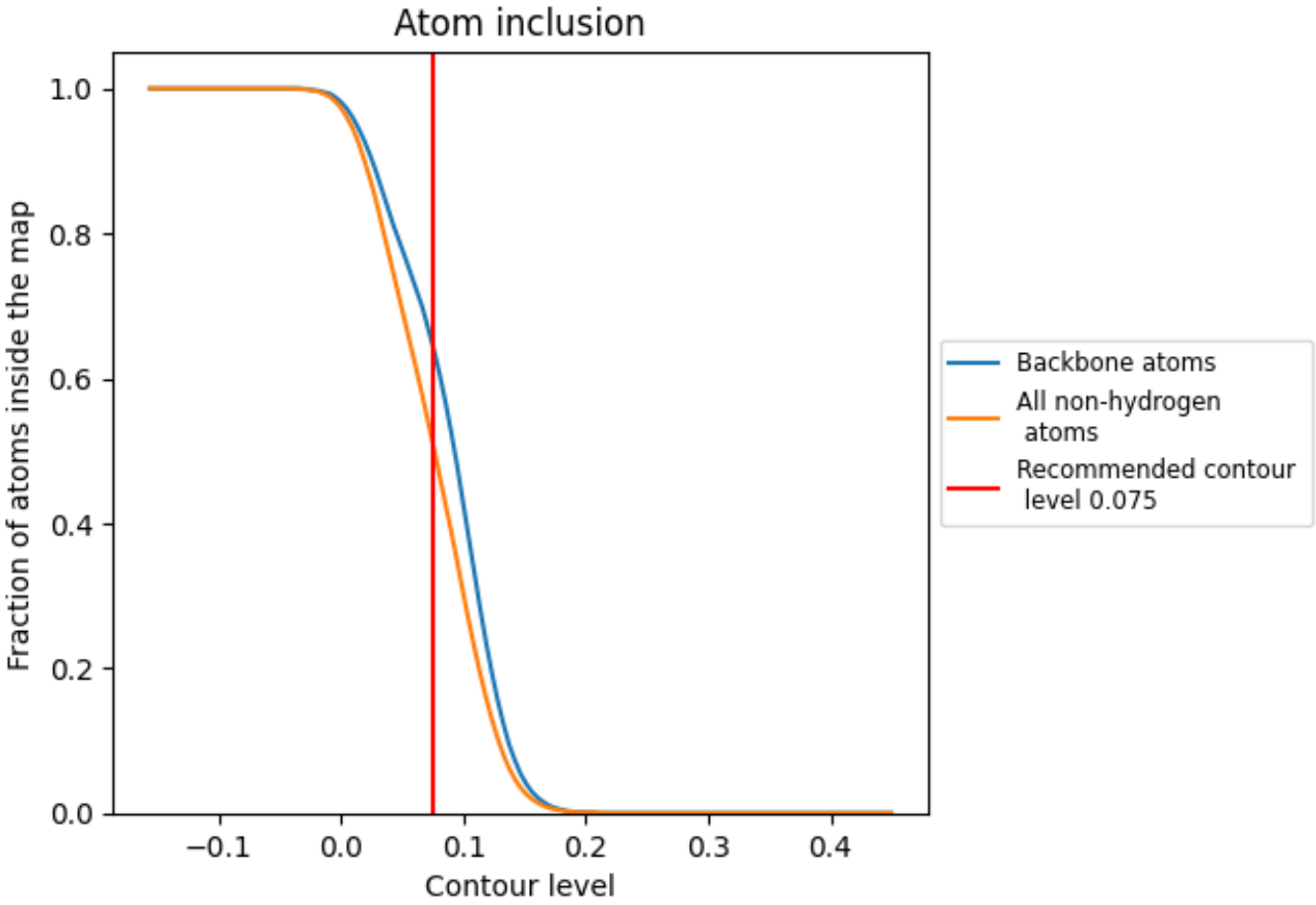
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.075).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5100	0.4690
A	0.5090	0.4820
B	0.6560	0.5030
C	0.6030	0.4980
D	0.6180	0.5020
E	0.4470	0.4570
F	0.4940	0.4600
G	0.5380	0.4760
H	0.5600	0.4960
I	0.6520	0.5070
J	0.4830	0.4650
K	0.5650	0.4900
L	0.4970	0.4760
M	0.5580	0.5020
N	0.5770	0.4920
O	0.5030	0.4640
P	0.5170	0.4680
Q	0.5330	0.4850
R	0.5400	0.4850
S	0.4140	0.4400
T	0.1780	0.3630
U	0.3540	0.4140
V	0.4730	0.4550
W	0.4950	0.4640
X	0.5180	0.4720
Y	0.4350	0.4490
Z	0.5160	0.4500
a	0.5670	0.4960
b	0.4630	0.4310
c	0.3810	0.4180
d	0.4960	0.4650
e	0.5200	0.4630
f	0.4180	0.4250
g	0.4330	0.4570
h	0.5140	0.4690

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.3730	0.4220
j	0.3510	0.3870
k	0.3260	0.4250
l	0.4560	0.4470
m	0.4630	0.4640
n	0.4240	0.4110
o	0.3220	0.3870
p	0.4600	0.4440
q	0.5570	0.4780
r	0.4950	0.4560
s	0.3850	0.4410