Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 03:15 am GMT

PDB ID	:	7B93
EMDB ID	:	EMD-12095
Title	:	Cryo-EM structure of mitochondrial complex I from Mus musculus inhibited by IACS-2858 at 3.0 A
Authors	:	Chung, I.; Hirst, J.
Deposited on	:	2020-12-14
Resolution	:	3.04 Å(reported)
Based on initial model	:	6ZR2

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:

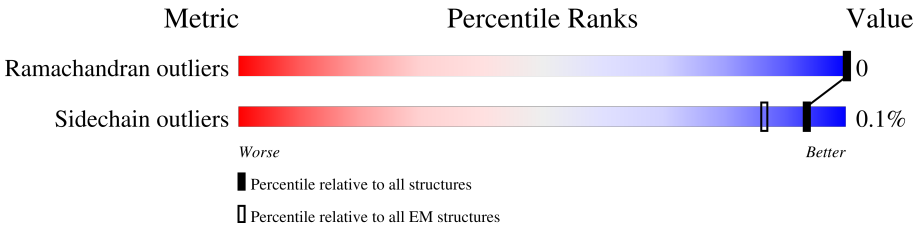
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.04 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	154571	4023
Sidechain outliers	154315	3826

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	100%
2	B	224	70% 30%
3	C	263	79% 21%
4	D	463	93% 7%
5	E	248	10% 87% 13%
6	F	464	92% 8%
7	G	727	95% 5%
8	H	318	100%
9	I	212	84% 16%

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Mol	Chain	Length	Quality of chain
10	J	172	6% 100%
11	K	98	99%
12	L	607	100%
13	M	459	100%
14	N	345	100%
15	O	355	90% 10%
16	P	377	90% 9%
17	Q	175	72% 28%
18	R	116	5% 83% 17%
19	S	99	13% 85% 15%
20	T	156	26% 51% 49%
20	U	156	6% 56% 44%
21	V	116	7% 99%
22	W	131	87% 13%
23	X	172	5% 99%
24	Y	143	98%
25	Z	144	99%
26	a	70	100%
27	b	84	8% 95% 5%
28	c	76	11% 64% 36%
29	d	120	100%
30	e	106	99%
31	f	57	26% 96%
32	g	151	5% 68% 32%
33	h	189	73% 27%

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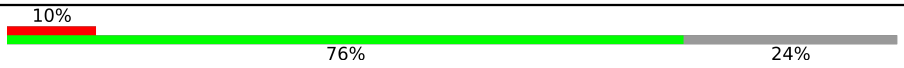
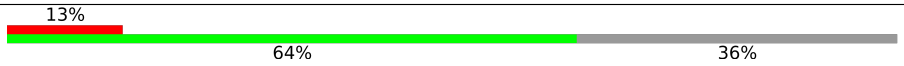
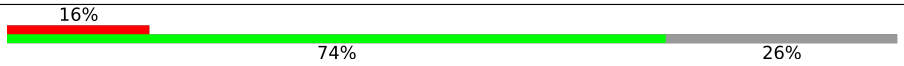
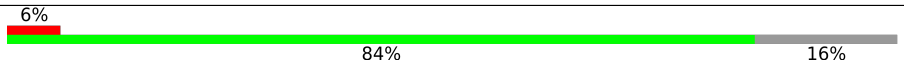
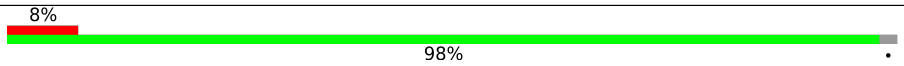
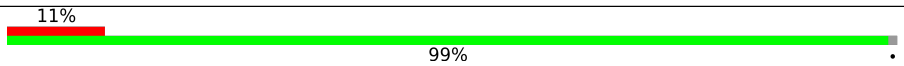
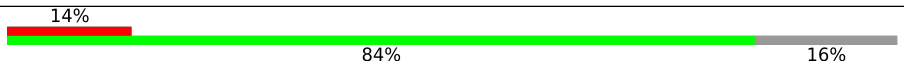
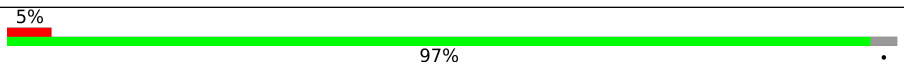
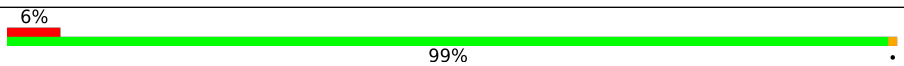
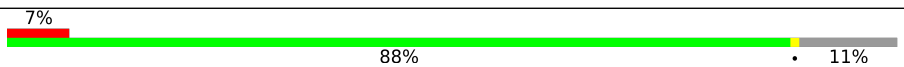
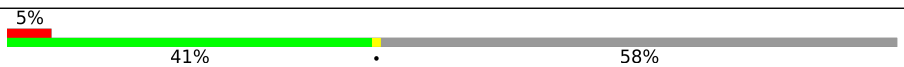
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 67491 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	156	1247	796	223	214	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	207	1721	1111	296	311	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	3464	2215	595	630	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	215	1664	1058	280	315	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	429	Total	C	N	O	S	0	0
			3310	2086	592	610	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	172	Total	C	N	O	S	0	0
			1308	878	186	229	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	607	Total	C	N	O	S	0	0
			4809	3187	747	830	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	345	Total	C	N	O	S	0	0
			2703	1795	417	454	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	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	79	Total	C	N	O	S	0	0
			637	410	95	127	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	115	Total	C	N	O	S	0	0
			932	607	155	167	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	143	Total	C	N	O	S	0	0
			1177	756	209	204	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	49	Total	C	N	O	S	0	0
			407	266	70	70	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	56	Total	C	N	O	S	0	0
			482	314	85	81	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			858	553	137	164	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	97	Total	C	N	O	S	0	0
			814	529	143	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			580	378	95	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	115	Total	C	N	O	S	0	0
			988	622	186	172	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	171	Total	C	N	O	S	0	0
			1444	907	259	270	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1212	779	215	213	5		

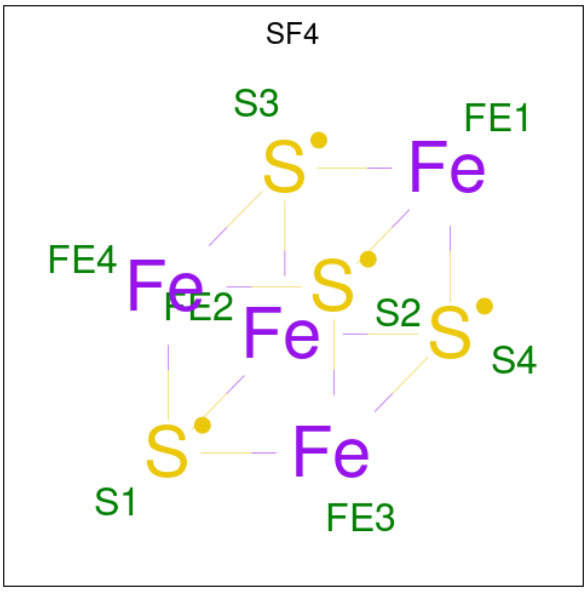
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	101	Total	C	N	O	S	0	0
			809	511	150	145	3		

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

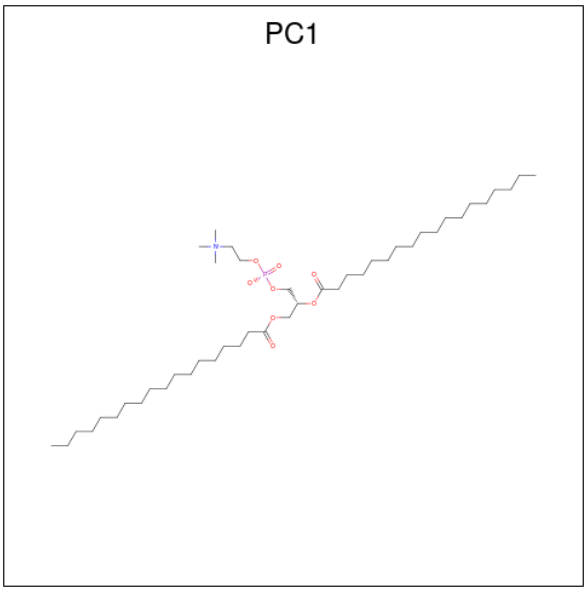
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	44	Total	C	N	O	0	0
			368	230	66	72		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



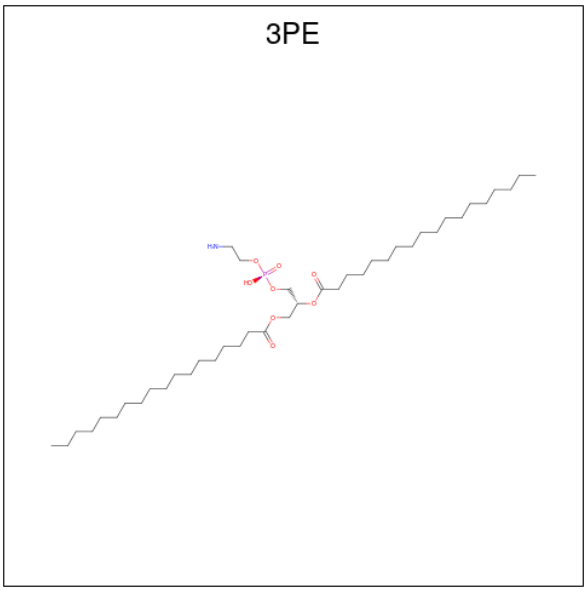
Mol	Chain	Residues	Atoms	AltConf
45	B	1	Total Fe S 8 4 4	0
45	F	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 16 8 8	0
45	G	1	Total Fe S 16 8 8	0
45	I	1	Total Fe S 16 8 8	0
45	I	1	Total Fe S 16 8 8	0

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



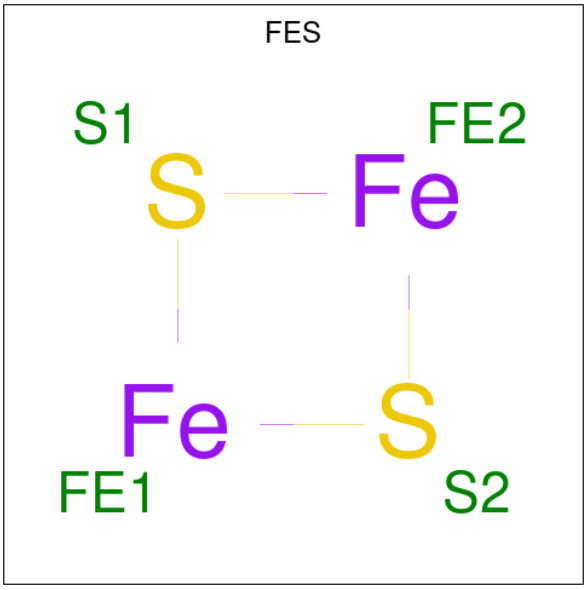
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			78	58	2	16	2	
46	B	1	Total	C	N	O	P	0
			78	58	2	16	2	
46	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	I	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



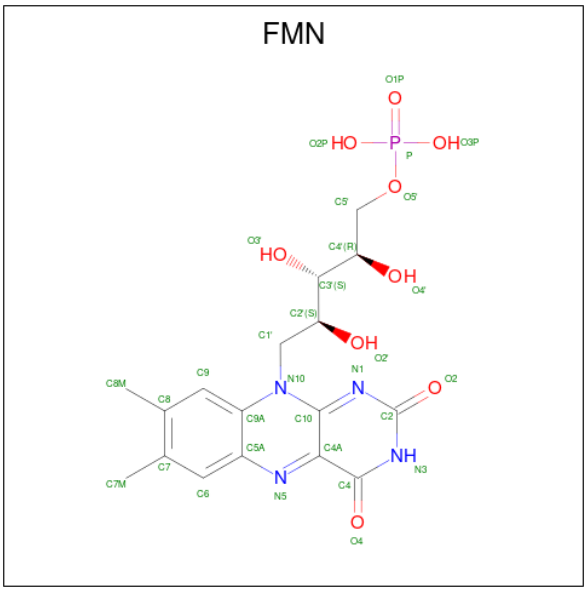
Mol	Chain	Residues	Atoms					AltConf
47	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	K	1	Total	C	N	O	P	0
			33	23	1	8	1	
47	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	Y	1	Total	C	N	O	P	0
			41	31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

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



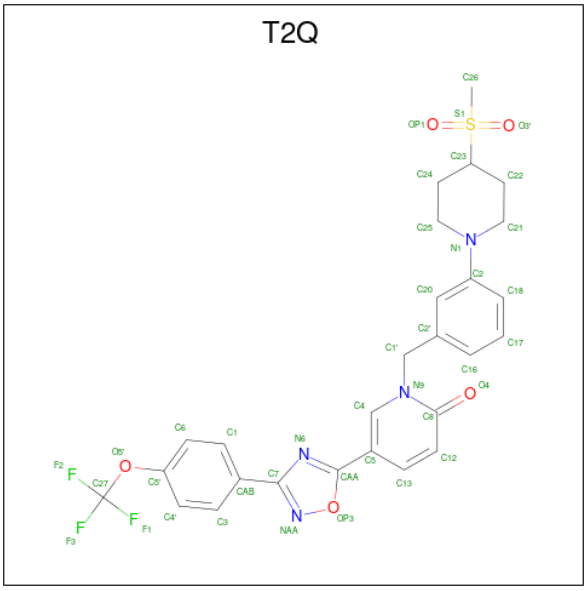
Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



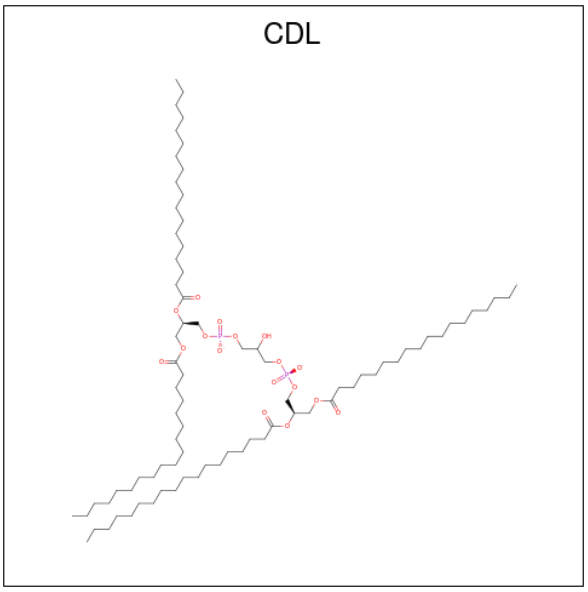
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is 1-[[3-(4-methylsulfonylpiperidin-1-yl)phenyl]methyl]-5-[3-[4-(trifluoromethyloxy)phenyl]-1,2,4-oxadiazol-5-yl]pyridin-2-one (three-letter code: T2Q) (formula: $C_{27}H_{25}F_3N_4O_5S$) (labeled as "Ligand of Interest" by depositor).



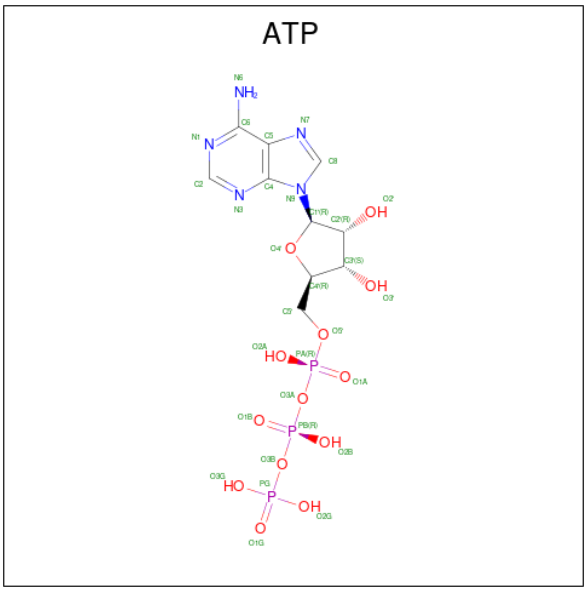
Mol	Chain	Residues	Atoms						AltConf
50	H	1	Total	C	F	N	O	S	0
			40	27	3	4	5	1	

- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



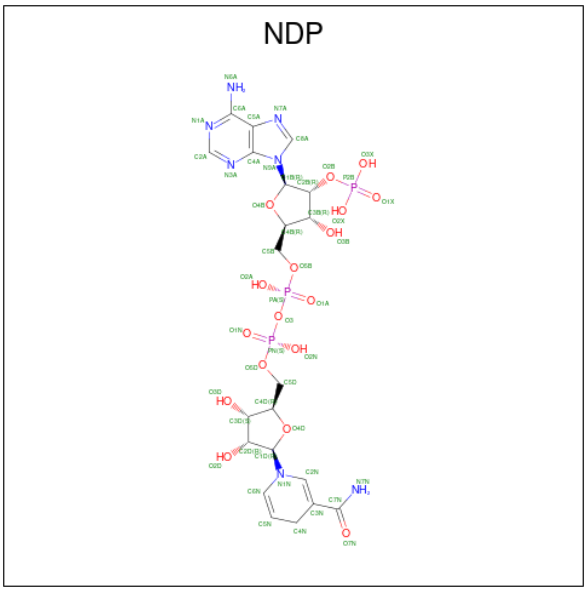
Mol	Chain	Residues	Atoms				AltConf
51	L	1	Total	C	O	P	0
			74	55	17	2	
51	N	1	Total	C	O	P	0
			65	46	17	2	
51	X	1	Total	C	O	P	0
			67	48	17	2	
51	d	1	Total	C	O	P	0
			122	85	33	4	
51	d	1	Total	C	O	P	0
			122	85	33	4	
51	h	1	Total	C	O	P	0
			70	51	17	2	
51	q	1	Total	C	O	P	0
			57	38	17	2	

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



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

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

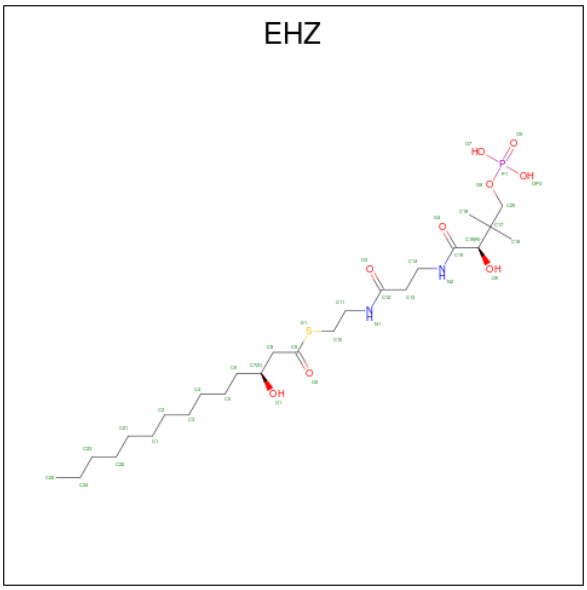


Mol	Chain	Residues	Atoms					AltConf
53	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 55 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



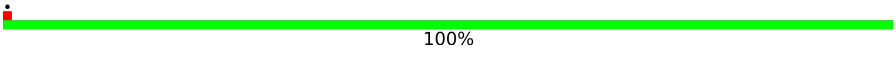
Mol	Chain	Residues	Atoms	AltConf
55	T	1	Total C N O P S 37 25 2 8 1 1	0
55	U	1	Total C N O P S 37 25 2 8 1 1	0

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.

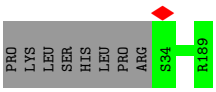
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



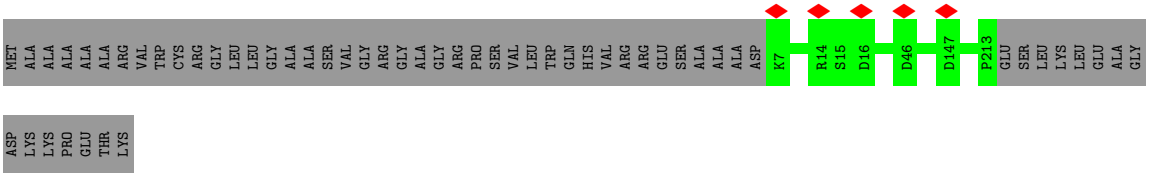
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



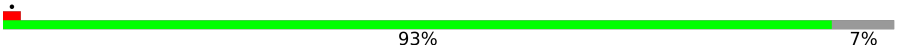
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

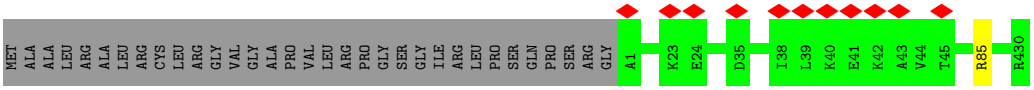
Chain C:



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

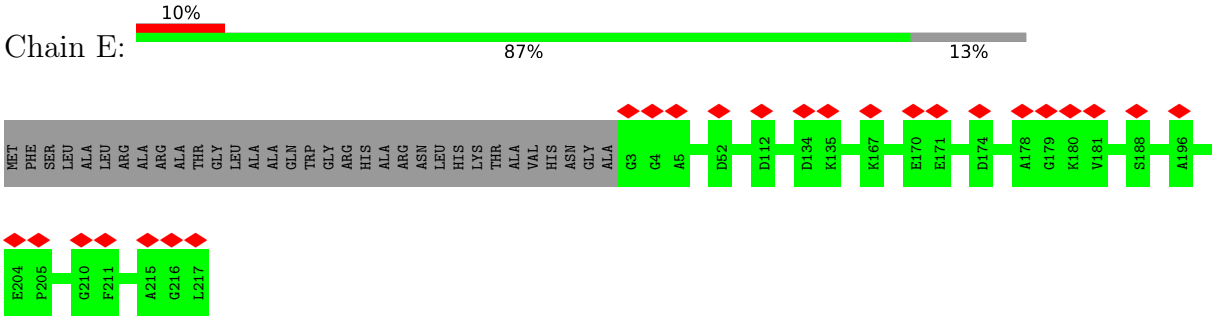
Chain D:





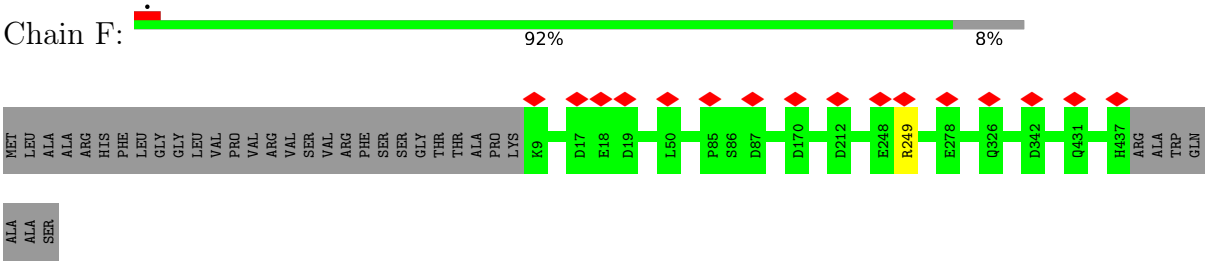
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



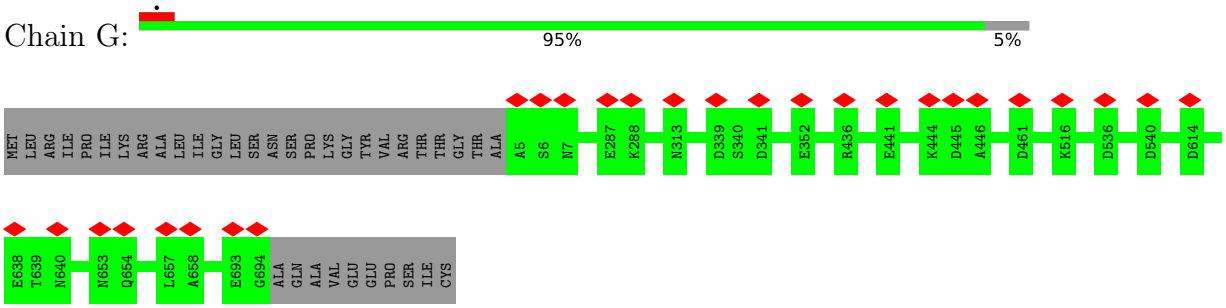
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



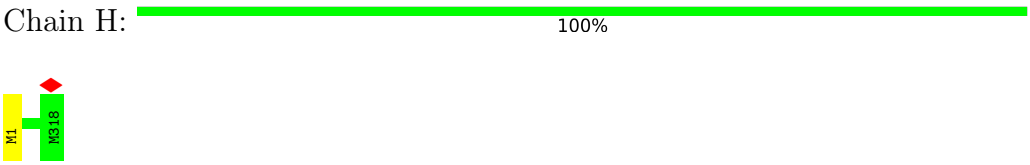
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



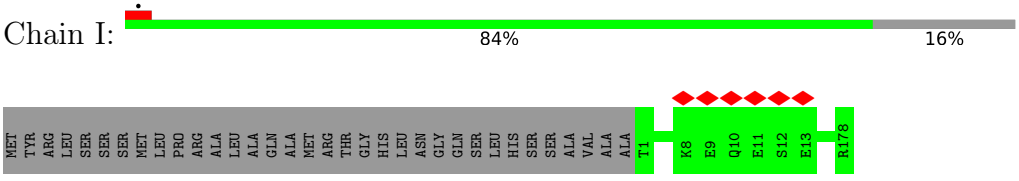
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



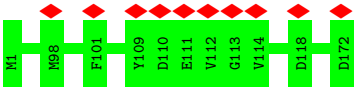
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



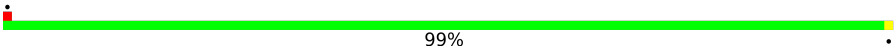
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



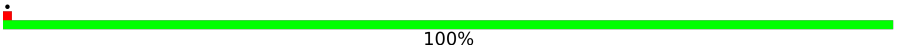
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

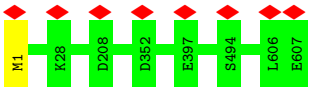
Chain K:



• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

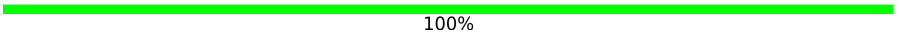
Chain L:

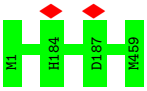




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

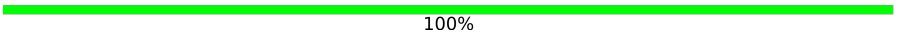
Chain M:





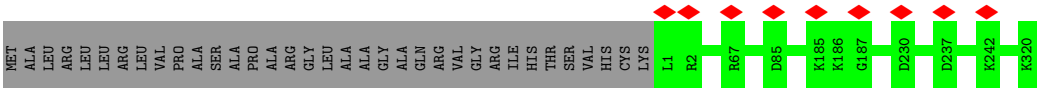
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



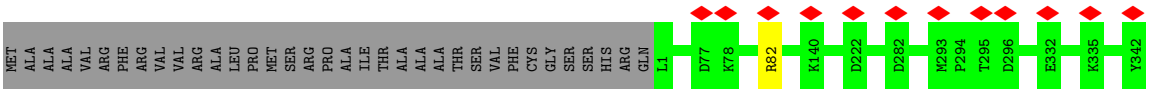
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



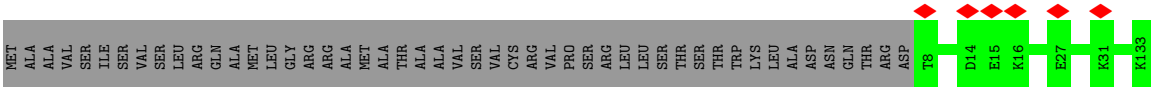
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



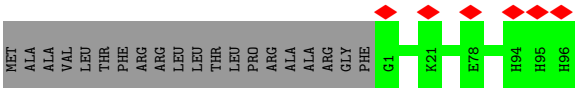
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



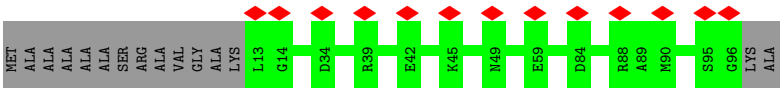
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



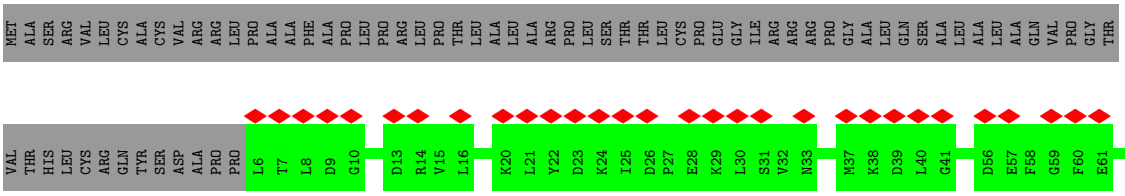
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



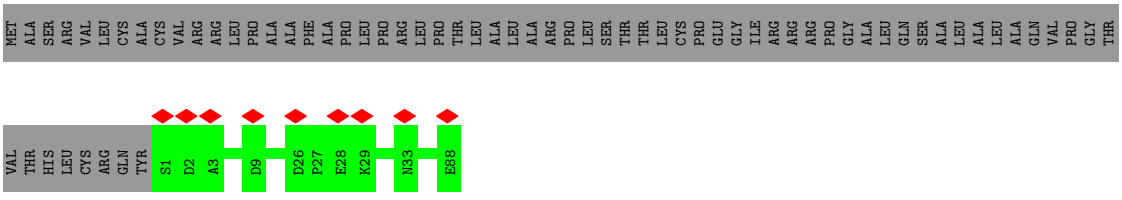
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



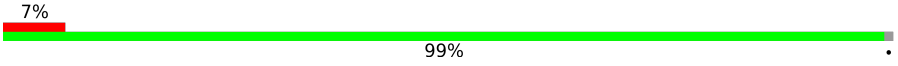
• Molecule 20: Acyl carrier protein, mitochondrial

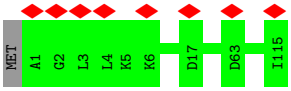
Chain U:



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

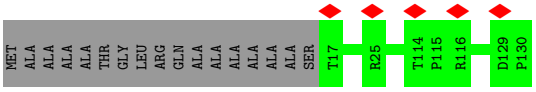
Chain V:





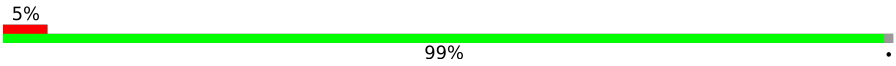
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

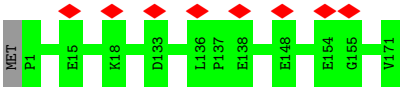
Chain W:



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

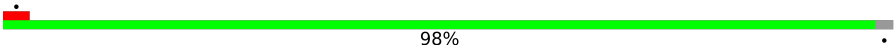
Chain X:

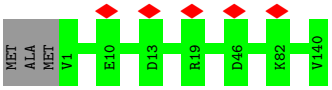




• Molecule 24: MCG5603

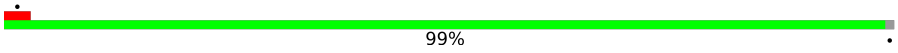
Chain Y:

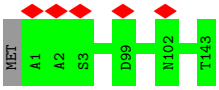




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

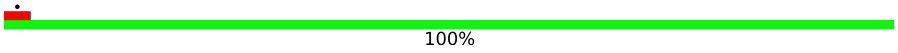
Chain Z:





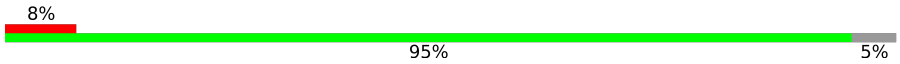
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

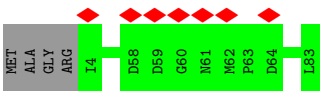
Chain a:



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

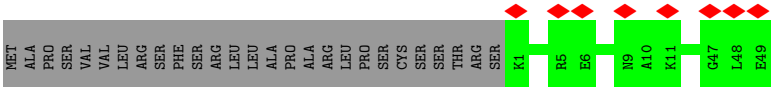
Chain b:





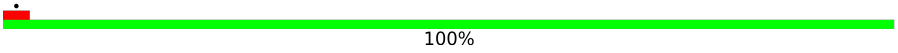
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

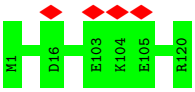
Chain c:



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

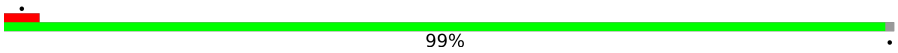
Chain d:

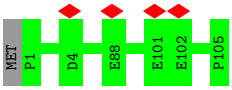




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

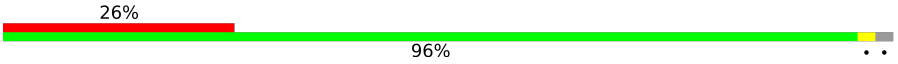
Chain e:

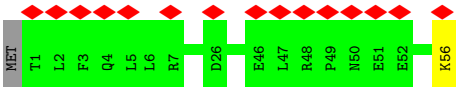




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

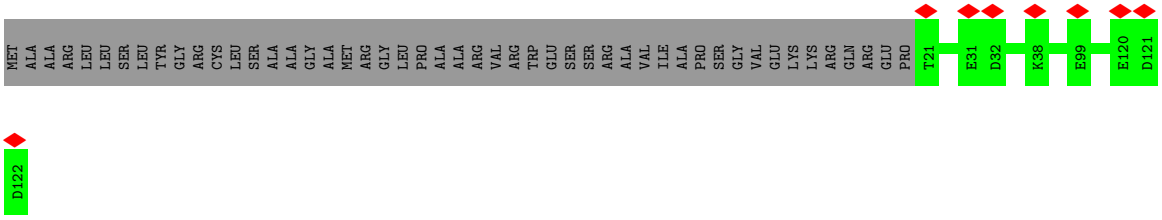
Chain f:





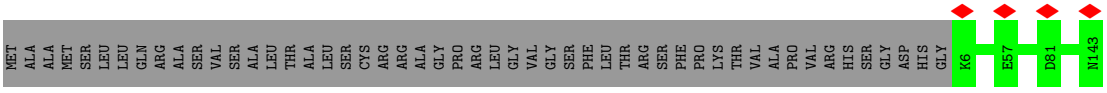
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



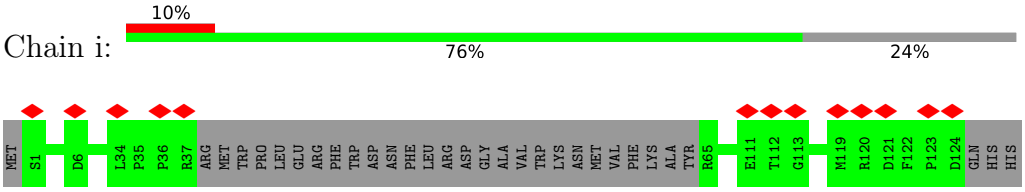
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



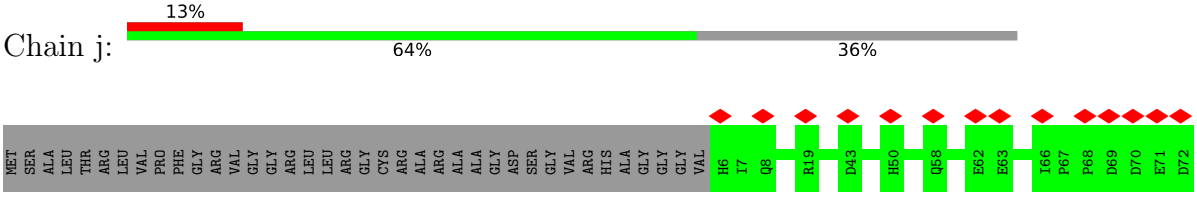
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



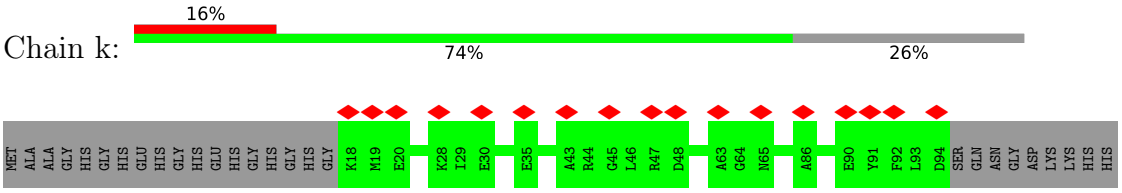
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



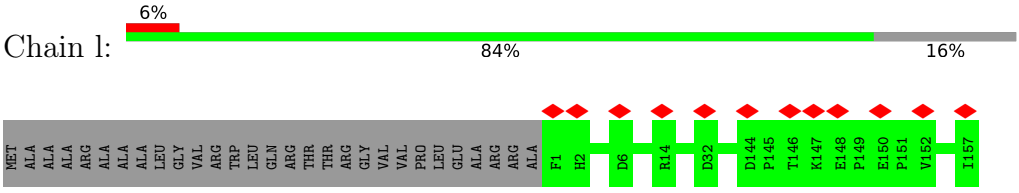
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



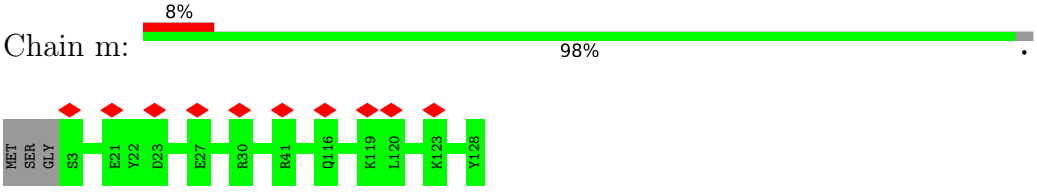
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



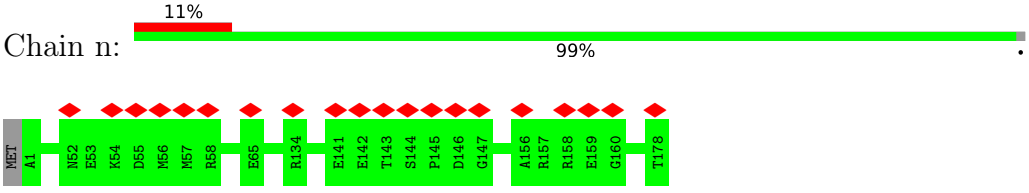
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



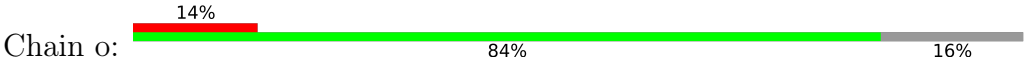
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

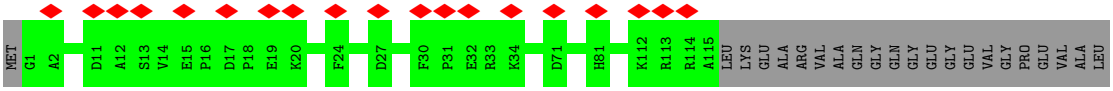
Chain n:



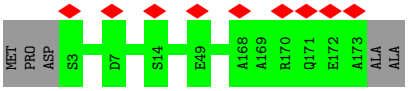
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:

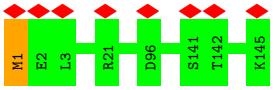




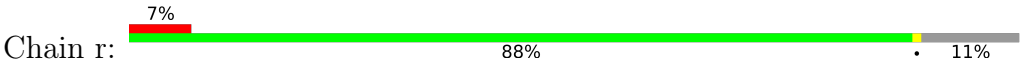
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

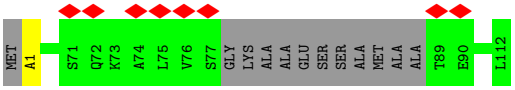


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

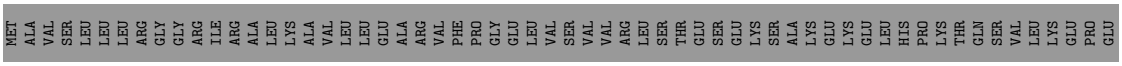


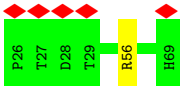
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





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





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44000	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	474.74997, 474.74997, 474.74997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, AYA, EHZ, T2Q, 2MR, SF4, NDP, PC1, FMN, ATP, FES, AME, CDL, FME, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/949	0.43	0/1297
2	B	0.39	0/1278	0.46	0/1730
3	C	0.33	0/1771	0.44	0/2412
4	D	0.34	0/3540	0.45	0/4795
5	E	0.31	0/1704	0.49	0/2321
6	F	0.29	0/3385	0.46	0/4572
7	G	0.31	0/5392	0.47	0/7305
8	H	0.31	0/2607	0.44	0/3564
9	I	0.34	0/1461	0.45	0/1974
10	J	0.30	0/1330	0.44	0/1810
11	K	0.28	0/738	0.42	0/1002
12	L	0.30	0/4922	0.43	0/6698
13	M	0.28	0/3709	0.44	0/5052
14	N	0.30	0/2755	0.45	0/3751
15	O	0.31	0/2674	0.44	0/3626
16	P	0.30	0/2823	0.45	0/3828
17	Q	0.30	0/1045	0.45	0/1411
18	R	0.34	0/773	0.44	0/1041
19	S	0.27	0/682	0.47	0/920
20	T	0.29	0/646	0.45	0/869
20	U	0.28	0/718	0.40	0/970
21	V	0.29	0/954	0.41	0/1293
22	W	0.29	0/993	0.41	0/1335
23	X	0.32	0/1434	0.43	0/1937
24	Y	0.27	0/1061	0.40	0/1439
25	Z	0.30	0/1208	0.44	0/1630
26	a	0.30	0/585	0.42	0/788
27	b	0.28	0/651	0.40	0/895
28	c	0.28	0/418	0.39	0/567
29	d	0.31	0/1028	0.42	0/1387
30	e	0.27	0/900	0.39	0/1199
31	f	0.29	0/495	0.43	0/667

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.31	0/886	0.39	0/1207
33	h	0.31	0/1197	0.41	0/1621
34	i	0.29	0/840	0.43	0/1141
35	j	0.27	0/605	0.41	0/828
36	k	0.28	0/646	0.39	0/873
37	l	0.29	0/1379	0.40	0/1882
38	m	0.29	0/1079	0.43	0/1463
39	n	0.29	0/1596	0.41	0/2162
40	o	0.27	0/1013	0.41	0/1360
41	p	0.30	0/1477	0.43	0/1996
42	q	0.31	0/1243	0.45	0/1692
43	r	0.29	0/819	0.45	0/1108
44	s	0.26	0/379	0.42	0/515
All	All	0.30	0/67788	0.44	0/91933

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	q	1	AME	Mainchain

5.2 Too-close contacts (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%)	107 (95%)	6 (5%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	205/263 (78%)	199 (97%)	6 (3%)	0	100	100
4	D	427/463 (92%)	408 (96%)	19 (4%)	0	100	100
5	E	213/248 (86%)	204 (96%)	9 (4%)	0	100	100
6	F	427/464 (92%)	410 (96%)	17 (4%)	0	100	100
7	G	688/727 (95%)	660 (96%)	28 (4%)	0	100	100
8	H	316/318 (99%)	301 (95%)	15 (5%)	0	100	100
9	I	176/212 (83%)	170 (97%)	6 (3%)	0	100	100
10	J	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	605/607 (100%)	569 (94%)	36 (6%)	0	100	100
13	M	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
14	N	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
15	O	318/355 (90%)	306 (96%)	12 (4%)	0	100	100
16	P	340/377 (90%)	331 (97%)	9 (3%)	0	100	100
17	Q	124/175 (71%)	121 (98%)	3 (2%)	0	100	100
18	R	94/116 (81%)	94 (100%)	0	0	100	100
19	S	82/99 (83%)	74 (90%)	8 (10%)	0	100	100
20	T	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
20	U	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
21	V	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
22	W	112/131 (86%)	108 (96%)	4 (4%)	0	100	100
23	X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
24	Y	138/143 (96%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
30	e	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	f	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
32	g	100/151 (66%)	97 (97%)	3 (3%)	0	100	100
33	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	i	93/128 (73%)	87 (94%)	6 (6%)	0	100	100
35	j	65/105 (62%)	60 (92%)	5 (8%)	0	100	100
36	k	75/104 (72%)	72 (96%)	3 (4%)	0	100	100
37	l	155/186 (83%)	147 (95%)	8 (5%)	0	100	100
38	m	124/129 (96%)	118 (95%)	6 (5%)	0	100	100
39	n	176/179 (98%)	165 (94%)	11 (6%)	0	100	100
40	o	113/137 (82%)	105 (93%)	8 (7%)	0	100	100
41	p	169/176 (96%)	159 (94%)	10 (6%)	0	100	100
42	q	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
43	r	97/113 (86%)	94 (97%)	3 (3%)	0	100	100
44	s	42/104 (40%)	39 (93%)	3 (7%)	0	100	100
All	All	8140/9214 (88%)	7804 (96%)	336 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	189/227 (83%)	189 (100%)	0	100	100
4	D	370/394 (94%)	370 (100%)	0	100	100
5	E	184/206 (89%)	184 (100%)	0	100	100
6	F	344/370 (93%)	343 (100%)	1 (0%)	92	97
7	G	580/610 (95%)	580 (100%)	0	100	100
8	H	279/279 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	137/137 (100%)	137 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	549/549 (100%)	549 (100%)	0	100	100
13	M	414/414 (100%)	414 (100%)	0	100	100
14	N	307/307 (100%)	307 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	299/325 (92%)	298 (100%)	1 (0%)	92	97
17	Q	113/153 (74%)	113 (100%)	0	100	100
18	R	81/96 (84%)	81 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	73/135 (54%)	73 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	122/123 (99%)	122 (100%)	0	100	100
26	a	60/60 (100%)	60 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	43/67 (64%)	43 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	52/53 (98%)	51 (98%)	1 (2%)	57	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	g	93/129 (72%)	93 (100%)	0	100 100
33	h	123/162 (76%)	123 (100%)	0	100 100
34	i	92/120 (77%)	92 (100%)	0	100 100
35	j	63/87 (72%)	63 (100%)	0	100 100
36	k	60/78 (77%)	60 (100%)	0	100 100
37	l	142/161 (88%)	142 (100%)	0	100 100
38	m	112/114 (98%)	112 (100%)	0	100 100
39	n	163/164 (99%)	163 (100%)	0	100 100
40	o	106/121 (88%)	106 (100%)	0	100 100
41	p	155/158 (98%)	155 (100%)	0	100 100
42	q	130/130 (100%)	130 (100%)	0	100 100
43	r	90/96 (94%)	90 (100%)	0	100 100
44	s	43/95 (45%)	42 (98%)	1 (2%)	50 78
All	All	7219/7948 (91%)	7215 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	249	ARG
16	P	82	ARG
31	f	56	LYS
44	s	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	149	ASN
7	G	336	ASN
7	G	654	GLN
12	L	135	ASN
12	L	194	ASN
12	L	199	GLN
12	L	209	ASN
14	N	134	GLN
14	N	144	GLN
15	O	200	GLN

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Mol	Chain	Res	Type
16	P	181	HIS
24	Y	43	ASN
31	f	50	ASN
37	l	135	ASN
40	o	109	GLN
41	p	90	GLN
41	p	99	GLN
41	p	106	GLN
42	q	12	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 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	$\#\|Z\|>2$
8	FME	H	1	8	8,9,10	0.94	0	7,9,11	1.05	1 (14%)
12	FME	L	1	12	8,9,10	0.90	0	7,9,11	1.42	1 (14%)
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	0.84	0
11	FME	K	1	11	8,9,10	0.98	0	7,9,11	1.19	1 (14%)
43	AYA	r	1	43	6,7,8	1.27	1 (16%)	5,8,10	1.28	1 (20%)
10	FME	J	1	10	8,9,10	0.90	0	7,9,11	0.96	0
4	2MR	D	85	4	10,12,13	2.38	3 (30%)	5,13,15	2.03	2 (40%)
14	FME	N	1	14	8,9,10	0.95	0	7,9,11	1.00	1 (14%)
42	AME	q	1	42	9,10,11	1.55	1 (11%)	9,11,13	2.35	5 (55%)
1	FME	A	1	1	8,9,10	0.94	0	7,9,11	0.64	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
8	FME	H	1	8	-	3/7/9/11	-
12	FME	L	1	12	-	4/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
10	FME	J	1	10	-	4/7/9/11	-
4	2MR	D	85	4	-	2/10/13/15	-
14	FME	N	1	14	-	5/7/9/11	-
42	AME	q	1	42	-	5/9/10/12	-
1	FME	A	1	1	-	3/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.15	1.45	1.34
4	D	85	2MR	CZ-NH2	4.70	1.43	1.33
42	q	1	AME	CT1-N	3.57	1.46	1.34
43	r	1	AYA	CA-N	-2.49	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.04	1.42	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	q	1	AME	CT2-CT1-N	5.08	124.69	116.10
4	D	85	2MR	NE-CZ-NH2	-3.31	116.44	119.48
4	D	85	2MR	CD-NE-CZ	3.02	129.07	123.41
12	L	1	FME	C-CA-N	2.91	114.98	109.73
43	r	1	AYA	CB-CA-N	2.56	112.46	109.61
11	K	1	FME	C-CA-N	2.54	114.32	109.73
42	q	1	AME	CE-SD-CG	2.44	108.77	100.40
42	q	1	AME	OT-CT1-CT2	-2.39	117.62	122.06
42	q	1	AME	OT-CT1-N	-2.32	117.68	121.95
8	H	1	FME	C-CA-N	2.14	113.58	109.73
14	N	1	FME	C-CA-N	2.05	113.44	109.73
42	q	1	AME	O-C-CA	-2.05	119.41	124.78

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O-C-CA-CB
8	H	1	FME	O-C-CA-CB
8	H	1	FME	CA-CB-CG-SD
10	J	1	FME	CB-CA-N-CN
11	K	1	FME	N-CA-CB-CG
12	L	1	FME	O1-CN-N-CA
12	L	1	FME	CB-CA-N-CN
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
14	N	1	FME	CA-CB-CG-SD
42	q	1	AME	CB-CA-N-CT1
4	D	85	2MR	NE-CD-CG-CB
42	q	1	AME	CT2-CT1-N-CA
42	q	1	AME	OT-CT1-N-CA
1	A	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
42	q	1	AME	CA-CB-CG-SD
10	J	1	FME	N-CA-CB-CG
4	D	85	2MR	CA-CB-CG-CD
11	K	1	FME	CA-CB-CG-SD
10	J	1	FME	CA-CB-CG-SD
8	H	1	FME	C-CA-CB-CG
12	L	1	FME	C-CA-CB-CG
13	M	1	FME	N-CA-CB-CG
14	N	1	FME	CB-CG-SD-CE
42	q	1	AME	C-CA-N-CT1
14	N	1	FME	CB-CA-N-CN
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
1	A	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	PC1	B	203	-	42,42,53	1.05	4 (9%)	48,50,61	0.98	2 (4%)
47	3PE	h	202	-	36,36,50	1.01	4 (11%)	39,41,55	1.08	2 (5%)
49	FMN	F	501	-	33,33,33	0.69	0	48,50,50	0.73	2 (4%)
47	3PE	D	501	-	48,48,50	0.87	3 (6%)	51,53,55	1.06	2 (3%)
47	3PE	H	401	-	43,43,50	0.91	4 (9%)	46,48,55	1.09	2 (4%)
45	SF4	G	802	7	0,12,12	-	-	-		
47	3PE	i	201	-	41,41,50	0.95	4 (9%)	44,46,55	1.06	2 (4%)
51	CDL	h	201	-	69,69,99	1.04	8 (11%)	75,81,111	1.12	4 (5%)
52	ATP	O	401	-	26,33,33	0.91	1 (3%)	31,52,52	1.56	5 (16%)
45	SF4	B	201	2	0,12,12	-	-	-		
45	SF4	I	204	9	0,12,12	-	-	-		
51	CDL	q	201	-	56,56,99	1.15	8 (14%)	62,68,111	1.16	4 (6%)
47	3PE	M	501	-	41,41,50	0.95	4 (9%)	44,46,55	1.01	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-		
51	CDL	L	702	-	73,73,99	1.02	8 (10%)	79,85,111	1.10	4 (5%)
51	CDL	d	201	-	58,58,99	1.02	6 (10%)	63,69,111	1.04	3 (4%)
46	PC1	I	202	-	44,44,53	1.02	4 (9%)	50,52,61	1.06	2 (4%)
55	EHZ	U	201	20	29,36,37	1.67	5 (17%)	35,44,47	8.60	5 (14%)
51	CDL	X	201	-	66,66,99	1.06	8 (12%)	72,78,111	1.14	4 (5%)
47	3PE	Y	401	-	40,40,50	0.96	4 (10%)	43,45,55	1.05	2 (4%)
45	SF4	G	801	7	0,12,12	-	-	-		
51	CDL	d	202	-	62,62,99	1.09	8 (12%)	68,74,111	1.14	4 (5%)
55	EHZ	T	201	20	29,36,37	1.67	5 (17%)	35,44,47	1.40	1 (2%)
48	FES	G	803	7	0,4,4	-	-	-		
45	SF4	F	502	6	0,12,12	-	-	-		
45	SF4	I	203	9	0,12,12	-	-	-		
46	PC1	B	202	-	34,34,53	1.16	4 (11%)	40,42,61	1.11	2 (5%)
50	T2Q	H	403	-	41,44,44	1.66	5 (12%)	52,65,65	2.54	9 (17%)
47	3PE	K	201	-	32,32,50	1.06	4 (12%)	35,37,55	1.05	2 (5%)
47	3PE	I	201	-	50,50,50	0.85	4 (8%)	53,55,55	1.09	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	CDL	N	401	-	64,64,99	1.08	8 (12%)	70,76,111	1.07	4 (5%)
46	PC1	H	402	-	41,41,53	1.06	4 (9%)	47,49,61	1.04	2 (4%)
53	NDP	P	501	-	45,52,52	2.26	4 (8%)	53,80,80	1.73	9 (16%)
47	3PE	L	701	-	48,48,50	0.89	4 (8%)	51,53,55	1.02	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
46	PC1	B	203	-	-	22/46/46/57	-
47	3PE	h	202	-	-	22/40/40/54	-
49	FMN	F	501	-	-	7/18/18/18	0/3/3/3
47	3PE	D	501	-	-	28/52/52/54	-
47	3PE	H	401	-	-	22/47/47/54	-
45	SF4	G	802	7	-	-	0/6/5/5
47	3PE	i	201	-	-	22/45/45/54	-
51	CDL	h	201	-	-	34/80/80/110	-
52	ATP	O	401	-	-	7/18/38/38	0/3/3/3
51	CDL	q	201	-	-	37/67/67/110	-
45	SF4	B	201	2	-	-	0/6/5/5
45	SF4	I	204	9	-	-	0/6/5/5
47	3PE	M	501	-	-	22/45/45/54	-
48	FES	E	301	5	-	-	0/1/1/1
51	CDL	L	702	-	-	40/84/84/110	-
51	CDL	d	201	-	-	27/67/67/110	-
46	PC1	I	202	-	-	17/48/48/57	-
55	EHZ	U	201	20	-	19/42/44/45	-
51	CDL	X	201	-	-	37/77/77/110	-
47	3PE	Y	401	-	-	15/44/44/54	-
45	SF4	G	801	7	-	-	0/6/5/5
51	CDL	d	202	-	-	27/73/73/110	-
55	EHZ	T	201	20	-	10/42/44/45	-
48	FES	G	803	7	-	-	0/1/1/1
45	SF4	F	502	6	-	-	0/6/5/5
45	SF4	I	203	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	B	202	-	-	17/38/38/57	-
50	T2Q	H	403	-	-	4/23/37/37	0/5/5/5
47	3PE	K	201	-	-	14/36/36/54	-
47	3PE	I	201	-	-	21/54/54/54	-
51	CDL	N	401	-	-	38/75/75/110	-
46	PC1	H	402	-	-	22/45/45/57	-
53	NDP	P	501	-	-	9/30/77/77	0/5/5/5
47	3PE	L	701	-	-	19/52/52/54	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	P	501	NDP	P2B-O2B	12.55	1.83	1.59
50	H	403	T2Q	O4-C8	7.69	1.40	1.23
55	U	201	EHZ	C15-N2	5.42	1.45	1.33
55	T	201	EHZ	C15-N2	5.39	1.45	1.33
55	U	201	EHZ	C12-N1	5.23	1.45	1.33
55	T	201	EHZ	C12-N1	5.23	1.45	1.33
53	P	501	NDP	PN-O5D	4.06	1.75	1.59
50	H	403	T2Q	C4-N9	3.44	1.44	1.37
53	P	501	NDP	O2B-C2B	-3.07	1.32	1.44
47	L	701	3PE	O21-C2	-2.73	1.39	1.46
51	h	201	CDL	OB6-CB4	-2.67	1.39	1.46
51	N	401	CDL	OA6-CA4	-2.61	1.40	1.46
51	q	201	CDL	OB6-CB4	-2.60	1.40	1.46
46	B	203	PC1	O21-C2	-2.59	1.40	1.46
47	M	501	3PE	O21-C2	-2.58	1.40	1.46
51	h	201	CDL	OA6-CA4	-2.57	1.40	1.46
47	I	201	3PE	O21-C2	-2.57	1.40	1.46
47	D	501	3PE	O31-C31	2.55	1.40	1.33
51	L	702	CDL	OA8-CA7	2.54	1.40	1.33
51	d	201	CDL	OB6-CB4	-2.54	1.40	1.46
51	L	702	CDL	OB6-CB4	-2.54	1.40	1.46
47	i	201	3PE	O21-C2	-2.54	1.40	1.46
51	X	201	CDL	OA8-CA7	2.53	1.40	1.33
51	N	401	CDL	OA8-CA7	2.53	1.40	1.33
51	q	201	CDL	OA8-CA7	2.52	1.40	1.33
46	B	202	PC1	O21-C2	-2.51	1.40	1.46
51	h	201	CDL	OA8-CA7	2.51	1.40	1.33
51	L	702	CDL	OB8-CB7	2.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	h	201	CDL	OB8-CB7	2.49	1.40	1.33
51	q	201	CDL	OB8-CB7	2.49	1.40	1.33
51	N	401	CDL	OB6-CB4	-2.48	1.40	1.46
51	d	201	CDL	OA8-CA7	2.48	1.40	1.33
51	d	201	CDL	OB8-CB7	2.48	1.40	1.33
46	H	402	PC1	O31-C31	2.48	1.40	1.33
51	N	401	CDL	OB8-CB7	2.47	1.40	1.33
51	d	202	CDL	OA8-CA7	2.47	1.40	1.33
47	h	202	3PE	O21-C2	-2.47	1.40	1.46
46	H	402	PC1	O21-C2	-2.46	1.40	1.46
47	Y	401	3PE	O31-C31	2.46	1.40	1.33
47	K	201	3PE	O21-C2	-2.45	1.40	1.46
51	L	702	CDL	OA6-CA4	-2.45	1.40	1.46
51	X	201	CDL	OB6-CB4	-2.43	1.40	1.46
51	X	201	CDL	OA6-CA4	-2.43	1.40	1.46
51	d	202	CDL	OB6-CB4	-2.43	1.40	1.46
51	d	202	CDL	OA6-CA4	-2.41	1.40	1.46
47	Y	401	3PE	O21-C2	-2.41	1.40	1.46
46	B	202	PC1	O31-C31	2.40	1.40	1.33
50	H	403	T2Q	C2-N1	2.40	1.45	1.38
51	X	201	CDL	OB8-CB7	2.40	1.40	1.33
47	M	501	3PE	O31-C31	2.39	1.40	1.33
46	I	202	PC1	O21-C2	-2.38	1.40	1.46
51	d	202	CDL	OB8-CB7	2.38	1.40	1.33
47	i	201	3PE	O31-C31	2.38	1.40	1.33
47	h	202	3PE	O31-C31	2.37	1.40	1.33
47	L	701	3PE	O31-C31	2.37	1.40	1.33
46	I	202	PC1	O31-C31	2.36	1.40	1.33
46	B	203	PC1	O31-C31	2.35	1.40	1.33
47	K	201	3PE	O31-C31	2.35	1.40	1.33
47	H	401	3PE	O31-C31	2.33	1.40	1.33
51	q	201	CDL	OA6-CA4	-2.32	1.40	1.46
55	T	201	EHZ	C9-S1	2.30	1.81	1.76
55	U	201	EHZ	O4-C15	-2.29	1.18	1.23
55	U	201	EHZ	O3-C12	-2.28	1.18	1.23
55	U	201	EHZ	C9-S1	2.28	1.81	1.76
51	X	201	CDL	OA6-CA5	2.28	1.40	1.34
50	H	403	T2Q	C4-C5	2.28	1.42	1.37
55	T	201	EHZ	O4-C15	-2.28	1.18	1.23
51	q	201	CDL	OA6-CA5	2.27	1.40	1.34
47	D	501	3PE	O21-C21	2.26	1.40	1.34
47	I	201	3PE	O31-C31	2.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	I	202	PC1	O31-C3	-2.25	1.40	1.45
46	I	202	PC1	O21-C21	2.25	1.40	1.34
47	H	401	3PE	O21-C21	2.25	1.40	1.34
55	T	201	EHZ	O3-C12	-2.23	1.18	1.23
47	K	201	3PE	O31-C3	-2.22	1.40	1.45
51	X	201	CDL	OB8-CB6	-2.22	1.40	1.45
52	O	401	ATP	C5-C4	2.21	1.46	1.40
51	N	401	CDL	OB6-CB5	2.21	1.40	1.34
47	I	201	3PE	O31-C3	-2.21	1.40	1.45
47	h	202	3PE	O21-C21	2.21	1.40	1.34
47	K	201	3PE	O21-C21	2.19	1.40	1.34
47	D	501	3PE	O21-C2	-2.19	1.41	1.46
51	d	202	CDL	OA6-CA5	2.19	1.40	1.34
47	Y	401	3PE	O21-C21	2.17	1.40	1.34
47	i	201	3PE	O31-C3	-2.17	1.40	1.45
46	B	202	PC1	O21-C21	2.17	1.40	1.34
47	i	201	3PE	O21-C21	2.17	1.40	1.34
51	L	702	CDL	OA6-CA5	2.17	1.40	1.34
47	H	401	3PE	O31-C3	-2.17	1.40	1.45
51	d	202	CDL	OB8-CB6	-2.16	1.40	1.45
46	H	402	PC1	O21-C21	2.16	1.40	1.34
51	d	202	CDL	OB6-CB5	2.16	1.40	1.34
46	B	203	PC1	O31-C3	-2.16	1.40	1.45
51	L	702	CDL	OB6-CB5	2.15	1.40	1.34
47	M	501	3PE	O31-C3	-2.15	1.40	1.45
47	H	401	3PE	O21-C2	-2.15	1.41	1.46
47	L	701	3PE	O31-C3	-2.14	1.40	1.45
47	h	202	3PE	O31-C3	-2.14	1.40	1.45
51	q	201	CDL	OB6-CB5	2.13	1.40	1.34
46	B	202	PC1	O31-C3	-2.12	1.40	1.45
51	X	201	CDL	OB6-CB5	2.12	1.40	1.34
51	h	201	CDL	OA6-CA5	2.12	1.40	1.34
51	q	201	CDL	OB8-CB6	-2.12	1.40	1.45
53	P	501	NDP	O5D-C5D	-2.11	1.36	1.44
51	d	201	CDL	OB8-CB6	-2.10	1.40	1.45
46	B	203	PC1	O21-C21	2.09	1.40	1.34
47	M	501	3PE	O21-C21	2.09	1.40	1.34
51	L	702	CDL	OA8-CA6	-2.09	1.40	1.45
51	N	401	CDL	OA6-CA5	2.09	1.40	1.34
51	d	201	CDL	OB6-CB5	2.09	1.40	1.34
51	L	702	CDL	OB8-CB6	-2.08	1.40	1.45
51	N	401	CDL	OB8-CB6	-2.07	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	h	201	CDL	OB8-CB6	-2.07	1.40	1.45
51	d	201	CDL	OA8-CA6	-2.06	1.40	1.45
47	Y	401	3PE	O31-C3	-2.06	1.40	1.45
46	H	402	PC1	O31-C3	-2.05	1.40	1.45
47	I	201	3PE	O21-C21	2.05	1.40	1.34
51	h	201	CDL	OB6-CB5	2.04	1.40	1.34
51	h	201	CDL	OA8-CA6	-2.04	1.40	1.45
51	q	201	CDL	OA8-CA6	-2.03	1.40	1.45
50	H	403	T2Q	CAA-C5	2.03	1.52	1.49
51	d	202	CDL	OA8-CA6	-2.03	1.40	1.45
51	N	401	CDL	OA8-CA6	-2.01	1.40	1.45
47	L	701	3PE	O21-C21	2.00	1.40	1.34
51	X	201	CDL	OA8-CA6	-2.00	1.40	1.45

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	U	201	EHZ	C8-C9-S1	37.87	160.49	113.63
55	U	201	EHZ	O2-C9-S1	-33.22	79.47	122.61
50	H	403	T2Q	OP1-S1-O3'	-11.59	101.34	117.72
50	H	403	T2Q	C7-N6-CAA	8.47	107.98	101.13
53	P	501	NDP	PN-O3-PA	-7.21	108.08	132.83
50	H	403	T2Q	CAB-C7-NAA	5.89	126.78	119.12
55	T	201	EHZ	C8-C9-S1	4.85	119.63	113.63
51	d	202	CDL	OB6-CB5-C51	4.37	120.92	111.50
47	D	501	3PE	O21-C21-C22	4.17	120.49	111.50
51	X	201	CDL	OB6-CB5-C51	4.17	120.49	111.50
47	H	401	3PE	O21-C21-C22	4.15	120.45	111.50
46	B	202	PC1	O21-C21-C22	4.11	120.35	111.50
51	L	702	CDL	OA6-CA5-C11	4.10	120.33	111.50
46	H	402	PC1	O21-C21-C22	4.09	120.31	111.50
51	X	201	CDL	OA6-CA5-C11	4.09	120.31	111.50
47	h	202	3PE	O21-C21-C22	4.08	120.30	111.50
46	I	202	PC1	O21-C21-C22	4.08	120.30	111.50
47	i	201	3PE	O21-C21-C22	4.01	120.14	111.50
51	L	702	CDL	OB6-CB5-C51	3.99	120.10	111.50
51	h	201	CDL	OB6-CB5-C51	3.90	119.90	111.50
51	d	202	CDL	OA6-CA5-C11	3.90	119.90	111.50
51	q	201	CDL	OB6-CB5-C51	3.89	119.88	111.50
47	I	201	3PE	O21-C21-C22	3.88	119.86	111.50
51	q	201	CDL	OA6-CA5-C11	3.87	119.84	111.50
51	d	201	CDL	OB6-CB5-C51	3.87	119.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	B	203	PC1	O21-C21-C22	3.86	119.82	111.50
51	h	201	CDL	OA6-CA5-C11	3.83	119.76	111.50
50	H	403	T2Q	C4-N9-C8	-3.82	120.34	122.50
52	O	401	ATP	PA-O3A-PB	-3.76	119.91	132.83
50	H	403	T2Q	C12-C8-N9	3.76	119.65	115.01
51	N	401	CDL	OA6-CA5-C11	3.76	119.60	111.50
47	Y	401	3PE	O21-C21-C22	3.71	119.49	111.50
52	O	401	ATP	N3-C2-N1	-3.67	122.94	128.68
47	K	201	3PE	O21-C21-C22	3.65	119.37	111.50
47	M	501	3PE	O21-C21-C22	3.55	119.16	111.50
47	L	701	3PE	O21-C21-C22	3.50	119.04	111.50
50	H	403	T2Q	C25-N1-C21	3.45	119.14	111.52
51	N	401	CDL	OB6-CB5-C51	3.39	118.80	111.50
53	P	501	NDP	O2B-P2B-O1X	-3.29	96.68	109.39
52	O	401	ATP	PB-O3B-PG	-3.27	121.59	132.83
53	P	501	NDP	PA-O5B-C5B	-2.99	104.17	121.68
51	q	201	CDL	OB8-CB7-C71	2.96	121.18	111.91
53	P	501	NDP	PN-O5D-C5D	-2.83	105.06	121.68
47	h	202	3PE	O31-C31-C32	2.82	120.77	111.91
47	I	201	3PE	O31-C31-C32	2.77	120.62	111.91
51	q	201	CDL	OA8-CA7-C31	2.76	120.58	111.91
51	d	201	CDL	OB8-CB7-C71	2.75	120.52	111.91
46	B	202	PC1	O31-C31-C32	2.73	120.46	111.91
51	h	201	CDL	OA8-CA7-C31	2.71	120.43	111.91
47	H	401	3PE	O31-C31-C32	2.71	120.41	111.91
47	D	501	3PE	O31-C31-C32	2.70	120.38	111.91
47	L	701	3PE	O31-C31-C32	2.69	120.34	111.91
51	X	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
51	X	201	CDL	OA8-CA7-C31	2.68	120.31	111.91
51	d	202	CDL	OA8-CA7-C31	2.67	120.27	111.91
53	P	501	NDP	C2A-N1A-C6A	-2.63	114.26	118.75
52	O	401	ATP	C4-C5-N7	-2.61	106.68	109.40
47	M	501	3PE	O31-C31-C32	2.60	120.07	111.91
47	Y	401	3PE	O31-C31-C32	2.60	120.06	111.91
51	L	702	CDL	OB8-CB7-C71	2.60	120.06	111.91
51	h	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
50	H	403	T2Q	OP1-S1-C26	2.54	111.76	108.61
51	N	401	CDL	OB8-CB7-C71	2.54	119.88	111.91
53	P	501	NDP	O3X-P2B-O2X	2.54	117.33	107.64
47	i	201	3PE	O31-C31-C32	2.53	119.86	111.91
46	I	202	PC1	O31-C31-C32	2.52	119.82	111.91
51	d	201	CDL	OA8-CA7-C31	2.52	119.82	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	U	201	EHZ	C13-C12-N1	2.49	120.61	116.42
51	N	401	CDL	OA8-CA7-C31	2.47	119.66	111.91
51	L	702	CDL	OA8-CA7-C31	2.47	119.66	111.91
46	H	402	PC1	O31-C31-C32	2.45	119.58	111.91
52	O	401	ATP	C3'-C2'-C1'	2.44	104.66	100.98
50	H	403	T2Q	O3'-S1-C26	2.44	111.64	108.61
47	K	201	3PE	O31-C31-C32	2.38	119.37	111.91
46	B	203	PC1	O31-C31-C32	2.34	119.24	111.91
50	H	403	T2Q	C2'-C1'-N9	-2.33	109.30	112.83
55	U	201	EHZ	C7-C8-C9	-2.32	108.60	113.89
51	d	202	CDL	OB8-CB7-C71	2.29	119.09	111.91
53	P	501	NDP	O2N-PN-O1N	2.27	123.47	112.24
53	P	501	NDP	N3A-C2A-N1A	2.21	132.13	128.68
49	F	501	FMN	C4-N3-C2	-2.13	121.71	125.64
53	P	501	NDP	O5D-PN-O1N	-2.11	100.81	109.07
55	U	201	EHZ	C14-C13-C12	-2.10	108.86	112.36
49	F	501	FMN	C4A-C4-N3	2.01	118.30	113.19

There are no chirality outliers.

All (559) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C1-O11-P-O12
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	C1-O11-P-O13
46	B	202	PC1	C22-C21-O21-C2
46	B	203	PC1	C22-C21-O21-C2
46	H	402	PC1	C11-O13-P-O12
46	H	402	PC1	C11-O13-P-O11
46	H	402	PC1	O13-C11-C12-N
46	I	202	PC1	O13-C11-C12-N
47	D	501	3PE	C1-O11-P-O12
47	D	501	3PE	C1-O11-P-O14
47	D	501	3PE	C22-C21-O21-C2
47	H	401	3PE	C1-O11-P-O14
47	H	401	3PE	C11-O13-P-O11
47	H	401	3PE	C11-O13-P-O12
47	H	401	3PE	C11-O13-P-O14
47	H	401	3PE	C22-C21-O21-C2
47	K	201	3PE	O13-C11-C12-N
47	L	701	3PE	C11-O13-P-O11
47	L	701	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
47	L	701	3PE	C11-O13-P-O14
47	L	701	3PE	O13-C11-C12-N
47	M	501	3PE	C11-O13-P-O11
47	M	501	3PE	C11-O13-P-O12
47	M	501	3PE	O13-C11-C12-N
47	Y	401	3PE	C11-O13-P-O14
47	Y	401	3PE	O13-C11-C12-N
47	Y	401	3PE	O21-C2-C3-O31
47	h	202	3PE	C1-O11-P-O12
47	h	202	3PE	C1-O11-P-O13
47	h	202	3PE	C1-O11-P-O14
47	h	202	3PE	O13-C11-C12-N
47	i	201	3PE	C1-O11-P-O12
47	i	201	3PE	C1-O11-P-O14
49	F	501	FMN	N10-C1'-C2'-O2'
49	F	501	FMN	N10-C1'-C2'-C3'
49	F	501	FMN	C1'-C2'-C3'-O3'
49	F	501	FMN	C1'-C2'-C3'-C4'
50	H	403	T2Q	C24-C23-S1-C26
51	L	702	CDL	CA2-OA2-PA1-OA3
51	L	702	CDL	CA2-OA2-PA1-OA5
51	L	702	CDL	C11-CA5-OA6-CA4
51	L	702	CDL	CB2-OB2-PB2-OB3
51	L	702	CDL	CB2-OB2-PB2-OB4
51	L	702	CDL	CB3-OB5-PB2-OB2
51	L	702	CDL	C51-CB5-OB6-CB4
51	N	401	CDL	CA2-OA2-PA1-OA3
51	N	401	CDL	CA2-OA2-PA1-OA4
51	N	401	CDL	CA3-OA5-PA1-OA4
51	N	401	CDL	OA7-CA5-OA6-CA4
51	N	401	CDL	CB2-OB2-PB2-OB3
51	N	401	CDL	CB2-OB2-PB2-OB5
51	X	201	CDL	CB2-C1-CA2-OA2
51	X	201	CDL	CA3-OA5-PA1-OA3
51	X	201	CDL	CA3-OA5-PA1-OA4
51	X	201	CDL	CB2-OB2-PB2-OB3
51	X	201	CDL	CB2-OB2-PB2-OB4
51	X	201	CDL	CB2-OB2-PB2-OB5
51	X	201	CDL	C51-CB5-OB6-CB4
51	d	201	CDL	OA5-CA3-CA4-CA6
51	d	201	CDL	C1-CB2-OB2-PB2
51	d	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
51	d	201	CDL	CB2-OB2-PB2-OB4
51	d	201	CDL	CB3-OB5-PB2-OB3
51	d	201	CDL	CB3-OB5-PB2-OB4
51	d	201	CDL	OB7-CB5-OB6-CB4
51	d	201	CDL	C51-CB5-OB6-CB4
51	d	202	CDL	CB2-C1-CA2-OA2
51	d	202	CDL	CB3-OB5-PB2-OB3
51	d	202	CDL	OB9-CB7-OB8-CB6
51	h	201	CDL	CA2-C1-CB2-OB2
51	h	201	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	OB6-CB4-CB6-OB8
51	h	201	CDL	C51-CB5-OB6-CB4
51	q	201	CDL	O1-C1-CB2-OB2
51	q	201	CDL	CA3-OA5-PA1-OA3
51	q	201	CDL	CB2-OB2-PB2-OB3
51	q	201	CDL	CB3-OB5-PB2-OB2
51	q	201	CDL	CB3-OB5-PB2-OB3
51	q	201	CDL	CB3-OB5-PB2-OB4
51	q	201	CDL	OB5-CB3-CB4-OB6
52	O	401	ATP	C5'-O5'-PA-O3A
52	O	401	ATP	C3'-C4'-C5'-O5'
53	P	501	NDP	C2B-O2B-P2B-O3X
55	T	201	EHZ	C5-C6-C7-C8
55	U	201	EHZ	C7-C8-C9-S1
55	U	201	EHZ	C15-C16-C17-C18
55	U	201	EHZ	C15-C16-C17-C19
55	U	201	EHZ	C15-C16-C17-C20
55	U	201	EHZ	O5-C16-C17-C19
55	U	201	EHZ	O5-C16-C17-C20
55	U	201	EHZ	O2-C9-S1-C10
55	U	201	EHZ	C8-C9-S1-C10
51	h	201	CDL	OB9-CB7-OB8-CB6
51	h	201	CDL	C71-CB7-OB8-CB6
51	q	201	CDL	C71-CB7-OB8-CB6
46	B	202	PC1	O32-C31-O31-C3
46	I	202	PC1	O32-C31-O31-C3
47	D	501	3PE	O32-C31-O31-C3
47	H	401	3PE	O32-C31-O31-C3
47	M	501	3PE	O32-C31-O31-C3
47	Y	401	3PE	O32-C31-O31-C3
47	h	202	3PE	O32-C31-O31-C3
51	L	702	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
51	N	401	CDL	OB9-CB7-OB8-CB6
51	q	201	CDL	OA9-CA7-OA8-CA6
51	q	201	CDL	OB9-CB7-OB8-CB6
46	B	202	PC1	O22-C21-O21-C2
46	B	203	PC1	O22-C21-O21-C2
47	D	501	3PE	O22-C21-O21-C2
47	H	401	3PE	O22-C21-O21-C2
51	L	702	CDL	OA7-CA5-OA6-CA4
51	L	702	CDL	OB7-CB5-OB6-CB4
51	X	201	CDL	OB7-CB5-OB6-CB4
46	I	202	PC1	C32-C31-O31-C3
47	H	401	3PE	C32-C31-O31-C3
47	M	501	3PE	C32-C31-O31-C3
47	Y	401	3PE	C32-C31-O31-C3
47	h	202	3PE	C32-C31-O31-C3
51	N	401	CDL	C71-CB7-OB8-CB6
51	d	202	CDL	C71-CB7-OB8-CB6
51	q	201	CDL	C31-CA7-OA8-CA6
51	N	401	CDL	C11-CA5-OA6-CA4
46	B	202	PC1	C32-C31-O31-C3
47	D	501	3PE	C32-C31-O31-C3
47	L	701	3PE	C32-C31-O31-C3
51	L	702	CDL	C31-CA7-OA8-CA6
51	h	201	CDL	OB7-CB5-OB6-CB4
51	X	201	CDL	OB9-CB7-OB8-CB6
51	X	201	CDL	O1-C1-CA2-OA2
51	d	202	CDL	O1-C1-CA2-OA2
51	h	201	CDL	O1-C1-CB2-OB2
51	d	201	CDL	C31-CA7-OA8-CA6
47	L	701	3PE	O32-C31-O31-C3
53	P	501	NDP	O4B-C4B-C5B-O5B
51	X	201	CDL	C71-CB7-OB8-CB6
51	d	201	CDL	C71-CB7-OB8-CB6
46	H	402	PC1	C2-C1-O11-P
51	d	201	CDL	OA9-CA7-OA8-CA6
51	d	202	CDL	C11-CA5-OA6-CA4
51	d	201	CDL	OB9-CB7-OB8-CB6
47	K	201	3PE	C32-C31-O31-C3
47	i	201	3PE	C32-C31-O31-C3
51	d	202	CDL	C31-CA7-OA8-CA6
53	P	501	NDP	O4D-C1D-N1N-C6N
46	B	203	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
51	d	201	CDL	OA5-CA3-CA4-OA6
51	q	201	CDL	O1-C1-CA2-OA2
47	K	201	3PE	O32-C31-O31-C3
47	i	201	3PE	O32-C31-O31-C3
47	h	202	3PE	C31-C32-C33-C34
46	B	203	PC1	C32-C31-O31-C3
47	M	501	3PE	C21-C22-C23-C24
46	B	202	PC1	C21-C22-C23-C24
46	B	202	PC1	C31-C32-C33-C34
47	I	201	3PE	C21-C22-C23-C24
51	L	702	CDL	CA5-C11-C12-C13
51	d	202	CDL	CA5-C11-C12-C13
55	T	201	EHZ	C5-C6-C7-O1
47	i	201	3PE	C21-C22-C23-C24
51	X	201	CDL	CA7-C31-C32-C33
51	d	202	CDL	OA9-CA7-OA8-CA6
51	d	202	CDL	OA7-CA5-OA6-CA4
46	B	203	PC1	O32-C31-O31-C3
46	I	202	PC1	C11-O13-P-O11
47	D	501	3PE	C1-O11-P-O13
47	D	501	3PE	C11-O13-P-O11
47	Y	401	3PE	C11-O13-P-O11
47	h	202	3PE	C11-O13-P-O11
47	i	201	3PE	C1-O11-P-O13
51	L	702	CDL	CB2-OB2-PB2-OB5
51	N	401	CDL	CA2-OA2-PA1-OA5
51	N	401	CDL	CA3-OA5-PA1-OA2
51	X	201	CDL	CA3-OA5-PA1-OA2
51	d	201	CDL	CA2-OA2-PA1-OA5
51	d	201	CDL	CB2-OB2-PB2-OB5
51	d	201	CDL	CB3-OB5-PB2-OB2
51	d	202	CDL	CB3-OB5-PB2-OB2
51	h	201	CDL	CB2-OB2-PB2-OB5
51	q	201	CDL	CA3-OA5-PA1-OA2
51	q	201	CDL	CB2-OB2-PB2-OB5
51	q	201	CDL	CA2-C1-CB2-OB2
49	F	501	FMN	O2'-C2'-C3'-O3'
47	D	501	3PE	C28-C29-C2A-C2B
51	h	201	CDL	C11-CA5-OA6-CA4
46	H	402	PC1	C37-C38-C39-C3A
47	H	401	3PE	C22-C23-C24-C25
47	L	701	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
47	Y	401	3PE	C35-C36-C37-C38
51	L	702	CDL	C74-C75-C76-C77
51	L	702	CDL	C71-CB7-OB8-CB6
51	L	702	CDL	C13-C14-C15-C16
51	d	201	CDL	C59-C60-C61-C62
51	q	201	CDL	C15-C16-C17-C18
51	q	201	CDL	C31-C32-C33-C34
47	H	401	3PE	C3-C2-O21-C21
51	h	201	CDL	OA7-CA5-OA6-CA4
49	F	501	FMN	O2'-C2'-C3'-C4'
47	M	501	3PE	C36-C37-C38-C39
47	L	701	3PE	C2E-C2F-C2G-C2H
51	L	702	CDL	C35-C36-C37-C38
51	L	702	CDL	O1-C1-CA2-OA2
46	B	203	PC1	C37-C38-C39-C3A
46	H	402	PC1	C22-C23-C24-C25
51	L	702	CDL	C52-C53-C54-C55
46	B	203	PC1	C22-C23-C24-C25
47	D	501	3PE	C38-C39-C3A-C3B
46	H	402	PC1	C33-C34-C35-C36
47	I	201	3PE	C24-C25-C26-C27
55	U	201	EHZ	C2-C1-C21-C22
55	U	201	EHZ	C1-C21-C22-C23
47	I	201	3PE	C2B-C2C-C2D-C2E
47	L	701	3PE	C22-C21-O21-C2
51	q	201	CDL	C51-CB5-OB6-CB4
46	I	202	PC1	C2C-C2D-C2E-C2F
47	D	501	3PE	C32-C33-C34-C35
47	I	201	3PE	C33-C34-C35-C36
51	X	201	CDL	C33-C34-C35-C36
47	I	201	3PE	C34-C35-C36-C37
47	M	501	3PE	C24-C25-C26-C27
47	i	201	3PE	C25-C26-C27-C28
51	N	401	CDL	C81-C82-C83-C84
51	X	201	CDL	C32-C33-C34-C35
55	T	201	EHZ	C2-C1-C21-C22
46	B	203	PC1	C3C-C3D-C3E-C3F
47	M	501	3PE	C3C-C3D-C3E-C3F
51	h	201	CDL	C18-C19-C20-C21
51	N	401	CDL	C52-C53-C54-C55
51	X	201	CDL	C51-C52-C53-C54
51	d	202	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
47	M	501	3PE	C32-C33-C34-C35
51	L	702	CDL	C33-C34-C35-C36
47	H	401	3PE	C3D-C3E-C3F-C3G
47	K	201	3PE	C25-C26-C27-C28
51	d	201	CDL	C56-C57-C58-C59
47	M	501	3PE	C23-C24-C25-C26
47	I	201	3PE	C1-C2-C3-O31
47	D	501	3PE	C3D-C3E-C3F-C3G
47	L	701	3PE	C2B-C2C-C2D-C2E
47	i	201	3PE	C2D-C2E-C2F-C2G
51	d	202	CDL	C73-C74-C75-C76
47	K	201	3PE	C31-C32-C33-C34
51	q	201	CDL	CA5-C11-C12-C13
47	H	401	3PE	C34-C35-C36-C37
47	i	201	3PE	C22-C21-O21-C2
51	N	401	CDL	C77-C78-C79-C80
47	H	401	3PE	C24-C25-C26-C27
47	Y	401	3PE	C3A-C3B-C3C-C3D
51	L	702	CDL	C78-C79-C80-C81
51	N	401	CDL	CA5-C11-C12-C13
47	I	201	3PE	C3D-C3E-C3F-C3G
51	d	201	CDL	C74-C75-C76-C77
47	L	701	3PE	O22-C21-O21-C2
51	q	201	CDL	OB7-CB5-OB6-CB4
47	D	501	3PE	C34-C35-C36-C37
47	i	201	3PE	C32-C33-C34-C35
51	L	702	CDL	OB9-CB7-OB8-CB6
47	i	201	3PE	C33-C34-C35-C36
46	H	402	PC1	C22-C21-O21-C2
47	I	201	3PE	C36-C37-C38-C39
47	M	501	3PE	C37-C38-C39-C3A
51	L	702	CDL	C15-C16-C17-C18
51	d	202	CDL	C11-C12-C13-C14
51	N	401	CDL	CB7-C71-C72-C73
47	h	202	3PE	C38-C39-C3A-C3B
51	N	401	CDL	OB7-CB5-OB6-CB4
51	N	401	CDL	C78-C79-C80-C81
47	D	501	3PE	C31-C32-C33-C34
51	q	201	CDL	CB5-C51-C52-C53
47	i	201	3PE	C29-C2A-C2B-C2C
51	X	201	CDL	C63-C64-C65-C66
51	h	201	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
47	M	501	3PE	C34-C35-C36-C37
47	M	501	3PE	C22-C21-O21-C2
47	h	202	3PE	C22-C21-O21-C2
51	N	401	CDL	C51-CB5-OB6-CB4
51	h	201	CDL	C11-C12-C13-C14
47	h	202	3PE	O22-C21-O21-C2
47	i	201	3PE	O22-C21-O21-C2
47	D	501	3PE	C3B-C3C-C3D-C3E
47	K	201	3PE	C34-C35-C36-C37
51	L	702	CDL	OB6-CB4-CB6-OB8
51	N	401	CDL	C31-C32-C33-C34
47	L	701	3PE	C38-C39-C3A-C3B
51	d	201	CDL	C72-C73-C74-C75
52	O	401	ATP	O4'-C4'-C5'-O5'
46	I	202	PC1	C26-C27-C28-C29
46	H	402	PC1	O22-C21-O21-C2
47	M	501	3PE	O22-C21-O21-C2
47	I	201	3PE	C22-C21-O21-C2
51	q	201	CDL	C17-C18-C19-C20
47	D	501	3PE	C21-C22-C23-C24
51	d	202	CDL	C1-CA2-OA2-PA1
51	X	201	CDL	C13-C14-C15-C16
46	I	202	PC1	O11-C1-C2-C3
47	L	701	3PE	O11-C1-C2-C3
51	q	201	CDL	OB5-CB3-CB4-CB6
47	h	202	3PE	C21-C22-C23-C24
51	X	201	CDL	CA5-C11-C12-C13
51	d	201	CDL	C31-C32-C33-C34
51	X	201	CDL	C11-C12-C13-C14
51	X	201	CDL	C53-C54-C55-C56
46	B	203	PC1	C3E-C3F-C3G-C3H
47	h	202	3PE	C1-C2-C3-O31
47	h	202	3PE	C22-C23-C24-C25
47	i	201	3PE	C1-C2-C3-O31
51	N	401	CDL	CA3-CA4-CA6-OA8
51	d	201	CDL	CB3-CB4-CB6-OB8
51	d	202	CDL	CB3-CB4-CB6-OB8
51	h	201	CDL	CA3-CA4-CA6-OA8
51	q	201	CDL	CA3-CA4-CA6-OA8
51	N	401	CDL	C82-C83-C84-C85
51	d	202	CDL	C77-C78-C79-C80
46	I	202	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
51	q	201	CDL	C18-C19-C20-C21
46	H	402	PC1	C3A-C3B-C3C-C3D
46	B	202	PC1	C24-C25-C26-C27
47	K	201	3PE	C32-C33-C34-C35
47	M	501	3PE	C3E-C3F-C3G-C3H
55	T	201	EHZ	C18-C17-C20-O6
55	T	201	EHZ	C19-C17-C20-O6
51	L	702	CDL	CA6-CA4-OA6-CA5
47	K	201	3PE	C22-C23-C24-C25
51	N	401	CDL	C1-CA2-OA2-PA1
46	I	202	PC1	C35-C36-C37-C38
47	D	501	3PE	C29-C2A-C2B-C2C
47	K	201	3PE	C27-C28-C29-C2A
55	T	201	EHZ	C1-C21-C22-C23
55	U	201	EHZ	C22-C23-C24-C25
51	X	201	CDL	C60-C61-C62-C63
55	U	201	EHZ	O5-C16-C17-C18
51	h	201	CDL	C24-C25-C26-C27
47	H	401	3PE	C36-C37-C38-C39
55	U	201	EHZ	C21-C1-C2-C3
47	I	201	3PE	C3E-C3F-C3G-C3H
55	U	201	EHZ	C5-C6-C7-C8
47	H	401	3PE	C32-C33-C34-C35
46	H	402	PC1	C32-C31-O31-C3
46	B	203	PC1	C3D-C3E-C3F-C3G
53	P	501	NDP	O4D-C4D-C5D-O5D
51	h	201	CDL	OA5-CA3-CA4-CA6
51	q	201	CDL	OA5-CA3-CA4-CA6
46	I	202	PC1	C29-C2A-C2B-C2C
55	U	201	EHZ	C3-C4-C5-C6
46	B	203	PC1	C34-C35-C36-C37
51	d	202	CDL	C33-C34-C35-C36
47	H	401	3PE	C31-C32-C33-C34
51	h	201	CDL	C1-CB2-OB2-PB2
46	B	202	PC1	C35-C36-C37-C38
47	H	401	3PE	C38-C39-C3A-C3B
47	L	701	3PE	C32-C33-C34-C35
47	Y	401	3PE	C1-C2-C3-O31
51	L	702	CDL	CB3-CB4-CB6-OB8
51	N	401	CDL	CB3-CB4-CB6-OB8
51	X	201	CDL	CA3-CA4-CA6-OA8
51	d	202	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
46	I	202	PC1	C33-C34-C35-C36
47	D	501	3PE	C2D-C2E-C2F-C2G
51	h	201	CDL	C53-C54-C55-C56
55	T	201	EHZ	N2-C15-C16-C17
47	I	201	3PE	C28-C29-C2A-C2B
51	h	201	CDL	CA5-C11-C12-C13
46	I	202	PC1	C34-C35-C36-C37
46	H	402	PC1	O11-C1-C2-O21
51	q	201	CDL	OA5-CA3-CA4-OA6
51	d	201	CDL	CB7-C71-C72-C73
55	U	201	EHZ	C5-C6-C7-O1
47	i	201	3PE	O21-C2-C3-O31
51	h	201	CDL	OA6-CA4-CA6-OA8
47	h	202	3PE	C36-C37-C38-C39
51	q	201	CDL	C52-C53-C54-C55
46	H	402	PC1	C34-C35-C36-C37
47	I	201	3PE	O22-C21-O21-C2
55	T	201	EHZ	C2-C3-C4-C5
51	N	401	CDL	CB4-CB3-OB5-PB2
51	d	202	CDL	C1-CB2-OB2-PB2
51	L	702	CDL	C37-C38-C39-C40
51	q	201	CDL	C12-C13-C14-C15
47	I	201	3PE	C2F-C2G-C2H-C2I
51	d	202	CDL	C76-C77-C78-C79
46	H	402	PC1	O11-C1-C2-C3
47	H	401	3PE	C25-C26-C27-C28
47	L	701	3PE	C22-C23-C24-C25
47	D	501	3PE	C3F-C3G-C3H-C3I
53	P	501	NDP	C3B-C4B-C5B-O5B
51	q	201	CDL	C51-C52-C53-C54
47	D	501	3PE	C3-C2-O21-C21
51	X	201	CDL	CB3-CB4-OB6-CB5
51	d	202	CDL	CA6-CA4-OA6-CA5
46	H	402	PC1	O32-C31-O31-C3
46	B	203	PC1	C1-C2-C3-O31
51	h	201	CDL	OA5-CA3-CA4-OA6
51	L	702	CDL	CB2-C1-CA2-OA2
47	D	501	3PE	C23-C24-C25-C26
46	B	202	PC1	C36-C37-C38-C39
46	H	402	PC1	C25-C26-C27-C28
47	I	201	3PE	O21-C2-C3-O31
51	d	202	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
53	P	501	NDP	C5B-O5B-PA-O3
51	N	401	CDL	C76-C77-C78-C79
51	h	201	CDL	C17-C18-C19-C20
51	N	401	CDL	CB5-C51-C52-C53
51	L	702	CDL	C76-C77-C78-C79
51	L	702	CDL	C14-C15-C16-C17
47	h	202	3PE	C2-C1-O11-P
46	H	402	PC1	C11-O13-P-O14
46	I	202	PC1	C11-O13-P-O12
46	I	202	PC1	C11-O13-P-O14
47	D	501	3PE	C11-O13-P-O12
47	D	501	3PE	C11-O13-P-O14
47	M	501	3PE	C11-O13-P-O14
47	Y	401	3PE	C11-O13-P-O12
47	h	202	3PE	C11-O13-P-O12
51	d	201	CDL	CA2-OA2-PA1-OA4
51	d	202	CDL	CB3-OB5-PB2-OB4
51	q	201	CDL	CA2-OA2-PA1-OA4
52	O	401	ATP	C5'-O5'-PA-O1A
47	Y	401	3PE	C37-C38-C39-C3A
51	L	702	CDL	OB5-CB3-CB4-CB6
47	D	501	3PE	C12-C11-O13-P
47	H	401	3PE	C12-C11-O13-P
47	K	201	3PE	C12-C11-O13-P
46	B	203	PC1	C3A-C3B-C3C-C3D
51	X	201	CDL	C14-C15-C16-C17
51	h	201	CDL	C51-C52-C53-C54
51	d	201	CDL	CB5-C51-C52-C53
51	h	201	CDL	C74-C75-C76-C77
46	I	202	PC1	O11-C1-C2-O21
47	L	701	3PE	O11-C1-C2-O21
51	L	702	CDL	OB5-CB3-CB4-OB6
47	K	201	3PE	C33-C34-C35-C36
51	L	702	CDL	C11-C12-C13-C14
46	B	202	PC1	O13-C11-C12-N
51	h	201	CDL	CB3-CB4-CB6-OB8
46	B	203	PC1	O21-C2-C3-O31
47	h	202	3PE	O21-C2-C3-O31
51	N	401	CDL	OA6-CA4-CA6-OA8
51	N	401	CDL	OB6-CB4-CB6-OB8
51	X	201	CDL	OA6-CA4-CA6-OA8
51	X	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
51	d	202	CDL	OB6-CB4-CB6-OB8
47	i	201	3PE	C2F-C2G-C2H-C2I
51	X	201	CDL	C52-C53-C54-C55
51	q	201	CDL	C72-C71-CB7-OB8
51	q	201	CDL	CB2-C1-CA2-OA2
55	U	201	EHZ	C2-C3-C4-C5
51	X	201	CDL	C62-C63-C64-C65
47	D	501	3PE	C2-C1-O11-P
46	B	203	PC1	C33-C34-C35-C36
47	I	201	3PE	C22-C23-C24-C25
50	H	403	T2Q	F1-C27-O5'-C5'
51	d	201	CDL	OB6-CB4-CB6-OB8
51	q	201	CDL	OA6-CA4-CA6-OA8
51	h	201	CDL	C54-C55-C56-C57
46	B	202	PC1	C11-O13-P-O11
46	B	203	PC1	C11-O13-P-O11
46	H	402	PC1	C1-O11-P-O13
46	I	202	PC1	C1-O11-P-O13
47	H	401	3PE	C1-O11-P-O13
47	K	201	3PE	C1-O11-P-O13
51	N	401	CDL	CB3-OB5-PB2-OB2
51	h	201	CDL	CA2-OA2-PA1-OA5
51	q	201	CDL	CA2-OA2-PA1-OA5
51	X	201	CDL	C32-C31-CA7-OA8
47	I	201	3PE	C3C-C3D-C3E-C3F
47	M	501	3PE	C2-C1-O11-P
51	d	202	CDL	CA4-CA3-OA5-PA1
47	M	501	3PE	C25-C26-C27-C28
51	X	201	CDL	C12-C13-C14-C15
51	h	201	CDL	C14-C15-C16-C17
47	H	401	3PE	O13-C11-C12-N
46	B	203	PC1	C32-C33-C34-C35
47	D	501	3PE	C2B-C2C-C2D-C2E
49	F	501	FMN	C4'-C5'-O5'-P
51	X	201	CDL	C1-CB2-OB2-PB2
47	L	701	3PE	O21-C21-C22-C23
46	I	202	PC1	C2B-C2C-C2D-C2E
47	D	501	3PE	C26-C27-C28-C29
55	U	201	EHZ	C4-C5-C6-C7
51	h	201	CDL	C19-C20-C21-C22
51	h	201	CDL	C73-C74-C75-C76
47	I	201	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
47	I	201	3PE	C3-C2-O21-C21
51	q	201	CDL	CA6-CA4-OA6-CA5
47	M	501	3PE	C33-C34-C35-C36
51	N	401	CDL	C74-C75-C76-C77
50	H	403	T2Q	C6-C5'-O5'-C27
46	B	203	PC1	C3B-C3C-C3D-C3E
55	U	201	EHZ	C21-C22-C23-C24
51	N	401	CDL	C75-C76-C77-C78
47	h	202	3PE	C23-C24-C25-C26
51	X	201	CDL	CA2-C1-CB2-OB2
50	H	403	T2Q	C4'-C5'-O5'-C27
47	i	201	3PE	C34-C35-C36-C37
52	O	401	ATP	PG-O3B-PB-O1B
53	P	501	NDP	PN-O3-PA-O1A
47	i	201	3PE	C27-C28-C29-C2A
51	N	401	CDL	C79-C80-C81-C82
47	h	202	3PE	O31-C31-C32-C33
47	I	201	3PE	O13-C11-C12-N
46	H	402	PC1	C28-C29-C2A-C2B
51	L	702	CDL	C54-C55-C56-C57
51	h	201	CDL	C15-C16-C17-C18
46	B	202	PC1	O21-C21-C22-C23
47	h	202	3PE	O21-C21-C22-C23
47	L	701	3PE	C26-C27-C28-C29
47	L	701	3PE	C34-C35-C36-C37
51	N	401	CDL	C83-C84-C85-C86
46	B	203	PC1	O11-C1-C2-O21
51	X	201	CDL	C12-C11-CA5-OA6
51	N	401	CDL	C55-C56-C57-C58
47	Y	401	3PE	C28-C29-C2A-C2B
46	H	402	PC1	O31-C31-C32-C33
46	B	203	PC1	C21-C22-C23-C24
51	L	702	CDL	C72-C71-CB7-OB8
46	B	203	PC1	O21-C21-C22-C23
47	H	401	3PE	C3B-C3C-C3D-C3E
47	i	201	3PE	C2C-C2D-C2E-C2F
47	D	501	3PE	C35-C36-C37-C38
46	H	402	PC1	C23-C24-C25-C26
47	Y	401	3PE	C22-C23-C24-C25
55	T	201	EHZ	C3-C4-C5-C6
53	P	501	NDP	C3D-C4D-C5D-O5D
52	O	401	ATP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
52	O	401	ATP	PB-O3A-PA-O1A
51	L	702	CDL	C52-C51-CB5-OB6
46	B	202	PC1	O22-C21-C22-C23
51	N	401	CDL	C72-C73-C74-C75
47	i	201	3PE	C28-C29-C2A-C2B
46	B	202	PC1	C33-C34-C35-C36
47	h	202	3PE	O22-C21-C22-C23
51	d	202	CDL	C32-C31-CA7-OA8
47	I	201	3PE	C11-O13-P-O14
51	N	401	CDL	CB3-OB5-PB2-OB3
51	h	201	CDL	CA3-OA5-PA1-OA4
51	h	201	CDL	CB3-OB5-PB2-OB3
53	P	501	NDP	C5B-O5B-PA-O1A
47	I	201	3PE	C35-C36-C37-C38
46	H	402	PC1	O32-C31-C32-C33
51	L	702	CDL	C72-C71-CB7-OB9
46	B	203	PC1	O22-C21-C22-C23
51	L	702	CDL	C12-C11-CA5-OA6
51	N	401	CDL	C84-C85-C86-C87
51	X	201	CDL	C12-C11-CA5-OA7
51	d	201	CDL	C33-C34-C35-C36
51	q	201	CDL	CA3-CA4-OA6-CA5
55	T	201	EHZ	O4-C15-C16-C17
47	M	501	3PE	C22-C23-C24-C25
47	K	201	3PE	O21-C21-C22-C23
47	Y	401	3PE	O31-C31-C32-C33
47	i	201	3PE	O31-C31-C32-C33
51	L	702	CDL	C1-CA2-OA2-PA1
47	M	501	3PE	C38-C39-C3A-C3B
47	i	201	3PE	O32-C31-C32-C33
51	X	201	CDL	C71-C72-C73-C74
51	X	201	CDL	O1-C1-CB2-OB2
47	K	201	3PE	O31-C31-C32-C33
47	Y	401	3PE	O32-C31-C32-C33
51	L	702	CDL	C52-C51-CB5-OB7

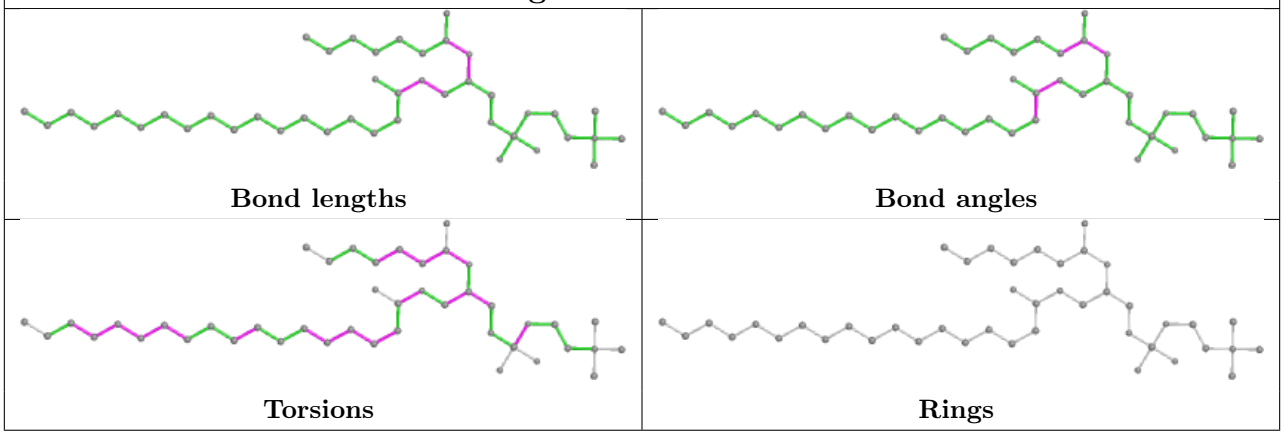
There are no ring outliers.

No monomer is involved in short contacts.

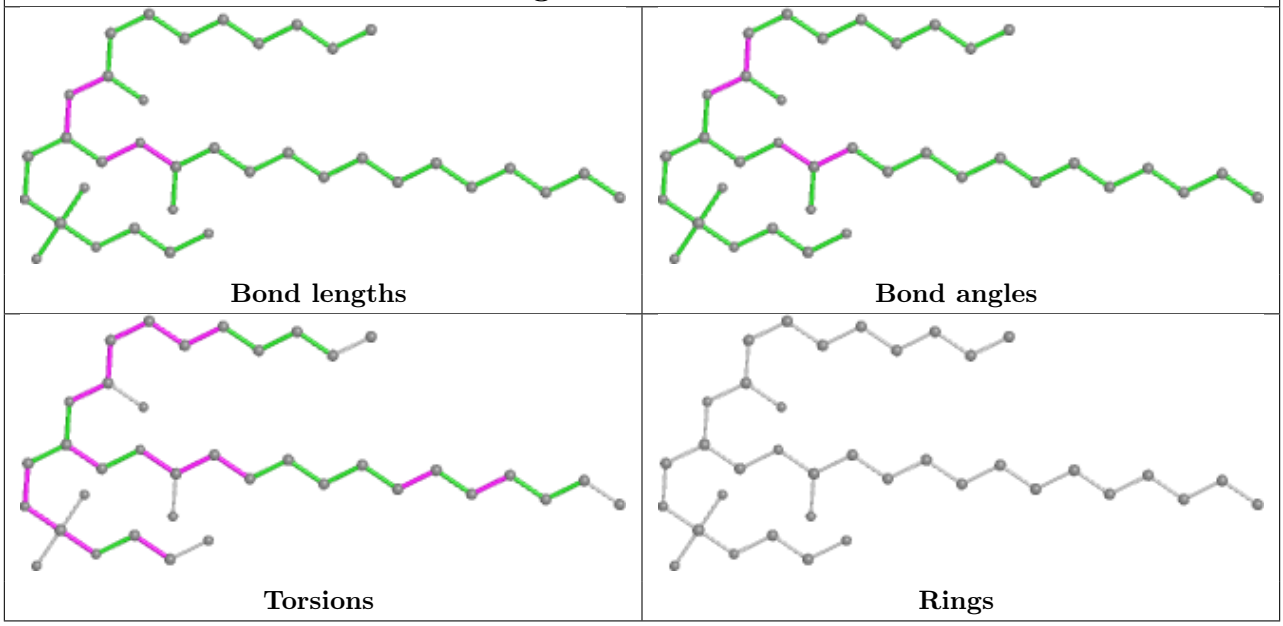
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

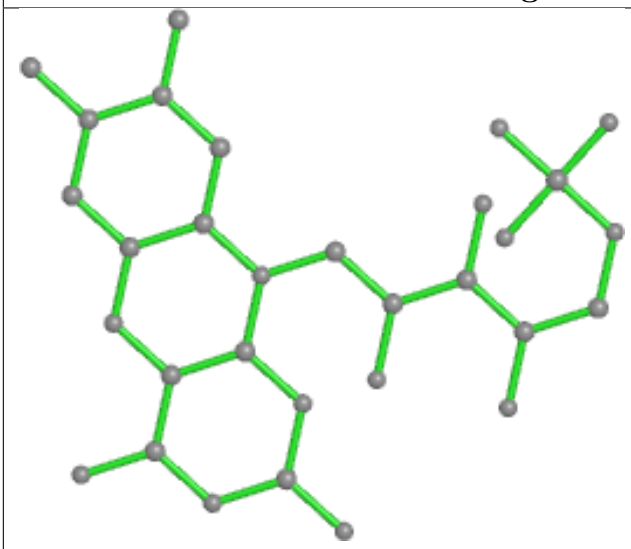
Ligand PC1 B 203



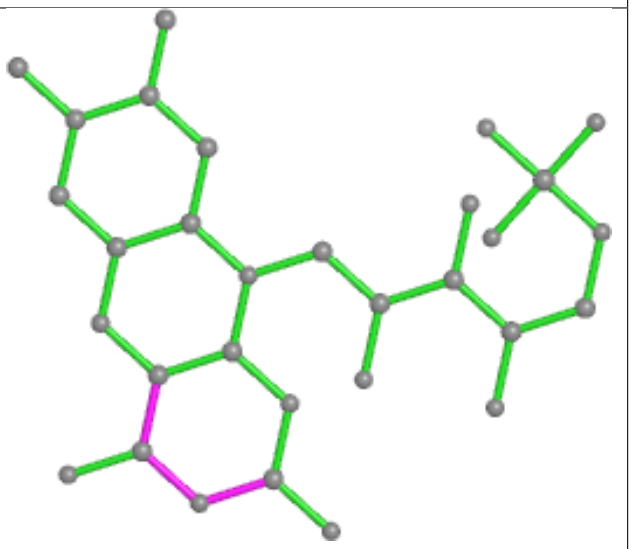
Ligand 3PE h 202



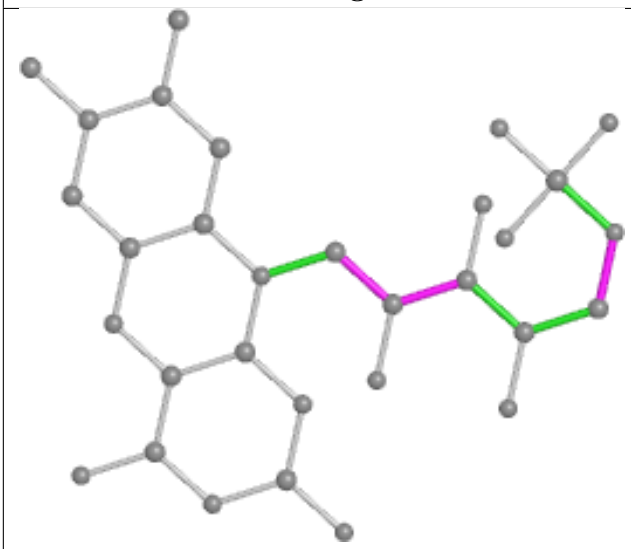
Ligand FMN F 501



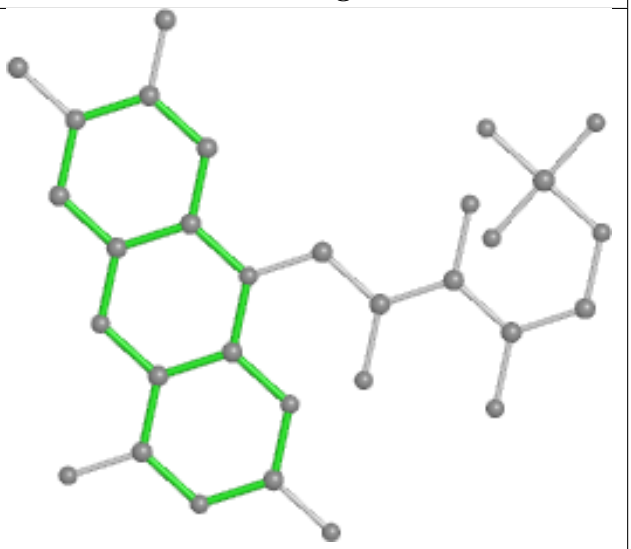
Bond lengths



Bond angles

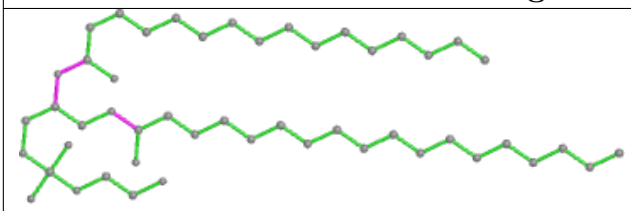


Torsions



Rings

Ligand 3PE D 501



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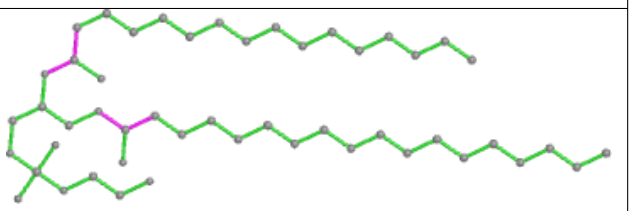

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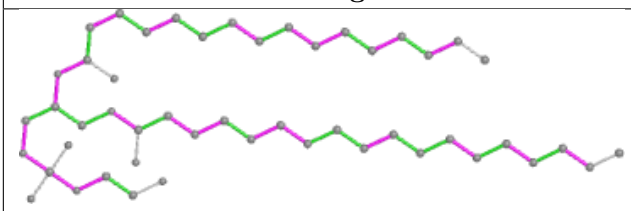

Torsions

Rings

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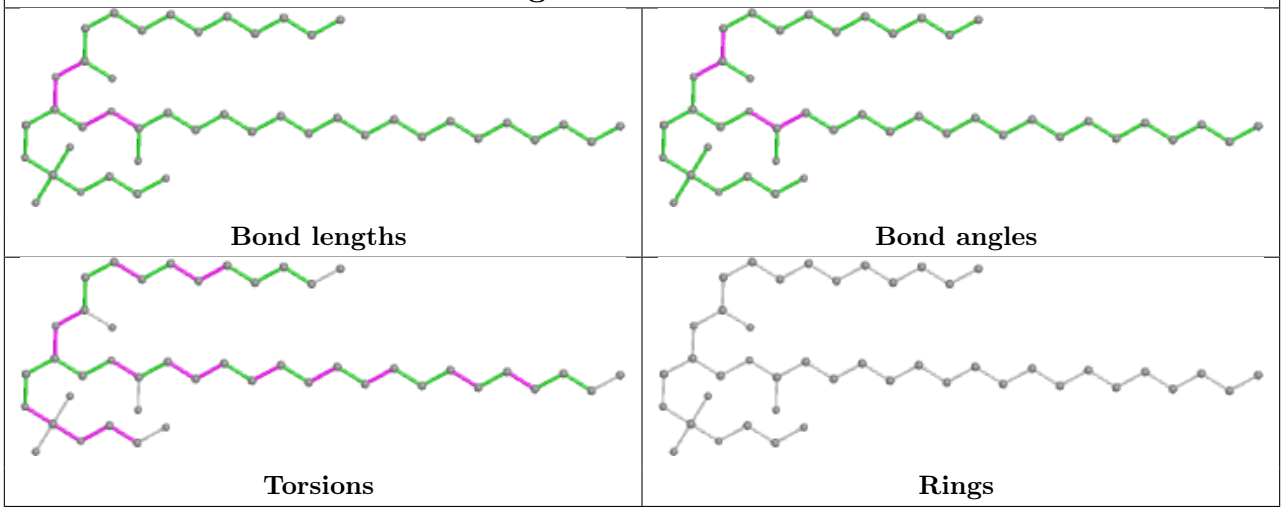

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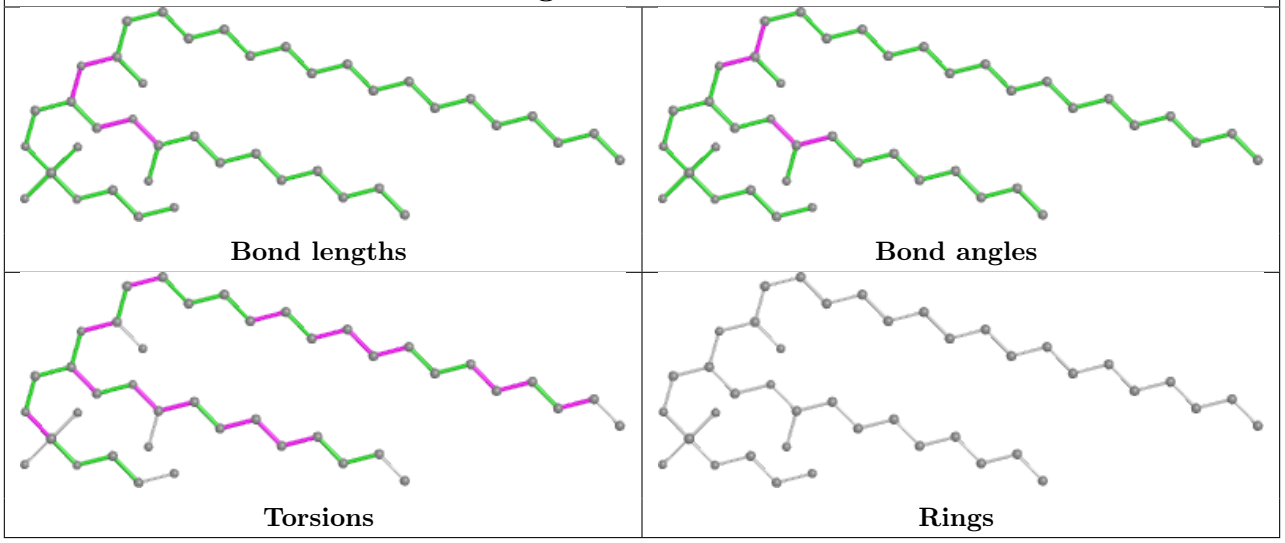

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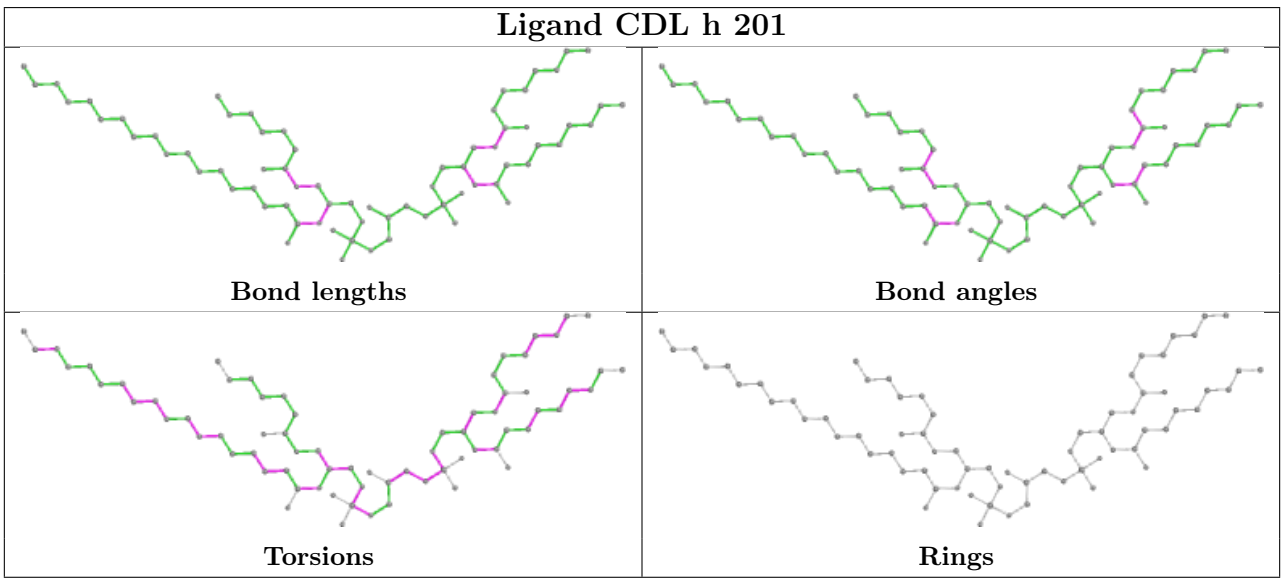

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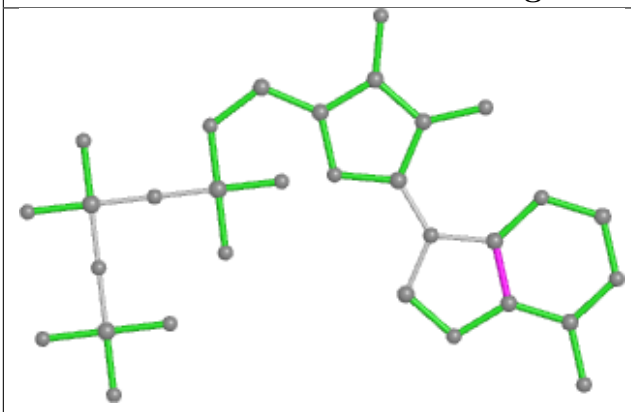

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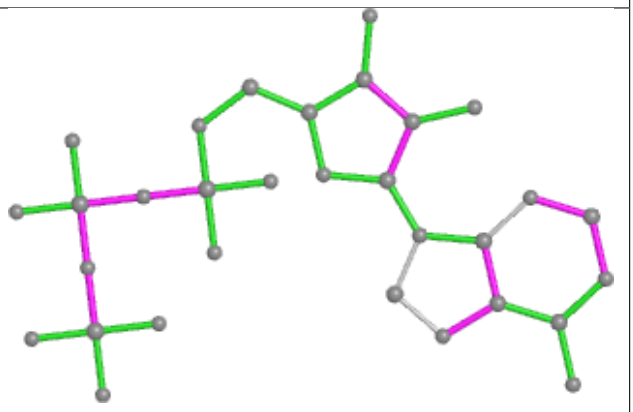

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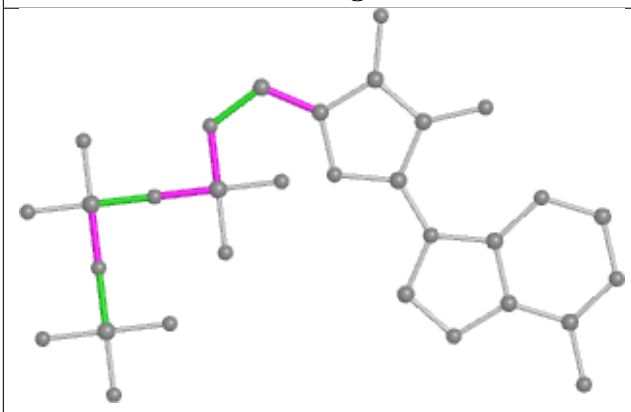

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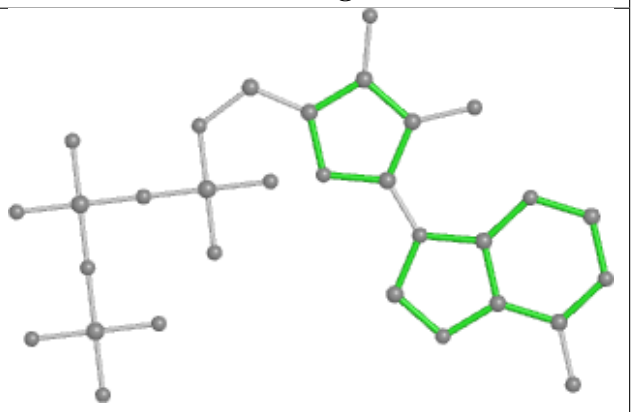

Rings

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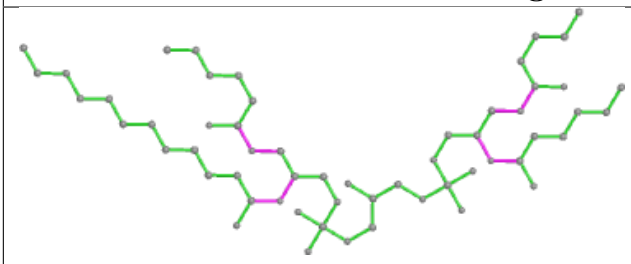

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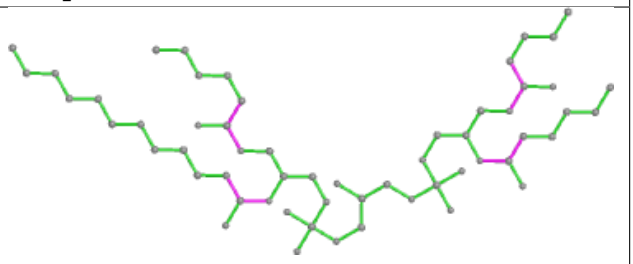

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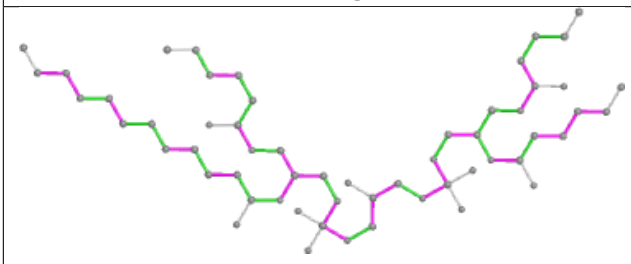

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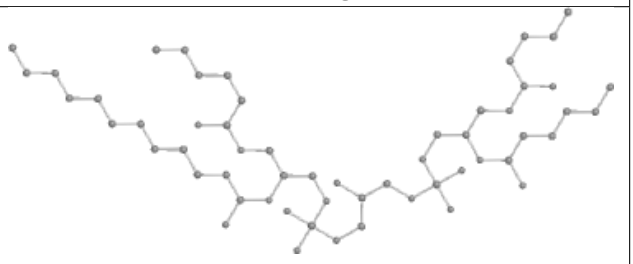

Rings

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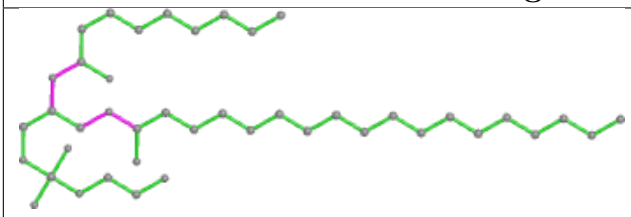

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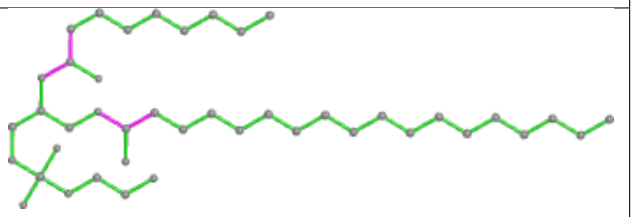

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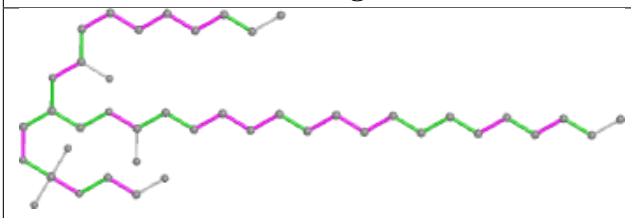

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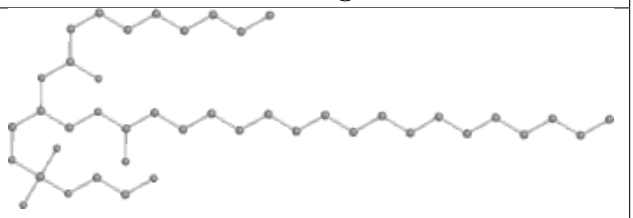
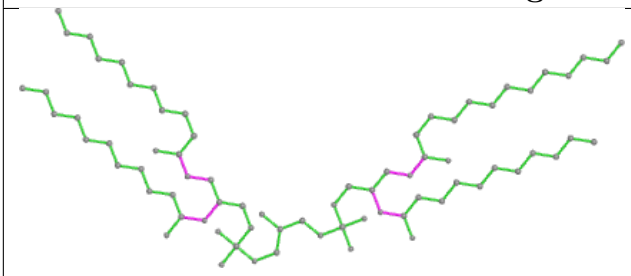


Rings

Ligand CDL L 702



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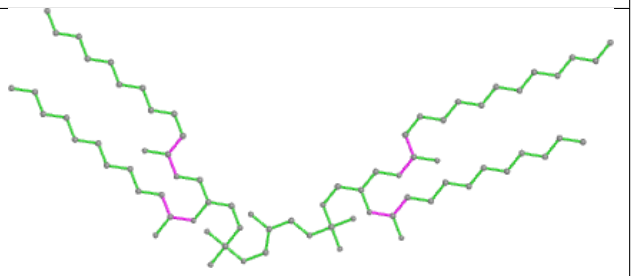

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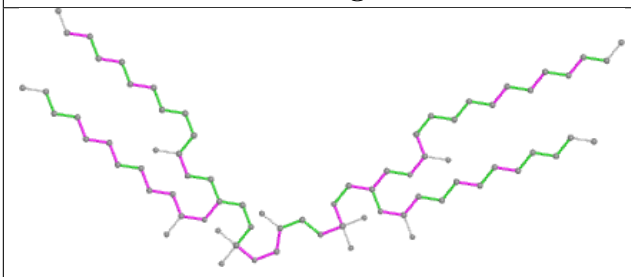

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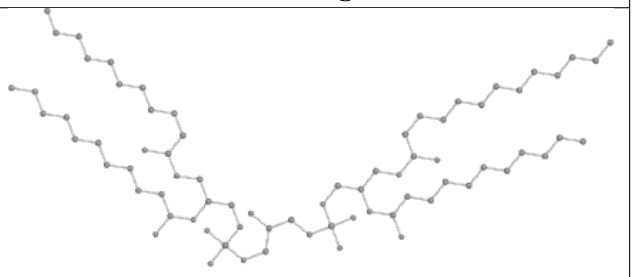
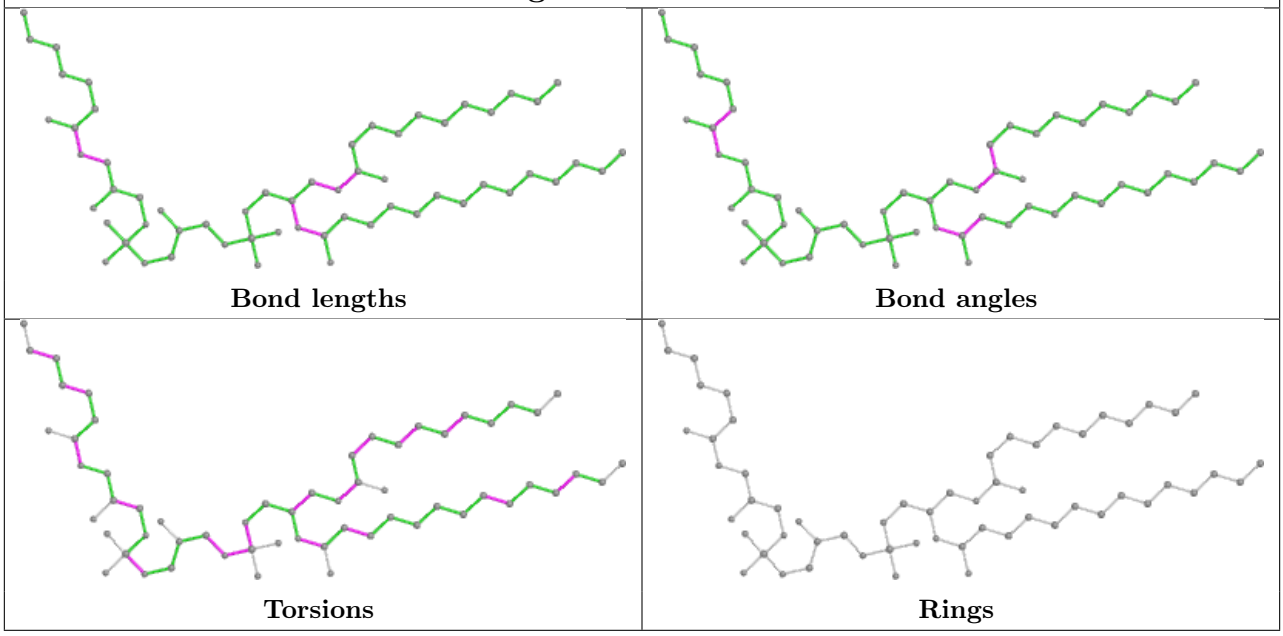


Rings

Ligand CDL d 201



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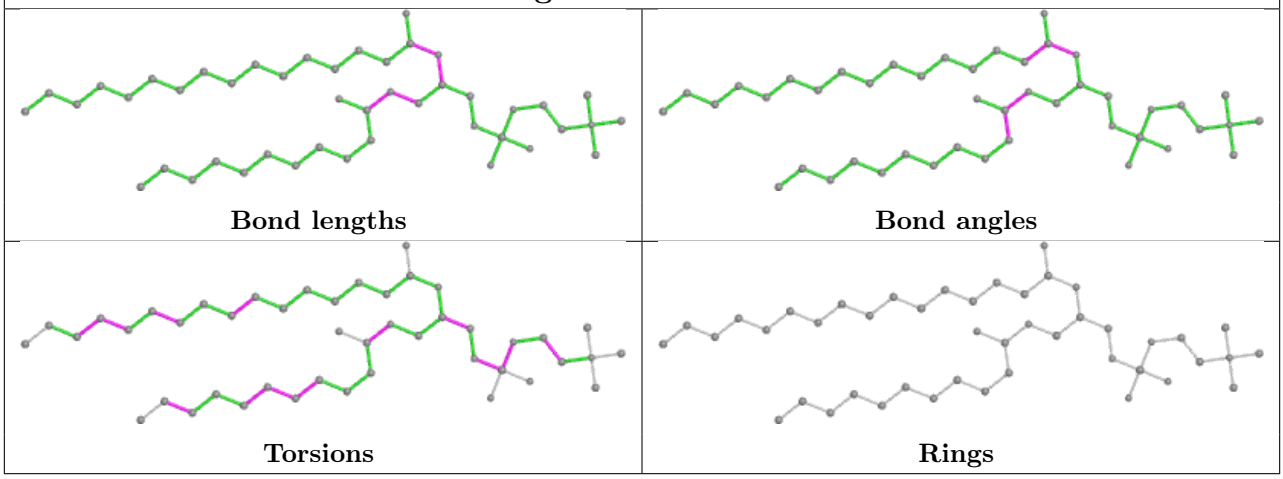

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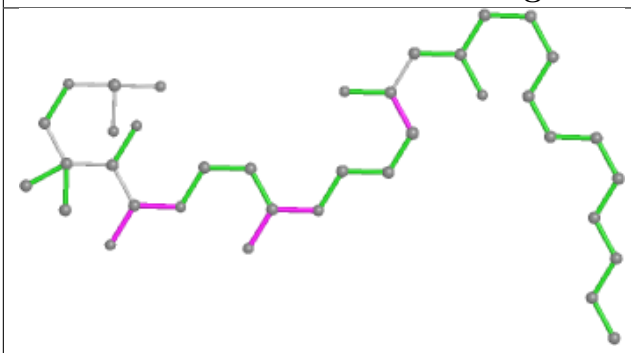

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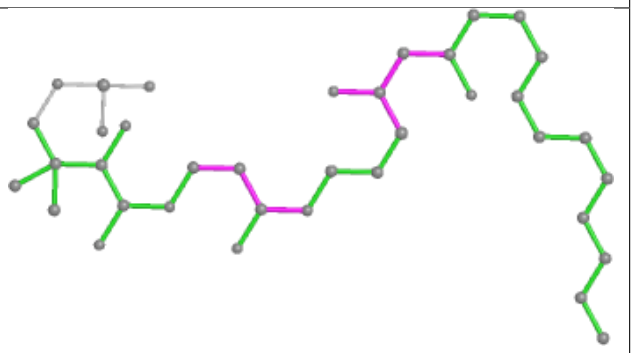

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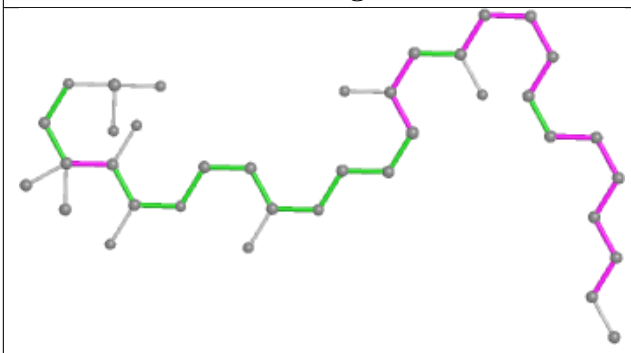

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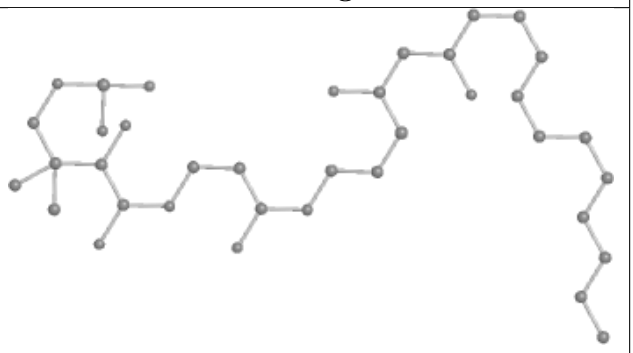

Rings

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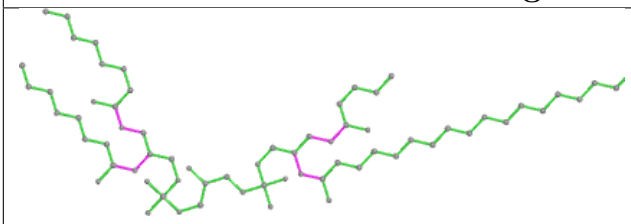

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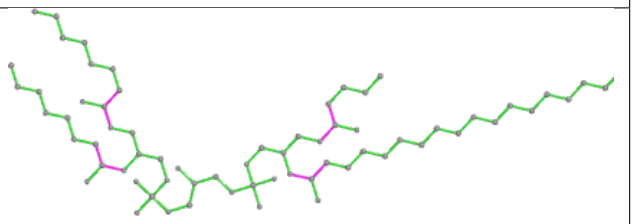

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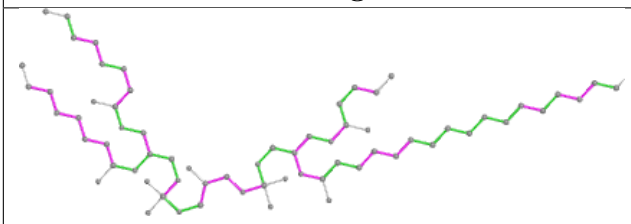

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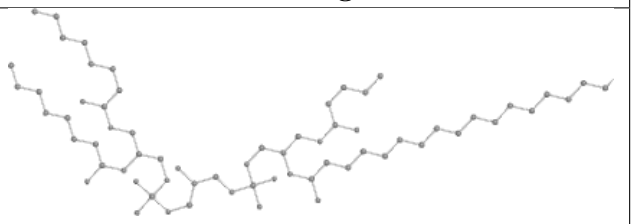

Rings

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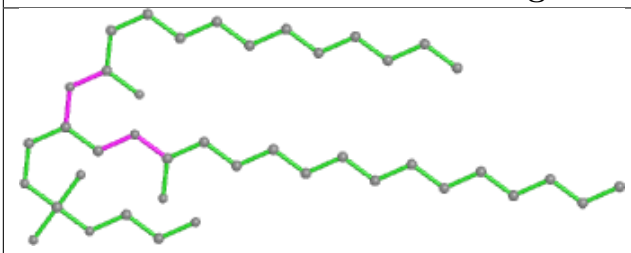

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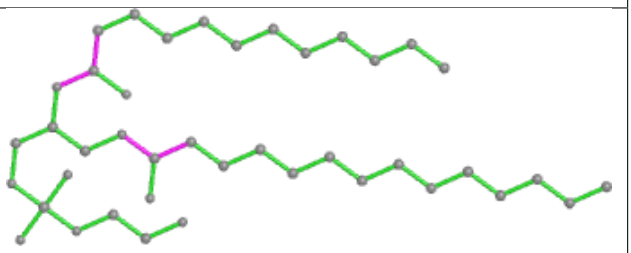

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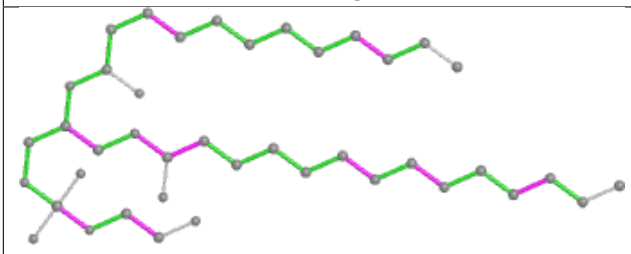

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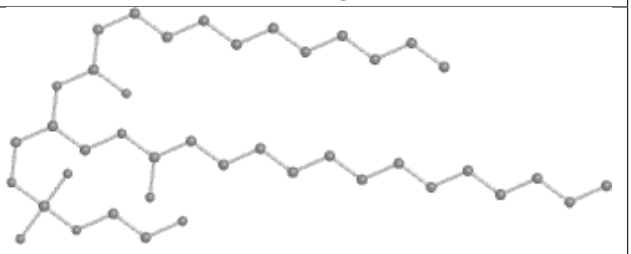
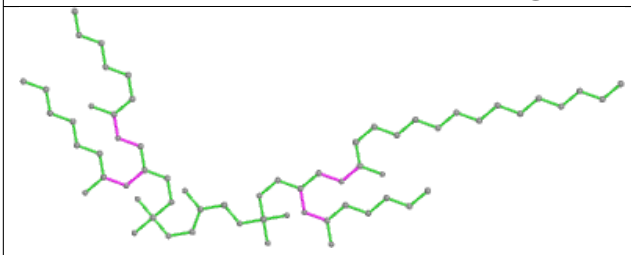


Rings

Ligand CDL d 202



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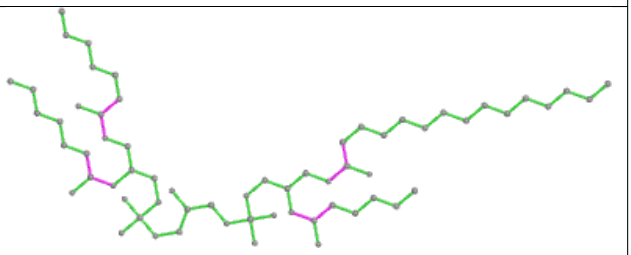

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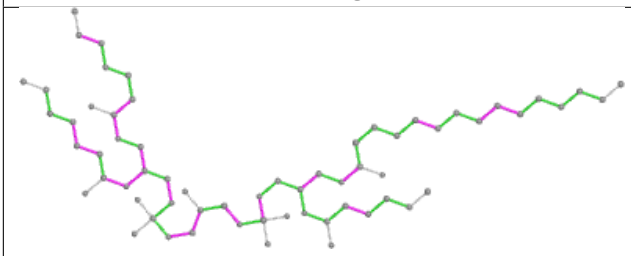

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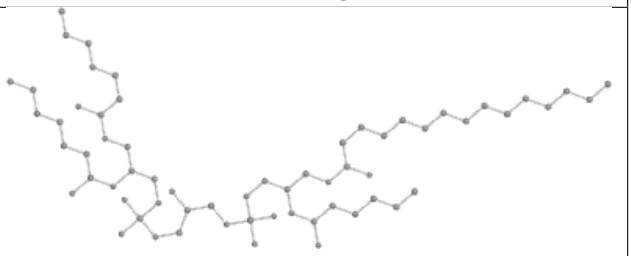
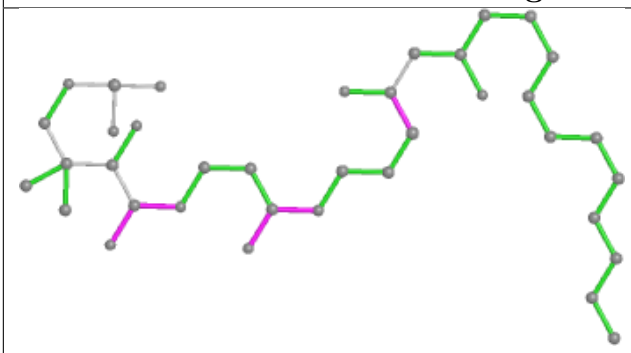


Rings

Ligand EHZ T 201



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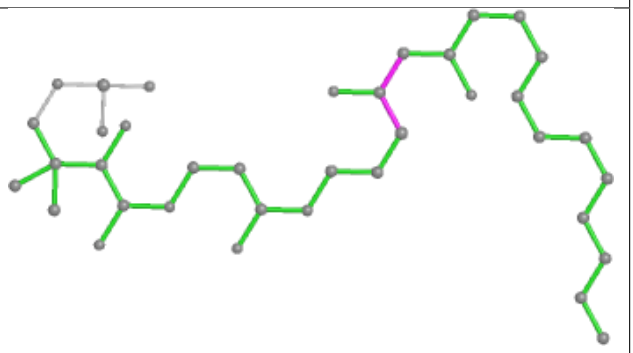
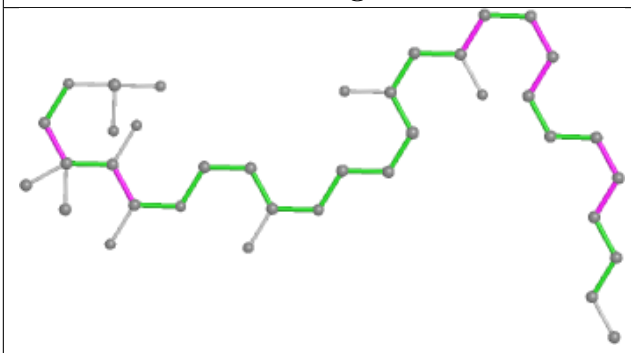


Bond angles



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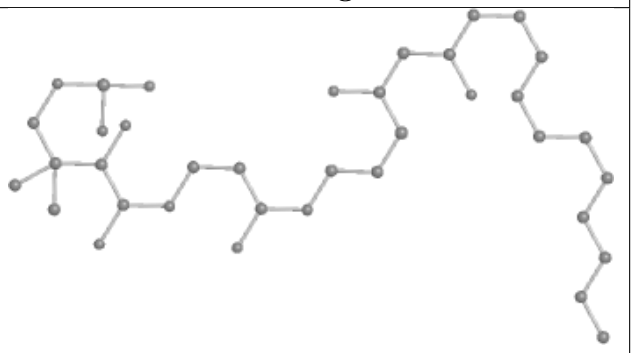
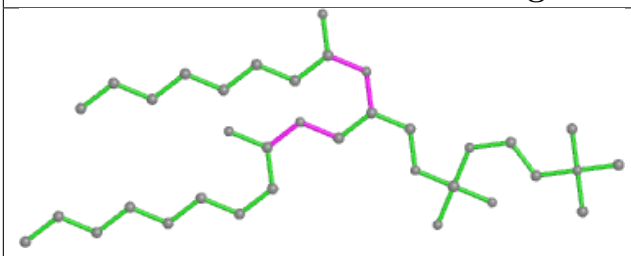


Rings

Ligand PC1 B 202



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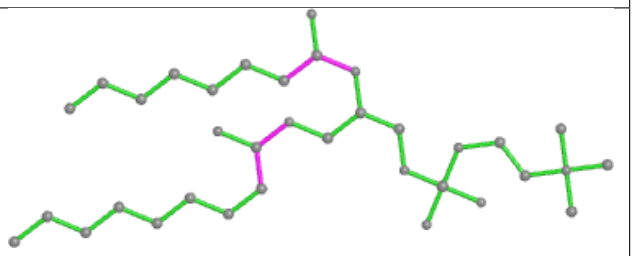

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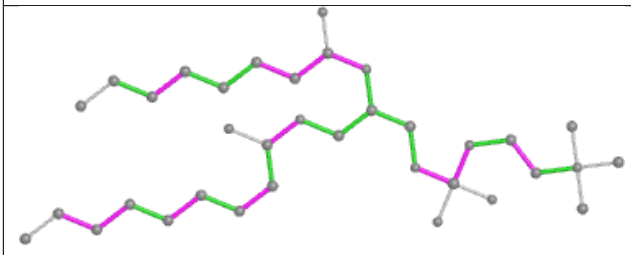

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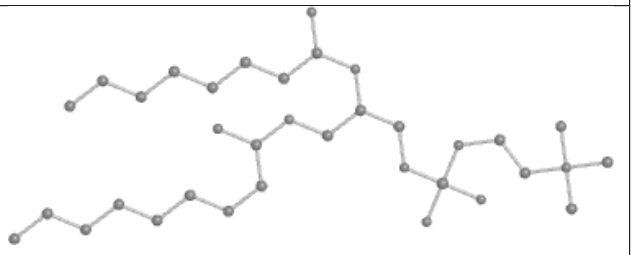
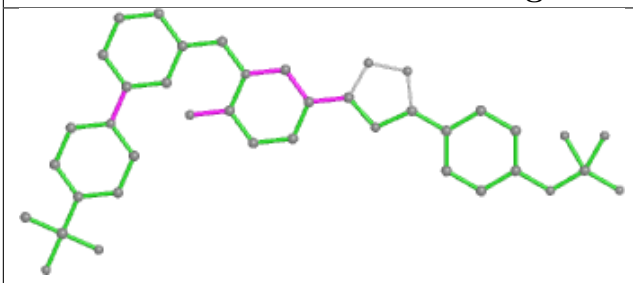


Rings

Ligand T2Q H 403



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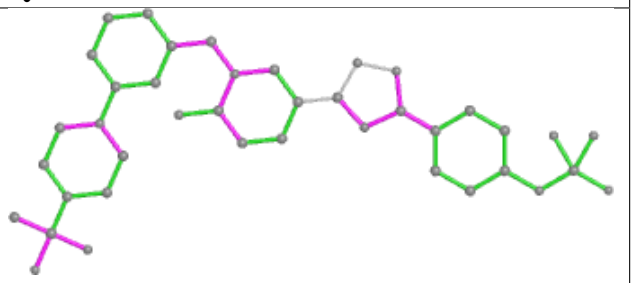
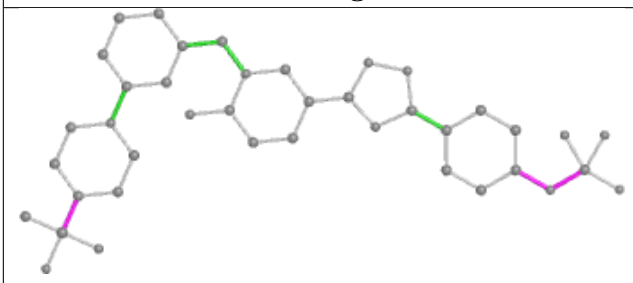


Bond angles



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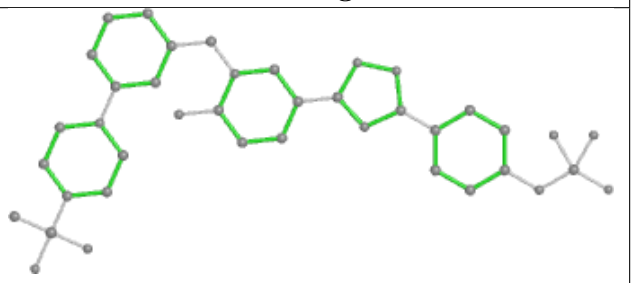
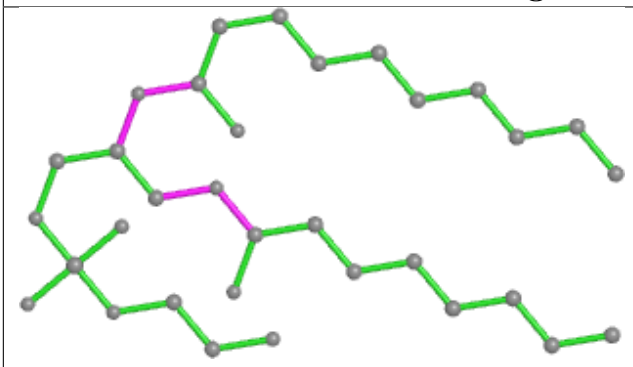


Rings

Ligand 3PE K 201



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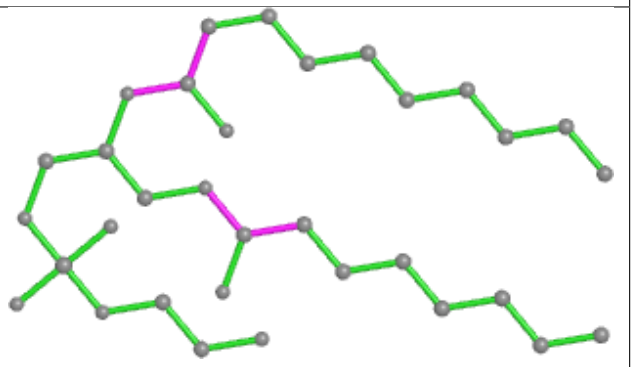
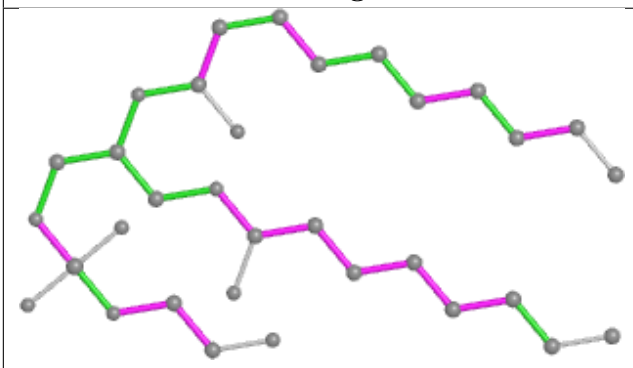
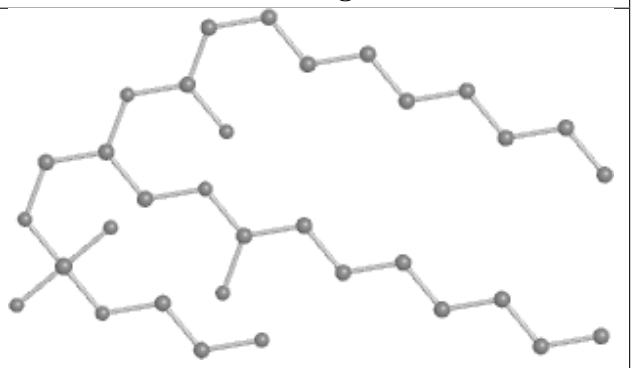


Bond angles

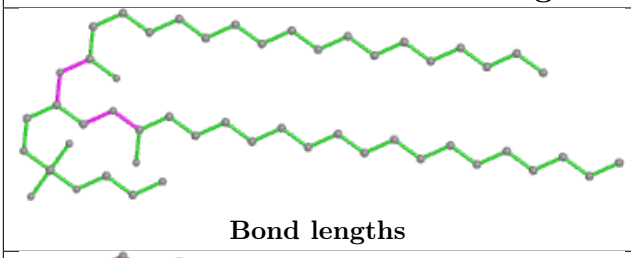


Torsions

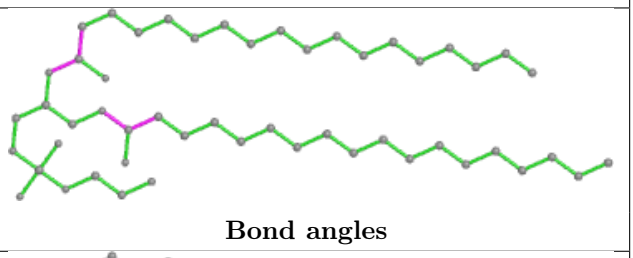


Rings

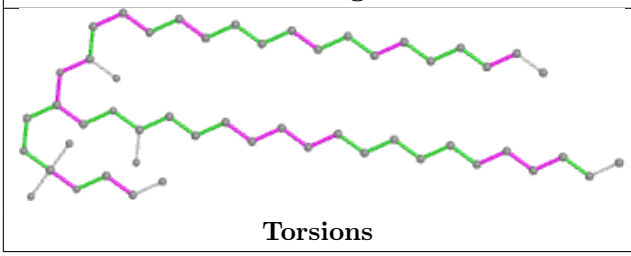
Ligand 3PE I 201



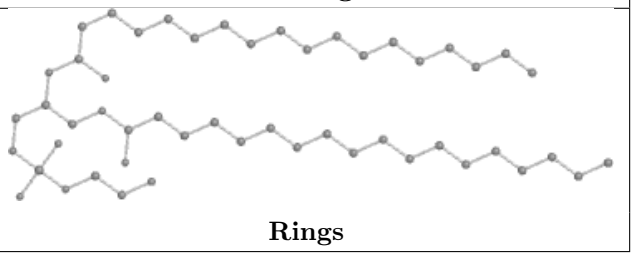
Bond lengths



Bond angles

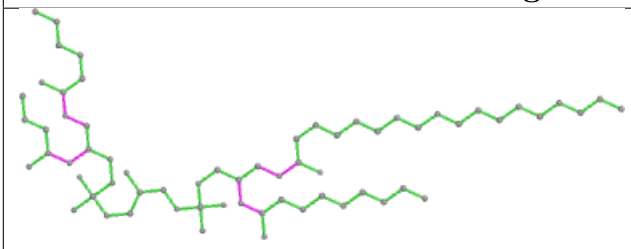


Torsions

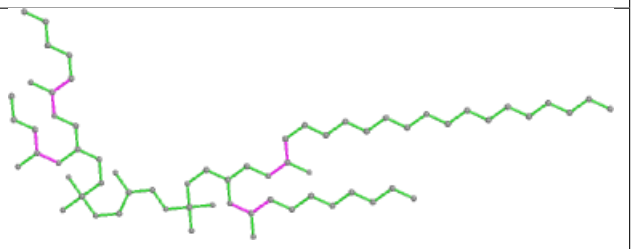


Rings

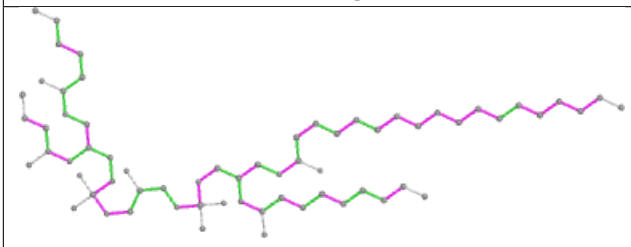
Ligand CDL N 401



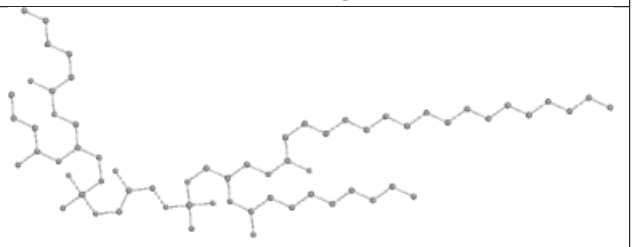
Bond lengths



Bond angles

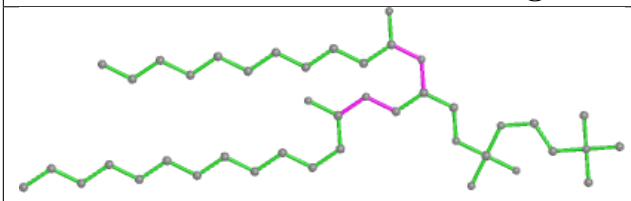


Torsions

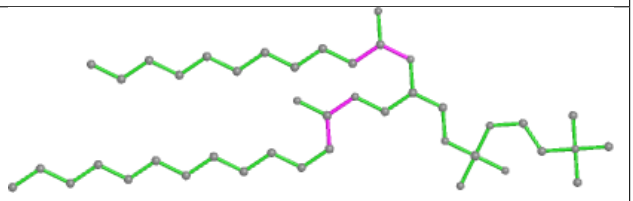


Rings

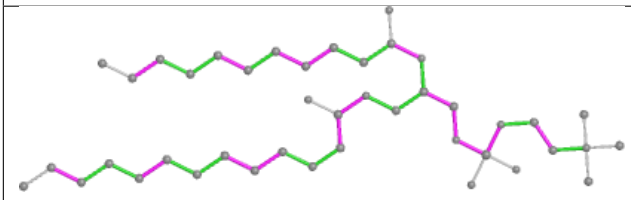
Ligand PC1 H 402



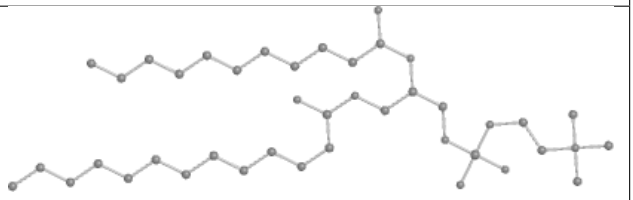
Bond lengths



Bond angles

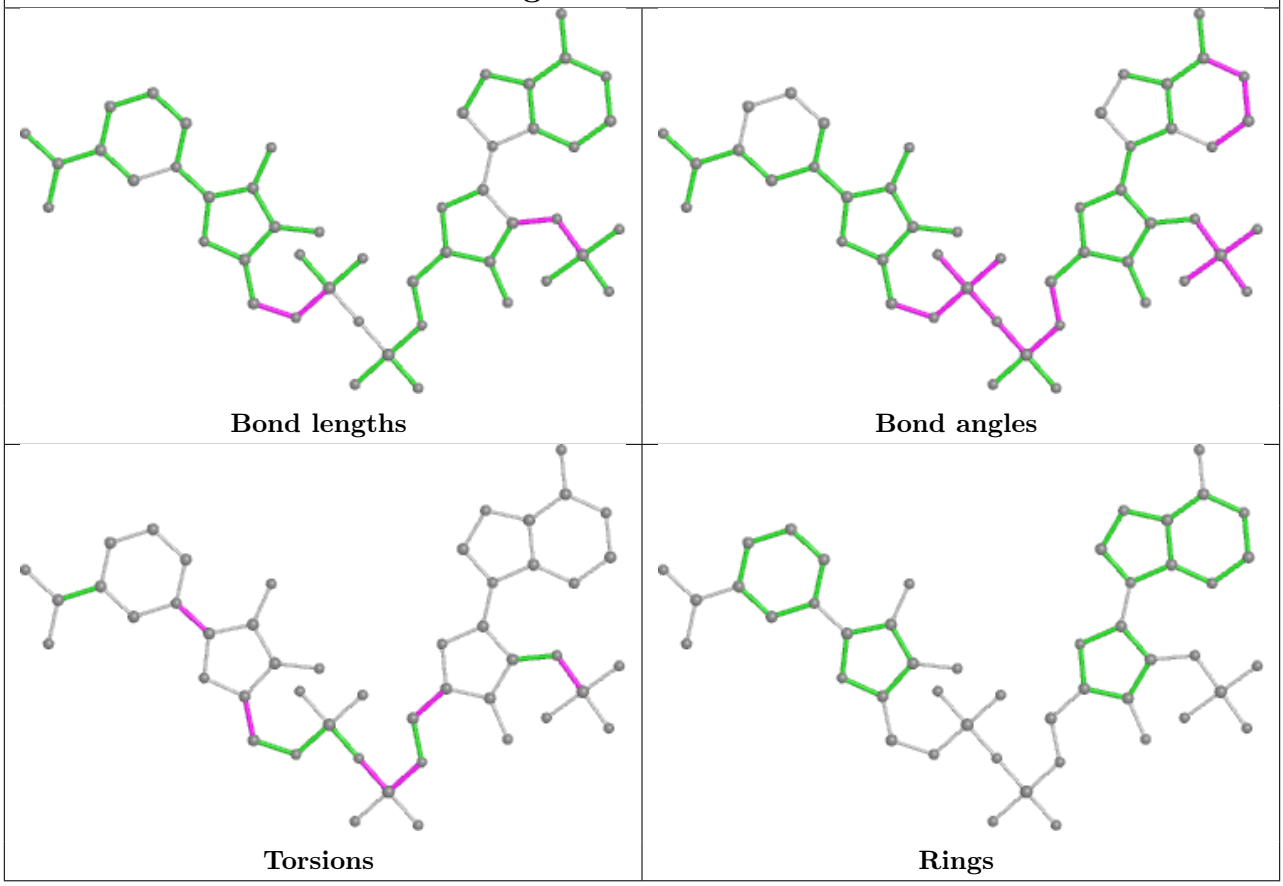


Torsions

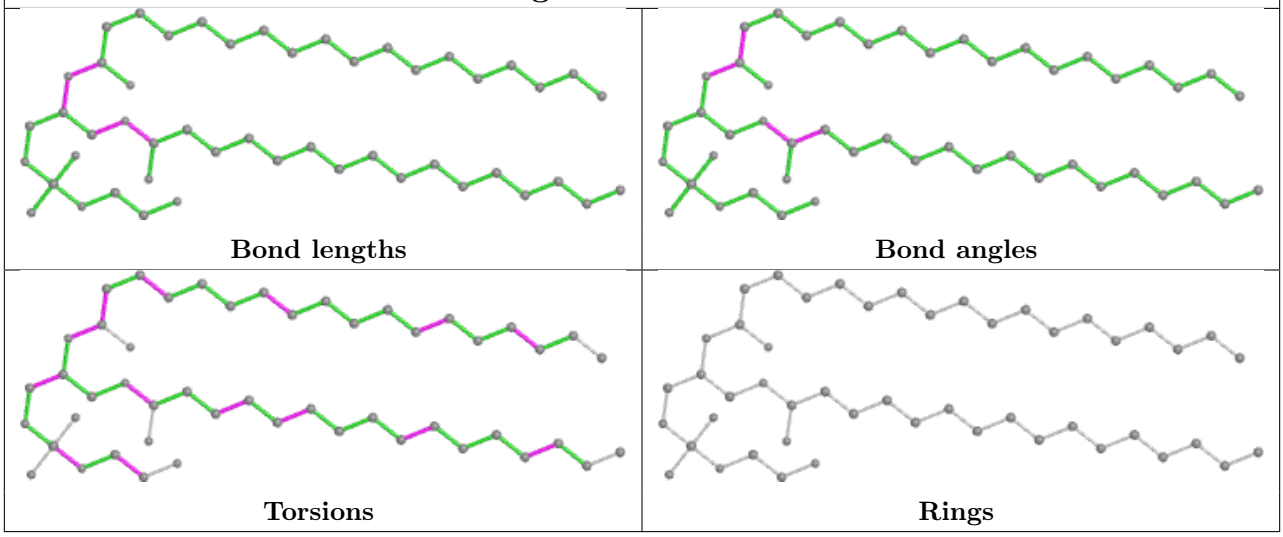


Rings

Ligand NDP P 501



Ligand 3PE L 701



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.

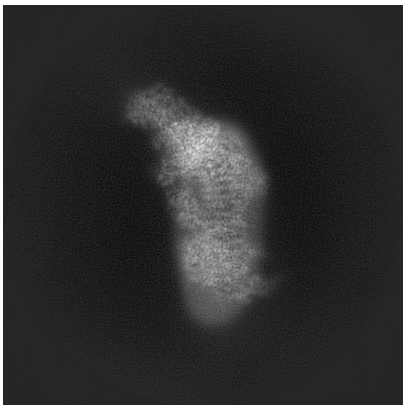
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12095. These allow visual inspection of the internal detail of the map and identification of artifacts.

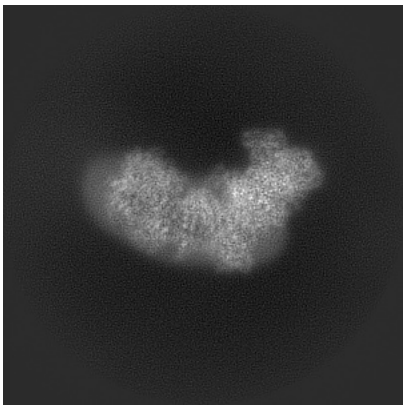
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

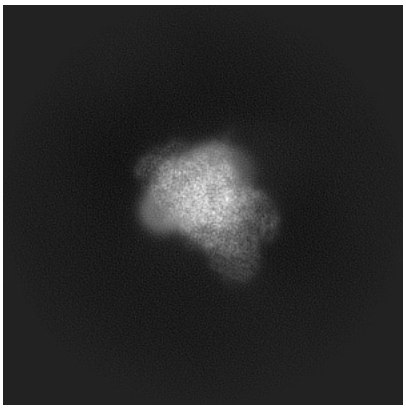
6.1.1 Primary map



X

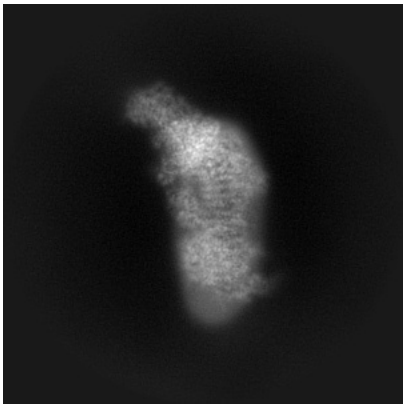


Y

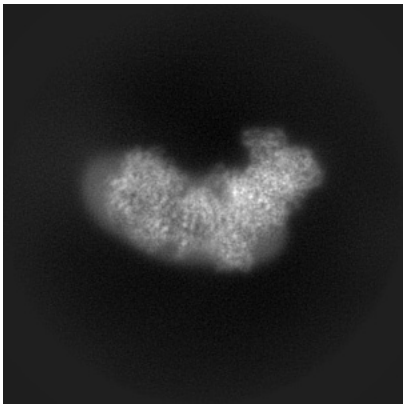


Z

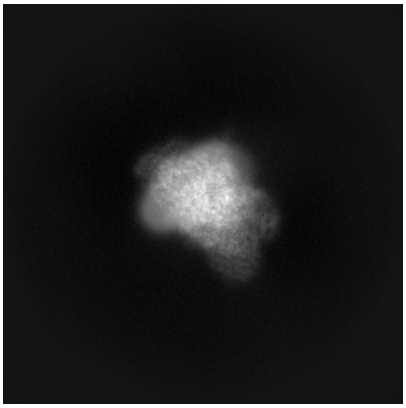
6.1.2 Raw map



X



Y

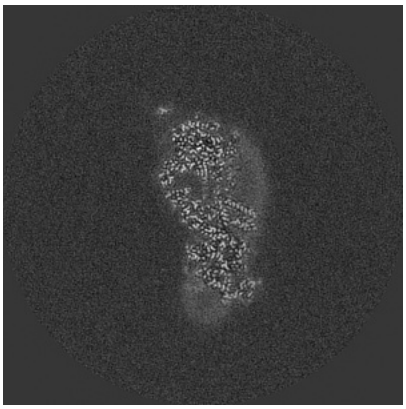


Z

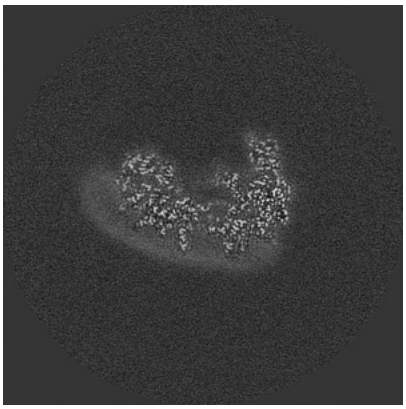
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

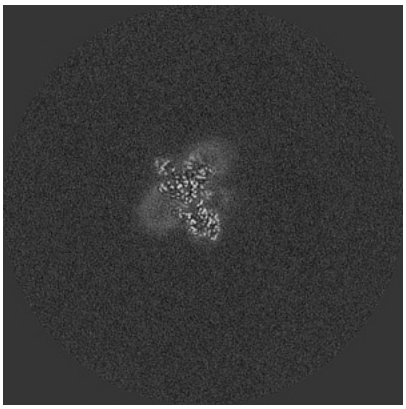
6.2.1 Primary map



X Index: 225

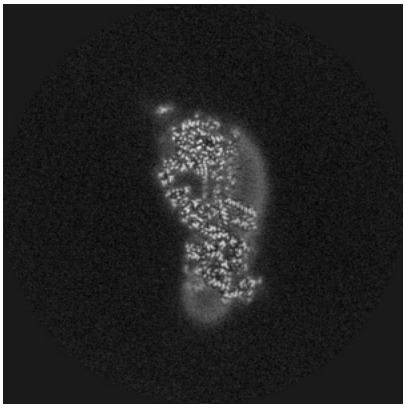


Y Index: 225

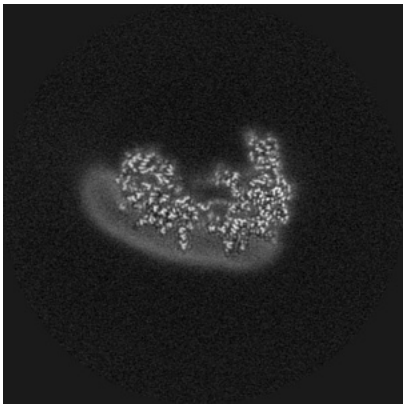


Z Index: 225

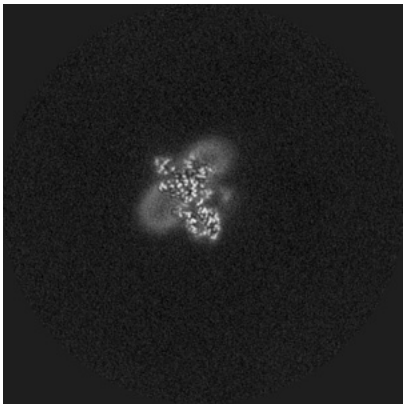
6.2.2 Raw map



X Index: 225



Y Index: 225

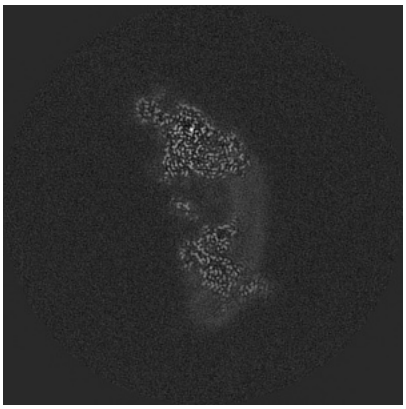


Z Index: 225

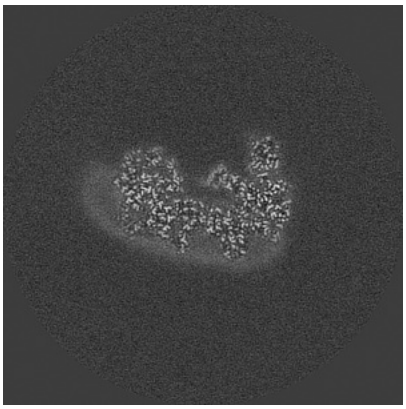
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

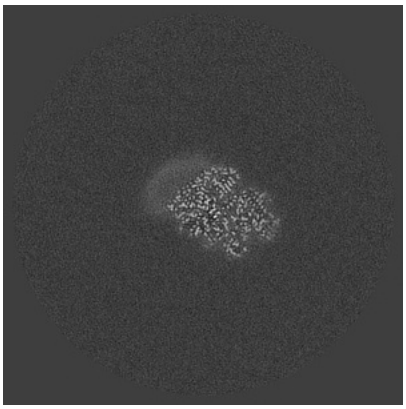
6.3.1 Primary map



X Index: 242

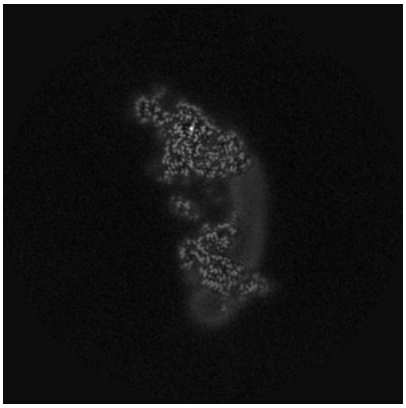


Y Index: 230

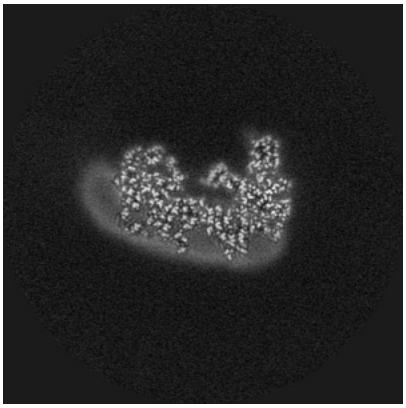


Z Index: 296

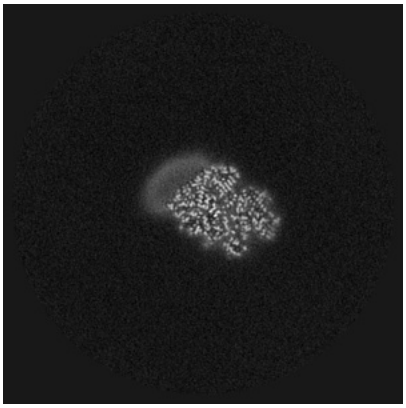
6.3.2 Raw map



X Index: 242



Y Index: 231



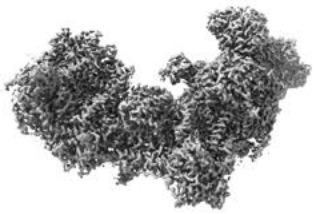
Z Index: 296

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

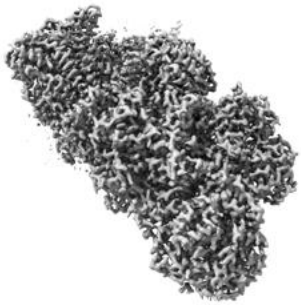
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

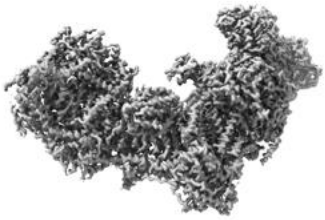


Z

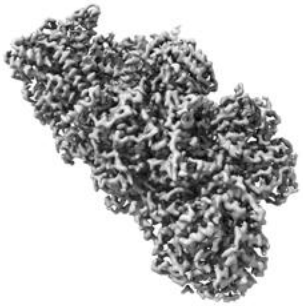
The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

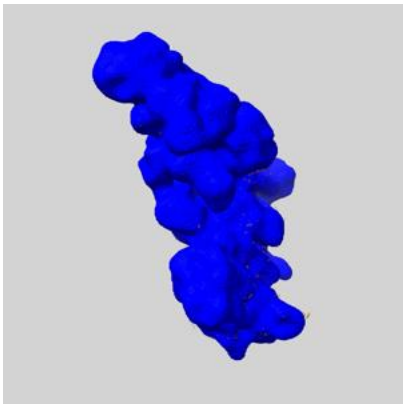
6.5 Mask visualisation

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

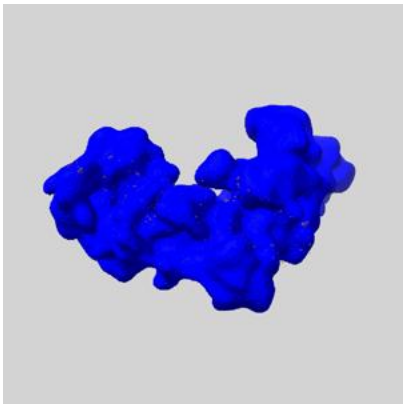
A mask typically either:

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

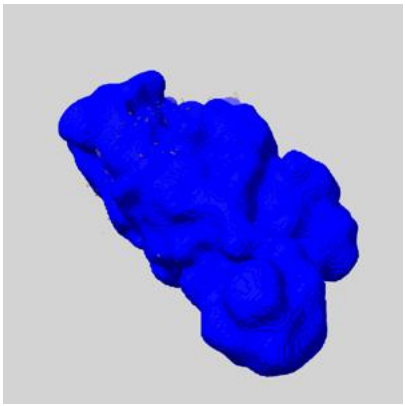
6.5.1 emd_12095_msk_1.map



X



Y

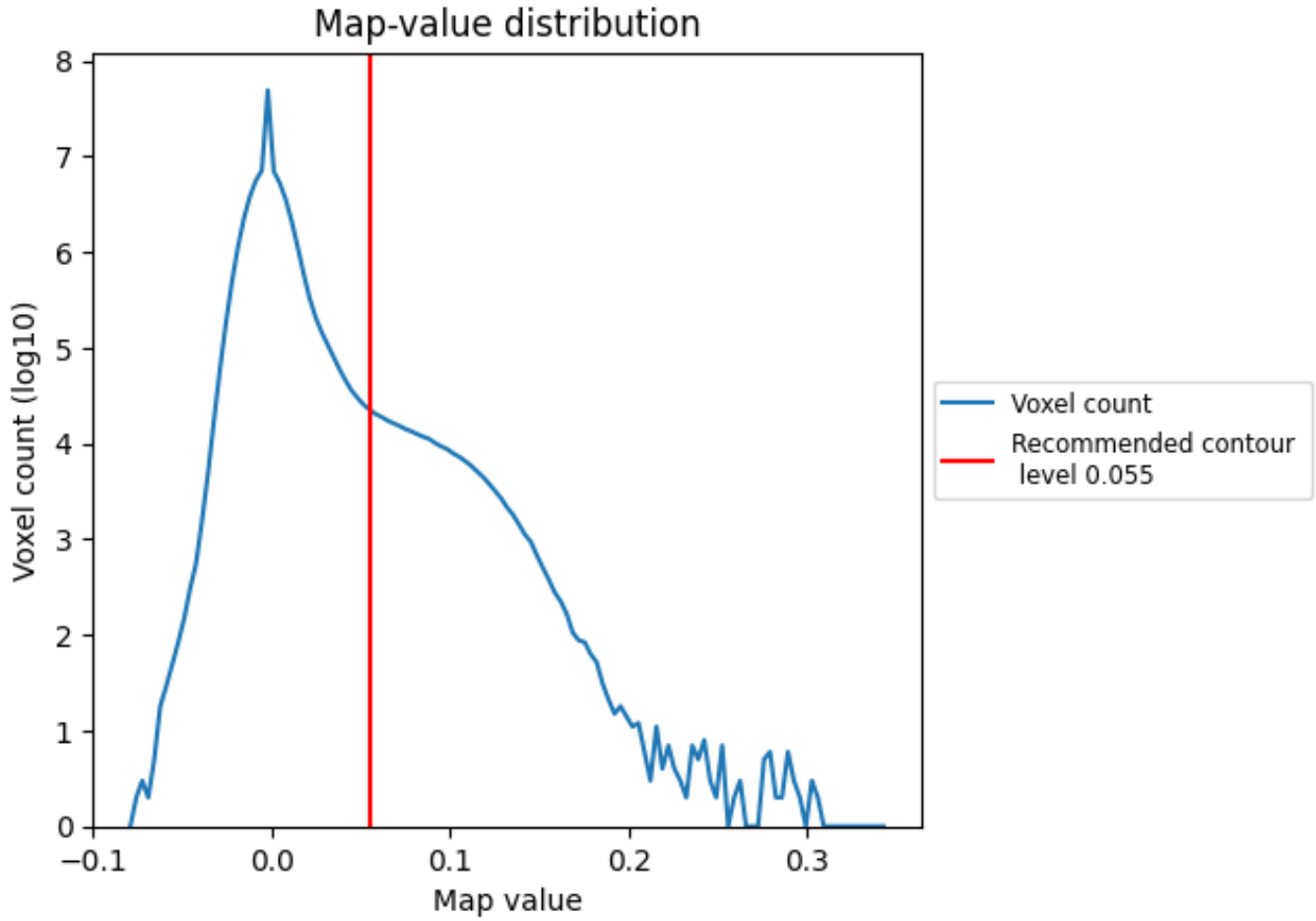


Z

7 Map analysis

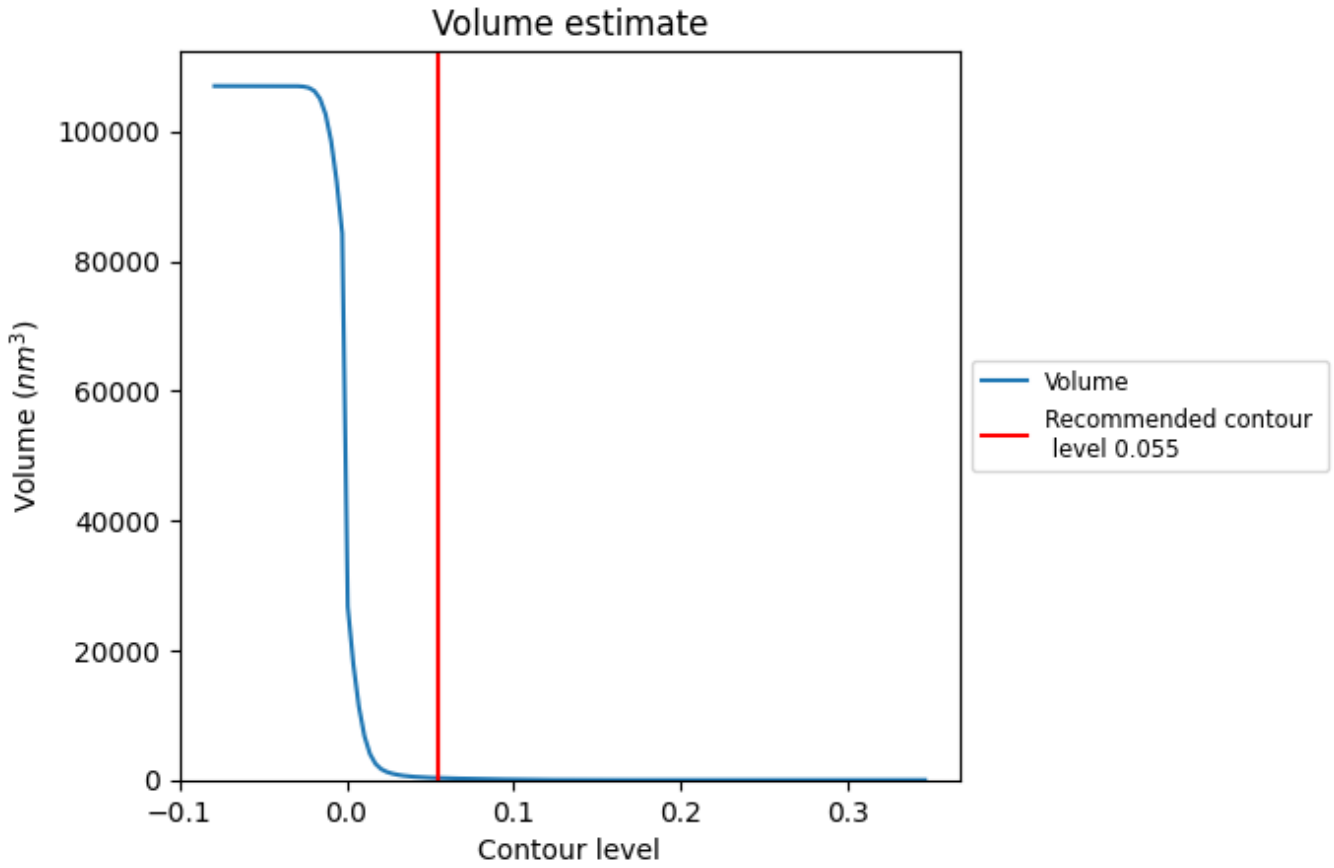
This section contains the results of statistical analysis of the map.

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.

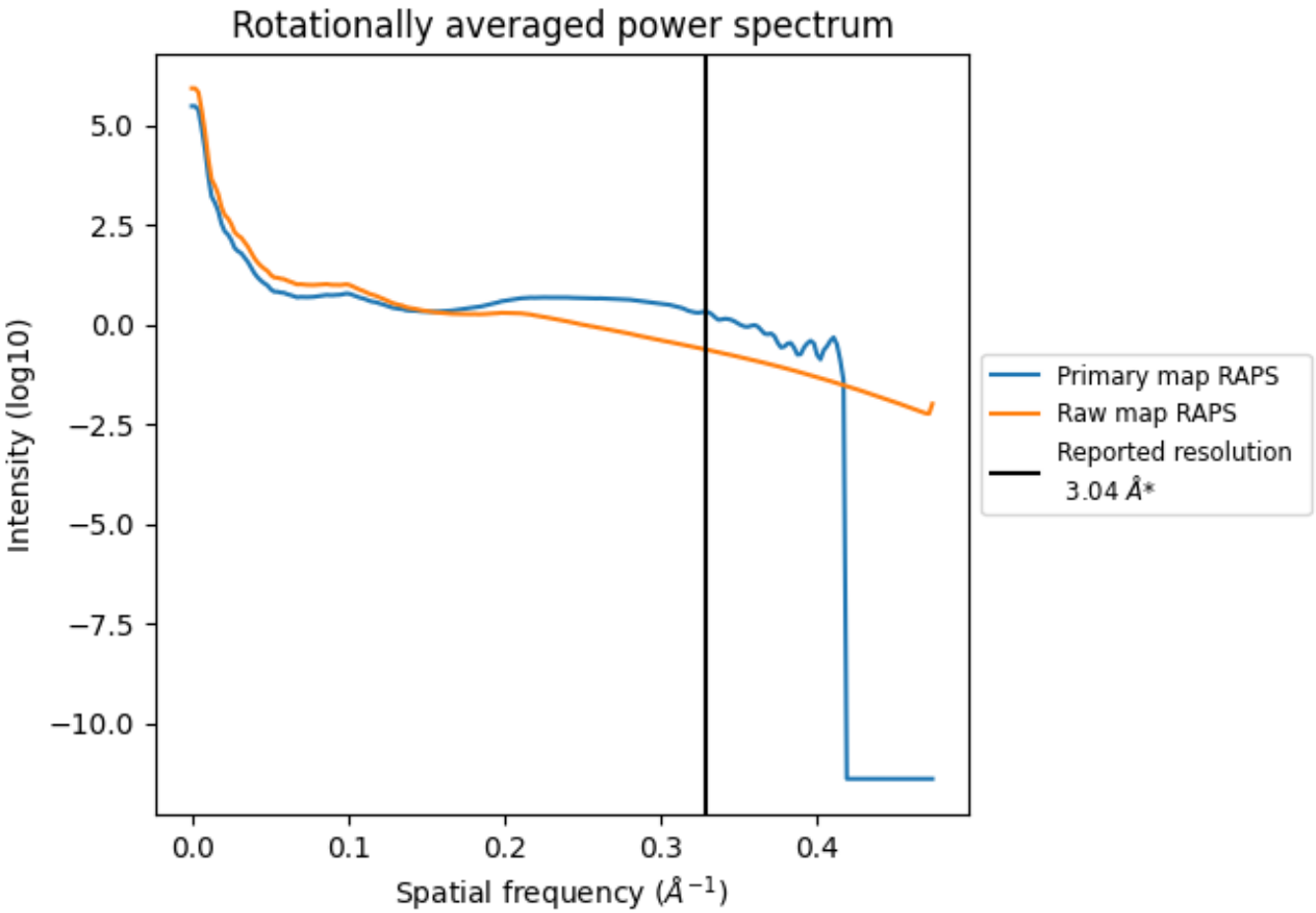
7.2 Volume estimate



The volume at the recommended contour level is 305 nm^3; this corresponds to an approximate mass of 276 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)

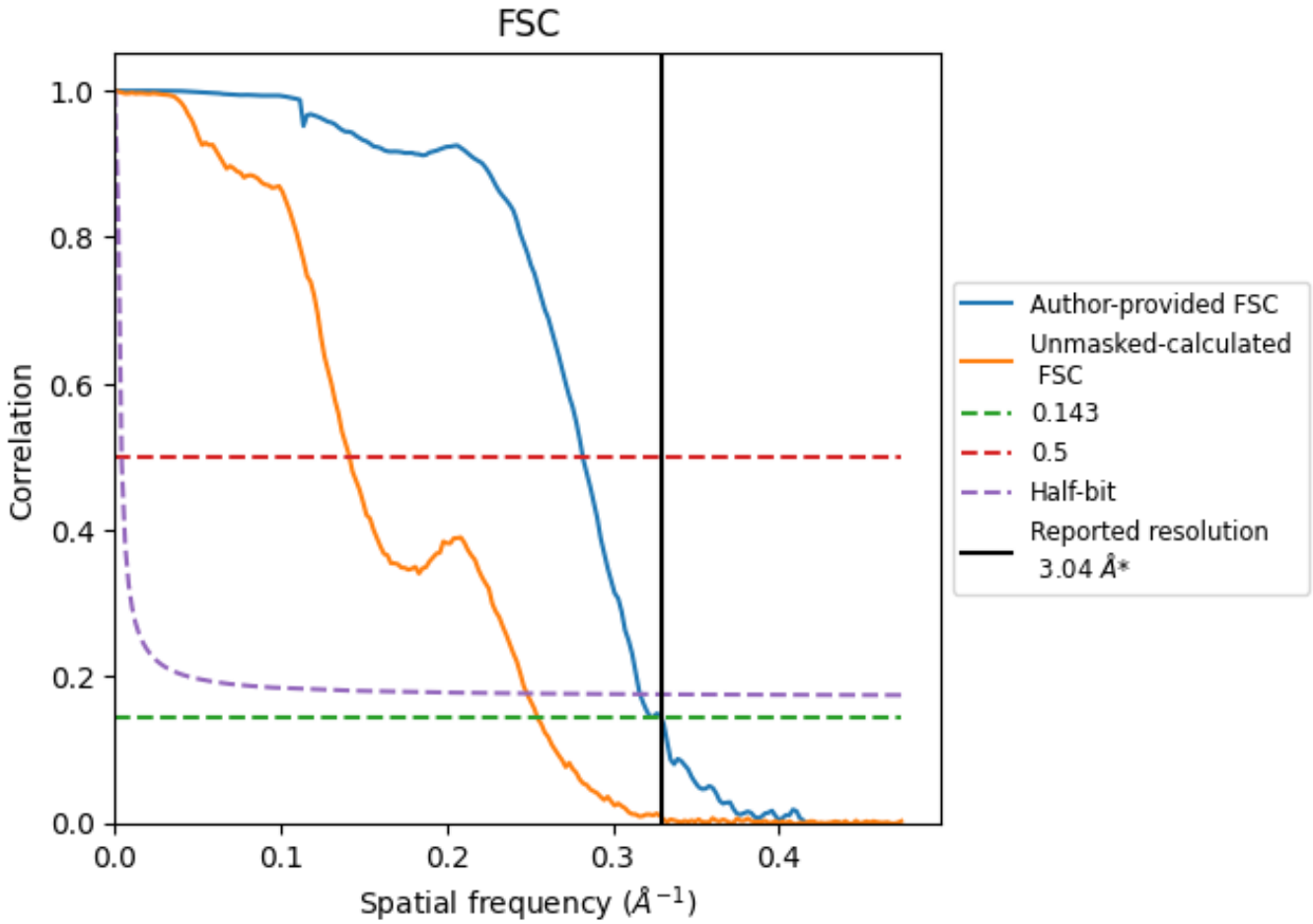


*Reported resolution corresponds to spatial frequency of 0.329 $Å^{-1}$

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 0.329 Å^{-1}

8.2 Resolution estimates (i)

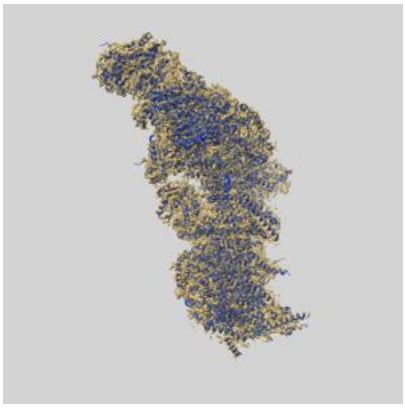
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.55	3.16
Unmasked-calculated*	3.93	7.07	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.04 by more than 10 %

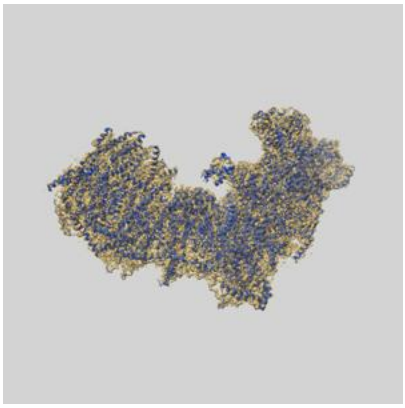
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12095 and PDB model 7B93. Per-residue inclusion information can be found in section 3 on page 19.

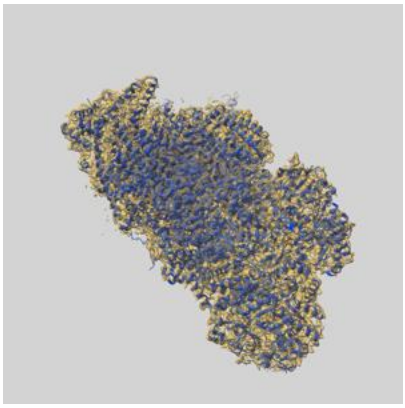
9.1 Map-model overlay



X



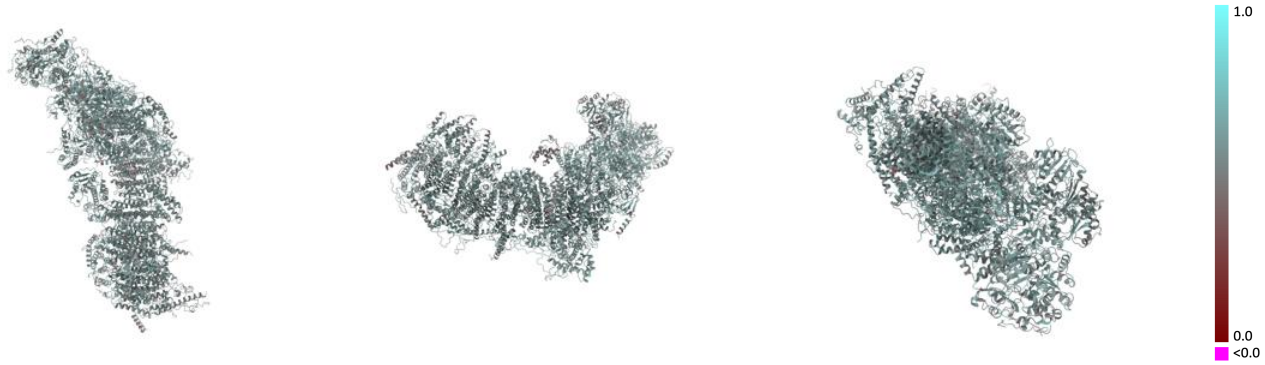
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

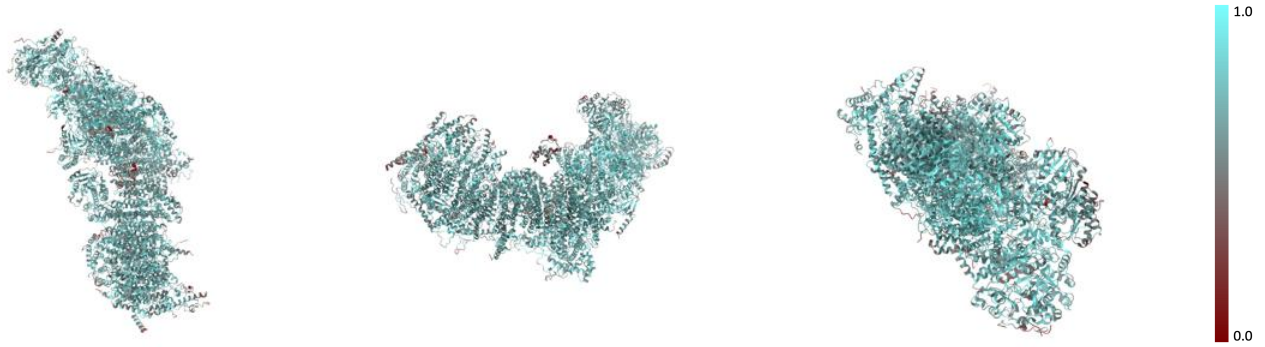
9.2 Q-score mapped to coordinate model (i)



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.

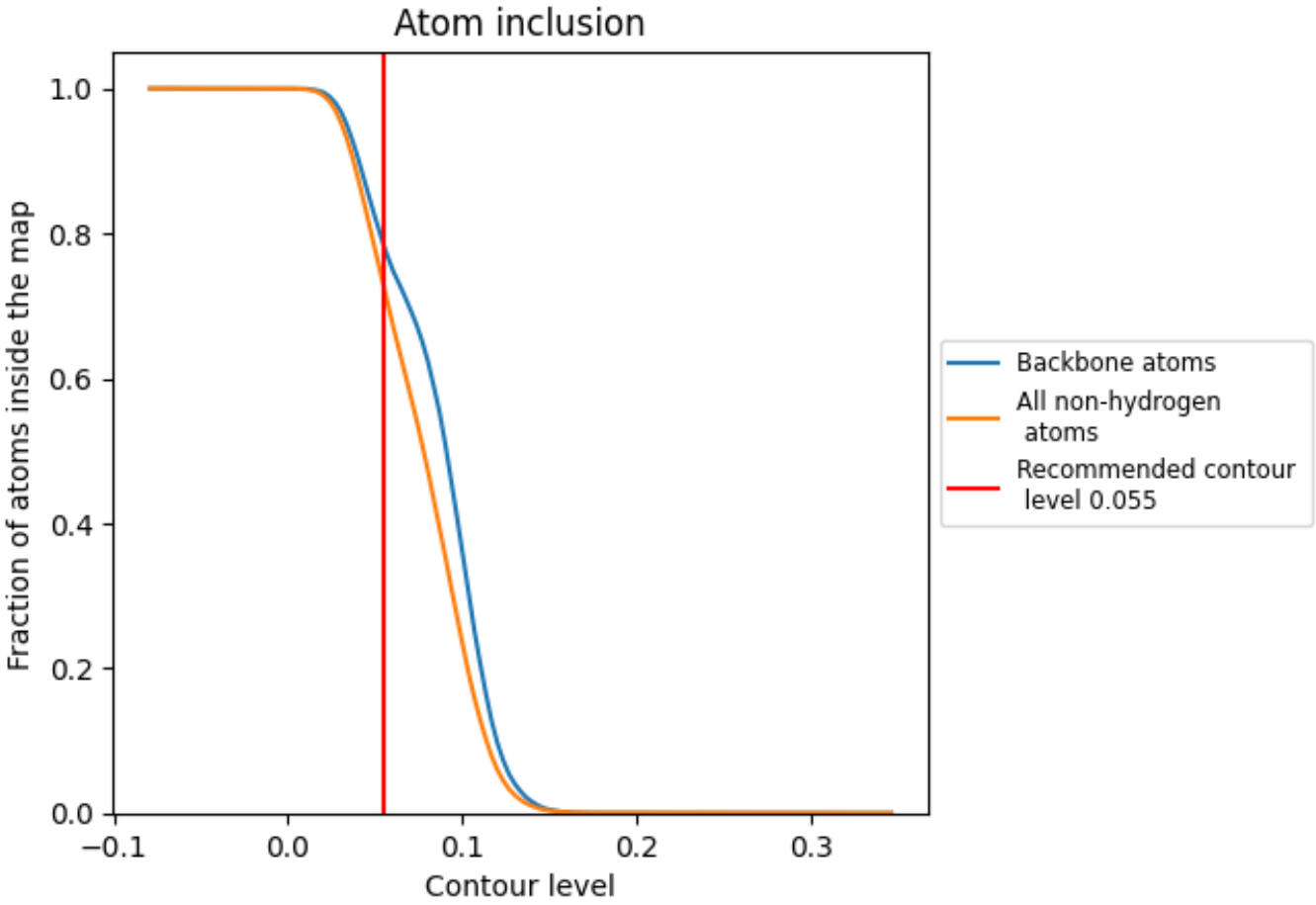
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.5650
A	0.7313	0.5770
B	0.8300	0.5940
C	0.8209	0.5990
D	0.8033	0.5870
E	0.6722	0.5500
F	0.7200	0.5550
G	0.7410	0.5680
H	0.7654	0.5750
I	0.8117	0.5890
J	0.6896	0.5480
K	0.7337	0.5740
L	0.7229	0.5590
M	0.7671	0.5740
N	0.7647	0.5760
O	0.7555	0.5760
P	0.7675	0.5760
Q	0.7512	0.5780
R	0.7409	0.5720
S	0.5982	0.5260
T	0.4350	0.4710
U	0.6431	0.5400
V	0.6921	0.5600
W	0.7407	0.5720
X	0.6971	0.5630
Y	0.6616	0.5540
Z	0.7276	0.5660
a	0.7505	0.5690
b	0.6769	0.5580
c	0.6111	0.5250
d	0.7042	0.5680
e	0.7263	0.5650
f	0.6013	0.5390
g	0.7025	0.5570
h	0.7130	0.5760

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Chain	Atom inclusion	Q-score
i	0.6522	0.5410
j	0.5894	0.5160
k	0.5993	0.5270
l	0.7185	0.5640
m	0.7082	0.5510
n	0.6960	0.5500
o	0.6212	0.5260
p	0.6819	0.5360
q	0.7403	0.5770
r	0.7052	0.5610
s	0.6351	0.5460