Full wwPDB EM Validation Report ⓘ

Sep 26, 2022 – 10:42 pm BST

PDB ID	:	7ZD6
EMDB ID	:	EMD-14637
Title	:	Complex I from Ovis aries, at pH7.4, Open state
Authors	:	Sazanov, L.; Petrova, O.
Deposited on	:	2022-03-29
Resolution	:	3.16 Å(reported)
Based on initial model	:	6ZKE

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:

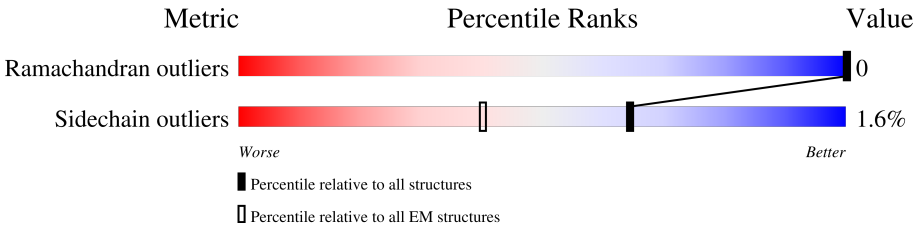
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.16 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.



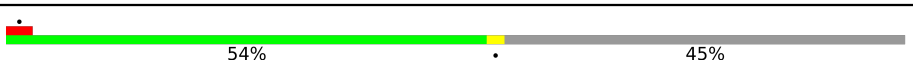
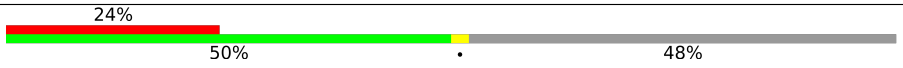
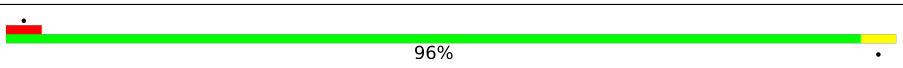
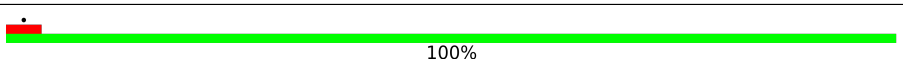
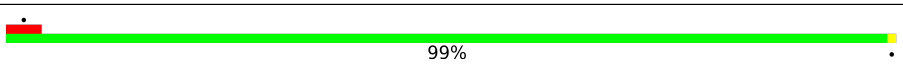
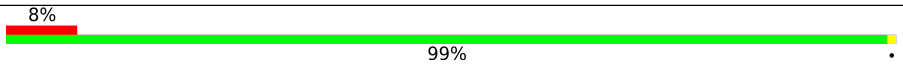
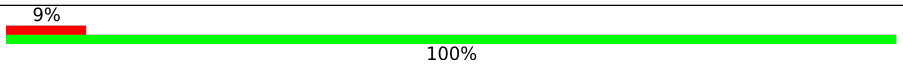
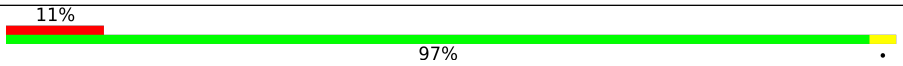
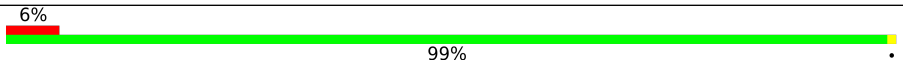
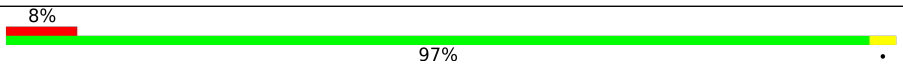
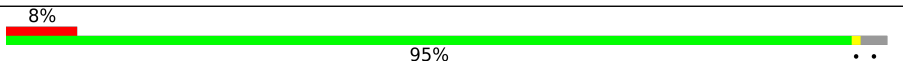
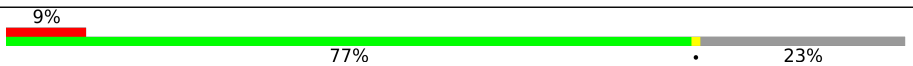
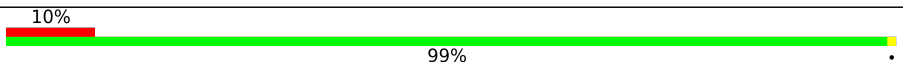
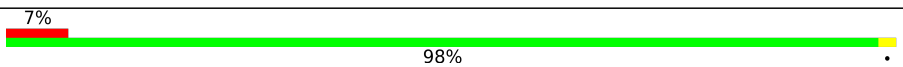
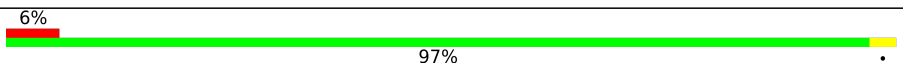
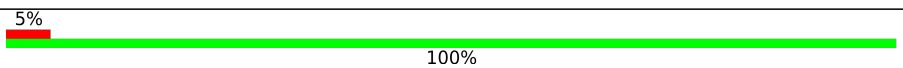
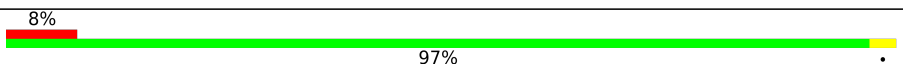
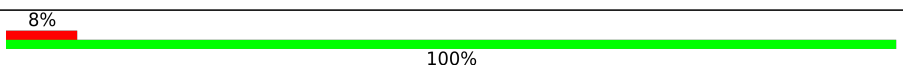
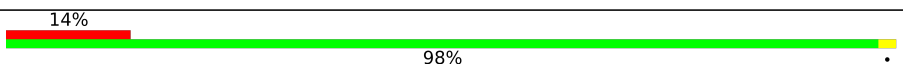
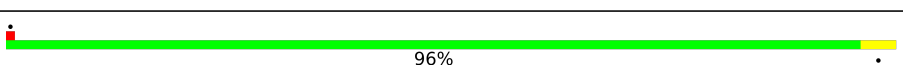
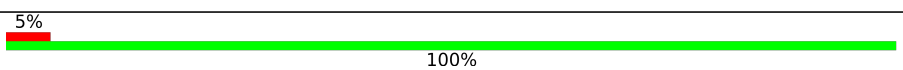
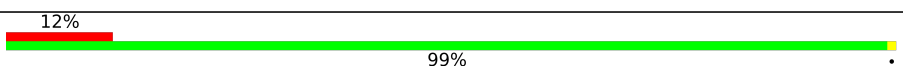
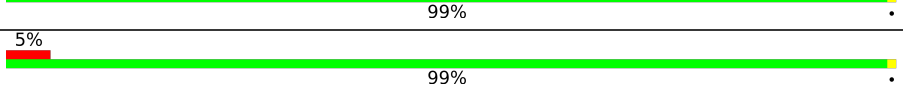
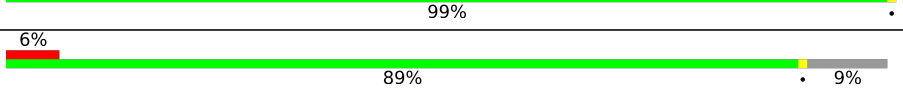
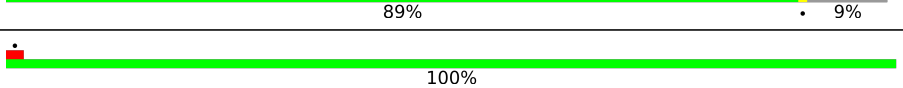
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	17% 95%
2	H	318	97%
3	J	175	9% 93%
4	K	98	97%
5	L	606	99%
6	M	459	100%
7	N	347	99%
8	V	140	6% 97%
9	W	139	99%

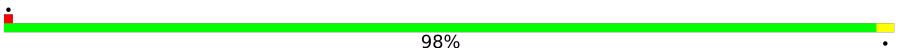
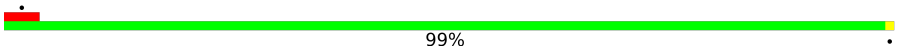
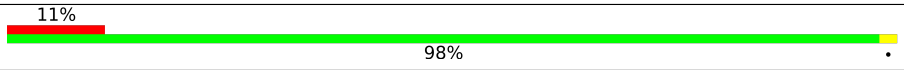
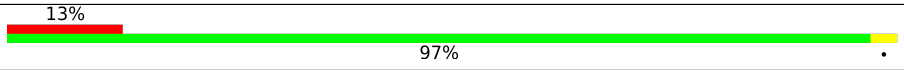
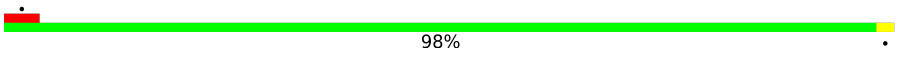
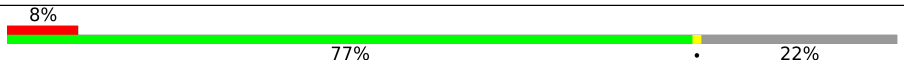
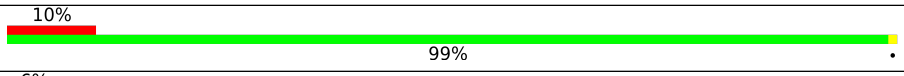
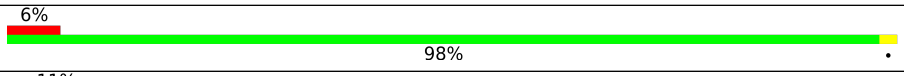
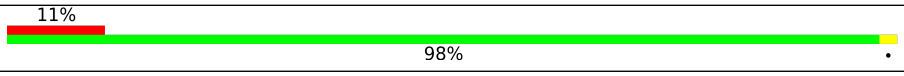
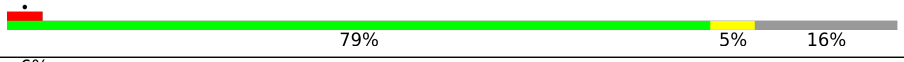
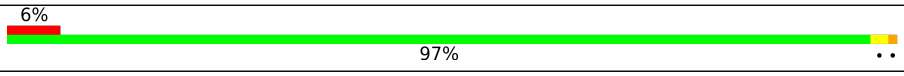
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	X	157	
10	j	157	
11	Y	171	
12	Z	171	
13	k	320	
14	l	105	
15	m	80	
16	n	79	
17	o	120	
18	p	128	
19	q	144	
20	r	128	
21	s	122	
22	t	177	
23	u	65	
24	v	155	
25	w	101	
26	x	49	
27	y	50	
28	z	70	
29	1	430	
30	2	213	
31	3	688	
32	4	463	
33	5	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	6	156	
35	9	176	
36	a	44	
37	b	95	
38	c	126	
39	d	380	
40	e	86	
41	f	113	
42	g	114	
43	h	114	
44	i	145	

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 66748 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	110	880	593	128	153	6	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	314	2498	1685	380	414	19	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	169	1294	870	185	226	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	98	749	490	112	132	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	606	4806	3187	746	829	44	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	459	3647	2429	571	607	40	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
10	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 12 is a protein called Complex I-PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 20 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	x	49	Total 412	C 271	N 70	O 71	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
27	y	50	Total 436	C 287	N 77	O 72	0	0

- Molecule 28 is a protein called Complex I-MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	z	70	Total 576	C 369	N 106	O 96	S 5	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1	430	Total 3312	C 2086	N 593	O 613	S 20	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	213	Total 1655	C 1058	N 278	O 309	S 10	0	0

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	688	Total 5275	C 3301	N 922	O 1011	S 41	0	0

- Molecule 32 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4	421	Total 3390	C 2165	N 581	O 619	S 25	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

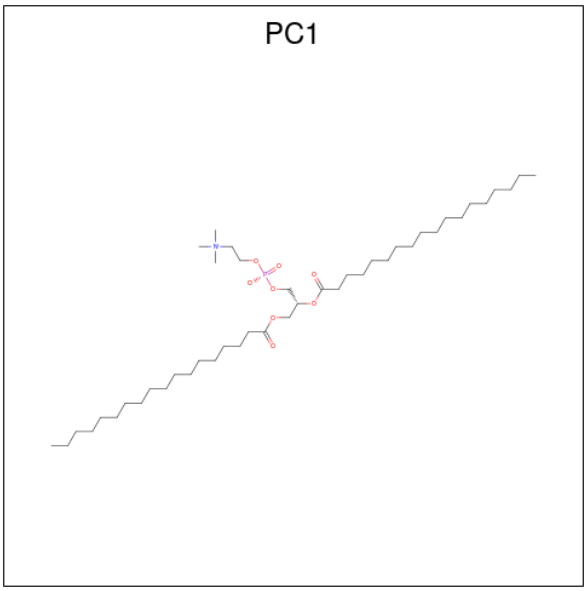
- Molecule 43 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

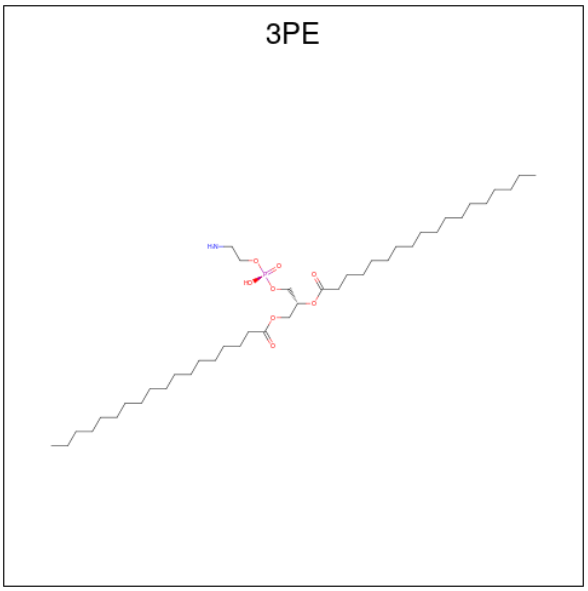
Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



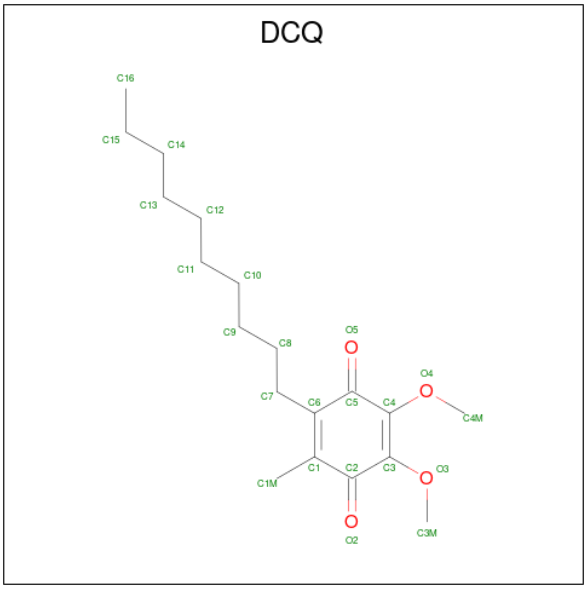
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			83	63	2	16	2	
45	A	1	Total	C	N	O	P	0
			83	63	2	16	2	
45	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	L	1	Total	C	N	O	P	0
			108	88	2	16	2	
45	L	1	Total	C	N	O	P	0
			108	88	2	16	2	
45	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



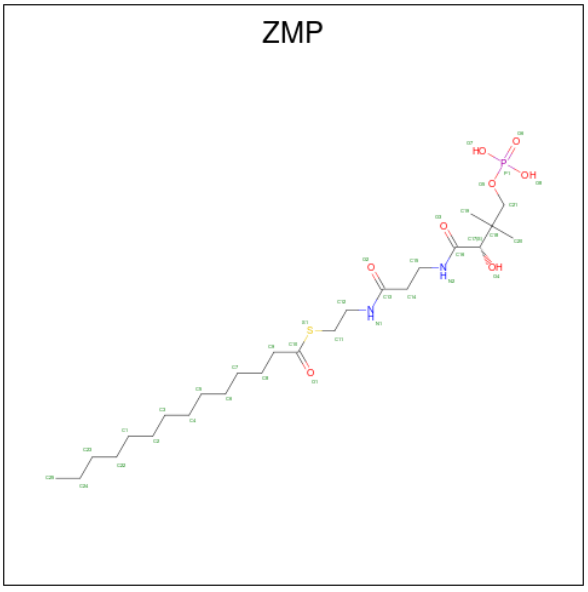
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	H	1	Total	C	N	O	P	0
			102	82	2	16	2	
46	H	1	Total	C	N	O	P	0
			102	82	2	16	2	
46	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	L	1	Total	C	N	O	P	0
			82	62	2	16	2	
46	L	1	Total	C	N	O	P	0
			82	62	2	16	2	
46	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	N	1	Total	C	N	O	P	0
			122	92	3	24	3	
46	N	1	Total	C	N	O	P	0
			122	92	3	24	3	
46	N	1	Total	C	N	O	P	0
			122	92	3	24	3	
46	V	1	Total	C	N	O	P	0
			99	70	2	24	3	
46	V	1	Total	C	N	O	P	0
			99	70	2	24	3	
46	V	1	Total	C	N	O	P	0
			99	70	2	24	3	
46	6	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 47 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: $C_{19}H_{30}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
47	H	1	23	19	4	0

- Molecule 48 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



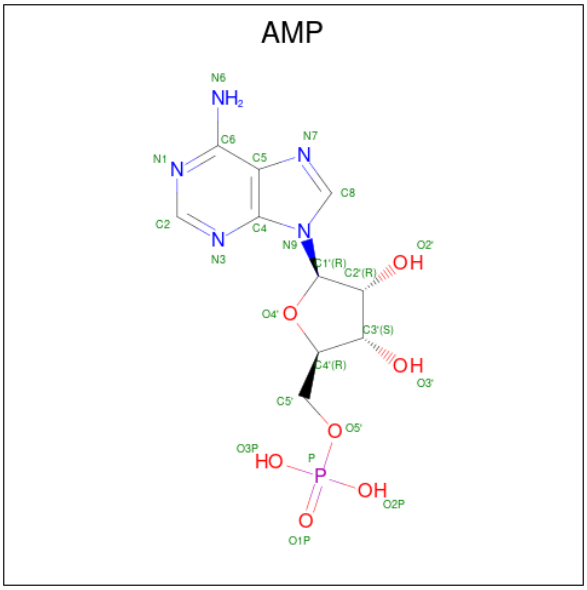
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
48	X	1	31	20	2	7	1	1	0

Continued on next page...

Continued from previous page...

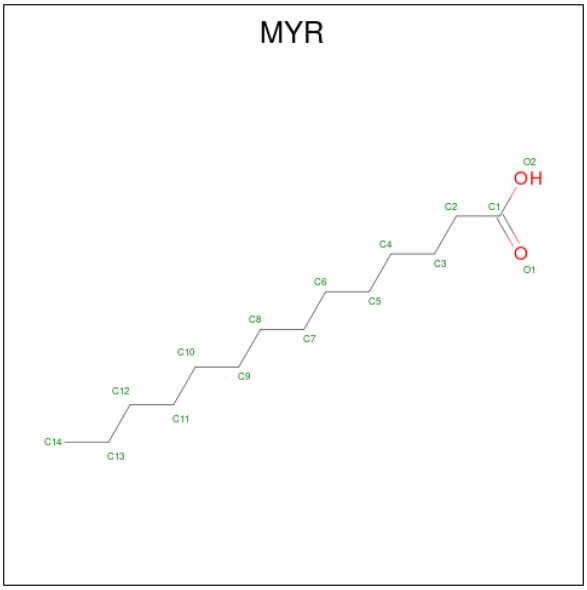
Mol	Chain	Residues	Atoms						AltConf
48	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 49 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



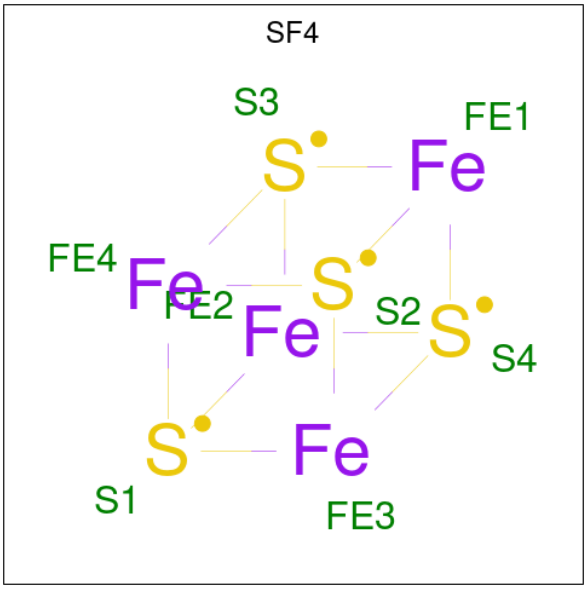
Mol	Chain	Residues	Atoms					AltConf
49	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 50 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



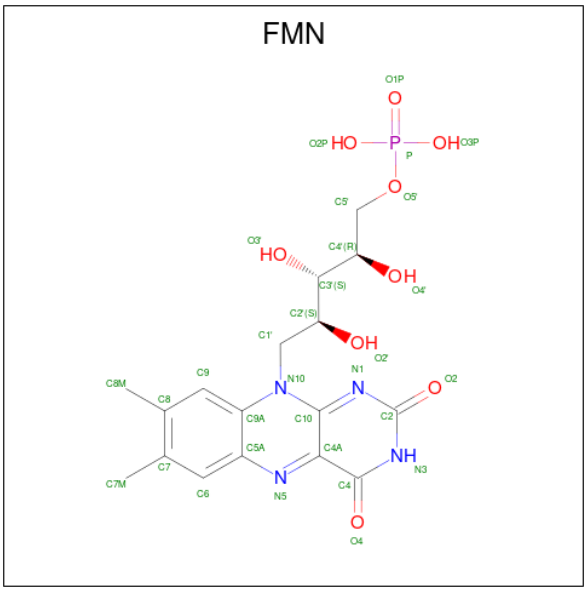
Mol	Chain	Residues	Atoms			AltConf
50	s	1	Total	C	O	0
			15	14	1	

- Molecule 51 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



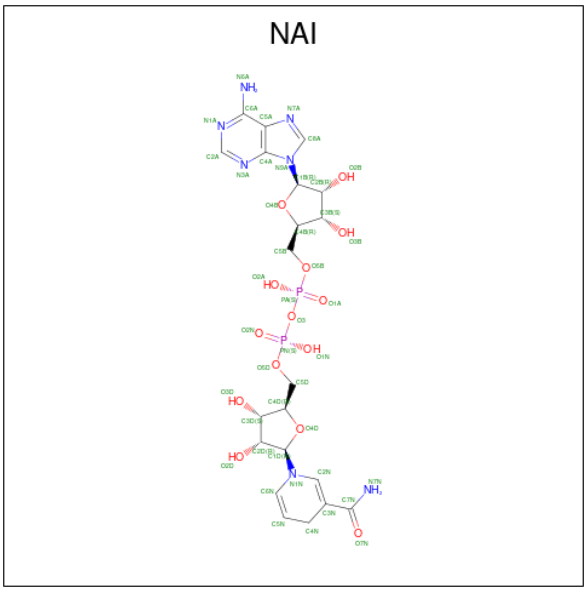
Mol	Chain	Residues	Atoms			AltConf
51	1	1	Total	Fe	S	0
			8	4	4	
51	3	1	Total	Fe	S	0
			16	8	8	
51	3	1	Total	Fe	S	0
			16	8	8	
51	6	1	Total	Fe	S	0
			8	4	4	
51	9	1	Total	Fe	S	0
			16	8	8	
51	9	1	Total	Fe	S	0
			16	8	8	

- Molecule 52 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



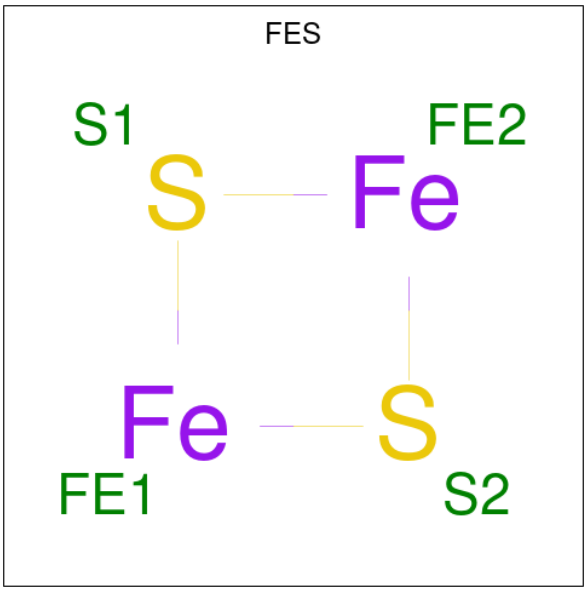
Mol	Chain	Residues	Atoms					AltConf
52	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 53 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
53	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
54	2	1	Total Fe S 4 2 2	0
54	3	1	Total Fe S 4 2 2	0

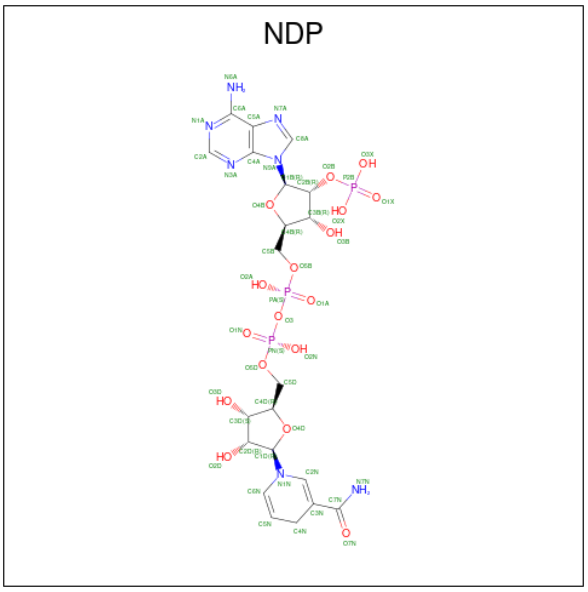
- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
55	3	1	Total K 1 1	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
56	b	1	Total Zn 1 1	0

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

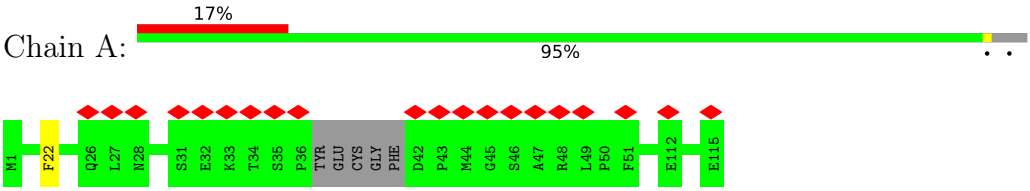


Mol	Chain	Residues	Atoms					AltConf
57	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

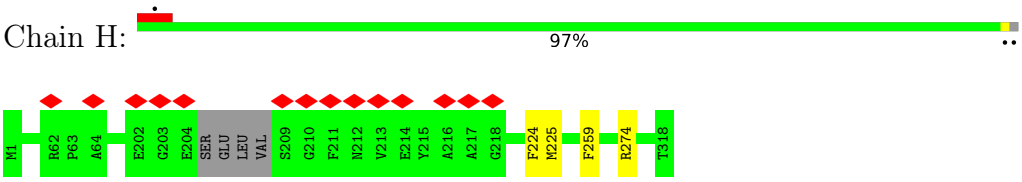
3 Residue-property plots (i)

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

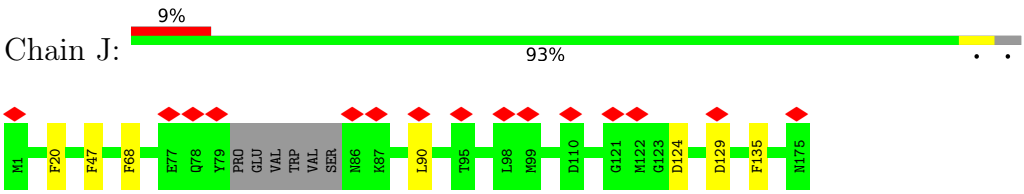
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



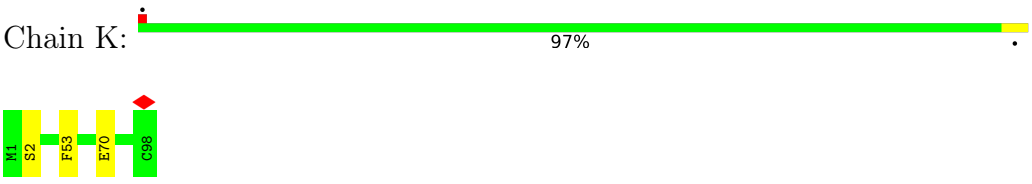
• Molecule 2: NADH-ubiquinone oxidoreductase chain 1



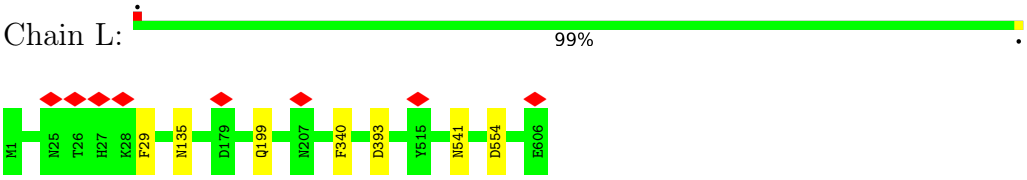
• Molecule 3: NADH-ubiquinone oxidoreductase chain 6



• Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

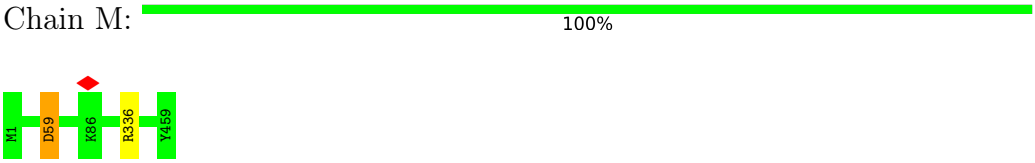


• Molecule 5: NADH-ubiquinone oxidoreductase chain 5



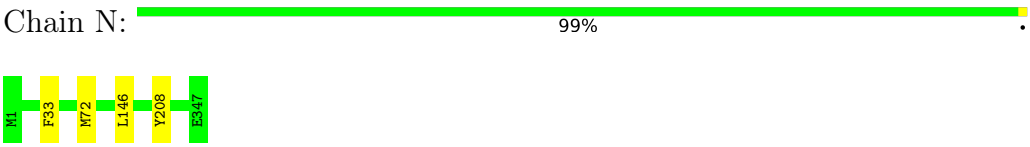
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4

Chain M:



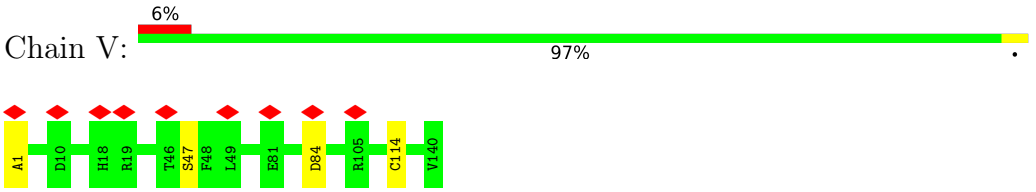
• Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain N:



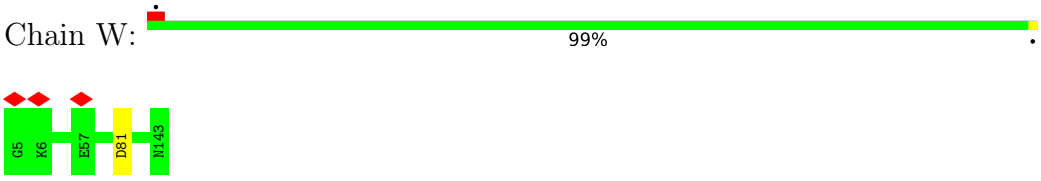
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:



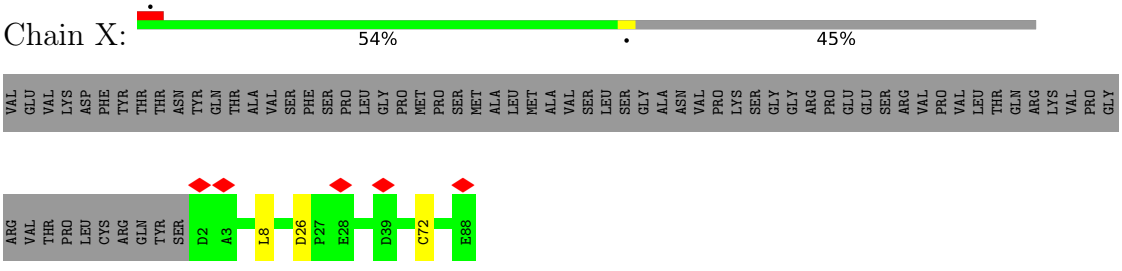
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain W:



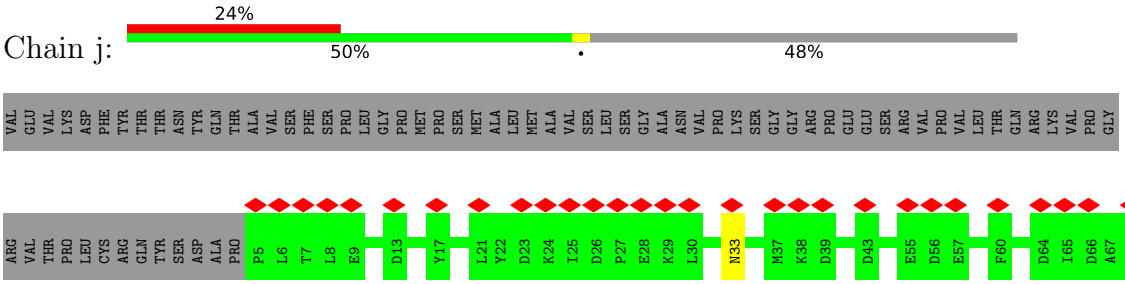
• Molecule 10: Acyl carrier protein

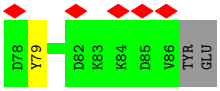
Chain X:



• Molecule 10: Acyl carrier protein

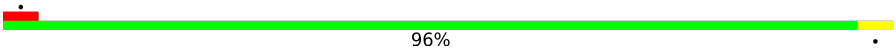
Chain j:





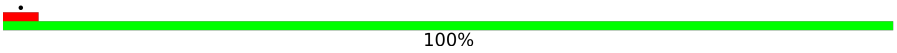
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

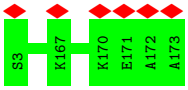
Chain Y:



• Molecule 12: Complex I-PDSW

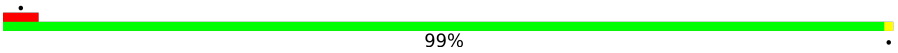
Chain Z:





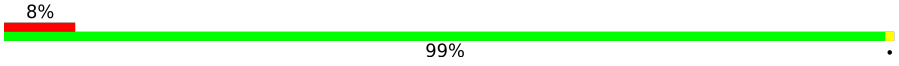
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

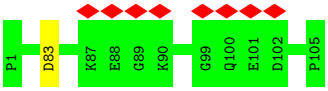
Chain k:



• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

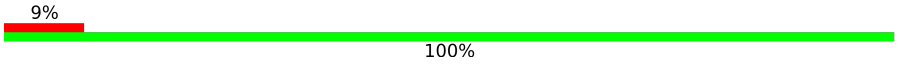
Chain l:

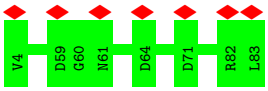




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

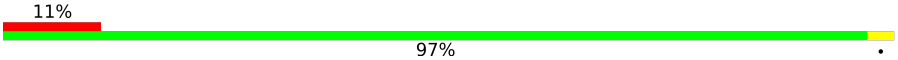
Chain m:

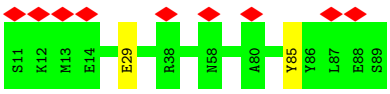




• Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

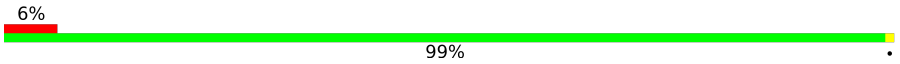
Chain n:

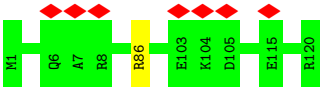




• Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2

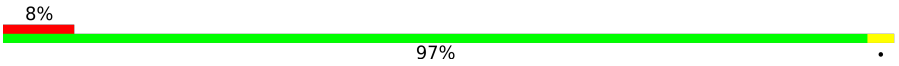
Chain o:





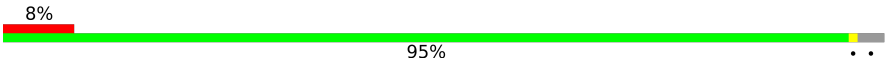
• Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

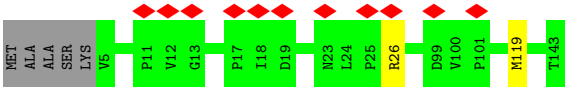
Chain p:



• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

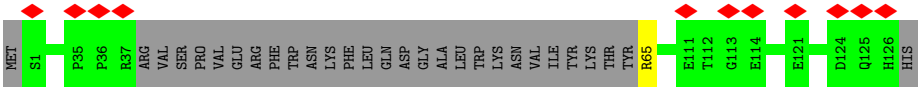
Chain q:





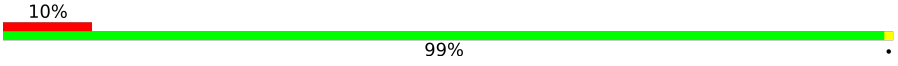
• Molecule 20: Mitochondrial complex I, B17 subunit

Chain r:



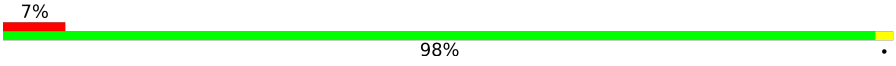
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

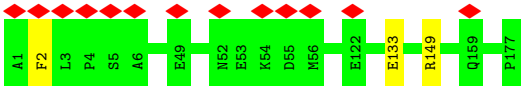
Chain s:



• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

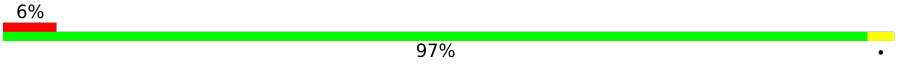
Chain t:

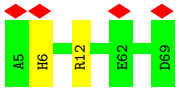




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

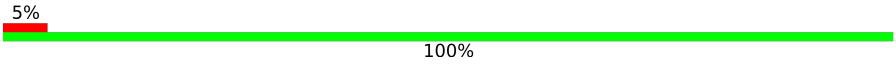
Chain u:

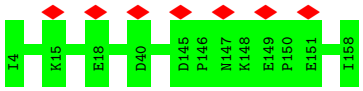




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

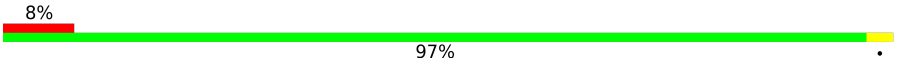
Chain v:

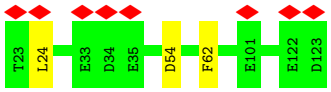




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

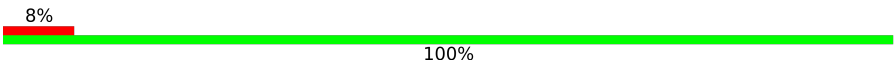
Chain w:

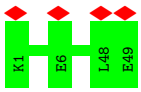




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

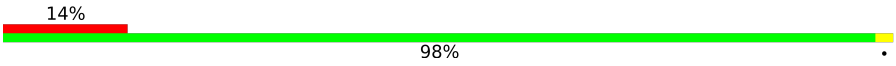
Chain x:

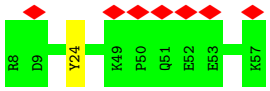




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

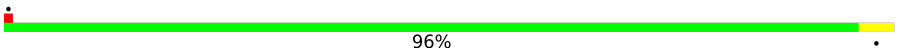
Chain y:





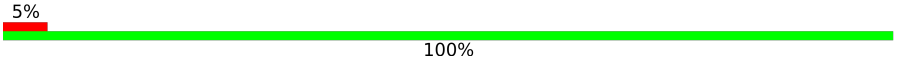
• Molecule 28: Complex I-MWFE

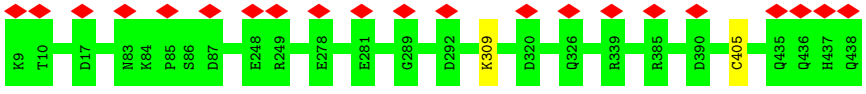
Chain z:



• Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

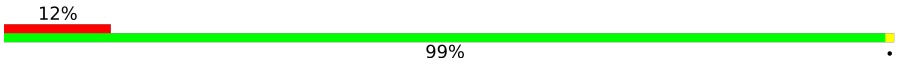
Chain 1:

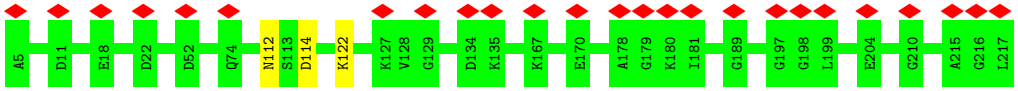




• Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

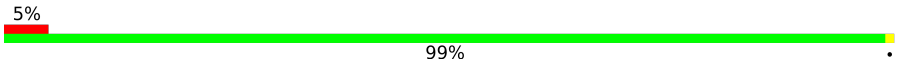
Chain 2:

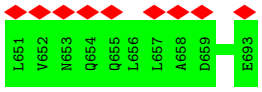




• Molecule 31: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

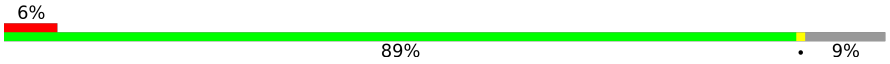
Chain 3:

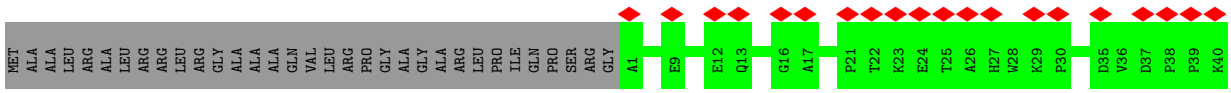


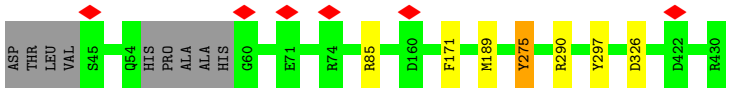


• Molecule 32: Complex I-49kD

Chain 4:

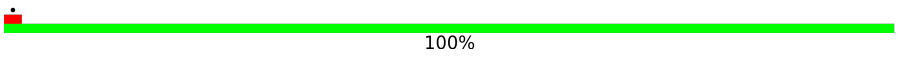


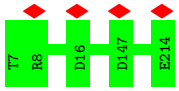




• Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

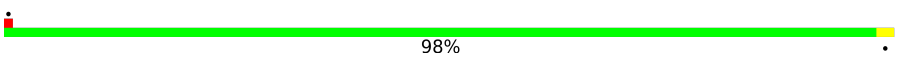
Chain 5:

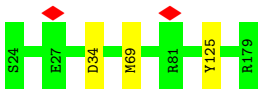




• Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

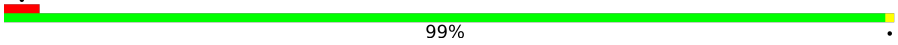
Chain 6:

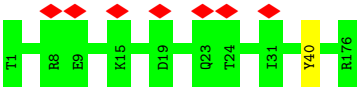




• Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

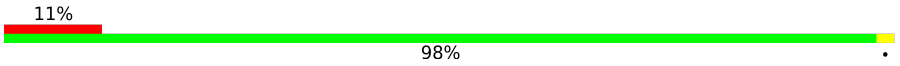
Chain 9:

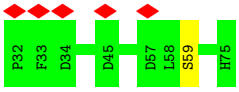




• Molecule 36: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

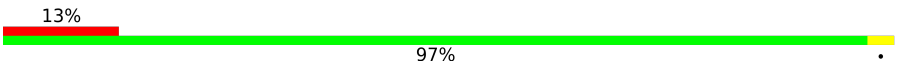
Chain a:

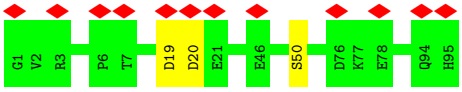




• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

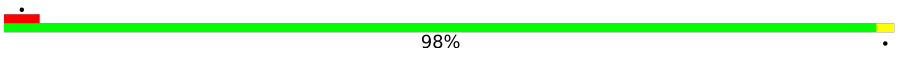
Chain b:

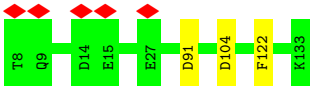




• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

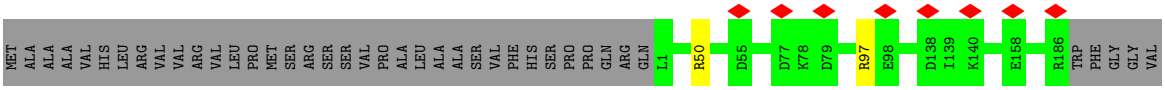
Chain c:

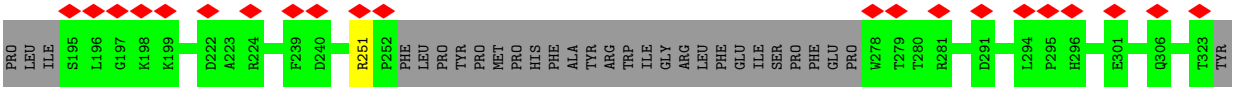


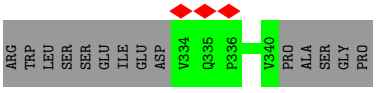


• Molecule 39: NADH:ubiquinone oxidoreductase subunit A9

Chain d:

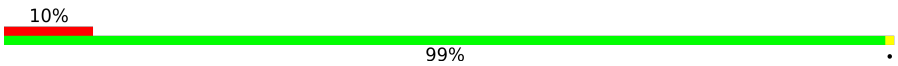


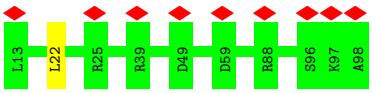




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

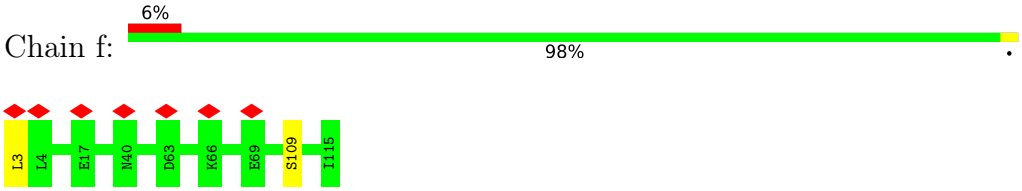
Chain e:





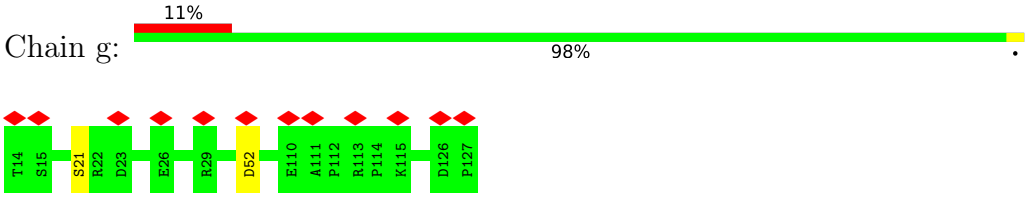
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain f:



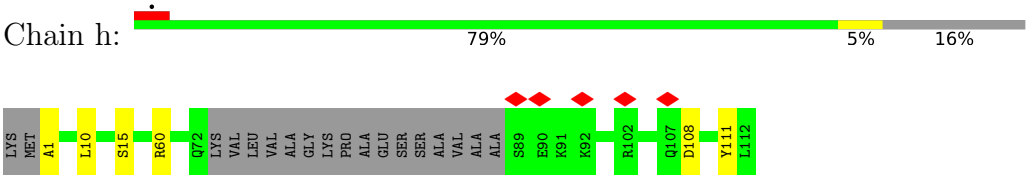
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain g:



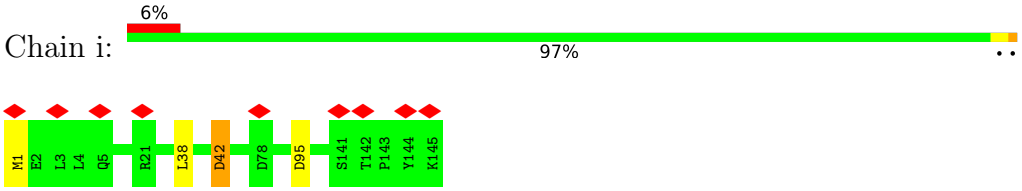
• Molecule 43: Mitochondrial complex I, B14.5a subunit

Chain h:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.556	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	173.24, 193.98001, 291.58002	wwPDB
Map dimensions	239, 159, 142	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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: ZMP, AMP, FME, FES, NDP, FMN, ZN, K, MYR, DCQ, 3PE, 2MR, AYA, SEP, PC1, NAI, SF4

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	0.30	0/902	0.57	0/1234
2	H	0.33	0/2572	0.55	0/3517
3	J	0.34	0/1324	0.50	0/1790
4	K	0.31	0/749	0.56	0/1014
5	L	0.31	0/4924	0.50	1/6698 (0.0%)
6	M	0.32	0/3731	0.54	1/5085 (0.0%)
7	N	0.31	0/2787	0.51	0/3795
8	V	0.28	0/1041	0.47	0/1412
9	W	0.31	0/1188	0.48	0/1607
10	X	0.33	0/713	0.52	1/963 (0.1%)
10	j	0.33	0/670	0.59	0/902
11	Y	0.31	0/1440	0.53	0/1942
12	Z	0.31	0/1475	0.49	0/1989
13	k	0.32	0/2646	0.47	0/3579
14	l	0.32	0/896	0.55	0/1200
15	m	0.30	0/647	0.49	0/890
16	n	0.32	0/653	0.53	0/882
17	o	0.35	0/1035	0.53	0/1398
18	p	0.31	0/1085	0.58	1/1467 (0.1%)
19	q	0.31	0/1171	0.57	0/1579
20	r	0.33	0/874	0.53	0/1188
21	s	0.31	0/1072	0.57	0/1436
22	t	0.31	0/1573	0.53	0/2130
23	u	0.29	0/590	0.44	0/810
24	v	0.32	0/1361	0.49	0/1861
25	w	0.31	0/872	0.56	2/1185 (0.2%)
26	x	0.33	0/425	0.46	0/576
27	y	0.33	0/449	0.53	0/605
28	z	0.34	0/591	0.73	1/795 (0.1%)
29	1	0.30	0/3386	0.52	0/4575
30	2	0.29	0/1695	0.49	0/2306
31	3	0.30	0/5362	0.53	0/7266

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	4	0.33	0/3463	0.51	0/4687
33	5	0.33	0/1776	0.54	0/2417
34	6	0.33	0/1278	0.56	0/1728
35	9	0.35	0/1445	0.56	0/1956
36	a	0.27	0/383	0.51	0/518
37	b	0.31	0/749	0.54	0/1009
38	c	0.29	0/1047	0.54	1/1415 (0.1%)
39	d	0.30	0/2424	0.53	0/3276
40	e	0.31	0/702	0.56	0/945
41	f	0.30	0/937	0.43	0/1271
42	g	0.31	0/993	0.52	0/1336
43	h	0.30	0/779	0.56	1/1053 (0.1%)
44	i	0.32	0/1250	0.55	1/1698 (0.1%)
All	All	0.31	0/67125	0.53	10/90985 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
31	3	0	1
32	4	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	z	51	ASP	CB-CG-OD1	8.47	125.93	118.30
18	p	23	ASP	CB-CG-OD1	7.55	125.09	118.30
6	M	59	ASP	CB-CG-OD1	7.15	124.74	118.30
44	i	42	ASP	CB-CG-OD1	6.61	124.25	118.30
38	c	104	ASP	CB-CG-OD1	6.21	123.89	118.30
5	L	393	ASP	CB-CG-OD1	5.98	123.68	118.30
25	w	24	LEU	CA-CB-CG	5.93	128.93	115.30
25	w	54	ASP	CB-CG-OD1	5.90	123.61	118.30
43	h	108	ASP	CB-CG-OD1	5.84	123.56	118.30
10	X	8	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	3	259	ASN	Peptide
32	4	275	TYR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	106/115 (92%)	100 (94%)	6 (6%)	0	100	100
2	H	310/318 (98%)	303 (98%)	7 (2%)	0	100	100
3	J	165/175 (94%)	159 (96%)	6 (4%)	0	100	100
4	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
5	L	604/606 (100%)	584 (97%)	20 (3%)	0	100	100
6	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
7	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
8	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	W	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
10	X	85/157 (54%)	82 (96%)	3 (4%)	0	100	100
10	j	80/157 (51%)	79 (99%)	1 (1%)	0	100	100
11	Y	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
12	Z	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
13	k	317/320 (99%)	303 (96%)	14 (4%)	0	100	100
14	l	103/105 (98%)	95 (92%)	8 (8%)	0	100	100
15	m	78/80 (98%)	72 (92%)	6 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	n	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
17	o	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
18	p	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
19	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
20	r	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
21	s	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
22	t	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
23	u	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
24	v	153/155 (99%)	149 (97%)	4 (3%)	0	100	100
25	w	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
26	x	47/49 (96%)	47 (100%)	0	0	100	100
27	y	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
28	z	68/70 (97%)	68 (100%)	0	0	100	100
29	1	428/430 (100%)	420 (98%)	8 (2%)	0	100	100
30	2	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
31	3	686/688 (100%)	665 (97%)	21 (3%)	0	100	100
32	4	414/463 (89%)	397 (96%)	17 (4%)	0	100	100
33	5	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
34	6	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
35	9	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
36	a	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
37	b	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
38	c	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
39	d	289/380 (76%)	282 (98%)	7 (2%)	0	100	100
40	e	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
41	f	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
42	g	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
43	h	92/114 (81%)	87 (95%)	5 (5%)	0	100	100
44	i	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
All	All	8048/8497 (95%)	7799 (97%)	249 (3%)	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	99/103 (96%)	98 (99%)	1 (1%)	76 89
2	H	274/278 (99%)	270 (98%)	4 (2%)	65 84
3	J	138/144 (96%)	131 (95%)	7 (5%)	24 56
4	K	86/86 (100%)	83 (96%)	3 (4%)	36 67
5	L	538/538 (100%)	532 (99%)	6 (1%)	73 88
6	M	411/411 (100%)	409 (100%)	2 (0%)	88 95
7	N	315/315 (100%)	311 (99%)	4 (1%)	69 86
8	V	101/101 (100%)	98 (97%)	3 (3%)	41 71
9	W	122/122 (100%)	121 (99%)	1 (1%)	81 92
10	X	80/141 (57%)	78 (98%)	2 (2%)	47 75
10	j	76/141 (54%)	73 (96%)	3 (4%)	32 64
11	Y	154/154 (100%)	148 (96%)	6 (4%)	32 64
12	Z	155/155 (100%)	155 (100%)	0	100 100
13	k	283/283 (100%)	280 (99%)	3 (1%)	73 88
14	l	94/94 (100%)	93 (99%)	1 (1%)	73 88
15	m	69/69 (100%)	69 (100%)	0	100 100
16	n	61/61 (100%)	59 (97%)	2 (3%)	38 69
17	o	107/107 (100%)	106 (99%)	1 (1%)	78 91
18	p	114/114 (100%)	111 (97%)	3 (3%)	46 74
19	q	119/122 (98%)	117 (98%)	2 (2%)	60 82
20	r	95/122 (78%)	94 (99%)	1 (1%)	73 88
21	s	110/110 (100%)	109 (99%)	1 (1%)	78 91
22	t	159/159 (100%)	156 (98%)	3 (2%)	57 80
23	u	59/59 (100%)	57 (97%)	2 (3%)	37 68
24	v	140/140 (100%)	140 (100%)	0	100 100
25	w	92/92 (100%)	91 (99%)	1 (1%)	73 88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	x	44/44 (100%)	44 (100%)	0	100 100
27	y	46/46 (100%)	45 (98%)	1 (2%)	52 77
28	z	59/59 (100%)	57 (97%)	2 (3%)	37 68
29	1	344/344 (100%)	342 (99%)	2 (1%)	86 94
30	2	183/183 (100%)	180 (98%)	3 (2%)	62 83
31	3	578/578 (100%)	569 (98%)	9 (2%)	62 83
32	4	363/391 (93%)	357 (98%)	6 (2%)	60 82
33	5	189/189 (100%)	189 (100%)	0	100 100
34	6	132/132 (100%)	129 (98%)	3 (2%)	50 76
35	9	151/151 (100%)	150 (99%)	1 (1%)	84 93
36	a	43/43 (100%)	42 (98%)	1 (2%)	50 76
37	b	79/79 (100%)	76 (96%)	3 (4%)	33 65
38	c	113/113 (100%)	111 (98%)	2 (2%)	59 81
39	d	255/326 (78%)	252 (99%)	3 (1%)	71 87
40	e	76/76 (100%)	75 (99%)	1 (1%)	69 86
41	f	101/101 (100%)	99 (98%)	2 (2%)	55 79
42	g	107/107 (100%)	105 (98%)	2 (2%)	57 80
43	h	84/96 (88%)	80 (95%)	4 (5%)	25 59
44	i	131/131 (100%)	127 (97%)	4 (3%)	40 70
All	All	7129/7410 (96%)	7018 (98%)	111 (2%)	64 83

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
2	H	224	PHE
2	H	225	MET
2	H	259	PHE
2	H	274	ARG
3	J	20	PHE
3	J	47	PHE
3	J	68	PHE
3	J	90	LEU
3	J	124	ASP
3	J	129	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	135	PHE
4	K	2	SER
4	K	53	PHE
4	K	70	GLU
5	L	29	PHE
5	L	135	ASN
5	L	199	GLN
5	L	340	PHE
5	L	541	ASN
5	L	554	ASP
6	M	59	ASP
6	M	336	ARG
7	N	33	PHE
7	N	72	MET
7	N	146	LEU
7	N	208	TYR
8	V	47	SER
8	V	84	ASP
8	V	114	CYS
9	W	81	ASP
10	X	26	ASP
10	X	72	CYS
11	Y	11	ASP
11	Y	47	TRP
11	Y	65	CYS
11	Y	111	LEU
11	Y	120	ASP
11	Y	133	ASP
13	k	196	SER
13	k	213	GLU
13	k	218	CYS
14	l	83	ASP
16	n	29	GLU
16	n	85	TYR
17	o	86	ARG
18	p	60	GLU
18	p	74	ASN
18	p	121	ASP
19	q	26	ARG
19	q	119	MET
20	r	65	ARG
21	s	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	t	2	PHE
22	t	133	GLU
22	t	149	ARG
23	u	6	HIS
23	u	12	ARG
25	w	62	PHE
27	y	24	TYR
28	z	31	ASN
28	z	60	TYR
29	1	309	LYS
29	1	405	CYS
30	2	112	ASN
30	2	114	ASP
30	2	122	LYS
31	3	35	MET
31	3	52	CYS
31	3	77	TRP
31	3	156	CYS
31	3	343	LEU
31	3	447	LYS
31	3	490	MET
31	3	598	LYS
31	3	613	TYR
32	4	171	PHE
32	4	189	MET
32	4	275	TYR
32	4	290	ARG
32	4	297	TYR
32	4	326	ASP
34	6	34	ASP
34	6	69	MET
34	6	125	TYR
35	9	40	TYR
36	a	59	SER
37	b	19	ASP
37	b	20	ASP
37	b	50	SER
38	c	91	ASP
38	c	122	PHE
39	d	50	ARG
39	d	97	ARG
39	d	251	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	e	22	LEU
41	f	3	LEU
41	f	109	SER
42	g	21	SER
42	g	52	ASP
43	h	10	LEU
43	h	15	SER
43	h	60	ARG
43	h	111	TYR
44	i	1	MET
44	i	38	LEU
44	i	42	ASP
44	i	95	ASP
10	j	33	ASN
10	j	72	CYS
10	j	79	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	J	120	ASN
14	l	76	ASN
20	r	88	HIS
44	i	91	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	2MR	4	85	32	10,12,13	2.41	2 (20%)	5,13,15	1.03	0
5	FME	L	1	5	8,9,10	0.95	0	7,9,11	0.88	0
8	AYA	V	1	8	6,7,8	1.20	1 (16%)	5,8,10	1.92	2 (40%)
4	FME	K	1	4	8,9,10	0.96	0	7,9,11	0.78	0
43	AYA	h	1	43	6,7,8	1.30	1 (16%)	5,8,10	1.37	1 (20%)
13	SEP	k	36	13	8,9,10	1.57	1 (12%)	8,12,14	1.65	2 (25%)
6	FME	M	1	6	8,9,10	0.97	0	7,9,11	0.99	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
32	2MR	4	85	32	-	2/10/13/15	-
5	FME	L	1	5	-	3/7/9/11	-
8	AYA	V	1	8	-	2/4/6/8	-
4	FME	K	1	4	-	4/7/9/11	-
43	AYA	h	1	43	-	0/4/6/8	-
13	SEP	k	36	13	-	3/5/8/10	-
6	FME	M	1	6	-	2/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	85	2MR	CZ-NE	5.18	1.45	1.34
32	4	85	2MR	CZ-NH2	4.91	1.44	1.33
13	k	36	SEP	P-O1P	3.39	1.61	1.50
43	h	1	AYA	CA-N	-2.61	1.43	1.46
8	V	1	AYA	CA-N	-2.21	1.44	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	1	AYA	CB-CA-N	3.19	113.16	109.61
13	k	36	SEP	OG-CB-CA	3.03	111.09	108.14
43	h	1	AYA	CB-CA-N	2.86	112.79	109.61
13	k	36	SEP	P-OG-CB	-2.84	110.48	118.30
8	V	1	AYA	CA-N-CT	2.43	125.06	121.52

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	FME	O1-CN-N-CA
5	L	1	FME	CA-CB-CG-SD
6	M	1	FME	C-CA-CB-CG
6	M	1	FME	O-C-CA-CB
13	k	36	SEP	CB-OG-P-O1P
13	k	36	SEP	CB-OG-P-O2P
13	k	36	SEP	CB-OG-P-O3P
32	4	85	2MR	C-CA-CB-CG
8	V	1	AYA	OT-CT-N-CA
8	V	1	AYA	CM-CT-N-CA
4	K	1	FME	CA-CB-CG-SD
4	K	1	FME	CB-CG-SD-CE
5	L	1	FME	CB-CG-SD-CE
5	L	1	FME	N-CA-CB-CG
32	4	85	2MR	CA-CB-CG-CD
4	K	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 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
50	MYR	s	201	21	14,14,15	0.20	0	13,13,15	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	FMN	1	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	7 (14%)
46	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.31	0
45	PC1	M	502	-	53,53,53	0.30	0	59,61,61	0.32	0
45	PC1	H	503	-	53,53,53	0.31	0	59,61,61	0.45	0
45	PC1	A	203	-	45,45,53	0.31	0	51,53,61	0.31	0
57	NDP	d	401	-	45,52,52	0.55	0	53,80,80	0.58	1 (1%)
45	PC1	L	1003	-	53,53,53	0.28	0	59,61,61	0.28	0
46	3PE	N	403	-	30,30,50	0.38	0	33,35,55	0.37	0
48	ZMP	X	101	10	24,30,36	0.74	1 (4%)	29,37,45	1.01	1 (3%)
49	AMP	k	501	-	22,25,25	0.88	1 (4%)	25,38,38	1.24	2 (8%)
47	DCQ	H	501	-	23,23,23	0.18	0	26,29,29	0.53	0
46	3PE	N	402	-	50,50,50	0.32	0	53,55,55	0.49	0
46	3PE	H	502	-	50,50,50	0.31	0	53,55,55	0.34	0
51	SF4	9	201	35	0,12,12	-	-	-		
46	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.34	0
51	SF4	1	501	29	0,12,12	-	-	-		
51	SF4	3	802	31	0,12,12	-	-	-		
51	SF4	9	202	35	0,12,12	-	-	-		
46	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.30	0
45	PC1	A	201	-	36,36,53	0.37	0	42,44,61	0.53	0
46	3PE	N	401	-	39,39,50	0.33	0	42,44,55	0.34	0
45	PC1	L	1002	-	53,53,53	0.30	0	59,61,61	0.53	2 (3%)
46	3PE	H	504	-	50,50,50	0.30	0	53,55,55	0.28	0
46	3PE	V	203	-	26,26,50	0.48	0	30,31,55	0.52	1 (3%)
51	SF4	3	801	31	0,12,12	-	-	-		
46	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.31	0
54	FES	2	300	30	0,4,4	-	-	-		
54	FES	3	803	31	0,4,4	-	-	-		
46	3PE	A	202	-	50,50,50	0.31	0	53,55,55	0.30	0
48	ZMP	j	101	10	27,33,36	0.64	1 (3%)	32,40,45	1.06	2 (6%)
51	SF4	6	201	34	0,12,12	-	-	-		
46	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.66	1 (3%)
46	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.30	0
53	NAI	1	503	-	42,48,48	0.59	1 (2%)	47,73,73	1.92	4 (8%)
46	3PE	6	202	-	50,50,50	0.30	0	53,55,55	0.30	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
50	MYR	s	201	21	-	2/11/12/13	-
52	FMN	1	502	-	-	5/18/18/18	0/3/3/3
46	3PE	V	202	-	-	11/40/40/54	-
45	PC1	M	502	-	-	17/57/57/57	-
45	PC1	H	503	-	-	10/57/57/57	-
45	PC1	A	203	-	-	13/49/49/57	-
57	NDP	d	401	-	-	3/30/77/77	0/5/5/5
45	PC1	L	1003	-	-	6/57/57/57	-
46	3PE	N	403	-	-	6/34/34/54	-
48	ZMP	X	101	10	-	8/35/37/43	-
49	AMP	k	501	-	-	2/6/26/26	0/3/3/3
47	DCQ	H	501	-	-	3/14/38/38	0/1/1/1
46	3PE	N	402	-	-	8/54/54/54	-
46	3PE	H	502	-	-	13/54/54/54	-
51	SF4	9	201	35	-	-	0/6/5/5
46	3PE	K	101	-	-	11/43/43/54	-
51	SF4	1	501	29	-	-	0/6/5/5
51	SF4	3	802	31	-	-	0/6/5/5
51	SF4	9	202	35	-	-	0/6/5/5
46	3PE	M	501	-	-	11/47/47/54	-
45	PC1	A	201	-	-	9/40/40/57	-
46	3PE	N	401	-	-	10/43/43/54	-
45	PC1	L	1002	-	-	13/57/57/57	-
46	3PE	H	504	-	-	7/54/54/54	-
46	3PE	V	203	-	-	1/27/27/54	-
51	SF4	3	801	31	-	-	0/6/5/5
46	3PE	L	1001	-	-	10/54/54/54	-
54	FES	2	300	30	-	-	0/1/1/1
54	FES	3	803	31	-	-	0/1/1/1
46	3PE	A	202	-	-	14/54/54/54	-
48	ZMP	j	101	10	-	1/38/40/43	-
53	NAI	1	503	-	-	9/25/72/72	0/5/5/5
46	3PE	L	1004	-	-	7/34/34/54	-
46	3PE	V	201	-	-	6/38/38/54	-
51	SF4	6	201	34	-	-	0/6/5/5
46	3PE	6	202	-	-	11/54/54/54	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	502	FMN	C4A-N5	3.54	1.37	1.30
49	k	501	AMP	C5-C4	2.51	1.47	1.40
48	X	101	ZMP	C9-C10	2.34	1.53	1.50
52	1	502	FMN	C10-N1	2.13	1.37	1.33
48	j	101	ZMP	C9-C10	2.07	1.53	1.50
53	1	503	NAI	PA-O5B	2.05	1.67	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	1	503	NAI	O5B-PA-O1A	-9.82	70.69	109.07
53	1	503	NAI	O2A-PA-O1A	-7.64	74.48	112.24
52	1	502	FMN	C4-N3-C2	-3.34	119.46	125.64
49	k	501	AMP	N3-C2-N1	-3.15	123.76	128.68
48	j	101	ZMP	O1-C10-C9	-3.03	120.41	123.99
52	1	502	FMN	C4A-C10-N10	2.89	120.71	116.48
52	1	502	FMN	C4A-C4-N3	2.71	120.08	113.19
48	X	101	ZMP	O1-C10-C9	-2.64	120.88	123.99
52	1	502	FMN	O4-C4-C4A	-2.60	119.70	126.60
49	k	501	AMP	C4-C5-N7	-2.48	106.81	109.40
52	1	502	FMN	C4A-C10-N1	-2.37	119.23	124.73
53	1	503	NAI	C5A-C6A-N6A	2.34	123.91	120.35
45	L	1002	PC1	C2-O21-C21	2.30	123.44	117.79
57	d	401	NDP	C5A-C6A-N6A	2.29	123.84	120.35
53	1	503	NAI	O2A-PA-O5B	2.24	118.15	107.75
52	1	502	FMN	C10-C4A-N5	-2.20	120.19	124.86
46	V	203	3PE	O12-P-O14	2.17	119.17	110.68
46	L	1004	3PE	C2-O21-C21	2.11	122.98	117.79
45	L	1002	PC1	O21-C2-C1	2.06	115.85	108.40
48	j	101	ZMP	C9-C10-S1	2.05	115.85	113.46
52	1	502	FMN	C4-C4A-C10	2.01	120.16	116.79

There are no chirality outliers.

All (227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	203	PC1	C11-O13-P-O12
45	A	203	PC1	C1-O11-P-O14
45	H	503	PC1	C1-O11-P-O13
45	L	1002	PC1	C1-O11-P-O12
45	L	1002	PC1	C1-O11-P-O14
45	M	502	PC1	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	502	PC1	C11-O13-P-O14
45	M	502	PC1	C11-O13-P-O11
45	M	502	PC1	C1-O11-P-O12
46	A	202	3PE	C1-O11-P-O12
46	A	202	3PE	C1-O11-P-O14
46	A	202	3PE	C11-O13-P-O12
46	H	502	3PE	C11-O13-P-O12
46	H	504	3PE	O13-C11-C12-N
46	K	101	3PE	C11-O13-P-O14
46	L	1001	3PE	C11-O13-P-O11
46	L	1001	3PE	C11-O13-P-O14
46	L	1004	3PE	C11-O13-P-O12
46	M	501	3PE	C11-O13-P-O14
46	N	401	3PE	C1-O11-P-O12
46	N	401	3PE	C1-O11-P-O13
46	N	401	3PE	C1-O11-P-O14
46	N	401	3PE	C11-O13-P-O11
46	N	401	3PE	C11-O13-P-O12
46	N	401	3PE	C11-O13-P-O14
46	N	402	3PE	C11-O13-P-O11
46	N	402	3PE	C11-O13-P-O14
46	N	403	3PE	C11-O13-P-O11
46	N	403	3PE	C11-O13-P-O12
46	N	403	3PE	C11-O13-P-O14
46	N	403	3PE	O13-C11-C12-N
46	V	201	3PE	C1-O11-P-O12
46	V	201	3PE	C1-O11-P-O14
46	V	202	3PE	C1-O11-P-O14
46	V	202	3PE	C11-O13-P-O11
46	V	202	3PE	C11-O13-P-O12
46	V	202	3PE	C11-O13-P-O14
46	V	202	3PE	O13-C11-C12-N
46	6	202	3PE	C1-O11-P-O12
46	6	202	3PE	C1-O11-P-O14
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O12
46	6	202	3PE	C11-O13-P-O14
48	X	101	ZMP	C16-C17-C18-C21
48	X	101	ZMP	C17-C16-N2-C15
48	j	101	ZMP	S1-C11-C12-N1
50	s	201	MYR	C1-C2-C3-C4
52	1	502	FMN	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	1	502	FMN	N10-C1'-C2'-C3'
52	1	502	FMN	C5'-O5'-P-O2P
52	1	502	FMN	C5'-O5'-P-O3P
53	1	503	NAI	C5D-O5D-PN-O3
53	1	503	NAI	C2D-C1D-N1N-C6N
57	d	401	NDP	C2B-O2B-P2B-O3X
48	X	101	ZMP	O3-C16-N2-C15
53	1	503	NAI	C2D-C1D-N1N-C2N
45	A	201	PC1	C11-O13-P-O11
45	A	203	PC1	C1-O11-P-O13
45	L	1002	PC1	C1-O11-P-O13
46	A	202	3PE	C1-O11-P-O13
46	H	502	3PE	C11-O13-P-O11
46	K	101	3PE	C1-O11-P-O13
46	L	1004	3PE	C11-O13-P-O11
46	V	201	3PE	C1-O11-P-O13
46	6	202	3PE	C1-O11-P-O13
45	M	502	PC1	C11-C12-N-C14
46	6	202	3PE	C36-C37-C38-C39
46	6	202	3PE	C3C-C3D-C3E-C3F
46	V	202	3PE	C2-C1-O11-P
45	A	203	PC1	C3B-C3C-C3D-C3E
46	N	402	3PE	C21-C22-C23-C24
45	A	203	PC1	C11-C12-N-C14
46	A	202	3PE	C2C-C2D-C2E-C2F
45	A	201	PC1	C11-C12-N-C13
46	V	203	3PE	C22-C23-C24-C25
46	A	202	3PE	C2E-C2F-C2G-C2H
45	A	203	PC1	C11-C12-N-C15
45	M	502	PC1	C11-C12-N-C15
45	M	502	PC1	C3A-C3B-C3C-C3D
47	H	501	DCQ	C11-C12-C13-C14
46	H	502	3PE	C1-O11-P-O13
46	V	202	3PE	C1-O11-P-O13
45	A	203	PC1	C11-C12-N-C13
45	M	502	PC1	C11-C12-N-C13
48	X	101	ZMP	O3-C16-C17-O4
52	1	502	FMN	C5'-O5'-P-O1P
45	A	201	PC1	C11-C12-N-C14
45	L	1002	PC1	C23-C24-C25-C26
46	N	401	3PE	C31-C32-C33-C34
45	A	201	PC1	C11-C12-N-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	L	1002	PC1	O11-C1-C2-C3
45	M	502	PC1	O11-C1-C2-C3
46	A	202	3PE	O13-C11-C12-N
46	M	501	3PE	C38-C39-C3A-C3B
45	L	1002	PC1	C2-C1-O11-P
46	K	101	3PE	C11-O13-P-O11
45	M	502	PC1	C25-C26-C27-C28
47	H	501	DCQ	C11-C10-C9-C8
46	6	202	3PE	C33-C34-C35-C36
45	H	503	PC1	C2B-C2C-C2D-C2E
46	L	1001	3PE	C2-C1-O11-P
46	L	1004	3PE	C2-C1-O11-P
46	M	501	3PE	C2-C1-O11-P
45	L	1002	PC1	C3B-C3C-C3D-C3E
53	1	503	NAI	PN-O3-PA-O5B
46	M	501	3PE	O11-C1-C2-C3
45	A	201	PC1	O21-C21-C22-C23
45	L	1003	PC1	C39-C3A-C3B-C3C
46	K	101	3PE	C2-C1-O11-P
53	1	503	NAI	PA-O3-PN-O2N
46	V	202	3PE	C32-C33-C34-C35
46	A	202	3PE	C11-O13-P-O11
46	M	501	3PE	C11-O13-P-O11
46	V	201	3PE	C11-O13-P-O11
53	1	503	NAI	O4D-C1D-N1N-C6N
57	d	401	NDP	O4D-C1D-N1N-C6N
45	M	502	PC1	C2-C1-O11-P
46	H	502	3PE	C2-C1-O11-P
45	A	201	PC1	C11-O13-P-O14
45	A	203	PC1	C1-O11-P-O12
45	H	503	PC1	C1-O11-P-O12
46	A	202	3PE	C11-O13-P-O14
46	K	101	3PE	C1-O11-P-O14
46	L	1004	3PE	C11-O13-P-O14
46	V	202	3PE	C1-O11-P-O12
53	1	503	NAI	C5B-O5B-PA-O2A
46	N	401	3PE	O13-C11-C12-N
47	H	501	DCQ	C5-C4-O4-C4M
46	A	202	3PE	C12-C11-O13-P
46	H	502	3PE	C12-C11-O13-P
45	A	203	PC1	C22-C23-C24-C25
45	A	201	PC1	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	502	PC1	O11-C1-C2-O21
46	M	501	3PE	O11-C1-C2-O21
45	A	203	PC1	C23-C24-C25-C26
45	H	503	PC1	O13-C11-C12-N
45	L	1002	PC1	O13-C11-C12-N
46	M	501	3PE	C39-C3A-C3B-C3C
45	L	1002	PC1	C2A-C2B-C2C-C2D
46	H	502	3PE	C29-C2A-C2B-C2C
45	M	502	PC1	O31-C31-C32-C33
49	k	501	AMP	C5'-O5'-P-O1P
45	M	502	PC1	C39-C3A-C3B-C3C
45	L	1002	PC1	C3E-C3F-C3G-C3H
45	H	503	PC1	C11-O13-P-O11
45	L	1003	PC1	C11-O13-P-O11
46	H	504	3PE	C11-O13-P-O11
49	k	501	AMP	C4'-C5'-O5'-P
46	V	201	3PE	C33-C34-C35-C36
46	K	101	3PE	C34-C35-C36-C37
46	K	101	3PE	C21-C22-C23-C24
46	L	1001	3PE	C36-C37-C38-C39
46	6	202	3PE	C23-C24-C25-C26
46	H	502	3PE	C2F-C2G-C2H-C2I
45	H	503	PC1	C3A-C3B-C3C-C3D
48	X	101	ZMP	N2-C16-C17-C18
45	H	503	PC1	C3-C2-O21-C21
46	L	1001	3PE	C35-C36-C37-C38
45	A	201	PC1	C22-C23-C24-C25
53	1	503	NAI	O4D-C1D-N1N-C2N
46	A	202	3PE	C2-C1-O11-P
46	N	402	3PE	O11-C1-C2-O21
45	A	203	PC1	C3F-C3G-C3H-C3I
45	M	502	PC1	C36-C37-C38-C39
46	L	1001	3PE	C34-C35-C36-C37
46	M	501	3PE	C35-C36-C37-C38
45	L	1003	PC1	C37-C38-C39-C3A
45	H	503	PC1	C2C-C2D-C2E-C2F
46	H	502	3PE	C26-C27-C28-C29
46	6	202	3PE	C32-C33-C34-C35
48	X	101	ZMP	N2-C16-C17-O4
46	N	402	3PE	O31-C31-C32-C33
45	L	1003	PC1	C3E-C3F-C3G-C3H
45	L	1002	PC1	C1-C2-O21-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	L	1004	3PE	C1-C2-O21-C21
46	L	1001	3PE	O31-C31-C32-C33
46	L	1004	3PE	O21-C21-C22-C23
50	s	201	MYR	C11-C10-C9-C8
46	H	502	3PE	O11-C1-C2-O21
46	N	401	3PE	O21-C21-C22-C23
45	H	503	PC1	C22-C23-C24-C25
46	N	403	3PE	C31-C32-C33-C34
48	X	101	ZMP	C16-C17-C18-C20
46	H	502	3PE	O11-C1-C2-C3
45	H	503	PC1	C35-C36-C37-C38
46	H	502	3PE	C28-C29-C2A-C2B
46	A	202	3PE	O21-C2-C3-O31
46	M	501	3PE	O31-C31-C32-C33
46	V	202	3PE	O31-C31-C32-C33
46	A	202	3PE	O21-C21-C22-C23
45	A	201	PC1	O22-C21-C22-C23
46	L	1001	3PE	O32-C31-C32-C33
46	L	1004	3PE	O22-C21-C22-C23
46	N	402	3PE	O32-C31-C32-C33
46	L	1001	3PE	C3B-C3C-C3D-C3E
46	N	401	3PE	O22-C21-C22-C23
46	H	504	3PE	C36-C37-C38-C39
45	M	502	PC1	C1-O11-P-O13
46	M	501	3PE	O32-C31-C32-C33
45	A	203	PC1	C11-O13-P-O14
45	L	1002	PC1	C11-O13-P-O14
45	M	502	PC1	C1-O11-P-O14
46	H	502	3PE	C1-O11-P-O14
46	H	504	3PE	C1-O11-P-O12
46	H	504	3PE	C1-O11-P-O14
46	V	201	3PE	C11-O13-P-O12
53	1	503	NAI	C2N-C3N-C7N-N7N
57	d	401	NDP	O4B-C4B-C5B-O5B
46	K	101	3PE	O13-C11-C12-N
46	A	202	3PE	O22-C21-C22-C23
46	L	1001	3PE	C26-C27-C28-C29
45	L	1003	PC1	C12-C11-O13-P
46	H	504	3PE	C12-C11-O13-P
46	K	101	3PE	C12-C11-O13-P
46	N	402	3PE	C12-C11-O13-P
46	N	402	3PE	C3-C2-O21-C21

Continued on next page...

Continued from previous page...

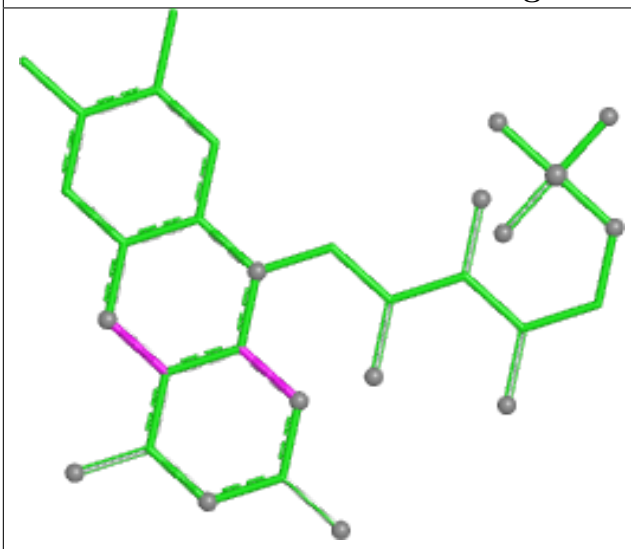
Mol	Chain	Res	Type	Atoms
48	X	101	ZMP	O3-C16-C17-C18
46	H	502	3PE	C32-C33-C34-C35
46	H	504	3PE	O21-C21-C22-C23
46	K	101	3PE	O31-C31-C32-C33
45	L	1002	PC1	C37-C38-C39-C3A
46	K	101	3PE	O32-C31-C32-C33
45	A	203	PC1	C26-C27-C28-C29
46	M	501	3PE	C3C-C3D-C3E-C3F
46	N	403	3PE	O31-C31-C32-C33
46	V	202	3PE	O32-C31-C32-C33
45	L	1003	PC1	C26-C27-C28-C29

There are no ring outliers.

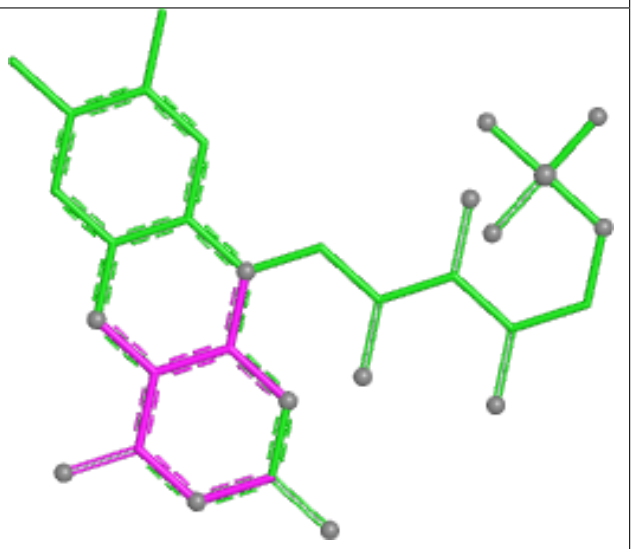
No monomer is involved in short contacts.

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.

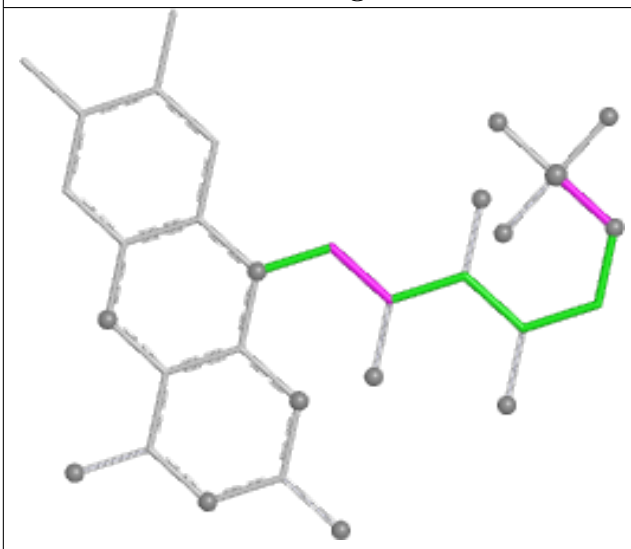
Ligand FMN 1 502



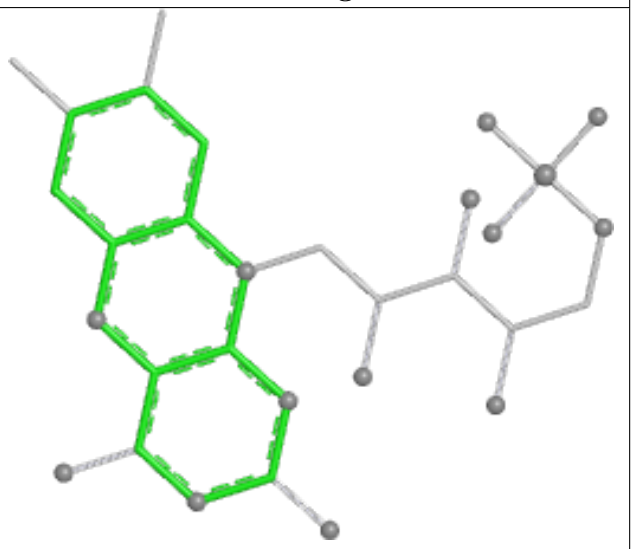
Bond lengths



Bond angles

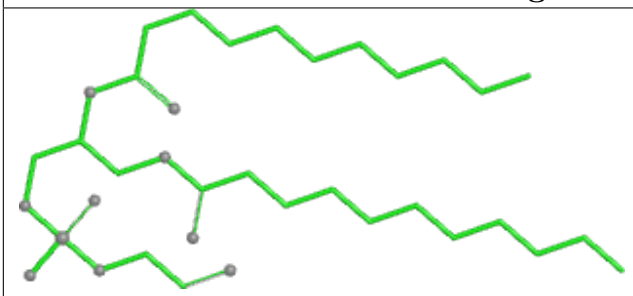


Torsions

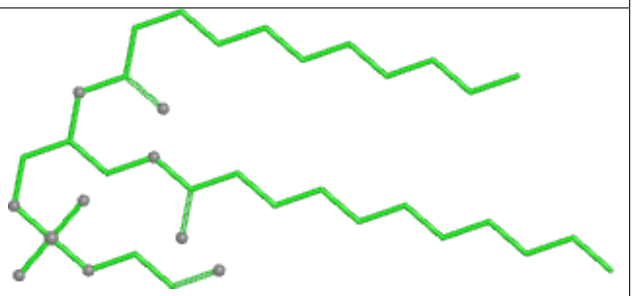


Rings

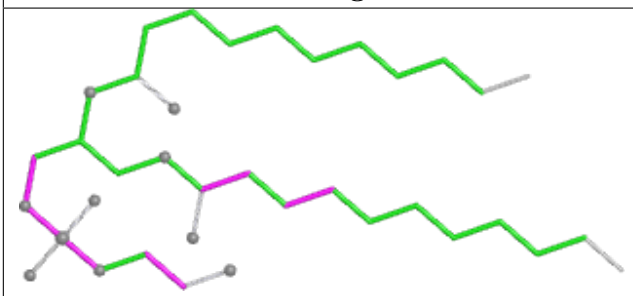
Ligand 3PE V 202



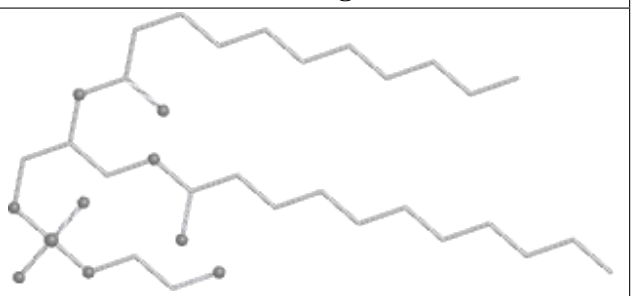
Bond lengths



Bond angles

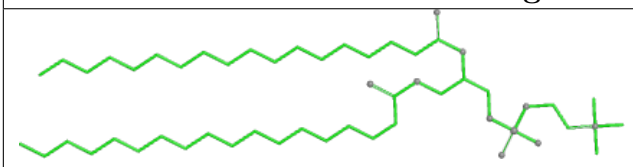


Torsions

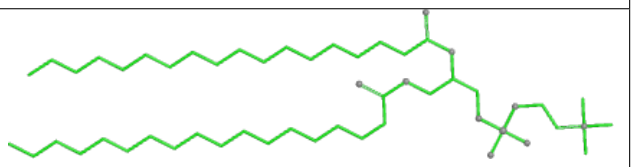


Rings

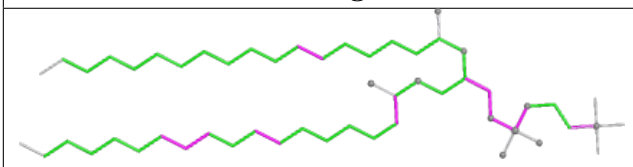
Ligand PC1 M 502



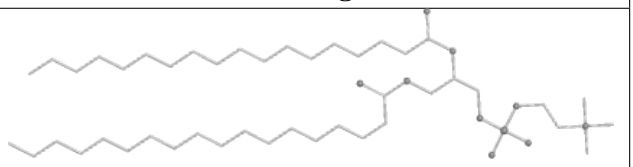
Bond lengths



Bond angles

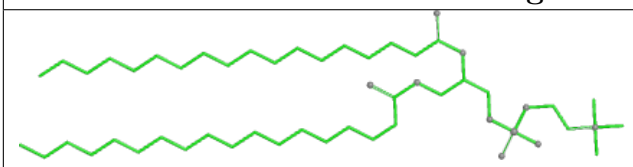


Torsions

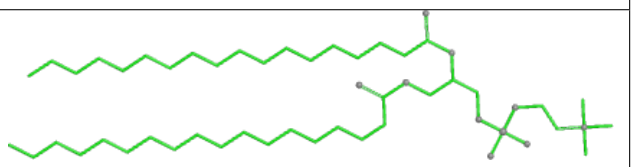


Rings

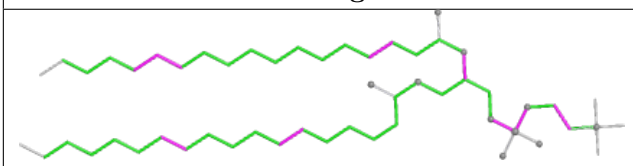
Ligand PC1 H 503



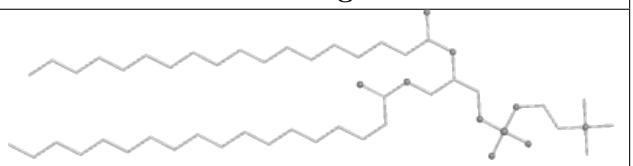
Bond lengths



Bond angles

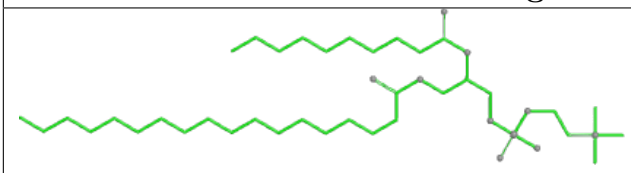


Torsions

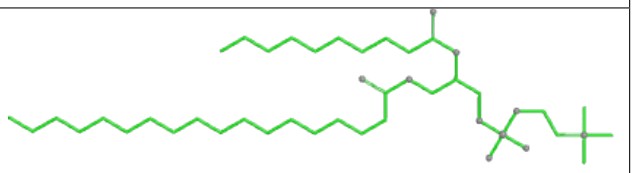


Rings

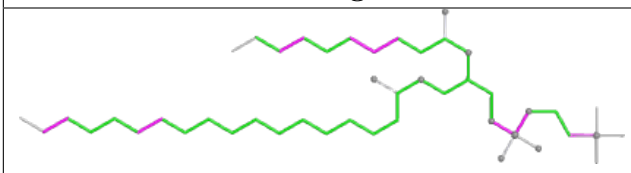
Ligand PC1 A 203



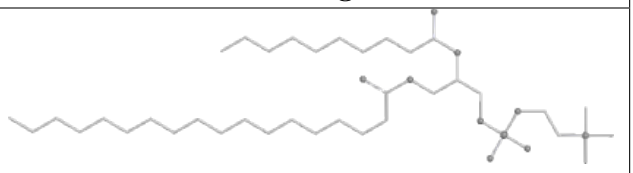
Bond lengths



Bond angles

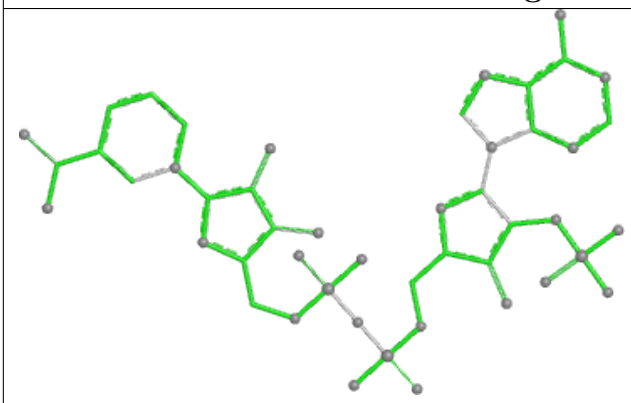


Torsions

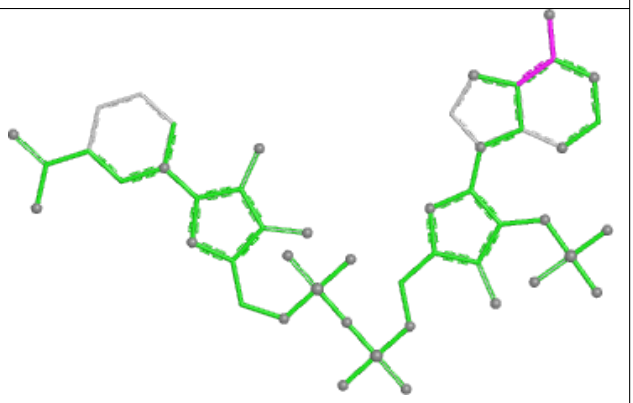


Rings

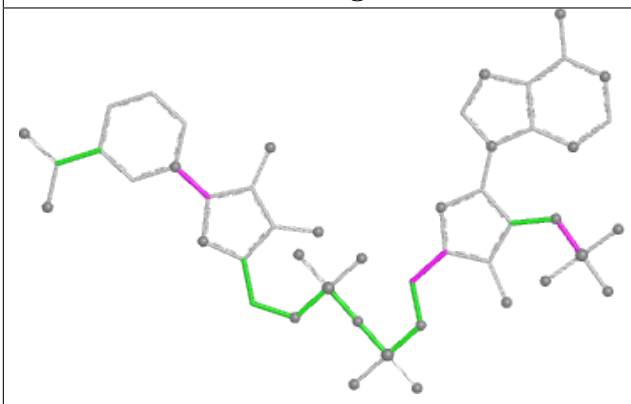
Ligand NDP d 401



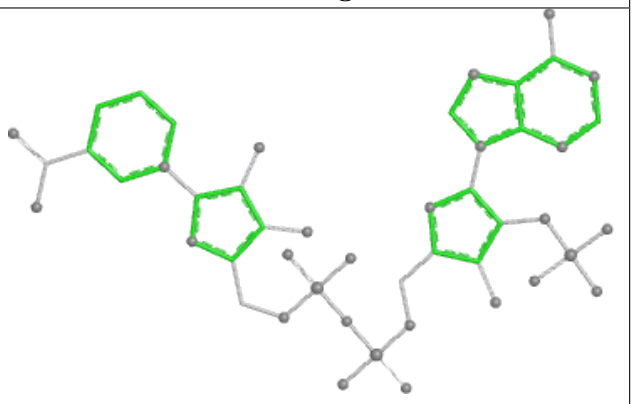
Bond lengths



Bond angles

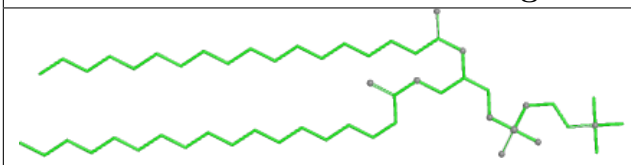


Torsions

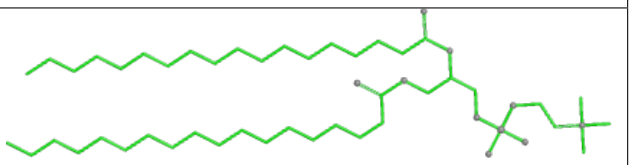


Rings

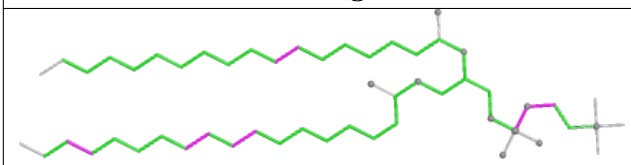
Ligand PC1 L 1003



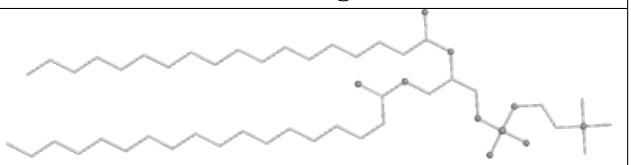
Bond lengths



Bond angles

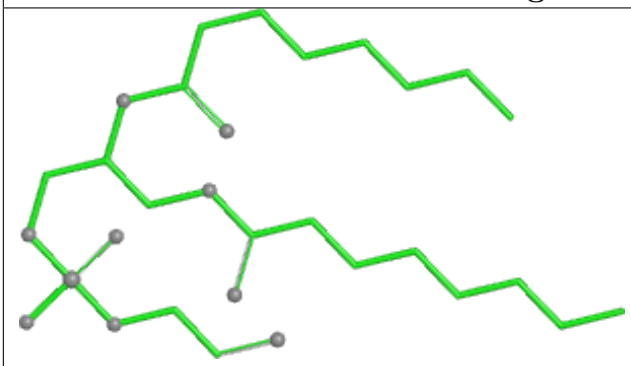


Torsions

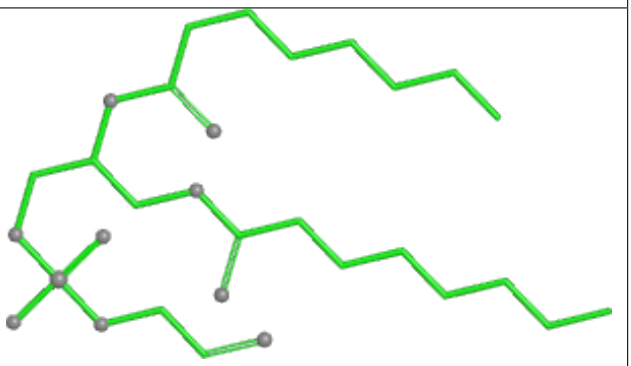


Rings

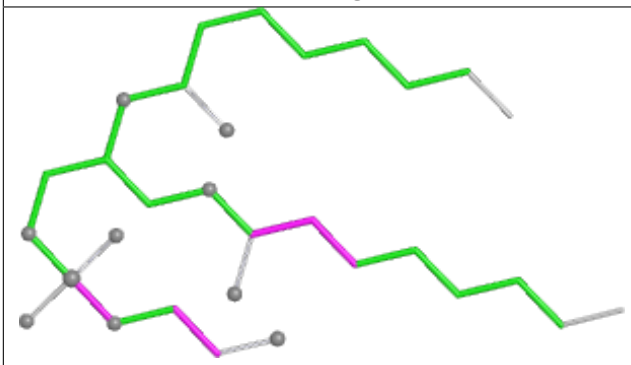
Ligand 3PE N 403



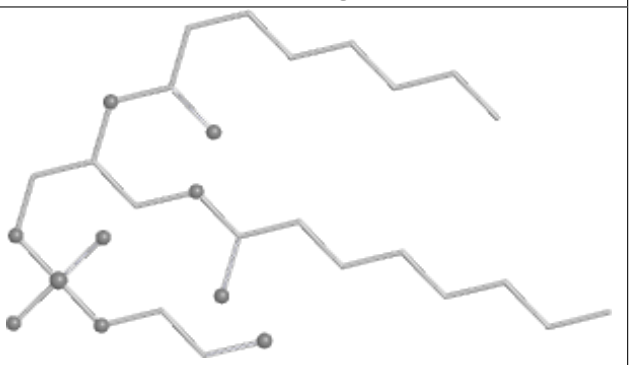
Bond lengths



Bond angles

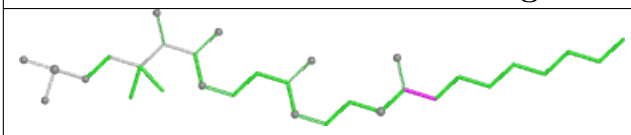


Torsions

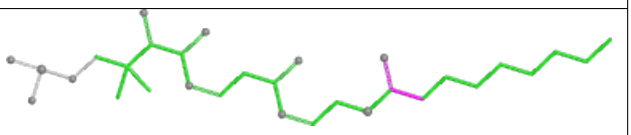


Rings

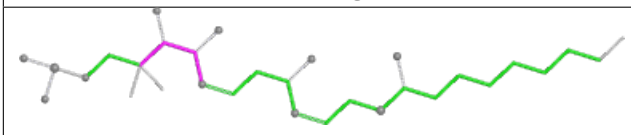
Ligand ZMP X 101



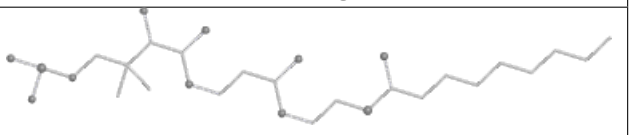
Bond lengths



Bond angles

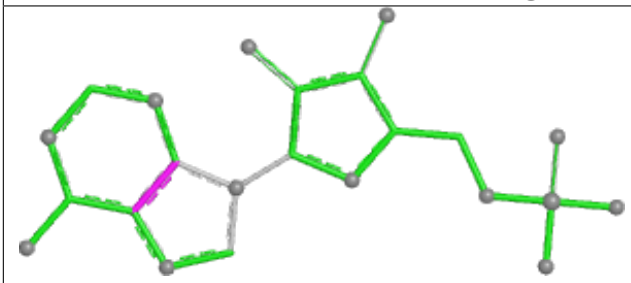


Torsions

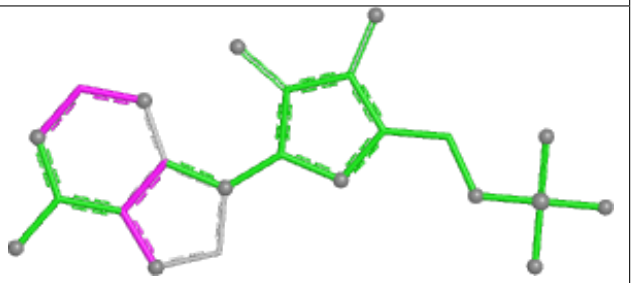


Rings

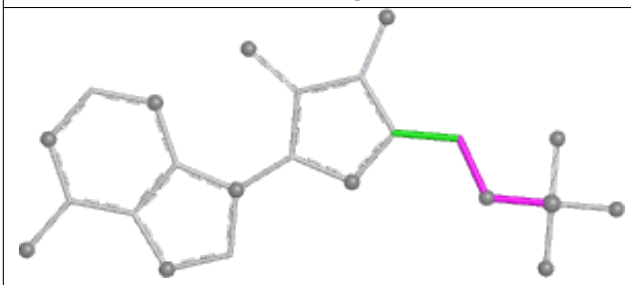
Ligand AMP k 501



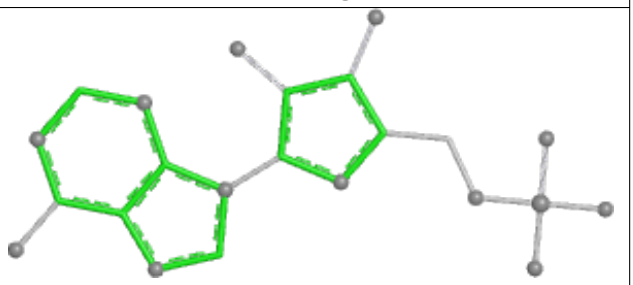
Bond lengths



Bond angles

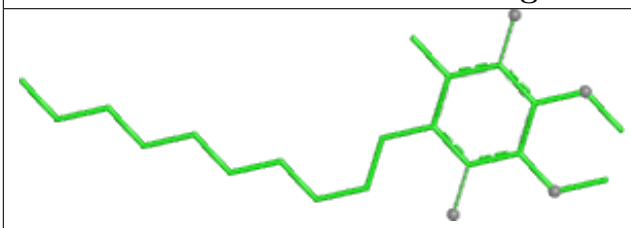


Torsions

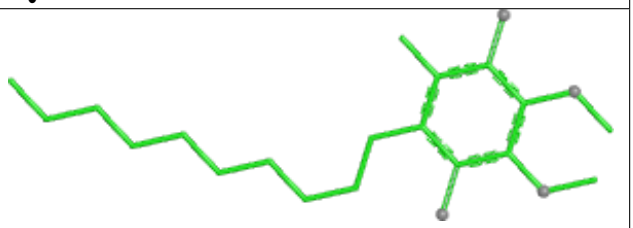


Rings

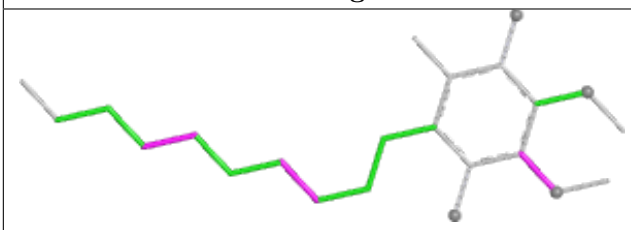
Ligand DCQ H 501



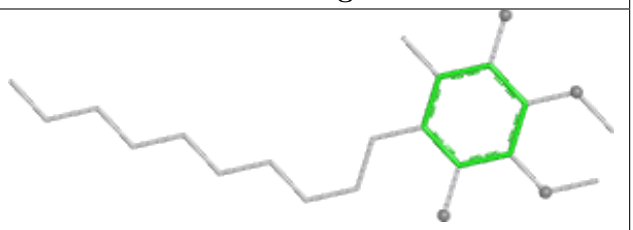
Bond lengths



Bond angles

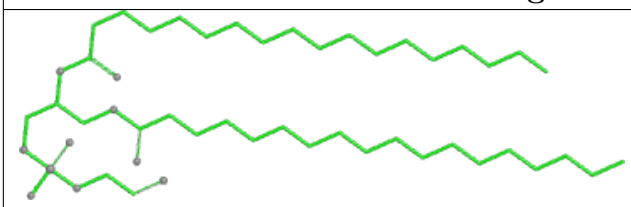


Torsions

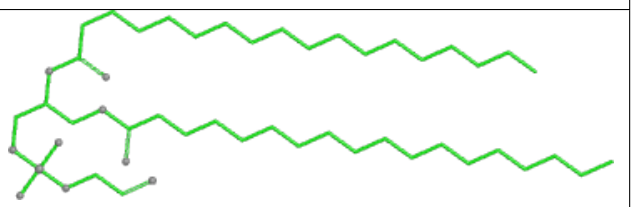


Rings

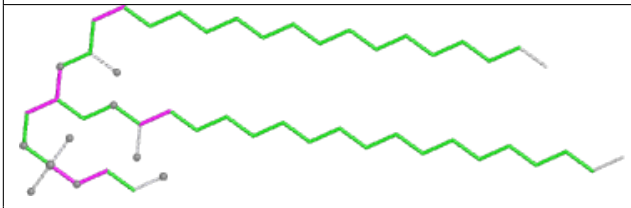
Ligand 3PE N 402



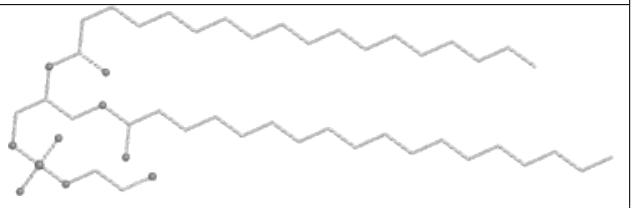
Bond lengths



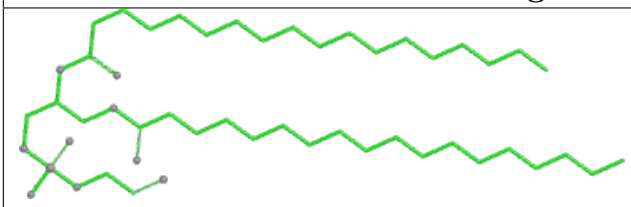
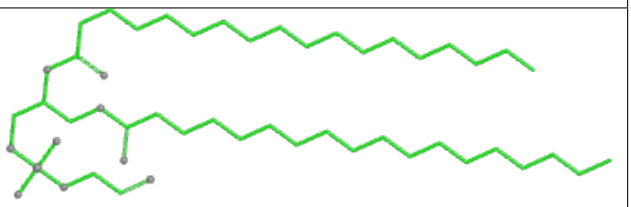
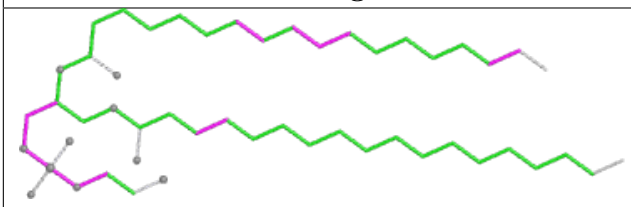
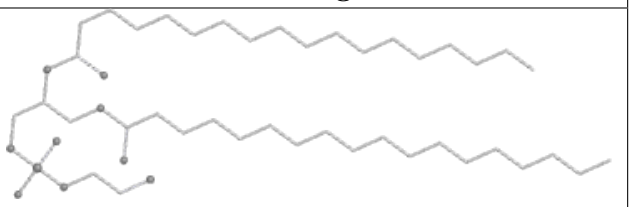
Bond angles

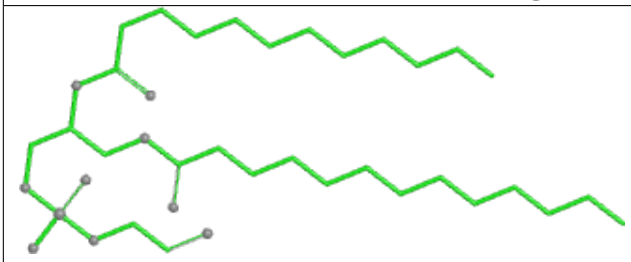
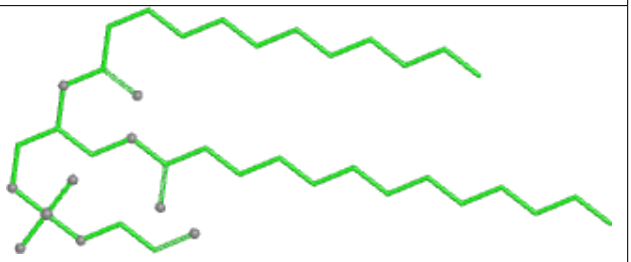
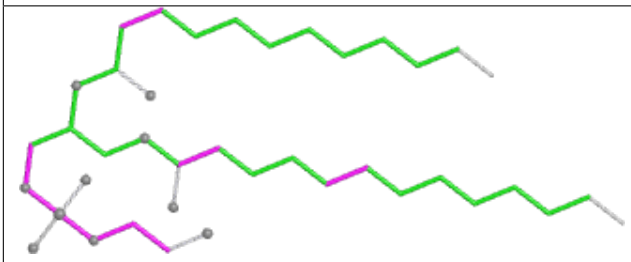
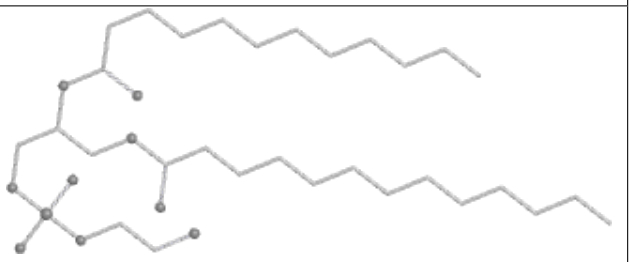


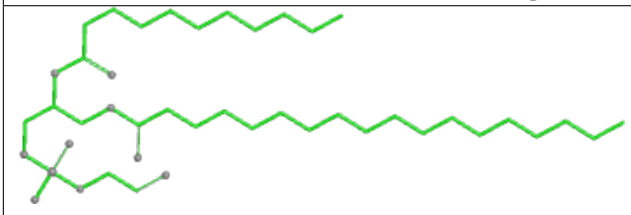
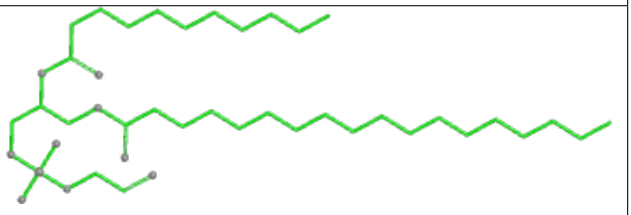
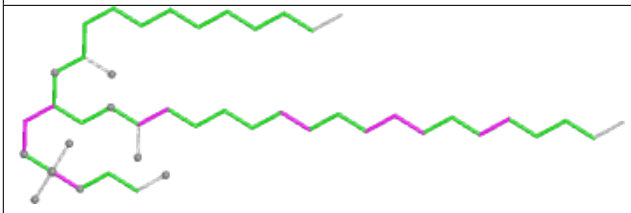
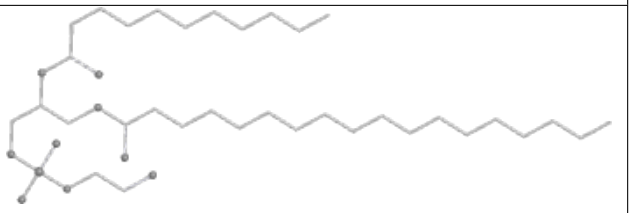
Torsions



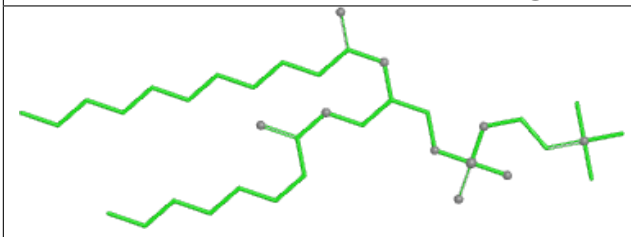
Rings

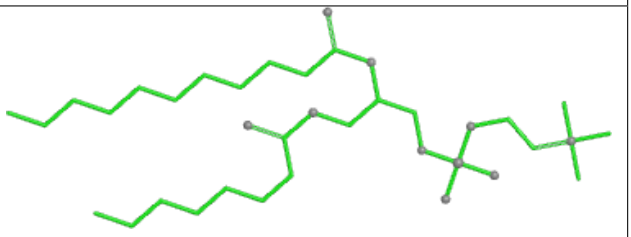
Ligand 3PE H 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

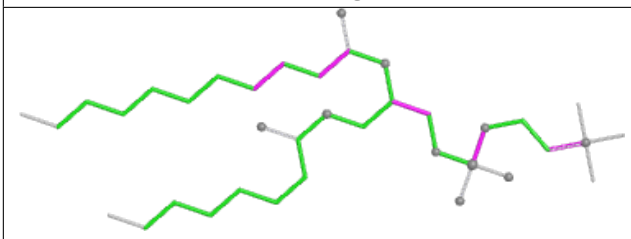
Ligand 3PE K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

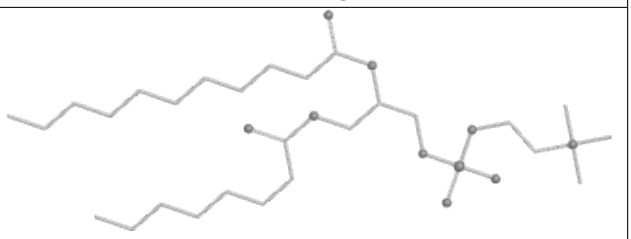
Ligand 3PE M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 A 201

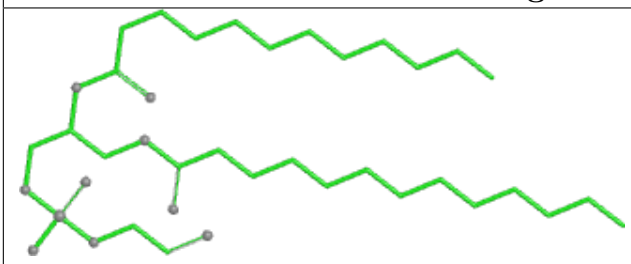

Bond lengths

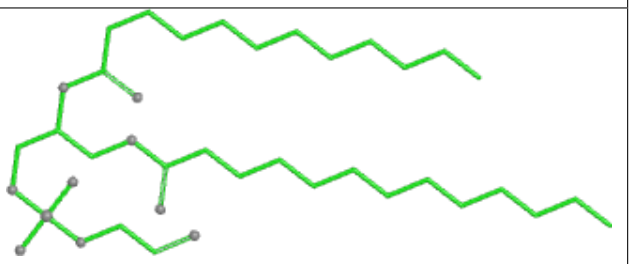

Bond angles

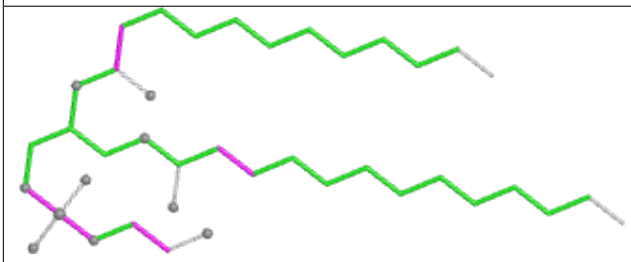

Torsions

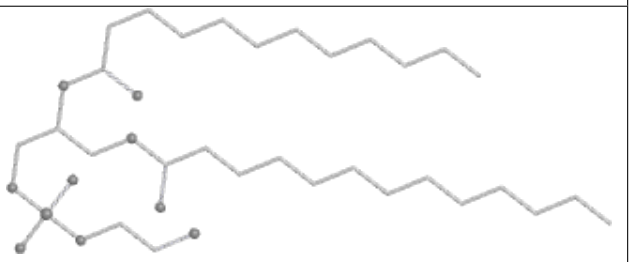

Rings

Ligand 3PE N 401

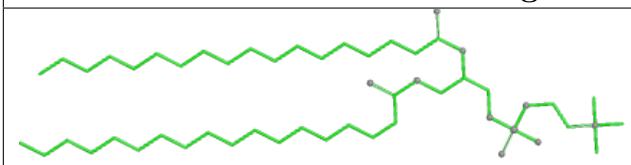

Bond lengths

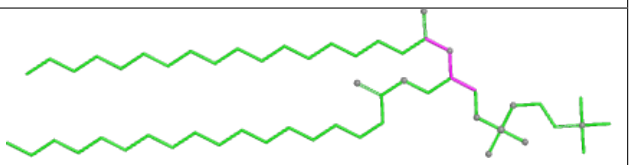

Bond angles

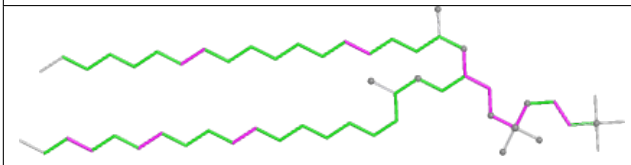

Torsions

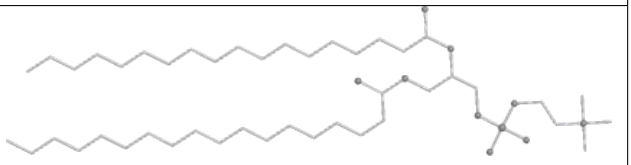

Rings

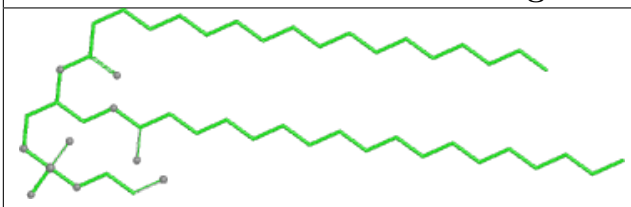
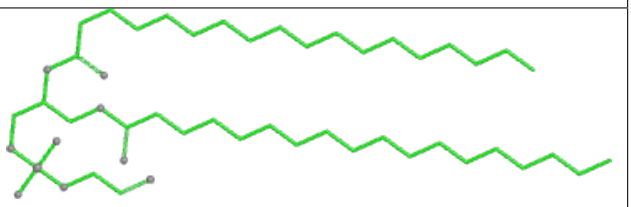
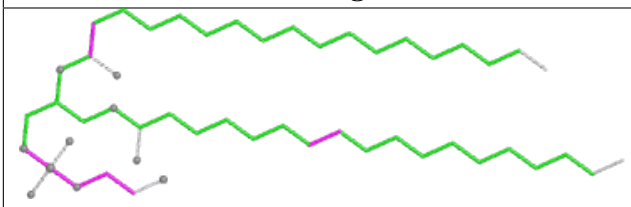
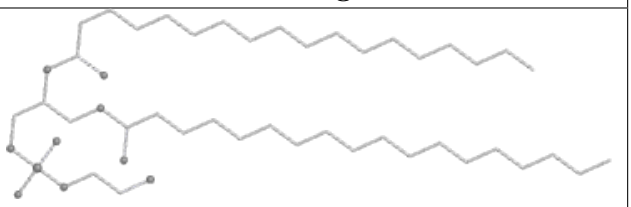
Ligand PC1 L 1002

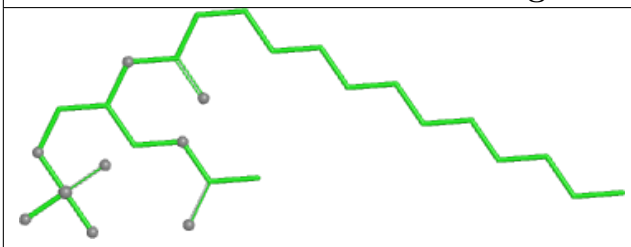
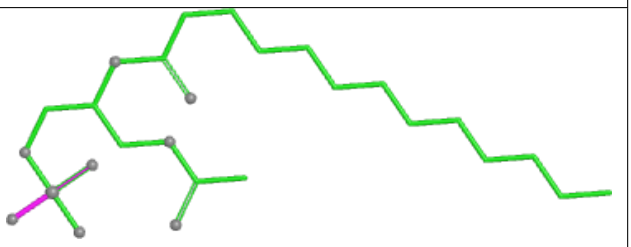
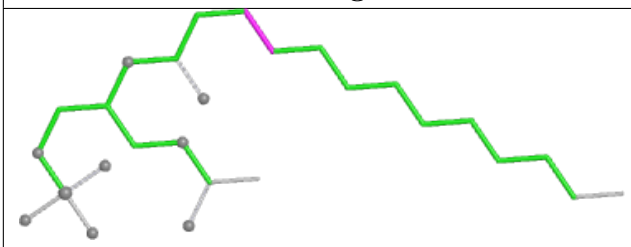
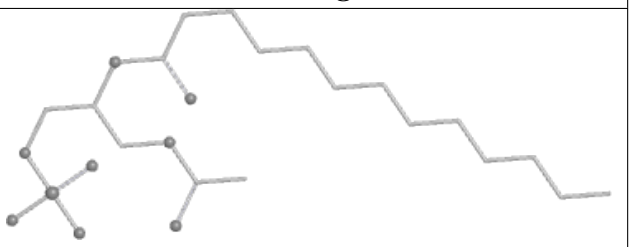

Bond lengths

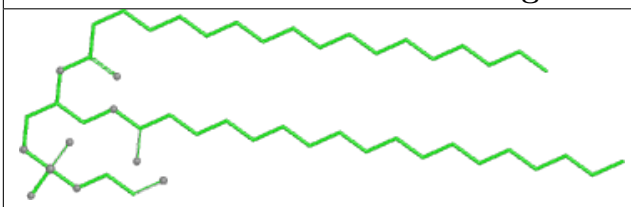
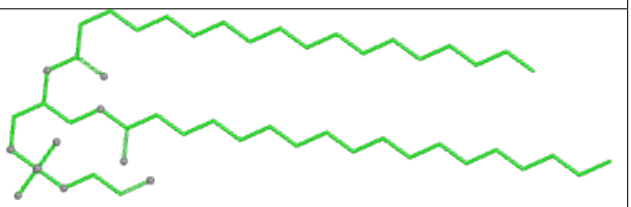
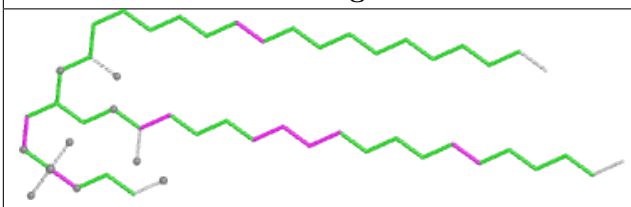
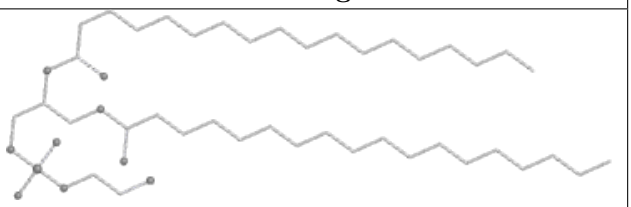

Bond angles


Torsions

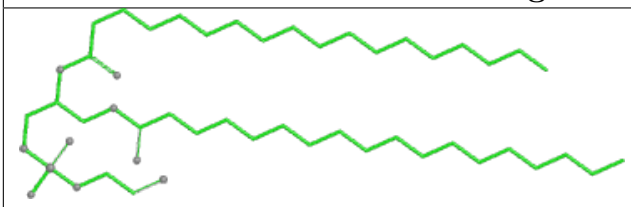

Rings

Ligand 3PE H 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

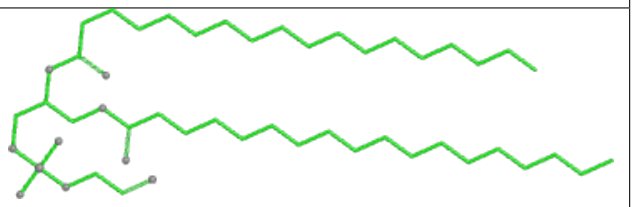
Ligand 3PE V 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

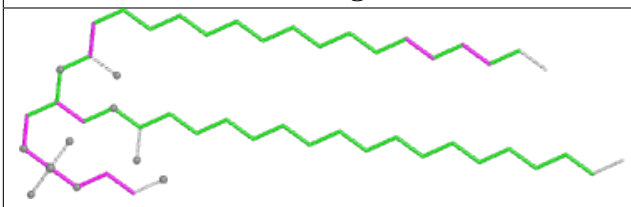
Ligand 3PE A 202



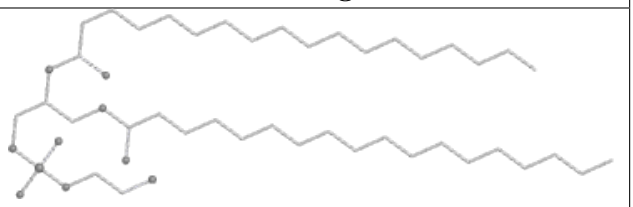
Bond lengths



Bond angles

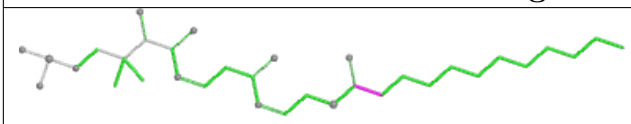


Torsions

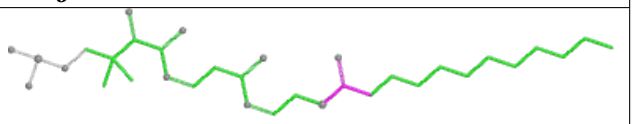


Rings

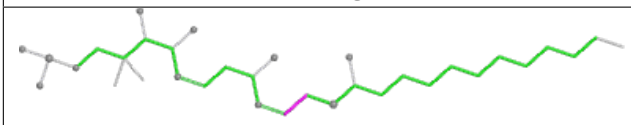
Ligand ZMP j 101



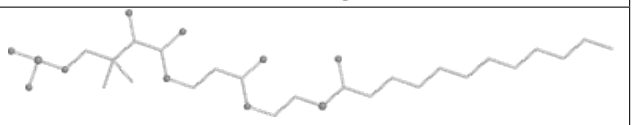
Bond lengths



Bond angles

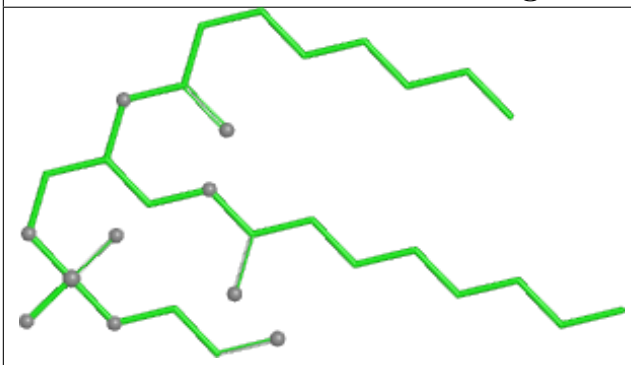


Torsions

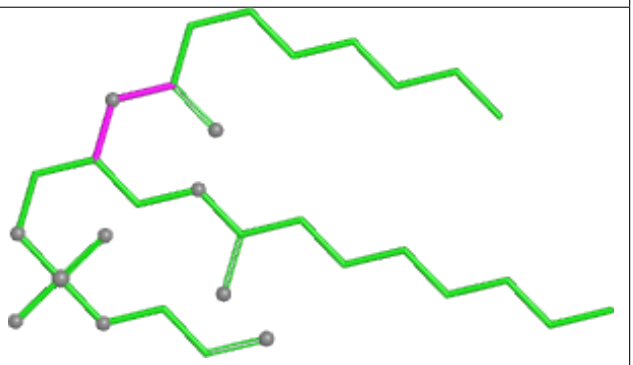


Rings

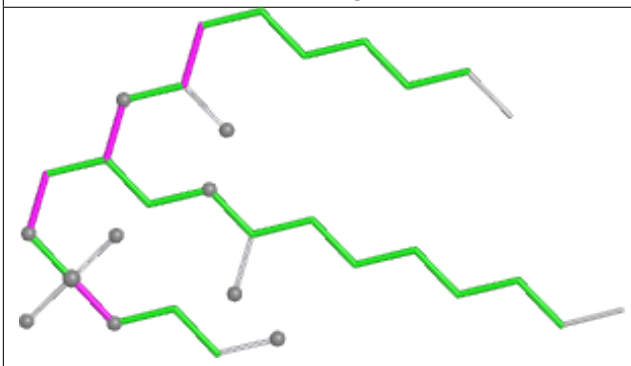
Ligand 3PE L 1004



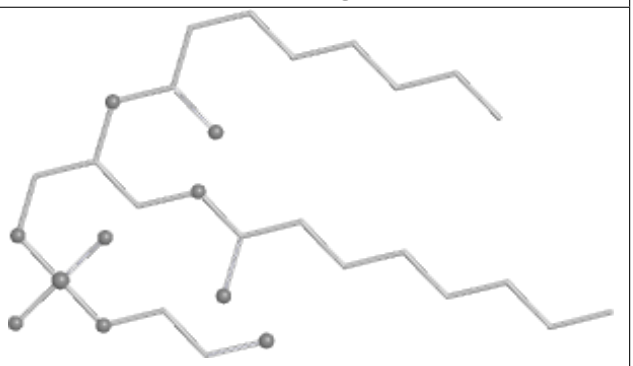
Bond lengths



Bond angles

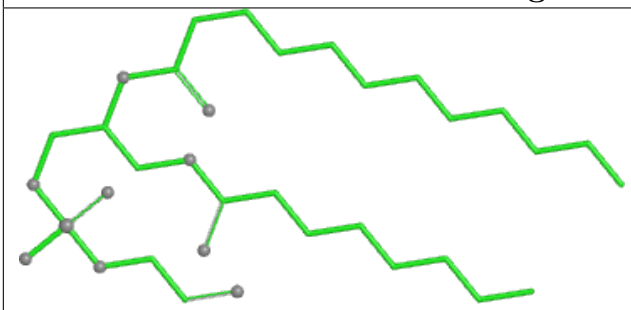


Torsions

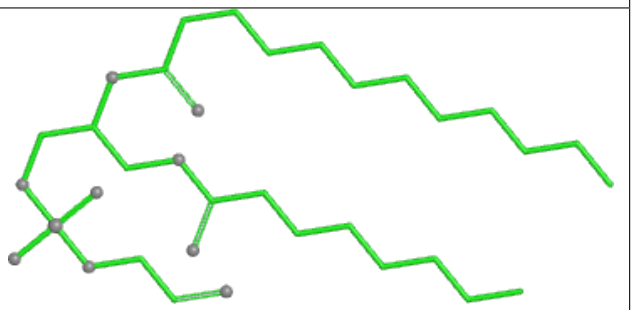


Rings

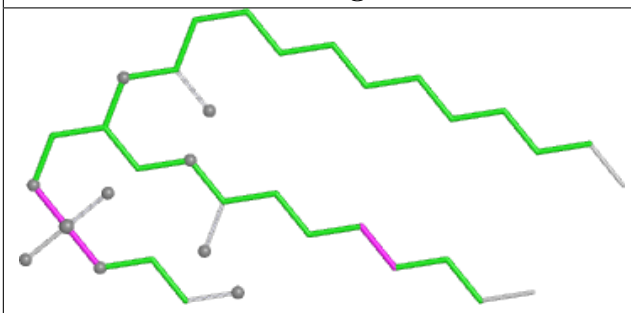
Ligand 3PE V 201



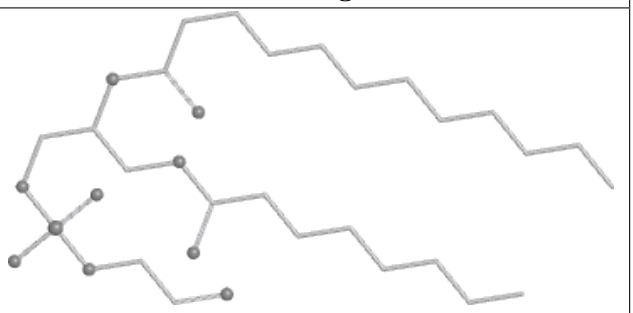
Bond lengths



Bond angles

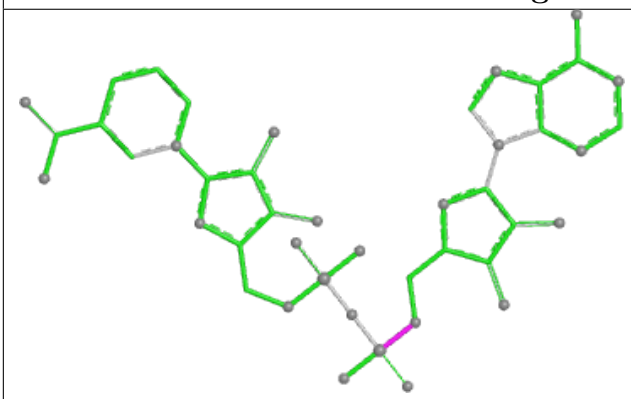


Torsions

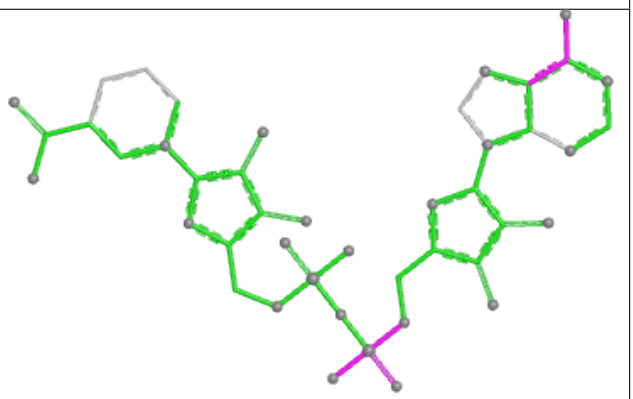


Rings

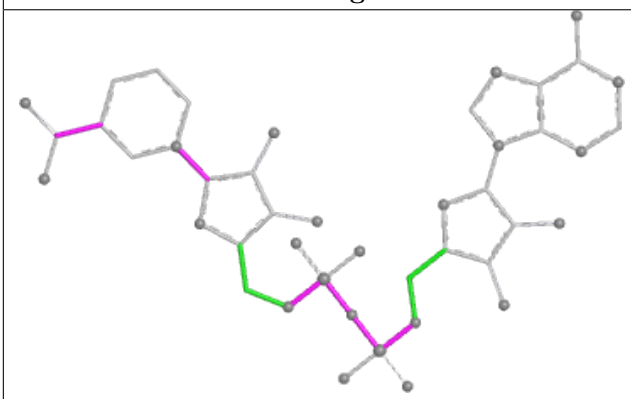
Ligand NAI 1 503



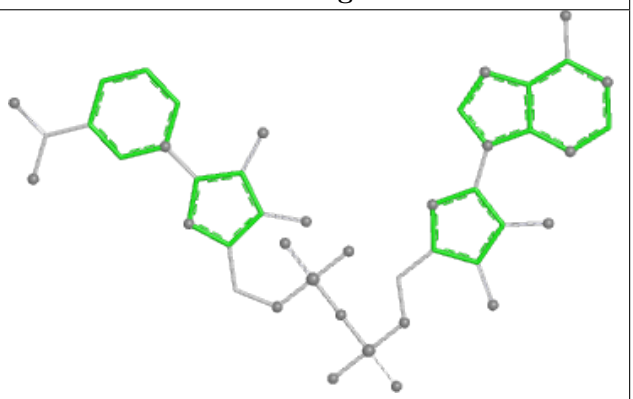
Bond lengths



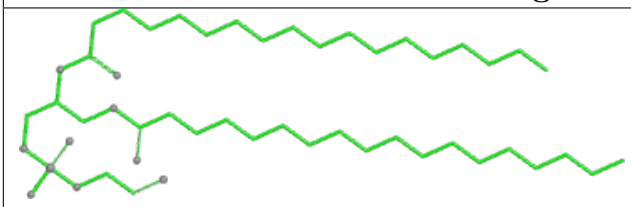
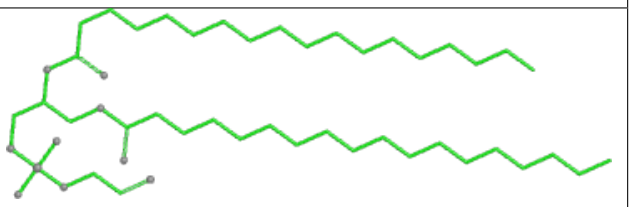
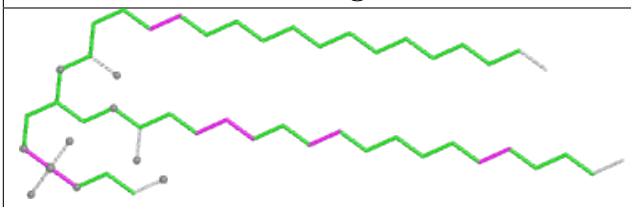
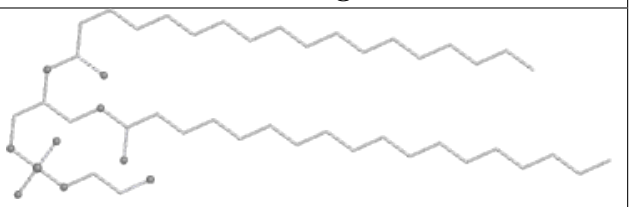
Bond angles



Torsions



Rings

Ligand 3PE 6 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

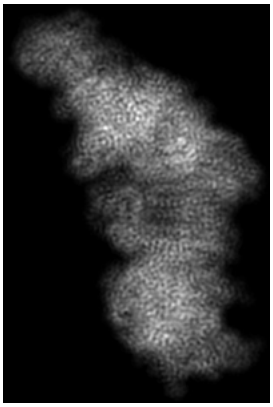
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14637. These allow visual inspection of the internal detail of the map and identification of artifacts.

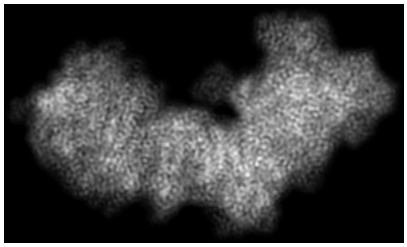
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

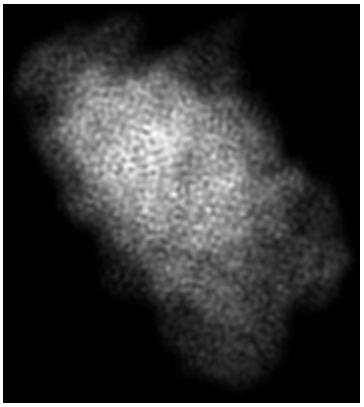
6.1.1 Primary map



X



Y

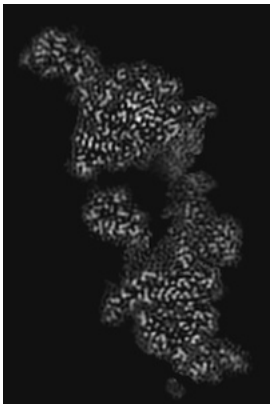


Z

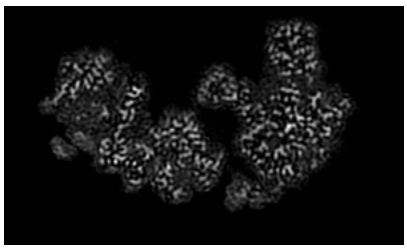
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 71



Y Index: 79

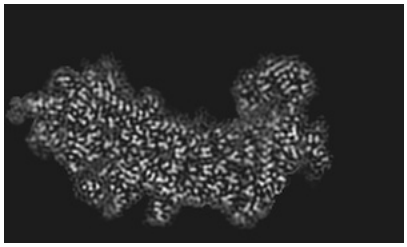
Z Index: 119

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

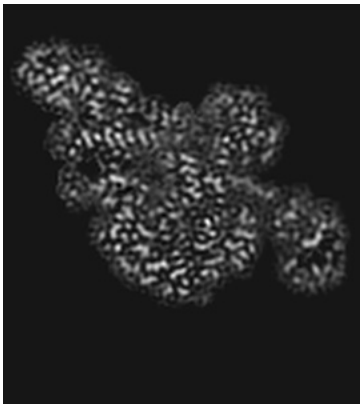
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 58



Y Index: 106



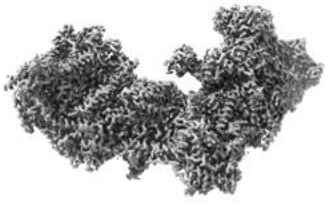
Z Index: 158

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

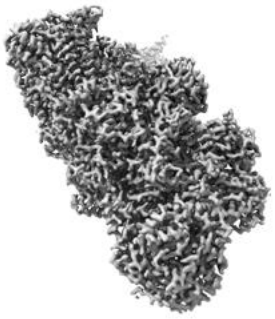
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

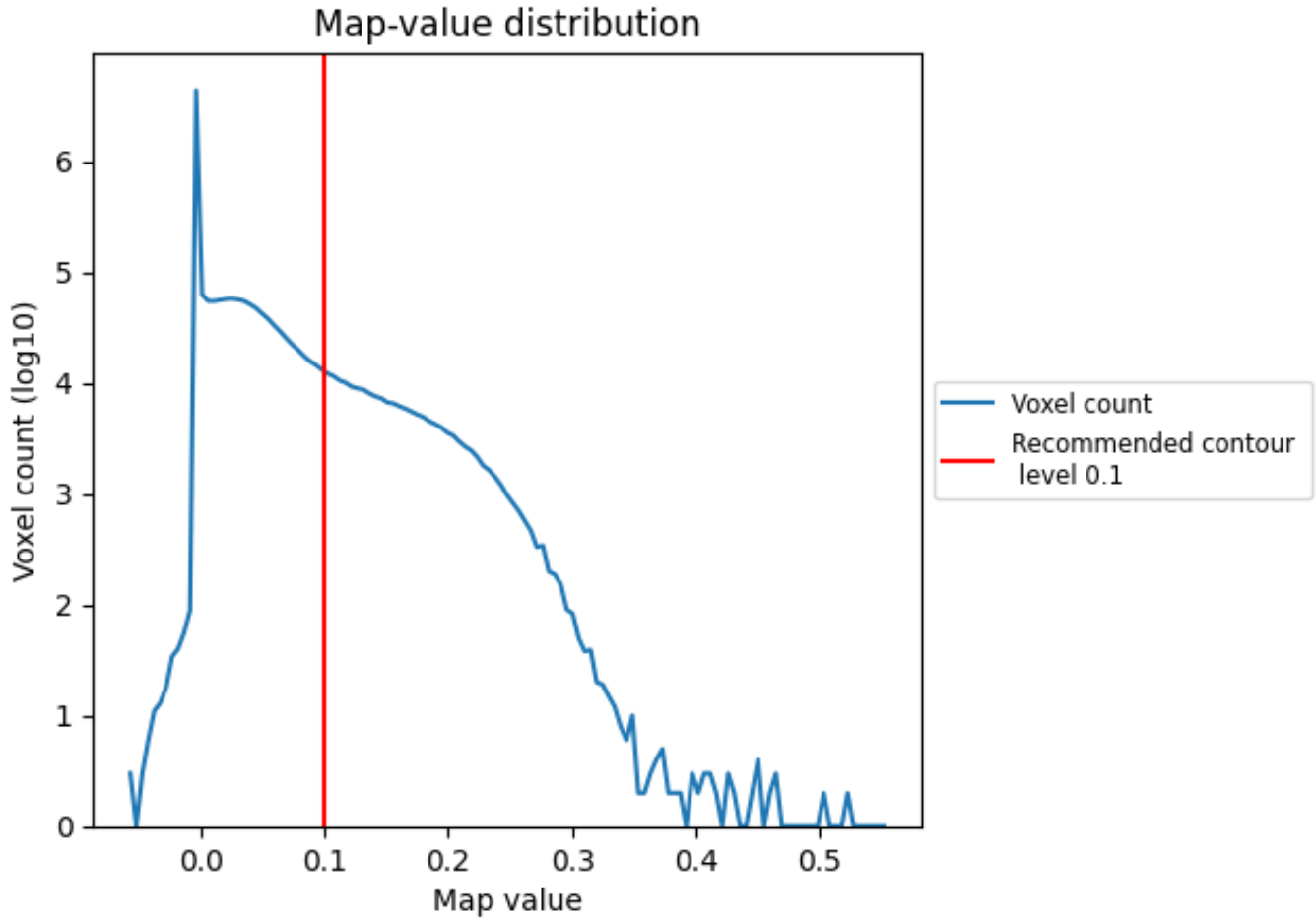
6.5 Mask visualisation (i)

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

7 Map analysis

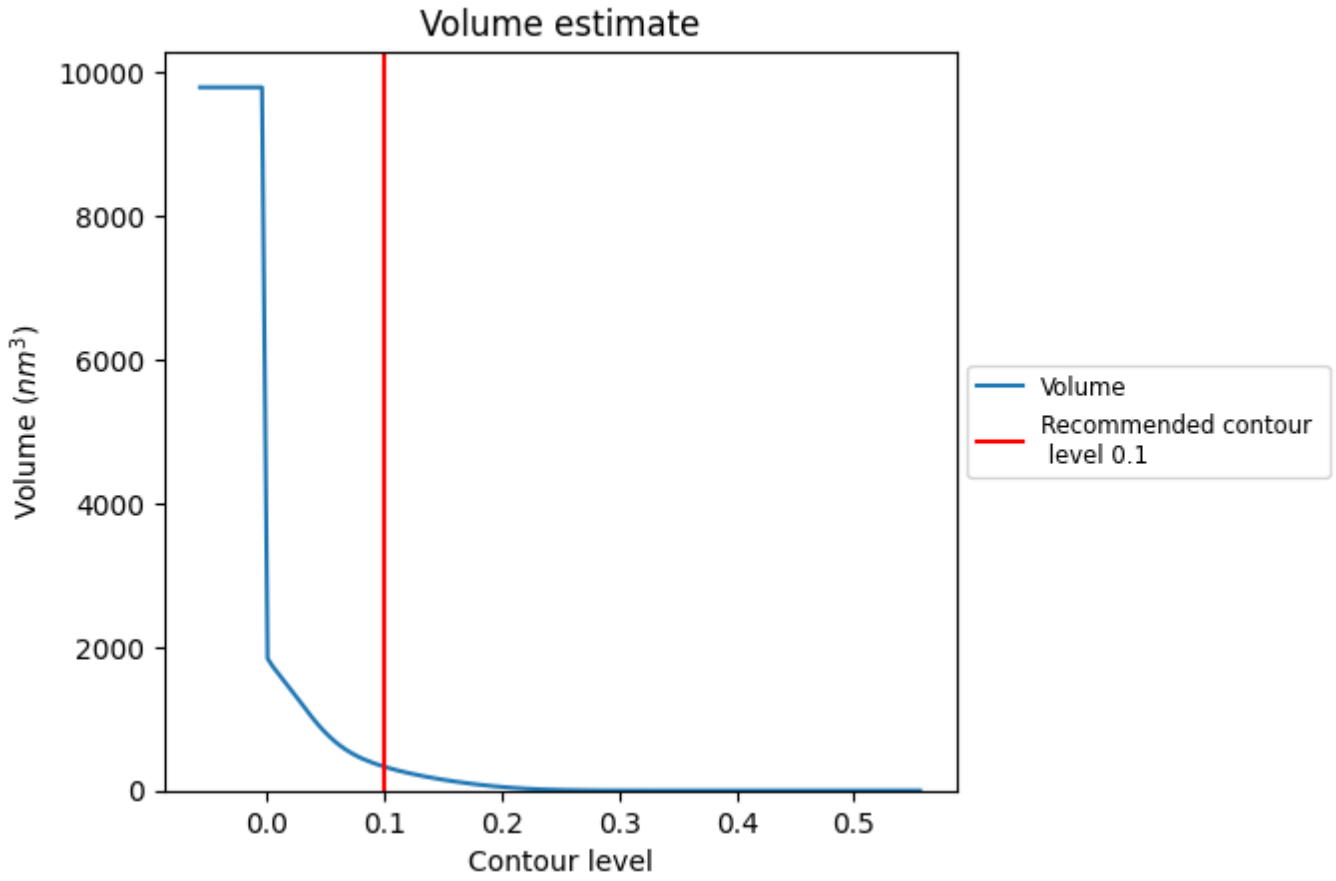
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate



The volume at the recommended contour level is 334 nm^3; this corresponds to an approximate mass of 302 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.

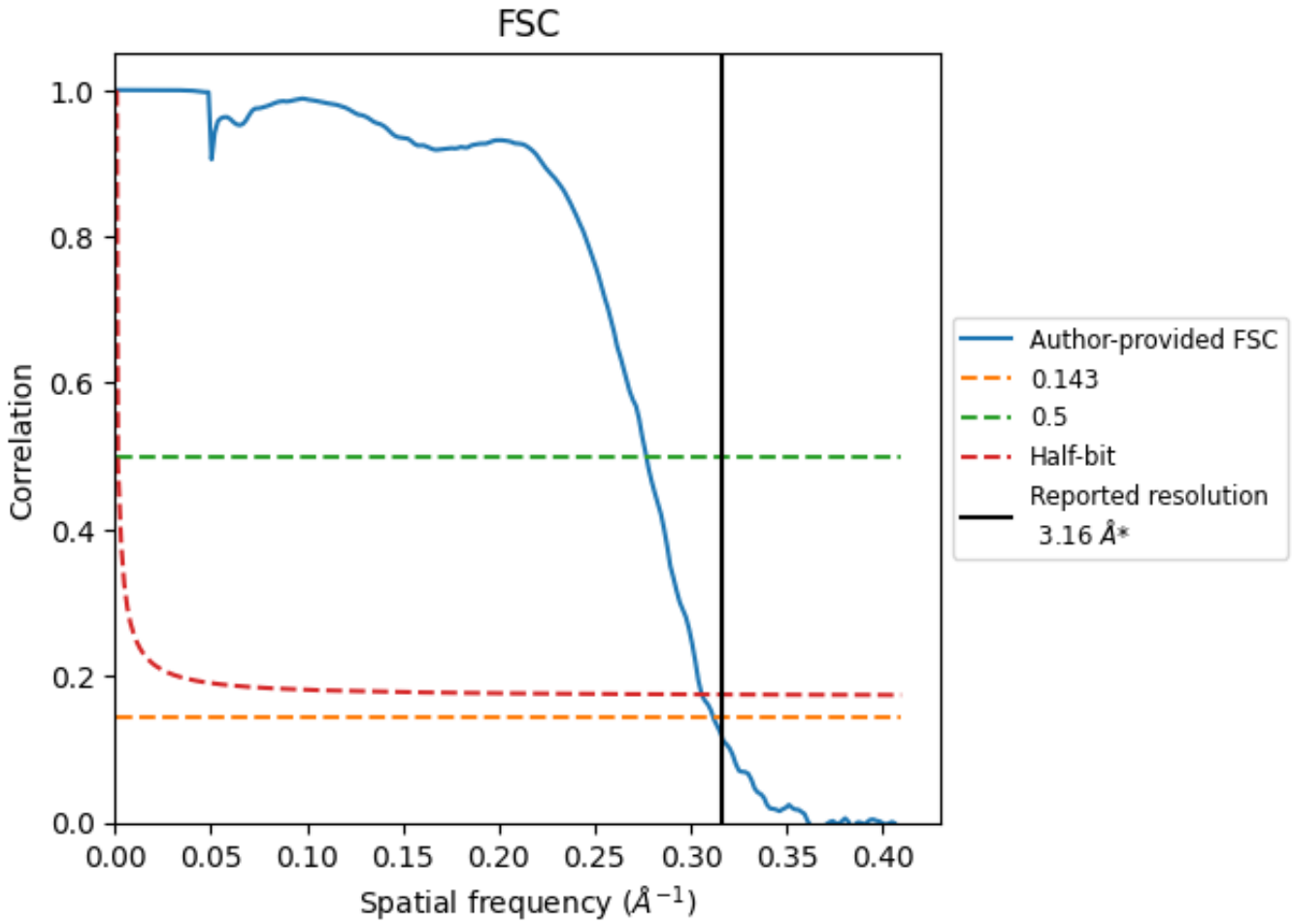
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.316 Å^{-1}

8.2 Resolution estimates (i)

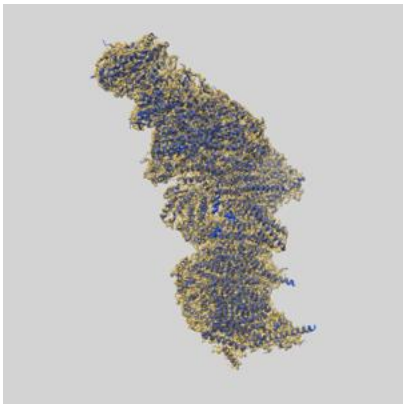
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.21	3.61	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

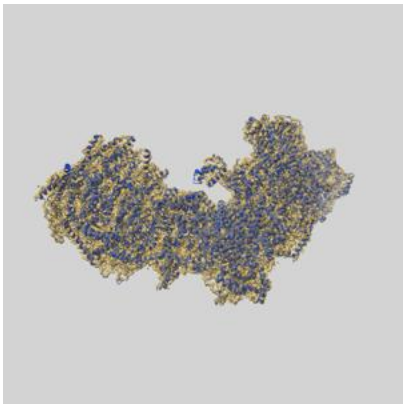
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14637 and PDB model 7ZD6. Per-residue inclusion information can be found in section 3 on page 20.

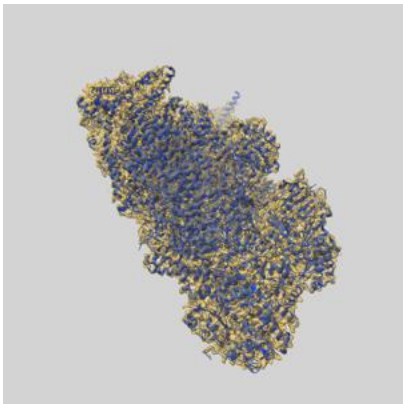
9.1 Map-model overlay



X



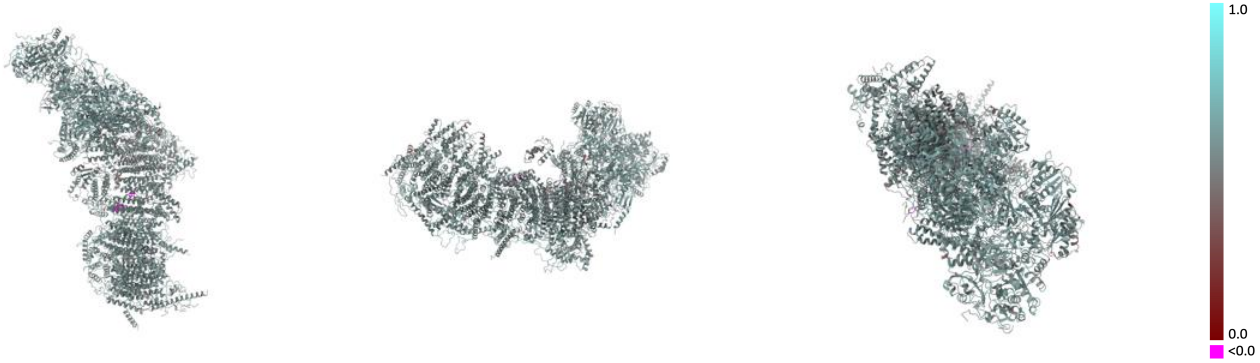
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

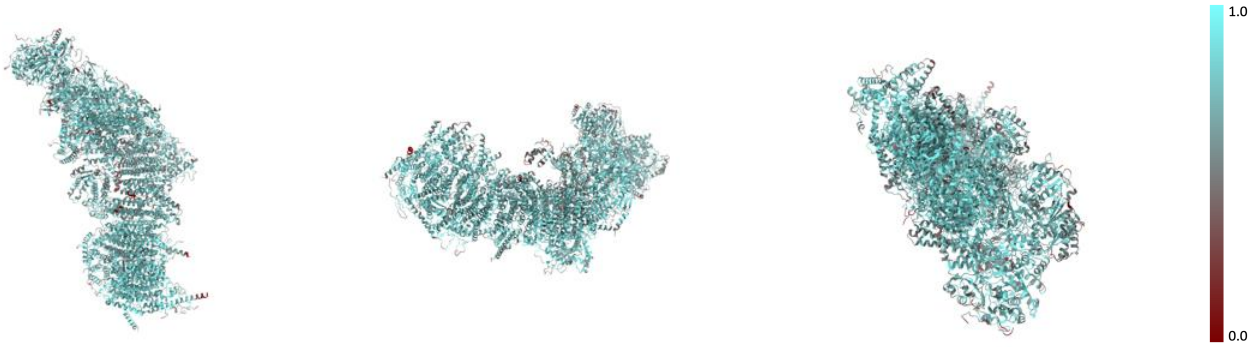
9.2 Q-score mapped to coordinate model (i)



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.

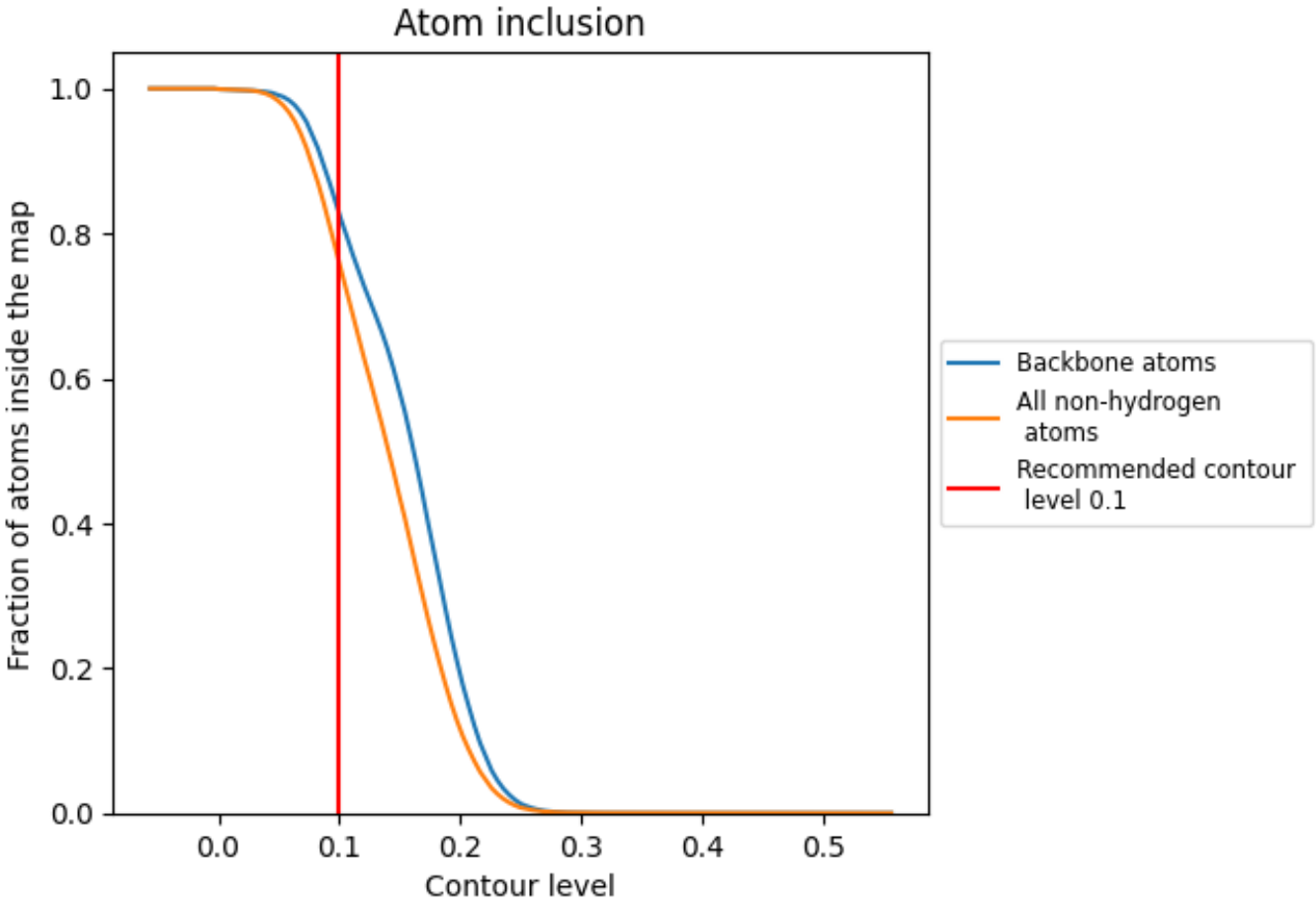
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7582	0.5610
1	0.7278	0.5640
2	0.6836	0.5530
3	0.7361	0.5710
4	0.7766	0.5600
5	0.8297	0.5920
6	0.8426	0.5840
9	0.8317	0.5790
A	0.6211	0.5020
H	0.7794	0.5480
J	0.7185	0.5370
K	0.7816	0.5550
L	0.8083	0.5620
M	0.8438	0.5770
N	0.8225	0.5710
V	0.6546	0.5350
W	0.8179	0.5770
X	0.7052	0.5400
Y	0.7615	0.5590
Z	0.7652	0.5610
a	0.6740	0.5640
b	0.7145	0.5840
c	0.7423	0.5820
d	0.6961	0.5560
e	0.6726	0.5650
f	0.7046	0.5680
g	0.7191	0.5650
h	0.7429	0.5770
i	0.7855	0.5880
j	0.4688	0.4970
k	0.7607	0.5610
l	0.7421	0.5500
m	0.7280	0.5400
n	0.7184	0.5310
o	0.8033	0.5680

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.7581	0.5610
q	0.7314	0.5450
r	0.7259	0.5520
s	0.7204	0.5350
t	0.7560	0.5590
u	0.7901	0.5480
v	0.7970	0.5680
w	0.7367	0.5520
x	0.7072	0.5430
y	0.7139	0.5540
z	0.8137	0.5520