Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 06:14 pm GMT

PDB ID	:	7AR7
EMDB ID	:	EMD-11875
Title	:	Cryo-EM structure of Arabidopsis thaliana complex-I (open conformation)
Authors	:	Klusch, N.; Kuelbrandt, W.
Deposited on	:	2020-10-23
Resolution	:	3.72 Å(reported)

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

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

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

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

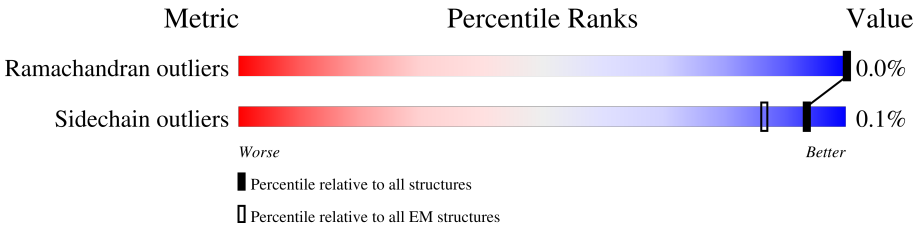
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.72 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	119	16% 77% 23%
2	B	157	100%
3	C	185	100%
4	D	385	100%
5	E	192	21% 100%
6	F	434	14% 100%
7	G	688	6% 100%
8	H	324	13% 100%
9	I	169	100%

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Mol	Chain	Length	Quality of chain
10	J	205	7% 67% 33%
11	K	88	9% 99%
12	L	615	87% 100%
13	M	487	28% 100%
14	N	488	9% 100%
15	P	331	24% 100%
16	Q	119	8% 99%
17	R	62	8% 100%
18	S	93	16% 99%
19	T	84	100% 100%
20	U	83	95% 100%
21	V	140	11% 100%
22	W	133	41% 81% 19%
23	X	96	15% 100%
24	Z	125	14% 99%
25	a	58	14% 100%
26	b	40	8% 100%
27	c	76	78% 99%
28	d	75	7% 99%
29	e	64	6% 100%
30	f	100	100%
31	g	72	53% 100%
32	i	85	16% 100%
33	j	51	98% 100%
34	k	47	100% 100%

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Mol	Chain	Length	Quality of chain
35	l	46	96% 100%
36	m	67	81% 100%
37	n	109	98% 100%
38	o	80	94% 100%
39	p	93	54% 100%
40	q	63	52% 100%
41	r	10	50% 100%
42	u	30	47% 100%
43	v	30	20% 100%
44	x	214	30% 100%
45	y	268	40% 100%
46	z	233	36% 100%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 60606 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	92	785	556	108	117	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	157	1244	797	218	215	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	185	1581	1021	271	283	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	385	3077	1954	542	557	24	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	LEU	SER	conflict	UNP P93306
D	227	SER	PRO	conflict	UNP P93306
D	309	LEU	SER	conflict	UNP P93306
D	363	SER	LEU	conflict	UNP P93306

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5252	3291	921	1001	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	324	Total	C	N	O	S	0	0
			2536	1719	386	416	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	126	ARG	TRP	conflict	UNP P92558

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	169	Total	C	N	O	S	0	0
			1381	869	234	268	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	138	Total	C	N	O	S	0	0
			1093	742	168	175	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	88	Total	C	N	O	S	0	0
			692	466	107	112	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	SER	conflict	UNP Q04614

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	615	Total	C	N	O	S	0	0
			4807	3191	748	832	36		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP P29388
L	288	PHE	SER	conflict	UNP P29388
L	537	LEU	PRO	conflict	UNP P29388

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	487	Total	C	N	O	S	0	0
			3887	2627	601	636	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	conflict	UNP P93313
M	326	LEU	PRO	conflict	UNP P93313
M	383	PHE	SER	conflict	UNP P93313

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	0	0
			3820	2573	577	642	28		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	331	Total	C	N	O	S	0	0
			2556	1641	438	462	15		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	119	Total	C	N	O	S	0	0
			939	600	163	175	1		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	62	Total	C	N	O	S	0	0
			482	304	84	89	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	93	Total	C	N	O	S	0	0
			728	459	129	134	6		

- Molecule 19 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	84	Total	C	N	O	S	0	0
			667	421	105	138	3		

- Molecule 20 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	83	Total	C	N	O	S	0	0
			650	411	103	135	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	108	Total 880	C 563	N 156	O 158	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	96	Total 763	C 478	N 131	O 142	S 12	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	125	Total 997	C 640	N 175	O 177	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	58	Total 470	C 302	N 84	O 79	S 5	0	0

- Molecule 26 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	40	Total 295	C 195	N 48	O 49	S 3	0	0

- Molecule 27 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	76	Total 617	C 396	N 115	O 100	S 6	0	0

- Molecule 28 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- Molecule 30 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	100	Total	C	N	O	S	0	0
			752	484	122	141	5		

- Molecule 31 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	72	Total	C	N	O	S	0	0
			586	379	100	104	3		

- Molecule 32 is a protein called At1g67350.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	85	Total	C	N	O	S	0	0
			737	466	135	131	5		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	47	Total	C	N	O	S	0	0
			374	238	71	62	3		

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

8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	l	46	Total	C	N	O	0	0
			360	241	57	62		

- Molecule 36 is a protein called AT2G31490 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	67	Total	C	N	O	S	0	0
			565	364	104	95	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	93	Total	C	N	O	S	0	0
			778	493	144	137	4		

- Molecule 40 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	63	Total	C	N	O	0	0
			520	332	92	96		

- Molecule 41 is a protein called B14.5a.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	r	10	Total	C	N	O	0	0
			87	58	17	12		

- Molecule 42 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	u	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 43 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	v	30	Total	C	N	O	0	0
			226	147	39	40		

- Molecule 44 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	x	214	Total	C	N	O	S	0	0
			1659	1063	285	306	5		

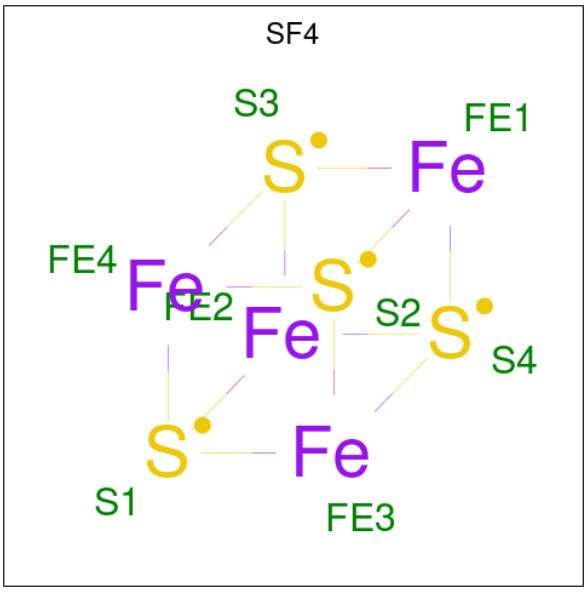
- Molecule 45 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	y	268	Total	C	N	O	S	0	0
			2032	1271	363	391	7		

- Molecule 46 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

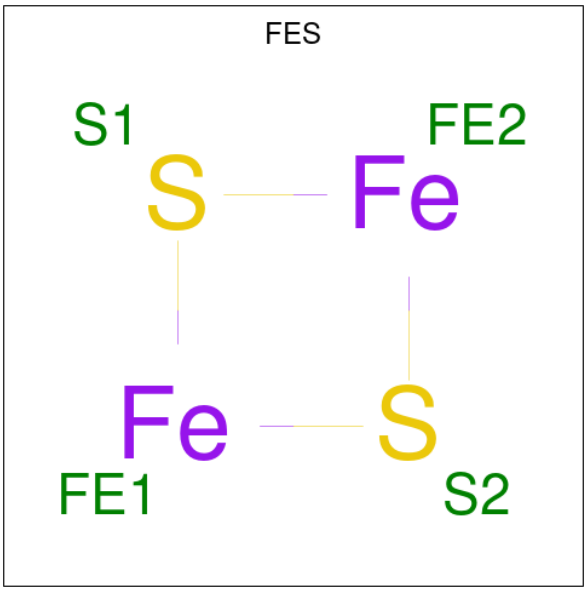
Mol	Chain	Residues	Atoms					AltConf	Trace
46	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



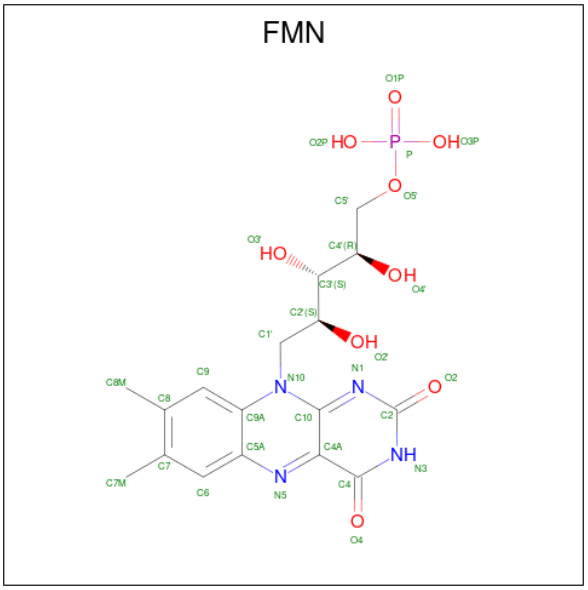
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			16	8	8	
47	G	1	Total	Fe	S	0
			16	8	8	
47	I	1	Total	Fe	S	0
			16	8	8	
47	I	1	Total	Fe	S	0
			16	8	8	

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



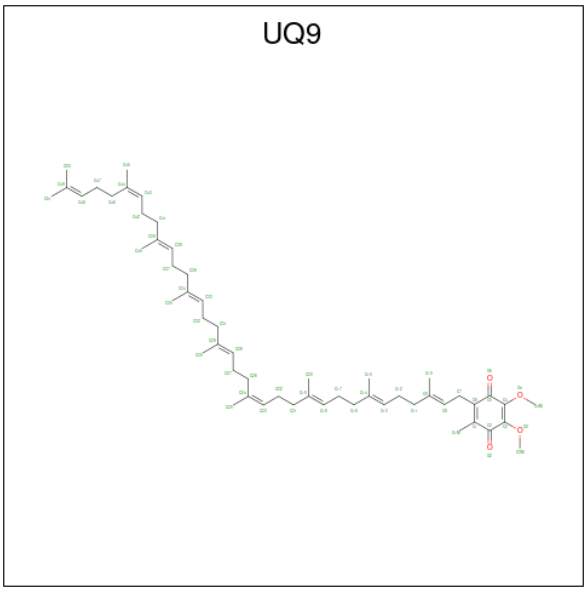
Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

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



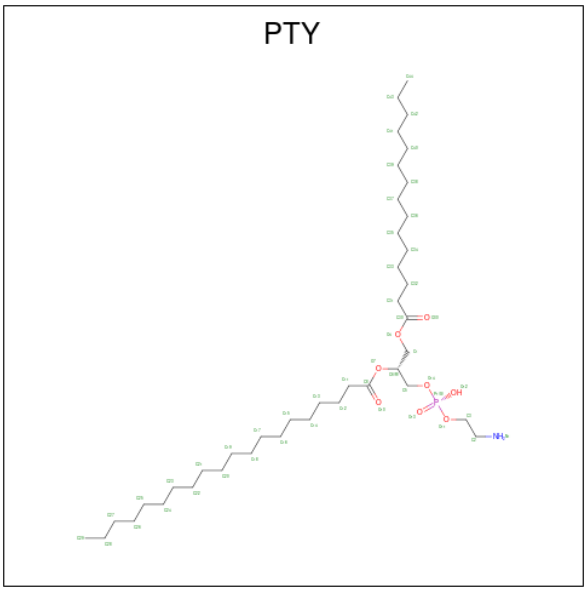
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$).



Mol	Chain	Residues	Atoms			AltConf
50	H	1	Total	C	O	0
			35	31	4	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
51	I	1	Total	C	N	O	P	0
			50	40	1	8	1	
51	M	1	Total	C	N	O	P	0
			50	40	1	8	1	

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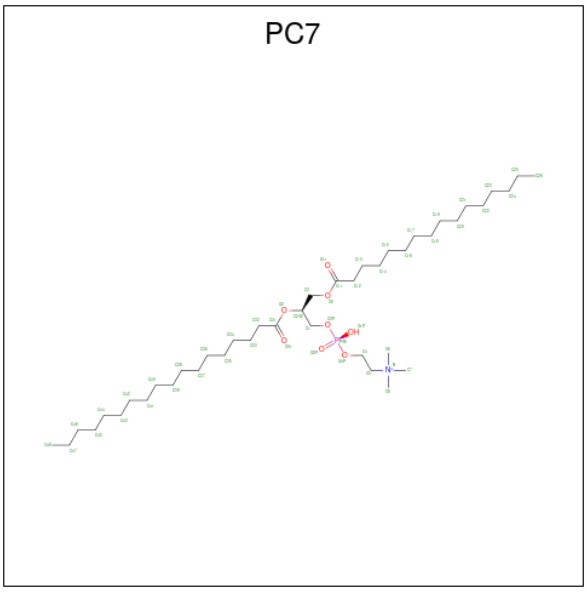
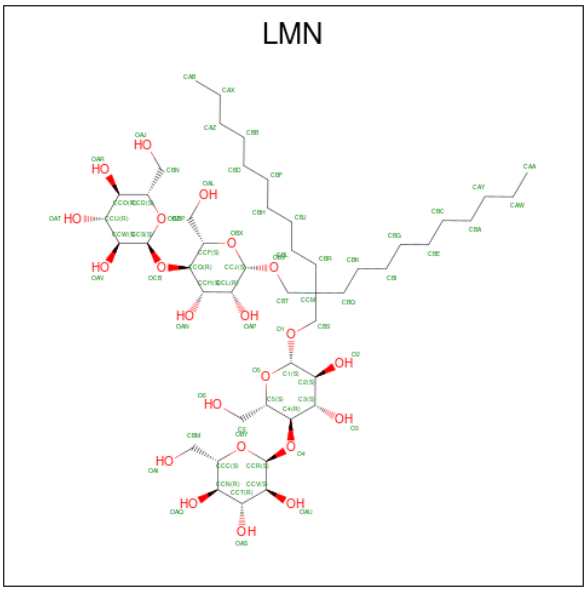
Mol	Chain	Residues	Atoms					AltConf
51	N	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 52 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$).



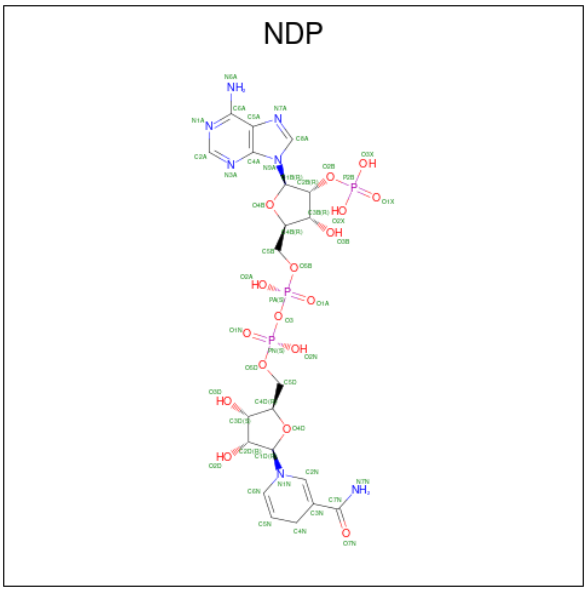
Mol	Chain	Residues	Atoms					AltConf
52	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	f	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 53 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	C	O	0
			69	47	22	

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

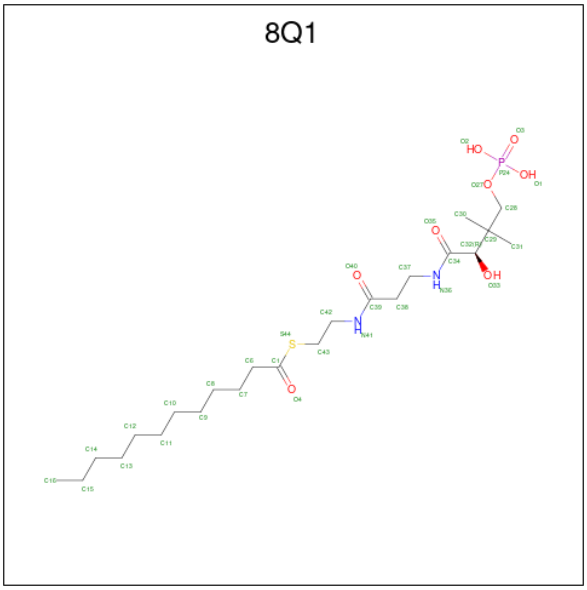


Mol	Chain	Residues	Atoms					AltConf
54	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

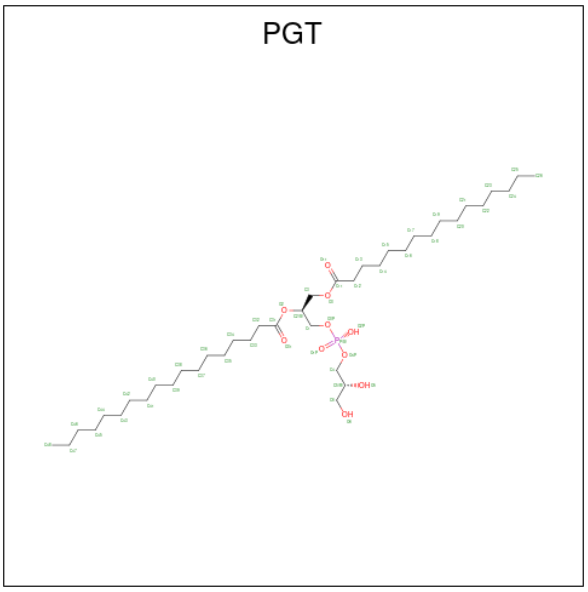
Mol	Chain	Residues	Atoms	AltConf
55	R	1	Total Zn 1 1	0
55	y	1	Total Zn 1 1	0

- Molecule 56 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



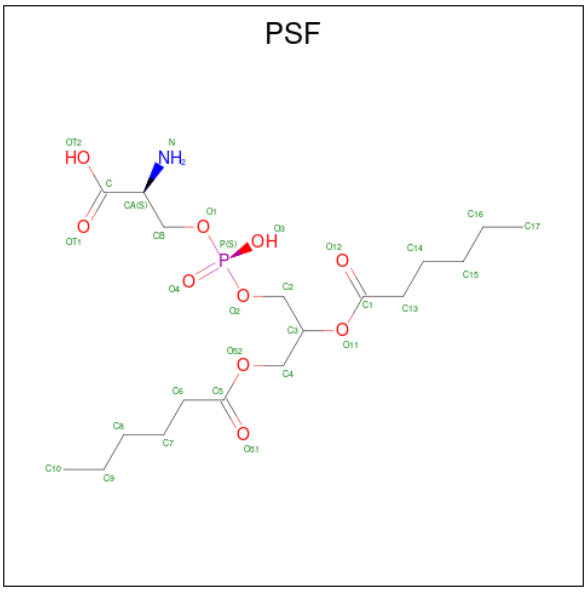
Mol	Chain	Residues	Atoms	AltConf
56	W	1	Total C N O P S 35 23 2 8 1 1	0
56	n	1	Total C N O P S 35 23 2 8 1 1	0

- Molecule 57 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



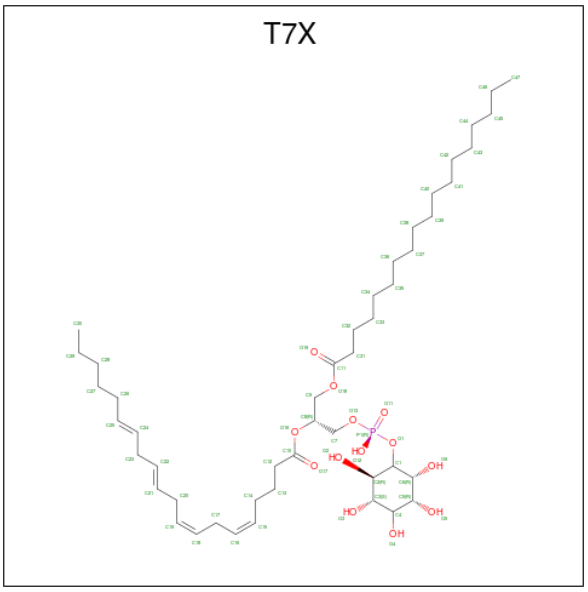
Mol	Chain	Residues	Atoms				AltConf
57	y	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 58 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
58	z	1	Total	C	N	O	P	0
			30	18	1	10	1	

- Molecule 59 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



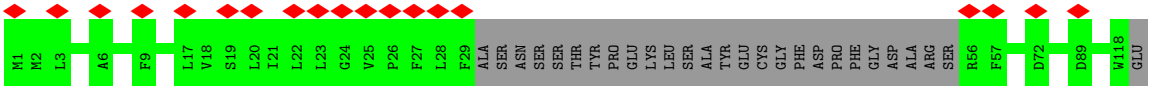
Mol	Chain	Residues	Atoms				AltConf
59	z	1	Total	C	O	P	0
			61	47	13	1	

3 Residue-property plots (i)

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

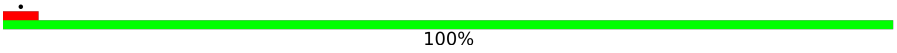
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

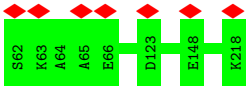
Chain A:



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

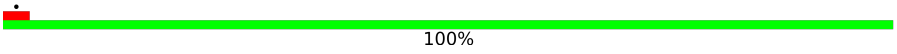
Chain B:

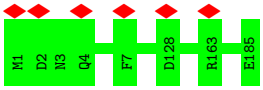




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

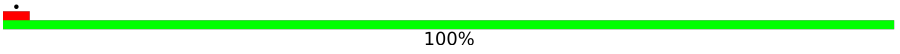
Chain C:

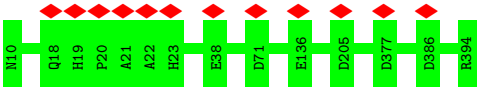




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2

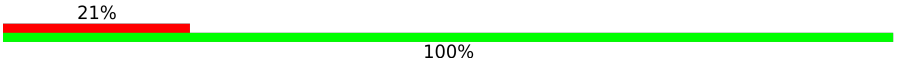
Chain D:

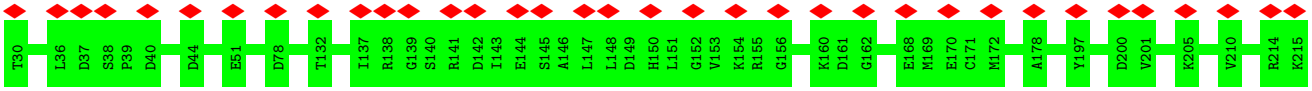


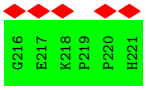


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

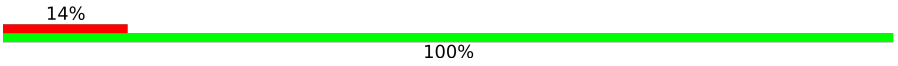


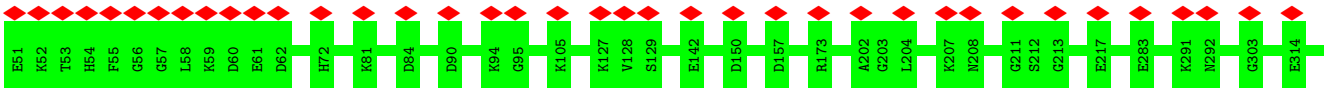


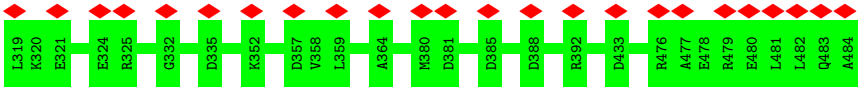


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

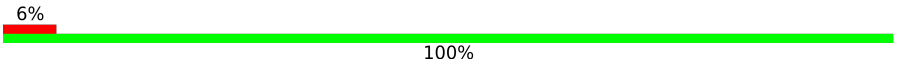


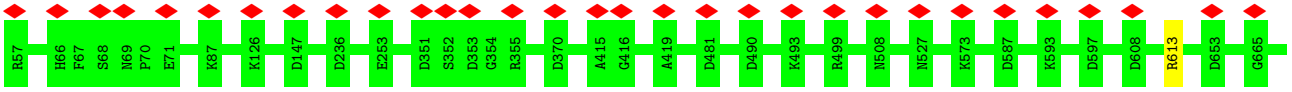


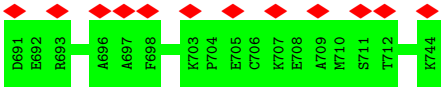


• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial

Chain G:

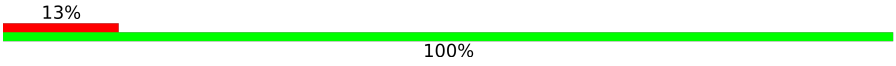


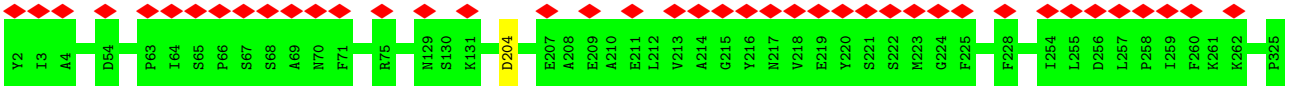




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

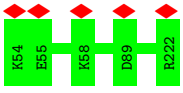
Chain H:





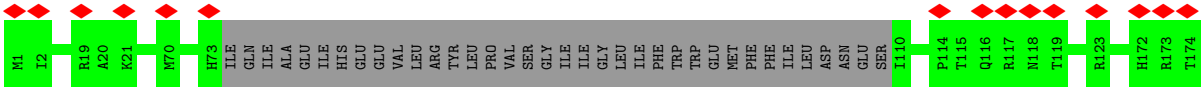
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

Chain I:



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

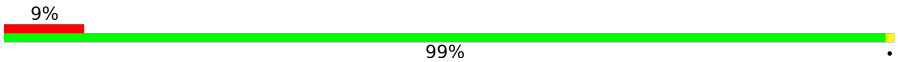
Chain J:



THR LYS VAL LYS ARG GLN ASP VAL PHE ARG ARG ASN ALA ILE ASP PHE ARG ARG THR ILE MET ARG ARG THR THR ASP PRO LEU THR ILE TYR

• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



M1 L22 R25 R26 N27 I28 R85 V86 R87 G88

• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:

M1 Y2 L3 L4 I5 V6 F7 L8 P9 L10 L11 G12 S13 S14 V15 F18 R21 F22 L23 G24 S25 E26 G27 S28 A29 I30 M31 C35 V36 S37 F38 S39 S40 I41 L42 S43 L44 I45 A46 F47 Y48 E49 V50 A51 L52 G53 A54 S55 A56 C57 Y58 L59 R60 I61 S66 S67

E68 M69 F70 D71 G75 F76 L77 F78 D79 S80 L81 T82 V83 V84 M85 L86 I87 V88 V89 T90 F91 I92 S93 S94 L95 V96 H97 L98 Y99 S100 I101 S102 Y103 M104 S105 E106 D107 P108 P111 R112 F113 M114 L117 S118 I119 F120 T121 F122 F123 M124 L127 G130 D131 L134

Q135 L136 F137 L138 G139 W140 E141 G142 V143 G144 L145 A146 S147 Y148 L149 L150 I151 H152 F153 W154 F155 T156 R157 L158 Q159 A160 D161 K162 A163 A164 I165 K166 A167 M168 L169 V170 N171 R172 V173 G174 D175 F176 G177 L178 A179 L180 G181 I182 L183 G184 C185 F186 F189 D193 F194 I197 F198

A199 C200 A201 S202 V203 P204 R205 N206 S207 W208 I209 F210 C211 N212 M213 R214 L215 N216 A217 I218 S219 L220 I221 C222 I223 L224 L225 F226 I227 G228 A229 V230 G231 K232 S233 A234 Q235 I236 G237 L238 H239 T240 W241 L242 P243 D244 A245 M246 E247 G248 P249 T250 P251 V252 S253 A254 L255 I256 H257 A258

A259 T260 M261 V262 T263 A264 G265 V266 F267 M268 I269 A270 R271 C272 L275 F276 E277 P280 T281 A282 L283 I284 V285 I286 T287 F288 A289 G290 A291 M292 T293 S294 F295 L296 A297 A298 T299 T300 G301 I302 L303 Q304 N305 D306 L307 K308 R309 V310 I311 A312 Y313 S314 T315 C316 S317 Q318 L319 G320

Y321 M322 I323 F324 A325 C326 G327 I328 S329 N330 Y331 S332 V333 S334 V335 F336 H337 L338 M339 N340 H341 A342 F343 F344 K345 A346 L347 L348 F349 L350 S351 A352 G353 S354 V355 I356 H357 A358 M359 S360 D361 E362 Q363 D364 M365 R366 K367 M368 G369 G370 L371 A372 S373 S374 F375 P376 L377 T378 Y379 A380

M381 M382 L383 I384 G385 S386 L387 S388 L389 I390 G391 F392 P393 F394 L395 T396 G397 F398 Y399 S400 K401 D402 V403 I404 L405 E406 L407 A408 Y409 T410 K411 Y412 T413 I414 S415 G416 N417 F418 A419 F420 W421 L422 G423 S424 V425 S426 V427 L428 F429 T430 S431 Y432 Y433 S434 F435 R436 L437 L438 F439 L440

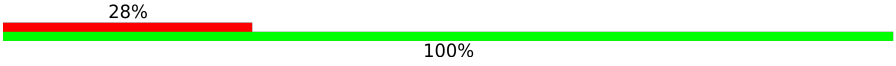
T441 F442 L443 V444 P445 T446 N447 S448 F449 G450 R451 D452 I453 S454 R455 C456 H457 D458 A459 P460 I461 P462 M463 A464 I465 P466 L467 I468 L469 L470 A471 L472 G473 S474 L475 F476 V477 G478 Y479 A539 D540 Q541 F542 Q543 R544 A545 F546 Q547 T548 S549 T550 F551 C552 N553 R554 L555 Y556 S557 F558 F559 N560

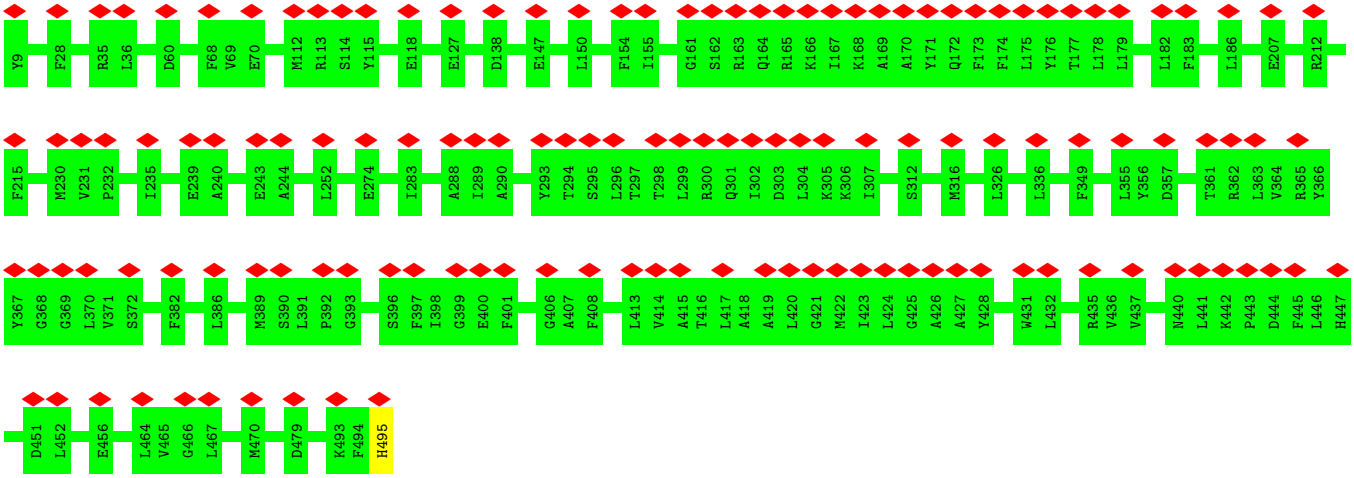
P501 K502 N503 E504 I505 L506 A507 E508 S509 E510 F511 A512 A513 P514 T515 I516 I517 K518 L519 I520 P521 I522 L523 F524 S525 T526 L527 G528 A529 F530 V531 A532 Y533 N534 V535 N536 L537 V538

K561 R562 W563 F564 F565 D566 Q567 V568 L569 W570 D571 F572 L573 V574 R575 S576 F577 L578 R579 F580 G581 Y582 E583 V584 S585 F586 E587 A588 L589 D590 K591 G592 A593 I594 E595 I596 L597 G598 P599 Y600 G601 I602 S603 Y604 T605 F606 R607 R608 L609 A610 E611 R612 I613 S614 Q615

• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

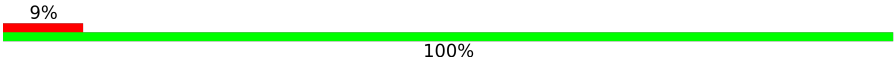
Chain M:

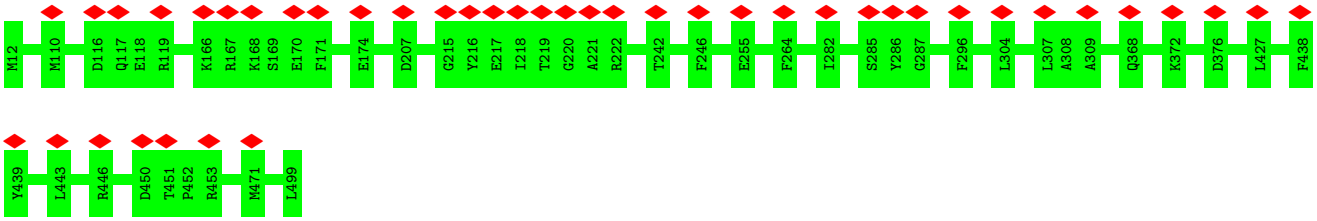




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

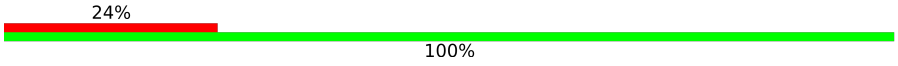
Chain N:

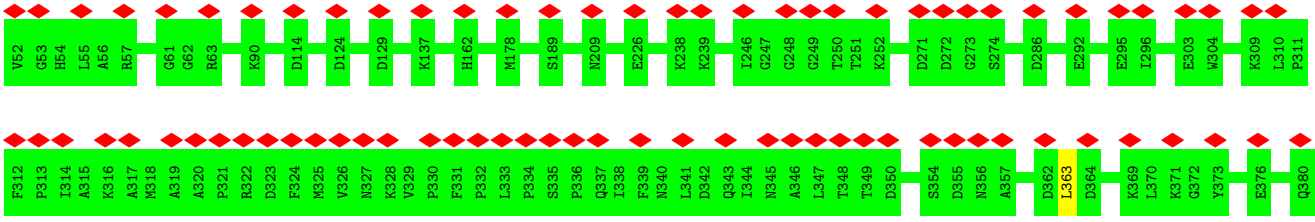




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

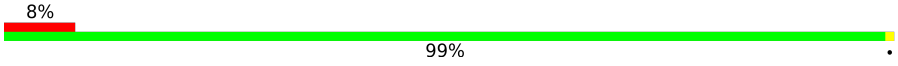
Chain P:

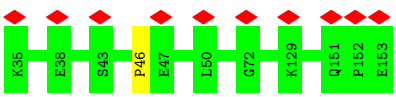




• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

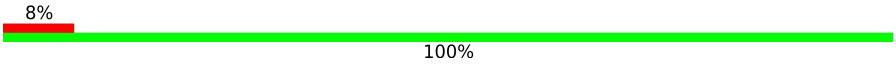
Chain Q:

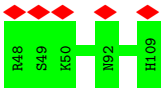




• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

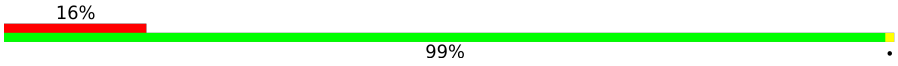
Chain R:

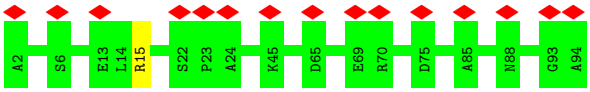




• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

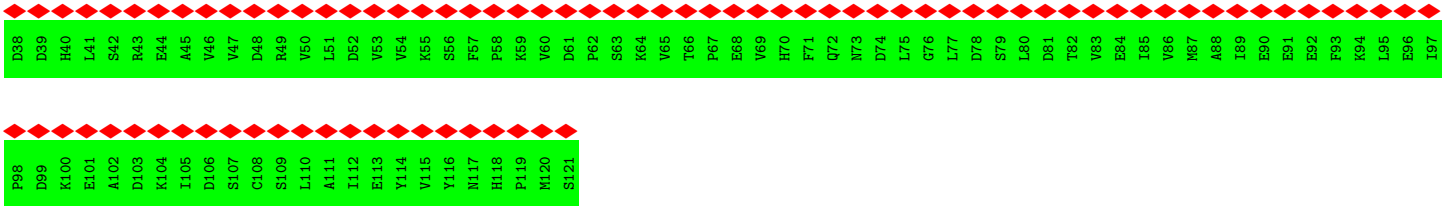
Chain S:





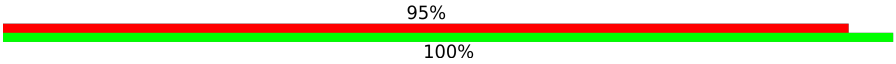
• Molecule 19: Acyl carrier protein 1, mitochondrial

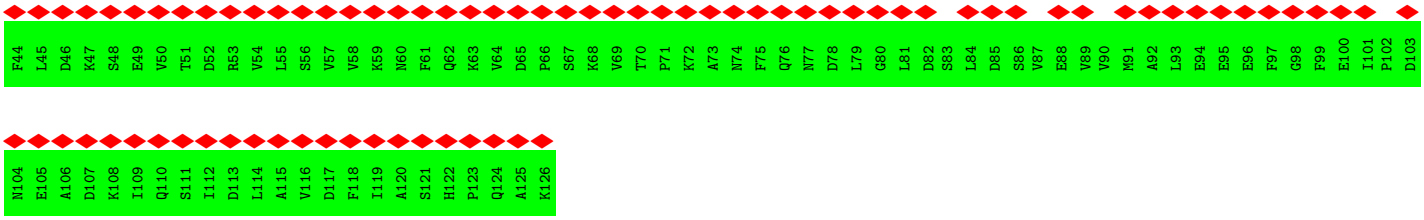
Chain T:



• Molecule 20: Acyl carrier protein 2, mitochondrial

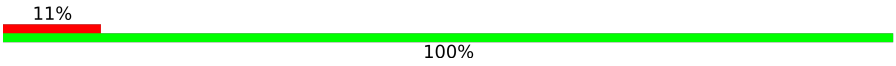
Chain U:

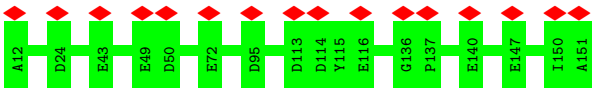




• Molecule 21: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial

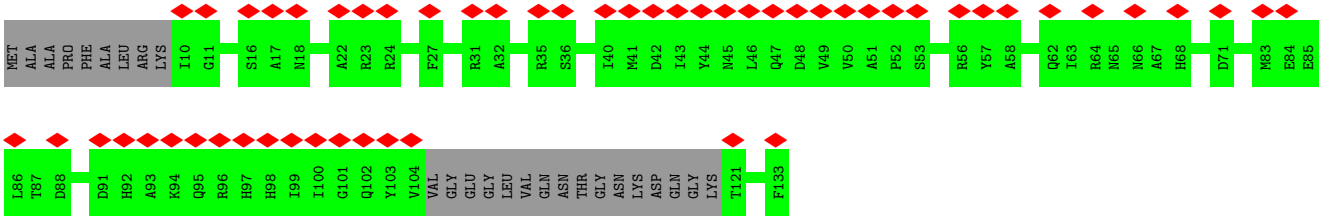
Chain V:



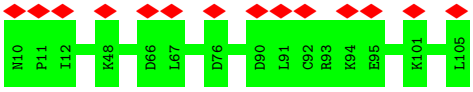


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

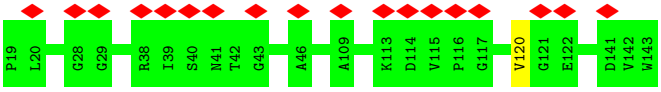
Chain W:



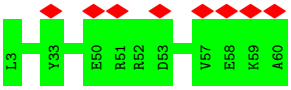
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



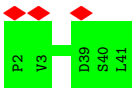
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



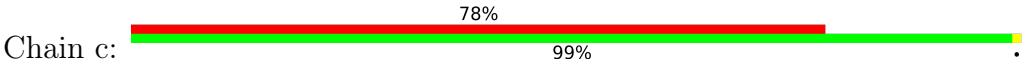
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

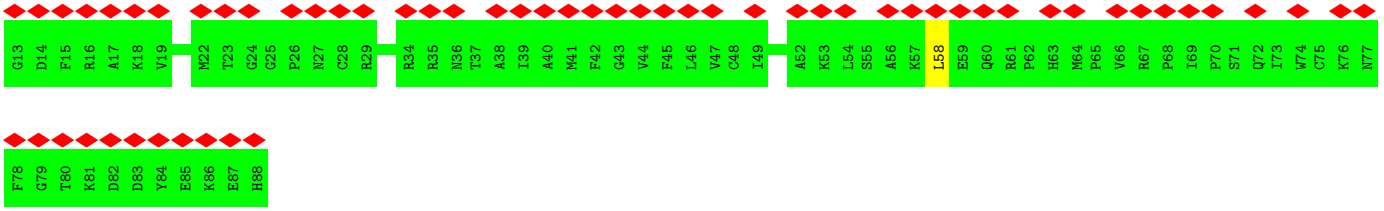


• Molecule 26: At2g46540/F11C10.23



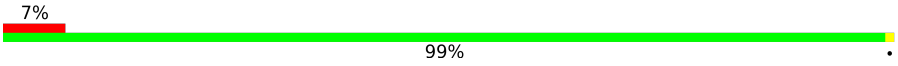
• Molecule 27: Transmembrane protein

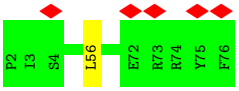




• Molecule 28: Excitatory amino acid transporter

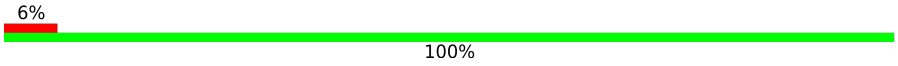
Chain d:

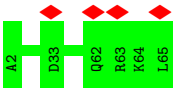




• Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-A

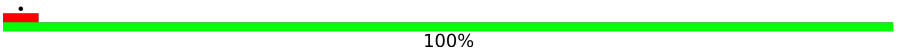
Chain e:

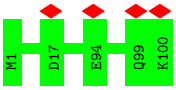




• Molecule 30: At4g16450

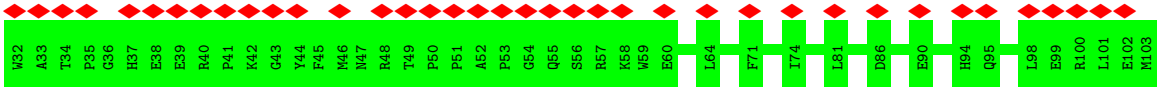
Chain f:





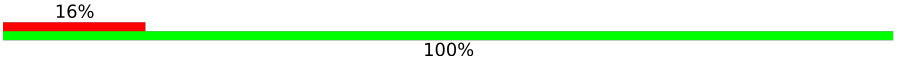
• Molecule 31: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein

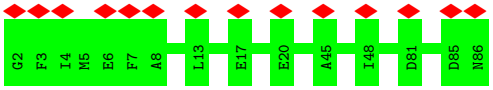
Chain g:



• Molecule 32: At1g67350

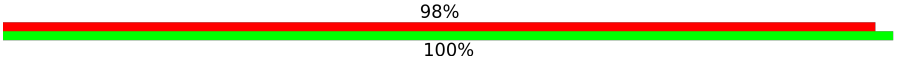
Chain i:

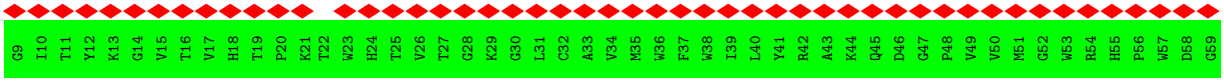




• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

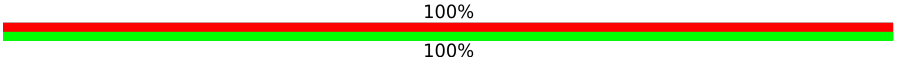
Chain j:

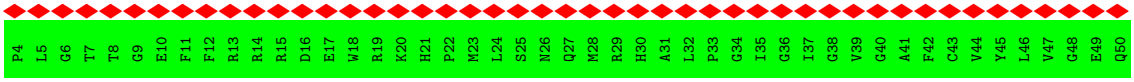




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A

Chain k:





• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l: 96% 100%

Y76 E77 A78 L79 A80 W81 L82 S83 G84 G85 L86 G87 F88 F89 V90 G91 L92 G93 L94 L95 A96 V97 L98 N99 D100 K101 A102 S103 K104 V105 P106 F107 T108 P109 R110 V111 Y112 P113 Y114 D115 N116 L117 R118 V119 E120 L121

• Molecule 36: AT2G31490 protein

Chain m: 81% 100%

M5 E6 T7 N8 K9 N10 K11 F12 I13 E14 D15 W16 G17 S18 A19 R20 E21 N22 L23 E24 H25 N26 F27 R28 W29 T30 R31 R32 N33 F34 A35 L36 I37 G38 I39 F40 G41 I42 A43 L44 P45 I46 G51 I52 H57 D60 E61 D62 A63 G64 R65 P66 H67 R68 K69 F70 L71

• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n: 98% 100%

A7 A8 Y9 F10 A11 R12 R13 A14 A15 Q16 K17 E18 R19 V20 R21 I22 L23 Y24 R25 R26 A27 L28 K29 D30 T31 L32 N33 W34 A35 V36 H37 R38 H39 I40 F41 Y42 R43 D44 A45 S46 D47 L48 R49 E50 K51 F52 N53 V54 N55 Q56 D57 V58 E59 D60 V61 D62 R63 I64 D65 K66

L67 I68 A69 H70 G71 E72 A73 E74 Y75 N76 K77 W78 R79 H80 P81 D82 P83 Y84 I85 V86 P87 W88 A89 P90 G91 G92 S93 K94 F95 C96 R97 N98 P99 T100 P101 P102 A103 G104 I105 E106 I107 N110 Y111 G112 L113 E114 D115

• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o: 94% 100%

K8 K9 M10 I11 A12 T13 Q14 E15 E16 M17 S18 A19 A20 K21 I22 A23 L24 G25 S26 R27 D28 M29 C30 A31 H32 L33 L34 I35 P36 L37 N38 K39 C40 R41 Q42 A43 E44 F45 Y46 L47 P48 W49 K50 C51 E52 D53 E54 R55 H56 V57 Y58 E59 K60 C61 E62 Y63 E64 L65 V66 M67

E68 R69 M70 L71 A72 M73 K74 K75 I76 R77 E78 E79 E80 A81 L82 A83 K84 Q85 N86 K87

• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B

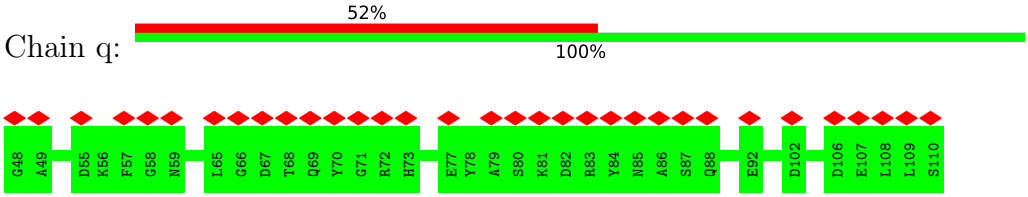
Chain p: 54% 100%

G2 R3 K4 K5 G6 L7 F10 E11 E12 S13 A14 P15 D16 G17 F18 D19 P20 E21 N22 K26 V31 E32 M33 R34 E35 I45 E46 K49 I50 L51 R52 E53 R60 V61 E62 G63 V64 N65 H66 Y67 Q68 R71 H72 Q75 Q76 D79 S80 T81 R82 G83 V84

G85 W86 G87 K88 D89 H90 R91 P92 I93 S94

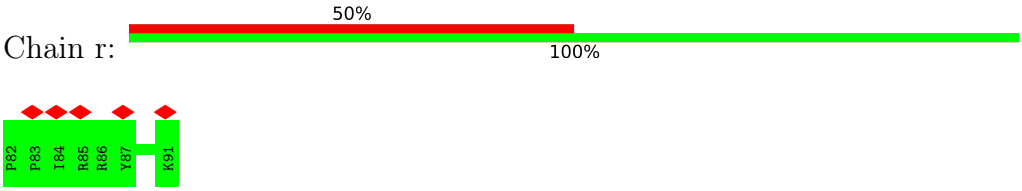
• Molecule 40: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



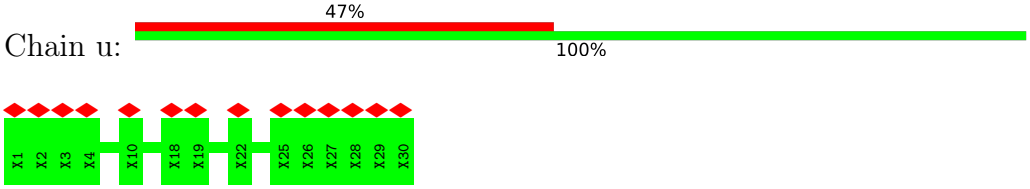
• Molecule 41: B14.5a

Chain r:



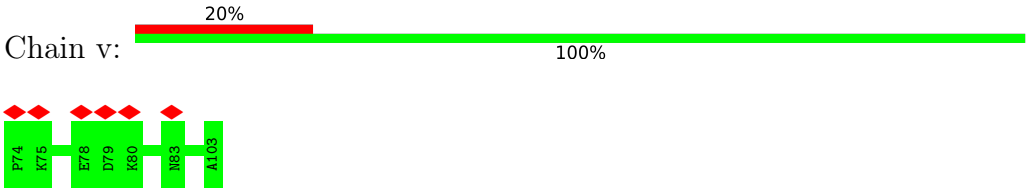
• Molecule 42: unknown

Chain u:



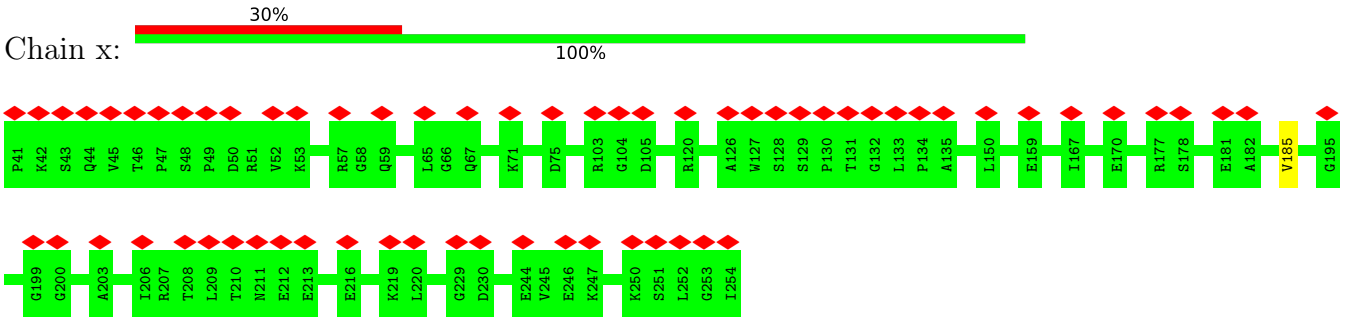
• Molecule 43: Uncharacterized protein At2g27730, mitochondrial

Chain v:



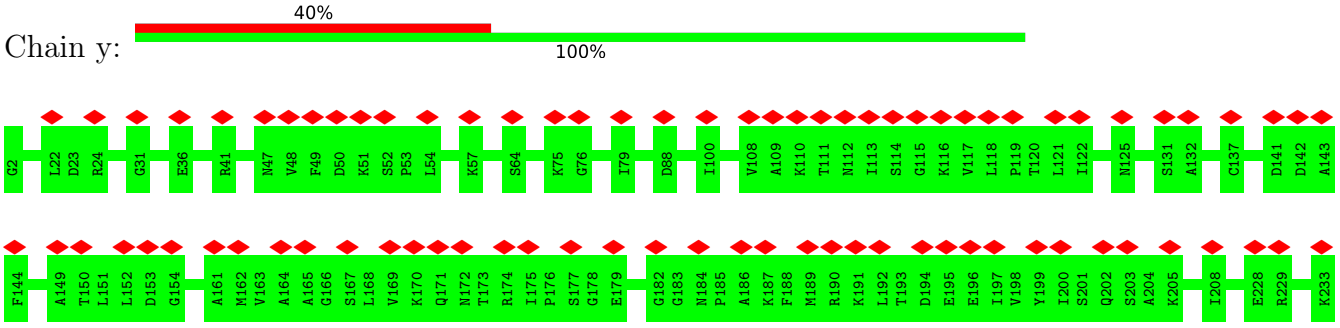
• Molecule 44: Gamma carbonic anhydrase-like 2, mitochondrial

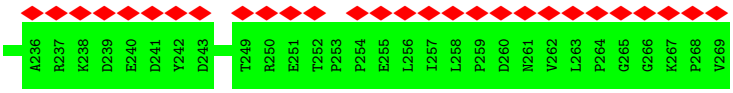
Chain x:



• Molecule 45: Gamma carbonic anhydrase 2, mitochondrial

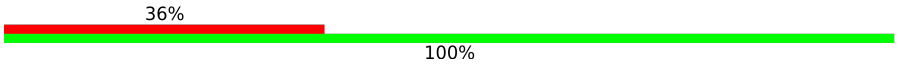
Chain y:

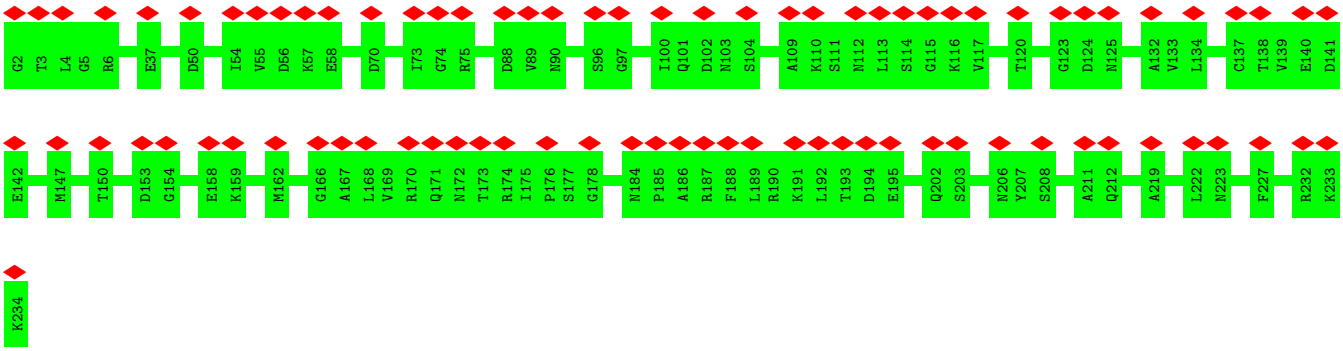




• Molecule 46: Gamma carbonic anhydrase 1, mitochondrial

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48933	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: NDP, UQ9, ZN, PGT, SF4, FMN, LMN, PC7, PSF, FES, 8Q1, T7X, PTY

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	0.28	0/813	0.46	0/1103
2	B	0.27	0/1279	0.48	0/1734
3	C	0.27	0/1629	0.52	0/2207
4	D	0.27	0/3147	0.52	0/4256
5	E	0.26	0/1535	0.48	0/2084
6	F	0.26	0/3441	0.51	0/4641
7	G	0.26	0/5347	0.51	0/7242
8	H	0.28	0/2609	0.52	1/3553 (0.0%)
9	I	0.28	0/1410	0.53	0/1904
10	J	0.26	0/1118	0.46	0/1523
11	K	0.26	0/702	0.50	0/948
12	L	0.26	0/4938	0.49	0/6706
13	M	0.27	0/3996	0.48	0/5431
14	N	0.27	0/3924	0.47	0/5327
15	P	0.26	0/2613	0.53	1/3539 (0.0%)
16	Q	0.27	0/966	0.50	1/1305 (0.1%)
17	R	0.26	0/493	0.49	0/668
18	S	0.25	0/740	0.52	0/996
19	T	0.23	0/679	0.43	0/922
20	U	0.25	0/660	0.47	0/892
21	V	0.25	0/1146	0.48	0/1555
22	W	0.26	0/899	0.51	0/1218
23	X	0.27	0/777	0.51	0/1044
24	Z	0.26	0/1027	0.54	0/1392
25	a	0.25	0/482	0.51	0/646
26	b	0.26	0/300	0.53	0/407
27	c	0.24	0/637	0.52	1/860 (0.1%)
28	d	0.26	0/605	0.54	1/815 (0.1%)
29	e	0.25	0/559	0.50	0/745
30	f	0.28	0/768	0.47	0/1038
31	g	0.24	0/606	0.50	0/826
32	i	0.26	0/757	0.52	0/1019

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	j	0.23	0/433	0.44	0/592
34	k	0.24	0/384	0.57	0/515
35	l	0.25	0/370	0.44	0/504
36	m	0.24	0/580	0.50	0/778
37	n	0.24	0/938	0.49	0/1273
38	o	0.28	0/666	0.60	0/886
39	p	0.25	0/799	0.49	0/1074
40	q	0.25	0/537	0.48	0/728
41	r	0.19	0/89	0.41	0/119
43	v	0.22	0/230	0.43	0/311
44	x	0.26	0/1700	0.54	1/2320 (0.0%)
45	y	0.25	0/2066	0.50	0/2800
46	z	0.26	0/1804	0.52	0/2441
All	All	0.26	0/61198	0.50	6/82887 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	204	ASP	CB-CG-OD2	6.32	123.98	118.30
16	Q	46	PRO	CA-N-CD	-6.27	102.72	111.50
44	x	185	VAL	C-N-CA	-5.59	107.72	121.70
15	P	363	LEU	CA-CB-CG	5.38	127.67	115.30
28	d	56	LEU	CA-CB-CG	5.28	127.44	115.30
27	c	58	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

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	88/119 (74%)	86 (98%)	2 (2%)	0	100	100
2	B	155/157 (99%)	142 (92%)	13 (8%)	0	100	100
3	C	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
4	D	383/385 (100%)	356 (93%)	27 (7%)	0	100	100
5	E	190/192 (99%)	170 (90%)	20 (10%)	0	100	100
6	F	432/434 (100%)	408 (94%)	24 (6%)	0	100	100
7	G	686/688 (100%)	637 (93%)	49 (7%)	0	100	100
8	H	322/324 (99%)	291 (90%)	31 (10%)	0	100	100
9	I	167/169 (99%)	162 (97%)	5 (3%)	0	100	100
10	J	134/205 (65%)	131 (98%)	3 (2%)	0	100	100
11	K	86/88 (98%)	85 (99%)	0	1 (1%)	13	48
12	L	613/615 (100%)	559 (91%)	54 (9%)	0	100	100
13	M	485/487 (100%)	465 (96%)	20 (4%)	0	100	100
14	N	486/488 (100%)	466 (96%)	20 (4%)	0	100	100
15	P	329/331 (99%)	309 (94%)	20 (6%)	0	100	100
16	Q	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
17	R	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	S	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
19	T	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
20	U	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
21	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
22	W	104/133 (78%)	100 (96%)	4 (4%)	0	100	100
23	X	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
24	Z	123/125 (98%)	114 (93%)	8 (6%)	1 (1%)	19	56
25	a	56/58 (97%)	56 (100%)	0	0	100	100
26	b	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
27	c	74/76 (97%)	59 (80%)	15 (20%)	0	100	100
28	d	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
29	e	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	g	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
32	i	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
33	j	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
34	k	45/47 (96%)	39 (87%)	6 (13%)	0	100	100
35	l	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
36	m	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
37	n	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
38	o	78/80 (98%)	70 (90%)	8 (10%)	0	100	100
39	p	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
40	q	61/63 (97%)	53 (87%)	8 (13%)	0	100	100
41	r	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
43	v	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
44	x	212/214 (99%)	196 (92%)	16 (8%)	0	100	100
45	y	266/268 (99%)	239 (90%)	27 (10%)	0	100	100
46	z	231/233 (99%)	212 (92%)	19 (8%)	0	100	100
All	All	7468/7683 (97%)	6980 (94%)	486 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	28	ILE
24	Z	120	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/106 (79%)	84 (100%)	0	100	100
2	B	132/132 (100%)	132 (100%)	0	100	100
3	C	175/175 (100%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	331/331 (100%)	331 (100%)	0	100	100
5	E	166/166 (100%)	166 (100%)	0	100	100
6	F	353/353 (100%)	353 (100%)	0	100	100
7	G	571/571 (100%)	570 (100%)	1 (0%)	93	97
8	H	271/271 (100%)	271 (100%)	0	100	100
9	I	151/151 (100%)	151 (100%)	0	100	100
10	J	123/186 (66%)	123 (100%)	0	100	100
11	K	76/76 (100%)	76 (100%)	0	100	100
12	L	518/518 (100%)	516 (100%)	2 (0%)	91	95
13	M	426/426 (100%)	425 (100%)	1 (0%)	93	97
14	N	406/406 (100%)	406 (100%)	0	100	100
15	P	273/273 (100%)	273 (100%)	0	100	100
16	Q	100/100 (100%)	100 (100%)	0	100	100
17	R	55/55 (100%)	55 (100%)	0	100	100
18	S	82/82 (100%)	81 (99%)	1 (1%)	71	84
19	T	79/79 (100%)	79 (100%)	0	100	100
20	U	75/75 (100%)	75 (100%)	0	100	100
21	V	123/123 (100%)	123 (100%)	0	100	100
22	W	96/114 (84%)	96 (100%)	0	100	100
23	X	87/87 (100%)	87 (100%)	0	100	100
24	Z	100/100 (100%)	100 (100%)	0	100	100
25	a	48/48 (100%)	48 (100%)	0	100	100
26	b	33/33 (100%)	33 (100%)	0	100	100
27	c	66/66 (100%)	66 (100%)	0	100	100
28	d	60/60 (100%)	60 (100%)	0	100	100
29	e	59/59 (100%)	59 (100%)	0	100	100
30	f	80/80 (100%)	80 (100%)	0	100	100
31	g	62/62 (100%)	62 (100%)	0	100	100
32	i	77/77 (100%)	77 (100%)	0	100	100
33	j	42/42 (100%)	42 (100%)	0	100	100
34	k	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	l	37/37 (100%)	37 (100%)	0	100	100
36	m	58/58 (100%)	58 (100%)	0	100	100
37	n	92/92 (100%)	92 (100%)	0	100	100
38	o	70/70 (100%)	70 (100%)	0	100	100
39	p	83/83 (100%)	83 (100%)	0	100	100
40	q	52/52 (100%)	52 (100%)	0	100	100
41	r	10/10 (100%)	10 (100%)	0	100	100
43	v	23/23 (100%)	23 (100%)	0	100	100
44	x	183/183 (100%)	183 (100%)	0	100	100
45	y	223/223 (100%)	223 (100%)	0	100	100
46	z	188/188 (100%)	188 (100%)	0	100	100
All	All	6437/6540 (98%)	6432 (100%)	5 (0%)	93	98

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

Mol	Chain	Res	Type
7	G	613	ARG
12	L	330	ASN
12	L	608	ARG
13	M	495	HIS
18	S	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	113	ASN
12	L	97	HIS
12	L	560	ASN
18	S	88	ASN
27	c	60	GLN
43	v	83	ASN
44	x	81	ASN
44	x	116	ASN
45	y	107	HIS
45	y	135	HIS
46	z	112	ASN
46	z	130	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	PC7	f	201	30	51,51,51	0.96	4 (7%)	57,59,59	1.03	2 (3%)
54	NDP	P	500	15	45,52,52	2.25	4 (8%)	53,80,80	1.75	9 (16%)
47	SF4	G	802	7	0,12,12	-	-	-		
47	SF4	I	301	9	0,12,12	-	-	-		
47	SF4	I	302	9	0,12,12	-	-	-		
53	LMN	M	503	-	72,72,72	1.67	13 (18%)	96,98,98	1.11	4 (4%)
49	FMN	F	500	-	33,33,33	1.08	2 (6%)	48,50,50	1.22	8 (16%)
56	8Q1	W	200	-	31,34,34	1.70	6 (19%)	40,43,43	1.52	4 (10%)
47	SF4	F	501	6	0,12,12	-	-	-		
57	PGT	y	302	-	40,40,50	1.17	3 (7%)	43,46,56	1.09	2 (4%)
59	T7X	z	302	-	61,61,61	0.84	4 (6%)	71,73,73	1.04	2 (2%)
50	UQ9	H	500	8	35,35,58	2.55	12 (34%)	42,45,73	1.59	9 (21%)
52	PC7	M	501	12,13	51,51,51	0.96	4 (7%)	57,59,59	1.09	2 (3%)
47	SF4	B	500	2	0,12,12	-	-	-		
51	PTY	N	501	14	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	PTY	M	502	13	49,49,49	0.88	4 (8%)	52,54,54	1.10	2 (3%)
58	PSF	z	301	46	28,29,29	1.18	4 (14%)	32,36,36	1.24	2 (6%)
51	PTY	I	303	9	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
48	FES	G	801	7	0,4,4	-	-	-		
47	SF4	G	803	7	0,12,12	-	-	-		
48	FES	E	500	5	0,4,4	-	-	-		
56	8Q1	n	200	37	31,34,34	1.71	6 (19%)	40,43,43	1.50	5 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PC7	f	201	30	-	26/55/55/55	-
54	NDP	P	500	15	-	4/30/77/77	0/5/5/5
47	SF4	G	802	7	-	-	0/6/5/5
47	SF4	I	301	9	-	-	0/6/5/5
47	SF4	I	302	9	-	-	0/6/5/5
53	LMN	M	503	-	-	35/50/130/130	0/4/4/4
49	FMN	F	500	-	-	7/18/18/18	0/3/3/3
56	8Q1	W	200	-	-	21/41/41/41	-
47	SF4	F	501	6	-	-	0/6/5/5
57	PGT	y	302	-	-	27/45/45/55	-
59	T7X	z	302	-	-	24/56/80/80	0/1/1/1
50	UQ9	H	500	8	-	4/30/54/81	0/1/1/1
52	PC7	M	501	12,13	-	20/55/55/55	-
47	SF4	B	500	2	-	-	0/6/5/5
51	PTY	N	501	14	-	27/53/53/53	-
51	PTY	M	502	13	-	24/53/53/53	-
58	PSF	z	301	46	-	11/35/35/35	-
51	PTY	I	303	9	-	22/53/53/53	-
48	FES	G	801	7	-	-	0/1/1/1
47	SF4	G	803	7	-	-	0/6/5/5
48	FES	E	500	5	-	-	0/1/1/1
56	8Q1	n	200	37	-	7/41/41/41	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	500	NDP	P2B-O2B	12.51	1.82	1.59
50	H	500	UQ9	C6-C1	10.23	1.53	1.35
56	W	200	8Q1	C34-N36	5.55	1.45	1.33
56	n	200	8Q1	C34-N36	5.52	1.45	1.33
56	n	200	8Q1	C39-N41	5.38	1.45	1.33
56	W	200	8Q1	C39-N41	5.32	1.45	1.33
53	M	503	LMN	O5-C1	4.76	1.54	1.41
50	H	500	UQ9	C4-C3	4.33	1.53	1.36
53	M	503	LMN	CBS-CCM	4.31	1.63	1.53
50	H	500	UQ9	C7-C8	4.25	1.56	1.50
54	P	500	NDP	PN-O5D	4.19	1.76	1.59
53	M	503	LMN	CBT-CCM	4.18	1.63	1.53
53	M	503	LMN	CBR-CCM	3.73	1.61	1.54
49	F	500	FMN	C4A-N5	3.72	1.38	1.30
53	M	503	LMN	O1-C1	-3.36	1.34	1.40
57	y	302	PGT	O3-C11	3.07	1.42	1.33
57	y	302	PGT	O2-C31	2.96	1.42	1.34
53	M	503	LMN	OBZ-CCS	2.92	1.49	1.41
53	M	503	LMN	OBY-CCR	2.90	1.49	1.41
54	P	500	NDP	O2B-C2B	-2.89	1.33	1.44
53	M	503	LMN	O4-C4	2.82	1.51	1.43
53	M	503	LMN	OBX-CCF	2.68	1.50	1.44
50	H	500	UQ9	C11-C9	2.60	1.56	1.51
50	H	500	UQ9	C7-C6	2.60	1.55	1.51
52	f	201	PC7	O2-C2	-2.58	1.40	1.46
51	I	303	PTY	O7-C6	-2.55	1.40	1.46
51	M	502	PTY	O7-C6	-2.53	1.40	1.46
58	z	301	PSF	O11-C3	-2.53	1.40	1.46
52	M	501	PC7	O2-C2	-2.52	1.40	1.46
49	F	500	FMN	C10-N1	2.51	1.38	1.33
53	M	503	LMN	OBX-CCJ	2.47	1.48	1.41
50	H	500	UQ9	C16-C14	2.47	1.56	1.51
56	W	200	8Q1	C1-S44	2.46	1.82	1.76
56	n	200	8Q1	C1-S44	2.45	1.82	1.76
51	N	501	PTY	O4-C30	2.41	1.40	1.33
58	z	301	PSF	O52-C5	2.40	1.40	1.33
52	M	501	PC7	O3-C11	2.40	1.40	1.33
50	H	500	UQ9	C21-C19	2.40	1.56	1.51
50	H	500	UQ9	C26-C24	2.40	1.56	1.51
59	z	302	T7X	O18-C11	2.39	1.40	1.33
51	I	303	PTY	O4-C30	2.39	1.40	1.33
51	M	502	PTY	O4-C30	2.39	1.40	1.33
52	f	201	PC7	O3-C11	2.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	z	302	T7X	O16-C10	2.30	1.40	1.34
50	H	500	UQ9	O4-C4M	-2.28	1.39	1.45
56	n	200	8Q1	C6-C1	2.27	1.53	1.50
53	M	503	LMN	C3-C4	-2.26	1.46	1.52
51	N	501	PTY	O7-C8	2.25	1.40	1.34
56	W	200	8Q1	O40-C39	-2.22	1.18	1.23
57	y	302	PGT	P-O3P	2.21	1.68	1.59
51	N	501	PTY	O7-C6	-2.21	1.41	1.46
52	f	201	PC7	O3-C3	-2.20	1.40	1.45
51	I	303	PTY	O4-C1	-2.19	1.40	1.45
56	n	200	8Q1	O35-C34	-2.19	1.19	1.23
56	W	200	8Q1	O35-C34	-2.18	1.19	1.23
52	M	501	PC7	O3-C3	-2.18	1.40	1.45
59	z	302	T7X	O16-C8	-2.17	1.41	1.46
53	M	503	LMN	O5-C5	2.17	1.49	1.44
51	M	502	PTY	O4-C1	-2.17	1.40	1.45
52	M	501	PC7	O2-C31	2.16	1.40	1.34
52	f	201	PC7	O2-C31	2.16	1.40	1.34
51	N	501	PTY	O4-C1	-2.15	1.40	1.45
56	n	200	8Q1	O40-C39	-2.15	1.18	1.23
50	H	500	UQ9	C6-C5	2.15	1.52	1.46
51	M	502	PTY	O7-C8	2.14	1.40	1.34
58	z	301	PSF	O11-C1	2.14	1.40	1.34
58	z	301	PSF	O52-C4	-2.13	1.40	1.45
51	I	303	PTY	O7-C8	2.12	1.40	1.34
56	W	200	8Q1	C6-C1	2.12	1.53	1.50
59	z	302	T7X	O18-C9	-2.11	1.40	1.45
53	M	503	LMN	CBQ-CCM	2.11	1.58	1.54
54	P	500	NDP	C2A-N1A	2.09	1.37	1.33
50	H	500	UQ9	O5-C5	-2.06	1.18	1.23
50	H	500	UQ9	C17-C18	2.05	1.57	1.50

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	P	500	NDP	PN-O3-PA	-7.18	108.20	132.83
56	n	200	8Q1	C6-C1-S44	5.55	119.92	113.46
56	W	200	8Q1	C6-C1-S44	5.43	119.78	113.46
50	H	500	UQ9	C7-C8-C9	-4.16	119.86	126.79
59	z	302	T7X	O16-C10-C12	4.13	120.41	111.50
52	M	501	PC7	O2-C31-C32	4.12	120.38	111.50
51	M	502	PTY	O7-C8-C11	4.03	120.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	N	501	PTY	O7-C8-C11	4.01	120.14	111.50
58	z	301	PSF	O11-C1-C13	3.99	120.11	111.50
57	y	302	PGT	O2-C31-C32	3.99	120.10	111.50
52	f	201	PC7	O2-C31-C32	3.93	119.97	111.50
53	M	503	LMN	CCR-O4-C4	-3.88	108.35	117.96
51	I	303	PTY	O7-C8-C11	3.84	119.78	111.50
56	W	200	8Q1	O4-C1-C6	-3.59	119.75	123.99
56	n	200	8Q1	O4-C1-C6	-3.33	120.06	123.99
54	P	500	NDP	O2B-P2B-O1X	-3.32	96.58	109.39
50	H	500	UQ9	C12-C13-C14	-3.21	119.94	127.66
49	F	500	FMN	C4-N3-C2	-3.15	119.83	125.64
50	H	500	UQ9	C17-C18-C19	-3.13	120.13	127.66
54	P	500	NDP	PA-O5B-C5B	-3.02	104.00	121.68
54	P	500	NDP	PN-O5D-C5D	-2.96	104.33	121.68
50	H	500	UQ9	C27-C26-C24	-2.80	110.04	114.62
53	M	503	LMN	CCS-OCB-CCQ	-2.79	111.06	117.96
50	H	500	UQ9	C15-C14-C16	2.77	119.94	115.27
50	H	500	UQ9	C22-C23-C24	-2.77	120.98	127.66
50	H	500	UQ9	C25-C24-C26	2.75	119.90	115.27
49	F	500	FMN	C4A-C4-N3	2.72	120.10	113.19
49	F	500	FMN	O4-C4-C4A	-2.70	119.42	126.60
50	H	500	UQ9	C20-C19-C21	2.68	119.79	115.27
51	M	502	PTY	O4-C30-C31	2.66	120.26	111.91
56	W	200	8Q1	C43-S44-C1	2.66	110.14	101.87
54	P	500	NDP	O5D-PN-O1N	-2.65	98.71	109.07
54	P	500	NDP	O2N-PN-O1N	2.62	125.17	112.24
51	I	303	PTY	O4-C30-C31	2.61	120.10	111.91
51	N	501	PTY	O4-C30-C31	2.59	120.05	111.91
59	z	302	T7X	O18-C11-C31	2.57	119.96	111.91
52	M	501	PC7	O3-C11-C12	2.56	119.94	111.91
58	z	301	PSF	O52-C5-C6	2.55	119.92	111.91
54	P	500	NDP	O3X-P2B-O2X	2.54	117.34	107.64
57	y	302	PGT	O3-C11-C12	2.53	119.86	111.91
50	H	500	UQ9	C10-C9-C11	2.49	119.45	115.27
52	f	201	PC7	O3-C11-C12	2.42	119.52	111.91
54	P	500	NDP	C2A-N1A-C6A	-2.34	114.75	118.75
56	n	200	8Q1	C43-S44-C1	2.32	109.11	101.87
49	F	500	FMN	C4A-C10-N1	-2.28	119.43	124.73
49	F	500	FMN	C4A-C10-N10	2.27	119.80	116.48
56	W	200	8Q1	C38-C39-N41	2.27	120.24	116.42
49	F	500	FMN	C9A-C5A-N5	-2.27	119.97	122.43
49	F	500	FMN	C5A-C9A-N10	2.23	120.25	117.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	P	500	NDP	C5D-C4D-C3D	-2.20	106.94	115.18
53	M	503	LMN	OBX-CCF-CCQ	2.19	114.37	109.75
53	M	503	LMN	OBX-CCJ-CCL	2.12	114.83	110.35
49	F	500	FMN	C10-C4A-N5	-2.09	120.43	124.86
56	n	200	8Q1	C38-C39-N41	2.06	119.89	116.42
56	n	200	8Q1	O4-C1-S44	-2.00	120.02	122.61

There are no chirality outliers.

All (259) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	F	500	FMN	N10-C1'-C2'-O2'
49	F	500	FMN	N10-C1'-C2'-C3'
49	F	500	FMN	C1'-C2'-C3'-O3'
49	F	500	FMN	C1'-C2'-C3'-C4'
50	H	500	UQ9	C9-C11-C12-C13
50	H	500	UQ9	C12-C11-C9-C10
50	H	500	UQ9	C12-C11-C9-C8
51	I	303	PTY	N1-C2-C3-O11
51	I	303	PTY	O14-C5-C6-O7
51	I	303	PTY	C5-O14-P1-O13
51	M	502	PTY	O10-C8-O7-C6
51	M	502	PTY	C11-C8-O7-C6
51	M	502	PTY	C5-O14-P1-O13
51	N	501	PTY	O10-C8-O7-C6
51	N	501	PTY	C3-O11-P1-O13
51	N	501	PTY	C3-O11-P1-O14
51	N	501	PTY	C5-O14-P1-O13
52	M	501	PC7	C4-O4P-P-O1P
52	M	501	PC7	C4-O4P-P-O2P
52	M	501	PC7	O4P-C4-C5-N
52	f	201	PC7	C32-C31-O2-C2
52	f	201	PC7	O31-C31-O2-C2
52	f	201	PC7	O2-C2-C3-O3
52	f	201	PC7	C4-O4P-P-O1P
52	f	201	PC7	C5-C4-O4P-P
53	M	503	LMN	O5-C1-O1-CBS
53	M	503	LMN	CBK-CBQ-CCM-CBR
53	M	503	LMN	CBK-CBQ-CCM-CBS
53	M	503	LMN	CBK-CBQ-CCM-CBT
53	M	503	LMN	CBL-CBR-CCM-CBQ
53	M	503	LMN	OBV-CBT-CCM-CBQ

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Mol	Chain	Res	Type	Atoms
53	M	503	LMN	OBV-CBT-CCM-CBR
53	M	503	LMN	OBX-CCJ-OBV-CBT
53	M	503	LMN	CCL-CCJ-OBV-CBT
54	P	500	NDP	C5B-O5B-PA-O3
56	W	200	8Q1	S44-C1-C6-C7
56	W	200	8Q1	O4-C1-S44-C43
56	W	200	8Q1	C6-C1-S44-C43
56	W	200	8Q1	C28-C29-C32-C34
56	W	200	8Q1	C31-C29-C32-C34
56	W	200	8Q1	C29-C32-C34-N36
56	W	200	8Q1	C29-C32-C34-O35
56	W	200	8Q1	O33-C32-C34-N36
56	W	200	8Q1	N36-C37-C38-C39
56	W	200	8Q1	C28-O27-P24-O2
56	W	200	8Q1	C28-O27-P24-O1
56	n	200	8Q1	O27-C28-C29-C30
56	n	200	8Q1	O27-C28-C29-C31
56	n	200	8Q1	O27-C28-C29-C32
56	n	200	8Q1	C42-C43-S44-C1
57	y	302	PGT	C32-C31-O2-C2
57	y	302	PGT	C4-O4P-P-O3P
57	y	302	PGT	C4-O4P-P-O1P
57	y	302	PGT	O4P-C4-C5-C6
58	z	301	PSF	CB-O1-P-O4
58	z	301	PSF	CB-O1-P-O3
58	z	301	PSF	C13-C1-O11-C3
58	z	301	PSF	N-CA-CB-O1
58	z	301	PSF	C-CA-CB-O1
59	z	302	T7X	C12-C10-O16-C8
59	z	302	T7X	O17-C10-O16-C8
59	z	302	T7X	C21-C22-C23-C24
51	M	502	PTY	O30-C30-O4-C1
52	M	501	PC7	O11-C11-O3-C3
53	M	503	LMN	OBZ-CCS-OCB-CCQ
58	z	301	PSF	O12-C1-O11-C3
53	M	503	LMN	CCW-CCS-OCB-CCQ
52	M	501	PC7	C12-C11-O3-C3
51	N	501	PTY	C11-C8-O7-C6
51	M	502	PTY	C31-C30-O4-C1
57	y	302	PGT	O31-C31-O2-C2
54	P	500	NDP	O4D-C1D-N1N-C6N
53	M	503	LMN	OAJ-CBN-CCD-CCO

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Mol	Chain	Res	Type	Atoms
53	M	503	LMN	OAI-CBM-CCC-OBY
57	y	302	PGT	C14-C15-C16-C17
53	M	503	LMN	OAI-CBM-CCC-CCN
52	f	201	PC7	C18-C19-C20-C21
57	y	302	PGT	O4P-C4-C5-O5
53	M	503	LMN	OAJ-CBN-CCD-OBZ
53	M	503	LMN	OAL-CBP-CCF-OBX
52	M	501	PC7	C11-C12-C13-C14
52	f	201	PC7	C31-C32-C33-C34
52	f	201	PC7	C11-C12-C13-C14
59	z	302	T7X	C11-C31-C32-C33
53	M	503	LMN	CBJ-CBL-CBR-CCM
53	M	503	LMN	OBV-CBT-CCM-CBS
51	I	303	PTY	C35-C36-C37-C38
51	I	303	PTY	C5-O14-P1-O11
51	M	502	PTY	C5-O14-P1-O11
52	M	501	PC7	C4-O4P-P-O3P
52	f	201	PC7	C1-O3P-P-O4P
52	f	201	PC7	C4-O4P-P-O3P
57	y	302	PGT	C1-O3P-P-O4P
58	z	301	PSF	CB-O1-P-O2
51	N	501	PTY	C15-C16-C17-C18
53	M	503	LMN	CBE-CBG-CBI-CBK
52	f	201	PC7	C40-C41-C42-C43
51	I	303	PTY	C23-C24-C25-C26
57	y	302	PGT	C18-C19-C20-C21
51	M	502	PTY	C22-C23-C24-C25
57	y	302	PGT	C35-C36-C37-C38
53	M	503	LMN	C2-C1-O1-CBS
52	f	201	PC7	C13-C14-C15-C16
53	M	503	LMN	CBC-CBE-CBG-CBI
53	M	503	LMN	CBD-CBF-CBH-CBJ
51	M	502	PTY	C19-C20-C21-C22
57	y	302	PGT	C15-C16-C17-C18
51	I	303	PTY	C31-C32-C33-C34
52	M	501	PC7	C32-C33-C34-C35
53	M	503	LMN	OAL-CBP-CCF-CCQ
51	I	303	PTY	C12-C13-C14-C15
52	f	201	PC7	C19-C20-C21-C22
57	y	302	PGT	C17-C18-C19-C20
53	M	503	LMN	CAY-CBA-CBC-CBE
59	z	302	T7X	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
51	M	502	PTY	O14-C5-C6-O7
53	M	503	LMN	CBG-CBI-CBK-CBQ
51	N	501	PTY	C32-C33-C34-C35
53	M	503	LMN	CBB-CBD-CBF-CBH
51	M	502	PTY	C18-C19-C20-C21
53	M	503	LMN	CCF-CCQ-OCB-CCS
49	F	500	FMN	O2'-C2'-C3'-C4'
51	N	501	PTY	C5-O14-P1-O11
51	I	303	PTY	C30-C31-C32-C33
51	I	303	PTY	O14-C5-C6-C1
53	M	503	LMN	CCH-CCQ-OCB-CCS
51	I	303	PTY	C37-C38-C39-C40
52	M	501	PC7	C35-C36-C37-C38
59	z	302	T7X	C33-C34-C35-C36
56	W	200	8Q1	O33-C32-C34-O35
59	z	302	T7X	C1-O1-P1-O13
53	M	503	LMN	O5-C5-C6-O6
56	n	200	8Q1	C13-C14-C15-C16
56	W	200	8Q1	C30-C29-C32-O33
56	W	200	8Q1	C31-C29-C32-O33
51	N	501	PTY	C31-C30-O4-C1
51	M	502	PTY	O14-C5-C6-C1
51	N	501	PTY	O14-C5-C6-C1
51	M	502	PTY	N1-C2-C3-O11
52	M	501	PC7	C41-C42-C43-C44
51	I	303	PTY	C11-C12-C13-C14
51	M	502	PTY	C21-C22-C23-C24
51	N	501	PTY	O4-C1-C6-C5
51	N	501	PTY	C22-C23-C24-C25
59	z	302	T7X	C15-C16-C17-C18
59	z	302	T7X	C16-C17-C18-C19
59	z	302	T7X	C19-C20-C21-C22
51	N	501	PTY	O14-C5-C6-O7
59	z	302	T7X	O13-C7-C8-O16
49	F	500	FMN	O2'-C2'-C3'-O3'
59	z	302	T7X	C41-C42-C43-C44
51	N	501	PTY	O4-C1-C6-O7
52	M	501	PC7	O2-C2-C3-O3
57	y	302	PGT	C13-C14-C15-C16
51	N	501	PTY	O30-C30-O4-C1
52	f	201	PC7	C36-C37-C38-C39
56	W	200	8Q1	O4-C1-C6-C7

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Mol	Chain	Res	Type	Atoms
57	y	302	PGT	O3P-C1-C2-C3
57	y	302	PGT	C16-C17-C18-C19
51	N	501	PTY	C1-C6-O7-C8
59	z	302	T7X	C9-C8-O16-C10
51	I	303	PTY	C8-C11-C12-C13
52	f	201	PC7	C1-C2-C3-O3
52	f	201	PC7	O3P-C1-C2-O2
53	M	503	LMN	OBY-CCR-O4-C4
58	z	301	PSF	OT1-C-CA-CB
52	M	501	PC7	C23-C24-C25-C26
51	I	303	PTY	C3-O11-P1-O14
51	N	501	PTY	C3-O11-P1-O12
51	N	501	PTY	C5-O14-P1-O12
52	f	201	PC7	C1-O3P-P-O1P
54	P	500	NDP	C5B-O5B-PA-O1A
57	y	302	PGT	C1-O3P-P-O2P
59	z	302	T7X	C7-O13-P1-O11
52	f	201	PC7	O3P-C1-C2-C3
59	z	302	T7X	O13-C7-C8-C9
52	f	201	PC7	C33-C34-C35-C36
52	f	201	PC7	C42-C43-C44-C45
57	y	302	PGT	C19-C20-C21-C22
51	N	501	PTY	C33-C34-C35-C36
57	y	302	PGT	O3P-C1-C2-O2
51	I	303	PTY	C18-C19-C20-C21
52	M	501	PC7	C19-C20-C21-C22
53	M	503	LMN	CBL-CBR-CCM-CBT
56	n	200	8Q1	C43-C42-N41-C39
52	f	201	PC7	O4P-C4-C5-N
53	M	503	LMN	CCM-CBT-OBV-CCJ
56	W	200	8Q1	C28-C29-C32-O33
57	y	302	PGT	C1-C2-C3-O3
51	M	502	PTY	O4-C1-C6-O7
57	y	302	PGT	O2-C2-C3-O3
51	N	501	PTY	C14-C15-C16-C17
53	M	503	LMN	CAX-CAZ-CBB-CBD
52	M	501	PC7	C18-C19-C20-C21
51	N	501	PTY	C30-C31-C32-C33
52	f	201	PC7	O3-C11-C12-C13
51	I	303	PTY	C15-C16-C17-C18
49	F	500	FMN	C5'-O5'-P-O1P
57	y	302	PGT	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
57	y	302	PGT	C12-C11-O3-C3
51	I	303	PTY	C13-C14-C15-C16
51	M	502	PTY	C37-C38-C39-C40
59	z	302	T7X	C7-O13-P1-O1
52	M	501	PC7	C36-C37-C38-C39
52	M	501	PC7	C38-C39-C40-C41
56	W	200	8Q1	C7-C8-C9-C10
57	y	302	PGT	O11-C11-O3-C3
50	H	500	UQ9	C24-C26-C27-C28
53	M	503	LMN	CCV-CCR-O4-C4
52	f	201	PC7	C16-C17-C18-C19
52	M	501	PC7	O3P-C1-C2-O2
51	N	501	PTY	C11-C12-C13-C14
59	z	302	T7X	C39-C40-C41-C42
57	y	302	PGT	C5-C4-O4P-P
52	f	201	PC7	C35-C36-C37-C38
58	z	301	PSF	OT2-C-CA-CB
59	z	302	T7X	C35-C36-C37-C38
51	M	502	PTY	C8-C11-C12-C13
56	n	200	8Q1	C9-C10-C11-C12
59	z	302	T7X	C13-C14-C15-C16
59	z	302	T7X	C43-C44-C45-C46
59	z	302	T7X	C31-C32-C33-C34
56	W	200	8Q1	C12-C13-C14-C15
53	M	503	LMN	CBL-CBR-CCM-CBS
52	M	501	PC7	C31-C32-C33-C34
59	z	302	T7X	O18-C11-C31-C32
57	y	302	PGT	O3-C11-C12-C13
56	W	200	8Q1	C1-C6-C7-C8
51	N	501	PTY	C25-C26-C27-C28
51	N	501	PTY	O4-C30-C31-C32
51	M	502	PTY	C33-C34-C35-C36
51	M	502	PTY	C39-C40-C41-C42
51	M	502	PTY	O4-C1-C6-C5
56	W	200	8Q1	C28-O27-P24-O3
51	M	502	PTY	C34-C35-C36-C37
56	W	200	8Q1	C30-C29-C32-C34
51	M	502	PTY	C12-C11-C8-O7
52	f	201	PC7	C32-C33-C34-C35
51	M	502	PTY	C31-C32-C33-C34
58	z	301	PSF	O11-C1-C13-C14
51	I	303	PTY	C38-C39-C40-C41

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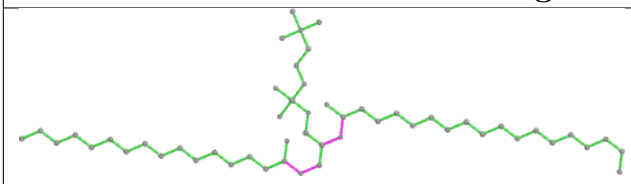
Mol	Chain	Res	Type	Atoms
57	y	302	PGT	O2-C31-C32-C33
51	I	303	PTY	C40-C41-C42-C43
59	z	302	T7X	O16-C10-C12-C13
51	N	501	PTY	O30-C30-C31-C32
51	M	502	PTY	C12-C11-C8-O10
52	M	501	PC7	C1-C2-C3-O3
51	I	303	PTY	C5-O14-P1-O12
52	M	501	PC7	C1-O3P-P-O2P
54	P	500	NDP	C5D-O5D-PN-O1N
51	N	501	PTY	C36-C37-C38-C39
59	z	302	T7X	O17-C10-C12-C13
52	f	201	PC7	C15-C16-C17-C18
51	I	303	PTY	C2-C3-O11-P1
51	N	501	PTY	C2-C3-O11-P1
57	y	302	PGT	O31-C31-C32-C33
58	z	301	PSF	O12-C1-C13-C14
51	I	303	PTY	C33-C34-C35-C36
51	M	502	PTY	C11-C12-C13-C14

There are no ring outliers.

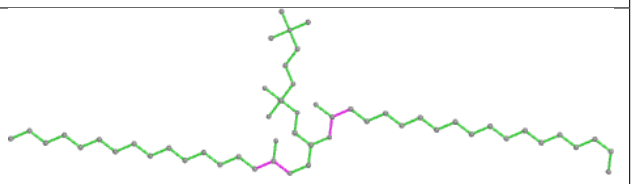
No monomer is involved in short contacts.

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.

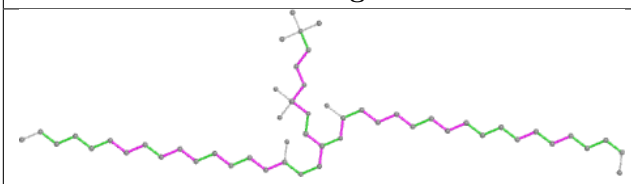
Ligand PC7 f 201



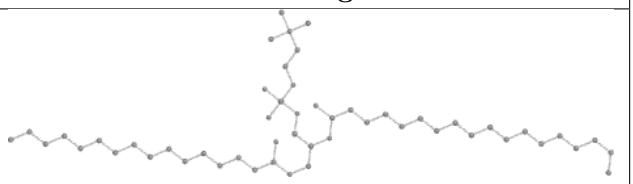
Bond lengths



Bond angles

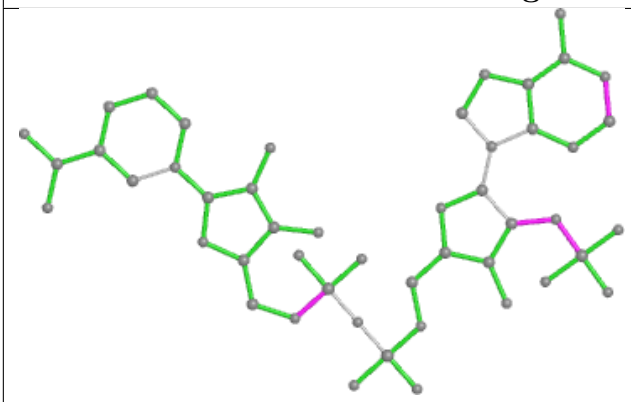


Torsions

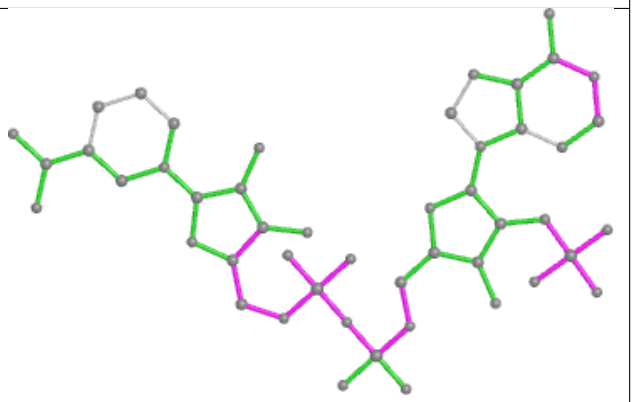


Rings

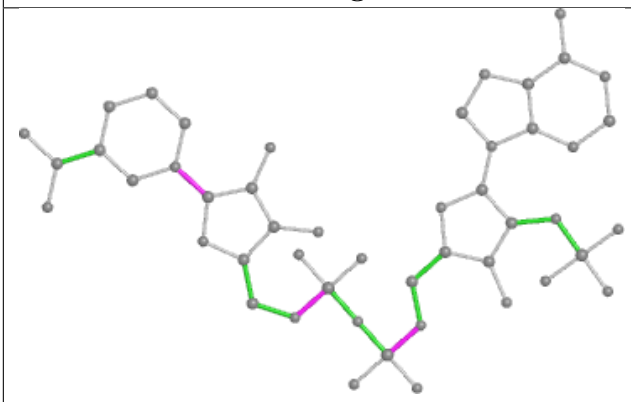
Ligand NDP P 500



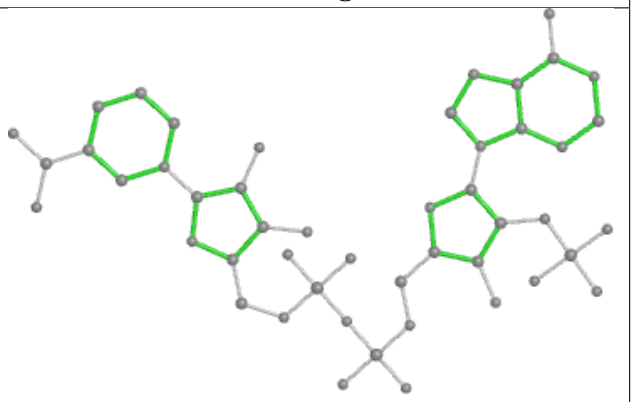
Bond lengths



Bond angles

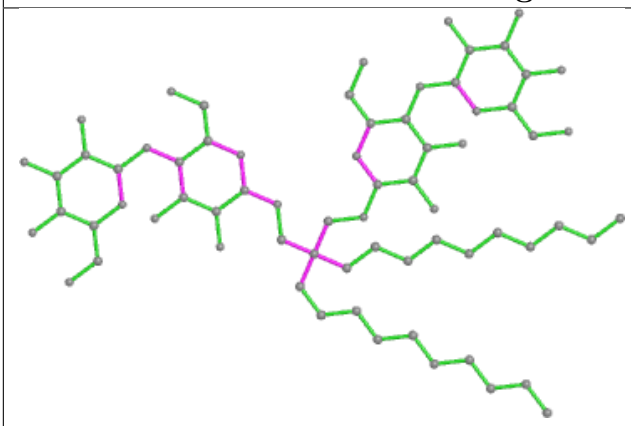


Torsions

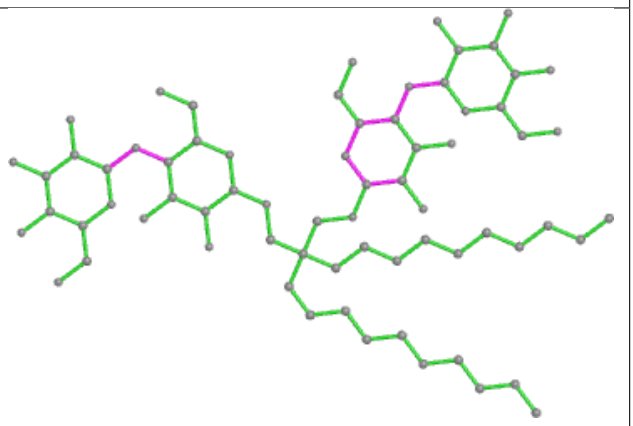


Rings

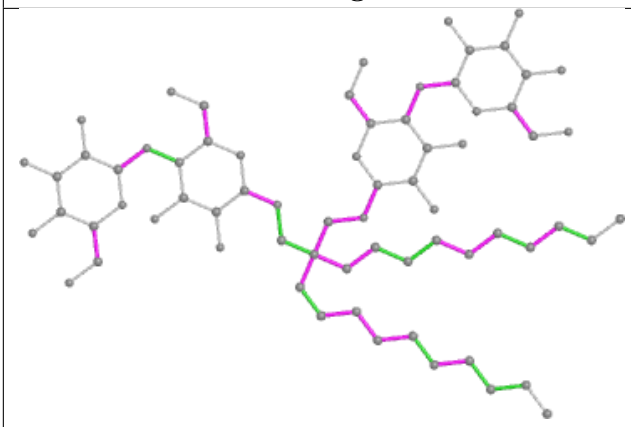
Ligand LMN M 503



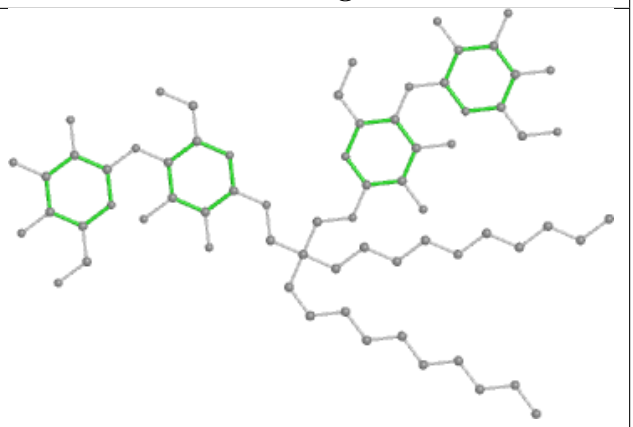
Bond lengths



Bond angles

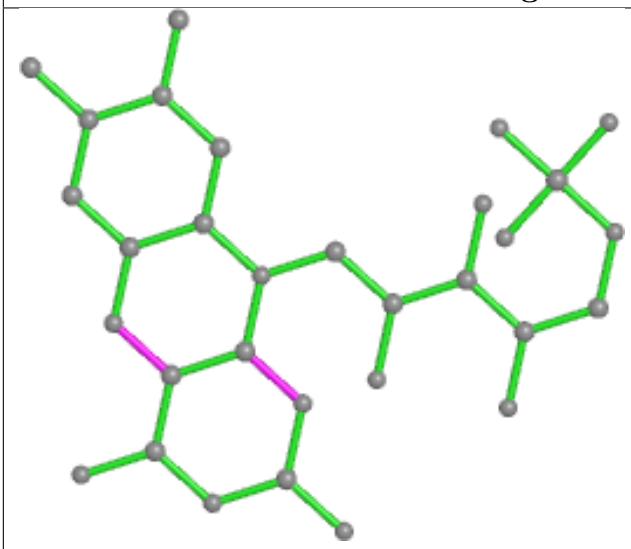


Torsions

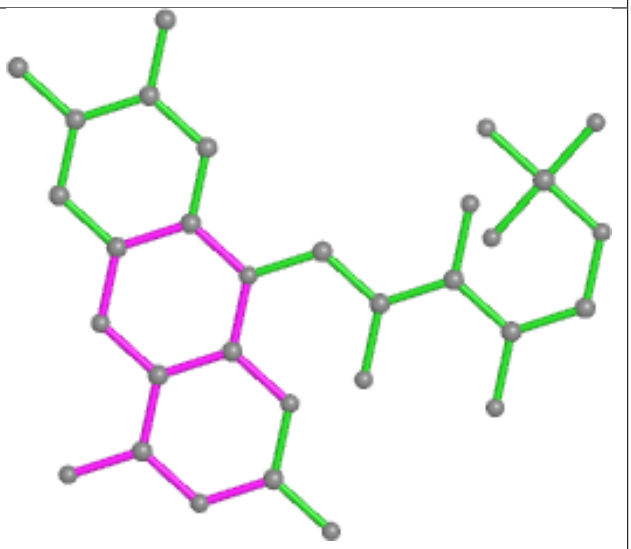


Rings

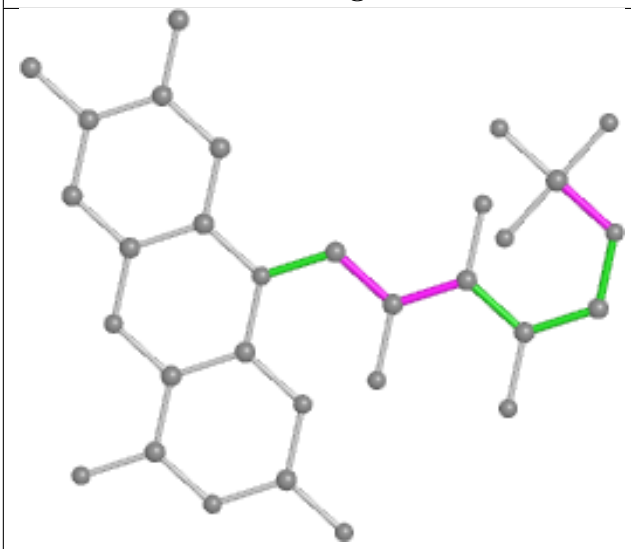
Ligand FMN F 500



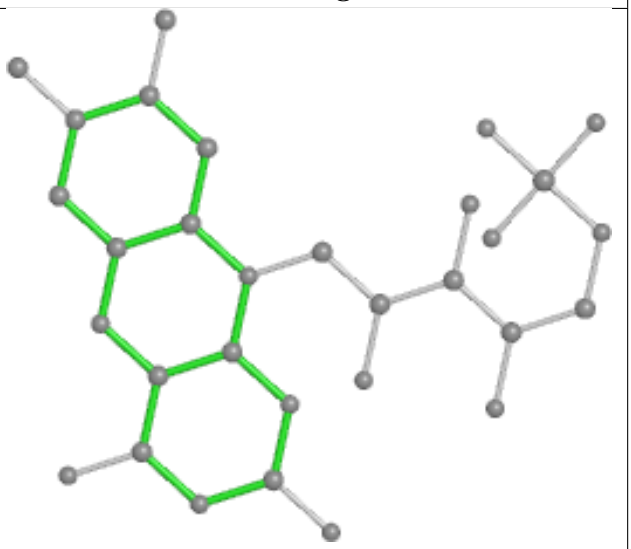
Bond lengths



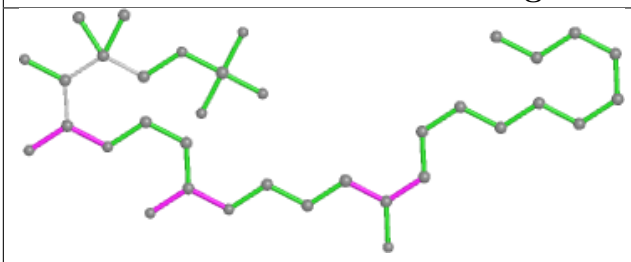
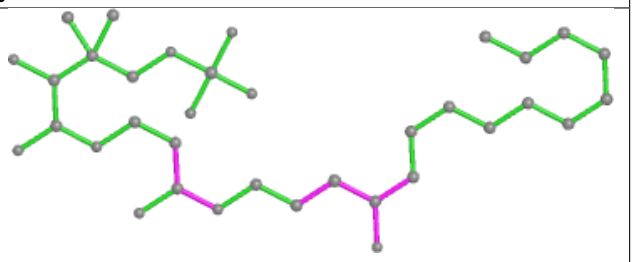
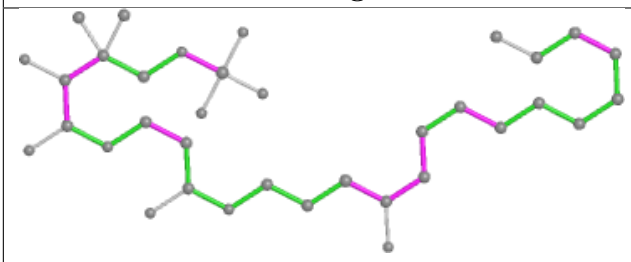
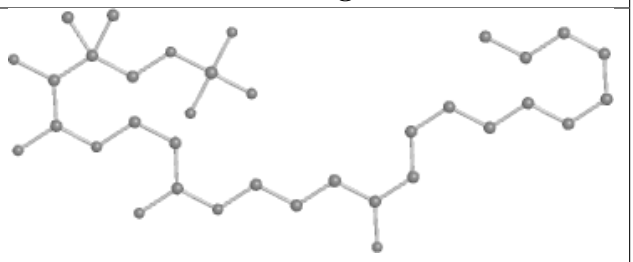
Bond angles

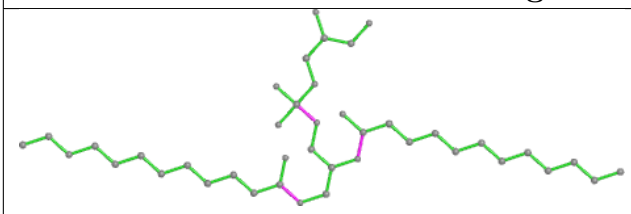
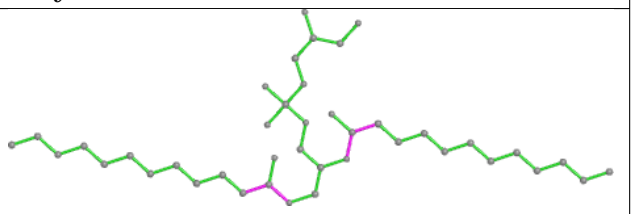
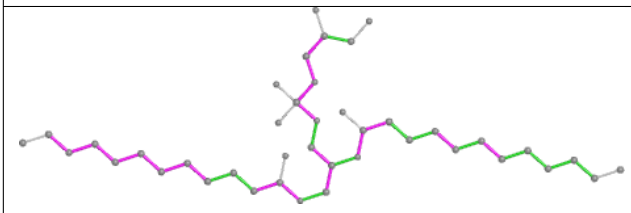
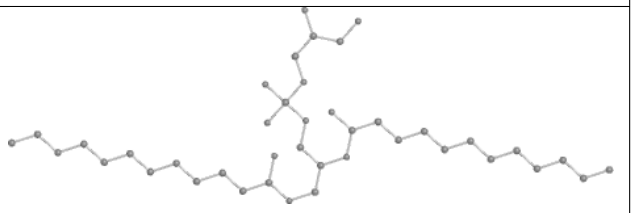


Torsions

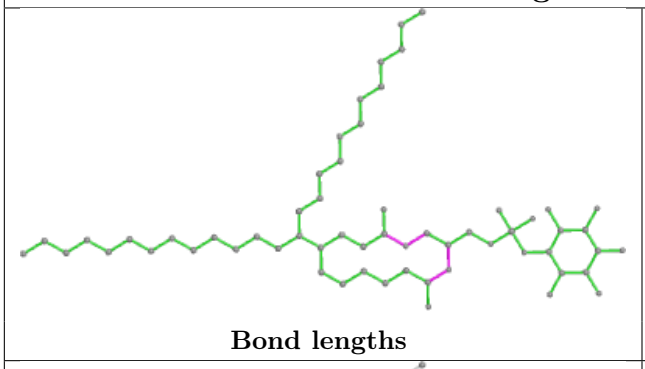


Rings

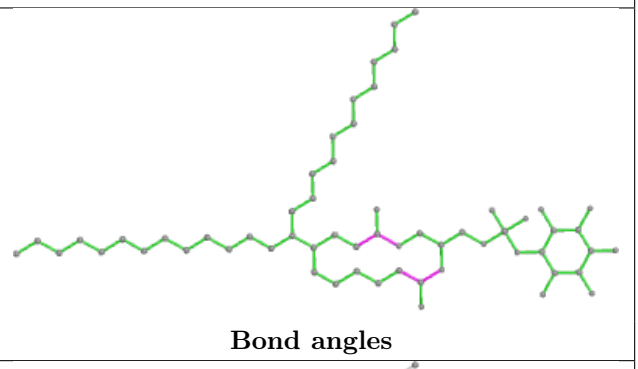
Ligand 8Q1 W 200	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGT y 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

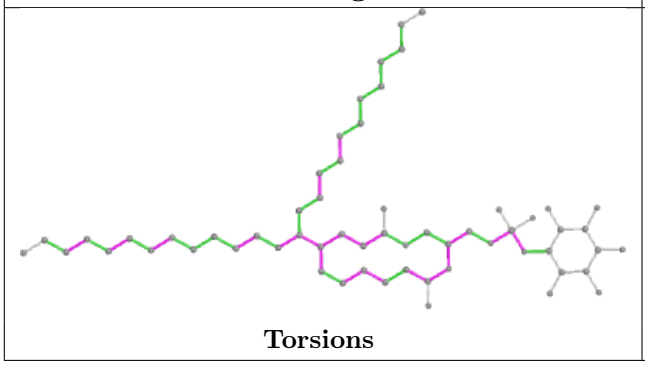
Ligand T7X z 302



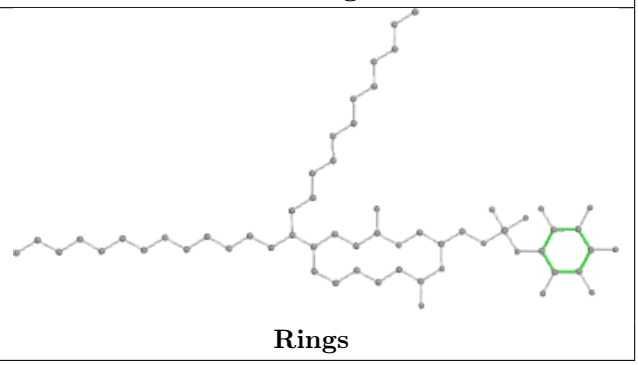
Bond lengths



Bond angles

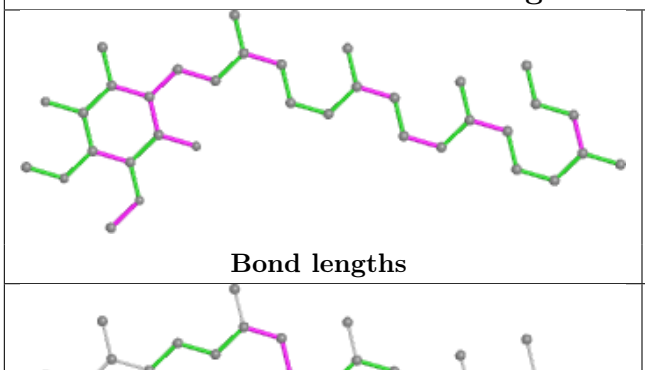


Torsions

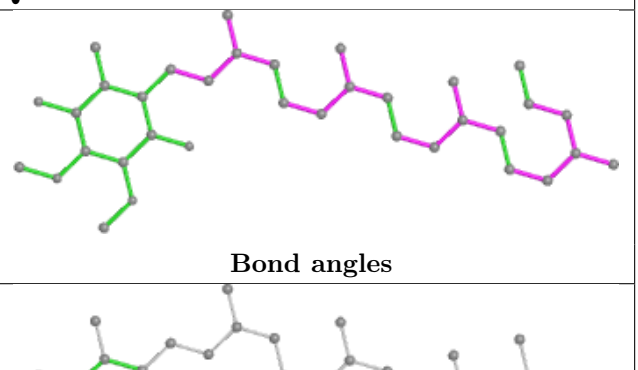


Rings

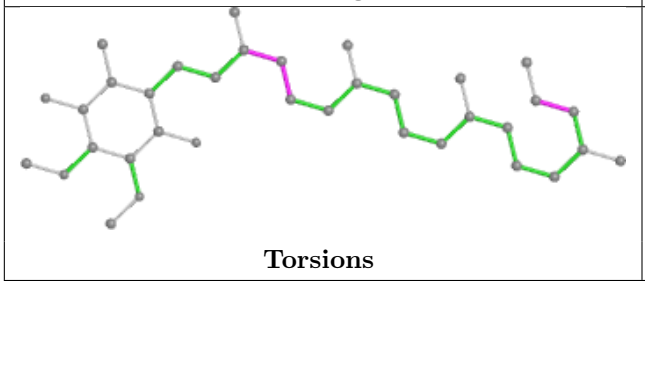
Ligand UQ9 H 500



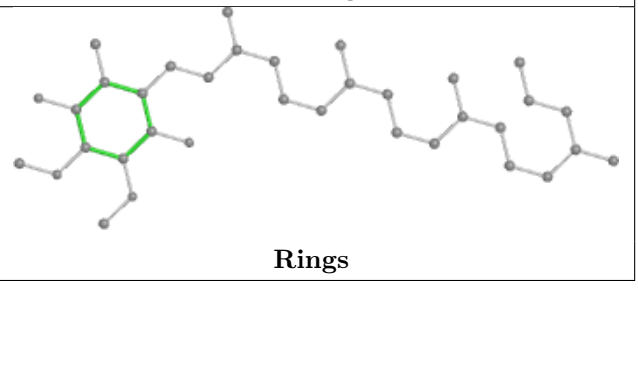
Bond lengths



Bond angles

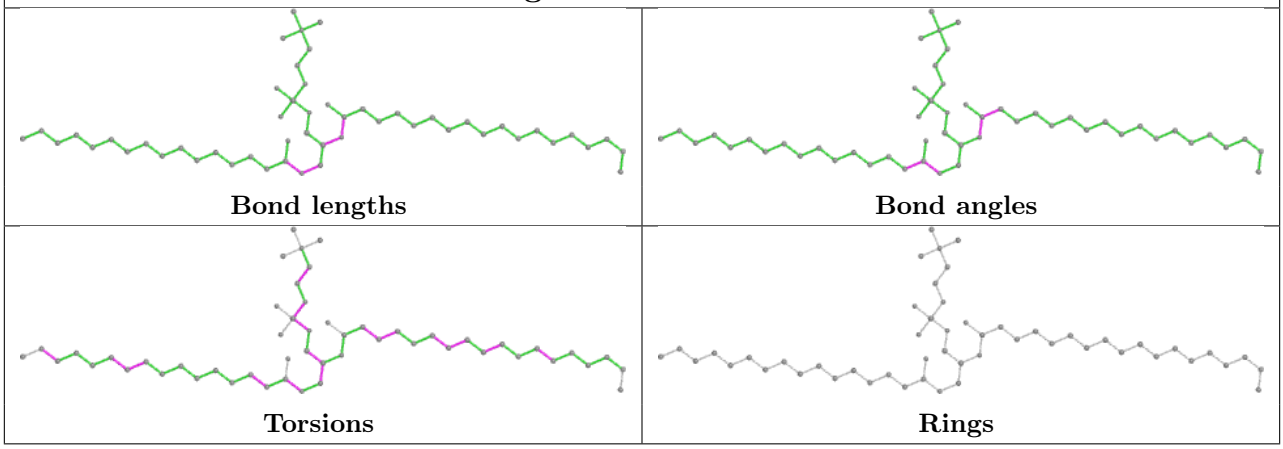


Torsions

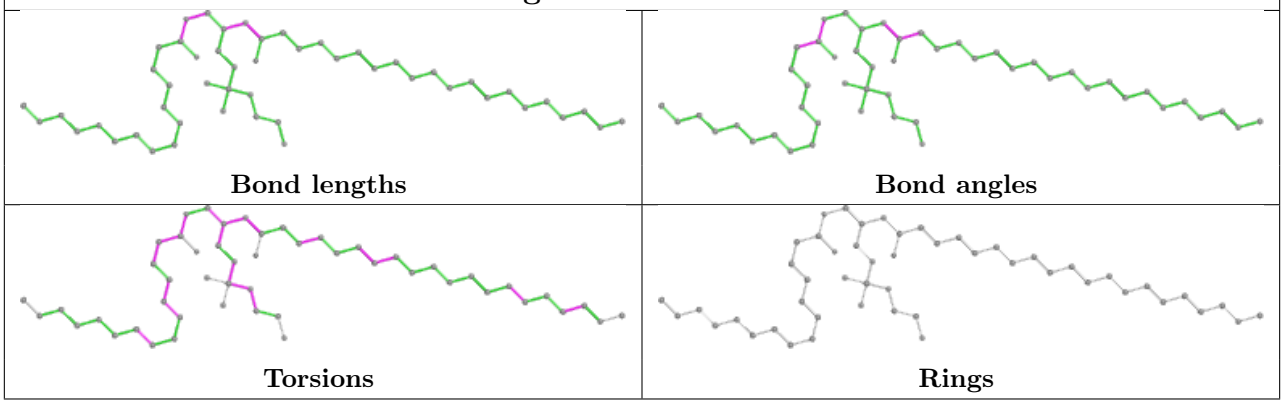


Rings

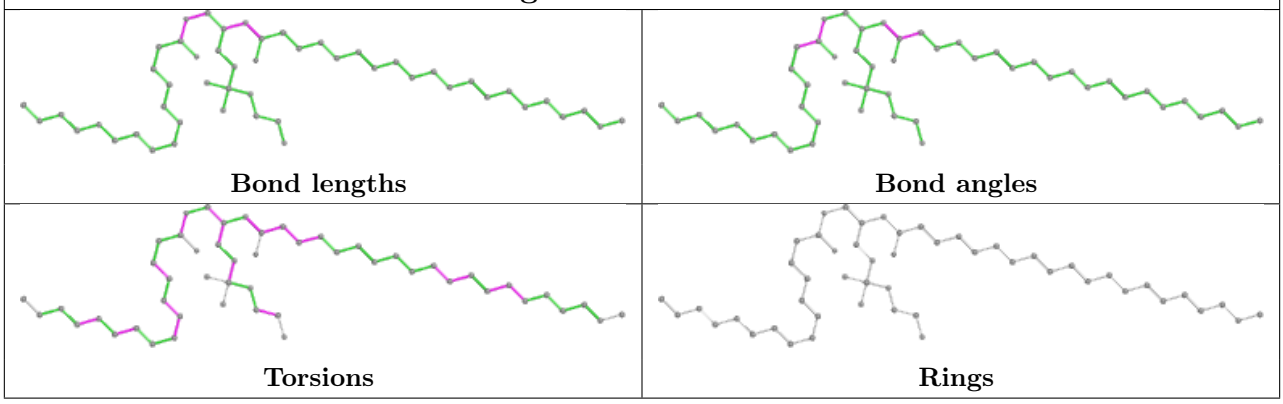
Ligand PC7 M 501



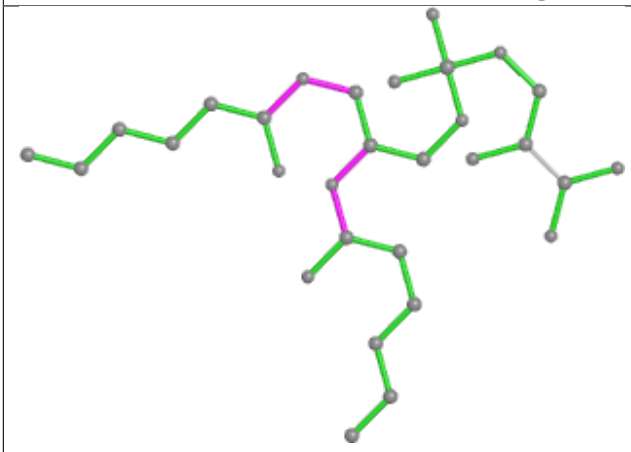
Ligand PTY N 501



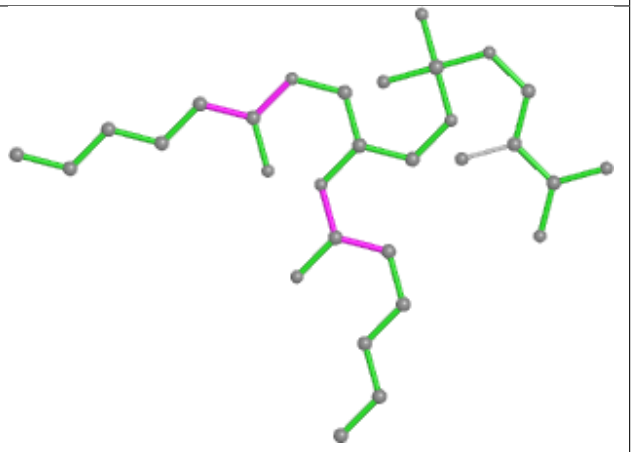
Ligand PTY M 502



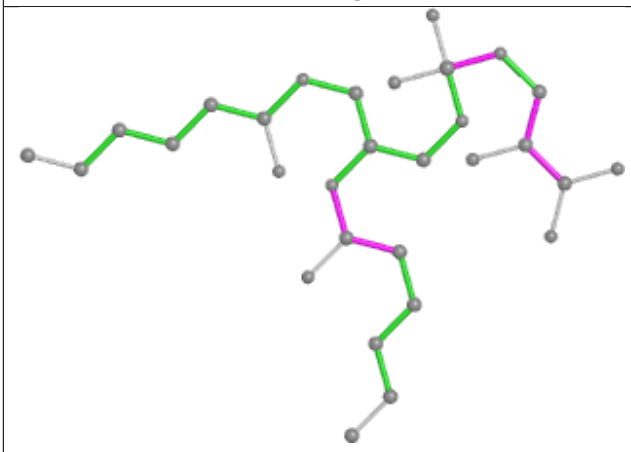
Ligand PSF z 301



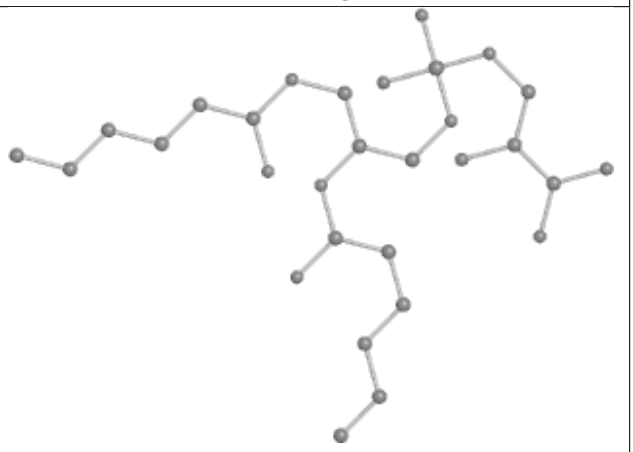
Bond lengths



Bond angles

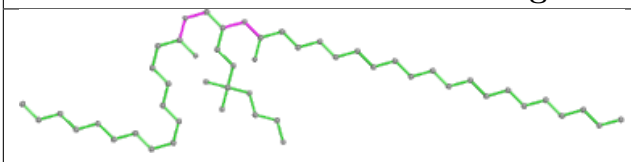


Torsions

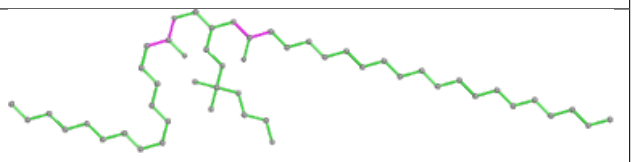


Rings

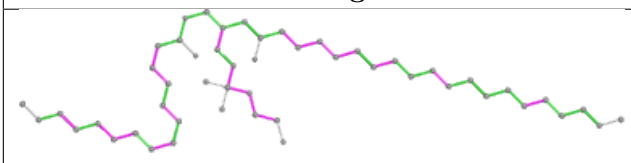
Ligand PTY I 303



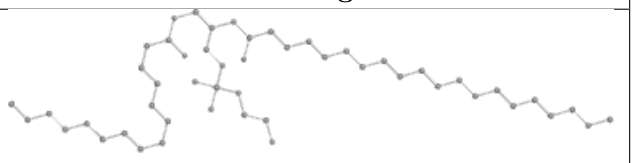
Bond lengths



Bond angles

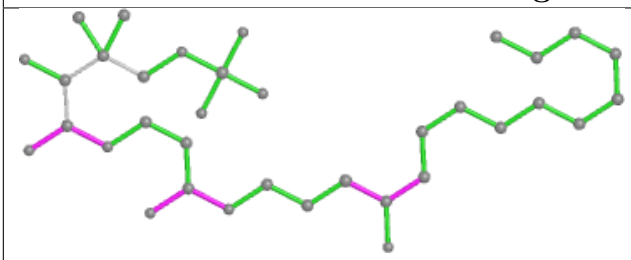


Torsions

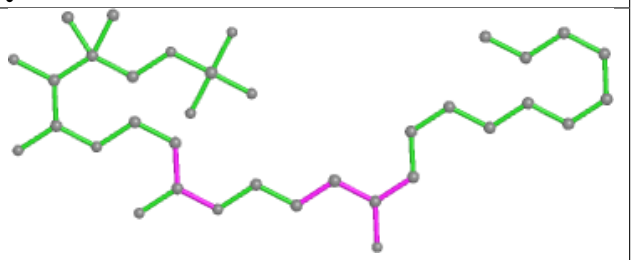


Rings

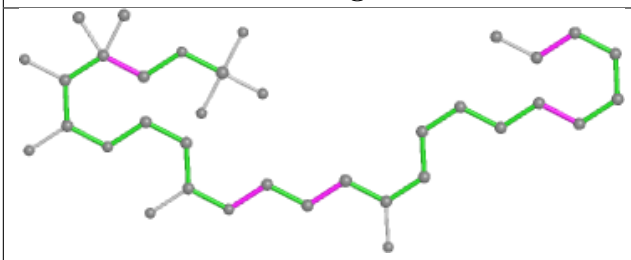
Ligand 8Q1 n 200



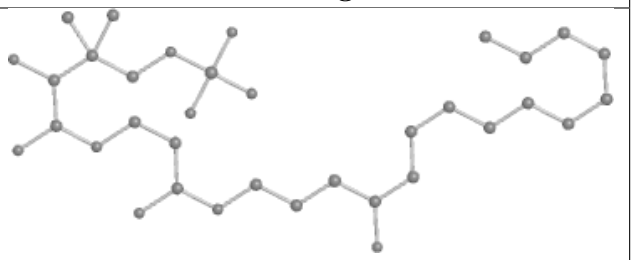
Bond lengths



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.

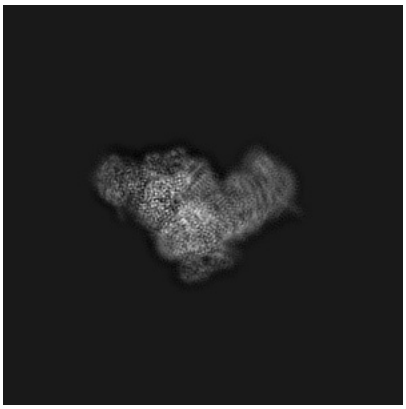
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11875. These allow visual inspection of the internal detail of the map and identification of artifacts.

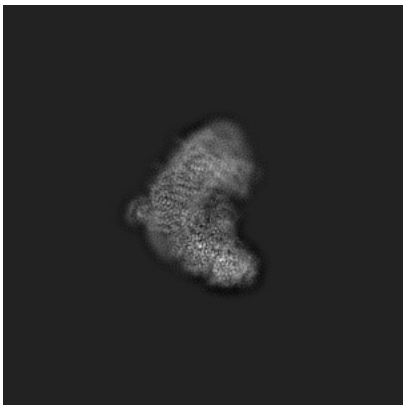
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

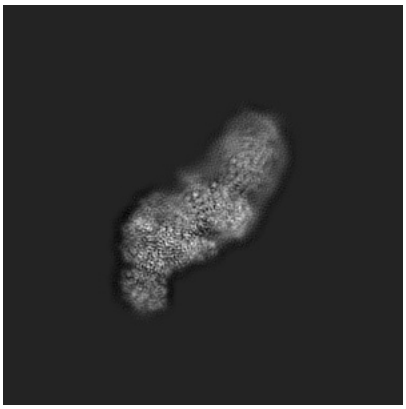
6.1.1 Primary map



X

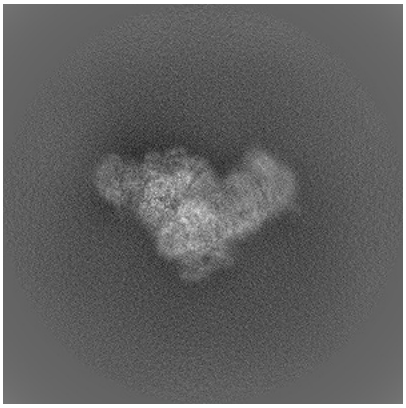


Y

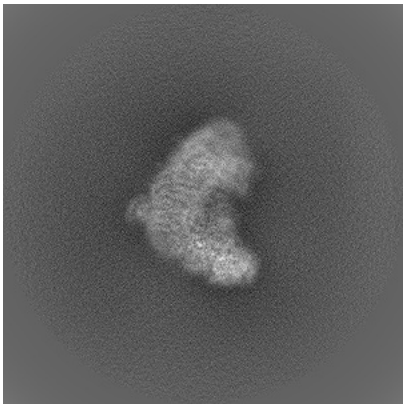


Z

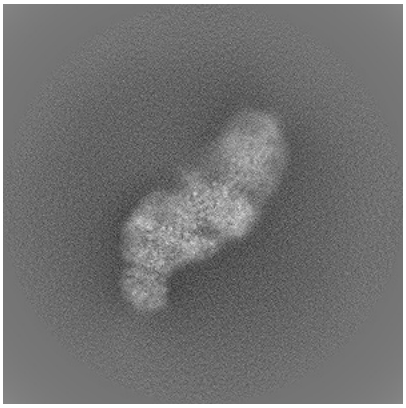
6.1.2 Raw map



X



Y

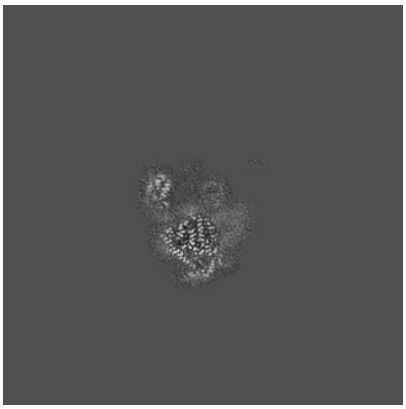


Z

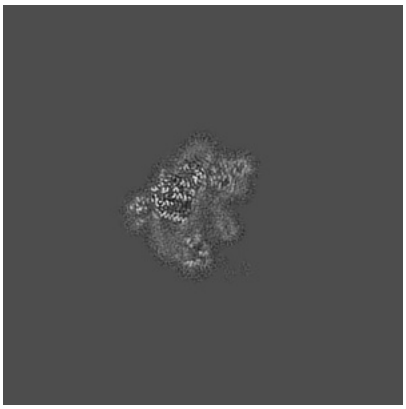
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

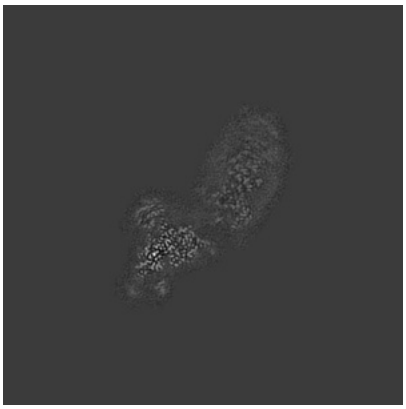
6.2.1 Primary map



X Index: 300

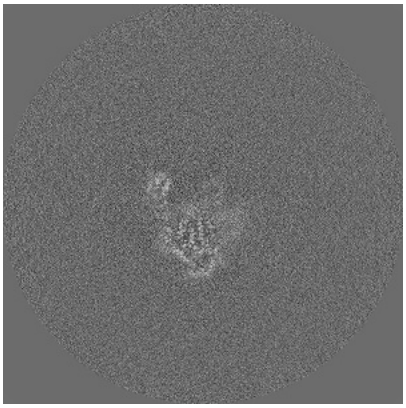


Y Index: 300

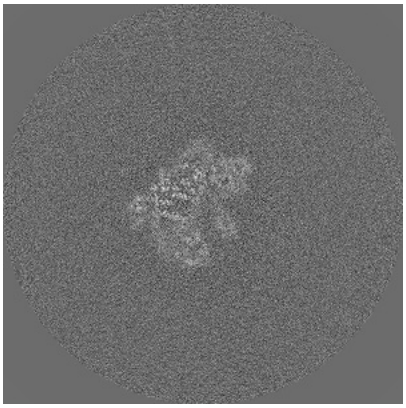


Z Index: 300

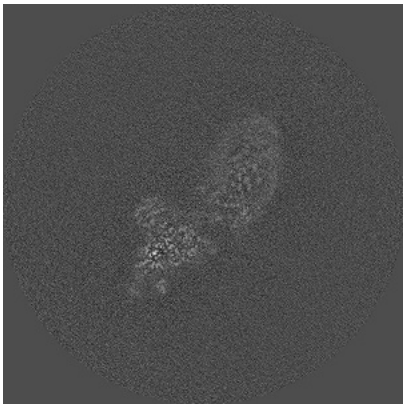
6.2.2 Raw map



X Index: 300



Y Index: 300



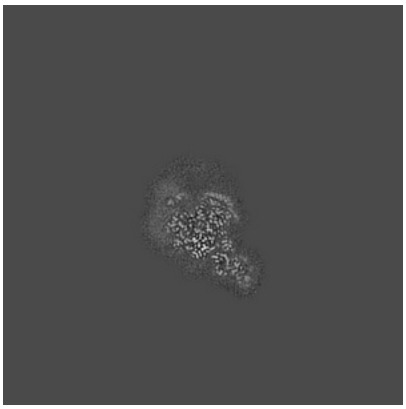
Z Index: 300

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

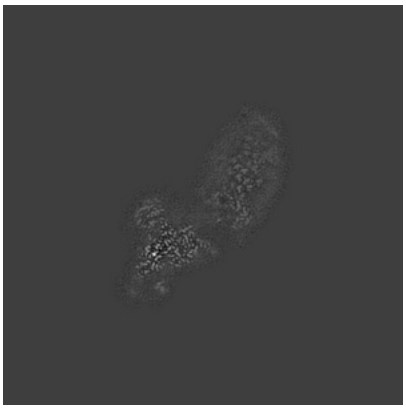
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 224

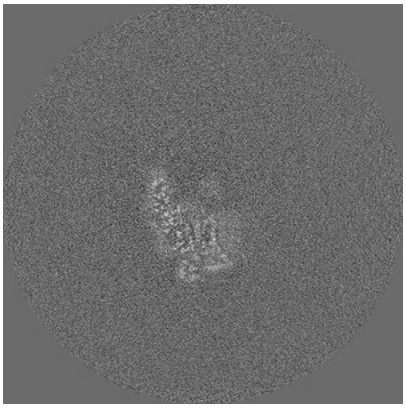


Y Index: 240

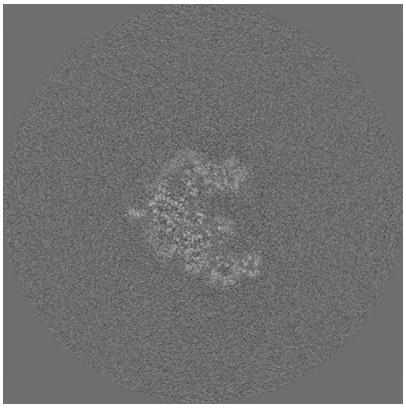


Z Index: 299

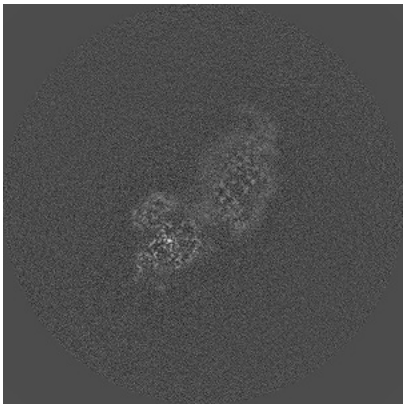
6.3.2 Raw map



X Index: 287



Y Index: 268

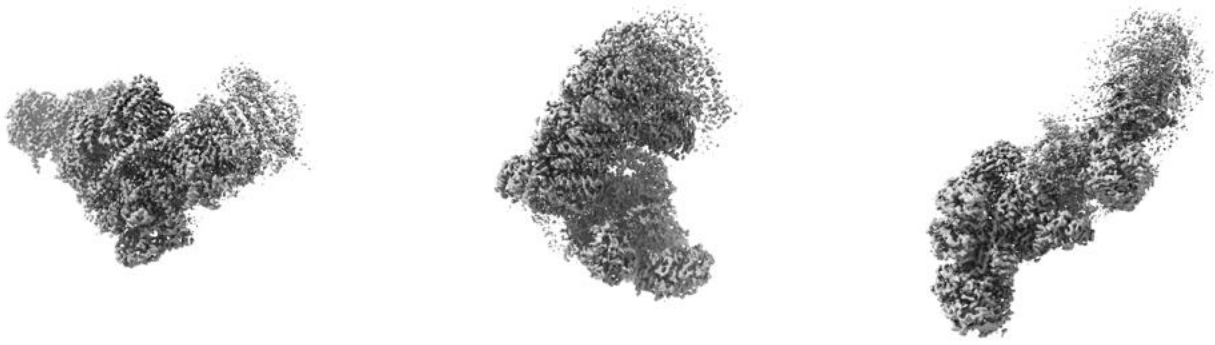


Z Index: 291

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

6.4 Orthogonal surface views (i)

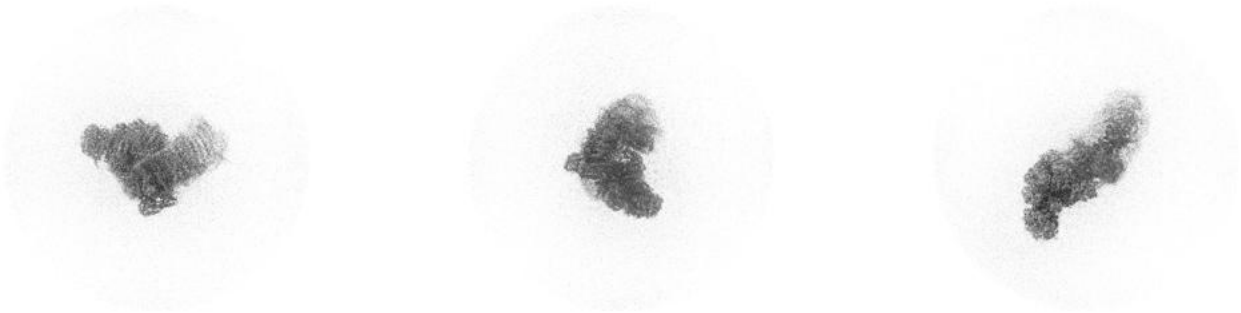
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

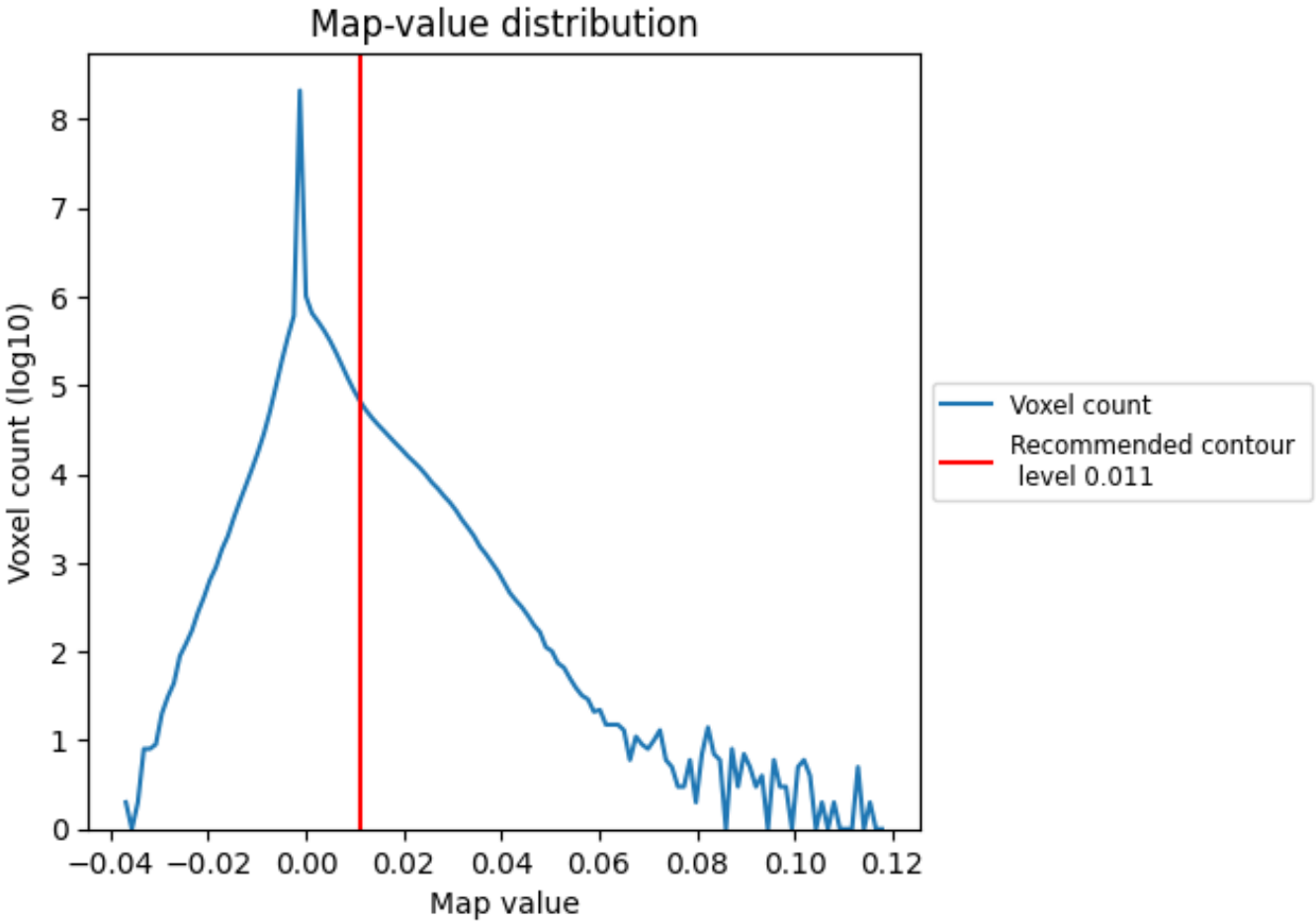
6.5 Mask visualisation (i)

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

7 Map analysis

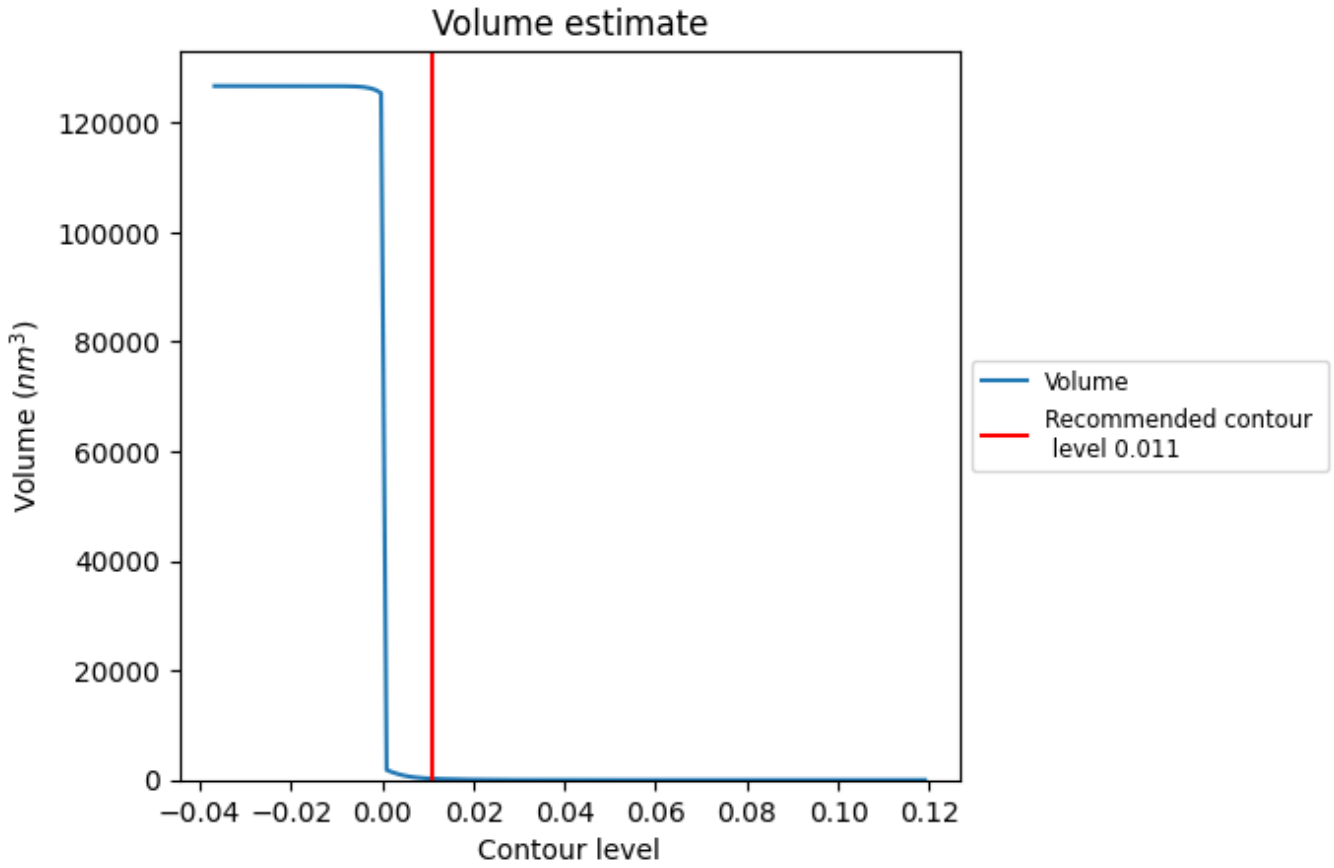
This section contains the results of statistical analysis of the map.

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.

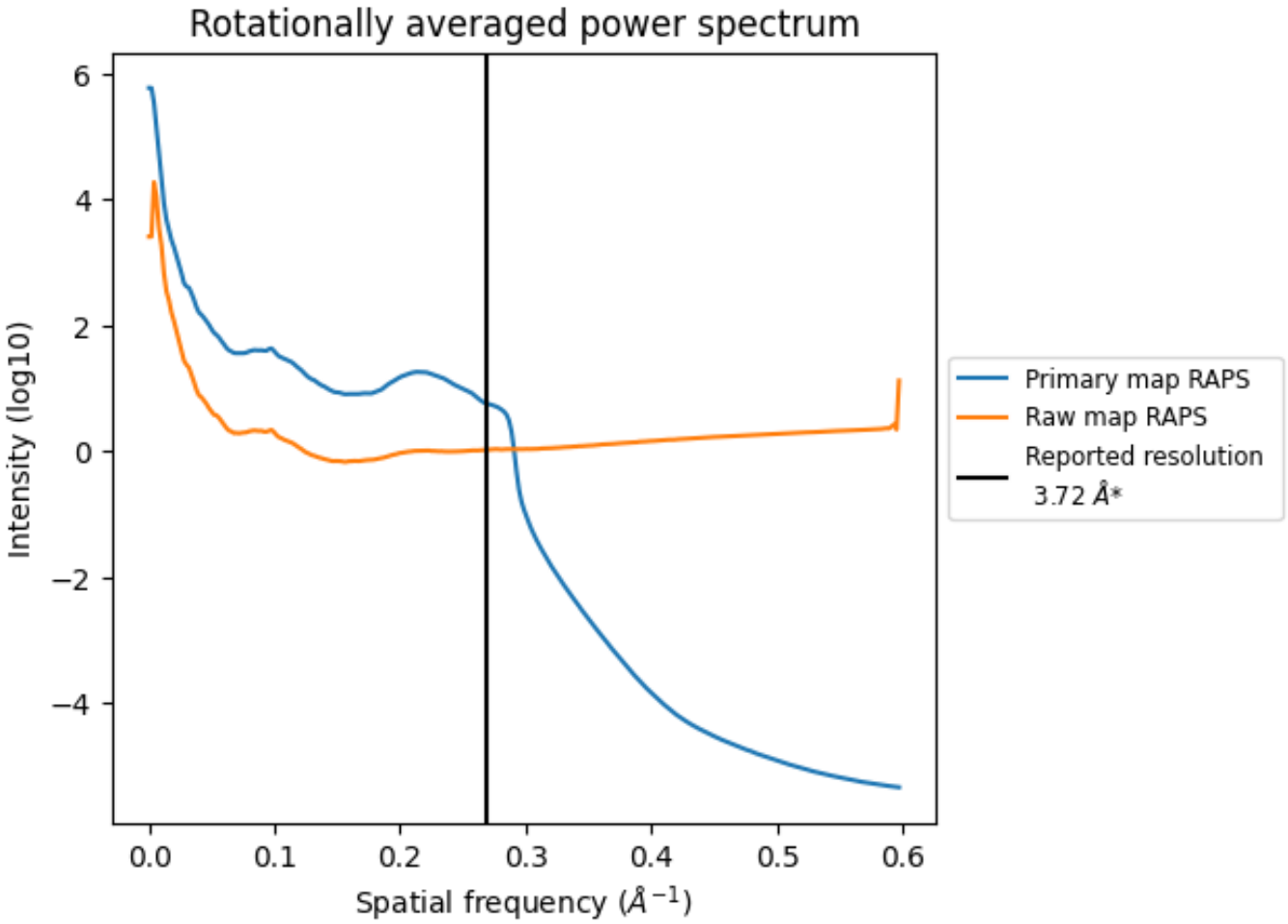
7.2 Volume estimate



The volume at the recommended contour level is 234 nm^3; this corresponds to an approximate mass of 211 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

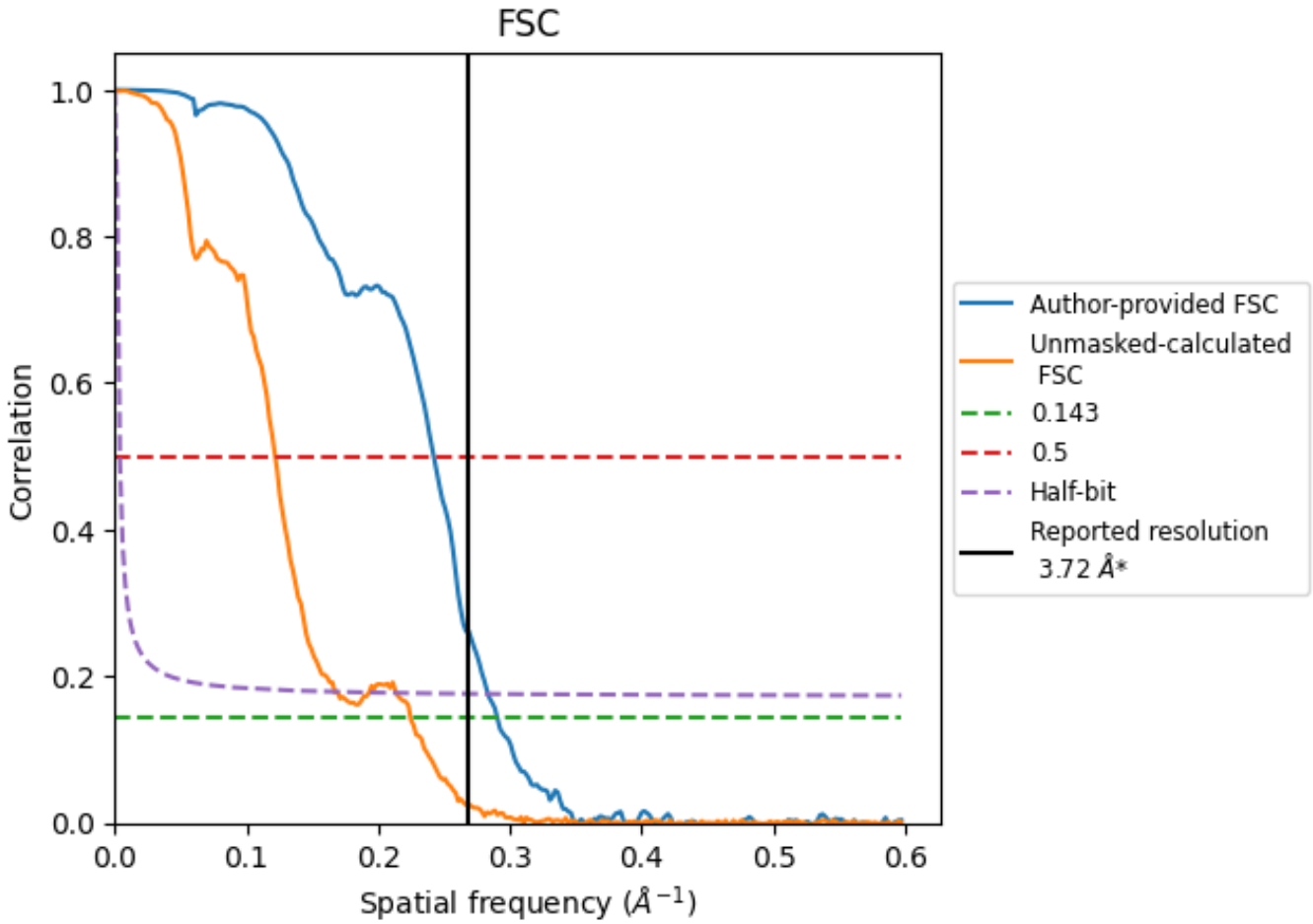


*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.269 Å^{-1}

8.2 Resolution estimates (i)

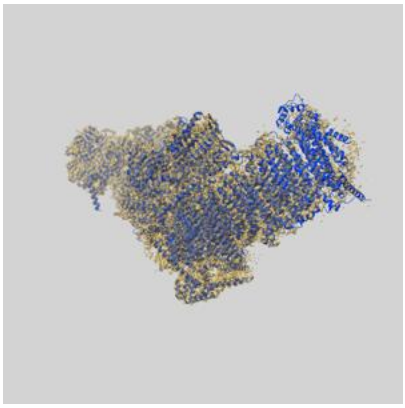
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.44	4.13	3.53
Unmasked-calculated*	4.45	8.20	5.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.45 differs from the reported value 3.72 by more than 10 %

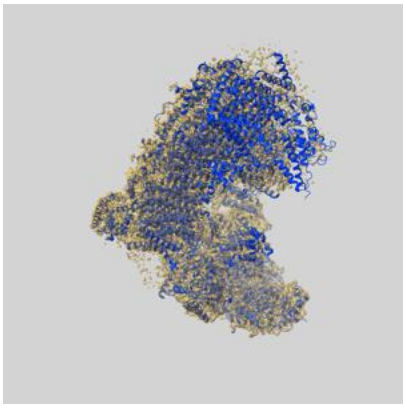
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11875 and PDB model 7AR7. Per-residue inclusion information can be found in section 3 on page 21.

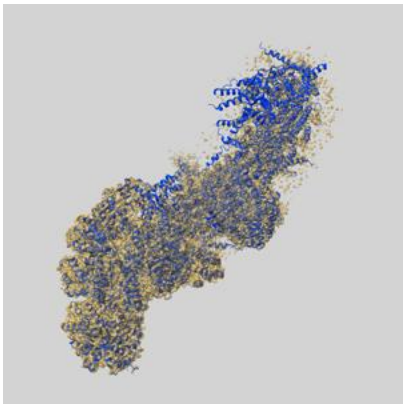
9.1 Map-model overlay



X



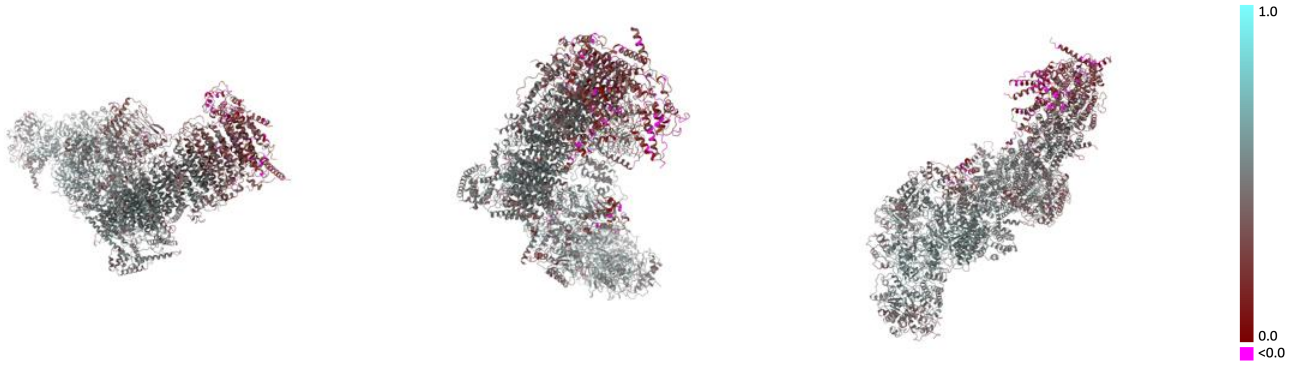
Y



Z

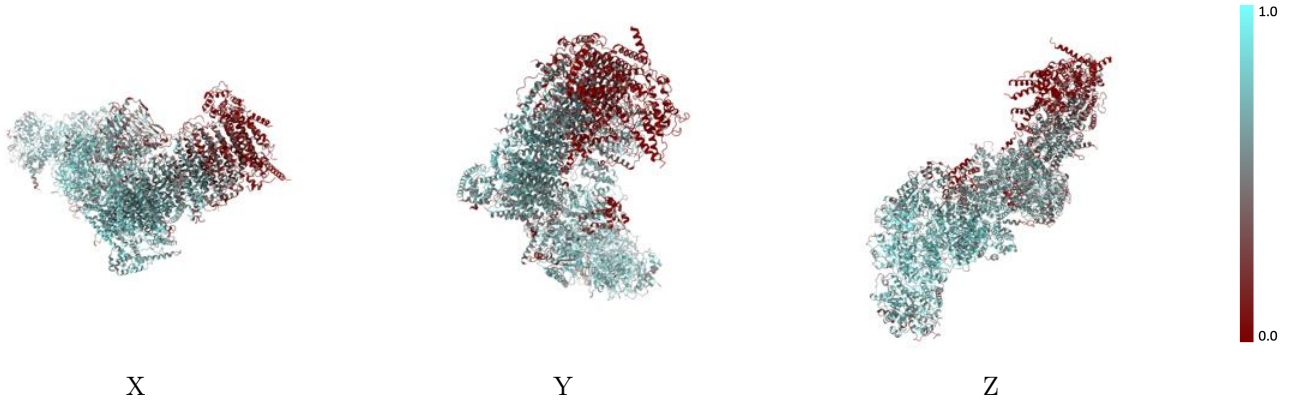
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



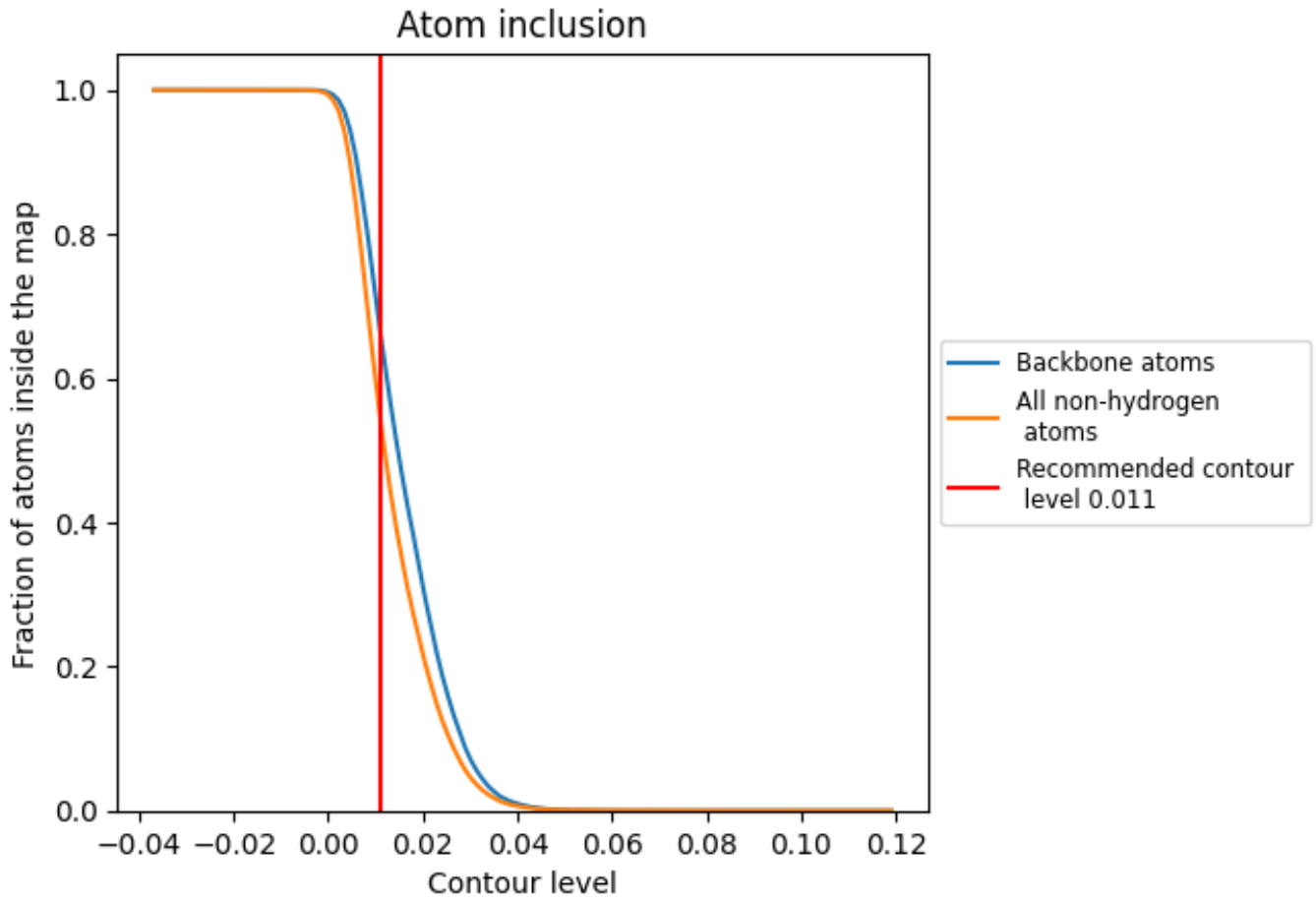
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 54% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5446	0.4380
A	0.6347	0.4980
B	0.7592	0.5290
C	0.7649	0.5350
D	0.7749	0.5320
E	0.6193	0.4410
F	0.6440	0.4680
G	0.7301	0.5110
H	0.6606	0.4930
I	0.7865	0.5380
J	0.6456	0.5010
K	0.5982	0.4920
L	0.1766	0.2760
M	0.5096	0.4500
N	0.6407	0.4990
P	0.5622	0.4460
Q	0.6909	0.5240
R	0.7116	0.5120
S	0.6475	0.4530
T	0.0166	0.1250
U	0.0772	0.2080
V	0.6597	0.4710
W	0.4340	0.3980
X	0.6365	0.4590
Z	0.6594	0.4850
a	0.6558	0.4840
b	0.6323	0.4870
c	0.2446	0.3200
d	0.6378	0.4850
e	0.7021	0.4760
f	0.6755	0.5020
g	0.3899	0.3800
i	0.5977	0.4490
j	0.1089	0.2500
k	0.0635	0.2160

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Chain	Atom inclusion	Q-score
l	0.0767	0.2590
m	0.1764	0.2650
n	0.0493	0.1900
o	0.0980	0.2180
p	0.3815	0.3740
q	0.4032	0.4550
r	0.3415	0.4450
u	0.5133	0.3280
v	0.5747	0.4650
x	0.5154	0.4390
y	0.4453	0.3960
z	0.4978	0.4200