wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 11:58 PM JST

PDB ID	:	7V3M / pdb_00007v3m
EMDB ID	:	EMD-31652
Title	:	Deactive state complex I from rotenone-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-10
Resolution	:	2.90 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

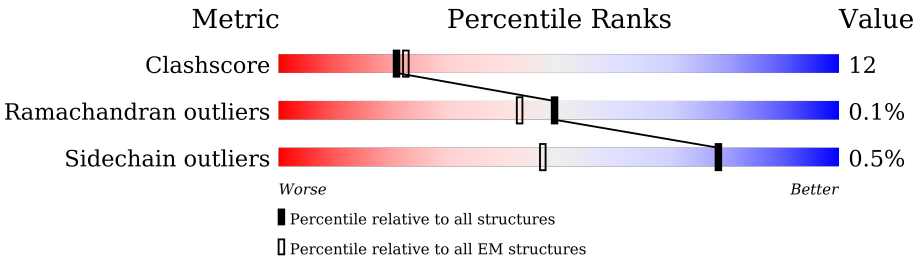
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

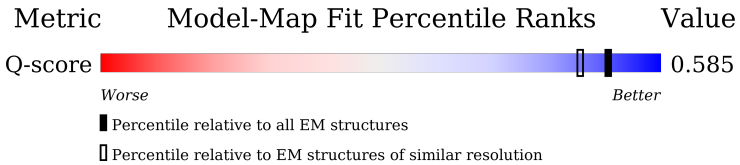
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	431	71% 28%
2	B	176	78% 22%
3	C	156	78% 21%
4	E	115	5% 75% 25%

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Mol	Chain	Length	Quality of chain
5	F	86	9% 64% 36%
6	G	88	33% 56% 43%
6	X	88	6% 76% 24%
7	H	112	73% 27%
8	I	112	68% 19% 13%
9	J	341	5% 65% 22% 13%
10	K	42	5% 74% 26%
11	L	125	6% 85% 15%
12	M	690	82% 18%
13	N	144	75% 25%
14	O	217	73% 27%
15	P	208	80% 19%
16	Q	430	75% 22%
17	S	70	89% 11%
18	T	96	6% 93% 7%
19	U	83	89% 11%
20	V	140	13% 84% 16%
21	W	142	80% 20%
22	Y	70	17% 71% 26%
23	Z	84	27% 88% 12%
24	a	140	80% 19%
25	b	126	14% 58% 23% 18%
26	c	156	10% 72% 28%
27	d	175	9% 81% 19%
28	e	107	17% 76% 24%

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Mol	Chain	Length	Quality of chain
29	f	42	12% 86% 14%
30	g	121	90% 10%
31	h	105	83% 17%
32	i	347	76% 24%
33	j	113	12% 60% 27% 12%
34	k	98	77% 23%
35	l	603	73% 27%
36	m	175	6% 56% 18% 26%
37	n	56	20% 68% 29%
38	o	128	7% 90% 10%
39	p	178	6% 71% 25%
40	r	459	75% 24%
41	s	318	75% 20% 5%
42	u	171	75% 18% 6%
43	v	131	20% 71% 24% 5%
44	w	320	7% 70% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
48	PEE	Q	501	-	-	X	-
48	PEE	l	704	-	-	X	-
51	CDL	a	201	-	-	X	-
51	CDL	l	701	-	-	X	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 66644 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3318	2095	591	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7,mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0
6	X	88	696	449	103	139	5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	112	910	588	154	165	3	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	97	762	479	144	136	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	297	2359	1514	421	416	8	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	42	355	219	67	68	1	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	125	1016	642	181	190	3	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	690	5296	3320	923	1014	39	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	144	1204	770	218	212	4	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1671	1065	281	315	10	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1738	1124	298	314	2	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	419	3377	2162	578	613	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	567	364	104	94	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	96	741	452	140	146	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	83	643	417	110	115	1	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	140	1021	651	174	190	6	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1161	749	197	206	9	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	70	583	386	98	98	1	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	84	674	437	116	120	1	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	140	1152	754	196	199	3	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	103	875	571	158	145	1	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	156	1315	853	213	241	8	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	175	1461	916	265	272	8	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	107	890	568	145	173	4	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	42	342	225	58	59	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	121	1000	650	173	171	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	105	867	550	161	150	6	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2706	1779	419	462	46	0	0

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	99	800	545	118	132	5	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	98	748	493	113	128	14	0	0

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4785	3173	741	820	51	0	0

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	129	948	636	138	166	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	456	295	83	77	1	0	0

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

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	o	128	1058	688	181	189	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	178	1534	982	279	265	8	0	0

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3631	2412	572	609	38	0	0

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	303	2394	1607	369	397	21	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	171	1398	887	250	251	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1020	637	189	185	9	0	0

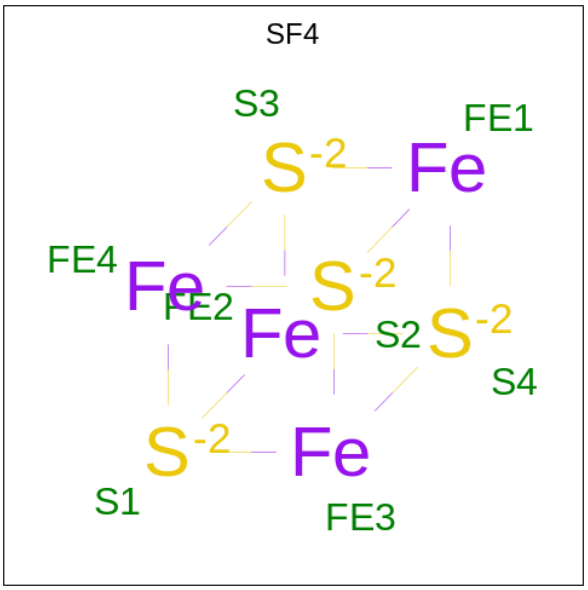
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

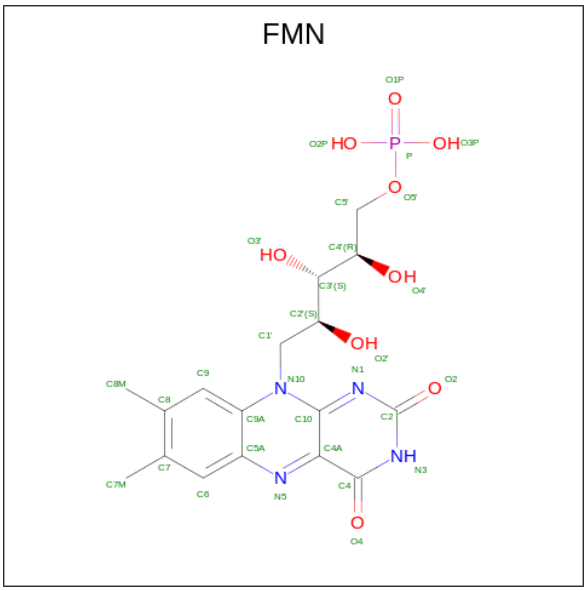
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2574	1638	437	489	10	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



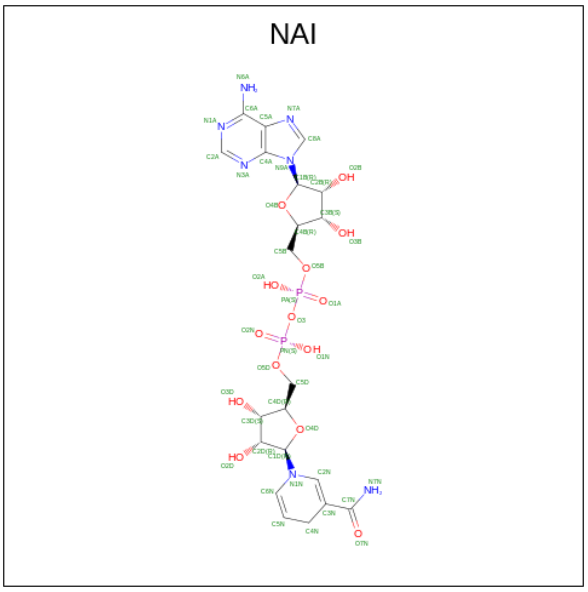
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	8	4	4	0
45	B	1	8	4	4	0
45	C	1	8	4	4	0
45	M	1	8	4	4	0
45	M	1	8	4	4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

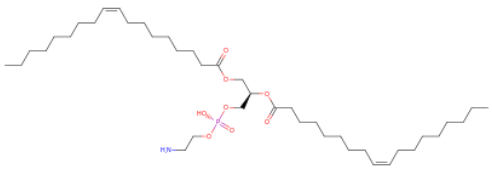
- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).

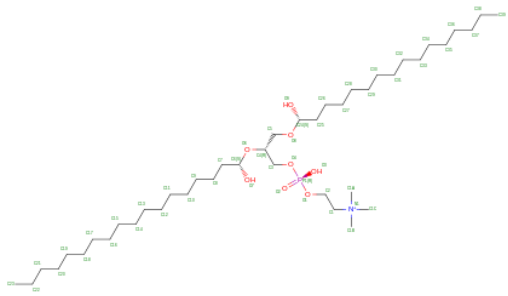
PEE



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	51	41	1	8	1	0
			Total	C	N	O	P	
48	C	1	47	37	1	8	1	0
			Total	C	N	O	P	
48	Q	1	47	37	1	8	1	0
			Total	C	N	O	P	
48	W	1	41	31	1	8	1	0
			Total	C	N	O	P	
48	j	1	51	41	1	8	1	0
			Total	C	N	O	P	
48	l	1	46	36	1	8	1	0
			Total	C	N	O	P	
48	l	1	46	36	1	8	1	0
			Total	C	N	O	P	
48	r	1	51	41	1	8	1	0

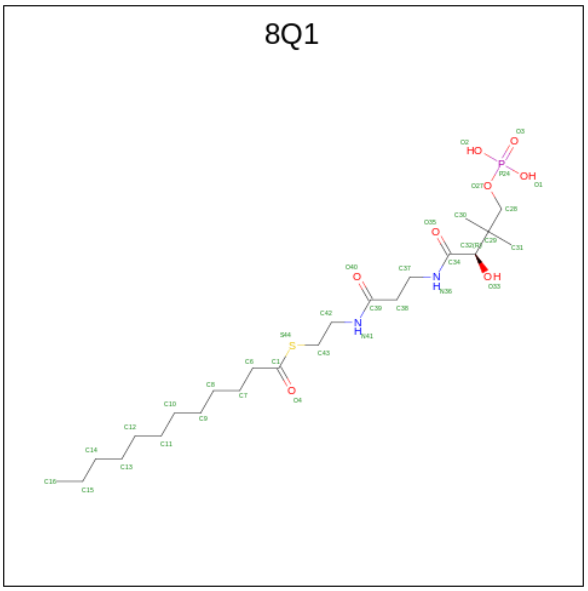
- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).

PLX



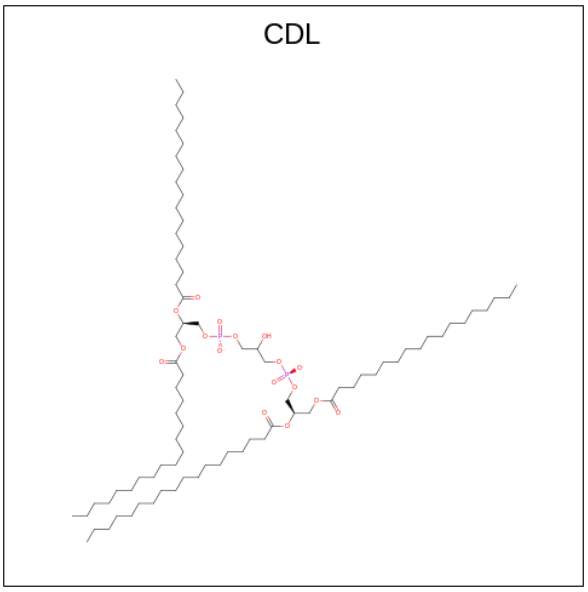
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	52	42	1	8	1	0
49	a	1	52	42	1	8	1	0
49	g	1	52	42	1	8	1	0
49	j	1	52	42	1	8	1	0
49	r	1	52	42	1	8	1	0
49	r	1	52	42	1	8	1	0

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
50	G	1	35	23	2	8	1	1	0
50	X	1	35	23	2	8	1	1	0

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	I	1	51	32	17	2	0

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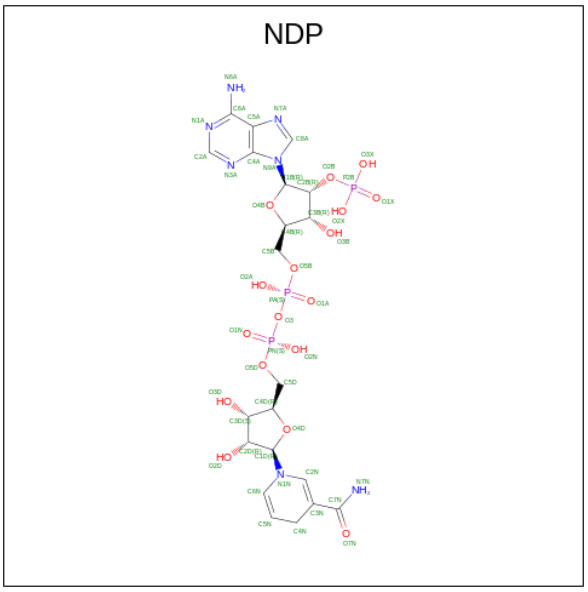
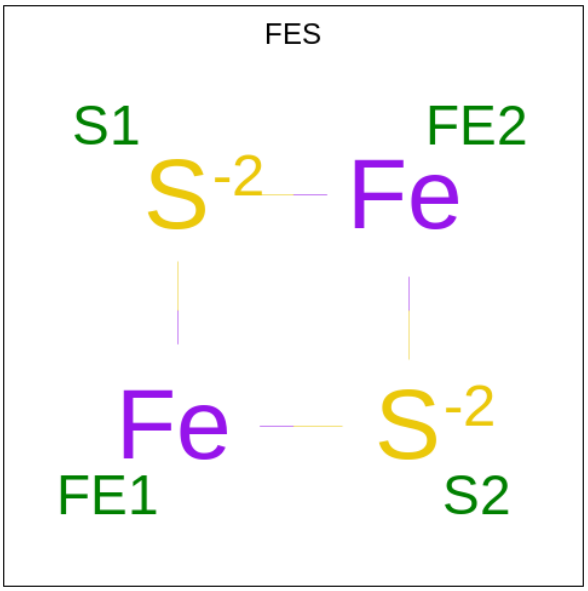
Mol	Chain	Residues	Atoms				AltConf
51	a	1	Total 91	C 72	O 17	P 2	0
51	i	1	Total 66	C 47	O 17	P 2	0
51	l	1	Total 99	C 80	O 17	P 2	0
51	l	1	Total 100	C 81	O 17	P 2	0
51	r	1	Total 100	C 81	O 17	P 2	0
51	u	1	Total 78	C 59	O 17	P 2	0

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
53	M	1	4	2	2	0
53	O	1	4	2	2	0

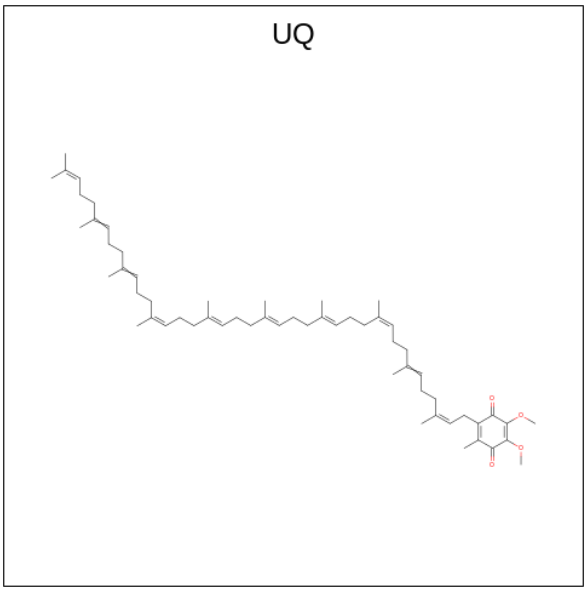
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	M	1	1	1	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

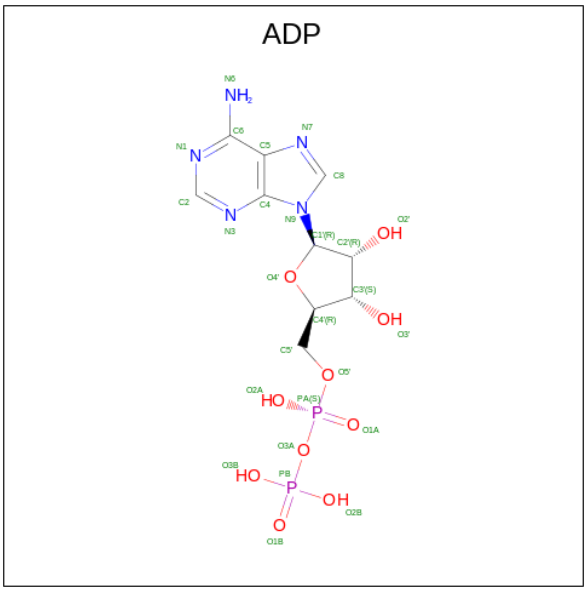
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	T	1	1	1	0

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
56	s	1	28	24	4	0

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



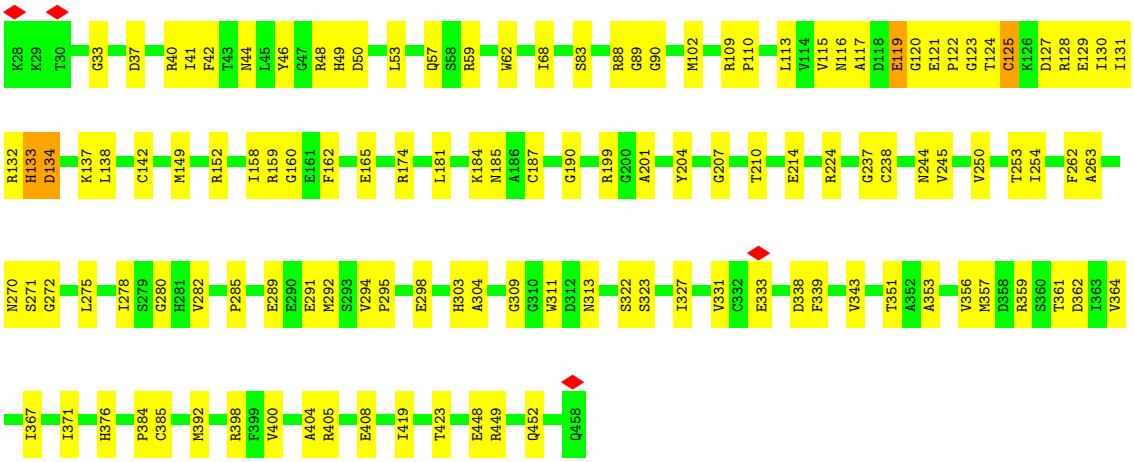
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

3 Residue-property plots (i)

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

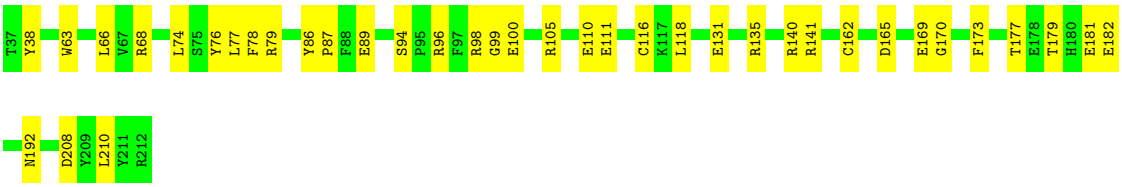
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A: 71% 28%



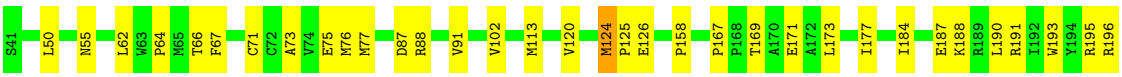
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B: 78% 22%



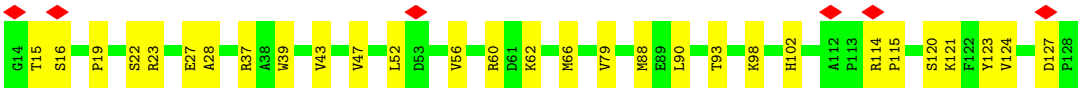
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7,mitochondrial

Chain C: 78% 21%



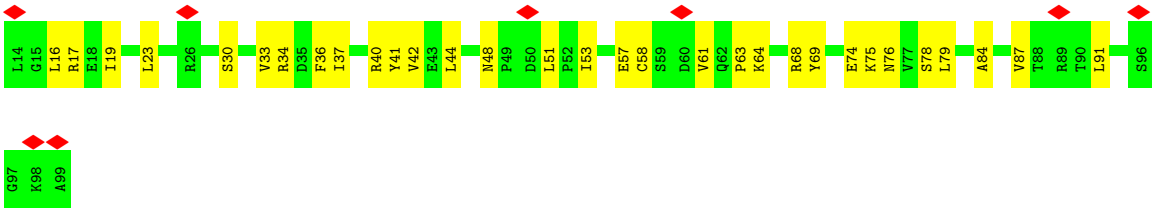
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 5% 75% 25%



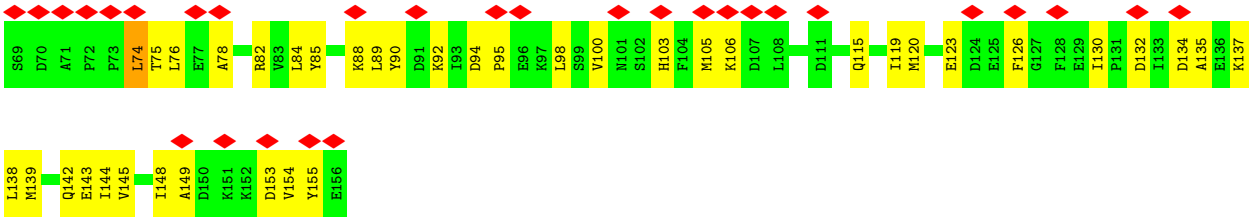
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 9% 64% 36%



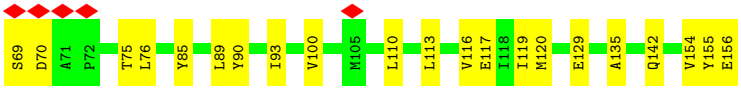
• Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 33% 56% 43%



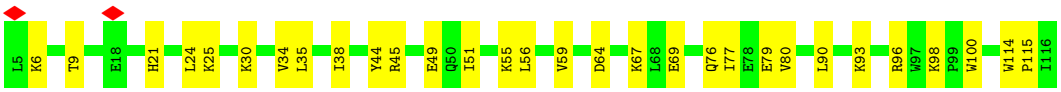
• Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 6% 76% 24%



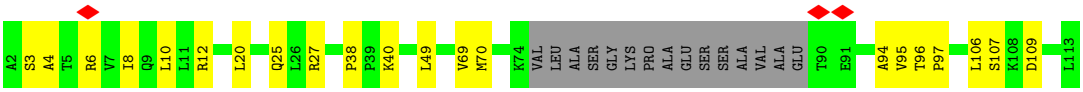
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H: 73% 27%



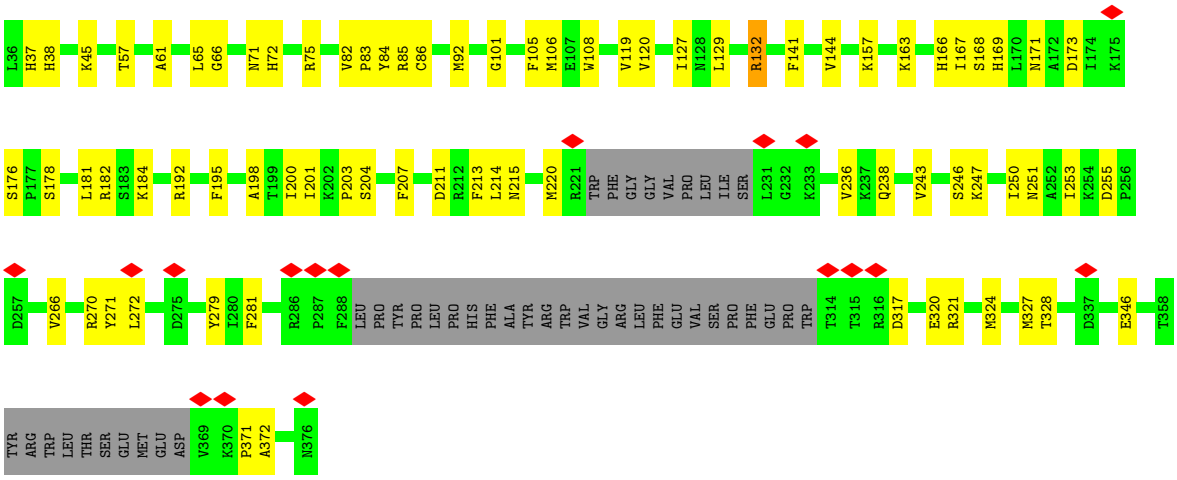
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 68% 19% 13%



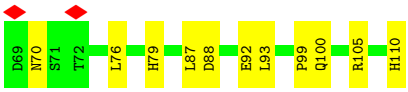
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J:



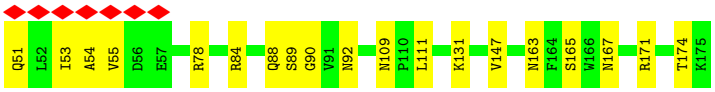
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K:



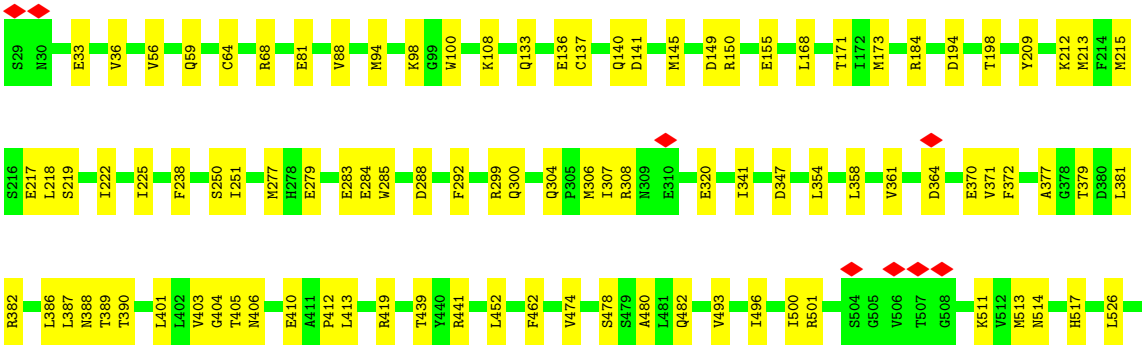
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



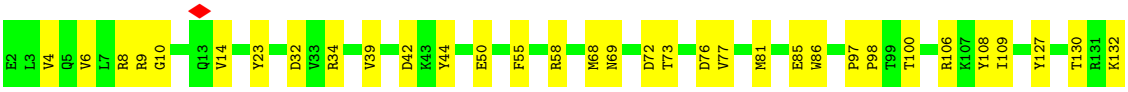
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

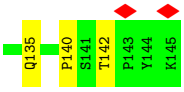
Chain M:



• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

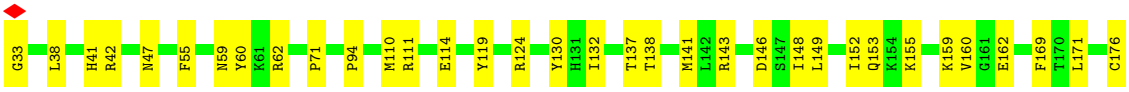
Chain N:

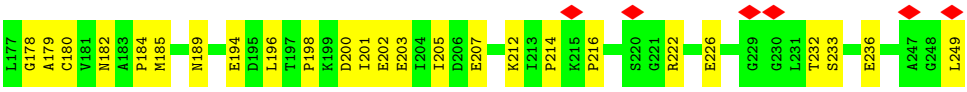




• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

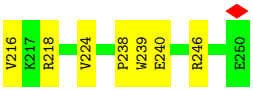
Chain O:





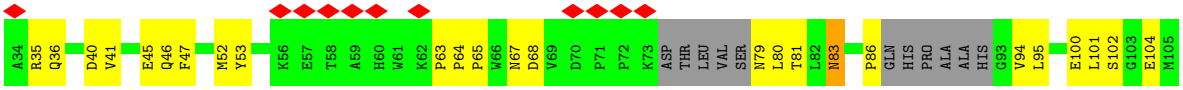
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

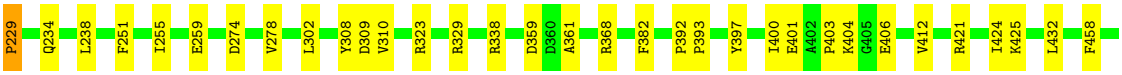
Chain P:



• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

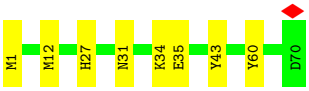
Chain Q:





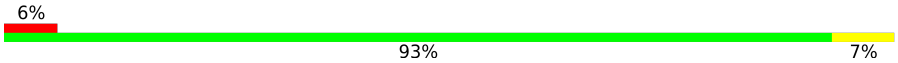
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

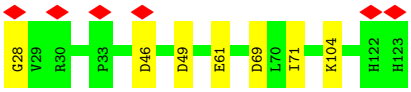
Chain S:



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

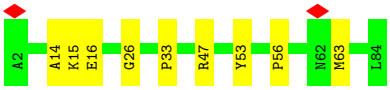
Chain T:





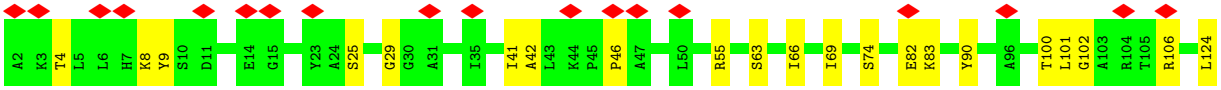
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:



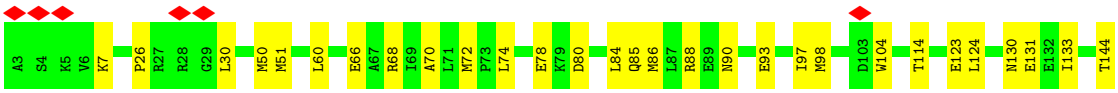
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:



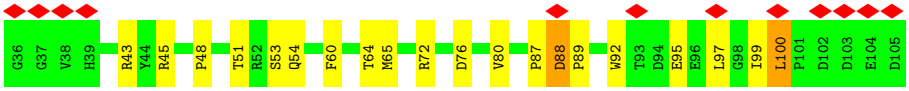
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:



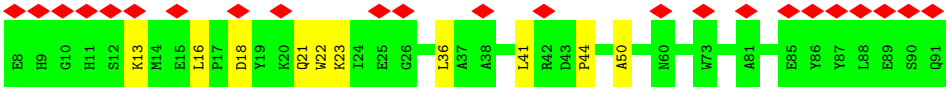
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:



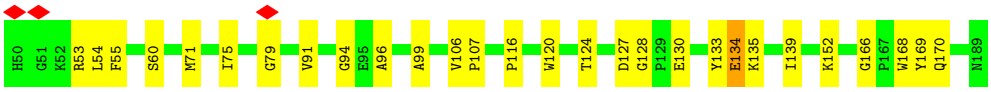
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:



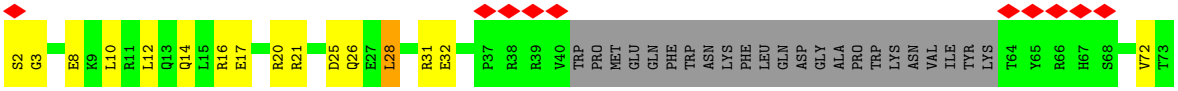
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

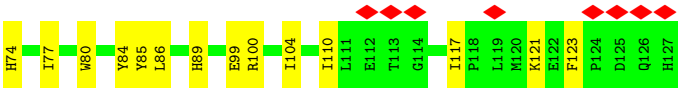
Chain a:



• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

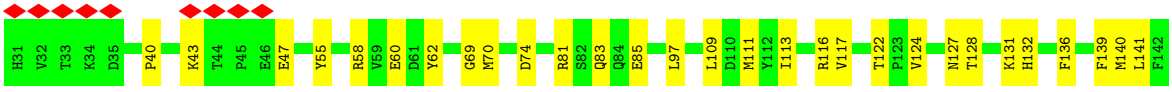
Chain b:

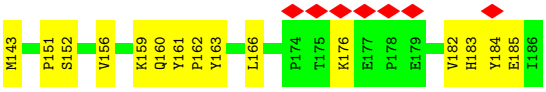




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

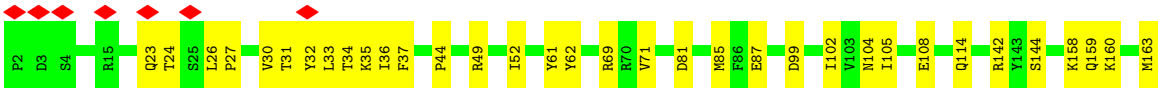
Chain c:

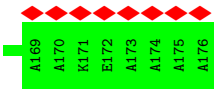




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

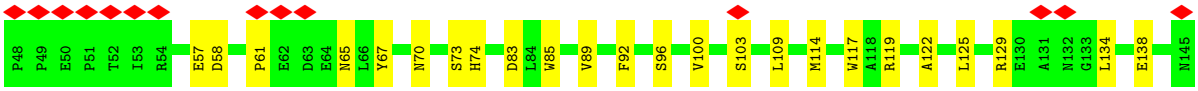
Chain d:

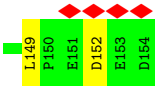




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

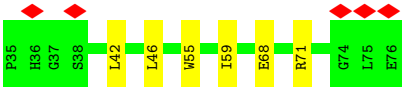
Chain e:





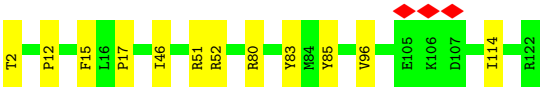
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:



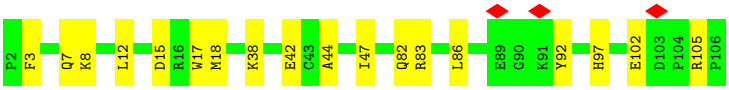
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:



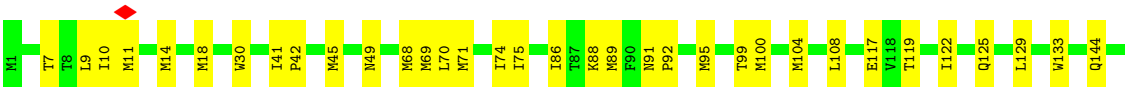
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

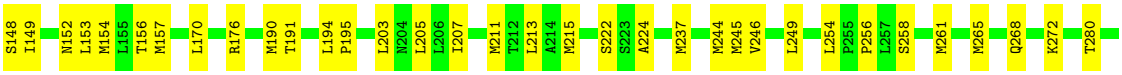
Chain h:



• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

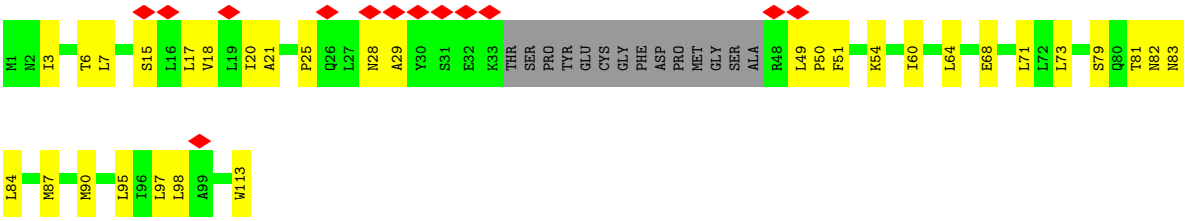
Chain i:





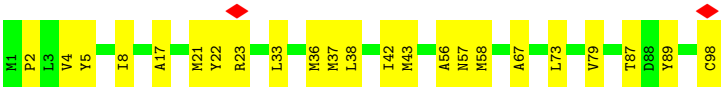
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:



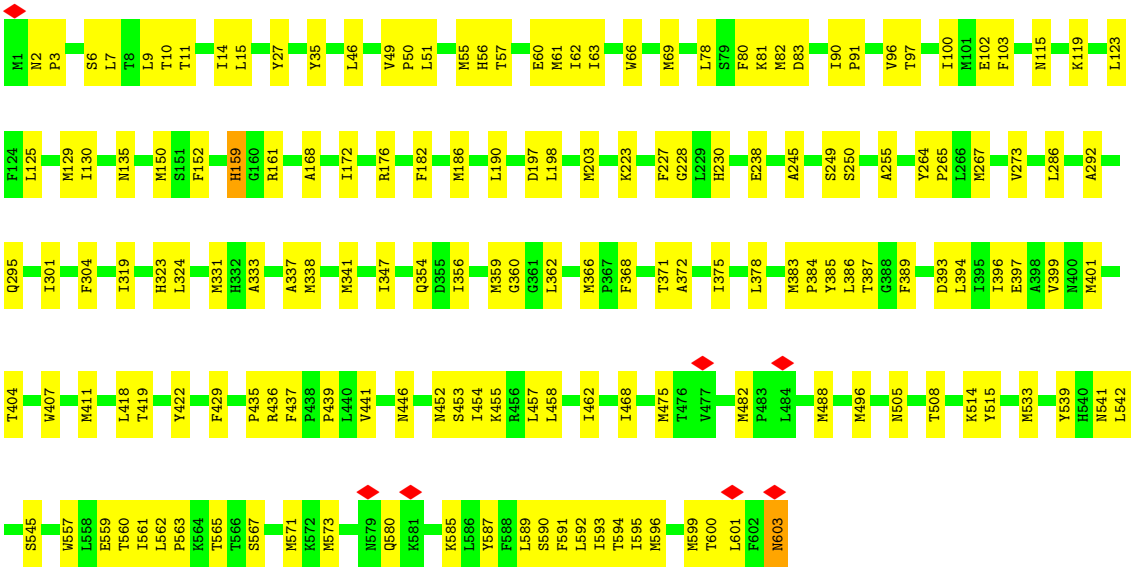
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:



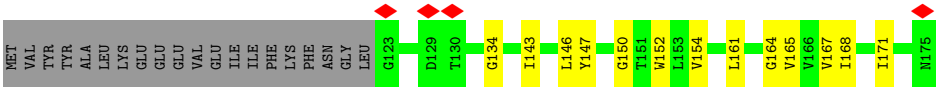
• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:

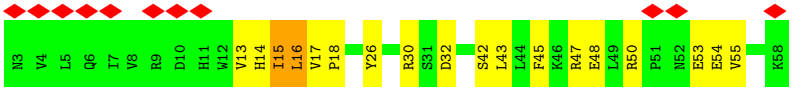


• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

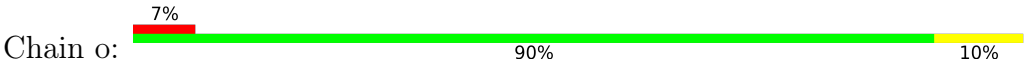
Chain m:

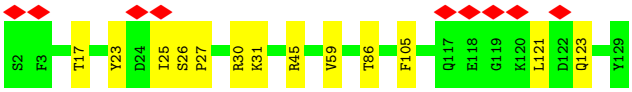


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

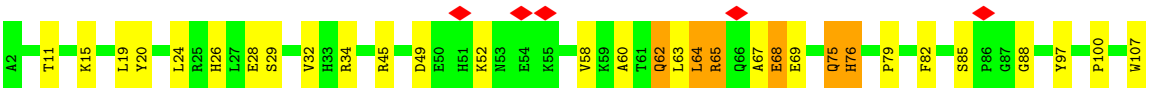


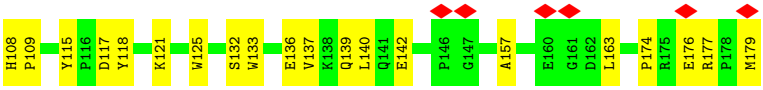
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



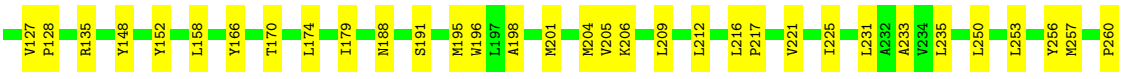


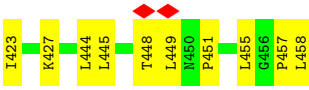
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



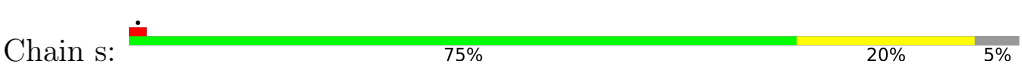


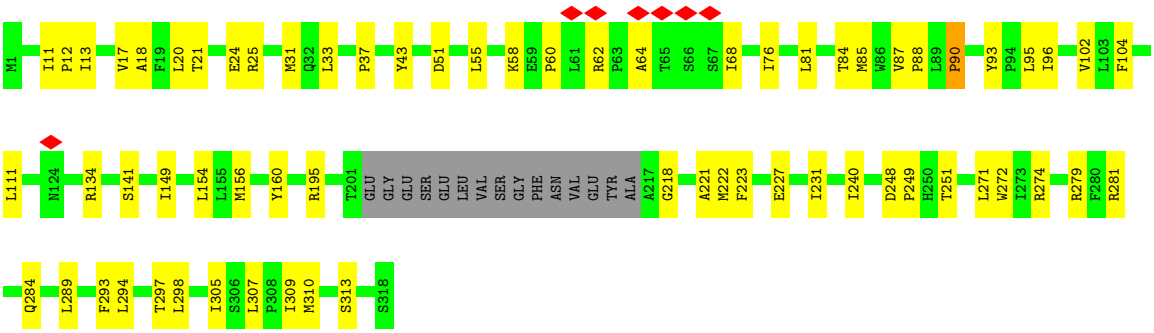
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4





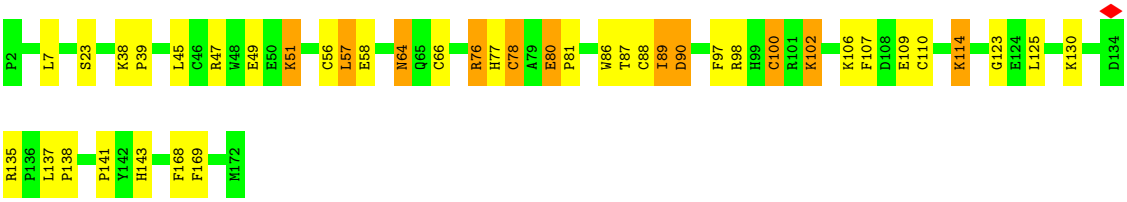
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1





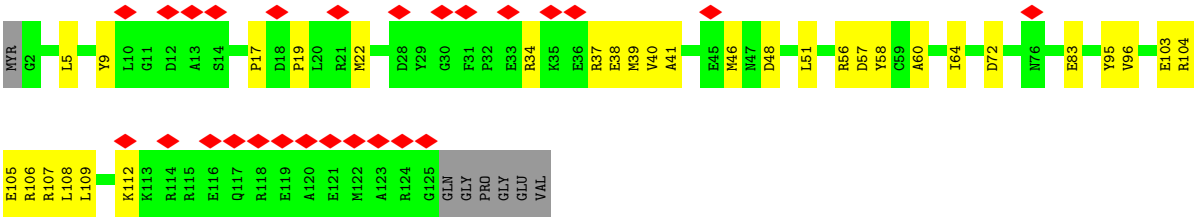
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:



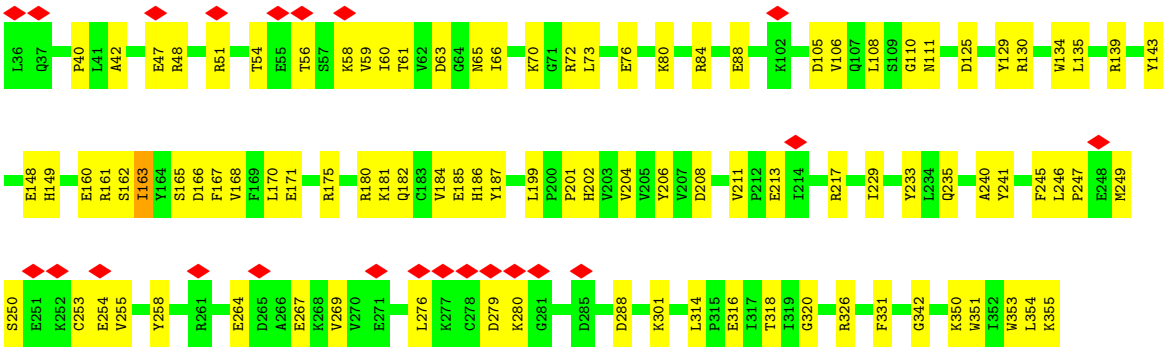
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169835	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0243	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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: ZN, NDP, UQ, CDL, FMN, ADP, 8Q1, PEE, PLX, SF4, FES, NAI, 2MR, MG

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	0.23	0/3393	0.48	5/4584 (0.1%)
2	B	0.27	0/1443	0.41	0/1952
3	C	0.26	0/1279	0.51	2/1730 (0.1%)
4	E	0.18	0/995	0.34	0/1340
5	F	0.19	0/702	0.46	0/945
6	G	0.19	0/705	0.47	0/956
6	X	0.18	0/708	0.42	0/959
7	H	0.19	0/929	0.34	0/1258
8	I	0.29	0/780	0.54	0/1059
9	J	0.21	0/2411	0.45	1/3254 (0.0%)
10	K	0.17	0/365	0.44	0/493
11	L	0.22	0/1039	0.36	0/1403
12	M	0.22	0/5384	0.38	0/7295
13	N	0.19	0/1245	0.38	0/1694
14	O	0.20	0/1711	0.41	0/2328
15	P	0.24	0/1789	0.43	0/2436
16	Q	0.27	0/3451	0.48	3/4672 (0.1%)
17	S	0.25	0/582	0.46	0/783
18	T	0.17	0/755	0.32	0/1018
19	U	0.17	0/664	0.33	0/912
20	V	0.17	0/1042	0.37	0/1411
21	W	0.20	0/1192	0.31	0/1610
22	Y	0.21	0/609	0.56	2/835 (0.2%)
23	Z	0.13	0/695	0.30	0/939
24	a	0.24	0/1185	0.47	2/1606 (0.1%)
25	b	0.22	0/902	0.47	0/1227
26	c	0.20	0/1371	0.37	0/1875
27	d	0.18	0/1494	0.37	0/2015
28	e	0.18	0/916	0.37	0/1246
29	f	0.15	0/350	0.27	0/473
30	g	0.18	0/1031	0.33	0/1394
31	h	0.19	0/889	0.35	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.26	0/2769	0.47	0/3764
33	j	0.26	0/819	0.47	0/1117
34	k	0.23	0/759	0.41	0/1029
35	l	0.23	0/4914	0.46	2/6683 (0.0%)
36	m	0.23	0/970	0.43	0/1316
37	n	0.25	0/468	0.65	1/633 (0.2%)
38	o	0.17	0/1088	0.33	0/1477
39	p	0.22	0/1590	0.55	3/2155 (0.1%)
40	r	0.26	0/3723	0.47	0/5078
41	s	0.25	0/2464	0.49	2/3369 (0.1%)
42	u	0.27	0/1436	0.53	2/1938 (0.1%)
43	v	0.20	0/1044	0.45	0/1403
44	w	0.21	0/2634	0.48	1/3571 (0.0%)
All	All	0.22	0/66684	0.44	26/90425 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	p	75	GLN	N-CA-C	9.47	121.60	111.28
39	p	62	GLN	N-CA-C	-9.05	101.41	111.28
1	A	120	GLY	N-CA-C	8.29	122.68	112.73
39	p	65	ARG	N-CA-C	-7.66	103.55	113.12
35	l	600	THR	N-CA-C	7.55	119.30	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	126	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	100	0
2	B	1412	0	1363	41	0
3	C	1248	0	1254	39	0
4	E	971	0	975	21	0
5	F	691	0	704	21	0
6	G	693	0	671	35	0
6	X	696	0	680	18	0
7	H	910	0	950	20	0
8	I	762	0	766	21	0
9	J	2359	0	2402	56	0
10	K	355	0	329	11	0
11	L	1016	0	1016	16	0
12	M	5296	0	5326	81	0
13	N	1204	0	1162	27	0
14	O	1671	0	1673	47	0
15	P	1738	0	1693	32	0
16	Q	3377	0	3320	76	0
17	S	567	0	565	7	0
18	T	741	0	702	7	0
19	U	643	0	642	8	0
20	V	1021	0	1027	16	0
21	W	1161	0	1144	33	0
22	Y	583	0	525	57	0
23	Z	674	0	643	7	0
24	a	1152	0	1154	29	0
25	b	875	0	895	45	0
26	c	1315	0	1208	40	0
27	d	1461	0	1429	34	0
28	e	890	0	837	26	0
29	f	342	0	341	3	0
30	g	1000	0	994	10	0
31	h	867	0	871	14	0
32	i	2706	0	2863	84	0
33	j	800	0	855	44	0
34	k	748	0	799	24	0
35	l	4785	0	4933	145	0
36	m	948	0	960	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	456	0	433	22	0
38	o	1058	0	1061	13	0
39	p	1534	0	1470	51	0
40	r	3631	0	3839	104	0
41	s	2394	0	2508	61	0
42	u	1398	0	1380	42	0
43	v	1020	0	957	71	0
44	w	2574	0	2516	71	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	0	0
46	A	31	0	19	2	0
47	A	44	0	27	7	0
48	B	51	0	82	1	0
48	C	47	0	71	16	0
48	Q	47	0	71	22	0
48	W	41	0	59	16	0
48	j	51	0	82	5	0
48	l	92	0	138	31	0
48	r	51	0	82	12	0
49	C	52	0	88	2	0
49	a	52	0	88	6	0
49	g	52	0	88	5	0
49	j	52	0	88	4	0
49	r	104	0	176	10	0
50	G	35	0	0	0	0
50	X	35	0	0	0	0
51	I	51	0	46	12	0
51	a	91	0	132	44	0
51	i	66	0	76	18	0
51	l	199	0	307	65	0
51	r	100	0	156	11	0
51	u	78	0	103	18	0
52	J	48	0	23	6	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	T	1	0	0	0	0
56	s	28	0	31	6	0
57	w	27	0	11	1	0
All	All	66644	0	67159	1596	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1596 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:99:ILE:CD1	43:v:108:LEU:HD23	1.15	1.54
22:Y:99:ILE:HD13	43:v:108:LEU:CD2	1.36	1.52
22:Y:97:LEU:HD12	43:v:104:ARG:CA	1.50	1.40
33:j:68:GLU:OE2	33:j:98:LEU:CD1	1.78	1.30
1:A:119:GLU:OE2	1:A:127:ASP:CB	1.83	1.24

There are no symmetry-related clashes.

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	429/431 (100%)	417 (97%)	12 (3%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	86 (100%)	0	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	80 (86%)	12 (13%)	1 (1%)	11	36
9	J	289/341 (85%)	277 (96%)	11 (4%)	1 (0%)	36	65
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	688/690 (100%)	665 (97%)	22 (3%)	1 (0%)	48	77
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	13 (3%)	1 (0%)	43	72
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18	48
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
29	f	40/42 (95%)	40 (100%)	0	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
33	j	95/113 (84%)	88 (93%)	7 (7%)	0	100	100
34	k	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
35	l	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
36	m	125/175 (71%)	112 (90%)	12 (10%)	1 (1%)	16	44
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	165 (94%)	9 (5%)	2 (1%)	11	36
40	r	457/459 (100%)	441 (96%)	14 (3%)	2 (0%)	30	59
41	s	299/318 (94%)	284 (95%)	14 (5%)	1 (0%)	36	65
42	u	169/171 (99%)	160 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	v	122/131 (93%)	112 (92%)	10 (8%)	0	100	100
44	w	318/320 (99%)	300 (94%)	18 (6%)	0	100	100
All	All	8029/8315 (97%)	7699 (96%)	319 (4%)	11 (0%)	49	77

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	r	112	ALA
8	I	69	VAL
40	r	43	ASN
12	M	283	GLU
39	p	76	HIS

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	345/345 (100%)	341 (99%)	4 (1%)	63	86
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	75 (99%)	1 (1%)	61	86
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	82/97 (84%)	81 (99%)	1 (1%)	63	86
9	J	255/295 (86%)	254 (100%)	1 (0%)	84	94
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	580 (100%)	0	100	100
13	N	130/130 (100%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	93
16	Q	361/370 (98%)	359 (99%)	2 (1%)	78	93
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	58/63 (92%)	57 (98%)	1 (2%)	53	82
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	119/122 (98%)	118 (99%)	1 (1%)	73	90
25	b	97/119 (82%)	96 (99%)	1 (1%)	68	89
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	310/311 (100%)	310 (100%)	0	100	100
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/537 (100%)	535 (100%)	2 (0%)	84	94
36	m	98/141 (70%)	98 (100%)	0	100	100
37	n	46/53 (87%)	45 (98%)	1 (2%)	45	77
38	o	112/113 (99%)	112 (100%)	0	100	100
39	p	159/159 (100%)	156 (98%)	3 (2%)	50	79
40	r	410/410 (100%)	409 (100%)	1 (0%)	87	96
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	153/153 (100%)	138 (90%)	15 (10%)	7	25
43	v	103/115 (90%)	103 (100%)	0	100	100
44	w	279/283 (99%)	278 (100%)	1 (0%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7039/7238 (97%)	7003 (100%)	36 (0%)	78 93

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	u	89	ILE
44	w	163	ILE
42	u	90	ASP
42	u	106	LYS
25	b	28	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
37	n	14	HIS
43	v	76	ASN
39	p	12	HIS
41	s	284	GLN
15	P	196	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	2.00	2 (20%)	5,13,15	6.46	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.40	1.45	1.34
16	Q	118	2MR	CQ2-NH2	-2.18	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	13.33	131.70	119.48
16	Q	118	2MR	CD-NE-CZ	4.60	132.01	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.87	130.20	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
49	PLX	r	502	-	51,51,51	1.12	4 (7%)	55,59,59	0.62	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-		
52	NDP	J	401	-	49,52,52	4.36	22 (44%)	66,80,80	2.23	12 (18%)
45	SF4	M	801	12	0,12,12	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
49	PLX	j	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
51	CDL	r	504	-	99,99,99	1.07	8 (8%)	105,111,111	0.85	4 (3%)
47	NAI	A	503	-	45,48,48	3.91	20 (44%)	60,73,73	1.73	11 (18%)
48	PEE	C	302	-	46,46,50	1.22	6 (13%)	49,51,55	1.00	2 (4%)
48	PEE	Q	501	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
48	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.02	2 (4%)
45	SF4	C	301	3	0,12,12	-	-	-		
51	CDL	l	702	-	99,99,99	1.08	8 (8%)	105,111,111	0.88	4 (3%)
49	PLX	C	303	-	51,51,51	1.12	3 (5%)	55,59,59	0.62	1 (1%)
51	CDL	I	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.32	7 (12%)
51	CDL	l	701	-	98,98,99	0.92	4 (4%)	104,110,111	1.18	9 (8%)
57	ADP	w	401	-	27,29,29	2.97	8 (29%)	42,45,45	1.97	9 (21%)
48	PEE	l	703	-	45,45,50	1.23	6 (13%)	48,50,55	1.00	2 (4%)
49	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.63	1 (1%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
51	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.07	6 (6%)
45	SF4	M	802	12	0,12,12	-	-	-		
53	FES	O	301	14	0,4,4	-	-	-		
50	8Q1	G	201	6	31,34,34	2.00	6 (19%)	40,43,43	1.59	8 (20%)
48	PEE	B	303	-	50,50,50	1.15	6 (12%)	53,55,55	0.98	2 (3%)
48	PEE	r	501	-	50,50,50	1.14	6 (12%)	53,55,55	0.95	2 (3%)
49	PLX	a	202	-	51,51,51	0.61	0	55,59,59	0.73	0
46	FMN	A	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.28	8 (16%)
51	CDL	u	201	-	77,77,99	1.03	4 (5%)	83,89,111	1.13	4 (4%)
45	SF4	B	301	2	0,12,12	-	-	-		
56	UQ	s	401	-	28,28,63	3.26	6 (21%)	34,37,79	2.84	11 (32%)
50	8Q1	X	201	-	31,34,34	2.06	6 (19%)	40,43,43	1.76	9 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
49	PLX	r	503	-	51,51,51	1.13	3 (5%)	55,59,59	0.60	1 (1%)
53	FES	M	803	12	0,4,4	-	-	-		
51	CDL	i	401	-	65,65,99	1.13	4 (6%)	71,77,111	1.22	7 (9%)
48	PEE	j	201	-	50,50,50	1.15	5 (10%)	53,55,55	1.00	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PLX	r	502	-	-	24/55/55/55	-
52	NDP	J	401	-	-	6/34/77/77	0/4/5/5
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	j	202	-	-	28/55/55/55	-
51	CDL	r	504	-	-	75/110/110/110	-
47	NAI	A	503	-	-	9/29/72/72	0/5/5/5
48	PEE	C	302	-	-	29/50/50/54	-
48	PEE	Q	501	-	-	19/50/50/54	-
48	PEE	W	201	-	-	23/44/44/54	-
45	SF4	C	301	3	-	-	0/6/5/5
51	CDL	l	702	-	-	56/110/110/110	-
49	PLX	C	303	-	-	29/55/55/55	-
51	CDL	l	701	-	-	40/109/109/110	-
57	ADP	w	401	-	-	3/16/32/32	0/3/3/3
48	PEE	j	201	-	-	24/54/54/54	-
48	PEE	l	703	-	-	22/49/49/54	-
49	PLX	g	201	-	-	31/55/55/55	-
48	PEE	l	704	-	-	24/49/49/54	-
51	CDL	a	201	-	-	28/101/101/110	-
45	SF4	M	802	12	-	-	0/6/5/5
53	FES	O	301	14	-	-	0/1/1/1
50	8Q1	G	201	6	-	19/41/41/41	-
48	PEE	B	303	-	-	24/54/54/54	-
48	PEE	r	501	-	-	28/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PLX	a	202	-	-	21/55/55/55	-
46	FMN	A	502	-	-	9/18/18/18	0/3/3/3
51	CDL	u	201	-	-	23/88/88/110	-
45	SF4	B	301	2	-	-	0/6/5/5
56	UQ	s	401	-	-	9/21/45/87	0/1/1/1
50	8Q1	X	201	-	-	21/41/41/41	-
49	PLX	r	503	-	-	35/55/55/55	-
53	FES	M	803	12	-	-	0/1/1/1
51	CDL	i	401	-	-	30/76/76/110	-
51	CDL	I	201	-	-	24/61/61/110	-

The worst 5 of 169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C3B-C2B	-12.43	1.25	1.52
52	J	401	NDP	C6N-C5N	12.38	1.55	1.33
52	J	401	NDP	O4D-C4D	10.72	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.21	1.26	1.53
52	J	401	NDP	C3D-C4D	-10.05	1.27	1.53

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C7-C8-C9	-9.51	110.95	126.79
52	J	401	NDP	C3N-C2N-N1N	-9.27	109.86	123.10
56	s	401	UQ	C12-C13-C14	-6.25	112.61	127.66
52	J	401	NDP	C1D-N1N-C2N	-6.11	110.95	121.11
52	J	401	NDP	C5A-C4A-N3A	-5.90	119.05	126.75

There are no chirality outliers.

5 of 713 torsion outliers are listed below:

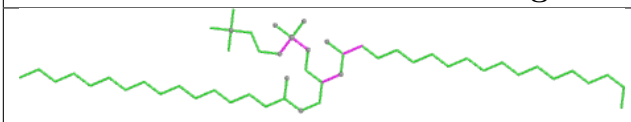
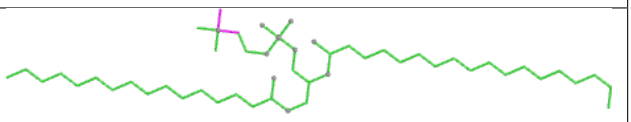
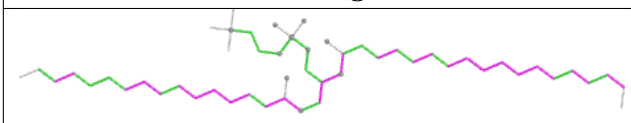
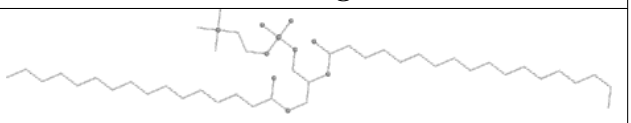
Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'

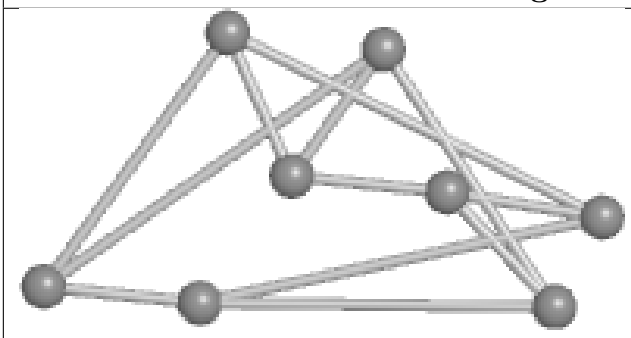
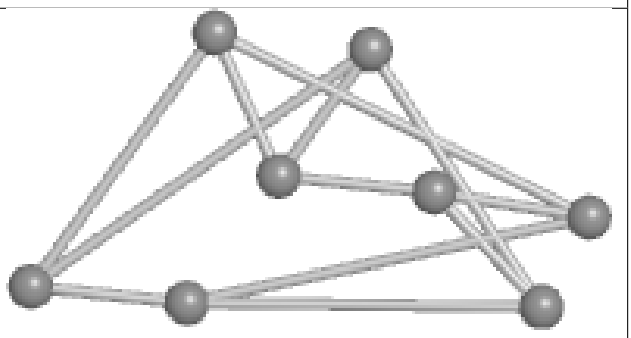
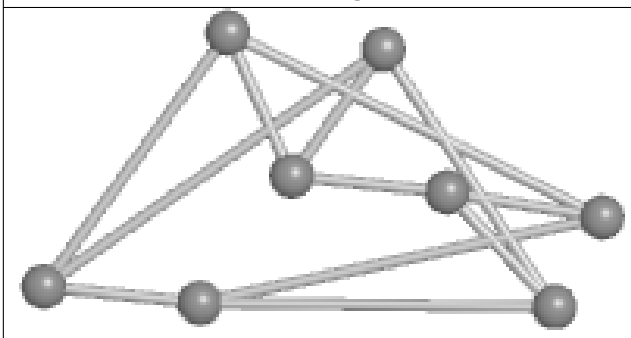
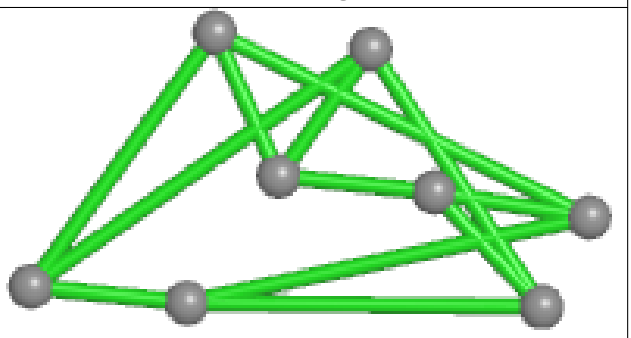
There are no ring outliers.

27 monomers are involved in 303 short contacts:

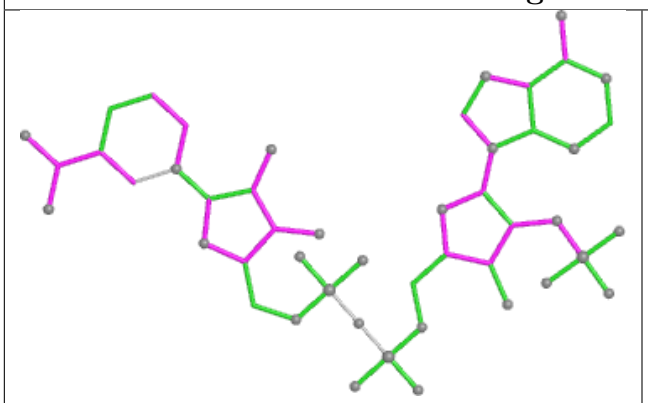
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	r	502	PLX	4	0
45	A	501	SF4	2	0
52	J	401	NDP	6	0
49	j	202	PLX	4	0
51	r	504	CDL	11	0
47	A	503	NAI	7	0
48	C	302	PEE	16	0
48	Q	501	PEE	22	0
48	W	201	PEE	16	0
51	l	702	CDL	7	0
49	C	303	PLX	2	0
51	I	201	CDL	12	0
51	l	701	CDL	58	0
57	w	401	ADP	1	0
48	l	703	PEE	6	0
49	g	201	PLX	5	0
48	l	704	PEE	25	0
51	a	201	CDL	44	0
48	B	303	PEE	1	0
48	r	501	PEE	12	0
49	a	202	PLX	6	0
46	A	502	FMN	2	0
51	u	201	CDL	18	0
56	s	401	UQ	6	0
49	r	503	PLX	6	0
51	i	401	CDL	18	0
48	j	201	PEE	5	0

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

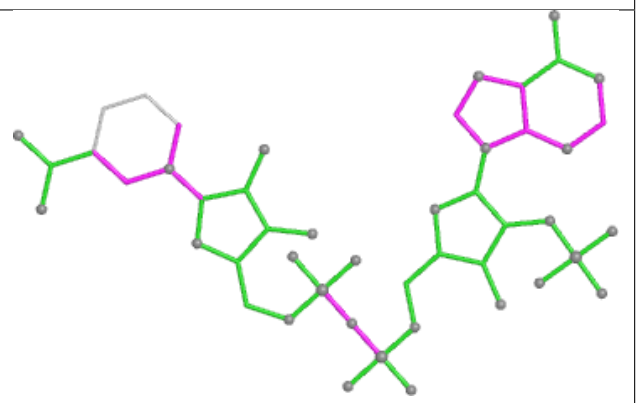
Ligand PLX r 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

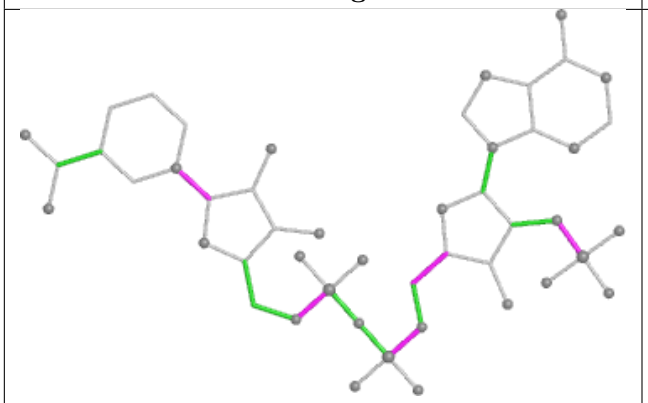
Ligand NDP J 401



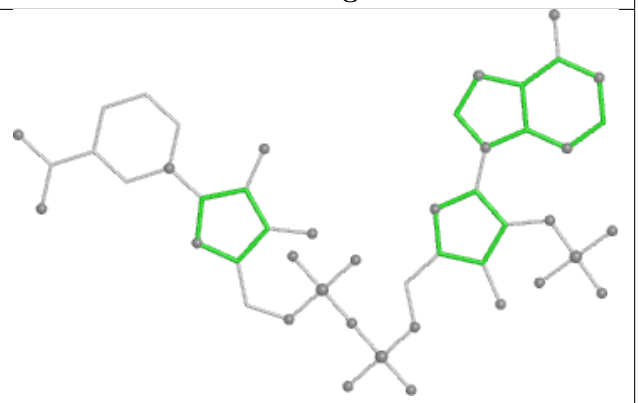
Bond lengths



Bond angles

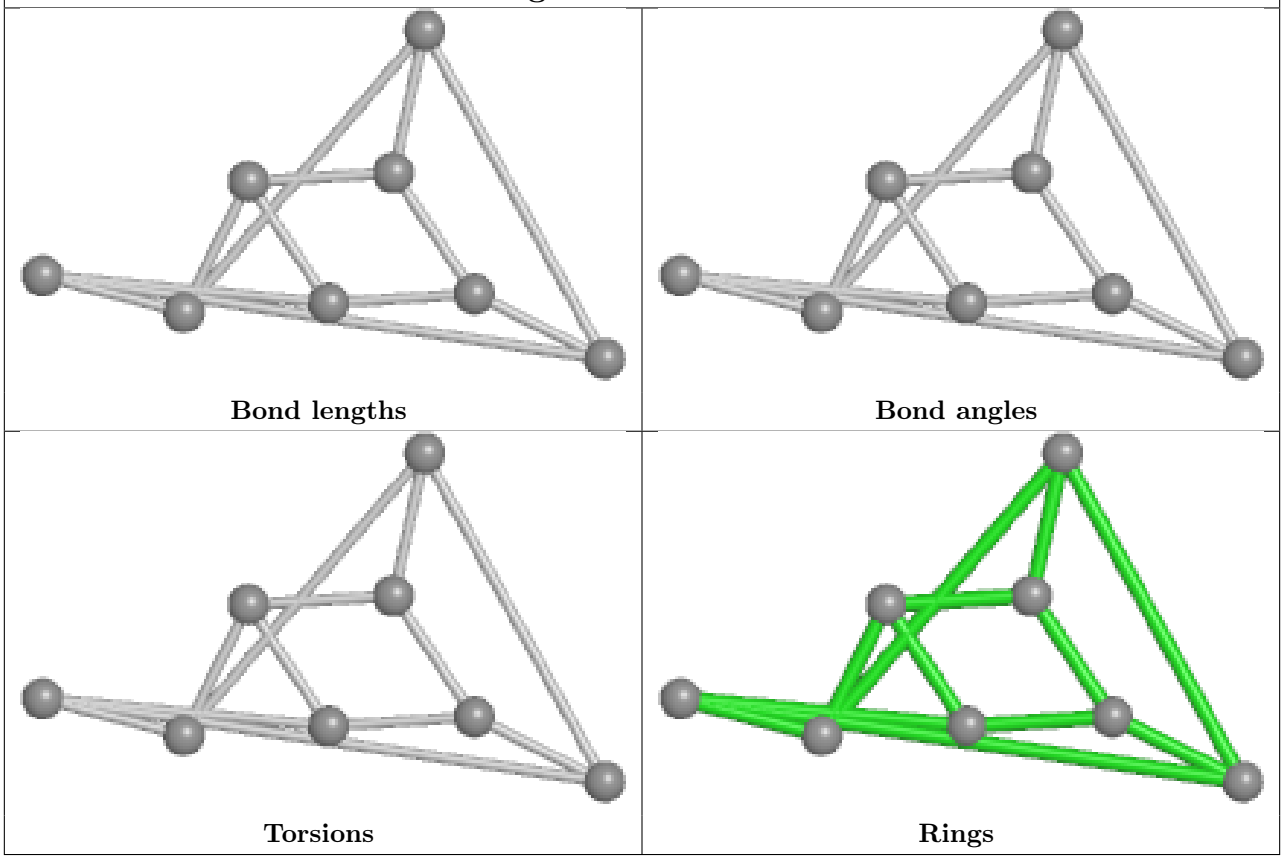


Torsions

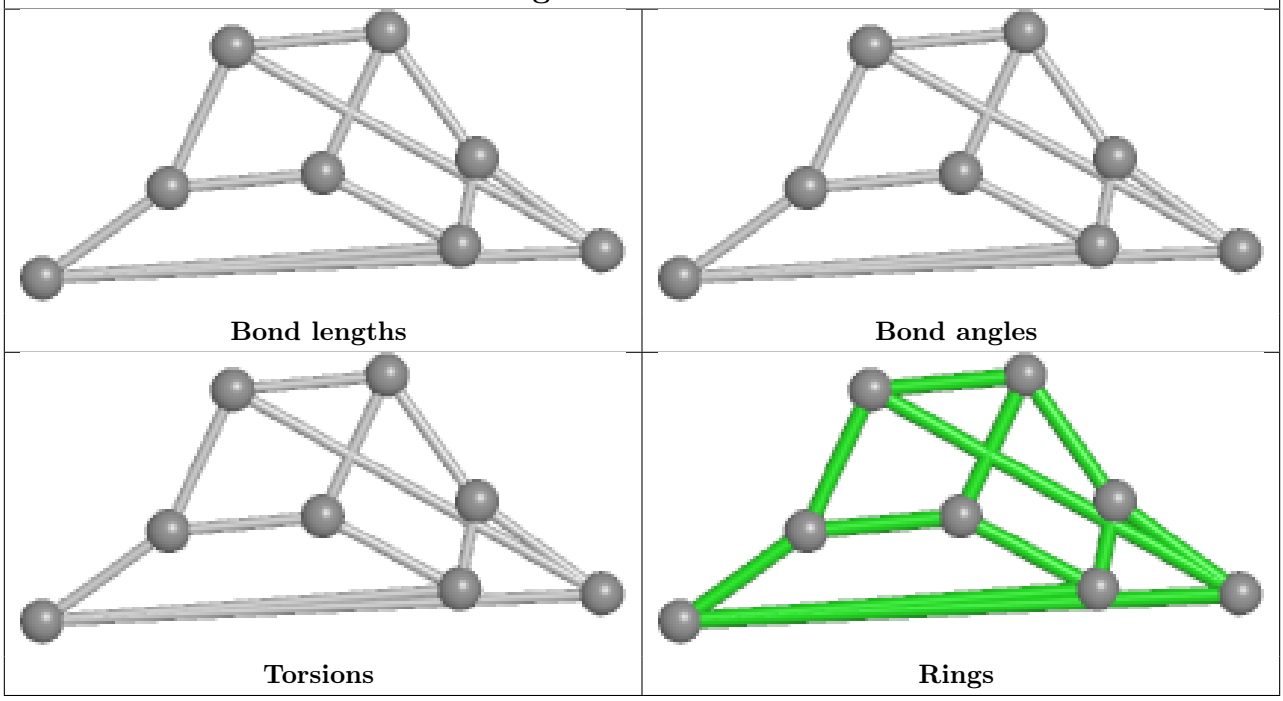


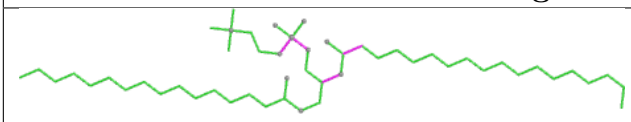
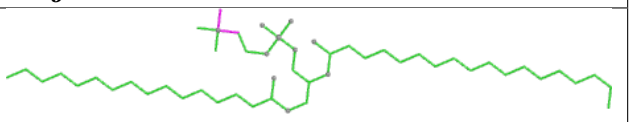
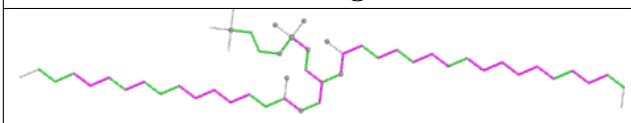
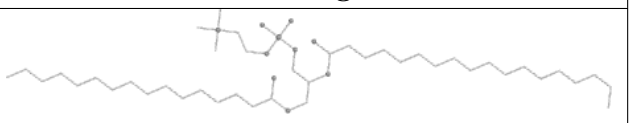
Rings

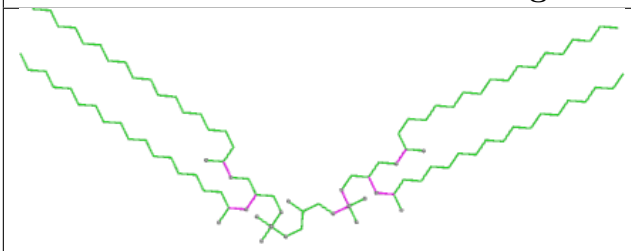
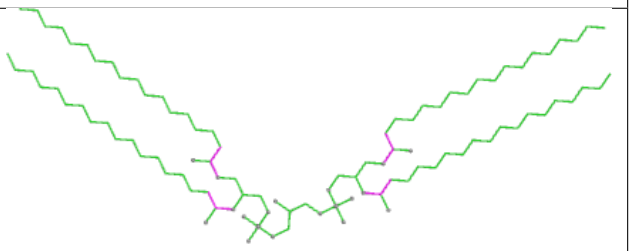
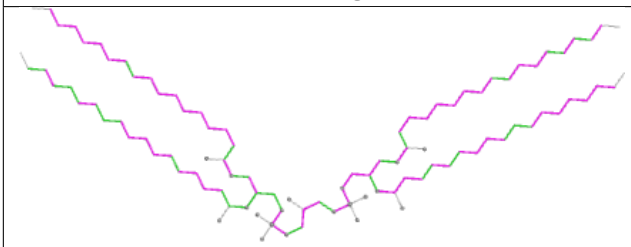
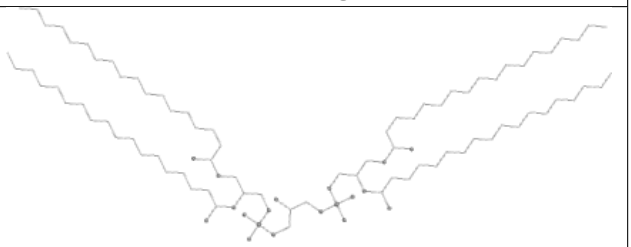
Ligand SF4 M 801



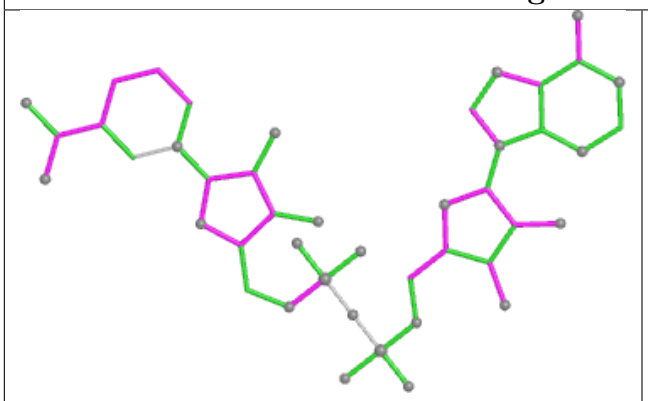
Ligand SF4 B 302



Ligand PLX j 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL r 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI A 503



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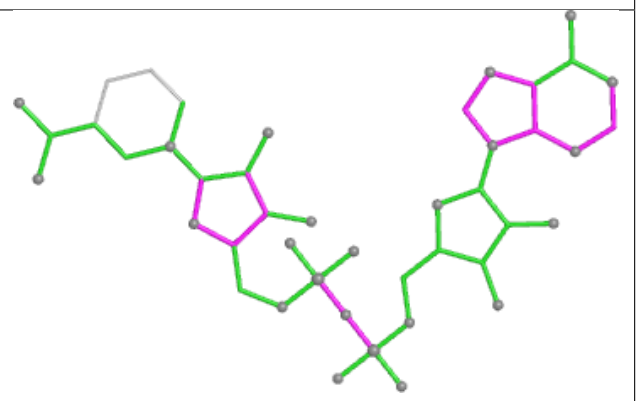
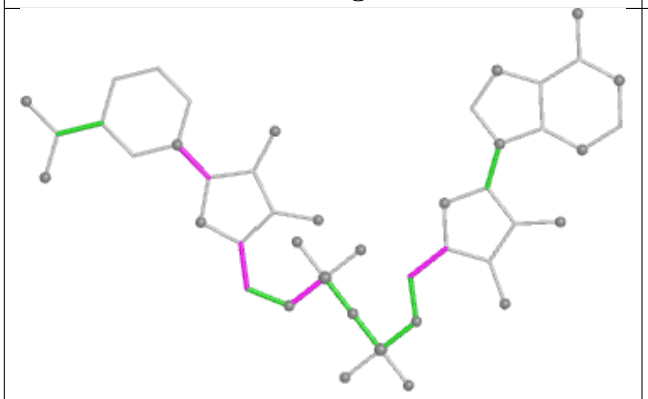


Bond angles



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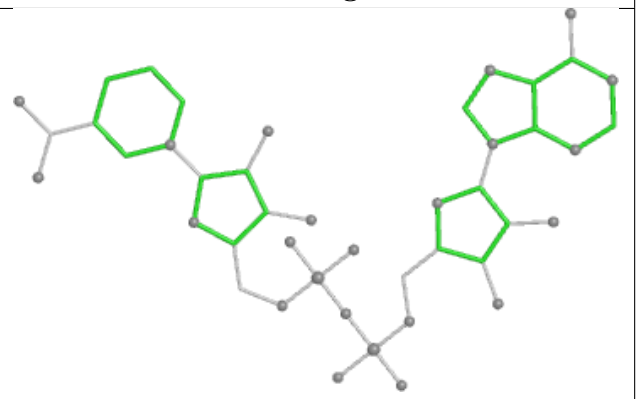
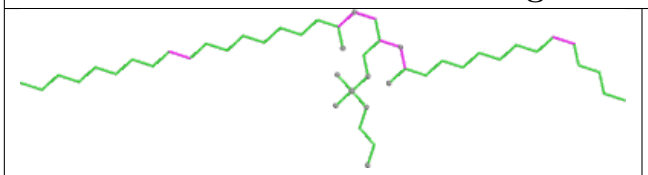


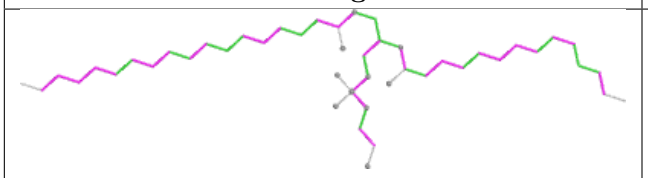
Rings

Ligand PEE C 302



Bond lengths

Bond angles



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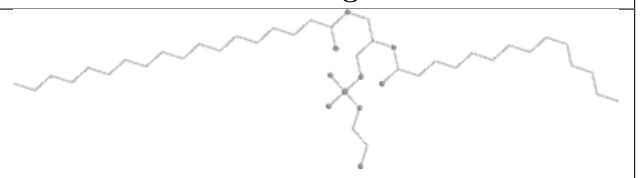
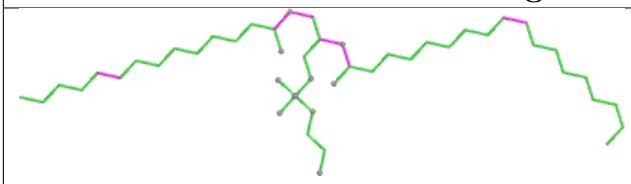


Rings

Ligand PEE Q 501



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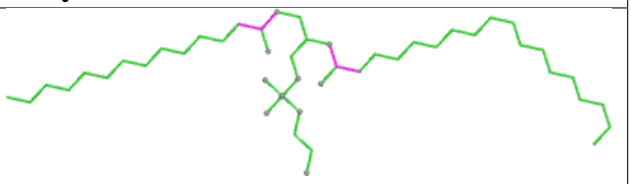

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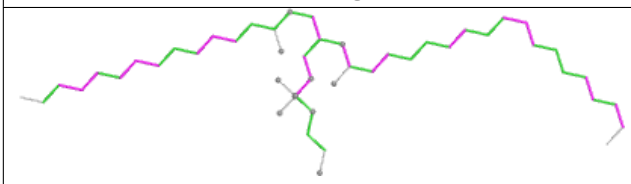

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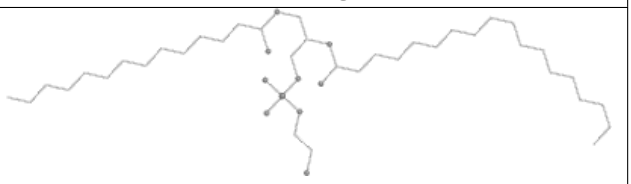
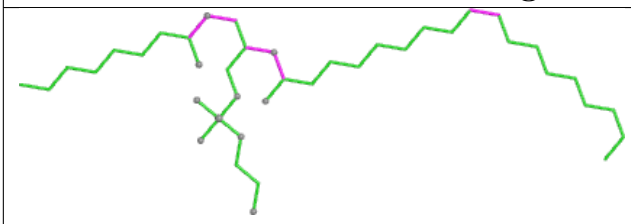


Rings

Ligand PEE W 201



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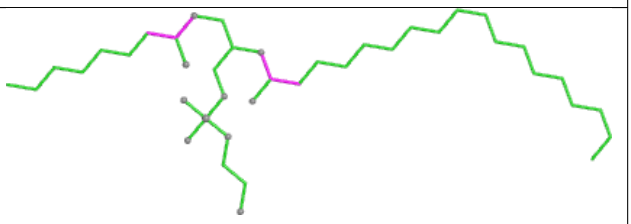

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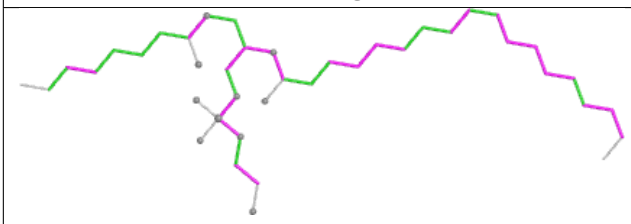

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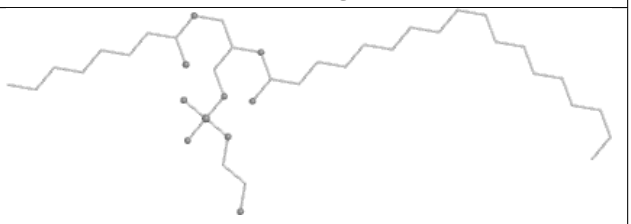
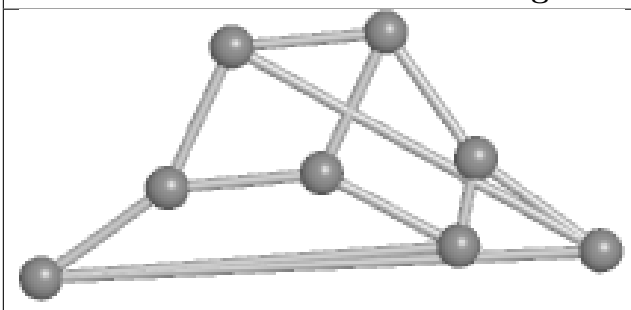


Rings

Ligand SF4 C 301



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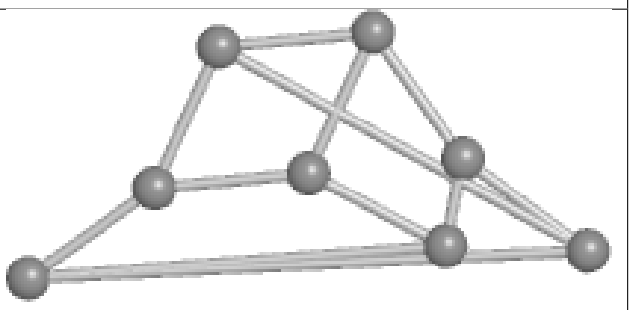
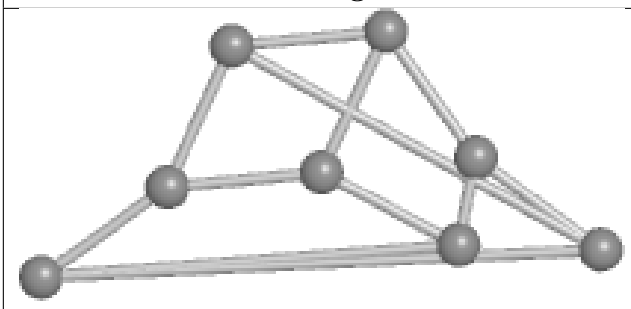


Bond angles



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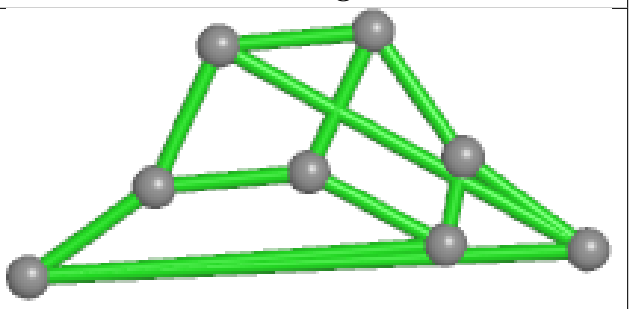
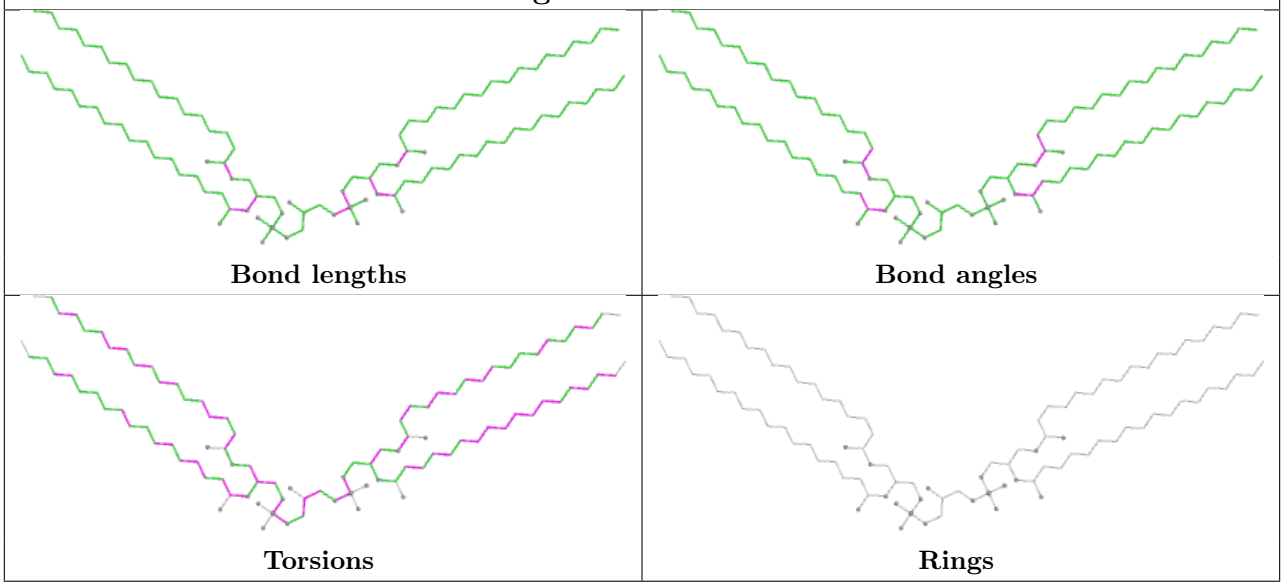
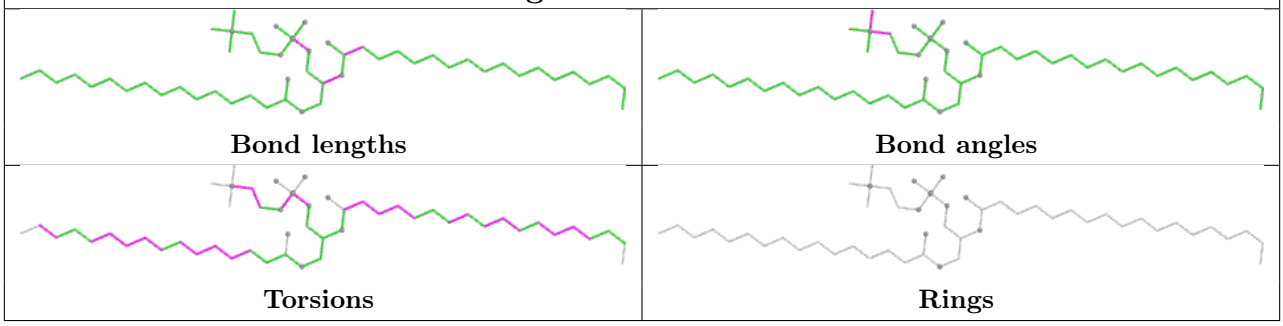


Rings

Ligand CDL l 702



Ligand PLX C 303



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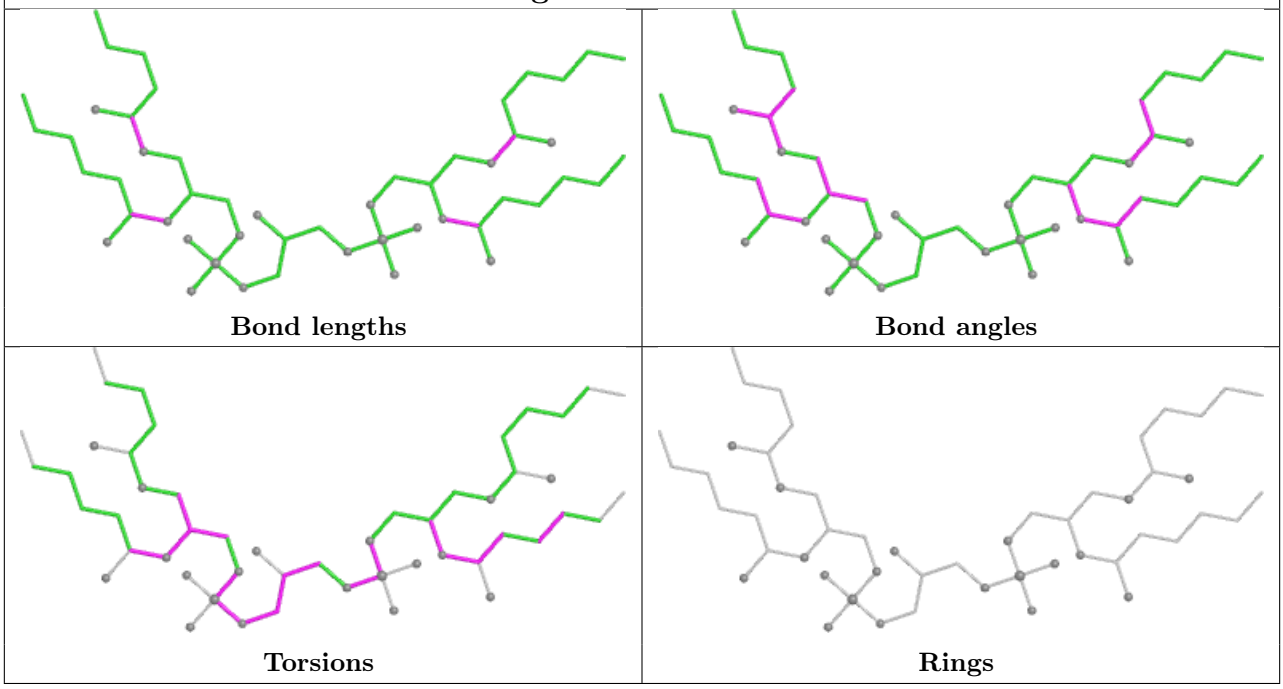

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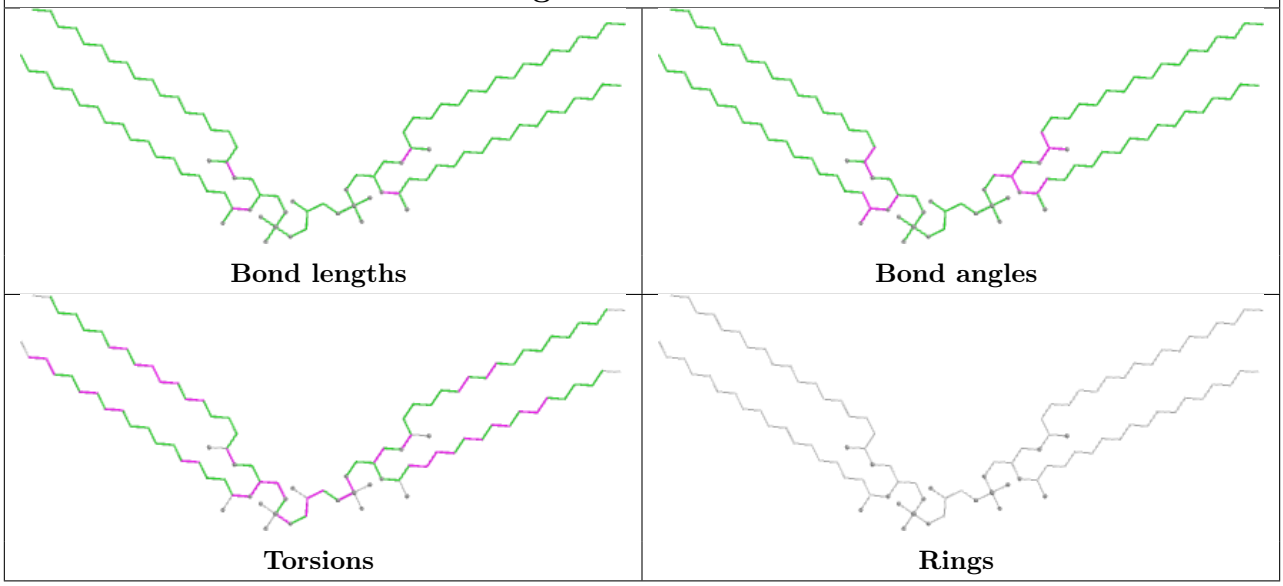
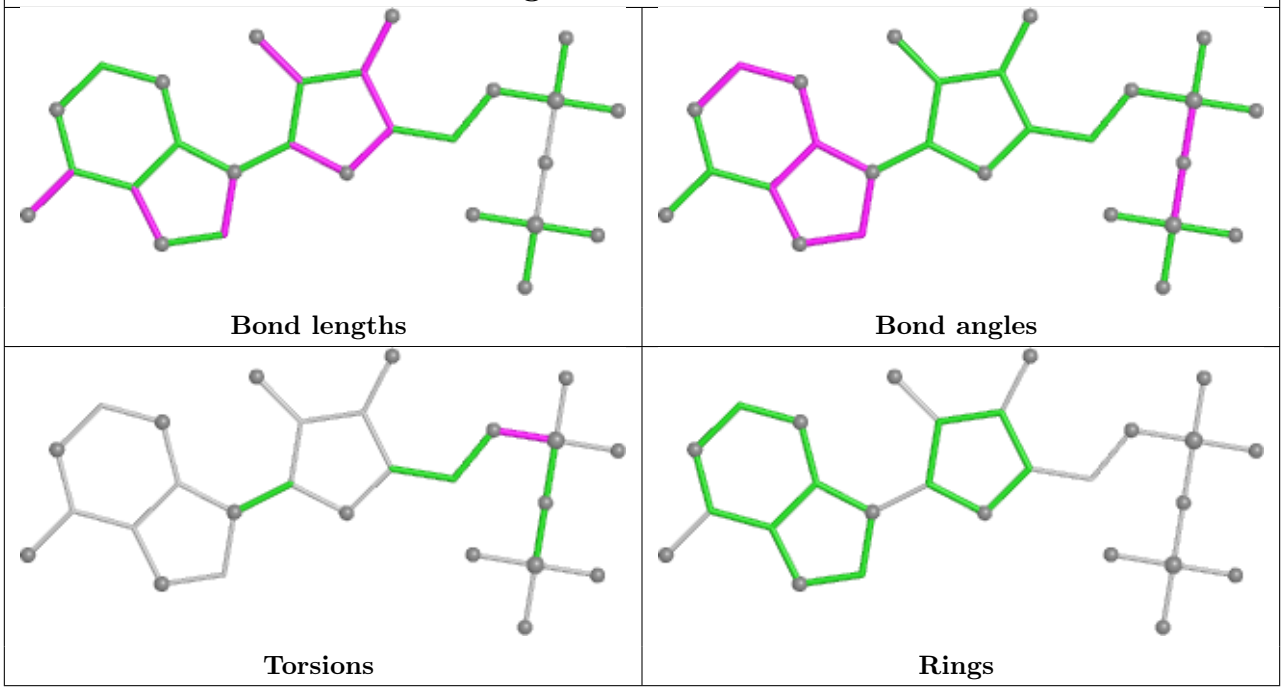
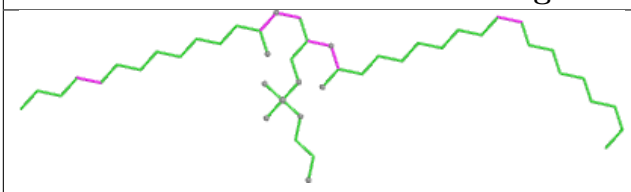
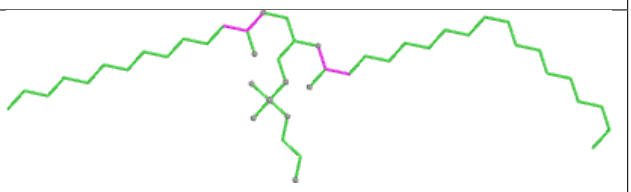
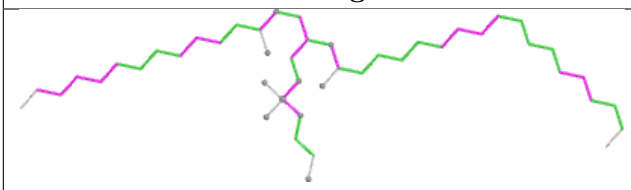
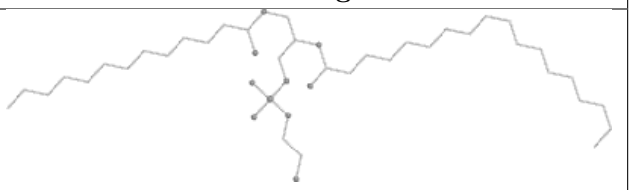
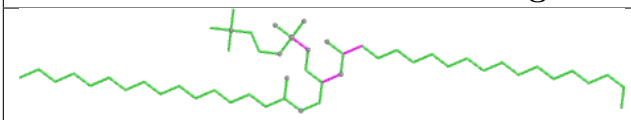
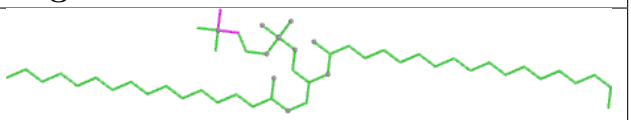
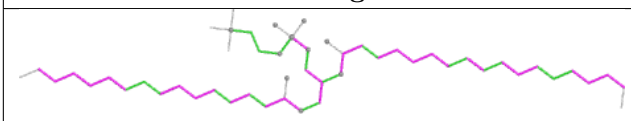
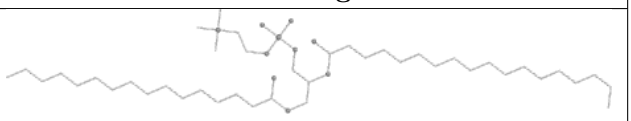
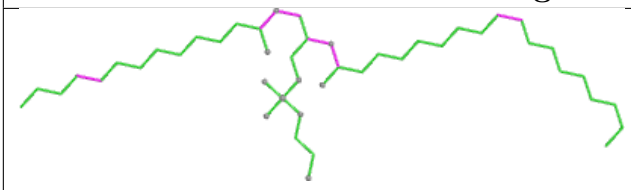
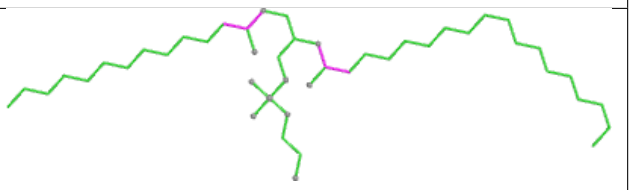
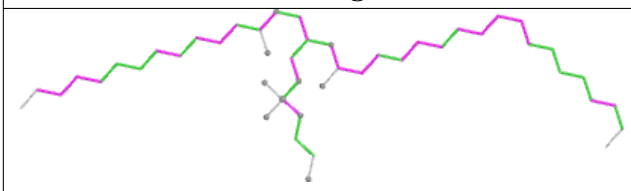
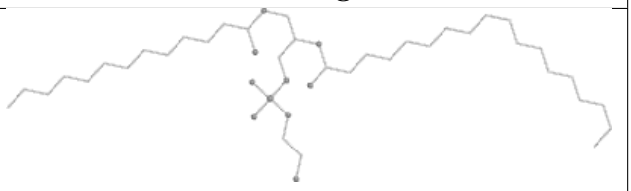


Ligand ADP w 401

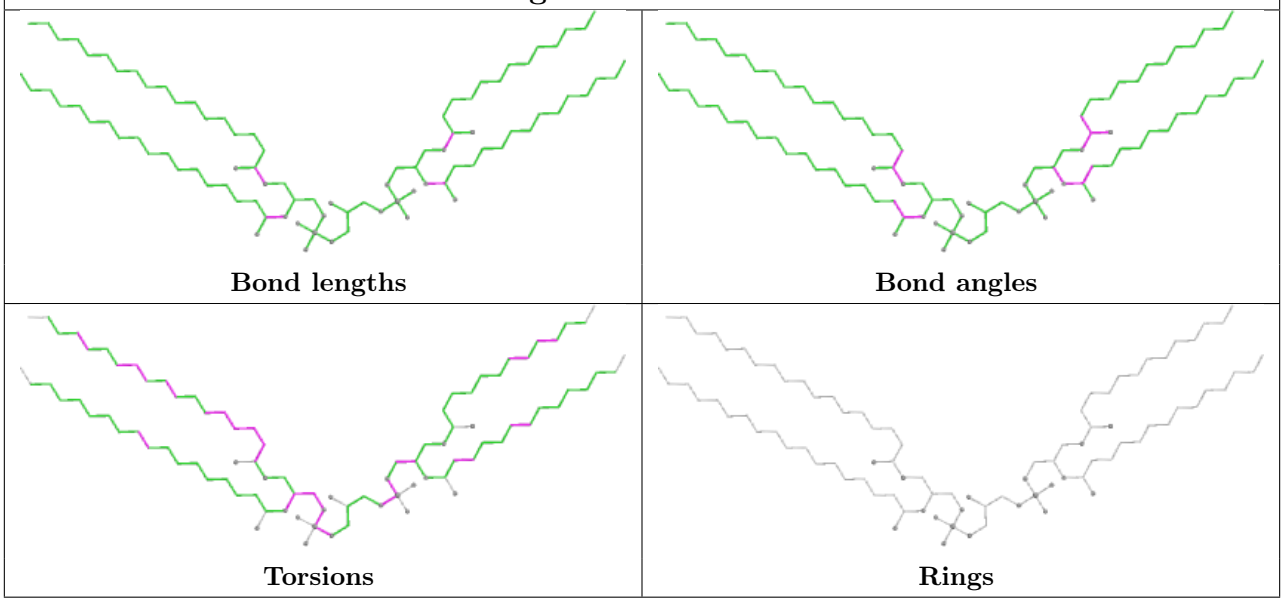


Ligand PEE l 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

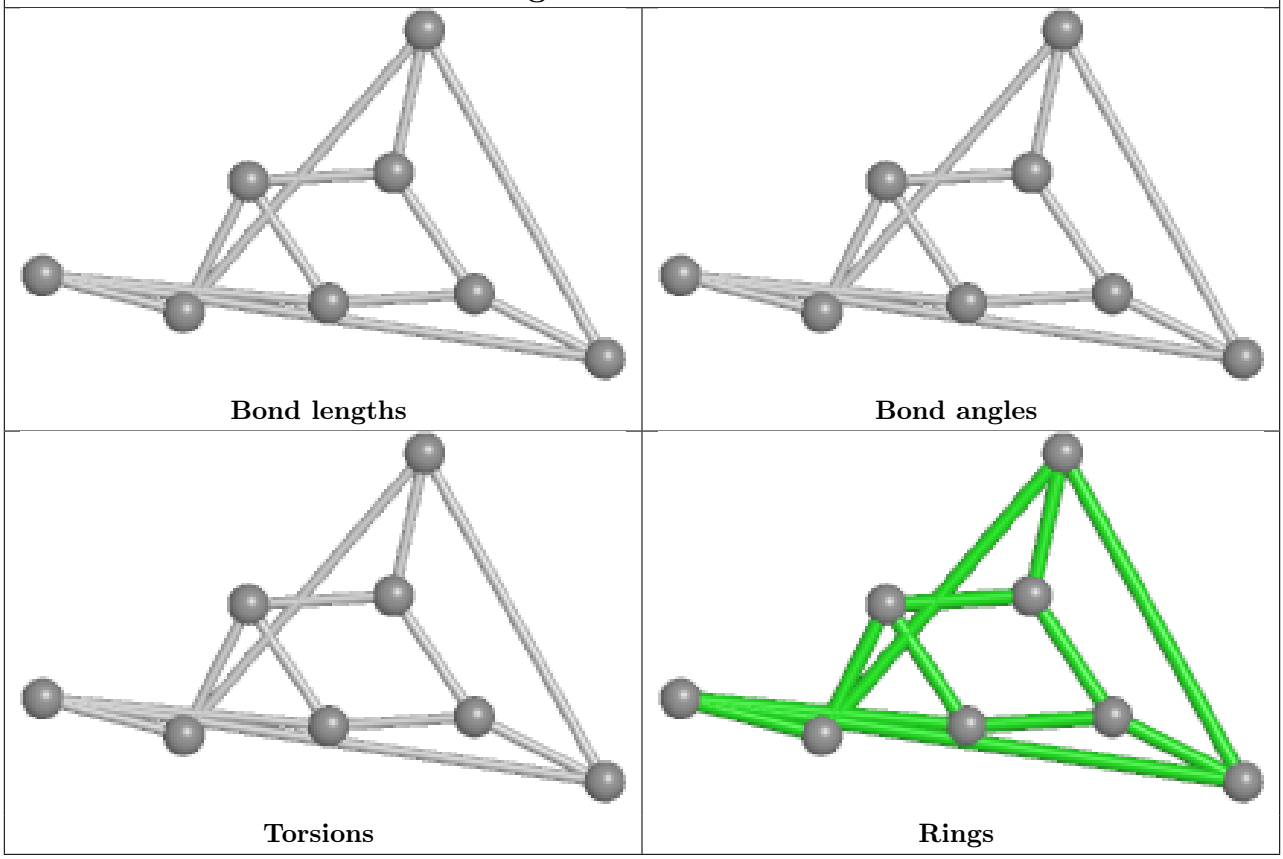
Ligand PLX g 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE l 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

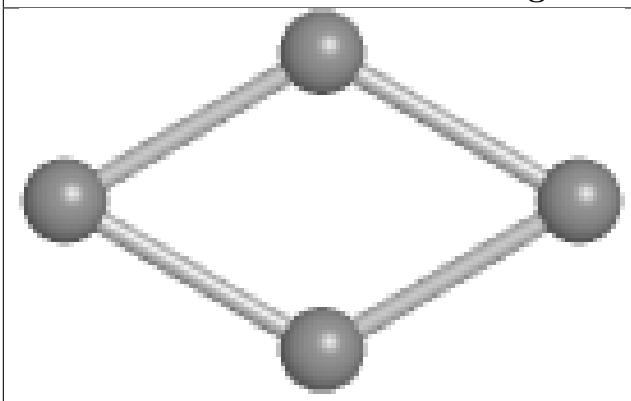
Ligand CDL a 201



Ligand SF4 M 802



Ligand FES O 301



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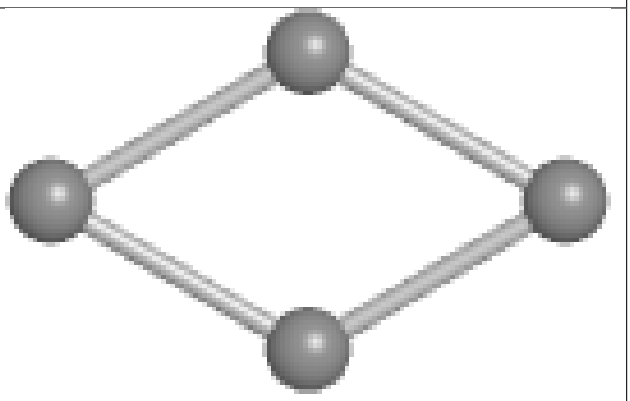
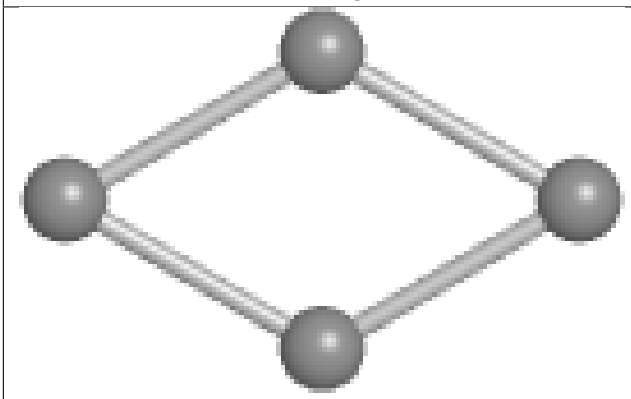
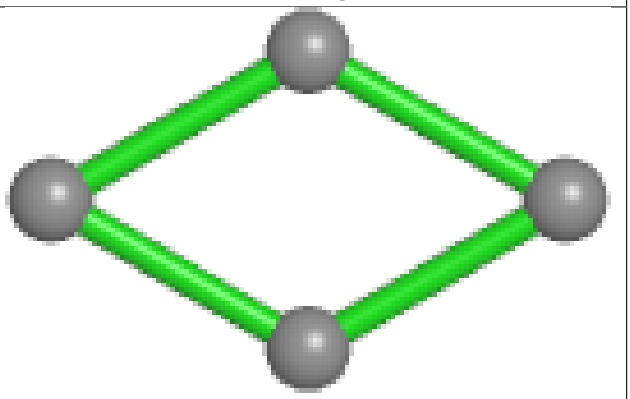


Bond angles

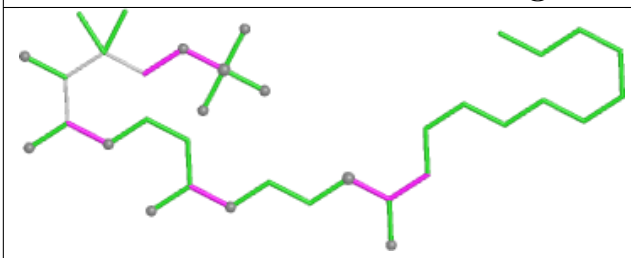


Torsions



Rings

Ligand 8Q1 G 201



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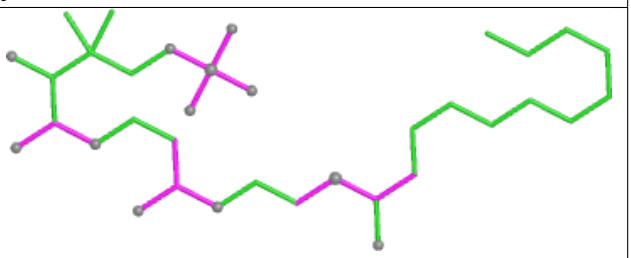
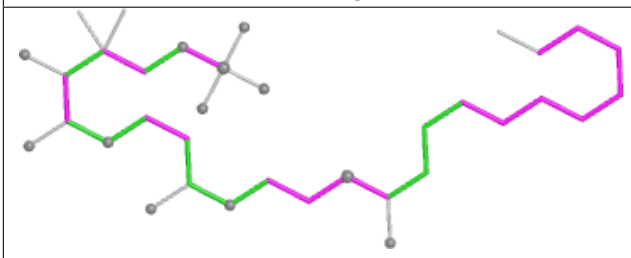


Bond angles



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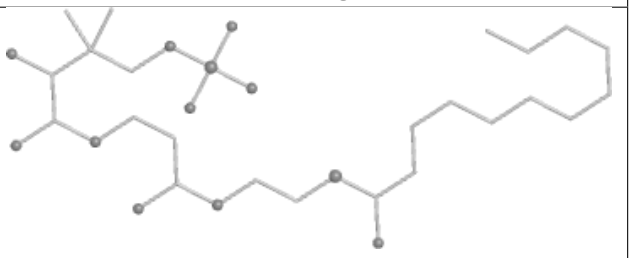
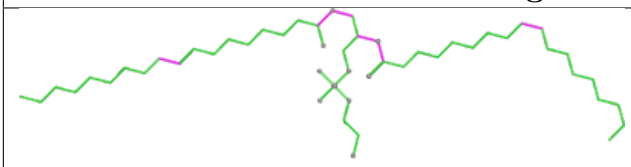
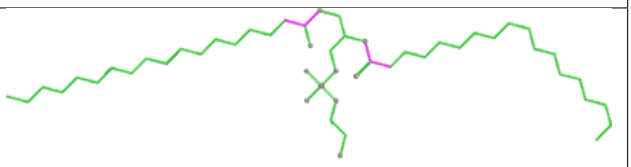
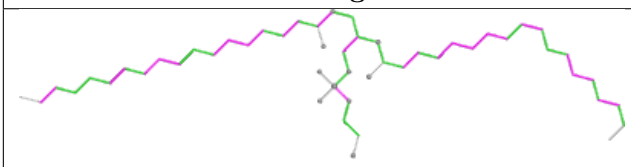
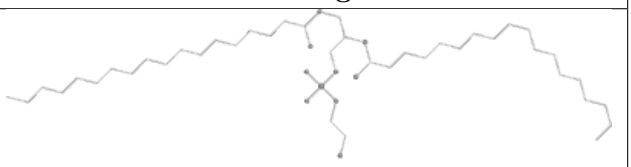
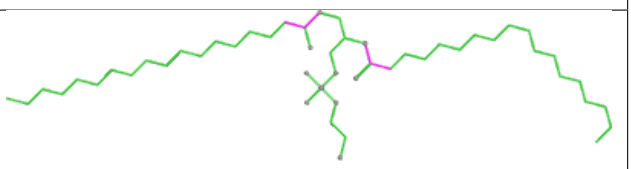
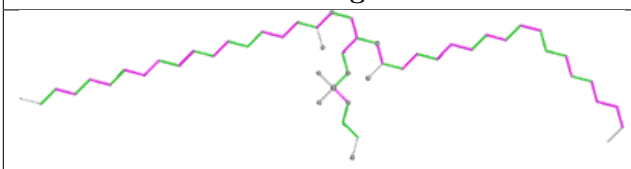
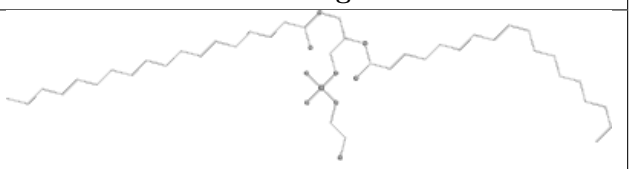
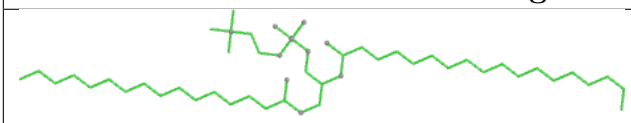
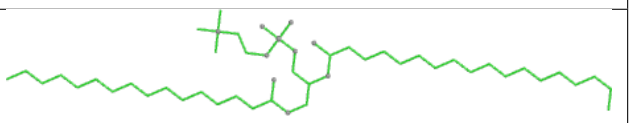
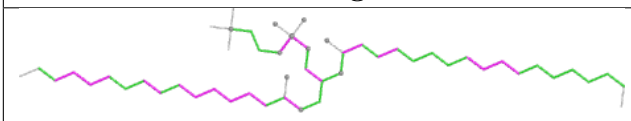
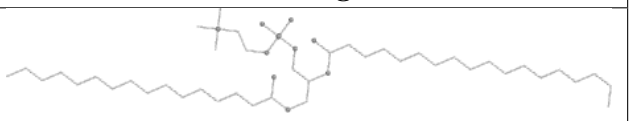


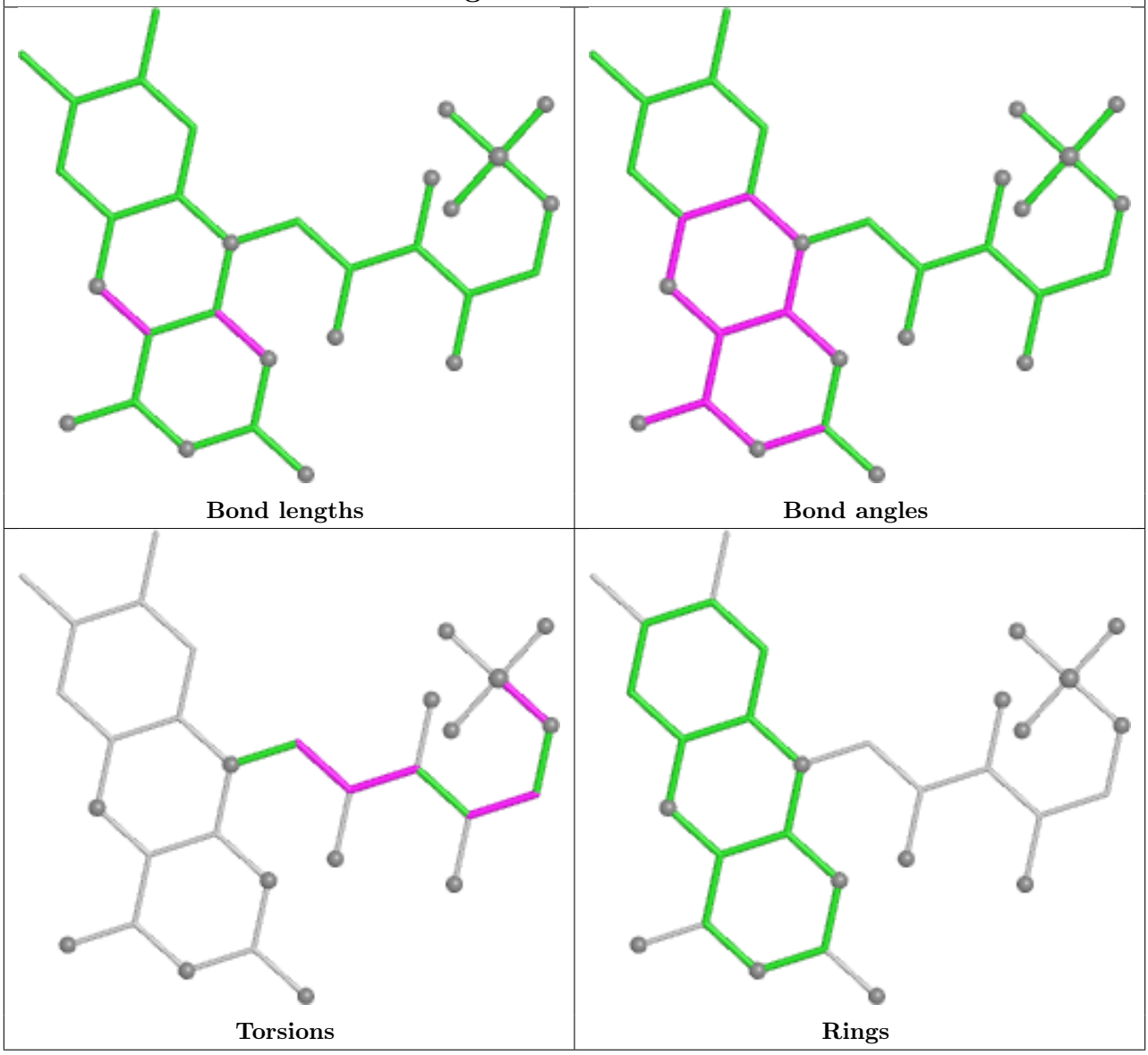
Rings

Ligand PEE B 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

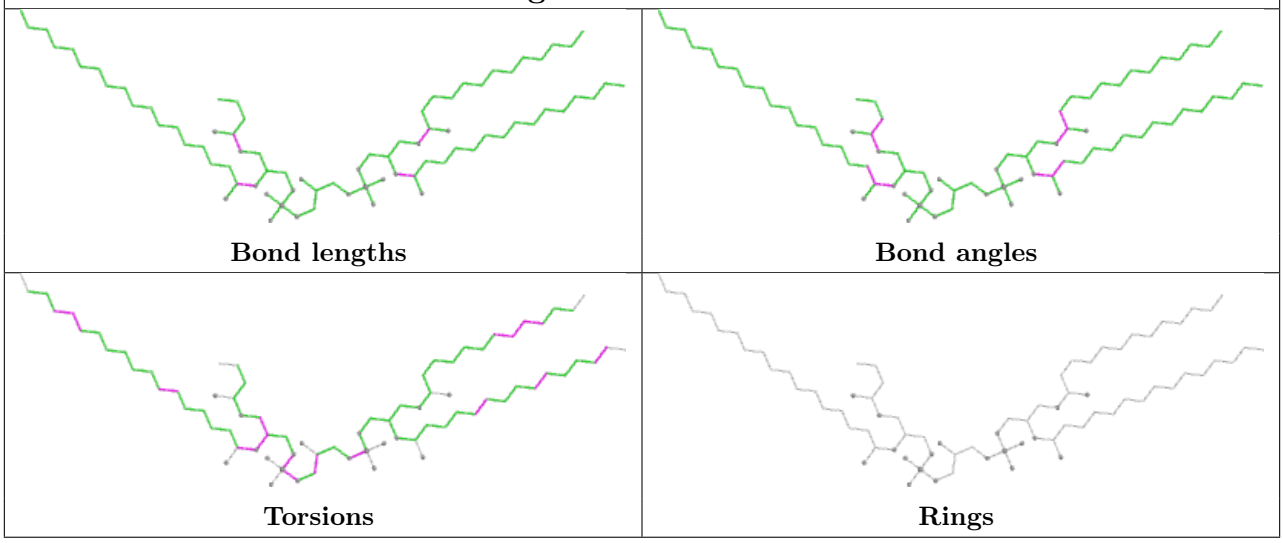
Ligand PEE r 501	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX a 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

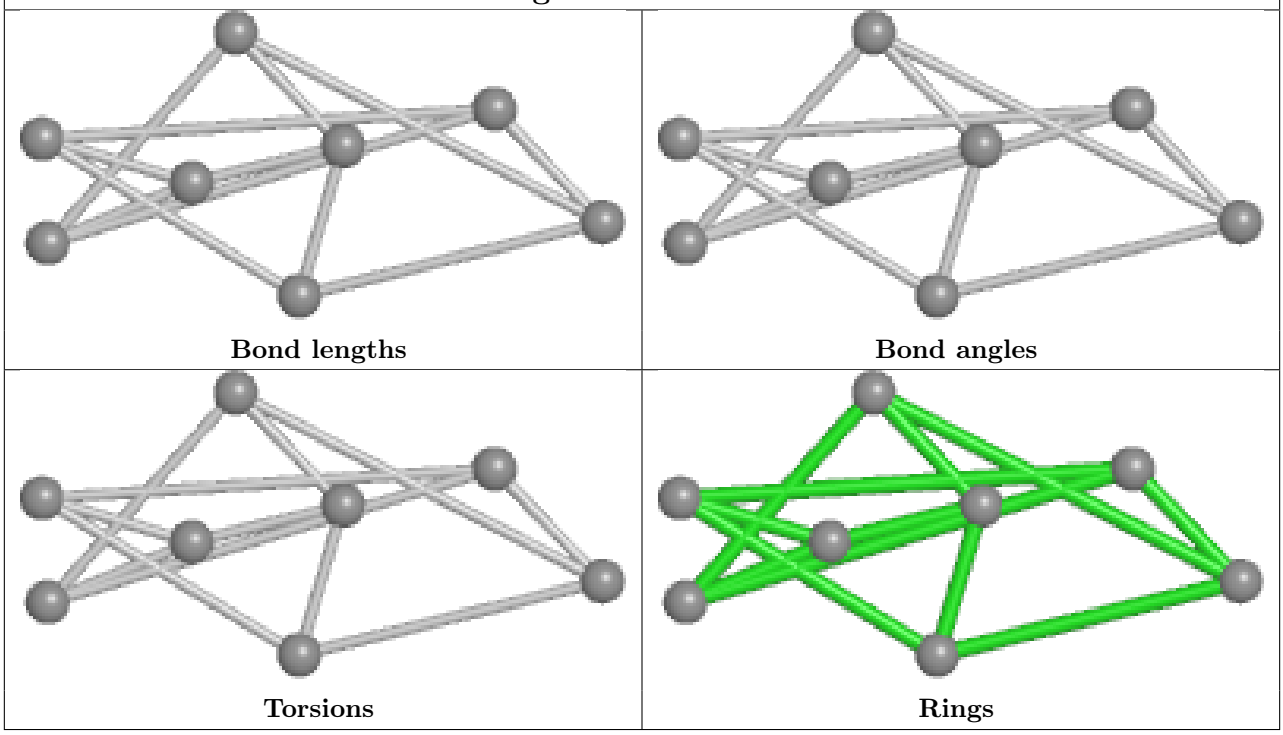
Ligand FMN A 502



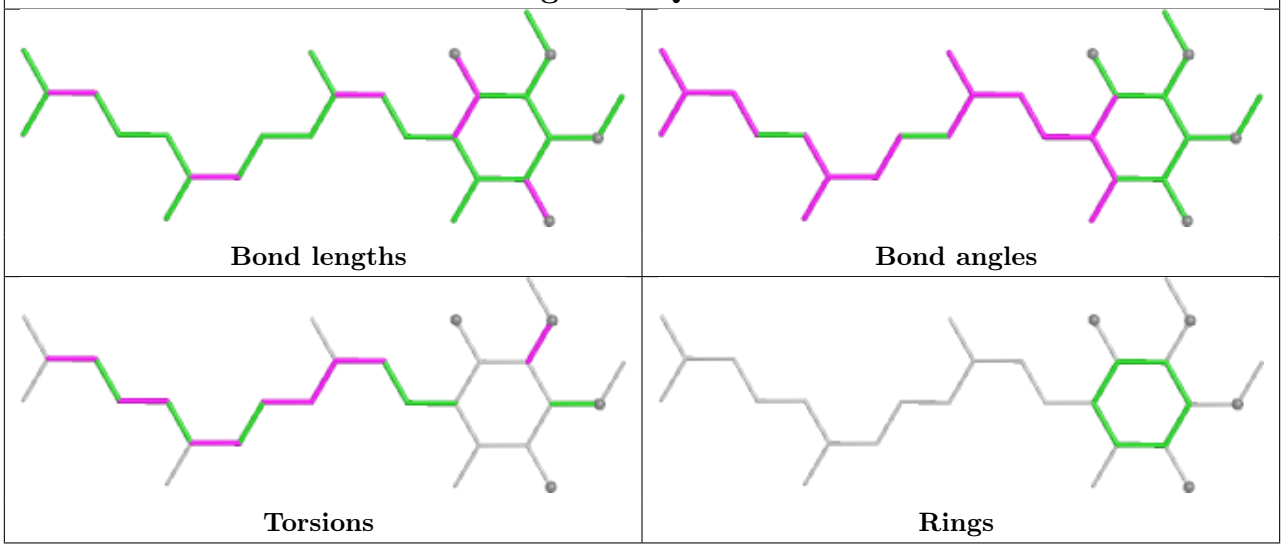
Ligand CDL u 201

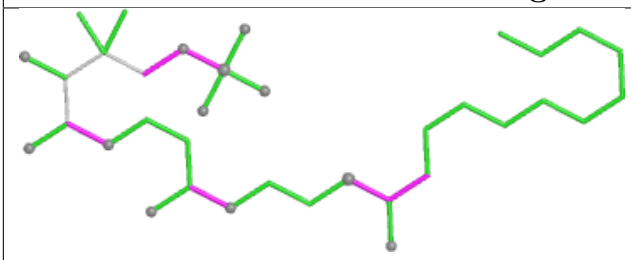
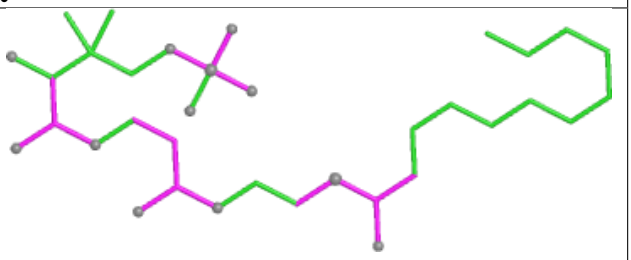
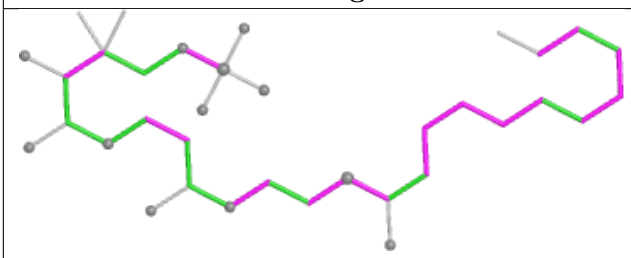
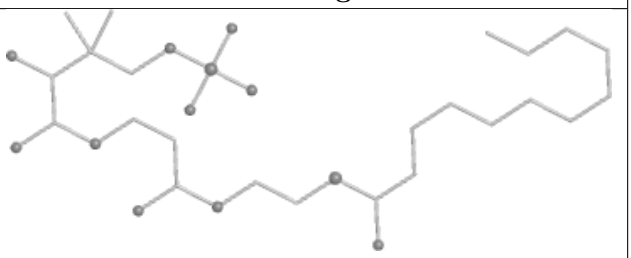


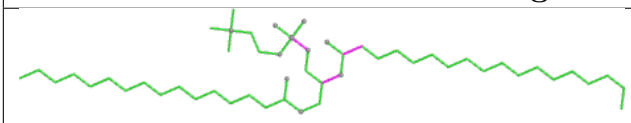
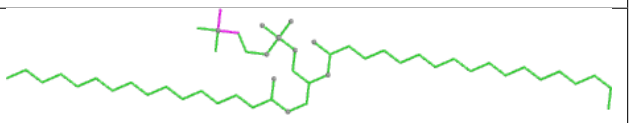
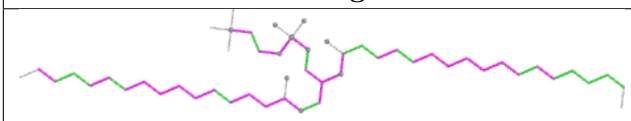
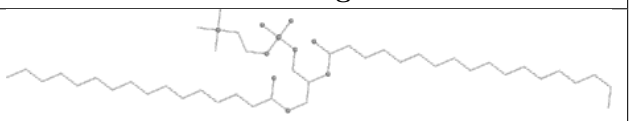
Ligand SF4 B 301



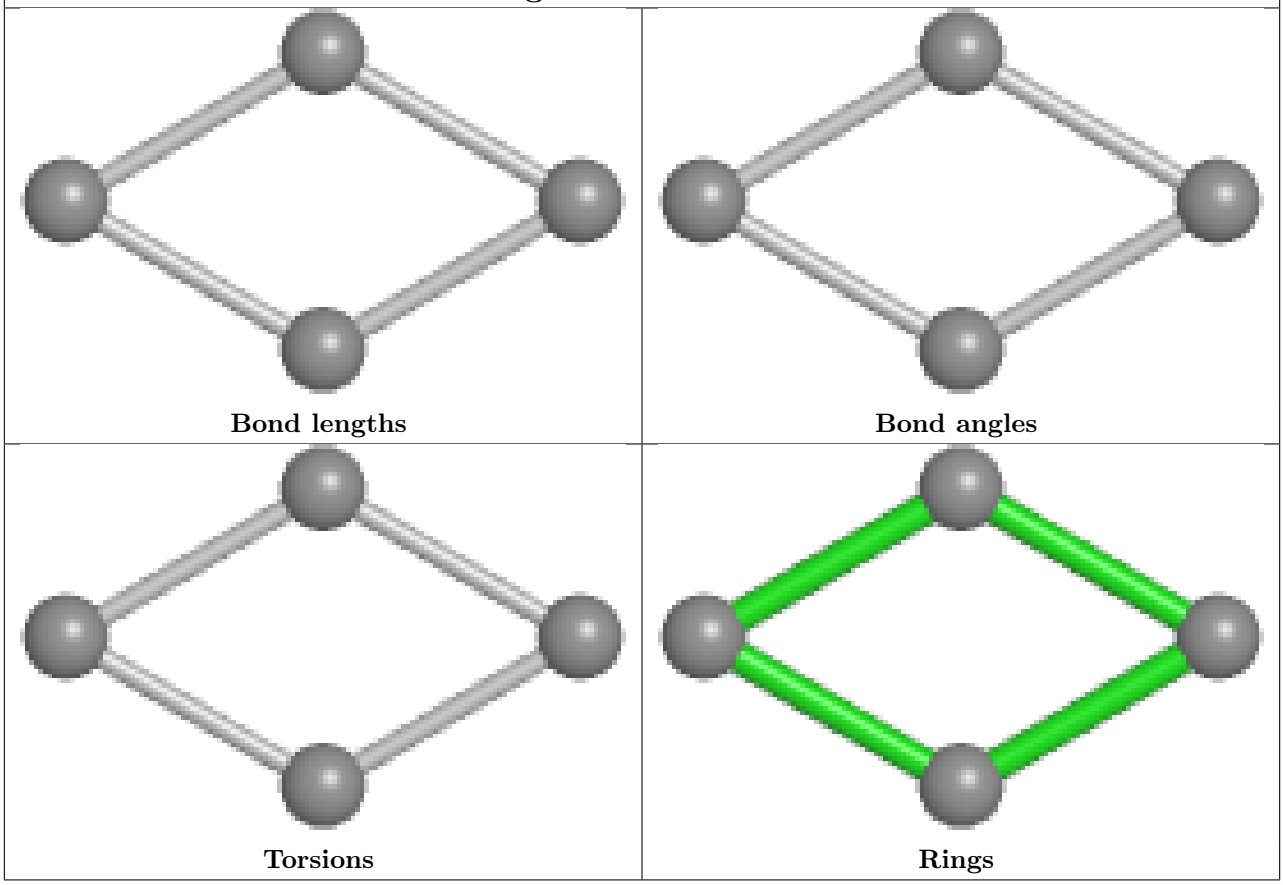
Ligand UQ s 401



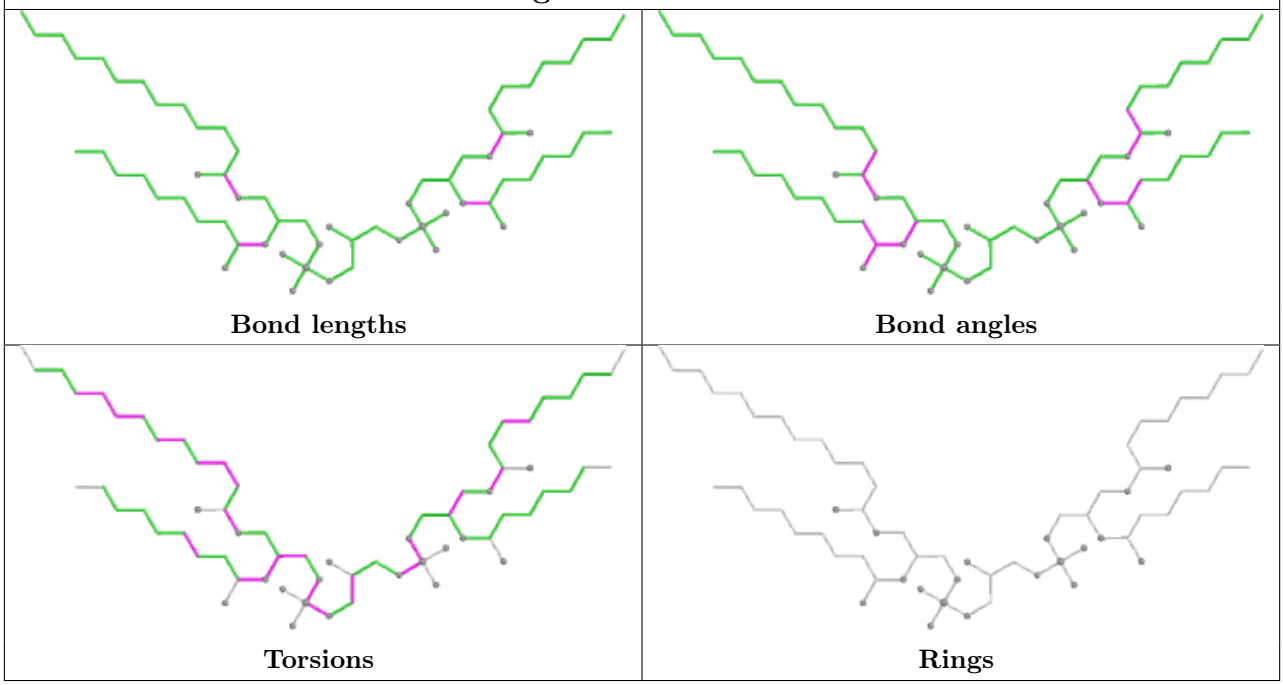
Ligand 8Q1 X 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

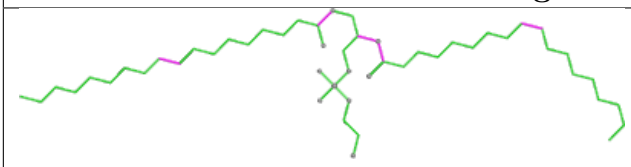
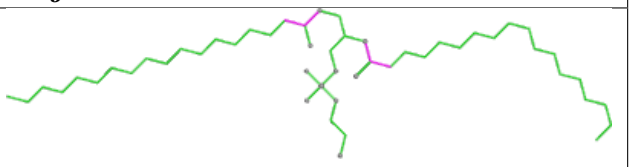
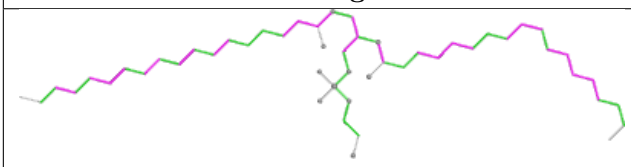
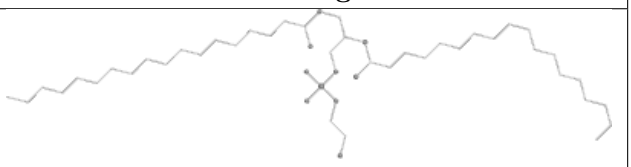
Ligand PLX r 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES M 803



Ligand CDL i 401



Ligand PEE j 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

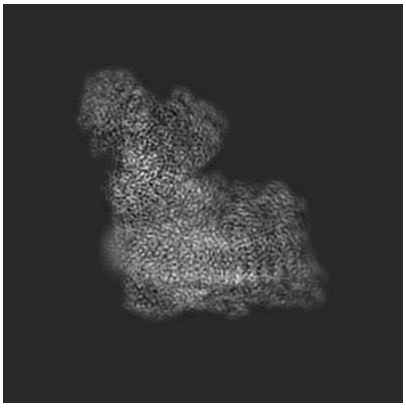
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31652. These allow visual inspection of the internal detail of the map and identification of artifacts.

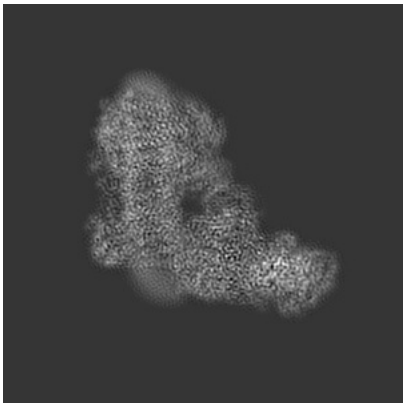
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

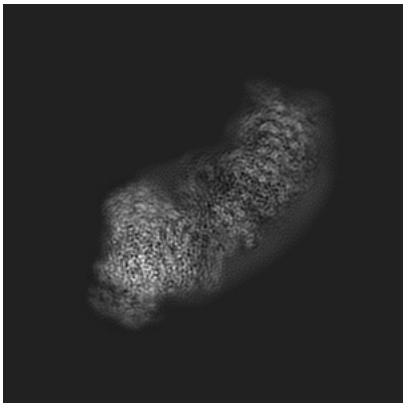
6.1.1 Primary map



X



Y

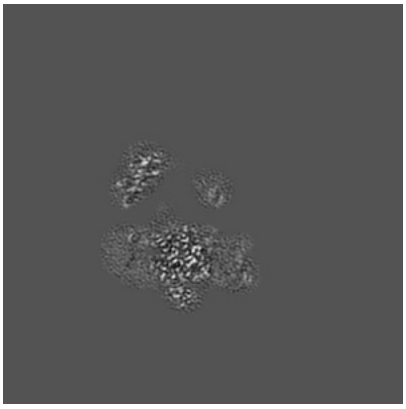


Z

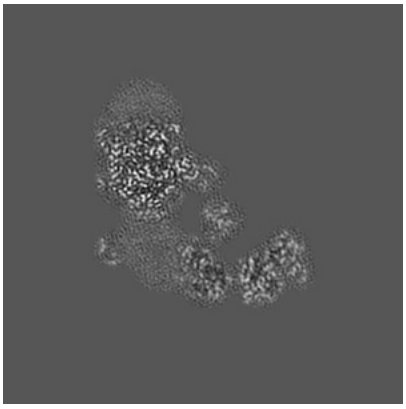
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

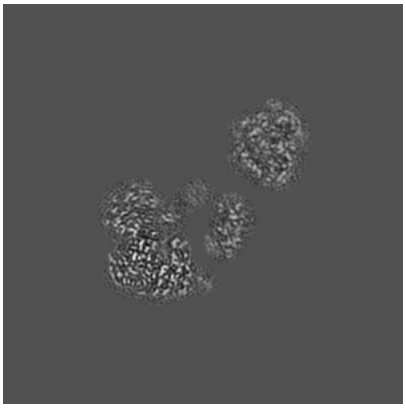
6.2.1 Primary map



X Index: 155



Y Index: 155



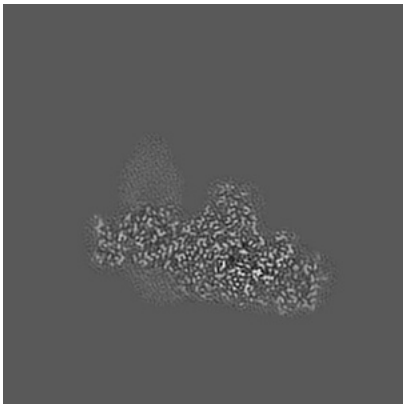
Z Index: 155

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

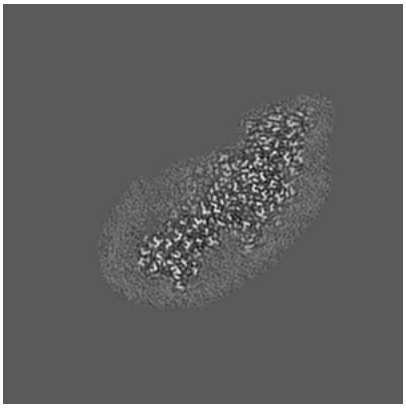
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 107



Y Index: 105

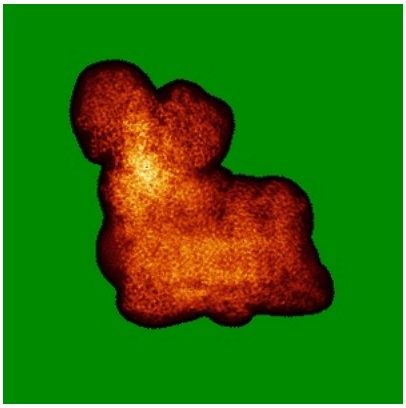


Z Index: 121

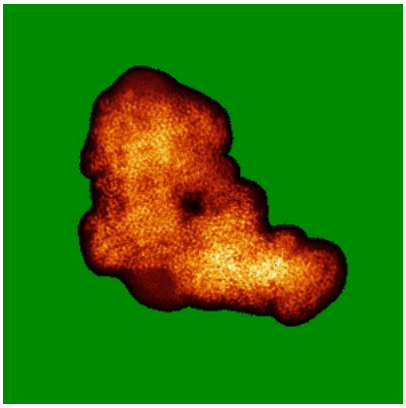
The images above show the largest variance slices of the map in three orthogonal directions.

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

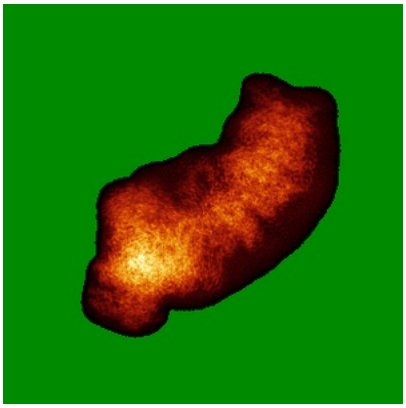
6.4.1 Primary map



X



Y

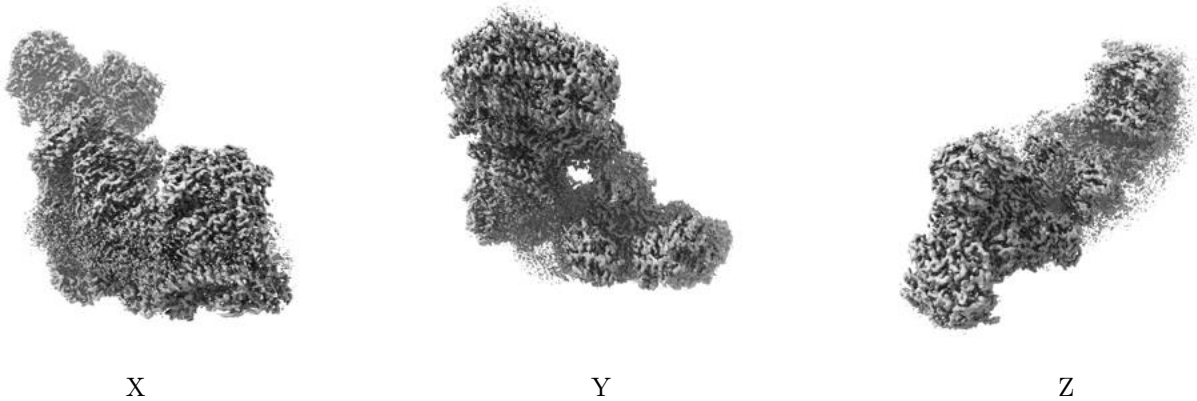


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

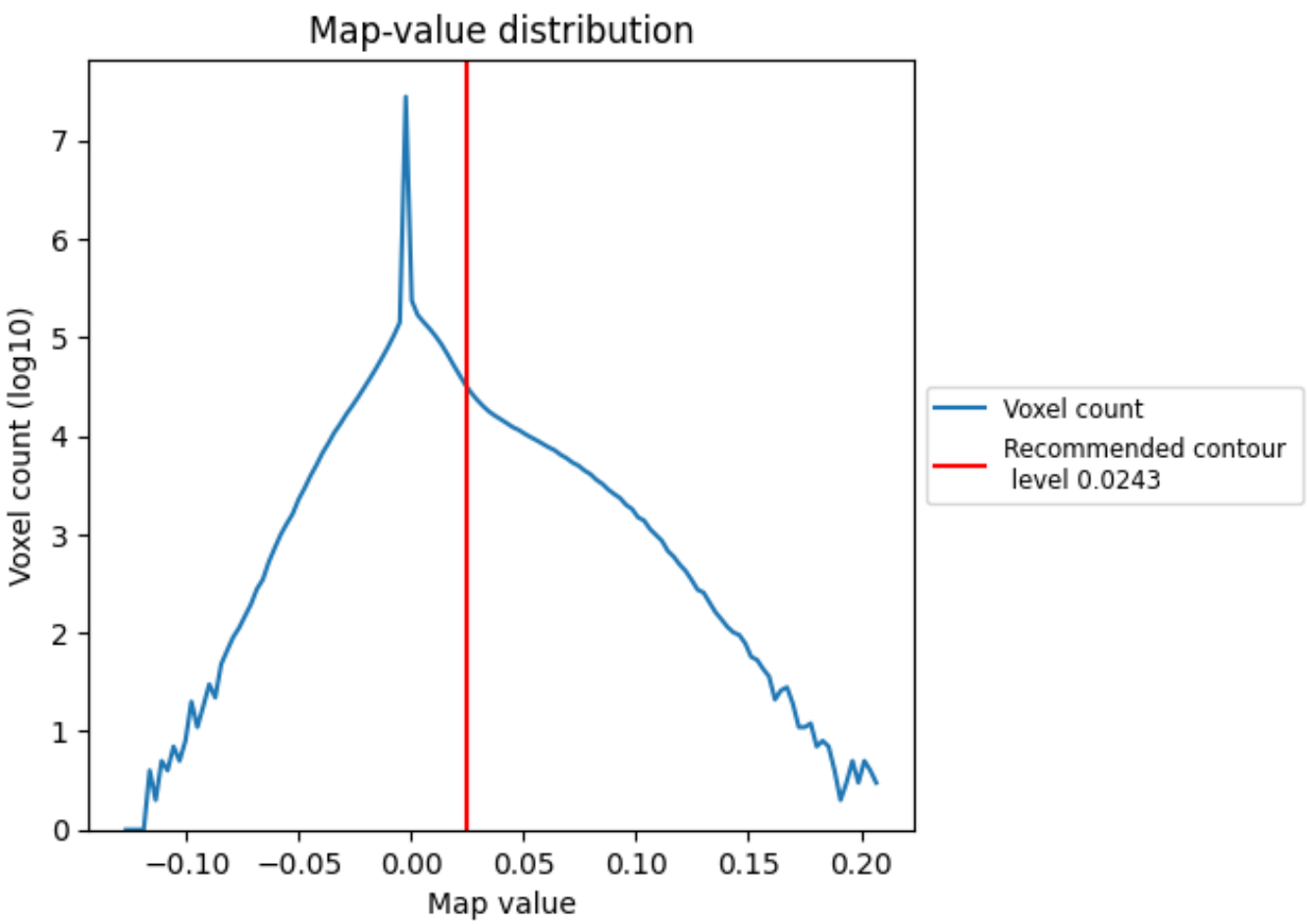
6.6 Mask visualisation (i)

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

7 Map analysis (i)

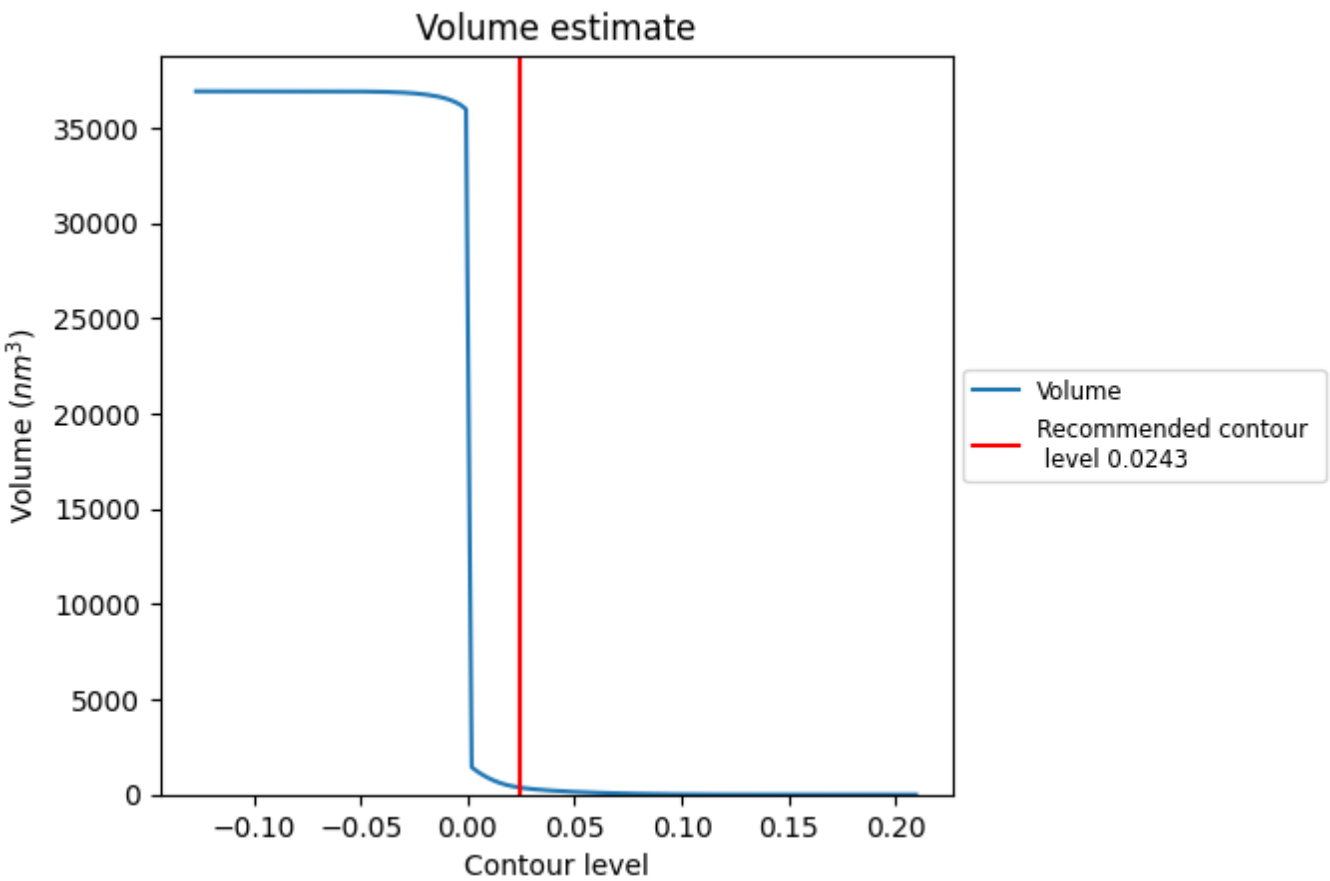
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

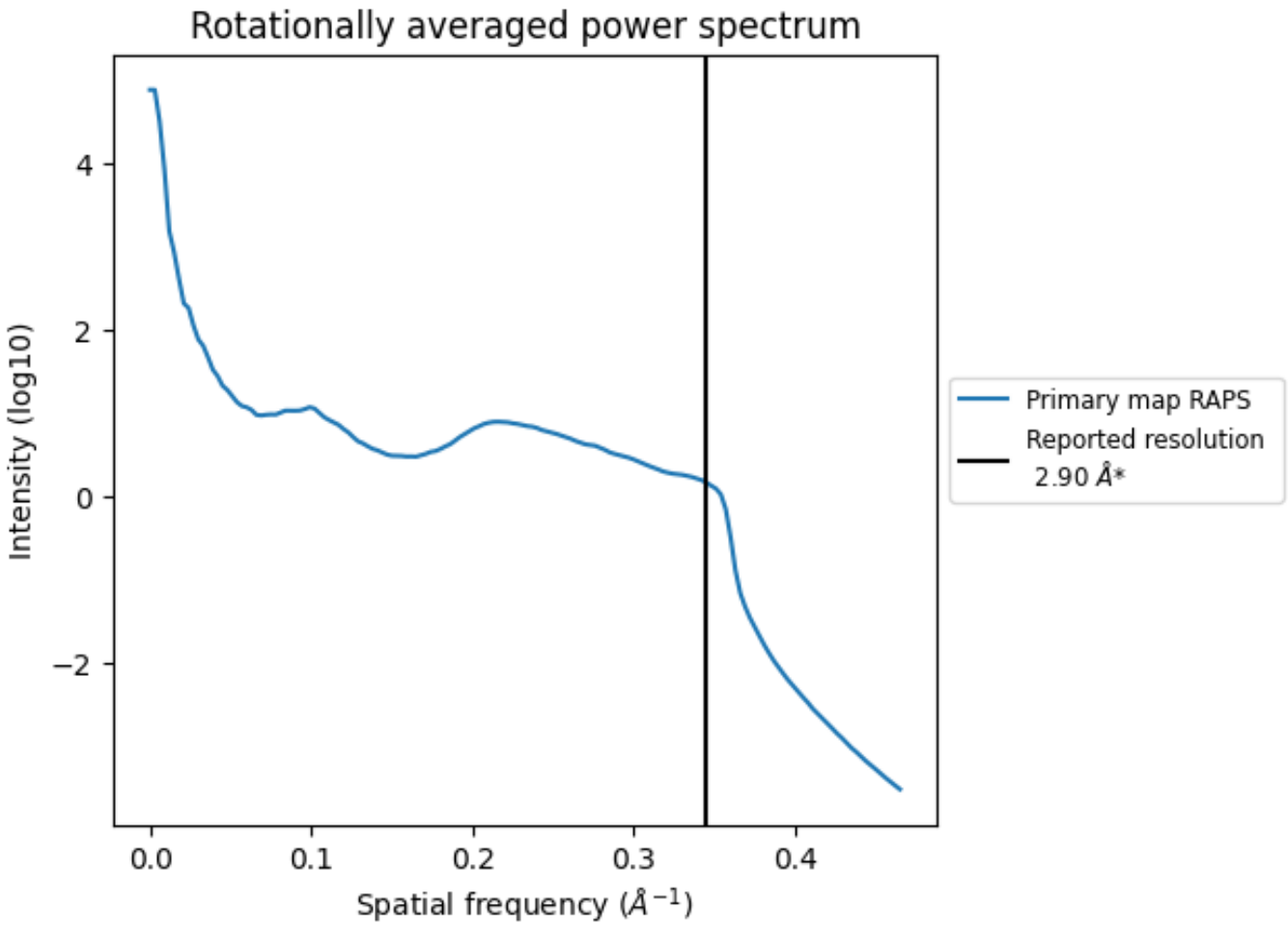
7.2 Volume estimate (i)



The volume at the recommended contour level is 370 nm^3; this corresponds to an approximate mass of 335 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 0.345 Å^{-1}

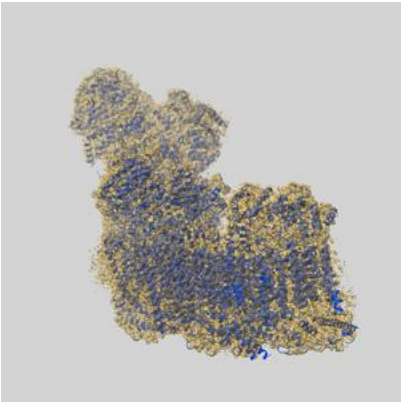
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

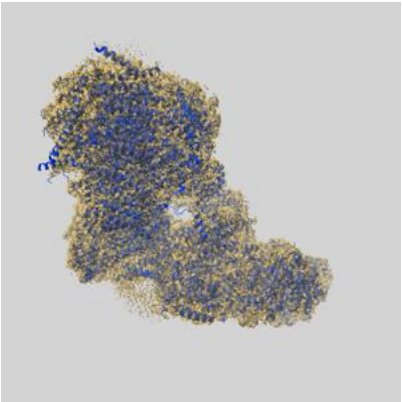
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31652 and PDB model 7V3M. Per-residue inclusion information can be found in section 3 on page 20.

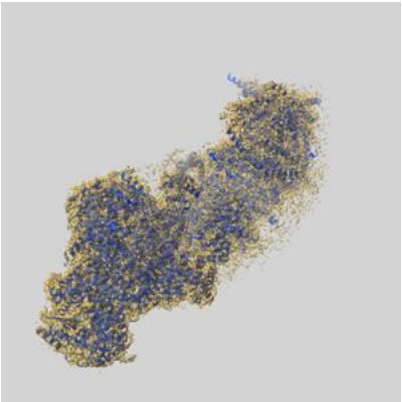
9.1 Map-model overlay (i)



X



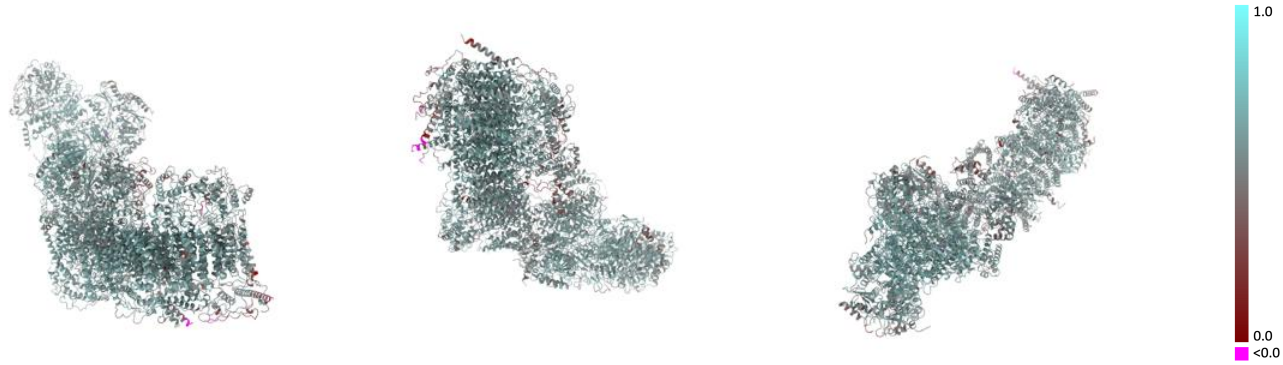
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

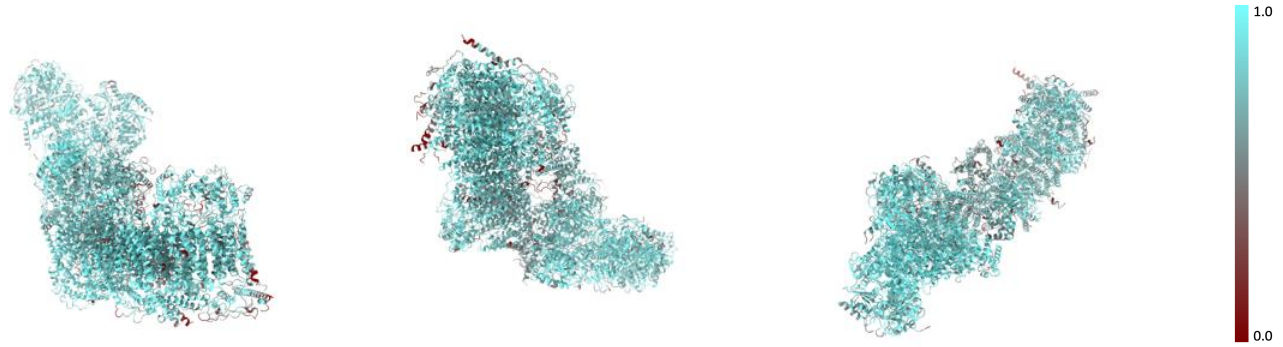
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

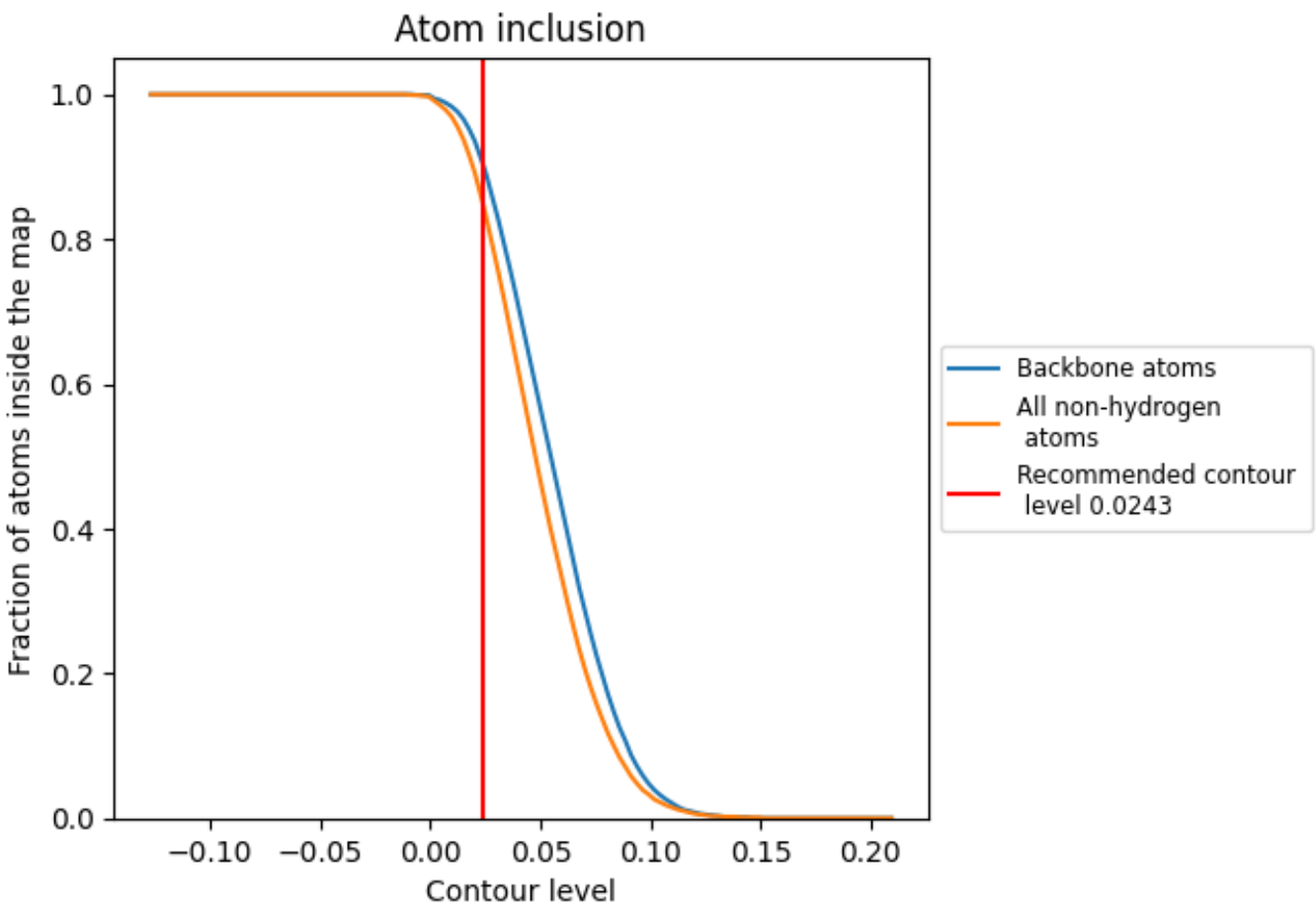
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0243).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.5850
A	0.8610	0.5810
B	0.9650	0.6460
C	0.9000	0.6260
E	0.8220	0.5680
F	0.7340	0.5050
G	0.5550	0.4150
H	0.8450	0.5660
I	0.8190	0.5940
J	0.8210	0.5660
K	0.7990	0.5470
L	0.8910	0.6180
M	0.8940	0.6040
N	0.8670	0.6080
O	0.8180	0.5520
P	0.9390	0.6330
Q	0.9190	0.6290
S	0.9370	0.6250
T	0.8680	0.6060
U	0.8540	0.5850
V	0.6450	0.5180
W	0.8720	0.5970
X	0.7480	0.5260
Y	0.7080	0.5110
Z	0.6110	0.4640
a	0.8560	0.6060
b	0.7020	0.5040
c	0.7650	0.5460
d	0.7940	0.5580
e	0.7310	0.5330
f	0.7510	0.5530
g	0.8850	0.6110
h	0.8910	0.6050
i	0.9270	0.6320
j	0.7490	0.5680

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Chain	Atom inclusion	Q-score
k	0.8520	0.5960
l	0.8490	0.5990
m	0.8070	0.5700
n	0.7200	0.5490
o	0.7840	0.5660
p	0.8080	0.5530
r	0.9120	0.6240
s	0.9130	0.6190
u	0.8780	0.6110
v	0.6610	0.4690
w	0.7830	0.5470