Full wwPDB EM Validation Report ⓘ

Jun 22, 2023 – 12:00 PM JST

PDB ID	:	7W4K
EMDB ID	:	EMD-32306
Title	:	Deactive state CI from Q1-NADH dataset, Subclass 2
Authors	:	Gu, J.; Yang, M.
Deposited on	:	2021-11-28
Resolution	:	3.20 Å(reported)

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

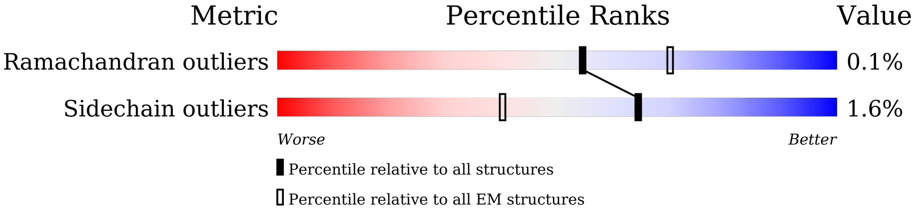
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance ⓘ

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

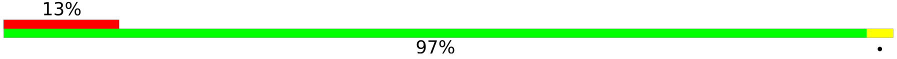
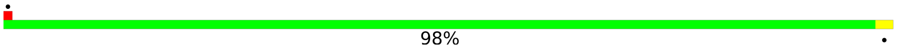
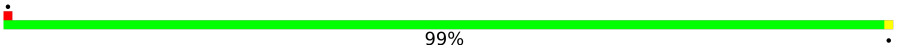
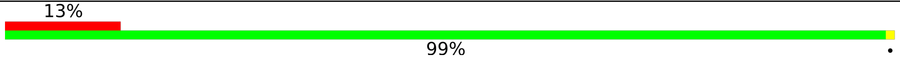
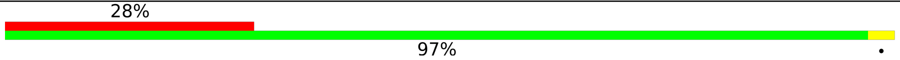
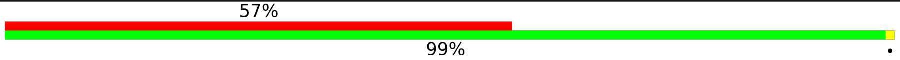
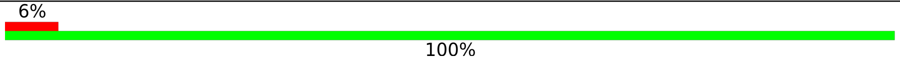
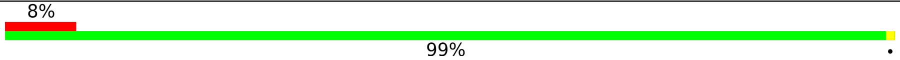
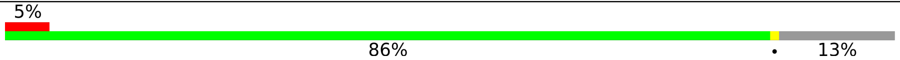
The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



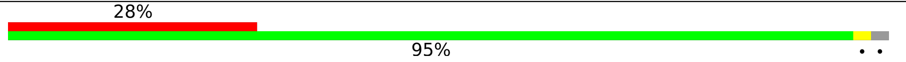
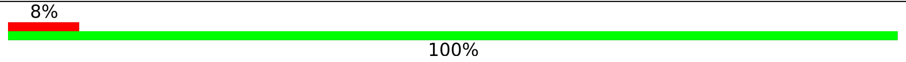
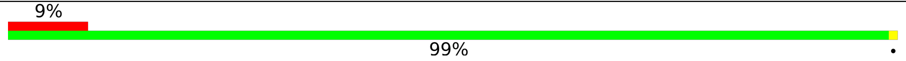
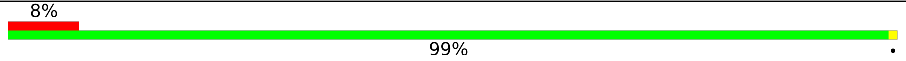
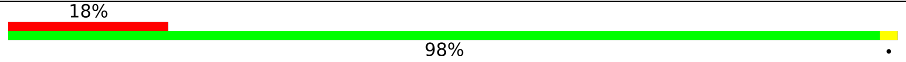
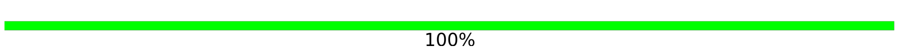
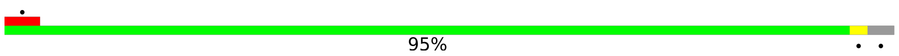
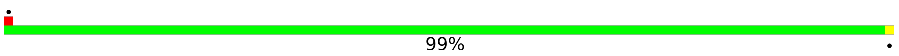
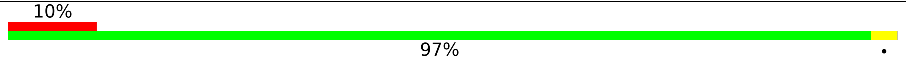
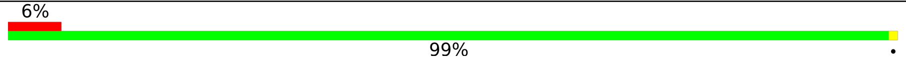
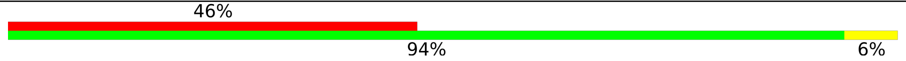
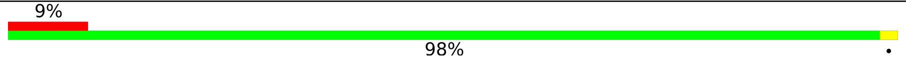
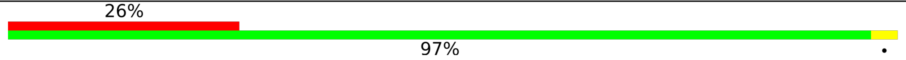
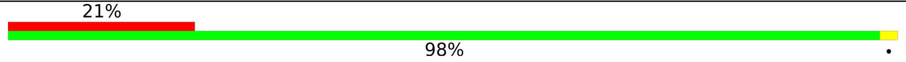
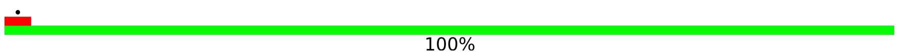
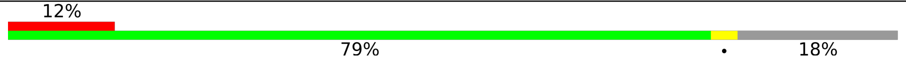
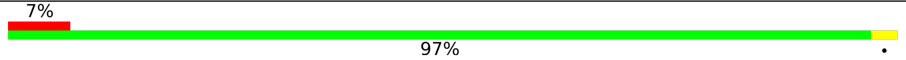
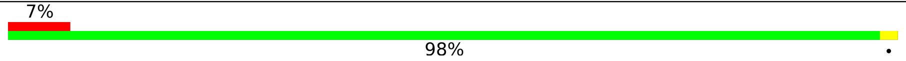
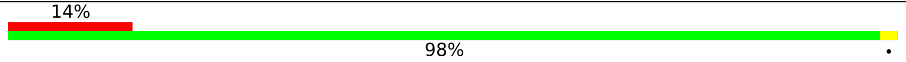
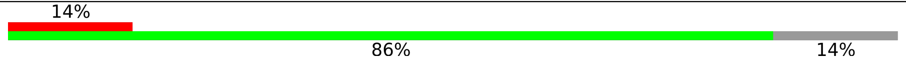
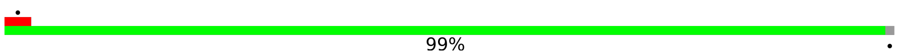
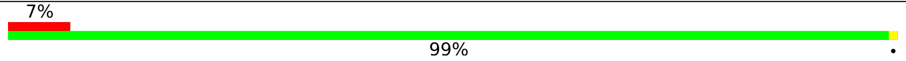
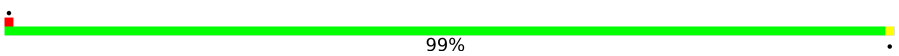
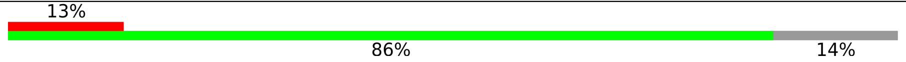
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	

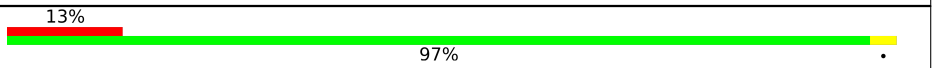
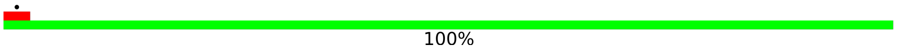
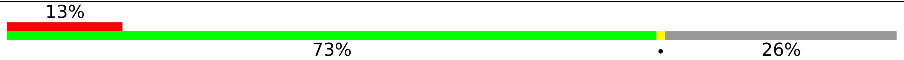
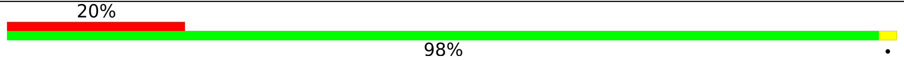
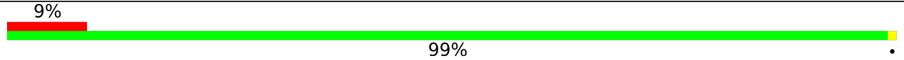
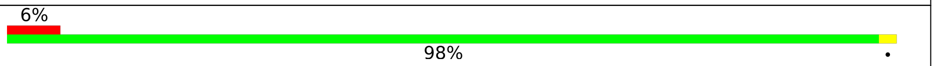
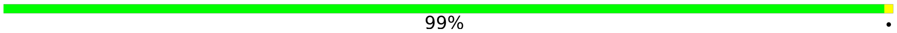
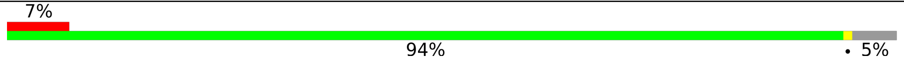
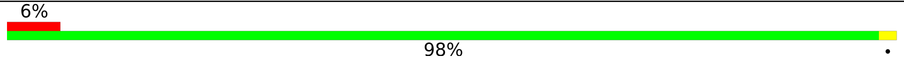
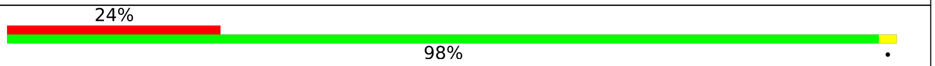
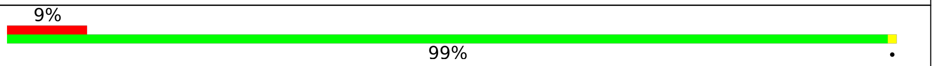
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	124	
44	w	320	

2 Entry composition ⓘ

There are 57 unique types of molecules in this entry. The entry contains 66374 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	3314	2094	590	610	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	672	425	122	123	2	0	0

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total 690	C 446	N 102	O 137	S 5	0	0
6	X	88	Total 696	C 449	N 103	O 139	S 5	0	0

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total 906	C 586	N 154	O 163	S 3	0	0

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total 780	C 491	N 147	O 139	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total 2355	C 1512	N 421	O 414	S 8	0	0

- Molecule 10 is a protein called Complex I-9kD.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total 5296	C 3320	N 923	O 1014	S 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 Complex I-30kD.

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 Complex I-49kD.

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		
19	U	83	640	415	110	115	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	1015	648	171	190	6	0	0

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1173	755	203	206	9	0	0

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	70	597	392	98	106	1	0	0

- Molecule 23 is a protein called Complex I-B12.

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 Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	140	1165	762	199	201	3	0	0

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	103	870	569	158	142	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total 1311	C 851	N 213	O 239	S 8	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total 2706	C 1780	N 420	O 460	S 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	4782	3172	740	819	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	466	305	84	76	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	1062	691	182	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	1529	979	277	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

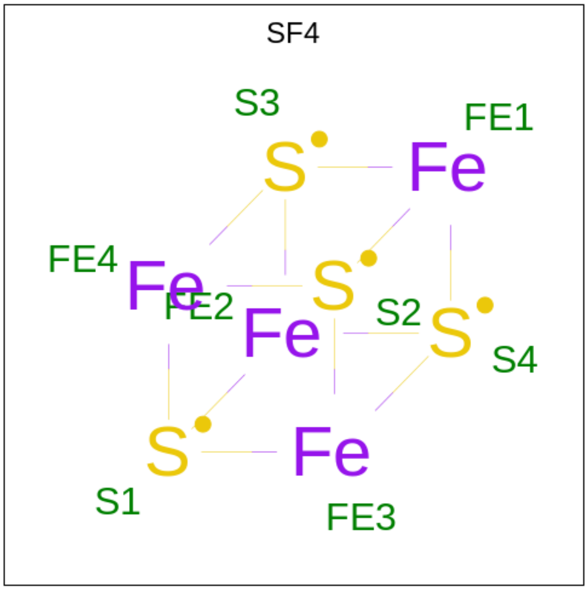
- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1028	642	195	182	9	0	0

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

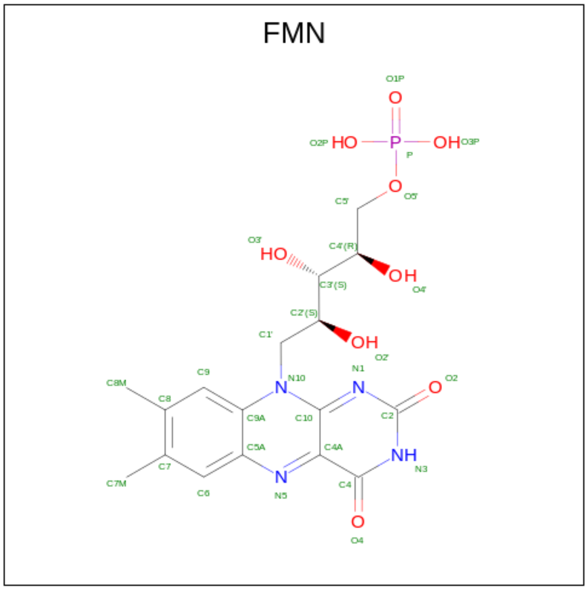
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2579	1642	438	489	10	0	0

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



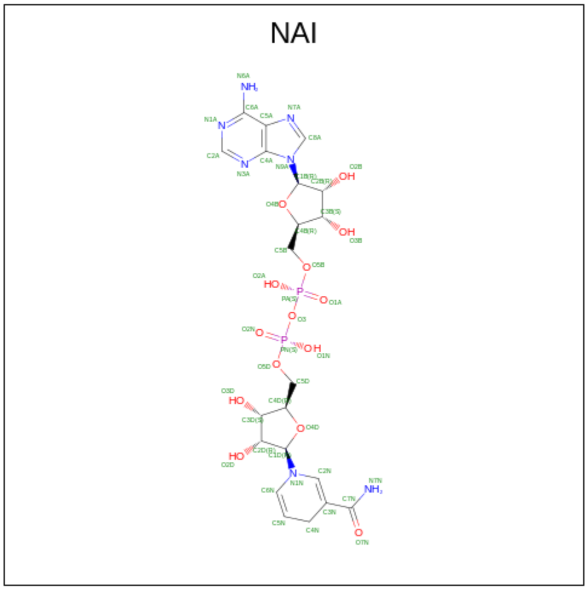
Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total Fe S 8 4 4	0
45	B	1	Total Fe S 8 4 4	0
45	B	1	Total Fe S 8 4 4	0
45	C	1	Total Fe S 8 4 4	0
45	M	1	Total Fe S 8 4 4	0
45	M	1	Total Fe S 8 4 4	0

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



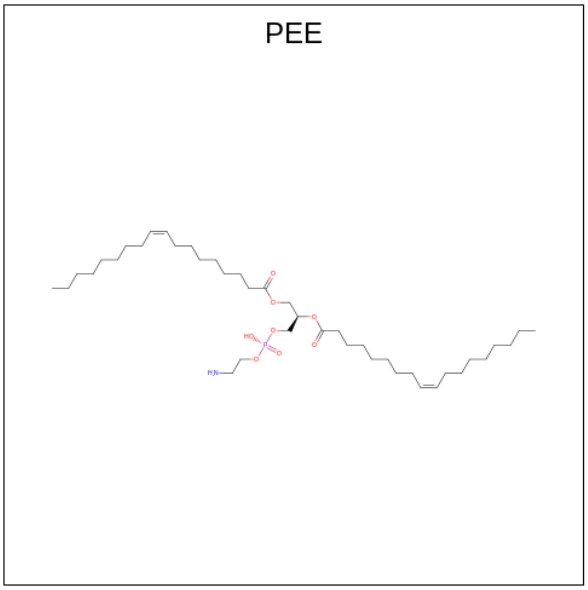
Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 31 17 4 9 1	0

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



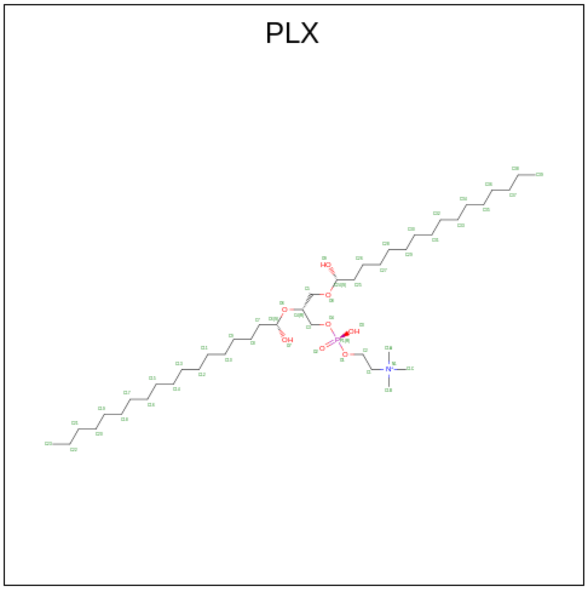
Mol	Chain	Residues	Atoms	AltConf
47	A	1	Total C N O P 44 21 7 14 2	0

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



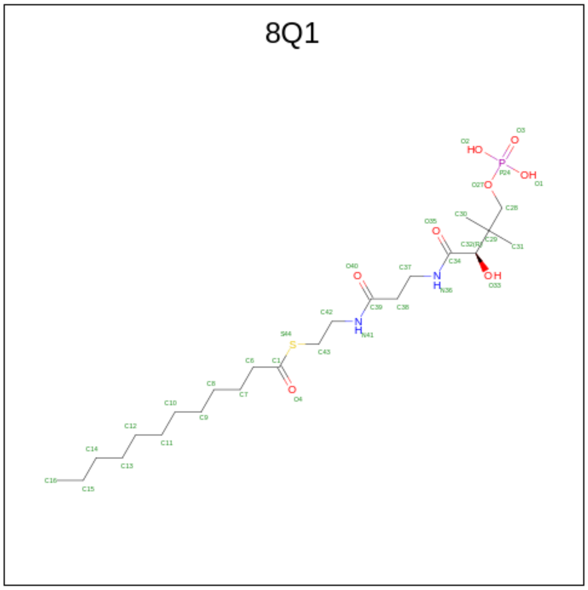
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total 47	C 37	N 1	O 8	P 1	0
48	Q	1	Total 47	C 37	N 1	O 8	P 1	0
48	Q	1	Total 51	C 41	N 1	O 8	P 1	0
48	U	1	Total 51	C 41	N 1	O 8	P 1	0
48	l	1	Total 46	C 36	N 1	O 8	P 1	0
48	l	1	Total 46	C 36	N 1	O 8	P 1	0
48	m	1	Total 41	C 31	N 1	O 8	P 1	0
48	r	1	Total 51	C 41	N 1	O 8	P 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 (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



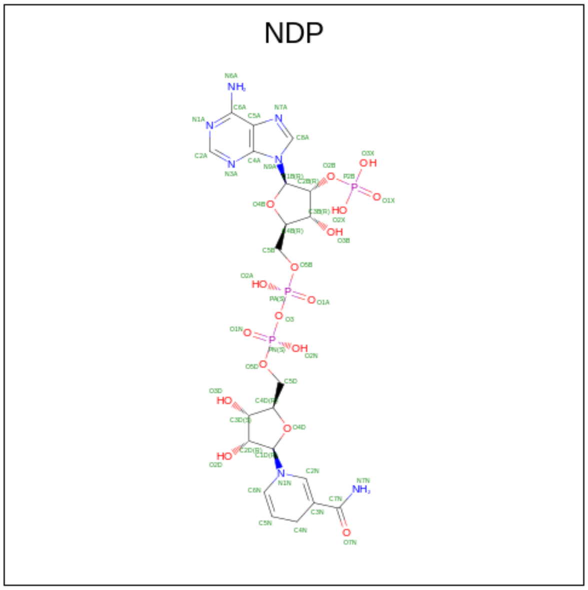
Mol	Chain	Residues	Atoms	AltConf
49	C	1	Total C N O P 52 42 1 8 1	0
49	a	1	Total C N O P 52 42 1 8 1	0
49	i	1	Total C N O P 52 42 1 8 1	0
49	j	1	Total C N O P 52 42 1 8 1	0
49	r	1	Total C N O P 52 42 1 8 1	0
49	r	1	Total C N O P 52 42 1 8 1	0

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



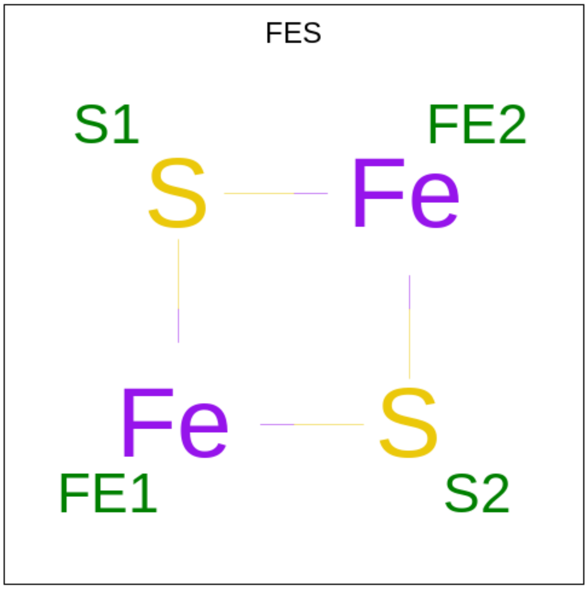
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
50	G	1	35	23	2	8	1	1	0
50	X	1	35	23	2	8	1	1	0

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_{7}O_{17}P_{3}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

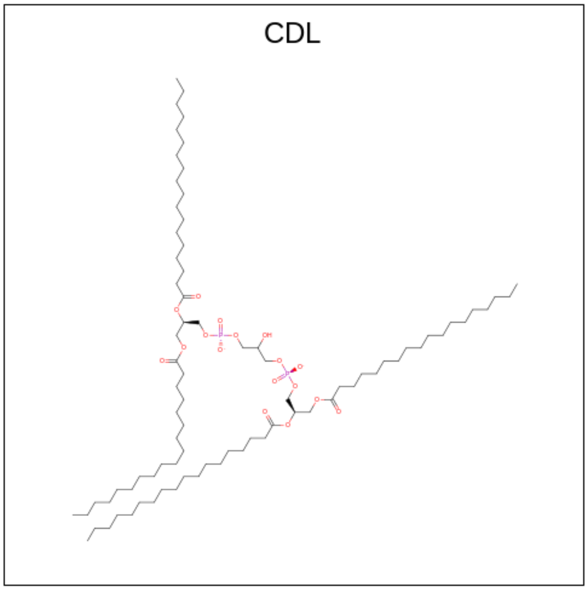
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

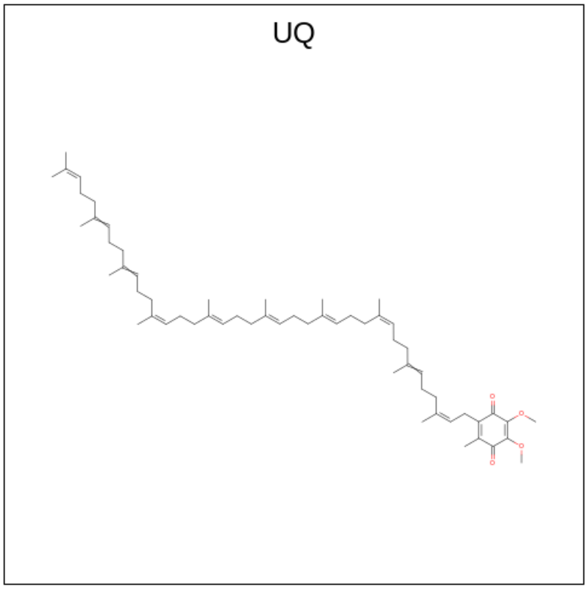
Mol	Chain	Residues	Atoms	AltConf
54	T	1	Total Zn 1 1	0

- Molecule 55 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



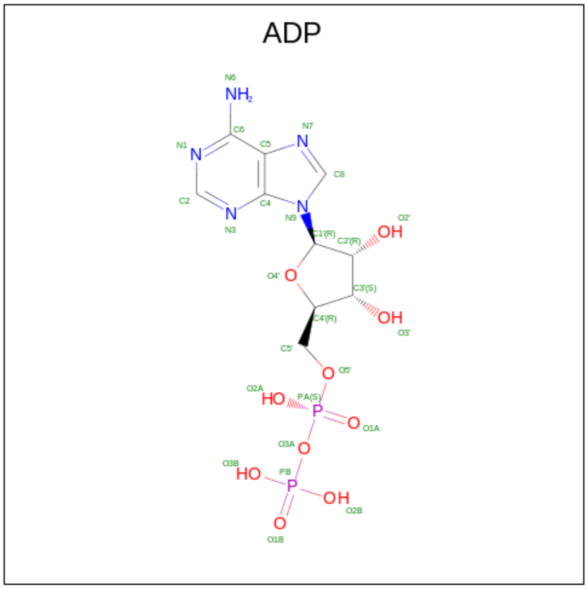
Mol	Chain	Residues	Atoms				AltConf
55	a	1	Total 91	C 72	O 17	P 2	0
55	i	1	Total 100	C 81	O 17	P 2	0
55	l	1	Total 100	C 81	O 17	P 2	0

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



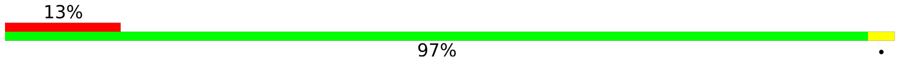
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

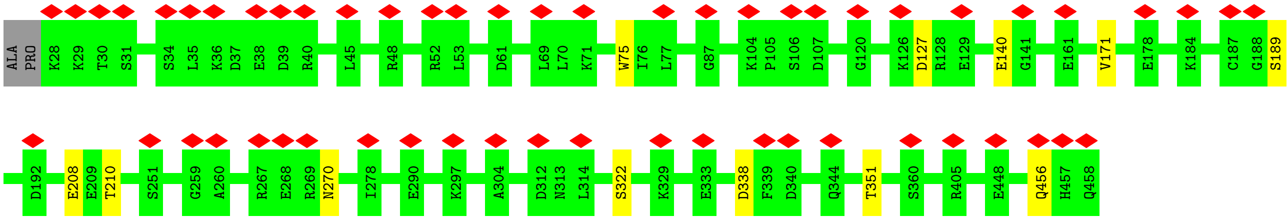
3 Residue-property plots ⓘ

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

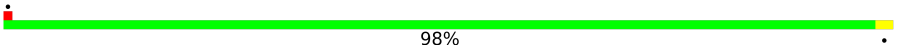
Chain A:

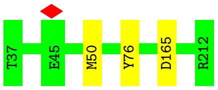




- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

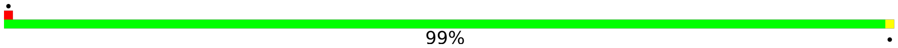
Chain B:

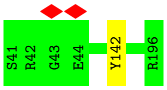




- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

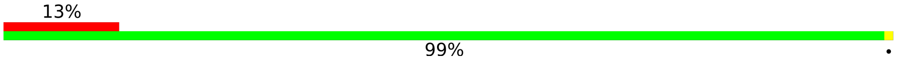
Chain C:

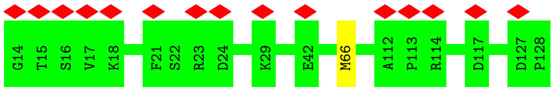




- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

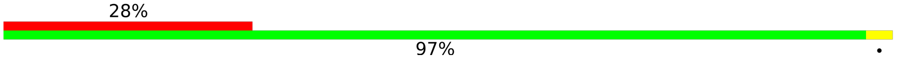
Chain E:

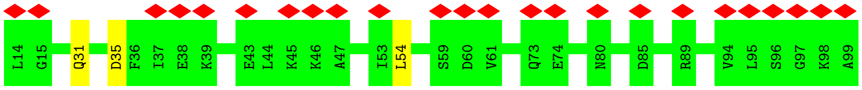




- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

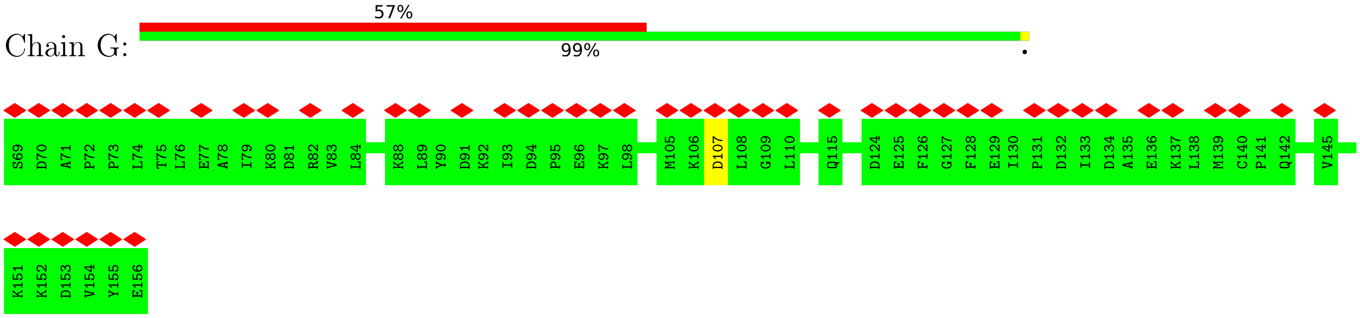
Chain F:





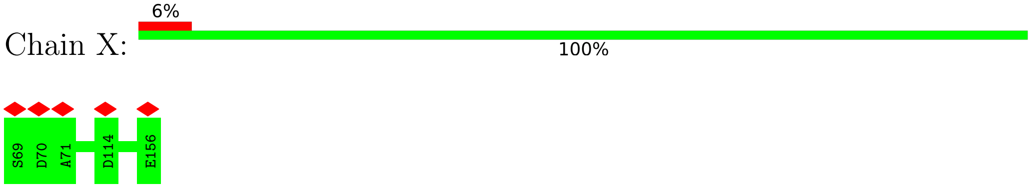
- Molecule 6: Acyl carrier protein

Chain G:



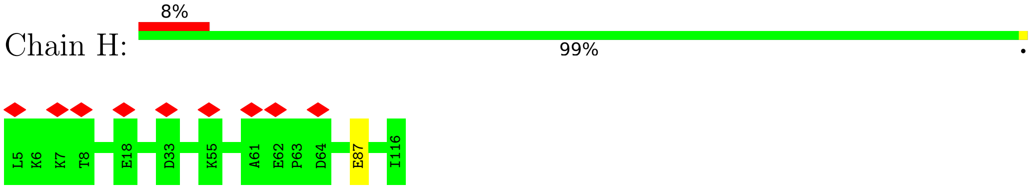
- Molecule 6: Acyl carrier protein

Chain X:



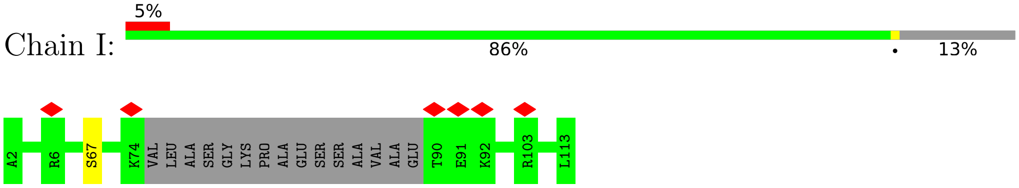
- Molecule 7: Complex I subunit B13

Chain H:



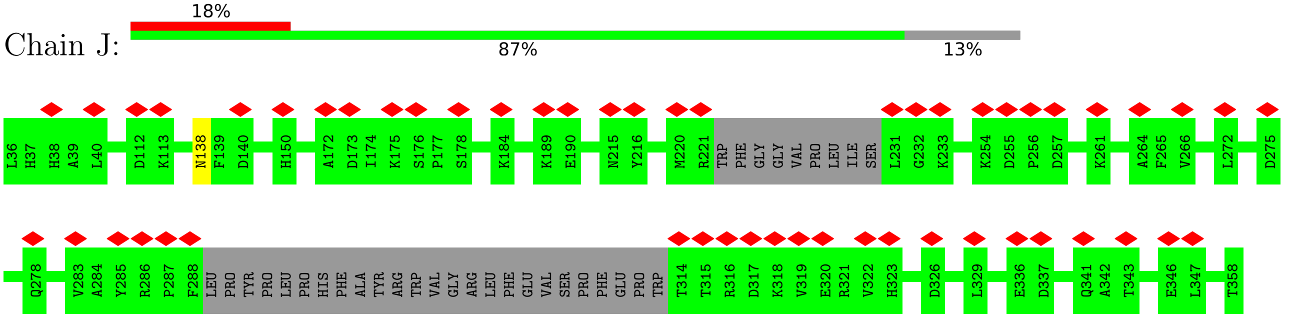
- Molecule 8: Complex I-B14.5a

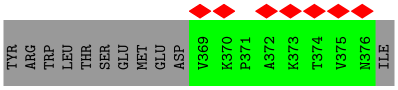
Chain I:



- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

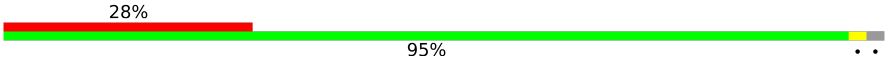
Chain J:

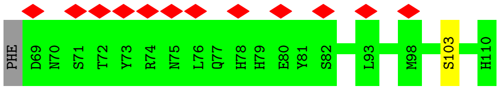




- Molecule 10: Complex I-9kD

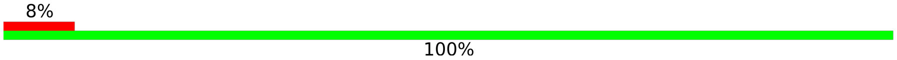
Chain K:

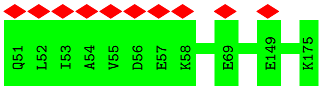




- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

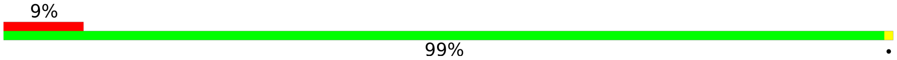
Chain L:

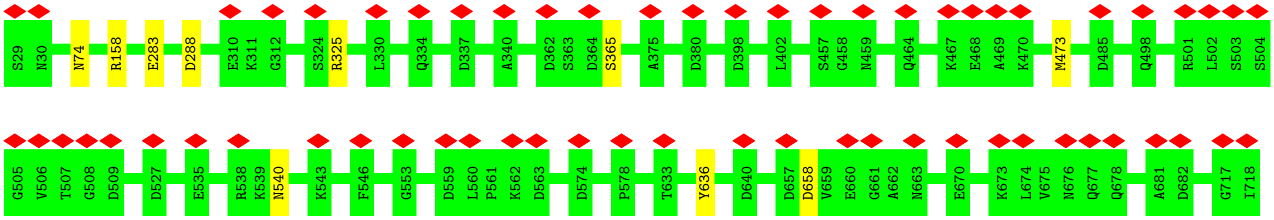




- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

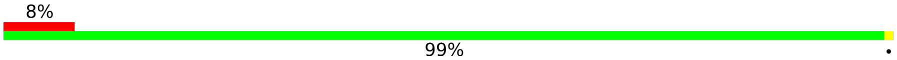
Chain M:

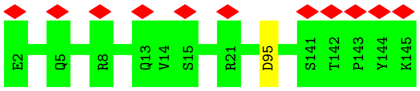




- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

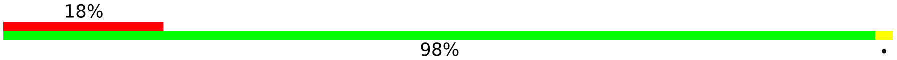
Chain N:

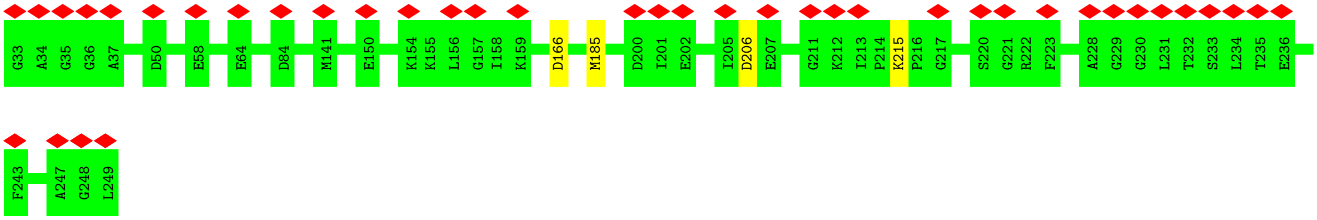




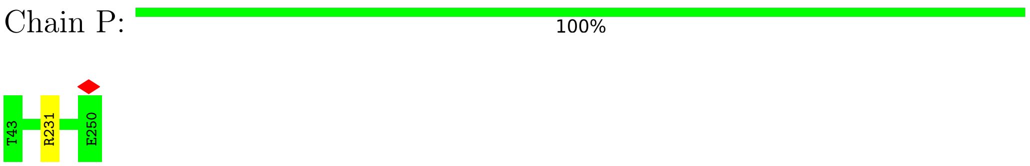
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:

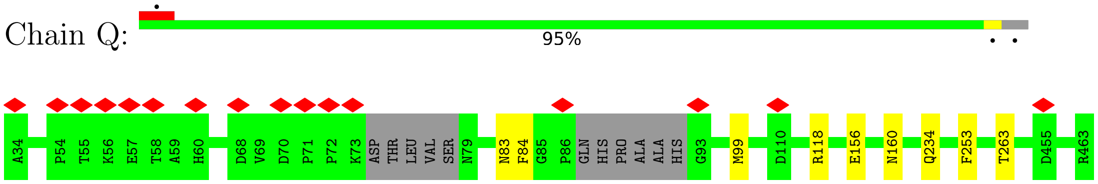




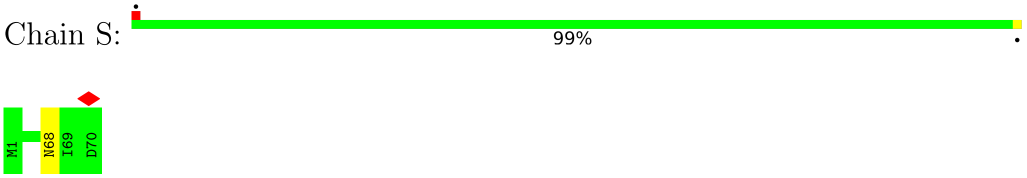
- Molecule 15: Complex I-30kD



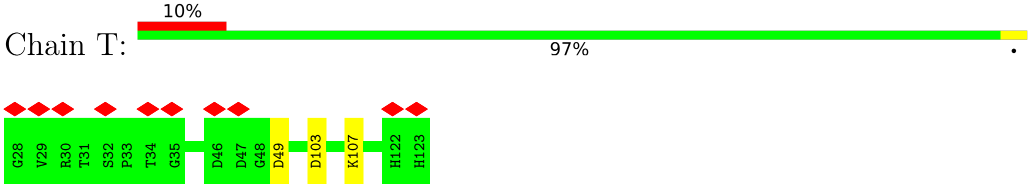
- Molecule 16: Complex I-49kD



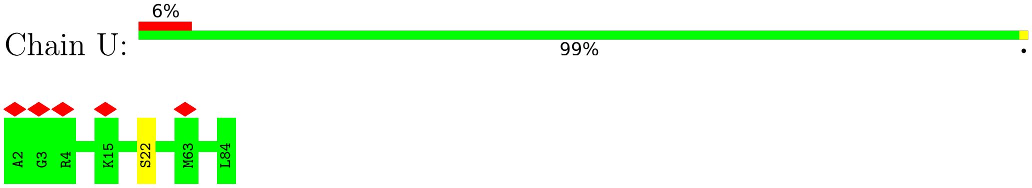
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



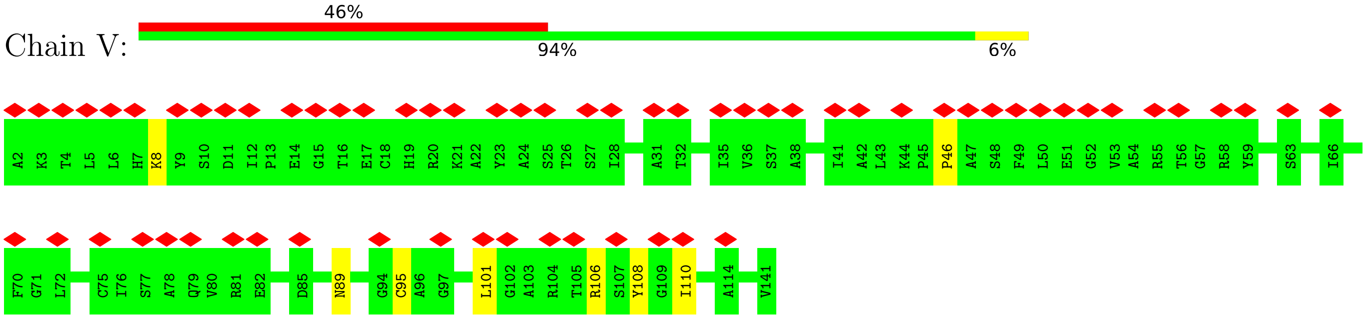
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

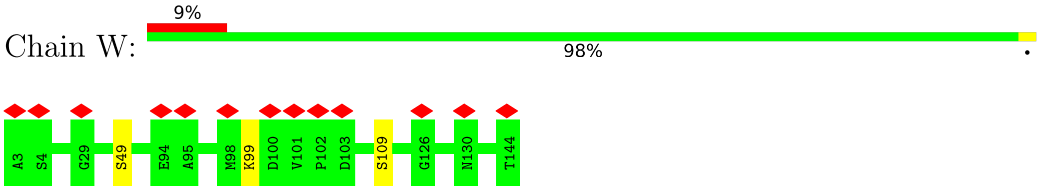


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



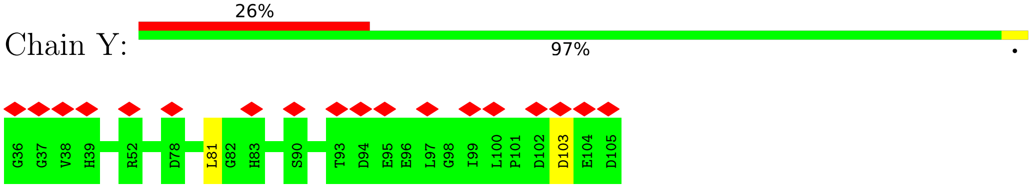
- Molecule 21: Complex I-B16.6

Chain W:



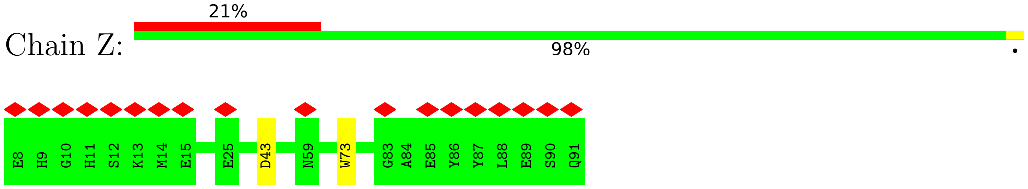
- Molecule 22: Complex I-AGGG

Chain Y:



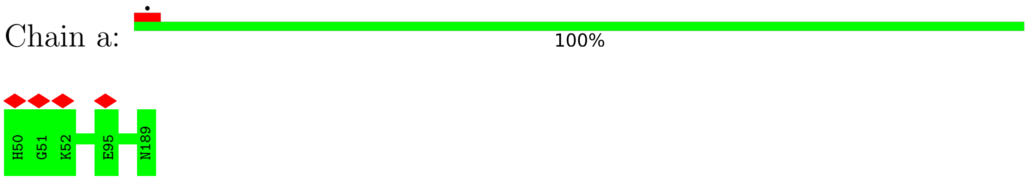
- Molecule 23: Complex I-B12

Chain Z:



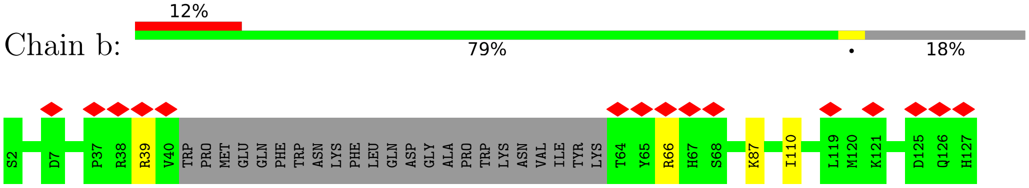
- Molecule 24: Complex I-SGDH

Chain a:



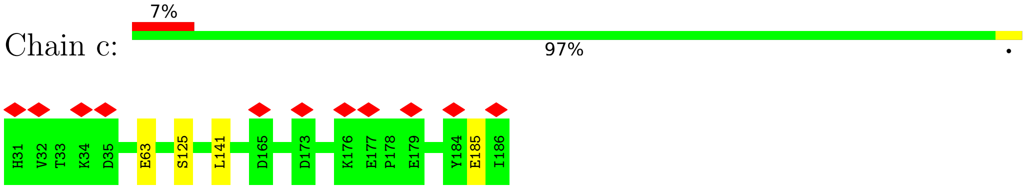
- Molecule 25: Complex I-B17

Chain b:



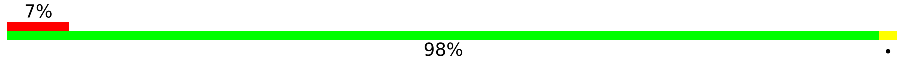
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

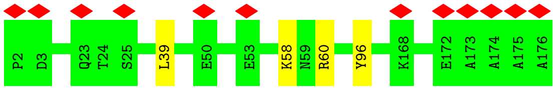
Chain c:



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

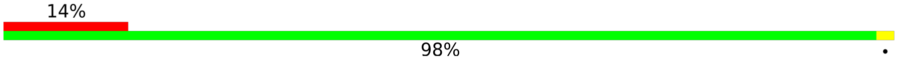
Chain d:

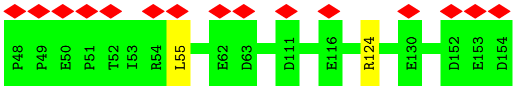




- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

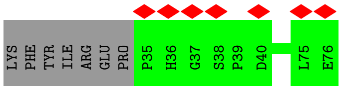
Chain e:





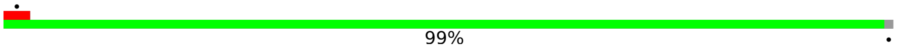
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

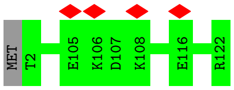
Chain f:



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

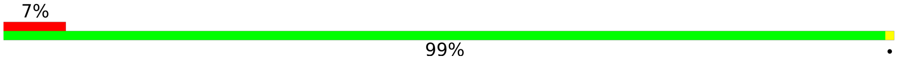
Chain g:

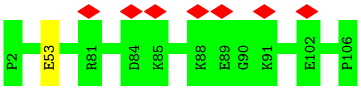




- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

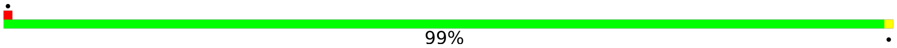
Chain h:

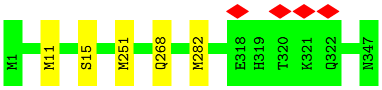




- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

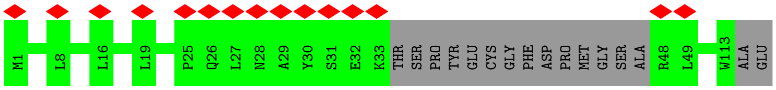
Chain i:





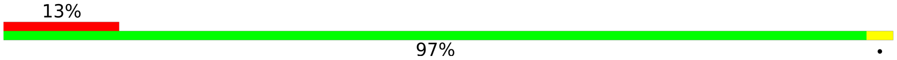
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

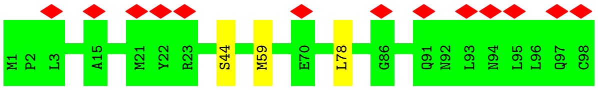
Chain j:



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

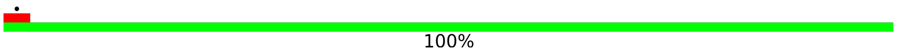
Chain k:

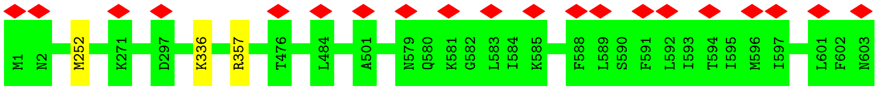




- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

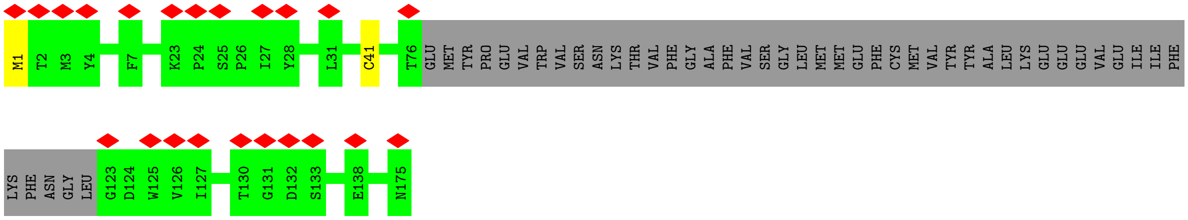
Chain l:





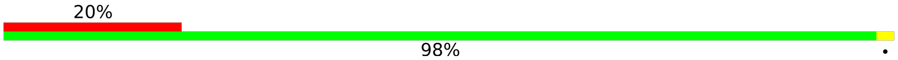
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

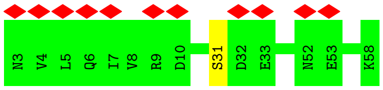
Chain m:



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

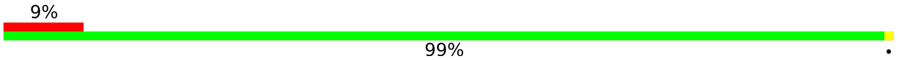
Chain n:

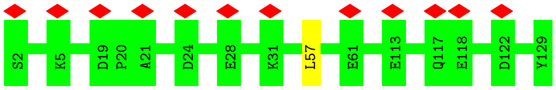




- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

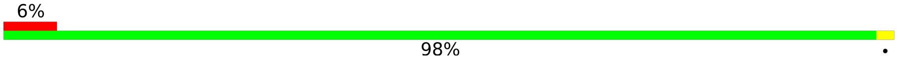
Chain o:

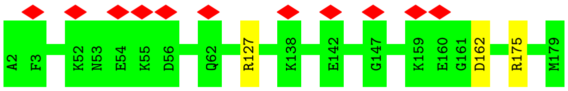




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

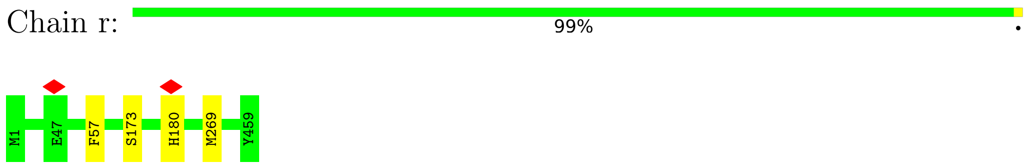
Chain p:





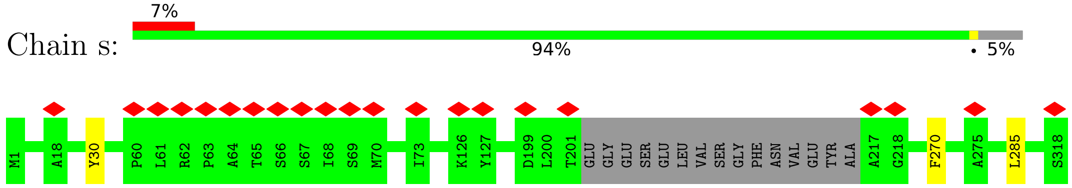
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:



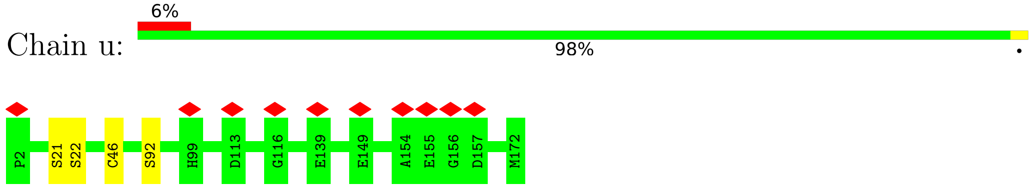
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:



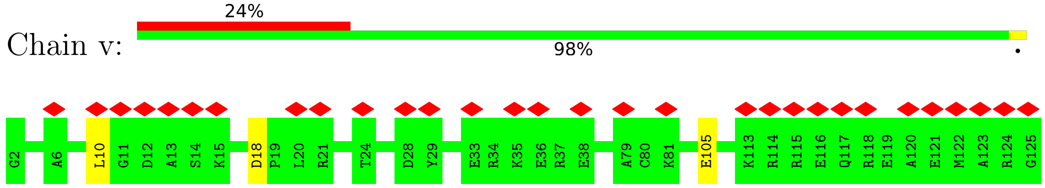
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:



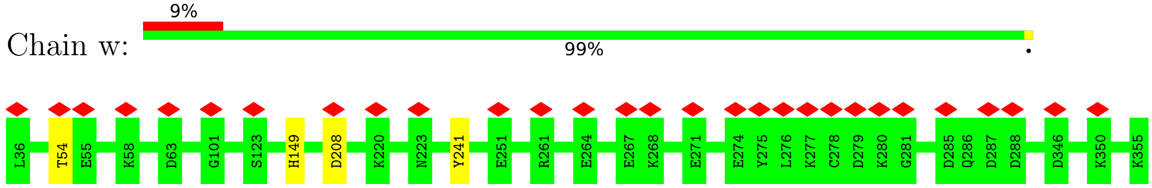
• Molecule 43: Complex I-B18

Chain v:



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

Chain w:



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23715	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 ($e^-/\text{Å}^2$)	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	0.230	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0282	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, PEE, ZN, PLX, UQ, CDL, MG, 2MR, SF4, FES, NDP, 8Q1, FMN, NAI

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	0.27	0/3389	0.50	0/4579
2	B	0.31	0/1443	0.51	0/1952
3	C	0.30	0/1279	0.53	0/1730
4	E	0.26	0/995	0.53	0/1340
5	F	0.28	0/683	0.53	0/922
6	G	0.28	0/702	0.43	0/952
6	X	0.26	0/708	0.45	0/959
7	H	0.25	0/925	0.46	0/1253
8	I	0.25	0/798	0.54	0/1079
9	J	0.26	0/2407	0.49	0/3249
10	K	0.23	0/365	0.47	0/493
11	L	0.25	0/1039	0.49	0/1403
12	M	0.25	0/5384	0.50	0/7295
13	N	0.25	0/1245	0.50	0/1694
14	O	0.26	0/1711	0.47	0/2328
15	P	0.29	0/1789	0.51	0/2436
16	Q	0.29	0/3451	0.51	0/4672
17	S	0.26	0/582	0.50	0/783
18	T	0.27	0/755	0.51	0/1018
19	U	0.26	0/661	0.46	0/909
20	V	0.34	1/1036 (0.1%)	0.46	0/1404
21	W	0.28	0/1204	0.51	0/1624
22	Y	0.26	0/623	0.47	0/853
23	Z	0.25	0/695	0.46	0/939
24	a	0.29	0/1199	0.51	0/1623
25	b	0.26	0/897	0.55	0/1221
26	c	0.29	0/1367	0.48	0/1870
27	d	0.27	0/1494	0.51	0/2015
28	e	0.27	0/916	0.52	0/1246
29	f	0.27	0/350	0.50	0/473
30	g	0.29	0/1031	0.49	0/1394
31	h	0.25	0/889	0.48	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
32	i	0.26	0/2769	0.44	0/3763
33	j	0.27	0/819	0.46	0/1117
34	k	0.27	0/759	0.44	0/1029
35	l	0.27	0/4911	0.45	0/6679
36	m	0.31	0/970	0.47	0/1316
37	n	0.24	0/478	0.50	0/647
38	o	0.27	0/1092	0.52	1/1481 (0.1%)
39	p	0.27	0/1584	0.51	0/2147
40	r	0.26	0/3723	0.45	0/5078
41	s	0.28	0/2464	0.47	0/3369
42	u	0.27	0/1436	0.50	0/1938
43	v	0.27	0/1052	0.55	0/1411
44	w	0.27	0/2639	0.48	0/3576
All	All	0.27	1/66708 (0.0%)	0.49	1/90449 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	8	LYS	CE-NZ	-5.91	1.34	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	o	57	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	429/433 (99%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	13	49
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/342 (84%)	276 (96%)	13 (4%)	0	100	100
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	669 (97%)	18 (3%)	1 (0%)	51	83
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	13 (3%)	1 (0%)	47	79
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%)	131 (95%)	6 (4%)	1 (1%)	22	61
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
23	Z	82/84 (98%)	82 (100%)	0	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	93 (94%)	5 (5%)	1 (1%)	15	54
26	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
29	f	40/49 (82%)	40 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	570 (95%)	31 (5%)	0	100	100
36	m	125/175 (71%)	115 (92%)	10 (8%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	25	64
40	r	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
41	s	299/318 (94%)	282 (94%)	17 (6%)	0	100	100
42	u	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
43	v	122/124 (98%)	115 (94%)	7 (6%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8322 (96%)	7702 (96%)	321 (4%)	6 (0%)	54	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	31	GLN
39	p	175	ARG
12	M	283	GLU
16	Q	160	ASN
25	b	110	ILE
20	V	46	PRO

5.3.2 Protein sidechains ⓘ

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	343/346 (99%)	331 (96%)	12 (4%)	36	69
2	B	151/151 (100%)	148 (98%)	3 (2%)	55	80
3	C	132/132 (100%)	131 (99%)	1 (1%)	81	93
4	E	107/107 (100%)	106 (99%)	1 (1%)	78	91
5	F	72/76 (95%)	70 (97%)	2 (3%)	43	74
6	G	75/81 (93%)	74 (99%)	1 (1%)	69	87
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	98/99 (99%)	97 (99%)	1 (1%)	76	90
8	I	87/97 (90%)	86 (99%)	1 (1%)	73	88
9	J	254/296 (86%)	253 (100%)	1 (0%)	91	95
10	K	41/42 (98%)	40 (98%)	1 (2%)	49	77
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	571 (98%)	9 (2%)	62	84
13	N	130/130 (100%)	129 (99%)	1 (1%)	81	93
14	O	183/183 (100%)	179 (98%)	4 (2%)	52	79
15	P	190/190 (100%)	189 (100%)	1 (0%)	88	95
16	Q	361/370 (98%)	354 (98%)	7 (2%)	57	81
17	S	58/58 (100%)	57 (98%)	1 (2%)	60	83
18	T	79/79 (100%)	76 (96%)	3 (4%)	33	67
19	U	68/69 (99%)	67 (98%)	1 (2%)	65	85
20	V	100/101 (99%)	94 (94%)	6 (6%)	19	54
21	W	123/123 (100%)	120 (98%)	3 (2%)	49	77
22	Y	62/63 (98%)	60 (97%)	2 (3%)	39	71
23	Z	65/65 (100%)	63 (97%)	2 (3%)	40	72
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	95/119 (80%)	92 (97%)	3 (3%)	39	71
26	c	140/141 (99%)	136 (97%)	4 (3%)	42	74
27	d	155/155 (100%)	151 (97%)	4 (3%)	46	76
28	e	99/99 (100%)	97 (98%)	2 (2%)	55	80
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/109 (99%)	108 (100%)	0	100	100
31	h	93/93 (100%)	92 (99%)	1 (1%)	73	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	310/311 (100%)	305 (98%)	5 (2%)	62	84
33	j	88/100 (88%)	88 (100%)	0	100	100
34	k	85/85 (100%)	82 (96%)	3 (4%)	36	69
35	l	536/537 (100%)	533 (99%)	3 (1%)	86	94
36	m	98/141 (70%)	96 (98%)	2 (2%)	55	80
37	n	50/53 (94%)	49 (98%)	1 (2%)	55	80
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	158/159 (99%)	156 (99%)	2 (1%)	69	87
40	r	410/410 (100%)	406 (99%)	4 (1%)	76	90
41	s	263/275 (96%)	260 (99%)	3 (1%)	73	88
42	u	153/153 (100%)	149 (97%)	4 (3%)	46	76
43	v	104/111 (94%)	101 (97%)	3 (3%)	42	74
44	w	280/283 (99%)	276 (99%)	4 (1%)	67	86
All	All	7044/7246 (97%)	6932 (98%)	112 (2%)	64	84

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	TRP
1	A	127	ASP
1	A	140	GLU
1	A	171	VAL
1	A	189	SER
1	A	208	GLU
1	A	210	THR
1	A	270	ASN
1	A	322	SER
1	A	338	ASP
1	A	351	THR
1	A	456	GLN
2	B	50	MET
2	B	76	TYR
2	B	165	ASP
3	C	142	TYR
4	E	66	MET
5	F	35	ASP
5	F	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	G	107	ASP
7	H	87	GLU
8	I	67	SER
9	J	138	ASN
10	K	103	SER
12	M	74	ASN
12	M	158	ARG
12	M	288	ASP
12	M	325	ARG
12	M	365	SER
12	M	473	MET
12	M	540	ASN
12	M	636	TYR
12	M	658	ASP
13	N	95	ASP
14	O	166	ASP
14	O	185	MET
14	O	206	ASP
14	O	215	LYS
15	P	231	ARG
16	Q	83	ASN
16	Q	84	PHE
16	Q	99	MET
16	Q	156	GLU
16	Q	234	GLN
16	Q	253	PHE
16	Q	263	THR
17	S	68	ASN
18	T	49	ASP
18	T	103	ASP
18	T	107	LYS
19	U	22	SER
20	V	89	ASN
20	V	95	CYS
20	V	101	LEU
20	V	106	ARG
20	V	108	TYR
20	V	110	ILE
21	W	49	SER
21	W	99	LYS
21	W	109	SER
22	Y	81	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Y	103	ASP
23	Z	43	ASP
23	Z	73	TRP
25	b	39	ARG
25	b	66	ARG
25	b	87	LYS
26	c	63	GLU
26	c	125	SER
26	c	141	LEU
26	c	185	GLU
27	d	39	LEU
27	d	58	LYS
27	d	60	ARG
27	d	96	TYR
28	e	55	LEU
28	e	124	ARG
31	h	53	GLU
32	i	11	MET
32	i	15	SER
32	i	251	MET
32	i	268	GLN
32	i	282	MET
34	k	44	SER
34	k	59	MET
34	k	78	LEU
35	l	252	MET
35	l	336	LYS
35	l	357	ARG
36	m	1	MET
36	m	41	CYS
37	n	31	SER
39	p	127	ARG
39	p	162	ASP
40	r	57	PHE
40	r	173	SER
40	r	180	HIS
40	r	269	MET
41	s	30	TYR
41	s	270	PHE
41	s	285	LEU
42	u	21	SER
42	u	22	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	u	46	CYS
42	u	92	SER
43	v	10	LEU
43	v	18	ASP
43	v	105	GLU
44	w	54	THR
44	w	149	HIS
44	w	208	ASP
44	w	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
3	C	123	GLN
14	O	69	ASN
14	O	133	GLN
15	P	51	ASN
27	d	134	GLN
31	h	27	HIS
32	i	268	GLN
35	l	400	ASN
38	o	50	GLN
38	o	123	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.18	1 (10%)	5,13,15	1.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	5/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NH2	-3.20	1.26	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NH1-CZ-NE-CD
16	Q	118	2MR	NH2-CZ-NE-CD
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	C	303	-	51,51,51	1.15	3 (5%)	55,59,59	0.62	1 (1%)
50	8Q1	G	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.55	6 (15%)
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.45	5 (17%)
48	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
48	PEE	Q	501	-	46,46,50	1.20	6 (13%)	49,51,55	0.99	2 (4%)
48	PEE	U	101	-	50,50,50	1.15	6 (12%)	53,55,55	0.95	2 (3%)
55	CDL	l	701	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
50	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.51	6 (15%)
48	PEE	C	302	-	46,46,50	1.22	6 (13%)	49,51,55	0.97	2 (4%)
55	CDL	a	201	-	90,90,99	1.13	9 (10%)	96,102,111	0.93	4 (4%)
47	NAI	A	503	-	42,48,48	4.95	18 (42%)	47,73,73	1.33	6 (12%)
49	PLX	i	401	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
49	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
48	PEE	l	702	-	45,45,50	1.21	6 (13%)	48,50,55	0.96	2 (4%)
49	PLX	j	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
48	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.95	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
48	PEE	Q	502	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
51	NDP	J	401	-	45,52,52	4.57	20 (44%)	53,80,80	1.95	8 (15%)
45	SF4	M	802	12	0,12,12	-	-	-		
52	FES	O	301	14	0,4,4	-	-	-		
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
49	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.58	1 (1%)
45	SF4	C	301	16,3	0,12,12	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
56	UQ	s	401	-	28,28,63	3.27	7 (25%)	34,37,79	2.74	10 (29%)
55	CDL	i	402	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
46	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.22	8 (16%)
52	FES	M	803	12	0,4,4	-	-	-		
49	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)

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	C	303	-	-	25/55/55/55	-
50	8Q1	G	201	-	-	20/41/41/41	-
57	ADP	w	401	-	-	4/12/32/32	0/3/3/3
48	PEE	m	201	-	-	18/44/44/54	-
48	PEE	Q	501	-	-	25/50/50/54	-
48	PEE	U	101	-	-	26/54/54/54	-
55	CDL	l	701	-	-	54/110/110/110	-
50	8Q1	X	201	-	-	21/41/41/41	-
48	PEE	C	302	-	-	20/50/50/54	-
55	CDL	a	201	-	-	41/101/101/110	-
47	NAI	A	503	-	-	6/25/72/72	0/5/5/5
49	PLX	i	401	-	-	27/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	a	202	-	-	20/55/55/55	-
48	PEE	l	702	-	-	28/49/49/54	-
49	PLX	j	201	-	-	26/55/55/55	-
48	PEE	l	703	-	-	25/49/49/54	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	Q	502	-	-	19/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
51	NDP	J	401	-	-	9/30/77/77	0/4/5/5
45	SF4	M	802	12	-	-	0/6/5/5
52	FES	O	301	14	-	-	0/1/1/1
48	PEE	r	501	-	-	25/54/54/54	-
49	PLX	r	503	-	-	33/55/55/55	-
45	SF4	C	301	16,3	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
56	UQ	s	401	-	-	9/21/45/87	0/1/1/1
55	CDL	i	402	-	-	63/110/110/110	-
46	FMN	A	502	-	-	4/18/18/18	0/3/3/3
52	FES	M	803	12	-	-	0/1/1/1
49	PLX	r	502	-	-	33/55/55/55	-

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.23	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.53	1.30	1.53
51	J	401	NDP	C3B-C2B	-12.71	1.24	1.52
51	J	401	NDP	C6N-C5N	12.47	1.55	1.33
51	J	401	NDP	O4D-C4D	10.66	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.30	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.85	1.27	1.53
56	s	401	UQ	C13-C14	9.34	1.55	1.33
57	w	401	ADP	C3'-C4'	-8.86	1.30	1.53
56	s	401	UQ	C8-C9	8.86	1.54	1.33
47	A	503	NAI	O4B-C4B	-8.34	1.26	1.45
56	s	401	UQ	C18-C19	8.28	1.56	1.32
51	J	401	NDP	O4B-C1B	8.24	1.52	1.41
51	J	401	NDP	O4B-C4B	-8.01	1.27	1.45
57	w	401	ADP	O4'-C4'	7.64	1.62	1.45
51	J	401	NDP	C2N-C3N	7.60	1.56	1.34
47	A	503	NAI	C2D-C1D	-7.56	1.29	1.53
47	A	503	NAI	O4D-C4D	6.90	1.60	1.45
57	w	401	ADP	O4'-C1'	-6.87	1.31	1.41
47	A	503	NAI	C2D-C3D	5.99	1.69	1.53
47	A	503	NAI	C7N-N7N	5.76	1.48	1.33
51	J	401	NDP	P2B-O2B	5.73	1.70	1.59
47	A	503	NAI	O4D-C1D	5.46	1.54	1.42
51	J	401	NDP	C3B-C4B	5.46	1.66	1.53
50	G	201	8Q1	C34-N36	5.45	1.45	1.33
50	X	201	8Q1	C34-N36	5.38	1.45	1.33
50	X	201	8Q1	C39-N41	5.35	1.45	1.33
50	G	201	8Q1	C39-N41	5.28	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.06	1.40	1.49
51	J	401	NDP	C6N-N1N	4.96	1.49	1.37
51	J	401	NDP	O4D-C1D	-4.94	1.30	1.42
47	A	503	NAI	O2B-C2B	4.52	1.53	1.43
51	J	401	NDP	C7N-N7N	4.20	1.44	1.33
51	J	401	NDP	O2D-C2D	-4.13	1.33	1.43
51	J	401	NDP	C6A-N6A	4.09	1.49	1.34
47	A	503	NAI	C6N-C5N	3.94	1.40	1.33
46	A	502	FMN	C4A-N5	3.89	1.38	1.30
57	w	401	ADP	C6-N6	3.81	1.48	1.34
48	C	302	PEE	C18-C19	3.76	1.53	1.31
48	m	201	PEE	C18-C19	3.75	1.53	1.31
48	l	703	PEE	C18-C19	3.74	1.53	1.31
48	r	501	PEE	C18-C19	3.72	1.53	1.31
48	l	702	PEE	C18-C19	3.71	1.53	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	501	PEE	C18-C19	3.71	1.53	1.31
48	Q	502	PEE	C18-C19	3.71	1.53	1.31
48	U	101	PEE	C18-C19	3.69	1.53	1.31
48	C	302	PEE	C39-C38	3.69	1.53	1.31
48	Q	501	PEE	C39-C38	3.66	1.53	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	l	702	PEE	C39-C38	3.64	1.52	1.31
48	U	101	PEE	C39-C38	3.63	1.52	1.31
48	l	703	PEE	C39-C38	3.63	1.52	1.31
47	A	503	NAI	C6A-N6A	3.63	1.47	1.34
48	Q	502	PEE	C39-C38	3.62	1.52	1.31
47	A	503	NAI	C7N-C3N	3.58	1.56	1.48
55	l	701	CDL	OA8-CA7	3.42	1.43	1.33
55	i	402	CDL	OA8-CA7	3.41	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.37	1.40	1.48
57	w	401	ADP	O2’-C2’	-3.37	1.35	1.43
55	a	201	CDL	OA8-CA7	3.36	1.43	1.33
51	J	401	NDP	C7N-C3N	3.21	1.55	1.48
57	w	401	ADP	O3’-C3’	3.12	1.50	1.43
51	J	401	NDP	O3D-C3D	3.09	1.50	1.43
55	i	402	CDL	OB6-CB5	3.08	1.43	1.34
55	l	701	CDL	OB6-CB5	3.05	1.42	1.34
55	a	201	CDL	OB6-CB5	3.04	1.42	1.34
55	l	701	CDL	OA6-CA5	3.04	1.42	1.34
55	a	201	CDL	OB8-CB7	3.03	1.42	1.33
55	i	402	CDL	OB8-CB7	2.98	1.42	1.33
55	l	701	CDL	OB8-CB7	2.96	1.42	1.33
55	a	201	CDL	OA6-CA5	2.95	1.42	1.34
55	i	402	CDL	OA6-CA5	2.94	1.42	1.34
49	a	202	PLX	O6-C4	-2.79	1.40	1.44
49	i	401	PLX	O6-C4	-2.78	1.40	1.44
49	C	303	PLX	O6-C4	-2.75	1.40	1.44
49	r	503	PLX	O6-C4	-2.71	1.41	1.44
56	s	401	UQ	C6-C1	2.63	1.54	1.46
48	l	703	PEE	O3-C30	2.55	1.40	1.33
49	j	201	PLX	O6-C4	-2.54	1.41	1.44
48	Q	502	PEE	O2-C2	-2.52	1.40	1.46
48	Q	501	PEE	O3-C30	2.51	1.40	1.33
48	C	302	PEE	O2-C2	-2.47	1.40	1.46
48	r	501	PEE	O2-C2	-2.47	1.40	1.46
48	Q	502	PEE	O3-C30	2.46	1.40	1.33
48	r	501	PEE	O3-C30	2.46	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	302	PEE	O3-C30	2.45	1.40	1.33
47	A	503	NAI	PN-O5D	2.45	1.69	1.59
55	i	402	CDL	OA6-CA4	-2.45	1.40	1.46
51	J	401	NDP	O2B-C2B	2.43	1.52	1.44
48	U	101	PEE	O3-C30	2.43	1.40	1.33
48	Q	501	PEE	O2-C2	-2.42	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.41	1.37	1.43
48	l	702	PEE	O3-C30	2.41	1.40	1.33
48	m	201	PEE	O2-C10	2.40	1.41	1.34
49	r	502	PLX	C7-C6	2.40	1.55	1.50
48	m	201	PEE	O3-C30	2.40	1.40	1.33
55	a	201	CDL	OA6-CA4	-2.39	1.40	1.46
46	A	502	FMN	C10-N1	2.39	1.38	1.33
48	l	703	PEE	O2-C2	-2.39	1.40	1.46
50	X	201	8Q1	C1-S44	2.39	1.81	1.76
48	U	101	PEE	O2-C2	-2.38	1.40	1.46
50	G	201	8Q1	C1-S44	2.37	1.81	1.76
51	J	401	NDP	C2D-C3D	2.37	1.59	1.53
48	l	702	PEE	O2-C2	-2.33	1.40	1.46
49	j	201	PLX	C7-C6	2.33	1.55	1.50
49	r	502	PLX	O6-C4	-2.33	1.41	1.44
48	l	702	PEE	O2-C10	2.32	1.40	1.34
49	C	303	PLX	C7-C6	2.31	1.55	1.50
55	l	701	CDL	OA6-CA4	-2.30	1.40	1.46
50	G	201	8Q1	O40-C39	-2.30	1.18	1.23
49	a	202	PLX	C7-C6	2.29	1.55	1.50
49	r	503	PLX	C7-C6	2.29	1.55	1.50
49	i	401	PLX	C7-C6	2.28	1.55	1.50
48	U	101	PEE	O2-C10	2.27	1.40	1.34
48	Q	501	PEE	O2-C10	2.26	1.40	1.34
48	C	302	PEE	O2-C10	2.25	1.40	1.34
48	l	703	PEE	O2-C10	2.25	1.40	1.34
48	m	201	PEE	O2-C2	-2.24	1.41	1.46
48	Q	502	PEE	O2-C10	2.24	1.40	1.34
50	X	201	8Q1	O40-C39	-2.23	1.18	1.23
50	X	201	8Q1	C6-C1	2.22	1.53	1.50
55	l	701	CDL	OB6-CB4	-2.21	1.41	1.46
50	G	201	8Q1	O35-C34	-2.20	1.19	1.23
55	a	201	CDL	PB2-OB2	2.20	1.68	1.59
55	i	402	CDL	PB2-OB2	2.19	1.68	1.59
56	s	401	UQ	O4-C4	-2.19	1.18	1.23
55	l	701	CDL	PB2-OB2	2.19	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	i	402	CDL	PB2-OB5	2.18	1.68	1.59
50	X	201	8Q1	O35-C34	-2.17	1.19	1.23
48	r	501	PEE	O2-C10	2.16	1.40	1.34
49	j	201	PLX	P1-O4	2.16	1.68	1.59
47	A	503	NAI	C5B-C4B	2.16	1.58	1.51
50	G	201	8Q1	C6-C1	2.16	1.53	1.50
56	s	401	UQ	C7-C8	2.15	1.53	1.50
55	a	201	CDL	PB2-OB5	2.14	1.68	1.59
48	U	101	PEE	O3-C3	-2.12	1.40	1.45
51	J	401	NDP	PA-O5B	2.12	1.67	1.59
48	l	702	PEE	O3-C3	-2.11	1.40	1.45
48	Q	502	PEE	O3-C3	-2.11	1.40	1.45
49	r	502	PLX	P1-O4	2.10	1.67	1.59
51	J	401	NDP	O7N-C7N	-2.10	1.19	1.24
49	a	202	PLX	P1-O4	2.10	1.67	1.59
49	r	503	PLX	P1-O4	2.09	1.67	1.59
48	m	201	PEE	O3-C3	-2.09	1.40	1.45
49	C	303	PLX	P1-O4	2.09	1.67	1.59
48	C	302	PEE	O3-C3	-2.08	1.40	1.45
49	i	401	PLX	P1-O4	2.08	1.67	1.59
55	i	402	CDL	OB6-CB4	-2.08	1.41	1.46
55	l	701	CDL	PB2-OB5	2.08	1.67	1.59
48	r	501	PEE	O3-C3	-2.07	1.40	1.45
49	r	502	PLX	P1-O1	2.06	1.67	1.59
49	r	503	PLX	P1-O1	2.06	1.67	1.59
55	a	201	CDL	OB6-CB4	-2.05	1.41	1.46
48	l	703	PEE	O3-C3	-2.05	1.40	1.45
49	j	201	PLX	P1-O1	2.05	1.67	1.59
56	s	401	UQ	O1-C1	-2.04	1.18	1.23
48	Q	501	PEE	O3-C3	-2.02	1.40	1.45
49	a	202	PLX	P1-O1	2.02	1.67	1.59
55	l	701	CDL	C11-CA5	2.00	1.56	1.50
55	a	201	CDL	C11-CA5	2.00	1.56	1.50

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C7-C8-C9	-9.34	111.24	126.79
51	J	401	NDP	C3N-C2N-N1N	-7.60	112.25	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.47	110.34	121.11
50	G	201	8Q1	C6-C1-S44	5.90	120.33	113.46
56	s	401	UQ	C12-C13-C14	-5.88	113.50	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	X	201	8Q1	C6-C1-S44	5.83	120.24	113.46
51	J	401	NDP	C1D-N1N-C6N	-5.48	109.02	120.83
56	s	401	UQ	C11-C9-C8	-4.64	111.72	121.12
56	s	401	UQ	C10-C9-C8	-4.62	111.82	123.68
57	w	401	ADP	N3-C2-N1	-4.47	121.69	128.68
47	A	503	NAI	N3A-C2A-N1A	-4.29	121.97	128.68
55	a	201	CDL	OA6-CA5-C11	4.22	120.60	111.50
55	a	201	CDL	OB6-CB5-C51	4.19	120.53	111.50
48	m	201	PEE	O2-C10-C11	4.17	120.49	111.50
55	i	402	CDL	OB6-CB5-C51	4.11	120.37	111.50
51	J	401	NDP	N3A-C2A-N1A	-4.05	122.35	128.68
55	l	701	CDL	OA6-CA5-C11	4.04	120.22	111.50
48	r	501	PEE	O2-C10-C11	4.03	120.18	111.50
56	s	401	UQ	C15-C14-C13	-4.02	113.36	123.68
48	Q	501	PEE	O2-C10-C11	3.99	120.09	111.50
56	s	401	UQ	C17-C18-C19	-3.98	114.14	127.75
48	C	302	PEE	O2-C10-C11	3.96	120.04	111.50
56	s	401	UQ	C16-C14-C13	-3.95	113.13	121.12
55	i	402	CDL	OA6-CA5-C11	3.94	119.99	111.50
48	U	101	PEE	O2-C10-C11	3.86	119.82	111.50
48	Q	502	PEE	O2-C10-C11	3.83	119.76	111.50
48	l	703	PEE	O2-C10-C11	3.79	119.67	111.50
48	l	702	PEE	O2-C10-C11	3.71	119.49	111.50
55	l	701	CDL	OB6-CB5-C51	3.66	119.38	111.50
50	G	201	8Q1	C37-C38-C39	3.47	118.14	112.36
50	X	201	8Q1	O4-C1-C6	-3.45	119.92	123.99
47	A	503	NAI	C3D-C2D-C1D	3.42	107.92	101.43
56	s	401	UQ	C21-C19-C18	-3.39	112.84	122.65
50	G	201	8Q1	O4-C1-C6	-3.35	120.04	123.99
51	J	401	NDP	PN-O3-PA	-3.13	122.08	132.83
46	A	502	FMN	C4-N3-C2	-3.07	119.96	125.64
56	s	401	UQ	C20-C19-C18	-2.97	114.07	122.65
57	w	401	ADP	PA-O3A-PB	-2.94	122.74	132.83
56	s	401	UQ	CM5-C5-C6	-2.78	119.86	124.40
47	A	503	NAI	C4A-C5A-N7A	-2.74	106.54	109.40
48	r	501	PEE	O3-C30-C31	2.73	120.48	111.91
47	A	503	NAI	PN-O3-PA	-2.72	123.49	132.83
47	A	503	NAI	C2D-C3D-C4D	2.72	107.92	102.64
46	A	502	FMN	C4A-C4-N3	2.67	119.98	113.19
48	l	702	PEE	O3-C30-C31	2.67	120.30	111.91
55	a	201	CDL	OB8-CB7-C71	2.65	120.22	111.91
51	J	401	NDP	C2B-C3B-C4B	2.64	107.73	101.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	m	201	PEE	O3-C30-C31	2.62	120.13	111.91
48	C	302	PEE	O3-C30-C31	2.61	120.11	111.91
48	l	703	PEE	O3-C30-C31	2.60	120.07	111.91
48	Q	501	PEE	O3-C30-C31	2.58	120.01	111.91
46	A	502	FMN	O4-C4-C4A	-2.58	119.76	126.60
55	l	701	CDL	OB8-CB7-C71	2.57	119.98	111.91
48	Q	502	PEE	O3-C30-C31	2.56	119.95	111.91
55	i	402	CDL	OA8-CA7-C31	2.55	119.91	111.91
55	i	402	CDL	OB8-CB7-C71	2.49	119.73	111.91
47	A	503	NAI	C4D-O4D-C1D	-2.49	103.99	109.47
48	U	101	PEE	O3-C30-C31	2.48	119.68	111.91
55	a	201	CDL	OA8-CA7-C31	2.46	119.61	111.91
55	l	701	CDL	OA8-CA7-C31	2.45	119.60	111.91
49	r	502	PLX	C1A-N1-C1	2.41	119.78	109.92
49	i	401	PLX	C1A-N1-C1	2.41	119.78	109.92
49	j	201	PLX	C1A-N1-C1	2.38	119.64	109.92
49	a	202	PLX	C1A-N1-C1	2.37	119.61	109.92
46	A	502	FMN	C4A-C10-N10	2.33	119.88	116.48
51	J	401	NDP	C4A-C5A-N7A	-2.32	106.98	109.40
49	r	503	PLX	C1A-N1-C1	2.31	119.37	109.92
50	X	201	8Q1	C37-C38-C39	2.30	116.19	112.36
50	G	201	8Q1	O4-C1-S44	-2.29	119.63	122.61
50	X	201	8Q1	C38-C39-N41	2.29	120.28	116.42
46	A	502	FMN	C9A-C5A-N5	-2.25	119.99	122.43
50	G	201	8Q1	C38-C39-N41	2.23	120.18	116.42
57	w	401	ADP	O4'-C1'-C2'	-2.20	103.72	106.93
49	C	303	PLX	C1A-N1-C1	2.19	118.89	109.92
50	X	201	8Q1	C43-S44-C1	2.18	108.65	101.87
46	A	502	FMN	C5A-C9A-N10	2.18	120.20	117.95
46	A	502	FMN	C10-C4A-N5	-2.14	120.31	124.86
50	X	201	8Q1	O4-C1-S44	-2.14	119.84	122.61
57	w	401	ADP	C4-C5-N7	-2.12	107.19	109.40
46	A	502	FMN	C4A-C10-N1	-2.10	119.85	124.73
50	G	201	8Q1	C43-S44-C1	2.05	108.26	101.87
51	J	401	NDP	O4B-C1B-C2B	-2.04	103.04	106.59
57	w	401	ADP	C2'-C3'-C4'	2.02	106.58	102.64

There are no chirality outliers.

All (581) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	C5B-O5B-PA-O1A
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O1P
48	Q	501	PEE	C11-C10-O2-C2
48	Q	501	PEE	C4-O4P-P-O1P
48	Q	502	PEE	C1-O3P-P-O1P
48	U	101	PEE	C17-C18-C19-C20
48	U	101	PEE	C1-O3P-P-O2P
48	U	101	PEE	C1-O3P-P-O1P
48	U	101	PEE	C1-O3P-P-O4P
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	l	702	PEE	C4-O4P-P-O3P
48	l	702	PEE	C4-O4P-P-O2P
48	l	702	PEE	C4-O4P-P-O1P
48	l	703	PEE	C37-C38-C39-C40
48	m	201	PEE	C11-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
48	m	201	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
48	m	201	PEE	O4P-C4-C5-N
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
49	C	303	PLX	C3-C4-O6-C6
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-C7-C8
49	i	401	PLX	O7-C6-O6-C4
49	j	201	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O9-C24-O8-C5
49	r	503	PLX	O9-C24-C25-C26
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	O27-C28-C29-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	N41-C42-C43-S44
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	O27-C28-C29-C31
50	X	201	8Q1	O27-C28-C29-C32
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C5B-O5B-PA-O3
51	J	401	NDP	O4B-C4B-C5B-O5B
51	J	401	NDP	C2B-O2B-P2B-O3X
51	J	401	NDP	C2N-C3N-C7N-N7N
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB3-OB5-PB2-OB3
55	i	402	CDL	CA2-OA2-PA1-OA3
55	i	402	CDL	CA2-OA2-PA1-OA4
55	i	402	CDL	CA3-OA5-PA1-OA2
55	i	402	CDL	CA3-OA5-PA1-OA3
55	i	402	CDL	CA3-OA5-PA1-OA4
55	i	402	CDL	CB3-OB5-PB2-OB4
55	l	701	CDL	CA2-OA2-PA1-OA3
55	l	701	CDL	CA2-OA2-PA1-OA4
55	l	701	CDL	CA2-OA2-PA1-OA5
55	l	701	CDL	CB2-OB2-PB2-OB3
55	l	701	CDL	CB2-OB2-PB2-OB4
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C10
56	s	401	UQ	C12-C13-C14-C16
56	s	401	UQ	C13-C14-C16-C17
56	s	401	UQ	C14-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
56	s	401	UQ	C17-C18-C19-C21
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
48	l	703	PEE	C31-C30-O3-C3
48	Q	502	PEE	C37-C38-C39-C40
48	r	501	PEE	C17-C18-C19-C20
56	s	401	UQ	C7-C8-C9-C10
48	Q	501	PEE	O4-C10-O2-C2
55	l	701	CDL	C59-C60-C61-C62
48	l	702	PEE	C31-C30-O3-C3
48	m	201	PEE	C31-C30-O3-C3
55	i	402	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	O5-C30-O3-C3
51	J	401	NDP	C2D-C1D-N1N-C6N
49	r	502	PLX	C9-C10-C11-C12
49	a	202	PLX	C33-C34-C35-C36
49	i	401	PLX	C7-C8-C9-C10
49	r	503	PLX	C12-C13-C14-C15
49	j	201	PLX	C28-C29-C30-C31
48	l	702	PEE	O5-C30-O3-C3
48	m	201	PEE	O5-C30-O3-C3
55	i	402	CDL	OB9-CB7-OB8-CB6
56	s	401	UQ	C9-C11-C12-C13
48	Q	502	PEE	C12-C13-C14-C15
55	a	201	CDL	C34-C35-C36-C37
55	i	402	CDL	CB2-C1-CA2-OA2
49	r	502	PLX	C30-C31-C32-C33
48	U	101	PEE	C31-C30-O3-C3
55	a	201	CDL	C71-CB7-OB8-CB6
55	l	701	CDL	C71-CB7-OB8-CB6
49	i	401	PLX	C31-C32-C33-C34
55	i	402	CDL	C78-C79-C80-C81
55	l	701	CDL	C35-C36-C37-C38
55	i	402	CDL	OA6-CA4-CA6-OA8
49	j	201	PLX	C34-C35-C36-C37
49	r	502	PLX	C11-C12-C13-C14
49	j	201	PLX	C15-C16-C17-C18
55	i	402	CDL	C74-C75-C76-C77
49	C	303	PLX	C28-C29-C30-C31
48	r	501	PEE	C10-C11-C12-C13
48	U	101	PEE	C34-C35-C36-C37
48	U	101	PEE	O5-C30-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	a	201	CDL	CA7-C31-C32-C33
55	i	402	CDL	CB7-C71-C72-C73
51	J	401	NDP	C3B-C4B-C5B-O5B
55	l	701	CDL	C11-C12-C13-C14
55	a	201	CDL	OB9-CB7-OB8-CB6
55	l	701	CDL	C39-C40-C41-C42
55	l	701	CDL	OB9-CB7-OB8-CB6
55	i	402	CDL	O1-C1-CA2-OA2
48	C	302	PEE	C1-O3P-P-O4P
49	r	502	PLX	C3-O4-P1-O1
49	r	503	PLX	C3-O4-P1-O1
49	r	503	PLX	C2-O1-P1-O4
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CA3-OA5-PA1-OA2
55	i	402	CDL	CA2-OA2-PA1-OA5
55	i	402	CDL	CB2-OB2-PB2-OB5
55	i	402	CDL	CB3-OB5-PB2-OB2
55	l	701	CDL	CA3-OA5-PA1-OA2
55	l	701	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	CB3-OB5-PB2-OB2
55	i	402	CDL	CB5-C51-C52-C53
49	C	303	PLX	O6-C6-C7-C8
55	l	701	CDL	C51-C52-C53-C54
48	U	101	PEE	C40-C41-C42-C43
55	i	402	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C28-C29-C30-C31
49	r	503	PLX	C33-C34-C35-C36
55	a	201	CDL	C73-C74-C75-C76
50	G	201	8Q1	O27-C28-C29-C30
50	X	201	8Q1	O27-C28-C29-C30
48	Q	502	PEE	C14-C15-C16-C17
49	C	303	PLX	C17-C18-C19-C20
49	i	401	PLX	C10-C11-C12-C13
49	r	503	PLX	C13-C14-C15-C16
55	l	701	CDL	C75-C76-C77-C78
55	i	402	CDL	OB7-CB5-OB6-CB4
49	i	401	PLX	C11-C10-C9-C8
49	r	502	PLX	C27-C28-C29-C30
55	l	701	CDL	C52-C53-C54-C55
48	Q	501	PEE	C17-C18-C19-C20
48	l	703	PEE	C33-C34-C35-C36
49	a	202	PLX	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	i	401	PLX	C27-C28-C29-C30
49	j	201	PLX	C7-C8-C9-C10
55	a	201	CDL	C35-C36-C37-C38
55	i	402	CDL	C17-C18-C19-C20
48	r	501	PEE	C31-C32-C33-C34
49	a	202	PLX	C10-C11-C12-C13
49	i	401	PLX	C25-C26-C27-C28
55	l	701	CDL	C37-C38-C39-C40
55	a	201	CDL	CB5-C51-C52-C53
48	Q	502	PEE	C34-C35-C36-C37
49	r	503	PLX	C14-C15-C16-C17
50	G	201	8Q1	C7-C8-C9-C10
55	i	402	CDL	C73-C74-C75-C76
55	l	701	CDL	C73-C74-C75-C76
55	i	402	CDL	CA7-C31-C32-C33
48	Q	502	PEE	C33-C34-C35-C36
49	C	303	PLX	C14-C15-C16-C17
49	a	202	PLX	C14-C15-C16-C17
49	i	401	PLX	C9-C10-C11-C12
49	i	401	PLX	C32-C33-C34-C35
49	i	401	PLX	C33-C34-C35-C36
49	r	502	PLX	C7-C8-C9-C10
55	a	201	CDL	C17-C18-C19-C20
55	a	201	CDL	C75-C76-C77-C78
55	i	402	CDL	C71-C72-C73-C74
55	i	402	CDL	C75-C76-C77-C78
48	r	501	PEE	C11-C10-O2-C2
48	m	201	PEE	C11-C12-C13-C14
49	i	401	PLX	C30-C31-C32-C33
49	j	201	PLX	C10-C11-C12-C13
49	r	503	PLX	C25-C26-C27-C28
55	i	402	CDL	C55-C56-C57-C58
48	Q	501	PEE	C35-C36-C37-C38
48	C	302	PEE	C42-C43-C44-C45
48	Q	501	PEE	C22-C23-C24-C25
48	l	703	PEE	C12-C13-C14-C15
48	r	501	PEE	C12-C13-C14-C15
49	a	202	PLX	C7-C8-C9-C10
49	a	202	PLX	C29-C30-C31-C32
49	i	401	PLX	C28-C29-C30-C31
49	r	503	PLX	C28-C29-C30-C31
50	X	201	8Q1	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	l	701	CDL	C40-C41-C42-C43
48	Q	501	PEE	C21-C22-C23-C24
49	C	303	PLX	C16-C17-C18-C19
55	a	201	CDL	C11-C12-C13-C14
49	j	201	PLX	C27-C28-C29-C30
48	Q	502	PEE	C30-C31-C32-C33
55	l	701	CDL	CB7-C71-C72-C73
48	U	101	PEE	C21-C22-C23-C24
55	i	402	CDL	C56-C57-C58-C59
55	l	701	CDL	CB3-CB4-CB6-OB8
48	r	501	PEE	O4-C10-O2-C2
48	C	302	PEE	C37-C38-C39-C40
49	C	303	PLX	C9-C10-C11-C12
49	i	401	PLX	C14-C15-C16-C17
49	r	503	PLX	C11-C12-C13-C14
55	a	201	CDL	C21-C22-C23-C24
55	a	201	CDL	C37-C38-C39-C40
48	C	302	PEE	C11-C10-O2-C2
48	U	101	PEE	C11-C10-O2-C2
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	C13-C14-C15-C16
49	C	303	PLX	C25-C26-C27-C28
49	r	503	PLX	C27-C28-C29-C30
55	a	201	CDL	C31-C32-C33-C34
55	i	402	CDL	C43-C44-C45-C46
49	j	201	PLX	C25-C26-C27-C28
55	a	201	CDL	C52-C53-C54-C55
49	r	503	PLX	C29-C30-C31-C32
48	C	302	PEE	O4-C10-O2-C2
48	U	101	PEE	O4-C10-O2-C2
49	a	202	PLX	C25-C26-C27-C28
49	r	502	PLX	C28-C29-C30-C31
48	l	702	PEE	C31-C32-C33-C34
48	l	703	PEE	C31-C32-C33-C34
49	r	503	PLX	C2-C1-N1-C1A
48	Q	501	PEE	C10-C11-C12-C13
55	i	402	CDL	C59-C60-C61-C62
49	C	303	PLX	C7-C8-C9-C10
49	C	303	PLX	C33-C34-C35-C36
49	r	503	PLX	C10-C11-C12-C13
48	l	702	PEE	C30-C31-C32-C33
49	j	201	PLX	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C16-C17-C18-C19
49	r	503	PLX	C31-C32-C33-C34
55	i	402	CDL	C62-C63-C64-C65
55	l	701	CDL	C58-C59-C60-C61
49	a	202	PLX	C9-C10-C11-C12
49	j	201	PLX	C35-C36-C37-C38
48	r	501	PEE	C20-C21-C22-C23
55	a	201	CDL	C32-C33-C34-C35
55	i	402	CDL	C41-C42-C43-C44
55	l	701	CDL	C32-C33-C34-C35
55	l	701	CDL	C55-C56-C57-C58
48	Q	502	PEE	C42-C43-C44-C45
48	l	702	PEE	C23-C24-C25-C26
49	a	202	PLX	C11-C10-C9-C8
55	l	701	CDL	C51-CB5-OB6-CB4
48	l	702	PEE	O3P-C1-C2-O2
55	l	701	CDL	C60-C61-C62-C63
48	C	302	PEE	C13-C14-C15-C16
49	C	303	PLX	C27-C28-C29-C30
55	a	201	CDL	C33-C34-C35-C36
55	l	701	CDL	OB7-CB5-OB6-CB4
50	G	201	8Q1	C11-C12-C13-C14
48	U	101	PEE	O2-C2-C3-O3
55	l	701	CDL	OA6-CA4-CA6-OA8
55	l	701	CDL	OB6-CB4-CB6-OB8
49	r	503	PLX	C30-C31-C32-C33
49	r	503	PLX	C2-C1-N1-C1C
48	r	501	PEE	C40-C41-C42-C43
49	j	201	PLX	C13-C14-C15-C16
48	Q	501	PEE	C19-C20-C21-C22
48	Q	502	PEE	C19-C20-C21-C22
48	Q	502	PEE	C20-C21-C22-C23
48	U	101	PEE	C36-C37-C38-C39
48	l	702	PEE	C14-C15-C16-C17
49	r	502	PLX	C33-C34-C35-C36
55	i	402	CDL	C14-C15-C16-C17
48	Q	502	PEE	C31-C30-O3-C3
55	i	402	CDL	C60-C61-C62-C63
49	a	202	PLX	C30-C31-C32-C33
49	r	503	PLX	C18-C19-C20-C21
48	r	501	PEE	C36-C37-C38-C39
49	a	202	PLX	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	j	201	PLX	C33-C34-C35-C36
55	i	402	CDL	C52-C53-C54-C55
48	C	302	PEE	C11-C12-C13-C14
49	j	201	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
55	i	402	CDL	CA3-CA4-CA6-OA8
55	i	402	CDL	CB3-CB4-CB6-OB8
49	r	502	PLX	C12-C13-C14-C15
55	l	701	CDL	C64-C65-C66-C67
49	r	502	PLX	C18-C19-C20-C21
55	i	402	CDL	C84-C85-C86-C87
50	G	201	8Q1	C12-C13-C14-C15
55	l	701	CDL	C56-C57-C58-C59
48	C	302	PEE	C15-C16-C17-C18
48	Q	501	PEE	C15-C16-C17-C18
49	i	401	PLX	C13-C14-C15-C16
50	G	201	8Q1	C6-C7-C8-C9
55	a	201	CDL	C71-C72-C73-C74
50	G	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O3
55	a	201	CDL	OA5-CA3-CA4-OA6
49	r	503	PLX	C2-C1-N1-C1B
55	i	402	CDL	C13-C14-C15-C16
55	i	402	CDL	C23-C24-C25-C26
48	C	302	PEE	O2-C2-C3-O3
55	i	402	CDL	OB6-CB4-CB6-OB8
48	Q	501	PEE	C31-C32-C33-C34
48	Q	502	PEE	C21-C22-C23-C24
48	Q	502	PEE	O5-C30-O3-C3
49	r	502	PLX	C14-C15-C16-C17
55	i	402	CDL	C35-C36-C37-C38
48	Q	502	PEE	C17-C18-C19-C20
48	l	703	PEE	C17-C18-C19-C20
55	l	701	CDL	C77-C78-C79-C80
48	l	702	PEE	O3P-C1-C2-C3
55	l	701	CDL	OA5-CA3-CA4-CA6
49	r	502	PLX	C31-C32-C33-C34
48	r	501	PEE	O4P-C4-C5-N
49	j	201	PLX	C9-C10-C11-C12
49	j	201	PLX	C14-C15-C16-C17
49	j	201	PLX	C31-C32-C33-C34
55	i	402	CDL	C82-C83-C84-C85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	m	201	PEE	C24-C25-C26-C27
55	i	402	CDL	C64-C65-C66-C67
48	l	702	PEE	C11-C12-C13-C14
55	i	402	CDL	C31-CA7-OA8-CA6
48	l	702	PEE	C32-C33-C34-C35
48	C	302	PEE	C1-C2-C3-O3
48	Q	501	PEE	C1-C2-C3-O3
48	U	101	PEE	C1-C2-C3-O3
49	i	401	PLX	C3-C4-C5-O8
55	l	701	CDL	CA3-CA4-CA6-OA8
49	r	502	PLX	C13-C14-C15-C16
50	X	201	8Q1	C10-C11-C12-C13
49	C	303	PLX	C11-C12-C13-C14
49	C	303	PLX	C30-C31-C32-C33
48	Q	501	PEE	C32-C33-C34-C35
49	r	502	PLX	C15-C16-C17-C18
49	i	401	PLX	O9-C24-C25-C26
49	r	503	PLX	C7-C8-C9-C10
55	i	402	CDL	C42-C43-C44-C45
48	C	302	PEE	C39-C40-C41-C42
49	r	502	PLX	C32-C33-C34-C35
49	i	401	PLX	C19-C20-C21-C22
49	j	201	PLX	C30-C31-C32-C33
49	r	503	PLX	C15-C16-C17-C18
48	r	501	PEE	C38-C39-C40-C41
49	j	201	PLX	C18-C19-C20-C21
48	Q	502	PEE	O3P-C1-C2-C3
49	j	201	PLX	O4-C3-C4-C5
55	a	201	CDL	OA5-CA3-CA4-CA6
48	m	201	PEE	O3-C30-C31-C32
49	r	502	PLX	C29-C30-C31-C32
50	G	201	8Q1	C1-C6-C7-C8
49	C	303	PLX	C31-C32-C33-C34
49	i	401	PLX	C12-C13-C14-C15
55	l	701	CDL	C62-C63-C64-C65
50	X	201	8Q1	C7-C8-C9-C10
48	m	201	PEE	C3-C2-O2-C10
55	i	402	CDL	C20-C21-C22-C23
49	r	503	PLX	C26-C27-C28-C29
48	Q	501	PEE	C30-C31-C32-C33
48	r	501	PEE	C1-C2-C3-O3
49	r	503	PLX	C3-C4-C5-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	i	402	CDL	CB4-CB3-OB5-PB2
48	Q	502	PEE	O3P-C1-C2-O2
49	j	201	PLX	O4-C3-C4-O6
55	l	701	CDL	OA5-CA3-CA4-OA6
50	G	201	8Q1	C31-C29-C32-C34
55	i	402	CDL	OA9-CA7-OA8-CA6
49	i	401	PLX	C17-C18-C19-C20
48	Q	501	PEE	O2-C2-C3-O3
49	j	201	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
48	U	101	PEE	C23-C24-C25-C26
55	a	201	CDL	C54-C55-C56-C57
55	i	402	CDL	CA5-C11-C12-C13
47	A	503	NAI	C5B-O5B-PA-O3
49	i	401	PLX	C35-C36-C37-C38
48	r	501	PEE	C41-C42-C43-C44
48	Q	501	PEE	C23-C24-C25-C26
49	C	303	PLX	C11-C10-C9-C8
48	U	101	PEE	C41-C42-C43-C44
48	l	702	PEE	C24-C25-C26-C27
48	l	703	PEE	C21-C22-C23-C24
55	l	701	CDL	O1-C1-CB2-OB2
46	A	502	FMN	C3'-C4'-C5'-O5'
48	m	201	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	C3-O4-P1-O3
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O2
49	r	503	PLX	C2-O1-P1-O3
51	J	401	NDP	C5B-O5B-PA-O2A
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB4
55	i	402	CDL	CB2-OB2-PB2-OB3
55	i	402	CDL	CB2-OB2-PB2-OB4
55	i	402	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CA3-OA5-PA1-OA4
55	l	701	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	w	401	ADP	C5'-O5'-PA-O1A
49	i	401	PLX	O4-C3-C4-C5
55	a	201	CDL	C55-C56-C57-C58
50	G	201	8Q1	C11-C10-C9-C8
55	i	402	CDL	C81-C82-C83-C84
48	r	501	PEE	C24-C25-C26-C27
49	j	201	PLX	C25-C24-O8-C5
48	U	101	PEE	C19-C20-C21-C22
55	i	402	CDL	C31-C32-C33-C34
49	i	401	PLX	O4-C3-C4-O6
48	U	101	PEE	C38-C39-C40-C41
55	l	701	CDL	C76-C77-C78-C79
55	l	701	CDL	C14-C15-C16-C17
51	J	401	NDP	C2N-C3N-C7N-O7N
55	a	201	CDL	CB3-CB4-CB6-OB8
48	l	702	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	i	401	PLX	O6-C4-C5-O8
55	a	201	CDL	OB6-CB4-CB6-OB8
48	U	101	PEE	C37-C38-C39-C40
49	a	202	PLX	C27-C28-C29-C30
49	j	201	PLX	C26-C27-C28-C29
48	r	501	PEE	C31-C30-O3-C3
48	l	702	PEE	C34-C35-C36-C37
49	C	303	PLX	O8-C24-C25-C26
49	a	202	PLX	O6-C6-C7-C8
49	r	503	PLX	O8-C24-C25-C26
48	l	703	PEE	C18-C19-C20-C21
48	l	703	PEE	C16-C17-C18-C19
49	C	303	PLX	O9-C24-C25-C26
48	l	703	PEE	C14-C15-C16-C17
49	C	303	PLX	C15-C16-C17-C18
48	l	702	PEE	C19-C20-C21-C22
48	Q	501	PEE	C13-C14-C15-C16
48	l	702	PEE	C13-C14-C15-C16
49	r	502	PLX	C20-C21-C22-C23
55	l	701	CDL	C44-C45-C46-C47
49	r	503	PLX	C9-C10-C11-C12
48	r	501	PEE	O5-C30-O3-C3
48	Q	501	PEE	C14-C15-C16-C17
55	l	701	CDL	C72-C73-C74-C75
48	l	703	PEE	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	l	701	CDL	C33-C34-C35-C36
48	l	703	PEE	C11-C12-C13-C14
55	l	701	CDL	C15-C16-C17-C18
48	C	302	PEE	C41-C42-C43-C44
49	r	502	PLX	O6-C4-C5-O8
49	a	202	PLX	C2-O1-P1-O4
49	i	401	PLX	C3-O4-P1-O1
55	a	201	CDL	CB2-OB2-PB2-OB5
48	Q	502	PEE	C10-C11-C12-C13
49	a	202	PLX	C16-C17-C18-C19
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-O33
48	l	702	PEE	C1-C2-C3-O3
48	l	703	PEE	C1-C2-C3-O3
47	A	503	NAI	O4D-C1D-N1N-C2N
55	l	701	CDL	C12-C13-C14-C15
48	Q	501	PEE	C2-C1-O3P-P
49	j	201	PLX	C11-C12-C13-C14
55	i	402	CDL	C39-C40-C41-C42
48	Q	502	PEE	C39-C40-C41-C42
48	r	501	PEE	C39-C40-C41-C42
47	A	503	NAI	C2D-C1D-N1N-C2N
49	C	303	PLX	O4-C3-C4-O6
48	l	703	PEE	C15-C16-C17-C18
48	r	501	PEE	C34-C35-C36-C37
49	a	202	PLX	C19-C20-C21-C22
49	i	401	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
48	Q	501	PEE	C18-C19-C20-C21
48	l	702	PEE	C38-C39-C40-C41
48	l	703	PEE	O4-C10-O2-C2
55	a	201	CDL	C60-C61-C62-C63
55	i	402	CDL	C72-C73-C74-C75
48	l	702	PEE	C1-C2-O2-C10
48	l	702	PEE	C3-C2-O2-C10
48	r	501	PEE	C4-O4P-P-O3P
49	r	502	PLX	C2-O1-P1-O4
55	i	402	CDL	C44-C45-C46-C47
48	Q	501	PEE	C38-C39-C40-C41
48	m	201	PEE	C16-C17-C18-C19
55	a	201	CDL	C59-C60-C61-C62
50	G	201	8Q1	C42-C43-S44-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O2-C2-C3-O3
49	r	503	PLX	C16-C17-C18-C19
49	i	401	PLX	C36-C37-C38-C39
55	a	201	CDL	C41-C42-C43-C44
57	w	401	ADP	PB-O3A-PA-O1A
55	l	701	CDL	C31-C32-C33-C34
55	a	201	CDL	C36-C37-C38-C39
49	a	202	PLX	C13-C14-C15-C16
55	a	201	CDL	C76-C77-C78-C79
55	a	201	CDL	C74-C75-C76-C77
55	l	701	CDL	C71-C72-C73-C74
50	X	201	8Q1	C13-C14-C15-C16
48	m	201	PEE	C13-C14-C15-C16
48	l	703	PEE	O4P-C4-C5-N
55	i	402	CDL	C33-C34-C35-C36
48	Q	502	PEE	C15-C16-C17-C18
48	m	201	PEE	C18-C19-C20-C21
48	U	101	PEE	O3-C30-C31-C32
56	s	401	UQ	C12-C11-C9-C8
48	l	702	PEE	C10-C11-C12-C13
48	U	101	PEE	C22-C23-C24-C25
48	l	702	PEE	C20-C21-C22-C23
49	a	202	PLX	C6-C7-C8-C9
55	l	701	CDL	C52-C51-CB5-OB6
48	r	501	PEE	C18-C19-C20-C21
48	m	201	PEE	C10-C11-C12-C13
55	a	201	CDL	C22-C23-C24-C25
48	C	302	PEE	O3-C30-C31-C32
48	l	702	PEE	C35-C36-C37-C38
49	j	201	PLX	C7-C6-O6-C4
55	i	402	CDL	C32-C33-C34-C35
48	C	302	PEE	C18-C19-C20-C21
48	U	101	PEE	C16-C17-C18-C19
55	a	201	CDL	C43-C44-C45-C46
48	l	703	PEE	C11-C10-O2-C2
48	Q	501	PEE	C24-C25-C26-C27
49	r	503	PLX	C36-C37-C38-C39
48	Q	501	PEE	C36-C37-C38-C39
48	l	703	PEE	C38-C39-C40-C41
49	j	201	PLX	C32-C33-C34-C35
48	U	101	PEE	O2-C10-C11-C12
55	i	402	CDL	C83-C84-C85-C86

Continued on next page...

Continued from previous page...

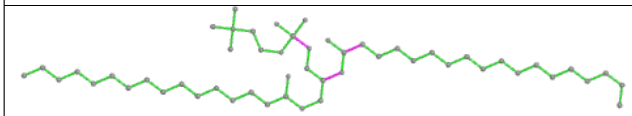
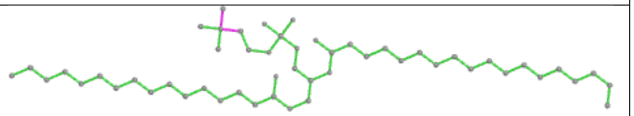
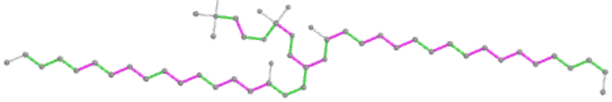
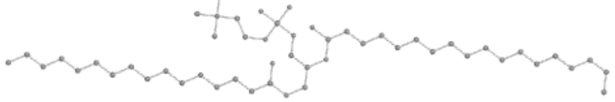
Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O3-C30-C31-C32
48	C	302	PEE	C38-C39-C40-C41
48	l	702	PEE	C16-C17-C18-C19
47	A	503	NAI	C3D-C4D-C5D-O5D
48	C	302	PEE	O5-C30-C31-C32
55	i	402	CDL	C37-C38-C39-C40
48	U	101	PEE	O5-C30-C31-C32
50	G	201	8Q1	C9-C10-C11-C12
48	U	101	PEE	C31-C32-C33-C34
48	Q	501	PEE	C4-O4P-P-O3P
49	r	502	PLX	C4-C3-O4-P1
48	l	703	PEE	O5-C30-C31-C32
49	r	502	PLX	C26-C27-C28-C29
48	Q	501	PEE	C1-O3P-P-O1P
48	l	703	PEE	C1-O3P-P-O1P
49	i	401	PLX	C3-O4-P1-O2
55	l	701	CDL	C34-C35-C36-C37
49	C	303	PLX	C24-C25-C26-C27
48	U	101	PEE	O4-C10-C11-C12
48	m	201	PEE	O5-C30-C31-C32
55	i	402	CDL	C76-C77-C78-C79
48	l	703	PEE	C5-C4-O4P-P
49	r	502	PLX	C25-C24-O8-C5
48	C	302	PEE	C43-C44-C45-C46
47	A	503	NAI	C2D-C1D-N1N-C6N
48	l	703	PEE	C39-C40-C41-C42
49	r	502	PLX	C25-C26-C27-C28
55	i	402	CDL	C72-C71-CB7-OB8
55	l	701	CDL	C32-C31-CA7-OA8
46	A	502	FMN	O2'-C2'-C3'-C4'
48	C	302	PEE	C32-C33-C34-C35
49	r	503	PLX	C24-C25-C26-C27
55	l	701	CDL	C32-C31-CA7-OA9
55	a	201	CDL	C12-C11-CA5-OA6

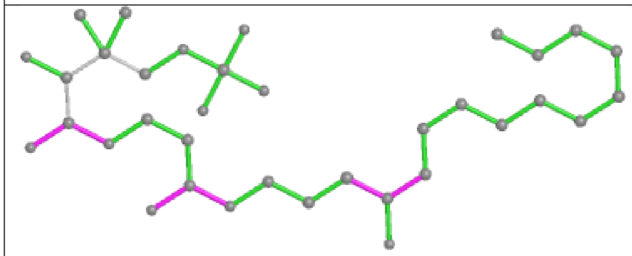
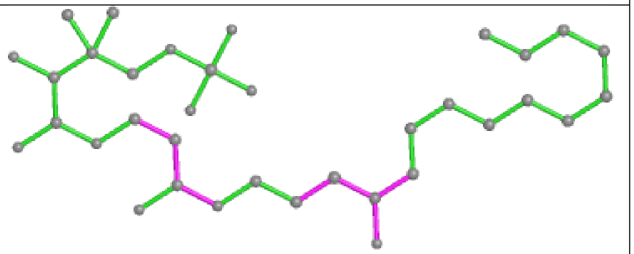
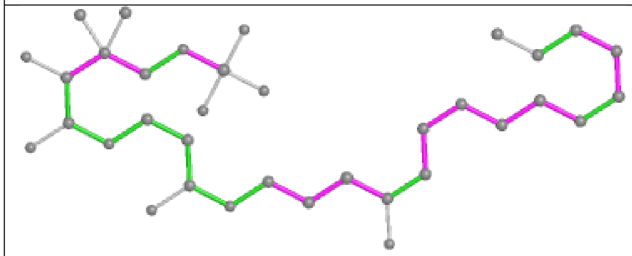
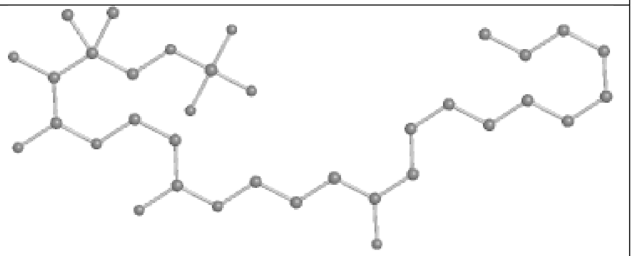
There are no ring outliers.

No monomer is involved in short contacts.

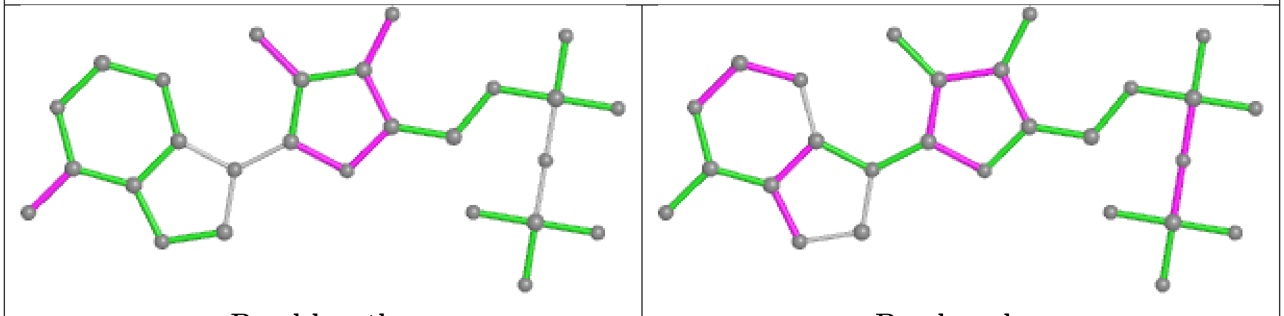
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

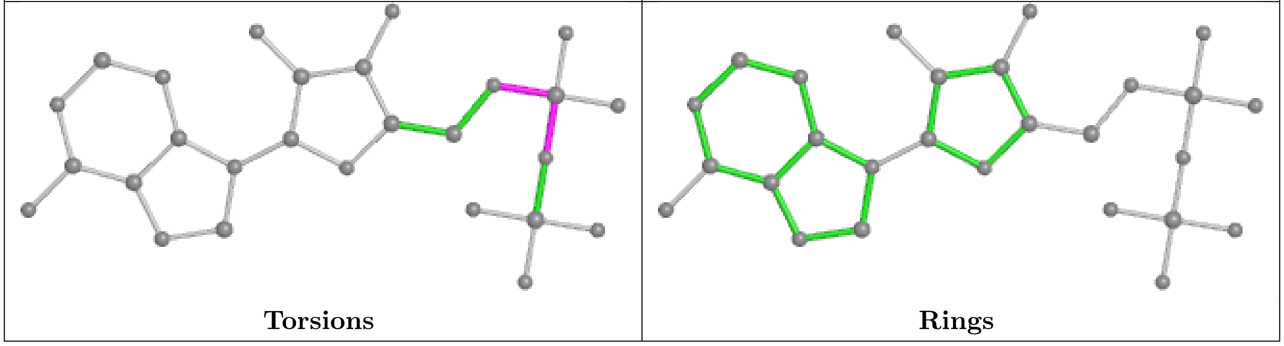
Ligand PLX C 303	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand 8Q1 G 201	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand ADP w 401

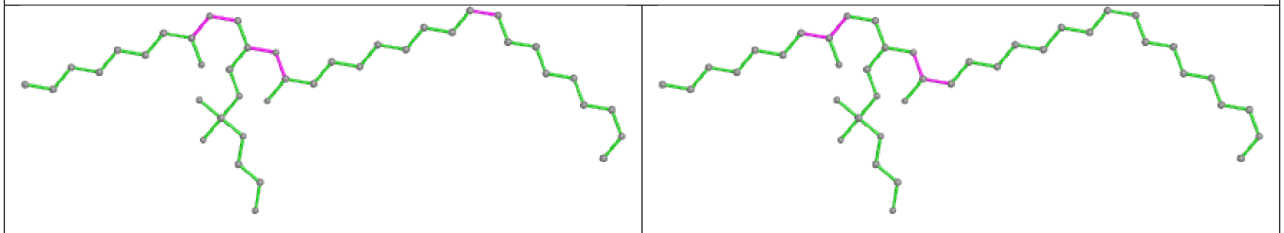


Bond lengths Bond angles

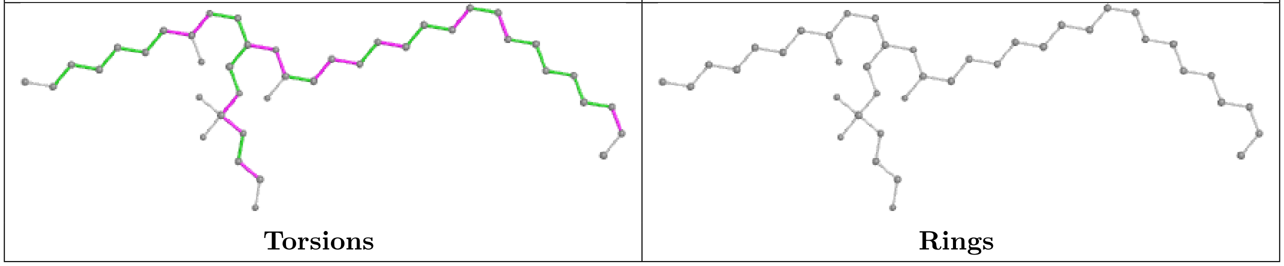


Torsions Rings

Ligand PEE m 201

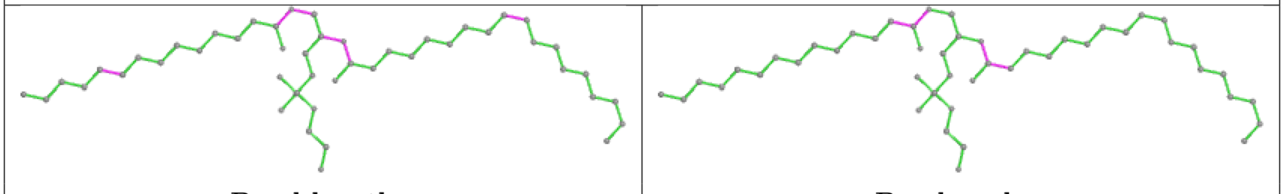


Bond lengths Bond angles

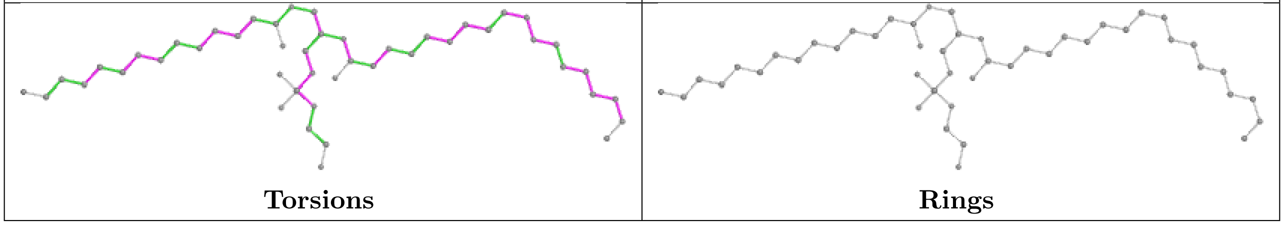


Torsions Rings

Ligand PEE Q 501

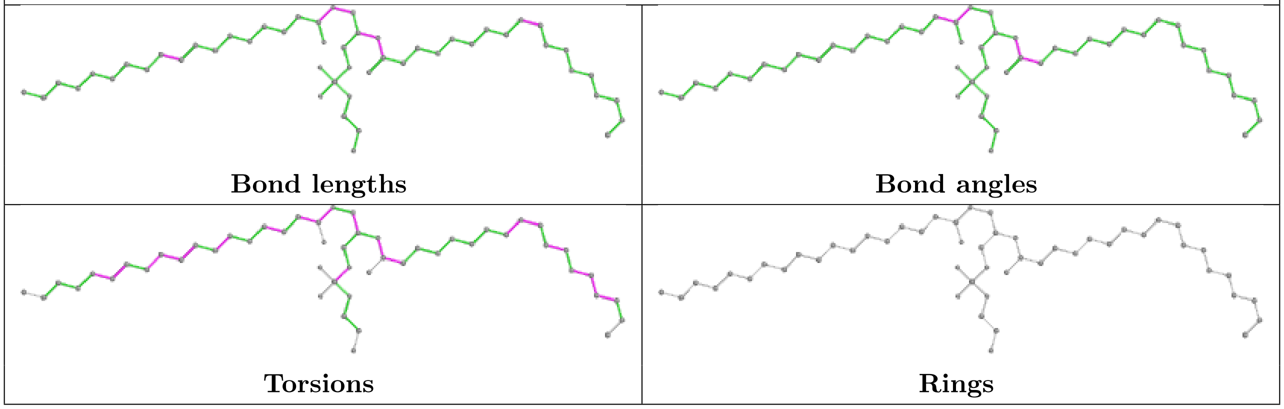


Bond lengths Bond angles

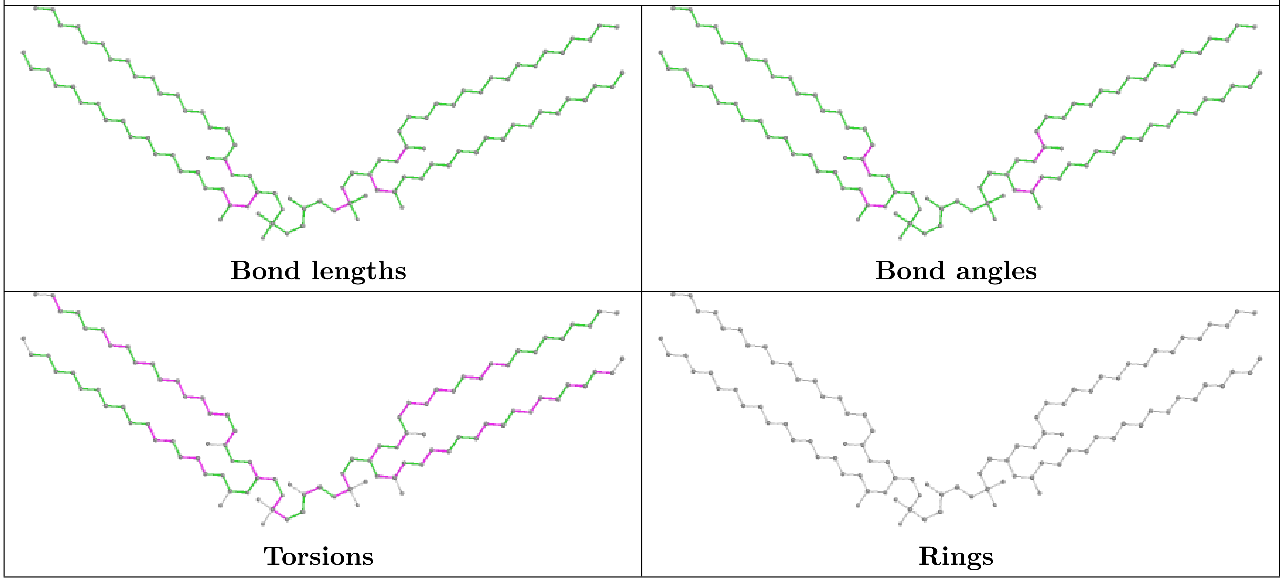


Torsions Rings

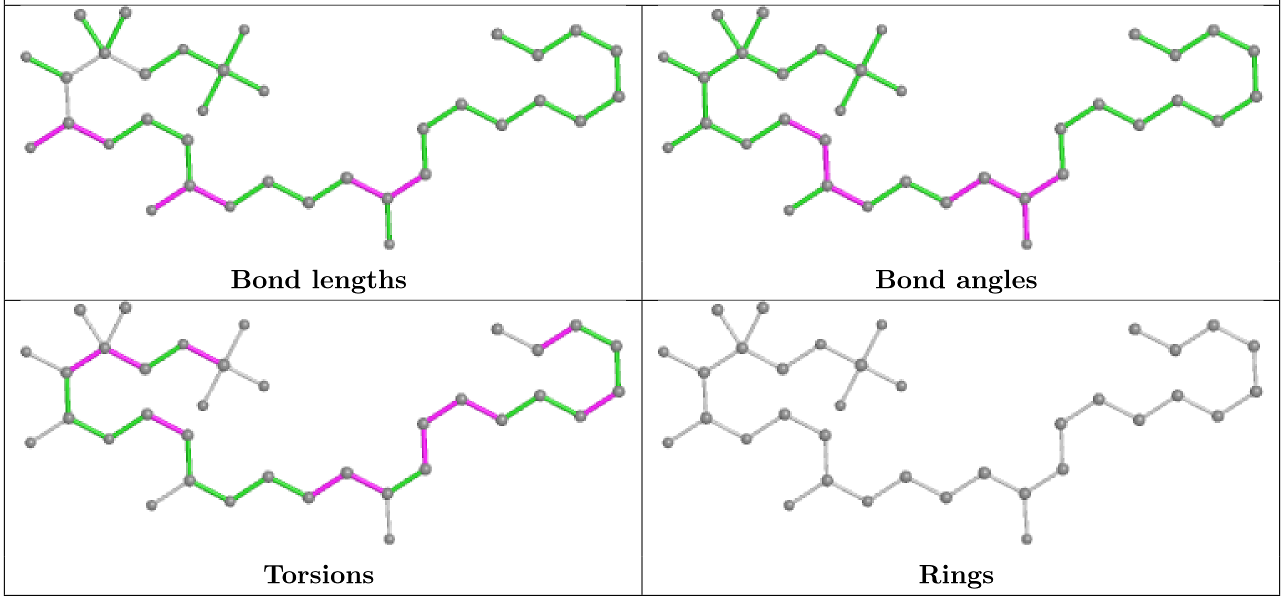
Ligand PEE U 101



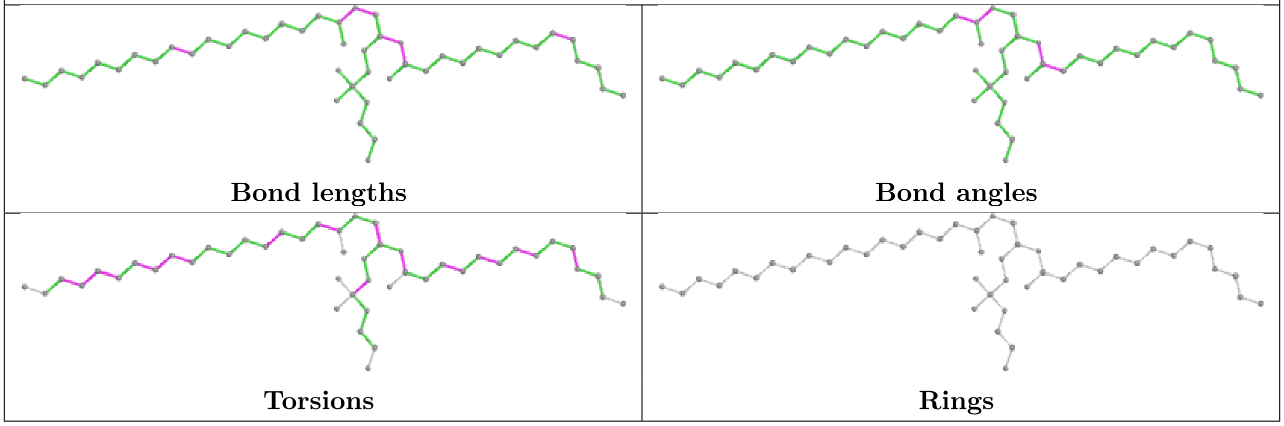
Ligand CDL l 701



Ligand 8Q1 X 201



Ligand PEE C 302



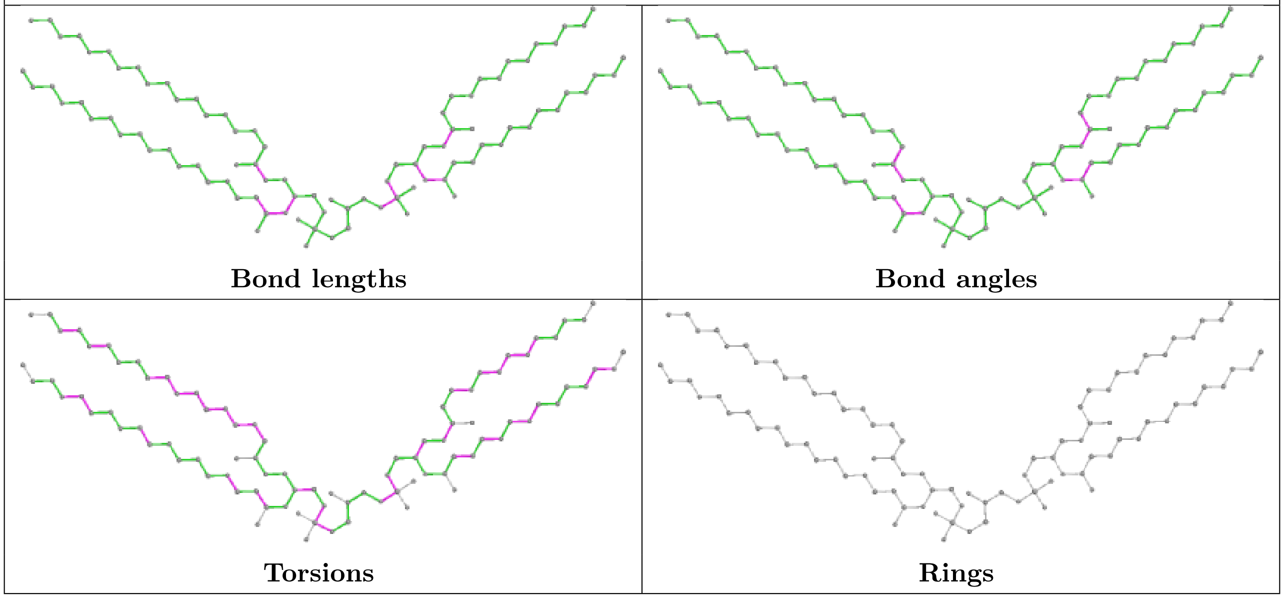
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL a 201



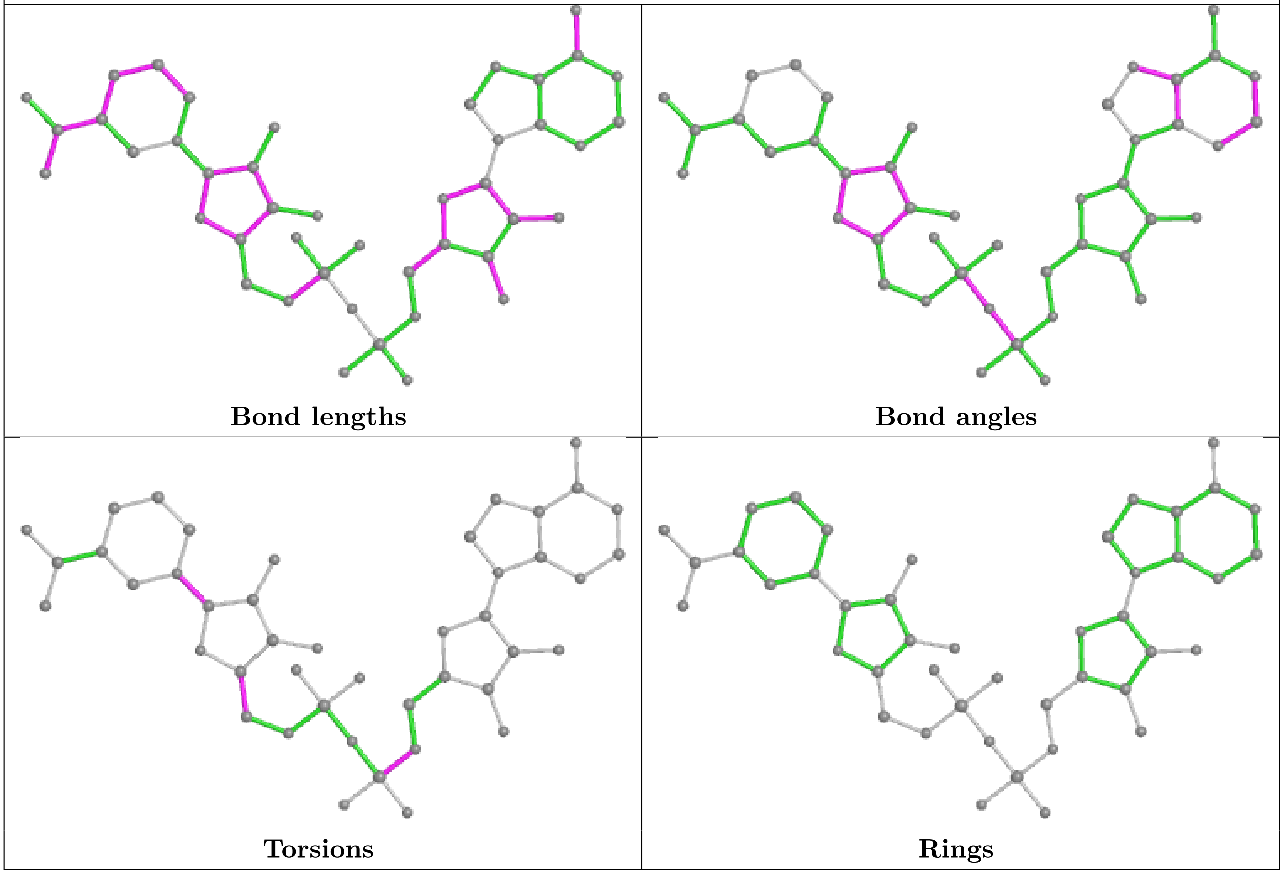
Bond lengths

Bond angles

Torsions

Rings

Ligand NAI A 503



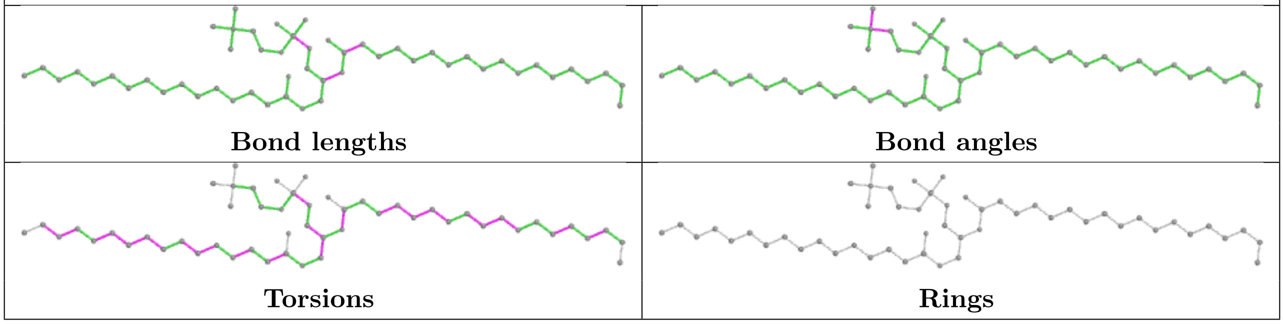
Bond lengths

Bond angles

Torsions

Rings

Ligand PLX i 401



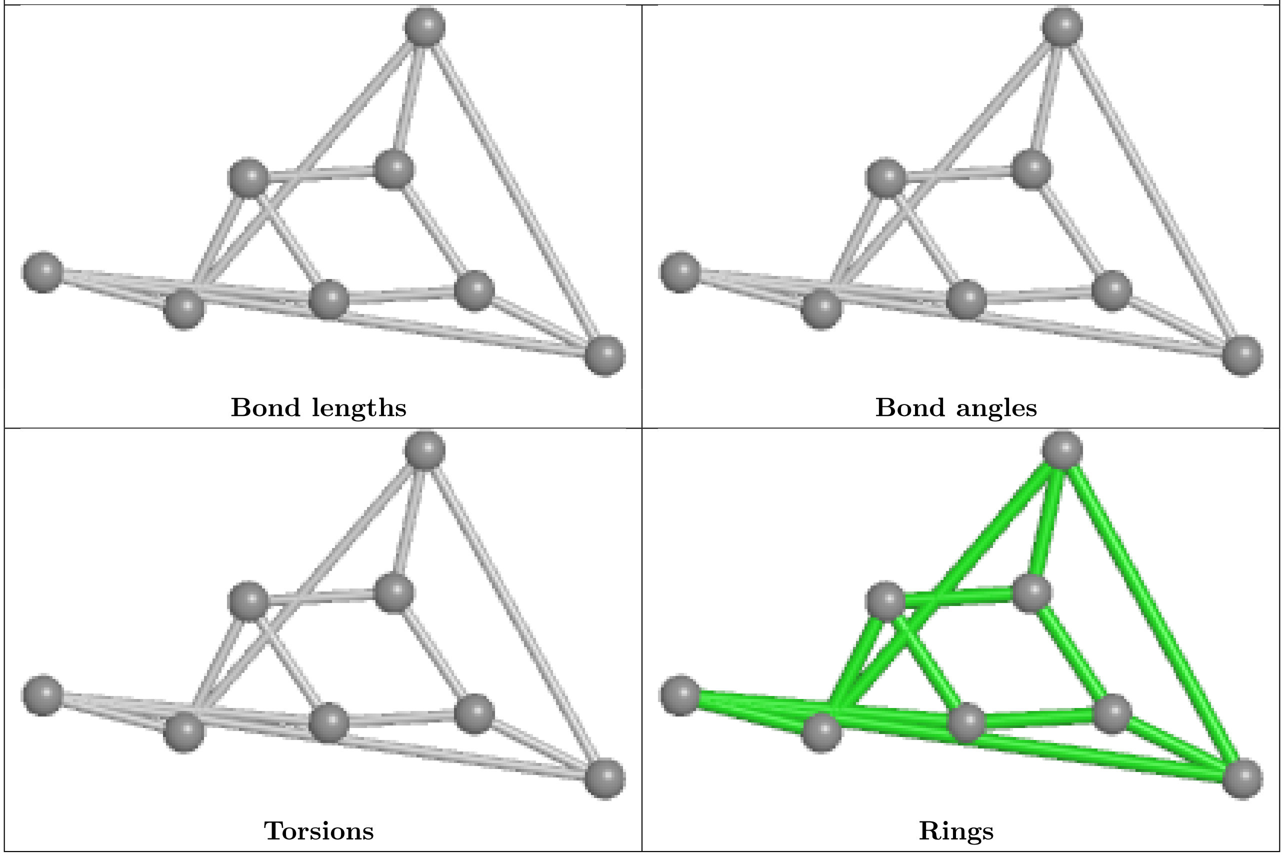
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 M 801



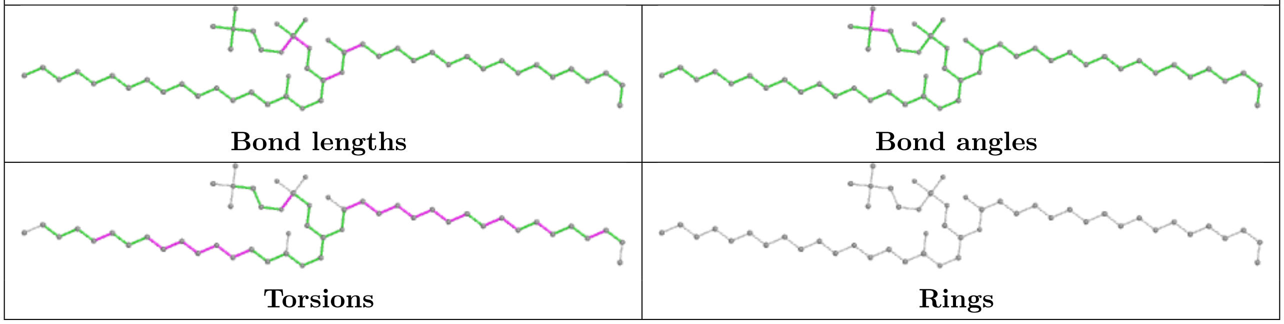
Bond lengths

Bond angles

Torsions

Rings

Ligand PLX a 202



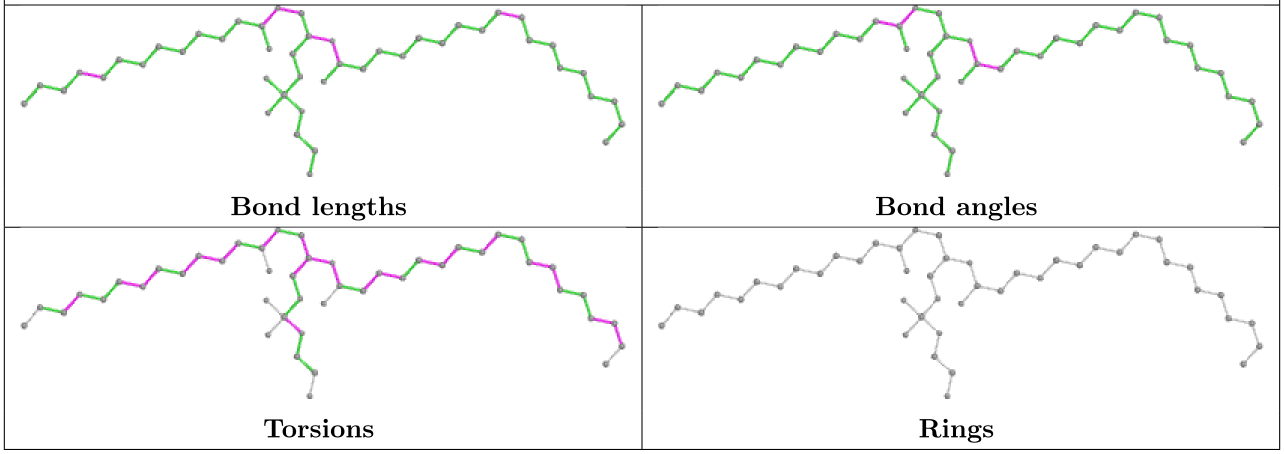
Bond lengths

Bond angles

Torsions

Rings

Ligand PEE l 702



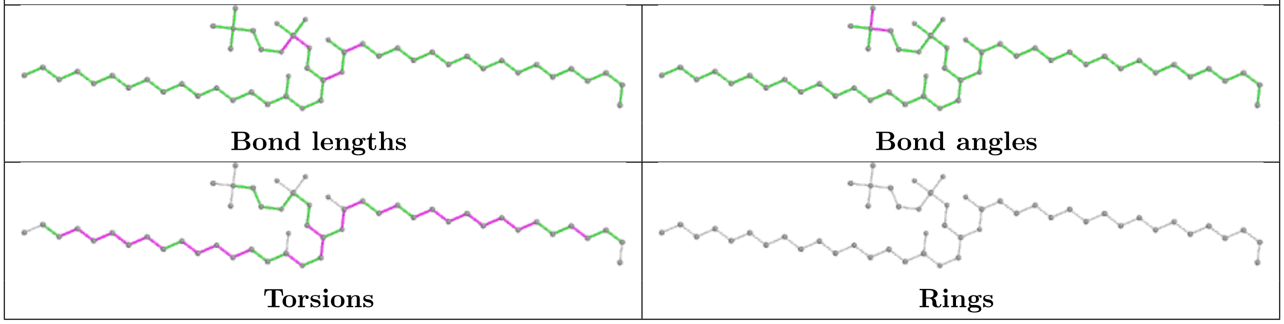
Bond lengths

Bond angles

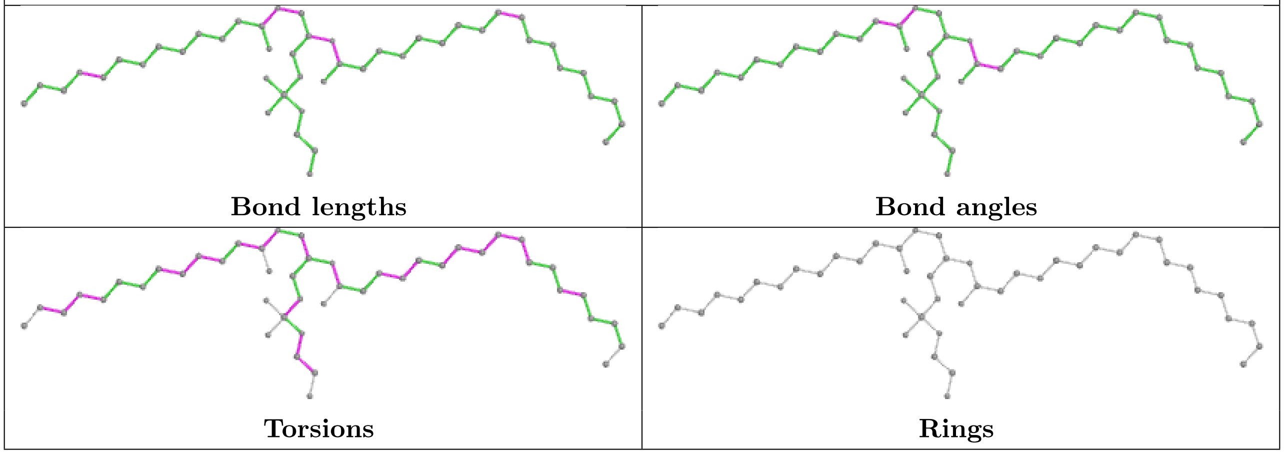
Torsions

Rings

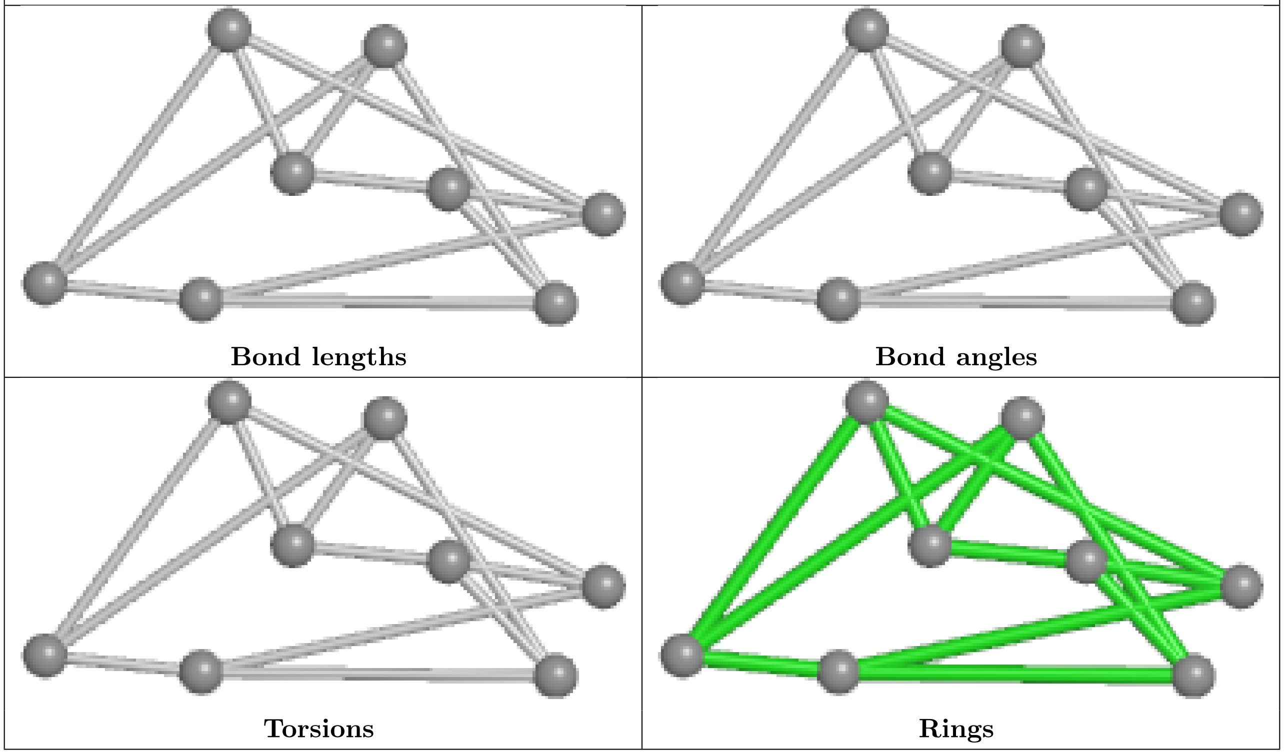
Ligand PLX j 201



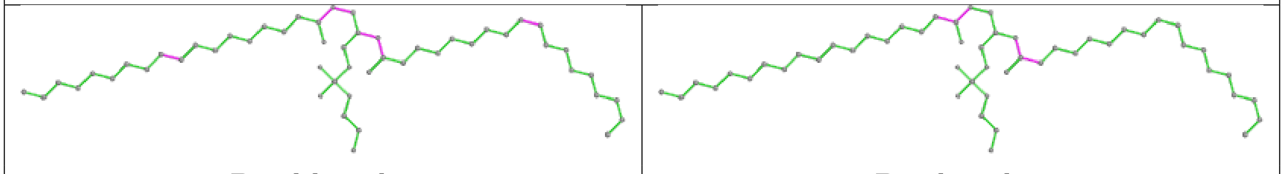
Ligand PEE l 703



Ligand SF4 A 501

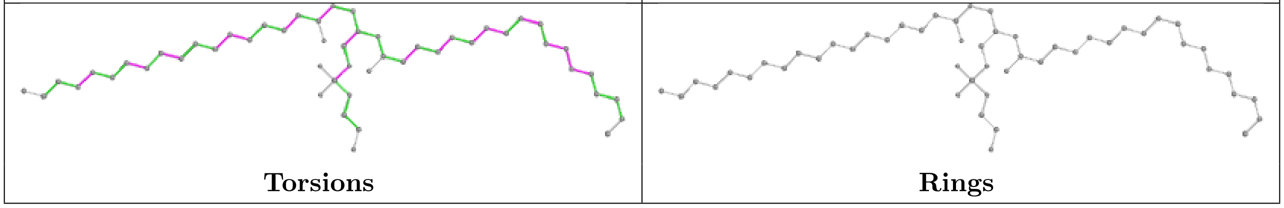


Ligand PEE Q 502



Bond lengths

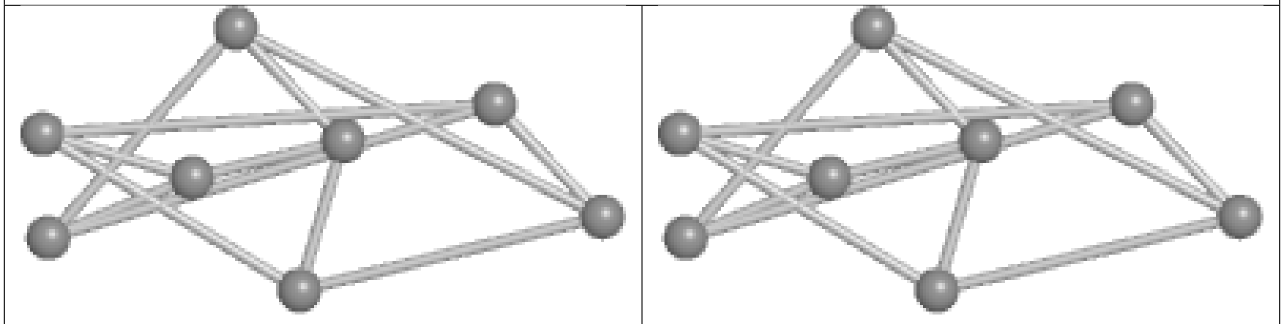
Bond angles



Torsions

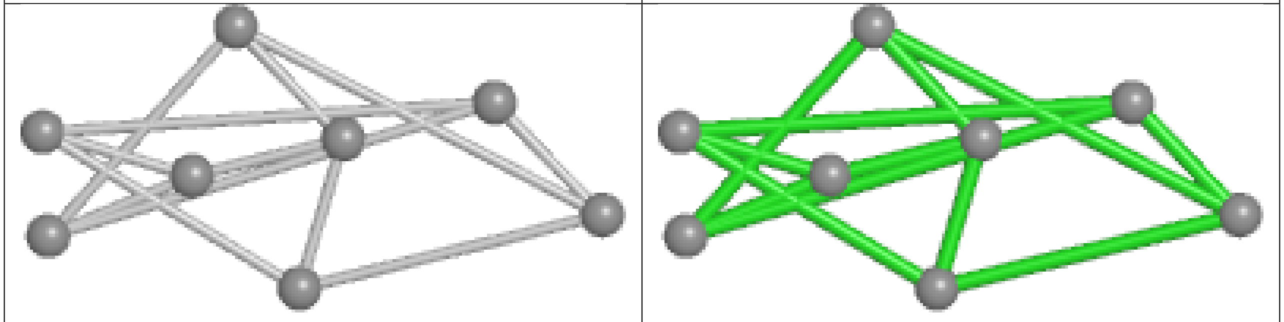
Rings

Ligand SF4 B 301



Bond lengths

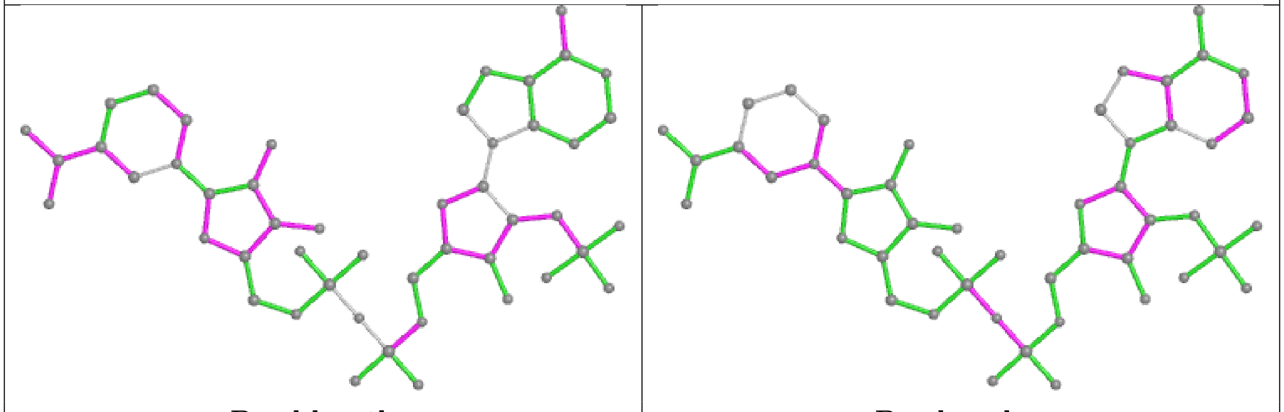
Bond angles



Torsions

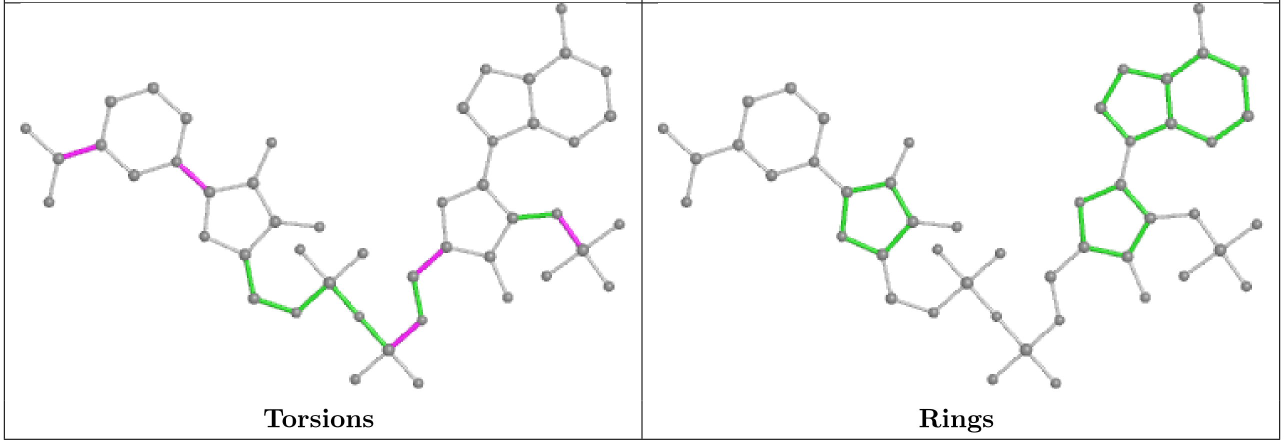
Rings

Ligand NDP J 401



Bond lengths

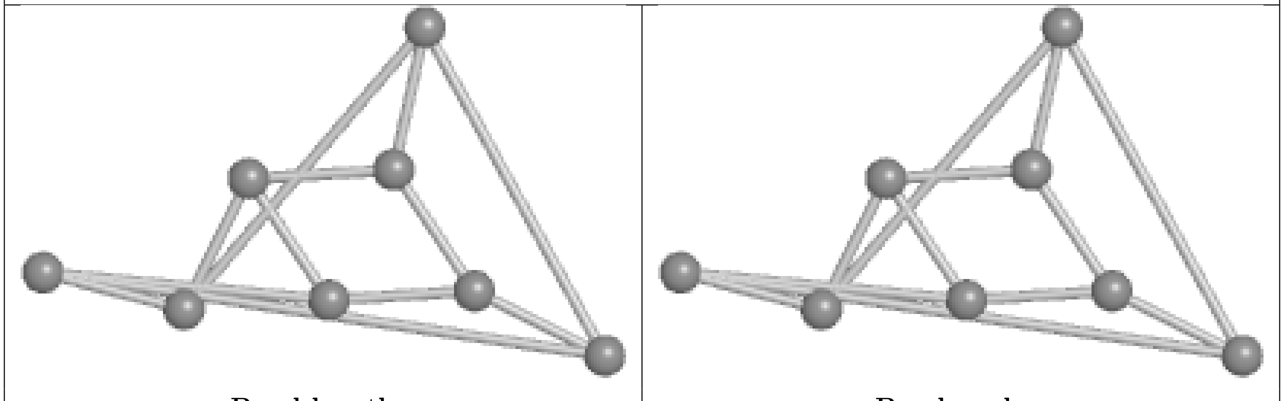
Bond angles



Torsions

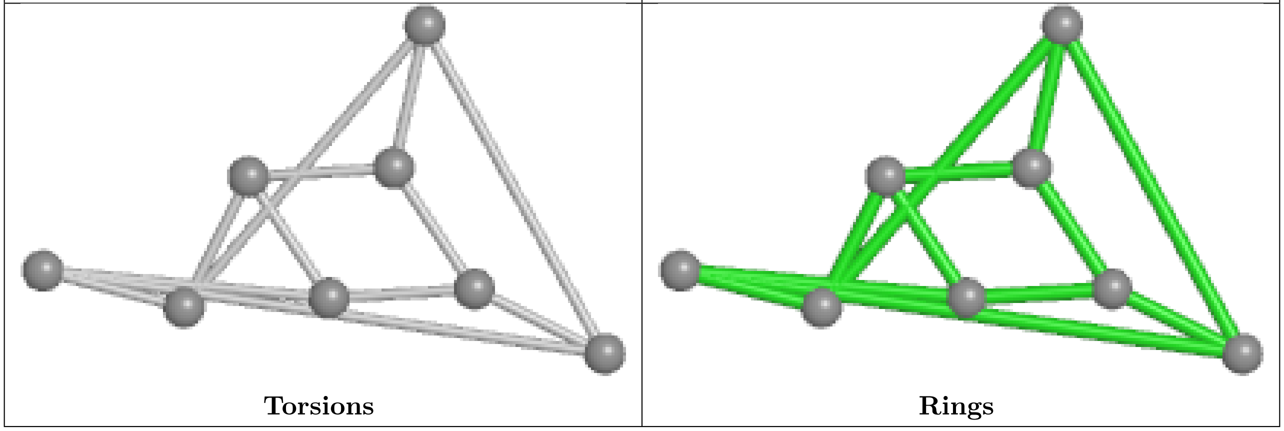
Rings

Ligand SF4 M 802



Bond lengths

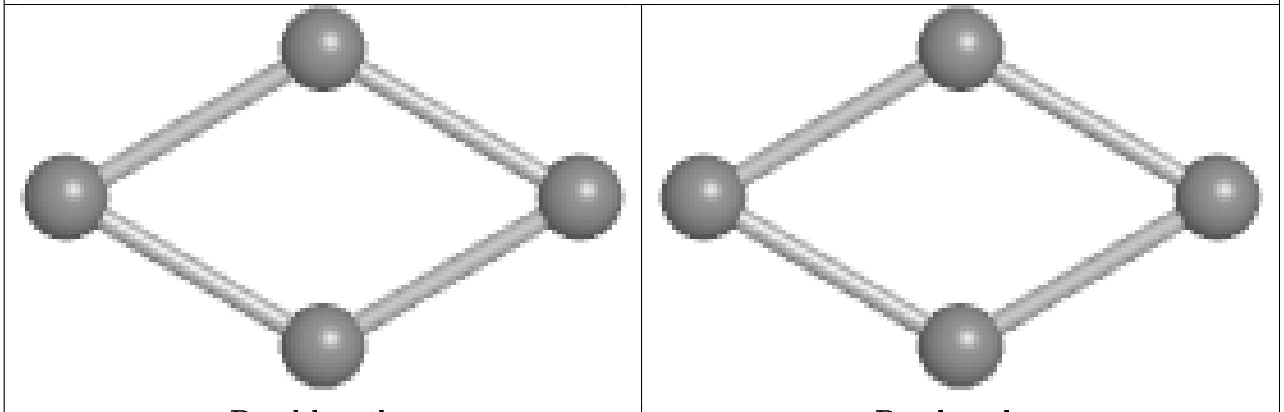
Bond angles



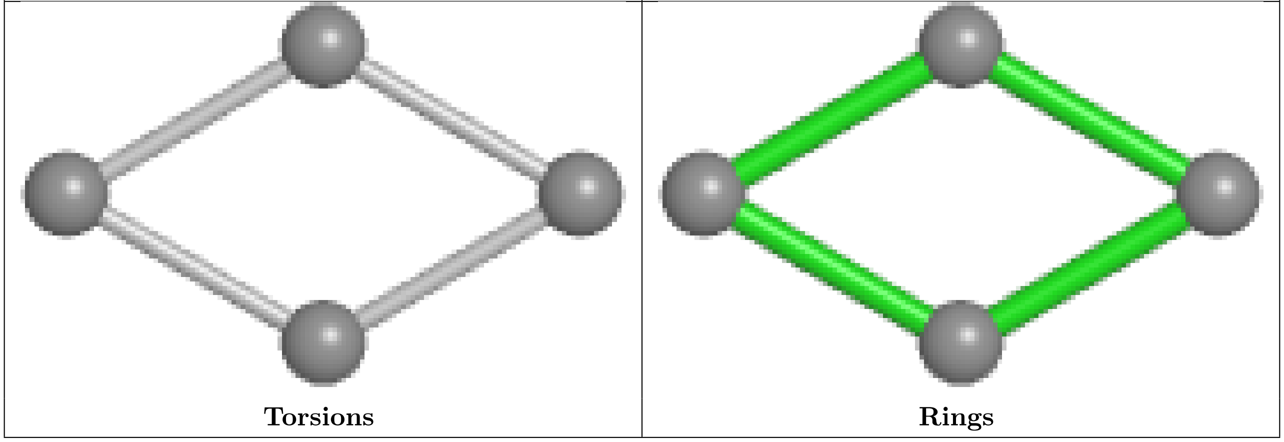
Torsions

Rings

Ligand FES O 301

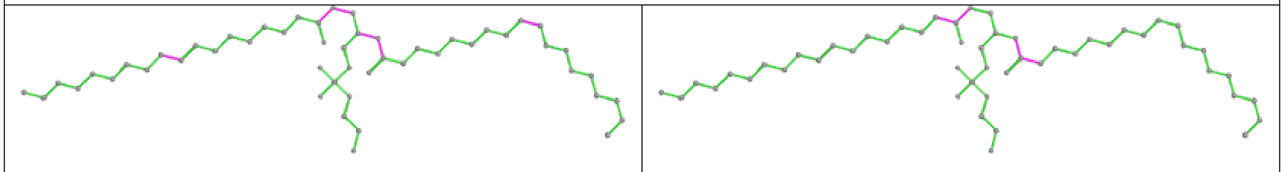


Bond lengths Bond angles

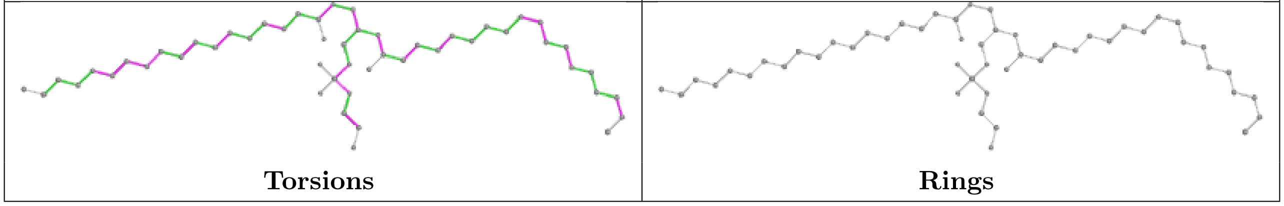


Torsions Rings

Ligand PEE r 501

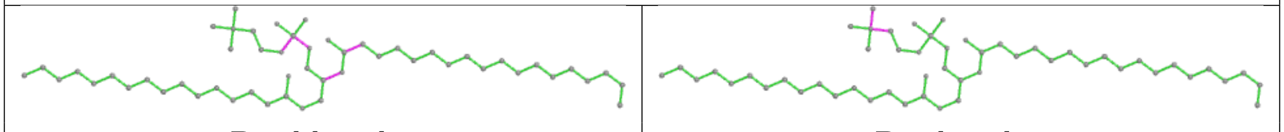


Bond lengths Bond angles

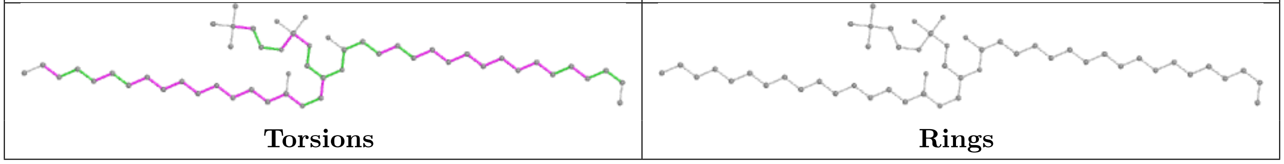


Torsions Rings

Ligand PLX r 503

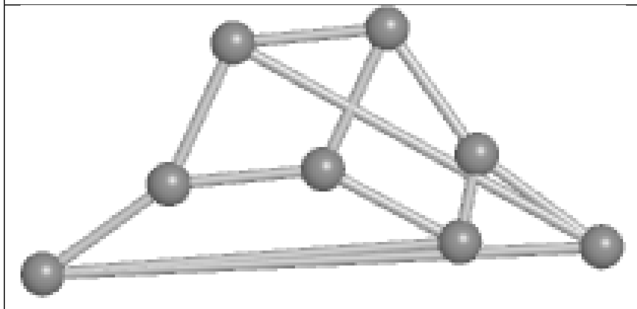


Bond lengths Bond angles

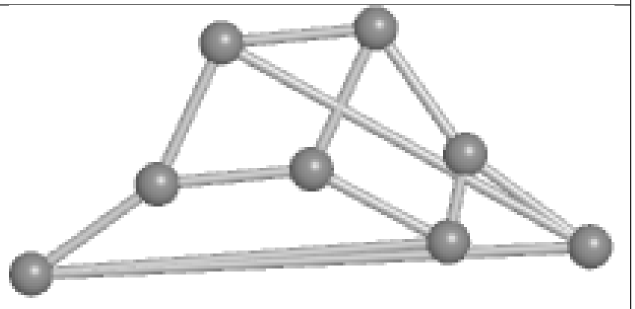


Torsions Rings

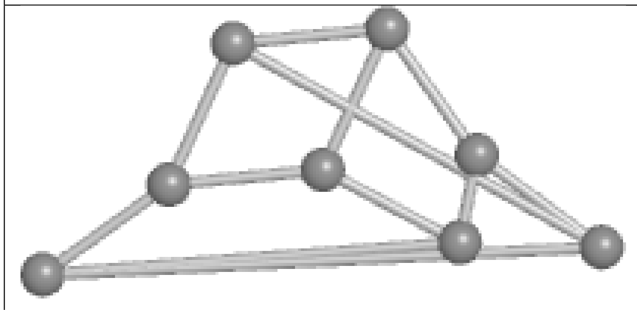
Ligand SF4 C 301



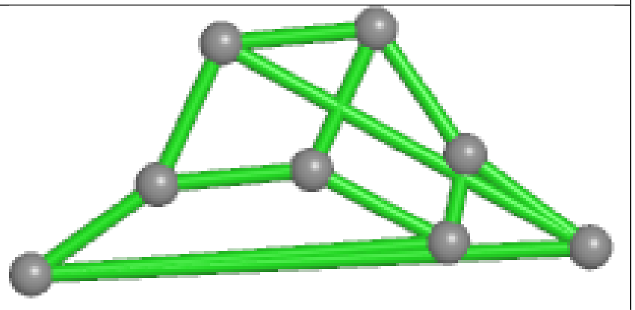
Bond lengths



Bond angles

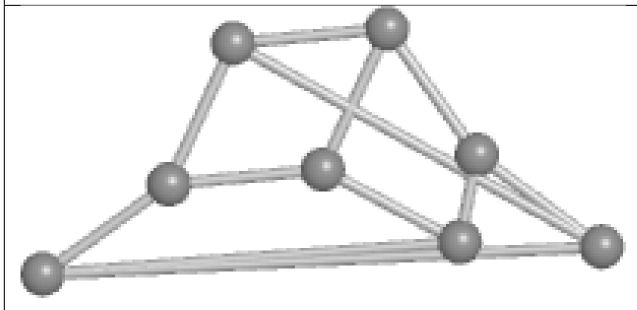


Torsions

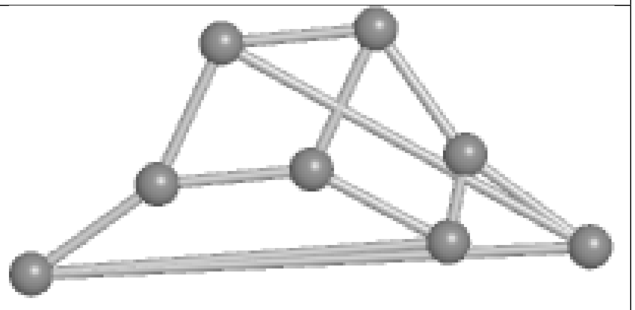


Rings

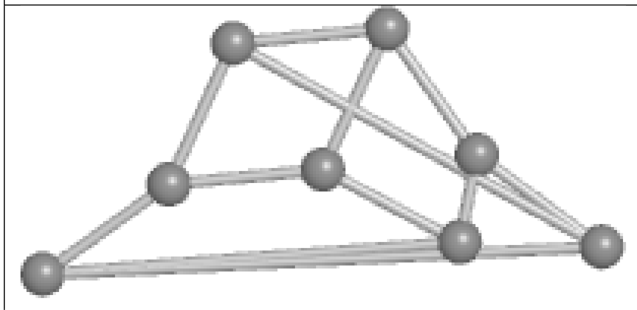
Ligand SF4 B 302



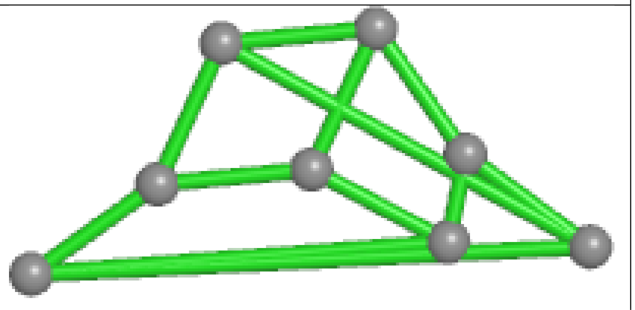
Bond lengths



Bond angles

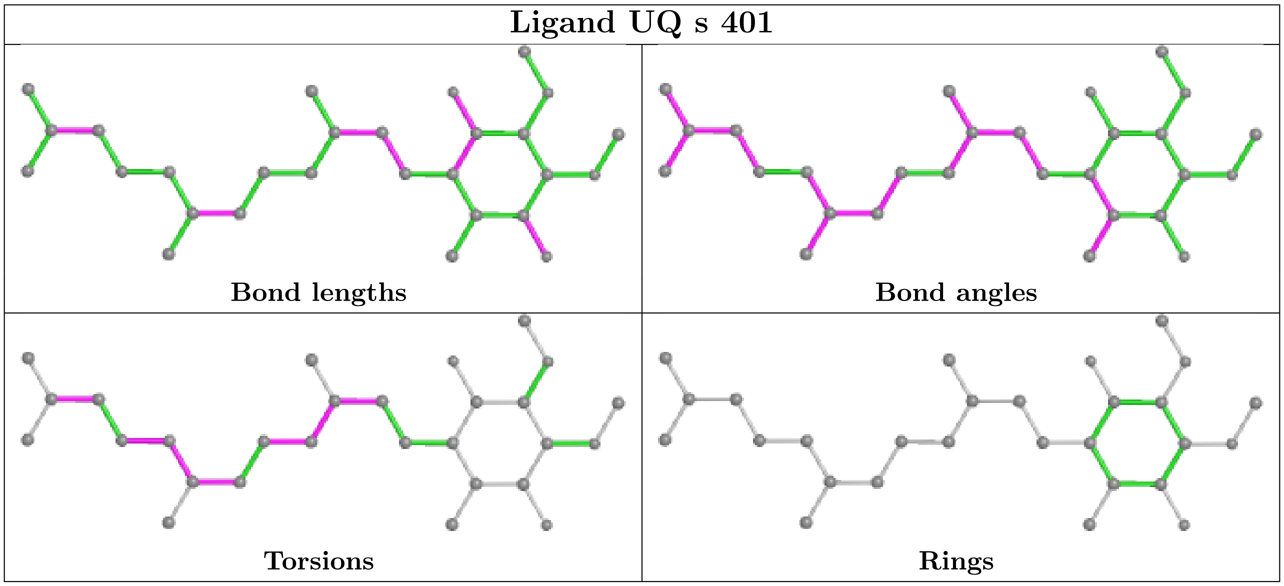


Torsions

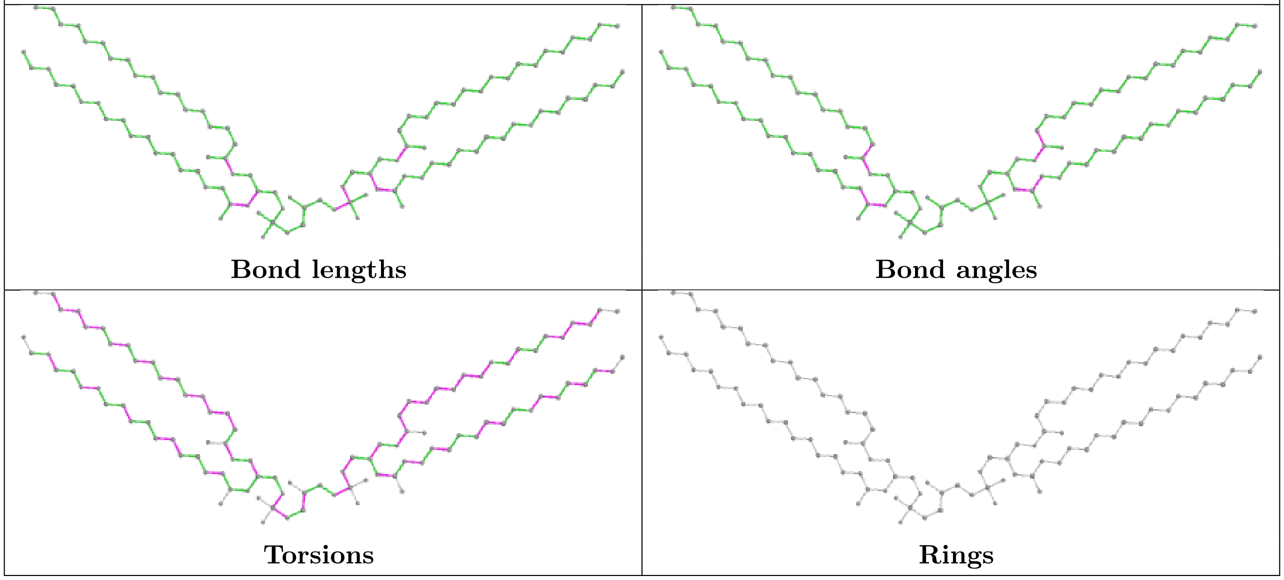


Rings

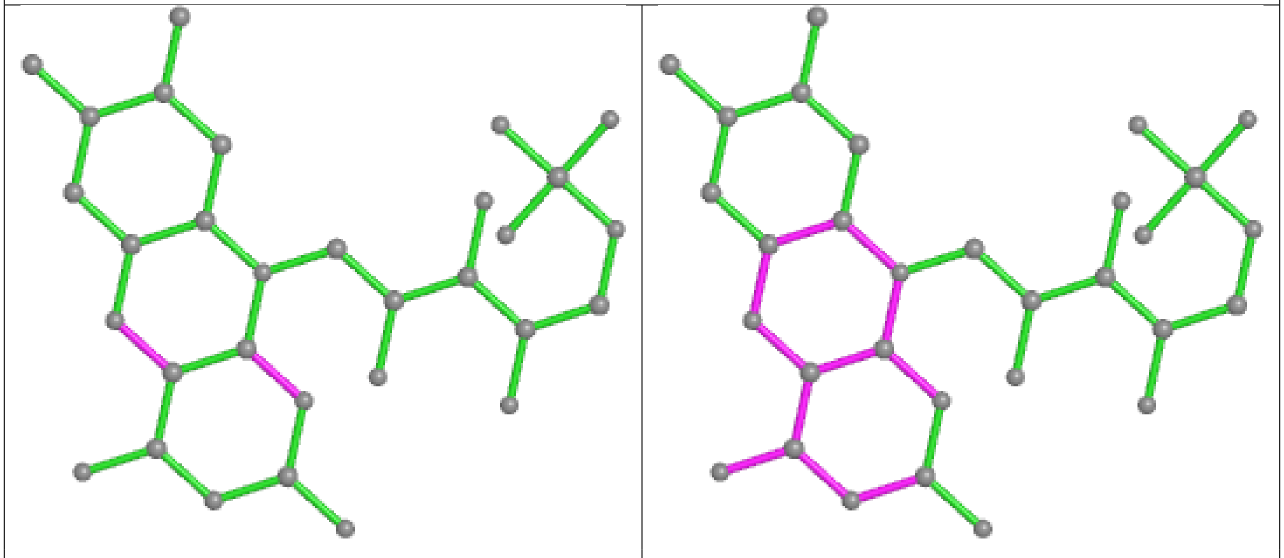
Ligand UQ s 401



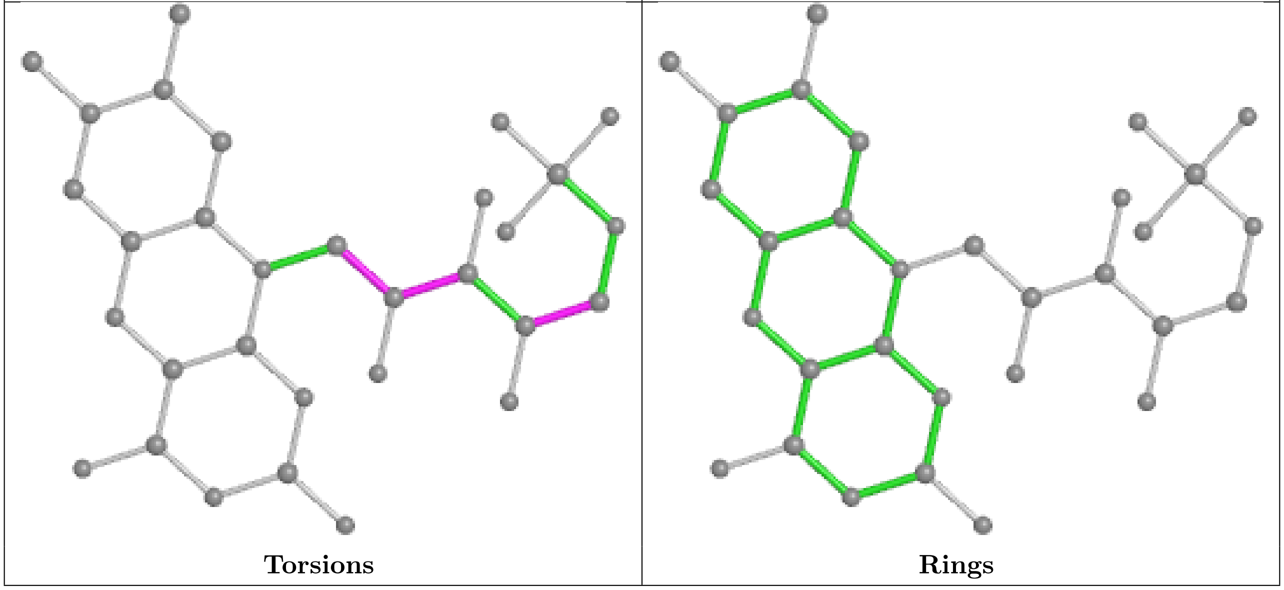
Ligand CDL i 402



Ligand FMN A 502

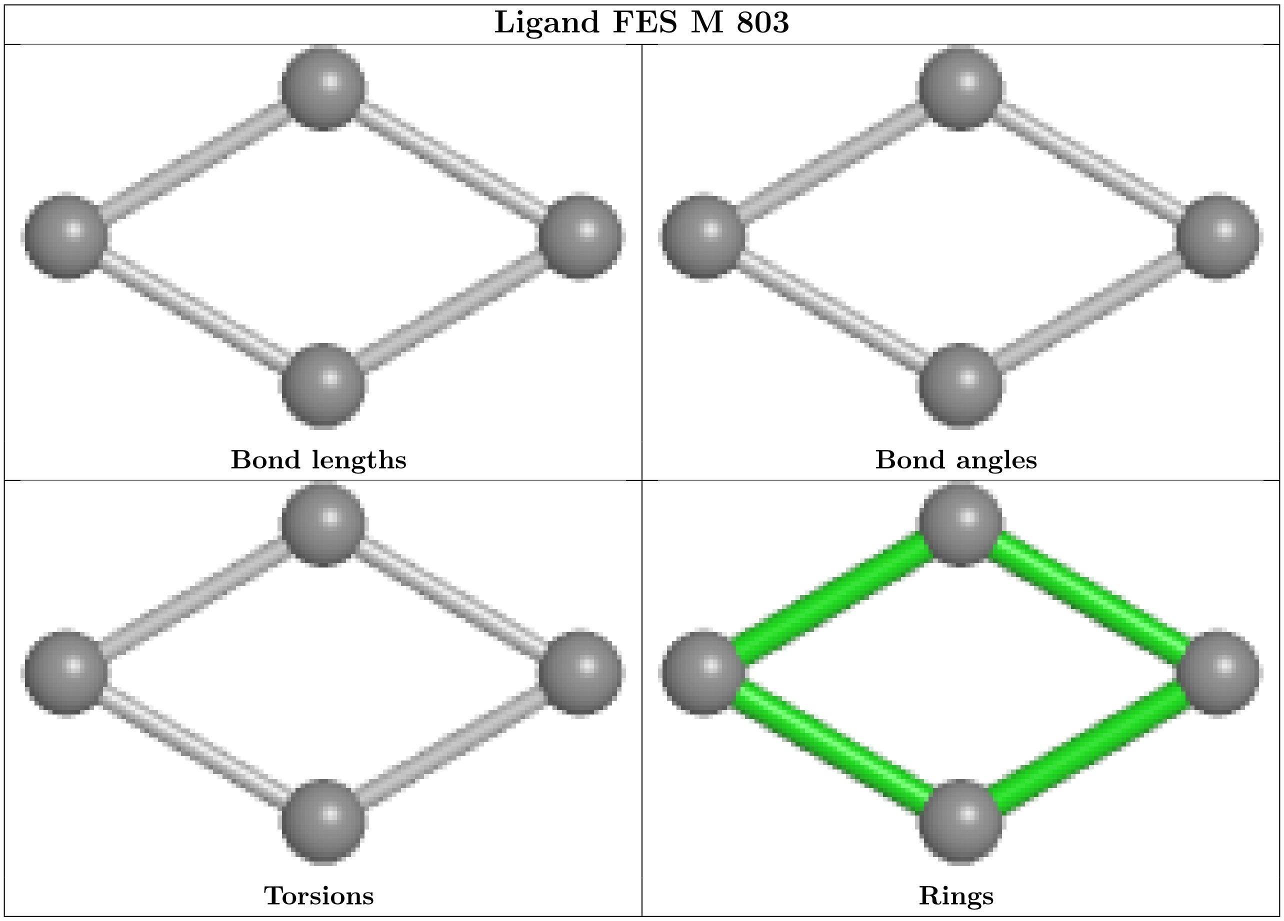


Bond lengths Bond angles

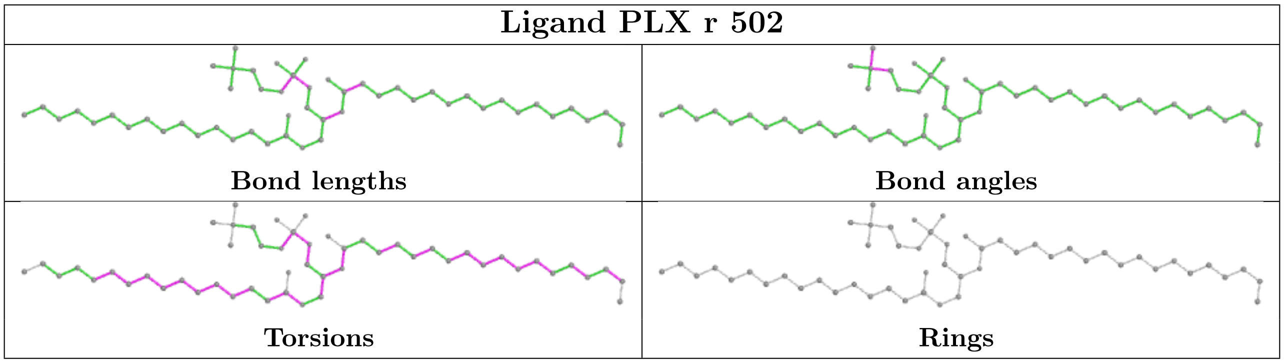


Torsions Rings

Ligand FES M 803



Ligand PLX r 502



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

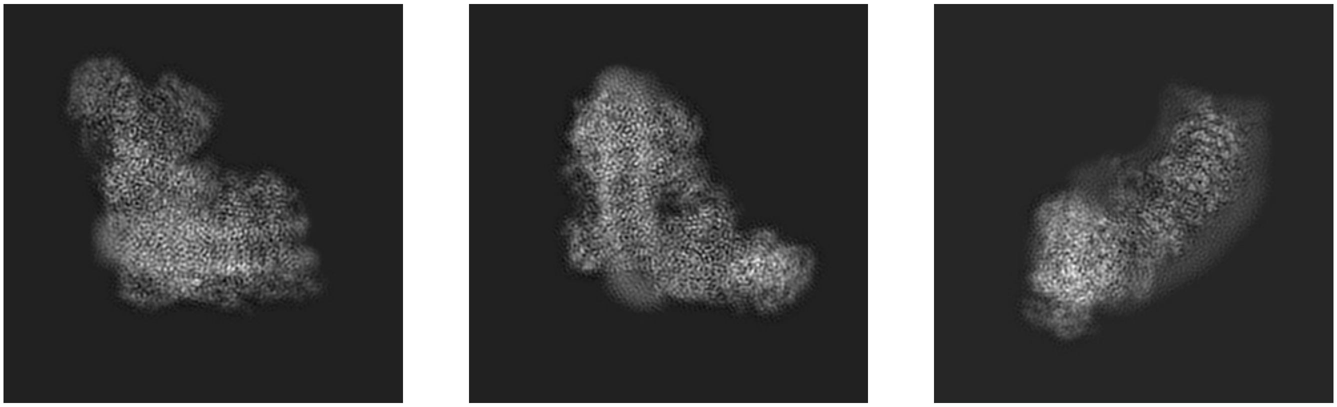
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-32306. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

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

6.2 Central slices ⓘ

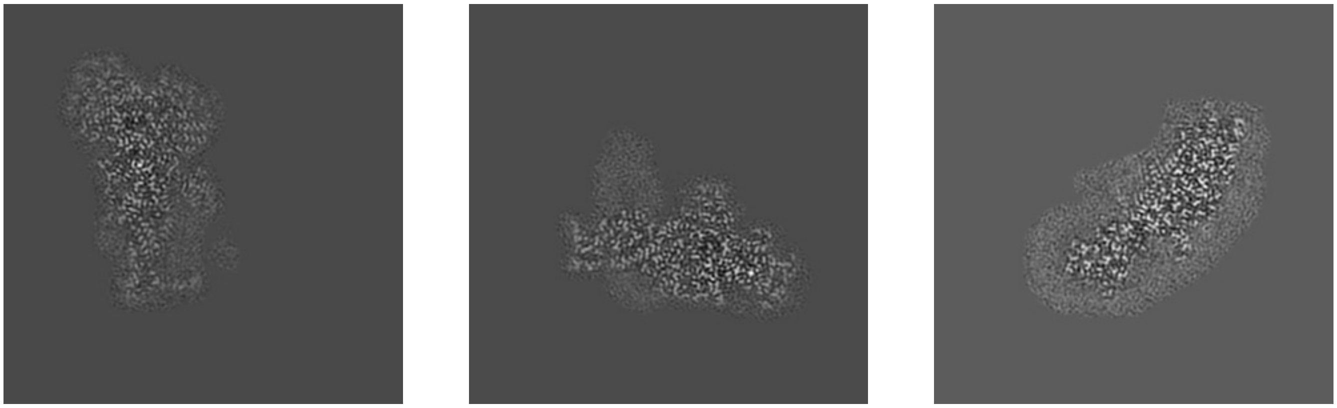
6.2.1 Primary map

X Index: 152 Y Index: 152 Z Index: 152

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

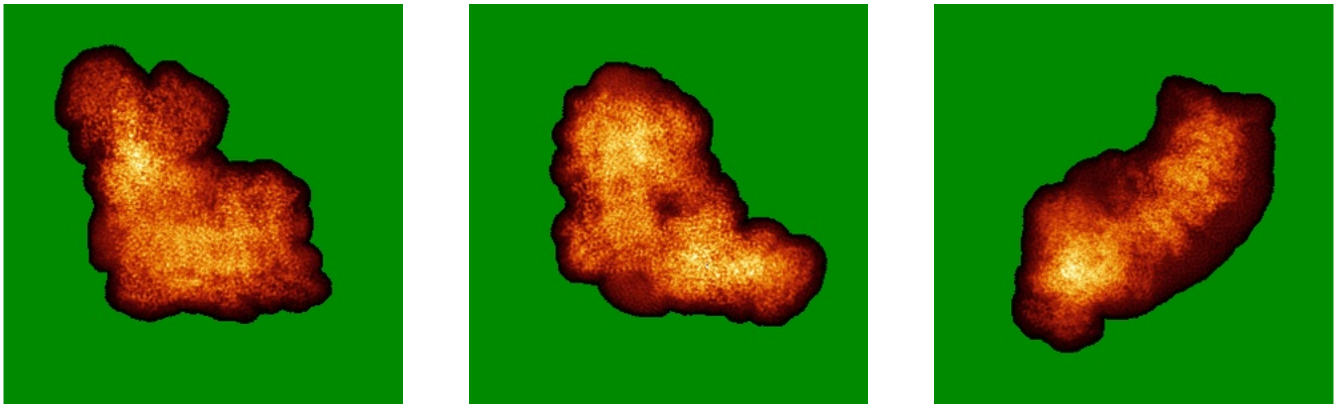


X Index: 105 Y Index: 98 Z Index: 128

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

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

6.4.1 Primary map

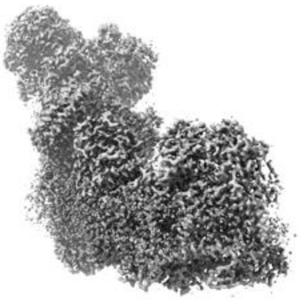


X Y Z

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.

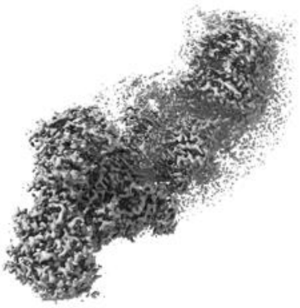
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0282. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

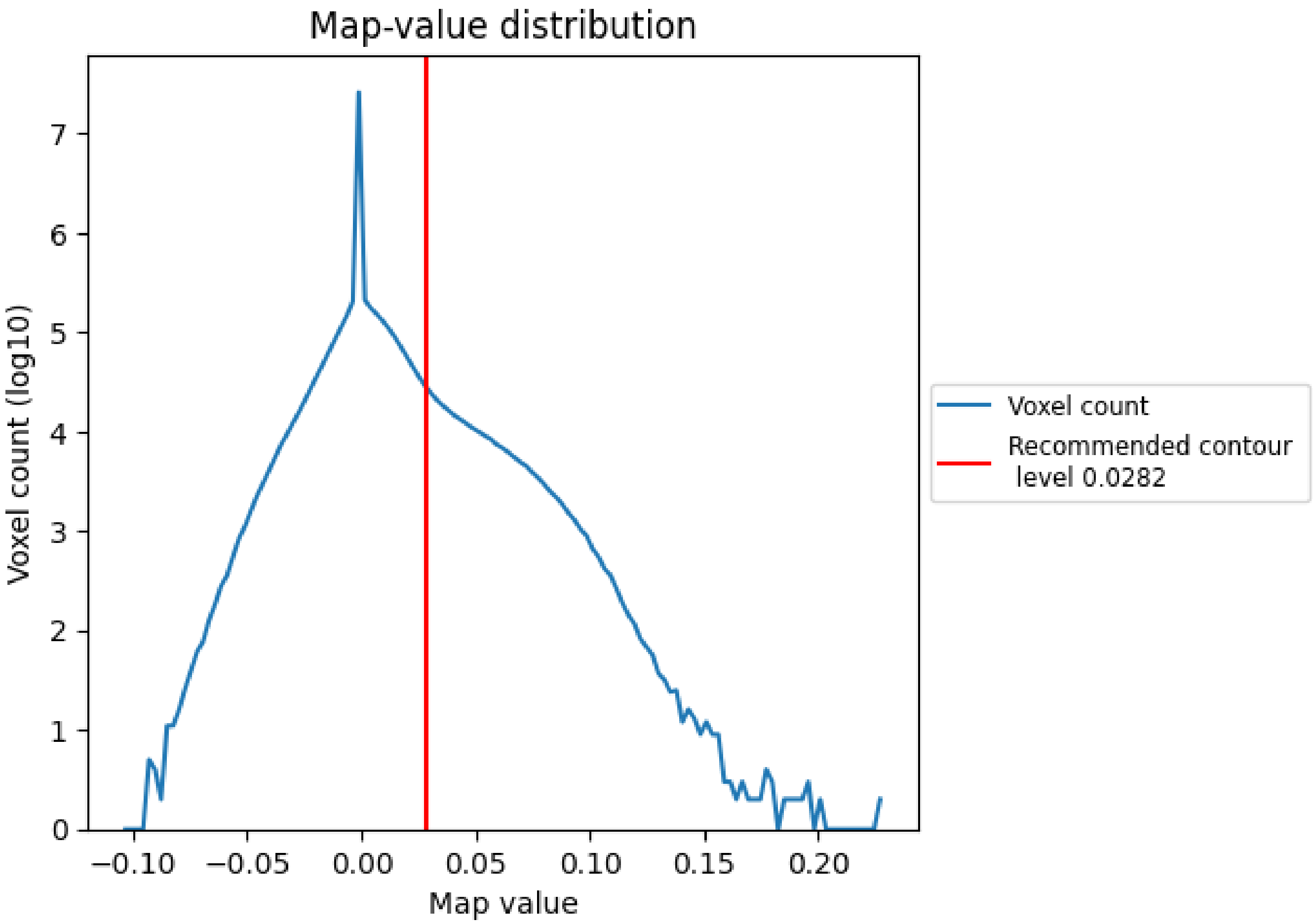
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

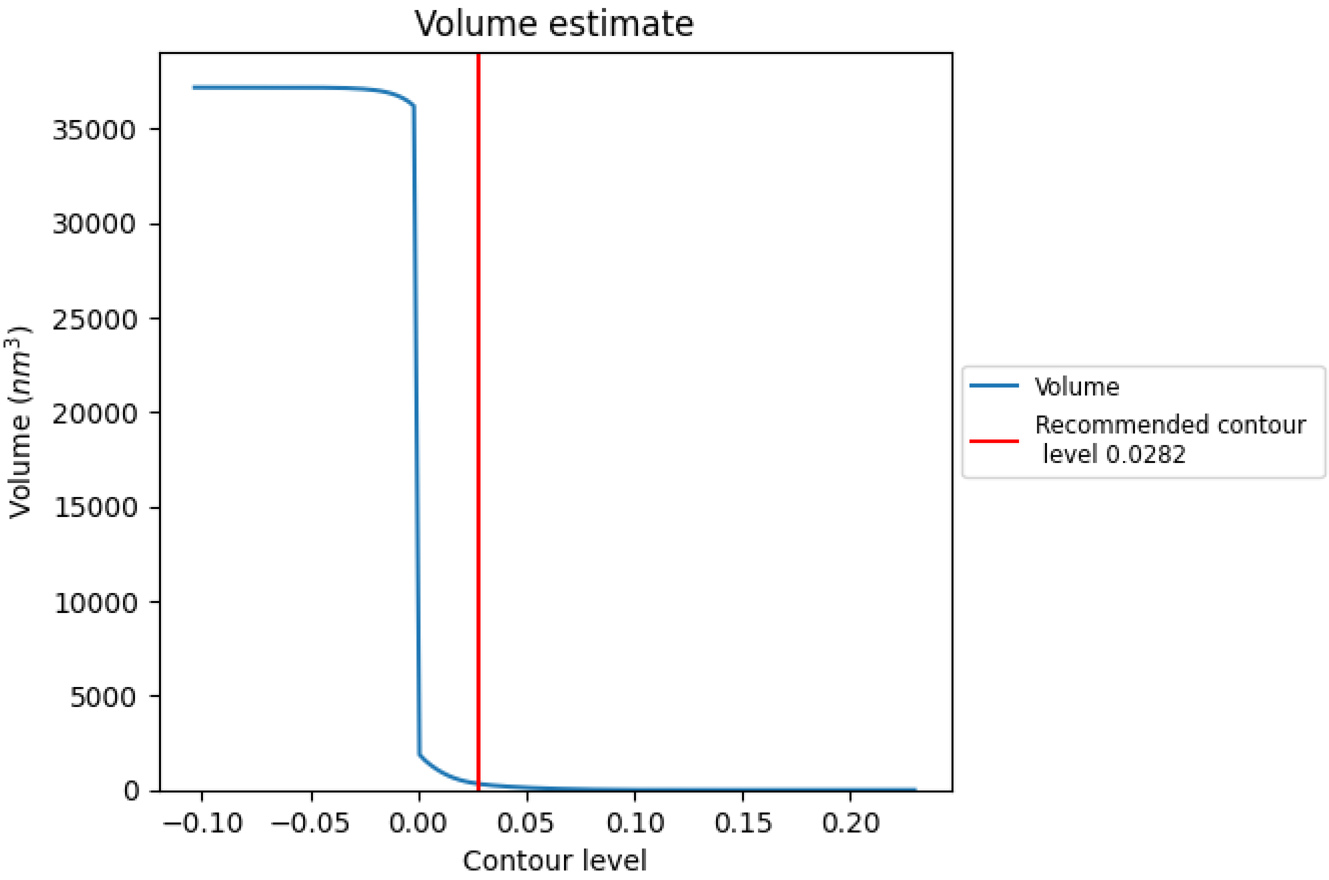
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

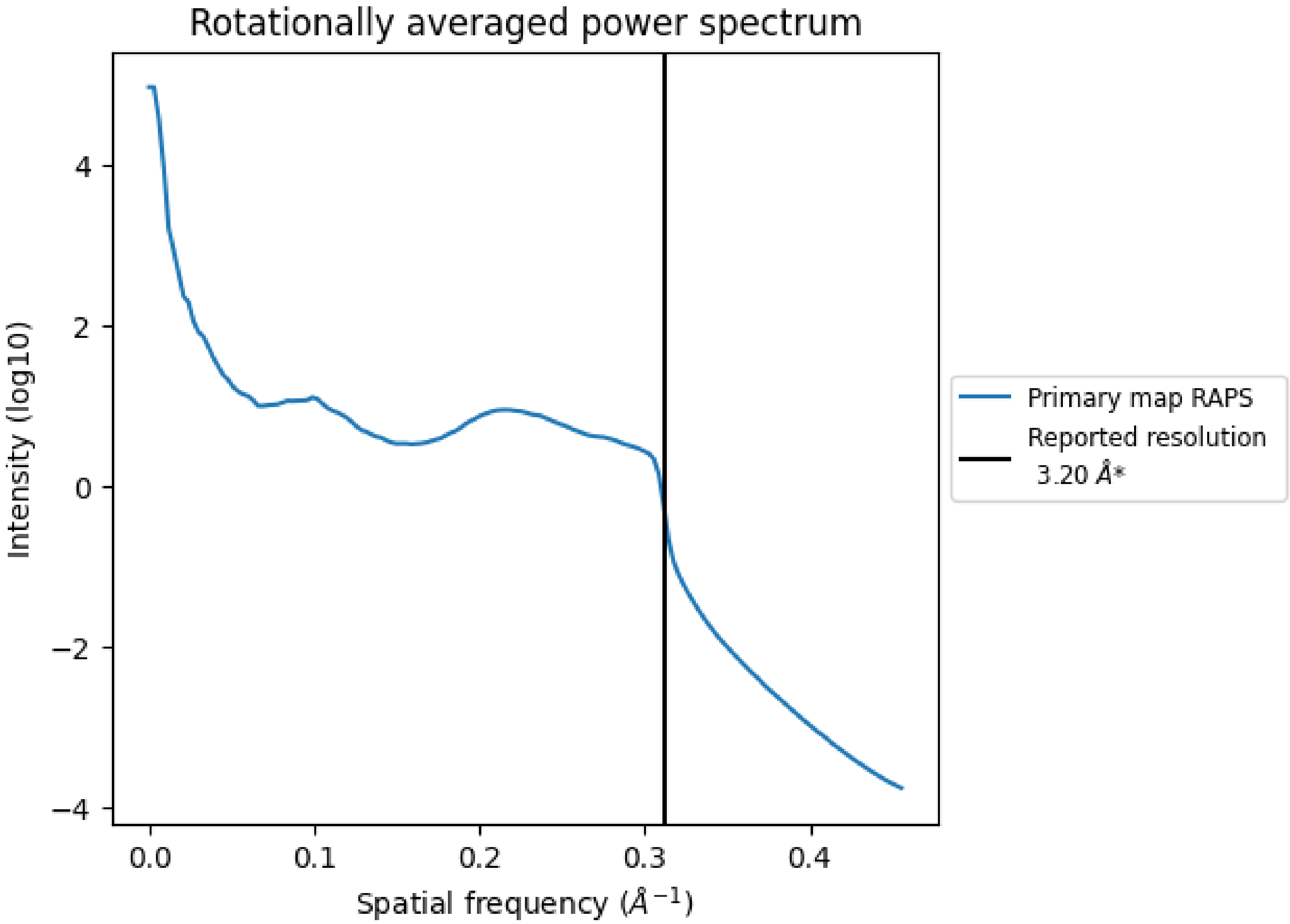
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 321 nm^3; this corresponds to an approximate mass of 290 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

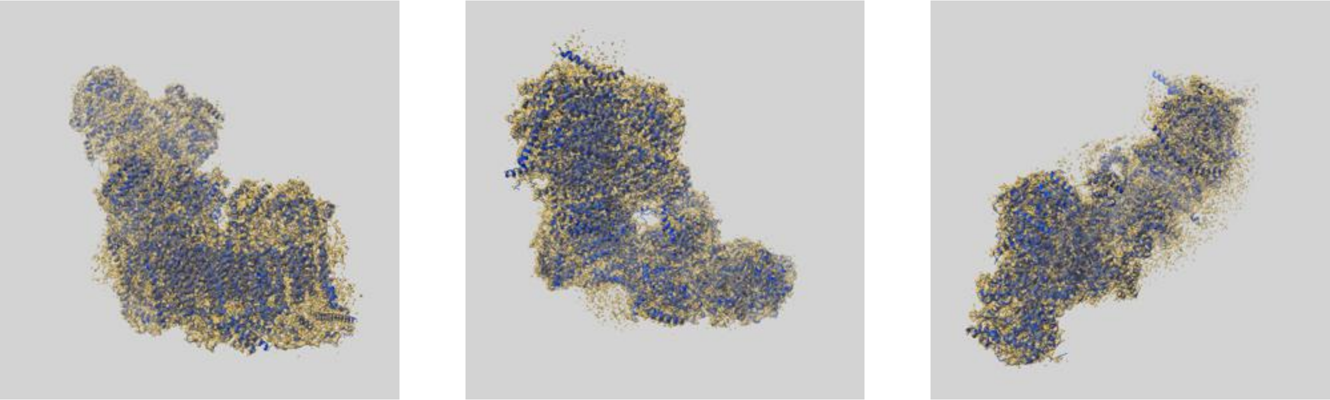
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32306 and PDB model 7W4K. Per-residue inclusion information can be found in section 3 on page 20.

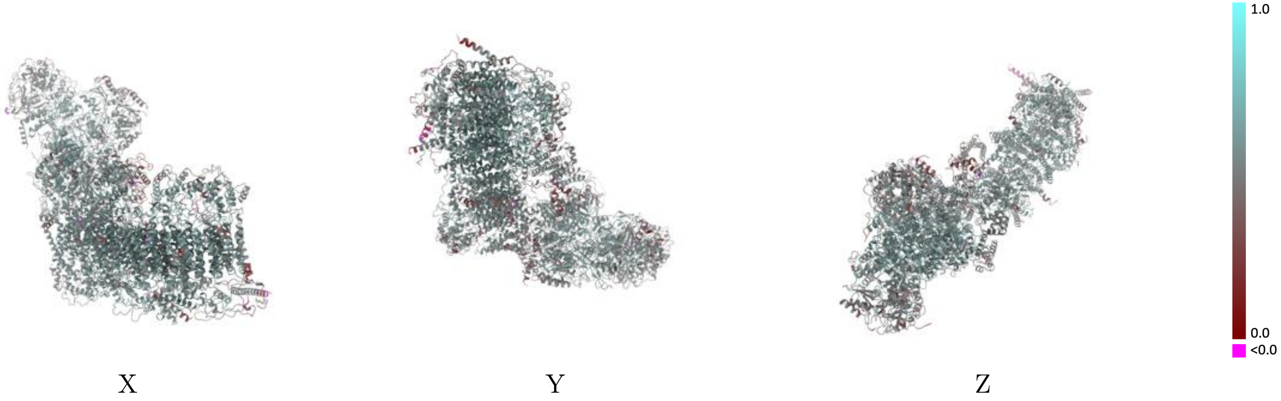
9.1 Map-model overlay ⓘ



X Y Z

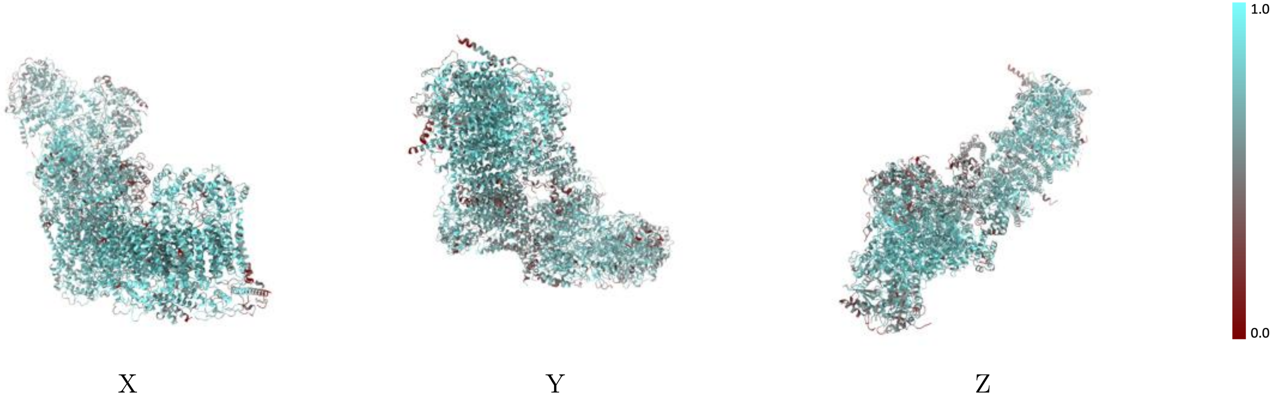
The images above show the 3D surface view of the map at the recommended contour level 0.0282 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



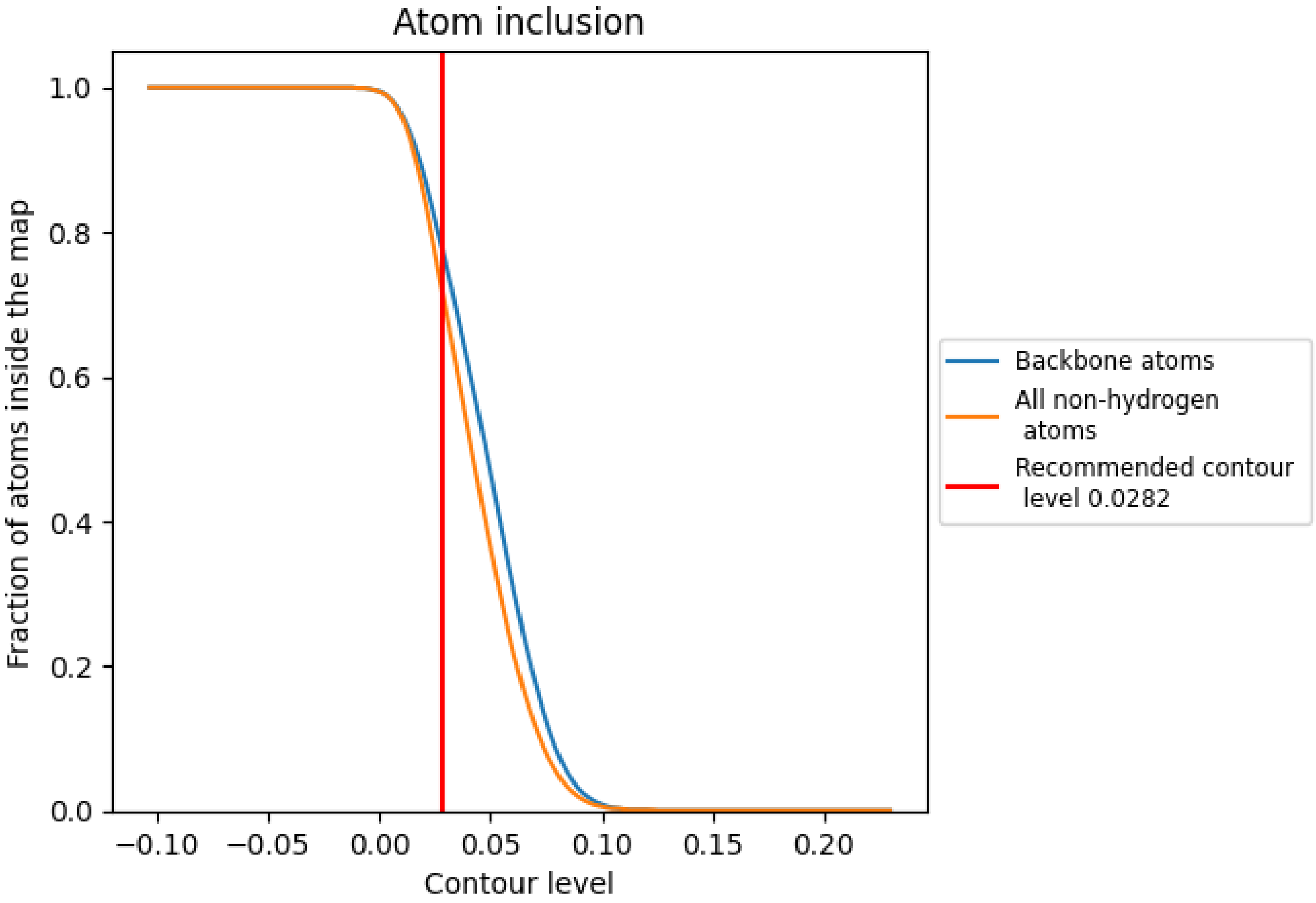
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.0282).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0282) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	■ 0.7210	■ 0.5310
A	■ 0.6420	■ 0.5000
B	■ 0.8720	■ 0.5840
C	■ 0.8040	■ 0.5650
E	■ 0.6730	■ 0.5210
F	■ 0.5170	■ 0.4330
G	■ 0.4060	■ 0.3590
H	■ 0.6700	■ 0.5030
I	■ 0.7390	■ 0.5420
J	■ 0.6040	■ 0.4900
K	■ 0.5550	■ 0.4610
L	■ 0.7440	■ 0.5530
M	■ 0.7190	■ 0.5380
N	■ 0.7600	■ 0.5490
O	■ 0.6180	■ 0.4960
P	■ 0.8390	■ 0.5790
Q	■ 0.8140	■ 0.5760
S	■ 0.7850	■ 0.5440
T	■ 0.7180	■ 0.5400
U	■ 0.6820	■ 0.5020
V	■ 0.4510	■ 0.4430
W	■ 0.7250	■ 0.5310
X	■ 0.7020	■ 0.5020
Y	■ 0.6120	■ 0.4700
Z	■ 0.5610	■ 0.4580
a	■ 0.7650	■ 0.5510
b	■ 0.6800	■ 0.4870
c	■ 0.7540	■ 0.5360
d	■ 0.7310	■ 0.5210
e	■ 0.6750	■ 0.5140
f	■ 0.6350	■ 0.4820
g	■ 0.8010	■ 0.5550
h	■ 0.7420	■ 0.5310
i	■ 0.8020	■ 0.5700
j	■ 0.6300	■ 0.5010

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	▬ 0.6760	▬ 0.5330
l	▬ 0.7690	▬ 0.5560
m	▬ 0.6440	▬ 0.5010
n	▬ 0.6510	▬ 0.5010
o	▬ 0.7200	▬ 0.5290
p	▬ 0.7540	▬ 0.5310
r	▬ 0.8250	▬ 0.5740
s	▬ 0.7560	▬ 0.5430
u	▬ 0.7340	▬ 0.5250
v	▬ 0.6180	▬ 0.4730
w	▬ 0.7030	▬ 0.5210