Full wwPDB EM Validation Report (i)

Jun 22, 2023 – 10:36 AM JST

PDB ID	:	7W1O
EMDB ID	:	EMD-32253
Title	:	Deactive state CI from Q10-NADH dataset, Subclass 1
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-19
Resolution	:	3.50 Å(reported)

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

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

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

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

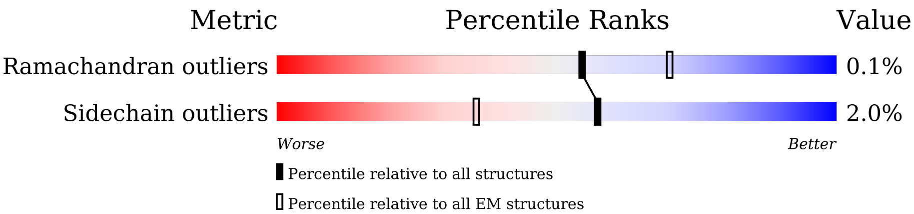
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	431	14% / 100%
2	B	176	• / 98% •
3	C	156	• / 98% •
4	E	115	13% / 99% •
5	F	86	24% / 97% •
6	G	88	57% / 98% •
6	X	88	25% / 95% 5%
7	H	112	16% / 97% •
8	I	112	17% / 84% • 13%

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Mol	Chain	Length	Quality of chain
9	J	341	13% 85% • 13%
10	K	42	14% 93% 7%
11	L	125	9% 98% •
12	M	690	7% 98% •
13	N	144	19% 98% •
14	O	217	18% 99% •
15	P	208	• 98% •
16	Q	430	7% 95% • •
17	S	70	• 99% •
18	T	96	10% 98% ••
19	U	83	19% 100%
20	V	140	50% 98% •
21	W	142	8% 96% •
22	Y	70	34% 94% 6%
23	Z	84	40% 99% •
24	a	140	7% 98% •
25	b	126	18% 80% • 18%
26	c	156	13% 99% •
27	d	175	13% 99% •
28	e	107	17% 95% • •
29	f	42	14% 98% •
30	g	121	7% 99% •
31	h	105	11% 100%
32	i	347	• 99% •
33	j	113	19% 85% • 12%

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Mol	Chain	Length	Quality of chain
34	k	98	27% 97% •
35	l	603	8% 98% •
36	m	175	19% 71% • 26%
37	n	56	27% 100%
38	o	128	12% 99% •
39	p	178	12% 97% •
40	r	459	• 99% •
41	s	318	6% 94% • 5%
42	u	171	9% 98% •
43	v	125	33% 92% 7% •
44	w	320	16% 99% •

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 66536 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
1	A	431	Total 3315	C 2094	N 590	O 611	S 20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total 1405	C 881	N 243	O 268	S 13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total 1239	C 790	N 224	O 211	S 14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total 959	C 614	N 176	O 164	S 5	0	0

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

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0
6	X	88	697	448	103	141	5	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	297	2337	1502	419	408	8	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total 1668	C 1064	N 280	O 314	S 10	0	0

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total 1731	C 1121	N 298	O 310	S 2	0	0

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total 3362	C 2155	N 578	O 605	S 24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total 560	C 359	N 104	O 92	S 5	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1167	752	200	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	600	393	98	108	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	879	573	158	147	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 1441	C 903	N 260	O 270	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 889	C 568	N 145	O 172	S 4	0	0

- Molecule 29 is a protein called Complex I-KFYI.

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 2707	C 1781	N 419	O 461	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	4784	3173	741	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	951	637	138	168	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	479	311	88	79	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	1045	679	182	184	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total 3628	C 2411	N 571	O 608	S 38	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total 1378	C 878	N 244	O 246	S 10	0	0

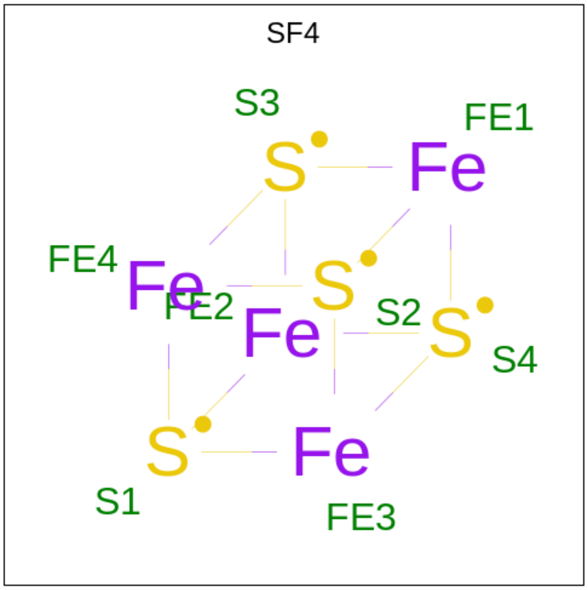
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total 1012	C 633	N 188	O 182	S 9	0	0

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

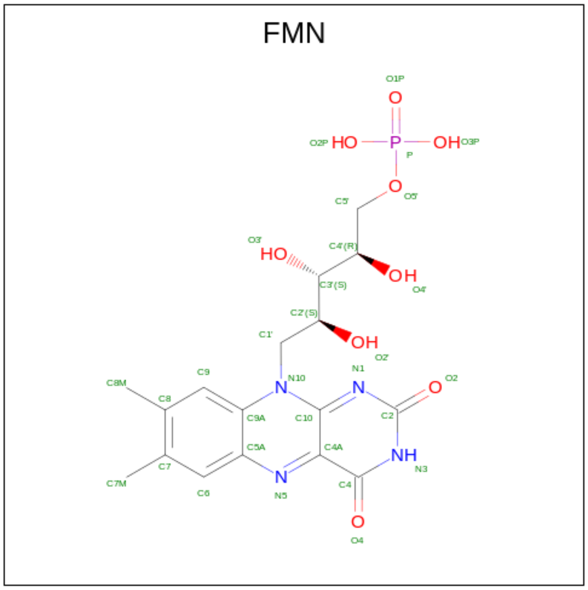
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total 2583	C 1646	N 437	O 491	S 9	0	0

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



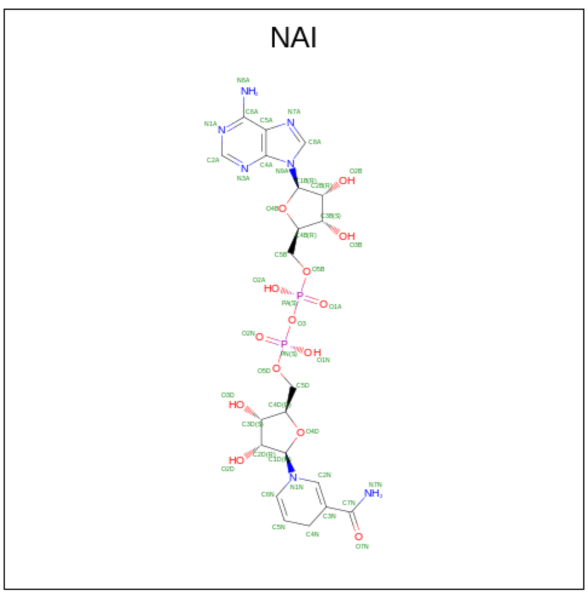
Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total Fe S 8 4 4	0
45	B	1	Total Fe S 8 4 4	0
45	B	1	Total Fe S 8 4 4	0
45	C	1	Total Fe S 8 4 4	0
45	M	1	Total Fe S 8 4 4	0
45	M	1	Total Fe S 8 4 4	0

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



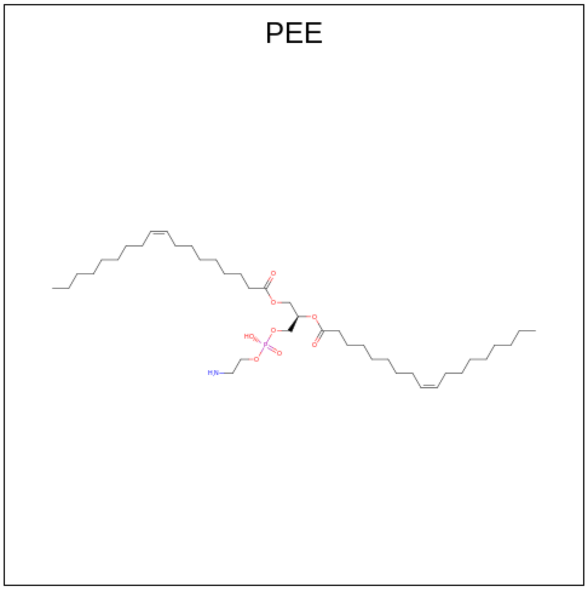
Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 31 17 4 9 1	0

- 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).



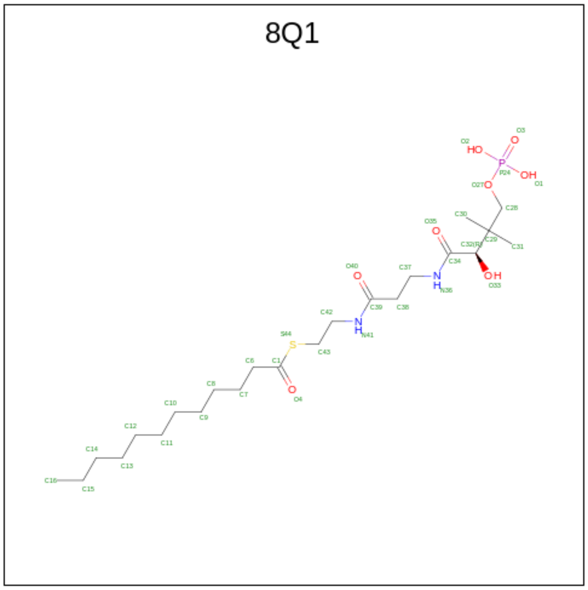
Mol	Chain	Residues	Atoms	AltConf
47	A	1	Total C N O P 44 21 7 14 2	0

- 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).



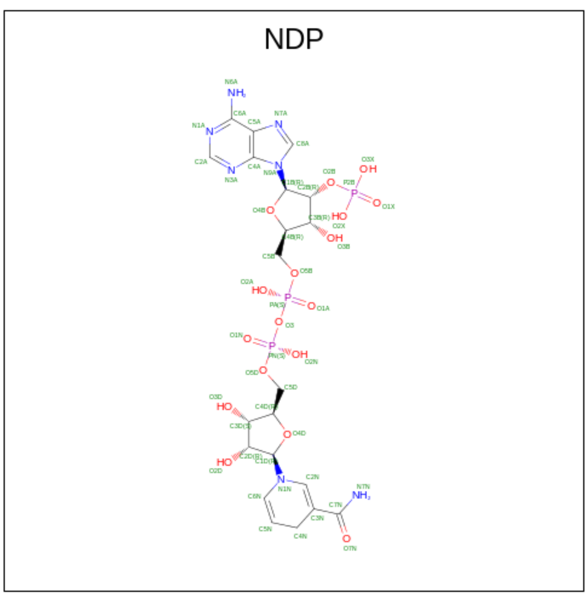
Mol	Chain	Residues	Atoms	AltConf
48	B	1	Total C N O P 51 41 1 8 1	0
48	Q	1	Total N 1 1	0
48	V	1	Total C N O P 40 30 1 8 1	0
48	j	1	Total N 1 1	0
48	j	1	Total C N O P 51 41 1 8 1	0
48	l	1	Total C N O P 46 36 1 8 1	0
48	l	1	Total C N O P 46 36 1 8 1	0
48	m	1	Total C N O P 41 31 1 8 1	0
48	r	1	Total C N O P 51 41 1 8 1	0

- Molecule 49 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).



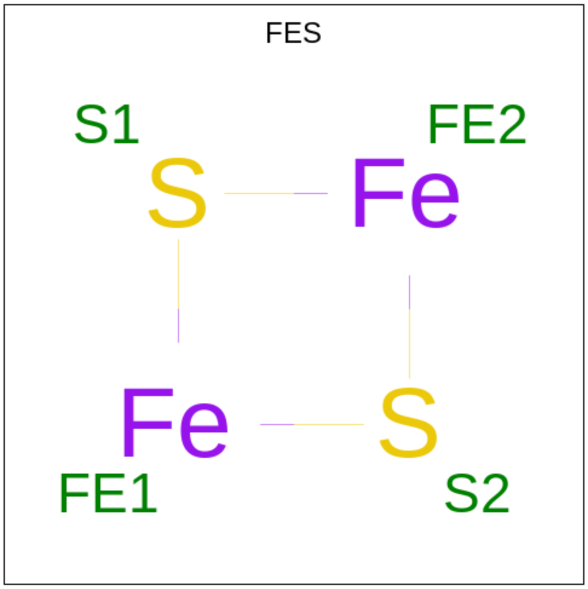
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total 35	C 23	N 2	O 8	P 1	S 1	0
49	X	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 51 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
51	M	1	Total Fe S 4 2 2	0
51	O	1	Total Fe S 4 2 2	0

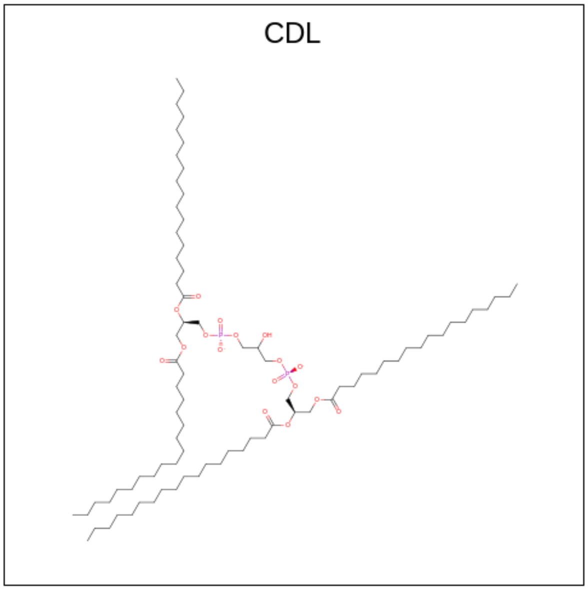
- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

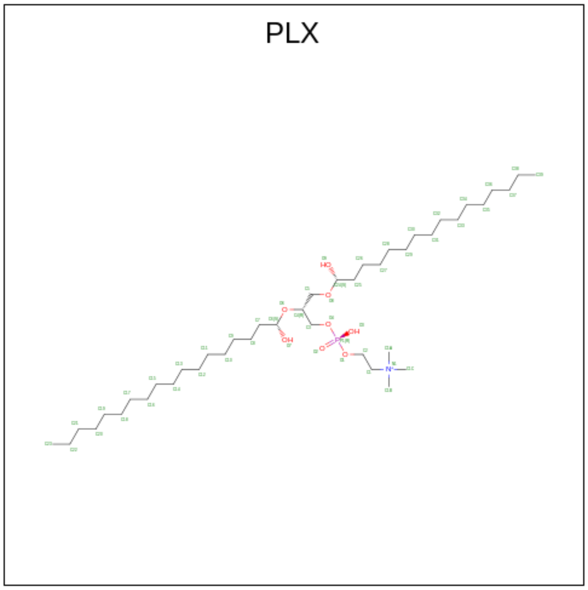
Mol	Chain	Residues	Atoms	AltConf
53	T	1	Total Zn 1 1	0

- Molecule 54 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



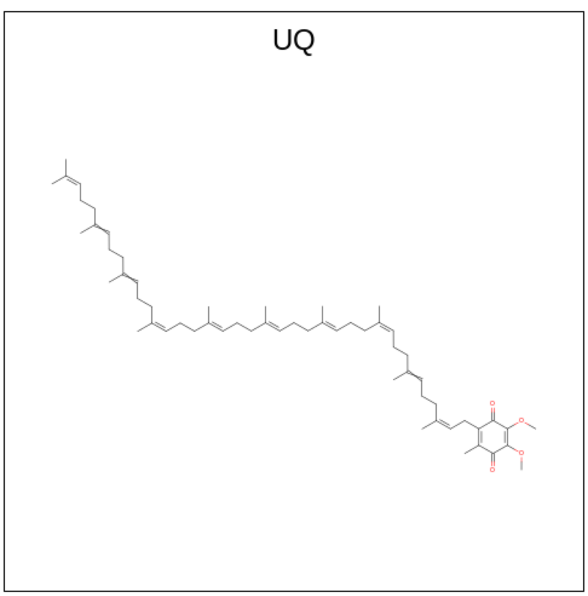
Mol	Chain	Residues	Atoms	AltConf
54	V	1	Total C O P 94 75 17 2	0
54	V	1	Total C O P 68 49 17 2	0
54	a	1	Total C O P 91 72 17 2	0
54	g	1	Total C O P 97 78 17 2	0
54	i	1	Total C O P 66 47 17 2	0
54	l	1	Total C O P 99 80 17 2	0
54	l	1	Total C O P 100 81 17 2	0
54	u	1	Total C O P 78 59 17 2	0

- Molecule 55 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).



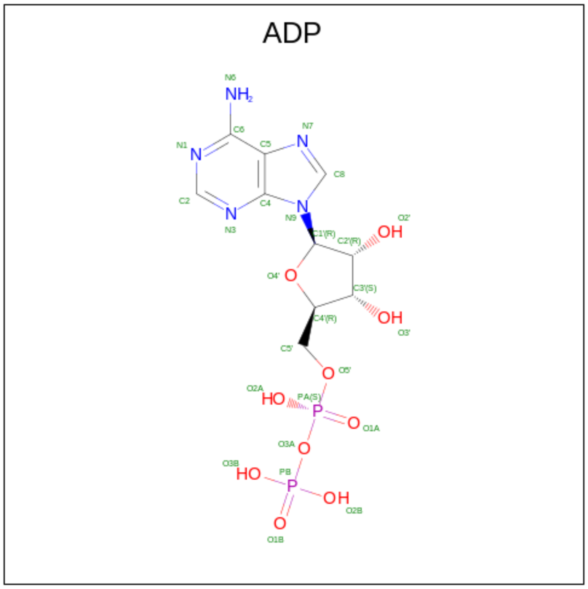
Mol	Chain	Residues	Atoms					AltConf
55	a	1	Total 52	C 42	N 1	O 8	P 1	0
55	g	1	Total 52	C 42	N 1	O 8	P 1	0
55	j	1	Total 52	C 42	N 1	O 8	P 1	0
55	r	1	Total 52	C 42	N 1	O 8	P 1	0

- 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
56	s	1	Total 28	C 24	O 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).



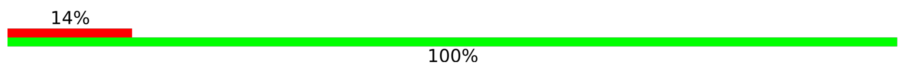
Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total 27	C 10	N 5	O 10	P 2	0

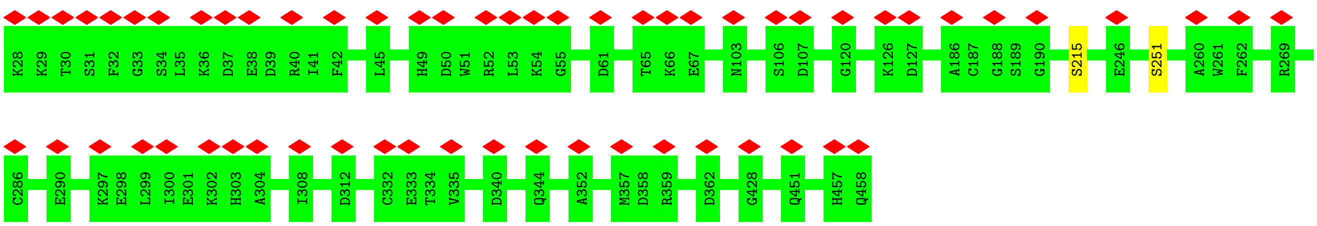
3 Residue-property plots (i)

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

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

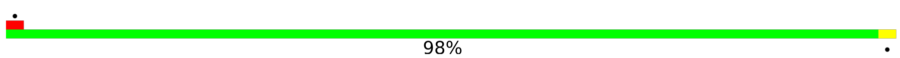
Chain A:

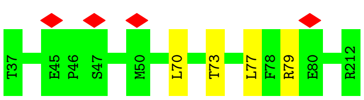




- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

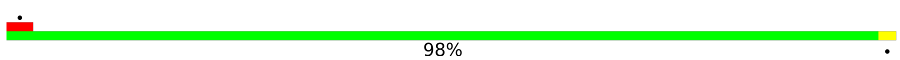
Chain B:

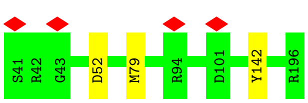




- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

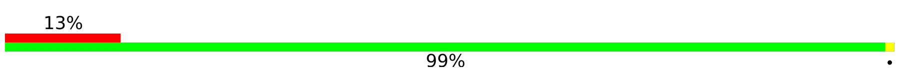
Chain C:

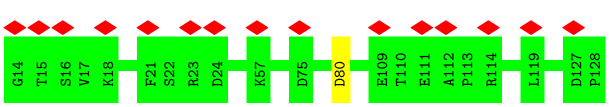




- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

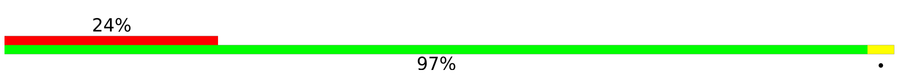
Chain E:





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

Chain F:



L14 R17 L23 C24 Q25 R26 S27 R34 D35 F36 I37 E38 E43 L51 P52 I53 S59 D60 V61 Q62 A84 R89 E92 L95 S96 G97 K98 A99

• Molecule 6: Acyl carrier protein

Chain G: 57% 98% •

S69 D70 A71 P72 P73 L74 E77 A78 I79 K80 D81 R82 V83 L84 K88 L89 Y90 D91 K92 I93 D94 P95 E96 K97 L98 N101 S102 K106 D107 L108 G109 L110 D111 M122 E123 D124 F128 E129 D132 I133 D134 A135 E136 K137 Q142 E143 I144 V145 D146 Y147 I148 A149

D150 K151 K152 D153 V154 Y155 E156

• Molecule 6: Acyl carrier protein

Chain X: 25% 95% 5%

S69 D70 A71 P72 P73 L74 E77 D91 D94 P95 E96 M105 K106 D107 D114 D124 E129 D132 I133 D134 M139 D146 D150 D153 E156

• Molecule 7: Complex I subunit B13

Chain H: 16% 97% •

L5 K6 K7 A15 V16 C17 E18 E22 R23 L24 N41 Y44 I51 M58 E62 P63 D64 V65 K66 G74 I77 E78 E79 L95 W100 E101 P102 I116

• Molecule 8: Complex I-B14.5a

Chain I: 17% 84% • 13%

A2 S3 A4 T5 R6 V7 L10 L11 R18 D19 N51 R61 M64 Q73 K74 VAL LEU ALA SER GLY LYS PRO ALA GLU SER SER ALA VAL ALA GLU T90 E91 K92 K102 R103 W104 E105 D109 L113

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

Chain J: 13% 85% • 13%

L36 H37 H38 W108 N109 G110 K111 D114 K137 E142 I148 D173 I174 K175 S178 R179 K184 G187 G208 D211 R212 R221 TRP PHE GLY GLY VAL PRO LEU ILE SER L231 G232 K233 E234 D257 D275 L276 V277 Q278 A282 R286 P287 F288

LEU PRO TYR PRO LEU PRO HIS PHE ALA TYR ARG TRP VAL GLY ARG LEU PHE GLU VAL SER PRO PHE GLU PRO TRP T314 T315 R321 V322 D326 M327 T328 L329 P330 H331 Q341 E346 E351 R357 T358 TYR ARG TRP LEU THR SER GLU MET GLU ASP V369 K370 P371 A372

K373 T374 V375 N376

• Molecule 10: Complex I-9kD

Chain K: 14% 93% 7%

D69 T72 Y73 R74 N75 L76 H79 S82 L87 S103 R109 H110

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

Chain L: 9% 98% •

Q51 L52 I53 A54 V55 D56 E57 K58 L59 D60 E69 D146 K154 K175

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

Chain M: 7% 98% •

S29 N30 M58 M117 L126 D127 I130 D162 D194 M213 E310 K311 L330 D337 G343 D362 S363 D364 E370 A375 G376 A377 T405 E410 D426 R441 Y442 D443 S448 H460 E468 S479 L502 S503 S504 G505 V506

T507 K539 L560 P561 K562 D563 D581 Y636 E648 E660 G661 A662 N663 A668 L674 V675 N676 Q677 Q678 A681 D682 G717 I718

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

Chain N: 19% 98% •

E2 L3 V4 Q5 V6 L7 R8 R9 Q12 Q13 V14 S15 G16 H17 G18 G19 L20 R21 G22 Y23 L24 F28 N31 D32 K47 N52 R71 D78 D95 D96 K133 K145

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

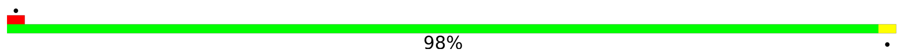
Chain O: 18% 99% •

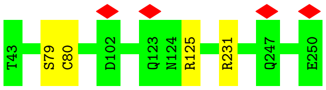
G33 A34 G35 G36 A37 R42 D43 D50 E58 D84 H131 M141 E150 K159 M185 D190 D195 L196 T197 P198 K199 D200 I201 E202 I205 D206 E207 A210 G211 K212 I213 P214 K215 S220 A228 G229 G230 S233 L234 T235 E236 K239 G240

F243 A247 G248 L249

• Molecule 15: Complex I-30kD

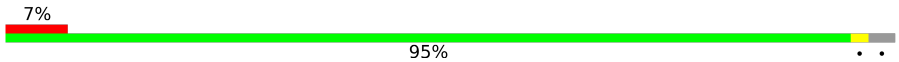
Chain P:

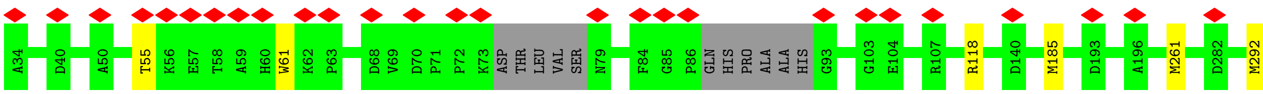


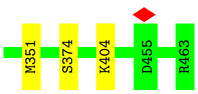


- Molecule 16: Complex I-49kD

Chain Q:

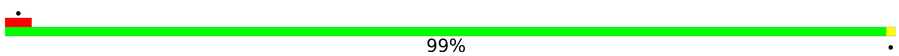


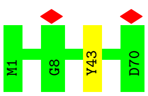




- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

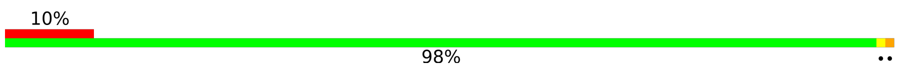
Chain S:

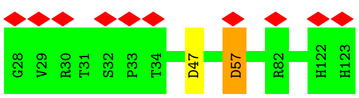




- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

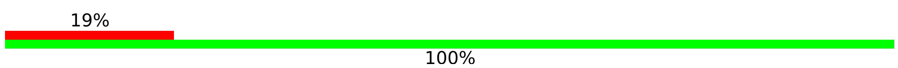
Chain T:

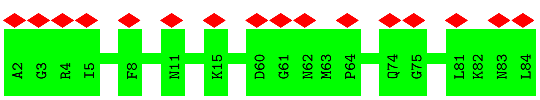




- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

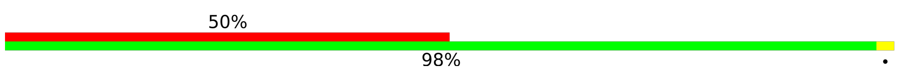
Chain U:

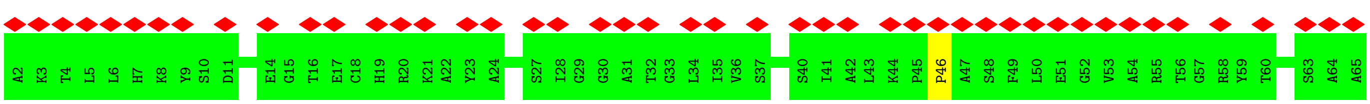


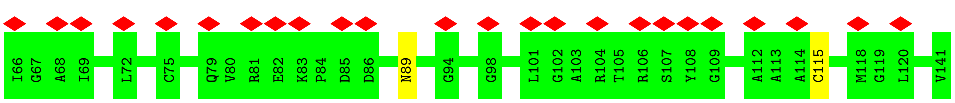


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

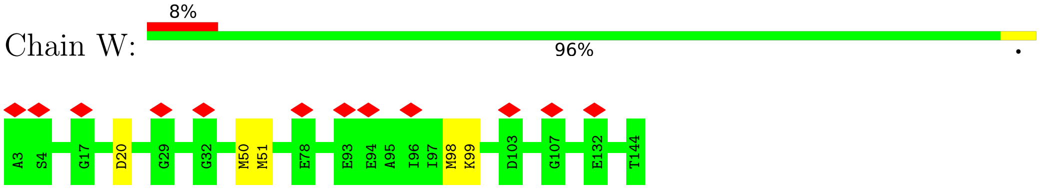
Chain V:



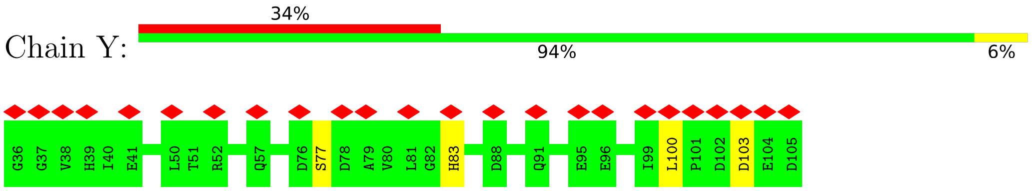




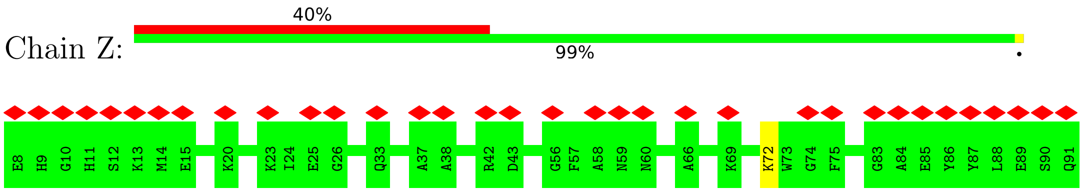
• Molecule 21: Complex I-B16.6



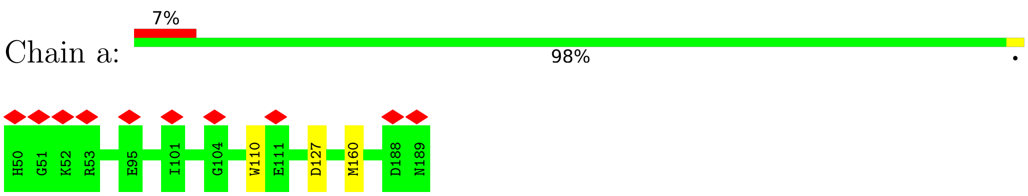
• Molecule 22: Complex I-AGGG



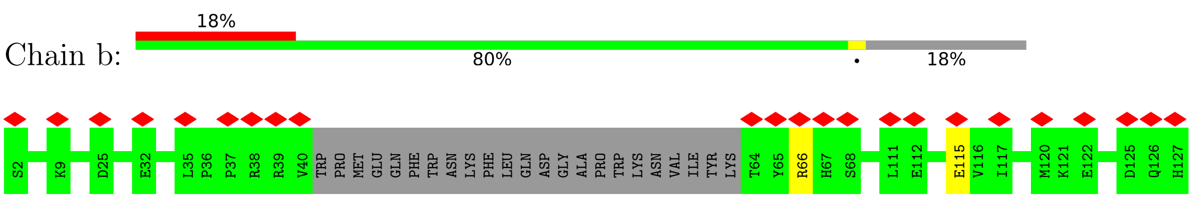
• Molecule 23: Complex I-B12



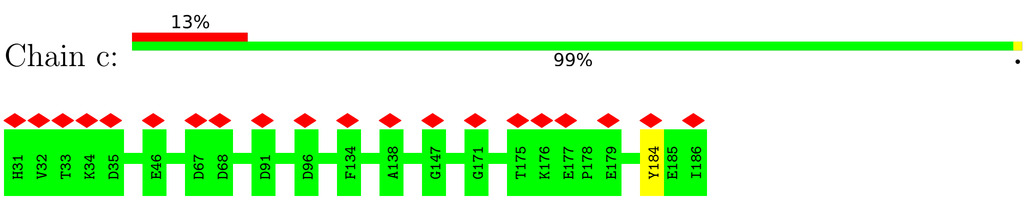
• Molecule 24: Complex I-SGDH



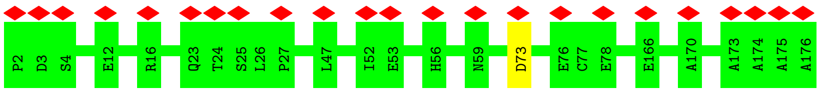
• Molecule 25: Complex I-B17



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

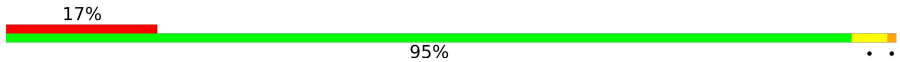


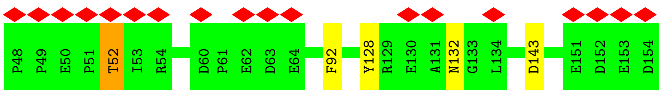
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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

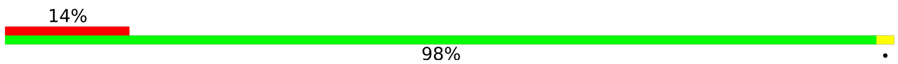
Chain e:

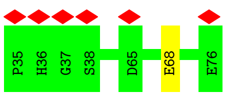




• Molecule 29: Complex I-KFYI

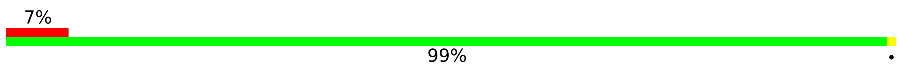
Chain f:

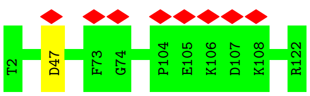




• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

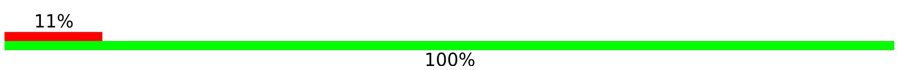
Chain g:

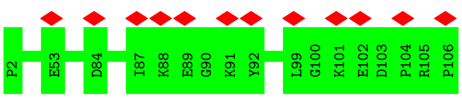




• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

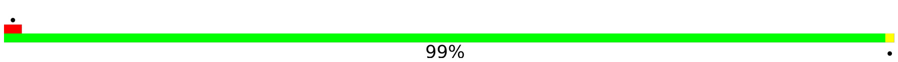
Chain h:

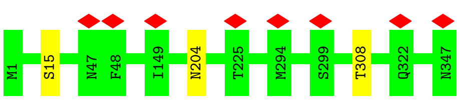




• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

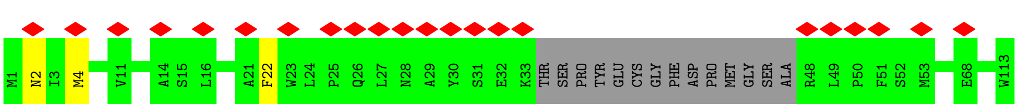
Chain i:





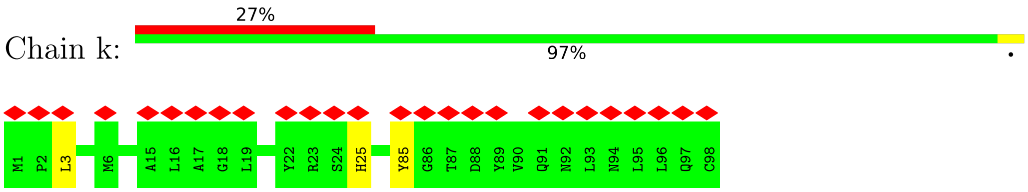
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:



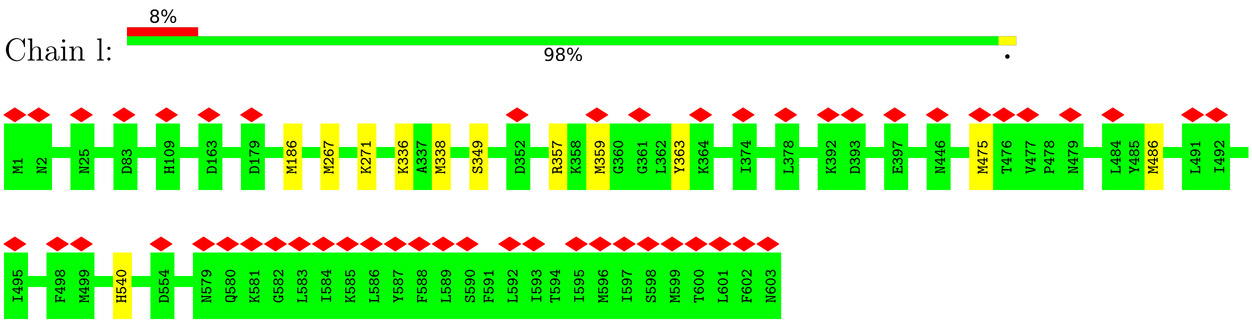
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:



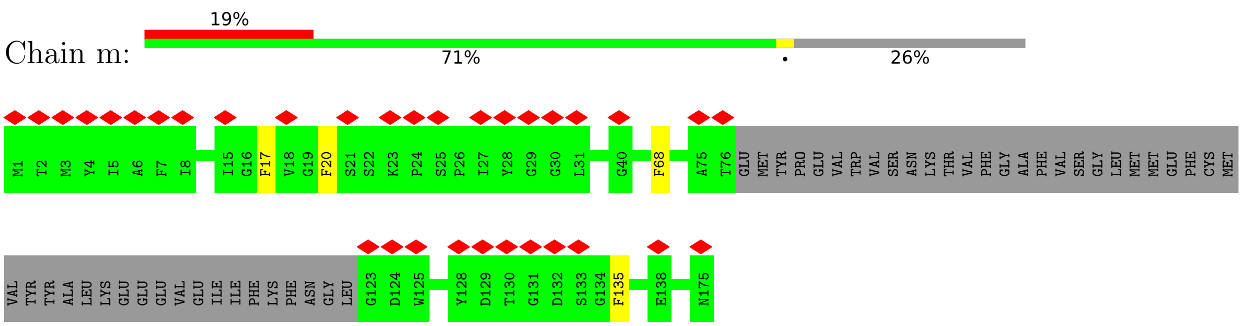
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:



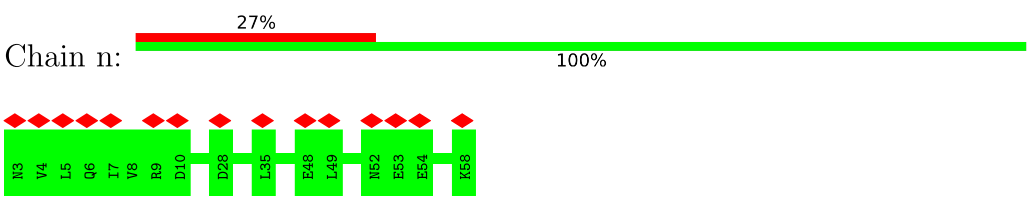
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:



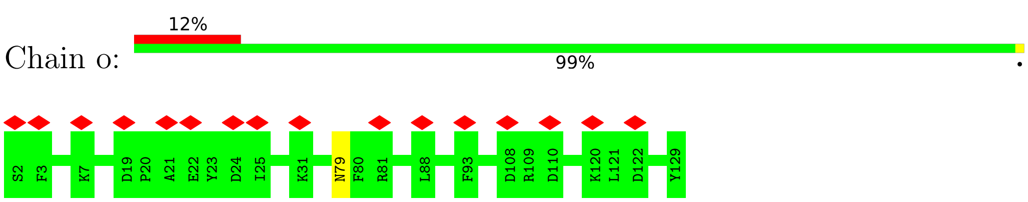
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:



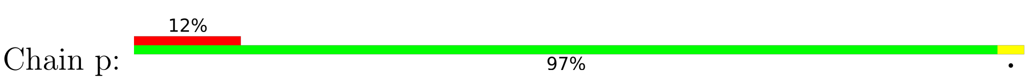
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

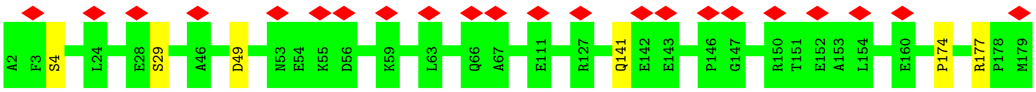
Chain o:



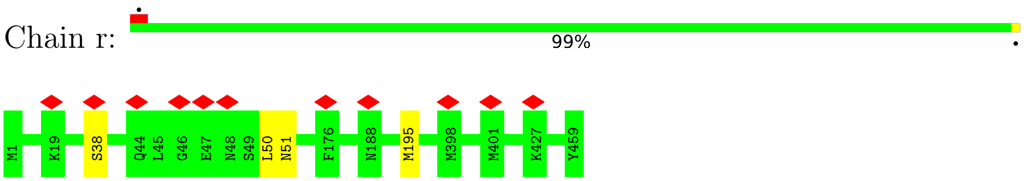
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:

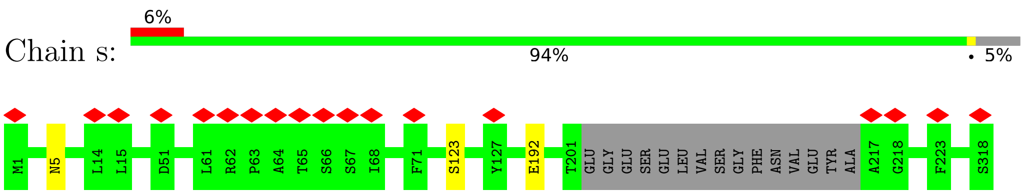




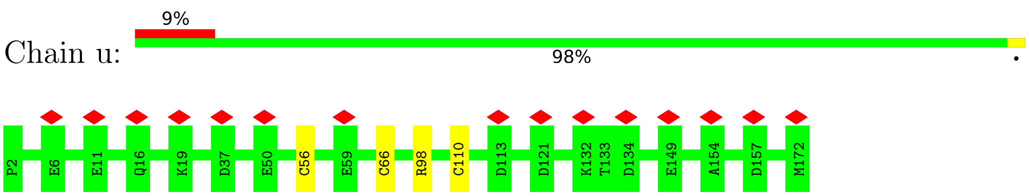
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4



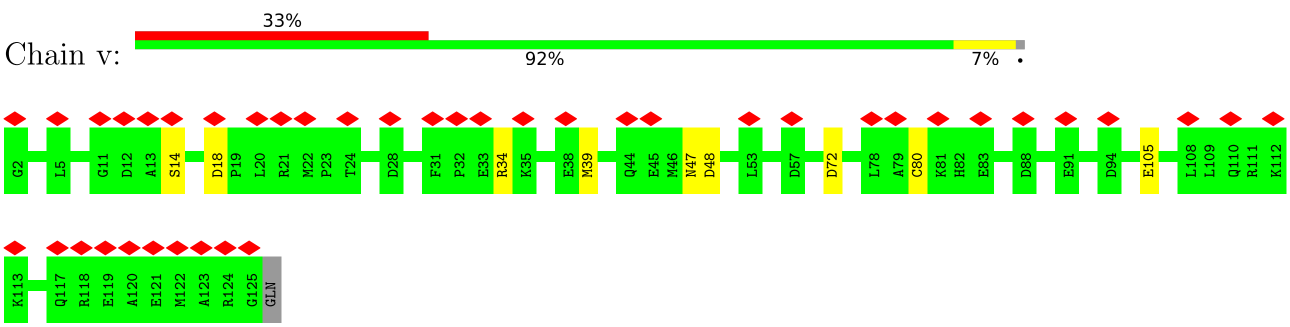
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



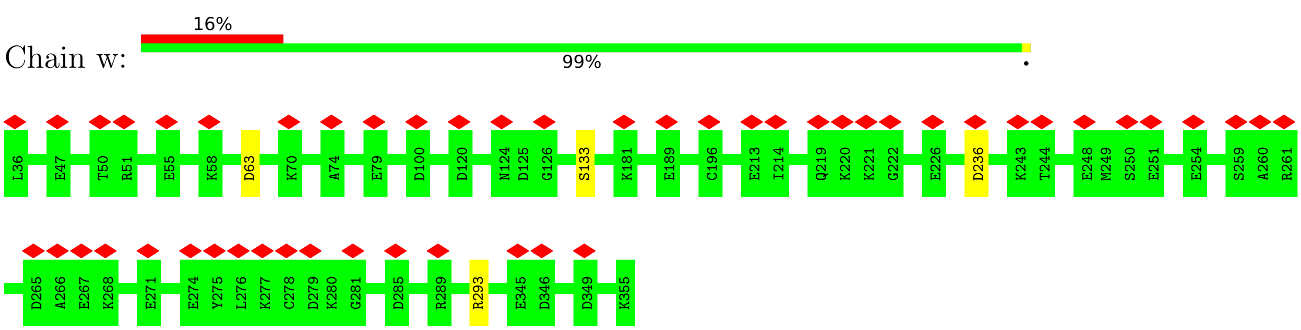
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24886	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	0.239	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0267	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0/3390	0.52	0/4580
2	B	0.27	0/1435	0.53	0/1941
3	C	0.28	0/1270	0.53	0/1719
4	E	0.26	0/983	0.54	0/1325
5	F	0.30	0/702	0.61	0/945
6	G	0.28	0/705	0.53	0/956
6	X	0.30	0/709	0.52	0/960
7	H	0.30	0/929	0.53	0/1258
8	I	0.27	0/798	0.55	0/1079
9	J	0.26	0/2388	0.53	0/3225
10	K	0.25	0/365	0.52	0/493
11	L	0.27	0/1039	0.55	0/1403
12	M	0.26	0/5384	0.52	0/7295
13	N	0.26	0/1245	0.53	0/1694
14	O	0.27	0/1708	0.51	0/2324
15	P	0.28	0/1782	0.54	0/2427
16	Q	0.28	0/3436	0.52	0/4653
17	S	0.27	0/575	0.53	0/774
18	T	0.26	0/755	0.55	1/1018 (0.1%)
19	U	0.28	0/664	0.51	0/912
20	V	0.28	0/1042	0.50	0/1411
21	W	0.28	0/1198	0.52	0/1617
22	Y	0.30	0/626	0.59	0/857
23	Z	0.28	0/695	0.51	0/939
24	a	0.28	0/1199	0.52	0/1623
25	b	0.30	0/906	0.57	0/1232
26	c	0.29	0/1367	0.53	0/1870
27	d	0.27	0/1473	0.55	0/1989
28	e	0.29	0/915	0.55	0/1245
29	f	0.26	0/350	0.43	0/473
30	g	0.29	0/1031	0.53	1/1394 (0.1%)
31	h	0.27	0/889	0.52	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.27	0/2770	0.49	0/3764
33	j	0.30	0/819	0.55	0/1117
34	k	0.27	0/759	0.52	1/1029 (0.1%)
35	l	0.28	0/4913	0.50	0/6682
36	m	0.29	0/973	0.48	0/1320
37	n	0.25	0/491	0.53	0/663
38	o	0.28	0/1074	0.55	0/1457
39	p	0.28	0/1590	0.55	0/2155
40	r	0.27	0/3720	0.50	0/5074
41	s	0.28	0/2464	0.49	0/3369
42	u	0.26	0/1416	0.50	0/1913
43	v	0.29	0/1036	0.56	0/1393
44	w	0.27	0/2643	0.50	0/3580
All	All	0.28	0/66621	0.52	3/90337 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	k	3	LEU	CA-CB-CG	5.37	127.65	115.30
18	T	57	ASP	CB-CG-OD1	5.32	123.08	118.30
30	g	47	ASP	CB-CG-OD1	5.27	123.04	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	414 (96%)	15 (4%)	0	100	100
2	B	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/341 (85%)	267 (92%)	20 (7%)	2 (1%)	22	61
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
12	M	688/690 (100%)	663 (96%)	24 (4%)	1 (0%)	51	84
13	N	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	186 (90%)	19 (9%)	1 (0%)	29	68
16	Q	412/430 (96%)	399 (97%)	11 (3%)	2 (0%)	29	68
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	61
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	97 (98%)	2 (2%)	0	100	100
26	c	154/156 (99%)	141 (92%)	13 (8%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	98 (93%)	6 (6%)	1 (1%)	15	54
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	328 (95%)	17 (5%)	0	100	100
33	j	95/113 (84%)	91 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
35	l	601/603 (100%)	567 (94%)	34 (6%)	0	100	100
36	m	125/175 (71%)	109 (87%)	16 (13%)	0	100	100
37	n	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	25	64
40	r	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
41	s	299/318 (94%)	279 (93%)	20 (7%)	0	100	100
42	u	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
43	v	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	301 (95%)	17 (5%)	0	100	100
All	All	8029/8309 (97%)	7637 (95%)	383 (5%)	9 (0%)	54	84

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	357	ARG
28	e	52	THR
15	P	125	ARG
12	M	126	LEU
16	Q	61	TRP
20	V	46	PRO
9	J	38	HIS
16	Q	404	LYS
39	p	174	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/345 (100%)	342 (99%)	2 (1%)	86	94
2	B	150/151 (99%)	146 (97%)	4 (3%)	44	73
3	C	130/132 (98%)	127 (98%)	3 (2%)	50	77
4	E	103/107 (96%)	102 (99%)	1 (1%)	76	88
5	F	76/76 (100%)	73 (96%)	3 (4%)	32	64
6	G	76/81 (94%)	74 (97%)	2 (3%)	46	74
6	X	76/81 (94%)	72 (95%)	4 (5%)	22	55
7	H	99/99 (100%)	96 (97%)	3 (3%)	41	71
8	I	87/97 (90%)	84 (97%)	3 (3%)	37	68
9	J	248/295 (84%)	242 (98%)	6 (2%)	49	76
10	K	41/41 (100%)	38 (93%)	3 (7%)	14	45
11	L	113/113 (100%)	111 (98%)	2 (2%)	59	81
12	M	580/580 (100%)	570 (98%)	10 (2%)	60	82
13	N	130/130 (100%)	127 (98%)	3 (2%)	50	77
14	O	182/183 (100%)	180 (99%)	2 (1%)	73	88
15	P	188/190 (99%)	185 (98%)	3 (2%)	62	83
16	Q	357/370 (96%)	351 (98%)	6 (2%)	60	82
17	S	56/58 (97%)	55 (98%)	1 (2%)	59	81
18	T	79/79 (100%)	77 (98%)	2 (2%)	47	75
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	99 (98%)	2 (2%)	55	79
21	W	122/123 (99%)	117 (96%)	5 (4%)	30	63
22	Y	63/63 (100%)	59 (94%)	4 (6%)	18	51
23	Z	65/65 (100%)	64 (98%)	1 (2%)	65	84
24	a	122/122 (100%)	119 (98%)	3 (2%)	47	75
25	b	98/119 (82%)	96 (98%)	2 (2%)	55	79
26	c	140/141 (99%)	139 (99%)	1 (1%)	84	93
27	d	151/155 (97%)	150 (99%)	1 (1%)	84	93
28	e	98/99 (99%)	93 (95%)	5 (5%)	24	57
29	f	35/38 (92%)	34 (97%)	1 (3%)	42	71
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	310/311 (100%)	307 (99%)	3 (1%)	76	88
33	j	88/99 (89%)	85 (97%)	3 (3%)	37	68
34	k	85/85 (100%)	83 (98%)	2 (2%)	49	76
35	l	536/537 (100%)	524 (98%)	12 (2%)	52	78
36	m	99/141 (70%)	95 (96%)	4 (4%)	31	64
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	109/113 (96%)	108 (99%)	1 (1%)	78	90
39	p	159/159 (100%)	154 (97%)	5 (3%)	40	70
40	r	409/410 (100%)	405 (99%)	4 (1%)	76	88
41	s	263/275 (96%)	260 (99%)	3 (1%)	73	88
42	u	148/153 (97%)	144 (97%)	4 (3%)	44	73
43	v	101/112 (90%)	92 (91%)	9 (9%)	9	37
44	w	281/283 (99%)	277 (99%)	4 (1%)	67	85
All	All	7021/7235 (97%)	6879 (98%)	142 (2%)	57	79

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	SER
1	A	251	SER
2	B	70	LEU
2	B	73	THR
2	B	77	LEU
2	B	79	ARG
3	C	52	ASP
3	C	79	MET
3	C	142	TYR
4	E	80	ASP
5	F	23	LEU
5	F	36	PHE
5	F	38	GLU
6	G	90	TYR
6	G	132	ASP
7	H	17	CYS
7	H	44	TYR
7	H	100	TRP
8	I	51	ASN

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Mol	Chain	Res	Type
8	I	61	ARG
8	I	64	MET
9	J	108	TRP
9	J	109	ASN
9	J	212	ARG
9	J	278	GLN
9	J	288	PHE
9	J	327	MET
10	K	74	ARG
10	K	103	SER
10	K	109	ARG
11	L	60	ASP
11	L	146	ASP
12	M	58	MET
12	M	117	MET
12	M	127	ASP
12	M	130	ILE
12	M	213	MET
12	M	426	ASP
12	M	448	SER
12	M	460	HIS
12	M	479	SER
12	M	636	TYR
13	N	47	LYS
13	N	52	ASN
13	N	71	ARG
14	O	42	ARG
14	O	195	ASP
15	P	79	SER
15	P	80	CYS
15	P	231	ARG
16	Q	55	THR
16	Q	185	MET
16	Q	261	MET
16	Q	292	MET
16	Q	351	MET
16	Q	374	SER
17	S	43	TYR
18	T	47	ASP
18	T	57	ASP
20	V	89	ASN
20	V	115	CYS

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Mol	Chain	Res	Type
21	W	20	ASP
21	W	50	MET
21	W	51	MET
21	W	98	MET
21	W	99	LYS
6	X	107	ASP
6	X	114	ASP
6	X	129	GLU
6	X	139	MET
22	Y	77	SER
22	Y	83	HIS
22	Y	100	LEU
22	Y	103	ASP
23	Z	72	LYS
24	a	110	TRP
24	a	127	ASP
24	a	160	MET
25	b	66	ARG
25	b	115	GLU
26	c	184	TYR
27	d	73	ASP
28	e	52	THR
28	e	92	PHE
28	e	128	TYR
28	e	132	ASN
28	e	143	ASP
29	f	68	GLU
32	i	15	SER
32	i	204	ASN
32	i	308	THR
33	j	2	ASN
33	j	4	MET
33	j	22	PHE
34	k	25	HIS
34	k	85	TYR
35	l	186	MET
35	l	267	MET
35	l	271	LYS
35	l	336	LYS
35	l	338	MET
35	l	349	SER
35	l	357	ARG

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Mol	Chain	Res	Type
35	l	359	MET
35	l	363	TYR
35	l	475	MET
35	l	486	MET
35	l	540	HIS
36	m	17	PHE
36	m	20	PHE
36	m	68	PHE
36	m	135	PHE
38	o	79	ASN
39	p	4	SER
39	p	29	SER
39	p	49	ASP
39	p	141	GLN
39	p	177	ARG
40	r	38	SER
40	r	50	LEU
40	r	51	ASN
40	r	195	MET
41	s	5	ASN
41	s	123	SER
41	s	192	GLU
42	u	56	CYS
42	u	66	CYS
42	u	98	ARG
42	u	110	CYS
43	v	14	SER
43	v	18	ASP
43	v	34	ARG
43	v	39	MET
43	v	47	ASN
43	v	48	ASP
43	v	72	ASP
43	v	80	CYS
43	v	105	GLU
44	w	63	ASP
44	w	133	SER
44	w	236	ASP
44	w	293	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
7	H	21	HIS
8	I	25	GLN
9	J	37	HIS
10	K	77	GLN
12	M	425	ASN
22	Y	83	HIS
24	a	132	ASN
26	c	154	GLN
26	c	183	HIS
27	d	23	GLN
32	i	347	ASN
39	p	62	GLN
40	r	44	GLN
40	r	51	ASN
41	s	5	ASN
43	v	47	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	6.32	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.61	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	13.00	131.40	119.48
16	Q	118	2MR	CD-NE-CZ	4.76	132.32	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.73	129.91	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 2 are modelled with single atom and 2 are monoatomic - leaving 34 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
56	UQ	s	401	-	28,28,63	3.30	7 (25%)	34,37,79	2.99	11 (32%)
54	CDL	u	201	-	77,77,99	1.19	8 (10%)	83,89,111	0.94	4 (4%)
47	NAI	A	503	-	42,48,48	4.97	19 (45%)	47,73,73	1.29	5 (10%)
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.46	4 (13%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.02	2 (3%)
54	CDL	l	701	-	98,98,99	1.08	8 (8%)	104,110,111	0.93	5 (4%)
48	PEE	V	203	-	39,39,50	1.31	6 (15%)	41,44,55	1.02	2 (4%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.22	8 (16%)
48	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
50	NDP	J	401	-	45,52,52	4.58	20 (44%)	53,80,80	1.93	9 (16%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.56	8 (20%)
54	CDL	V	202	-	67,67,99	1.25	9 (13%)	73,79,111	1.00	4 (5%)
55	PLX	r	502	-	51,51,51	1.14	3 (5%)	55,59,59	0.65	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
45	SF4	M	802	12	0,12,12	-	-	-		
55	PLX	j	203	-	51,51,51	1.16	4 (7%)	55,59,59	0.58	1 (1%)
54	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.91	4 (4%)
54	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
54	CDL	i	401	-	65,65,99	1.27	8 (12%)	71,77,111	1.03	5 (7%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.96	2 (4%)
55	PLX	a	202	-	51,51,51	1.16	5 (9%)	55,59,59	0.62	1 (1%)
51	FES	M	803	12	0,4,4	-	-	-		
45	SF4	C	301	3,16	0,12,12	-	-	-		
54	CDL	a	201	-	90,90,99	1.12	8 (8%)	96,102,111	0.94	4 (4%)
54	CDL	g	202	-	96,96,99	1.10	8 (8%)	102,108,111	0.85	4 (3%)
51	FES	O	301	14	0,4,4	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
49	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.60	5 (12%)
55	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.63	1 (1%)
48	PEE	j	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
48	PEE	m	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.04	3 (6%)

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
56	UQ	s	401	-	-	12/21/45/87	0/1/1/1
54	CDL	u	201	-	-	42/88/88/110	-
47	NAI	A	503	-	-	7/25/72/72	0/5/5/5
57	ADP	w	401	-	-	2/12/32/32	0/3/3/3
48	PEE	B	303	-	-	28/54/54/54	-
54	CDL	l	701	-	-	56/109/109/110	-
48	PEE	V	203	-	-	19/43/43/54	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
48	PEE	l	703	-	-	27/49/49/54	-
50	NDP	J	401	-	-	10/30/77/77	0/4/5/5
49	8Q1	X	201	-	-	7/41/41/41	-
45	SF4	B	301	2	-	-	0/6/5/5
54	CDL	V	202	-	-	45/78/78/110	-
55	PLX	r	502	-	-	35/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	r	501	-	-	22/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5
55	PLX	j	203	-	-	26/55/55/55	-
54	CDL	V	201	-	-	62/104/104/110	-
54	CDL	l	702	-	-	69/110/110/110	-
54	CDL	i	401	-	-	45/76/76/110	-
48	PEE	l	704	-	-	31/49/49/54	-
55	PLX	a	202	-	-	25/55/55/55	-
51	FES	M	803	12	-	-	0/1/1/1
45	SF4	B	302	2	-	-	0/6/5/5
54	CDL	a	201	-	-	50/101/101/110	-
45	SF4	C	301	3,16	-	-	0/6/5/5
54	CDL	g	202	-	-	60/107/107/110	-
51	FES	O	301	14	-	-	0/1/1/1
48	PEE	m	201	-	-	22/44/44/54	-
49	8Q1	G	201	6	-	18/41/41/41	-
55	PLX	g	201	-	-	21/55/55/55	-
48	PEE	j	202	-	-	28/54/54/54	-

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.29	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.56	1.30	1.53
50	J	401	NDP	C3B-C2B	-12.80	1.24	1.52
50	J	401	NDP	C6N-C5N	12.50	1.55	1.33
50	J	401	NDP	O4D-C4D	10.56	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.29	1.26	1.53
50	J	401	NDP	C3D-C4D	-9.85	1.27	1.53
56	s	401	UQ	C13-C14	9.27	1.55	1.33
56	s	401	UQ	C8-C9	9.07	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.82	1.30	1.53
50	J	401	NDP	O4B-C1B	8.56	1.53	1.41
56	s	401	UQ	C18-C19	8.22	1.56	1.32
47	A	503	NAI	O4B-C4B	-8.17	1.26	1.45
50	J	401	NDP	O4B-C4B	-7.87	1.27	1.45
57	w	401	ADP	O4'-C4'	7.78	1.62	1.45
50	J	401	NDP	C2N-C3N	7.53	1.56	1.34
47	A	503	NAI	C2D-C1D	-7.51	1.29	1.53
47	A	503	NAI	O4D-C4D	7.00	1.60	1.45
57	w	401	ADP	O4'-C1'	-6.85	1.31	1.41
47	A	503	NAI	C2D-C3D	5.99	1.69	1.53
47	A	503	NAI	C7N-N7N	5.79	1.48	1.33
50	J	401	NDP	P2B-O2B	5.74	1.70	1.59
47	A	503	NAI	O4D-C1D	5.59	1.55	1.42
49	G	201	8Q1	C34-N36	5.48	1.45	1.33
49	X	201	8Q1	C39-N41	5.43	1.45	1.33
49	X	201	8Q1	C34-N36	5.41	1.45	1.33
50	J	401	NDP	C3B-C4B	5.40	1.66	1.53
49	G	201	8Q1	C39-N41	5.33	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.03	1.40	1.49
50	J	401	NDP	C6N-N1N	4.96	1.49	1.37
50	J	401	NDP	O4D-C1D	-4.93	1.30	1.42
47	A	503	NAI	O2B-C2B	4.53	1.53	1.43
50	J	401	NDP	C7N-N7N	4.22	1.44	1.33
50	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
50	J	401	NDP	C6A-N6A	4.11	1.49	1.34
46	A	502	FMN	C4A-N5	4.01	1.38	1.30
47	A	503	NAI	C6N-C5N	3.97	1.40	1.33
57	w	401	ADP	C6-N6	3.79	1.47	1.34
48	r	501	PEE	C18-C19	3.75	1.53	1.31
48	l	704	PEE	C18-C19	3.75	1.53	1.31
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	l	703	PEE	C18-C19	3.74	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	V	203	PEE	C18-C19	3.73	1.53	1.31
48	j	202	PEE	C18-C19	3.73	1.53	1.31
48	m	201	PEE	C18-C19	3.72	1.53	1.31
47	A	503	NAI	C7N-C3N	3.69	1.56	1.48
48	l	704	PEE	C39-C38	3.66	1.53	1.31
48	j	202	PEE	C39-C38	3.65	1.53	1.31
48	V	203	PEE	C39-C38	3.65	1.52	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
48	l	703	PEE	C39-C38	3.63	1.52	1.31
47	A	503	NAI	C6A-N6A	3.61	1.47	1.34
54	i	401	CDL	OA8-CA7	3.52	1.43	1.33
54	l	702	CDL	OA8-CA7	3.48	1.43	1.33
54	a	201	CDL	OA8-CA7	3.45	1.43	1.33
54	u	201	CDL	OA8-CA7	3.42	1.43	1.33
54	V	202	CDL	OA8-CA7	3.39	1.43	1.33
54	V	201	CDL	OA8-CA7	3.39	1.43	1.33
54	g	202	CDL	OA8-CA7	3.36	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.34	1.40	1.48
54	l	701	CDL	OA8-CA7	3.33	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.33	1.35	1.43
50	J	401	NDP	C7N-C3N	3.11	1.55	1.48
54	a	201	CDL	OA6-CA5	3.09	1.43	1.34
54	l	702	CDL	OB6-CB5	3.09	1.43	1.34
50	J	401	NDP	O3D-C3D	3.09	1.50	1.43
57	w	401	ADP	O3'-C3'	3.08	1.50	1.43
54	V	201	CDL	OA6-CA5	3.08	1.43	1.34
54	g	202	CDL	OB6-CB5	3.06	1.42	1.34
54	u	201	CDL	OB6-CB5	3.05	1.42	1.34
54	i	401	CDL	OB6-CB5	3.02	1.42	1.34
54	V	201	CDL	OB6-CB5	3.02	1.42	1.34
54	g	202	CDL	OB8-CB7	3.01	1.42	1.33
54	V	202	CDL	OA6-CA5	3.00	1.42	1.34
54	V	201	CDL	OB8-CB7	2.99	1.42	1.33
54	g	202	CDL	OA6-CA5	2.99	1.42	1.34
54	l	702	CDL	OB8-CB7	2.99	1.42	1.33
54	u	201	CDL	OB8-CB7	2.99	1.42	1.33
54	i	401	CDL	OB8-CB7	2.99	1.42	1.33
54	V	202	CDL	OB6-CB5	2.99	1.42	1.34
54	l	701	CDL	OB8-CB7	2.97	1.42	1.33
54	a	201	CDL	OB6-CB5	2.95	1.42	1.34
54	V	202	CDL	OB8-CB7	2.95	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	l	701	CDL	OA6-CA5	2.94	1.42	1.34
55	r	502	PLX	O6-C4	-2.93	1.40	1.44
54	l	701	CDL	OB6-CB5	2.92	1.42	1.34
54	l	702	CDL	OA6-CA5	2.92	1.42	1.34
54	a	201	CDL	OB8-CB7	2.91	1.41	1.33
54	u	201	CDL	OA6-CA5	2.87	1.42	1.34
54	i	401	CDL	OA6-CA5	2.86	1.42	1.34
55	a	202	PLX	O6-C4	-2.83	1.40	1.44
55	g	201	PLX	O6-C4	-2.77	1.40	1.44
56	s	401	UQ	C6-C1	2.74	1.54	1.46
55	j	203	PLX	O6-C4	-2.58	1.41	1.44
48	l	704	PEE	O3-C30	2.51	1.40	1.33
50	J	401	NDP	C2D-C3D	2.50	1.60	1.53
47	A	503	NAI	PN-O5D	2.49	1.69	1.59
54	i	401	CDL	OA6-CA4	-2.48	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.48	1.37	1.43
50	J	401	NDP	O2B-C2B	2.47	1.53	1.44
48	l	703	PEE	O2-C2	-2.46	1.40	1.46
48	B	303	PEE	O3-C30	2.46	1.40	1.33
49	G	201	8Q1	C1-S44	2.45	1.82	1.76
48	r	501	PEE	O3-C30	2.45	1.40	1.33
54	u	201	CDL	OA6-CA4	-2.45	1.40	1.46
48	l	703	PEE	O3-C30	2.44	1.40	1.33
54	l	701	CDL	OA6-CA4	-2.43	1.40	1.46
48	j	202	PEE	O3-C30	2.42	1.40	1.33
48	l	704	PEE	O2-C2	-2.42	1.40	1.46
48	r	501	PEE	O2-C2	-2.42	1.40	1.46
48	j	202	PEE	O2-C2	-2.42	1.40	1.46
48	V	203	PEE	O2-C2	-2.40	1.40	1.46
54	l	702	CDL	OA6-CA4	-2.40	1.40	1.46
54	g	202	CDL	OA6-CA4	-2.39	1.40	1.46
48	m	201	PEE	O2-C10	2.39	1.41	1.34
47	A	503	NAI	C5B-C4B	2.39	1.59	1.51
48	B	303	PEE	O2-C10	2.38	1.41	1.34
55	j	203	PLX	C7-C6	2.38	1.55	1.50
46	A	502	FMN	C10-N1	2.37	1.38	1.33
48	V	203	PEE	O3-C30	2.36	1.40	1.33
49	X	201	8Q1	C1-S44	2.36	1.81	1.76
48	m	201	PEE	O3-C30	2.35	1.40	1.33
48	V	203	PEE	O2-C10	2.33	1.40	1.34
55	g	201	PLX	C7-C6	2.33	1.55	1.50
54	V	202	CDL	OA6-CA4	-2.32	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	B	303	PEE	O2-C2	-2.31	1.40	1.46
48	m	201	PEE	O2-C2	-2.30	1.40	1.46
49	G	201	8Q1	C6-C1	2.29	1.53	1.50
55	r	502	PLX	C7-C6	2.29	1.55	1.50
48	r	501	PEE	O2-C10	2.26	1.40	1.34
54	a	201	CDL	OA6-CA4	-2.25	1.41	1.46
48	l	703	PEE	O2-C10	2.25	1.40	1.34
48	l	704	PEE	O2-C10	2.25	1.40	1.34
54	V	202	CDL	PB2-OB2	2.25	1.68	1.59
54	V	201	CDL	PB2-OB2	2.24	1.68	1.59
55	a	202	PLX	C7-C6	2.24	1.55	1.50
56	s	401	UQ	O4-C4	-2.23	1.18	1.23
48	j	202	PEE	O2-C10	2.22	1.40	1.34
54	a	201	CDL	OB6-CB4	-2.22	1.41	1.46
54	g	202	CDL	PB2-OB5	2.21	1.68	1.59
54	V	202	CDL	OB6-CB4	-2.21	1.41	1.46
54	l	701	CDL	OB6-CB4	-2.21	1.41	1.46
56	s	401	UQ	C7-C8	2.21	1.53	1.50
54	g	202	CDL	PB2-OB2	2.21	1.68	1.59
54	l	701	CDL	PB2-OB2	2.21	1.68	1.59
54	l	702	CDL	PB2-OB2	2.21	1.68	1.59
49	X	201	8Q1	O35-C34	-2.20	1.19	1.23
55	j	203	PLX	P1-O4	2.20	1.68	1.59
54	V	201	CDL	PB2-OB5	2.20	1.68	1.59
49	X	201	8Q1	O40-C39	-2.19	1.18	1.23
48	j	202	PEE	O3-C3	-2.19	1.40	1.45
54	u	201	CDL	PB2-OB2	2.18	1.68	1.59
54	V	201	CDL	OB6-CB4	-2.18	1.41	1.46
49	G	201	8Q1	O40-C39	-2.18	1.18	1.23
54	i	401	CDL	OB6-CB4	-2.18	1.41	1.46
48	V	203	PEE	O3-C3	-2.18	1.40	1.45
54	i	401	CDL	PB2-OB5	2.18	1.68	1.59
54	a	201	CDL	PB2-OB2	2.18	1.68	1.59
48	m	201	PEE	O3-C3	-2.18	1.40	1.45
49	G	201	8Q1	O35-C34	-2.18	1.19	1.23
54	V	202	CDL	PB2-OB5	2.18	1.68	1.59
49	X	201	8Q1	C6-C1	2.17	1.53	1.50
56	s	401	UQ	O1-C1	-2.16	1.18	1.23
54	i	401	CDL	PB2-OB2	2.16	1.68	1.59
54	u	201	CDL	OB6-CB4	-2.16	1.41	1.46
54	l	702	CDL	PB2-OB5	2.15	1.68	1.59
50	J	401	NDP	PA-O5B	2.15	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	u	201	CDL	PB2-OB5	2.15	1.68	1.59
54	l	701	CDL	PB2-OB5	2.12	1.67	1.59
54	l	702	CDL	OB6-CB4	-2.12	1.41	1.46
48	B	303	PEE	O3-C3	-2.12	1.40	1.45
54	a	201	CDL	PB2-OB5	2.11	1.67	1.59
50	J	401	NDP	O7N-C7N	-2.10	1.19	1.24
54	V	201	CDL	C11-CA5	2.10	1.56	1.50
48	l	704	PEE	O3-C3	-2.10	1.40	1.45
47	A	503	NAI	C2N-C3N	2.09	1.40	1.34
55	j	203	PLX	P1-O1	2.09	1.67	1.59
48	l	703	PEE	O3-C3	-2.09	1.40	1.45
55	g	201	PLX	P1-O4	2.08	1.67	1.59
48	r	501	PEE	O3-C3	-2.08	1.40	1.45
55	a	202	PLX	P1-O1	2.08	1.67	1.59
55	a	202	PLX	P1-O4	2.08	1.67	1.59
54	V	201	CDL	OA6-CA4	-2.06	1.41	1.46
54	g	202	CDL	OB6-CB4	-2.06	1.41	1.46
55	a	202	PLX	C25-C24	2.05	1.55	1.50
54	V	202	CDL	C11-CA5	2.04	1.56	1.50
55	r	502	PLX	P1-O1	2.02	1.67	1.59

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C7-C8-C9	-10.56	109.22	126.79
50	J	401	NDP	C3N-C2N-N1N	-7.77	112.01	123.10
50	J	401	NDP	C1D-N1N-C2N	-6.35	110.54	121.11
49	G	201	8Q1	C6-C1-S44	6.05	120.50	113.46
49	X	201	8Q1	C6-C1-S44	5.82	120.23	113.46
56	s	401	UQ	C12-C13-C14	-5.65	114.06	127.66
50	J	401	NDP	C1D-N1N-C6N	-5.06	109.94	120.83
56	s	401	UQ	C11-C9-C8	-4.82	111.37	121.12
56	s	401	UQ	C10-C9-C8	-4.53	112.07	123.68
57	w	401	ADP	N3-C2-N1	-4.50	121.64	128.68
48	B	303	PEE	O2-C10-C11	4.40	120.99	111.50
54	l	701	CDL	OB6-CB5-C51	4.36	120.90	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.34	121.89	128.68
54	V	202	CDL	OA6-CA5-C11	4.25	120.66	111.50
54	i	401	CDL	OA6-CA5-C11	4.17	120.49	111.50
54	a	201	CDL	OA6-CA5-C11	4.15	120.44	111.50
56	s	401	UQ	C17-C18-C19	-4.13	113.62	127.75
56	s	401	UQ	C16-C14-C13	-4.12	112.78	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	V	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
54	a	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
54	l	702	CDL	OA6-CA5-C11	4.07	120.28	111.50
54	l	701	CDL	OA6-CA5-C11	4.07	120.26	111.50
54	g	202	CDL	OB6-CB5-C51	4.06	120.25	111.50
48	r	501	PEE	O2-C10-C11	4.02	120.16	111.50
48	m	201	PEE	O2-C10-C11	4.01	120.14	111.50
54	V	201	CDL	OA6-CA5-C11	4.01	120.13	111.50
54	u	201	CDL	OA6-CA5-C11	3.97	120.06	111.50
50	J	401	NDP	N3A-C2A-N1A	-3.95	122.50	128.68
54	l	702	CDL	OB6-CB5-C51	3.95	120.01	111.50
48	j	202	PEE	O2-C10-C11	3.88	119.87	111.50
56	s	401	UQ	C15-C14-C13	-3.85	113.79	123.68
48	V	203	PEE	O2-C10-C11	3.85	119.80	111.50
48	l	703	PEE	O2-C10-C11	3.84	119.78	111.50
54	V	202	CDL	OB6-CB5-C51	3.82	119.74	111.50
48	l	704	PEE	O2-C10-C11	3.81	119.72	111.50
56	s	401	UQ	C7-C6-C1	3.80	123.05	118.48
54	i	401	CDL	OB6-CB5-C51	3.71	119.51	111.50
54	u	201	CDL	OB6-CB5-C51	3.64	119.35	111.50
49	G	201	8Q1	C37-C38-C39	3.61	118.37	112.36
54	g	202	CDL	OA6-CA5-C11	3.61	119.28	111.50
49	G	201	8Q1	O4-C1-C6	-3.45	119.91	123.99
56	s	401	UQ	C21-C19-C18	-3.44	112.69	122.65
49	X	201	8Q1	O4-C1-C6	-3.41	119.96	123.99
57	w	401	ADP	O4'-C1'-C2'	-3.35	102.03	106.93
56	s	401	UQ	CM5-C5-C6	-3.30	119.02	124.40
47	A	503	NAI	C3D-C2D-C1D	3.29	107.68	101.43
56	s	401	UQ	C20-C19-C18	-3.29	113.14	122.65
46	A	502	FMN	C4-N3-C2	-3.22	119.70	125.64
47	A	503	NAI	C4D-O4D-C1D	-3.09	102.65	109.47
50	J	401	NDP	PN-O3-PA	-3.03	122.44	132.83
49	X	201	8Q1	C37-C38-C39	2.93	117.23	112.36
54	V	201	CDL	OB8-CB7-C71	2.90	121.02	111.91
48	r	501	PEE	O3-C30-C31	2.88	120.93	111.91
46	A	502	FMN	C4A-C4-N3	2.77	120.21	113.19
48	B	303	PEE	O3-C30-C31	2.73	120.48	111.91
54	i	401	CDL	OB8-CB7-C71	2.71	120.42	111.91
48	l	703	PEE	O3-C30-C31	2.69	120.33	111.91
55	r	502	PLX	C1A-N1-C1	2.65	120.77	109.92
54	V	202	CDL	OB8-CB7-C71	2.64	120.21	111.91
54	i	401	CDL	OA8-CA7-C31	2.62	120.14	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	l	702	CDL	OB8-CB7-C71	2.59	120.03	111.91
54	u	201	CDL	OB8-CB7-C71	2.58	120.02	111.91
48	m	201	PEE	O3-C30-C31	2.57	119.98	111.91
47	A	503	NAI	C4A-C5A-N7A	-2.56	106.73	109.40
54	l	701	CDL	OB8-CB7-C71	2.56	119.94	111.91
57	w	401	ADP	PA-O3A-PB	-2.55	124.09	132.83
54	a	201	CDL	OB8-CB7-C71	2.53	119.86	111.91
54	u	201	CDL	OA8-CA7-C31	2.53	119.85	111.91
54	g	202	CDL	OA8-CA7-C31	2.53	119.83	111.91
54	a	201	CDL	OA8-CA7-C31	2.52	119.82	111.91
48	j	202	PEE	O3-C30-C31	2.52	119.81	111.91
48	m	201	PEE	C3-C2-C1	-2.51	105.84	111.79
48	l	704	PEE	O3-C30-C31	2.51	119.79	111.91
54	l	701	CDL	CB4-OB6-CB5	-2.51	111.62	117.79
54	g	202	CDL	OB8-CB7-C71	2.48	119.70	111.91
54	l	701	CDL	OA8-CA7-C31	2.47	119.64	111.91
46	A	502	FMN	C4A-C10-N10	2.43	120.04	116.48
54	V	201	CDL	OA8-CA7-C31	2.43	119.55	111.91
54	l	702	CDL	OA8-CA7-C31	2.42	119.51	111.91
46	A	502	FMN	O4-C4-C4A	-2.42	120.18	126.60
55	g	201	PLX	C1A-N1-C1	2.41	119.76	109.92
49	X	201	8Q1	C32-C34-N36	2.37	121.30	116.58
46	A	502	FMN	C9A-C5A-N5	-2.36	119.87	122.43
47	A	503	NAI	C2D-C3D-C4D	2.35	107.20	102.64
50	J	401	NDP	C4A-C5A-N7A	-2.34	106.96	109.40
55	j	203	PLX	C1A-N1-C1	2.33	119.46	109.92
46	A	502	FMN	C10-C4A-N5	-2.33	119.91	124.86
49	G	201	8Q1	O4-C1-S44	-2.33	119.59	122.61
50	J	401	NDP	C2B-C3B-C4B	2.32	107.04	101.99
48	V	203	PEE	O3-C30-C31	2.32	119.18	111.91
55	a	202	PLX	C1A-N1-C1	2.29	119.27	109.92
54	V	202	CDL	OA8-CA7-C31	2.28	119.05	111.91
49	G	201	8Q1	C43-S44-C1	2.23	108.80	101.87
49	X	201	8Q1	C43-S44-C1	2.17	108.62	101.87
49	X	201	8Q1	O4-C1-S44	-2.16	119.80	122.61
54	i	401	CDL	CA4-OA6-CA5	-2.16	112.48	117.79
50	J	401	NDP	C2D-C3D-C4D	2.10	106.73	102.64
46	A	502	FMN	C4A-C10-N1	-2.10	119.87	124.73
49	X	201	8Q1	C37-N36-C34	-2.09	118.86	122.59
49	X	201	8Q1	C38-C39-N41	2.09	119.93	116.42
57	w	401	ADP	C4-C5-N7	-2.05	107.26	109.40
46	A	502	FMN	C5A-C9A-N10	2.03	120.05	117.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	J	401	NDP	C3D-C2D-C1D	2.01	105.25	101.43

There are no chirality outliers.

All (774) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	PN-O3-PA-O5B
47	A	503	NAI	C5D-O5D-PN-O3
47	A	503	NAI	O4D-C4D-C5D-O5D
47	A	503	NAI	C3D-C4D-C5D-O5D
48	B	303	PEE	C11-C10-O2-C2
48	B	303	PEE	C4-O4P-P-O2P
48	V	203	PEE	C11-C10-O2-C2
48	V	203	PEE	C1-O3P-P-O2P
48	V	203	PEE	C1-O3P-P-O1P
48	V	203	PEE	C1-O3P-P-O4P
48	V	203	PEE	C4-O4P-P-O1P
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O2P
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	O4P-C4-C5-N
48	l	704	PEE	C1-O3P-P-O1P
48	l	704	PEE	O4P-C4-C5-N
48	l	704	PEE	C37-C38-C39-C40
48	m	201	PEE	C4-O4P-P-O1P
48	r	501	PEE	C11-C10-O2-C2
49	G	201	8Q1	C1-C6-C7-C8
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	C31-C29-C32-O33
49	G	201	8Q1	C28-O27-P24-O2
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	C42-C43-S44-C1
50	J	401	NDP	C5D-O5D-PN-O1N
50	J	401	NDP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
50	J	401	NDP	C2N-C3N-C7N-N7N
54	V	201	CDL	O1-C1-CA2-OA2
54	V	201	CDL	CA2-C1-CB2-OB2
54	V	201	CDL	CA2-OA2-PA1-OA3
54	V	201	CDL	CA2-OA2-PA1-OA4
54	V	201	CDL	CA3-OA5-PA1-OA2
54	V	201	CDL	CA3-OA5-PA1-OA3
54	V	201	CDL	CA3-OA5-PA1-OA4
54	V	201	CDL	OA7-CA5-OA6-CA4
54	V	201	CDL	C11-CA5-OA6-CA4
54	V	201	CDL	CB2-OB2-PB2-OB3
54	V	201	CDL	CB2-OB2-PB2-OB4
54	V	201	CDL	CB2-OB2-PB2-OB5
54	V	201	CDL	CB3-OB5-PB2-OB3
54	V	201	CDL	CB3-OB5-PB2-OB4
54	V	202	CDL	CA2-C1-CB2-OB2
54	V	202	CDL	CB2-OB2-PB2-OB3
54	V	202	CDL	CB3-OB5-PB2-OB2
54	V	202	CDL	CB3-OB5-PB2-OB3
54	V	202	CDL	CB3-OB5-PB2-OB4
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB3
54	a	201	CDL	CB3-OB5-PB2-OB4
54	g	202	CDL	CA2-OA2-PA1-OA3
54	g	202	CDL	CA2-OA2-PA1-OA4
54	g	202	CDL	OA6-CA4-CA6-OA8
54	g	202	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	CA2-OA2-PA1-OA5
54	i	401	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CA3-OA5-PA1-OA3
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB3
54	i	401	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CB2-OB2-PB2-OB5
54	i	401	CDL	CB3-OB5-PB2-OB3
54	l	701	CDL	O1-C1-CA2-OA2
54	l	701	CDL	CB2-OB2-PB2-OB3
54	l	701	CDL	CB2-OB2-PB2-OB4
54	l	701	CDL	CB3-OB5-PB2-OB2
54	l	701	CDL	CB3-OB5-PB2-OB3
54	l	701	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
54	l	702	CDL	O1-C1-CA2-OA2
54	l	702	CDL	CA2-OA2-PA1-OA3
54	l	702	CDL	CA2-OA2-PA1-OA4
54	l	702	CDL	CA2-OA2-PA1-OA5
54	l	702	CDL	CB2-OB2-PB2-OB4
54	l	702	CDL	OB6-CB4-CB6-OB8
54	u	201	CDL	O1-C1-CA2-OA2
54	u	201	CDL	CB2-C1-CA2-OA2
54	u	201	CDL	CA2-OA2-PA1-OA5
54	u	201	CDL	CB2-OB2-PB2-OB3
54	u	201	CDL	CB3-OB5-PB2-OB3
54	u	201	CDL	CB3-OB5-PB2-OB4
55	a	202	PLX	O7-C6-O6-C4
55	a	202	PLX	C3-O4-P1-O2
55	a	202	PLX	C2-O1-P1-O2
55	a	202	PLX	N1-C1-C2-O1
55	g	201	PLX	O7-C6-O6-C4
55	g	201	PLX	C3-O4-P1-O2
55	g	201	PLX	C3-O4-P1-O3
55	j	203	PLX	O7-C6-C7-C8
55	j	203	PLX	O7-C6-O6-C4
55	j	203	PLX	O9-C24-C25-C26
55	r	502	PLX	O7-C6-O6-C4
55	r	502	PLX	C3-O4-P1-O1
55	r	502	PLX	C2-O1-P1-O3
55	r	502	PLX	O9-C24-C25-C26
56	s	401	UQ	C7-C8-C9-C10
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C8
56	s	401	UQ	C12-C13-C14-C16
56	s	401	UQ	C13-C14-C16-C17
56	s	401	UQ	C14-C16-C17-C18
56	s	401	UQ	C17-C18-C19-C21
48	l	704	PEE	O5-C30-O3-C3
54	i	401	CDL	OA9-CA7-OA8-CA6
48	B	303	PEE	O4-C10-O2-C2
48	V	203	PEE	O4-C10-O2-C2
48	j	202	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
48	j	202	PEE	C11-C10-O2-C2
54	l	701	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
56	s	401	UQ	C12-C11-C9-C10
54	V	201	CDL	OA9-CA7-OA8-CA6
48	l	703	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
54	g	202	CDL	C71-CB7-OB8-CB6
54	i	401	CDL	C31-CA7-OA8-CA6
54	l	701	CDL	C31-CA7-OA8-CA6
48	j	202	PEE	C17-C18-C19-C20
54	V	201	CDL	C59-C60-C61-C62
48	l	703	PEE	O5-C30-O3-C3
54	g	202	CDL	OB9-CB7-OB8-CB6
54	l	702	CDL	C11-C12-C13-C14
54	V	201	CDL	C32-C33-C34-C35
54	V	202	CDL	C51-CB5-OB6-CB4
54	g	202	CDL	C51-CB5-OB6-CB4
48	j	202	PEE	C30-C31-C32-C33
50	J	401	NDP	C2D-C1D-N1N-C6N
54	V	202	CDL	C80-C81-C82-C83
54	l	701	CDL	C14-C15-C16-C17
54	l	701	CDL	C58-C59-C60-C61
55	j	203	PLX	C28-C29-C30-C31
54	V	202	CDL	C32-C33-C34-C35
54	l	702	CDL	C59-C60-C61-C62
54	i	401	CDL	C31-C32-C33-C34
54	l	702	CDL	C75-C76-C77-C78
55	r	502	PLX	C30-C31-C32-C33
54	V	201	CDL	C31-CA7-OA8-CA6
54	V	202	CDL	OB7-CB5-OB6-CB4
54	l	702	CDL	C39-C40-C41-C42
55	g	201	PLX	C7-C8-C9-C10
54	u	201	CDL	C71-C72-C73-C74
54	V	201	CDL	C11-C12-C13-C14
54	g	202	CDL	C78-C79-C80-C81
54	V	201	CDL	CB2-C1-CA2-OA2
54	a	201	CDL	CB2-C1-CA2-OA2
54	a	201	CDL	CA2-C1-CB2-OB2
54	g	202	CDL	CB2-C1-CA2-OA2
54	i	401	CDL	CA2-C1-CB2-OB2
54	l	701	CDL	CB2-C1-CA2-OA2
54	l	701	CDL	CA2-C1-CB2-OB2
54	l	702	CDL	CB2-C1-CA2-OA2
54	g	202	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
54	l	701	CDL	OB9-CB7-OB8-CB6
54	l	701	CDL	C71-CB7-OB8-CB6
54	l	702	CDL	C71-CB7-OB8-CB6
54	V	201	CDL	C62-C63-C64-C65
48	m	201	PEE	C31-C32-C33-C34
54	a	201	CDL	C34-C35-C36-C37
54	i	401	CDL	C14-C15-C16-C17
55	r	502	PLX	C35-C36-C37-C38
48	V	203	PEE	O3P-C1-C2-O2
48	m	201	PEE	C13-C14-C15-C16
54	V	201	CDL	C34-C35-C36-C37
54	l	701	CDL	C55-C56-C57-C58
54	l	702	CDL	C35-C36-C37-C38
54	l	702	CDL	C54-C55-C56-C57
54	a	201	CDL	O1-C1-CB2-OB2
54	l	702	CDL	O1-C1-CB2-OB2
54	V	201	CDL	OB6-CB4-CB6-OB8
54	V	202	CDL	OB6-CB4-CB6-OB8
48	m	201	PEE	C33-C34-C35-C36
54	l	701	CDL	C72-C73-C74-C75
55	r	502	PLX	C12-C13-C14-C15
54	u	201	CDL	CB7-C71-C72-C73
54	l	702	CDL	OB9-CB7-OB8-CB6
54	l	702	CDL	CB5-C51-C52-C53
48	B	303	PEE	C17-C18-C19-C20
54	V	202	CDL	CB7-C71-C72-C73
54	g	202	CDL	CA5-C11-C12-C13
54	g	202	CDL	CA7-C31-C32-C33
54	g	202	CDL	CB7-C71-C72-C73
54	i	401	CDL	CA7-C31-C32-C33
54	i	401	CDL	CB7-C71-C72-C73
54	l	701	CDL	CB5-C51-C52-C53
54	l	701	CDL	CB7-C71-C72-C73
54	u	201	CDL	CB5-C51-C52-C53
54	u	201	CDL	C52-C53-C54-C55
55	g	201	PLX	C12-C13-C14-C15
50	J	401	NDP	C3D-C4D-C5D-O5D
48	V	203	PEE	C31-C30-O3-C3
54	g	202	CDL	C57-C58-C59-C60
54	u	201	CDL	C75-C76-C77-C78
55	r	502	PLX	C2-C1-N1-C1C
55	r	502	PLX	C2-C1-N1-C1A

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	CA7-C31-C32-C33
54	g	202	CDL	CB5-C51-C52-C53
54	l	702	CDL	CB7-C71-C72-C73
54	g	202	CDL	C23-C24-C25-C26
48	l	703	PEE	C30-C31-C32-C33
54	V	202	CDL	O1-C1-CB2-OB2
54	a	201	CDL	O1-C1-CA2-OA2
54	g	202	CDL	O1-C1-CA2-OA2
54	i	401	CDL	O1-C1-CB2-OB2
54	l	701	CDL	O1-C1-CB2-OB2
54	V	201	CDL	CB7-C71-C72-C73
48	V	203	PEE	C17-C18-C19-C20
48	l	703	PEE	C37-C38-C39-C40
48	m	201	PEE	C17-C18-C19-C20
54	u	201	CDL	C11-CA5-OA6-CA4
54	l	701	CDL	C20-C21-C22-C23
48	l	703	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O3P
54	V	201	CDL	CA2-OA2-PA1-OA5
54	V	202	CDL	CA2-OA2-PA1-OA5
54	V	202	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CB2-OB2-PB2-OB5
54	a	201	CDL	CB3-OB5-PB2-OB2
54	g	202	CDL	CA2-OA2-PA1-OA5
54	g	202	CDL	CB2-OB2-PB2-OB5
54	g	202	CDL	CB3-OB5-PB2-OB2
54	l	701	CDL	CB2-OB2-PB2-OB5
54	l	702	CDL	CB2-OB2-PB2-OB5
54	l	702	CDL	CB3-OB5-PB2-OB2
54	u	201	CDL	CB2-OB2-PB2-OB5
54	u	201	CDL	CB3-OB5-PB2-OB2
55	a	202	PLX	C2-O1-P1-O4
55	g	201	PLX	C3-O4-P1-O1
55	r	502	PLX	C2-O1-P1-O4
54	V	201	CDL	C71-CB7-OB8-CB6
54	u	201	CDL	OA7-CA5-OA6-CA4
54	l	701	CDL	C42-C43-C44-C45
55	j	203	PLX	C34-C35-C36-C37
54	V	202	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
54	V	202	CDL	C78-C79-C80-C81
54	l	701	CDL	C23-C24-C25-C26
48	l	704	PEE	C33-C34-C35-C36
54	V	201	CDL	C74-C75-C76-C77
54	l	702	CDL	C55-C56-C57-C58
55	g	201	PLX	C28-C29-C30-C31
54	V	201	CDL	C31-C32-C33-C34
54	V	201	CDL	C52-C53-C54-C55
54	g	202	CDL	C60-C61-C62-C63
54	u	201	CDL	C59-C60-C61-C62
55	a	202	PLX	C12-C13-C14-C15
55	g	201	PLX	C32-C33-C34-C35
55	r	502	PLX	C33-C34-C35-C36
48	l	704	PEE	C22-C23-C24-C25
54	g	202	CDL	C43-C44-C45-C46
54	g	202	CDL	C75-C76-C77-C78
54	u	201	CDL	C55-C56-C57-C58
55	a	202	PLX	C33-C34-C35-C36
55	g	201	PLX	C11-C10-C9-C8
55	j	203	PLX	C13-C14-C15-C16
48	r	501	PEE	C20-C21-C22-C23
54	a	201	CDL	C17-C18-C19-C20
54	a	201	CDL	C73-C74-C75-C76
55	a	202	PLX	C34-C35-C36-C37
55	r	502	PLX	C28-C29-C30-C31
48	V	203	PEE	O5-C30-O3-C3
48	B	303	PEE	C21-C22-C23-C24
48	l	704	PEE	C31-C32-C33-C34
54	g	202	CDL	C12-C13-C14-C15
54	i	401	CDL	C73-C74-C75-C76
54	l	701	CDL	C73-C74-C75-C76
54	l	702	CDL	C72-C73-C74-C75
55	j	203	PLX	C7-C8-C9-C10
54	V	201	CDL	O1-C1-CB2-OB2
54	V	201	CDL	C72-C73-C74-C75
54	g	202	CDL	C55-C56-C57-C58
54	V	202	CDL	C31-CA7-OA8-CA6
54	V	202	CDL	C79-C80-C81-C82
54	a	201	CDL	C75-C76-C77-C78
54	g	202	CDL	C32-C33-C34-C35
54	g	202	CDL	C63-C64-C65-C66
54	g	202	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
55	j	203	PLX	C12-C13-C14-C15
55	r	502	PLX	C15-C16-C17-C18
54	V	202	CDL	C52-C53-C54-C55
54	i	401	CDL	C32-C33-C34-C35
54	l	702	CDL	C40-C41-C42-C43
55	r	502	PLX	C13-C14-C15-C16
49	G	201	8Q1	C7-C8-C9-C10
54	l	702	CDL	C52-C53-C54-C55
54	l	702	CDL	C56-C57-C58-C59
55	g	201	PLX	C33-C34-C35-C36
48	l	703	PEE	C31-C32-C33-C34
48	l	704	PEE	C13-C14-C15-C16
48	m	201	PEE	O4-C10-O2-C2
48	m	201	PEE	C11-C10-O2-C2
54	a	201	CDL	C71-C72-C73-C74
55	a	202	PLX	C7-C8-C9-C10
55	r	502	PLX	C32-C33-C34-C35
54	V	201	CDL	CA7-C31-C32-C33
48	l	704	PEE	C14-C15-C16-C17
54	g	202	CDL	C62-C63-C64-C65
54	u	201	CDL	C13-C14-C15-C16
55	r	502	PLX	C10-C11-C12-C13
54	V	202	CDL	OB9-CB7-OB8-CB6
48	B	303	PEE	C14-C15-C16-C17
55	g	201	PLX	C9-C10-C11-C12
55	r	502	PLX	C11-C10-C9-C8
48	r	501	PEE	C12-C13-C14-C15
54	V	202	CDL	C75-C76-C77-C78
54	g	202	CDL	C71-C72-C73-C74
54	l	701	CDL	C39-C40-C41-C42
54	l	702	CDL	C60-C61-C62-C63
54	l	702	CDL	C81-C82-C83-C84
54	V	202	CDL	C81-C82-C83-C84
54	i	401	CDL	C74-C75-C76-C77
55	j	203	PLX	C27-C28-C29-C30
55	j	203	PLX	C35-C36-C37-C38
54	a	201	CDL	C22-C23-C24-C25
54	l	701	CDL	C35-C36-C37-C38
54	l	701	CDL	C56-C57-C58-C59
55	a	202	PLX	C19-C20-C21-C22
54	V	201	CDL	OB9-CB7-OB8-CB6
55	g	201	PLX	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
55	j	203	PLX	C26-C27-C28-C29
54	V	201	CDL	C37-C38-C39-C40
54	i	401	CDL	C52-C53-C54-C55
55	r	502	PLX	C14-C15-C16-C17
54	a	201	CDL	C37-C38-C39-C40
54	l	701	CDL	C52-C53-C54-C55
54	l	701	CDL	C75-C76-C77-C78
48	l	704	PEE	C11-C10-O2-C2
55	r	502	PLX	O7-C6-C7-C8
48	l	703	PEE	C21-C22-C23-C24
54	i	401	CDL	C37-C38-C39-C40
54	u	201	CDL	C14-C15-C16-C17
54	u	201	CDL	CA7-C31-C32-C33
48	B	303	PEE	C35-C36-C37-C38
55	j	203	PLX	C14-C15-C16-C17
54	l	702	CDL	C53-C54-C55-C56
55	j	203	PLX	C25-C26-C27-C28
48	V	203	PEE	C11-C12-C13-C14
48	l	704	PEE	O4-C10-O2-C2
54	i	401	CDL	C11-C12-C13-C14
54	V	202	CDL	CB5-C51-C52-C53
54	a	201	CDL	CB7-C71-C72-C73
54	a	201	CDL	C32-C33-C34-C35
54	g	202	CDL	C74-C75-C76-C77
54	V	202	CDL	OA9-CA7-OA8-CA6
48	m	201	PEE	C22-C23-C24-C25
54	V	201	CDL	C54-C55-C56-C57
54	g	202	CDL	C13-C14-C15-C16
48	B	303	PEE	C37-C38-C39-C40
48	l	703	PEE	C19-C20-C21-C22
54	a	201	CDL	C71-CB7-OB8-CB6
55	j	203	PLX	C15-C16-C17-C18
55	j	203	PLX	C10-C11-C12-C13
54	g	202	CDL	C61-C62-C63-C64
55	r	502	PLX	C31-C32-C33-C34
54	a	201	CDL	CA5-C11-C12-C13
54	V	202	CDL	C71-C72-C73-C74
48	j	202	PEE	C32-C33-C34-C35
48	j	202	PEE	C41-C42-C43-C44
54	l	701	CDL	C59-C60-C61-C62
54	V	201	CDL	C51-CB5-OB6-CB4
48	l	703	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	OA5-CA3-CA4-OA6
49	X	201	8Q1	C9-C10-C11-C12
54	g	202	CDL	OB6-CB4-CB6-OB8
54	i	401	CDL	OB6-CB4-CB6-OB8
55	r	502	PLX	C2-C1-N1-C1B
48	m	201	PEE	C12-C13-C14-C15
54	V	201	CDL	C14-C15-C16-C17
54	l	701	CDL	C81-C82-C83-C84
48	V	203	PEE	C12-C13-C14-C15
54	a	201	CDL	C43-C44-C45-C46
54	V	202	CDL	C55-C56-C57-C58
54	l	702	CDL	C32-C33-C34-C35
54	V	201	CDL	OB7-CB5-OB6-CB4
54	l	701	CDL	C74-C75-C76-C77
54	l	702	CDL	C37-C38-C39-C40
48	B	303	PEE	C4-O4P-P-O3P
48	V	203	PEE	C4-O4P-P-O3P
54	V	201	CDL	CB3-OB5-PB2-OB2
54	i	401	CDL	CB3-OB5-PB2-OB2
48	l	704	PEE	O3P-C1-C2-C3
48	r	501	PEE	C42-C43-C44-C45
55	r	502	PLX	C9-C10-C11-C12
54	u	201	CDL	C19-C20-C21-C22
54	l	701	CDL	C82-C83-C84-C85
54	l	702	CDL	C43-C44-C45-C46
55	a	202	PLX	C11-C12-C13-C14
54	a	201	CDL	OB9-CB7-OB8-CB6
48	B	303	PEE	C33-C34-C35-C36
54	V	201	CDL	CA3-CA4-CA6-OA8
54	V	202	CDL	CB3-CB4-CB6-OB8
54	g	202	CDL	CA3-CA4-CA6-OA8
54	g	202	CDL	CB3-CB4-CB6-OB8
54	l	702	CDL	C33-C34-C35-C36
55	j	203	PLX	C3-C4-C5-O8
48	l	704	PEE	C10-C11-C12-C13
56	s	401	UQ	C5-C6-C7-C8
54	u	201	CDL	C78-C79-C80-C81
55	r	502	PLX	C16-C17-C18-C19
55	a	202	PLX	O6-C6-C7-C8
48	B	303	PEE	C44-C45-C46-C47
48	r	501	PEE	C19-C20-C21-C22
54	V	202	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
54	l	702	CDL	C64-C65-C66-C67
55	g	201	PLX	C13-C14-C15-C16
55	r	502	PLX	C7-C8-C9-C10
54	l	702	CDL	C14-C15-C16-C17
54	u	201	CDL	C53-C54-C55-C56
48	V	203	PEE	C30-C31-C32-C33
48	j	202	PEE	C31-C30-O3-C3
54	l	702	CDL	C31-CA7-OA8-CA6
56	s	401	UQ	C1-C6-C7-C8
48	B	303	PEE	C12-C13-C14-C15
54	u	201	CDL	C11-C12-C13-C14
49	G	201	8Q1	C28-O27-P24-O3
54	l	701	CDL	C11-C12-C13-C14
54	l	701	CDL	C79-C80-C81-C82
54	V	201	CDL	OB5-CB3-CB4-OB6
54	V	202	CDL	OB5-CB3-CB4-OB6
48	l	703	PEE	C33-C34-C35-C36
54	V	201	CDL	C13-C14-C15-C16
54	g	202	CDL	C59-C60-C61-C62
48	r	501	PEE	C10-C11-C12-C13
54	u	201	CDL	C73-C74-C75-C76
54	i	401	CDL	OA6-CA4-CA6-OA8
54	l	701	CDL	C37-C38-C39-C40
49	G	201	8Q1	C30-C29-C32-O33
54	V	201	CDL	C33-C34-C35-C36
54	a	201	CDL	CB5-C51-C52-C53
55	a	202	PLX	C10-C11-C12-C13
48	l	704	PEE	C23-C24-C25-C26
54	V	201	CDL	C71-C72-C73-C74
54	a	201	CDL	C24-C25-C26-C27
54	i	401	CDL	C36-C37-C38-C39
54	g	202	CDL	C39-C40-C41-C42
54	g	202	CDL	C42-C43-C44-C45
48	B	303	PEE	C31-C30-O3-C3
48	r	501	PEE	C17-C18-C19-C20
48	j	202	PEE	C44-C45-C46-C47
50	J	401	NDP	O4B-C4B-C5B-O5B
48	V	203	PEE	O3P-C1-C2-C3
48	l	703	PEE	O3P-C1-C2-C3
54	V	201	CDL	OA5-CA3-CA4-CA6
54	V	201	CDL	OB5-CB3-CB4-CB6
54	a	201	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
54	g	202	CDL	OA5-CA3-CA4-CA6
54	i	401	CDL	OB5-CB3-CB4-CB6
56	s	401	UQ	C9-C11-C12-C13
54	g	202	CDL	C54-C55-C56-C57
48	B	303	PEE	C22-C23-C24-C25
54	l	702	CDL	C73-C74-C75-C76
48	l	704	PEE	C32-C33-C34-C35
55	a	202	PLX	C27-C28-C29-C30
48	l	704	PEE	C12-C13-C14-C15
48	j	202	PEE	C36-C37-C38-C39
54	i	401	CDL	C12-C13-C14-C15
55	j	203	PLX	C9-C10-C11-C12
56	s	401	UQ	C17-C18-C19-C20
48	j	202	PEE	C19-C20-C21-C22
48	m	201	PEE	C31-C30-O3-C3
54	i	401	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	C1-C2-C3-O3
48	l	704	PEE	C1-C2-C3-O3
48	m	201	PEE	C1-C2-C3-O3
54	i	401	CDL	CB3-CB4-CB6-OB8
54	u	201	CDL	CA3-CA4-CA6-OA8
55	r	502	PLX	C3-C4-C5-O8
48	l	704	PEE	C17-C18-C19-C20
54	l	702	CDL	OA9-CA7-OA8-CA6
54	V	201	CDL	C22-C23-C24-C25
49	X	201	8Q1	C7-C8-C9-C10
55	j	203	PLX	C33-C34-C35-C36
48	j	202	PEE	O5-C30-O3-C3
49	G	201	8Q1	C11-C10-C9-C8
54	l	702	CDL	C12-C13-C14-C15
55	a	202	PLX	C5-C4-O6-C6
55	r	502	PLX	C5-C4-O6-C6
54	l	701	CDL	C84-C85-C86-C87
54	u	201	CDL	C54-C55-C56-C57
48	l	704	PEE	O3P-C1-C2-O2
54	V	201	CDL	OA5-CA3-CA4-OA6
54	i	401	CDL	OB5-CB3-CB4-OB6
48	j	202	PEE	C24-C25-C26-C27
54	l	702	CDL	C51-C52-C53-C54
48	l	704	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
54	V	202	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	OB6-CB4-CB6-OB8
54	l	702	CDL	OA6-CA4-CA6-OA8
55	j	203	PLX	O6-C4-C5-O8
54	l	702	CDL	C20-C21-C22-C23
54	i	401	CDL	CB2-C1-CA2-OA2
54	l	702	CDL	CA2-C1-CB2-OB2
54	u	201	CDL	C22-C23-C24-C25
48	m	201	PEE	O3-C30-C31-C32
54	a	201	CDL	C14-C15-C16-C17
54	l	701	CDL	CA7-C31-C32-C33
55	g	201	PLX	C34-C35-C36-C37
48	m	201	PEE	C23-C24-C25-C26
54	a	201	CDL	C52-C53-C54-C55
54	l	701	CDL	C18-C19-C20-C21
54	l	702	CDL	C74-C75-C76-C77
54	V	202	CDL	OB5-CB3-CB4-CB6
54	i	401	CDL	OA5-CA3-CA4-CA6
48	j	202	PEE	C38-C39-C40-C41
48	V	203	PEE	C10-C11-C12-C13
48	B	303	PEE	O5-C30-O3-C3
54	a	201	CDL	C36-C37-C38-C39
54	i	401	CDL	C51-C52-C53-C54
54	V	201	CDL	CA6-CA4-OA6-CA5
54	V	202	CDL	C33-C34-C35-C36
48	l	703	PEE	C14-C15-C16-C17
48	r	501	PEE	C1-C2-C3-O3
54	V	201	CDL	CB3-CB4-CB6-OB8
54	g	202	CDL	CB4-CB3-OB5-PB2
54	l	702	CDL	CB3-CB4-CB6-OB8
54	u	201	CDL	CB4-CB3-OB5-PB2
48	r	501	PEE	O3P-C1-C2-O2
54	g	202	CDL	OA5-CA3-CA4-OA6
54	i	401	CDL	OA5-CA3-CA4-OA6
48	B	303	PEE	C36-C37-C38-C39
49	G	201	8Q1	C31-C29-C32-C34
54	i	401	CDL	OB9-CB7-OB8-CB6
54	i	401	CDL	C13-C14-C15-C16
48	l	703	PEE	O2-C2-C3-O3
48	m	201	PEE	O2-C2-C3-O3
54	V	201	CDL	OA6-CA4-CA6-OA8
54	a	201	CDL	OA6-CA4-CA6-OA8
57	w	401	ADP	C5’-O5’-PA-O3A

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Mol	Chain	Res	Type	Atoms
48	m	201	PEE	O5-C30-O3-C3
55	r	502	PLX	C24-C25-C26-C27
54	V	201	CDL	C64-C65-C66-C67
48	l	704	PEE	C11-C12-C13-C14
54	a	201	CDL	C39-C40-C41-C42
54	a	201	CDL	C60-C61-C62-C63
46	A	502	FMN	O2'-C2'-C3'-C4'
48	j	202	PEE	C1-O3P-P-O4P
54	l	702	CDL	CA3-OA5-PA1-OA2
54	u	201	CDL	CA3-OA5-PA1-OA2
55	a	202	PLX	C3-O4-P1-O1
48	r	501	PEE	C13-C14-C15-C16
47	A	503	NAI	C5D-O5D-PN-O1N
48	B	303	PEE	C4-O4P-P-O1P
48	V	203	PEE	C4-O4P-P-O2P
48	j	202	PEE	C1-O3P-P-O2P
48	j	202	PEE	C1-O3P-P-O1P
48	j	202	PEE	C4-O4P-P-O1P
48	r	501	PEE	C4-O4P-P-O2P
54	V	202	CDL	CA2-OA2-PA1-OA4
54	V	202	CDL	CB2-OB2-PB2-OB4
54	a	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CB2-OB2-PB2-OB4
54	a	201	CDL	CB3-OB5-PB2-OB3
54	g	202	CDL	CB2-OB2-PB2-OB3
54	g	202	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CA2-OA2-PA1-OA4
54	i	401	CDL	CB3-OB5-PB2-OB4
54	l	702	CDL	CB2-OB2-PB2-OB3
54	l	702	CDL	CB3-OB5-PB2-OB3
54	l	702	CDL	CB3-OB5-PB2-OB4
54	u	201	CDL	CA3-OA5-PA1-OA3
54	u	201	CDL	CA3-OA5-PA1-OA4
54	u	201	CDL	CB2-OB2-PB2-OB4
55	a	202	PLX	C2-O1-P1-O3
55	r	502	PLX	C3-O4-P1-O3
55	r	502	PLX	C2-O1-P1-O2
48	B	303	PEE	C31-C32-C33-C34
48	B	303	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
54	a	201	CDL	OB5-CB3-CB4-CB6
54	l	702	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
55	j	203	PLX	O4-C3-C4-C5
48	j	202	PEE	O4P-C4-C5-N
48	B	303	PEE	C23-C24-C25-C26
46	A	502	FMN	C1'-C2'-C3'-O3'
55	a	202	PLX	C25-C24-O8-C5
55	g	201	PLX	C25-C24-O8-C5
55	j	203	PLX	C25-C24-O8-C5
55	r	502	PLX	C25-C24-O8-C5
48	l	703	PEE	C23-C24-C25-C26
48	B	303	PEE	C15-C16-C17-C18
54	V	202	CDL	CB2-C1-CA2-OA2
48	m	201	PEE	C20-C21-C22-C23
48	B	303	PEE	O3P-C1-C2-O2
54	a	201	CDL	OB5-CB3-CB4-OB6
54	l	702	CDL	OA5-CA3-CA4-OA6
55	j	203	PLX	O4-C3-C4-O6
54	V	201	CDL	C38-C39-C40-C41
48	r	501	PEE	C36-C37-C38-C39
54	V	202	CDL	C83-C84-C85-C86
55	r	502	PLX	C25-C26-C27-C28
54	l	701	CDL	C51-CB5-OB6-CB4
55	r	502	PLX	C18-C19-C20-C21
54	V	202	CDL	C72-C73-C74-C75
50	J	401	NDP	C2N-C3N-C7N-O7N
54	a	201	CDL	CA3-CA4-CA6-OA8
54	i	401	CDL	CA3-CA4-CA6-OA8
54	u	201	CDL	OA6-CA4-CA6-OA8
55	r	502	PLX	O6-C4-C5-O8
54	g	202	CDL	C37-C38-C39-C40
48	r	501	PEE	C23-C24-C25-C26
54	g	202	CDL	C56-C57-C58-C59
48	B	303	PEE	C34-C35-C36-C37
54	l	702	CDL	C58-C59-C60-C61
55	r	502	PLX	C26-C27-C28-C29
54	a	201	CDL	C55-C56-C57-C58
48	r	501	PEE	C14-C15-C16-C17
54	l	702	CDL	C15-C16-C17-C18
55	r	502	PLX	O8-C24-C25-C26
54	g	202	CDL	C41-C42-C43-C44
54	V	202	CDL	C32-C31-CA7-OA8
48	l	704	PEE	C16-C17-C18-C19
55	a	202	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C39-C40-C41-C42
48	m	201	PEE	C19-C20-C21-C22
55	a	202	PLX	C11-C10-C9-C8
54	l	701	CDL	C71-C72-C73-C74
48	B	303	PEE	C42-C43-C44-C45
54	l	701	CDL	C54-C55-C56-C57
54	V	201	CDL	C75-C76-C77-C78
54	V	201	CDL	C80-C81-C82-C83
54	l	701	CDL	CA4-CA3-OA5-PA1
54	l	701	CDL	C40-C41-C42-C43
54	a	201	CDL	C13-C14-C15-C16
48	l	704	PEE	C1-O3P-P-O4P
54	l	701	CDL	CA2-OA2-PA1-OA5
55	j	203	PLX	C3-O4-P1-O1
54	l	702	CDL	C57-C58-C59-C60
54	l	702	CDL	CA3-CA4-CA6-OA8
48	l	703	PEE	C18-C19-C20-C21
48	m	201	PEE	C16-C17-C18-C19
54	l	702	CDL	C11-CA5-OA6-CA4
48	j	202	PEE	C10-C11-C12-C13
54	V	201	CDL	C1-CB2-OB2-PB2
55	a	202	PLX	C13-C14-C15-C16
54	l	702	CDL	C77-C78-C79-C80
55	a	202	PLX	C18-C19-C20-C21
48	j	202	PEE	C13-C14-C15-C16
48	l	704	PEE	C18-C19-C20-C21
55	a	202	PLX	C29-C30-C31-C32
54	l	701	CDL	OB7-CB5-OB6-CB4
55	g	201	PLX	C36-C37-C38-C39
48	l	704	PEE	C36-C37-C38-C39
54	V	201	CDL	C78-C79-C80-C81
54	g	202	CDL	C64-C65-C66-C67
54	u	201	CDL	C18-C19-C20-C21
48	l	704	PEE	C39-C40-C41-C42
55	j	203	PLX	O8-C24-C25-C26
54	l	702	CDL	C62-C63-C64-C65
55	g	201	PLX	C26-C27-C28-C29
54	g	202	CDL	CA4-CA3-OA5-PA1
49	G	201	8Q1	N41-C42-C43-S44
48	V	203	PEE	C13-C14-C15-C16
54	l	702	CDL	OA7-CA5-OA6-CA4
54	V	202	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	O4D-C1D-N1N-C2N
54	i	401	CDL	C33-C34-C35-C36
55	g	201	PLX	C31-C32-C33-C34
48	r	501	PEE	C21-C22-C23-C24
54	a	201	CDL	C53-C54-C55-C56
54	g	202	CDL	C17-C18-C19-C20
54	g	202	CDL	C36-C37-C38-C39
54	l	702	CDL	C84-C85-C86-C87
55	a	202	PLX	C15-C16-C17-C18
55	g	201	PLX	C27-C28-C29-C30
54	V	202	CDL	CB4-CB3-OB5-PB2
54	u	201	CDL	C61-C62-C63-C64
55	g	201	PLX	C30-C31-C32-C33
48	l	703	PEE	C15-C16-C17-C18
54	V	202	CDL	C77-C78-C79-C80
48	j	202	PEE	C21-C22-C23-C24
54	l	701	CDL	C34-C35-C36-C37
54	i	401	CDL	O1-C1-CA2-OA2
54	a	201	CDL	C58-C59-C60-C61
54	i	401	CDL	C15-C16-C17-C18
47	A	503	NAI	C2D-C1D-N1N-C2N
48	l	703	PEE	C13-C14-C15-C16
54	l	702	CDL	C44-C45-C46-C47
54	V	202	CDL	C12-C11-CA5-OA6
54	V	201	CDL	C58-C59-C60-C61
48	V	203	PEE	C38-C39-C40-C41
54	V	202	CDL	OA5-CA3-CA4-OA6
48	B	303	PEE	C20-C21-C22-C23
54	l	702	CDL	C61-C62-C63-C64
48	m	201	PEE	C21-C22-C23-C24
55	j	203	PLX	O6-C6-C7-C8
48	B	303	PEE	C24-C25-C26-C27
55	j	203	PLX	C11-C10-C9-C8
54	l	701	CDL	C61-C62-C63-C64
46	A	502	FMN	O2'-C2'-C3'-O3'
49	G	201	8Q1	C11-C12-C13-C14
54	l	702	CDL	C32-C31-CA7-OA8
50	J	401	NDP	C3B-C4B-C5B-O5B
54	V	201	CDL	C43-C44-C45-C46
48	l	703	PEE	O2-C10-C11-C12
49	X	201	8Q1	O27-C28-C29-C30
54	l	701	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
48	j	202	PEE	C16-C17-C18-C19
48	l	703	PEE	C16-C17-C18-C19
49	G	201	8Q1	C6-C7-C8-C9
49	X	201	8Q1	C13-C14-C15-C16
48	j	202	PEE	C40-C41-C42-C43
54	a	201	CDL	C41-C42-C43-C44
54	l	701	CDL	C51-C52-C53-C54
54	l	702	CDL	C41-C42-C43-C44
48	l	703	PEE	C36-C37-C38-C39
54	V	202	CDL	CA3-CA4-CA6-OA8
54	a	201	CDL	CB3-CB4-CB6-OB8
55	a	202	PLX	C7-C6-O6-C4
54	l	701	CDL	OB5-CB3-CB4-OB6
48	j	202	PEE	C37-C38-C39-C40
48	j	202	PEE	O2-C10-C11-C12
54	l	701	CDL	C16-C17-C18-C19
54	g	202	CDL	C12-C11-CA5-OA6
48	m	201	PEE	C18-C19-C20-C21
49	G	201	8Q1	C30-C29-C32-C34
54	l	702	CDL	C12-C11-CA5-OA6
49	G	201	8Q1	C13-C14-C15-C16
48	m	201	PEE	O5-C30-C31-C32
50	J	401	NDP	C5D-O5D-PN-O3
54	u	201	CDL	C31-CA7-OA8-CA6
54	u	201	CDL	OA9-CA7-OA8-CA6
48	l	704	PEE	C30-C31-C32-C33
54	l	701	CDL	C72-C71-CB7-OB8
54	l	702	CDL	C32-C31-CA7-OA9
54	l	701	CDL	C12-C11-CA5-OA7
48	l	703	PEE	O4-C10-C11-C12
48	l	704	PEE	C38-C39-C40-C41
54	g	202	CDL	C53-C54-C55-C56
54	l	702	CDL	C17-C18-C19-C20
48	r	501	PEE	C30-C31-C32-C33
54	i	401	CDL	C53-C54-C55-C56
48	B	303	PEE	C1-O3P-P-O1P
48	l	703	PEE	C4-O4P-P-O1P
50	J	401	NDP	C5B-O5B-PA-O2A
54	l	701	CDL	CA2-OA2-PA1-OA3
57	w	401	ADP	C5'-O5'-PA-O2A
54	V	201	CDL	C21-C22-C23-C24
54	g	202	CDL	C12-C11-CA5-OA7

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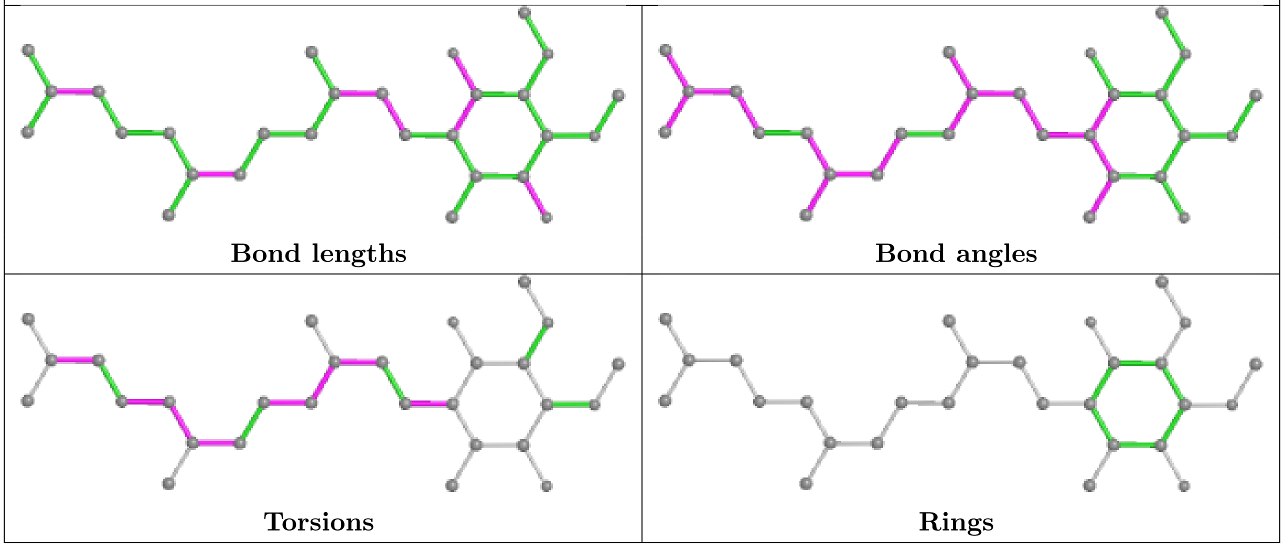
Mol	Chain	Res	Type	Atoms
54	l	702	CDL	C12-C11-CA5-OA7
54	V	201	CDL	C55-C56-C57-C58
54	g	202	CDL	C34-C35-C36-C37
54	l	702	CDL	C31-C32-C33-C34
48	l	704	PEE	C5-C4-O4P-P
54	u	201	CDL	CA3-CA4-OA6-CA5
54	u	201	CDL	CA6-CA4-OA6-CA5
48	j	202	PEE	O4-C10-C11-C12
54	l	702	CDL	C21-C22-C23-C24
48	r	501	PEE	C16-C17-C18-C19
54	V	201	CDL	C17-C18-C19-C20
55	g	201	PLX	C25-C26-C27-C28
48	l	704	PEE	O3-C30-C31-C32
54	u	201	CDL	CA2-C1-CB2-OB2
54	g	202	CDL	OB5-CB3-CB4-OB6
54	g	202	CDL	C33-C34-C35-C36
54	g	202	CDL	C72-C71-CB7-OB8
54	i	401	CDL	C52-C51-CB5-OB6
54	u	201	CDL	C72-C71-CB7-OB8
54	l	701	CDL	C72-C71-CB7-OB9
54	V	202	CDL	O1-C1-CA2-OA2
54	a	201	CDL	C16-C17-C18-C19
54	g	202	CDL	C72-C71-CB7-OB9
48	r	501	PEE	C33-C34-C35-C36

There are no ring outliers.

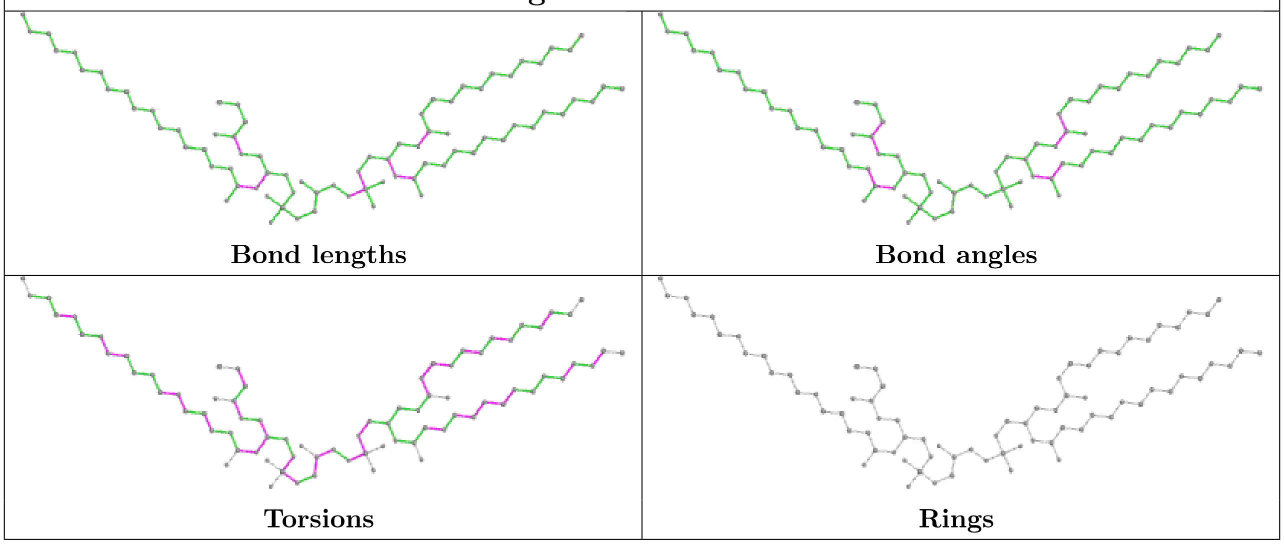
No monomer is involved in short contacts.

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.

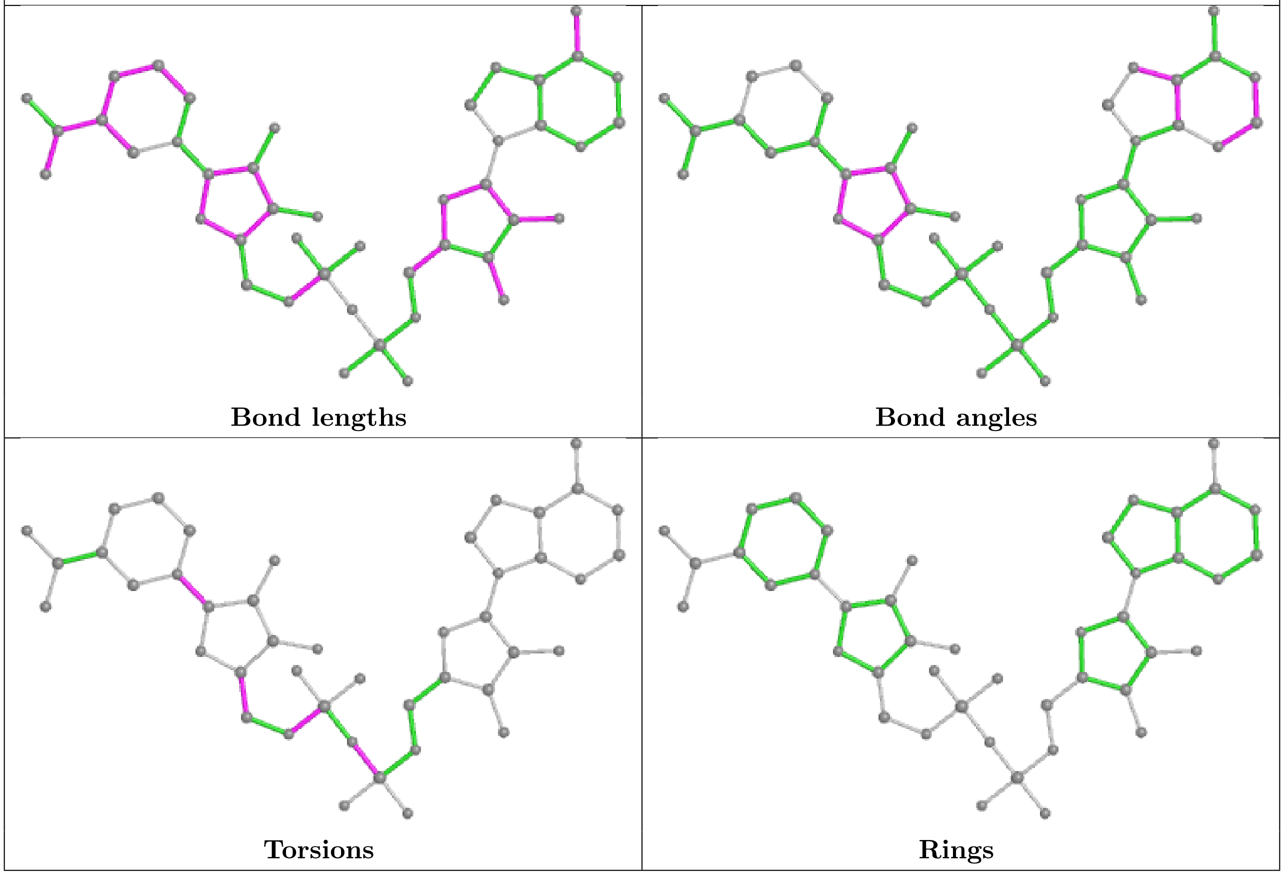
Ligand UQ s 401



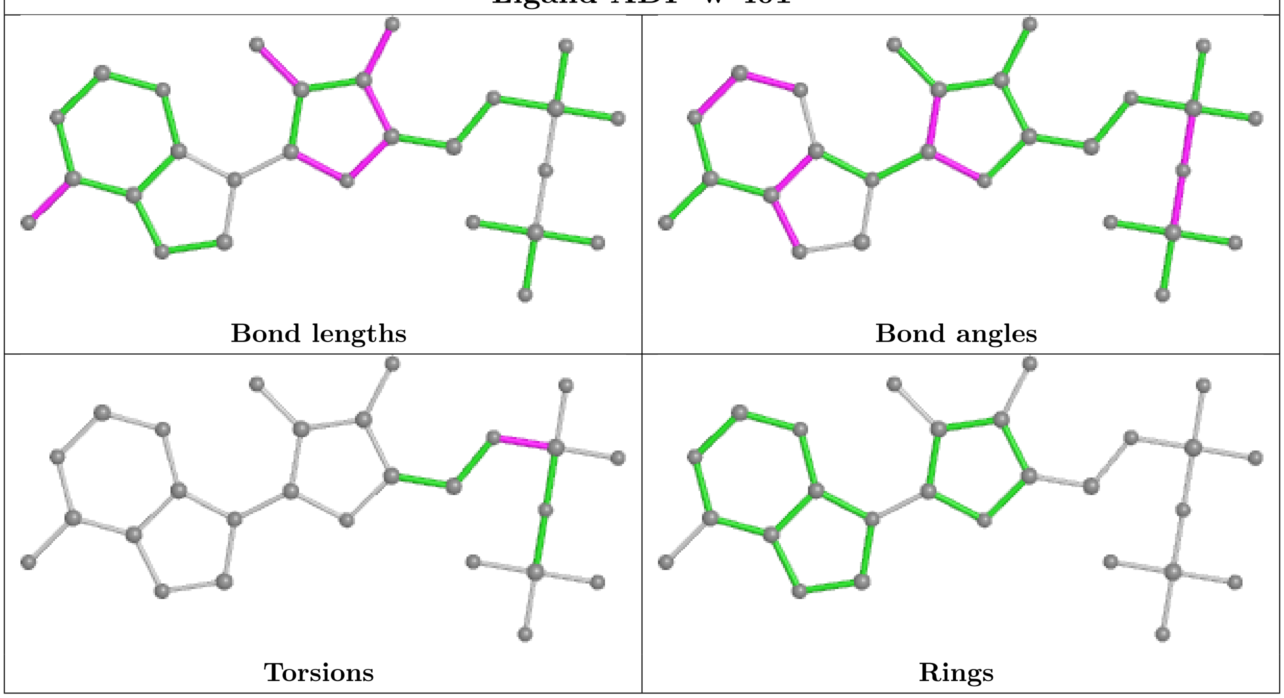
Ligand CDL u 201



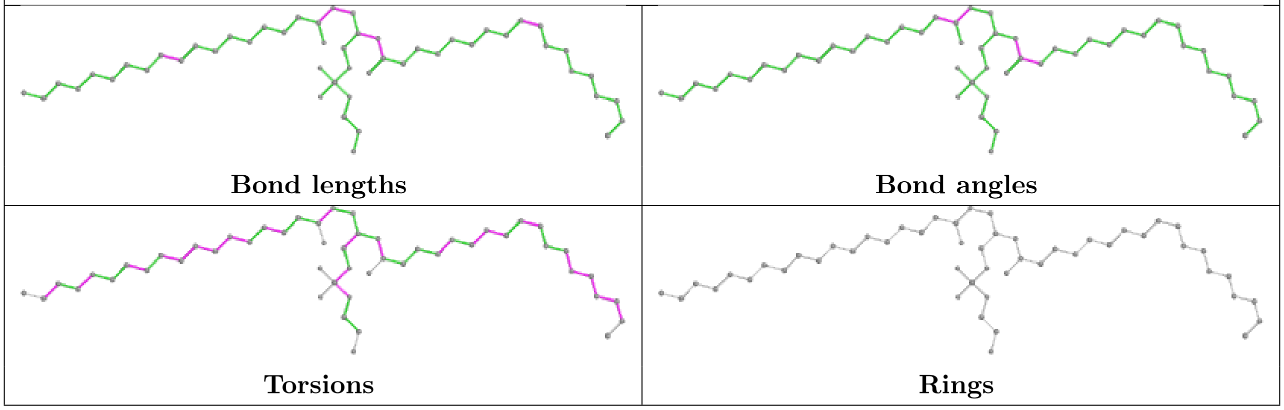
Ligand NAI A 503



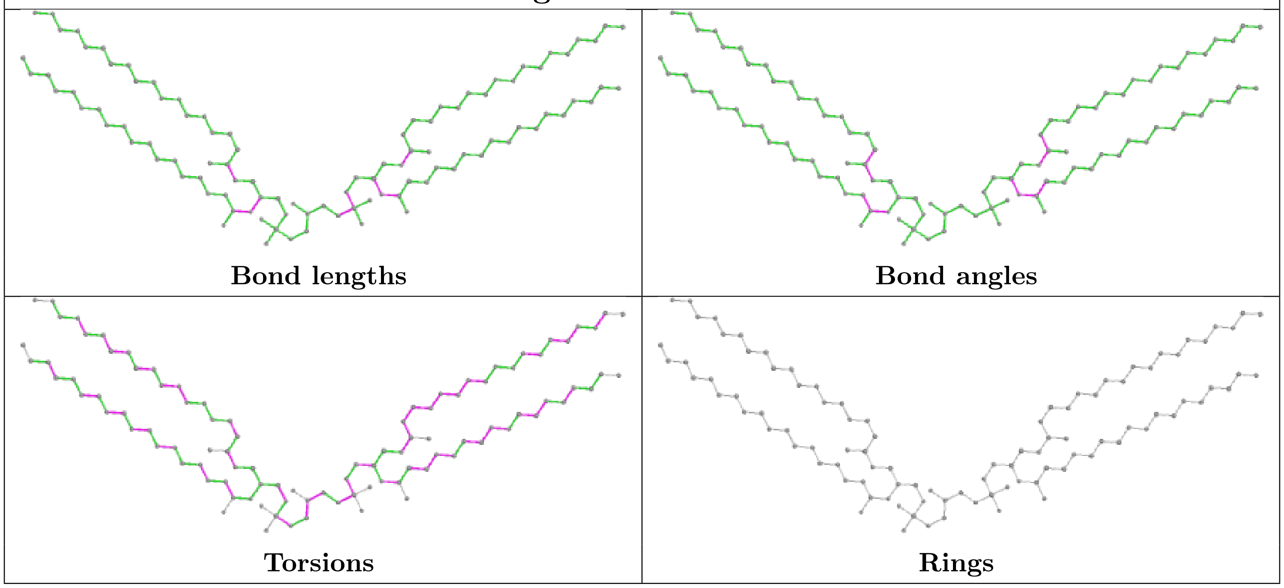
Ligand ADP w 401



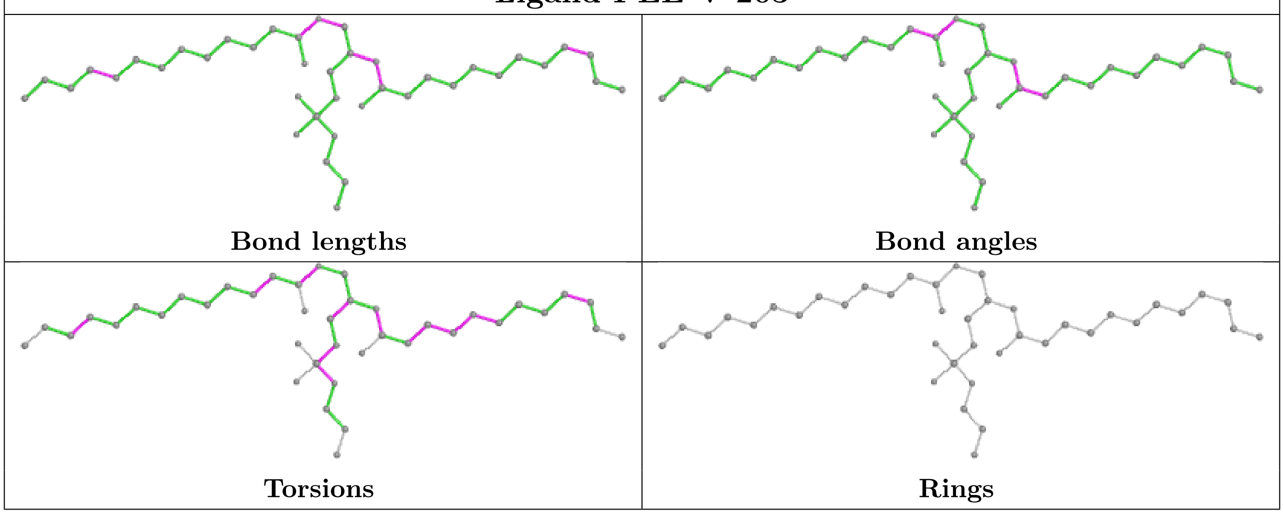
Ligand PEE B 303



Ligand CDL l 701



Ligand PEE V 203



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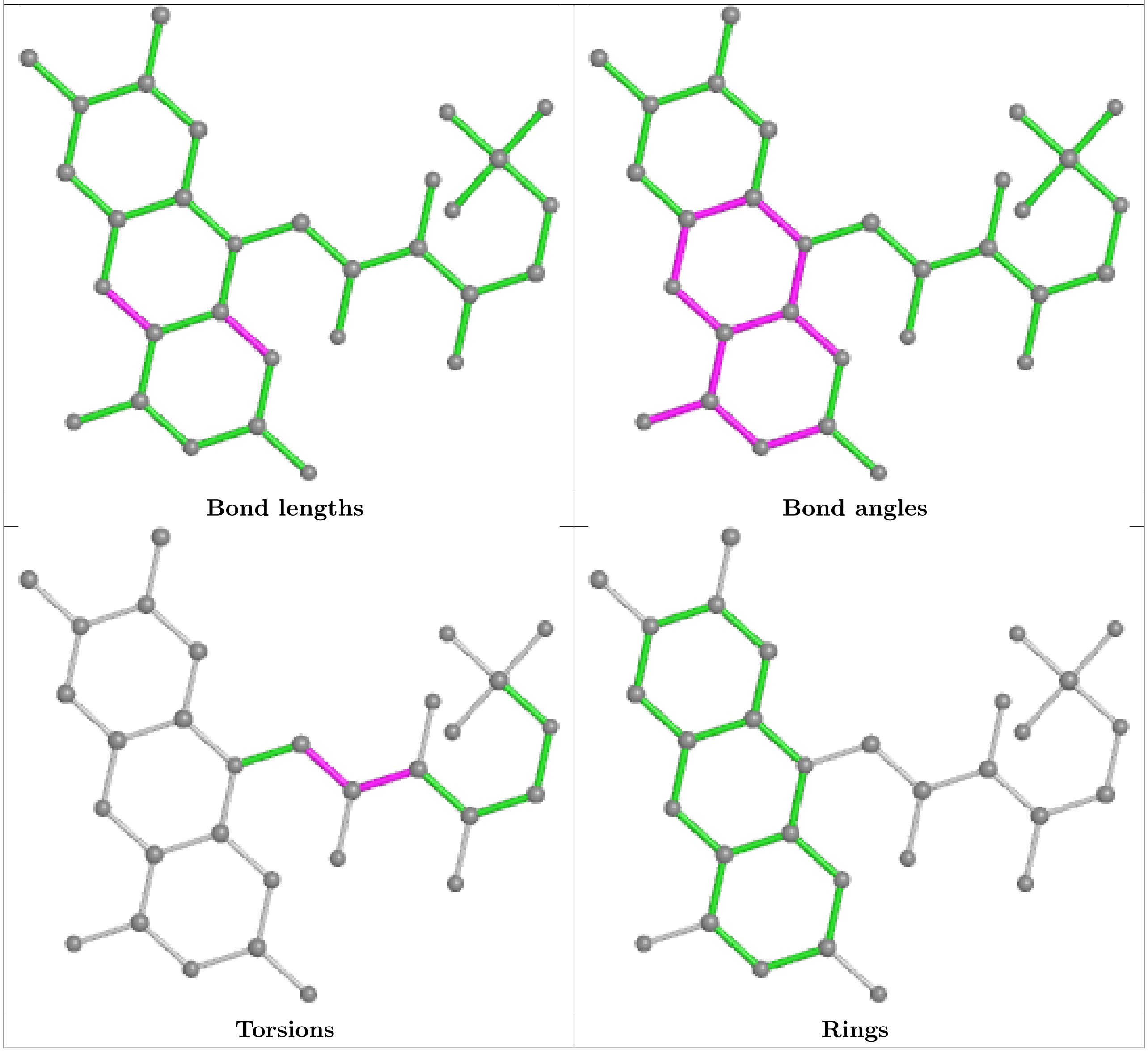
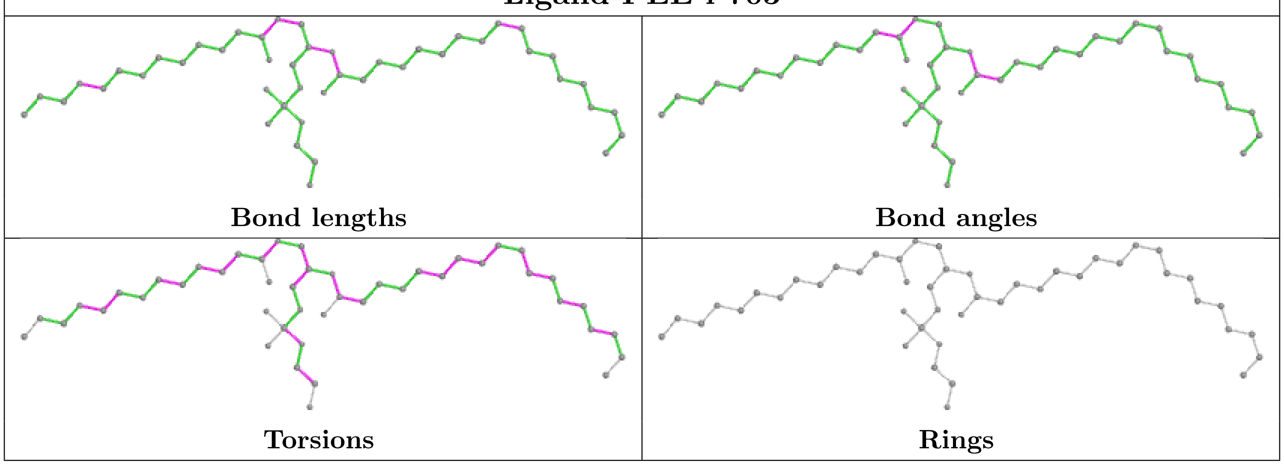
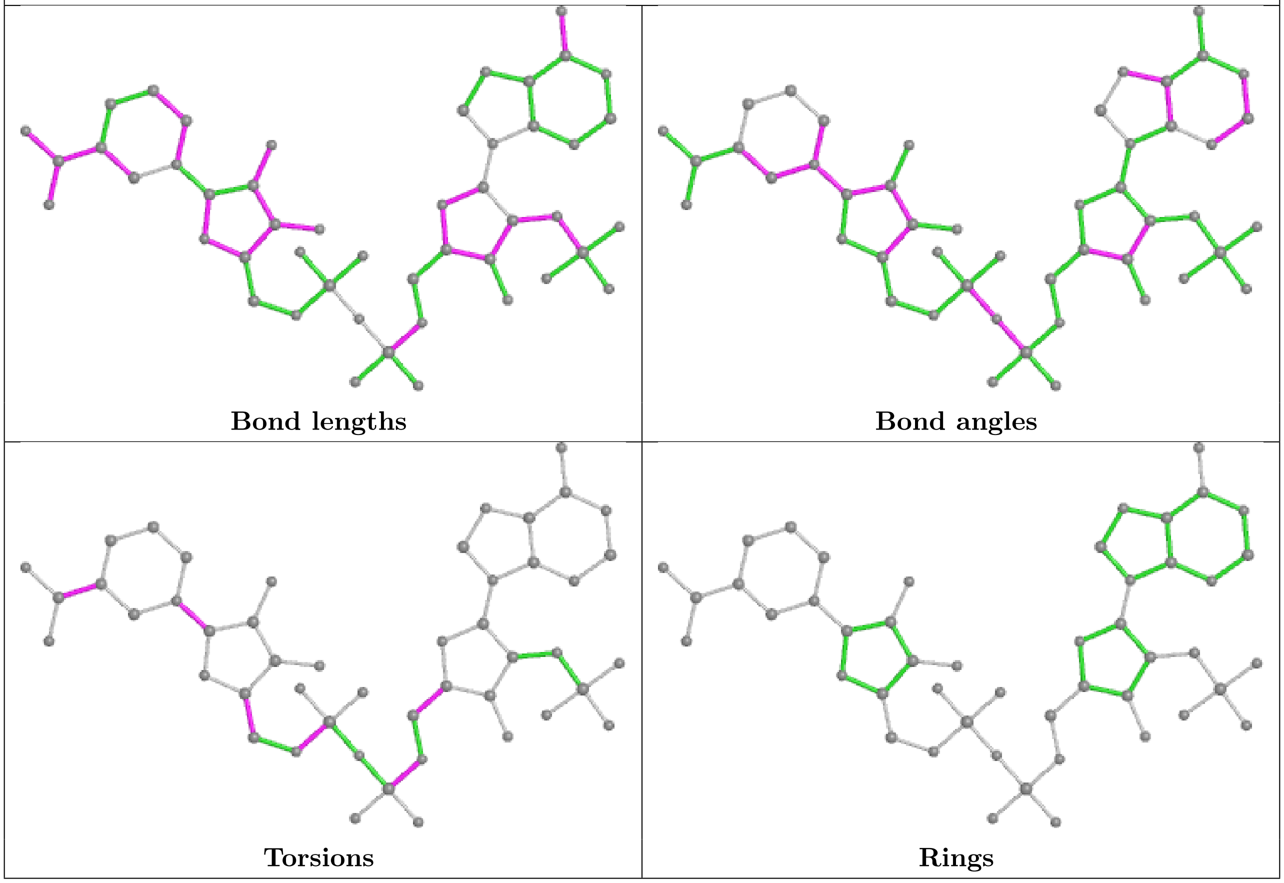


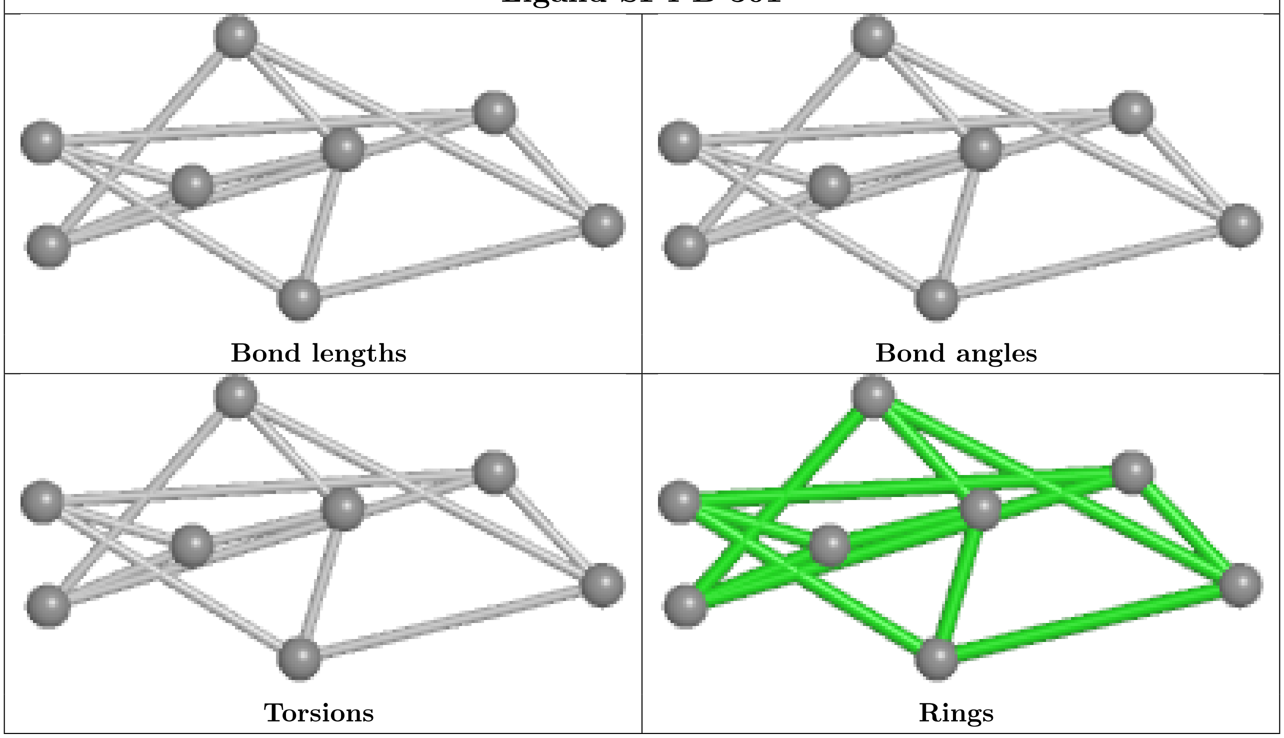
Ligand PEE l 703



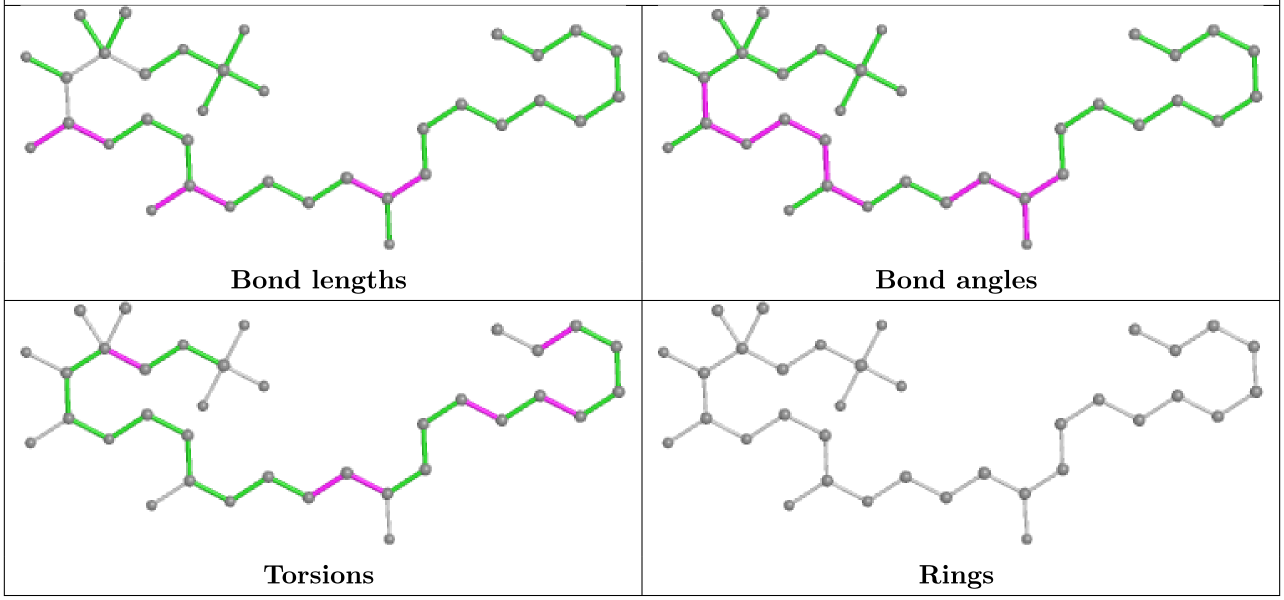
Ligand NDP J 401



Ligand SF4 B 301



Ligand 8Q1 X 201



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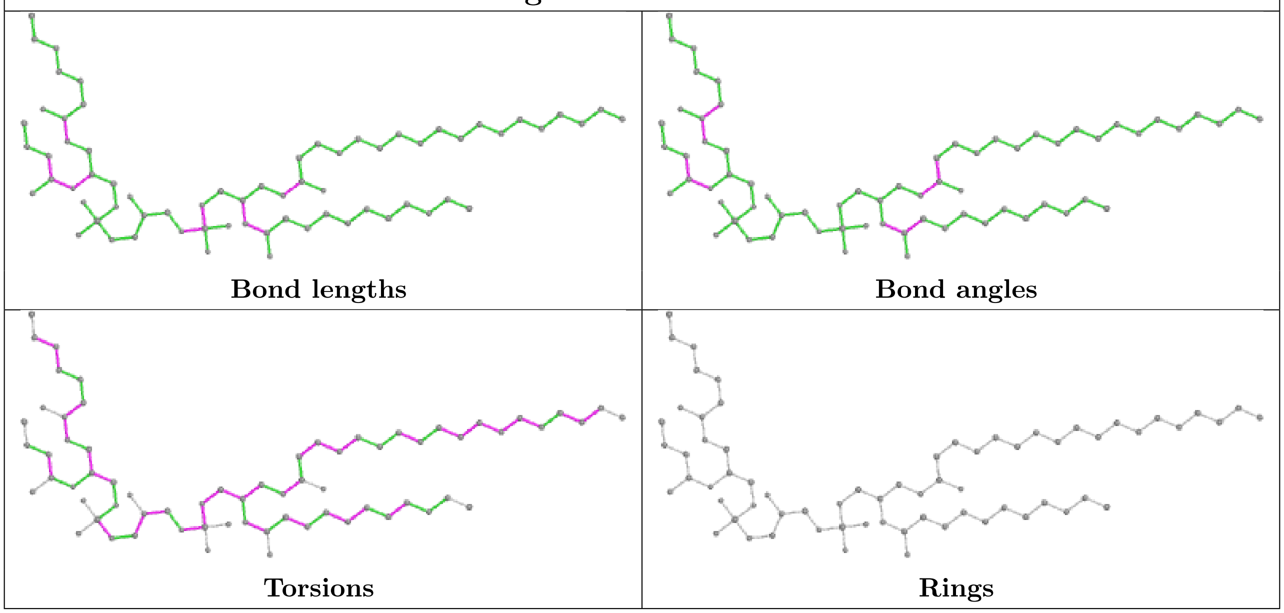
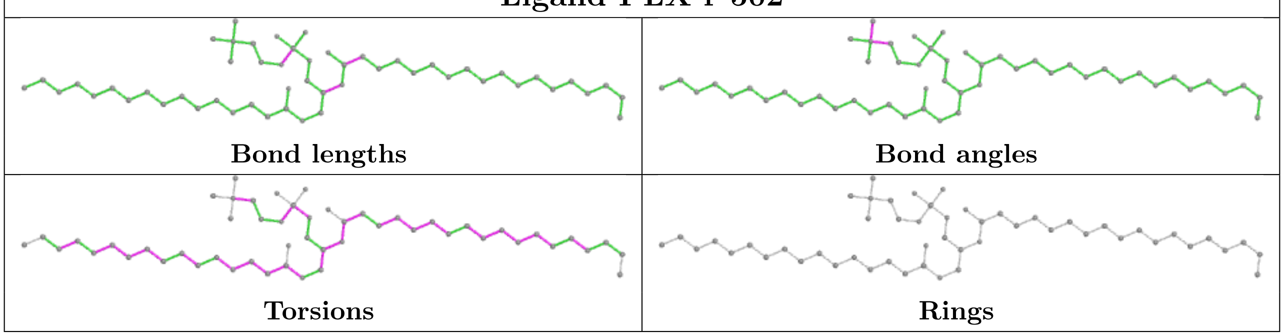
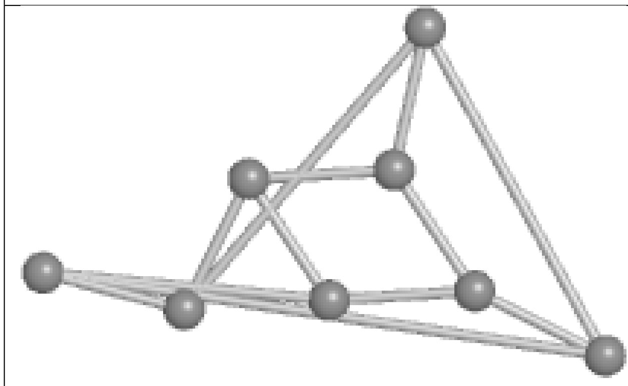
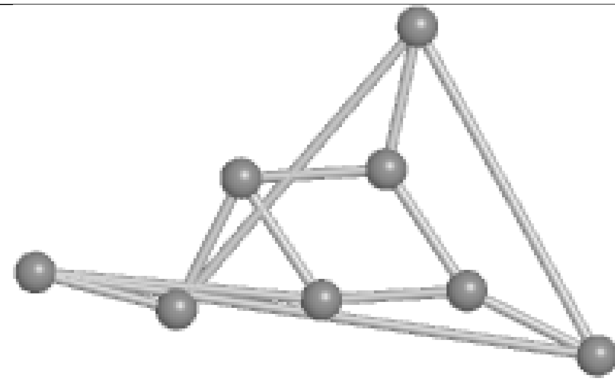


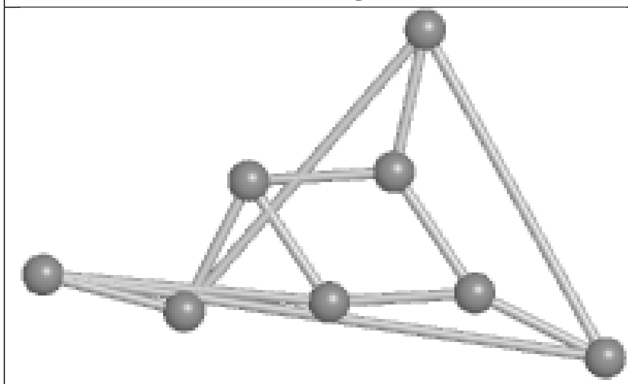
Ligand PLX r 502

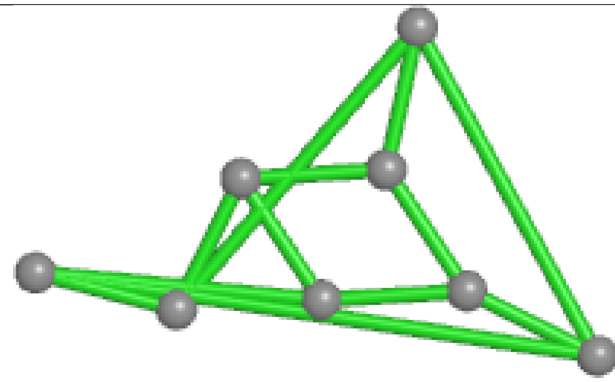


Ligand SF4 M 801

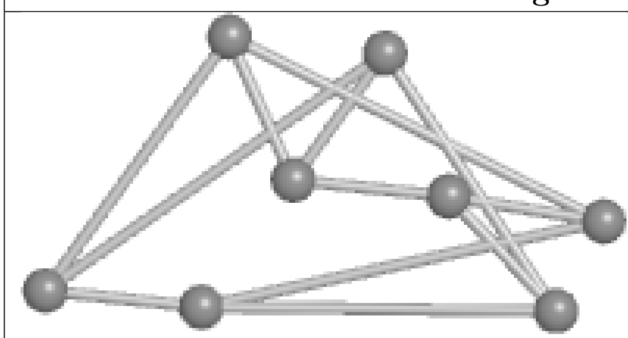

Bond lengths

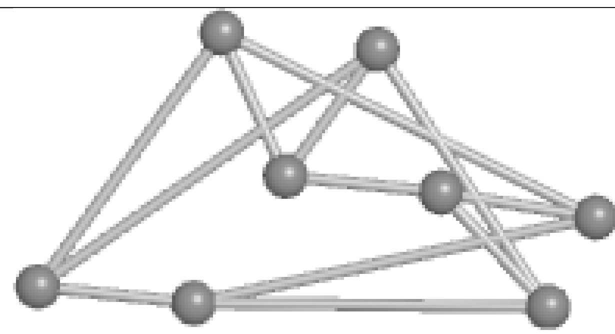

Bond angles

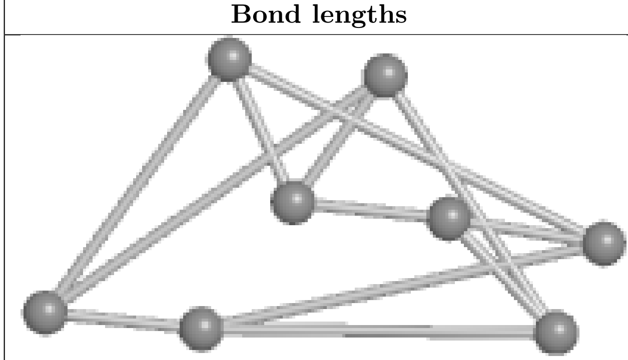

Torsions

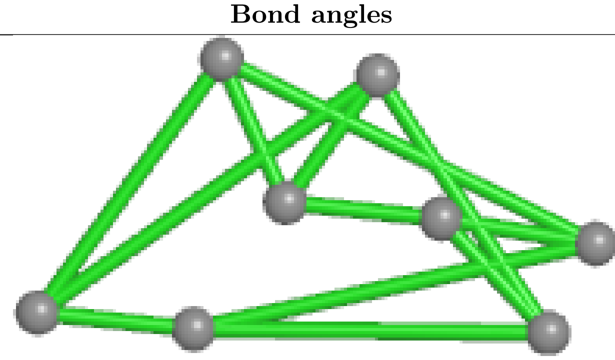

Rings

Ligand SF4 A 501

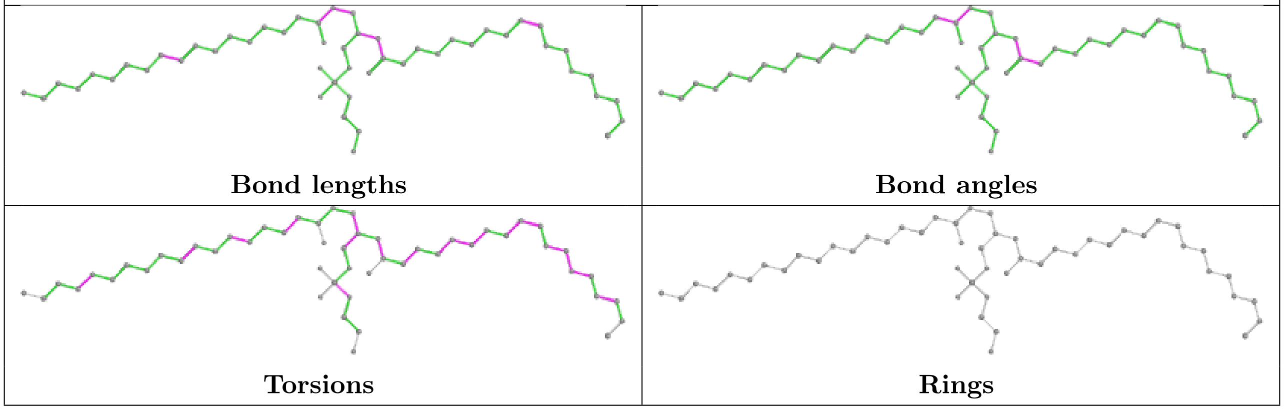

Bond lengths


Bond angles


Torsions

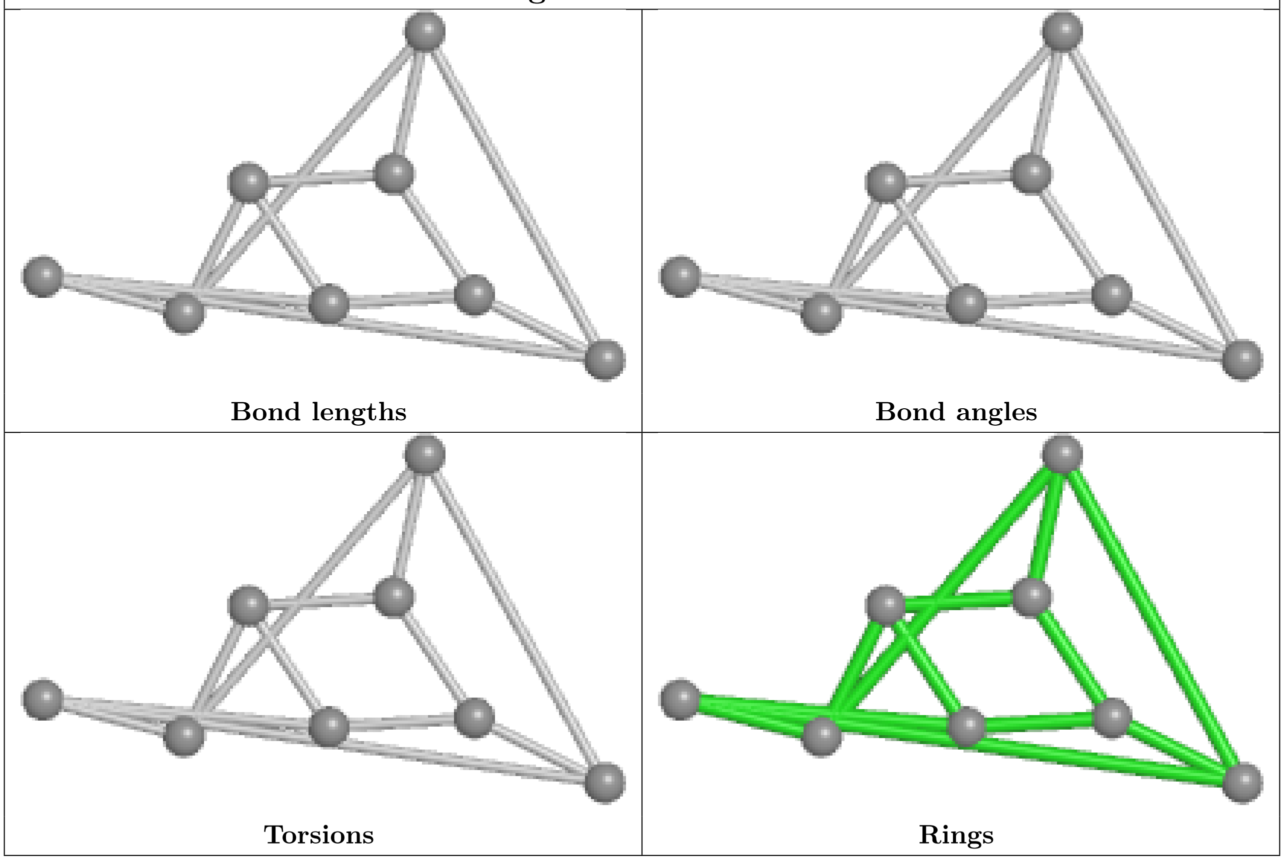

Rings

Ligand PEE r 501



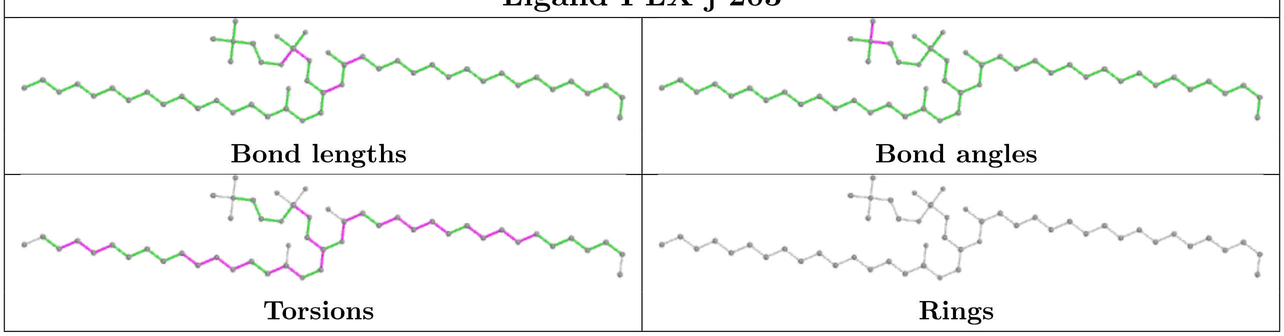
Bond lengths | Bond angles | Torsions | Rings

Ligand SF4 M 802



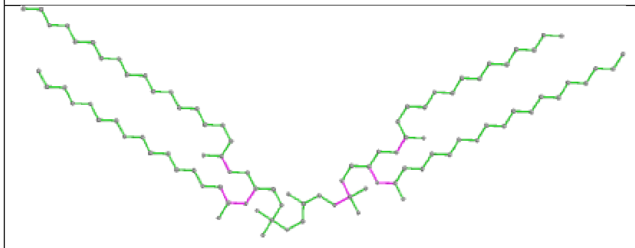
Bond lengths | Bond angles | Torsions | Rings

Ligand PLX j 203

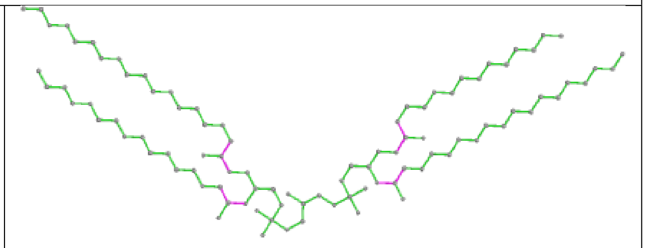


Bond lengths | Bond angles | Torsions | Rings

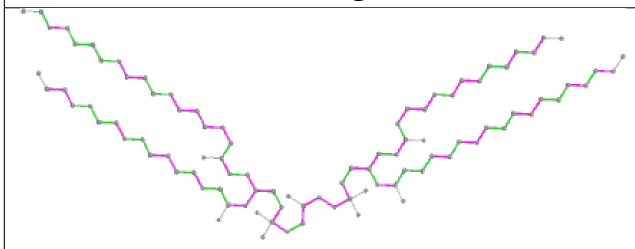
Ligand CDL V 201



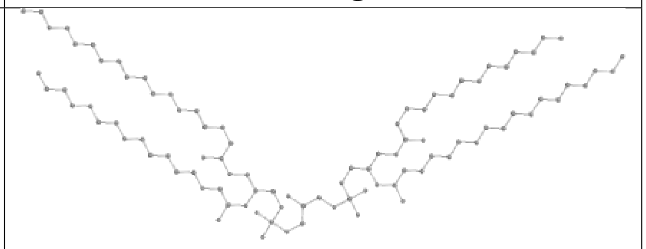
Bond lengths



Bond angles

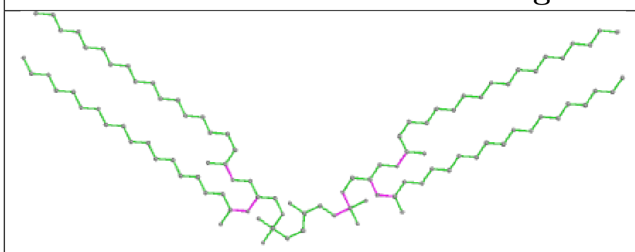


Torsions

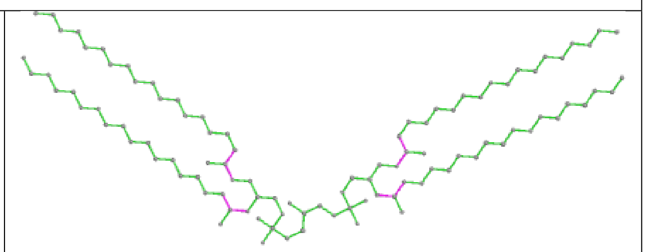


Rings

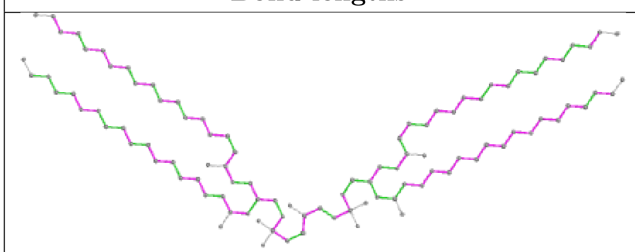
Ligand CDL l 702



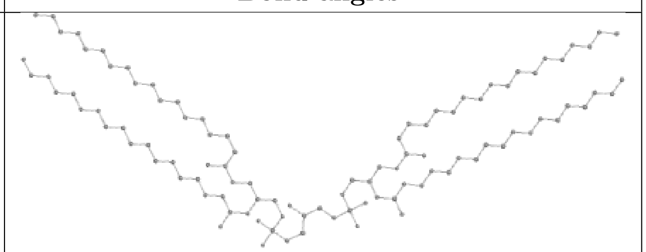
Bond lengths



Bond angles

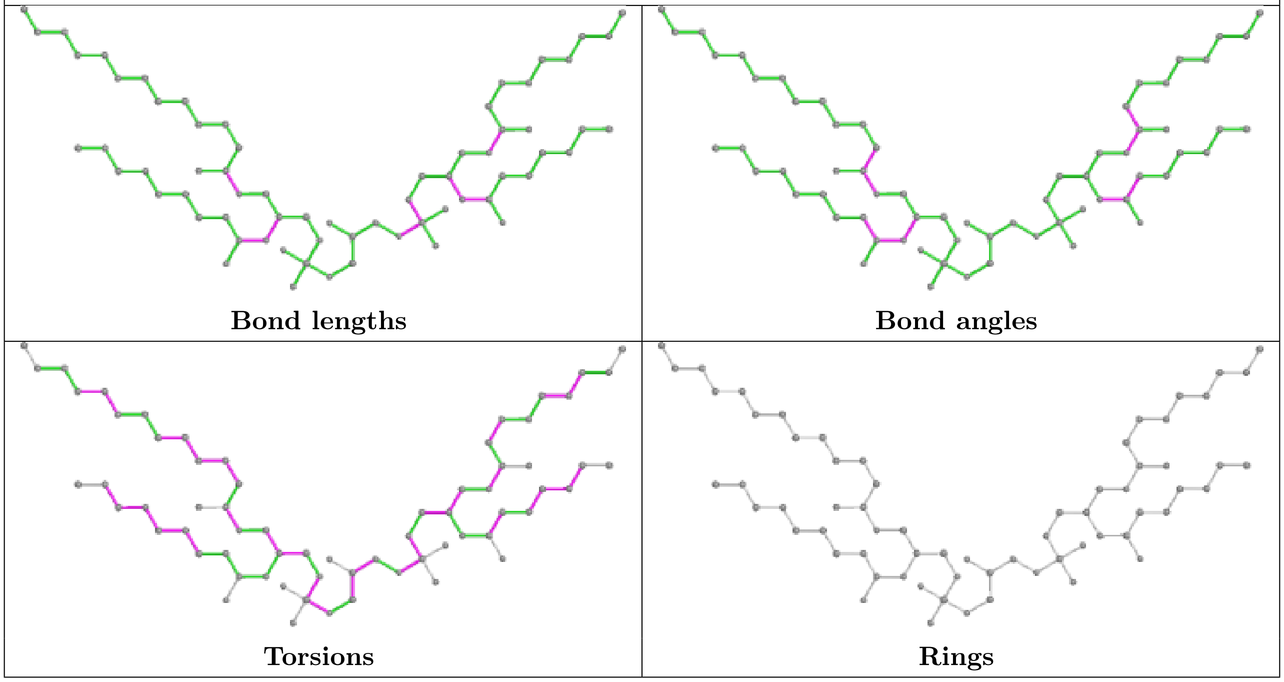


Torsions



Rings

Ligand CDL i 401



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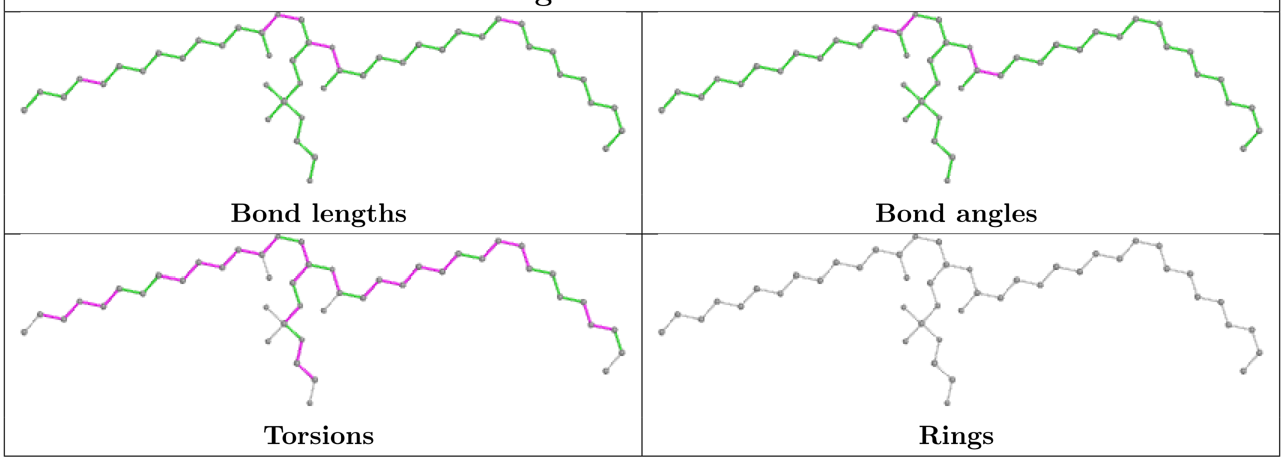
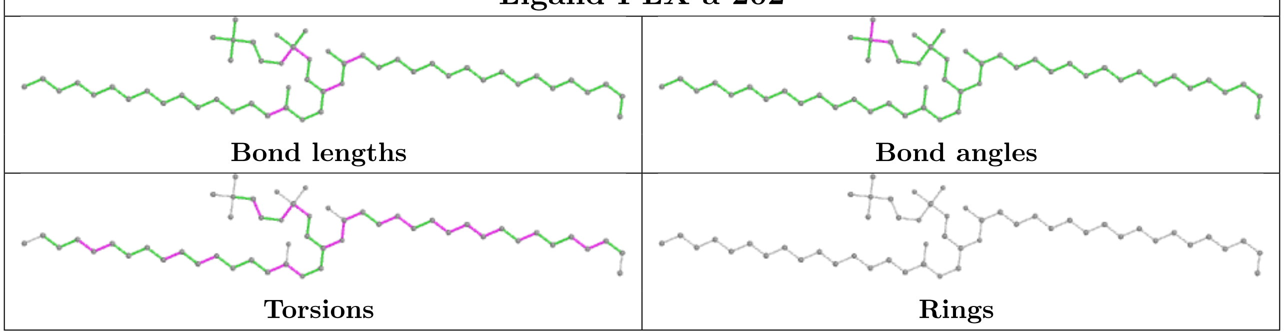
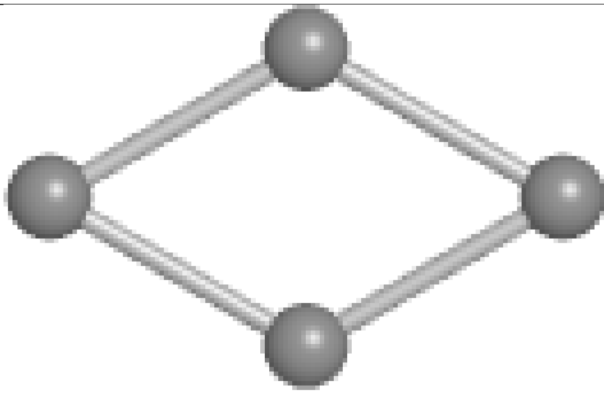
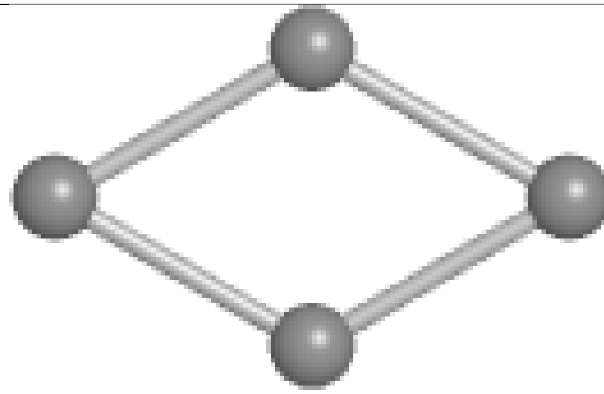
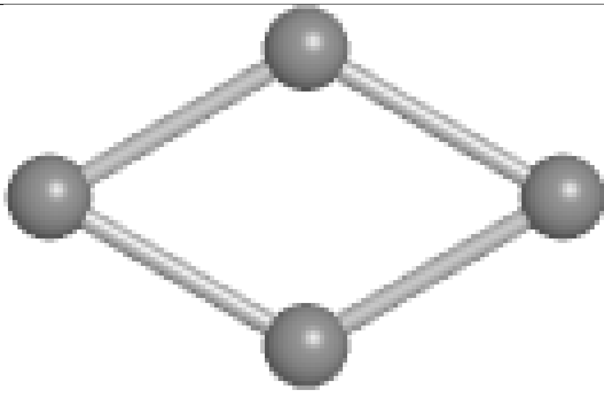
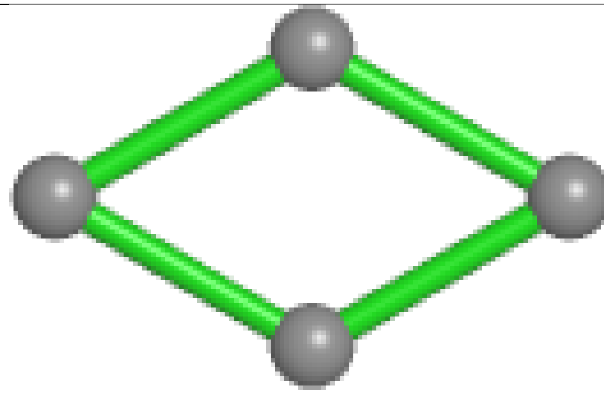
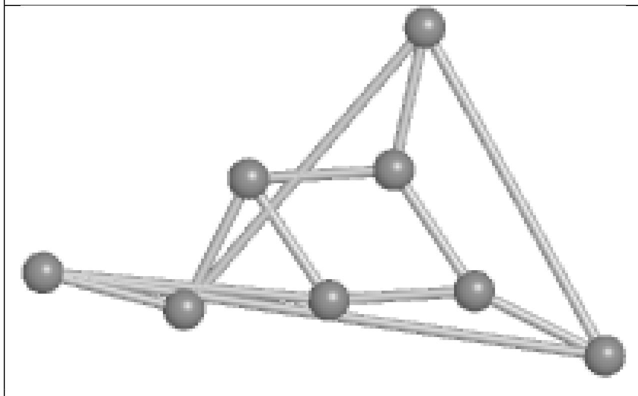


Ligand PLX a 202

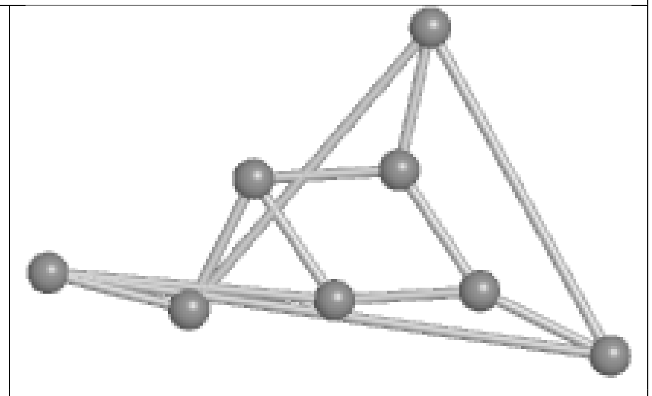


Ligand FES M 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

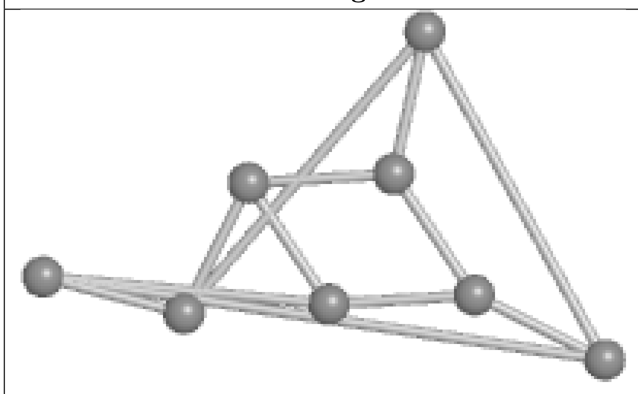
Ligand SF4 C 301



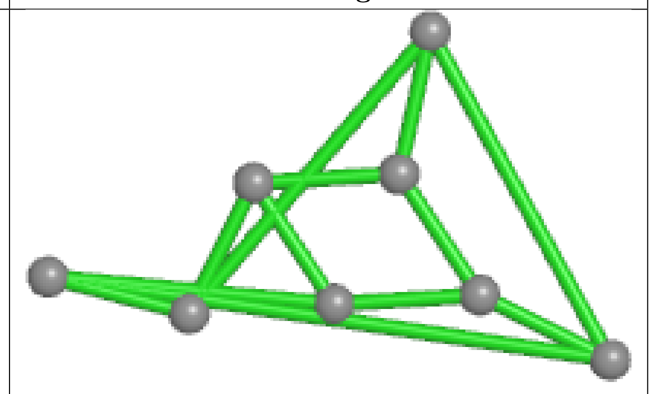
Bond lengths



Bond angles

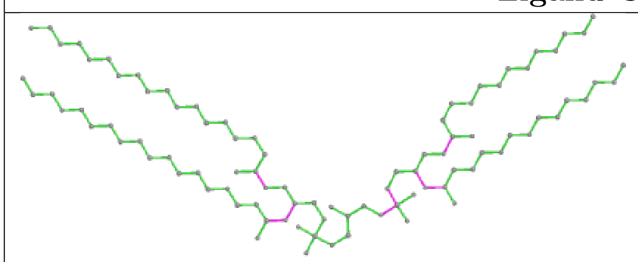


Torsions

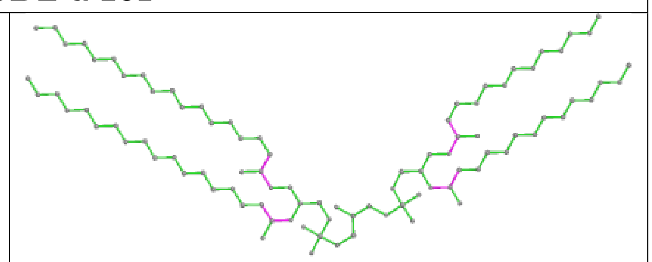


Rings

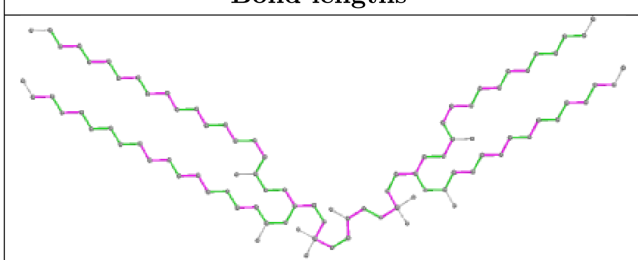
Ligand CDL a 201



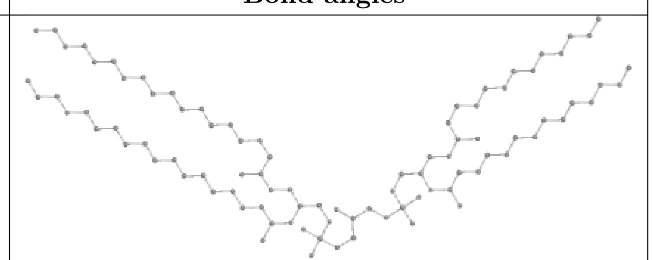
Bond lengths



Bond angles

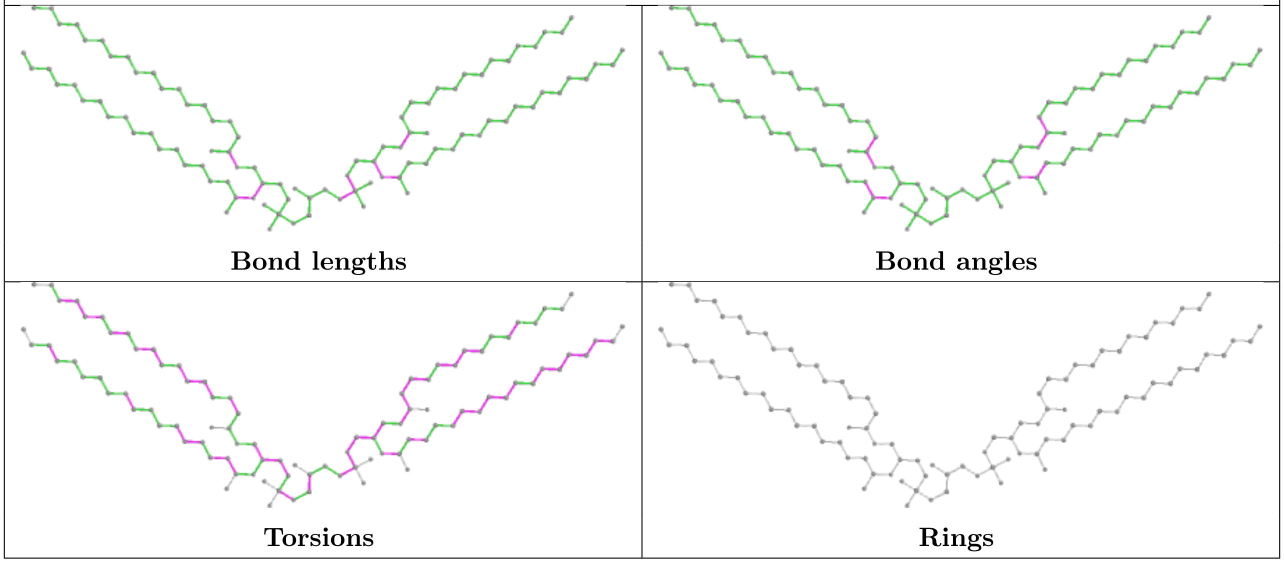


Torsions

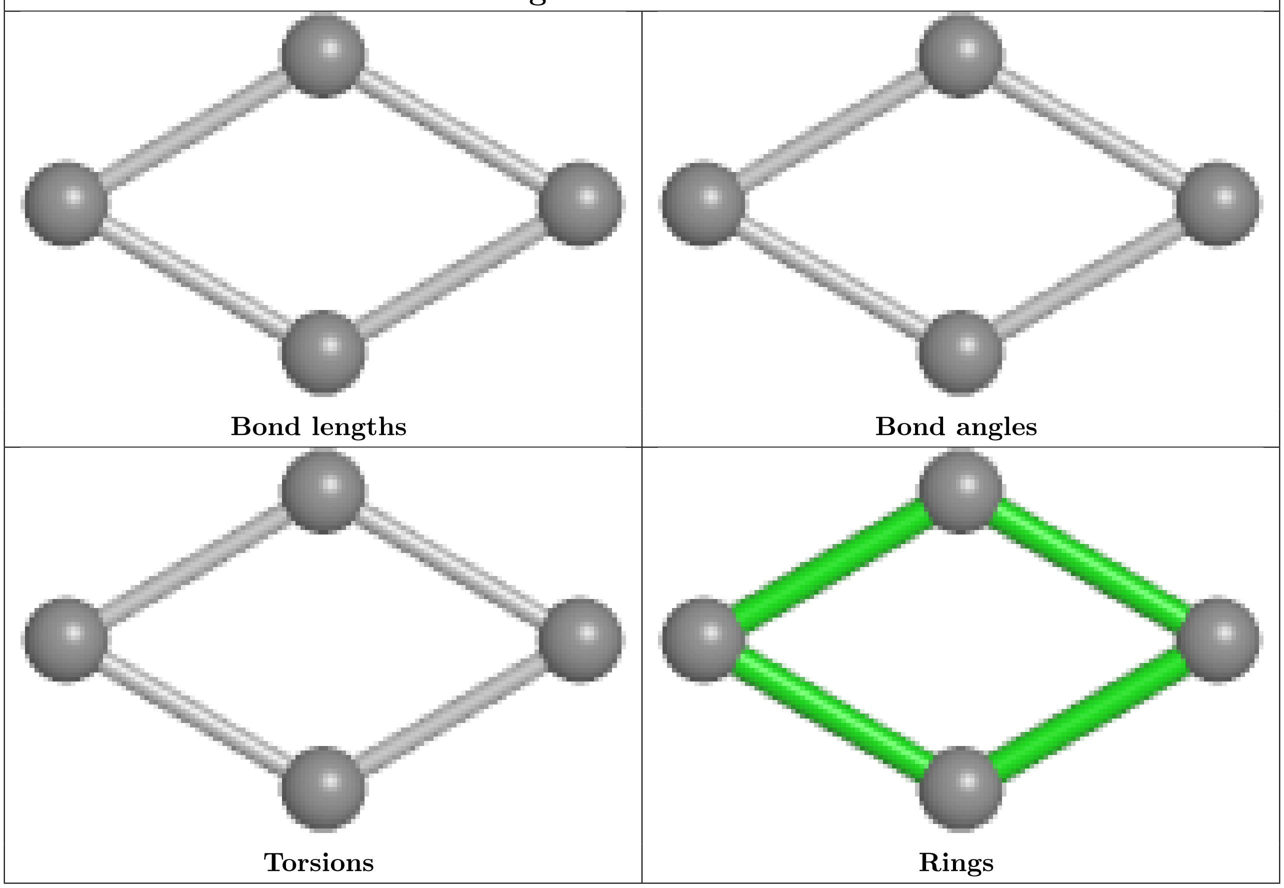


Rings

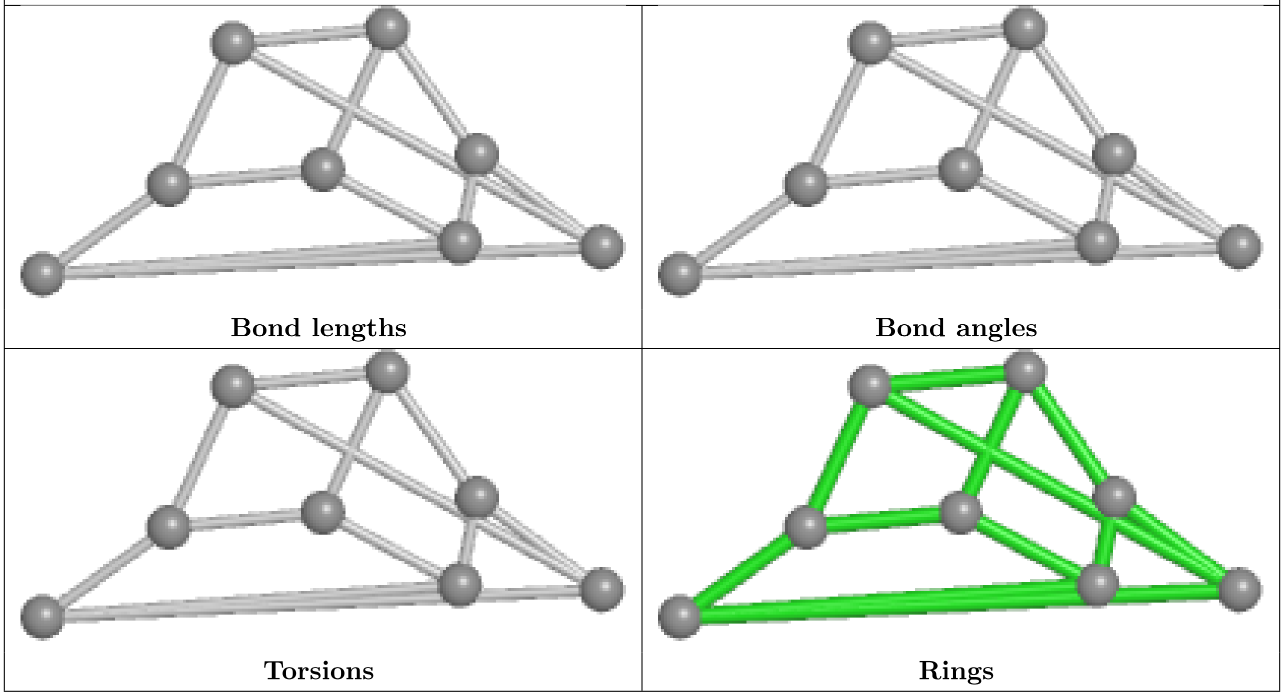
Ligand CDL g 202



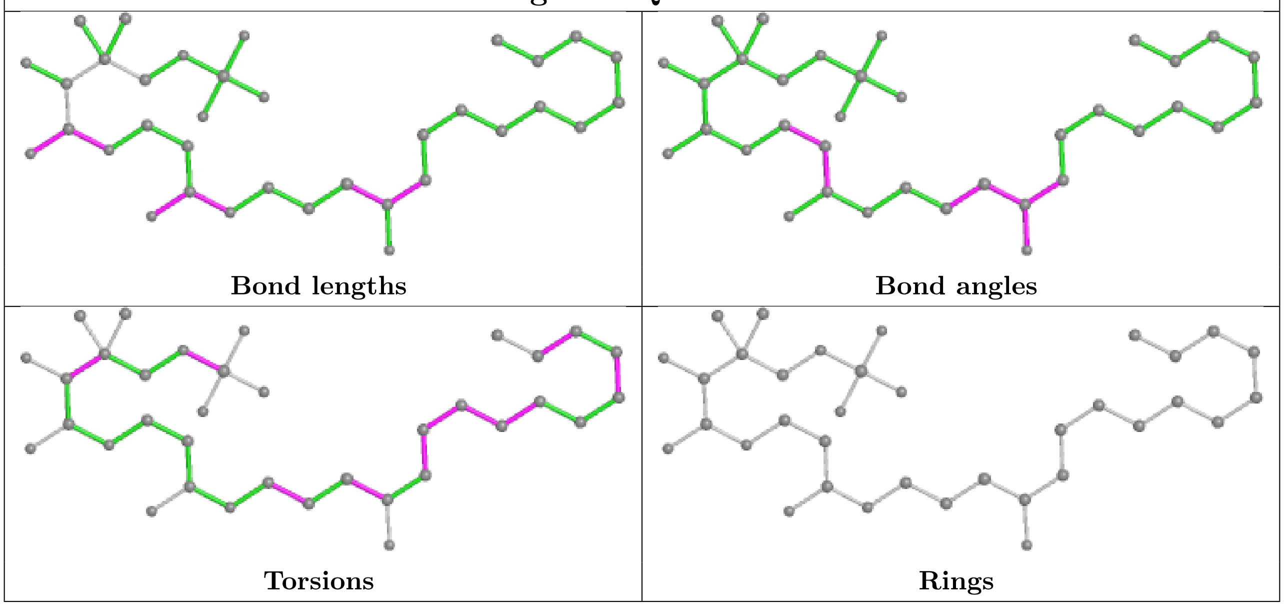
Ligand FES O 301



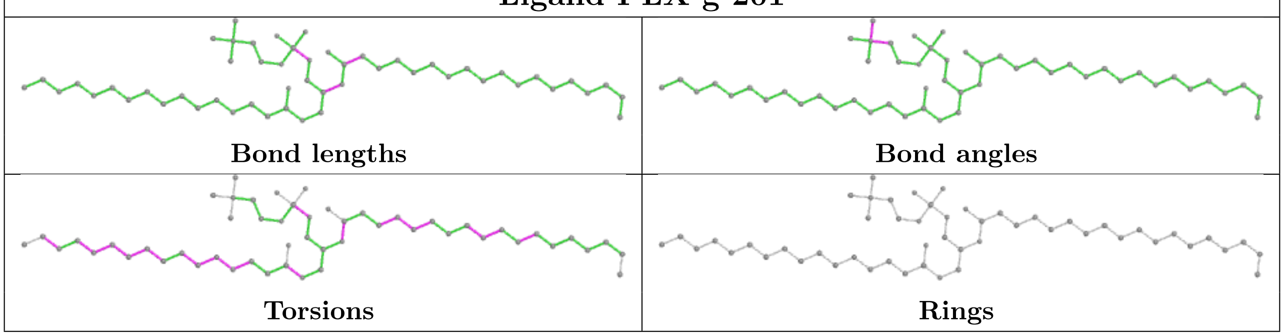
Ligand SF4 B 302

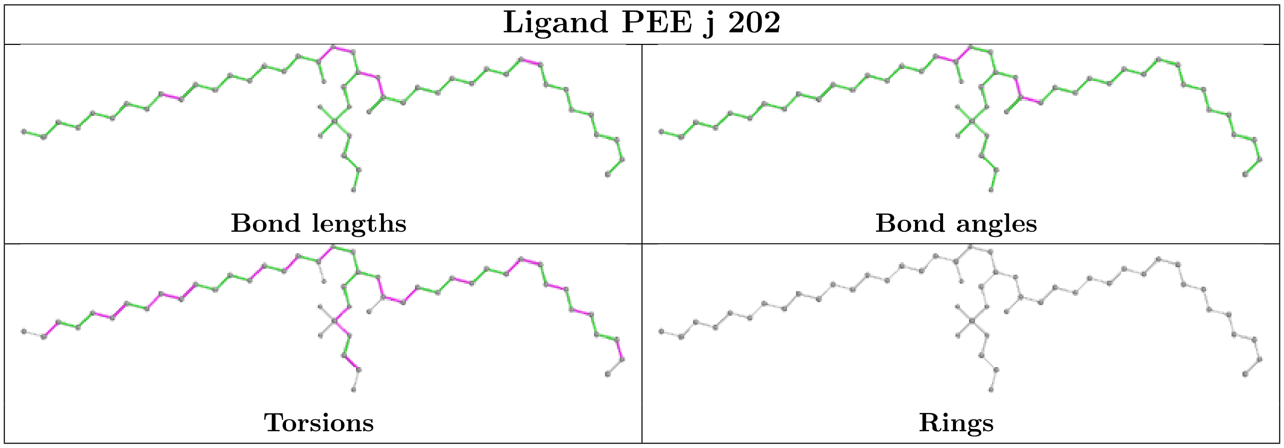


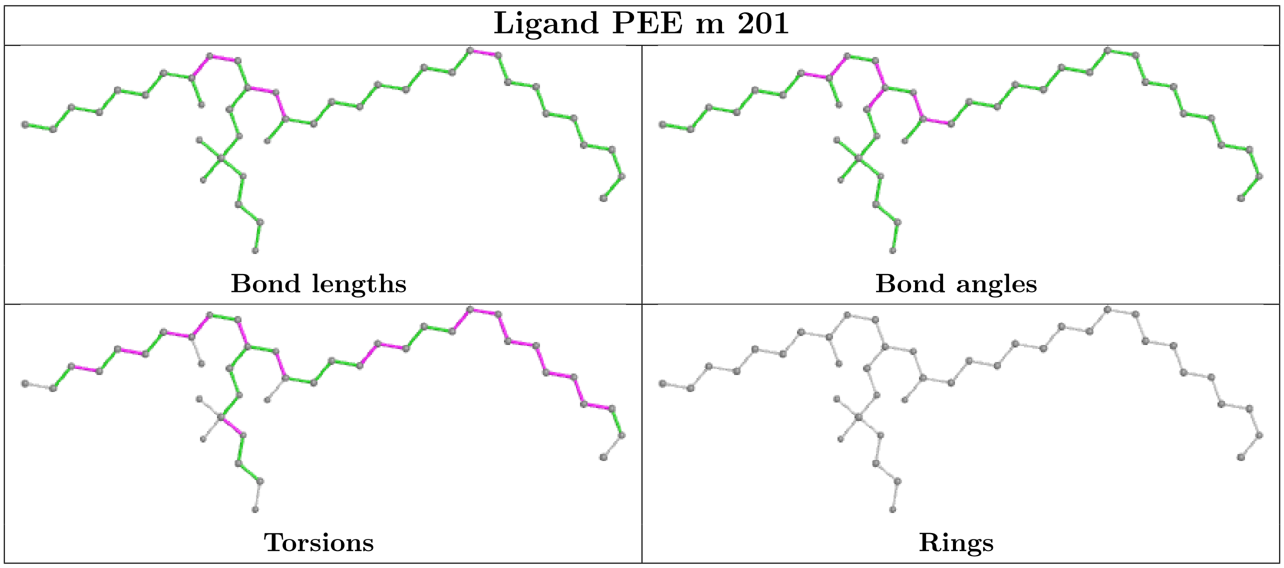
Ligand 8Q1 G 201



Ligand PLX g 201







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

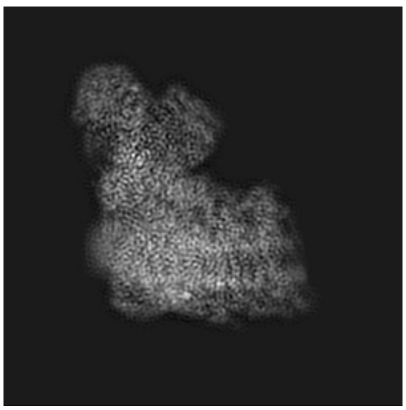
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32253. These allow visual inspection of the internal detail of the map and identification of artifacts.

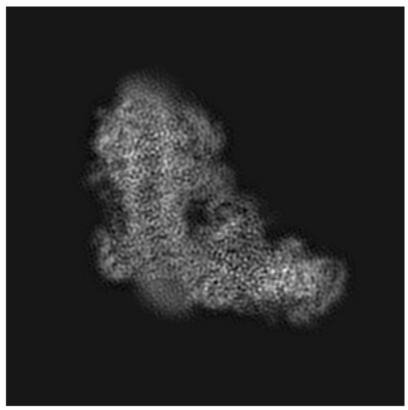
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

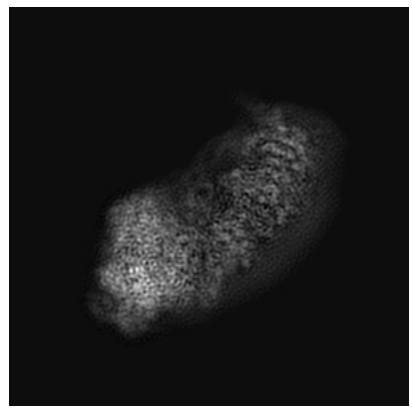
6.1.1 Primary map



X



Y

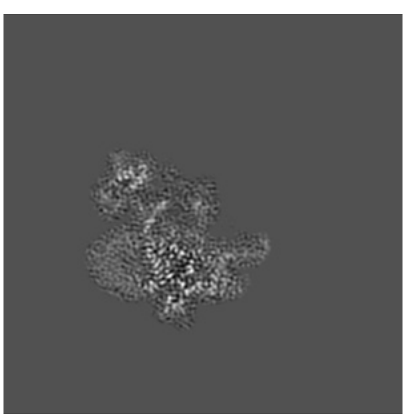


Z

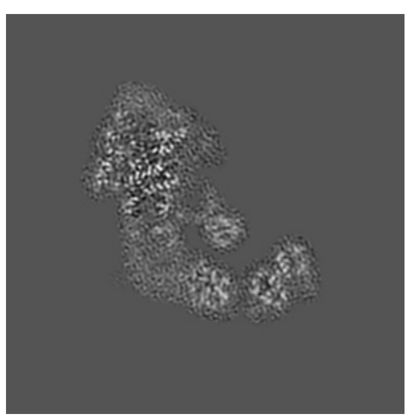
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

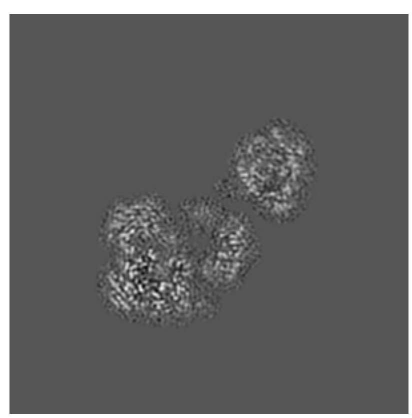
6.2.1 Primary map



X Index: 155



Y Index: 155

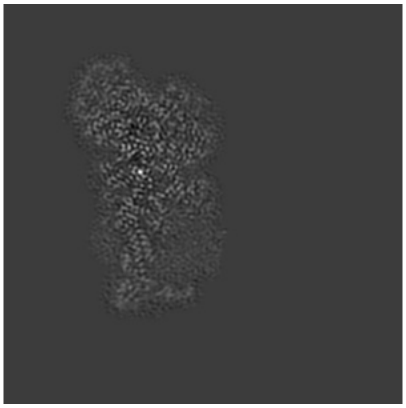


Z Index: 155

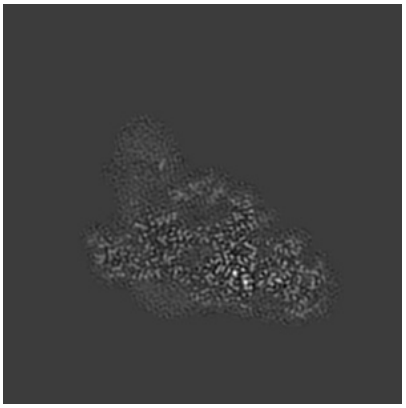
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

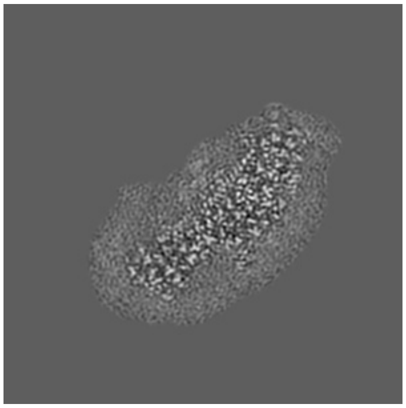
6.3.1 Primary map



X Index: 101



Y Index: 105

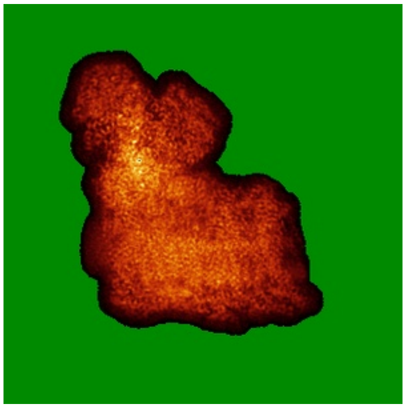


Z Index: 121

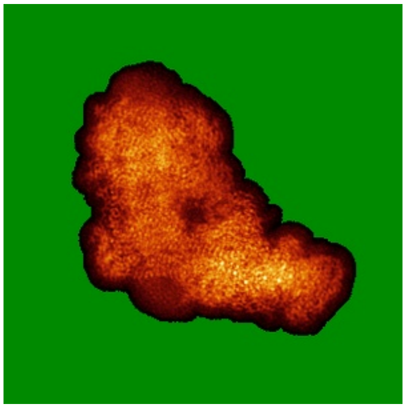
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

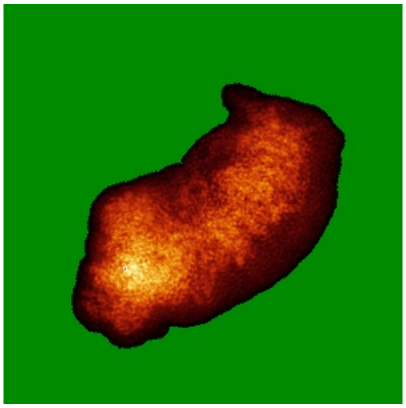
6.4.1 Primary map



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 0.0267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

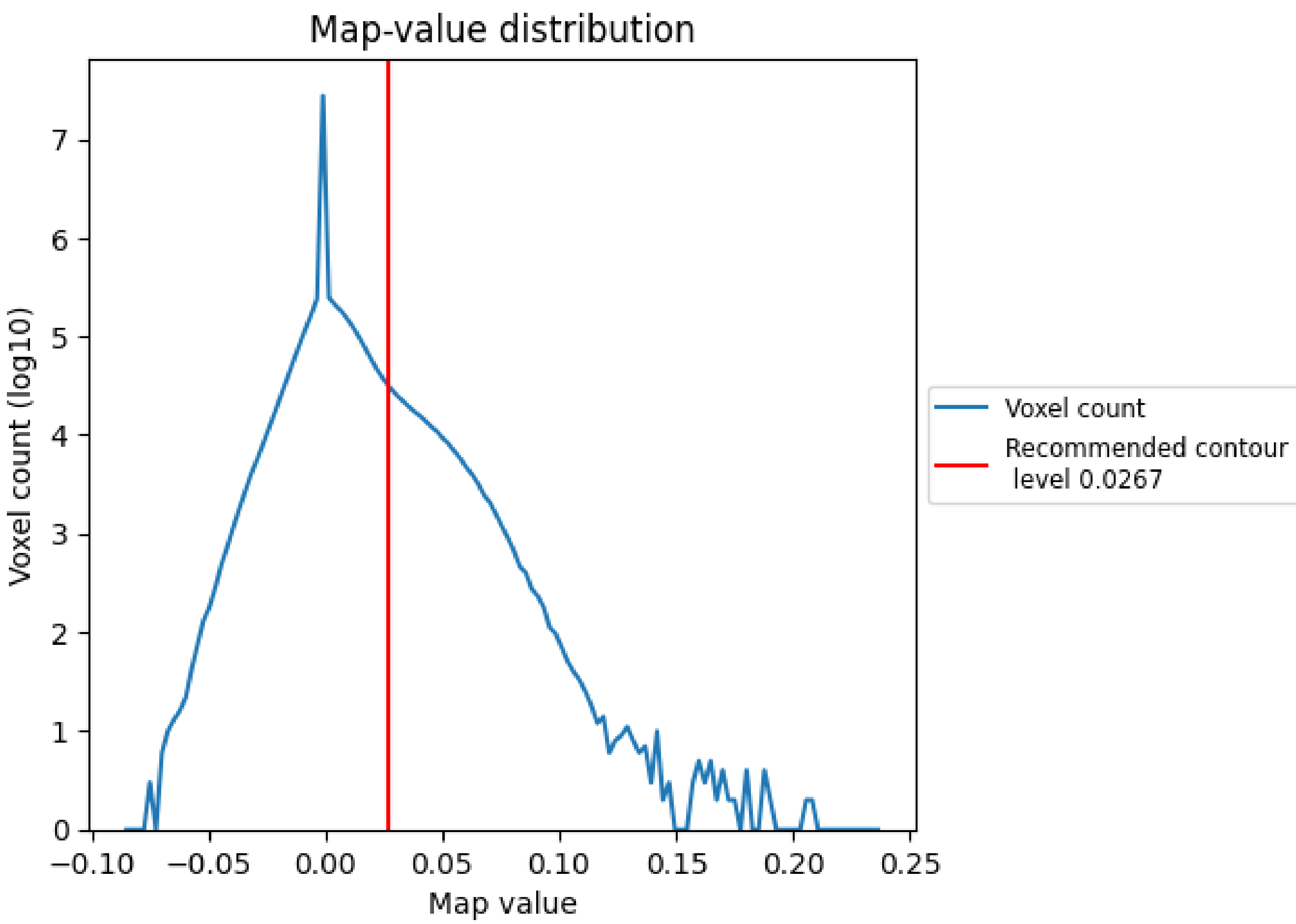
6.6 Mask visualisation (i)

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

7 Map analysis (i)

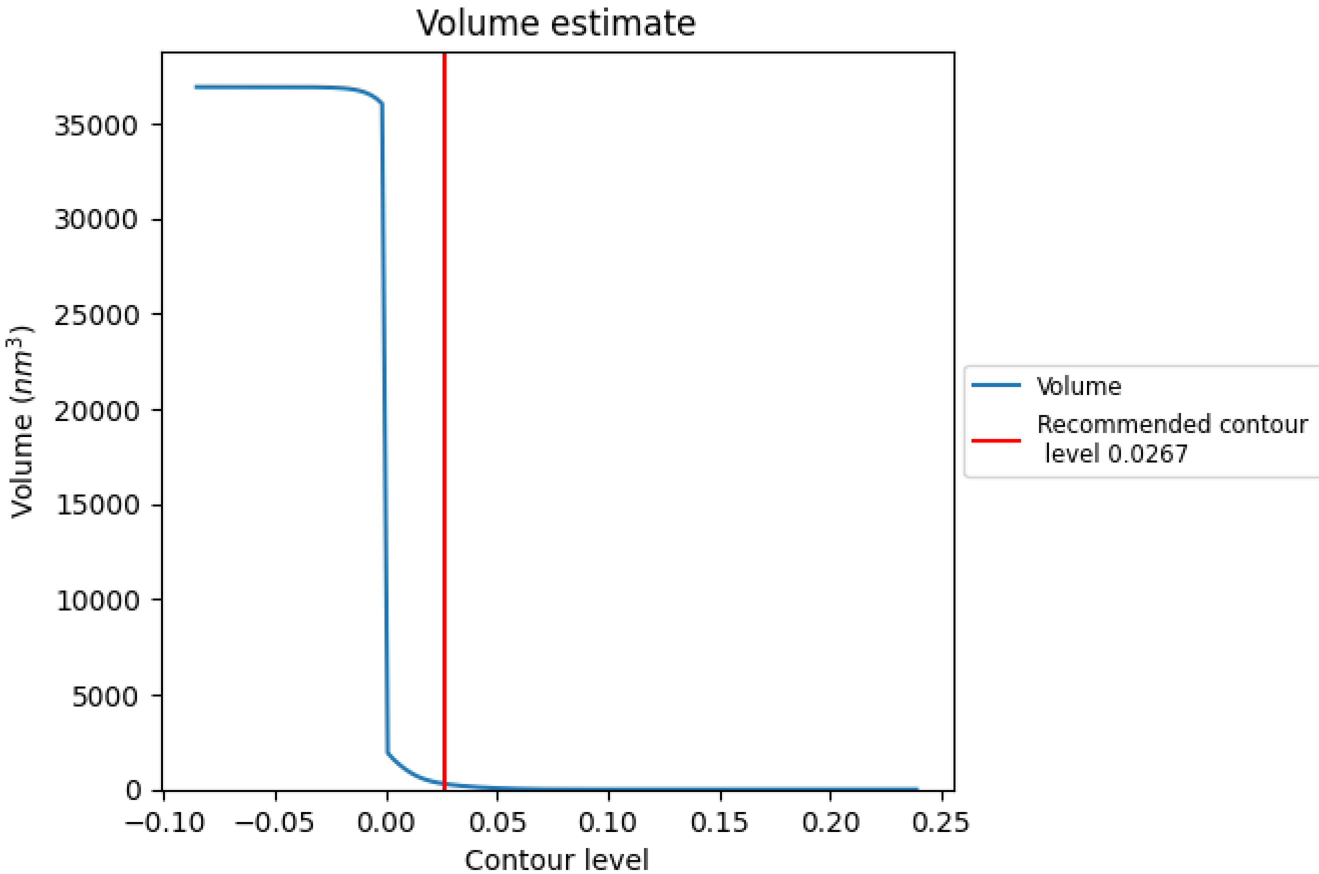
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

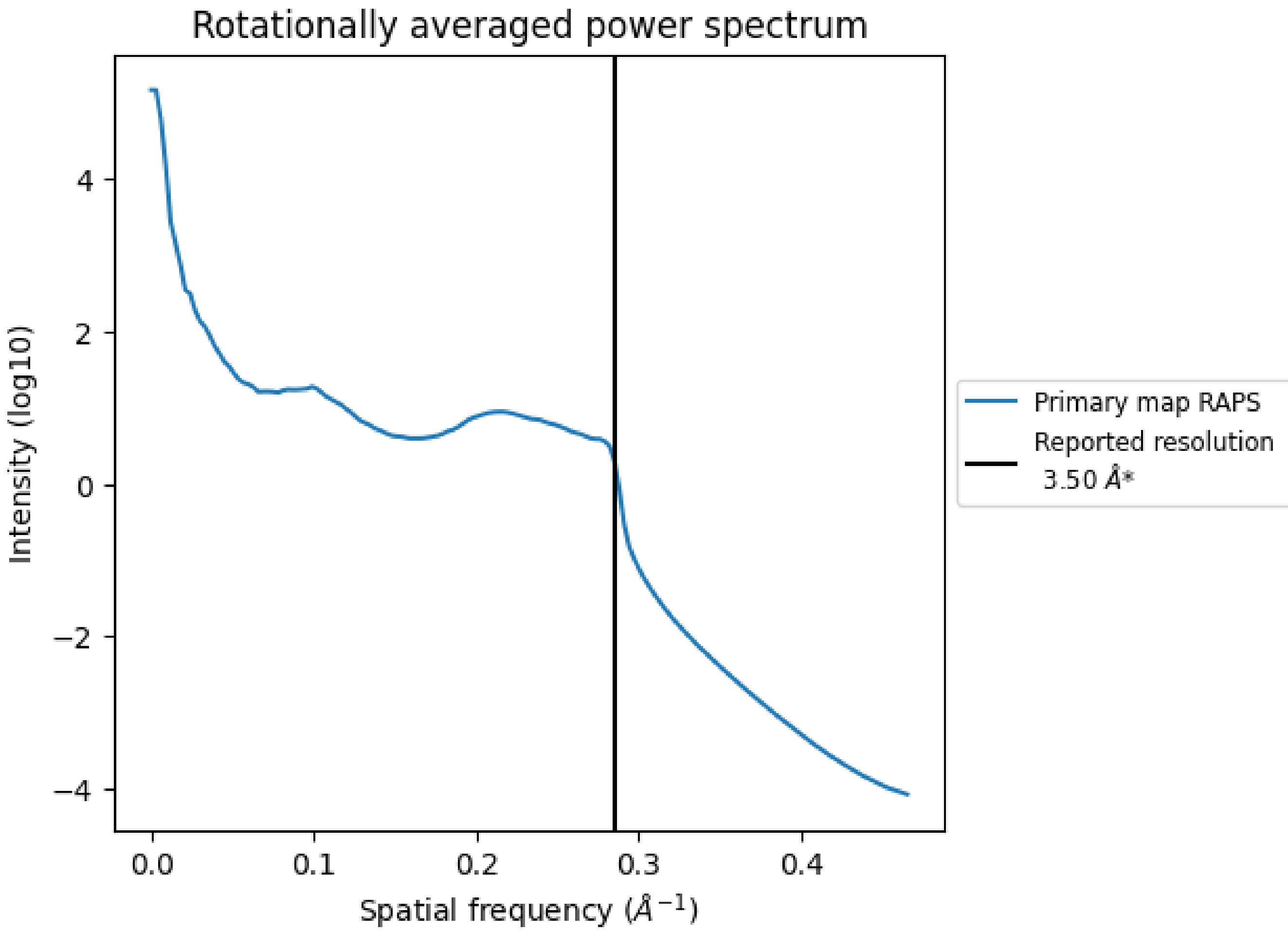
7.2 Volume estimate (i)



The volume at the recommended contour level is 289 nm^3; this corresponds to an approximate mass of 261 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

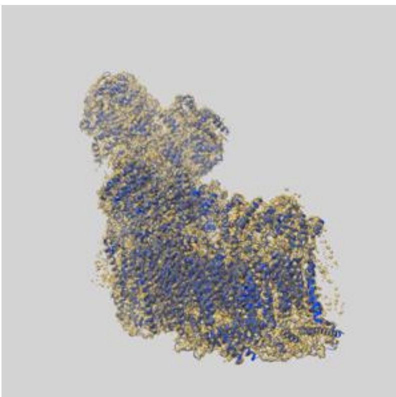
8 Fourier-Shell correlation (i)

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

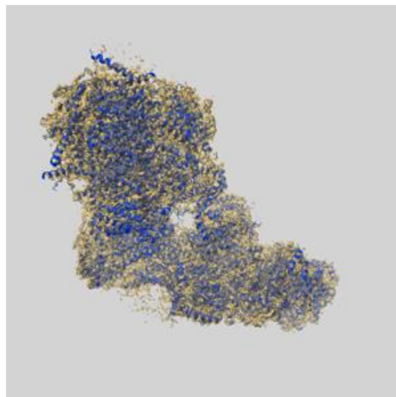
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32253 and PDB model 7W1O. Per-residue inclusion information can be found in section 3 on page 20.

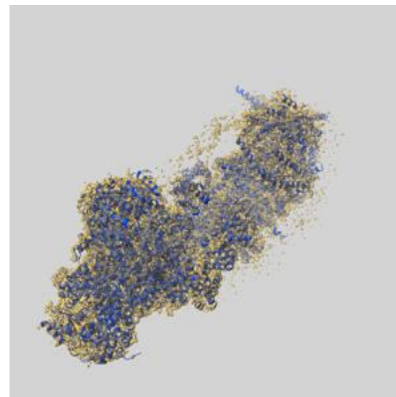
9.1 Map-model overlay (i)



X



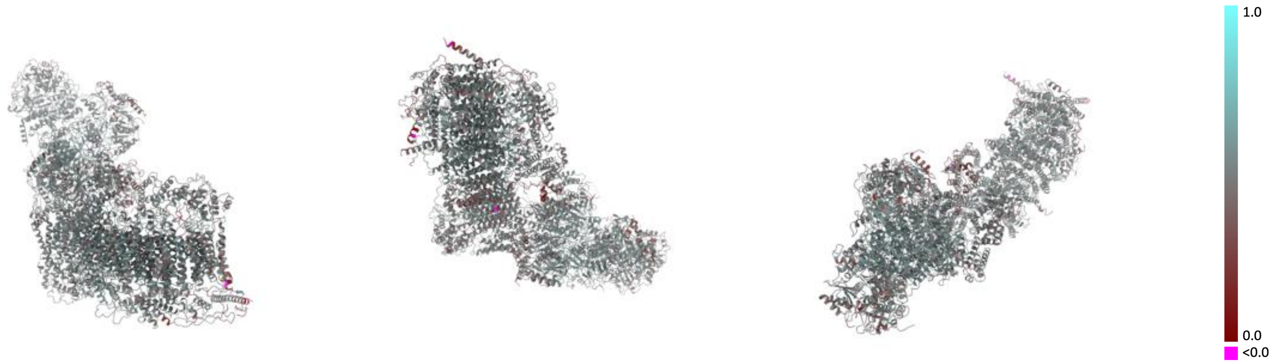
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

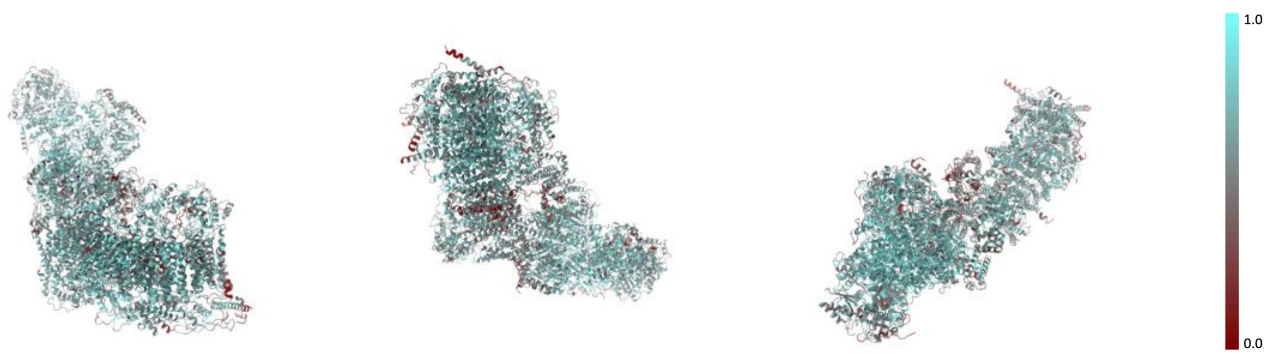
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

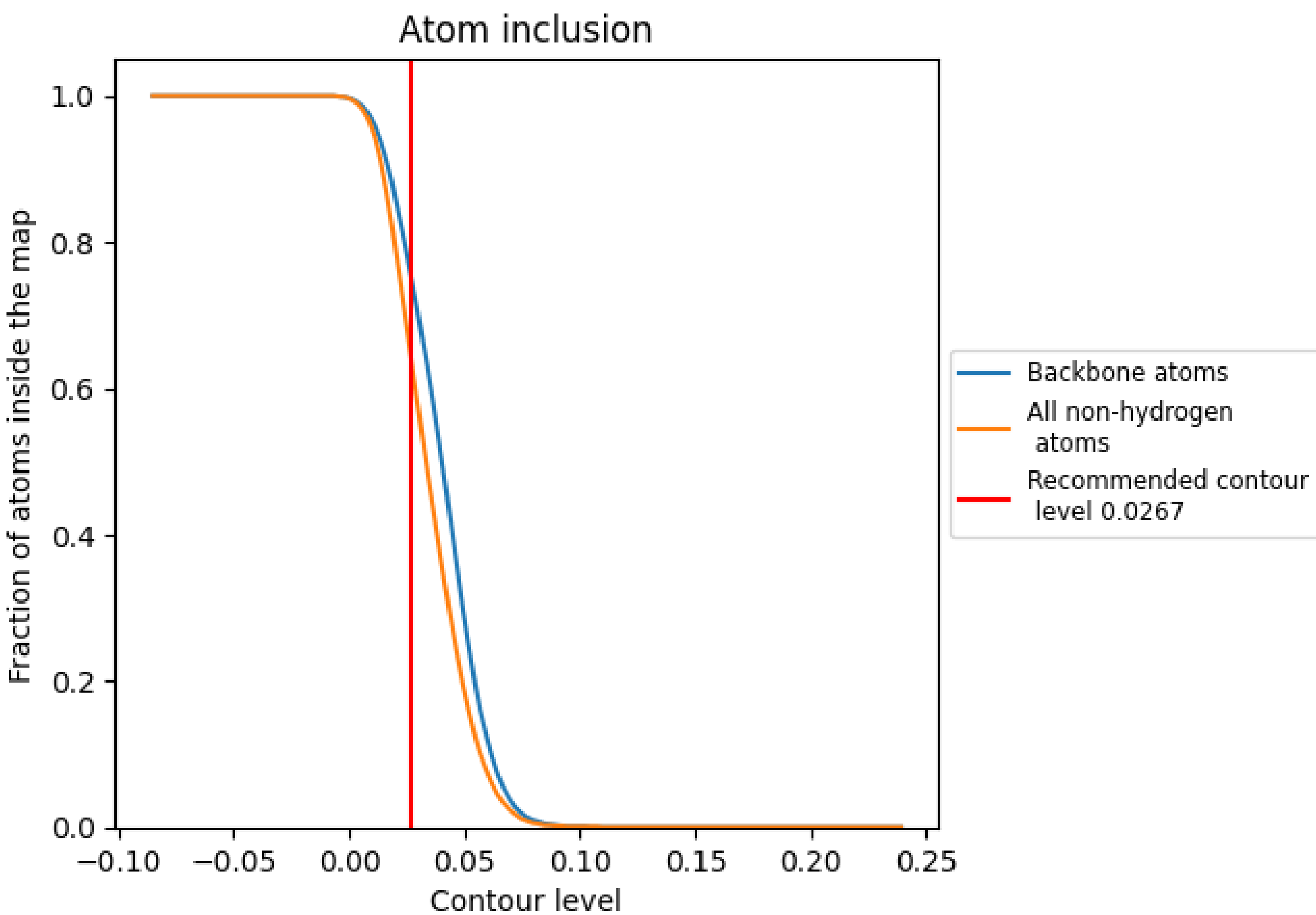
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0267).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6440	0.5020
A	0.6230	0.4850
B	0.7710	0.5530
C	0.7660	0.5350
E	0.6670	0.5000
F	0.5370	0.4390
G	0.3860	0.3860
H	0.6160	0.4880
I	0.6390	0.5110
J	0.6210	0.4870
K	0.6160	0.4970
L	0.6980	0.5360
M	0.7020	0.5200
N	0.6460	0.5080
O	0.6160	0.4840
P	0.7670	0.5420
Q	0.7420	0.5390
S	0.7030	0.5140
T	0.6870	0.5260
U	0.6250	0.4820
V	0.3520	0.4240
W	0.6730	0.5070
X	0.5500	0.4730
Y	0.4960	0.4390
Z	0.4620	0.3890
a	0.6520	0.5090
b	0.5710	0.4670
c	0.6520	0.5010
d	0.6270	0.4840
e	0.5990	0.4880
f	0.5810	0.4700
g	0.6470	0.5170
h	0.6430	0.4920
i	0.7130	0.5320
j	0.5140	0.4740

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Chain	Atom inclusion	Q-score
k	0.5460	0.4780
l	0.6250	0.5070
m	0.5370	0.4710
n	0.5520	0.4760
o	0.6400	0.5010
p	0.6410	0.4980
r	0.7070	0.5340
s	0.6800	0.5120
u	0.6440	0.5040
v	0.5440	0.4520
w	0.6140	0.4850