Full wwPDB EM Validation Report ⓘ

Jan 24, 2023 – 06:33 PM JST

PDB ID	:	7W2L
EMDB ID	:	EMD-32264
Title	:	Deactive state CI from Rotenone-NADH dataset, Subclass 2
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-24
Resolution	:	3.00 Å(reported)

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

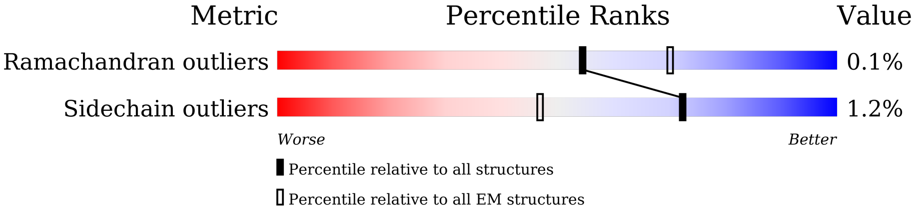
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

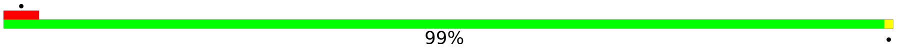
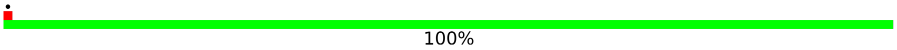
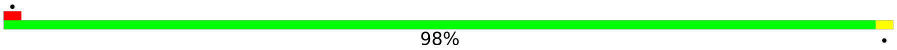
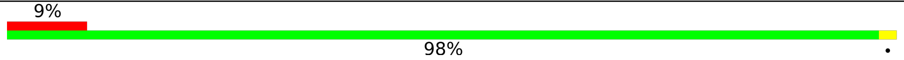
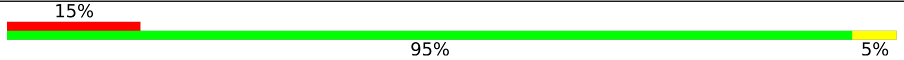
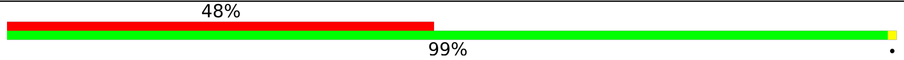
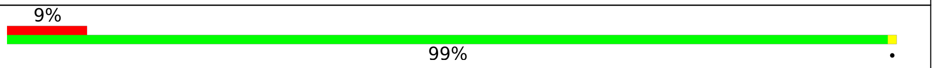
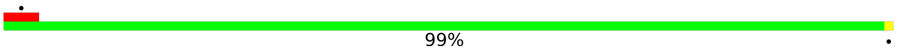
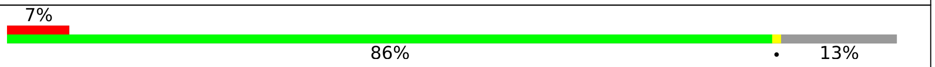
The reported resolution of this entry is 3.00 Å.

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	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	

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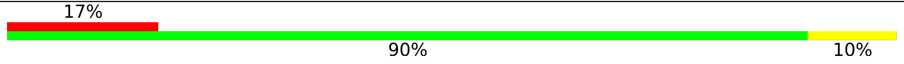
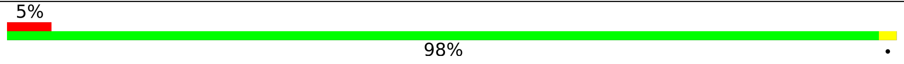
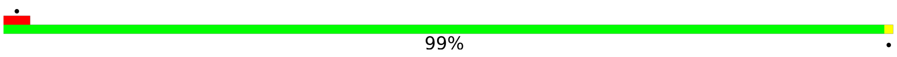
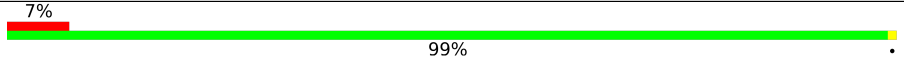
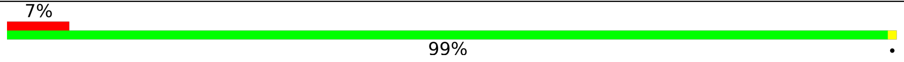
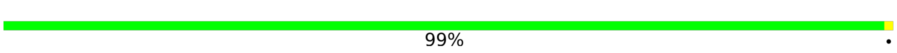
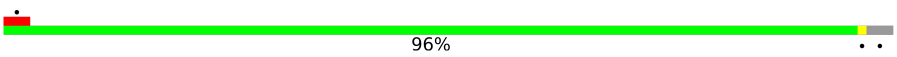
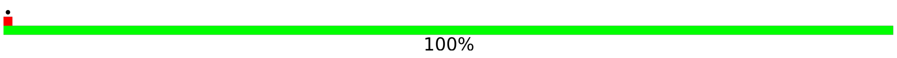
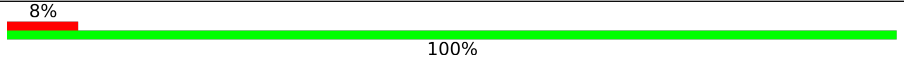
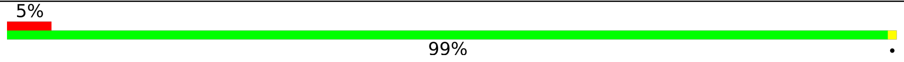
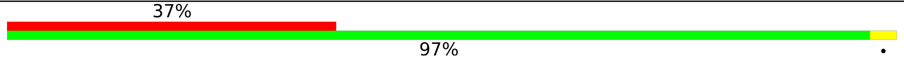
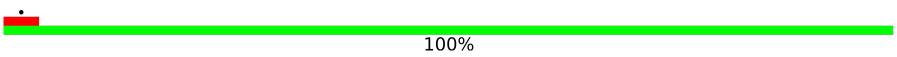
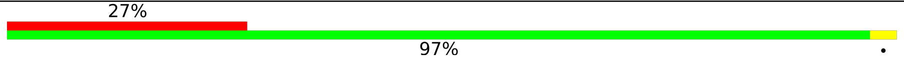
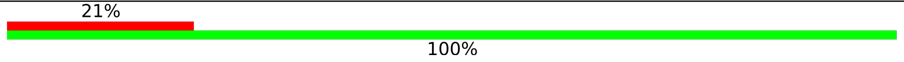
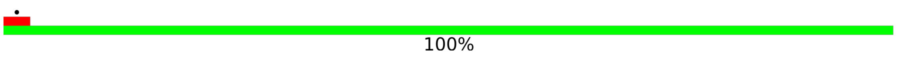
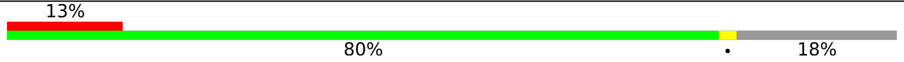
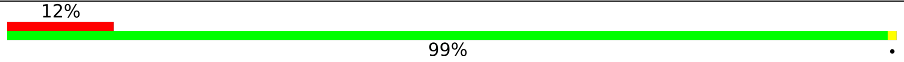
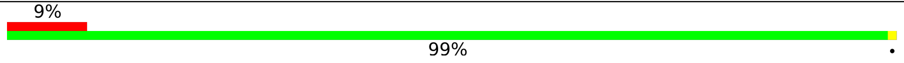
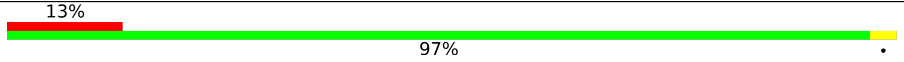
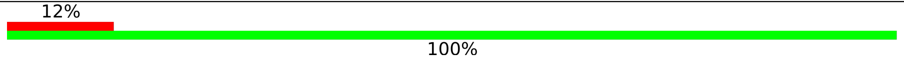
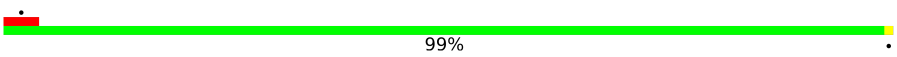
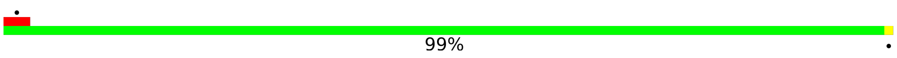
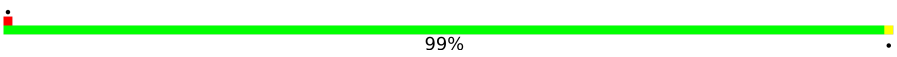
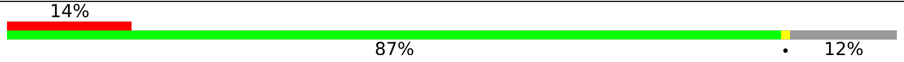
Mol	Chain	Length	Quality of chain
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	

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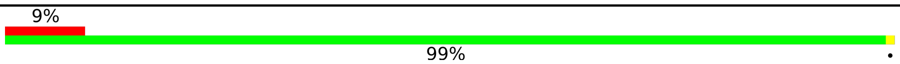
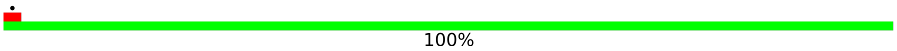
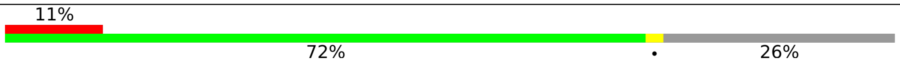
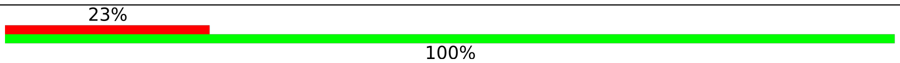
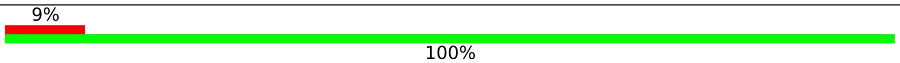
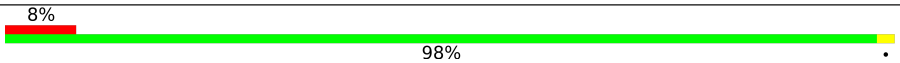
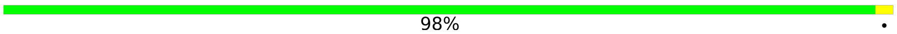
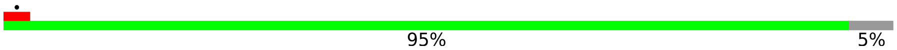
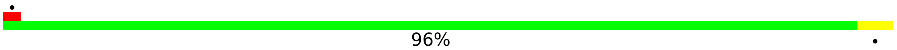
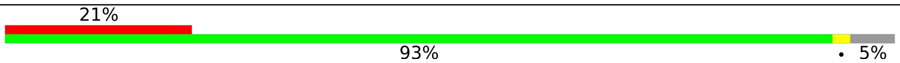
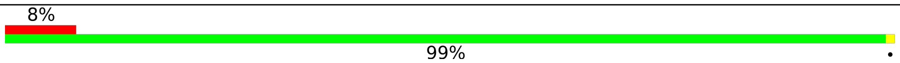
Mol	Chain	Length	Quality of chain
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	131	
44	w	320	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66472 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	C	N	O	S	0	0
			3314	2092	590	612	20		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			963	615	176	167	5		

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

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	683	440	102	137	4	0	0
6	X	88	696	449	103	139	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	762	479	144	136	3	0	0

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

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

- Molecule 10 is a protein called 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	1013	639	181	190	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	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	1017	649	174	188	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	1154	746	197	202	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	577	383	95	98	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	663	430	114	118	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	1152	754	196	199	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	875	571	158	145	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1457	914	265	270	8		

- 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	C	N	O	S	0	0
			890	568	145	173	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total 1054	C 685	N 180	O 189	0	0

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

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

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

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

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

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

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

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

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

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

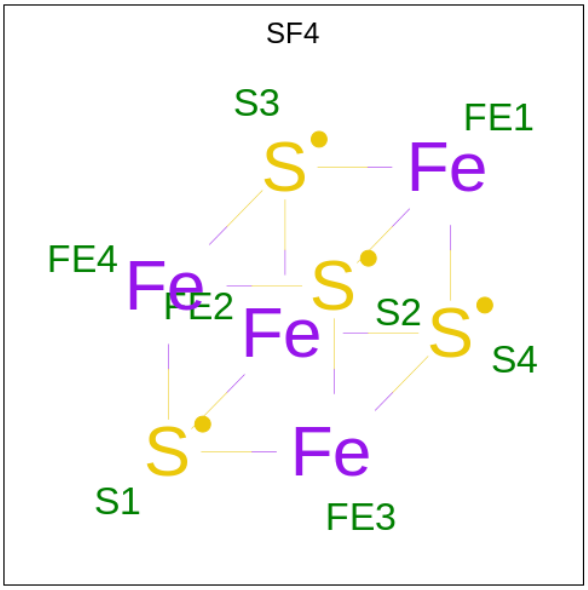
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1
v	126	ALA	GLN	conflict	UNP F1SCH1
v	128	ALA	PRO	conflict	UNP F1SCH1
v	130	ALA	GLU	conflict	UNP F1SCH1
v	131	ALA	VAL	conflict	UNP F1SCH1

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

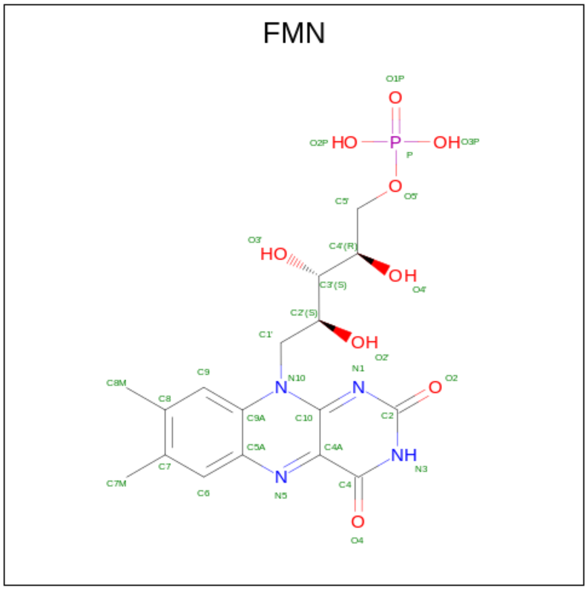
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2567	1632	437	488	10	0	0

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



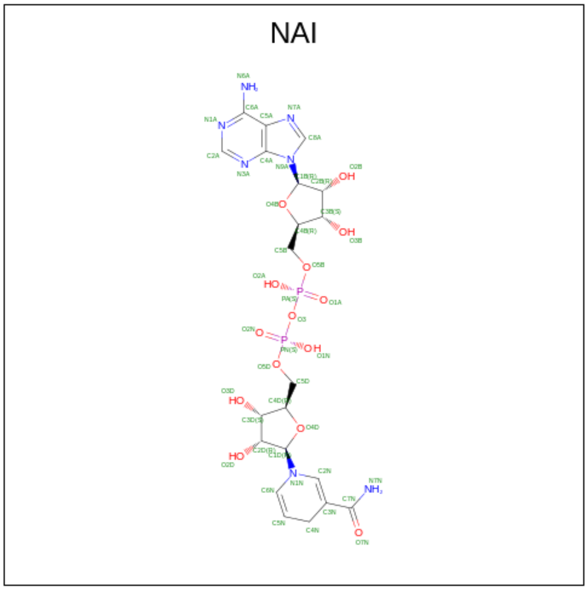
Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total Fe S 8 4 4	0
45	B	1	Total Fe S 16 8 8	0
45	B	1	Total Fe S 16 8 8	0
45	C	1	Total Fe S 8 4 4	0
45	M	1	Total Fe S 16 8 8	0
45	M	1	Total Fe S 16 8 8	0

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



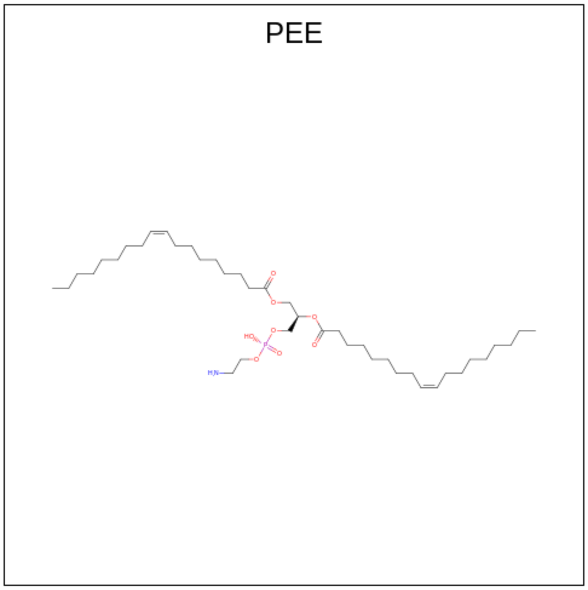
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

- 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).



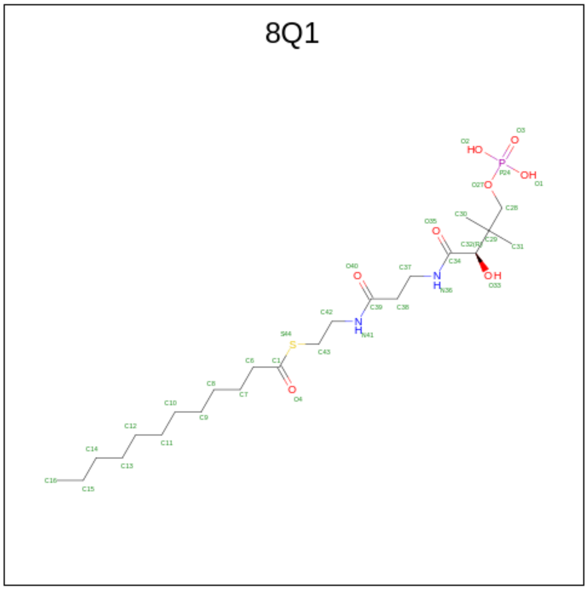
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

- 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).



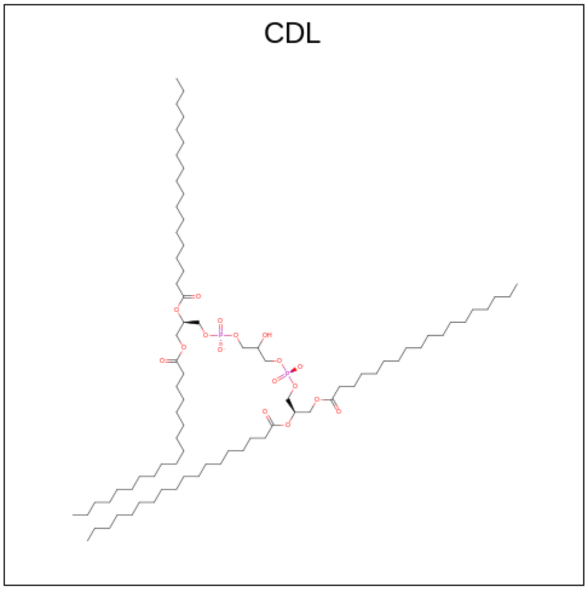
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	51	41	1	8	1	0
48	Q	1	47	37	1	8	1	0
48	U	1	51	41	1	8	1	0
48	j	1	47	37	1	8	1	0
48	l	1	92	72	2	16	2	0
48	l	1	92	72	2	16	2	0
48	m	1	41	31	1	8	1	0
48	r	1	51	41	1	8	1	0

- 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 C N O P S 35 23 2 8 1 1	0
49	X	1	Total C N O P S 35 23 2 8 1 1	0

- Molecule 50 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
50	I	1	Total C O P 51 32 17 2	0

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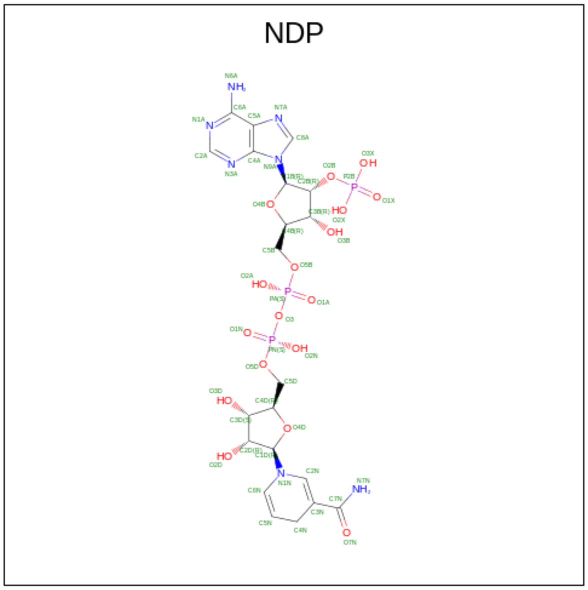
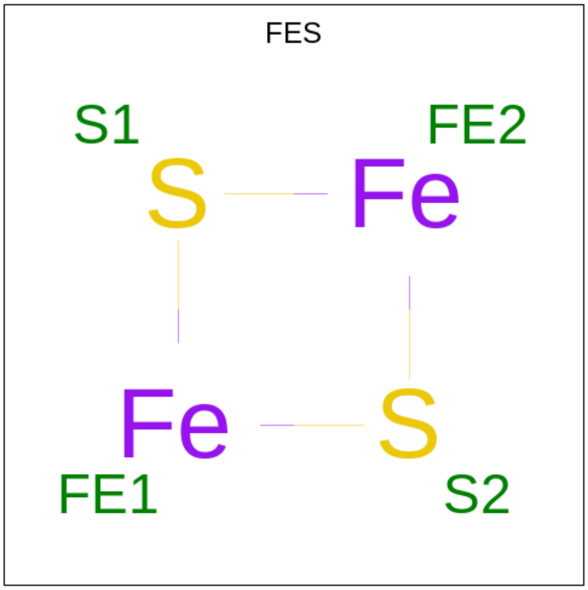
Mol	Chain	Residues	Atoms				AltConf
50	a	1	Total 91	C 72	O 17	P 2	0
50	g	1	Total 78	C 59	O 17	P 2	0
50	i	1	Total 66	C 47	O 17	P 2	0
50	l	1	Total 199	C 161	O 34	P 4	0
50	l	1	Total 199	C 161	O 34	P 4	0
50	r	1	Total 100	C 81	O 17	P 2	0

- Molecule 51 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
51	J	1	Total 48	C 21	N 7	O 17	P 3	0

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



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

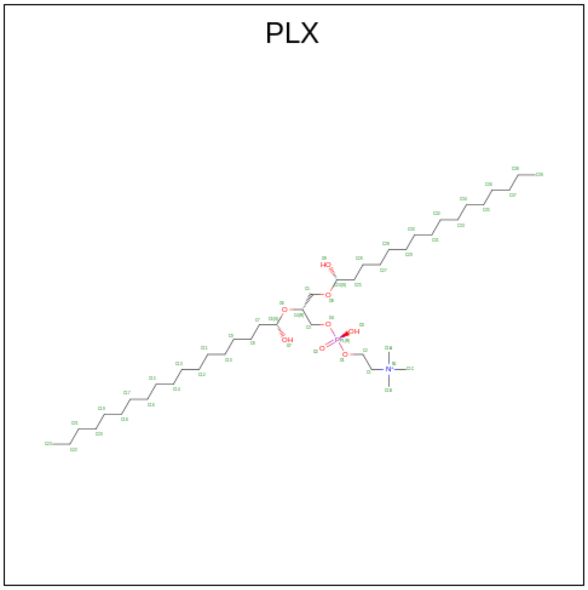
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

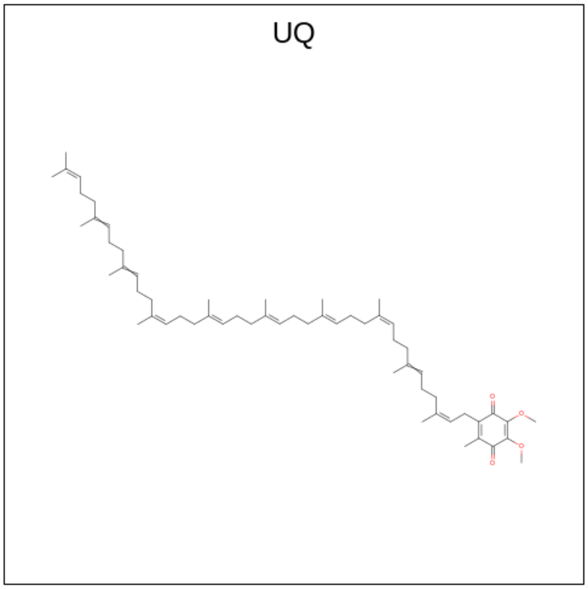
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total 1	Zn 1	0

- 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).



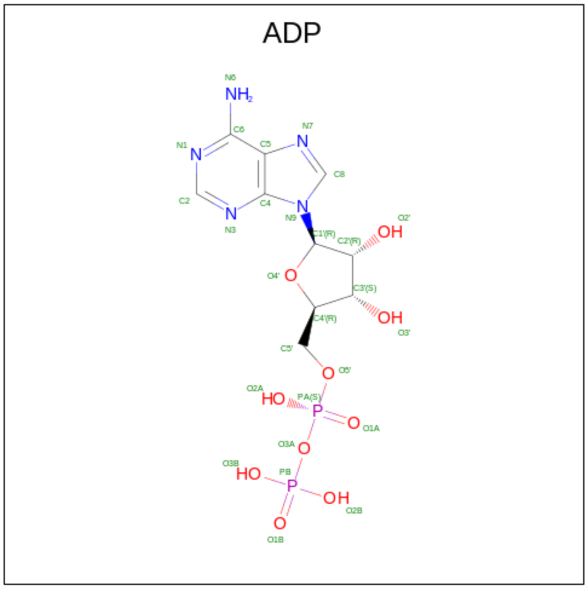
Mol	Chain	Residues	Atoms	AltConf
55	a	1	Total C N O P 52 42 1 8 1	0
55	g	1	Total C N O P 52 42 1 8 1	0
55	j	1	Total C N O P 52 42 1 8 1	0
55	r	1	Total C N O P 52 42 1 8 1	0

- 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
			Total	C	O	
56	s	1	28	24	4	0

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



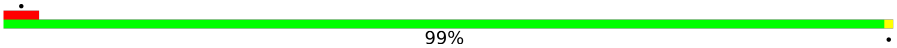
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

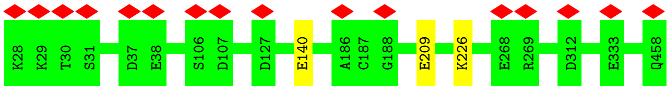
3 Residue-property plots ⓘ

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

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

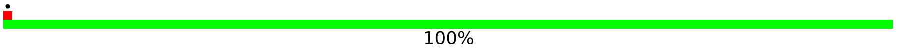
Chain A:

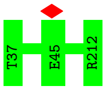




- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

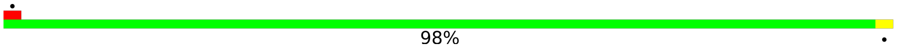
Chain B:

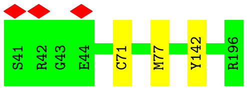




- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

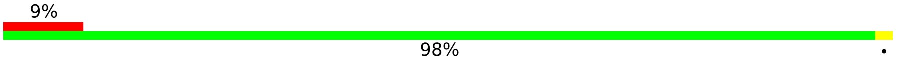
Chain C:

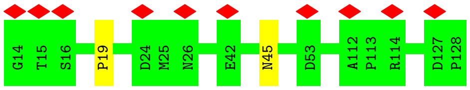




- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

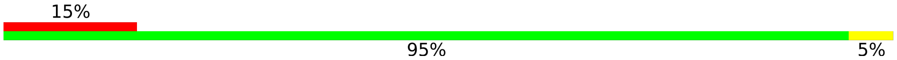
Chain E:

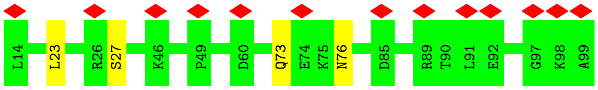




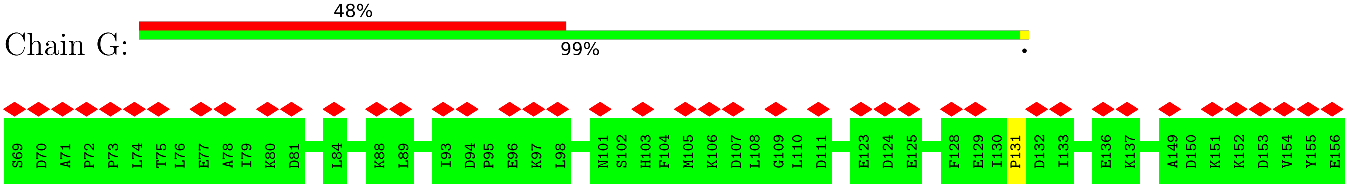
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:

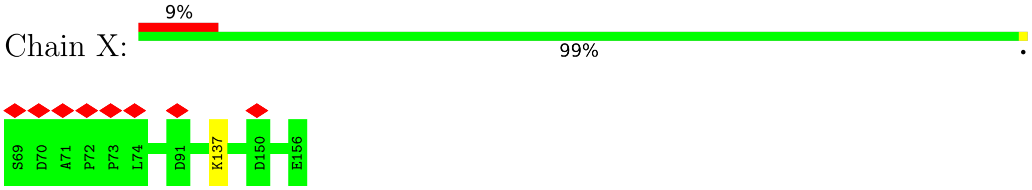




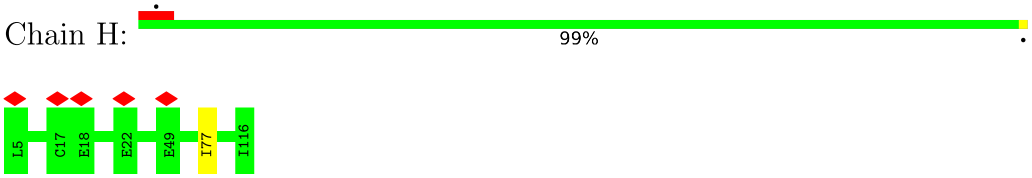
- Molecule 6: Acyl carrier protein



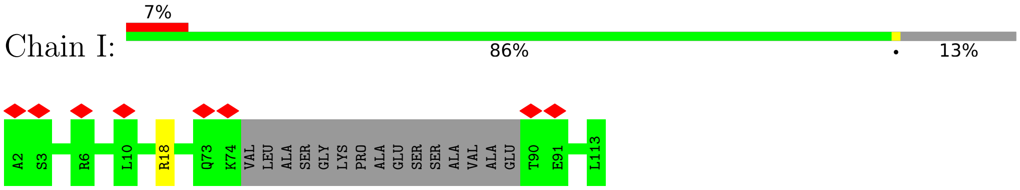
- Molecule 6: Acyl carrier protein



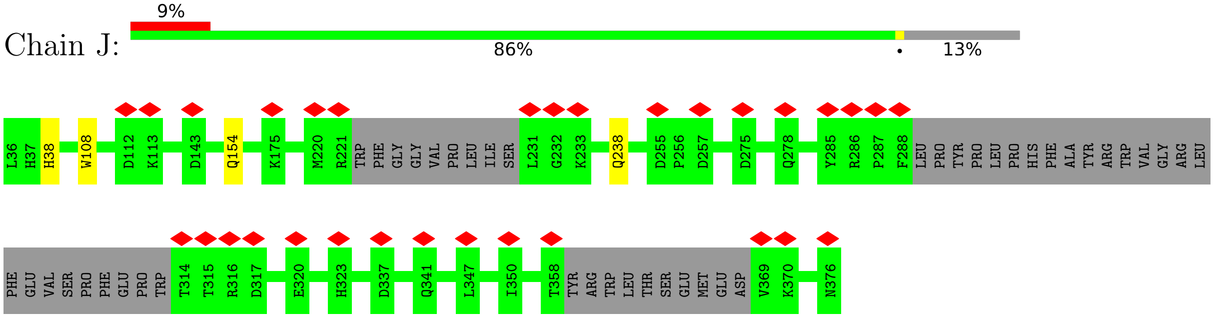
- Molecule 7: Complex I subunit B13



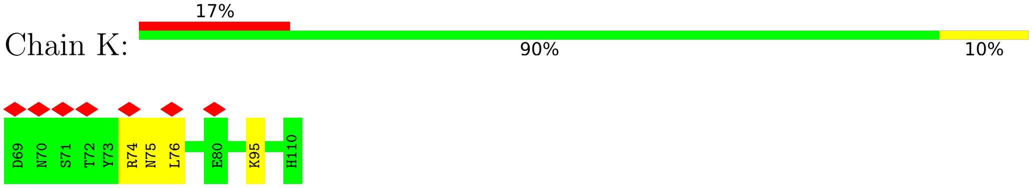
- Molecule 8: Complex I-B14.5a



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

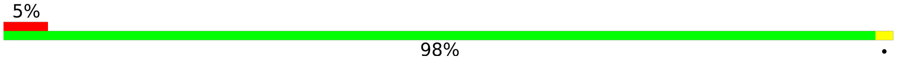


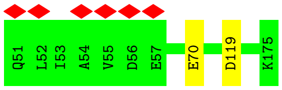
- Molecule 10: Complex I-9kD



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

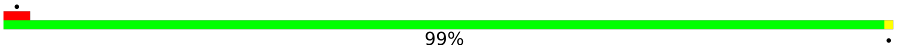
Chain L:

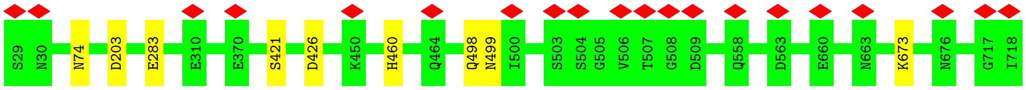




- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

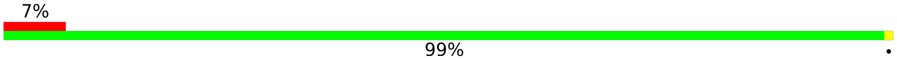
Chain M:

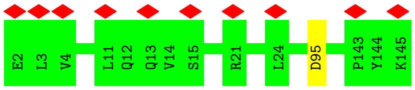




- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

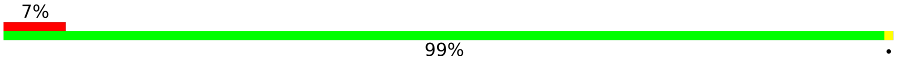
Chain N:

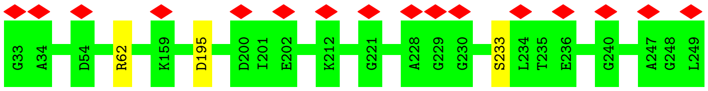




- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

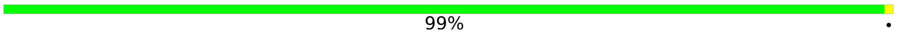
Chain O:

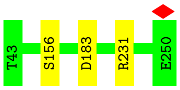




- Molecule 15: Complex I-30kD

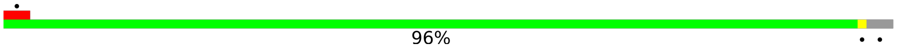
Chain P:

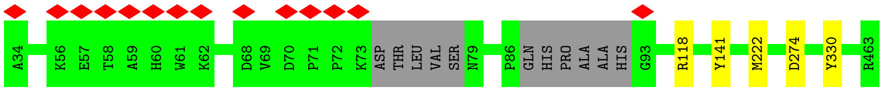




- Molecule 16: Complex I-49kD

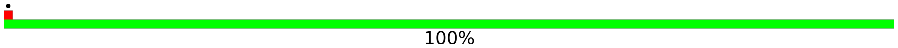
Chain Q:

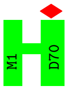




- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

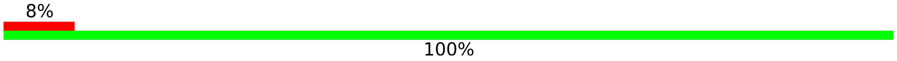
Chain S:

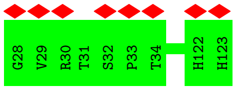




- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

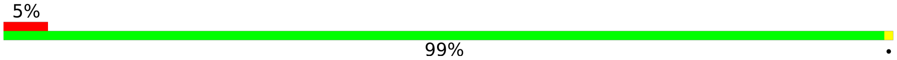
Chain T:

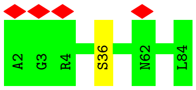




- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

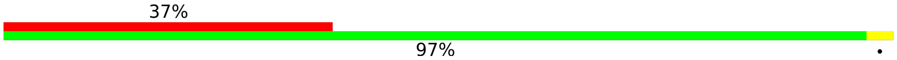
Chain U:

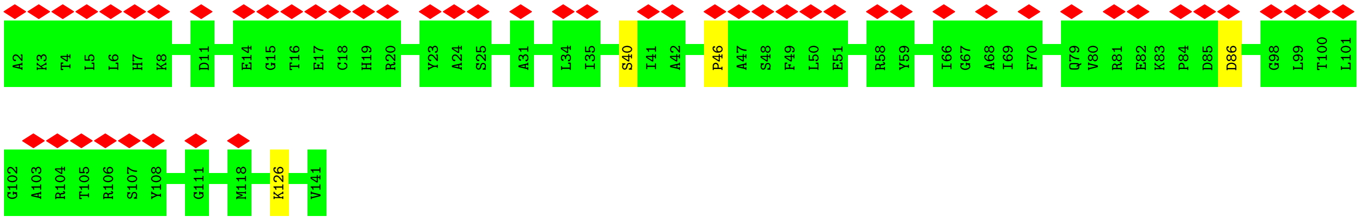




- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

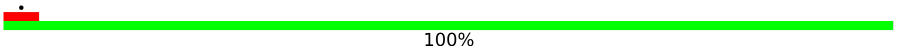
Chain V:

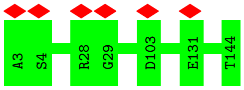




- Molecule 21: Complex I-B16.6

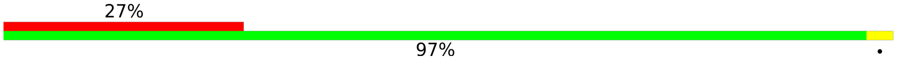
Chain W:

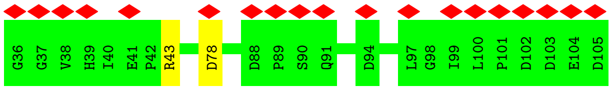




- Molecule 22: Complex I-AGGG

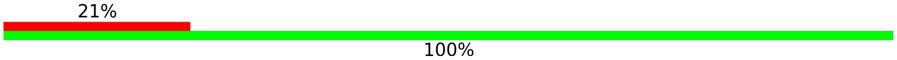
Chain Y:

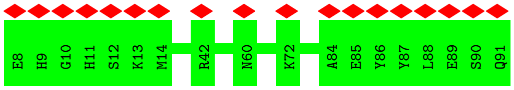




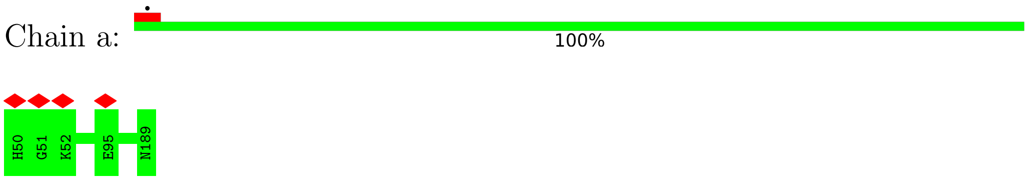
- Molecule 23: Complex I-B12

Chain Z:

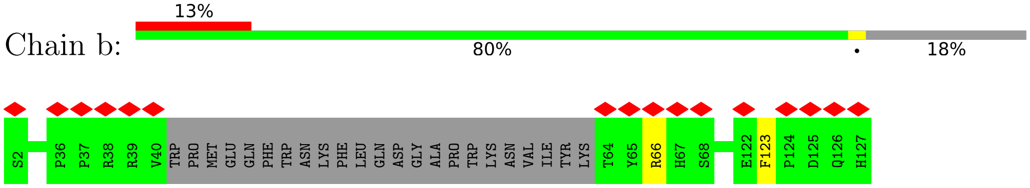




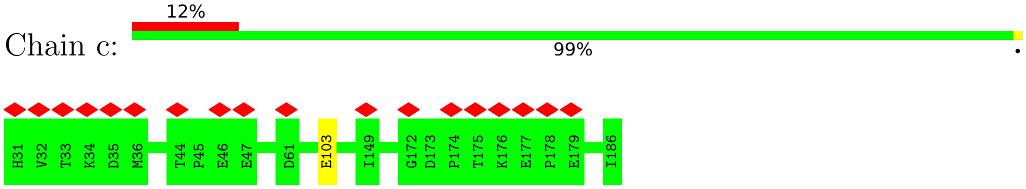
- Molecule 24: Complex I-SGDH



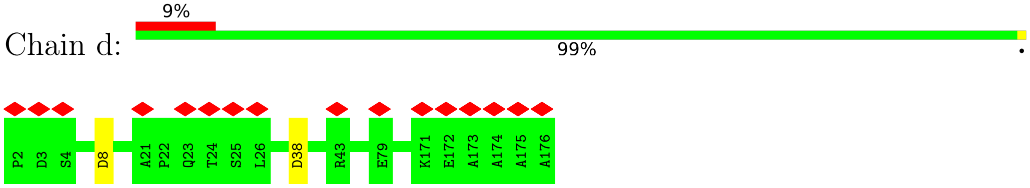
- Molecule 25: Complex I-B17



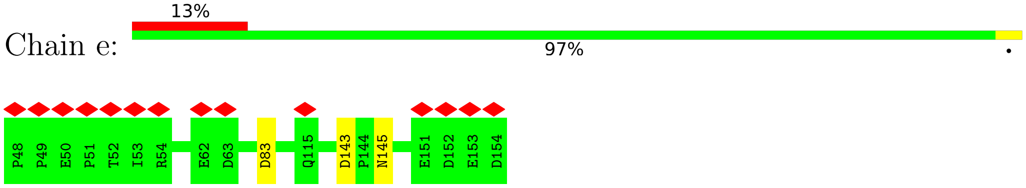
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



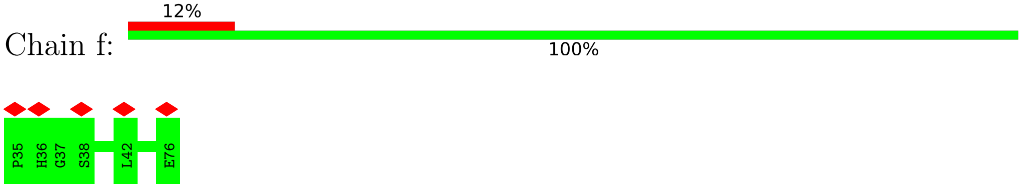
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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

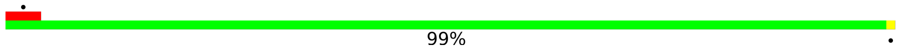


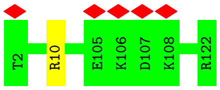
- Molecule 29: Complex I-KFYI



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

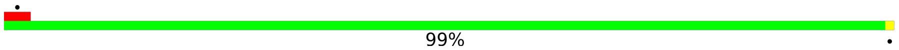
Chain g:

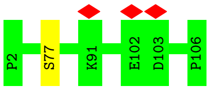




- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

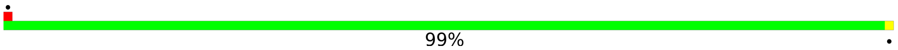
Chain h:

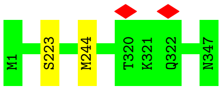




- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

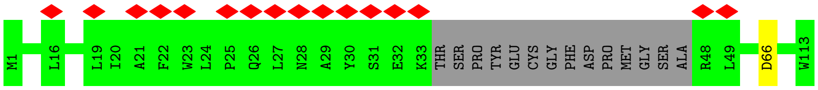
Chain i:





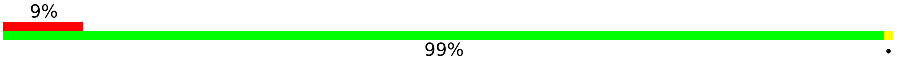
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

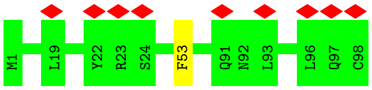
Chain j:



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

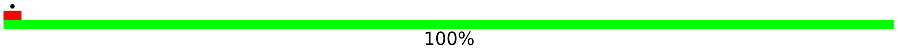
Chain k:

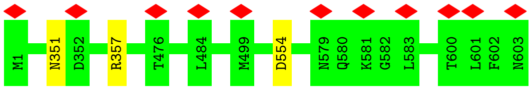




- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

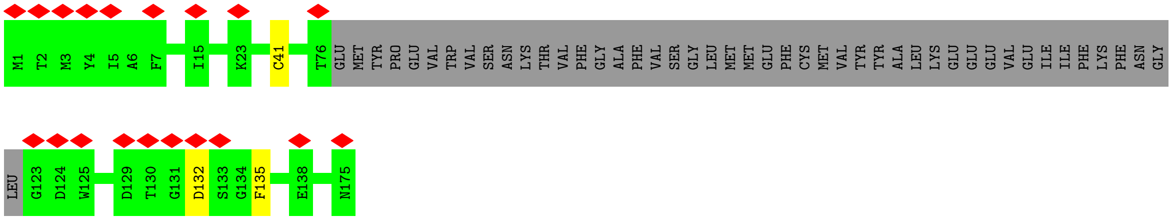
Chain l:





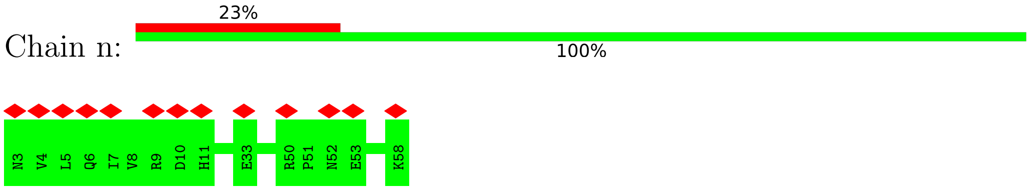
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:



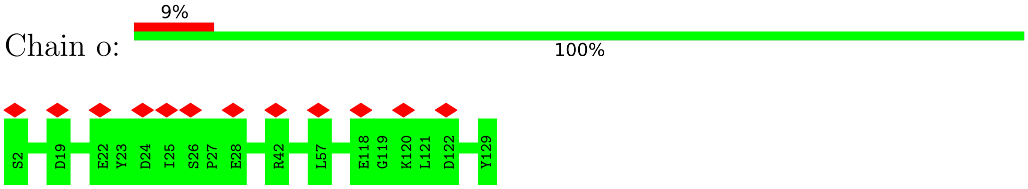
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:



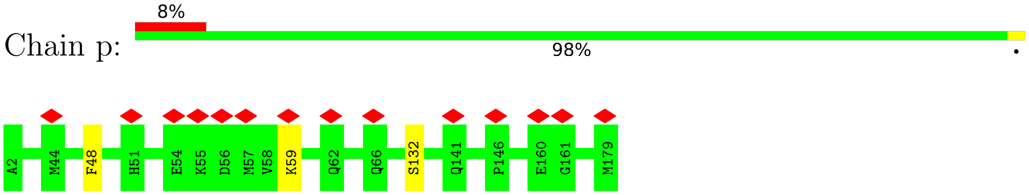
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:



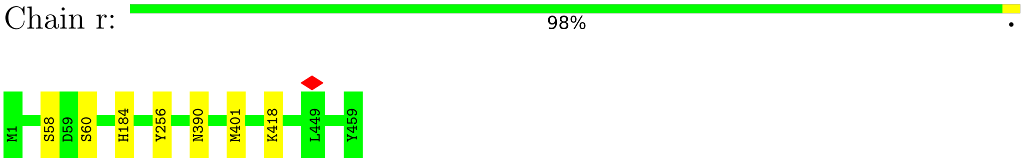
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:



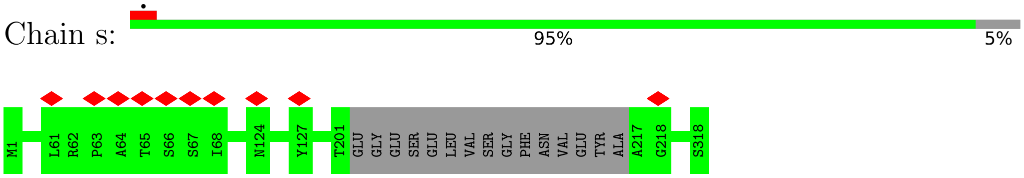
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:



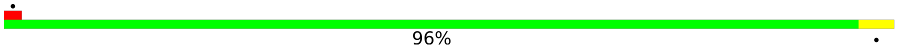
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

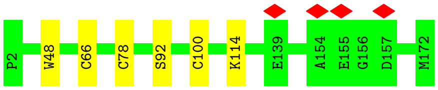
Chain s:



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

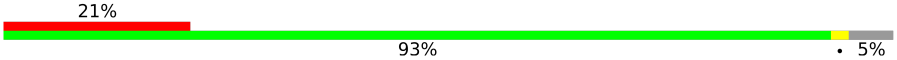
Chain u:

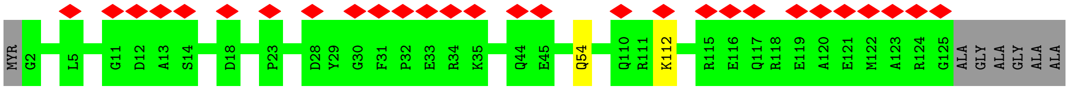




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

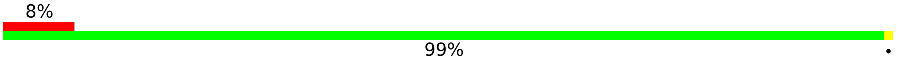
Chain v:

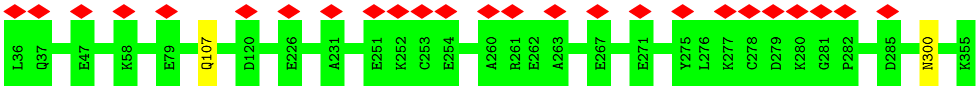




- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65171	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	0.213	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.029	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.26	0/3389	0.51	0/4580
2	B	0.26	0/1443	0.52	0/1952
3	C	0.26	0/1279	0.53	0/1730
4	E	0.25	0/987	0.53	0/1330
5	F	0.26	0/702	0.57	0/945
6	G	0.32	1/695 (0.1%)	0.49	0/944
6	X	0.26	0/708	0.46	0/959
7	H	0.24	0/929	0.44	0/1258
8	I	0.25	0/780	0.53	0/1059
9	J	0.25	0/2411	0.50	0/3254
10	K	0.25	0/365	0.51	0/493
11	L	0.25	0/1036	0.51	0/1399
12	M	0.25	0/5384	0.51	0/7295
13	N	0.26	0/1245	0.53	0/1694
14	O	0.27	0/1711	0.51	0/2328
15	P	0.27	0/1789	0.53	0/2436
16	Q	0.27	0/3451	0.51	0/4672
17	S	0.26	0/582	0.50	0/783
18	T	0.25	0/755	0.51	0/1018
19	U	0.25	0/664	0.45	0/912
20	V	0.27	0/1038	0.49	0/1406
21	W	0.26	0/1185	0.48	0/1601
22	Y	0.27	0/603	0.46	0/828
23	Z	0.25	0/684	0.45	0/927
24	a	0.26	0/1185	0.50	0/1606
25	b	0.25	0/902	0.52	0/1227
26	c	0.25	0/1371	0.46	0/1875
27	d	0.25	0/1490	0.51	0/2010
28	e	0.26	0/916	0.48	0/1246
29	f	0.24	0/350	0.43	0/473
30	g	0.27	0/1031	0.49	0/1394
31	h	0.26	0/889	0.51	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\lvert Z \rvert$ >5	RMSZ	#$\lvert Z \rvert$ >5
32	i	0.26	0/2769	0.45	0/3764
33	j	0.27	0/819	0.48	0/1117
34	k	0.26	0/759	0.48	0/1029
35	l	0.27	0/4914	0.47	0/6683
36	m	0.28	0/970	0.47	0/1316
37	n	0.27	0/468	0.51	0/633
38	o	0.27	0/1084	0.51	0/1473
39	p	0.27	0/1590	0.54	0/2155
40	r	0.26	0/3723	0.46	0/5078
41	s	0.28	0/2464	0.50	0/3369
42	u	0.25	0/1436	0.47	0/1938
43	v	0.26	0/1044	0.54	0/1403
44	w	0.26	0/2626	0.49	0/3560
All	All	0.26	1/66615 (0.0%)	0.50	0/90342

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	131	PRO	N-CD	5.54	1.55	1.47

There are no bond angle outliers.

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%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	17	55
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
6	G	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	H	110/112 (98%)	101 (92%)	8 (7%)	1 (1%)	17	55
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	289/341 (85%)	277 (96%)	11 (4%)	1 (0%)	41	76
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	665 (97%)	22 (3%)	1 (0%)	51	85
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	412/430 (96%)	399 (97%)	13 (3%)	0	100	100
17	S	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	60
21	W	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
22	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
27	d	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
28	e	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
29	f	40/42 (95%)	40 (100%)	0	0	100	100
30	g	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	575 (96%)	26 (4%)	0	100	100
36	m	125/175 (71%)	113 (90%)	12 (10%)	0	100	100
37	n	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
39	p	176/178 (99%)	166 (94%)	10 (6%)	0	100	100
40	r	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
41	s	299/318 (94%)	284 (95%)	15 (5%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/131 (93%)	116 (95%)	6 (5%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8029/8315 (97%)	7721 (96%)	303 (4%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
12	M	283	GLU
20	V	46	PRO
4	E	19	PRO
7	H	77	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/345 (100%)	341 (99%)	3 (1%)	78	92
2	B	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	132/132 (100%)	129 (98%)	3 (2%)	50	80
4	E	105/107 (98%)	104 (99%)	1 (1%)	76	91
5	F	76/76 (100%)	72 (95%)	4 (5%)	22	58
6	G	73/81 (90%)	73 (100%)	0	100	100
6	X	77/81 (95%)	76 (99%)	1 (1%)	69	89
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	82/97 (84%)	81 (99%)	1 (1%)	71	90
9	J	255/295 (86%)	252 (99%)	3 (1%)	71	90
10	K	41/41 (100%)	37 (90%)	4 (10%)	8	30
11	L	112/113 (99%)	110 (98%)	2 (2%)	59	85
12	M	580/580 (100%)	572 (99%)	8 (1%)	67	88
13	N	130/130 (100%)	129 (99%)	1 (1%)	81	93
14	O	183/183 (100%)	180 (98%)	3 (2%)	62	86
15	P	190/190 (100%)	187 (98%)	3 (2%)	62	86
16	Q	361/370 (98%)	357 (99%)	4 (1%)	73	90
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	68 (99%)	1 (1%)	67	88
20	V	100/101 (99%)	97 (97%)	3 (3%)	41	75
21	W	119/123 (97%)	119 (100%)	0	100	100
22	Y	57/63 (90%)	55 (96%)	2 (4%)	36	71
23	Z	62/65 (95%)	62 (100%)	0	100	100
24	a	119/122 (98%)	119 (100%)	0	100	100
25	b	97/119 (82%)	95 (98%)	2 (2%)	53	82
26	c	141/141 (100%)	140 (99%)	1 (1%)	84	94
27	d	154/155 (99%)	152 (99%)	2 (1%)	69	89
28	e	99/99 (100%)	96 (97%)	3 (3%)	41	75
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	107 (99%)	1 (1%)	78	92
31	h	93/93 (100%)	92 (99%)	1 (1%)	73	90
32	i	310/311 (100%)	308 (99%)	2 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	j	88/99 (89%)	87 (99%)	1 (1%)	73	90
34	k	85/85 (100%)	84 (99%)	1 (1%)	71	90
35	l	537/537 (100%)	534 (99%)	3 (1%)	86	95
36	m	98/141 (70%)	95 (97%)	3 (3%)	40	75
37	n	46/53 (87%)	46 (100%)	0	100	100
38	o	111/113 (98%)	111 (100%)	0	100	100
39	p	159/159 (100%)	156 (98%)	3 (2%)	57	84
40	r	410/410 (100%)	403 (98%)	7 (2%)	60	85
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	153/153 (100%)	147 (96%)	6 (4%)	32	69
43	v	103/111 (93%)	101 (98%)	2 (2%)	57	84
44	w	278/283 (98%)	276 (99%)	2 (1%)	84	94
All	All	7022/7234 (97%)	6935 (99%)	87 (1%)	72	90

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLU
1	A	209	GLU
1	A	226	LYS
3	C	71	CYS
3	C	77	MET
3	C	142	TYR
4	E	45	ASN
5	F	23	LEU
5	F	27	SER
5	F	73	GLN
5	F	76	ASN
8	I	18	ARG
9	J	108	TRP
9	J	154	GLN
9	J	238	GLN
10	K	74	ARG
10	K	75	ASN
10	K	76	LEU
10	K	95	LYS
11	L	70	GLU
11	L	119	ASP

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Mol	Chain	Res	Type
12	M	74	ASN
12	M	203	ASP
12	M	421	SER
12	M	426	ASP
12	M	460	HIS
12	M	498	GLN
12	M	499	ASN
12	M	673	LYS
13	N	95	ASP
14	O	62	ARG
14	O	195	ASP
14	O	233	SER
15	P	156	SER
15	P	183	ASP
15	P	231	ARG
16	Q	141	TYR
16	Q	222	MET
16	Q	274	ASP
16	Q	330	TYR
19	U	36	SER
20	V	40	SER
20	V	86	ASP
20	V	126	LYS
6	X	137	LYS
22	Y	43	ARG
22	Y	78	ASP
25	b	66	ARG
25	b	123	PHE
26	c	103	GLU
27	d	8	ASP
27	d	38	ASP
28	e	83	ASP
28	e	143	ASP
28	e	145	ASN
30	g	10	ARG
31	h	77	SER
32	i	223	SER
32	i	244	MET
33	j	66	ASP
34	k	53	PHE
35	l	351	ASN
35	l	357	ARG

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Mol	Chain	Res	Type
35	l	554	ASP
36	m	41	CYS
36	m	132	ASP
36	m	135	PHE
39	p	48	PHE
39	p	59	LYS
39	p	132	SER
40	r	58	SER
40	r	60	SER
40	r	184	HIS
40	r	256	TYR
40	r	390	ASN
40	r	401	MET
40	r	418	LYS
42	u	48	TRP
42	u	66	CYS
42	u	78	CYS
42	u	92	SER
42	u	100	CYS
42	u	114	LYS
43	v	54	GLN
43	v	112	LYS
44	w	107	GLN
44	w	300	ASN

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

Mol	Chain	Res	Type
1	A	133	HIS
3	C	99	GLN
6	G	142	GLN
12	M	652	ASN
16	Q	182	ASN
20	V	79	GLN
22	Y	54	GLN
35	l	446	ASN
39	p	76	HIS
41	s	250	HIS
42	u	99	HIS
44	w	155	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	2.00	1 (10%)	5,13,15	6.14	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	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.68	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	12.56	130.99	119.48
16	Q	118	2MR	CD-NE-CZ	4.73	132.27	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.81	130.06	123.86

There are no chirality outliers.

All (2) 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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 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	$\#\|Z\| > 2$
55	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
48	PEE	U	101	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
52	FES	O	301	14	0,4,4	-	-	-		
55	PLX	j	202	-	51,51,51	1.16	4 (7%)	55,59,59	0.60	1 (1%)
49	8Q1	X	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.54	6 (15%)
50	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.87	4 (3%)
50	CDL	i	401	-	65,65,99	1.27	8 (12%)	71,77,111	0.99	4 (5%)
45	SF4	B	302	2	0,12,12	-	-	-		
51	NDP	J	401	-	45,52,52	4.57	20 (44%)	53,80,80	2.02	7 (13%)
48	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	1.01	2 (4%)
48	PEE	Q	501	-	46,46,50	1.20	6 (13%)	49,51,55	0.99	2 (4%)
50	CDL	a	201	-	90,90,99	1.13	8 (8%)	96,102,111	0.93	4 (4%)
47	NAI	A	503	-	42,48,48	4.95	19 (45%)	47,73,73	1.33	7 (14%)
45	SF4	M	801	12	0,12,12	-	-	-		
50	CDL	I	201	-	50,50,99	1.39	8 (16%)	56,62,111	1.12	4 (7%)

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	8 (28%)	34,37,79	2.79	11 (32%)
45	SF4	M	802	12	0,12,12	-	-	-		
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
48	PEE	j	201	-	46,46,50	1.21	6 (13%)	49,51,55	1.00	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.05	3 (5%)
50	CDL	l	702	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
50	CDL	g	202	-	77,77,99	1.20	8 (10%)	83,89,111	0.96	4 (4%)
55	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.64	1 (1%)
50	CDL	r	503	-	99,99,99	1.09	8 (8%)	105,111,111	0.86	4 (3%)
49	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.58	5 (12%)
52	FES	M	803	12	0,4,4	-	-	-		
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.25	7 (14%)
55	PLX	r	502	-	51,51,51	1.13	4 (7%)	55,59,59	0.64	1 (1%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.45	4 (13%)
48	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.07	3 (6%)
45	SF4	C	301	3,16	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PLX	a	202	-	-	29/55/55/55	-
48	PEE	U	101	-	-	24/54/54/54	-
55	PLX	j	202	-	-	33/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
52	FES	O	301	14	-	-	0/1/1/1
49	8Q1	X	201	6	-	21/41/41/41	-
50	CDL	l	701	-	-	52/109/109/110	-
50	CDL	i	401	-	-	38/76/76/110	-
51	NDP	J	401	-	-	9/30/77/77	0/4/5/5
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	l	703	-	-	26/49/49/54	-
48	PEE	Q	501	-	-	23/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CDL	a	201	-	-	55/101/101/110	-
47	NAI	A	503	-	-	9/25/72/72	0/5/5/5
50	CDL	I	201	-	-	33/61/61/110	-
45	SF4	M	801	12	-	-	0/6/5/5
56	UQ	s	401	-	-	9/21/45/87	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	l	704	-	-	32/49/49/54	-
48	PEE	j	201	-	-	22/50/50/54	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	r	501	-	-	20/54/54/54	-
50	CDL	l	702	-	-	57/110/110/110	-
50	CDL	g	202	-	-	43/88/88/110	-
55	PLX	g	201	-	-	32/55/55/55	-
50	CDL	r	503	-	-	72/110/110/110	-
49	8Q1	G	201	6	-	20/41/41/41	-
52	FES	M	803	12	-	-	0/1/1/1
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
55	PLX	r	502	-	-	32/55/55/55	-
48	PEE	B	303	-	-	27/54/54/54	-
57	ADP	w	401	-	-	3/12/32/32	0/3/3/3
48	PEE	m	201	-	-	17/44/44/54	-
45	SF4	C	301	3,16	-	-	0/6/5/5

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.32	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.40	1.30	1.53
51	J	401	NDP	C3B-C2B	-12.75	1.24	1.52
51	J	401	NDP	C6N-C5N	12.56	1.55	1.33
51	J	401	NDP	O4D-C4D	10.69	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.17	1.27	1.53
51	J	401	NDP	C3D-C4D	-9.84	1.27	1.53
56	s	401	UQ	C13-C14	9.34	1.55	1.33
56	s	401	UQ	C8-C9	9.01	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.84	1.30	1.53
51	J	401	NDP	O4B-C1B	8.35	1.52	1.41
56	s	401	UQ	C18-C19	8.24	1.56	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C4B	-8.22	1.26	1.45
51	J	401	NDP	O4B-C4B	-7.98	1.27	1.45
57	w	401	ADP	O4'-C4'	7.72	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.63	1.29	1.53
51	J	401	NDP	C2N-C3N	7.40	1.55	1.34
47	A	503	NAI	O4D-C4D	7.06	1.60	1.45
57	w	401	ADP	O4'-C1'	-6.86	1.31	1.41
47	A	503	NAI	C2D-C3D	5.94	1.69	1.53
51	J	401	NDP	P2B-O2B	5.79	1.70	1.59
47	A	503	NAI	C7N-N7N	5.74	1.48	1.33
49	G	201	8Q1	C34-N36	5.49	1.45	1.33
49	X	201	8Q1	C39-N41	5.46	1.45	1.33
47	A	503	NAI	O4D-C1D	5.45	1.54	1.42
51	J	401	NDP	C3B-C4B	5.41	1.66	1.53
49	X	201	8Q1	C34-N36	5.40	1.45	1.33
49	G	201	8Q1	C39-N41	5.38	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.07	1.40	1.49
51	J	401	NDP	O4D-C1D	-4.89	1.30	1.42
51	J	401	NDP	C6N-N1N	4.77	1.49	1.37
47	A	503	NAI	O2B-C2B	4.56	1.53	1.43
51	J	401	NDP	C7N-N7N	4.22	1.44	1.33
51	J	401	NDP	O2D-C2D	-4.14	1.33	1.43
51	J	401	NDP	C6A-N6A	4.10	1.49	1.34
47	A	503	NAI	C6N-C5N	4.00	1.40	1.33
46	A	502	FMN	C4A-N5	3.96	1.38	1.30
57	w	401	ADP	C6-N6	3.85	1.48	1.34
48	r	501	PEE	C18-C19	3.75	1.53	1.31
48	U	101	PEE	C18-C19	3.75	1.53	1.31
48	m	201	PEE	C18-C19	3.74	1.53	1.31
48	j	201	PEE	C18-C19	3.74	1.53	1.31
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	l	704	PEE	C18-C19	3.73	1.53	1.31
48	Q	501	PEE	C18-C19	3.73	1.53	1.31
48	l	703	PEE	C18-C19	3.73	1.53	1.31
47	A	503	NAI	C7N-C3N	3.67	1.56	1.48
48	Q	501	PEE	C39-C38	3.66	1.53	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	l	704	PEE	C39-C38	3.65	1.52	1.31
48	l	703	PEE	C39-C38	3.64	1.52	1.31
48	U	101	PEE	C39-C38	3.64	1.52	1.31
48	j	201	PEE	C39-C38	3.63	1.52	1.31
48	B	303	PEE	C39-C38	3.62	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C6A-N6A	3.59	1.47	1.34
50	i	401	CDL	OA8-CA7	3.51	1.43	1.33
50	g	202	CDL	OA8-CA7	3.46	1.43	1.33
50	l	702	CDL	OA8-CA7	3.44	1.43	1.33
50	r	503	CDL	OA8-CA7	3.44	1.43	1.33
50	I	201	CDL	OA8-CA7	3.43	1.43	1.33
50	a	201	CDL	OA8-CA7	3.39	1.43	1.33
50	l	701	CDL	OA8-CA7	3.37	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.31	1.40	1.48
57	w	401	ADP	O2'-C2'	-3.31	1.35	1.43
57	w	401	ADP	O3'-C3'	3.13	1.50	1.43
50	l	702	CDL	OB6-CB5	3.10	1.43	1.34
51	J	401	NDP	O3D-C3D	3.09	1.50	1.43
50	l	701	CDL	OB6-CB5	3.07	1.43	1.34
51	J	401	NDP	C7N-C3N	3.07	1.55	1.48
50	r	503	CDL	OA6-CA5	3.03	1.42	1.34
50	g	202	CDL	OB8-CB7	3.03	1.42	1.33
50	l	701	CDL	OB8-CB7	3.03	1.42	1.33
50	i	401	CDL	OB6-CB5	3.02	1.42	1.34
50	g	202	CDL	OB6-CB5	3.02	1.42	1.34
50	I	201	CDL	OB6-CB5	3.01	1.42	1.34
50	i	401	CDL	OB8-CB7	3.01	1.42	1.33
50	a	201	CDL	OB6-CB5	3.00	1.42	1.34
50	a	201	CDL	OA6-CA5	3.00	1.42	1.34
50	r	503	CDL	OB6-CB5	3.00	1.42	1.34
50	r	503	CDL	OB8-CB7	3.00	1.42	1.33
50	a	201	CDL	OB8-CB7	2.99	1.42	1.33
50	l	702	CDL	OB8-CB7	2.95	1.42	1.33
50	l	702	CDL	OA6-CA5	2.94	1.42	1.34
50	I	201	CDL	OB8-CB7	2.92	1.41	1.33
50	g	202	CDL	OA6-CA5	2.90	1.42	1.34
50	I	201	CDL	OA6-CA5	2.90	1.42	1.34
50	l	701	CDL	OA6-CA5	2.88	1.42	1.34
50	i	401	CDL	OA6-CA5	2.82	1.42	1.34
55	g	201	PLX	O6-C4	-2.77	1.40	1.44
56	s	401	UQ	C6-C1	2.72	1.54	1.46
55	r	502	PLX	O6-C4	-2.70	1.41	1.44
55	a	202	PLX	O6-C4	-2.65	1.41	1.44
48	l	704	PEE	O3-C30	2.56	1.40	1.33
46	A	502	FMN	C10-N1	2.54	1.38	1.33
48	l	703	PEE	O3-C30	2.52	1.40	1.33
50	i	401	CDL	OA6-CA4	-2.50	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	j	201	PEE	O3-C30	2.49	1.40	1.33
50	I	201	CDL	OA6-CA4	-2.49	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.48	1.37	1.43
48	Q	501	PEE	O3-C30	2.48	1.40	1.33
47	A	503	NAI	PN-O5D	2.47	1.69	1.59
48	m	201	PEE	O3-C30	2.47	1.40	1.33
51	J	401	NDP	O2B-C2B	2.47	1.53	1.44
55	j	202	PLX	C7-C6	2.47	1.56	1.50
55	j	202	PLX	O6-C4	-2.47	1.41	1.44
50	g	202	CDL	OA6-CA4	-2.46	1.40	1.46
50	l	701	CDL	OA6-CA4	-2.46	1.40	1.46
48	B	303	PEE	O3-C30	2.45	1.40	1.33
51	J	401	NDP	C2D-C3D	2.43	1.60	1.53
48	U	101	PEE	O3-C30	2.43	1.40	1.33
49	X	201	8Q1	C1-S44	2.43	1.82	1.76
49	G	201	8Q1	C1-S44	2.41	1.82	1.76
48	U	101	PEE	O2-C2	-2.41	1.40	1.46
48	r	501	PEE	O3-C30	2.40	1.40	1.33
48	j	201	PEE	O2-C10	2.40	1.41	1.34
48	m	201	PEE	O2-C10	2.38	1.41	1.34
48	l	703	PEE	O2-C2	-2.38	1.40	1.46
48	l	704	PEE	O2-C2	-2.38	1.40	1.46
48	B	303	PEE	O2-C2	-2.38	1.40	1.46
50	l	702	CDL	OA6-CA4	-2.36	1.40	1.46
50	r	503	CDL	OA6-CA4	-2.34	1.40	1.46
50	a	201	CDL	OA6-CA4	-2.34	1.40	1.46
55	a	202	PLX	C7-C6	2.34	1.55	1.50
48	Q	501	PEE	O2-C2	-2.34	1.40	1.46
56	s	401	UQ	O4-C4	-2.33	1.18	1.23
48	j	201	PEE	O2-C2	-2.33	1.40	1.46
48	r	501	PEE	O2-C2	-2.33	1.40	1.46
56	s	401	UQ	C7-C8	2.31	1.54	1.50
48	U	101	PEE	O2-C10	2.30	1.40	1.34
55	g	201	PLX	C7-C6	2.30	1.55	1.50
48	B	303	PEE	O2-C10	2.30	1.40	1.34
49	G	201	8Q1	C6-C1	2.29	1.53	1.50
48	Q	501	PEE	O2-C10	2.28	1.40	1.34
48	l	703	PEE	O2-C10	2.28	1.40	1.34
48	m	201	PEE	O2-C2	-2.27	1.40	1.46
48	l	704	PEE	O2-C10	2.26	1.40	1.34
48	r	501	PEE	O2-C10	2.26	1.40	1.34
47	A	503	NAI	C5B-C4B	2.23	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r	502	PLX	C7-C6	2.22	1.55	1.50
50	l	702	CDL	PB2-OB2	2.22	1.68	1.59
49	X	201	8Q1	C6-C1	2.22	1.53	1.50
50	r	503	CDL	PB2-OB2	2.21	1.68	1.59
55	j	202	PLX	P1-O4	2.21	1.68	1.59
50	l	701	CDL	PB2-OB2	2.20	1.68	1.59
50	l	701	CDL	PB2-OB5	2.20	1.68	1.59
50	i	401	CDL	PB2-OB2	2.19	1.68	1.59
50	i	401	CDL	OB6-CB4	-2.19	1.41	1.46
50	l	702	CDL	PB2-OB5	2.19	1.68	1.59
50	i	401	CDL	PB2-OB5	2.18	1.68	1.59
50	a	201	CDL	PB2-OB2	2.18	1.68	1.59
50	r	503	CDL	PB2-OB5	2.18	1.68	1.59
50	g	202	CDL	PB2-OB5	2.18	1.68	1.59
49	G	201	8Q1	O35-C34	-2.18	1.19	1.23
50	g	202	CDL	PB2-OB2	2.17	1.68	1.59
50	I	201	CDL	OB6-CB4	-2.17	1.41	1.46
49	G	201	8Q1	O40-C39	-2.16	1.18	1.23
50	a	201	CDL	PB2-OB5	2.16	1.68	1.59
49	X	201	8Q1	O40-C39	-2.15	1.18	1.23
49	X	201	8Q1	O35-C34	-2.15	1.19	1.23
55	a	202	PLX	P1-O4	2.15	1.68	1.59
50	r	503	CDL	OB6-CB4	-2.15	1.41	1.46
50	I	201	CDL	PB2-OB2	2.13	1.67	1.59
55	g	201	PLX	P1-O4	2.11	1.67	1.59
50	a	201	CDL	OB6-CB4	-2.10	1.41	1.46
50	g	202	CDL	OB6-CB4	-2.10	1.41	1.46
48	U	101	PEE	O3-C3	-2.10	1.40	1.45
50	I	201	CDL	PB2-OB5	2.10	1.67	1.59
50	l	702	CDL	OB6-CB4	-2.10	1.41	1.46
51	J	401	NDP	O7N-C7N	-2.10	1.19	1.24
51	J	401	NDP	PA-O5B	2.10	1.67	1.59
50	l	701	CDL	OB6-CB4	-2.09	1.41	1.46
56	s	401	UQ	O1-C1	-2.09	1.18	1.23
48	B	303	PEE	O3-C3	-2.09	1.40	1.45
55	j	202	PLX	P1-O1	2.08	1.67	1.59
48	r	501	PEE	O3-C3	-2.07	1.40	1.45
55	r	502	PLX	P1-O4	2.06	1.67	1.59
47	A	503	NAI	C2N-C3N	2.06	1.40	1.34
48	j	201	PEE	O3-C3	-2.05	1.40	1.45
48	Q	501	PEE	O3-C3	-2.04	1.40	1.45
55	a	202	PLX	P1-O1	2.03	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r	502	PLX	P1-O1	2.03	1.67	1.59
48	l	704	PEE	O3-C3	-2.03	1.40	1.45
48	l	703	PEE	O3-C3	-2.02	1.40	1.45
48	m	201	PEE	O3-C3	-2.02	1.40	1.45
56	s	401	UQ	O3-CM3	-2.01	1.40	1.45
50	l	702	CDL	C11-CA5	2.01	1.56	1.50

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C7-C8-C9	-9.69	110.65	126.79
51	J	401	NDP	C3N-C2N-N1N	-8.38	111.14	123.10
51	J	401	NDP	C1D-N1N-C2N	-7.02	109.43	121.11
49	G	201	8Q1	C6-C1-S44	6.00	120.44	113.46
49	X	201	8Q1	C6-C1-S44	5.90	120.33	113.46
56	s	401	UQ	C12-C13-C14	-5.64	114.09	127.66
51	J	401	NDP	C1D-N1N-C6N	-5.00	110.06	120.83
56	s	401	UQ	C10-C9-C8	-4.58	111.92	123.68
57	w	401	ADP	N3-C2-N1	-4.47	121.70	128.68
47	A	503	NAI	N3A-C2A-N1A	-4.44	121.74	128.68
50	a	201	CDL	OA6-CA5-C11	4.43	121.05	111.50
56	s	401	UQ	C11-C9-C8	-4.38	112.25	121.12
48	r	501	PEE	O2-C10-C11	4.32	120.80	111.50
50	g	202	CDL	OB6-CB5-C51	4.27	120.71	111.50
50	a	201	CDL	OB6-CB5-C51	4.22	120.59	111.50
48	B	303	PEE	O2-C10-C11	4.20	120.56	111.50
48	m	201	PEE	O2-C10-C11	4.11	120.35	111.50
56	s	401	UQ	C15-C14-C13	-4.10	113.16	123.68
48	Q	501	PEE	O2-C10-C11	4.01	120.15	111.50
48	j	201	PEE	O2-C10-C11	4.01	120.15	111.50
48	l	703	PEE	O2-C10-C11	4.00	120.12	111.50
50	r	503	CDL	OB6-CB5-C51	4.00	120.12	111.50
50	l	702	CDL	OA6-CA5-C11	3.99	120.09	111.50
49	G	201	8Q1	C37-C38-C39	3.98	118.98	112.36
51	J	401	NDP	N3A-C2A-N1A	-3.96	122.49	128.68
50	l	702	CDL	OB6-CB5-C51	3.96	120.03	111.50
56	s	401	UQ	C16-C14-C13	-3.96	113.11	121.12
50	I	201	CDL	OB6-CB5-C51	3.95	120.02	111.50
50	r	503	CDL	OA6-CA5-C11	3.94	119.99	111.50
48	l	704	PEE	O2-C10-C11	3.92	119.95	111.50
50	l	701	CDL	OB6-CB5-C51	3.89	119.89	111.50
56	s	401	UQ	C17-C18-C19	-3.89	114.45	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	U	101	PEE	O2-C10-C11	3.89	119.88	111.50
50	l	701	CDL	OA6-CA5-C11	3.82	119.73	111.50
50	g	202	CDL	OA6-CA5-C11	3.81	119.71	111.50
50	i	401	CDL	OB6-CB5-C51	3.76	119.61	111.50
50	I	201	CDL	OA6-CA5-C11	3.73	119.54	111.50
50	i	401	CDL	OA6-CA5-C11	3.59	119.24	111.50
56	s	401	UQ	C21-C19-C18	-3.46	112.64	122.65
49	X	201	8Q1	O4-C1-C6	-3.44	119.92	123.99
49	G	201	8Q1	O4-C1-C6	-3.41	119.96	123.99
46	A	502	FMN	C4-N3-C2	-3.23	119.67	125.64
48	m	201	PEE	O3-C30-C31	3.01	121.36	111.91
56	s	401	UQ	C20-C19-C18	-2.99	113.99	122.65
51	J	401	NDP	PN-O3-PA	-2.97	122.64	132.83
56	s	401	UQ	CM5-C5-C6	-2.91	119.64	124.40
47	A	503	NAI	PN-O3-PA	-2.91	122.83	132.83
48	r	501	PEE	O3-C30-C31	2.89	120.97	111.91
46	A	502	FMN	C4A-C4-N3	2.86	120.45	113.19
57	w	401	ADP	PA-O3A-PB	-2.83	123.10	132.83
50	i	401	CDL	OA8-CA7-C31	2.74	120.52	111.91
47	A	503	NAI	C2D-C3D-C4D	2.74	107.97	102.64
48	l	703	PEE	O3-C30-C31	2.73	120.47	111.91
48	l	704	PEE	O3-C30-C31	2.71	120.40	111.91
57	w	401	ADP	O4'-C1'-C2'	-2.69	102.99	106.93
50	g	202	CDL	OB8-CB7-C71	2.68	120.33	111.91
50	l	701	CDL	OB8-CB7-C71	2.68	120.31	111.91
51	J	401	NDP	C2B-C3B-C4B	2.67	107.79	101.99
50	l	701	CDL	OA8-CA7-C31	2.65	120.22	111.91
50	i	401	CDL	OB8-CB7-C71	2.63	120.18	111.91
48	B	303	PEE	O3-C30-C31	2.61	120.11	111.91
48	j	201	PEE	O3-C30-C31	2.61	120.09	111.91
50	I	201	CDL	OA8-CA7-C31	2.59	120.03	111.91
50	r	503	CDL	OA8-CA7-C31	2.58	120.00	111.91
46	A	502	FMN	O4-C4-C4A	-2.57	119.77	126.60
47	A	503	NAI	C4A-C5A-N7A	-2.57	106.72	109.40
47	A	503	NAI	C3B-C2B-C1B	2.56	104.84	100.98
55	r	502	PLX	C1A-N1-C1	2.56	120.38	109.92
56	s	401	UQ	C7-C6-C1	2.56	121.55	118.48
55	g	201	PLX	C1A-N1-C1	2.55	120.37	109.92
47	A	503	NAI	C3D-C2D-C1D	2.55	106.27	101.43
48	U	101	PEE	O3-C30-C31	2.54	119.88	111.91
48	Q	501	PEE	O3-C30-C31	2.51	119.79	111.91
50	r	503	CDL	OB8-CB7-C71	2.51	119.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	503	NAI	C4D-O4D-C1D	-2.50	103.95	109.47
50	I	201	CDL	OB8-CB7-C71	2.50	119.76	111.91
50	a	201	CDL	OB8-CB7-C71	2.48	119.69	111.91
50	l	702	CDL	OA8-CA7-C31	2.47	119.66	111.91
50	g	202	CDL	OA8-CA7-C31	2.44	119.56	111.91
50	l	702	CDL	OB8-CB7-C71	2.42	119.51	111.91
49	X	201	8Q1	C37-C38-C39	2.41	116.38	112.36
50	a	201	CDL	OA8-CA7-C31	2.40	119.43	111.91
46	A	502	FMN	C9A-C5A-N5	-2.38	119.84	122.43
46	A	502	FMN	C4A-C10-N10	2.38	119.96	116.48
49	X	201	8Q1	C38-C39-N41	2.37	120.41	116.42
51	J	401	NDP	C4A-C5A-N7A	-2.34	106.96	109.40
48	m	201	PEE	C3-C2-C1	-2.34	106.26	111.79
46	A	502	FMN	C4A-C10-N1	-2.32	119.34	124.73
49	G	201	8Q1	O4-C1-S44	-2.32	119.60	122.61
55	j	202	PLX	C1A-N1-C1	2.30	119.32	109.92
55	a	202	PLX	C1A-N1-C1	2.29	119.30	109.92
46	A	502	FMN	C10-C4A-N5	-2.29	120.00	124.86
48	r	501	PEE	C2-O2-C10	-2.27	112.21	117.79
57	w	401	ADP	C4-C5-N7	-2.22	107.08	109.40
49	X	201	8Q1	C43-S44-C1	2.21	108.75	101.87
49	X	201	8Q1	O4-C1-S44	-2.20	119.75	122.61
49	G	201	8Q1	C43-S44-C1	2.13	108.50	101.87

There are no chirality outliers.

All (746) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1’-C2’-O2’
46	A	502	FMN	N10-C1’-C2’-C3’
46	A	502	FMN	C1’-C2’-C3’-O3’
46	A	502	FMN	C1’-C2’-C3’-C4’
48	B	303	PEE	C4-O4P-P-O3P
48	B	303	PEE	C4-O4P-P-O2P
48	B	303	PEE	C4-O4P-P-O1P
48	Q	501	PEE	C11-C10-O2-C2
48	U	101	PEE	C17-C18-C19-C20
48	j	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C4-O4P-P-O1P
48	j	201	PEE	O4P-C4-C5-N
48	l	703	PEE	C11-C10-O2-C2
48	l	704	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	l	704	PEE	C1-O3P-P-O1P
48	l	704	PEE	C1-O3P-P-O4P
48	m	201	PEE	C11-C10-O2-C2
48	m	201	PEE	O4P-C4-C5-N
48	r	501	PEE	O3P-C1-C2-O2
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	N36-C37-C38-C39
49	G	201	8Q1	N41-C42-C43-S44
49	G	201	8Q1	C42-C43-S44-C1
49	G	201	8Q1	C28-O27-P24-O3
49	G	201	8Q1	C28-O27-P24-O2
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C31-C29-C32-O33
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	I	201	CDL	O1-C1-CA2-OA2
50	I	201	CDL	CB2-C1-CA2-OA2
50	I	201	CDL	CA2-OA2-PA1-OA3
50	I	201	CDL	CA2-OA2-PA1-OA4
50	I	201	CDL	CA2-OA2-PA1-OA5
50	I	201	CDL	CA3-OA5-PA1-OA3
50	I	201	CDL	CB2-OB2-PB2-OB3
50	I	201	CDL	CB2-OB2-PB2-OB4
50	I	201	CDL	CB2-OB2-PB2-OB5
50	a	201	CDL	CA2-C1-CB2-OB2
50	a	201	CDL	CA2-OA2-PA1-OA3
50	a	201	CDL	CA2-OA2-PA1-OA4
50	a	201	CDL	CB2-OB2-PB2-OB3
50	a	201	CDL	CB2-OB2-PB2-OB4
50	a	201	CDL	CB3-OB5-PB2-OB2
50	a	201	CDL	CB3-OB5-PB2-OB3
50	g	202	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
50	g	202	CDL	CA2-OA2-PA1-OA5
50	g	202	CDL	CB2-OB2-PB2-OB3
50	g	202	CDL	CB2-OB2-PB2-OB4
50	i	401	CDL	CB2-C1-CA2-OA2
50	i	401	CDL	CA3-OA5-PA1-OA2
50	i	401	CDL	CA3-OA5-PA1-OA3
50	i	401	CDL	CA3-OA5-PA1-OA4
50	i	401	CDL	CB3-OB5-PB2-OB3
50	l	701	CDL	O1-C1-CB2-OB2
50	l	701	CDL	CA2-C1-CB2-OB2
50	l	701	CDL	CA2-OA2-PA1-OA4
50	l	701	CDL	CB3-OB5-PB2-OB3
50	l	701	CDL	CB3-OB5-PB2-OB4
50	l	702	CDL	O1-C1-CA2-OA2
50	l	702	CDL	CA3-OA5-PA1-OA3
50	l	702	CDL	CA3-OA5-PA1-OA4
50	l	702	CDL	OA6-CA4-CA6-OA8
50	l	702	CDL	CB2-OB2-PB2-OB4
50	r	503	CDL	CA2-OA2-PA1-OA3
50	r	503	CDL	CA2-OA2-PA1-OA4
50	r	503	CDL	CA3-OA5-PA1-OA3
50	r	503	CDL	CA3-OA5-PA1-OA4
50	r	503	CDL	OA6-CA4-CA6-OA8
50	r	503	CDL	CB2-OB2-PB2-OB3
50	r	503	CDL	CB3-OB5-PB2-OB2
50	r	503	CDL	CB3-OB5-PB2-OB4
51	J	401	NDP	C5B-O5B-PA-O3
51	J	401	NDP	C2B-O2B-P2B-O1X
55	a	202	PLX	O7-C6-C7-C8
55	a	202	PLX	O7-C6-O6-C4
55	a	202	PLX	O4-C3-C4-O6
55	a	202	PLX	C2-O1-P1-O4
55	a	202	PLX	C2-O1-P1-O3
55	a	202	PLX	N1-C1-C2-O1
55	g	201	PLX	O7-C6-O6-C4
55	g	201	PLX	O9-C24-O8-C5
55	g	201	PLX	O9-C24-C25-C26
55	j	202	PLX	O7-C6-C7-C8
55	j	202	PLX	C3-O4-P1-O3
55	j	202	PLX	O9-C24-C25-C26
55	r	502	PLX	O7-C6-O6-C4
55	r	502	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
55	r	502	PLX	O9-C24-C25-C26
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C10
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
48	m	201	PEE	O5-C30-O3-C3
48	m	201	PEE	C31-C30-O3-C3
56	s	401	UQ	C17-C18-C19-C21
50	i	401	CDL	OA9-CA7-OA8-CA6
50	l	701	CDL	OA9-CA7-OA8-CA6
50	l	702	CDL	OB9-CB7-OB8-CB6
48	Q	501	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
50	i	401	CDL	C31-CA7-OA8-CA6
50	l	701	CDL	C31-CA7-OA8-CA6
50	l	702	CDL	C71-CB7-OB8-CB6
50	r	503	CDL	C71-CB7-OB8-CB6
48	l	704	PEE	C37-C38-C39-C40
48	r	501	PEE	C17-C18-C19-C20
56	s	401	UQ	C7-C8-C9-C10
50	r	503	CDL	OB7-CB5-OB6-CB4
50	l	701	CDL	O1-C1-CA2-OA2
50	l	702	CDL	O1-C1-CB2-OB2
48	l	703	PEE	C31-C30-O3-C3
50	l	702	CDL	C75-C76-C77-C78
48	U	101	PEE	C11-C10-O2-C2
50	g	202	CDL	C11-CA5-OA6-CA4
50	r	503	CDL	C51-CB5-OB6-CB4
50	g	202	CDL	C71-C72-C73-C74
51	J	401	NDP	C2D-C1D-N1N-C6N
50	a	201	CDL	C38-C39-C40-C41
50	i	401	CDL	C31-C32-C33-C34
50	l	701	CDL	C32-C33-C34-C35
50	l	702	CDL	C11-C12-C13-C14
55	a	202	PLX	C10-C11-C12-C13
50	g	202	CDL	C75-C76-C77-C78
50	l	702	CDL	C59-C60-C61-C62
55	g	201	PLX	C7-C8-C9-C10
50	I	201	CDL	C11-C12-C13-C14
47	A	503	NAI	C3B-C4B-C5B-O5B
51	J	401	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
50	l	701	CDL	C55-C56-C57-C58
55	j	202	PLX	C34-C35-C36-C37
50	r	503	CDL	OB9-CB7-OB8-CB6
55	j	202	PLX	C28-C29-C30-C31
48	l	703	PEE	O5-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
50	i	401	CDL	C71-CB7-OB8-CB6
50	l	701	CDL	C58-C59-C60-C61
50	a	201	CDL	C40-C41-C42-C43
55	a	202	PLX	C11-C10-C9-C8
50	g	202	CDL	CA2-C1-CB2-OB2
48	U	101	PEE	O4-C10-O2-C2
48	l	704	PEE	O5-C30-O3-C3
50	i	401	CDL	OB9-CB7-OB8-CB6
48	l	703	PEE	O3P-C1-C2-O2
50	g	202	CDL	O1-C1-CA2-OA2
50	i	401	CDL	O1-C1-CA2-OA2
50	r	503	CDL	CB5-C51-C52-C53
50	l	701	CDL	OB6-CB4-CB6-OB8
50	l	702	CDL	OB6-CB4-CB6-OB8
56	s	401	UQ	C12-C11-C9-C8
50	i	401	CDL	C14-C15-C16-C17
50	l	702	CDL	C54-C55-C56-C57
48	j	201	PEE	C11-C10-O2-C2
48	r	501	PEE	C11-C10-O2-C2
50	l	701	CDL	C20-C21-C22-C23
50	i	401	CDL	CB7-C71-C72-C73
48	U	101	PEE	C40-C41-C42-C43
48	j	201	PEE	C31-C30-O3-C3
48	B	303	PEE	C30-C31-C32-C33
50	i	401	CDL	CA7-C31-C32-C33
50	l	701	CDL	CB5-C51-C52-C53
50	r	503	CDL	CB7-C71-C72-C73
55	a	202	PLX	C29-C30-C31-C32
46	A	502	FMN	O2'-C2'-C3'-O3'
48	r	501	PEE	C10-C11-C12-C13
47	A	503	NAI	O4B-C4B-C5B-O5B
50	l	701	CDL	C71-CB7-OB8-CB6
50	r	503	CDL	C36-C37-C38-C39
50	g	202	CDL	OA7-CA5-OA6-CA4
46	A	502	FMN	O2'-C2'-C3'-C4'
50	a	201	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
50	r	503	CDL	CA7-C31-C32-C33
48	l	703	PEE	C33-C34-C35-C36
50	l	702	CDL	C35-C36-C37-C38
56	s	401	UQ	C9-C11-C12-C13
50	i	401	CDL	CA5-C11-C12-C13
50	a	201	CDL	O1-C1-CA2-OA2
50	a	201	CDL	O1-C1-CB2-OB2
50	g	202	CDL	O1-C1-CB2-OB2
50	r	503	CDL	O1-C1-CA2-OA2
48	B	303	PEE	C37-C38-C39-C40
48	Q	501	PEE	C17-C18-C19-C20
48	Q	501	PEE	C37-C38-C39-C40
55	g	201	PLX	C12-C13-C14-C15
48	j	201	PEE	O5-C30-O3-C3
55	r	502	PLX	C12-C13-C14-C15
48	j	201	PEE	C1-O3P-P-O4P
48	l	703	PEE	C4-O4P-P-O3P
50	a	201	CDL	CA2-OA2-PA1-OA5
50	a	201	CDL	CA3-OA5-PA1-OA2
50	a	201	CDL	CB2-OB2-PB2-OB5
50	g	202	CDL	CB2-OB2-PB2-OB5
50	i	401	CDL	CB3-OB5-PB2-OB2
50	l	701	CDL	CA2-OA2-PA1-OA5
50	l	701	CDL	CB3-OB5-PB2-OB2
50	l	702	CDL	CA3-OA5-PA1-OA2
50	l	702	CDL	CB2-OB2-PB2-OB5
50	r	503	CDL	CA2-OA2-PA1-OA5
50	r	503	CDL	CA3-OA5-PA1-OA2
55	a	202	PLX	C3-O4-P1-O1
55	g	201	PLX	C3-O4-P1-O1
55	j	202	PLX	C3-O4-P1-O1
55	r	502	PLX	C3-O4-P1-O1
55	r	502	PLX	C2-O1-P1-O4
50	a	201	CDL	CB2-C1-CA2-OA2
50	l	702	CDL	CB2-C1-CA2-OA2
50	l	702	CDL	CA2-C1-CB2-OB2
48	j	201	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
50	l	701	CDL	OB9-CB7-OB8-CB6
48	U	101	PEE	C31-C30-O3-C3
50	I	201	CDL	CA7-C31-C32-C33
50	a	201	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
50	r	503	CDL	C74-C75-C76-C77
50	l	702	CDL	C39-C40-C41-C42
48	l	704	PEE	C11-C10-O2-C2
50	I	201	CDL	C11-CA5-OA6-CA4
48	l	704	PEE	C33-C34-C35-C36
50	i	401	CDL	C11-C12-C13-C14
50	l	701	CDL	C75-C76-C77-C78
50	l	702	CDL	C56-C57-C58-C59
50	r	503	CDL	C11-C12-C13-C14
55	r	502	PLX	C28-C29-C30-C31
48	l	703	PEE	C21-C22-C23-C24
49	G	201	8Q1	C7-C8-C9-C10
50	i	401	CDL	C36-C37-C38-C39
50	r	503	CDL	C56-C57-C58-C59
55	j	202	PLX	C27-C28-C29-C30
48	l	704	PEE	O4-C10-O2-C2
50	I	201	CDL	OA7-CA5-OA6-CA4
50	l	702	CDL	CB7-C71-C72-C73
48	Q	501	PEE	C14-C15-C16-C17
49	X	201	8Q1	C11-C12-C13-C14
50	l	701	CDL	C82-C83-C84-C85
50	r	503	CDL	C73-C74-C75-C76
55	r	502	PLX	C11-C12-C13-C14
48	l	704	PEE	C17-C18-C19-C20
48	l	703	PEE	C22-C23-C24-C25
50	a	201	CDL	C72-C73-C74-C75
50	g	202	CDL	C59-C60-C61-C62
55	a	202	PLX	C28-C29-C30-C31
55	j	202	PLX	C14-C15-C16-C17
50	a	201	CDL	C32-C33-C34-C35
50	r	503	CDL	C43-C44-C45-C46
55	g	201	PLX	C28-C29-C30-C31
55	r	502	PLX	C25-C26-C27-C28
48	l	704	PEE	C12-C13-C14-C15
50	g	202	CDL	C14-C15-C16-C17
50	l	702	CDL	C55-C56-C57-C58
55	j	202	PLX	C9-C10-C11-C12
55	j	202	PLX	C25-C26-C27-C28
50	a	201	CDL	C37-C38-C39-C40
50	r	503	CDL	C62-C63-C64-C65
55	g	201	PLX	C10-C11-C12-C13
50	g	202	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
48	Q	501	PEE	C21-C22-C23-C24
50	r	503	CDL	C63-C64-C65-C66
50	r	503	CDL	C71-C72-C73-C74
50	r	503	CDL	C75-C76-C77-C78
55	g	201	PLX	C9-C10-C11-C12
55	r	502	PLX	C14-C15-C16-C17
48	B	303	PEE	C23-C24-C25-C26
48	j	201	PEE	C13-C14-C15-C16
48	l	703	PEE	C31-C32-C33-C34
50	a	201	CDL	C11-C12-C13-C14
50	r	503	CDL	C23-C24-C25-C26
55	g	201	PLX	C27-C28-C29-C30
50	i	401	CDL	C35-C36-C37-C38
50	l	701	CDL	C59-C60-C61-C62
50	l	702	CDL	C14-C15-C16-C17
50	r	503	CDL	C41-C42-C43-C44
50	r	503	CDL	C52-C53-C54-C55
55	g	201	PLX	C18-C19-C20-C21
55	g	201	PLX	C14-C15-C16-C17
55	r	502	PLX	C29-C30-C31-C32
48	U	101	PEE	O5-C30-O3-C3
48	U	101	PEE	C21-C22-C23-C24
50	l	702	CDL	C60-C61-C62-C63
50	l	702	CDL	C72-C73-C74-C75
50	l	702	CDL	C73-C74-C75-C76
55	a	202	PLX	C33-C34-C35-C36
55	g	201	PLX	C11-C10-C9-C8
55	j	202	PLX	C13-C14-C15-C16
48	l	704	PEE	O4P-C4-C5-N
48	B	303	PEE	C20-C21-C22-C23
48	B	303	PEE	C42-C43-C44-C45
49	X	201	8Q1	C7-C8-C9-C10
50	a	201	CDL	C22-C23-C24-C25
50	g	202	CDL	C54-C55-C56-C57
50	l	701	CDL	C35-C36-C37-C38
50	l	702	CDL	C58-C59-C60-C61
55	a	202	PLX	C7-C8-C9-C10
55	j	202	PLX	C12-C13-C14-C15
55	r	502	PLX	C10-C11-C12-C13
48	r	501	PEE	C13-C14-C15-C16
48	r	501	PEE	C12-C13-C14-C15
50	i	401	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
50	r	503	CDL	C37-C38-C39-C40
55	g	201	PLX	C30-C31-C32-C33
55	j	202	PLX	C7-C8-C9-C10
50	l	702	CDL	CB5-C51-C52-C53
50	r	503	CDL	C15-C16-C17-C18
50	a	201	CDL	C42-C43-C44-C45
48	U	101	PEE	C22-C23-C24-C25
48	m	201	PEE	C33-C34-C35-C36
48	r	501	PEE	C41-C42-C43-C44
50	l	702	CDL	C57-C58-C59-C60
50	r	503	CDL	C35-C36-C37-C38
50	a	201	CDL	C73-C74-C75-C76
50	r	503	CDL	C17-C18-C19-C20
50	r	503	CDL	C55-C56-C57-C58
50	r	503	CDL	C59-C60-C61-C62
48	m	201	PEE	C19-C20-C21-C22
48	r	501	PEE	C30-C31-C32-C33
50	I	201	CDL	O1-C1-CB2-OB2
49	G	201	8Q1	C9-C10-C11-C12
50	l	702	CDL	C62-C63-C64-C65
48	U	101	PEE	C43-C44-C45-C46
50	r	503	CDL	C12-C13-C14-C15
48	m	201	PEE	C11-C12-C13-C14
55	r	502	PLX	C33-C34-C35-C36
55	r	502	PLX	C2-C1-N1-C1A
48	B	303	PEE	C11-C10-O2-C2
50	I	201	CDL	C51-CB5-OB6-CB4
48	l	704	PEE	C31-C32-C33-C34
50	l	701	CDL	CA7-C31-C32-C33
48	B	303	PEE	C13-C14-C15-C16
55	a	202	PLX	C12-C13-C14-C15
48	U	101	PEE	C36-C37-C38-C39
48	r	501	PEE	C36-C37-C38-C39
48	l	703	PEE	C12-C13-C14-C15
49	G	201	8Q1	C11-C10-C9-C8
48	j	201	PEE	C15-C16-C17-C18
48	j	201	PEE	C39-C40-C41-C42
55	g	201	PLX	C35-C36-C37-C38
50	a	201	CDL	C17-C18-C19-C20
50	a	201	CDL	C20-C21-C22-C23
50	a	201	CDL	CA7-C31-C32-C33
50	a	201	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
55	a	202	PLX	C14-C15-C16-C17
55	g	201	PLX	C25-C26-C27-C28
50	i	401	CDL	C13-C14-C15-C16
48	m	201	PEE	C21-C22-C23-C24
50	l	701	CDL	C61-C62-C63-C64
50	r	503	CDL	CA5-C11-C12-C13
50	a	201	CDL	OA5-CA3-CA4-OA6
48	B	303	PEE	O4-C10-O2-C2
50	g	202	CDL	C13-C14-C15-C16
48	j	201	PEE	C32-C33-C34-C35
50	l	702	CDL	C12-C13-C14-C15
55	r	502	PLX	C2-C1-N1-C1C
50	l	701	CDL	C36-C37-C38-C39
50	l	701	CDL	C81-C82-C83-C84
48	l	703	PEE	C15-C16-C17-C18
48	Q	501	PEE	C10-C11-C12-C13
56	s	401	UQ	C13-C14-C16-C17
50	r	503	CDL	C20-C21-C22-C23
50	l	701	CDL	C23-C24-C25-C26
50	l	701	CDL	C52-C53-C54-C55
50	g	202	CDL	CA5-C11-C12-C13
55	r	502	PLX	C27-C28-C29-C30
50	I	201	CDL	OB7-CB5-OB6-CB4
50	i	401	CDL	C11-CA5-OA6-CA4
55	g	201	PLX	C32-C33-C34-C35
50	l	702	CDL	CB3-OB5-PB2-OB2
50	i	401	CDL	C32-C33-C34-C35
55	r	502	PLX	C7-C8-C9-C10
48	r	501	PEE	O3P-C1-C2-C3
48	Q	501	PEE	C22-C23-C24-C25
50	l	702	CDL	C52-C53-C54-C55
48	B	303	PEE	C14-C15-C16-C17
50	l	701	CDL	C56-C57-C58-C59
55	j	202	PLX	C26-C27-C28-C29
48	m	201	PEE	C31-C32-C33-C34
48	l	704	PEE	C16-C17-C18-C19
50	l	702	CDL	C40-C41-C42-C43
48	B	303	PEE	C33-C34-C35-C36
50	a	201	CDL	C52-C53-C54-C55
50	a	201	CDL	C75-C76-C77-C78
50	r	503	CDL	C60-C61-C62-C63
48	Q	501	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
50	I	201	CDL	CA3-CA4-CA6-OA8
50	g	202	CDL	CA3-CA4-CA6-OA8
50	l	701	CDL	CB3-CB4-CB6-OB8
48	m	201	PEE	C24-C25-C26-C27
55	r	502	PLX	C36-C37-C38-C39
50	l	702	CDL	CA7-C31-C32-C33
50	g	202	CDL	C22-C23-C24-C25
55	r	502	PLX	O8-C24-C25-C26
50	l	702	CDL	C64-C65-C66-C67
48	j	201	PEE	C18-C19-C20-C21
55	j	202	PLX	C33-C34-C35-C36
48	B	303	PEE	C15-C16-C17-C18
48	Q	501	PEE	C19-C20-C21-C22
48	Q	501	PEE	C30-C31-C32-C33
50	l	701	CDL	C37-C38-C39-C40
48	j	201	PEE	C10-C11-C12-C13
47	A	503	NAI	C2D-C1D-N1N-C2N
50	I	201	CDL	C31-CA7-OA8-CA6
50	l	701	CDL	C54-C55-C56-C57
55	j	202	PLX	C35-C36-C37-C38
50	I	201	CDL	C31-C32-C33-C34
50	l	701	CDL	C14-C15-C16-C17
50	g	202	CDL	C76-C77-C78-C79
49	X	201	8Q1	C28-O27-P24-O3
50	l	701	CDL	C19-C20-C21-C22
50	l	701	CDL	C84-C85-C86-C87
48	j	201	PEE	O3P-C1-C2-O2
48	B	303	PEE	C17-C18-C19-C20
55	r	502	PLX	C2-C1-N1-C1B
50	l	702	CDL	C79-C80-C81-C82
55	j	202	PLX	C10-C11-C12-C13
48	l	703	PEE	O2-C2-C3-O3
50	I	201	CDL	OA6-CA4-CA6-OA8
55	j	202	PLX	O6-C4-C5-O8
50	r	503	CDL	C76-C77-C78-C79
50	g	202	CDL	C57-C58-C59-C60
50	g	202	CDL	C19-C20-C21-C22
50	r	503	CDL	C32-C33-C34-C35
50	l	701	CDL	CB2-C1-CA2-OA2
50	r	503	CDL	CB2-C1-CA2-OA2
50	l	701	CDL	C73-C74-C75-C76
50	l	702	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
50	r	503	CDL	C54-C55-C56-C57
55	r	502	PLX	C35-C36-C37-C38
50	I	201	CDL	OA9-CA7-OA8-CA6
48	Q	501	PEE	C13-C14-C15-C16
48	B	303	PEE	C10-C11-C12-C13
48	B	303	PEE	C32-C33-C34-C35
48	Q	501	PEE	C24-C25-C26-C27
48	Q	501	PEE	C31-C32-C33-C34
50	l	702	CDL	C17-C18-C19-C20
48	U	101	PEE	C38-C39-C40-C41
55	a	202	PLX	C25-C26-C27-C28
51	J	401	NDP	C3B-C4B-C5B-O5B
48	l	703	PEE	O3P-C1-C2-C3
50	a	201	CDL	OA5-CA3-CA4-CA6
50	a	201	CDL	OB5-CB3-CB4-CB6
50	r	503	CDL	OB5-CB3-CB4-CB6
55	a	202	PLX	O4-C3-C4-C5
49	X	201	8Q1	C6-C7-C8-C9
50	l	701	CDL	C39-C40-C41-C42
50	r	503	CDL	C34-C35-C36-C37
55	a	202	PLX	C9-C10-C11-C12
48	l	703	PEE	C30-C31-C32-C33
55	a	202	PLX	C31-C32-C33-C34
50	r	503	CDL	C13-C14-C15-C16
55	r	502	PLX	C13-C14-C15-C16
50	a	201	CDL	C41-C42-C43-C44
50	l	701	CDL	C71-C72-C73-C74
50	l	702	CDL	C37-C38-C39-C40
50	r	503	CDL	C64-C65-C66-C67
50	a	201	CDL	C31-CA7-OA8-CA6
48	r	501	PEE	C1-C2-C3-O3
50	l	702	CDL	CB3-CB4-CB6-OB8
50	r	503	CDL	CA3-CA4-CA6-OA8
50	r	503	CDL	CB3-CB4-CB6-OB8
55	a	202	PLX	C3-C4-C5-O8
55	r	502	PLX	C3-C4-C5-O8
50	i	401	CDL	OA7-CA5-OA6-CA4
50	a	201	CDL	C60-C61-C62-C63
55	r	502	PLX	C16-C17-C18-C19
56	s	401	UQ	C12-C13-C14-C16
49	X	201	8Q1	C9-C10-C11-C12
50	r	503	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
50	r	503	CDL	CB2-OB2-PB2-OB5
55	r	502	PLX	C5-C4-O6-C6
48	B	303	PEE	O3P-C1-C2-O2
50	I	201	CDL	OA5-CA3-CA4-OA6
50	i	401	CDL	OB5-CB3-CB4-OB6
50	l	702	CDL	OA5-CA3-CA4-OA6
50	r	503	CDL	OB5-CB3-CB4-OB6
50	i	401	CDL	CB5-C51-C52-C53
50	g	202	CDL	C56-C57-C58-C59
49	X	201	8Q1	C10-C11-C12-C13
48	U	101	PEE	C44-C45-C46-C47
50	r	503	CDL	C33-C34-C35-C36
48	U	101	PEE	O2-C2-C3-O3
50	g	202	CDL	OA6-CA4-CA6-OA8
50	r	503	CDL	OB6-CB4-CB6-OB8
55	a	202	PLX	O6-C4-C5-O8
50	r	503	CDL	C82-C83-C84-C85
48	r	501	PEE	C20-C21-C22-C23
50	a	201	CDL	C77-C78-C79-C80
49	G	201	8Q1	O4-C1-S44-C43
48	r	501	PEE	C33-C34-C35-C36
55	g	201	PLX	C33-C34-C35-C36
47	A	503	NAI	PN-O3-PA-O5B
50	g	202	CDL	C55-C56-C57-C58
48	j	201	PEE	O3P-C1-C2-C3
50	i	401	CDL	OB5-CB3-CB4-CB6
55	j	202	PLX	O4-C3-C4-C5
55	r	502	PLX	C34-C35-C36-C37
48	r	501	PEE	C31-C32-C33-C34
55	g	201	PLX	C36-C37-C38-C39
48	U	101	PEE	C31-C32-C33-C34
50	a	201	CDL	C39-C40-C41-C42
50	l	702	CDL	C22-C23-C24-C25
50	I	201	CDL	C51-C52-C53-C54
50	a	201	CDL	C71-CB7-OB8-CB6
48	m	201	PEE	C3-C2-O2-C10
49	G	201	8Q1	C6-C1-S44-C43
50	a	201	CDL	C78-C79-C80-C81
49	G	201	8Q1	C6-C7-C8-C9
55	a	202	PLX	C34-C35-C36-C37
50	l	702	CDL	CA3-CA4-CA6-OA8
50	r	503	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
55	g	201	PLX	C3-C4-C5-O8
50	a	201	CDL	C43-C44-C45-C46
50	a	201	CDL	OB5-CB3-CB4-OB6
55	g	201	PLX	O4-C3-C4-O6
48	Q	501	PEE	C32-C33-C34-C35
48	r	501	PEE	O2-C2-C3-O3
48	B	303	PEE	C31-C30-O3-C3
50	a	201	CDL	OA9-CA7-OA8-CA6
47	A	503	NAI	C5B-O5B-PA-O3
55	r	502	PLX	C31-C32-C33-C34
48	l	703	PEE	C35-C36-C37-C38
48	l	704	PEE	C19-C20-C21-C22
48	l	704	PEE	C15-C16-C17-C18
50	i	401	CDL	C51-C52-C53-C54
50	l	701	CDL	C31-C32-C33-C34
50	a	201	CDL	OB9-CB7-OB8-CB6
50	l	701	CDL	C44-C45-C46-C47
48	U	101	PEE	C41-C42-C43-C44
50	r	503	CDL	C31-CA7-OA8-CA6
55	g	201	PLX	C17-C18-C19-C20
48	l	704	PEE	C4-O4P-P-O3P
50	g	202	CDL	CA3-OA5-PA1-OA2
50	a	201	CDL	C34-C35-C36-C37
50	g	202	CDL	C52-C53-C54-C55
50	r	503	CDL	O1-C1-CB2-OB2
47	A	503	NAI	C2D-C1D-N1N-C6N
48	Q	501	PEE	C2-C1-O3P-P
50	i	401	CDL	CA4-CA3-OA5-PA1
46	A	502	FMN	C3'-C4'-C5'-O5'
47	A	503	NAI	C5B-O5B-PA-O2A
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O1P
48	l	703	PEE	C4-O4P-P-O2P
48	l	704	PEE	C4-O4P-P-O1P
50	a	201	CDL	CA3-OA5-PA1-OA4
50	g	202	CDL	CA2-OA2-PA1-OA4
50	g	202	CDL	CA3-OA5-PA1-OA3
50	i	401	CDL	CB3-OB5-PB2-OB4
50	l	701	CDL	CA2-OA2-PA1-OA3
50	l	701	CDL	CB2-OB2-PB2-OB3
50	l	702	CDL	CB2-OB2-PB2-OB3
50	l	702	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
50	l	702	CDL	CB3-OB5-PB2-OB4
50	r	503	CDL	CB3-OB5-PB2-OB3
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C5B-O5B-PA-O2A
55	a	202	PLX	C3-O4-P1-O2
55	a	202	PLX	C2-O1-P1-O2
55	g	201	PLX	C3-O4-P1-O2
55	g	201	PLX	C2-O1-P1-O3
55	j	202	PLX	C3-O4-P1-O2
55	r	502	PLX	C3-O4-P1-O2
55	r	502	PLX	C2-O1-P1-O2
55	r	502	PLX	C2-O1-P1-O3
57	w	401	ADP	C5'-O5'-PA-O1A
55	j	202	PLX	C31-C32-C33-C34
48	B	303	PEE	O3P-C1-C2-C3
50	I	201	CDL	OB5-CB3-CB4-CB6
50	l	702	CDL	OA5-CA3-CA4-CA6
55	g	201	PLX	O4-C3-C4-C5
56	s	401	UQ	C14-C16-C17-C18
55	a	202	PLX	C25-C24-O8-C5
55	j	202	PLX	C25-C24-O8-C5
48	B	303	PEE	O5-C30-O3-C3
50	I	201	CDL	OB5-CB3-CB4-OB6
50	i	401	CDL	OA5-CA3-CA4-OA6
55	j	202	PLX	O4-C3-C4-O6
48	l	704	PEE	C13-C14-C15-C16
47	A	503	NAI	O4D-C1D-N1N-C2N
49	G	201	8Q1	C10-C11-C12-C13
48	l	704	PEE	C1-C2-C3-O3
55	j	202	PLX	C3-C4-C5-O8
48	Q	501	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
55	r	502	PLX	O6-C4-C5-O8
50	r	503	CDL	C78-C79-C80-C81
50	I	201	CDL	CB7-C71-C72-C73
48	U	101	PEE	C12-C13-C14-C15
50	r	503	CDL	C79-C80-C81-C82
50	r	503	CDL	OA9-CA7-OA8-CA6
50	l	701	CDL	C51-C52-C53-C54
55	a	202	PLX	C27-C28-C29-C30
50	g	202	CDL	C61-C62-C63-C64
55	g	201	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
48	U	101	PEE	C42-C43-C44-C45
50	l	701	CDL	C72-C73-C74-C75
50	i	401	CDL	OA5-CA3-CA4-CA6
48	r	501	PEE	C31-C30-O3-C3
55	g	201	PLX	C29-C30-C31-C32
46	A	502	FMN	C5'-O5'-P-O1P
48	r	501	PEE	O5-C30-O3-C3
55	j	202	PLX	C17-C18-C19-C20
48	B	303	PEE	C21-C22-C23-C24
50	l	701	CDL	C11-CA5-OA6-CA4
50	I	201	CDL	C12-C13-C14-C15
50	i	401	CDL	CA2-OA2-PA1-OA5
50	l	702	CDL	CA2-OA2-PA1-OA5
50	a	201	CDL	C21-C22-C23-C24
49	G	201	8Q1	C30-C29-C32-O33
48	l	703	PEE	C1-C2-C3-O3
48	m	201	PEE	C16-C17-C18-C19
50	i	401	CDL	C52-C53-C54-C55
50	r	503	CDL	C80-C81-C82-C83
48	j	201	PEE	C33-C34-C35-C36
48	m	201	PEE	C15-C16-C17-C18
55	g	201	PLX	C19-C20-C21-C22
48	j	201	PEE	C11-C12-C13-C14
48	B	303	PEE	C38-C39-C40-C41
48	l	704	PEE	C18-C19-C20-C21
50	g	202	CDL	OA9-CA7-OA8-CA6
50	a	201	CDL	C55-C56-C57-C58
55	j	202	PLX	C15-C16-C17-C18
48	B	303	PEE	C39-C40-C41-C42
50	g	202	CDL	C31-CA7-OA8-CA6
48	r	501	PEE	C38-C39-C40-C41
50	l	701	CDL	OA7-CA5-OA6-CA4
48	l	703	PEE	C13-C14-C15-C16
50	g	202	CDL	C60-C61-C62-C63
48	l	704	PEE	C39-C40-C41-C42
49	X	201	8Q1	C11-C10-C9-C8
55	a	202	PLX	O6-C6-C7-C8
55	j	202	PLX	O6-C6-C7-C8
49	X	201	8Q1	N41-C42-C43-S44
50	l	702	CDL	C32-C33-C34-C35
55	j	202	PLX	C30-C31-C32-C33
48	B	303	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
55	g	201	PLX	C11-C12-C13-C14
48	U	101	PEE	C1-C2-C3-O3
55	j	202	PLX	C18-C19-C20-C21
49	G	201	8Q1	O27-C28-C29-C30
55	j	202	PLX	C24-C25-C26-C27
50	I	201	CDL	CA3-CA4-OA6-CA5
50	a	201	CDL	C32-C31-CA7-OA8
47	A	503	NAI	O4D-C1D-N1N-C6N
48	B	303	PEE	C24-C25-C26-C27
50	g	202	CDL	C74-C75-C76-C77
48	j	201	PEE	C14-C15-C16-C17
50	l	701	CDL	C72-C71-CB7-OB8
48	Q	501	PEE	O3P-C1-C2-C3
50	l	702	CDL	C80-C81-C82-C83
49	X	201	8Q1	C42-C43-S44-C1
55	g	201	PLX	O6-C4-C5-O8
48	U	101	PEE	C37-C38-C39-C40
48	l	703	PEE	C37-C38-C39-C40
50	r	503	CDL	C31-C32-C33-C34
50	l	701	CDL	C74-C75-C76-C77
51	J	401	NDP	PN-O3-PA-O1A
50	g	202	CDL	C78-C79-C80-C81
55	a	202	PLX	C24-C25-C26-C27
48	l	704	PEE	C32-C33-C34-C35
55	j	202	PLX	O8-C24-C25-C26
50	I	201	CDL	OA5-CA3-CA4-CA6
50	i	401	CDL	C52-C51-CB5-OB6
48	U	101	PEE	O4P-C4-C5-N
48	l	703	PEE	C38-C39-C40-C41
50	i	401	CDL	C12-C13-C14-C15
49	G	201	8Q1	O27-C28-C29-C31
55	r	502	PLX	C24-C25-C26-C27
48	l	703	PEE	C32-C33-C34-C35
48	l	703	PEE	C19-C20-C21-C22
48	m	201	PEE	C13-C14-C15-C16
50	r	503	CDL	C52-C51-CB5-OB6
48	l	703	PEE	C36-C37-C38-C39
48	l	704	PEE	C38-C39-C40-C41
48	l	704	PEE	C24-C25-C26-C27
50	i	401	CDL	C15-C16-C17-C18
50	I	201	CDL	CA6-CA4-OA6-CA5
50	g	202	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
50	g	202	CDL	CA6-CA4-OA6-CA5
48	j	201	PEE	C42-C43-C44-C45
50	g	202	CDL	C12-C11-CA5-OA6
48	Q	501	PEE	C36-C37-C38-C39
48	Q	501	PEE	C38-C39-C40-C41
48	m	201	PEE	C18-C19-C20-C21
48	Q	501	PEE	C11-C12-C13-C14
50	a	201	CDL	C18-C19-C20-C21
55	j	202	PLX	C7-C6-O6-C4
48	l	704	PEE	O3P-C1-C2-O2
50	l	701	CDL	OB5-CB3-CB4-OB6
50	a	201	CDL	C31-C32-C33-C34
48	l	704	PEE	C30-C31-C32-C33
50	l	702	CDL	C32-C31-CA7-OA8
55	j	202	PLX	C32-C33-C34-C35
49	G	201	8Q1	C31-C29-C32-C34
50	g	202	CDL	C51-C52-C53-C54
50	l	701	CDL	C12-C13-C14-C15
55	g	201	PLX	C15-C16-C17-C18
55	a	202	PLX	C13-C14-C15-C16
50	i	401	CDL	C38-C39-C40-C41
50	l	702	CDL	C12-C11-CA5-OA6
49	G	201	8Q1	C31-C29-C32-O33
48	U	101	PEE	C16-C17-C18-C19
50	I	201	CDL	C72-C71-CB7-OB8
50	l	702	CDL	C71-C72-C73-C74
50	g	202	CDL	C12-C11-CA5-OA7
48	U	101	PEE	C34-C35-C36-C37
50	g	202	CDL	C11-C12-C13-C14
48	U	101	PEE	O3-C30-C31-C32
50	a	201	CDL	C24-C25-C26-C27
50	a	201	CDL	C53-C54-C55-C56
50	l	701	CDL	C62-C63-C64-C65
50	l	702	CDL	C32-C31-CA7-OA9
50	r	503	CDL	C40-C41-C42-C43
48	l	704	PEE	C20-C21-C22-C23
55	g	201	PLX	C31-C32-C33-C34
50	a	201	CDL	CA4-CA3-OA5-PA1
48	Q	501	PEE	C1-O3P-P-O1P
48	l	704	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O1P

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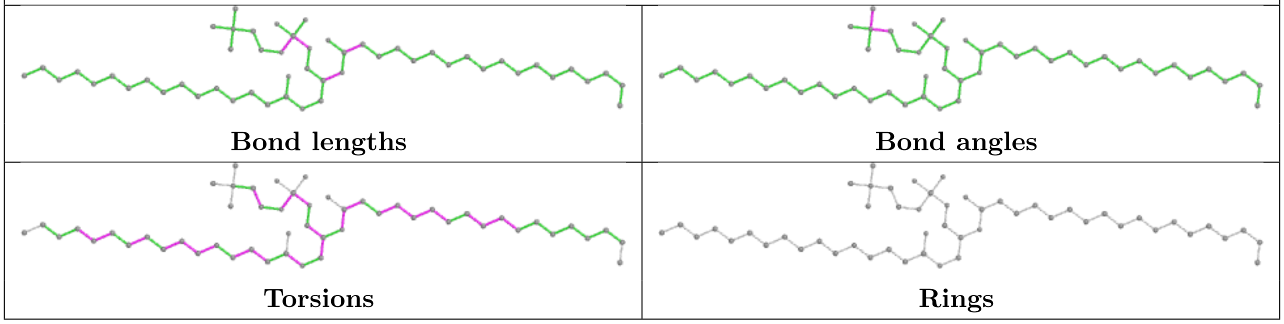
Mol	Chain	Res	Type	Atoms
51	J	401	NDP	C2N-C3N-C7N-N7N
50	l	702	CDL	C12-C11-CA5-OA7
50	r	503	CDL	C52-C51-CB5-OB7
48	l	704	PEE	C34-C35-C36-C37
48	l	704	PEE	C5-C4-O4P-P
48	l	703	PEE	O2-C10-C11-C12
50	g	202	CDL	C72-C71-CB7-OB8
50	r	503	CDL	C72-C71-CB7-OB8
48	B	303	PEE	C34-C35-C36-C37
50	I	201	CDL	CA2-C1-CB2-OB2
48	l	703	PEE	C34-C35-C36-C37
48	Q	501	PEE	C16-C17-C18-C19
50	r	503	CDL	C83-C84-C85-C86
48	U	101	PEE	O5-C30-C31-C32
50	l	702	CDL	C15-C16-C17-C18
50	I	201	CDL	C72-C71-CB7-OB9
50	a	201	CDL	C54-C55-C56-C57
50	r	503	CDL	C72-C71-CB7-OB9

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PLX a 202



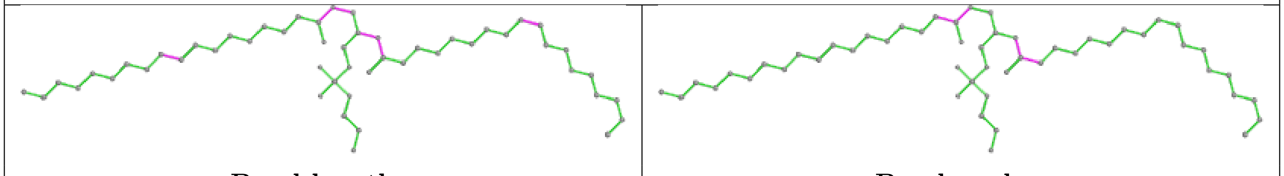
Bond lengths

Bond angles

Torsions

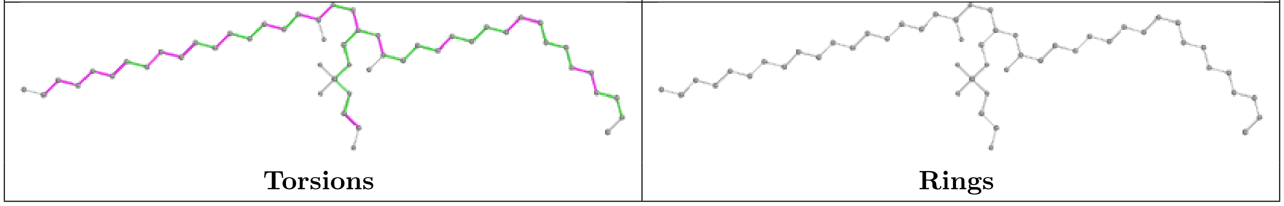
Rings

Ligand PEE U 101



Bond lengths

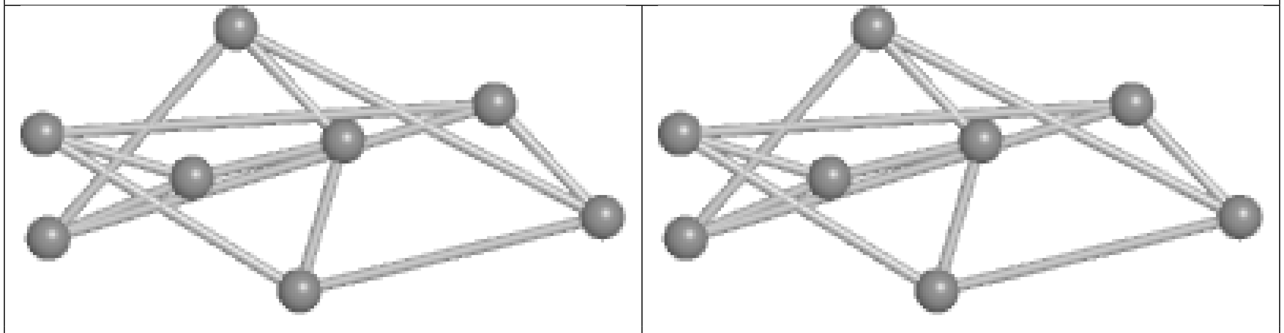
Bond angles



Torsions

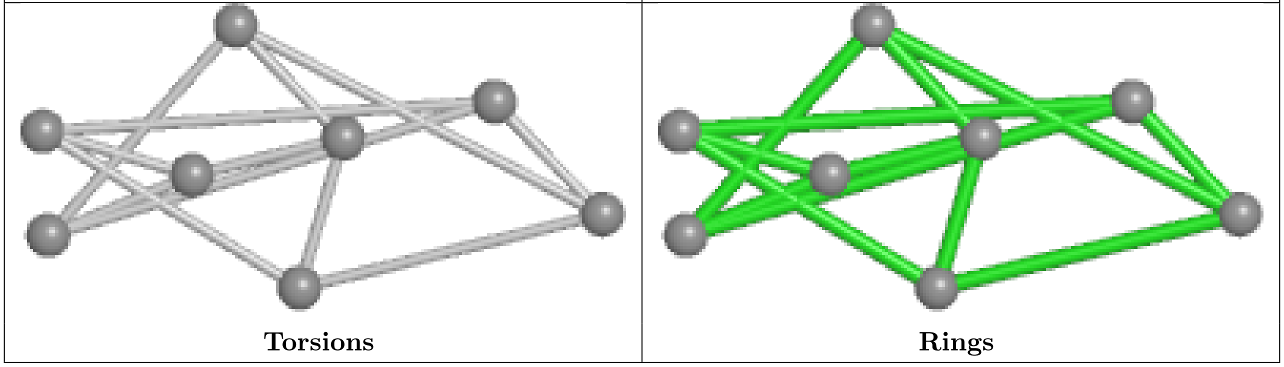
Rings

Ligand SF4 B 301



Bond lengths

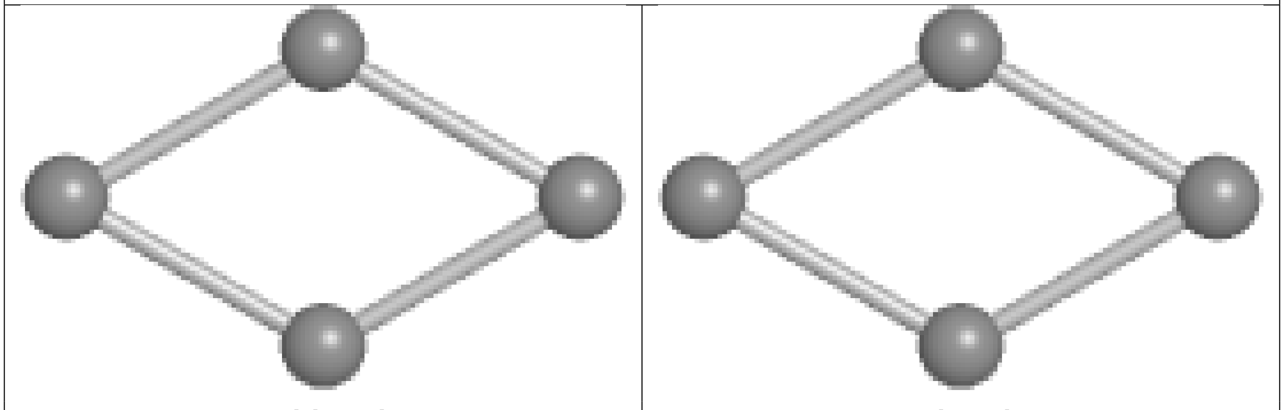
Bond angles



Torsions

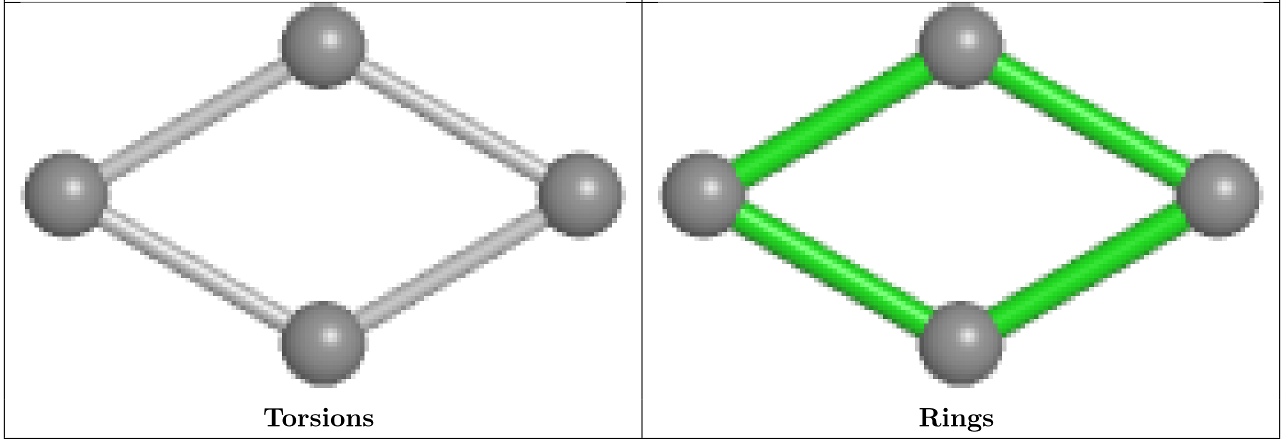
Rings

Ligand FES O 301



Bond lengths

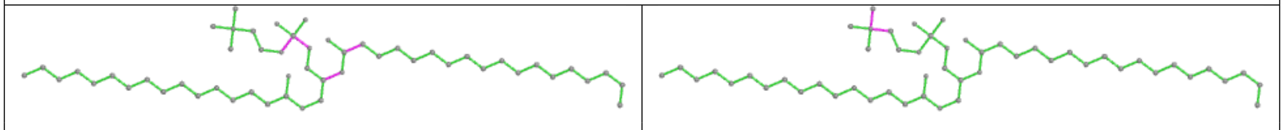
Bond angles



Torsions

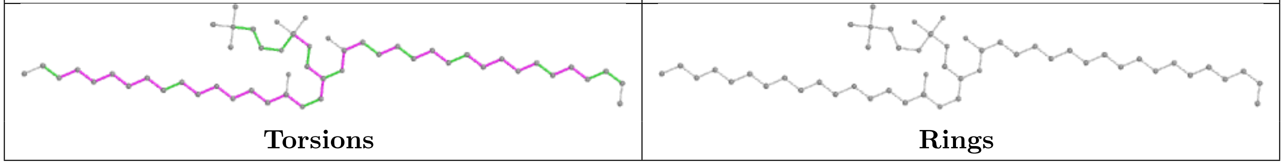
Rings

Ligand PLX j 202



Bond lengths

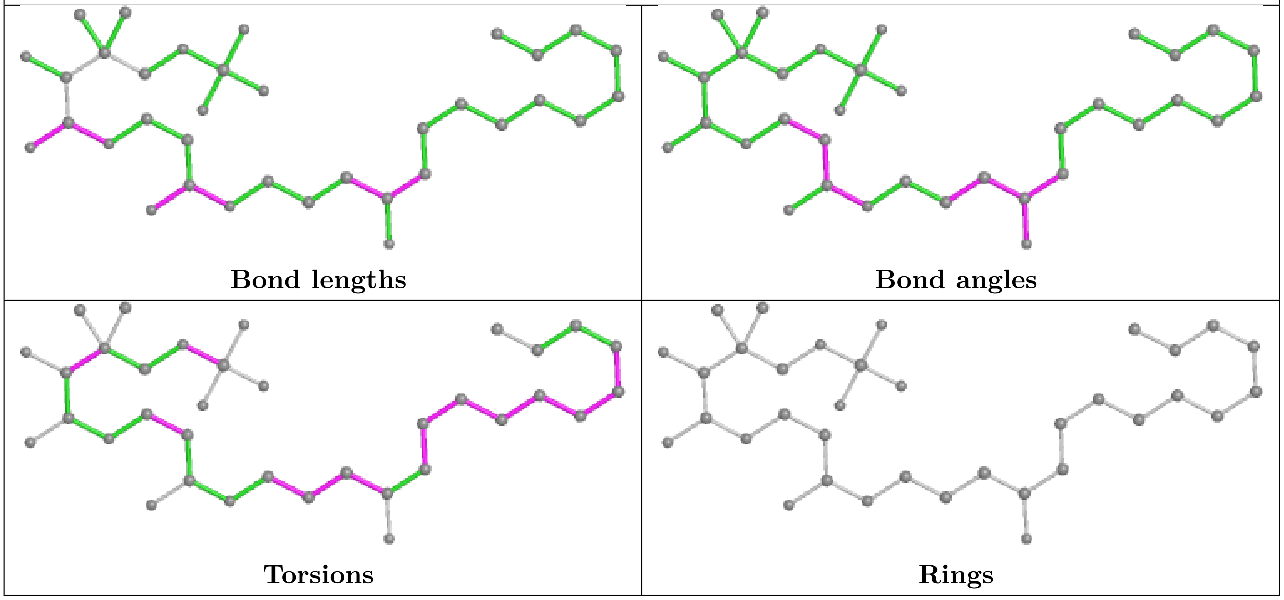
Bond angles



Torsions

Rings

Ligand 8Q1 X 201



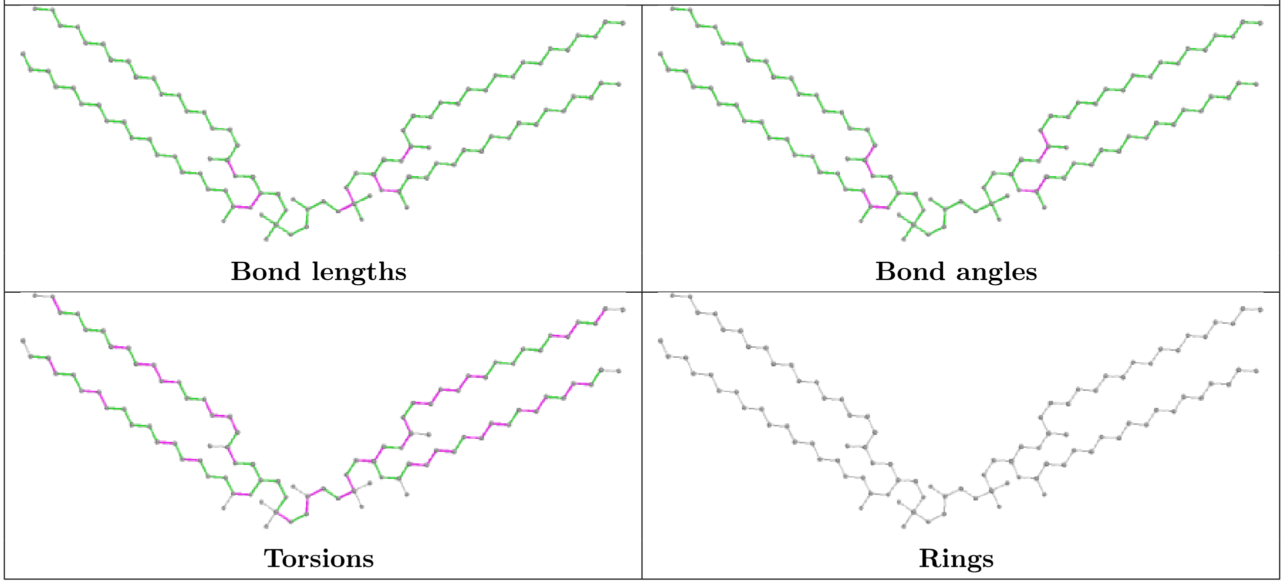
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL l 701



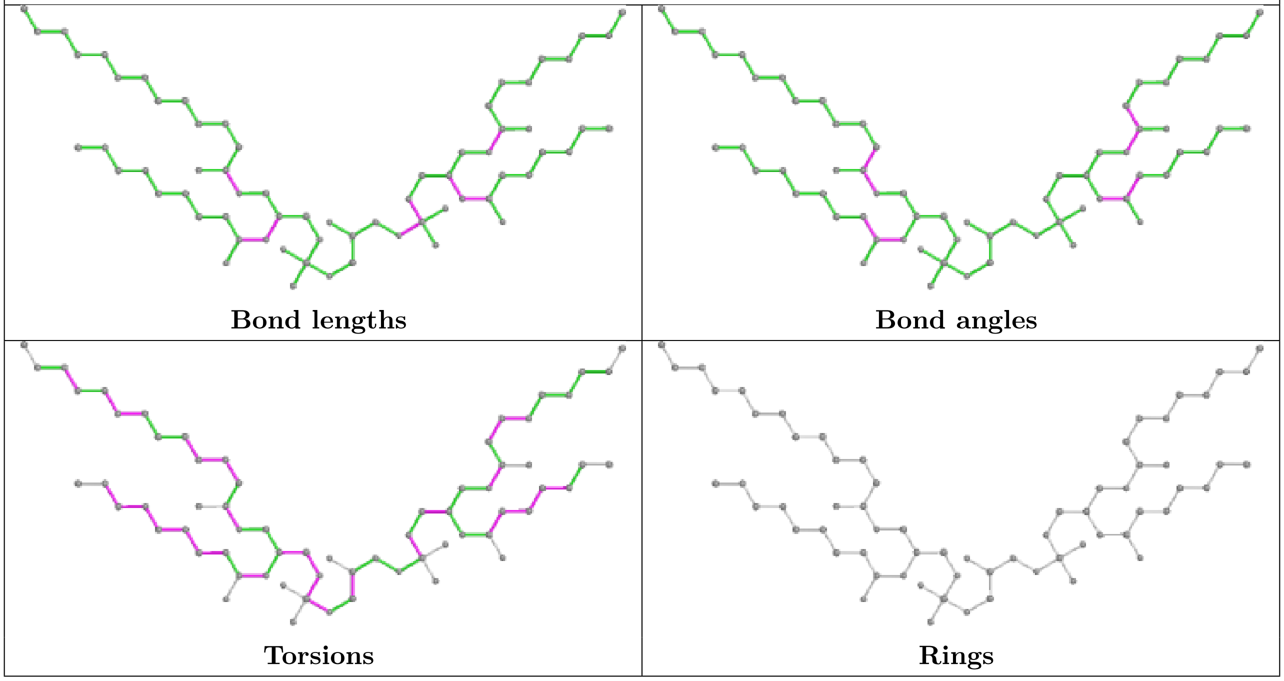
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL i 401



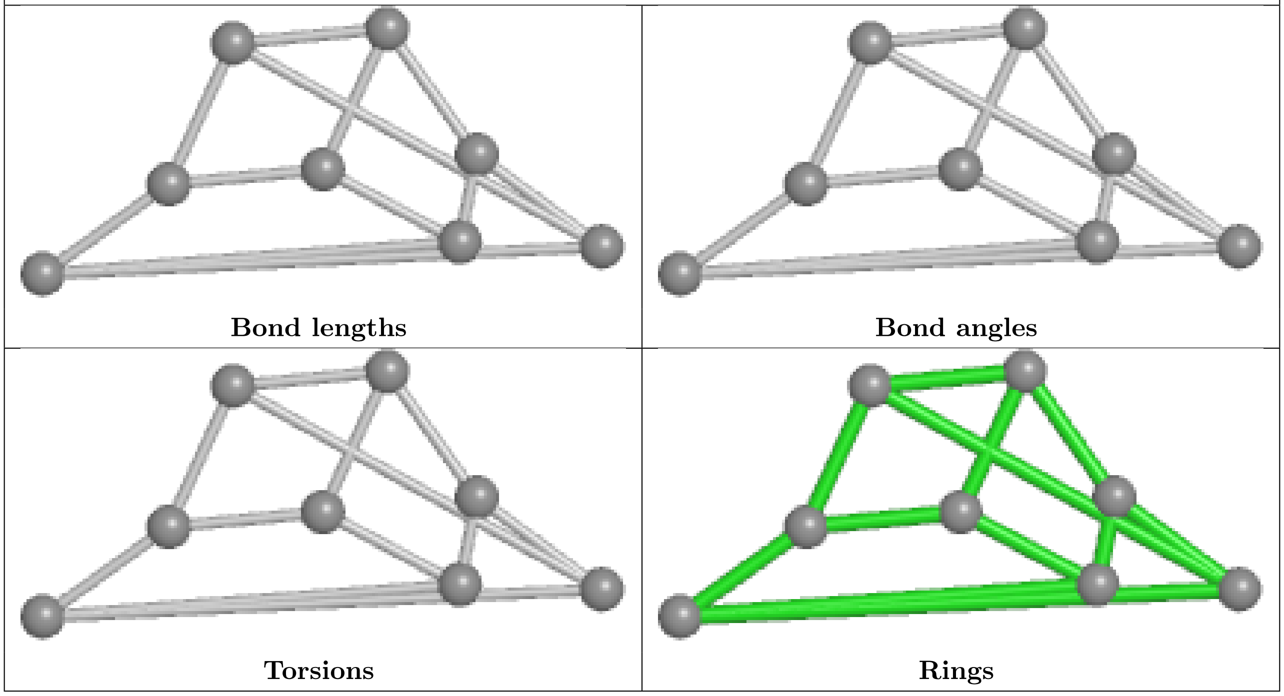
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 B 302



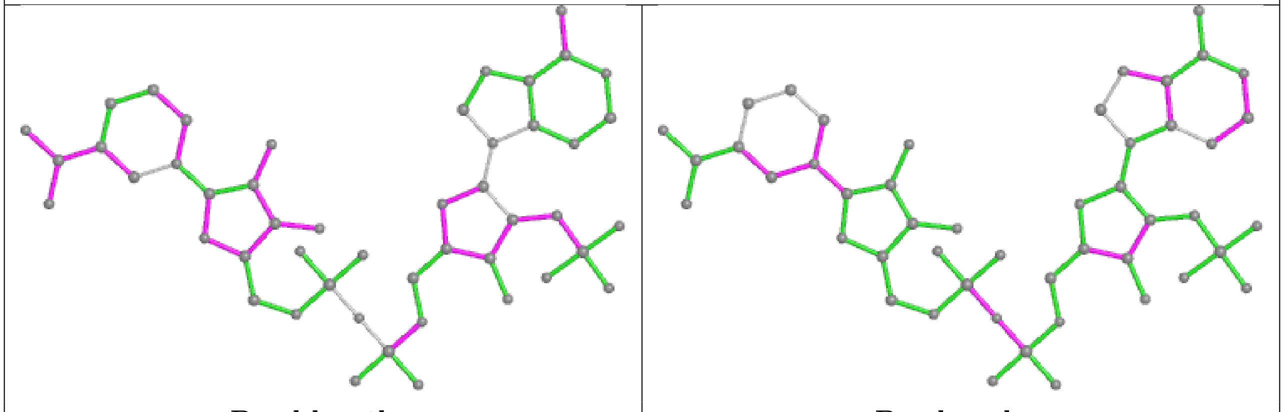
Bond lengths

Bond angles

Torsions

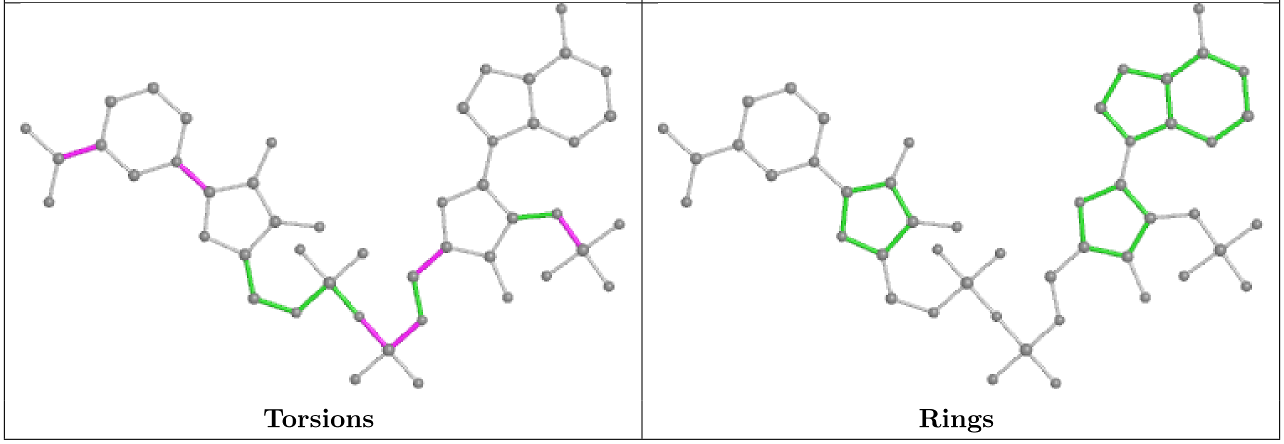
Rings

Ligand NDP J 401



Bond lengths

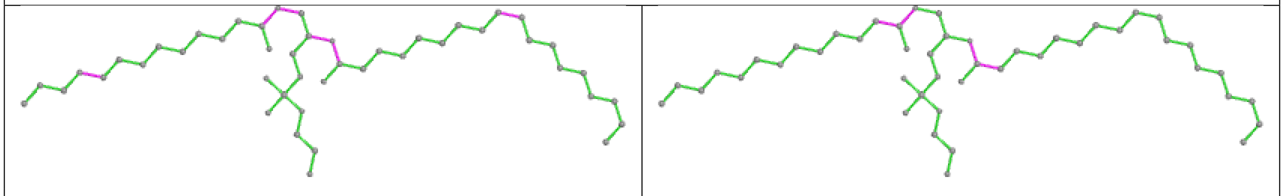
Bond angles



Torsions

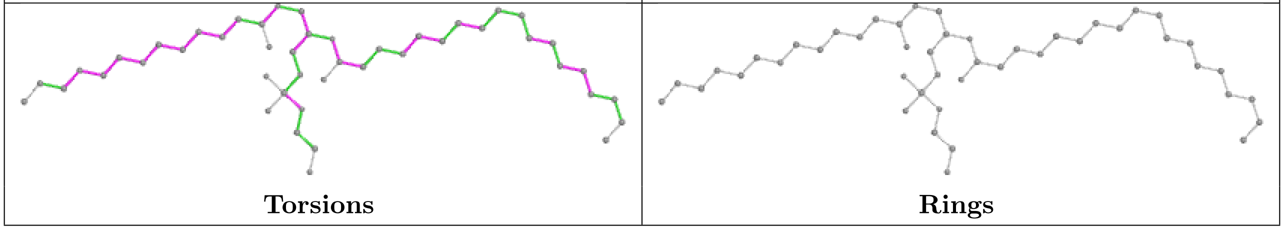
Rings

Ligand PEE l 703



Bond lengths

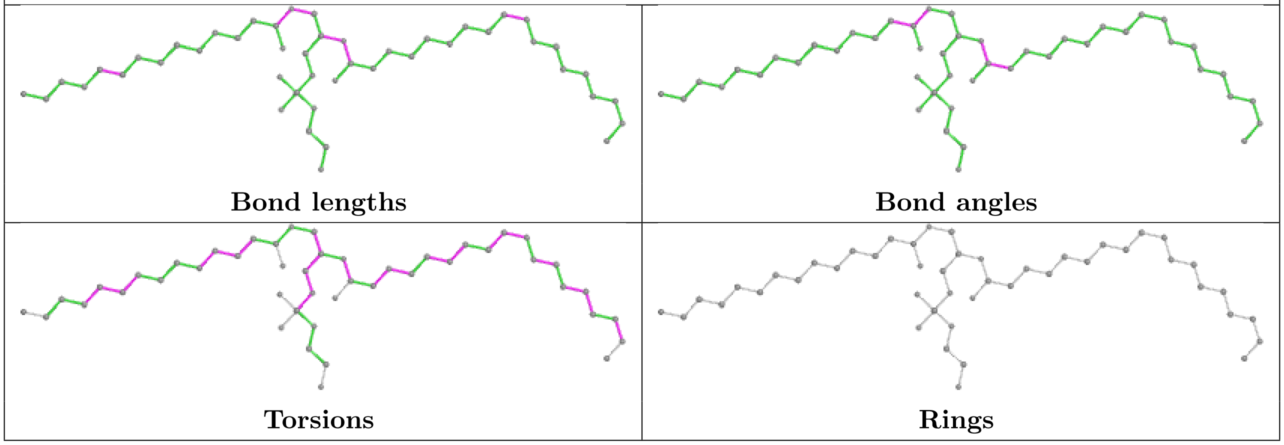
Bond angles



Torsions

Rings

Ligand PEE Q 501



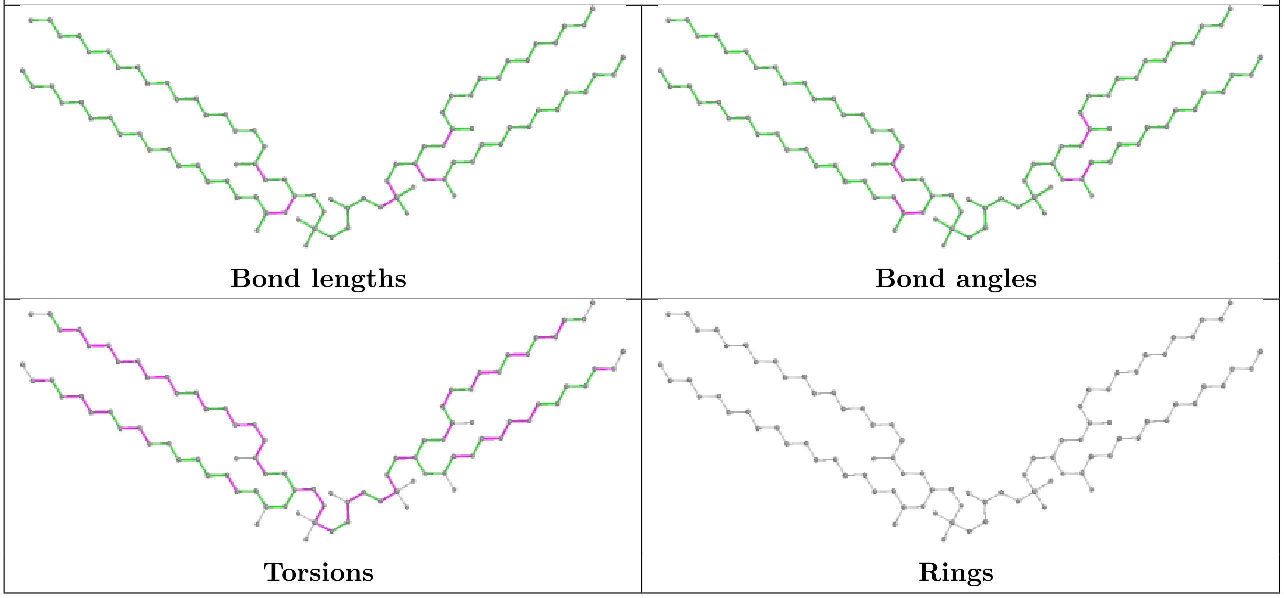
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL a 201



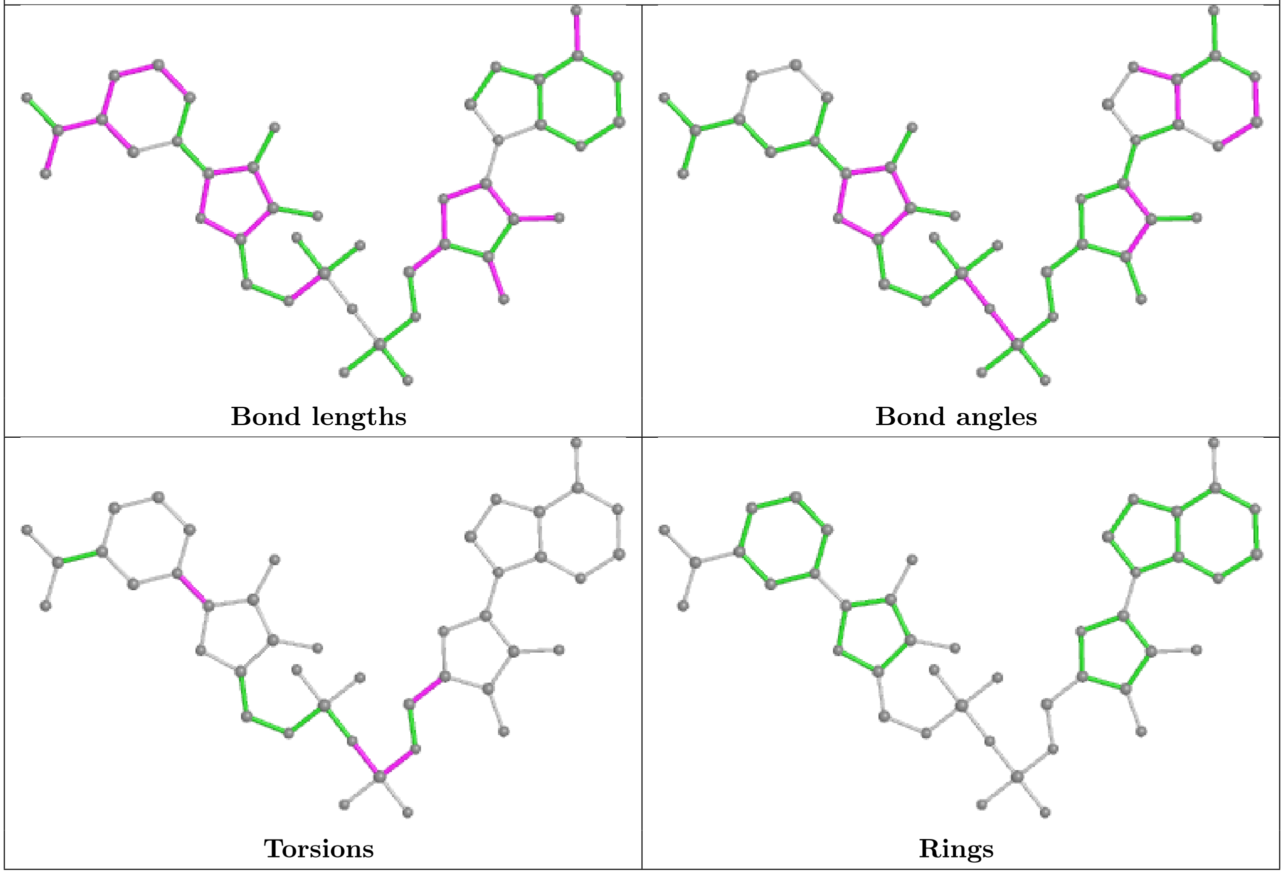
Bond lengths

Bond angles

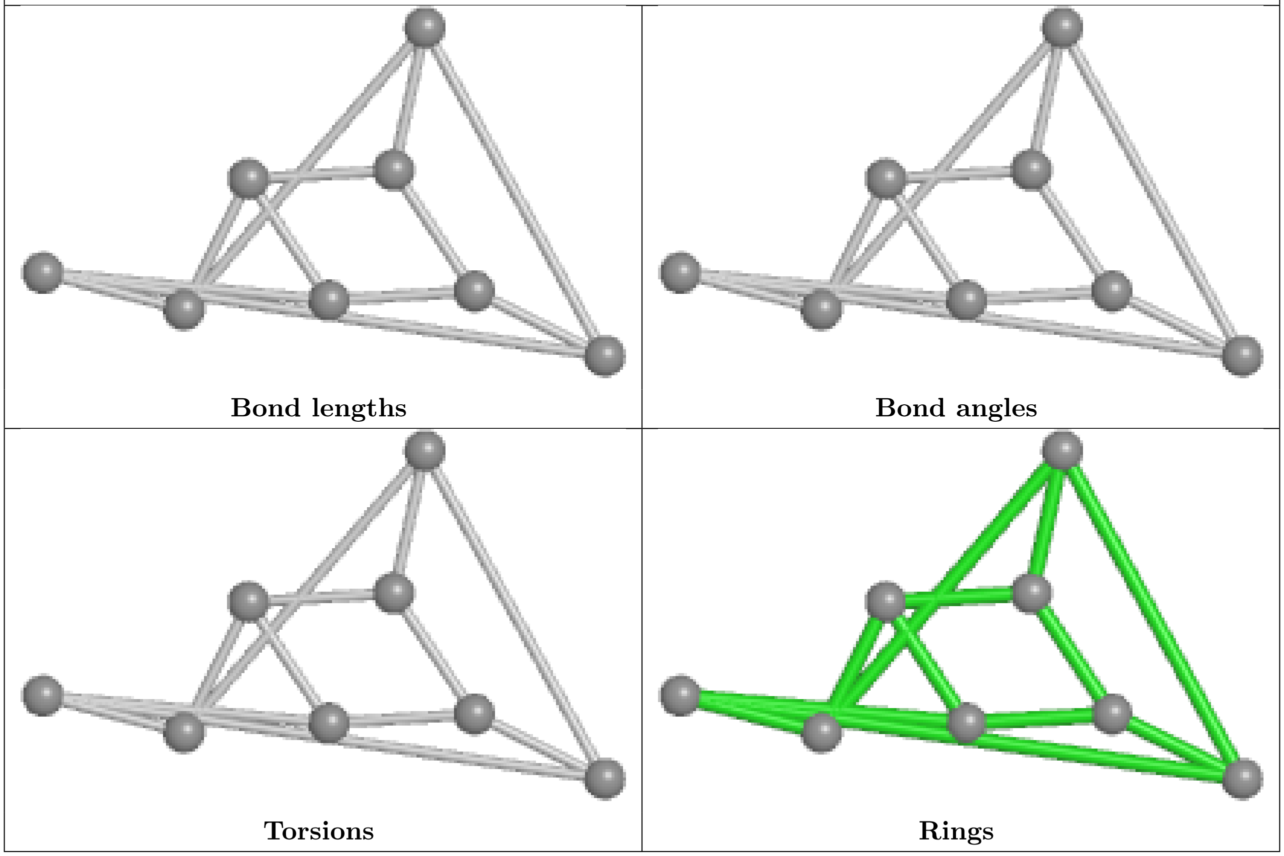
Torsions

Rings

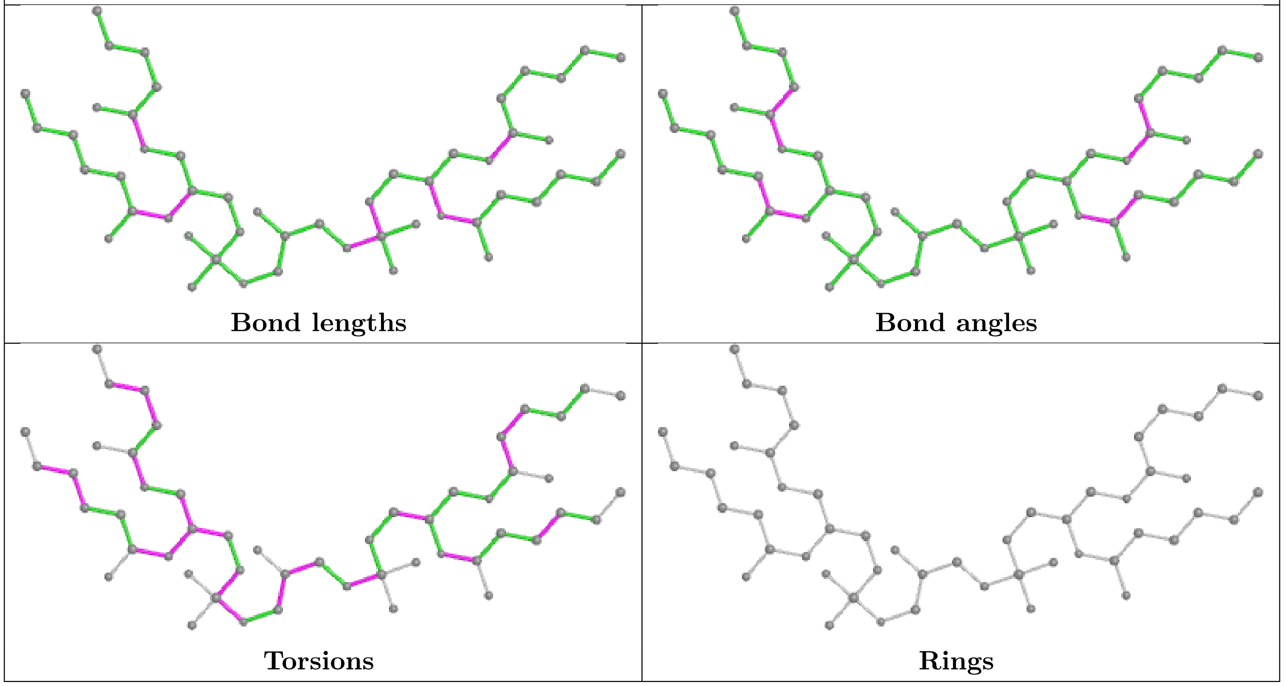
Ligand NAI A 503


Bond lengths
Bond angles
Torsions
Rings

Ligand SF4 M 801


Bond lengths
Bond angles
Torsions
Rings

Ligand CDL I 201



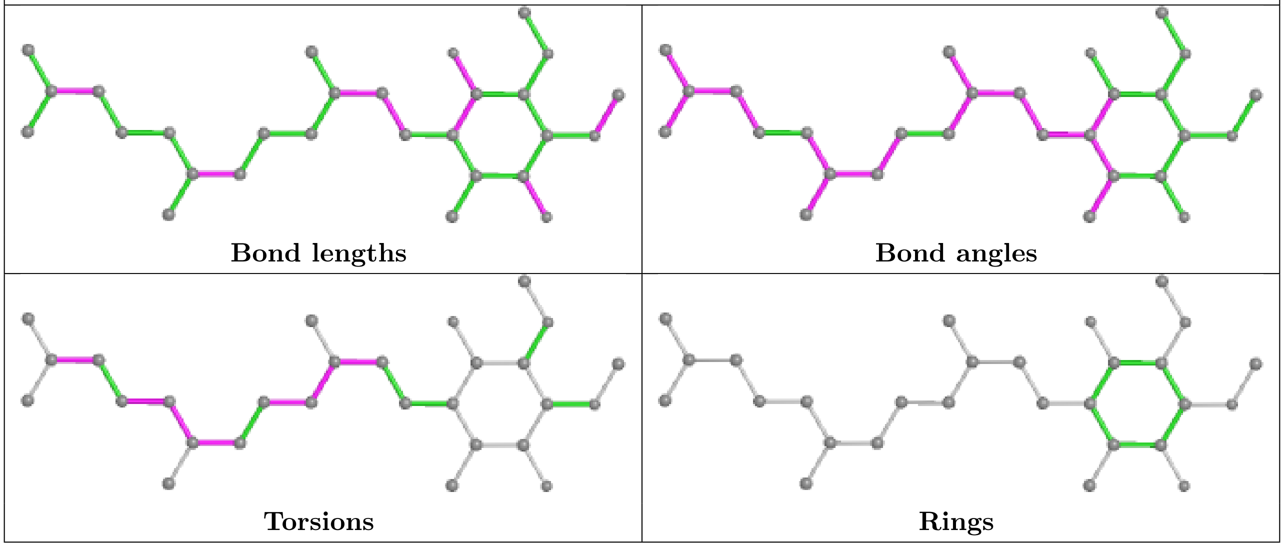
Bond lengths

Bond angles

Torsions

Rings

Ligand UQ s 401



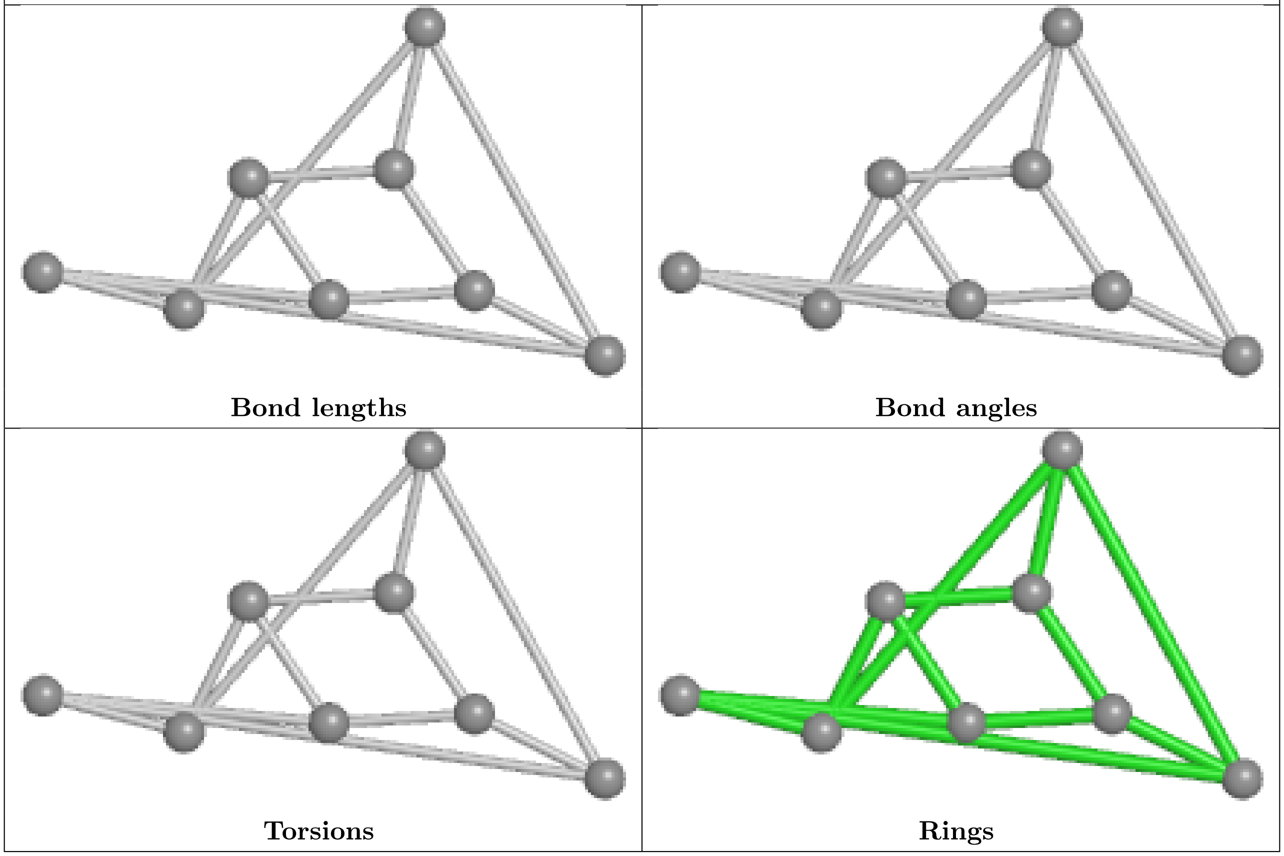
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 M 802



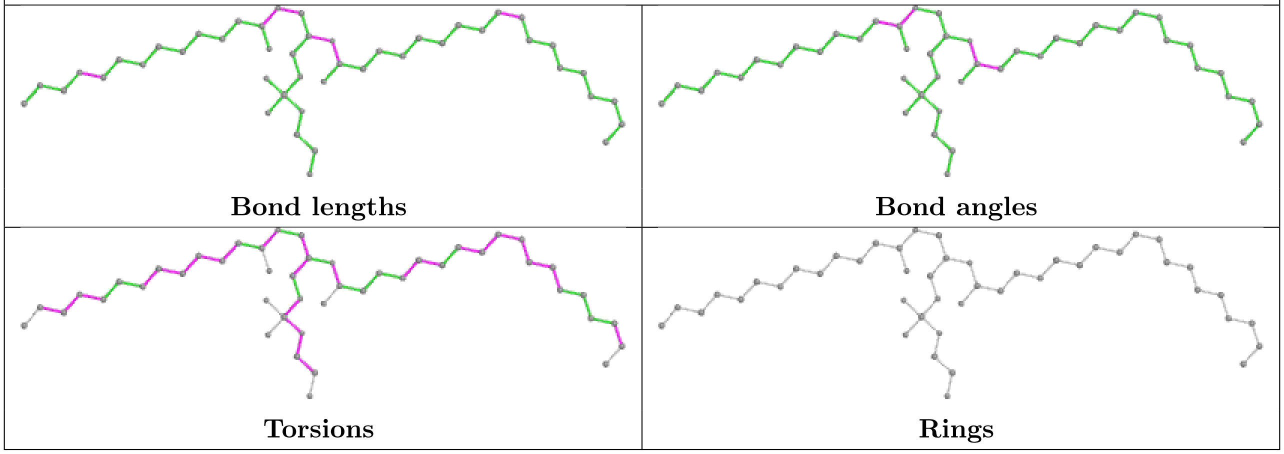
Bond lengths

Bond angles

Torsions

Rings

Ligand PEE l 704



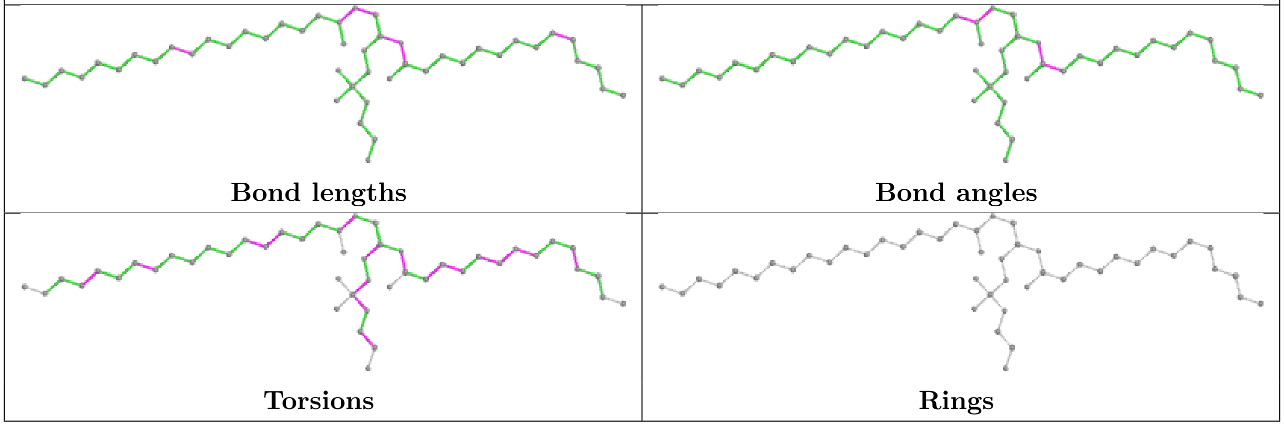
Bond lengths

Bond angles

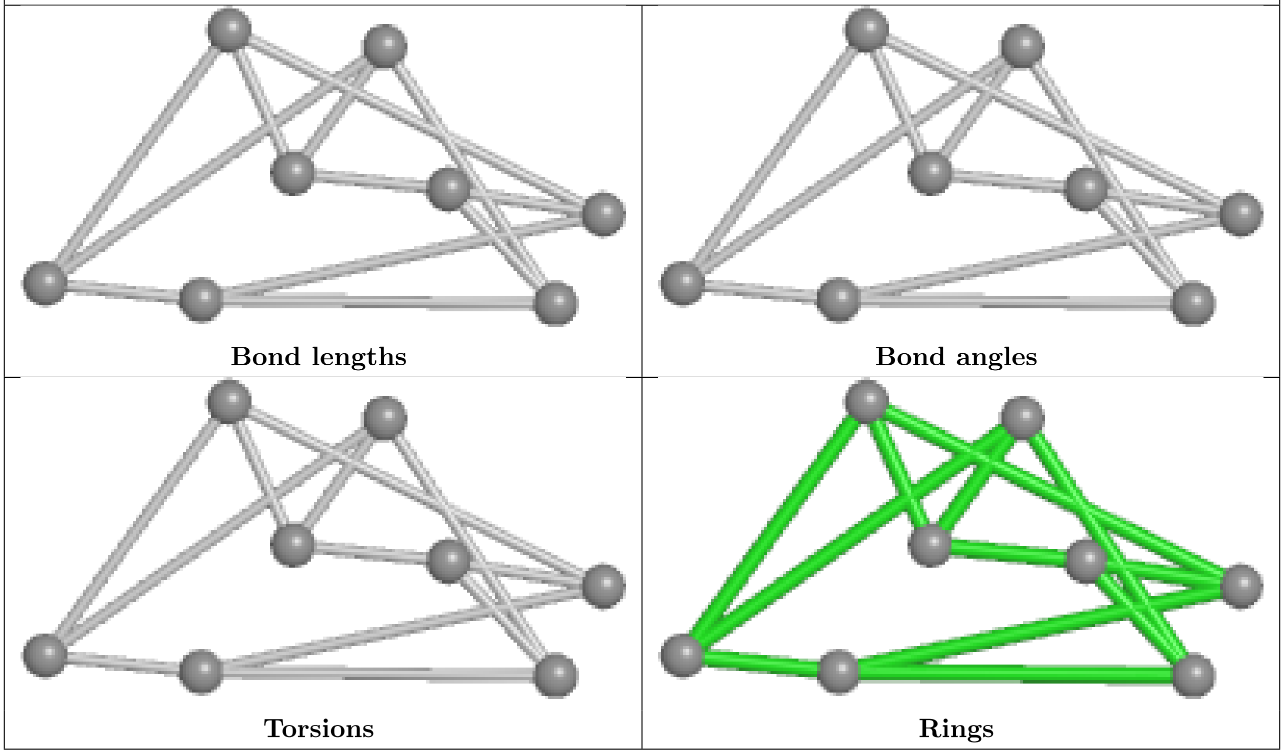
Torsions

Rings

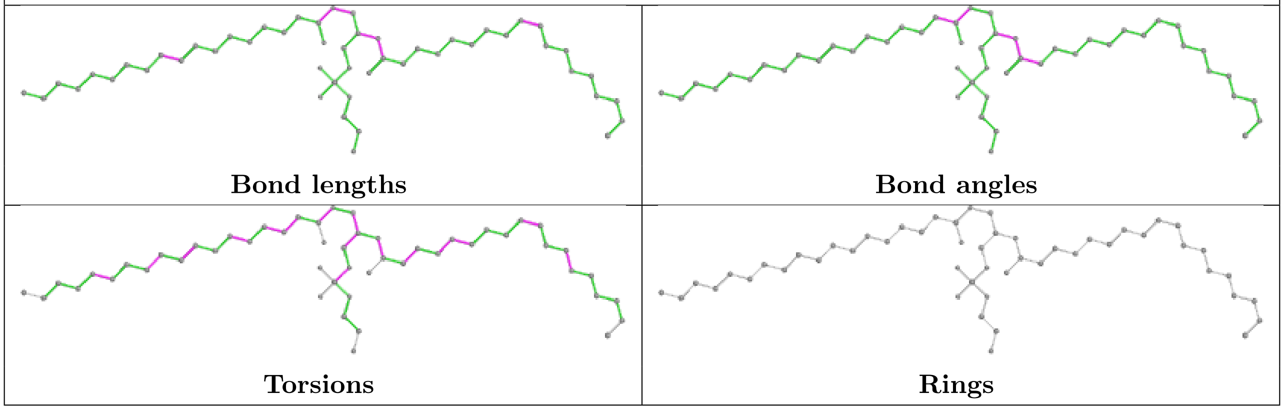
Ligand PEE j 201



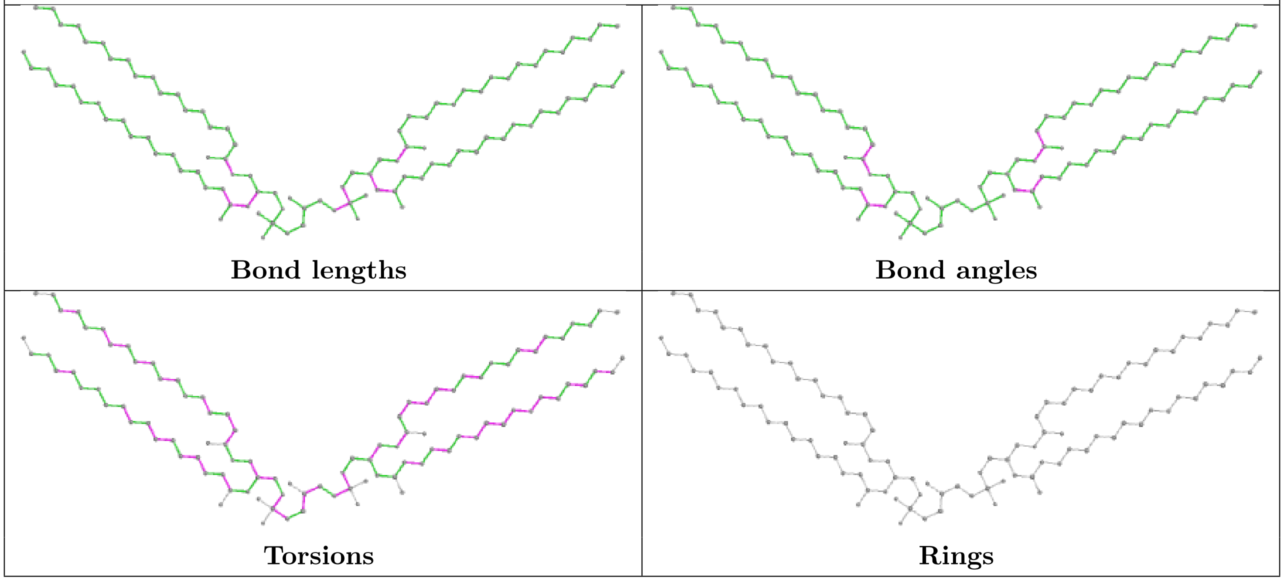
Ligand SF4 A 501



Ligand PEE r 501



Ligand CDL l 702



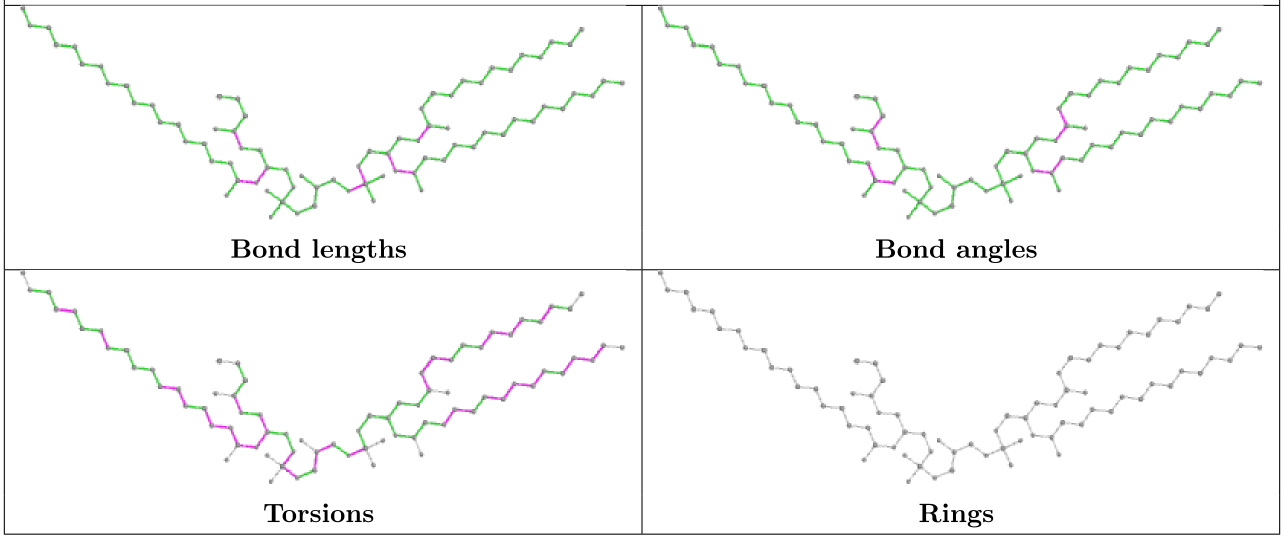
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL g 202



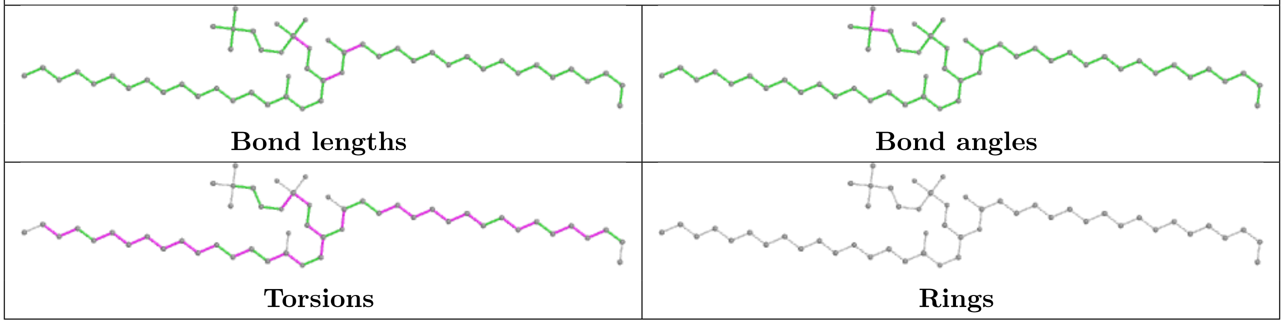
Bond lengths

Bond angles

Torsions

Rings

Ligand PLX g 201



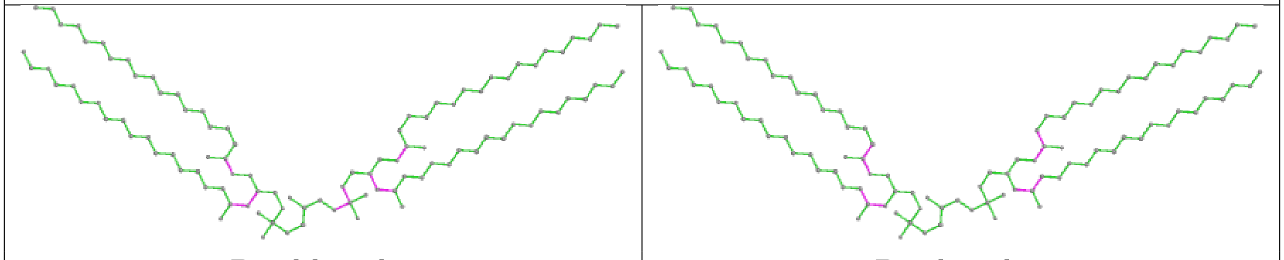
Bond lengths

Bond angles

Torsions

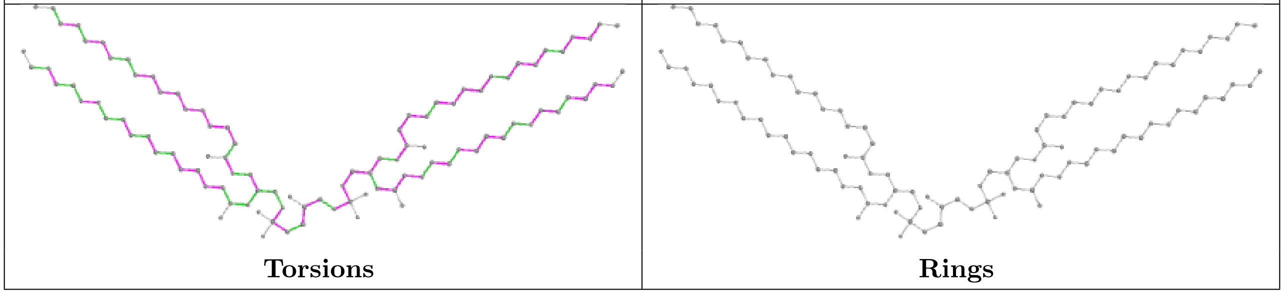
Rings

Ligand CDL r 503



Bond lengths

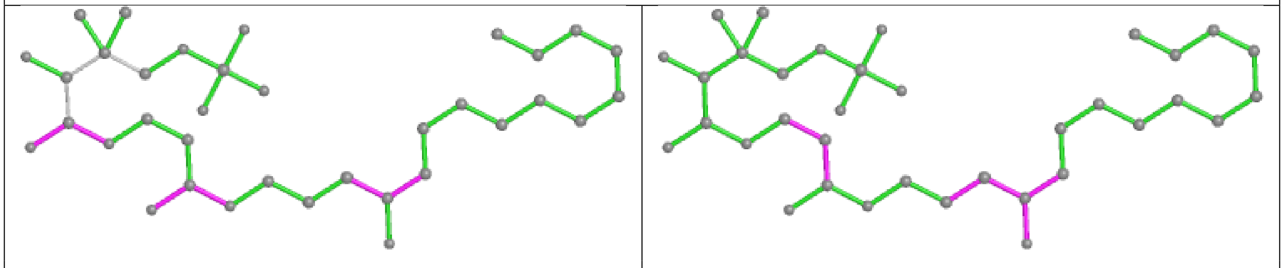
Bond angles



Torsions

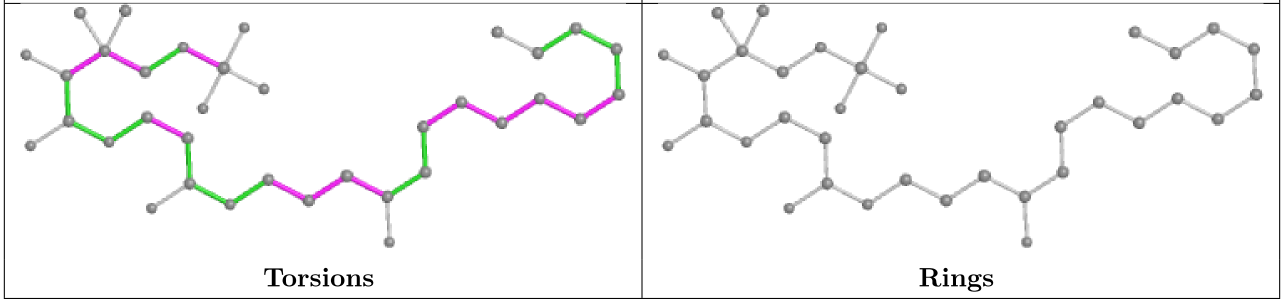
Rings

Ligand 8Q1 G 201



Bond lengths

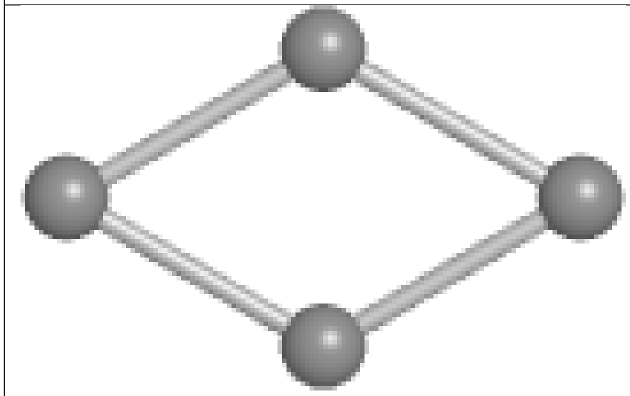
Bond angles



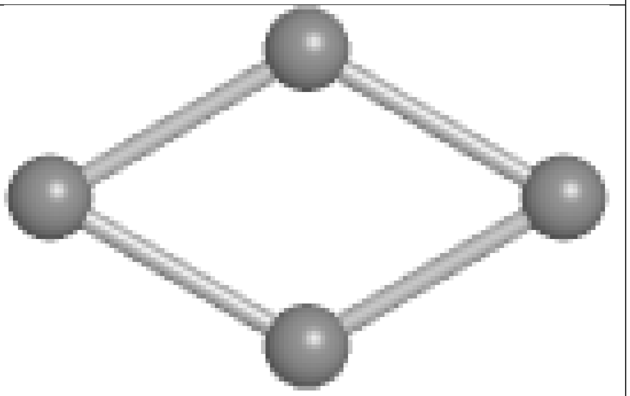
Torsions

Rings

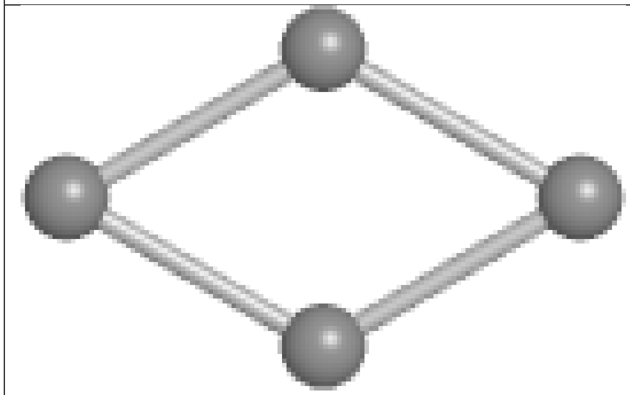
Ligand FES M 803



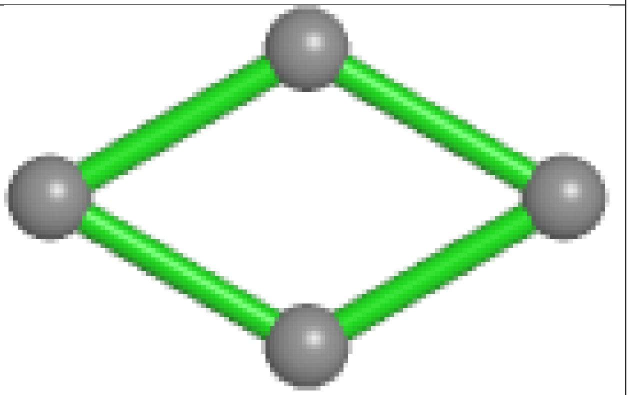
Bond lengths



Bond angles

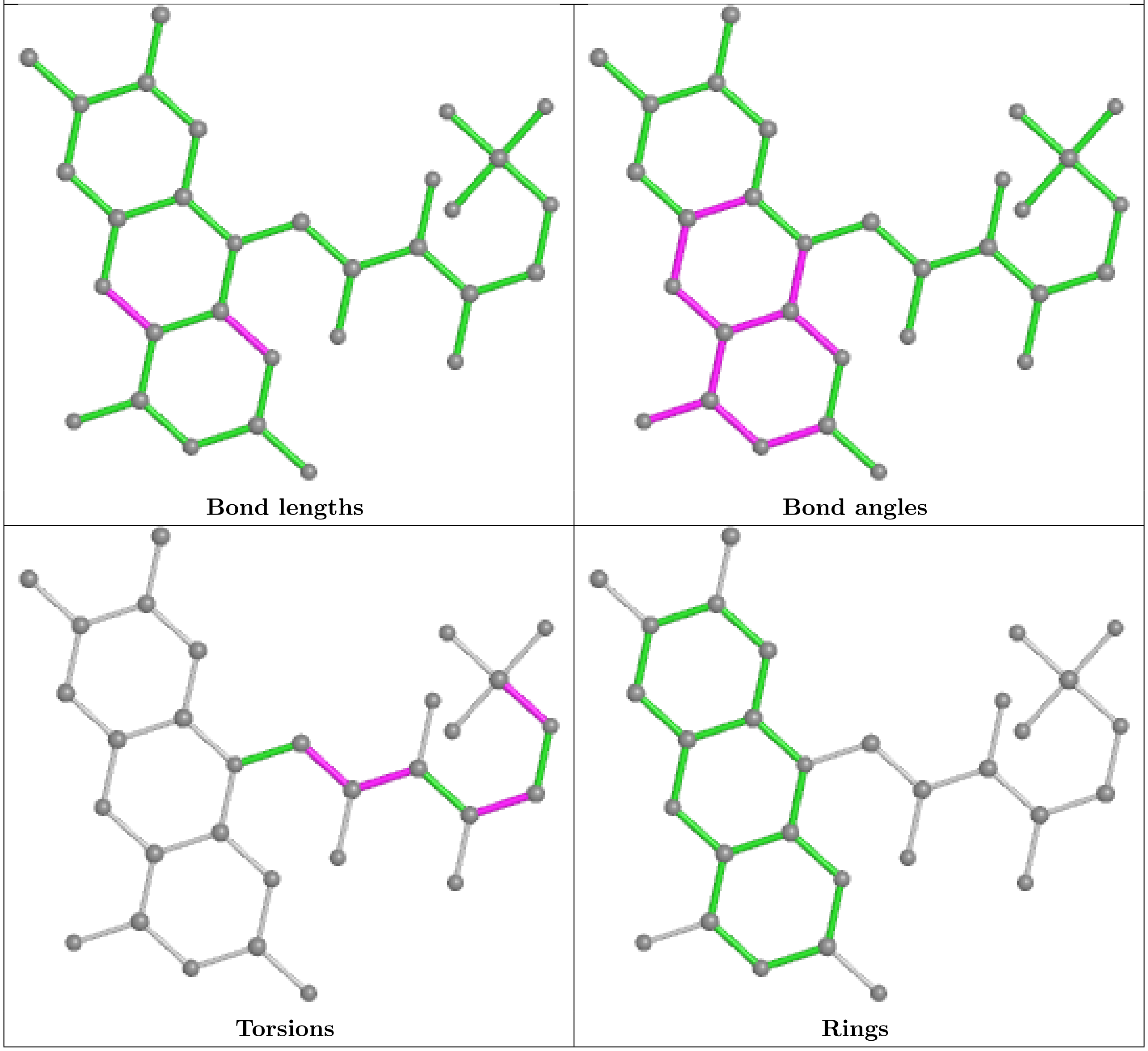


Torsions



Rings

Ligand FMN A 502



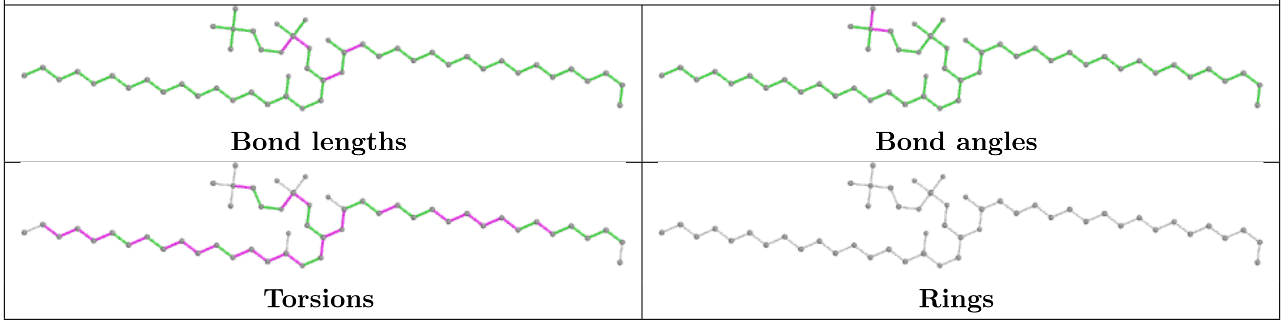
Bond lengths

Bond angles

Torsions

Rings

Ligand PLX r 502



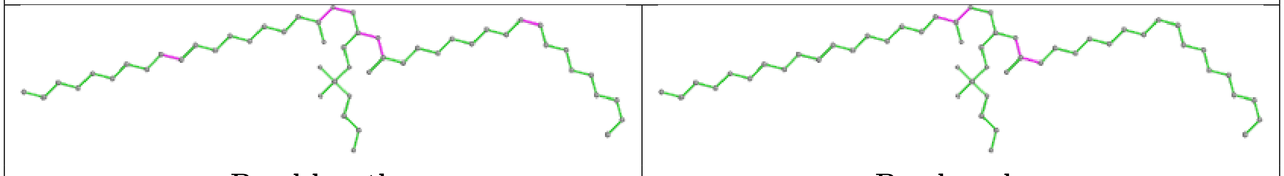
Bond lengths

Bond angles

Torsions

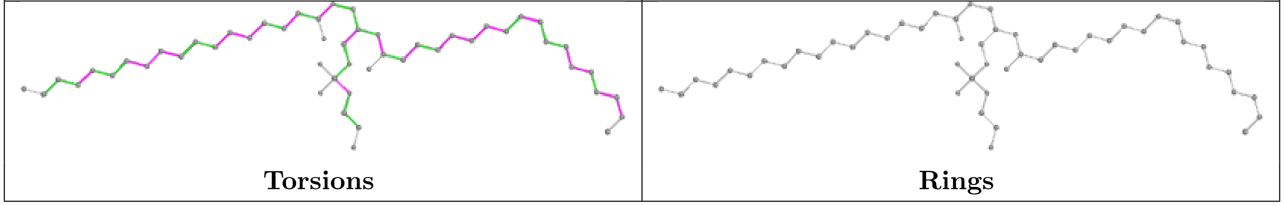
Rings

Ligand PEE B 303



Bond lengths

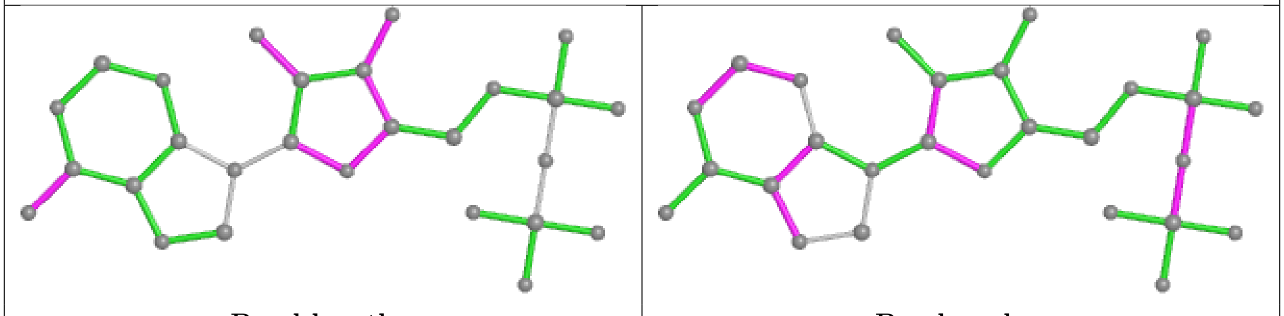
Bond angles



Torsions

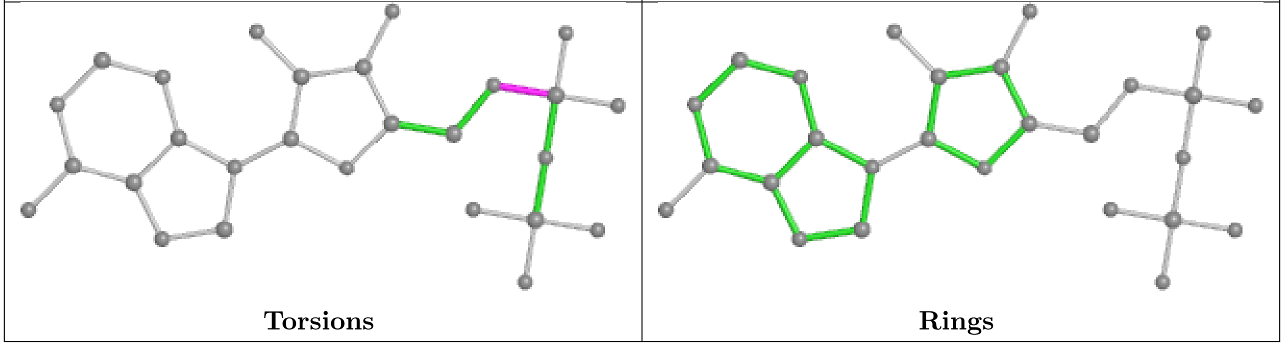
Rings

Ligand ADP w 401



Bond lengths

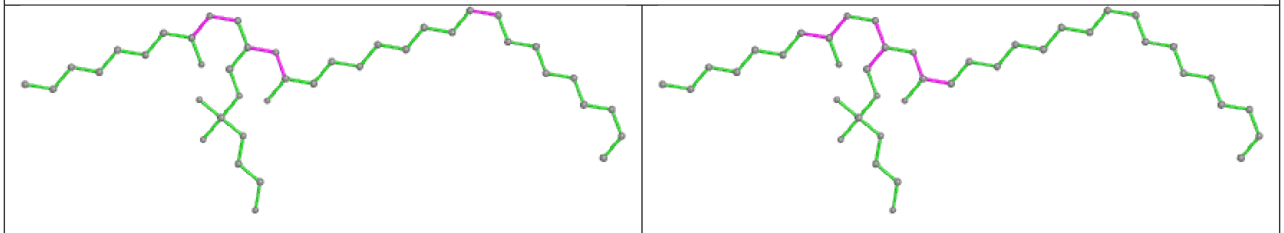
Bond angles



Torsions

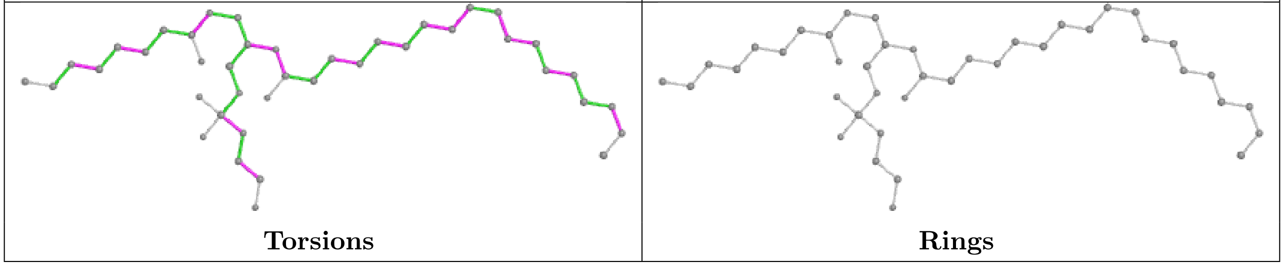
Rings

Ligand PEE m 201



Bond lengths

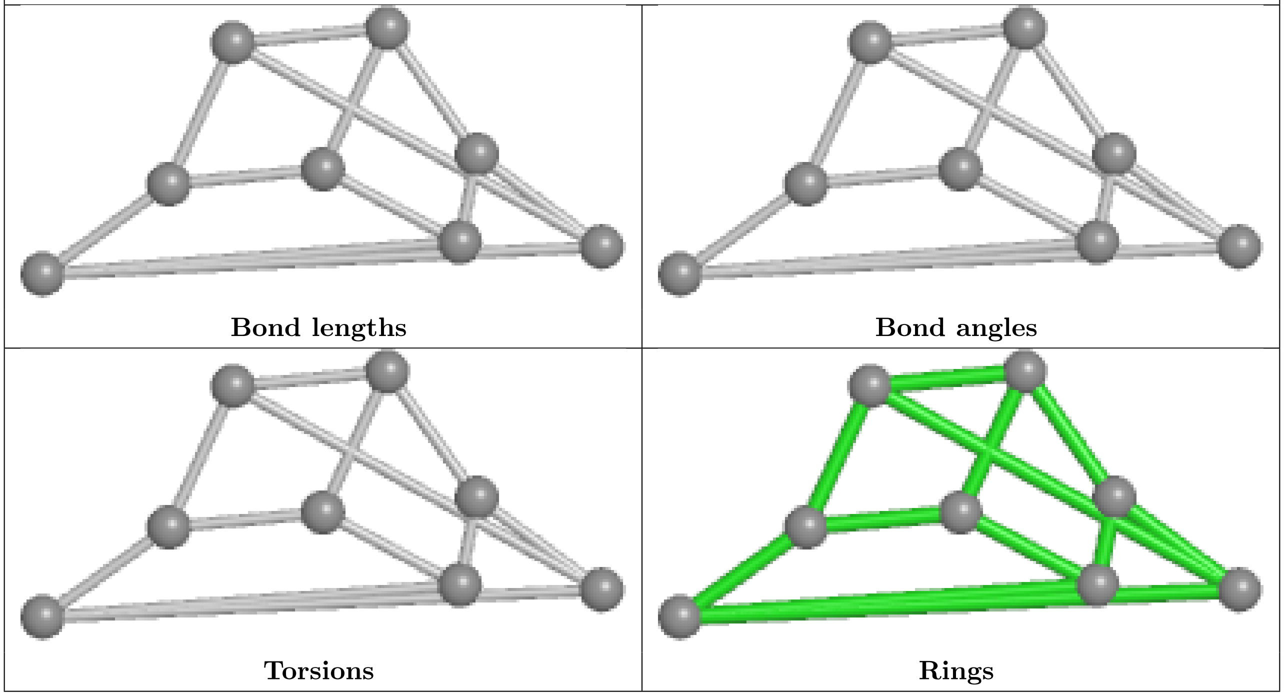
Bond angles



Torsions

Rings

Ligand SF4 C 301



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

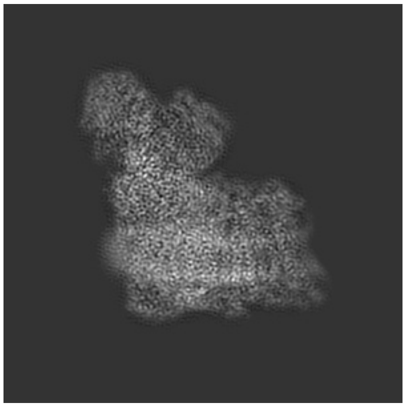
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-32264. These allow visual inspection of the internal detail of the map and identification of artifacts.

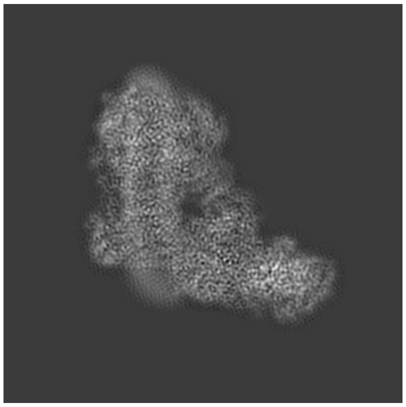
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

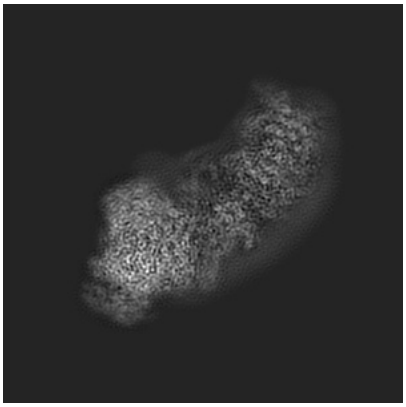
6.1.1 Primary map



X



Y

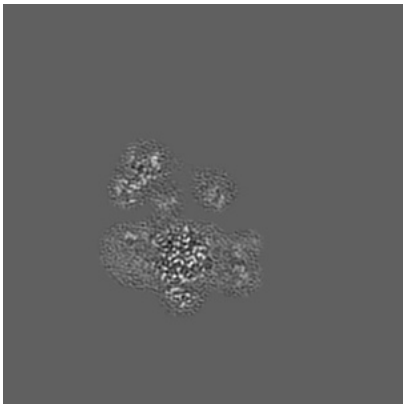


Z

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

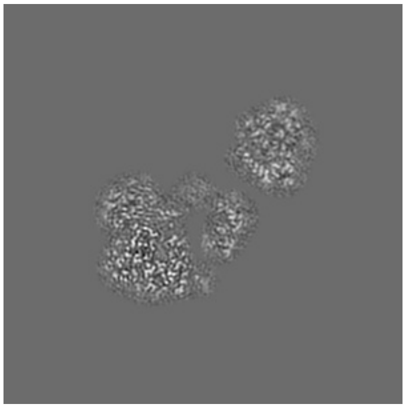
6.2 Central slices ⓘ

6.2.1 Primary map



X Index: 155

Y Index: 155

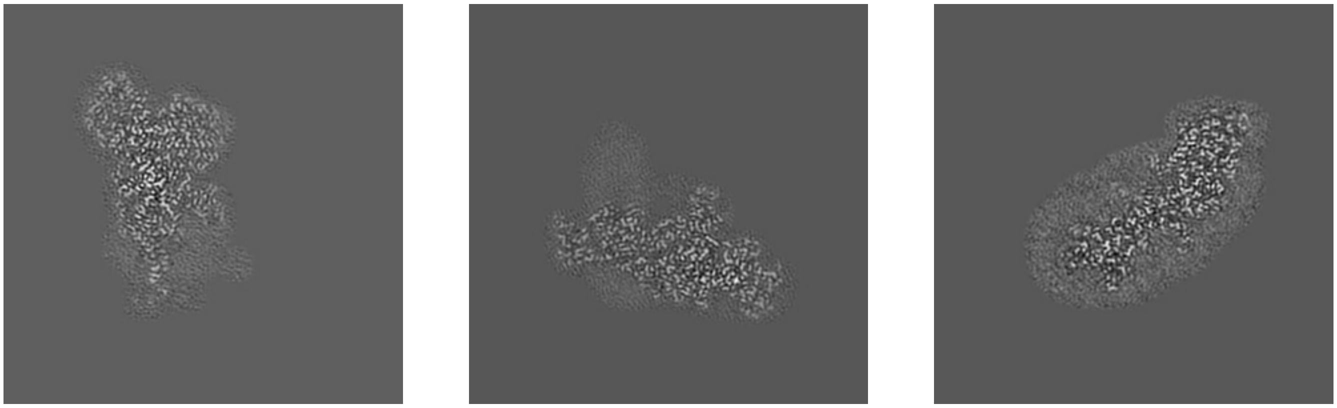


Z Index: 155

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

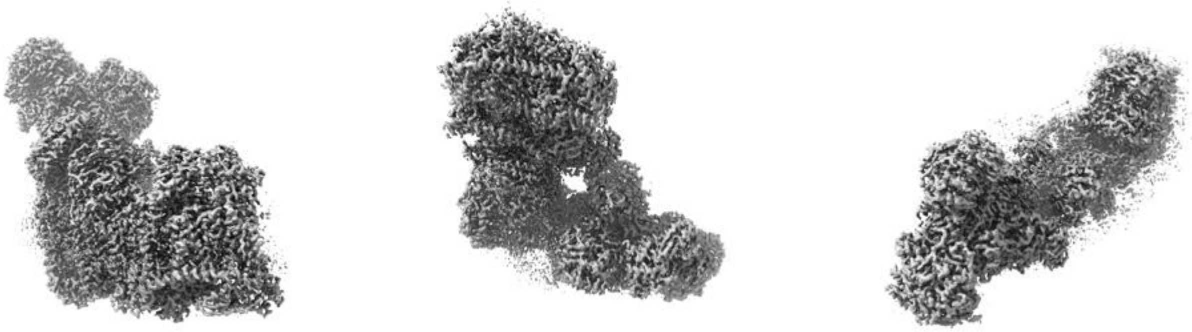


X Index: 105 Y Index: 111 Z Index: 126

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

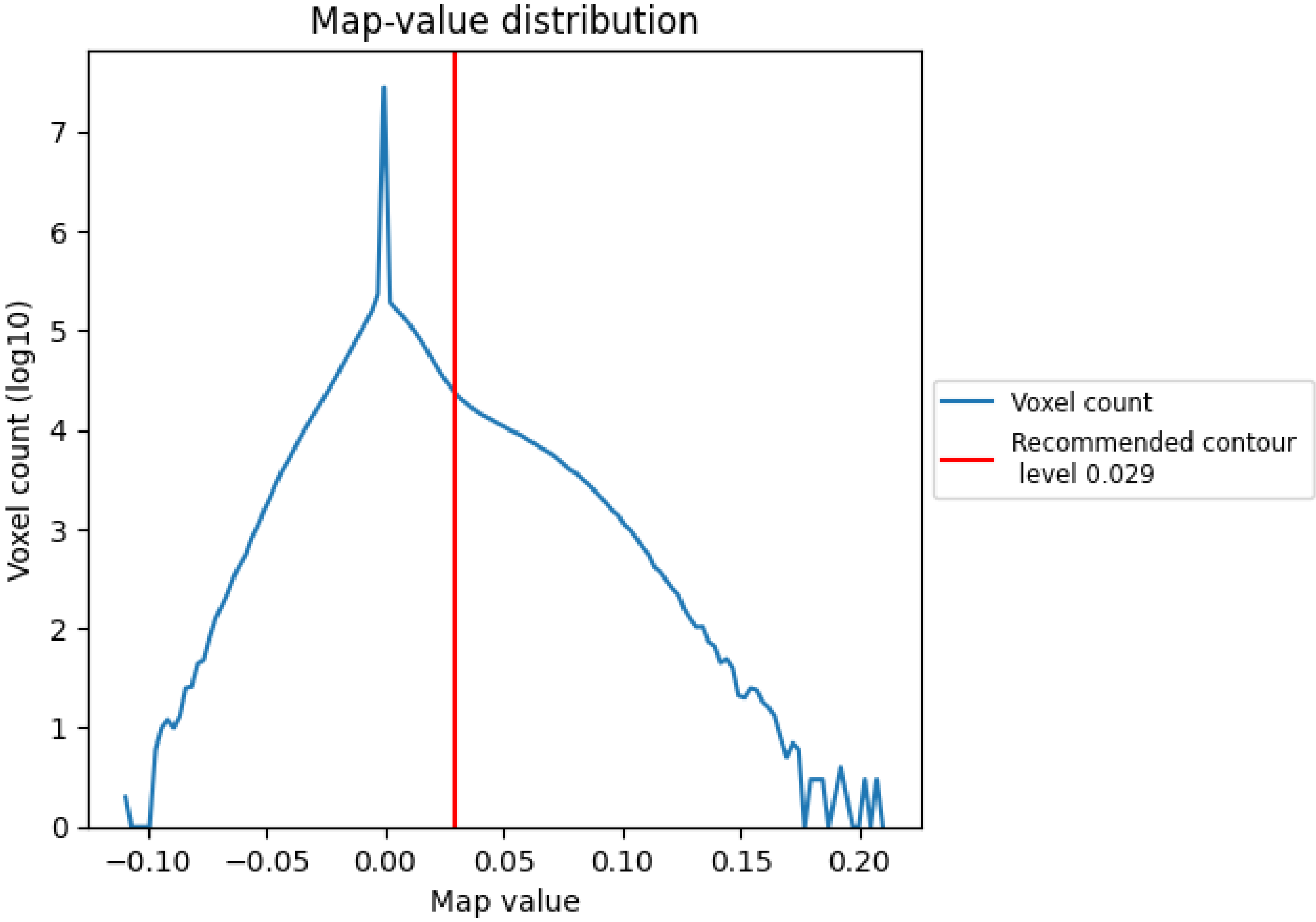
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

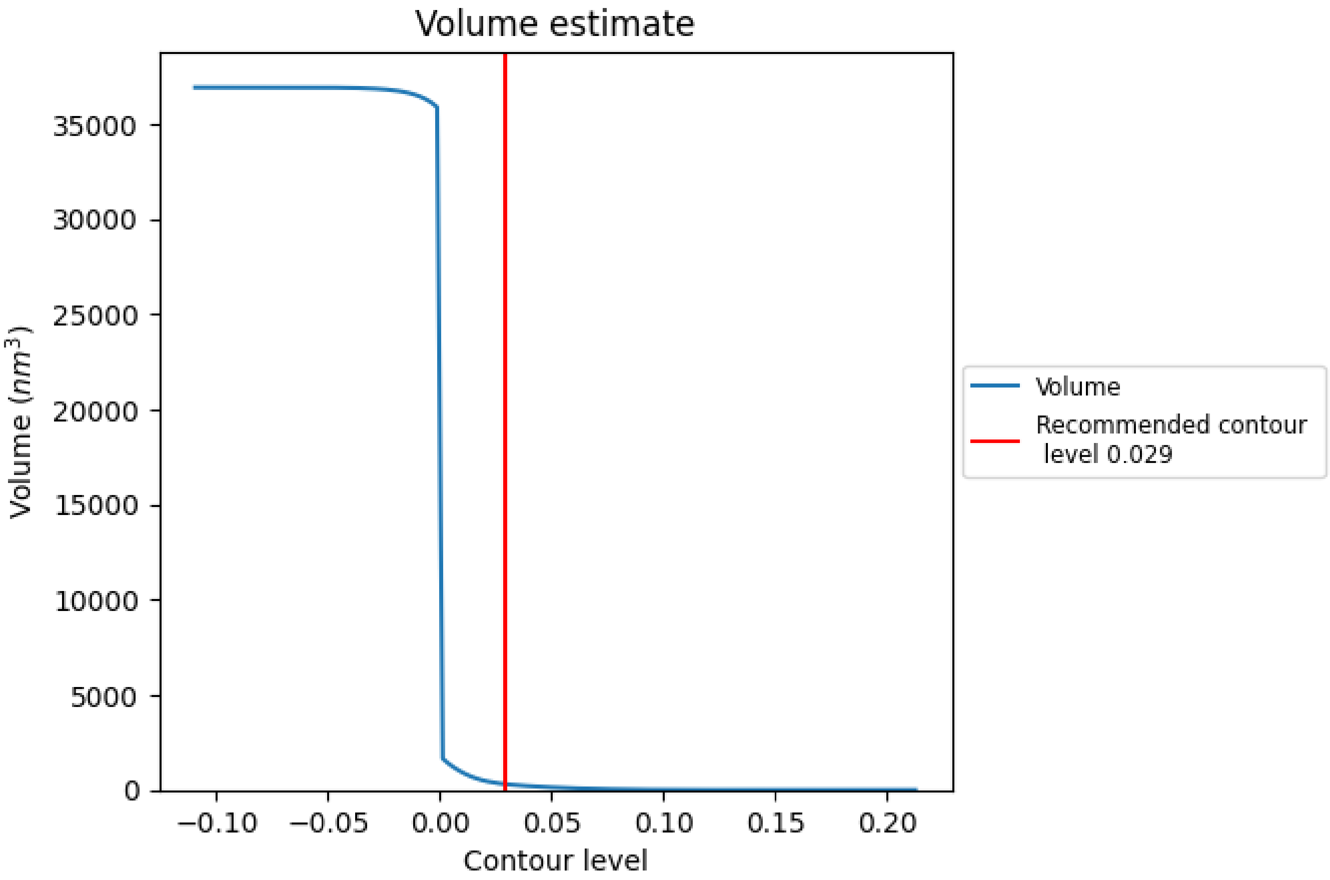
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

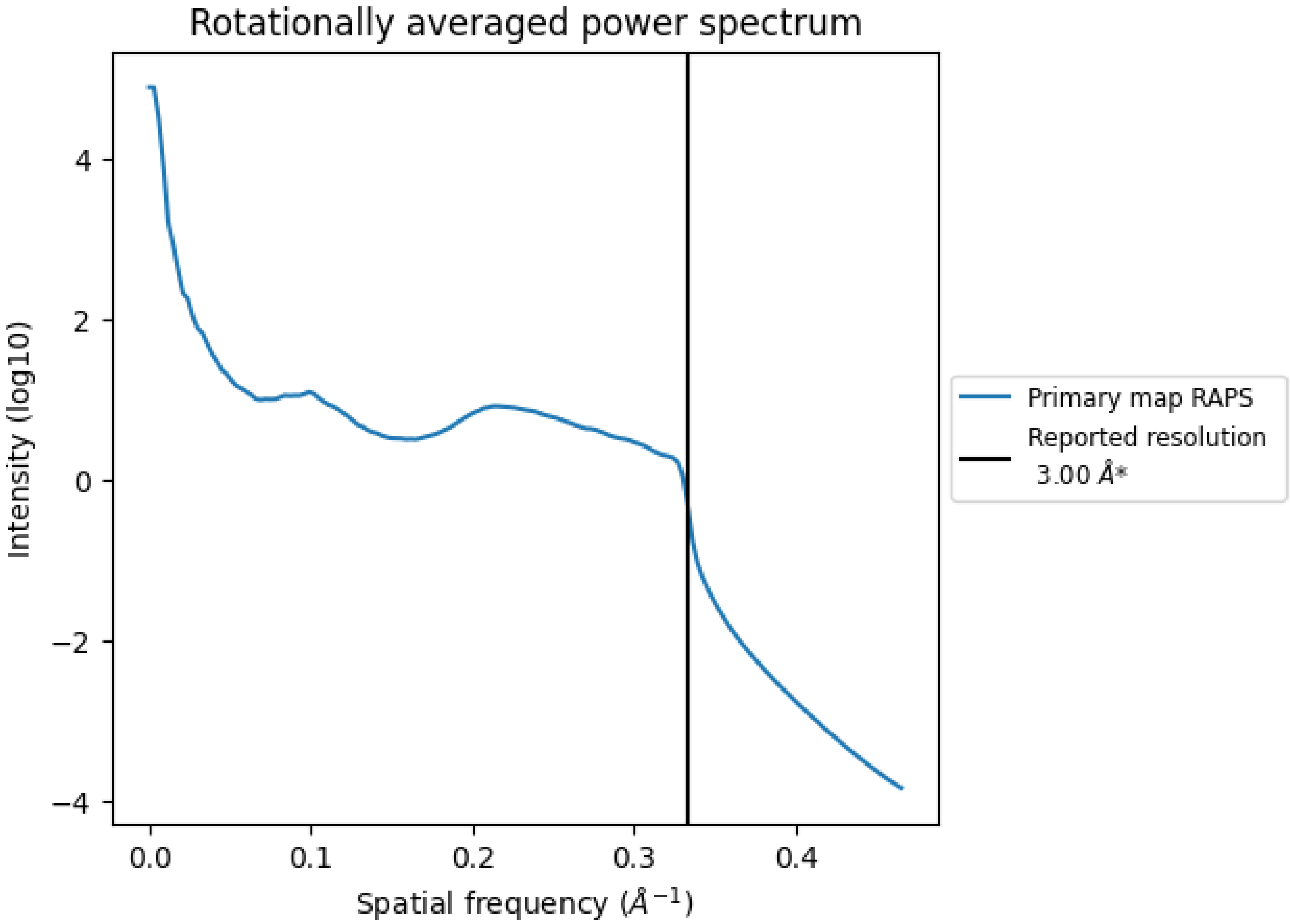
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 308 nm^3; this corresponds to an approximate mass of 278 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 0.333 $Å^{-1}$

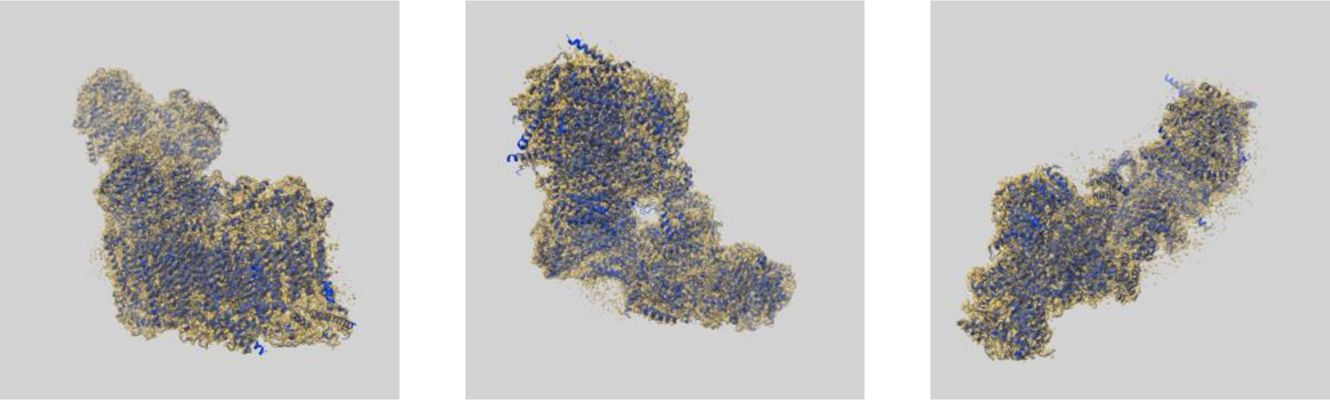
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32264 and PDB model 7W2L. Per-residue inclusion information can be found in section 3 on page 20.

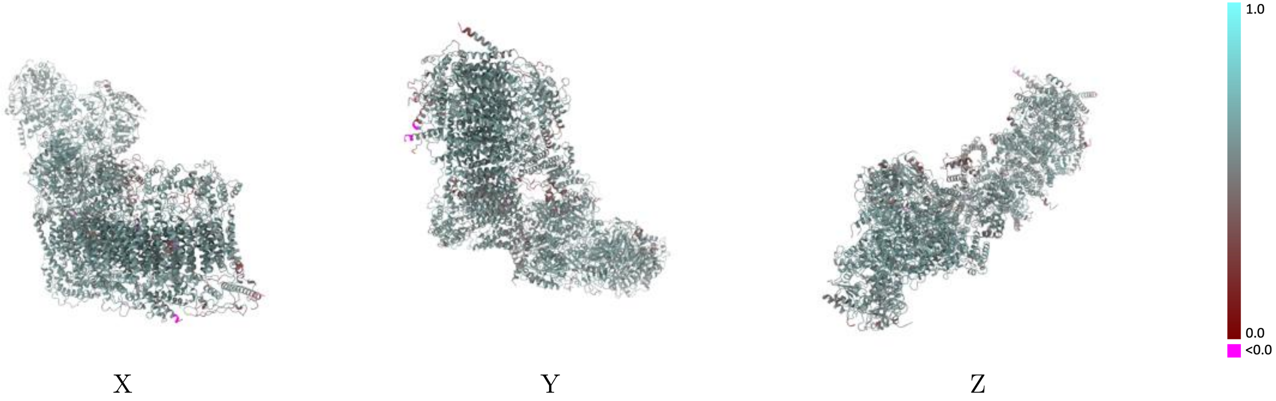
9.1 Map-model overlay ⓘ



X Y Z

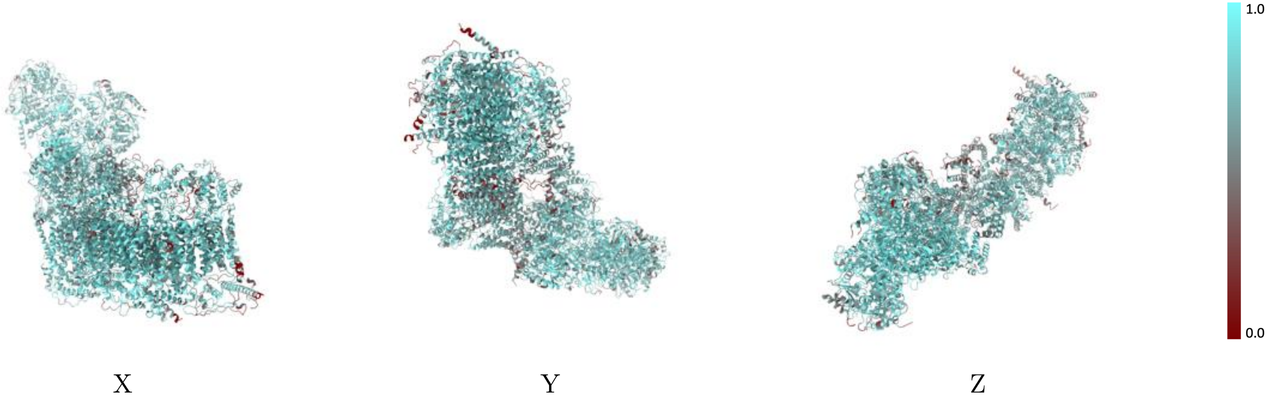
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



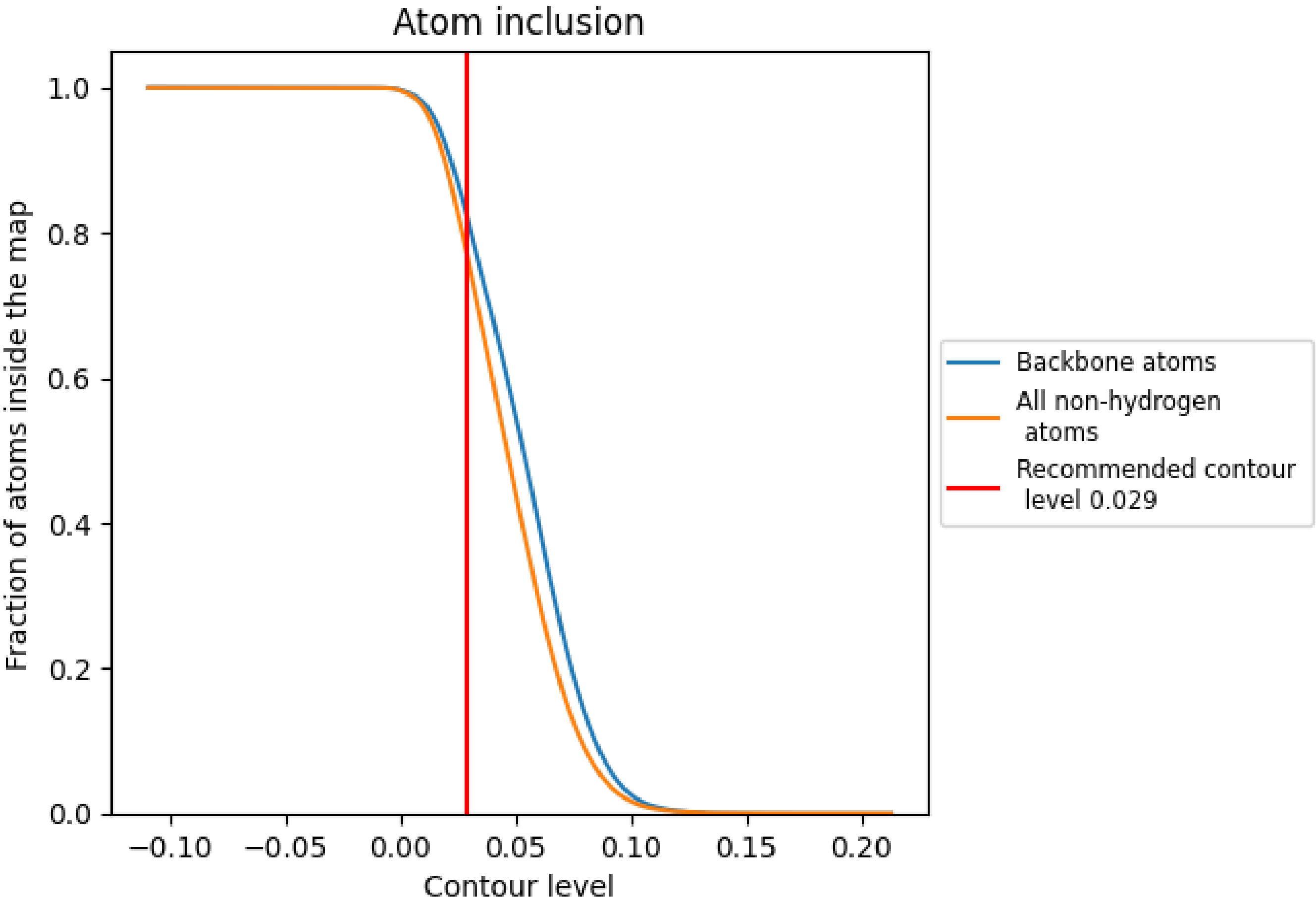
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.029).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7660	0.5700
A	0.7771	0.5610
B	0.9035	0.6210
C	0.8717	0.6060
E	0.7564	0.5660
F	0.6473	0.5100
G	0.4677	0.4090
H	0.7531	0.5560
I	0.7478	0.5700
J	0.7228	0.5520
K	0.6657	0.5380
L	0.8234	0.5970
M	0.8181	0.5840
N	0.7691	0.5820
O	0.7224	0.5530
P	0.8865	0.6120
Q	0.8424	0.6050
S	0.8318	0.5890
T	0.7881	0.5800
U	0.7750	0.5680
V	0.4895	0.4840
W	0.8205	0.5780
X	0.6648	0.5320
Y	0.6294	0.5070
Z	0.5564	0.4800
a	0.7662	0.5830
b	0.6509	0.5100
c	0.7349	0.5510
d	0.7342	0.5490
e	0.7089	0.5450
f	0.6557	0.5200
g	0.7753	0.5800
h	0.7849	0.5790
i	0.8442	0.6050
j	0.6532	0.5380

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Chain	Atom inclusion	Q-score
k	0.7480	0.5720
l	0.7734	0.5840
m	0.6810	0.5510
n	0.6704	0.5330
o	0.7120	0.5610
p	0.7414	0.5610
r	0.8383	0.6010
s	0.8106	0.5850
u	0.7987	0.5810
v	0.6350	0.5040
w	0.7065	0.5490