Full wwPDB EM Validation Report (i)

Jan 25, 2023 – 12:36 PM JST

PDB ID	:	7W31
EMDB ID	:	EMD-32269
Title	:	Deactive state CI from DQ-NADH dataset, Subclass 1
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-24
Resolution	:	3.10 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

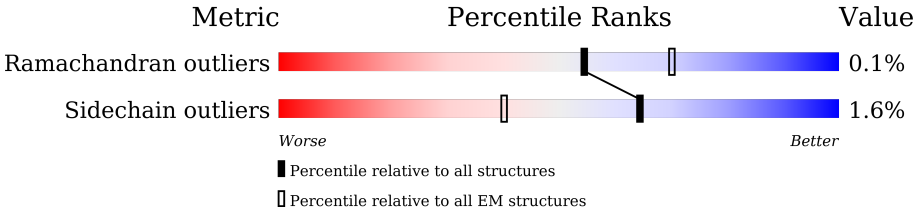
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	433	99%
2	B	176	99%
3	C	156	99%
4	E	115	97%
5	F	86	8%, 99%
6	G	88	52%, 94%, 6%
6	X	88	50%, 97%
7	H	112	98%
8	I	112	8%, 87%, 13%

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Mol	Chain	Length	Quality of chain
9	J	342	94%
10	K	43	12%, 98%
11	L	125	6%, 99%
12	M	690	99%
13	N	144	7%, 98%
14	O	217	99%
15	P	208	99%
16	Q	430	9%, 97%
17	S	70	100%
18	T	96	9%, 99%
19	U	83	5%, 96%
20	V	140	79%, 99%
21	W	142	99%
22	Y	70	54%, 99%
23	Z	84	65%, 99%
24	a	140	6%, 99%
25	b	126	33%, 77%, 5%, 18%
26	c	156	32%, 98%
27	d	175	19%, 98%
28	e	107	27%, 96%
29	f	49	22%, 84%, 14%
30	g	122	98%
31	h	105	98%
32	i	347	7%, 98%
33	j	115	10%, 85%, 14%

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Mol	Chain	Length	Quality of chain
34	k	98	21% 99%
35	l	603	17% 98%
36	m	175	14% 71% 26%
37	n	56	27% 98%
38	o	128	30% 100%
39	p	178	32% 100%
40	r	459	99%
41	s	318	95% 5%
42	u	171	96%
43	v	125	51% 97%
44	w	320	63% 98%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 66476 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3314	2093	591	610	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1402	882	240	267	13	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	968	618	179	166	5	0	0

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

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0
6	X	88	692	447	103	137	5	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	331	2611	1693	459	451	8	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	690	5290	3317	923	1011	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	1636	1042	272	312	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	1735	1123	298	312	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	1021	651	174	190	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1167	752	200	206	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	70	571	379	88	103	1	0	0

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

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

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	140	1159	759	199	198	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	847	553	154	139	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	156	1287	834	209	236	8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	107	889	568	145	172	4	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2710	1782	420	462	46	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4704	3106	738	812	48	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	129	915	611	137	159	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	479	311	88	79	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	o	128	1052	686	180	186	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	178	1491	954	273	257	7	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	3629	2412	572	607	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	1396	886	250	250	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	987	619	178	181	9	0	0

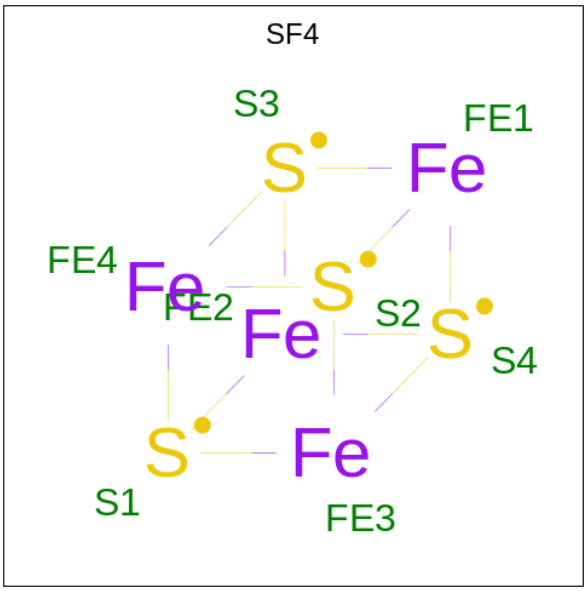
There is a discrepancy between the modelled and reference sequences:

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

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

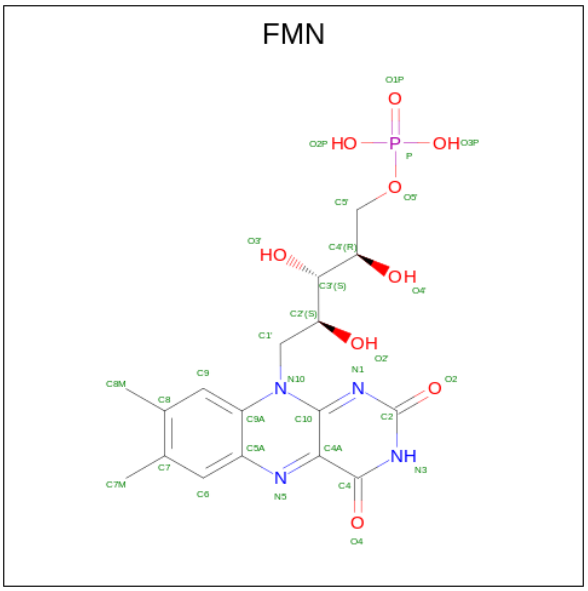
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2582	1643	438	491	10	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



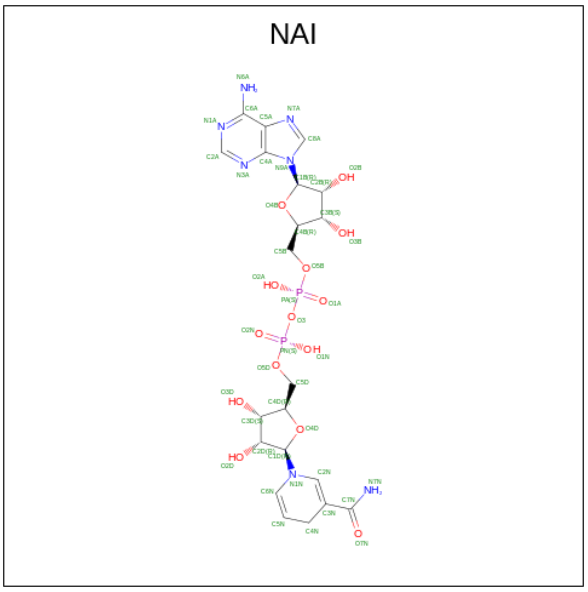
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
			Total	Fe	S	
45	B	1	16	8	8	0
			Total	Fe	S	
45	B	1	16	8	8	0
			Total	Fe	S	
45	C	1	8	4	4	0
			Total	Fe	S	
45	M	1	16	8	8	0
			Total	Fe	S	
45	M	1	16	8	8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



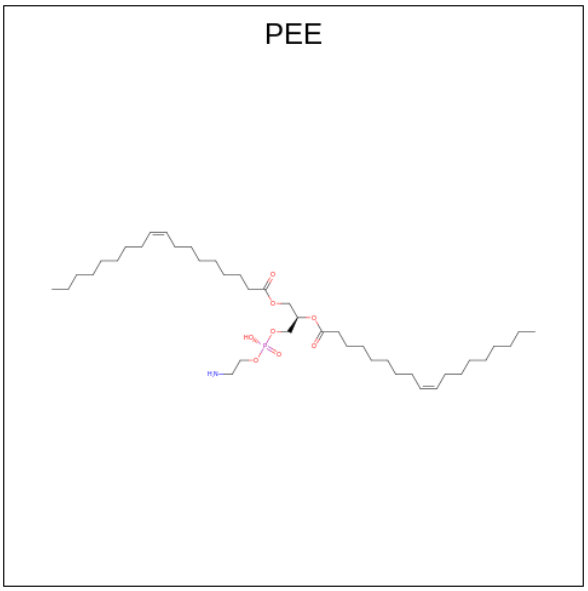
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



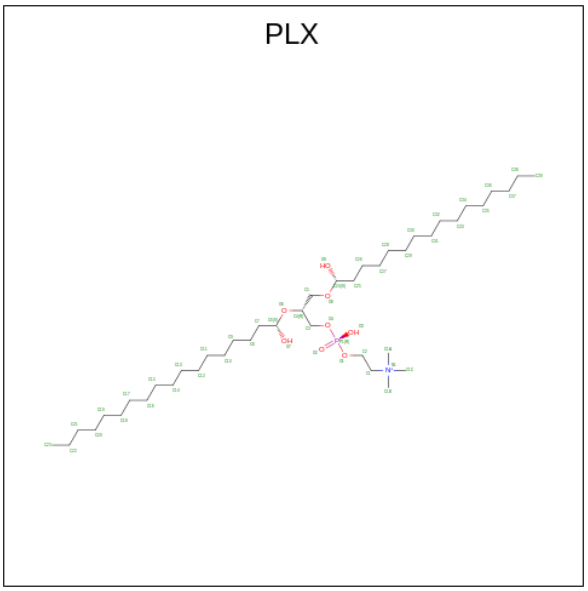
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



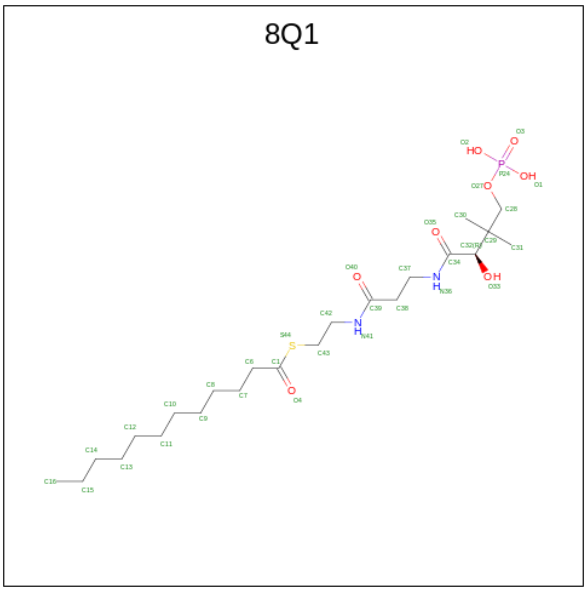
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31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

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$).



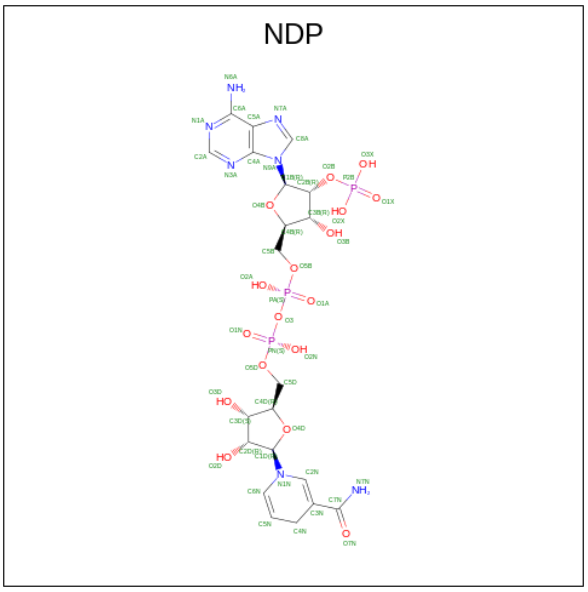
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	52	42	1	8	1	0
			Total	C	N	O	P	
49	g	1	52	42	1	8	1	0
			Total	C	N	O	P	
49	j	1	52	42	1	8	1	0
			Total	C	N	O	P	
49	l	1	52	42	1	8	1	0
			Total	C	N	O	P	
49	r	1	52	42	1	8	1	0

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



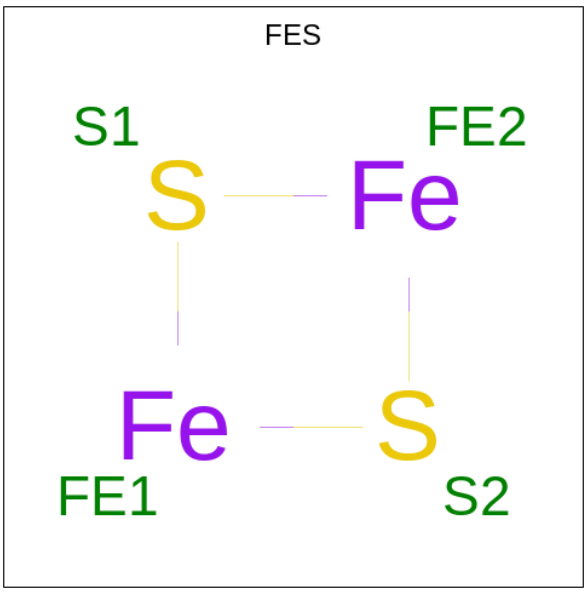
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
50	G	1	35	23	2	8	1	1	0
			Total	C	N	O	P	S	
50	X	1	35	23	2	8	1	1	0

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

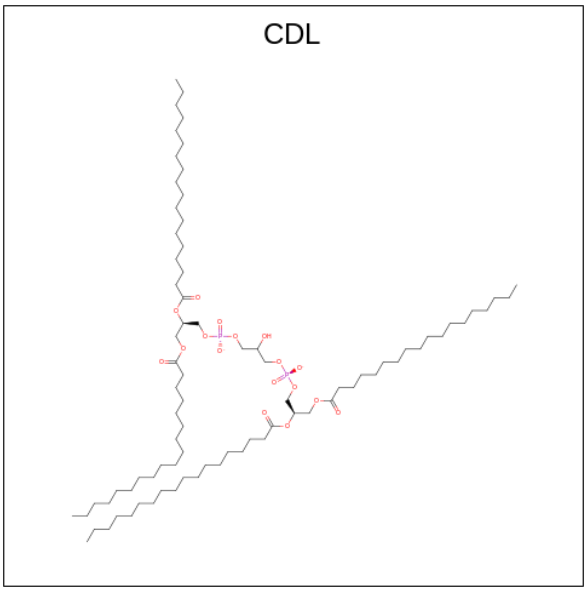


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
52	M	1	4	2	2	0
			Total	Fe	S	
52	O	1	4	2	2	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 54 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

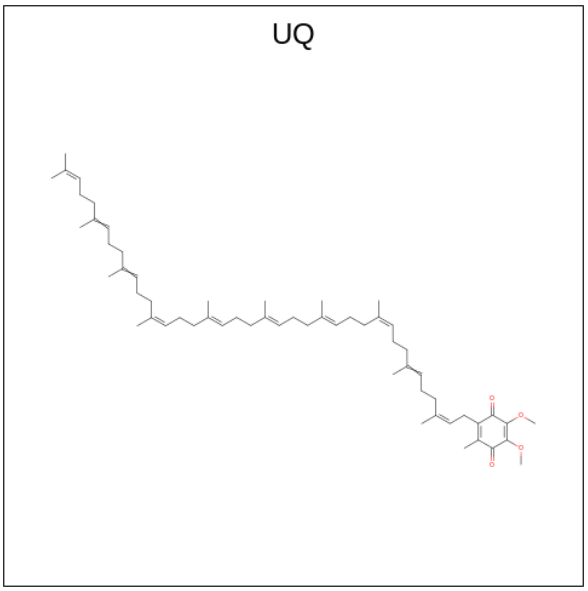


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
54	N	1	51	32	17	2	0
			Total	C	O	P	
54	a	1	91	72	17	2	0
			Total	C	O	P	
54	i	1	66	47	17	2	0
			Total	C	O	P	
54	r	1	199	161	34	4	0
			Total	C	O	P	
54	r	1	199	161	34	4	0
			Total	C	O	P	
54	u	1	78	59	17	2	0

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

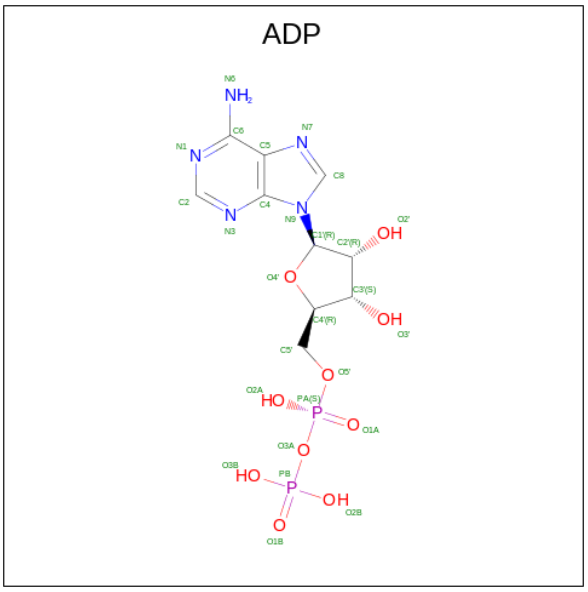
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	T	1	1	1	0

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



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: $C_{10}H_{15}N_5O_{10}P_2$).



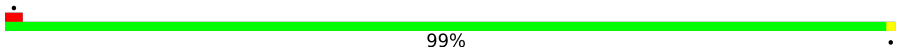
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

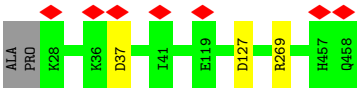
3 Residue-property plots (i)

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

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

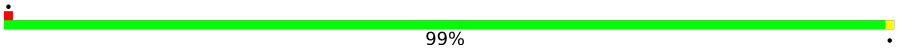
Chain A:





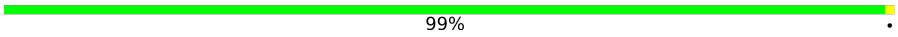
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

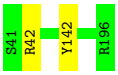
Chain B:



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

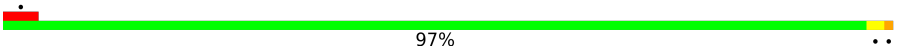
Chain C:

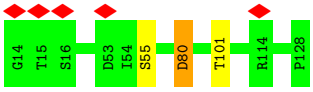




• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

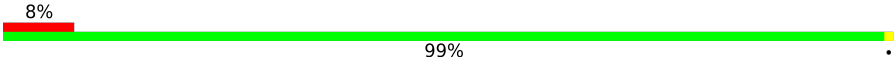
Chain E:

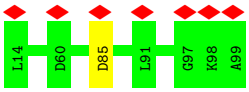




• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

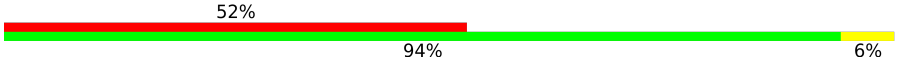
Chain F:

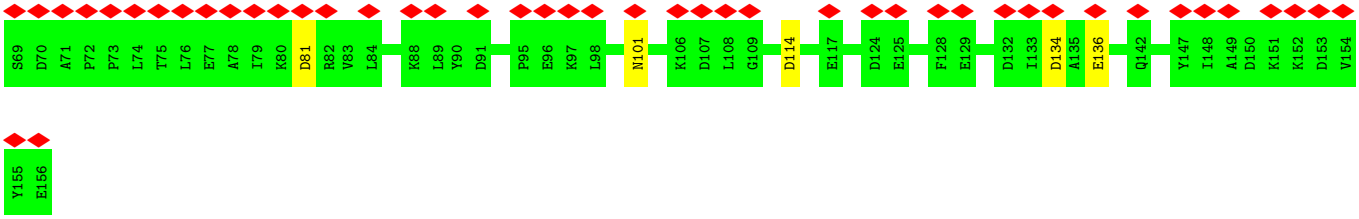




• Molecule 6: Acyl carrier protein

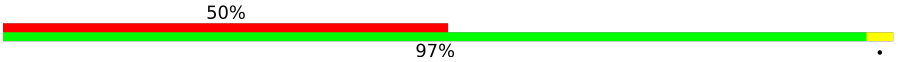
Chain G:

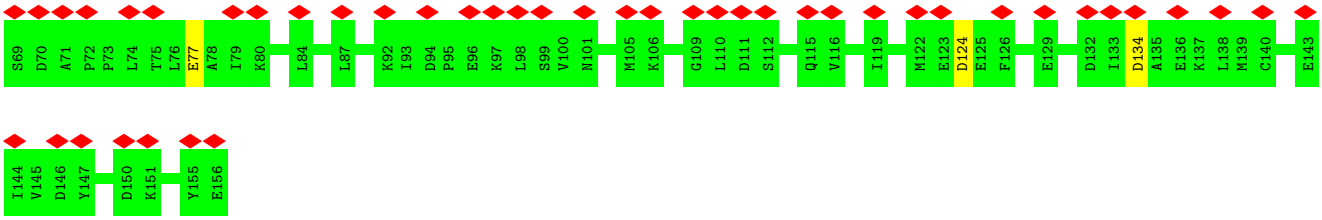




• Molecule 6: Acyl carrier protein

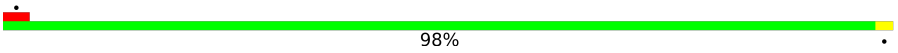
Chain X:

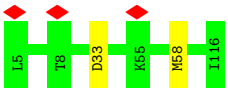




• Molecule 7: Complex I subunit B13

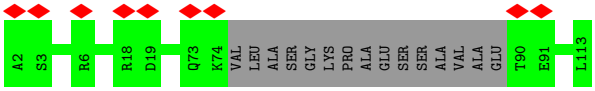
Chain H:





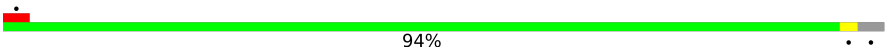
• Molecule 8: Complex I-B14.5a

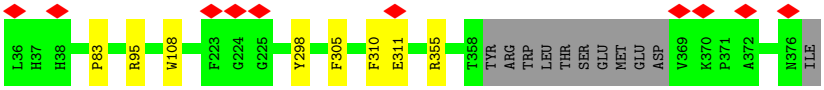
Chain I:



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

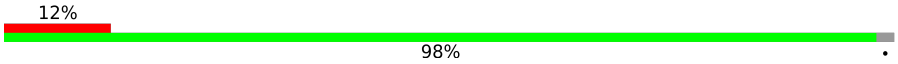
Chain J:

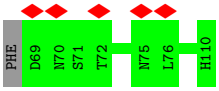




• Molecule 10: Complex I-9kD

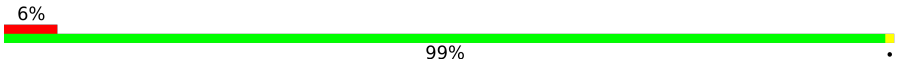
Chain K:

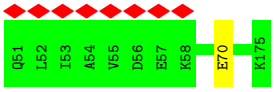




• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

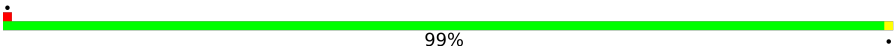
Chain L:

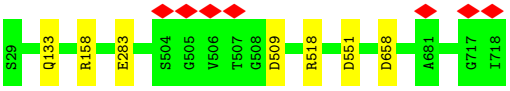




• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

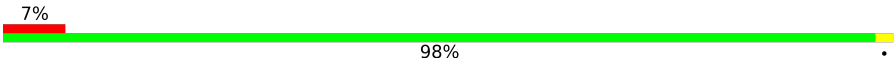
Chain M:

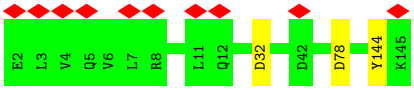




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

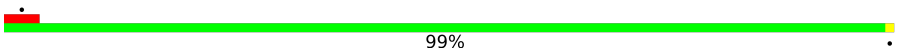
Chain N:

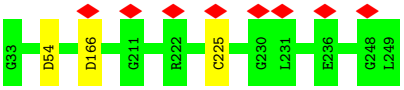




• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

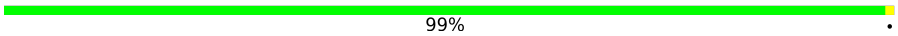
Chain O:

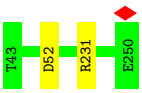




• Molecule 15: Complex I-30kD

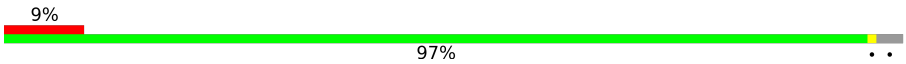
Chain P:

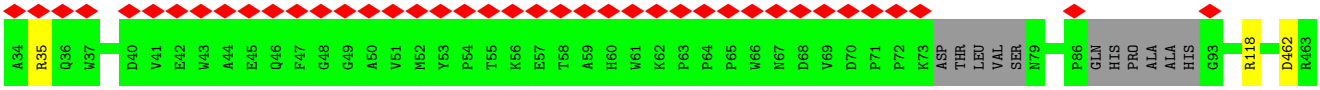




• Molecule 16: Complex I-49kD

Chain Q:



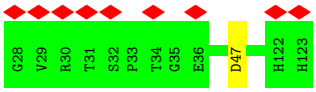


• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 100%

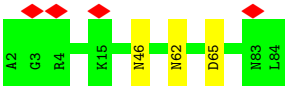
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 9% 99%



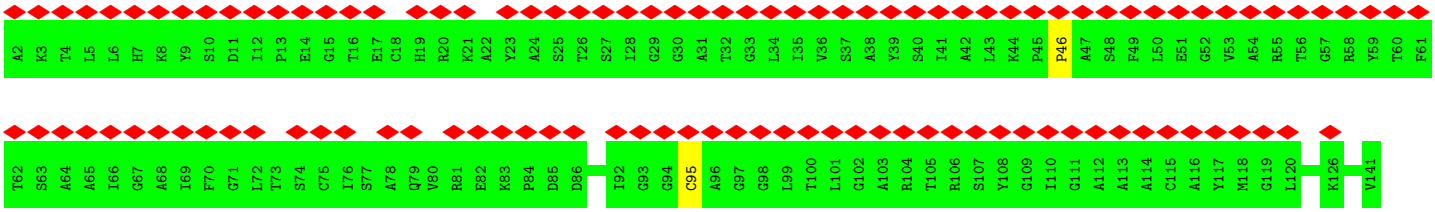
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 5% 96%



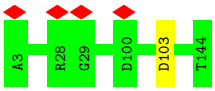
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 79% 99%



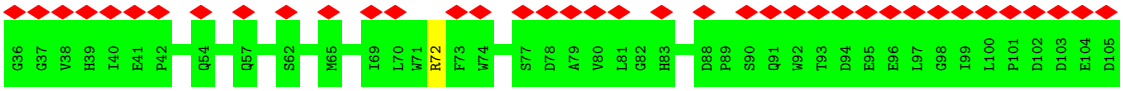
• Molecule 21: Complex I-B16.6

Chain W: 99%



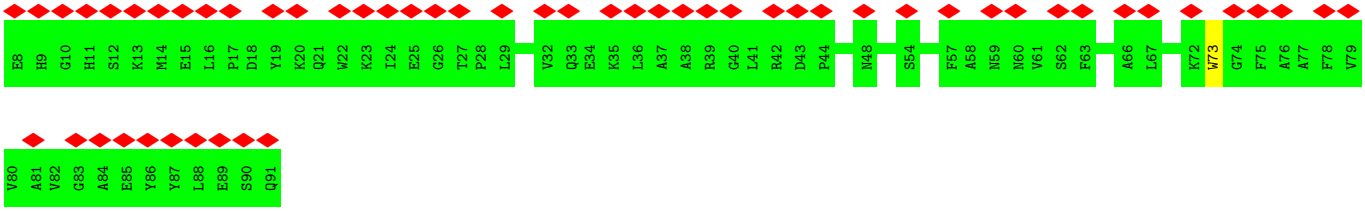
• Molecule 22: Complex I-AGGG

Chain Y: 54% 99%



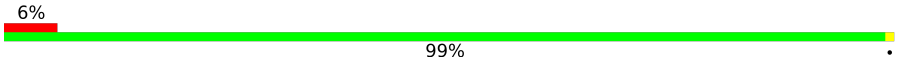
• Molecule 23: Complex I-B12

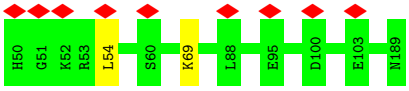
Chain Z: 65% 99%



• Molecule 24: Complex I-SGDH

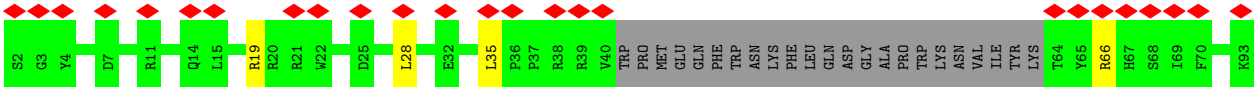
Chain a:

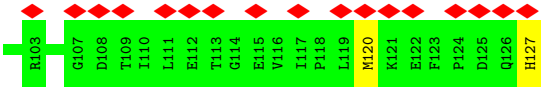




• Molecule 25: Complex I-B17

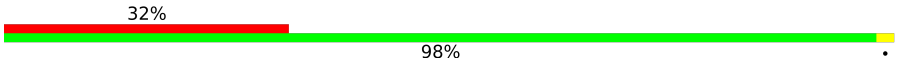
Chain b:

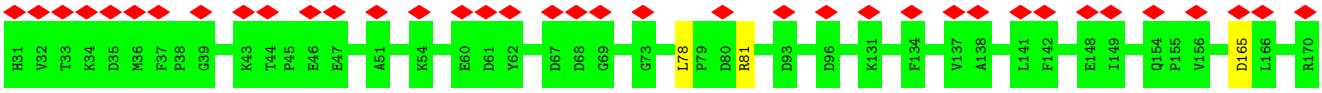


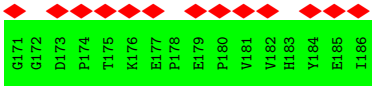


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:

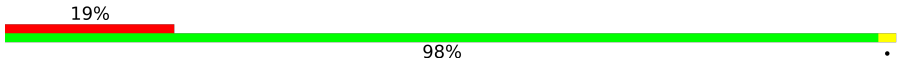


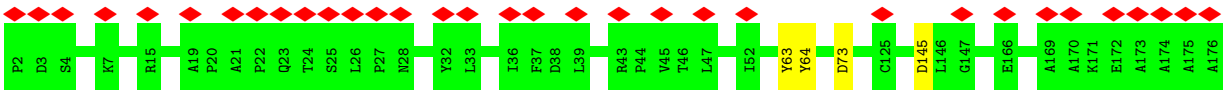




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

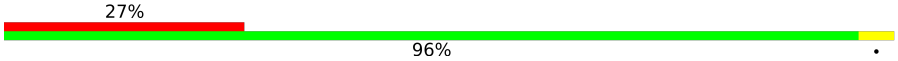
Chain d:

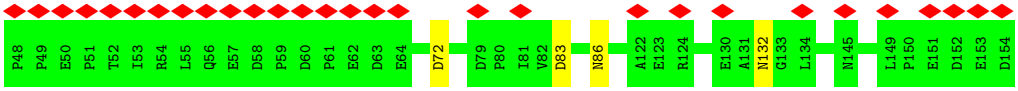




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

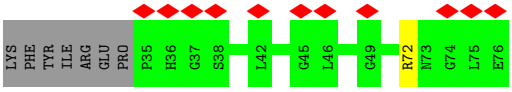
Chain e:





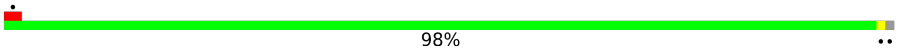
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

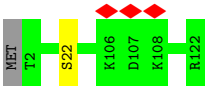
Chain f:



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

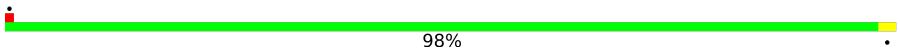
Chain g:

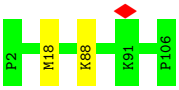




• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

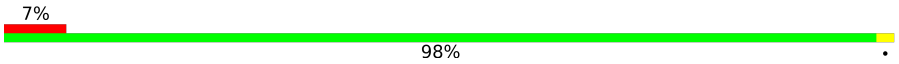
Chain h:

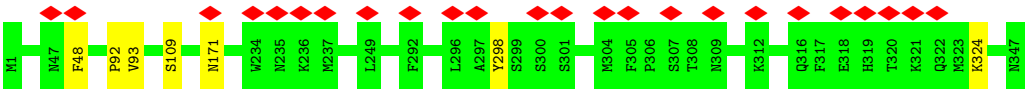




• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

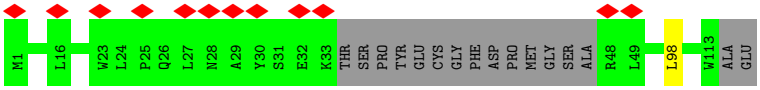
Chain i:





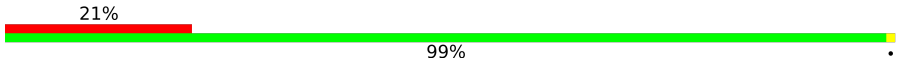
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

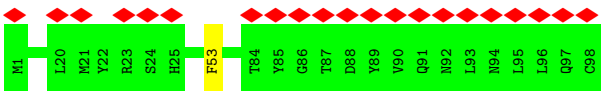
Chain j:



• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

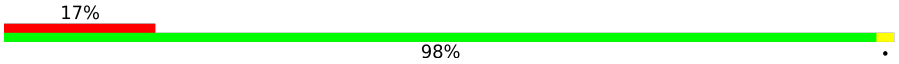
Chain k:

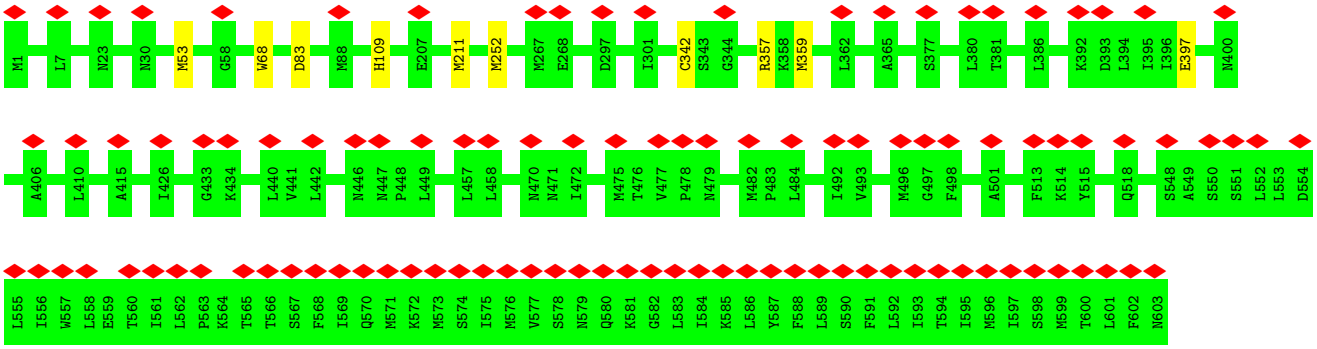




• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

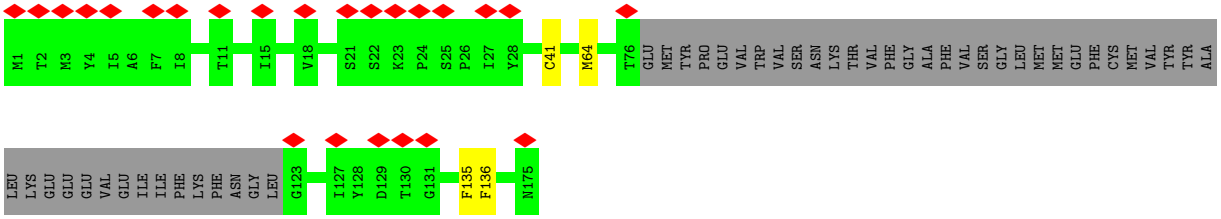
Chain l:





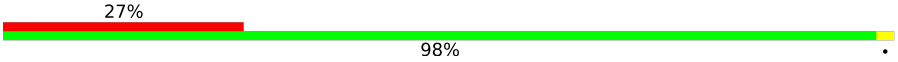
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

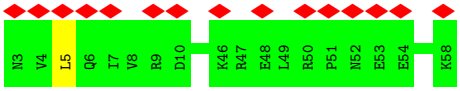
Chain m:



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

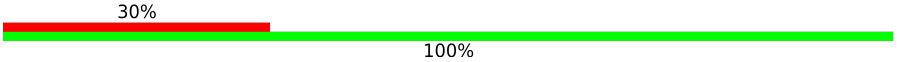
Chain n:

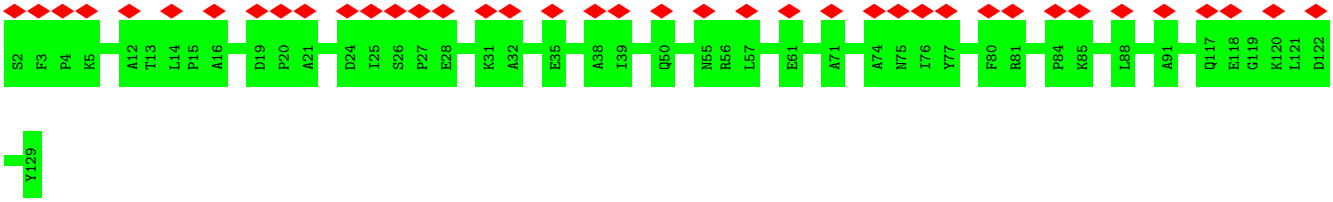




- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

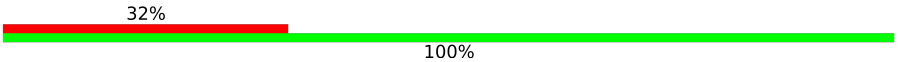
Chain o:

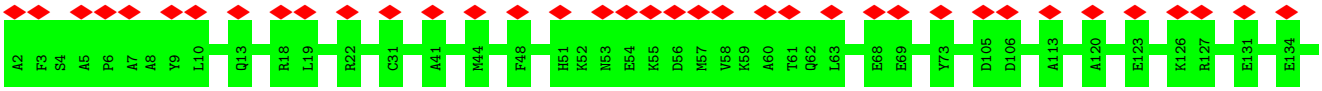


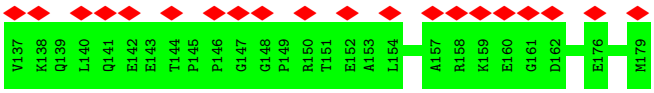


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:

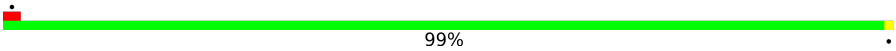


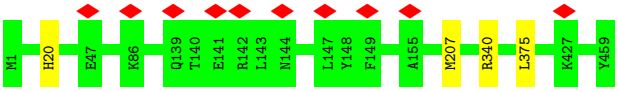




• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

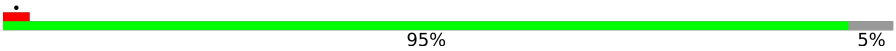
Chain r:

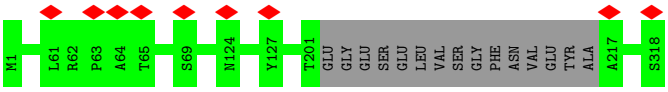




• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

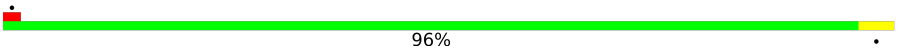
Chain s:

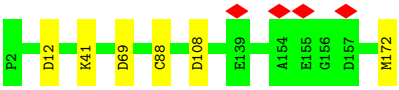




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

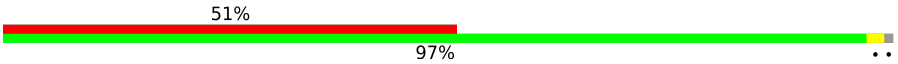
Chain u:

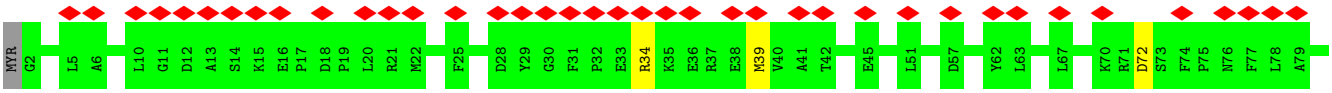


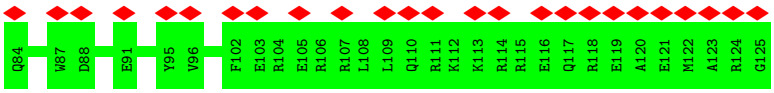


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:

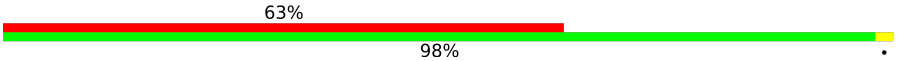


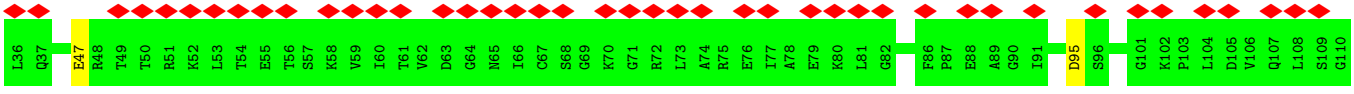


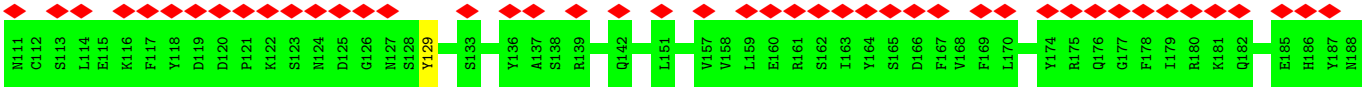


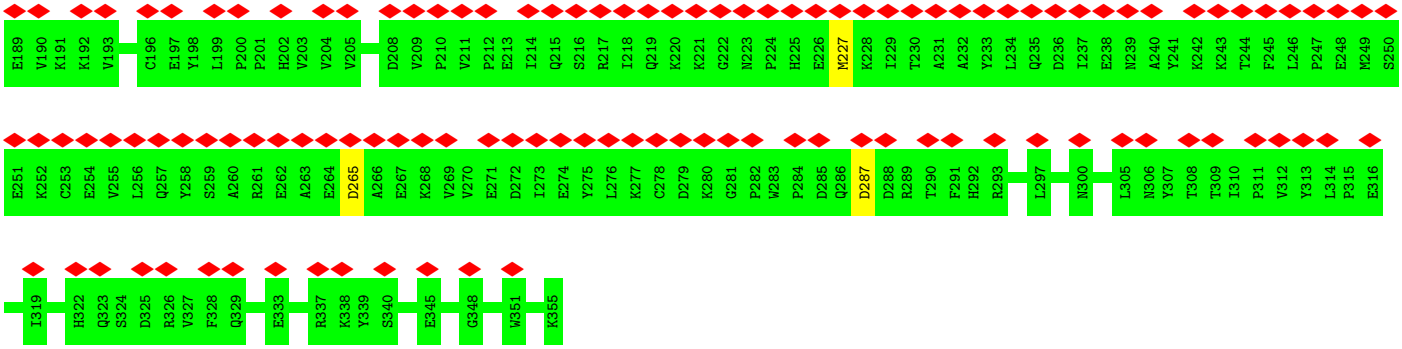
• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:








E189 V190 K191 K192 V193
C196 E197 Y198 L199 P200 P201 H202 V203 V204 V205
D208 V209 P210 V211 P212 E213 I214 Q215 S216 R217 I218 Q219 K220 K221 G222 N223 P224 H225 E226 M227 K228 I229 T230 A231 A232 Y233 L234 Q235 D236 I237 E238 N239 A240 Y241 K242 K243 T244 F245 L246 P247 E248 M249 S250
E251 K252 C253 E254 V255 L256 Q257 Y258 S259 A260 R261 E262 A263 E264 D265 A266 E267 K268 V269 V270 E271 D272 I273 E274 Y275 L276 K277 C278 D279 K280 G281 P282 W283 P284 D285 Q286 D287 D288 R289 T290 F291 H292 R293 L297 N300 L305 N306 Y307 T308 T309 I310 P311 V312 Y313 L314 P315 E316
T319 H322 Q323 S324 D325 R326 V327 F328 Q329 E333 R337 K338 Y339 S340 E345 G348 W351 K355

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0208	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0/4579
2	B	0.26	0/1433	0.49	0/1940
3	C	0.25	0/1279	0.52	0/1730
4	E	0.24	0/992	0.53	1/1336 (0.1%)
5	F	0.26	0/702	0.56	0/945
6	G	0.26	0/705	0.46	0/956
6	X	0.33	0/704	0.57	1/954 (0.1%)
7	H	0.26	0/929	0.45	0/1258
8	I	0.24	0/798	0.53	0/1079
9	J	0.25	0/2680	0.49	0/3633
10	K	0.27	0/365	0.55	0/493
11	L	0.24	0/1039	0.49	0/1403
12	M	0.25	0/5378	0.50	1/7287 (0.0%)
13	N	0.26	0/1245	0.56	1/1694 (0.1%)
14	O	0.26	0/1675	0.50	0/2287
15	P	0.26	0/1786	0.51	0/2432
16	Q	0.26	0/3451	0.51	0/4672
17	S	0.26	0/582	0.48	0/783
18	T	0.24	0/755	0.50	0/1018
19	U	0.25	0/664	0.47	0/912
20	V	0.25	0/1042	0.47	0/1411
21	W	0.25	0/1198	0.50	0/1617
22	Y	0.26	0/595	0.49	0/818
23	Z	0.26	0/695	0.47	0/939
24	a	0.26	0/1193	0.49	0/1615
25	b	0.26	0/873	0.57	1/1191 (0.1%)
26	c	0.27	0/1341	0.51	1/1836 (0.1%)
27	d	0.25	0/1494	0.51	0/2015
28	e	0.26	0/915	0.54	1/1245 (0.1%)
29	f	0.23	0/350	0.42	0/473
30	g	0.26	0/1031	0.49	0/1394
31	h	0.25	0/889	0.49	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.25	0/2773	0.44	0/3768
33	j	0.28	0/819	0.52	1/1117 (0.1%)
34	k	0.25	0/759	0.46	0/1029
35	l	0.26	0/4828	0.47	0/6573
36	m	0.27	0/934	0.48	0/1266
37	n	0.24	0/491	0.52	1/663 (0.2%)
38	o	0.29	0/1082	0.51	0/1469
39	p	0.25	0/1545	0.53	0/2099
40	r	0.25	0/3721	0.47	0/5076
41	s	0.28	0/2464	0.48	0/3369
42	u	0.25	0/1434	0.50	0/1935
43	v	0.32	0/1010	0.57	0/1362
44	w	0.26	0/2642	0.50	0/3580
All	All	0.26	0/66669	0.50	9/90441 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	N	78	ASP	CB-CG-OD1	5.91	123.62	118.30
26	c	165	ASP	CB-CG-OD1	5.87	123.58	118.30
37	n	5	LEU	CA-CB-CG	5.86	128.78	115.30
12	M	658	ASP	CB-CG-OD1	5.74	123.47	118.30
4	E	80	ASP	CB-CG-OD1	5.52	123.27	118.30
6	X	124	ASP	CB-CG-OD1	5.29	123.06	118.30
28	e	83	ASP	CB-CG-OD1	5.23	123.00	118.30
25	b	28	LEU	CB-CG-CD1	-5.11	102.31	111.00
33	j	98	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	327/342 (96%)	314 (96%)	13 (4%)	0	100	100
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	21 (3%)	1 (0%)	51	83
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	57
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
23	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	144 (94%)	9 (6%)	1 (1%)	25	59
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
30	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	332 (96%)	11 (3%)	2 (1%)	25	59
33	j	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	86 (90%)	10 (10%)	0	100	100
35	l	601/603 (100%)	572 (95%)	29 (5%)	0	100	100
36	m	125/175 (71%)	116 (93%)	9 (7%)	0	100	100
37	n	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	166 (94%)	10 (6%)	0	100	100
40	r	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
41	s	299/318 (94%)	285 (95%)	14 (5%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
All	All	8067/8323 (97%)	7746 (96%)	316 (4%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	c	81	ARG
32	i	93	VAL
32	i	92	PRO
12	M	283	GLU
20	V	46	PRO

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/346 (99%)	341 (99%)	3 (1%)	78	91
2	B	149/151 (99%)	147 (99%)	2 (1%)	69	87
3	C	132/132 (100%)	130 (98%)	2 (2%)	65	85
4	E	106/107 (99%)	103 (97%)	3 (3%)	43	73
5	F	76/76 (100%)	75 (99%)	1 (1%)	69	87
6	G	76/81 (94%)	71 (93%)	5 (7%)	16	47
6	X	74/81 (91%)	72 (97%)	2 (3%)	44	74
7	H	99/99 (100%)	97 (98%)	2 (2%)	55	80
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	276/296 (93%)	268 (97%)	8 (3%)	42	72
10	K	41/42 (98%)	41 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	91
12	M	578/580 (100%)	573 (99%)	5 (1%)	78	91
13	N	130/130 (100%)	128 (98%)	2 (2%)	65	85
14	O	175/183 (96%)	172 (98%)	3 (2%)	60	83
15	P	189/190 (100%)	187 (99%)	2 (1%)	73	89
16	Q	361/370 (98%)	359 (99%)	2 (1%)	86	94
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	69	87
19	U	69/69 (100%)	66 (96%)	3 (4%)	29	62
20	V	101/101 (100%)	100 (99%)	1 (1%)	76	90
21	W	122/123 (99%)	121 (99%)	1 (1%)	81	92
22	Y	56/63 (89%)	55 (98%)	1 (2%)	59	82
23	Z	65/65 (100%)	64 (98%)	1 (2%)	65	85
24	a	120/122 (98%)	118 (98%)	2 (2%)	60	83
25	b	90/119 (76%)	85 (94%)	5 (6%)	21	52
26	c	136/141 (96%)	135 (99%)	1 (1%)	84	93
27	d	155/155 (100%)	151 (97%)	4 (3%)	46	74
28	e	98/99 (99%)	95 (97%)	3 (3%)	40	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	f	35/45 (78%)	34 (97%)	1 (3%)	42	72
30	g	108/109 (99%)	107 (99%)	1 (1%)	78	91
31	h	93/93 (100%)	91 (98%)	2 (2%)	52	78
32	i	311/311 (100%)	306 (98%)	5 (2%)	62	84
33	j	88/100 (88%)	88 (100%)	0	100	100
34	k	85/85 (100%)	84 (99%)	1 (1%)	71	88
35	l	514/537 (96%)	504 (98%)	10 (2%)	57	81
36	m	89/141 (63%)	85 (96%)	4 (4%)	27	60
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	110/113 (97%)	110 (100%)	0	100	100
39	p	149/159 (94%)	149 (100%)	0	100	100
40	r	408/410 (100%)	404 (99%)	4 (1%)	76	90
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	152/153 (99%)	146 (96%)	6 (4%)	32	65
43	v	96/111 (86%)	93 (97%)	3 (3%)	40	70
44	w	281/283 (99%)	275 (98%)	6 (2%)	53	79
All	All	6990/7246 (96%)	6881 (98%)	109 (2%)	64	84

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	127	ASP
1	A	269	ARG
2	B	76	TYR
2	B	141	ARG
3	C	42	ARG
3	C	142	TYR
4	E	55	SER
4	E	80	ASP
4	E	101	THR
5	F	85	ASP
6	G	81	ASP
6	G	101	ASN
6	G	114	ASP
6	G	134	ASP

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Mol	Chain	Res	Type
6	G	136	GLU
7	H	33	ASP
7	H	58	MET
9	J	83	PRO
9	J	95	ARG
9	J	108	TRP
9	J	298	TYR
9	J	305	PHE
9	J	310	PHE
9	J	311	GLU
9	J	355	ARG
11	L	70	GLU
12	M	133	GLN
12	M	158	ARG
12	M	509	ASP
12	M	518	ARG
12	M	551	ASP
13	N	32	ASP
13	N	144	TYR
14	O	54	ASP
14	O	166	ASP
14	O	225	CYS
15	P	52	ASP
15	P	231	ARG
16	Q	35	ARG
16	Q	462	ASP
18	T	47	ASP
19	U	46	ASN
19	U	62	ASN
19	U	65	ASP
20	V	95	CYS
21	W	103	ASP
6	X	77	GLU
6	X	134	ASP
22	Y	72	ARG
23	Z	73	TRP
24	a	54	LEU
24	a	69	LYS
25	b	19	ARG
25	b	35	LEU
25	b	66	ARG
25	b	120	MET

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Mol	Chain	Res	Type
25	b	127	HIS
26	c	78	LEU
27	d	63	TYR
27	d	64	TYR
27	d	73	ASP
27	d	145	ASP
28	e	72	ASP
28	e	86	ASN
28	e	132	ASN
29	f	72	ARG
30	g	22	SER
31	h	18	MET
31	h	88	LYS
32	i	48	PHE
32	i	109	SER
32	i	171	ASN
32	i	298	TYR
32	i	324	LYS
34	k	53	PHE
35	l	53	MET
35	l	68	TRP
35	l	83	ASP
35	l	109	HIS
35	l	211	MET
35	l	252	MET
35	l	342	CYS
35	l	357	ARG
35	l	359	MET
35	l	397	GLU
36	m	41	CYS
36	m	64	MET
36	m	135	PHE
36	m	136	PHE
40	r	20	HIS
40	r	207	MET
40	r	340	ARG
40	r	375	LEU
42	u	12	ASP
42	u	41	LYS
42	u	69	ASP
42	u	88	CYS
42	u	108	ASP

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Mol	Chain	Res	Type
42	u	172	MET
43	v	34	ARG
43	v	39	MET
43	v	72	ASP
44	w	47	GLU
44	w	95	ASP
44	w	129	TYR
44	w	227	MET
44	w	265	ASP
44	w	287	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	123	GLN
7	H	50	GLN
8	I	29	GLN
9	J	72	HIS
10	K	79	HIS
12	M	278	HIS
12	M	453	GLN
14	O	187	GLN
15	P	124	ASN
20	V	89	ASN
22	Y	54	GLN
22	Y	57	GLN
23	Z	9	HIS
25	b	14	GLN
26	c	56	ASN
27	d	54	GLN
35	l	505	ASN
40	r	251	ASN
40	r	304	GLN
40	r	440	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	1.97	1 (10%)	5,13,15	6.09	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	5.65	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	12.41	130.85	119.48
16	Q	118	2MR	CD-NE-CZ	4.71	132.22	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.95	130.40	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
48	PEE	B	303	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)
52	FES	O	301	14	0,4,4	-	-	-		
48	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.97	2 (4%)
54	CDL	a	201	-	90,90,99	1.14	8 (8%)	96,102,111	0.88	4 (4%)
51	NDP	J	401	-	45,52,52	4.57	20 (44%)	53,80,80	1.97	8 (15%)
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.42	4 (13%)
49	PLX	l	701	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
49	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
48	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	0.98	2 (3%)
45	SF4	M	801	12	0,12,12	-	-	-		
48	PEE	i	402	-	46,46,50	1.21	6 (13%)	49,51,55	0.95	2 (4%)
49	PLX	g	201	-	51,51,51	1.15	3 (5%)	55,59,59	0.61	1 (1%)
50	8Q1	X	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.54	6 (15%)
54	CDL	r	504	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
49	PLX	C	303	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
54	CDL	N	201	-	50,50,99	1.40	9 (18%)	56,62,111	1.14	4 (7%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
48	PEE	l	702	-	45,45,50	1.22	6 (13%)	48,50,55	0.97	2 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
54	CDL	u	201	-	77,77,99	1.03	4 (5%)	83,89,111	1.08	4 (4%)
50	8Q1	G	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.62	6 (15%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.22	8 (16%)
52	FES	M	803	12	0,4,4	-	-	-		
56	UQ	s	401	-	28,28,63	3.24	6 (21%)	34,37,79	2.96	10 (29%)
54	CDL	r	503	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
48	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	0.98	2 (4%)
47	NAI	A	503	-	42,48,48	4.93	18 (42%)	47,73,73	1.31	7 (14%)
48	PEE	m	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.00	2 (4%)
54	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	1.01	4 (5%)
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
48	PEE	B	303	-	-	25/54/54/54	-
52	FES	O	301	14	-	-	0/1/1/1
48	PEE	b	201	-	-	29/49/49/54	-
54	CDL	a	201	-	-	37/101/101/110	-
51	NDP	J	401	-	-	5/30/77/77	0/4/5/5
57	ADP	w	401	-	-	3/12/32/32	0/3/3/3
49	PLX	l	701	-	-	32/55/55/55	-
49	PLX	r	502	-	-	28/55/55/55	-
48	PEE	r	501	-	-	28/54/54/54	-
48	PEE	i	402	-	-	23/50/50/54	-
49	PLX	g	201	-	-	22/55/55/55	-
50	8Q1	X	201	-	-	18/41/41/41	-
45	SF4	M	801	12	-	-	0/6/5/5
54	CDL	r	504	-	-	62/110/110/110	-
49	PLX	C	303	-	-	26/55/55/55	-
54	CDL	N	201	-	-	35/61/61/110	-
49	PLX	j	202	-	-	29/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	l	702	-	-	20/49/49/54	-
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	j	201	-	-	28/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
54	CDL	u	201	-	-	29/88/88/110	-
50	8Q1	G	201	-	-	14/41/41/41	-
46	FMN	A	502	-	-	9/18/18/18	0/3/3/3
52	FES	M	803	12	-	-	0/1/1/1
56	UQ	s	401	-	-	10/21/45/87	0/1/1/1
54	CDL	r	503	-	-	54/109/109/110	-
48	PEE	C	302	-	-	29/50/50/54	-
47	NAI	A	503	-	-	6/25/72/72	0/5/5/5
48	PEE	m	201	-	-	23/44/44/54	-
54	CDL	i	401	-	-	44/76/76/110	-
45	SF4	C	301	3,16	-	-	0/6/5/5

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.21	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.32	1.30	1.53
51	J	401	NDP	C3B-C2B	-12.84	1.24	1.52
51	J	401	NDP	C6N-C5N	12.42	1.55	1.33
51	J	401	NDP	O4D-C4D	10.69	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.08	1.27	1.53
51	J	401	NDP	C3D-C4D	-9.82	1.27	1.53
56	s	401	UQ	C13-C14	9.23	1.55	1.33
57	w	401	ADP	C3'-C4'	-8.99	1.30	1.53
56	s	401	UQ	C8-C9	8.83	1.54	1.33
51	J	401	NDP	O4B-C1B	8.56	1.53	1.41
47	A	503	NAI	O4B-C4B	-8.25	1.26	1.45
56	s	401	UQ	C18-C19	8.22	1.56	1.32
51	J	401	NDP	O4B-C4B	-7.77	1.27	1.45
47	A	503	NAI	C2D-C1D	-7.67	1.29	1.53
57	w	401	ADP	O4'-C4'	7.61	1.62	1.45
51	J	401	NDP	C2N-C3N	7.46	1.55	1.34
47	A	503	NAI	O4D-C4D	7.04	1.60	1.45
57	w	401	ADP	O4'-C1'	-6.87	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C2D-C3D	5.91	1.69	1.53
47	A	503	NAI	C7N-N7N	5.78	1.48	1.33
51	J	401	NDP	P2B-O2B	5.68	1.70	1.59
50	G	201	8Q1	C34-N36	5.51	1.45	1.33
47	A	503	NAI	O4D-C1D	5.45	1.54	1.42
51	J	401	NDP	C3B-C4B	5.44	1.66	1.53
50	X	201	8Q1	C39-N41	5.42	1.45	1.33
50	X	201	8Q1	C34-N36	5.41	1.45	1.33
50	G	201	8Q1	C39-N41	5.27	1.45	1.33
51	J	401	NDP	C6N-N1N	5.01	1.49	1.37
47	A	503	NAI	C4N-C3N	-5.00	1.40	1.49
51	J	401	NDP	O4D-C1D	-4.88	1.30	1.42
47	A	503	NAI	O2B-C2B	4.57	1.53	1.43
51	J	401	NDP	C7N-N7N	4.22	1.44	1.33
54	u	201	CDL	OA8-CA7	4.22	1.45	1.33
54	u	201	CDL	OB8-CB7	4.20	1.45	1.33
54	u	201	CDL	OA6-CA5	4.19	1.46	1.34
51	J	401	NDP	C6A-N6A	4.12	1.49	1.34
51	J	401	NDP	O2D-C2D	-4.11	1.33	1.43
47	A	503	NAI	C6N-C5N	4.07	1.40	1.33
54	u	201	CDL	OB6-CB5	3.97	1.45	1.34
57	w	401	ADP	C6-N6	3.85	1.48	1.34
46	A	502	FMN	C4A-N5	3.84	1.38	1.30
48	m	201	PEE	C18-C19	3.77	1.53	1.31
48	i	402	PEE	C18-C19	3.74	1.53	1.31
48	j	201	PEE	C18-C19	3.74	1.53	1.31
48	C	302	PEE	C18-C19	3.73	1.53	1.31
48	r	501	PEE	C18-C19	3.73	1.53	1.31
48	B	303	PEE	C18-C19	3.72	1.53	1.31
48	b	201	PEE	C18-C19	3.72	1.53	1.31
48	l	702	PEE	C18-C19	3.72	1.53	1.31
48	C	302	PEE	C39-C38	3.66	1.53	1.31
48	r	501	PEE	C39-C38	3.66	1.53	1.31
48	i	402	PEE	C39-C38	3.65	1.52	1.31
48	l	702	PEE	C39-C38	3.65	1.52	1.31
48	j	201	PEE	C39-C38	3.64	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
48	b	201	PEE	C39-C38	3.63	1.52	1.31
47	A	503	NAI	C7N-C3N	3.62	1.56	1.48
47	A	503	NAI	C6A-N6A	3.61	1.47	1.34
54	i	401	CDL	OA8-CA7	3.51	1.43	1.33
54	r	504	CDL	OA8-CA7	3.46	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	N	201	CDL	OA8-CA7	3.45	1.43	1.33
54	a	201	CDL	OA8-CA7	3.44	1.43	1.33
54	r	503	CDL	OA8-CA7	3.38	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.31	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.31	1.40	1.48
57	w	401	ADP	O3'-C3'	3.14	1.50	1.43
51	J	401	NDP	O3D-C3D	3.13	1.50	1.43
54	a	201	CDL	OB6-CB5	3.13	1.43	1.34
54	r	504	CDL	OB6-CB5	3.12	1.43	1.34
54	N	201	CDL	OA6-CA5	3.12	1.43	1.34
54	i	401	CDL	OB6-CB5	3.04	1.42	1.34
51	J	401	NDP	C7N-C3N	3.04	1.55	1.48
54	r	504	CDL	OB8-CB7	3.03	1.42	1.33
54	a	201	CDL	OA6-CA5	3.03	1.42	1.34
54	i	401	CDL	OB8-CB7	3.03	1.42	1.33
54	N	201	CDL	OB8-CB7	3.01	1.42	1.33
54	a	201	CDL	OB8-CB7	3.00	1.42	1.33
54	r	503	CDL	OB6-CB5	2.99	1.42	1.34
54	r	503	CDL	OB8-CB7	2.99	1.42	1.33
54	r	504	CDL	OA6-CA5	2.97	1.42	1.34
54	i	401	CDL	OA6-CA5	2.97	1.42	1.34
54	N	201	CDL	OB6-CB5	2.96	1.42	1.34
54	r	503	CDL	OA6-CA5	2.88	1.42	1.34
49	l	701	PLX	O6-C4	-2.79	1.40	1.44
49	C	303	PLX	O6-C4	-2.73	1.41	1.44
49	g	201	PLX	O6-C4	-2.71	1.41	1.44
56	s	401	UQ	C6-C1	2.58	1.53	1.46
49	j	202	PLX	O6-C4	-2.54	1.41	1.44
48	b	201	PEE	O3-C30	2.52	1.40	1.33
48	i	402	PEE	O3-C30	2.52	1.40	1.33
46	A	502	FMN	C10-N1	2.51	1.38	1.33
48	l	702	PEE	O3-C30	2.48	1.40	1.33
48	r	501	PEE	O2-C2	-2.47	1.40	1.46
47	A	503	NAI	PN-O5D	2.47	1.69	1.59
48	C	302	PEE	O3-C30	2.44	1.40	1.33
51	J	401	NDP	O2B-C2B	2.44	1.53	1.44
54	r	503	CDL	OA6-CA4	-2.43	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.42	1.37	1.43
48	r	501	PEE	O3-C30	2.41	1.40	1.33
50	X	201	8Q1	C1-S44	2.41	1.82	1.76
48	B	303	PEE	O3-C30	2.41	1.40	1.33
48	j	201	PEE	O3-C30	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C2D-C3D	2.40	1.59	1.53
48	B	303	PEE	O2-C2	-2.39	1.40	1.46
48	m	201	PEE	O2-C10	2.39	1.41	1.34
48	b	201	PEE	O2-C2	-2.39	1.40	1.46
48	C	302	PEE	O2-C2	-2.39	1.40	1.46
54	r	504	CDL	OA6-CA4	-2.38	1.40	1.46
49	g	201	PLX	C7-C6	2.38	1.55	1.50
48	m	201	PEE	O3-C30	2.37	1.40	1.33
49	r	502	PLX	C7-C6	2.37	1.55	1.50
48	l	702	PEE	O2-C2	-2.37	1.40	1.46
48	i	402	PEE	O2-C2	-2.36	1.40	1.46
54	i	401	CDL	OA6-CA4	-2.36	1.40	1.46
50	G	201	8Q1	C1-S44	2.36	1.81	1.76
49	j	202	PLX	C7-C6	2.36	1.55	1.50
48	j	201	PEE	O2-C2	-2.35	1.40	1.46
54	a	201	CDL	OA6-CA4	-2.34	1.40	1.46
50	G	201	8Q1	O35-C34	-2.30	1.18	1.23
49	l	701	PLX	C7-C6	2.30	1.55	1.50
49	C	303	PLX	C7-C6	2.29	1.55	1.50
48	i	402	PEE	O2-C10	2.28	1.40	1.34
50	X	201	8Q1	O35-C34	-2.27	1.18	1.23
48	C	302	PEE	O2-C10	2.27	1.40	1.34
48	l	702	PEE	O2-C10	2.27	1.40	1.34
48	j	201	PEE	O2-C10	2.27	1.40	1.34
48	b	201	PEE	O2-C10	2.26	1.40	1.34
50	G	201	8Q1	O40-C39	-2.25	1.18	1.23
48	m	201	PEE	O2-C2	-2.25	1.41	1.46
49	r	502	PLX	O6-C4	-2.25	1.41	1.44
47	A	503	NAI	C5B-C4B	2.25	1.58	1.51
48	B	303	PEE	O2-C10	2.23	1.40	1.34
50	X	201	8Q1	C6-C1	2.23	1.53	1.50
54	r	503	CDL	OB6-CB4	-2.22	1.41	1.46
50	G	201	8Q1	C6-C1	2.22	1.53	1.50
54	i	401	CDL	PB2-OB2	2.22	1.68	1.59
54	r	503	CDL	PB2-OB2	2.21	1.68	1.59
54	r	504	CDL	PB2-OB2	2.21	1.68	1.59
54	i	401	CDL	PB2-OB5	2.20	1.68	1.59
54	N	201	CDL	OB6-CB4	-2.19	1.41	1.46
54	r	504	CDL	PB2-OB5	2.19	1.68	1.59
48	r	501	PEE	O2-C10	2.18	1.40	1.34
54	a	201	CDL	PB2-OB2	2.18	1.68	1.59
54	N	201	CDL	PB2-OB5	2.18	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	r	502	PLX	P1-O4	2.18	1.68	1.59
54	r	503	CDL	PB2-OB5	2.17	1.68	1.59
49	j	202	PLX	P1-O4	2.17	1.68	1.59
54	a	201	CDL	PB2-OB5	2.16	1.68	1.59
54	N	201	CDL	PB2-OB2	2.16	1.68	1.59
56	s	401	UQ	C7-C8	2.15	1.53	1.50
50	X	201	8Q1	O40-C39	-2.14	1.18	1.23
48	m	201	PEE	O3-C3	-2.14	1.40	1.45
51	J	401	NDP	PA-O5B	2.13	1.67	1.59
48	r	501	PEE	O3-C3	-2.13	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.13	1.19	1.24
54	i	401	CDL	OB6-CB4	-2.12	1.41	1.46
56	s	401	UQ	O4-C4	-2.12	1.18	1.23
49	C	303	PLX	P1-O4	2.12	1.67	1.59
49	g	201	PLX	P1-O4	2.12	1.67	1.59
54	N	201	CDL	OA6-CA4	-2.11	1.41	1.46
54	a	201	CDL	OB6-CB4	-2.10	1.41	1.46
49	l	701	PLX	P1-O4	2.09	1.67	1.59
48	j	201	PEE	O3-C3	-2.07	1.40	1.45
49	r	502	PLX	P1-O1	2.07	1.67	1.59
48	l	702	PEE	O3-C3	-2.06	1.40	1.45
48	B	303	PEE	O3-C3	-2.05	1.40	1.45
49	j	202	PLX	P1-O1	2.05	1.67	1.59
48	C	302	PEE	O3-C3	-2.05	1.40	1.45
49	C	303	PLX	P1-O1	2.03	1.67	1.59
48	i	402	PEE	O3-C3	-2.03	1.40	1.45
48	b	201	PEE	O3-C3	-2.02	1.40	1.45
54	r	504	CDL	C11-CA5	2.02	1.56	1.50
54	r	504	CDL	OB6-CB4	-2.01	1.41	1.46
54	N	201	CDL	C11-CA5	2.01	1.56	1.50

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C7-C8-C9	-10.17	109.85	126.79
51	J	401	NDP	C3N-C2N-N1N	-7.62	112.22	123.10
51	J	401	NDP	C1D-N1N-C2N	-7.28	108.99	121.11
56	s	401	UQ	C12-C13-C14	-6.19	112.77	127.66
50	X	201	8Q1	C6-C1-S44	5.85	120.27	113.46
50	G	201	8Q1	C6-C1-S44	5.71	120.11	113.46
56	s	401	UQ	C11-C9-C8	-5.44	110.11	121.12
51	J	401	NDP	C1D-N1N-C6N	-5.27	109.47	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	401	UQ	C10-C9-C8	-4.83	111.29	123.68
47	A	503	NAI	N3A-C2A-N1A	-4.41	121.78	128.68
56	s	401	UQ	C16-C14-C13	-4.34	112.33	121.12
57	w	401	ADP	N3-C2-N1	-4.31	121.94	128.68
56	s	401	UQ	C15-C14-C13	-4.24	112.81	123.68
54	u	201	CDL	OA6-CA5-C11	4.23	120.62	111.50
54	N	201	CDL	OA6-CA5-C11	4.11	120.37	111.50
54	N	201	CDL	OB6-CB5-C51	4.11	120.36	111.50
51	J	401	NDP	N3A-C2A-N1A	-4.09	122.28	128.68
56	s	401	UQ	C17-C18-C19	-4.07	113.83	127.75
54	r	504	CDL	OB6-CB5-C51	4.02	120.17	111.50
54	a	201	CDL	OA6-CA5-C11	4.02	120.16	111.50
54	i	401	CDL	OA6-CA5-C11	4.01	120.15	111.50
48	r	501	PEE	O2-C10-C11	4.01	120.14	111.50
48	C	302	PEE	O2-C10-C11	3.95	120.01	111.50
48	j	201	PEE	O2-C10-C11	3.94	119.99	111.50
54	i	401	CDL	OB6-CB5-C51	3.93	119.96	111.50
54	r	503	CDL	OA6-CA5-C11	3.91	119.93	111.50
54	r	504	CDL	OA6-CA5-C11	3.90	119.91	111.50
48	B	303	PEE	O2-C10-C11	3.89	119.88	111.50
48	m	201	PEE	O2-C10-C11	3.88	119.87	111.50
48	i	402	PEE	O2-C10-C11	3.88	119.86	111.50
54	r	503	CDL	OB6-CB5-C51	3.87	119.84	111.50
54	a	201	CDL	OB6-CB5-C51	3.81	119.71	111.50
48	b	201	PEE	O2-C10-C11	3.79	119.66	111.50
48	l	702	PEE	O2-C10-C11	3.66	119.38	111.50
50	G	201	8Q1	C37-C38-C39	3.57	118.31	112.36
54	u	201	CDL	OB6-CB5-C51	3.55	119.16	111.50
50	G	201	8Q1	O4-C1-C6	-3.49	119.87	123.99
50	X	201	8Q1	O4-C1-C6	-3.39	119.99	123.99
56	s	401	UQ	C21-C19-C18	-3.37	112.90	122.65
50	G	201	8Q1	C31-C29-C32	3.27	114.50	108.82
56	s	401	UQ	C20-C19-C18	-3.13	113.61	122.65
56	s	401	UQ	CM5-C5-C6	-3.05	119.42	124.40
46	A	502	FMN	C4-N3-C2	-2.98	120.14	125.64
47	A	503	NAI	C3B-C2B-C1B	2.90	105.35	100.98
47	A	503	NAI	C2D-C3D-C4D	2.77	108.03	102.64
57	w	401	ADP	C3'-C2'-C1'	2.76	105.13	100.98
57	w	401	ADP	PA-O3A-PB	-2.73	123.44	132.83
48	r	501	PEE	O3-C30-C31	2.71	120.40	111.91
48	l	702	PEE	O3-C30-C31	2.70	120.38	111.91
54	i	401	CDL	OA8-CA7-C31	2.68	120.31	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	B	303	PEE	O3-C30-C31	2.67	120.28	111.91
54	u	201	CDL	OB8-CB7-C71	2.66	120.24	111.91
51	J	401	NDP	PN-O3-PA	-2.65	123.72	132.83
46	A	502	FMN	C4A-C4-N3	2.64	119.89	113.19
54	i	401	CDL	OB8-CB7-C71	2.63	120.17	111.91
48	b	201	PEE	O3-C30-C31	2.63	120.17	111.91
54	N	201	CDL	OB8-CB7-C71	2.63	120.16	111.91
47	A	503	NAI	C4A-C5A-N7A	-2.61	106.68	109.40
48	j	201	PEE	O3-C30-C31	2.58	119.99	111.91
54	r	503	CDL	OB8-CB7-C71	2.58	119.99	111.91
54	a	201	CDL	OB8-CB7-C71	2.57	119.98	111.91
47	A	503	NAI	C4D-O4D-C1D	-2.57	103.80	109.47
54	u	201	CDL	OA8-CA7-C31	2.56	119.93	111.91
54	r	503	CDL	OA8-CA7-C31	2.53	119.85	111.91
54	r	504	CDL	OB8-CB7-C71	2.53	119.84	111.91
54	N	201	CDL	OA8-CA7-C31	2.51	119.78	111.91
48	C	302	PEE	O3-C30-C31	2.50	119.76	111.91
46	A	502	FMN	O4-C4-C4A	-2.50	119.97	126.60
49	g	201	PLX	C1A-N1-C1	2.49	120.11	109.92
46	A	502	FMN	C4A-C10-N10	2.47	120.09	116.48
48	m	201	PEE	O3-C30-C31	2.47	119.66	111.91
51	J	401	NDP	C4A-C5A-N7A	-2.44	106.85	109.40
49	r	502	PLX	C1A-N1-C1	2.41	119.80	109.92
49	l	701	PLX	C1A-N1-C1	2.40	119.74	109.92
50	X	201	8Q1	C38-C39-N41	2.40	120.46	116.42
54	r	504	CDL	OA8-CA7-C31	2.40	119.42	111.91
54	a	201	CDL	OA8-CA7-C31	2.39	119.42	111.91
47	A	503	NAI	C3D-C2D-C1D	2.37	105.94	101.43
48	i	402	PEE	O3-C30-C31	2.37	119.35	111.91
57	w	401	ADP	C4-C5-N7	-2.37	106.93	109.40
50	G	201	8Q1	C43-S44-C1	2.34	109.16	101.87
49	j	202	PLX	C1A-N1-C1	2.31	119.38	109.92
47	A	503	NAI	PN-O3-PA	-2.31	124.90	132.83
46	A	502	FMN	C10-C4A-N5	-2.27	120.03	124.86
51	J	401	NDP	C2B-C3B-C4B	2.24	106.86	101.99
50	X	201	8Q1	C37-C38-C39	2.23	116.08	112.36
46	A	502	FMN	C9A-C5A-N5	-2.22	120.02	122.43
49	C	303	PLX	C1A-N1-C1	2.22	118.98	109.92
46	A	502	FMN	C4A-C10-N1	-2.21	119.59	124.73
50	X	201	8Q1	O4-C1-S44	-2.21	119.75	122.61
51	J	401	NDP	C2D-C3D-C4D	2.09	106.71	102.64
50	G	201	8Q1	C38-C39-N41	2.07	119.91	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	X	201	8Q1	C43-S44-C1	2.04	108.22	101.87
46	A	502	FMN	C5A-C9A-N10	2.02	120.03	117.95

There are no chirality outliers.

All (668) 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	C5'-O5'-P-O1P
47	A	503	NAI	C5B-O5B-PA-O1A
48	B	303	PEE	C37-C38-C39-C40
48	C	302	PEE	C1-O3P-P-O1P
48	b	201	PEE	O4P-C4-C5-N
48	i	402	PEE	C11-C10-O2-C2
48	i	402	PEE	C4-O4P-P-O1P
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	O3P-C1-C2-O2
48	l	702	PEE	C4-O4P-P-O3P
48	l	702	PEE	C4-O4P-P-O2P
48	l	702	PEE	C4-O4P-P-O1P
48	m	201	PEE	C11-C10-O2-C2
48	m	201	PEE	O4P-C4-C5-N
48	r	501	PEE	C17-C18-C19-C20
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O4-C3-C4-O6
49	C	303	PLX	C3-O4-P1-O2
49	C	303	PLX	C3-O4-P1-O3
49	g	201	PLX	O7-C6-O6-C4
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O7-C6-O6-C4
49	j	202	PLX	O9-C24-C25-C26
49	l	701	PLX	O7-C6-O6-C4
49	l	701	PLX	C25-C24-O8-C5
49	l	701	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	O9-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
51	J	401	NDP	C2B-O2B-P2B-O3X
54	N	201	CDL	CA2-C1-CB2-OB2
54	N	201	CDL	CA2-OA2-PA1-OA3
54	N	201	CDL	CA2-OA2-PA1-OA4
54	N	201	CDL	CA2-OA2-PA1-OA5
54	N	201	CDL	C11-CA5-OA6-CA4
54	N	201	CDL	CB2-OB2-PB2-OB3
54	N	201	CDL	CB2-OB2-PB2-OB4
54	N	201	CDL	CB2-OB2-PB2-OB5
54	N	201	CDL	CB3-OB5-PB2-OB2
54	N	201	CDL	CB3-OB5-PB2-OB3
54	N	201	CDL	CB3-OB5-PB2-OB4
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CB3-OB5-PB2-OB2
54	a	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	CA2-OA2-PA1-OA3
54	i	401	CDL	CA2-OA2-PA1-OA4
54	i	401	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CA3-OA5-PA1-OA3
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CB2-OB2-PB2-OB5
54	i	401	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	OB6-CB4-CB6-OB8
54	r	503	CDL	O1-C1-CA2-OA2
54	r	503	CDL	OA5-CA3-CA4-OA6
54	r	504	CDL	CA3-OA5-PA1-OA3
54	r	504	CDL	OA6-CA4-CA6-OA8
54	r	504	CDL	C51-CB5-OB6-CB4
54	u	201	CDL	CA2-OA2-PA1-OA3
54	u	201	CDL	CB3-OB5-PB2-OB3
56	s	401	UQ	C7-C8-C9-C10
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C8
56	s	401	UQ	C12-C13-C14-C16
56	s	401	UQ	C17-C18-C19-C21
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
54	r	503	CDL	C31-CA7-OA8-CA6
48	b	201	PEE	O5-C30-O3-C3
48	l	702	PEE	O5-C30-O3-C3
54	r	503	CDL	OA9-CA7-OA8-CA6
48	i	402	PEE	O4-C10-O2-C2
48	j	201	PEE	O4-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
54	N	201	CDL	OA7-CA5-OA6-CA4
54	r	504	CDL	OB7-CB5-OB6-CB4
54	i	401	CDL	OA9-CA7-OA8-CA6
49	g	201	PLX	C7-C8-C9-C10
48	b	201	PEE	C31-C30-O3-C3
48	l	702	PEE	C31-C30-O3-C3
48	b	201	PEE	C37-C38-C39-C40
48	i	402	PEE	C17-C18-C19-C20
48	j	201	PEE	C17-C18-C19-C20
49	l	701	PLX	C12-C13-C14-C15
54	N	201	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	O1-C1-CA2-OA2
54	r	504	CDL	C71-CB7-OB8-CB6
48	r	501	PEE	C11-C10-O2-C2
54	r	503	CDL	C62-C63-C64-C65
54	i	401	CDL	C14-C15-C16-C17
48	C	302	PEE	C14-C15-C16-C17
54	i	401	CDL	C31-CA7-OA8-CA6
48	m	201	PEE	C13-C14-C15-C16
54	i	401	CDL	C31-C32-C33-C34
49	j	202	PLX	C28-C29-C30-C31
54	r	504	CDL	OB9-CB7-OB8-CB6
54	r	503	CDL	C32-C33-C34-C35
48	m	201	PEE	C31-C30-O3-C3
49	r	502	PLX	C9-C10-C11-C12
54	i	401	CDL	C37-C38-C39-C40
48	r	501	PEE	C41-C42-C43-C44
56	s	401	UQ	C12-C13-C14-C15
54	r	503	CDL	CB2-C1-CA2-OA2
48	m	201	PEE	O5-C30-O3-C3
54	N	201	CDL	C31-CA7-OA8-CA6
49	r	502	PLX	C11-C12-C13-C14
54	a	201	CDL	C34-C35-C36-C37
49	r	502	PLX	C30-C31-C32-C33
49	j	202	PLX	C15-C16-C17-C18
48	r	501	PEE	O4-C10-O2-C2
48	b	201	PEE	C34-C35-C36-C37
49	C	303	PLX	C28-C29-C30-C31
54	a	201	CDL	CB5-C51-C52-C53
51	J	401	NDP	C2D-C1D-N1N-C6N
49	g	201	PLX	C12-C13-C14-C15
48	r	501	PEE	C10-C11-C12-C13
54	i	401	CDL	CA7-C31-C32-C33
54	u	201	CDL	C75-C76-C77-C78
48	B	303	PEE	C30-C31-C32-C33
54	N	201	CDL	CB5-C51-C52-C53
54	r	503	CDL	CB7-C71-C72-C73
49	l	701	PLX	C2-C1-N1-C1A
48	C	302	PEE	C30-C31-C32-C33
54	N	201	CDL	CA7-C31-C32-C33
54	r	504	CDL	CA7-C31-C32-C33
48	b	201	PEE	C10-C11-C12-C13
48	r	501	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C10-C11-C12-C13
48	i	402	PEE	C31-C30-O3-C3
54	a	201	CDL	C71-CB7-OB8-CB6
54	N	201	CDL	OA9-CA7-OA8-CA6
48	l	702	PEE	C30-C31-C32-C33
48	C	302	PEE	C1-O3P-P-O4P
48	i	402	PEE	C4-O4P-P-O3P
48	j	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O3P
48	r	501	PEE	C1-O3P-P-O4P
49	C	303	PLX	C3-O4-P1-O1
49	l	701	PLX	C2-O1-P1-O4
54	N	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CA2-OA2-PA1-OA5
54	r	504	CDL	CA3-OA5-PA1-OA2
54	r	504	CDL	CB2-OB2-PB2-OB5
54	u	201	CDL	CA2-OA2-PA1-OA5
54	u	201	CDL	CA3-OA5-PA1-OA2
54	u	201	CDL	CB3-OB5-PB2-OB2
48	r	501	PEE	C33-C34-C35-C36
54	i	401	CDL	CB2-C1-CA2-OA2
56	s	401	UQ	C12-C11-C9-C10
56	s	401	UQ	C13-C14-C16-C17
54	r	504	CDL	C78-C79-C80-C81
49	l	701	PLX	C2-C1-N1-C1C
54	r	503	CDL	C71-CB7-OB8-CB6
48	C	302	PEE	C15-C16-C17-C18
49	g	201	PLX	C11-C10-C9-C8
49	r	502	PLX	C27-C28-C29-C30
48	b	201	PEE	C11-C10-O2-C2
54	N	201	CDL	C51-CB5-OB6-CB4
48	j	201	PEE	C23-C24-C25-C26
49	C	303	PLX	C7-C8-C9-C10
49	j	202	PLX	C25-C26-C27-C28
49	j	202	PLX	C27-C28-C29-C30
54	a	201	CDL	C75-C76-C77-C78
54	a	201	CDL	C76-C77-C78-C79
54	i	401	CDL	C35-C36-C37-C38
54	r	504	CDL	C12-C13-C14-C15
49	g	201	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
49	l	701	PLX	C33-C34-C35-C36
54	r	503	CDL	C73-C74-C75-C76
48	b	201	PEE	O4-C10-O2-C2
54	N	201	CDL	OB7-CB5-OB6-CB4
48	b	201	PEE	C14-C15-C16-C17
49	C	303	PLX	C17-C18-C19-C20
49	r	502	PLX	C31-C32-C33-C34
54	i	401	CDL	C12-C13-C14-C15
54	r	503	CDL	C56-C57-C58-C59
48	C	302	PEE	C42-C43-C44-C45
49	j	202	PLX	C12-C13-C14-C15
49	j	202	PLX	C7-C8-C9-C10
54	r	504	CDL	C75-C76-C77-C78
54	r	503	CDL	O1-C1-CB2-OB2
54	r	504	CDL	O1-C1-CA2-OA2
48	C	302	PEE	C43-C44-C45-C46
48	b	201	PEE	C32-C33-C34-C35
49	l	701	PLX	C29-C30-C31-C32
54	r	503	CDL	C20-C21-C22-C23
54	r	503	CDL	C71-C72-C73-C74
54	r	504	CDL	C73-C74-C75-C76
54	N	201	CDL	C11-C12-C13-C14
54	a	201	CDL	C37-C38-C39-C40
54	r	503	CDL	C75-C76-C77-C78
49	j	202	PLX	C10-C11-C12-C13
54	r	504	CDL	C55-C56-C57-C58
48	m	201	PEE	C11-C12-C13-C14
49	g	201	PLX	C10-C11-C12-C13
49	g	201	PLX	C35-C36-C37-C38
54	a	201	CDL	C33-C34-C35-C36
54	r	503	CDL	C37-C38-C39-C40
54	r	504	CDL	C76-C77-C78-C79
54	a	201	CDL	OB9-CB7-OB8-CB6
50	X	201	8Q1	C7-C8-C9-C10
54	r	504	CDL	C52-C53-C54-C55
48	i	402	PEE	C22-C23-C24-C25
48	B	303	PEE	C39-C40-C41-C42
48	r	501	PEE	C19-C20-C21-C22
54	r	503	CDL	CB5-C51-C52-C53
48	B	303	PEE	C33-C34-C35-C36
48	b	201	PEE	C31-C32-C33-C34
49	l	701	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
54	r	504	CDL	C43-C44-C45-C46
48	j	201	PEE	C32-C33-C34-C35
48	l	702	PEE	C21-C22-C23-C24
48	m	201	PEE	C12-C13-C14-C15
49	g	201	PLX	C28-C29-C30-C31
54	i	401	CDL	C13-C14-C15-C16
54	r	503	CDL	C81-C82-C83-C84
54	r	503	CDL	OB9-CB7-OB8-CB6
49	l	701	PLX	C9-C10-C11-C12
54	i	401	CDL	C52-C53-C54-C55
54	r	504	CDL	C14-C15-C16-C17
54	r	504	CDL	C72-C73-C74-C75
48	b	201	PEE	C13-C14-C15-C16
49	l	701	PLX	C13-C14-C15-C16
54	r	504	CDL	C71-C72-C73-C74
49	C	303	PLX	C33-C34-C35-C36
54	i	401	CDL	C11-C12-C13-C14
48	i	402	PEE	O5-C30-O3-C3
49	j	202	PLX	C9-C10-C11-C12
49	r	502	PLX	C28-C29-C30-C31
54	a	201	CDL	C54-C55-C56-C57
54	r	503	CDL	CB3-CB4-CB6-OB8
49	C	303	PLX	C13-C14-C15-C16
49	l	701	PLX	C31-C32-C33-C34
54	i	401	CDL	C71-C72-C73-C74
54	r	504	CDL	C13-C14-C15-C16
49	r	502	PLX	C12-C13-C14-C15
54	u	201	CDL	C11-CA5-OA6-CA4
48	B	303	PEE	C23-C24-C25-C26
48	b	201	PEE	C22-C23-C24-C25
49	C	303	PLX	O7-C6-C7-C8
48	b	201	PEE	C33-C34-C35-C36
49	l	701	PLX	C11-C12-C13-C14
54	r	503	CDL	C42-C43-C44-C45
48	B	303	PEE	C15-C16-C17-C18
48	C	302	PEE	C39-C40-C41-C42
48	i	402	PEE	C19-C20-C21-C22
54	r	504	CDL	C80-C81-C82-C83
49	r	502	PLX	C33-C34-C35-C36
49	g	201	PLX	C9-C10-C11-C12
49	r	502	PLX	C14-C15-C16-C17
54	a	201	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C11-C12-C13-C14
54	r	504	CDL	C56-C57-C58-C59
54	r	504	CDL	C41-C42-C43-C44
49	l	701	PLX	C2-C1-N1-C1B
54	N	201	CDL	CB7-C71-C72-C73
49	l	701	PLX	C16-C17-C18-C19
48	B	303	PEE	C11-C10-O2-C2
48	j	201	PEE	C43-C44-C45-C46
48	i	402	PEE	C37-C38-C39-C40
48	l	702	PEE	C37-C38-C39-C40
48	i	402	PEE	C35-C36-C37-C38
54	r	503	CDL	OA7-CA5-OA6-CA4
54	u	201	CDL	OA7-CA5-OA6-CA4
48	B	303	PEE	C13-C14-C15-C16
48	m	201	PEE	C22-C23-C24-C25
54	r	504	CDL	CB7-C71-C72-C73
49	C	303	PLX	C27-C28-C29-C30
54	r	504	CDL	C60-C61-C62-C63
56	s	401	UQ	C14-C16-C17-C18
54	r	503	CDL	C51-C52-C53-C54
48	C	302	PEE	C11-C10-O2-C2
54	r	503	CDL	C11-CA5-OA6-CA4
54	a	201	CDL	OA5-CA3-CA4-OA6
48	r	501	PEE	C36-C37-C38-C39
54	r	503	CDL	C54-C55-C56-C57
54	r	504	CDL	C62-C63-C64-C65
54	r	503	CDL	OB6-CB4-CB6-OB8
48	l	702	PEE	C15-C16-C17-C18
48	l	702	PEE	C31-C32-C33-C34
49	l	701	PLX	C26-C27-C28-C29
54	r	503	CDL	C82-C83-C84-C85
48	j	201	PEE	C37-C38-C39-C40
54	r	504	CDL	C82-C83-C84-C85
48	B	303	PEE	O4-C10-O2-C2
48	C	302	PEE	O4-C10-O2-C2
48	j	201	PEE	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-C4'
54	i	401	CDL	CB3-OB5-PB2-OB2
54	u	201	CDL	CB2-OB2-PB2-OB5
49	r	502	PLX	C15-C16-C17-C18
50	G	201	8Q1	C12-C13-C14-C15
49	j	202	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C3'-C4'-C5'-O5'
48	l	702	PEE	O3P-C1-C2-C3
54	a	201	CDL	OA5-CA3-CA4-CA6
48	i	402	PEE	C14-C15-C16-C17
54	a	201	CDL	C14-C15-C16-C17
54	r	503	CDL	C58-C59-C60-C61
48	B	303	PEE	C34-C35-C36-C37
49	r	502	PLX	C13-C14-C15-C16
54	a	201	CDL	C72-C73-C74-C75
49	g	201	PLX	C30-C31-C32-C33
48	b	201	PEE	C1-C2-C3-O3
48	j	201	PEE	C44-C45-C46-C47
48	r	501	PEE	C1-C2-C3-O3
54	i	401	CDL	CB3-CB4-CB6-OB8
54	i	401	CDL	C73-C74-C75-C76
54	r	504	CDL	CA3-CA4-CA6-OA8
49	C	303	PLX	C31-C32-C33-C34
49	C	303	PLX	C36-C37-C38-C39
54	u	201	CDL	C57-C58-C59-C60
54	r	504	CDL	CB5-C51-C52-C53
49	j	202	PLX	C26-C27-C28-C29
48	B	303	PEE	C22-C23-C24-C25
49	g	201	PLX	C32-C33-C34-C35
54	i	401	CDL	C39-C40-C41-C42
48	B	303	PEE	C35-C36-C37-C38
48	r	501	PEE	C35-C36-C37-C38
54	i	401	CDL	C33-C34-C35-C36
54	i	401	CDL	C11-CA5-OA6-CA4
54	i	401	CDL	CB5-C51-C52-C53
48	j	201	PEE	C31-C30-O3-C3
54	a	201	CDL	C24-C25-C26-C27
54	r	503	CDL	C76-C77-C78-C79
54	N	201	CDL	CA6-CA4-OA6-CA5
54	u	201	CDL	CA6-CA4-OA6-CA5
49	j	202	PLX	C34-C35-C36-C37
48	C	302	PEE	C13-C14-C15-C16
49	l	701	PLX	C28-C29-C30-C31
50	X	201	8Q1	C9-C10-C11-C12
54	r	503	CDL	C78-C79-C80-C81
48	b	201	PEE	C17-C18-C19-C20
49	r	502	PLX	C10-C11-C12-C13
54	a	201	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	C32-C33-C34-C35
49	C	303	PLX	O4-C3-C4-C5
54	N	201	CDL	OA5-CA3-CA4-CA6
54	i	401	CDL	OA5-CA3-CA4-CA6
54	r	503	CDL	OA5-CA3-CA4-CA6
54	r	504	CDL	C35-C36-C37-C38
49	l	701	PLX	C25-C26-C27-C28
48	j	201	PEE	O5-C30-O3-C3
49	j	202	PLX	C13-C14-C15-C16
54	r	503	CDL	C11-C12-C13-C14
48	l	702	PEE	C13-C14-C15-C16
49	C	303	PLX	C30-C31-C32-C33
49	l	701	PLX	C30-C31-C32-C33
54	i	401	CDL	C15-C16-C17-C18
48	B	303	PEE	C20-C21-C22-C23
48	i	402	PEE	C20-C21-C22-C23
49	j	202	PLX	C3-C4-C5-O8
54	u	201	CDL	CA3-CA4-CA6-OA8
48	j	201	PEE	C30-C31-C32-C33
48	B	303	PEE	C17-C18-C19-C20
50	X	201	8Q1	C29-C32-C34-N36
49	j	202	PLX	C30-C31-C32-C33
54	r	503	CDL	CA7-C31-C32-C33
47	A	503	NAI	C2D-C1D-N1N-C2N
48	r	501	PEE	C24-C25-C26-C27
54	r	503	CDL	C35-C36-C37-C38
54	u	201	CDL	C53-C54-C55-C56
48	B	303	PEE	O3P-C1-C2-O2
48	C	302	PEE	C31-C30-O3-C3
54	i	401	CDL	CB7-C71-C72-C73
48	m	201	PEE	C31-C32-C33-C34
54	a	201	CDL	C58-C59-C60-C61
48	b	201	PEE	O2-C2-C3-O3
48	i	402	PEE	O2-C2-C3-O3
54	r	503	CDL	C21-C22-C23-C24
49	r	502	PLX	C25-C26-C27-C28
54	r	503	CDL	C33-C34-C35-C36
54	i	401	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C14-C15-C16-C17
48	b	201	PEE	C23-C24-C25-C26
49	l	701	PLX	C7-C8-C9-C10
54	a	201	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C25-C26-C27-C28
48	B	303	PEE	C31-C32-C33-C34
54	r	504	CDL	C59-C60-C61-C62
49	C	303	PLX	C11-C10-C9-C8
50	X	201	8Q1	O4-C1-S44-C43
54	r	503	CDL	C23-C24-C25-C26
54	u	201	CDL	CB7-C71-C72-C73
54	r	504	CDL	C64-C65-C66-C67
54	N	201	CDL	OB5-CB3-CB4-CB6
54	r	503	CDL	C84-C85-C86-C87
48	j	201	PEE	C38-C39-C40-C41
48	j	201	PEE	C15-C16-C17-C18
49	g	201	PLX	C25-C26-C27-C28
50	X	201	8Q1	O33-C32-C34-N36
54	r	504	CDL	C31-C32-C33-C34
54	r	504	CDL	C33-C34-C35-C36
54	r	503	CDL	C60-C61-C62-C63
48	m	201	PEE	C3-C2-O2-C10
50	X	201	8Q1	C6-C1-S44-C43
48	j	201	PEE	C34-C35-C36-C37
49	j	202	PLX	C31-C32-C33-C34
54	u	201	CDL	C77-C78-C79-C80
48	m	201	PEE	C14-C15-C16-C17
48	i	402	PEE	C1-C2-C3-O3
49	j	202	PLX	C7-C6-O6-C4
49	l	701	PLX	C3-C4-C5-O8
54	u	201	CDL	C22-C23-C24-C25
49	g	201	PLX	O4-C3-C4-O6
54	i	401	CDL	OA5-CA3-CA4-OA6
49	r	502	PLX	C20-C21-C22-C23
54	N	201	CDL	C71-CB7-OB8-CB6
54	r	504	CDL	C32-C33-C34-C35
54	i	401	CDL	C75-C76-C77-C78
49	j	202	PLX	O6-C4-C5-O8
49	l	701	PLX	O6-C4-C5-O8
48	C	302	PEE	O5-C30-O3-C3
54	a	201	CDL	C55-C56-C57-C58
48	m	201	PEE	C23-C24-C25-C26
49	C	303	PLX	C9-C10-C11-C12
49	r	502	PLX	C2-O1-P1-O4
54	r	503	CDL	C55-C56-C57-C58
54	N	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
49	C	303	PLX	C2-O1-P1-O3
49	l	701	PLX	C2-O1-P1-O2
49	l	701	PLX	C2-O1-P1-O3
49	r	502	PLX	C2-O1-P1-O3
54	N	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB3
54	r	503	CDL	CA3-OA5-PA1-OA4
54	r	504	CDL	CA2-OA2-PA1-OA3
54	r	504	CDL	CB2-OB2-PB2-OB3
54	r	504	CDL	CB2-OB2-PB2-OB4
54	u	201	CDL	CA2-OA2-PA1-OA4
54	u	201	CDL	CA3-OA5-PA1-OA3
54	u	201	CDL	CB2-OB2-PB2-OB4
54	u	201	CDL	CB3-OB5-PB2-OB4
57	w	401	ADP	C5'-O5'-PA-O1A
54	i	401	CDL	CA5-C11-C12-C13
49	g	201	PLX	O4-C3-C4-C5
49	j	202	PLX	O4-C3-C4-C5
54	u	201	CDL	C71-C72-C73-C74
48	C	302	PEE	C37-C38-C39-C40
46	A	502	FMN	C1'-C2'-C3'-O3'
49	g	201	PLX	C25-C24-O8-C5
49	j	202	PLX	C25-C24-O8-C5
49	l	701	PLX	C24-C25-C26-C27
48	l	702	PEE	C32-C33-C34-C35
54	r	504	CDL	C37-C38-C39-C40
49	C	303	PLX	C15-C16-C17-C18
54	a	201	CDL	C11-C12-C13-C14
54	r	504	CDL	CB2-C1-CA2-OA2
48	m	201	PEE	C21-C22-C23-C24
54	r	504	CDL	C40-C41-C42-C43
48	b	201	PEE	O3P-C1-C2-O2
48	r	501	PEE	O3P-C1-C2-O2
49	j	202	PLX	O4-C3-C4-O6
54	N	201	CDL	OB5-CB3-CB4-OB6
48	r	501	PEE	C16-C17-C18-C19
48	C	302	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	C20-C21-C22-C23
54	r	503	CDL	C17-C18-C19-C20
48	C	302	PEE	C1-C2-C3-O3
49	C	303	PLX	N1-C1-C2-O1
48	C	302	PEE	O2-C2-C3-O3
49	r	502	PLX	O6-C4-C5-O8
54	u	201	CDL	OA6-CA4-CA6-OA8
48	b	201	PEE	C18-C19-C20-C21
54	r	504	CDL	C39-C40-C41-C42
48	b	201	PEE	C11-C12-C13-C14
48	b	201	PEE	C30-C31-C32-C33
49	r	502	PLX	C7-C8-C9-C10
49	l	701	PLX	O8-C24-C25-C26
47	A	503	NAI	O4D-C1D-N1N-C2N
48	r	501	PEE	C12-C13-C14-C15
54	a	201	CDL	C60-C61-C62-C63
54	r	504	CDL	C15-C16-C17-C18
54	r	503	CDL	C61-C62-C63-C64
47	A	503	NAI	C2D-C1D-N1N-C6N
48	i	402	PEE	C34-C35-C36-C37
54	a	201	CDL	C35-C36-C37-C38
48	B	303	PEE	O3P-C1-C2-C3
48	b	201	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
48	j	201	PEE	C41-C42-C43-C44
50	G	201	8Q1	C11-C10-C9-C8
50	X	201	8Q1	C28-O27-P24-O3
48	j	201	PEE	C12-C13-C14-C15
48	m	201	PEE	O3-C30-C31-C32
54	N	201	CDL	C52-C53-C54-C55
48	C	302	PEE	C18-C19-C20-C21
48	m	201	PEE	C18-C19-C20-C21
50	G	201	8Q1	C11-C12-C13-C14
48	r	501	PEE	O2-C2-C3-O3
48	C	302	PEE	C4-O4P-P-O3P
49	g	201	PLX	C3-O4-P1-O1
49	l	701	PLX	C3-O4-P1-O1
54	r	503	CDL	CA2-OA2-PA1-OA5
54	r	503	CDL	CB3-OB5-PB2-OB2
54	r	504	CDL	CB3-OB5-PB2-OB2
54	r	504	CDL	CA5-C11-C12-C13
49	g	201	PLX	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
48	m	201	PEE	C24-C25-C26-C27
49	r	502	PLX	C16-C17-C18-C19
49	C	303	PLX	C19-C20-C21-C22
54	N	201	CDL	C31-C32-C33-C34
54	r	504	CDL	C74-C75-C76-C77
54	r	504	CDL	C1-CB2-OB2-PB2
48	C	302	PEE	C16-C17-C18-C19
48	b	201	PEE	C38-C39-C40-C41
48	r	501	PEE	C31-C30-O3-C3
54	r	504	CDL	C84-C85-C86-C87
54	a	201	CDL	C36-C37-C38-C39
48	b	201	PEE	C16-C17-C18-C19
54	a	201	CDL	OB5-CB3-CB4-CB6
54	u	201	CDL	OA5-CA3-CA4-OA6
48	B	303	PEE	C42-C43-C44-C45
54	a	201	CDL	C74-C75-C76-C77
49	j	202	PLX	C32-C33-C34-C35
48	r	501	PEE	O5-C30-O3-C3
54	r	503	CDL	C36-C37-C38-C39
54	r	504	CDL	C57-C58-C59-C60
49	r	502	PLX	O8-C24-C25-C26
48	C	302	PEE	C38-C39-C40-C41
48	j	201	PEE	C19-C20-C21-C22
48	i	402	PEE	C21-C22-C23-C24
49	l	701	PLX	C36-C37-C38-C39
49	C	303	PLX	C18-C19-C20-C21
56	s	401	UQ	C9-C11-C12-C13
48	i	402	PEE	C31-C32-C33-C34
48	m	201	PEE	C16-C17-C18-C19
54	r	504	CDL	C23-C24-C25-C26
48	j	201	PEE	C21-C22-C23-C24
49	l	701	PLX	C5-C4-O6-C6
49	j	202	PLX	C19-C20-C21-C22
54	N	201	CDL	C72-C73-C74-C75
48	r	501	PEE	C11-C12-C13-C14
48	B	303	PEE	C14-C15-C16-C17
54	r	504	CDL	C44-C45-C46-C47
54	a	201	CDL	OB7-CB5-OB6-CB4
54	i	401	CDL	C36-C37-C38-C39
51	J	401	NDP	O4D-C1D-N1N-C6N
54	r	503	CDL	CA2-C1-CB2-OB2
48	C	302	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C7-C8-C9-C10
48	i	402	PEE	C2-C1-O3P-P
48	i	402	PEE	C16-C17-C18-C19
49	r	502	PLX	C3-C4-C5-O8
51	J	401	NDP	O4B-C4B-C5B-O5B
47	A	503	NAI	O4D-C1D-N1N-C6N
48	B	303	PEE	C40-C41-C42-C43
49	j	202	PLX	C33-C34-C35-C36
48	r	501	PEE	C22-C23-C24-C25
49	j	202	PLX	O6-C6-C7-C8
49	j	202	PLX	O8-C24-C25-C26
54	r	503	CDL	C12-C11-CA5-OA6
46	A	502	FMN	O2'-C2'-C3'-O3'
49	l	701	PLX	C10-C11-C12-C13
46	A	502	FMN	C5'-O5'-P-O2P
50	X	201	8Q1	C28-O27-P24-O1
54	r	503	CDL	CA3-OA5-PA1-OA2
48	B	303	PEE	O5-C30-O3-C3
48	b	201	PEE	C15-C16-C17-C18
48	C	302	PEE	C36-C37-C38-C39
48	i	402	PEE	C38-C39-C40-C41
48	m	201	PEE	C33-C34-C35-C36
54	r	504	CDL	C20-C21-C22-C23
48	j	201	PEE	O2-C10-C11-C12
48	B	303	PEE	C31-C30-O3-C3
49	C	303	PLX	C12-C13-C14-C15
48	l	702	PEE	C16-C17-C18-C19
48	l	702	PEE	C1-C2-C3-O3
54	u	201	CDL	C17-C18-C19-C20
54	u	201	CDL	C55-C56-C57-C58
48	C	302	PEE	O3-C30-C31-C32
54	r	504	CDL	C52-C51-CB5-OB6
49	r	502	PLX	C35-C36-C37-C38
54	N	201	CDL	C12-C13-C14-C15
54	r	503	CDL	C79-C80-C81-C82
48	B	303	PEE	C18-C19-C20-C21
48	i	402	PEE	C36-C37-C38-C39
54	i	401	CDL	OA6-CA4-CA6-OA8
48	l	702	PEE	C36-C37-C38-C39
54	u	201	CDL	C12-C11-CA5-OA6
48	B	303	PEE	C41-C42-C43-C44
48	l	702	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
54	N	201	CDL	C72-C71-CB7-OB8
54	r	504	CDL	C42-C43-C44-C45
48	C	302	PEE	C32-C33-C34-C35
48	j	201	PEE	C16-C17-C18-C19
54	r	503	CDL	C74-C75-C76-C77
54	a	201	CDL	C51-CB5-OB6-CB4
48	r	501	PEE	C23-C24-C25-C26
54	i	401	CDL	CA3-CA4-CA6-OA8
49	C	303	PLX	C2-O1-P1-O4
54	r	504	CDL	CA2-OA2-PA1-OA5
54	r	503	CDL	C12-C11-CA5-OA7
48	j	201	PEE	O4-C10-C11-C12
54	r	504	CDL	C52-C51-CB5-OB7
49	j	202	PLX	C18-C19-C20-C21
54	u	201	CDL	C54-C55-C56-C57
47	A	503	NAI	C2N-C3N-C7N-N7N
48	b	201	PEE	C1-O3P-P-O1P
48	i	402	PEE	C1-O3P-P-O1P
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C2-O1-P1-O2
51	J	401	NDP	C5B-O5B-PA-O1A
54	r	503	CDL	CA2-OA2-PA1-OA3
54	r	504	CDL	CB3-OB5-PB2-OB3
54	a	201	CDL	C13-C14-C15-C16
48	C	302	PEE	C44-C45-C46-C47
48	C	302	PEE	O5-C30-C31-C32
49	g	201	PLX	C1-C2-O1-P1
54	N	201	CDL	C72-C71-CB7-OB9
54	u	201	CDL	C12-C11-CA5-OA7
54	r	504	CDL	C17-C18-C19-C20
48	b	201	PEE	C2-C3-O3-C30
54	u	201	CDL	C52-C51-CB5-OB6
49	g	201	PLX	C29-C30-C31-C32
54	r	503	CDL	C52-C53-C54-C55
54	a	201	CDL	CA4-CA3-OA5-PA1
48	m	201	PEE	C20-C21-C22-C23
48	r	501	PEE	C42-C43-C44-C45
54	r	504	CDL	C12-C11-CA5-OA6
54	r	504	CDL	C72-C71-CB7-OB8
48	r	501	PEE	C44-C45-C46-C47
54	i	401	CDL	C53-C54-C55-C56
46	A	502	FMN	O4'-C4'-C5'-O5'

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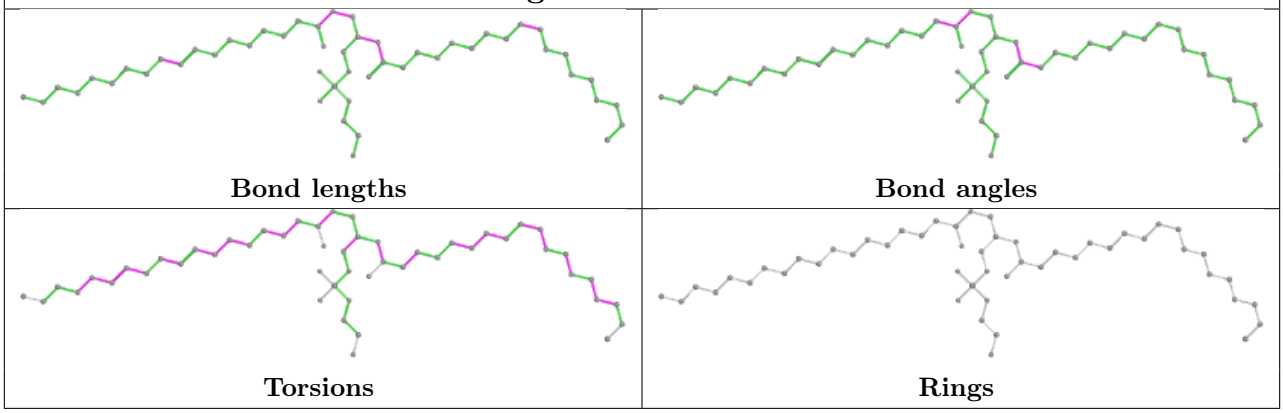
Mol	Chain	Res	Type	Atoms
48	b	201	PEE	O3-C30-C31-C32
49	l	701	PLX	C35-C36-C37-C38
49	r	502	PLX	C18-C19-C20-C21

There are no ring outliers.

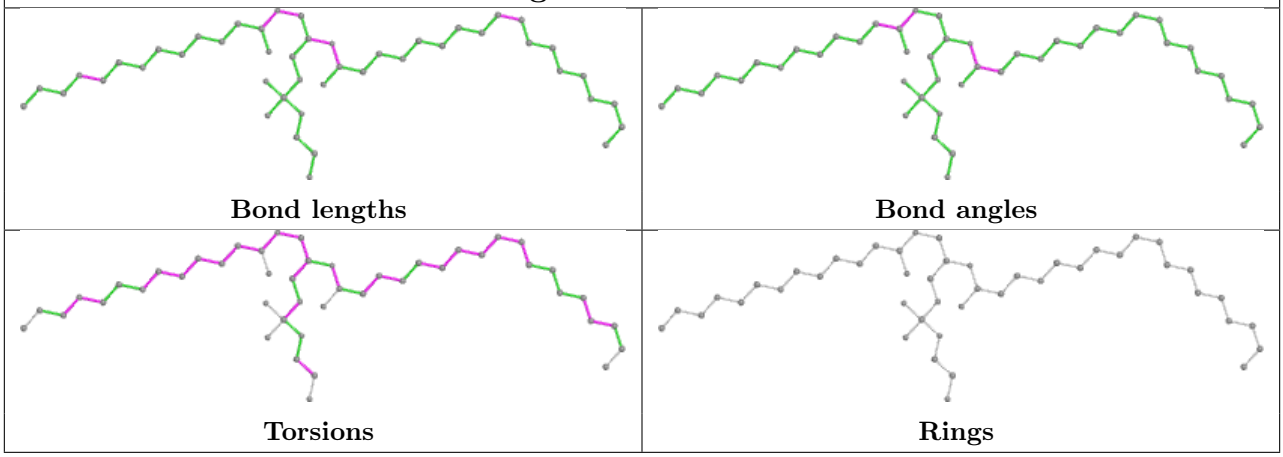
No monomer is involved in short contacts.

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.

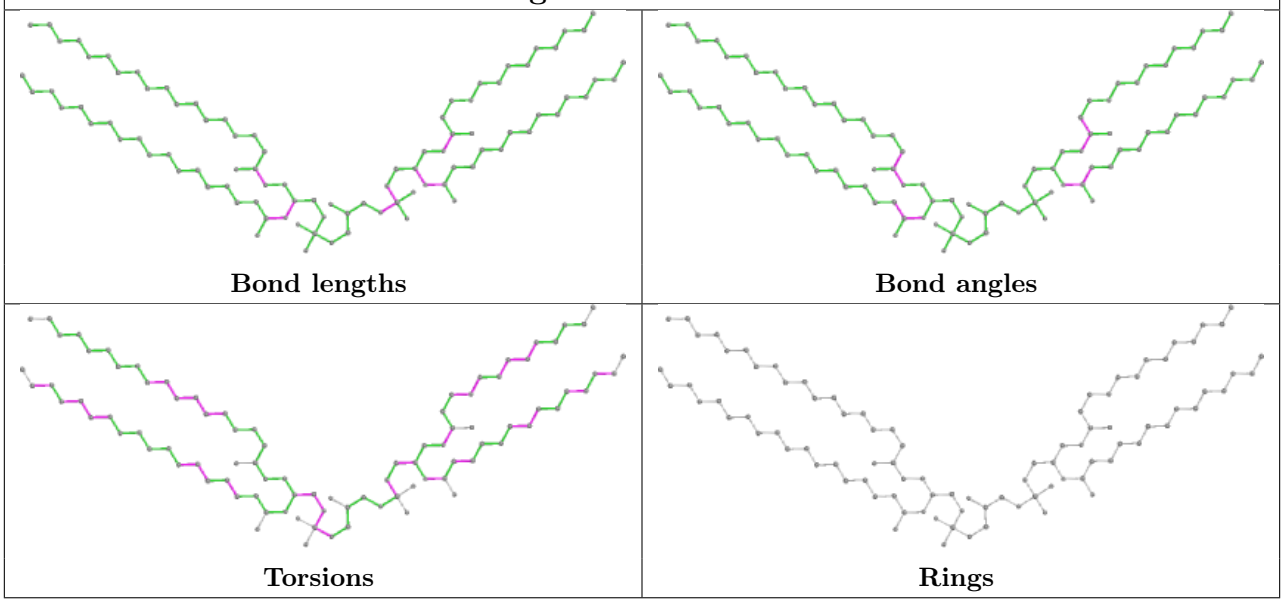
Ligand PEE B 303



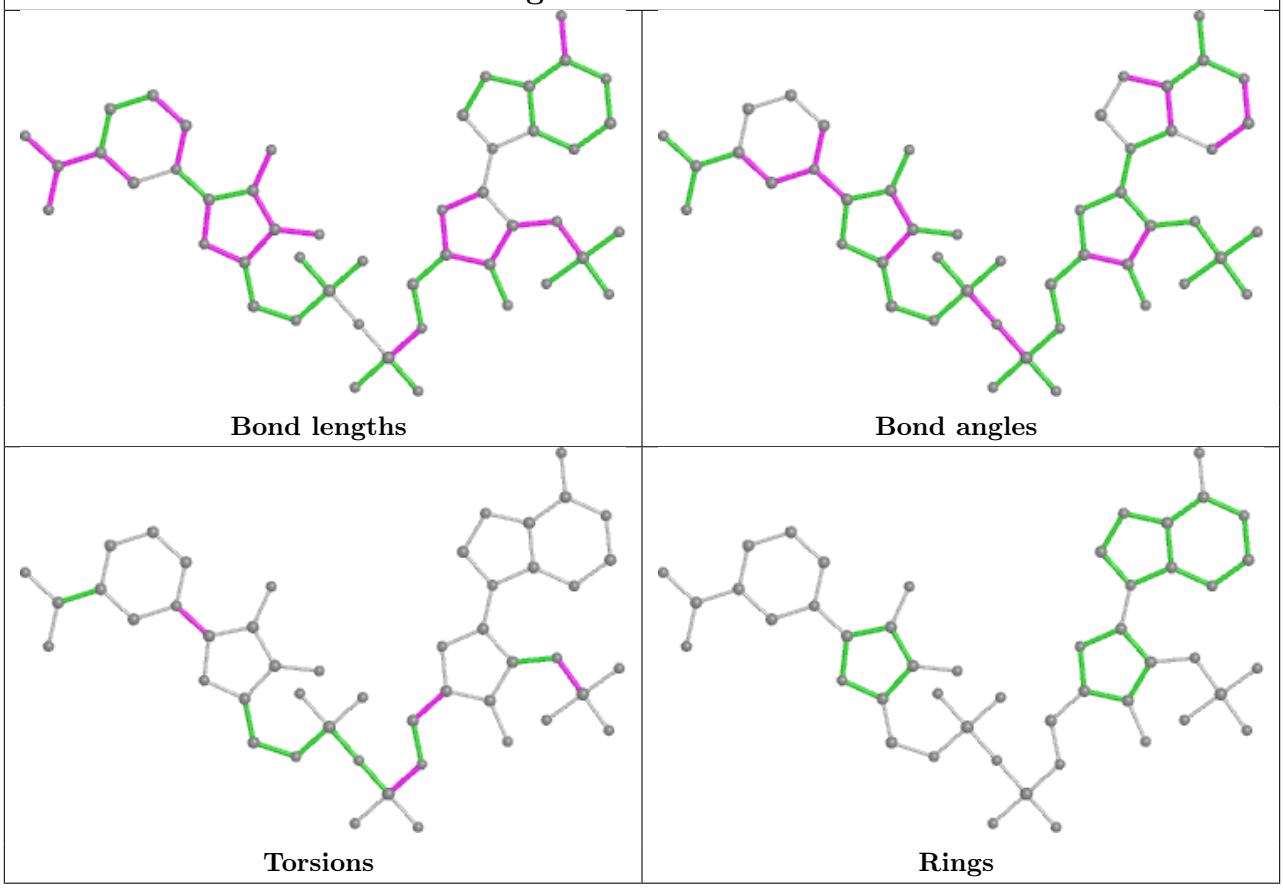
Ligand PEE b 201

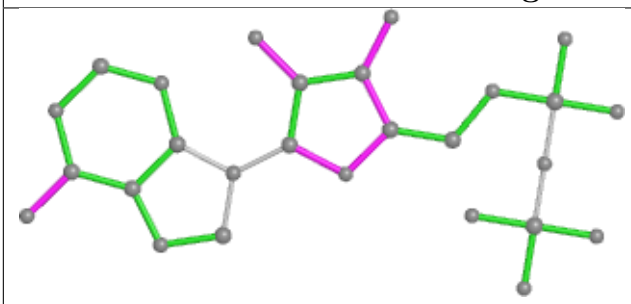
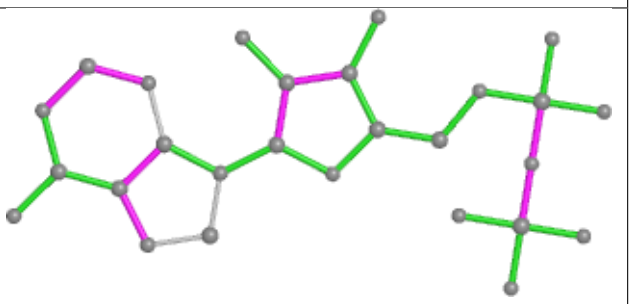
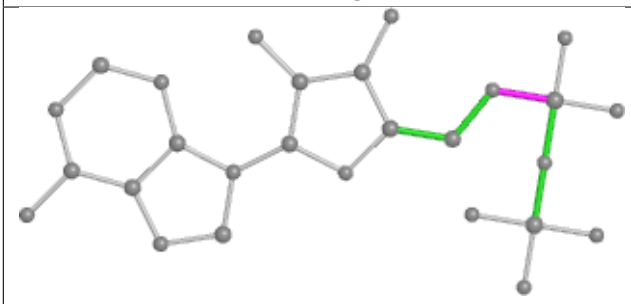
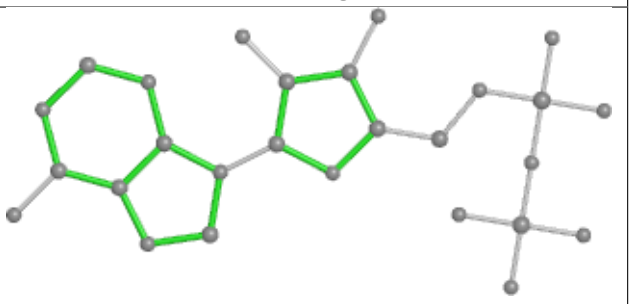


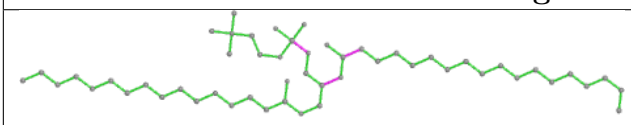
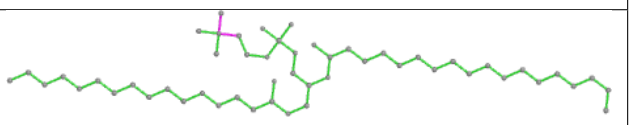
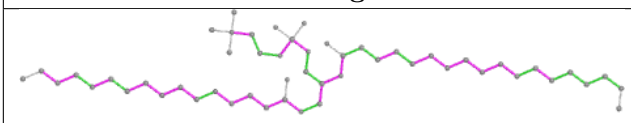
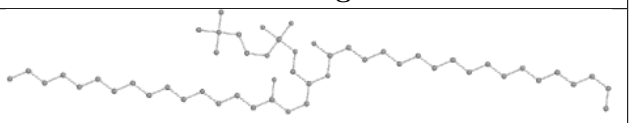
Ligand CDL a 201

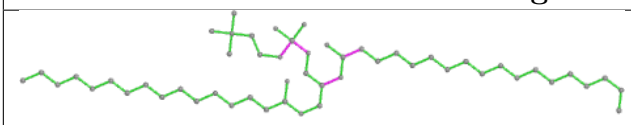
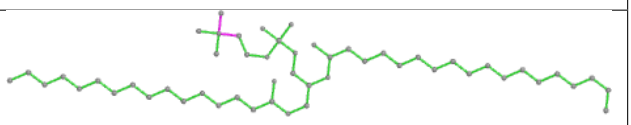
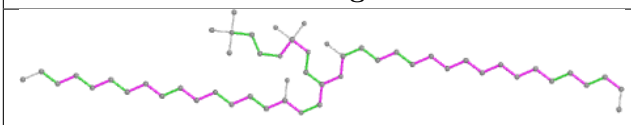
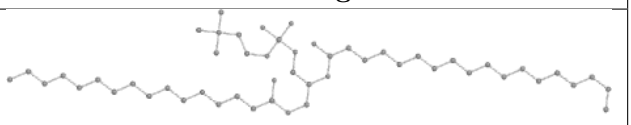


Ligand NDP J 401



Ligand ADP w 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX l 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX r 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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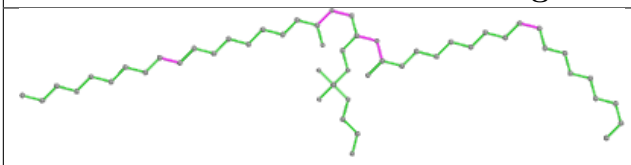
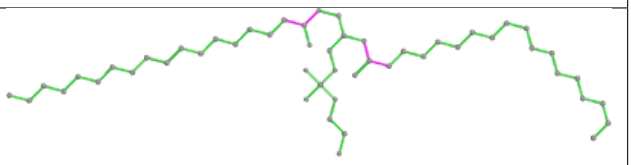
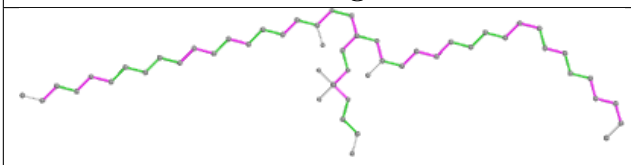
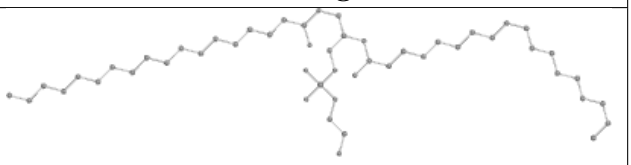
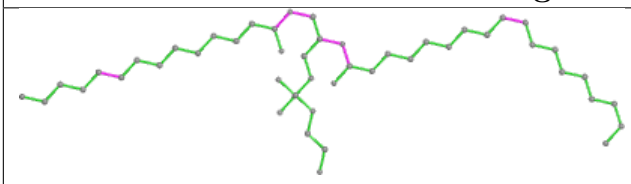
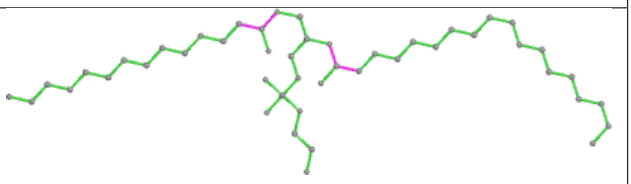
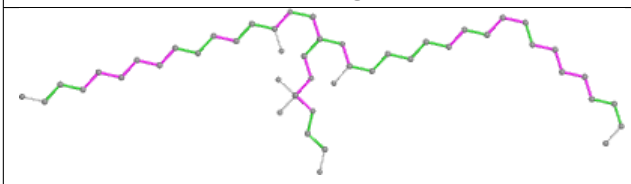
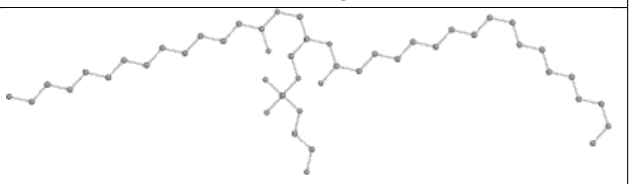
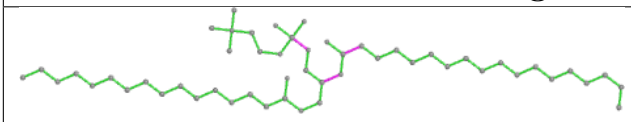
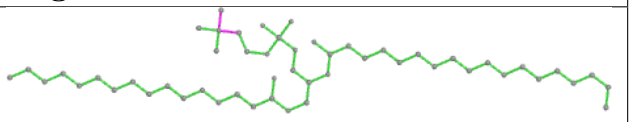
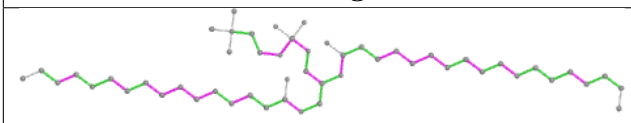
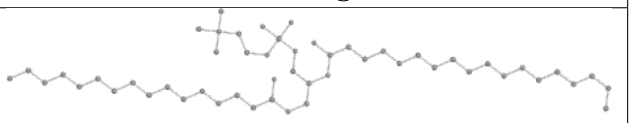
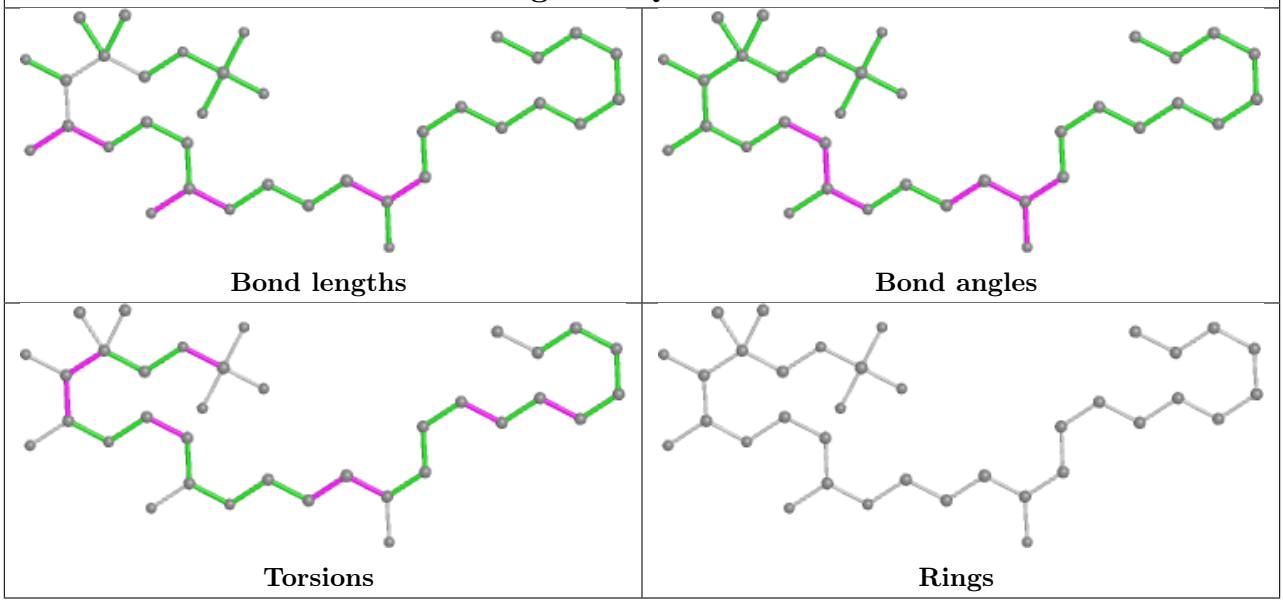
 Bond lengths	 Bond angles
 Torsions	 Rings

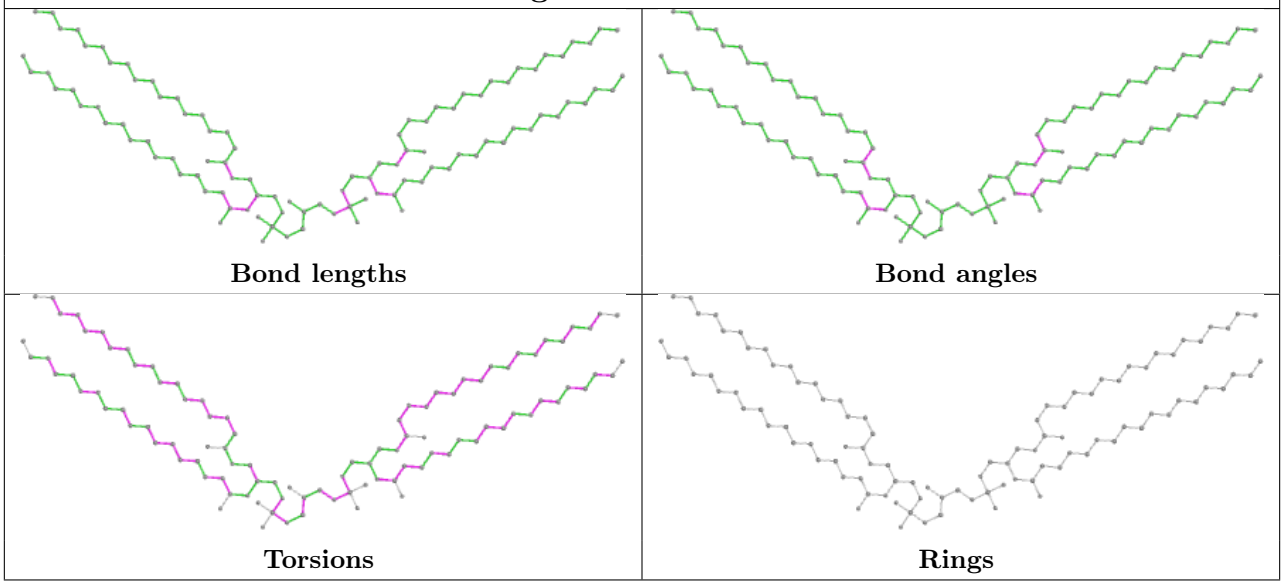
Ligand PEE i 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX g 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

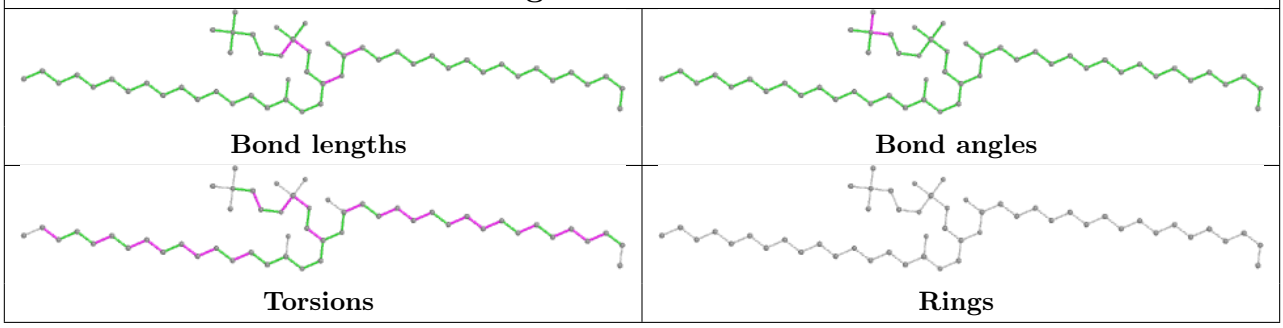
Ligand 8Q1 X 201



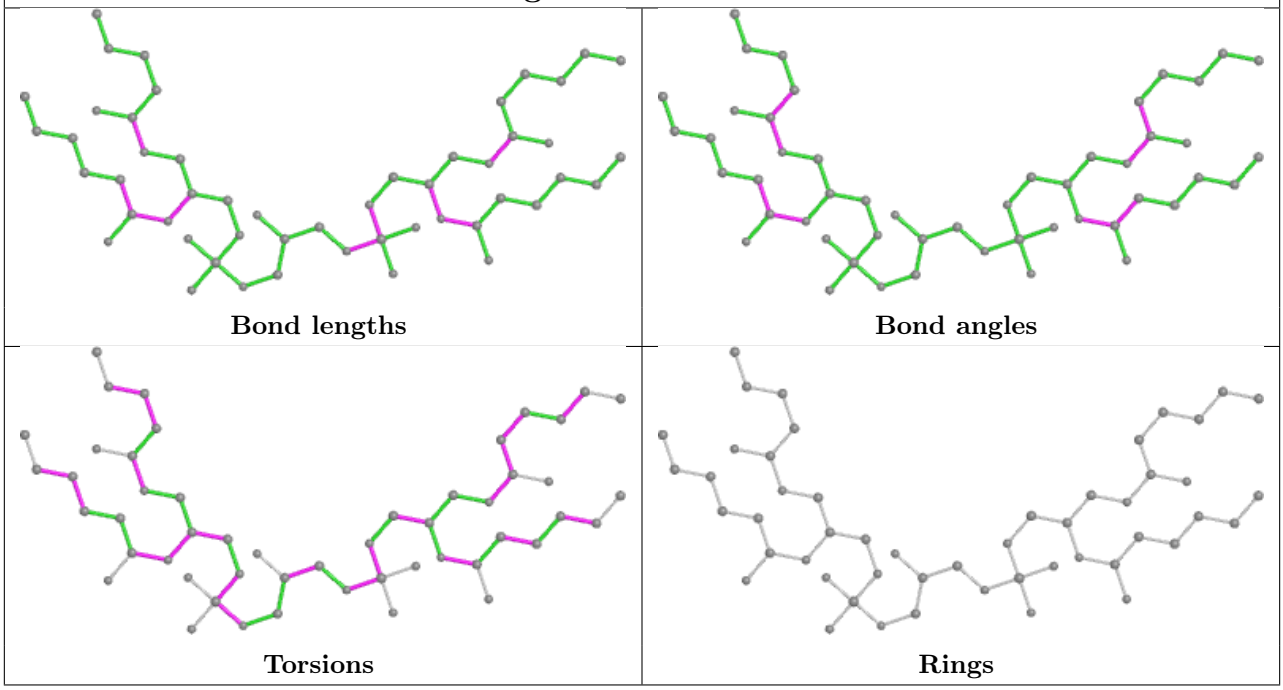
Ligand CDL r 504



Ligand PLX C 303



Ligand CDL N 201



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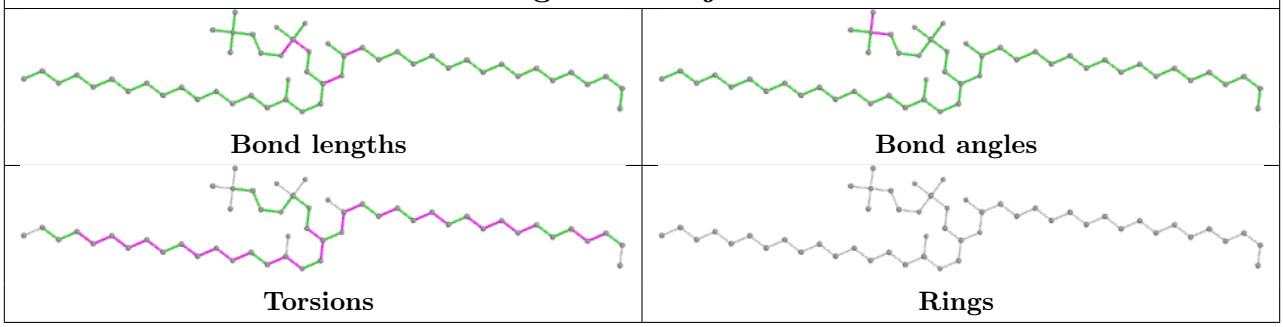
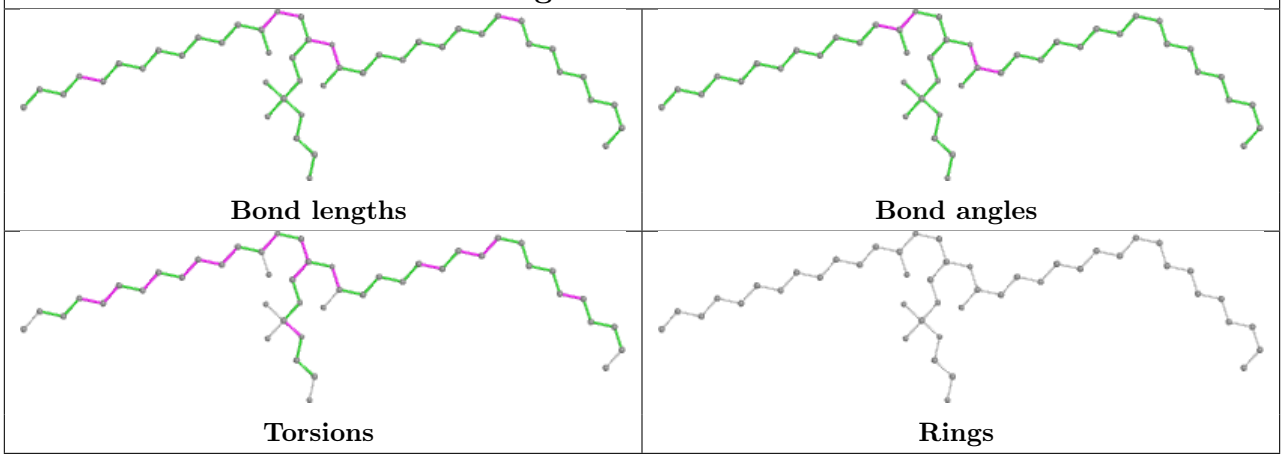


Ligand PEE l 702



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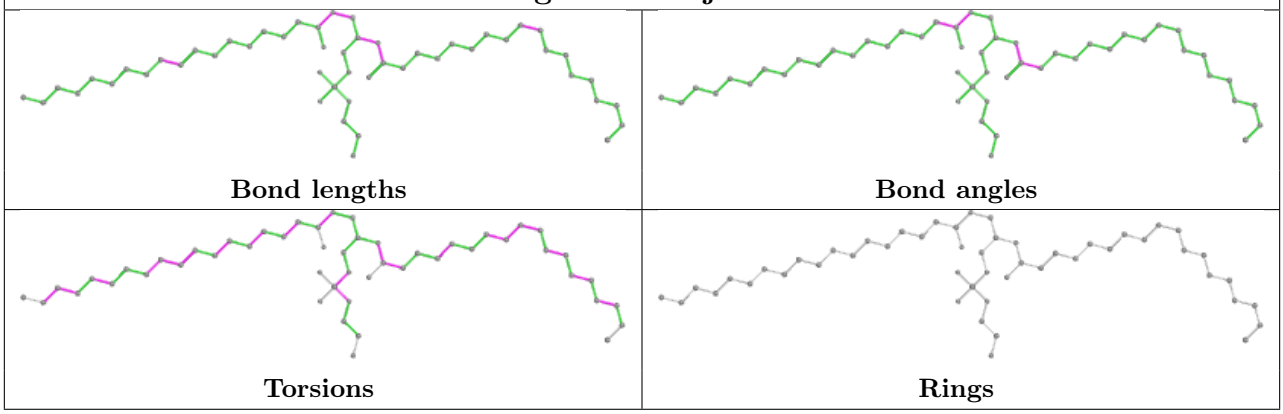
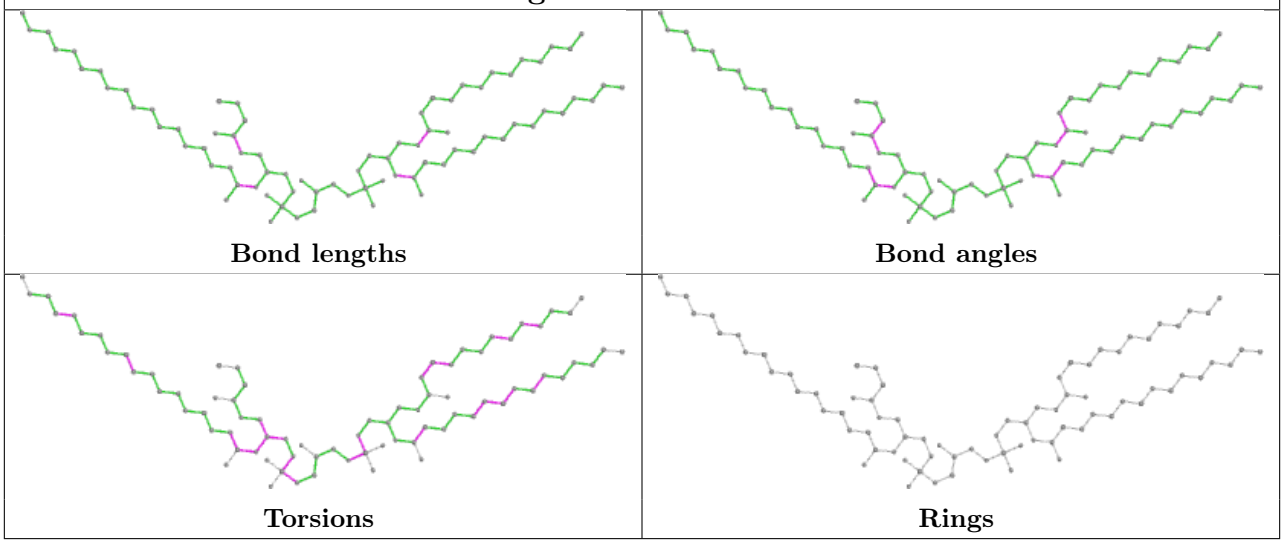
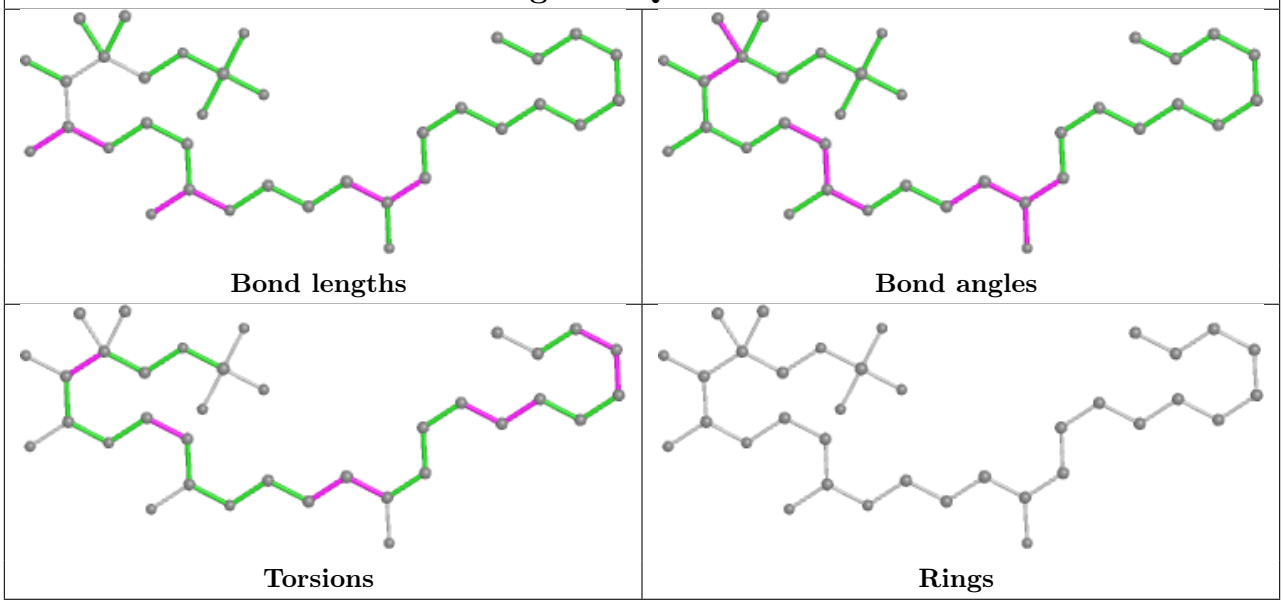


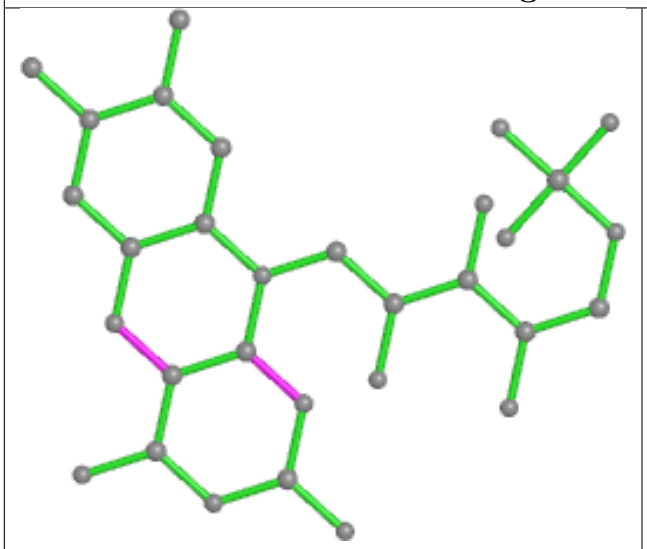
Ligand CDL u 201



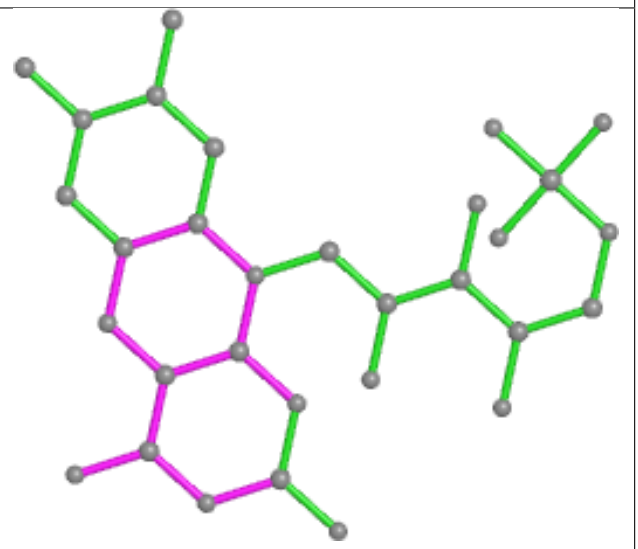
Ligand 8Q1 G 201



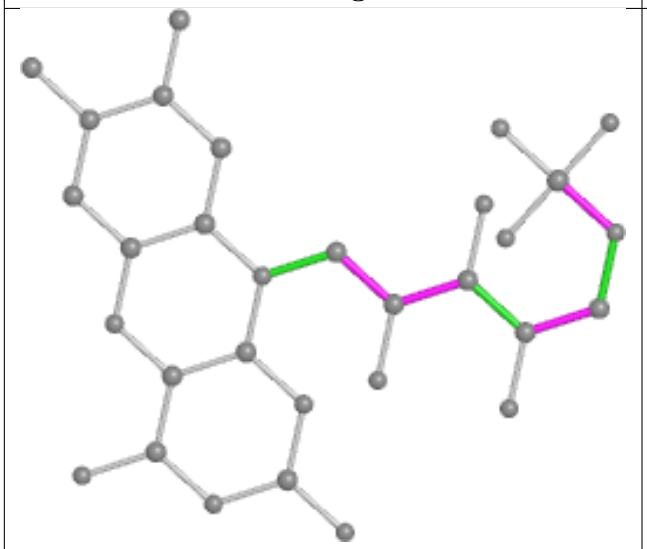
Ligand FMN A 502



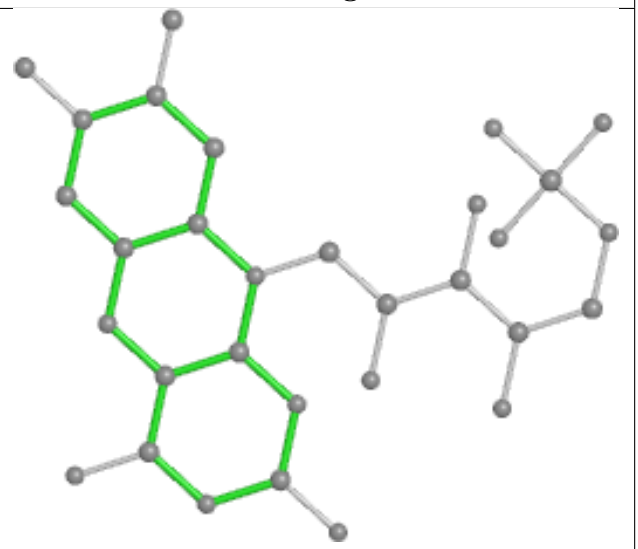
Bond lengths



Bond angles

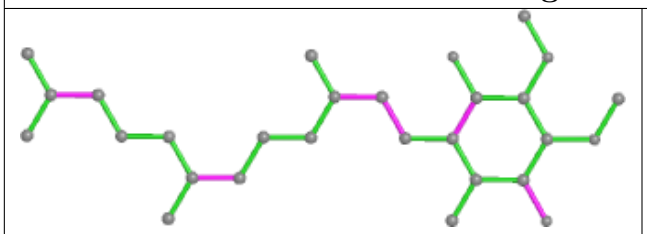


Torsions

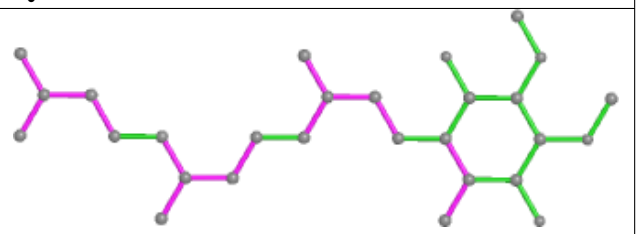


Rings

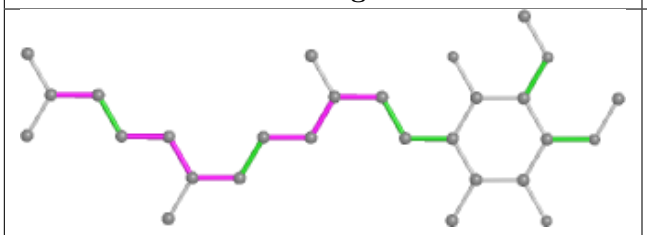
Ligand UQ s 401



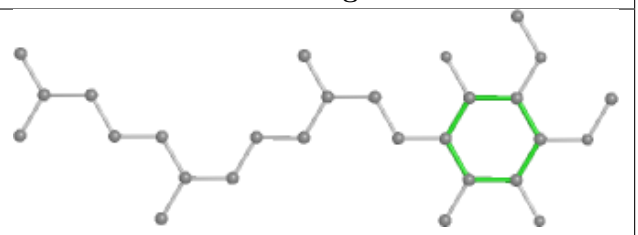
Bond lengths



Bond angles

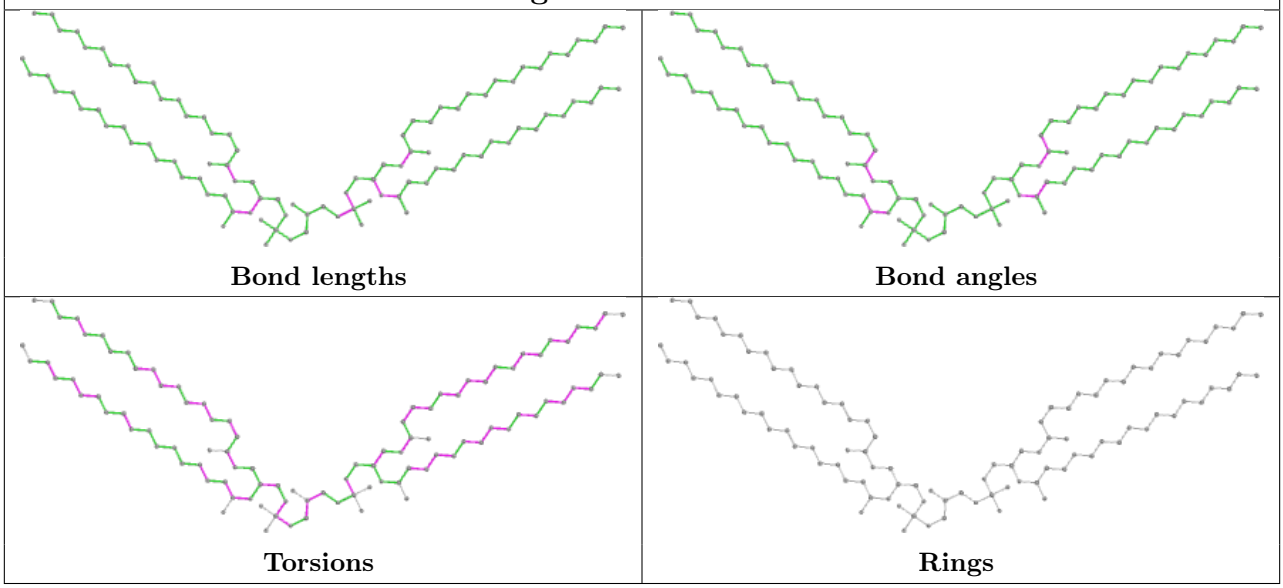


Torsions

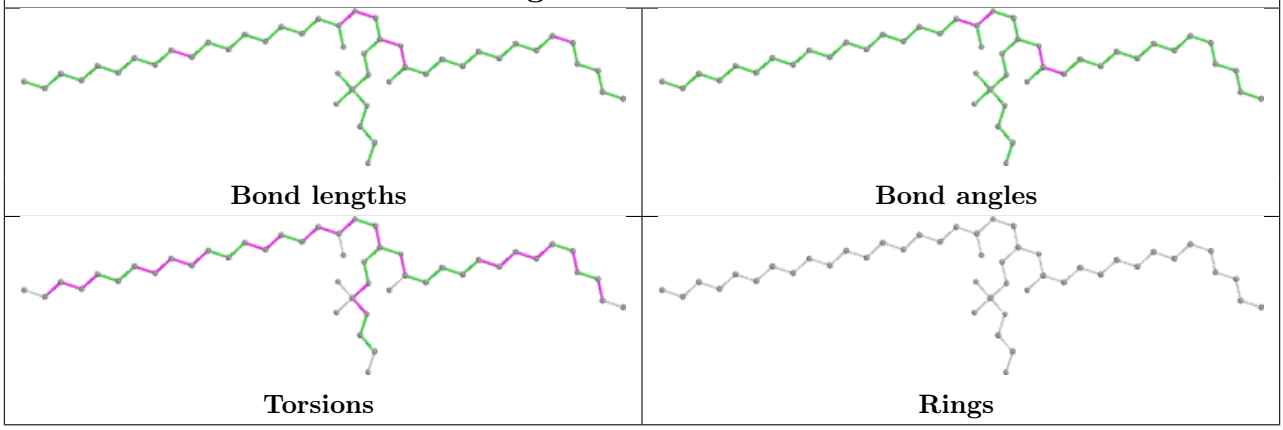


Rings

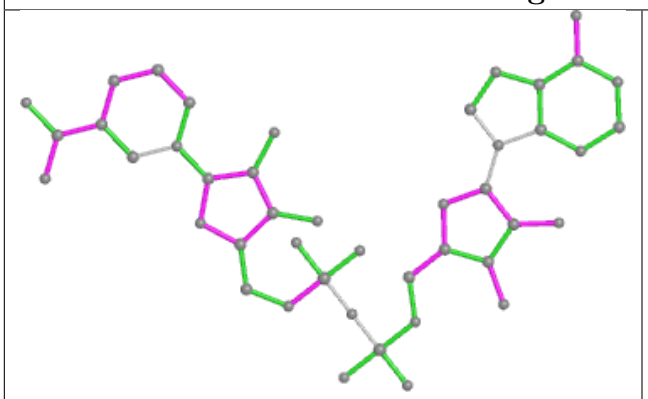
Ligand CDL r 503



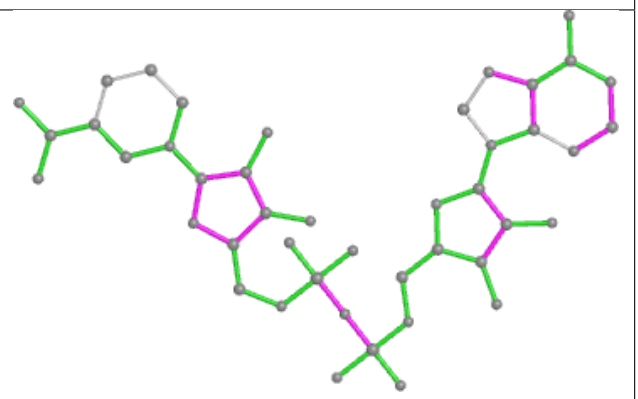
Ligand PEE C 302



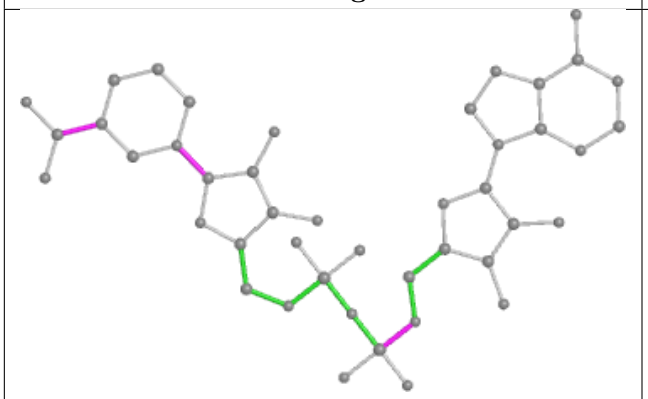
Ligand NAI A 503



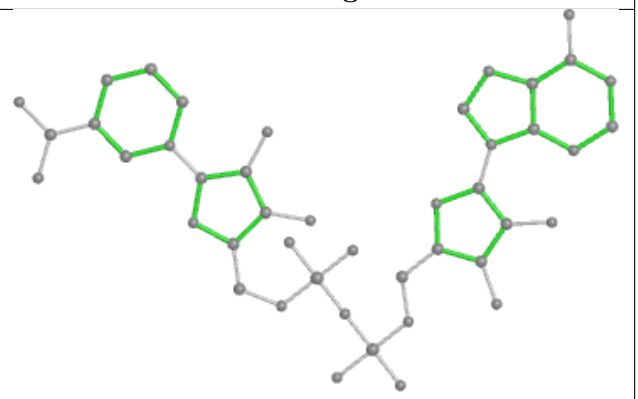
Bond lengths



Bond angles

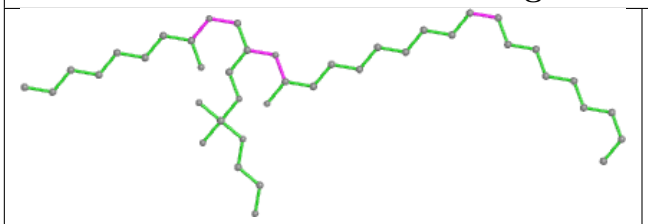


Torsions

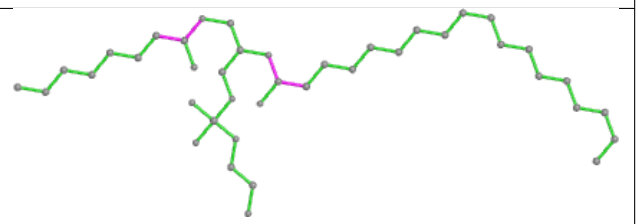


Rings

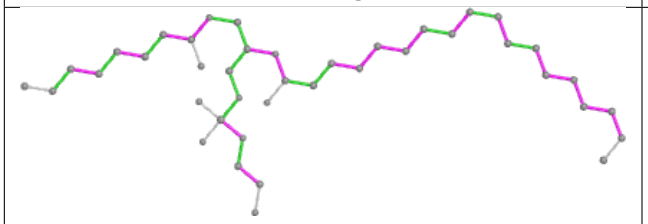
Ligand PEE m 201



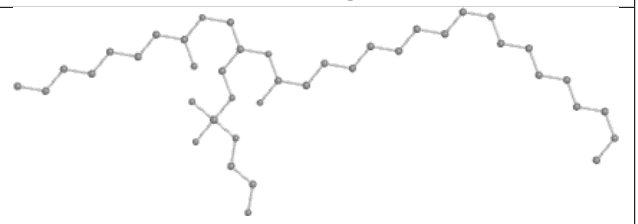
Bond lengths



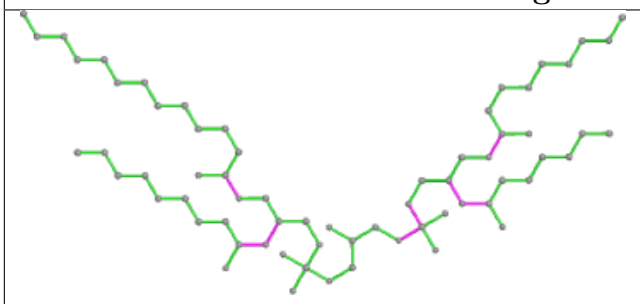
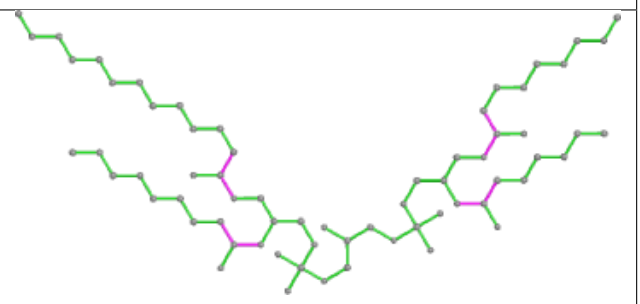
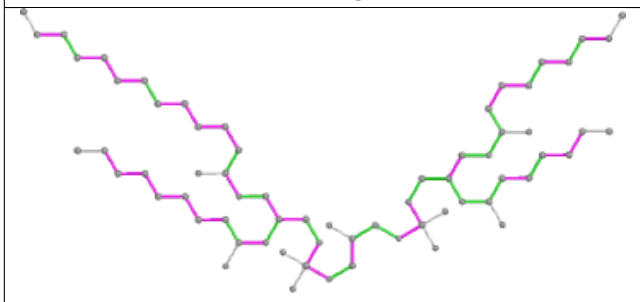
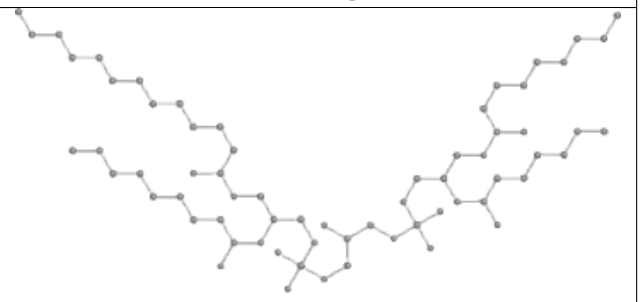
Bond angles



Torsions



Rings

Ligand CDL i 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

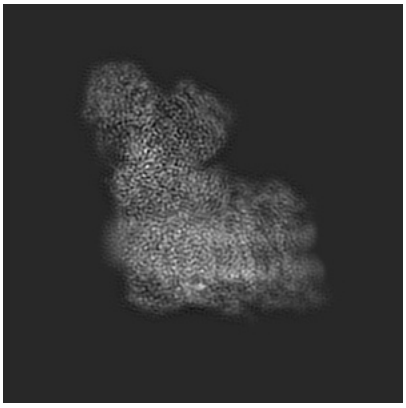
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32269. These allow visual inspection of the internal detail of the map and identification of artifacts.

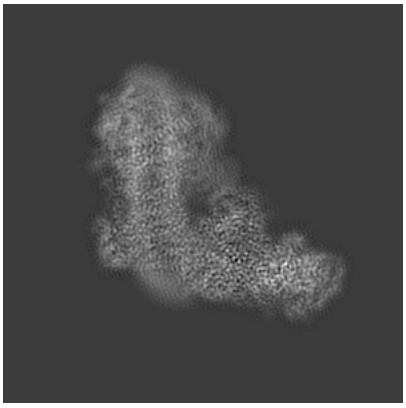
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

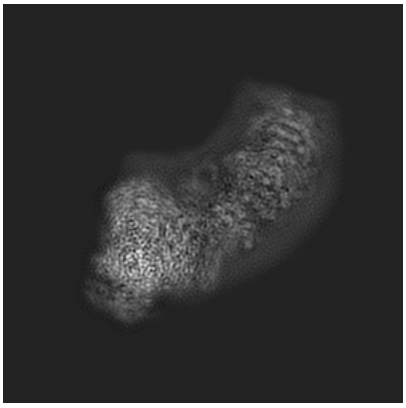
6.1.1 Primary map



X



Y

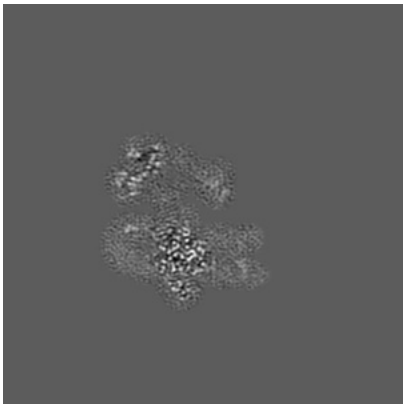


Z

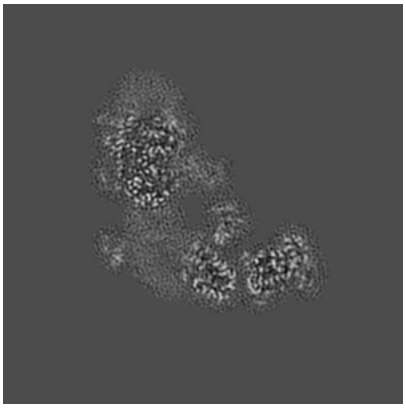
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 155



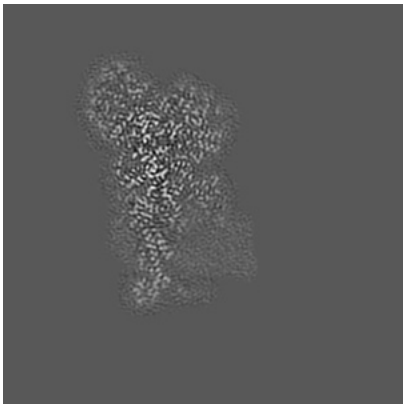
Y Index: 155

Z Index: 155

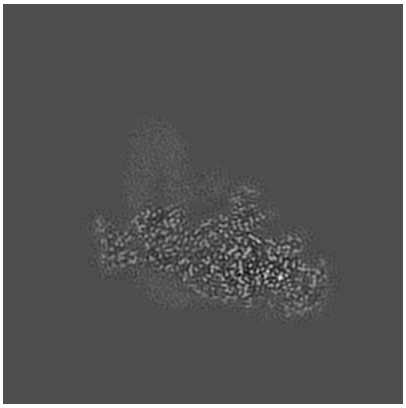
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

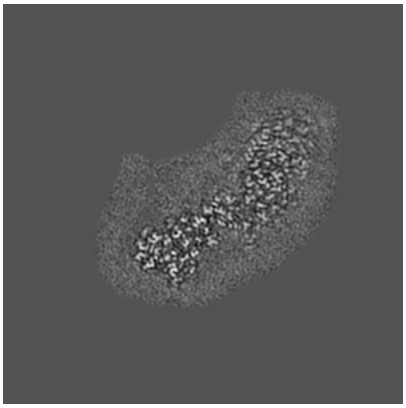
6.3.1 Primary map



X Index: 106



Y Index: 112



Z Index: 126

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0208. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

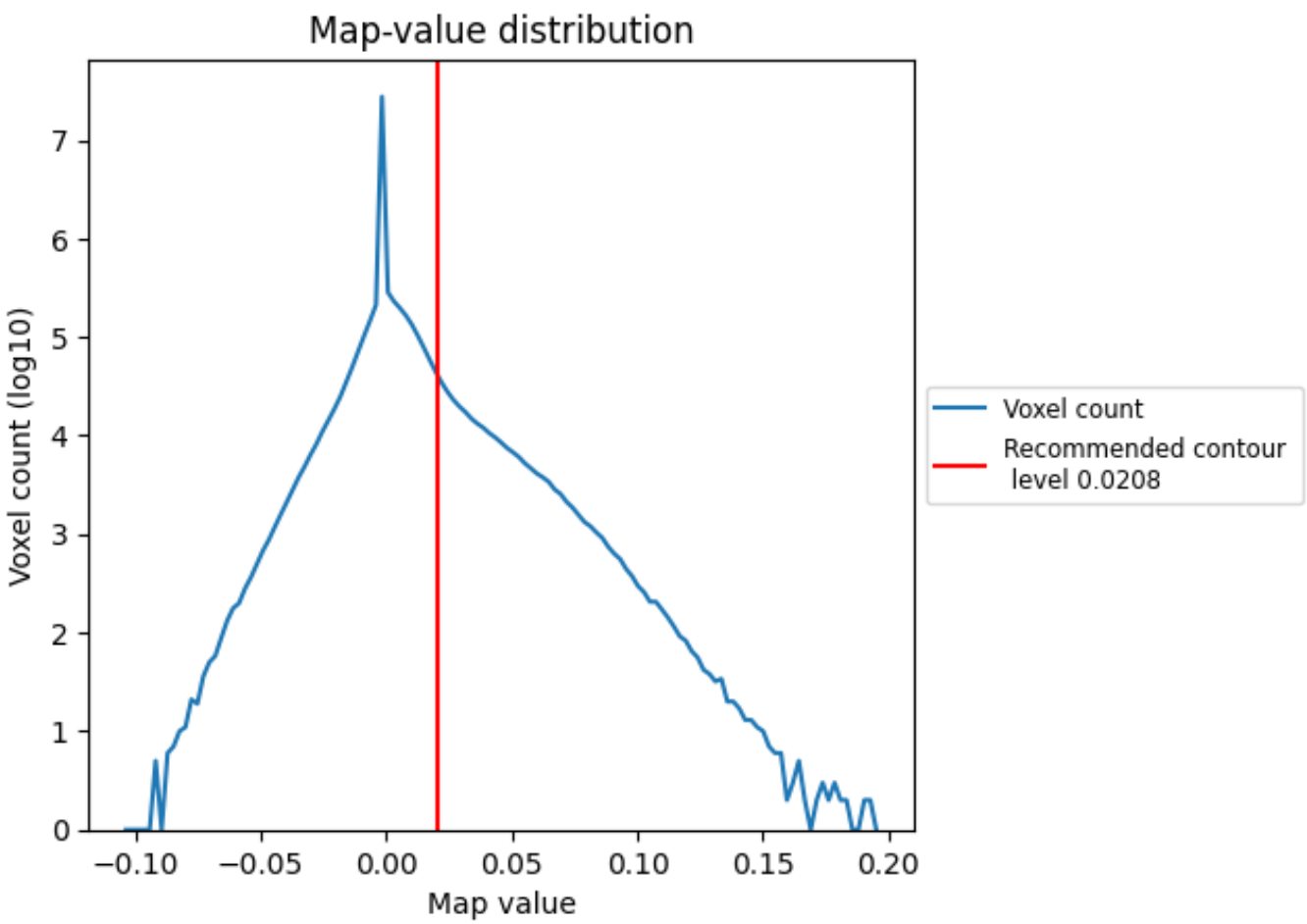
6.5 Mask visualisation (i)

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

7 Map analysis (i)

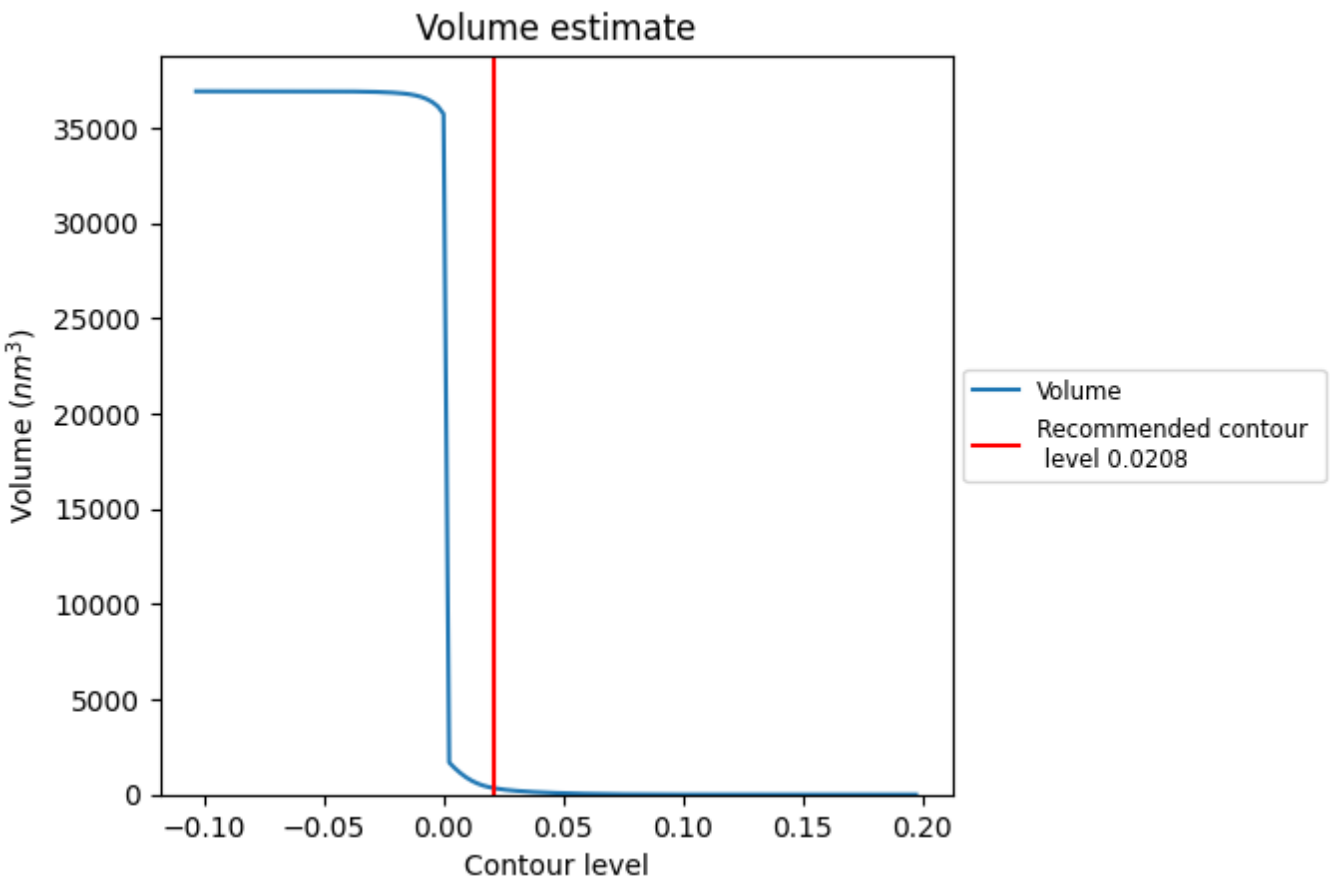
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

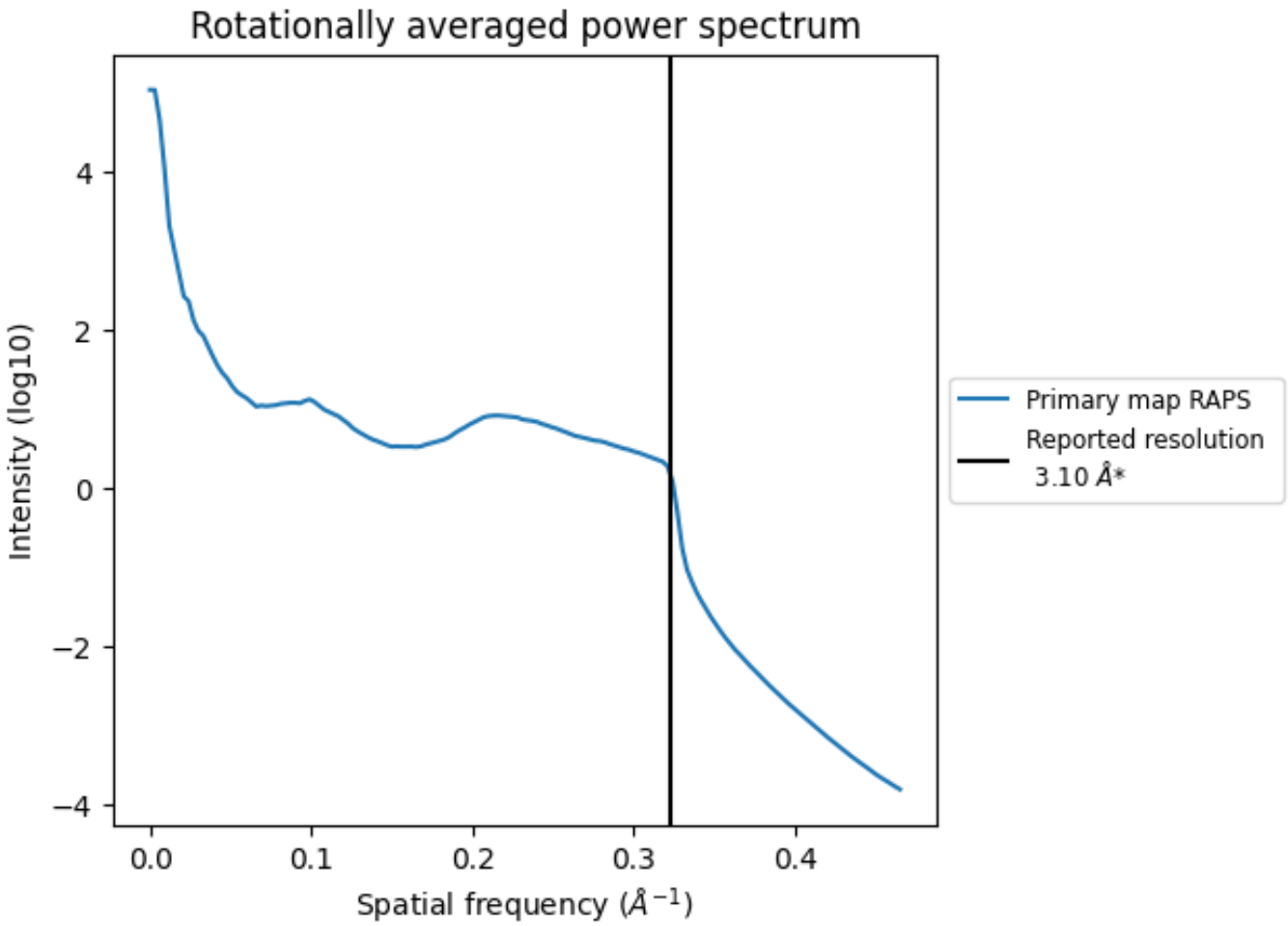
7.2 Volume estimate (i)



The volume at the recommended contour level is 342 nm^3; this corresponds to an approximate mass of 309 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 0.323 Å^{-1}

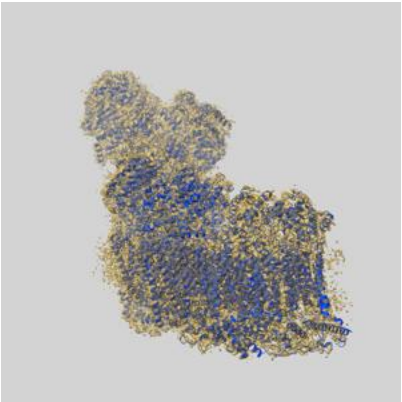
8 Fourier-Shell correlation (i)

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

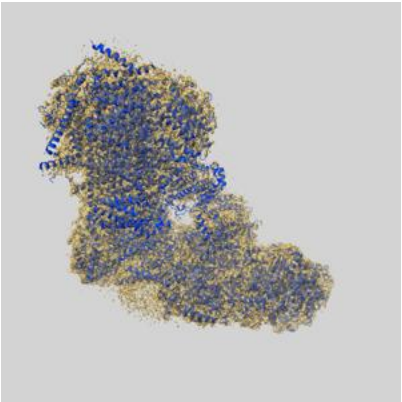
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32269 and PDB model 7W31. Per-residue inclusion information can be found in section 3 on page 20.

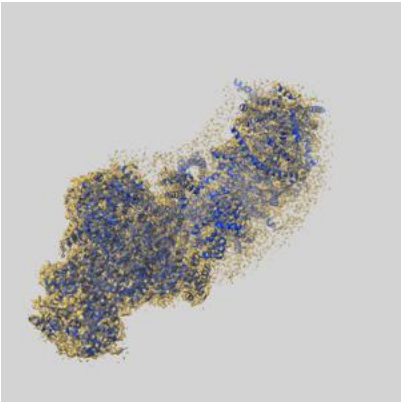
9.1 Map-model overlay (i)



X



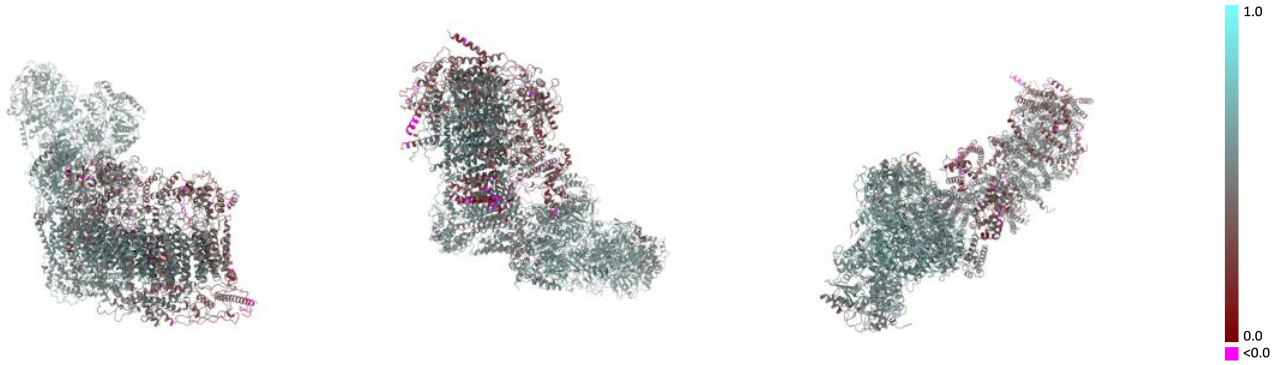
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0208 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

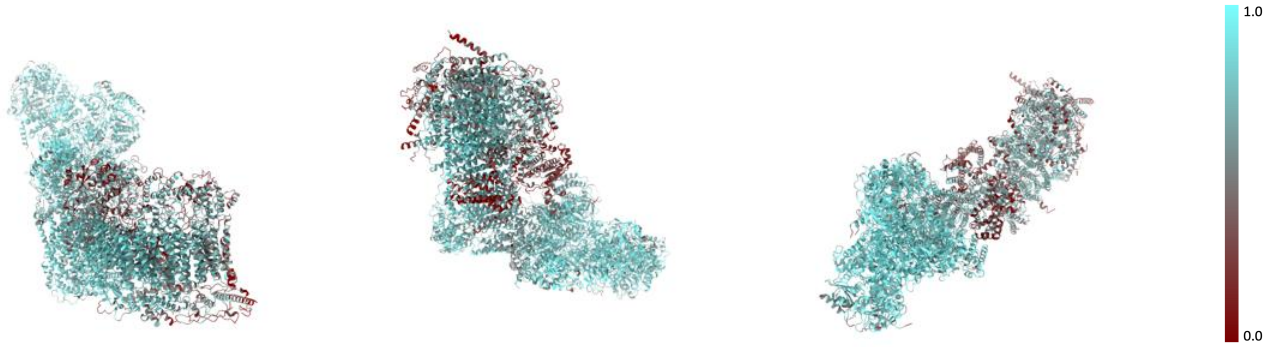
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

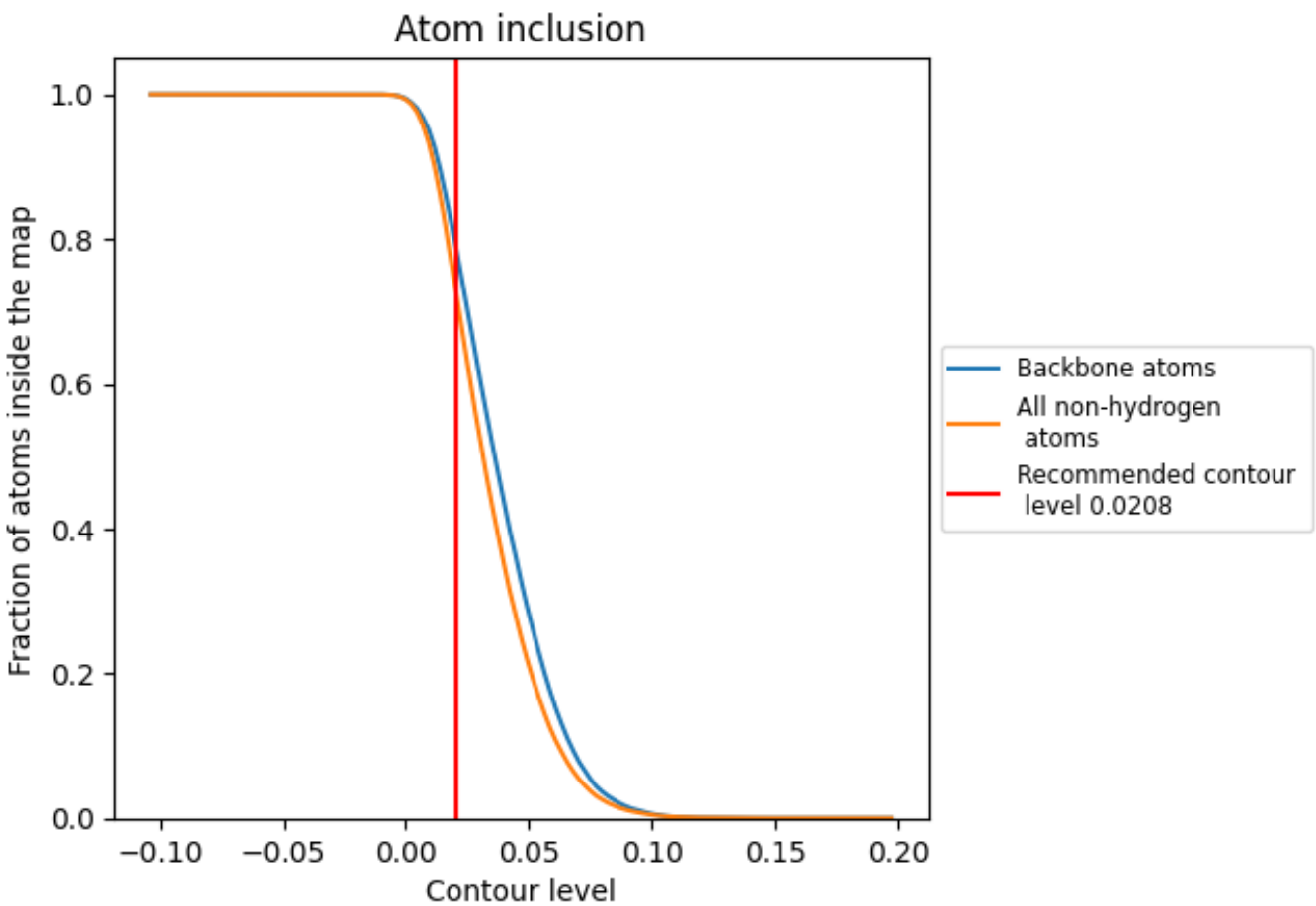
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0208).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0208) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7186	0.5090
A	0.8237	0.5510
B	0.9337	0.6080
C	0.8753	0.5920
E	0.7934	0.5490
F	0.7634	0.5070
G	0.4598	0.3520
H	0.7520	0.5110
I	0.7844	0.5550
J	0.7859	0.5440
K	0.7820	0.5320
L	0.8642	0.5860
M	0.8789	0.5830
N	0.7878	0.5620
O	0.7801	0.5250
P	0.9171	0.6000
Q	0.8286	0.5750
S	0.8662	0.5730
T	0.8019	0.5770
U	0.8156	0.5400
V	0.2408	0.2310
W	0.8285	0.5550
X	0.4397	0.3530
Y	0.3964	0.3240
Z	0.3267	0.2910
a	0.7165	0.5120
b	0.4469	0.3450
c	0.5665	0.4260
d	0.6389	0.4550
e	0.5714	0.4470
f	0.6078	0.4500
g	0.7845	0.5360
h	0.8227	0.5640
i	0.7756	0.5470
j	0.6827	0.5020

Continued on next page...

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Chain	Atom inclusion	Q-score
k	0.6496	0.4750
l	0.6296	0.4850
m	0.6822	0.5010
n	0.5841	0.4480
o	0.5604	0.4180
p	0.5372	0.3970
r	0.7664	0.5470
s	0.8374	0.5600
u	0.7961	0.5460
v	0.4125	0.3250
w	0.3307	0.3590