Full wwPDB EM Validation Report ⓘ

May 31, 2023 – 10:20 PM JST

PDB ID	:	7VXS
EMDB ID	:	EMD-32187
Title	:	Membrane arm of active state CI from Q10 dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-13
Resolution	:	2.90 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 ⓘ 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 ⓘ) were used in the production of this report:

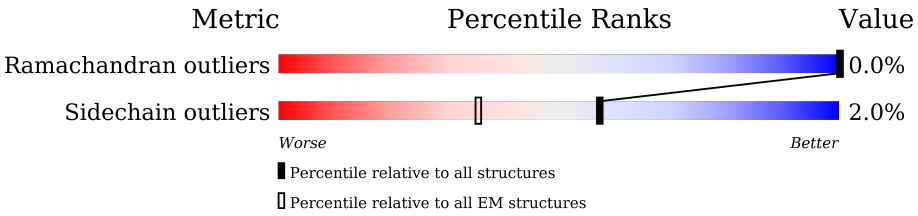
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	Q	44	9% 100%
2	S	70	100%
3	U	83	6% 98%
4	V	140	100%
5	W	113	98%
6	X	88	8% 98%
7	Y	67	9% 97%
8	Z	80	15% 95% 5%
9	a	138	99%

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Mol	Chain	Length	Quality of chain
10	b	126	7% 77% 22%
11	c	156	99%
12	d	175	5% 98%
13	e	104	9% 97%
14	f	49	27% 98%
15	g	121	98%
16	h	105	6% 100%
17	i	347	99%
18	j	115	97%
19	k	98	98%
20	l	606	98%
21	m	175	13% 98%
22	n	56	20% 96%
23	o	128	98%
24	p	178	98%
25	r	459	99%
26	s	318	99%
27	u	171	99%
28	v	124	10% 95% 5%
29	w	320	6% 98%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 39674 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] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	44	Total	C	N	O	S	0	0
			363	236	60	66	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

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

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	113	Total	C	N	O	S	0	0
			949	614	160	167	8		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			694	447	103	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 10 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	49	Total	C	N	O	0	0
			378	246	65	67		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	175	Total	C	N	O	S	0	0
			1291	861	188	229	13		

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

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	o	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

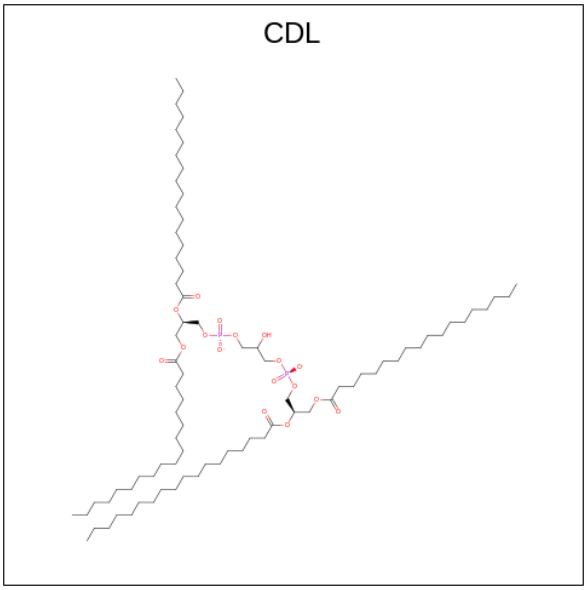
- Molecule 28 is a protein called Complex I-B18.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 30 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	V	1	Total	C	O	P	0
			94	75	17	2	
30	V	1	Total	C	O	P	0
			100	81	17	2	

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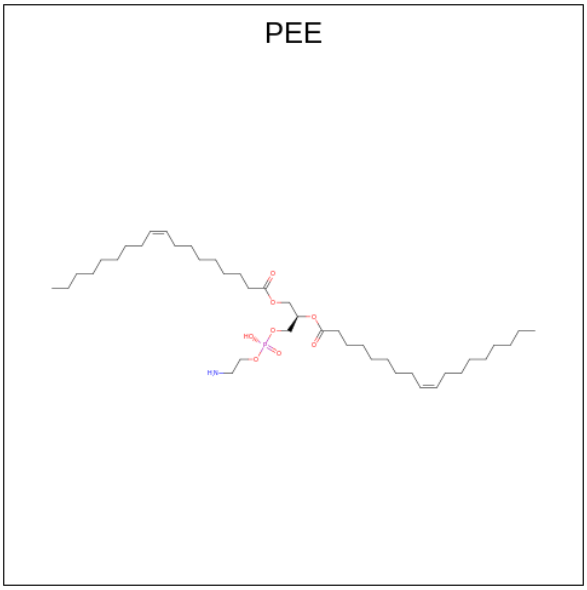
Mol	Chain	Residues	Atoms				AltConf
30	a	1	Total	C	O	P	0
			100	81	17	2	
30	i	1	Total	C	O	P	0
			68	49	17	2	
30	l	1	Total	C	O	P	0
			99	80	17	2	
30	l	1	Total	C	O	P	0
			100	81	17	2	
30	m	1	Total	C	O	P	0
			100	81	17	2	
30	n	1	Total	C	O	P	0
			55	36	17	2	
30	r	1	Total	C	O	P	0
			100	81	17	2	
30	s	1	Total	C	O	P	0
			89	70	17	2	

- Molecule 31 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
31	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
31	i	1	Total	C	N	O	P	0
			47	37	1	8	1	

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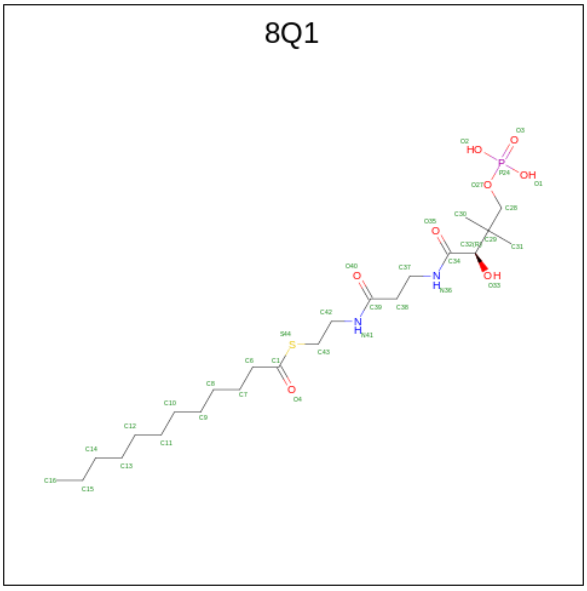
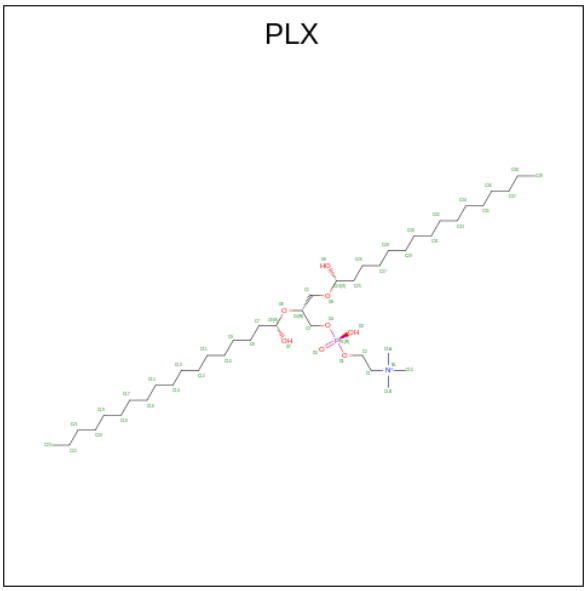
Mol	Chain	Residues	Atoms					AltConf
31	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
31	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
31	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
31	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
31	s	1	Total	C	N	O	P	0
			41	31	1	8	1	
31	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



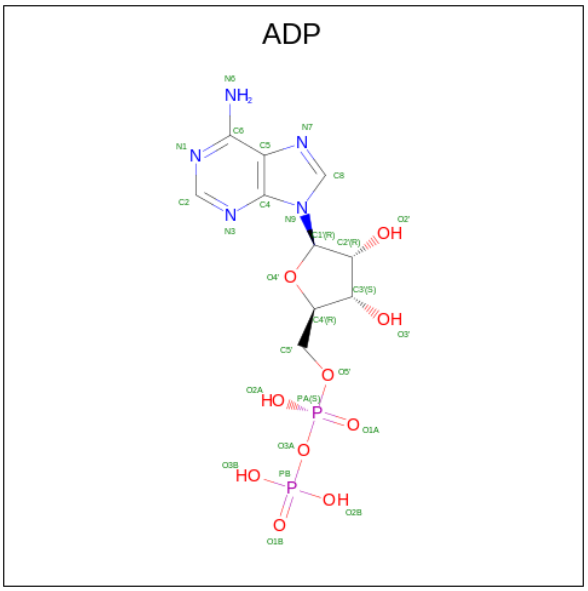
Mol	Chain	Residues	Atoms						AltConf
32	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 33 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



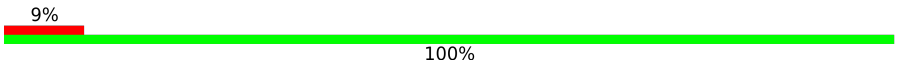
Mol	Chain	Residues	Atoms					AltConf
34	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

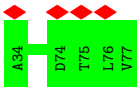
3 Residue-property plots (i)

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] iron-sulfur protein 2, mitochondrial

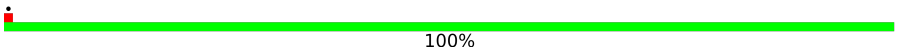
Chain Q:





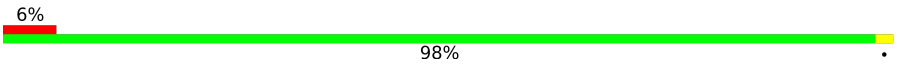
• Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

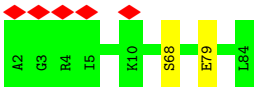
Chain S:



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

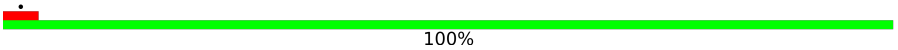
Chain U:

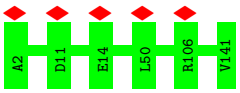




• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

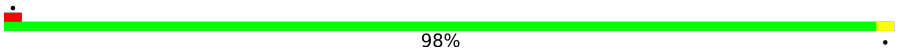
Chain V:

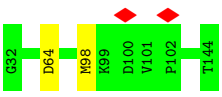




• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

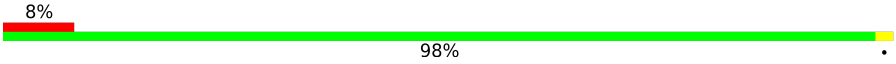
Chain W:





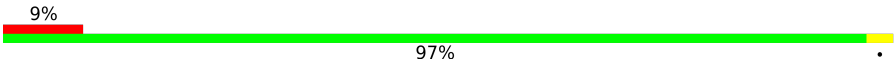
• Molecule 6: Acyl carrier protein

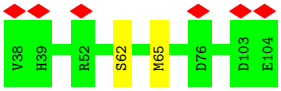
Chain X:



• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

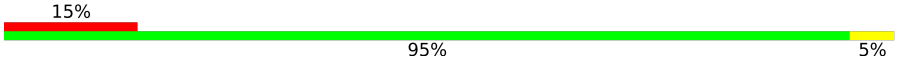
Chain Y:

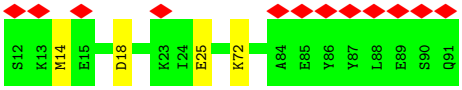




• Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

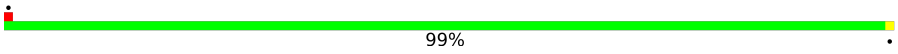
Chain Z:

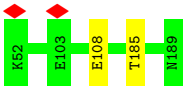




• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

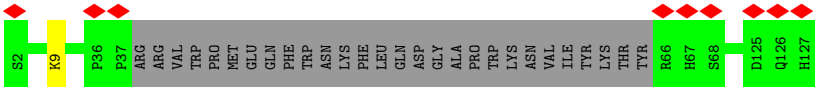
Chain a:





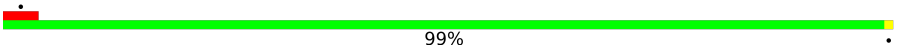
• Molecule 10: Complex I-B17

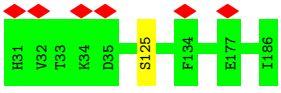
Chain b:



• Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

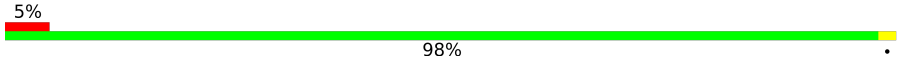
Chain c:

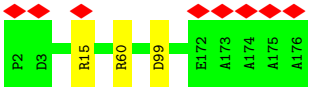




• Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

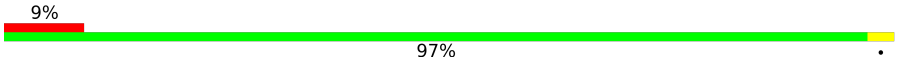
Chain d:

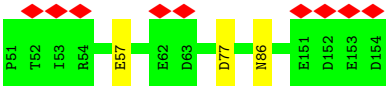




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

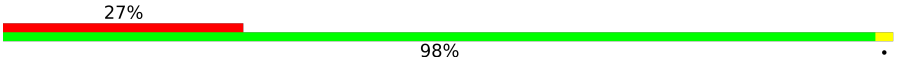
Chain e:

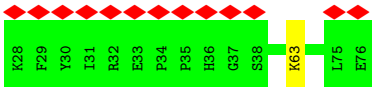




• Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

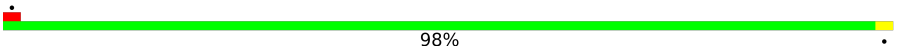
Chain f:

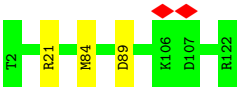




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

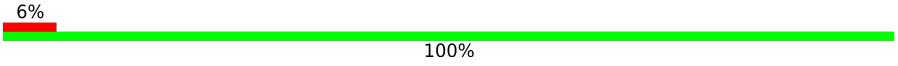
Chain g:

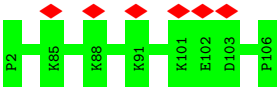




• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

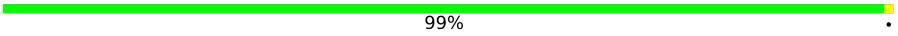
Chain h:

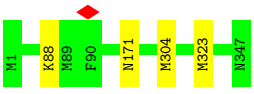




• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

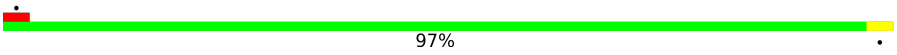
Chain i:

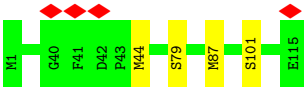




• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

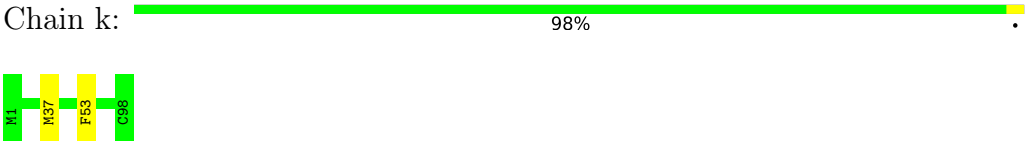
Chain j:





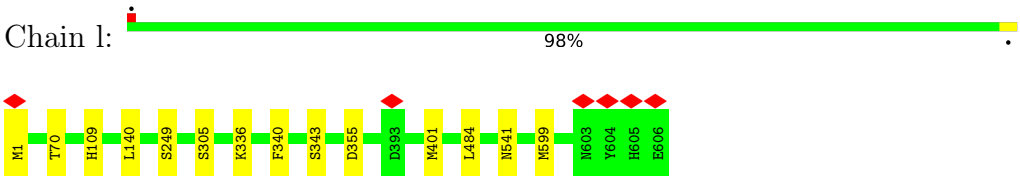
• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

Chain k:



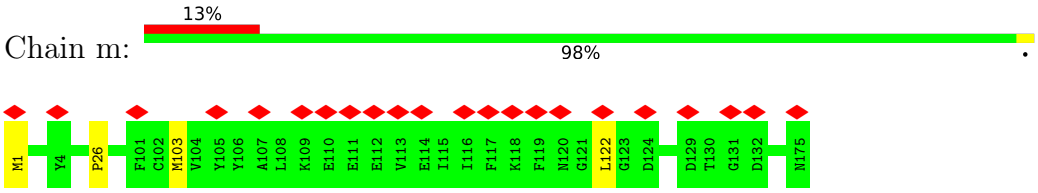
• Molecule 20: NADH-ubiquinone oxidoreductase chain 5

Chain l:



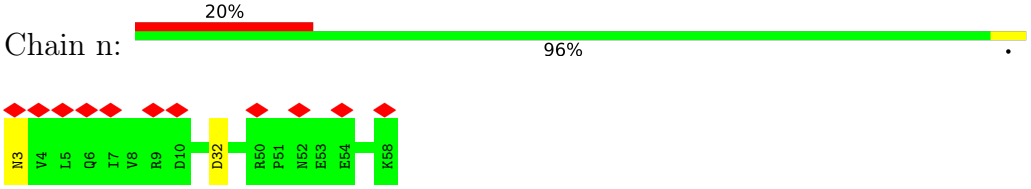
• Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain m:



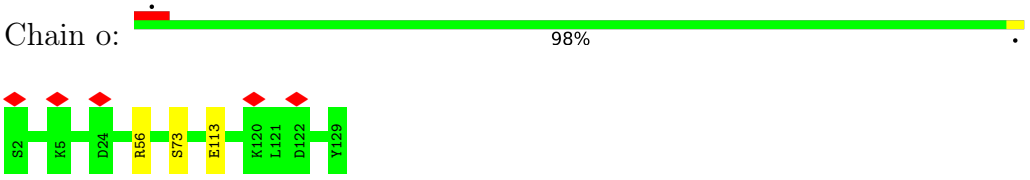
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:



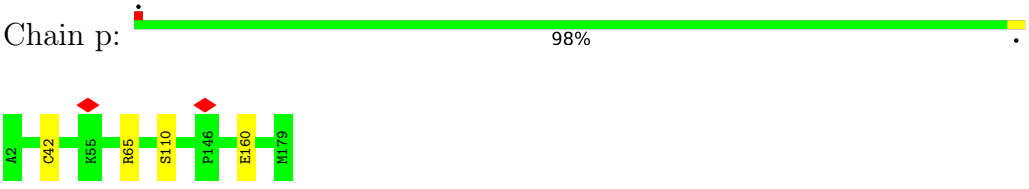
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:



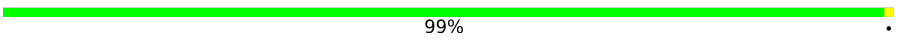
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

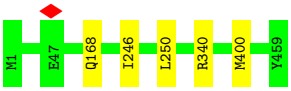
Chain p:



• Molecule 25: NADH-ubiquinone oxidoreductase chain 4

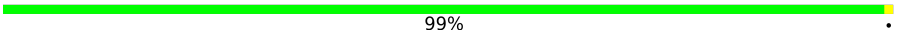
Chain r:

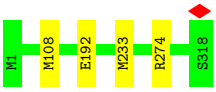




• Molecule 26: NADH-ubiquinone oxidoreductase chain 1

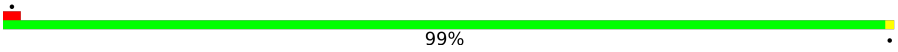
Chain s:

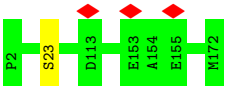




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

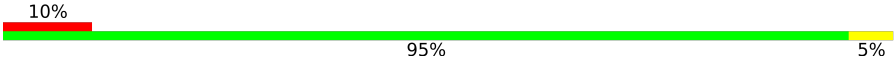
Chain u:

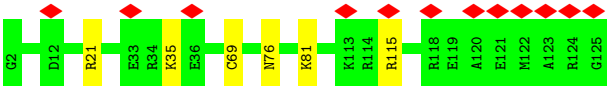




• Molecule 28: Complex I-B18

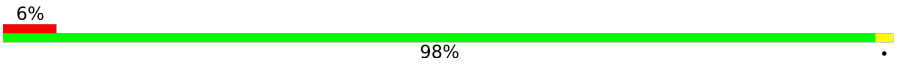
Chain v:

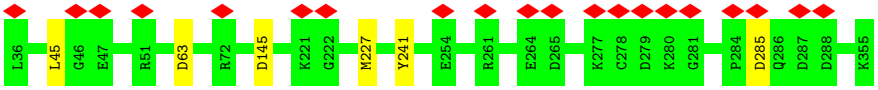




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252573	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	0.129	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	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: PEE, PLX, CDL, 8Q1, ADP

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	Q	0.23	0/380	0.42	0/525
2	S	0.24	0/581	0.50	0/781
3	U	0.26	0/664	0.45	0/912
4	V	0.25	0/1042	0.45	0/1411
5	W	0.25	0/973	0.47	0/1312
6	X	0.25	0/705	0.45	0/954
7	Y	0.25	0/610	0.43	0/836
8	Z	0.26	0/660	0.42	0/892
9	a	0.26	0/1184	0.49	0/1603
10	b	0.24	0/844	0.51	0/1149
11	c	0.27	0/1371	0.47	0/1875
12	d	0.25	0/1494	0.51	0/2015
13	e	0.25	0/891	0.48	0/1210
14	f	0.24	0/386	0.40	0/523
15	g	0.26	0/1031	0.48	0/1394
16	h	0.25	0/889	0.51	0/1190
17	i	0.25	0/2773	0.43	0/3768
18	j	0.24	0/938	0.45	0/1281
19	k	0.25	0/759	0.41	0/1029
20	l	0.26	0/4947	0.43	0/6728
21	m	0.27	0/1323	0.45	0/1797
22	n	0.26	0/491	0.48	0/663
23	o	0.27	0/1092	0.51	0/1481
24	p	0.25	0/1590	0.47	0/2155
25	r	0.25	0/3723	0.44	0/5078
26	s	0.26	0/2581	0.45	0/3529
27	u	0.25	0/1436	0.46	0/1938
28	v	0.26	0/1052	0.52	0/1411
29	w	0.25	0/2650	0.47	0/3588
All	All	0.25	0/39060	0.46	0/53028

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
4	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
5	W	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
9	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
10	b	94/126 (75%)	92 (98%)	2 (2%)	0	100	100
11	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
12	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
13	e	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
14	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
15	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
16	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	i	345/347 (99%)	328 (95%)	17 (5%)	0	100	100
18	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
19	k	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
20	l	604/606 (100%)	580 (96%)	24 (4%)	0	100	100
21	m	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	25	58
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
24	p	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
25	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
26	s	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
27	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
28	v	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
29	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	4666/4754 (98%)	4489 (96%)	176 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	m	26	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	Q	38/38 (100%)	38 (100%)	0	100	100
2	S	57/58 (98%)	57 (100%)	0	100	100
3	U	69/69 (100%)	67 (97%)	2 (3%)	42	76
4	V	101/101 (100%)	101 (100%)	0	100	100
5	W	99/99 (100%)	97 (98%)	2 (2%)	55	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	X	76/81 (94%)	74 (97%)	2 (3%)	46 77
7	Y	62/62 (100%)	60 (97%)	2 (3%)	39 73
8	Z	62/62 (100%)	58 (94%)	4 (6%)	17 45
9	a	121/121 (100%)	119 (98%)	2 (2%)	60 86
10	b	90/119 (76%)	89 (99%)	1 (1%)	73 92
11	c	141/141 (100%)	140 (99%)	1 (1%)	84 95
12	d	155/155 (100%)	152 (98%)	3 (2%)	57 84
13	e	96/96 (100%)	93 (97%)	3 (3%)	40 74
14	f	36/45 (80%)	35 (97%)	1 (3%)	43 76
15	g	108/108 (100%)	105 (97%)	3 (3%)	43 76
16	h	93/93 (100%)	93 (100%)	0	100 100
17	i	311/311 (100%)	307 (99%)	4 (1%)	69 90
18	j	100/100 (100%)	96 (96%)	4 (4%)	31 65
19	k	85/85 (100%)	83 (98%)	2 (2%)	49 79
20	l	540/540 (100%)	526 (97%)	14 (3%)	46 77
21	m	130/141 (92%)	127 (98%)	3 (2%)	50 80
22	n	53/53 (100%)	51 (96%)	2 (4%)	33 67
23	o	113/113 (100%)	110 (97%)	3 (3%)	44 77
24	p	159/159 (100%)	155 (98%)	4 (2%)	47 78
25	r	410/410 (100%)	405 (99%)	5 (1%)	71 91
26	s	275/275 (100%)	271 (98%)	4 (2%)	65 87
27	u	153/153 (100%)	152 (99%)	1 (1%)	84 95
28	v	104/111 (94%)	98 (94%)	6 (6%)	20 50
29	w	283/283 (100%)	277 (98%)	6 (2%)	53 81
All	All	4120/4182 (98%)	4036 (98%)	84 (2%)	57 82

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	U	68	SER
3	U	79	GLU
5	W	64	ASP
5	W	98	MET
6	X	98	LEU

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Mol	Chain	Res	Type
6	X	105	MET
7	Y	62	SER
7	Y	65	MET
8	Z	14	MET
8	Z	18	ASP
8	Z	25	GLU
8	Z	72	LYS
9	a	108	GLU
9	a	185	THR
10	b	9	LYS
11	c	125	SER
12	d	15	ARG
12	d	60	ARG
12	d	99	ASP
13	e	57	GLU
13	e	77	ASP
13	e	86	ASN
14	f	63	LYS
15	g	21	ARG
15	g	84	MET
15	g	89	ASP
17	i	88	LYS
17	i	171	ASN
17	i	304	MET
17	i	323	MET
18	j	44	MET
18	j	79	SER
18	j	87	MET
18	j	101	SER
19	k	37	MET
19	k	53	PHE
20	l	1	MET
20	l	70	THR
20	l	109	HIS
20	l	140	LEU
20	l	249	SER
20	l	305	SER
20	l	336	LYS
20	l	340	PHE
20	l	343	SER
20	l	355	ASP
20	l	401	MET

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Mol	Chain	Res	Type
20	l	484	LEU
20	l	541	ASN
20	l	599	MET
21	m	1	MET
21	m	103	MET
21	m	122	LEU
22	n	3	ASN
22	n	32	ASP
23	o	56	ARG
23	o	73	SER
23	o	113	GLU
24	p	42	CYS
24	p	65	ARG
24	p	110	SER
24	p	160	GLU
25	r	168	GLN
25	r	246	ILE
25	r	250	LEU
25	r	340	ARG
25	r	400	MET
26	s	108	MET
26	s	192	GLU
26	s	233	MET
26	s	274	ARG
27	u	23	SER
28	v	21	ARG
28	v	35	LYS
28	v	69	CYS
28	v	76	ASN
28	v	81	LYS
28	v	115	ARG
29	w	45	LEU
29	w	63	ASP
29	w	145	ASP
29	w	227	MET
29	w	241	TYR
29	w	285	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
9	a	189	ASN

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Mol	Chain	Res	Type
20	l	2	ASN
20	l	59	GLN
23	o	75	ASN
23	o	79	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are 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	$\#\|Z\| > 2$
31	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.02	2 (4%)
31	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
33	PLX	j	203	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
33	PLX	r	502	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
30	CDL	n	102	-	54,54,99	1.23	4 (7%)	60,66,111	1.25	4 (6%)
31	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
30	CDL	s	402	-	88,88,99	1.14	8 (9%)	94,100,111	0.91	4 (4%)
31	PEE	l	704	-	50,50,50	1.17	6 (12%)	53,55,55	0.93	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CDL	l	702	-	98,98,99	0.93	4 (4%)	104,110,111	1.09	7 (6%)
33	PLX	n	101	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
31	PEE	s	403	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
30	CDL	V	202	-	99,99,99	1.09	9 (9%)	105,111,111	0.86	4 (3%)
34	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.45	5 (17%)
31	PEE	s	401	-	40,40,50	1.16	4 (10%)	43,45,55	0.98	2 (4%)
30	CDL	l	703	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)
31	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.03	2 (4%)
33	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
33	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.63	1 (1%)
30	CDL	i	401	-	67,67,99	1.12	4 (5%)	73,79,111	1.16	5 (6%)
30	CDL	m	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
30	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
30	CDL	r	503	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)
32	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.54	7 (17%)
30	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.86	4 (4%)
31	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
31	PEE	i	402	-	46,46,50	1.20	6 (13%)	49,51,55	0.99	2 (4%)

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
31	PEE	W	201	-	-	25/44/44/54	-
31	PEE	r	501	-	-	27/54/54/54	-
33	PLX	j	203	-	-	25/55/55/55	-
33	PLX	r	502	-	-	28/55/55/55	-
30	CDL	n	102	-	-	24/65/65/110	-
31	PEE	j	201	-	-	25/54/54/54	-
30	CDL	s	402	-	-	50/99/99/110	-
31	PEE	l	704	-	-	27/54/54/54	-
30	CDL	l	702	-	-	38/109/109/110	-
33	PLX	n	101	-	-	25/55/55/55	-
31	PEE	s	403	-	-	26/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CDL	V	202	-	-	60/110/110/110	-
34	ADP	w	401	-	-	4/12/32/32	0/3/3/3
31	PEE	s	401	-	-	16/44/44/54	-
30	CDL	l	703	-	-	54/110/110/110	-
31	PEE	l	701	-	-	23/43/43/54	-
33	PLX	j	202	-	-	36/55/55/55	-
33	PLX	g	201	-	-	28/55/55/55	-
30	CDL	i	401	-	-	30/78/78/110	-
30	CDL	m	201	-	-	60/110/110/110	-
30	CDL	a	201	-	-	61/110/110/110	-
30	CDL	r	503	-	-	56/110/110/110	-
32	8Q1	X	201	-	-	18/41/41/41	-
30	CDL	V	201	-	-	48/104/104/110	-
31	PEE	b	201	-	-	26/49/49/54	-
31	PEE	i	402	-	-	27/50/50/54	-

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	w	401	ADP	C3'-C4'	-8.88	1.30	1.53
34	w	401	ADP	O4'-C4'	7.66	1.62	1.45
34	w	401	ADP	O4'-C1'	-6.95	1.31	1.41
32	X	201	8Q1	C34-N36	5.45	1.45	1.33
32	X	201	8Q1	C39-N41	5.31	1.45	1.33
30	i	401	CDL	OB8-CB7	4.27	1.45	1.33
30	i	401	CDL	OA8-CA7	4.27	1.45	1.33
30	n	102	CDL	OA8-CA7	4.23	1.45	1.33
30	l	702	CDL	OA8-CA7	4.23	1.45	1.33
30	l	702	CDL	OB8-CB7	4.20	1.45	1.33
30	n	102	CDL	OB8-CB7	4.20	1.45	1.33
30	l	702	CDL	OA6-CA5	4.19	1.46	1.34
30	n	102	CDL	OB6-CB5	4.18	1.46	1.34
30	i	401	CDL	OA6-CA5	4.18	1.46	1.34
30	i	401	CDL	OB6-CB5	4.16	1.46	1.34
30	n	102	CDL	OA6-CA5	4.12	1.45	1.34
30	l	702	CDL	OB6-CB5	4.05	1.45	1.34
34	w	401	ADP	C6-N6	3.83	1.48	1.34
31	r	501	PEE	C18-C19	3.75	1.53	1.31
31	l	701	PEE	C18-C19	3.75	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	201	PEE	C18-C19	3.74	1.53	1.31
31	s	401	PEE	C18-C19	3.73	1.53	1.31
31	b	201	PEE	C18-C19	3.73	1.53	1.31
31	l	704	PEE	C18-C19	3.73	1.53	1.31
31	s	403	PEE	C18-C19	3.73	1.53	1.31
31	W	201	PEE	C18-C19	3.73	1.53	1.31
31	i	402	PEE	C18-C19	3.71	1.53	1.31
31	l	701	PEE	C39-C38	3.66	1.53	1.31
31	r	501	PEE	C39-C38	3.66	1.53	1.31
31	j	201	PEE	C39-C38	3.66	1.53	1.31
31	i	402	PEE	C39-C38	3.65	1.52	1.31
31	l	704	PEE	C39-C38	3.65	1.52	1.31
31	b	201	PEE	C39-C38	3.64	1.52	1.31
31	s	403	PEE	C39-C38	3.64	1.52	1.31
30	s	402	CDL	OA8-CA7	3.47	1.43	1.33
30	m	201	CDL	OA8-CA7	3.46	1.43	1.33
30	V	201	CDL	OA8-CA7	3.45	1.43	1.33
30	V	202	CDL	OA8-CA7	3.45	1.43	1.33
30	a	201	CDL	OA8-CA7	3.42	1.43	1.33
30	r	503	CDL	OA8-CA7	3.40	1.43	1.33
30	l	703	CDL	OA8-CA7	3.36	1.43	1.33
34	w	401	ADP	O2'-C2'	-3.30	1.35	1.43
30	V	201	CDL	OA6-CA5	3.14	1.43	1.34
30	m	201	CDL	OA6-CA5	3.12	1.43	1.34
34	w	401	ADP	O3'-C3'	3.10	1.50	1.43
30	r	503	CDL	OB6-CB5	3.06	1.42	1.34
30	a	201	CDL	OB6-CB5	3.05	1.42	1.34
30	m	201	CDL	OB8-CB7	3.04	1.42	1.33
30	s	402	CDL	OB6-CB5	3.03	1.42	1.34
30	V	202	CDL	OB6-CB5	3.02	1.42	1.34
30	m	201	CDL	OB6-CB5	3.01	1.42	1.34
30	V	201	CDL	OB8-CB7	3.00	1.42	1.33
30	s	402	CDL	OA6-CA5	3.00	1.42	1.34
30	r	503	CDL	OB8-CB7	3.00	1.42	1.33
30	a	201	CDL	OB8-CB7	2.99	1.42	1.33
30	l	703	CDL	OB8-CB7	2.99	1.42	1.33
30	l	703	CDL	OB6-CB5	2.98	1.42	1.34
30	V	201	CDL	OB6-CB5	2.97	1.42	1.34
30	a	201	CDL	OA6-CA5	2.96	1.42	1.34
30	V	202	CDL	OB8-CB7	2.95	1.42	1.33
30	s	402	CDL	OB8-CB7	2.94	1.41	1.33
30	r	503	CDL	OA6-CA5	2.93	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	V	202	CDL	OA6-CA5	2.93	1.42	1.34
30	l	703	CDL	OA6-CA5	2.93	1.42	1.34
33	n	101	PLX	O6-C4	-2.76	1.40	1.44
33	r	502	PLX	O6-C4	-2.69	1.41	1.44
33	g	201	PLX	O6-C4	-2.67	1.41	1.44
31	s	401	PEE	O3-C30	2.65	1.41	1.33
33	j	203	PLX	O6-C4	-2.62	1.41	1.44
31	b	201	PEE	O3-C30	2.50	1.40	1.33
31	r	501	PEE	O3-C30	2.50	1.40	1.33
31	l	701	PEE	O3-C30	2.49	1.40	1.33
31	s	403	PEE	O3-C30	2.44	1.40	1.33
30	a	201	CDL	OA6-CA4	-2.44	1.40	1.46
31	j	201	PEE	O3-C30	2.43	1.40	1.33
31	l	704	PEE	O3-C30	2.43	1.40	1.33
31	i	402	PEE	O3-C30	2.43	1.40	1.33
31	s	403	PEE	O2-C2	-2.42	1.40	1.46
30	l	703	CDL	OA6-CA4	-2.41	1.40	1.46
31	i	402	PEE	O2-C2	-2.41	1.40	1.46
31	l	704	PEE	O2-C2	-2.41	1.40	1.46
31	j	201	PEE	O2-C2	-2.41	1.40	1.46
33	j	202	PLX	C7-C6	2.41	1.55	1.50
33	j	203	PLX	C7-C6	2.41	1.55	1.50
31	r	501	PEE	O2-C2	-2.40	1.40	1.46
32	X	201	8Q1	C1-S44	2.40	1.81	1.76
31	s	401	PEE	O2-C2	-2.40	1.40	1.46
30	r	503	CDL	OA6-CA4	-2.40	1.40	1.46
31	W	201	PEE	O3-C30	2.39	1.40	1.33
33	r	502	PLX	C7-C6	2.39	1.55	1.50
33	j	202	PLX	O6-C4	-2.39	1.41	1.44
30	s	402	CDL	OA6-CA4	-2.39	1.40	1.46
30	V	202	CDL	OA6-CA4	-2.39	1.40	1.46
31	l	701	PEE	O2-C2	-2.38	1.40	1.46
31	b	201	PEE	O2-C2	-2.35	1.40	1.46
31	W	201	PEE	O2-C2	-2.34	1.40	1.46
33	n	101	PLX	C7-C6	2.33	1.55	1.50
31	l	704	PEE	O2-C10	2.33	1.40	1.34
33	g	201	PLX	C7-C6	2.32	1.55	1.50
31	b	201	PEE	O2-C10	2.31	1.40	1.34
31	s	401	PEE	O2-C10	2.29	1.40	1.34
31	W	201	PEE	O2-C10	2.27	1.40	1.34
31	s	403	PEE	O2-C10	2.27	1.40	1.34
31	l	701	PEE	O2-C10	2.26	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	201	PEE	O2-C10	2.26	1.40	1.34
31	r	501	PEE	O2-C10	2.23	1.40	1.34
30	s	402	CDL	PB2-OB2	2.22	1.68	1.59
30	V	201	CDL	PB2-OB2	2.22	1.68	1.59
31	i	402	PEE	O2-C10	2.22	1.40	1.34
32	X	201	8Q1	O40-C39	-2.22	1.18	1.23
30	a	201	CDL	PB2-OB2	2.22	1.68	1.59
30	V	202	CDL	PB2-OB2	2.21	1.68	1.59
30	V	201	CDL	OB6-CB4	-2.21	1.41	1.46
30	l	703	CDL	PB2-OB2	2.21	1.68	1.59
30	m	201	CDL	PB2-OB2	2.20	1.68	1.59
30	r	503	CDL	PB2-OB2	2.20	1.68	1.59
30	m	201	CDL	OB6-CB4	-2.20	1.41	1.46
30	V	202	CDL	PB2-OB5	2.20	1.68	1.59
30	l	703	CDL	OB6-CB4	-2.19	1.41	1.46
32	X	201	8Q1	C6-C1	2.19	1.53	1.50
32	X	201	8Q1	O35-C34	-2.19	1.19	1.23
30	m	201	CDL	PB2-OB5	2.18	1.68	1.59
30	V	201	CDL	PB2-OB5	2.17	1.68	1.59
33	j	202	PLX	P1-O4	2.17	1.68	1.59
31	l	704	PEE	O3-C3	-2.17	1.40	1.45
30	l	703	CDL	PB2-OB5	2.16	1.68	1.59
30	a	201	CDL	PB2-OB5	2.16	1.68	1.59
33	g	201	PLX	P1-O4	2.15	1.68	1.59
30	a	201	CDL	OB6-CB4	-2.15	1.41	1.46
30	s	402	CDL	OB6-CB4	-2.15	1.41	1.46
30	r	503	CDL	PB2-OB5	2.15	1.68	1.59
30	s	402	CDL	PB2-OB5	2.15	1.68	1.59
33	j	203	PLX	P1-O4	2.14	1.68	1.59
31	W	201	PEE	O3-C3	-2.13	1.40	1.45
30	m	201	CDL	OA6-CA4	-2.13	1.41	1.46
30	V	202	CDL	OB6-CB4	-2.12	1.41	1.46
33	n	101	PLX	P1-O4	2.12	1.67	1.59
31	i	402	PEE	O3-C3	-2.10	1.40	1.45
30	r	503	CDL	OB6-CB4	-2.09	1.41	1.46
33	r	502	PLX	P1-O4	2.09	1.67	1.59
31	j	201	PEE	O3-C3	-2.08	1.40	1.45
30	V	201	CDL	OA6-CA4	-2.08	1.41	1.46
31	r	501	PEE	O3-C3	-2.07	1.40	1.45
31	l	701	PEE	O3-C3	-2.06	1.40	1.45
33	j	203	PLX	P1-O1	2.06	1.67	1.59
31	s	403	PEE	O3-C3	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	V	201	CDL	C11-CA5	2.05	1.56	1.50
31	b	201	PEE	O3-C3	-2.05	1.40	1.45
33	j	202	PLX	P1-O1	2.03	1.67	1.59
33	n	101	PLX	P1-O1	2.03	1.67	1.59
33	r	502	PLX	P1-O1	2.02	1.67	1.59
30	V	202	CDL	C11-CA5	2.00	1.56	1.50

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	201	8Q1	C6-C1-S44	5.52	119.88	113.46
30	l	702	CDL	OA6-CA5-C11	4.53	121.25	111.50
34	w	401	ADP	N3-C2-N1	-4.51	121.62	128.68
30	i	401	CDL	OA6-CA5-C11	4.26	120.68	111.50
30	a	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
31	b	201	PEE	O2-C10-C11	4.07	120.27	111.50
30	s	402	CDL	OB6-CB5-C51	4.04	120.21	111.50
31	W	201	PEE	O2-C10-C11	4.04	120.21	111.50
30	V	201	CDL	OA6-CA5-C11	4.01	120.15	111.50
30	l	702	CDL	OB6-CB5-C51	4.01	120.15	111.50
31	s	403	PEE	O2-C10-C11	4.00	120.11	111.50
31	j	201	PEE	O2-C10-C11	3.99	120.10	111.50
30	s	402	CDL	OA6-CA5-C11	3.99	120.09	111.50
30	m	201	CDL	OB6-CB5-C51	3.98	120.08	111.50
30	n	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
31	r	501	PEE	O2-C10-C11	3.97	120.06	111.50
31	s	401	PEE	O2-C10-C11	3.97	120.06	111.50
30	V	202	CDL	OB6-CB5-C51	3.96	120.03	111.50
30	r	503	CDL	OA6-CA5-C11	3.95	120.01	111.50
30	l	703	CDL	OA6-CA5-C11	3.95	120.00	111.50
31	i	402	PEE	O2-C10-C11	3.92	119.95	111.50
30	n	102	CDL	OA6-CA5-C11	3.90	119.90	111.50
30	r	503	CDL	OB6-CB5-C51	3.87	119.84	111.50
31	l	701	PEE	O2-C10-C11	3.86	119.83	111.50
30	i	401	CDL	OB6-CB5-C51	3.86	119.83	111.50
30	l	703	CDL	OB6-CB5-C51	3.85	119.81	111.50
30	V	202	CDL	OA6-CA5-C11	3.85	119.79	111.50
30	a	201	CDL	OA6-CA5-C11	3.83	119.77	111.50
30	V	201	CDL	OB6-CB5-C51	3.81	119.71	111.50
31	l	704	PEE	O2-C10-C11	3.76	119.61	111.50
30	m	201	CDL	OA6-CA5-C11	3.59	119.23	111.50
32	X	201	8Q1	O4-C1-C6	-3.42	119.95	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	102	CDL	OA8-CA7-C31	3.33	120.11	111.38
30	l	702	CDL	OB8-CB7-C71	2.91	121.05	111.91
30	l	702	CDL	OA8-CA7-C31	2.88	120.95	111.91
30	n	102	CDL	OB8-CB7-C71	2.80	120.71	111.91
30	m	201	CDL	OB8-CB7-C71	2.74	120.51	111.91
31	s	403	PEE	O3-C30-C31	2.73	120.47	111.91
30	a	201	CDL	OB8-CB7-C71	2.73	120.46	111.91
31	r	501	PEE	O3-C30-C31	2.72	120.46	111.91
30	r	503	CDL	OB8-CB7-C71	2.70	120.38	111.91
32	X	201	8Q1	C37-C38-C39	2.70	116.85	112.36
30	m	201	CDL	OA8-CA7-C31	2.69	120.33	111.91
30	i	401	CDL	OA8-CA7-C31	2.66	120.25	111.91
30	s	402	CDL	OA8-CA7-C31	2.65	120.23	111.91
30	V	202	CDL	OA8-CA7-C31	2.64	120.20	111.91
30	V	202	CDL	OB8-CB7-C71	2.64	120.19	111.91
31	j	201	PEE	O3-C30-C31	2.63	120.15	111.91
31	l	704	PEE	O3-C30-C31	2.62	120.13	111.91
31	l	701	PEE	O3-C30-C31	2.62	120.13	111.91
30	V	201	CDL	OB8-CB7-C71	2.60	120.08	111.91
31	b	201	PEE	O3-C30-C31	2.60	120.05	111.91
30	a	201	CDL	OA8-CA7-C31	2.59	120.04	111.91
30	l	703	CDL	OB8-CB7-C71	2.58	120.00	111.91
31	i	402	PEE	O3-C30-C31	2.58	119.99	111.91
33	g	201	PLX	C1A-N1-C1	2.57	120.44	109.92
31	s	401	PEE	O3-C30-C31	2.56	119.96	111.91
31	W	201	PEE	O3-C30-C31	2.56	119.94	111.91
34	w	401	ADP	O4'-C1'-C2'	-2.55	103.19	106.93
30	i	401	CDL	OB8-CB7-C71	2.55	119.90	111.91
30	r	503	CDL	OA8-CA7-C31	2.55	119.89	111.91
30	l	702	CDL	CA4-OA6-CA5	-2.51	111.62	117.79
30	s	402	CDL	OB8-CB7-C71	2.50	119.74	111.91
34	w	401	ADP	PA-O3A-PB	-2.49	124.27	132.83
30	V	201	CDL	OA8-CA7-C31	2.48	119.69	111.91
30	l	702	CDL	CB4-OB6-CB5	-2.45	111.77	117.79
32	X	201	8Q1	C38-C39-N41	2.42	120.50	116.42
33	j	203	PLX	C1A-N1-C1	2.41	119.76	109.92
30	l	703	CDL	OA8-CA7-C31	2.36	119.31	111.91
33	r	502	PLX	C1A-N1-C1	2.34	119.51	109.92
33	n	101	PLX	C1A-N1-C1	2.34	119.48	109.92
32	X	201	8Q1	C43-S44-C1	2.31	109.07	101.87
33	j	202	PLX	C1A-N1-C1	2.28	119.24	109.92
30	i	401	CDL	CA4-OA6-CA5	-2.21	112.34	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	w	401	ADP	C4-C5-N7	-2.15	107.16	109.40
34	w	401	ADP	C3'-C2'-C1'	2.09	104.13	100.98
32	X	201	8Q1	C42-N41-C39	-2.08	118.98	122.84
32	X	201	8Q1	O27-C28-C29	-2.00	107.33	110.55
30	l	702	CDL	OB8-CB7-OB9	-2.00	118.54	123.59

There are no chirality outliers.

All (867) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	V	201	CDL	CA2-OA2-PA1-OA5
30	V	201	CDL	OA7-CA5-OA6-CA4
30	V	201	CDL	C11-CA5-OA6-CA4
30	V	201	CDL	CB2-OB2-PB2-OB3
30	V	201	CDL	CB3-OB5-PB2-OB3
30	V	201	CDL	CB3-OB5-PB2-OB4
30	V	202	CDL	CA3-OA5-PA1-OA3
30	V	202	CDL	C51-CB5-OB6-CB4
30	a	201	CDL	CB2-C1-CA2-OA2
30	a	201	CDL	CA2-OA2-PA1-OA3
30	a	201	CDL	CB2-OB2-PB2-OB3
30	a	201	CDL	CB3-OB5-PB2-OB3
30	a	201	CDL	CB3-OB5-PB2-OB4
30	a	201	CDL	OB7-CB5-OB6-CB4
30	a	201	CDL	C51-CB5-OB6-CB4
30	i	401	CDL	CA2-OA2-PA1-OA3
30	i	401	CDL	CA2-OA2-PA1-OA5
30	i	401	CDL	CA3-OA5-PA1-OA4
30	i	401	CDL	CB2-OB2-PB2-OB3
30	i	401	CDL	CB2-OB2-PB2-OB4
30	i	401	CDL	CB2-OB2-PB2-OB5
30	l	702	CDL	CA2-OA2-PA1-OA3
30	l	702	CDL	CA2-OA2-PA1-OA4
30	l	702	CDL	CA2-OA2-PA1-OA5
30	l	702	CDL	CA3-OA5-PA1-OA3
30	l	702	CDL	CB3-OB5-PB2-OB4
30	l	703	CDL	O1-C1-CA2-OA2
30	l	703	CDL	CB2-C1-CA2-OA2
30	l	703	CDL	CB2-OB2-PB2-OB4
30	m	201	CDL	CB2-C1-CA2-OA2
30	m	201	CDL	CA2-OA2-PA1-OA3
30	m	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
30	m	201	CDL	CA2-OA2-PA1-OA5
30	m	201	CDL	CA3-OA5-PA1-OA3
30	m	201	CDL	CB3-OB5-PB2-OB2
30	m	201	CDL	CB3-OB5-PB2-OB3
30	m	201	CDL	CB3-OB5-PB2-OB4
30	n	102	CDL	O1-C1-CB2-OB2
30	n	102	CDL	CA2-OA2-PA1-OA5
30	n	102	CDL	CA3-OA5-PA1-OA4
30	n	102	CDL	CB3-OB5-PB2-OB4
30	r	503	CDL	CA2-OA2-PA1-OA3
30	r	503	CDL	CA3-OA5-PA1-OA2
30	r	503	CDL	CA3-OA5-PA1-OA3
30	r	503	CDL	CB2-OB2-PB2-OB3
30	r	503	CDL	CB2-OB2-PB2-OB4
30	r	503	CDL	CB2-OB2-PB2-OB5
30	r	503	CDL	CB3-OB5-PB2-OB3
30	r	503	CDL	C51-CB5-OB6-CB4
30	s	402	CDL	CB2-C1-CA2-OA2
30	s	402	CDL	CA2-OA2-PA1-OA3
30	s	402	CDL	CA2-OA2-PA1-OA4
30	s	402	CDL	OB6-CB4-CB6-OB8
31	W	201	PEE	C4-O4P-P-O3P
31	W	201	PEE	C4-O4P-P-O1P
31	W	201	PEE	O4P-C4-C5-N
31	b	201	PEE	O4P-C4-C5-N
31	b	201	PEE	C37-C38-C39-C40
31	i	402	PEE	C11-C10-O2-C2
31	i	402	PEE	C4-O4P-P-O1P
31	j	201	PEE	C1-O3P-P-O1P
31	l	701	PEE	C11-C10-O2-C2
31	l	701	PEE	C1-O3P-P-O2P
31	l	701	PEE	C1-O3P-P-O1P
31	l	701	PEE	C1-O3P-P-O4P
31	l	701	PEE	C4-O4P-P-O2P
31	l	704	PEE	O3P-C1-C2-O2
31	l	704	PEE	C4-O4P-P-O3P
31	r	501	PEE	C1-O3P-P-O1P
31	s	403	PEE	C11-C10-O2-C2
32	X	201	8Q1	C1-C6-C7-C8
32	X	201	8Q1	O4-C1-S44-C43
32	X	201	8Q1	C6-C1-S44-C43
32	X	201	8Q1	N41-C42-C43-S44

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Mol	Chain	Res	Type	Atoms
32	X	201	8Q1	C42-C43-S44-C1
32	X	201	8Q1	C28-O27-P24-O3
32	X	201	8Q1	C28-O27-P24-O2
33	g	201	PLX	C2-O1-P1-O4
33	j	202	PLX	O7-C6-O6-C4
33	j	202	PLX	C2-O1-P1-O2
33	j	203	PLX	O7-C6-C7-C8
33	n	101	PLX	O7-C6-C7-C8
33	n	101	PLX	O7-C6-O6-C4
33	n	101	PLX	C3-O4-P1-O3
33	r	502	PLX	C3-O4-P1-O2
33	r	502	PLX	C3-O4-P1-O3
34	w	401	ADP	C5'-O5'-PA-O2A
34	w	401	ADP	C5'-O5'-PA-O3A
30	i	401	CDL	OA9-CA7-OA8-CA6
30	s	402	CDL	OA9-CA7-OA8-CA6
30	V	202	CDL	OB7-CB5-OB6-CB4
30	r	503	CDL	OB7-CB5-OB6-CB4
30	s	402	CDL	OB7-CB5-OB6-CB4
31	l	701	PEE	O4-C10-O2-C2
31	l	704	PEE	O4-C10-O2-C2
31	s	403	PEE	O4-C10-O2-C2
30	s	402	CDL	C51-CB5-OB6-CB4
31	l	704	PEE	C11-C10-O2-C2
30	i	401	CDL	C31-CA7-OA8-CA6
30	s	402	CDL	C31-CA7-OA8-CA6
31	i	402	PEE	C31-C30-O3-C3
31	l	704	PEE	C31-C30-O3-C3
31	W	201	PEE	C17-C18-C19-C20
31	j	201	PEE	C17-C18-C19-C20
31	i	402	PEE	O4-C10-O2-C2
31	i	402	PEE	O5-C30-O3-C3
33	g	201	PLX	C2-C1-N1-C1A
30	a	201	CDL	O1-C1-CA2-OA2
30	a	201	CDL	O1-C1-CB2-OB2
30	l	702	CDL	O1-C1-CA2-OA2
30	r	503	CDL	O1-C1-CA2-OA2
30	s	402	CDL	O1-C1-CA2-OA2
30	s	402	CDL	O1-C1-CB2-OB2
30	V	201	CDL	C71-CB7-OB8-CB6
31	l	704	PEE	O5-C30-O3-C3
31	b	201	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
30	V	202	CDL	C11-C12-C13-C14
30	m	201	CDL	C73-C74-C75-C76
30	s	402	CDL	C37-C38-C39-C40
33	g	201	PLX	C9-C10-C11-C12
30	V	201	CDL	C62-C63-C64-C65
30	r	503	CDL	C74-C75-C76-C77
33	g	201	PLX	C7-C8-C9-C10
33	j	203	PLX	C13-C14-C15-C16
30	V	202	CDL	C32-C33-C34-C35
30	V	201	CDL	C32-C33-C34-C35
30	V	201	CDL	OB9-CB7-OB8-CB6
30	l	703	CDL	C71-CB7-OB8-CB6
30	m	201	CDL	C11-CA5-OA6-CA4
30	a	201	CDL	CA2-C1-CB2-OB2
30	n	102	CDL	CA2-C1-CB2-OB2
30	s	402	CDL	CA2-C1-CB2-OB2
31	b	201	PEE	O4-C10-O2-C2
30	l	703	CDL	C35-C36-C37-C38
30	l	702	CDL	C31-CA7-OA8-CA6
31	W	201	PEE	C31-C30-O3-C3
31	j	201	PEE	C31-C30-O3-C3
31	l	701	PEE	C31-C30-O3-C3
30	V	201	CDL	C59-C60-C61-C62
30	m	201	CDL	C62-C63-C64-C65
31	s	403	PEE	C42-C43-C44-C45
30	l	702	CDL	OA9-CA7-OA8-CA6
31	j	201	PEE	C11-C10-O2-C2
30	s	402	CDL	C31-C32-C33-C34
30	V	202	CDL	CB7-C71-C72-C73
31	r	501	PEE	C10-C11-C12-C13
31	j	201	PEE	O5-C30-O3-C3
31	l	701	PEE	O5-C30-O3-C3
30	m	201	CDL	C36-C37-C38-C39
30	n	102	CDL	C54-C55-C56-C57
30	s	402	CDL	CA7-C31-C32-C33
30	r	503	CDL	C60-C61-C62-C63
30	a	201	CDL	CA7-C31-C32-C33
30	i	401	CDL	CA7-C31-C32-C33
30	s	402	CDL	C14-C15-C16-C17
30	a	201	CDL	CA5-C11-C12-C13
30	s	402	CDL	CB7-C71-C72-C73
30	l	703	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	W	201	PEE	O5-C30-O3-C3
30	m	201	CDL	OA7-CA5-OA6-CA4
30	l	703	CDL	OB9-CB7-OB8-CB6
30	V	202	CDL	C72-C73-C74-C75
31	i	402	PEE	C37-C38-C39-C40
31	l	701	PEE	C17-C18-C19-C20
31	l	704	PEE	C37-C38-C39-C40
31	s	403	PEE	C17-C18-C19-C20
30	V	201	CDL	CB2-OB2-PB2-OB5
30	V	202	CDL	CB3-OB5-PB2-OB2
30	a	201	CDL	CB2-OB2-PB2-OB5
30	a	201	CDL	CB3-OB5-PB2-OB2
30	i	401	CDL	CA3-OA5-PA1-OA2
30	i	401	CDL	CB3-OB5-PB2-OB2
30	l	702	CDL	CB3-OB5-PB2-OB2
30	l	703	CDL	CA2-OA2-PA1-OA5
30	l	703	CDL	CA3-OA5-PA1-OA2
30	m	201	CDL	CA3-OA5-PA1-OA2
30	n	102	CDL	CA3-OA5-PA1-OA2
30	n	102	CDL	CB3-OB5-PB2-OB2
30	r	503	CDL	CA2-OA2-PA1-OA5
30	r	503	CDL	CB3-OB5-PB2-OB2
30	s	402	CDL	CA2-OA2-PA1-OA5
30	s	402	CDL	CA3-OA5-PA1-OA2
30	s	402	CDL	CB3-OB5-PB2-OB2
31	b	201	PEE	C1-O3P-P-O4P
31	j	201	PEE	C1-O3P-P-O4P
31	l	701	PEE	C4-O4P-P-O3P
33	j	202	PLX	C3-O4-P1-O1
33	j	202	PLX	C2-O1-P1-O4
33	n	101	PLX	C3-O4-P1-O1
33	r	502	PLX	C3-O4-P1-O1
31	i	402	PEE	C30-C31-C32-C33
31	b	201	PEE	C31-C30-O3-C3
30	m	201	CDL	C13-C14-C15-C16
30	r	503	CDL	CA5-C11-C12-C13
30	r	503	CDL	CB2-C1-CA2-OA2
31	j	201	PEE	O4-C10-O2-C2
33	g	201	PLX	C2-C1-N1-C1C
30	V	201	CDL	C58-C59-C60-C61
30	m	201	CDL	C32-C33-C34-C35
30	m	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
30	m	201	CDL	C60-C61-C62-C63
31	W	201	PEE	C21-C22-C23-C24
30	V	201	CDL	C51-CB5-OB6-CB4
31	r	501	PEE	C11-C10-O2-C2
30	V	201	CDL	C52-C53-C54-C55
30	V	201	CDL	C74-C75-C76-C77
30	V	202	CDL	C33-C34-C35-C36
30	a	201	CDL	C62-C63-C64-C65
30	a	201	CDL	C75-C76-C77-C78
30	l	702	CDL	C71-C72-C73-C74
30	s	402	CDL	C71-C72-C73-C74
33	g	201	PLX	C32-C33-C34-C35
33	j	202	PLX	C7-C8-C9-C10
33	j	203	PLX	C31-C32-C33-C34
33	n	101	PLX	C31-C32-C33-C34
30	a	201	CDL	C71-CB7-OB8-CB6
30	V	201	CDL	C37-C38-C39-C40
30	V	202	CDL	C37-C38-C39-C40
30	a	201	CDL	C17-C18-C19-C20
30	l	703	CDL	C11-C12-C13-C14
31	l	704	PEE	C21-C22-C23-C24
33	g	201	PLX	C11-C12-C13-C14
33	j	202	PLX	C31-C32-C33-C34
33	r	502	PLX	C13-C14-C15-C16
31	r	501	PEE	O4-C10-O2-C2
30	V	202	CDL	C59-C60-C61-C62
30	m	201	CDL	C11-C12-C13-C14
31	b	201	PEE	C33-C34-C35-C36
33	j	202	PLX	C30-C31-C32-C33
33	r	502	PLX	C25-C26-C27-C28
30	m	201	CDL	C61-C62-C63-C64
30	r	503	CDL	C35-C36-C37-C38
30	s	402	CDL	C75-C76-C77-C78
33	j	202	PLX	C28-C29-C30-C31
33	j	203	PLX	C16-C17-C18-C19
33	j	203	PLX	C7-C8-C9-C10
30	l	703	CDL	O1-C1-CB2-OB2
30	m	201	CDL	O1-C1-CA2-OA2
30	V	201	CDL	C33-C34-C35-C36
30	a	201	CDL	C60-C61-C62-C63
30	r	503	CDL	C57-C58-C59-C60
33	g	201	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	l	702	CDL	CA5-C11-C12-C13
30	l	702	CDL	CB5-C51-C52-C53
30	V	202	CDL	C71-CB7-OB8-CB6
30	a	201	CDL	C73-C74-C75-C76
30	m	201	CDL	C79-C80-C81-C82
30	r	503	CDL	C32-C33-C34-C35
31	b	201	PEE	C31-C32-C33-C34
31	i	402	PEE	C21-C22-C23-C24
31	l	701	PEE	C11-C12-C13-C14
33	j	203	PLX	C14-C15-C16-C17
33	n	101	PLX	C13-C14-C15-C16
30	V	201	CDL	C31-C32-C33-C34
30	a	201	CDL	C33-C34-C35-C36
30	i	401	CDL	C37-C38-C39-C40
30	s	402	CDL	C17-C18-C19-C20
31	s	401	PEE	C13-C14-C15-C16
33	g	201	PLX	C14-C15-C16-C17
30	V	202	CDL	C14-C15-C16-C17
30	V	202	CDL	C42-C43-C44-C45
30	m	201	CDL	C75-C76-C77-C78
30	s	402	CDL	C73-C74-C75-C76
31	W	201	PEE	C12-C13-C14-C15
33	g	201	PLX	C25-C26-C27-C28
33	n	101	PLX	C10-C11-C12-C13
33	n	101	PLX	C25-C26-C27-C28
33	r	502	PLX	C10-C11-C12-C13
31	b	201	PEE	O5-C30-O3-C3
30	V	202	CDL	C52-C53-C54-C55
30	a	201	CDL	C37-C38-C39-C40
30	m	201	CDL	C59-C60-C61-C62
33	j	203	PLX	C9-C10-C11-C12
33	n	101	PLX	C27-C28-C29-C30
30	V	201	CDL	OB7-CB5-OB6-CB4
30	V	201	CDL	C11-C12-C13-C14
30	V	202	CDL	C17-C18-C19-C20
30	m	201	CDL	C34-C35-C36-C37
31	s	401	PEE	C23-C24-C25-C26
31	W	201	PEE	C15-C16-C17-C18
31	l	701	PEE	C35-C36-C37-C38
30	r	503	CDL	CB7-C71-C72-C73
30	m	201	CDL	C71-C72-C73-C74
30	r	503	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	r	503	CDL	C14-C15-C16-C17
30	r	503	CDL	C73-C74-C75-C76
32	X	201	8Q1	C11-C12-C13-C14
33	j	202	PLX	C14-C15-C16-C17
33	j	202	PLX	C9-C10-C11-C12
33	j	203	PLX	C25-C26-C27-C28
33	j	203	PLX	C33-C34-C35-C36
33	g	201	PLX	C2-C1-N1-C1B
30	l	703	CDL	C55-C56-C57-C58
30	r	503	CDL	C37-C38-C39-C40
33	j	202	PLX	C33-C34-C35-C36
30	l	703	CDL	C14-C15-C16-C17
30	l	703	CDL	C59-C60-C61-C62
33	j	203	PLX	C12-C13-C14-C15
30	V	202	CDL	CA7-C31-C32-C33
30	V	202	CDL	C74-C75-C76-C77
30	s	402	CDL	C52-C53-C54-C55
33	j	202	PLX	C32-C33-C34-C35
30	r	503	CDL	C62-C63-C64-C65
31	l	704	PEE	C43-C44-C45-C46
30	l	703	CDL	C74-C75-C76-C77
30	r	503	CDL	C71-C72-C73-C74
31	b	201	PEE	C22-C23-C24-C25
33	g	201	PLX	C30-C31-C32-C33
30	V	202	CDL	C82-C83-C84-C85
30	l	702	CDL	C32-C33-C34-C35
31	r	501	PEE	C13-C14-C15-C16
33	j	203	PLX	C28-C29-C30-C31
31	i	402	PEE	C17-C18-C19-C20
31	r	501	PEE	C37-C38-C39-C40
30	s	402	CDL	C59-C60-C61-C62
33	n	101	PLX	C14-C15-C16-C17
33	r	502	PLX	C27-C28-C29-C30
30	V	201	CDL	C31-CA7-OA8-CA6
31	W	201	PEE	C11-C10-O2-C2
30	V	201	CDL	C71-C72-C73-C74
30	V	202	CDL	C73-C74-C75-C76
30	m	201	CDL	C14-C15-C16-C17
33	r	502	PLX	C14-C15-C16-C17
33	r	502	PLX	C11-C12-C13-C14
33	j	202	PLX	O9-C24-C25-C26
30	r	503	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
30	s	402	CDL	C55-C56-C57-C58
30	s	402	CDL	C82-C83-C84-C85
31	r	501	PEE	C40-C41-C42-C43
31	s	401	PEE	C19-C20-C21-C22
30	V	202	CDL	CB5-C51-C52-C53
30	V	202	CDL	C13-C14-C15-C16
31	s	403	PEE	C12-C13-C14-C15
33	j	202	PLX	C34-C35-C36-C37
30	V	201	CDL	C14-C15-C16-C17
30	s	402	CDL	C33-C34-C35-C36
33	g	201	PLX	C28-C29-C30-C31
30	V	201	CDL	C55-C56-C57-C58
33	g	201	PLX	C13-C14-C15-C16
33	j	202	PLX	C11-C12-C13-C14
31	W	201	PEE	O4-C10-O2-C2
30	a	201	CDL	C71-C72-C73-C74
30	l	702	CDL	C52-C53-C54-C55
30	r	503	CDL	C75-C76-C77-C78
30	r	503	CDL	C77-C78-C79-C80
31	r	501	PEE	C12-C13-C14-C15
33	j	202	PLX	C13-C14-C15-C16
33	j	203	PLX	C29-C30-C31-C32
30	V	202	CDL	OB9-CB7-OB8-CB6
30	a	201	CDL	OB9-CB7-OB8-CB6
30	V	202	CDL	C75-C76-C77-C78
31	l	701	PEE	C32-C33-C34-C35
31	s	403	PEE	C31-C32-C33-C34
33	r	502	PLX	C11-C10-C9-C8
31	W	201	PEE	C10-C11-C12-C13
30	V	202	CDL	C35-C36-C37-C38
30	l	703	CDL	C51-C52-C53-C54
30	r	503	CDL	C41-C42-C43-C44
30	s	402	CDL	C71-CB7-OB8-CB6
30	V	201	CDL	C72-C73-C74-C75
30	s	402	CDL	CB5-C51-C52-C53
31	l	701	PEE	C10-C11-C12-C13
30	m	201	CDL	C41-C42-C43-C44
33	r	502	PLX	C30-C31-C32-C33
31	l	701	PEE	C18-C19-C20-C21
30	V	201	CDL	OA9-CA7-OA8-CA6
30	s	402	CDL	OB9-CB7-OB8-CB6
30	a	201	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	g	201	PLX	C12-C13-C14-C15
31	s	403	PEE	C35-C36-C37-C38
31	s	403	PEE	C39-C40-C41-C42
30	r	503	CDL	C71-CB7-OB8-CB6
30	l	703	CDL	C32-C33-C34-C35
30	l	703	CDL	C37-C38-C39-C40
30	l	703	CDL	C73-C74-C75-C76
30	l	703	CDL	C79-C80-C81-C82
30	r	503	CDL	C31-C32-C33-C34
31	l	704	PEE	C31-C32-C33-C34
30	n	102	CDL	CB5-C51-C52-C53
30	a	201	CDL	C52-C53-C54-C55
31	W	201	PEE	C13-C14-C15-C16
32	X	201	8Q1	N36-C37-C38-C39
30	a	201	CDL	C21-C22-C23-C24
30	s	402	CDL	C35-C36-C37-C38
31	r	501	PEE	C20-C21-C22-C23
32	X	201	8Q1	C6-C7-C8-C9
30	l	703	CDL	C11-CA5-OA6-CA4
30	V	201	CDL	OB5-CB3-CB4-OB6
30	m	201	CDL	OA5-CA3-CA4-OA6
33	j	202	PLX	C11-C10-C9-C8
31	s	403	PEE	C36-C37-C38-C39
30	l	703	CDL	C31-C32-C33-C34
30	V	202	CDL	C62-C63-C64-C65
30	a	201	CDL	C31-C32-C33-C34
33	n	101	PLX	C9-C10-C11-C12
33	g	201	PLX	O6-C4-C5-O8
30	V	202	CDL	C34-C35-C36-C37
30	r	503	CDL	C83-C84-C85-C86
31	W	201	PEE	C24-C25-C26-C27
30	m	201	CDL	C18-C19-C20-C21
31	l	704	PEE	C34-C35-C36-C37
33	j	202	PLX	C27-C28-C29-C30
31	i	402	PEE	C19-C20-C21-C22
31	r	501	PEE	C39-C40-C41-C42
30	s	402	CDL	C36-C37-C38-C39
31	r	501	PEE	C41-C42-C43-C44
31	j	201	PEE	C34-C35-C36-C37
31	i	402	PEE	C20-C21-C22-C23
33	j	203	PLX	C27-C28-C29-C30
30	l	703	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
30	s	402	CDL	C51-C52-C53-C54
31	r	501	PEE	C36-C37-C38-C39
30	V	201	CDL	CB3-OB5-PB2-OB2
30	V	202	CDL	CA3-OA5-PA1-OA2
30	l	703	CDL	CB2-OB2-PB2-OB5
31	i	402	PEE	C4-O4P-P-O3P
30	V	201	CDL	C54-C55-C56-C57
30	r	503	CDL	OB9-CB7-OB8-CB6
30	a	201	CDL	OB5-CB3-CB4-CB6
31	i	402	PEE	O3P-C1-C2-C3
31	l	704	PEE	O3P-C1-C2-C3
31	j	201	PEE	C23-C24-C25-C26
31	s	401	PEE	C11-C12-C13-C14
31	s	403	PEE	C22-C23-C24-C25
33	r	502	PLX	C29-C30-C31-C32
30	m	201	CDL	C16-C17-C18-C19
30	l	702	CDL	CB2-C1-CA2-OA2
30	m	201	CDL	C19-C20-C21-C22
30	r	503	CDL	C59-C60-C61-C62
31	s	401	PEE	C12-C13-C14-C15
33	n	101	PLX	C28-C29-C30-C31
31	j	201	PEE	C38-C39-C40-C41
30	V	202	CDL	C40-C41-C42-C43
30	n	102	CDL	C11-CA5-OA6-CA4
31	b	201	PEE	C13-C14-C15-C16
33	j	203	PLX	C11-C12-C13-C14
30	m	201	CDL	CA3-CA4-CA6-OA8
30	n	102	CDL	CA3-CA4-CA6-OA8
31	W	201	PEE	C1-C2-C3-O3
33	j	202	PLX	C3-C4-C5-O8
33	j	202	PLX	C25-C26-C27-C28
33	j	203	PLX	C3-C4-C5-O8
33	n	101	PLX	C3-C4-C5-O8
33	r	502	PLX	C3-C4-C5-O8
30	V	202	CDL	C60-C61-C62-C63
30	m	201	CDL	C33-C34-C35-C36
33	g	201	PLX	C10-C11-C12-C13
33	g	201	PLX	C11-C10-C9-C8
30	V	202	CDL	C84-C85-C86-C87
30	a	201	CDL	C11-C12-C13-C14
30	l	703	CDL	C75-C76-C77-C78
33	r	502	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	a	201	CDL	C32-C33-C34-C35
31	l	704	PEE	C15-C16-C17-C18
30	n	102	CDL	C52-C53-C54-C55
31	r	501	PEE	C21-C22-C23-C24
30	V	202	CDL	C64-C65-C66-C67
30	l	703	CDL	CB7-C71-C72-C73
30	m	201	CDL	CA6-CA4-OA6-CA5
33	n	101	PLX	C26-C27-C28-C29
30	m	201	CDL	C20-C21-C22-C23
30	r	503	CDL	C33-C34-C35-C36
30	r	503	CDL	C56-C57-C58-C59
31	l	704	PEE	C24-C25-C26-C27
33	n	101	PLX	C16-C17-C18-C19
31	W	201	PEE	O3P-C1-C2-O2
31	l	704	PEE	C30-C31-C32-C33
30	V	202	CDL	C41-C42-C43-C44
30	r	503	CDL	C64-C65-C66-C67
31	s	403	PEE	C23-C24-C25-C26
30	V	202	CDL	OA6-CA4-CA6-OA8
30	i	401	CDL	OB6-CB4-CB6-OB8
30	m	201	CDL	OB6-CB4-CB6-OB8
33	n	101	PLX	O6-C4-C5-O8
33	j	202	PLX	C12-C13-C14-C15
31	r	501	PEE	C31-C32-C33-C34
33	r	502	PLX	C28-C29-C30-C31
33	r	502	PLX	C18-C19-C20-C21
30	l	703	CDL	C82-C83-C84-C85
30	r	503	CDL	C54-C55-C56-C57
30	m	201	CDL	C71-CB7-OB8-CB6
31	j	201	PEE	C32-C33-C34-C35
31	l	704	PEE	C11-C12-C13-C14
30	s	402	CDL	C54-C55-C56-C57
31	s	403	PEE	C34-C35-C36-C37
30	s	402	CDL	C34-C35-C36-C37
33	g	201	PLX	C33-C34-C35-C36
32	X	201	8Q1	C10-C11-C12-C13
30	V	201	CDL	OB5-CB3-CB4-CB6
30	l	703	CDL	OB5-CB3-CB4-CB6
30	m	201	CDL	OA5-CA3-CA4-CA6
30	a	201	CDL	C35-C36-C37-C38
31	j	201	PEE	C30-C31-C32-C33
30	a	201	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
30	s	402	CDL	C40-C41-C42-C43
30	r	503	CDL	CA7-C31-C32-C33
30	r	503	CDL	C42-C43-C44-C45
33	n	101	PLX	C29-C30-C31-C32
30	m	201	CDL	C52-C53-C54-C55
33	n	101	PLX	C30-C31-C32-C33
30	V	201	CDL	C1-CB2-OB2-PB2
30	m	201	CDL	CA4-CA3-OA5-PA1
30	r	503	CDL	C1-CB2-OB2-PB2
31	i	402	PEE	C18-C19-C20-C21
30	i	401	CDL	C71-C72-C73-C74
30	m	201	CDL	C17-C18-C19-C20
30	m	201	CDL	C64-C65-C66-C67
31	r	501	PEE	C14-C15-C16-C17
30	V	201	CDL	C75-C76-C77-C78
30	s	402	CDL	C12-C13-C14-C15
31	s	403	PEE	C44-C45-C46-C47
30	m	201	CDL	CB3-CB4-CB6-OB8
31	b	201	PEE	C1-C2-C3-O3
31	i	402	PEE	C1-C2-C3-O3
31	l	704	PEE	C1-C2-C3-O3
31	r	501	PEE	C1-C2-C3-O3
33	g	201	PLX	C3-C4-C5-O8
31	r	501	PEE	C17-C18-C19-C20
30	m	201	CDL	C82-C83-C84-C85
31	l	704	PEE	C32-C33-C34-C35
30	l	703	CDL	C12-C13-C14-C15
30	a	201	CDL	C36-C37-C38-C39
31	s	401	PEE	C22-C23-C24-C25
30	r	503	CDL	C84-C85-C86-C87
33	r	502	PLX	C36-C37-C38-C39
30	a	201	CDL	CA2-OA2-PA1-OA5
31	r	501	PEE	C1-O3P-P-O4P
33	j	202	PLX	C5-C4-O6-C6
30	l	703	CDL	C61-C62-C63-C64
31	s	403	PEE	C13-C14-C15-C16
33	g	201	PLX	O9-C24-C25-C26
33	r	502	PLX	O9-C24-C25-C26
30	V	201	CDL	OA5-CA3-CA4-OA6
30	a	201	CDL	OB5-CB3-CB4-OB6
30	n	102	CDL	OB5-CB3-CB4-OB6
31	b	201	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
30	l	703	CDL	C64-C65-C66-C67
31	s	403	PEE	C21-C22-C23-C24
30	m	201	CDL	OB9-CB7-OB8-CB6
33	j	202	PLX	C26-C27-C28-C29
31	b	201	PEE	O2-C2-C3-O3
31	i	402	PEE	O2-C2-C3-O3
31	r	501	PEE	O2-C2-C3-O3
33	r	502	PLX	O6-C4-C5-O8
30	V	202	CDL	C31-C32-C33-C34
33	n	101	PLX	C15-C16-C17-C18
30	V	202	CDL	CB2-C1-CA2-OA2
30	V	202	CDL	CA2-C1-CB2-OB2
31	s	401	PEE	C24-C25-C26-C27
30	n	102	CDL	OA7-CA5-OA6-CA4
30	l	703	CDL	C62-C63-C64-C65
31	l	704	PEE	C42-C43-C44-C45
32	X	201	8Q1	C12-C13-C14-C15
30	l	702	CDL	C51-C52-C53-C54
33	n	101	PLX	C12-C13-C14-C15
30	V	202	CDL	C55-C56-C57-C58
30	V	202	CDL	C15-C16-C17-C18
31	s	403	PEE	C38-C39-C40-C41
30	m	201	CDL	C31-C32-C33-C34
31	i	402	PEE	C24-C25-C26-C27
30	V	201	CDL	CA7-C31-C32-C33
30	l	703	CDL	C51-CB5-OB6-CB4
30	r	503	CDL	C51-C52-C53-C54
30	s	402	CDL	C84-C85-C86-C87
33	j	203	PLX	O6-C6-C7-C8
30	m	201	CDL	C84-C85-C86-C87
30	n	102	CDL	OB5-CB3-CB4-CB6
33	j	202	PLX	O4-C3-C4-C5
30	i	401	CDL	O1-C1-CB2-OB2
31	j	201	PEE	C36-C37-C38-C39
31	r	501	PEE	C38-C39-C40-C41
31	W	201	PEE	C11-C12-C13-C14
33	j	202	PLX	C10-C11-C12-C13
31	s	403	PEE	C20-C21-C22-C23
30	i	401	CDL	C71-CB7-OB8-CB6
31	i	402	PEE	C31-C32-C33-C34
30	r	503	CDL	C39-C40-C41-C42
32	X	201	8Q1	C28-O27-P24-O1

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Mol	Chain	Res	Type	Atoms
30	V	202	CDL	C12-C13-C14-C15
30	a	201	CDL	C54-C55-C56-C57
30	m	201	CDL	C15-C16-C17-C18
30	r	503	CDL	C82-C83-C84-C85
33	n	101	PLX	C11-C12-C13-C14
33	r	502	PLX	C26-C27-C28-C29
30	n	102	CDL	CA6-CA4-OA6-CA5
33	g	201	PLX	C31-C32-C33-C34
31	b	201	PEE	C10-C11-C12-C13
30	n	102	CDL	C1-CB2-OB2-PB2
31	W	201	PEE	C20-C21-C22-C23
30	V	202	CDL	OB5-CB3-CB4-OB6
30	l	703	CDL	OB5-CB3-CB4-OB6
30	m	201	CDL	OB5-CB3-CB4-OB6
31	i	402	PEE	O3P-C1-C2-O2
31	j	201	PEE	O3P-C1-C2-O2
31	l	701	PEE	O3P-C1-C2-O2
31	r	501	PEE	O3P-C1-C2-O2
33	j	202	PLX	O4-C3-C4-O6
30	l	703	CDL	C21-C22-C23-C24
30	V	202	CDL	O1-C1-CB2-OB2
30	l	703	CDL	OB7-CB5-OB6-CB4
30	l	703	CDL	C15-C16-C17-C18
30	m	201	CDL	OA6-CA4-CA6-OA8
30	n	102	CDL	OA6-CA4-CA6-OA8
31	l	704	PEE	O2-C2-C3-O3
30	a	201	CDL	C22-C23-C24-C25
31	j	201	PEE	C19-C20-C21-C22
30	a	201	CDL	C84-C85-C86-C87
33	j	202	PLX	C35-C36-C37-C38
30	i	401	CDL	OB9-CB7-OB8-CB6
33	r	502	PLX	C7-C8-C9-C10
30	i	401	CDL	C15-C16-C17-C18
30	V	202	CDL	CB2-OB2-PB2-OB5
30	l	702	CDL	CA3-OA5-PA1-OA2
30	n	102	CDL	CB2-OB2-PB2-OB5
30	l	702	CDL	CA4-CA3-OA5-PA1
30	V	201	CDL	CA3-OA5-PA1-OA3
30	V	201	CDL	CB2-OB2-PB2-OB4
30	V	202	CDL	CB2-OB2-PB2-OB3
30	V	202	CDL	CB2-OB2-PB2-OB4
30	V	202	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
30	V	202	CDL	CB3-OB5-PB2-OB4
30	a	201	CDL	CB2-OB2-PB2-OB4
30	i	401	CDL	CB3-OB5-PB2-OB3
30	l	702	CDL	CA3-OA5-PA1-OA4
30	l	703	CDL	CA2-OA2-PA1-OA4
30	l	703	CDL	CA3-OA5-PA1-OA4
30	l	703	CDL	CB2-OB2-PB2-OB3
30	m	201	CDL	CA3-OA5-PA1-OA4
30	n	102	CDL	CA2-OA2-PA1-OA4
30	n	102	CDL	CB3-OB5-PB2-OB3
30	r	503	CDL	CA2-OA2-PA1-OA4
30	r	503	CDL	CB3-OB5-PB2-OB4
30	s	402	CDL	CA3-OA5-PA1-OA3
30	s	402	CDL	CA3-OA5-PA1-OA4
30	s	402	CDL	CB3-OB5-PB2-OB4
31	W	201	PEE	C4-O4P-P-O2P
31	b	201	PEE	C1-O3P-P-O2P
31	b	201	PEE	C1-O3P-P-O1P
31	i	402	PEE	C4-O4P-P-O2P
31	j	201	PEE	C1-O3P-P-O2P
31	l	704	PEE	C4-O4P-P-O2P
31	r	501	PEE	C1-O3P-P-O2P
31	s	401	PEE	C1-O3P-P-O2P
33	j	202	PLX	C3-O4-P1-O2
33	j	202	PLX	C3-O4-P1-O3
33	j	202	PLX	C2-O1-P1-O3
33	j	203	PLX	C2-O1-P1-O3
33	n	101	PLX	C3-O4-P1-O2
33	n	101	PLX	C2-O1-P1-O3
34	w	401	ADP	C5'-O5'-PA-O1A
31	b	201	PEE	O3P-C1-C2-C3
31	j	201	PEE	O3P-C1-C2-C3
31	l	701	PEE	O3P-C1-C2-C3
30	V	202	CDL	C32-C31-CA7-OA8
31	s	403	PEE	C37-C38-C39-C40
31	W	201	PEE	C5-C4-O4P-P
33	g	201	PLX	C25-C24-O8-C5
33	j	203	PLX	C25-C24-O8-C5
30	l	703	CDL	C12-C11-CA5-OA6
30	r	503	CDL	C52-C53-C54-C55
31	b	201	PEE	C15-C16-C17-C18
30	l	702	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
30	i	401	CDL	CA5-C11-C12-C13
31	s	401	PEE	C31-C32-C33-C34
30	a	201	CDL	OA5-CA3-CA4-OA6
33	n	101	PLX	O4-C3-C4-O6
30	i	401	CDL	C35-C36-C37-C38
31	i	402	PEE	C11-C12-C13-C14
30	V	202	CDL	C58-C59-C60-C61
30	l	702	CDL	C82-C83-C84-C85
30	V	202	CDL	O1-C1-CA2-OA2
30	a	201	CDL	C74-C75-C76-C77
30	l	702	CDL	C55-C56-C57-C58
30	l	703	CDL	C81-C82-C83-C84
33	r	502	PLX	C16-C17-C18-C19
30	V	202	CDL	CA3-CA4-CA6-OA8
30	i	401	CDL	CB3-CB4-CB6-OB8
30	s	402	CDL	CB3-CB4-CB6-OB8
33	j	202	PLX	N1-C1-C2-O1
31	W	201	PEE	O2-C2-C3-O3
33	j	202	PLX	O6-C4-C5-O8
33	j	203	PLX	O6-C4-C5-O8
30	V	202	CDL	C71-C72-C73-C74
32	X	201	8Q1	C9-C10-C11-C12
30	V	201	CDL	C34-C35-C36-C37
30	l	702	CDL	C76-C77-C78-C79
30	l	703	CDL	C71-C72-C73-C74
30	r	503	CDL	C13-C14-C15-C16
30	l	703	CDL	C44-C45-C46-C47
33	g	201	PLX	O6-C6-C7-C8
33	g	201	PLX	O7-C6-C7-C8
33	r	502	PLX	O7-C6-C7-C8
30	i	401	CDL	O1-C1-CA2-OA2
30	l	702	CDL	C20-C21-C22-C23
30	l	702	CDL	C36-C37-C38-C39
30	V	201	CDL	CA6-CA4-OA6-CA5
30	i	401	CDL	CA6-CA4-OA6-CA5
30	l	702	CDL	CA6-CA4-OA6-CA5
31	l	704	PEE	C1-C2-O2-C10
30	V	201	CDL	OA5-CA3-CA4-CA6
30	V	202	CDL	OB5-CB3-CB4-CB6
31	W	201	PEE	O3P-C1-C2-C3
31	r	501	PEE	O3P-C1-C2-C3
33	n	101	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	O4-C3-C4-C5
30	i	401	CDL	C38-C39-C40-C41
30	V	201	CDL	CA4-CA3-OA5-PA1
31	j	201	PEE	C41-C42-C43-C44
32	X	201	8Q1	C11-C10-C9-C8
33	r	502	PLX	O4-C3-C4-O6
33	j	203	PLX	C32-C33-C34-C35
30	V	201	CDL	C40-C41-C42-C43
33	r	502	PLX	C33-C34-C35-C36
30	s	402	CDL	C72-C71-CB7-OB8
31	r	501	PEE	C11-C12-C13-C14
30	V	201	CDL	OB6-CB4-CB6-OB8
33	g	201	PLX	C15-C16-C17-C18
30	V	202	CDL	CA2-OA2-PA1-OA5
30	l	702	CDL	CB2-OB2-PB2-OB5
33	j	203	PLX	C2-O1-P1-O4
32	X	201	8Q1	C13-C14-C15-C16
30	m	201	CDL	CA5-C11-C12-C13
30	a	201	CDL	C12-C13-C14-C15
30	a	201	CDL	C64-C65-C66-C67
30	V	202	CDL	C57-C58-C59-C60
31	b	201	PEE	C16-C17-C18-C19
31	j	201	PEE	C16-C17-C18-C19
30	l	702	CDL	C11-C12-C13-C14
31	i	402	PEE	C39-C40-C41-C42
31	s	401	PEE	C15-C16-C17-C18
30	V	202	CDL	C54-C55-C56-C57
31	W	201	PEE	C34-C35-C36-C37
31	b	201	PEE	C18-C19-C20-C21
31	l	704	PEE	C13-C14-C15-C16
30	V	201	CDL	C64-C65-C66-C67
30	m	201	CDL	C42-C43-C44-C45
30	a	201	CDL	OA5-CA3-CA4-CA6
33	j	203	PLX	C18-C19-C20-C21
30	V	201	CDL	C21-C22-C23-C24
30	a	201	CDL	C14-C15-C16-C17
32	X	201	8Q1	C7-C8-C9-C10
30	l	702	CDL	C13-C14-C15-C16
30	a	201	CDL	C55-C56-C57-C58
33	r	502	PLX	C34-C35-C36-C37
33	j	203	PLX	C30-C31-C32-C33
31	s	403	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
31	i	402	PEE	C15-C16-C17-C18
31	s	401	PEE	C14-C15-C16-C17
30	a	201	CDL	C13-C14-C15-C16
30	m	201	CDL	C77-C78-C79-C80
31	b	201	PEE	C23-C24-C25-C26
30	V	201	CDL	CB2-C1-CA2-OA2
30	l	702	CDL	OB7-CB5-OB6-CB4
31	i	402	PEE	C33-C34-C35-C36
30	r	503	CDL	C15-C16-C17-C18
31	j	201	PEE	C12-C13-C14-C15
30	a	201	CDL	C43-C44-C45-C46
30	n	102	CDL	C57-C58-C59-C60
30	a	201	CDL	C16-C17-C18-C19
31	b	201	PEE	C11-C12-C13-C14
30	V	202	CDL	C44-C45-C46-C47
30	l	703	CDL	CB5-C51-C52-C53
30	l	702	CDL	C62-C63-C64-C65
31	l	701	PEE	C14-C15-C16-C17
31	l	701	PEE	C33-C34-C35-C36
31	s	403	PEE	C31-C30-O3-C3
30	m	201	CDL	C74-C75-C76-C77
31	s	401	PEE	O2-C2-C3-O3
30	V	201	CDL	C60-C61-C62-C63
30	a	201	CDL	C44-C45-C46-C47
31	s	403	PEE	O5-C30-O3-C3
30	l	703	CDL	CA2-C1-CB2-OB2
30	r	503	CDL	C20-C21-C22-C23
33	j	203	PLX	C24-C25-C26-C27
30	l	702	CDL	C51-CB5-OB6-CB4
31	l	704	PEE	C19-C20-C21-C22
31	i	402	PEE	C34-C35-C36-C37
31	s	401	PEE	C18-C19-C20-C21
30	n	102	CDL	C71-C72-C73-C74
31	s	403	PEE	C10-C11-C12-C13
30	a	201	CDL	C53-C54-C55-C56
30	s	402	CDL	C74-C75-C76-C77
31	b	201	PEE	C38-C39-C40-C41
30	l	703	CDL	C41-C42-C43-C44
33	j	202	PLX	O8-C24-C25-C26
30	m	201	CDL	OB5-CB3-CB4-CB6
32	X	201	8Q1	O33-C32-C34-O35
31	i	402	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
31	l	701	PEE	O3-C30-C31-C32
31	l	701	PEE	C2-C1-O3P-P
30	i	401	CDL	C12-C11-CA5-OA6
30	l	703	CDL	C72-C71-CB7-OB8
31	j	201	PEE	O2-C10-C11-C12
31	r	501	PEE	C16-C17-C18-C19
30	n	102	CDL	C74-C75-C76-C77
30	s	402	CDL	C12-C11-CA5-OA6
31	W	201	PEE	C16-C17-C18-C19
30	l	703	CDL	C39-C40-C41-C42
30	l	702	CDL	CA3-CA4-OA6-CA5
31	l	704	PEE	C3-C2-O2-C10
30	a	201	CDL	C51-C52-C53-C54
30	a	201	CDL	C32-C31-CA7-OA8
31	i	402	PEE	C36-C37-C38-C39
31	s	401	PEE	C16-C17-C18-C19
31	s	403	PEE	C16-C17-C18-C19
33	j	203	PLX	C7-C6-O6-C4
30	s	402	CDL	C19-C20-C21-C22
30	s	402	CDL	C15-C16-C17-C18
33	j	202	PLX	C29-C30-C31-C32
30	s	402	CDL	C16-C17-C18-C19
30	l	702	CDL	C72-C73-C74-C75
31	s	403	PEE	C18-C19-C20-C21
30	a	201	CDL	C12-C11-CA5-OA6
30	r	503	CDL	C72-C71-CB7-OB8
31	j	201	PEE	C24-C25-C26-C27
30	l	702	CDL	C72-C71-CB7-OB8
30	m	201	CDL	C12-C11-CA5-OA6
30	l	702	CDL	C38-C39-C40-C41
30	i	401	CDL	OA6-CA4-CA6-OA8
30	r	503	CDL	OA6-CA4-CA6-OA8
31	l	704	PEE	C18-C19-C20-C21
30	l	703	CDL	C56-C57-C58-C59
31	b	201	PEE	O3-C30-C31-C32
31	s	401	PEE	O3-C30-C31-C32
30	V	202	CDL	C63-C64-C65-C66
30	i	401	CDL	C32-C33-C34-C35
33	r	502	PLX	C9-C10-C11-C12
34	w	401	ADP	PB-O3A-PA-O2A
31	j	201	PEE	C44-C45-C46-C47
30	s	402	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
30	a	201	CDL	C82-C83-C84-C85
31	l	701	PEE	C38-C39-C40-C41
30	a	201	CDL	C39-C40-C41-C42
30	a	201	CDL	C76-C77-C78-C79
30	r	503	CDL	C21-C22-C23-C24
30	i	401	CDL	C12-C11-CA5-OA7
31	s	401	PEE	O5-C30-C31-C32
30	a	201	CDL	C12-C11-CA5-OA7
30	a	201	CDL	C32-C31-CA7-OA9
31	j	201	PEE	O4-C10-C11-C12
31	l	701	PEE	O5-C30-C31-C32
30	V	202	CDL	C22-C23-C24-C25
30	i	401	CDL	CA3-CA4-CA6-OA8
30	l	703	CDL	C43-C44-C45-C46
31	s	403	PEE	C41-C42-C43-C44
30	l	703	CDL	C72-C71-CB7-OB9
30	l	702	CDL	C72-C71-CB7-OB9
30	l	702	CDL	CB2-OB2-PB2-OB3
31	W	201	PEE	C1-O3P-P-O1P
31	s	403	PEE	C4-O4P-P-O1P
33	j	202	PLX	C36-C37-C38-C39
30	m	201	CDL	C12-C11-CA5-OA7
30	r	503	CDL	C12-C13-C14-C15
30	V	202	CDL	C24-C25-C26-C27
33	j	202	PLX	C1-C2-O1-P1
33	g	201	PLX	C6-C7-C8-C9
30	V	201	CDL	O1-C1-CA2-OA2
33	g	201	PLX	C18-C19-C20-C21
30	m	201	CDL	C35-C36-C37-C38
31	b	201	PEE	O5-C30-C31-C32
31	l	704	PEE	C22-C23-C24-C25
30	l	703	CDL	OA5-CA3-CA4-OA6
31	r	501	PEE	C44-C45-C46-C47
30	l	703	CDL	C36-C37-C38-C39
31	j	201	PEE	O3-C30-C31-C32
30	a	201	CDL	C18-C19-C20-C21
31	r	501	PEE	C42-C43-C44-C45

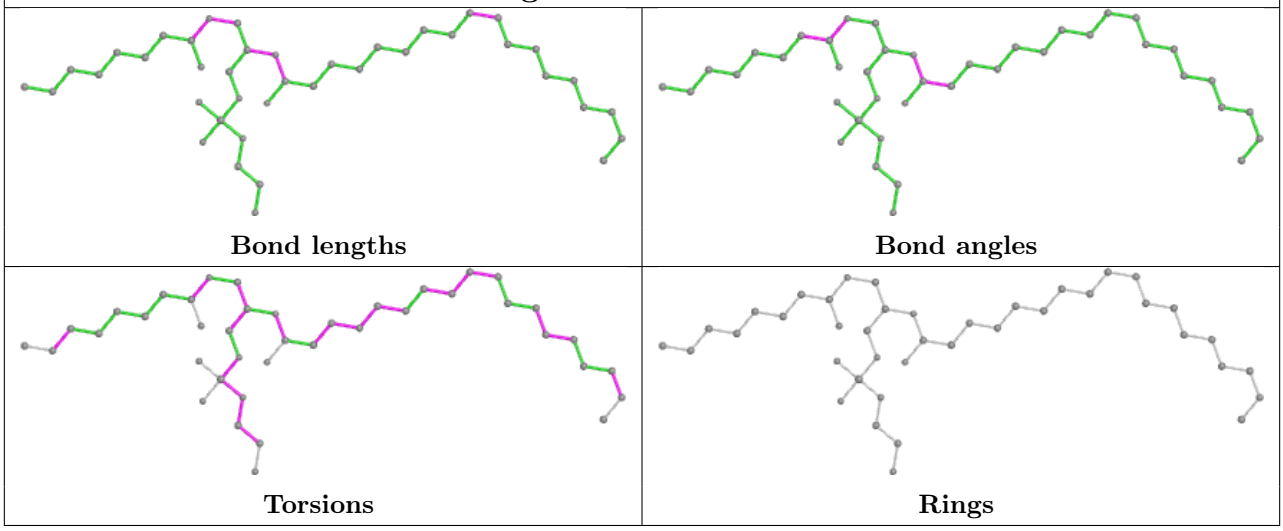
There are no ring outliers.

No monomer is involved in short contacts.

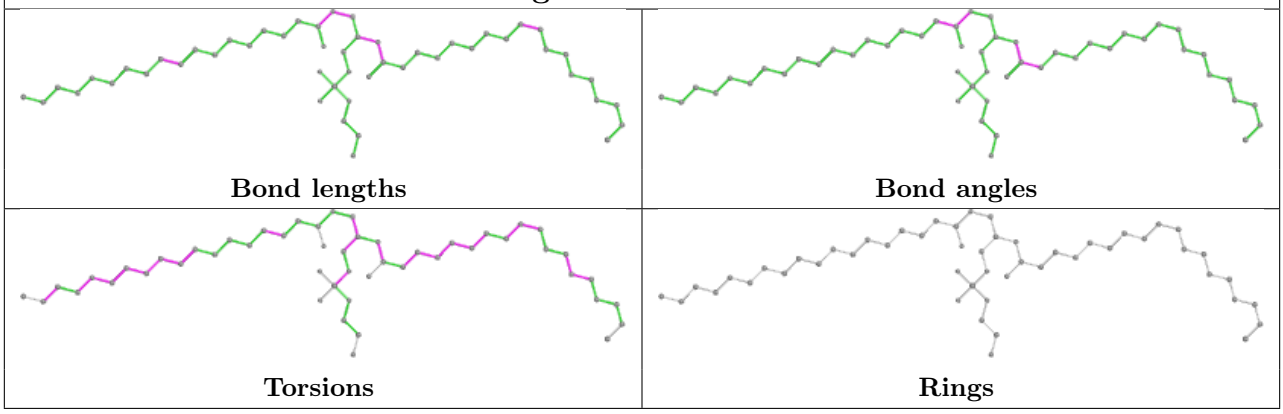
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

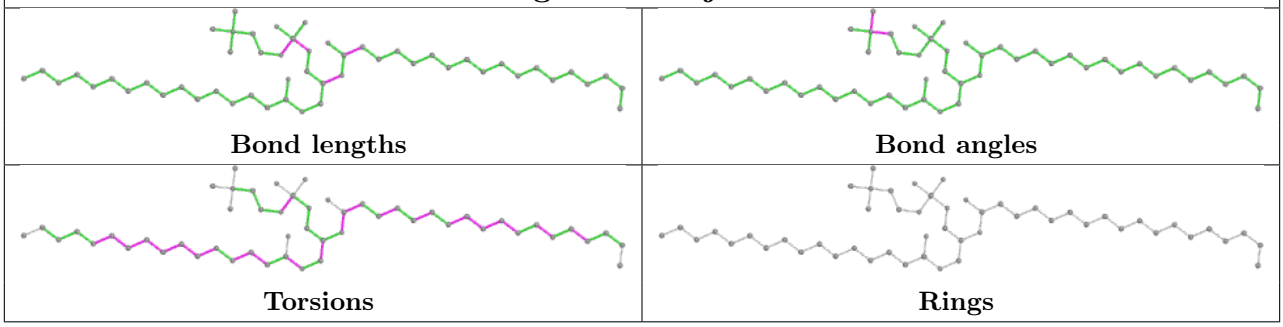
Ligand PEE W 201



Ligand PEE r 501



Ligand PLX j 203



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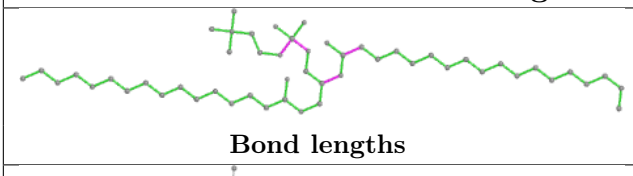
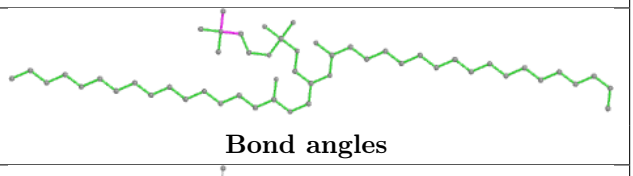
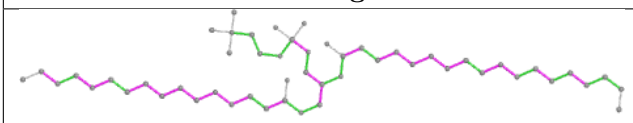
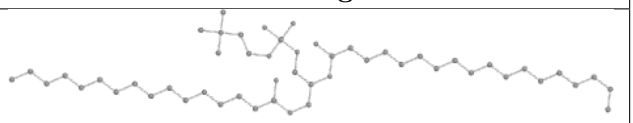
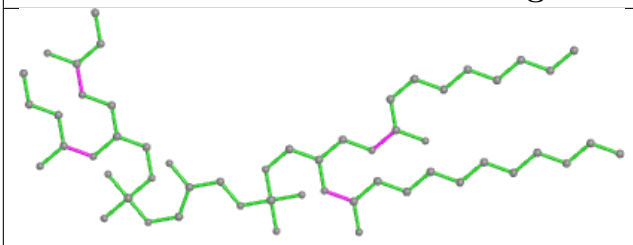

Bond lengths

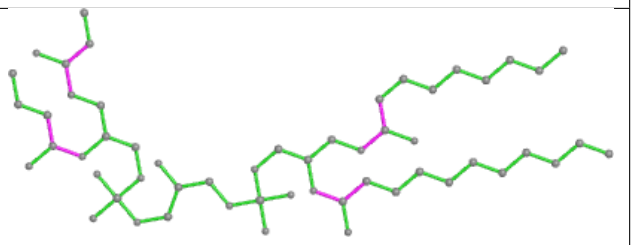

Bond angles

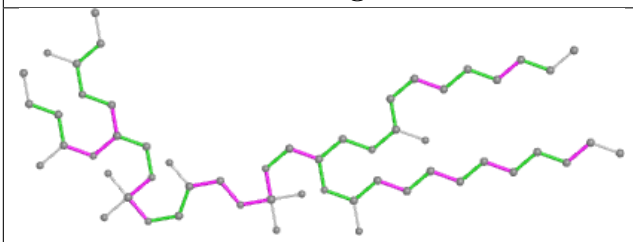

Torsions

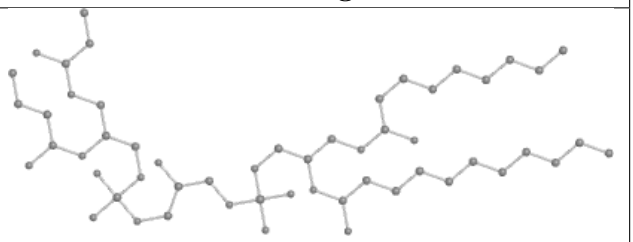

Rings

Ligand CDL n 102

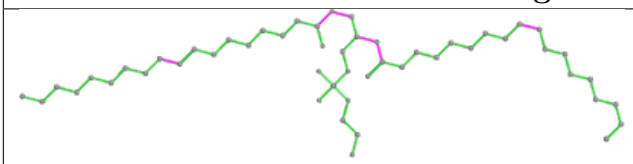

Bond lengths

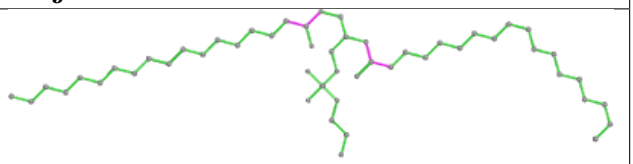

Bond angles

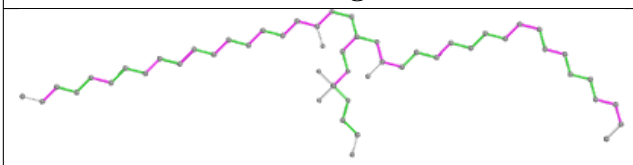

Torsions

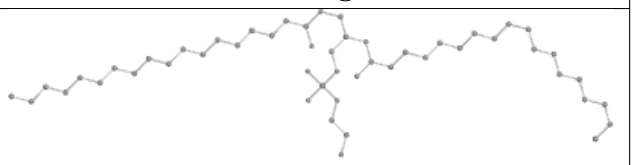

Rings

Ligand PEE j 201

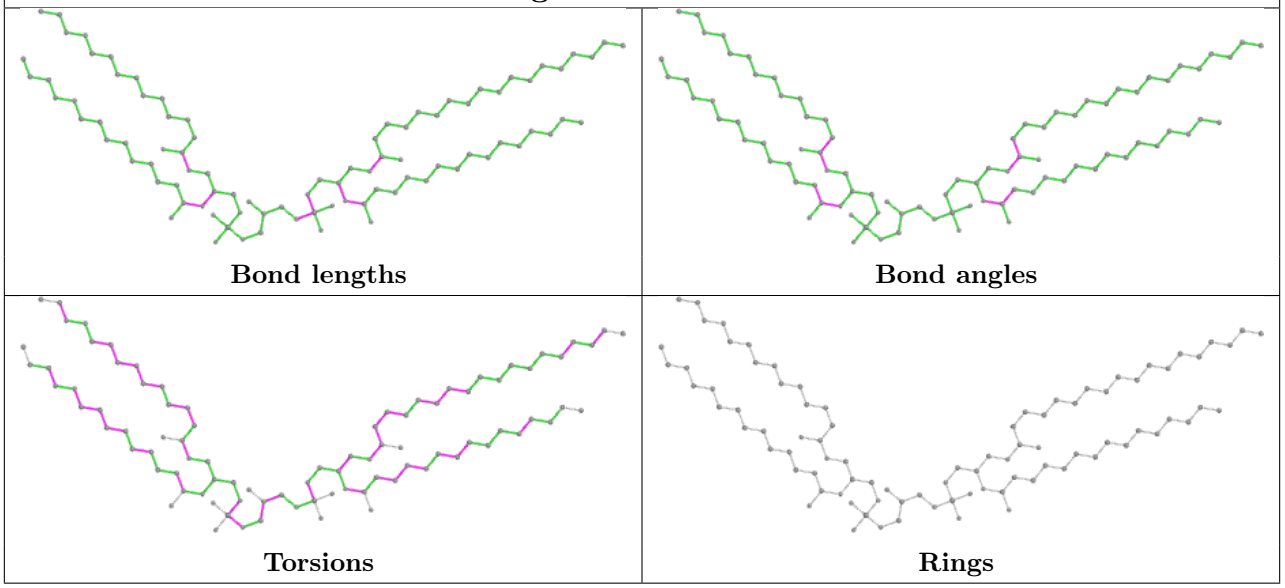

Bond lengths


Bond angles

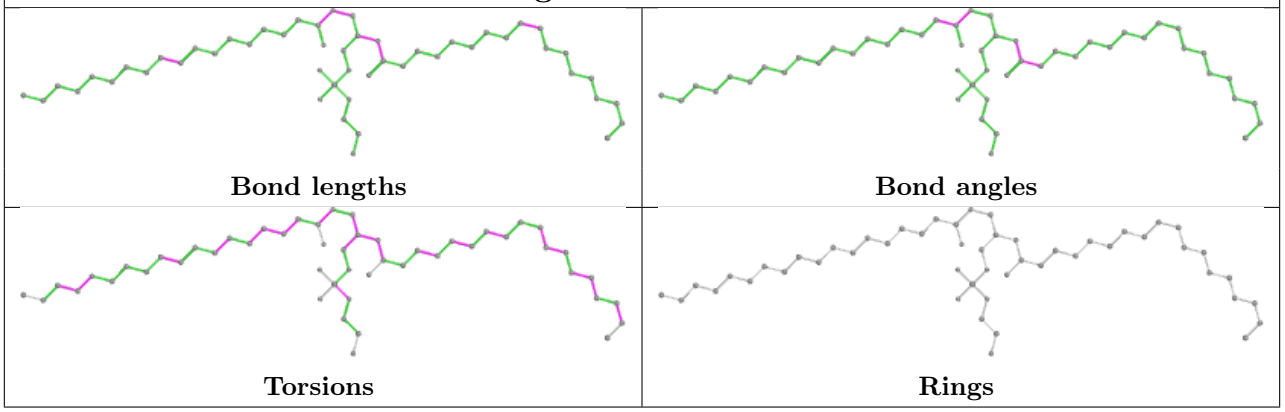

Torsions


Rings

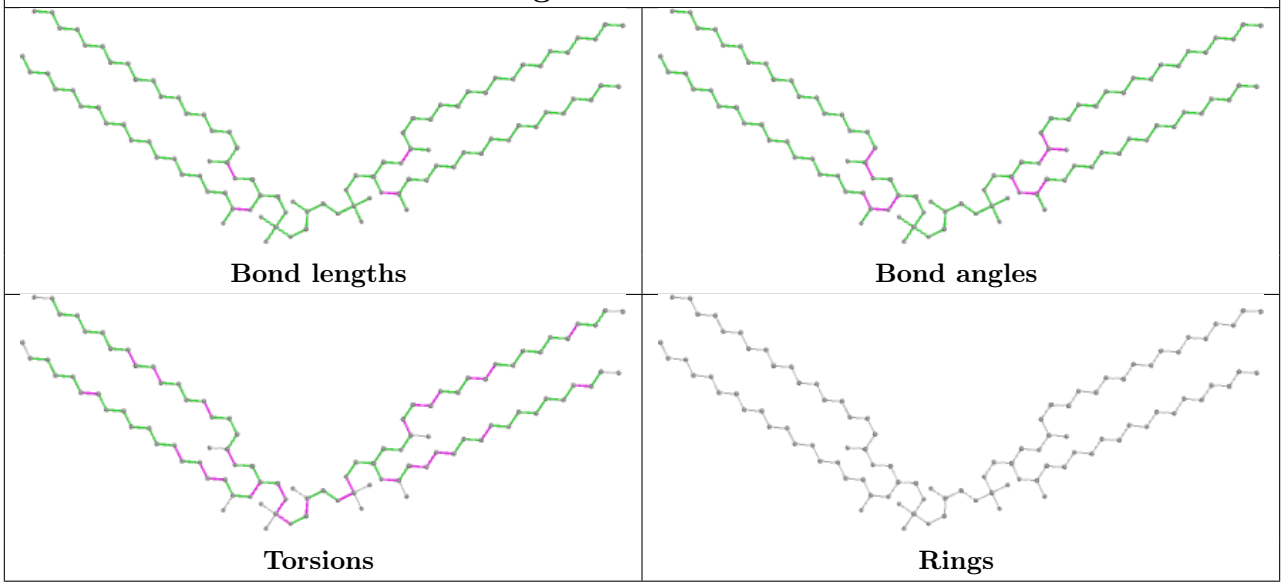
Ligand CDL s 402



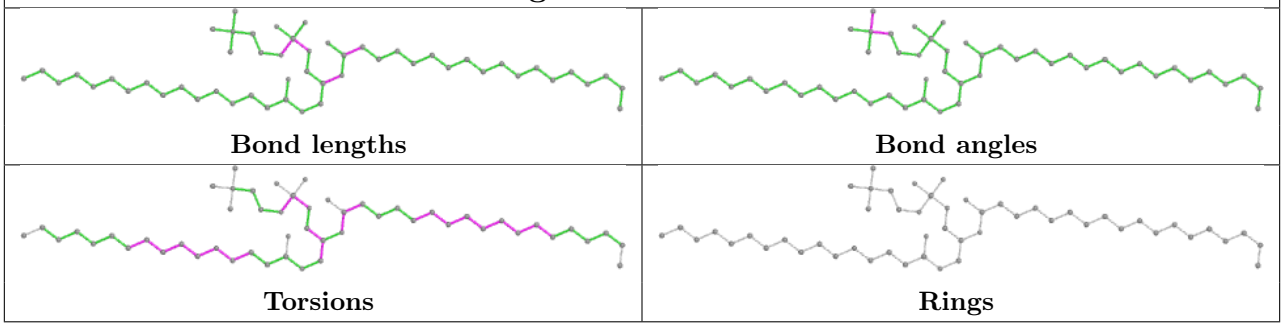
Ligand PEE l 704



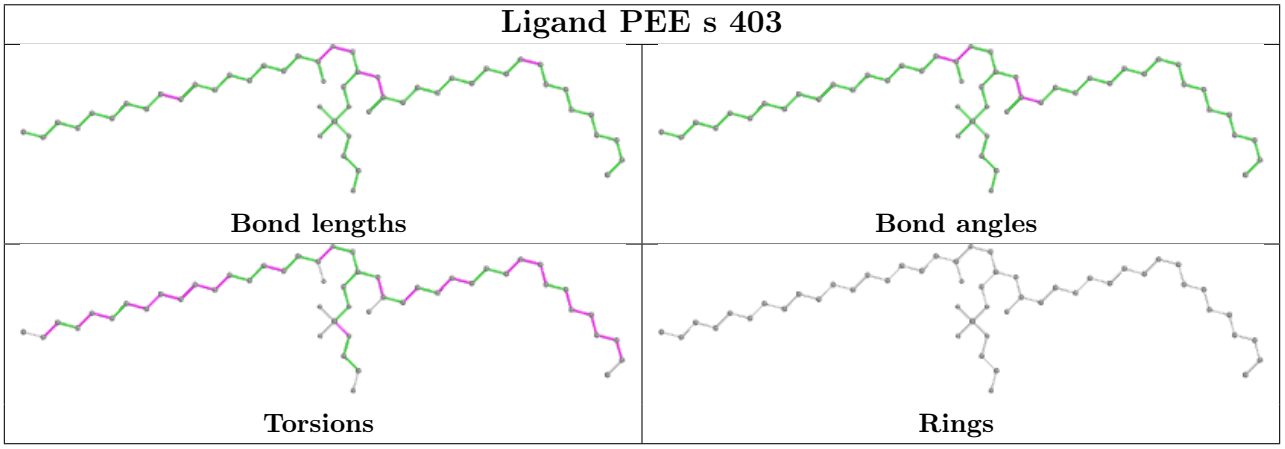
Ligand CDL l 702



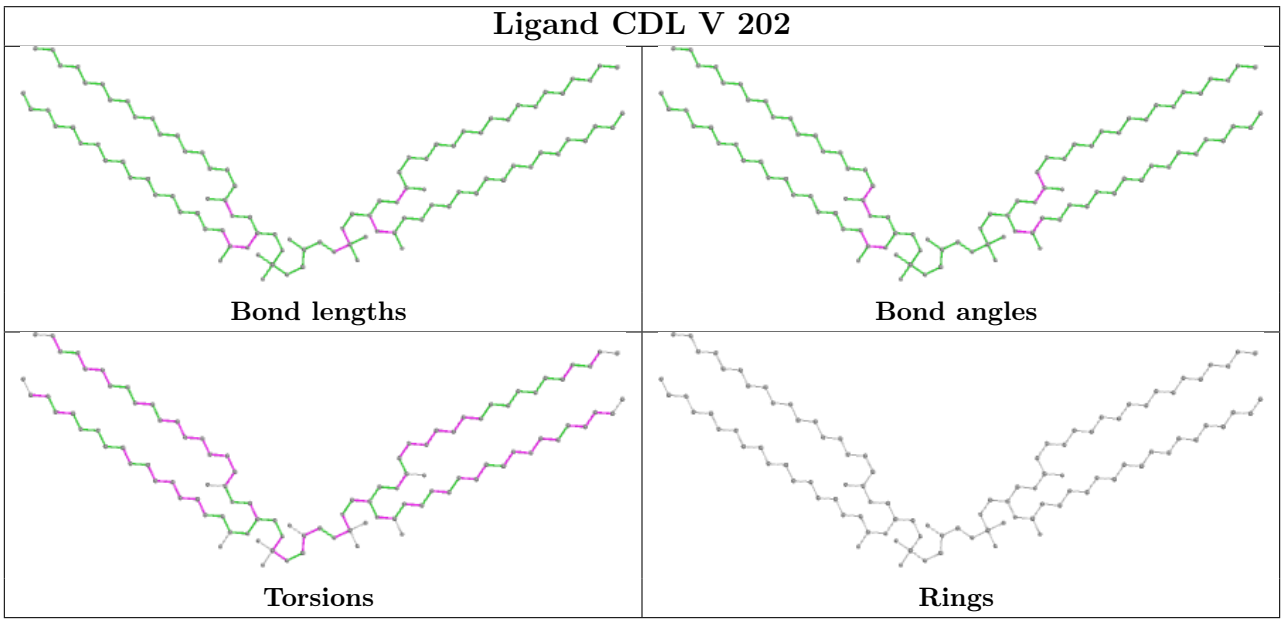
Ligand PLX n 101



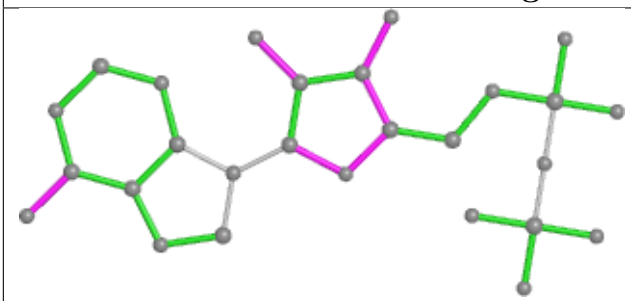
Ligand PEE s 403



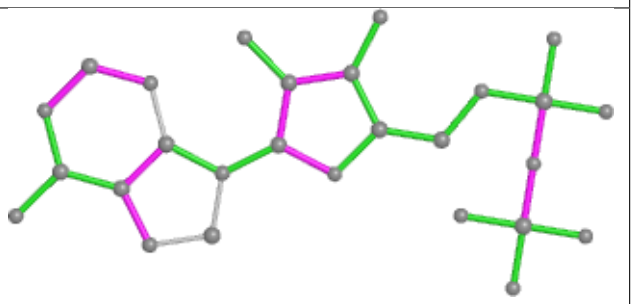
Ligand CDL V 202



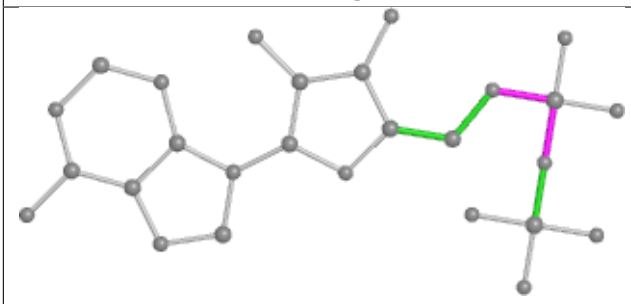
Ligand ADP w 401



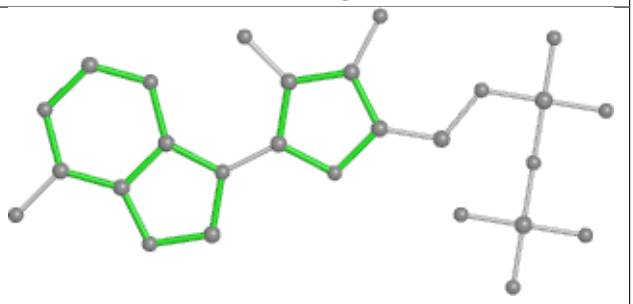
Bond lengths



Bond angles



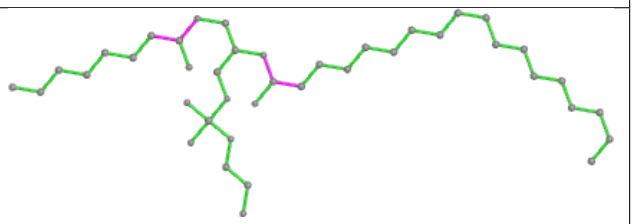
Torsions



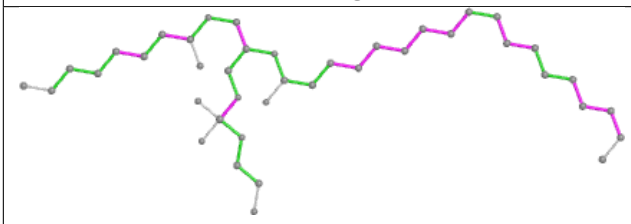
Rings

Ligand PEE s 401

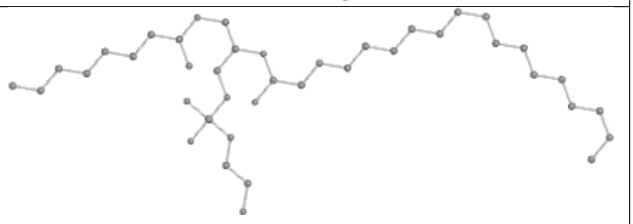
Bond lengths



Bond angles

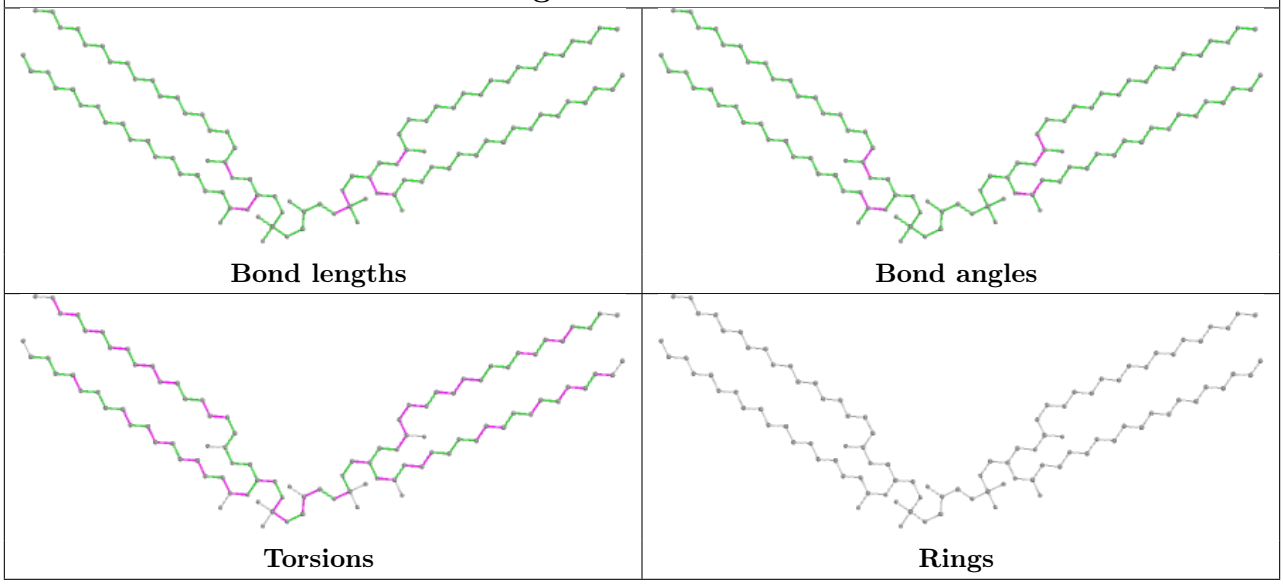


Torsions

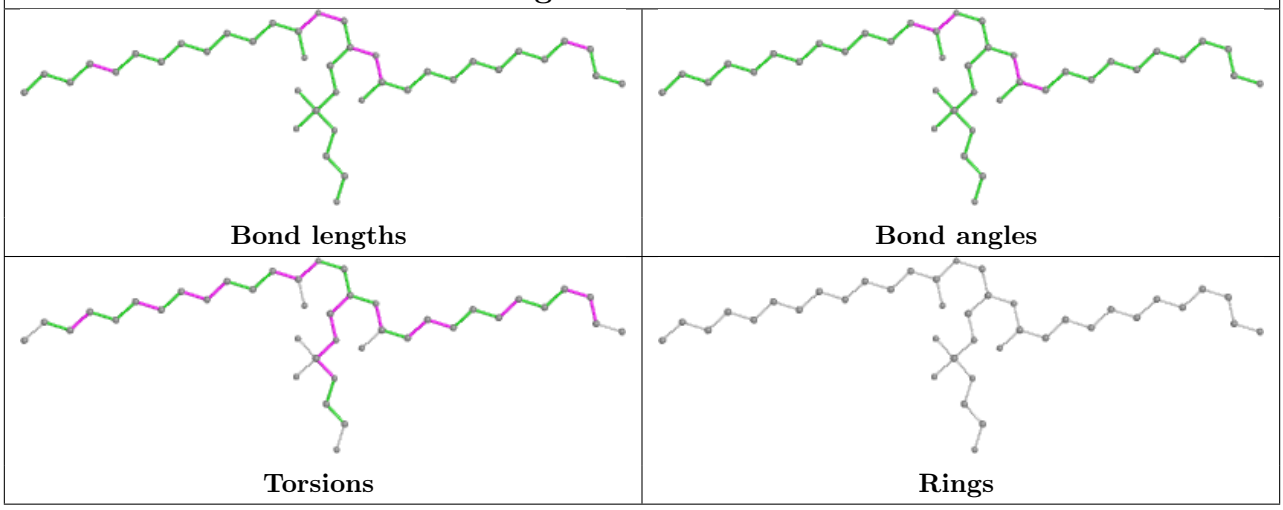


Rings

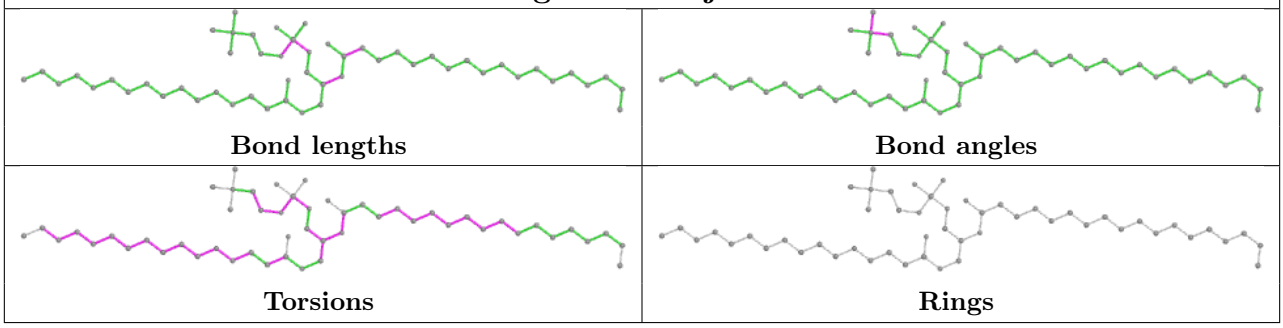
Ligand CDL l 703



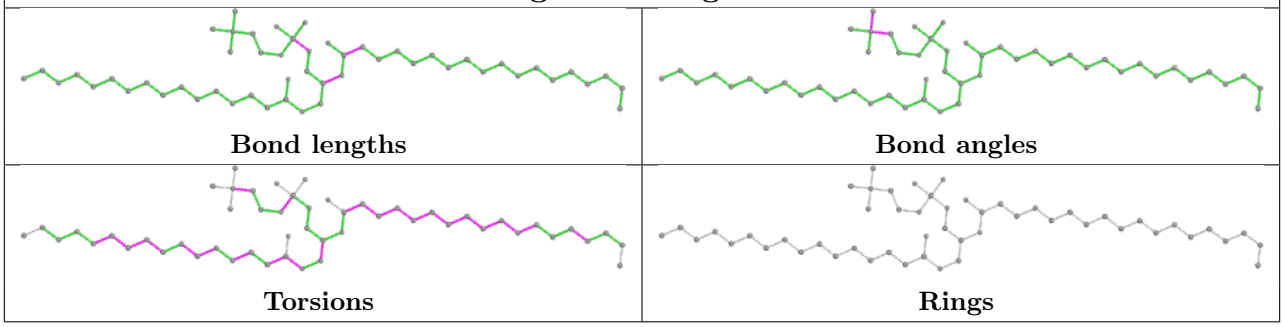
Ligand PEE l 701



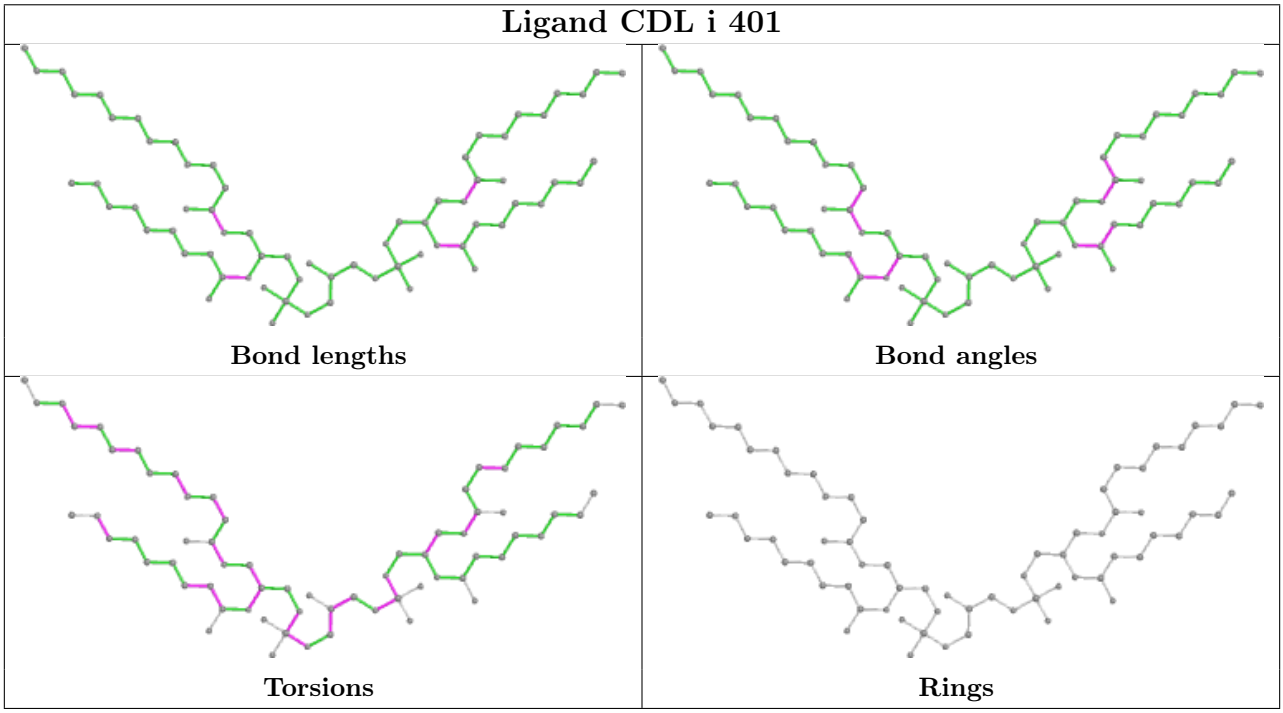
Ligand PLX j 202



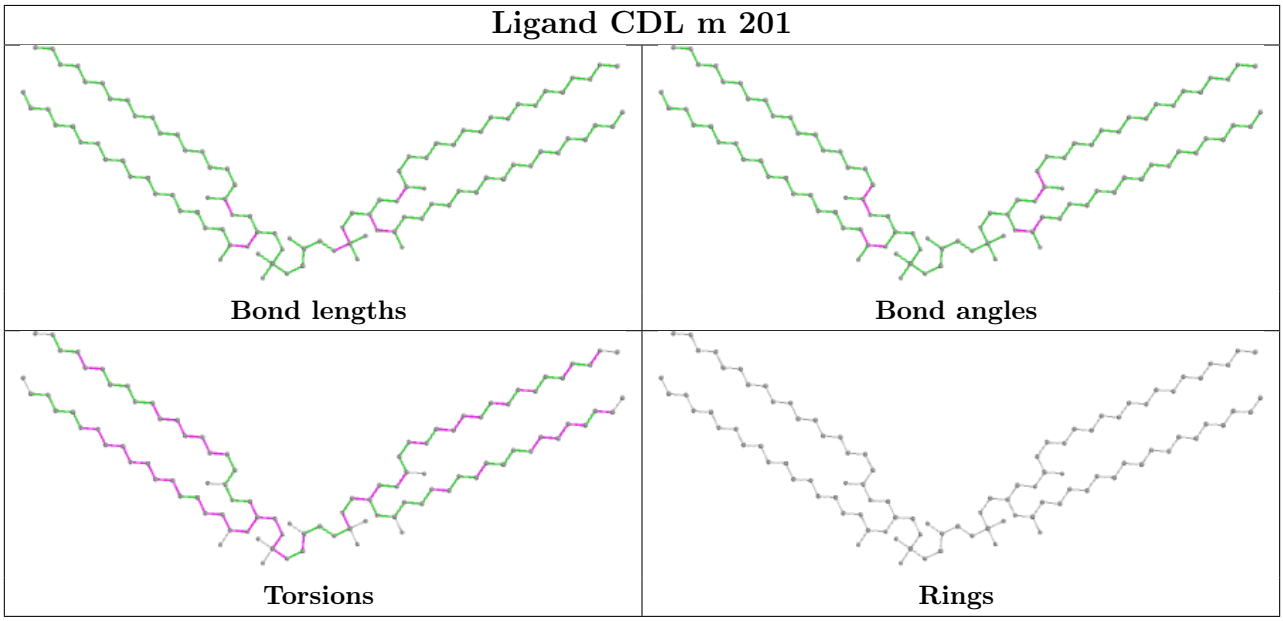
Ligand PLX g 201



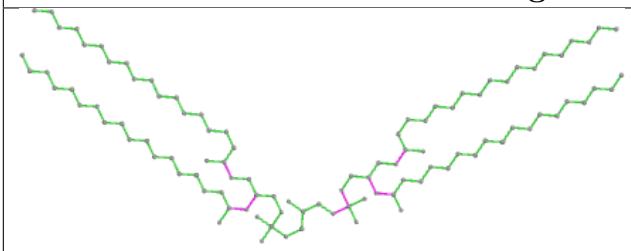
Ligand CDL i 401



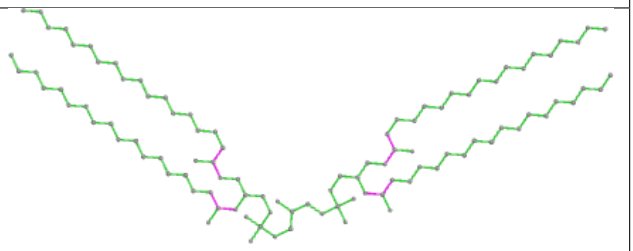
Ligand CDL m 201



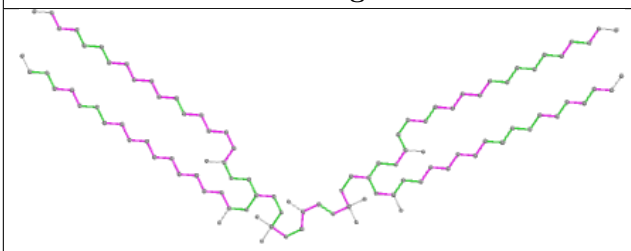
Ligand CDL a 201



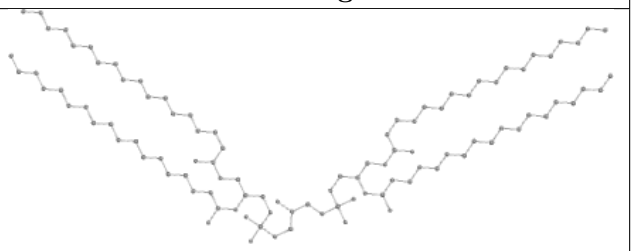
Bond lengths



Bond angles

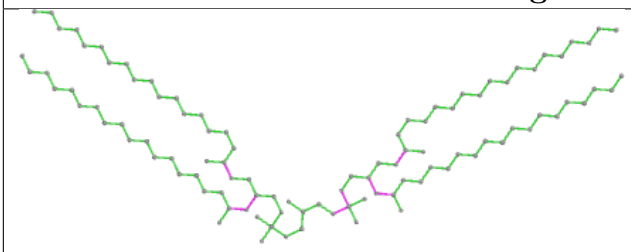


Torsions

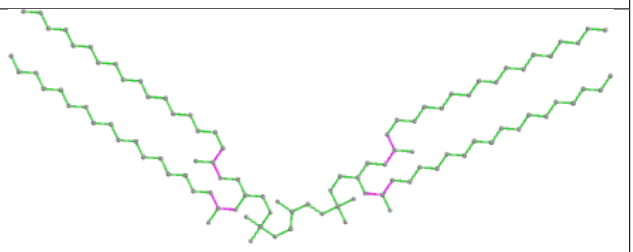


Rings

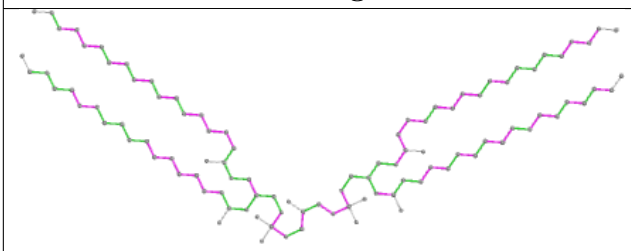
Ligand CDL r 503



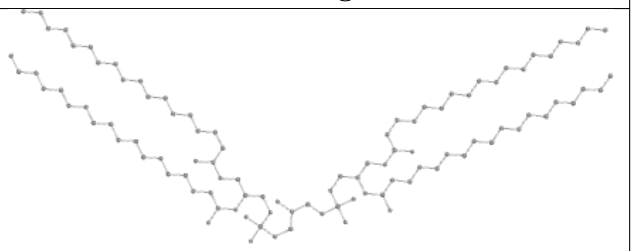
Bond lengths



Bond angles

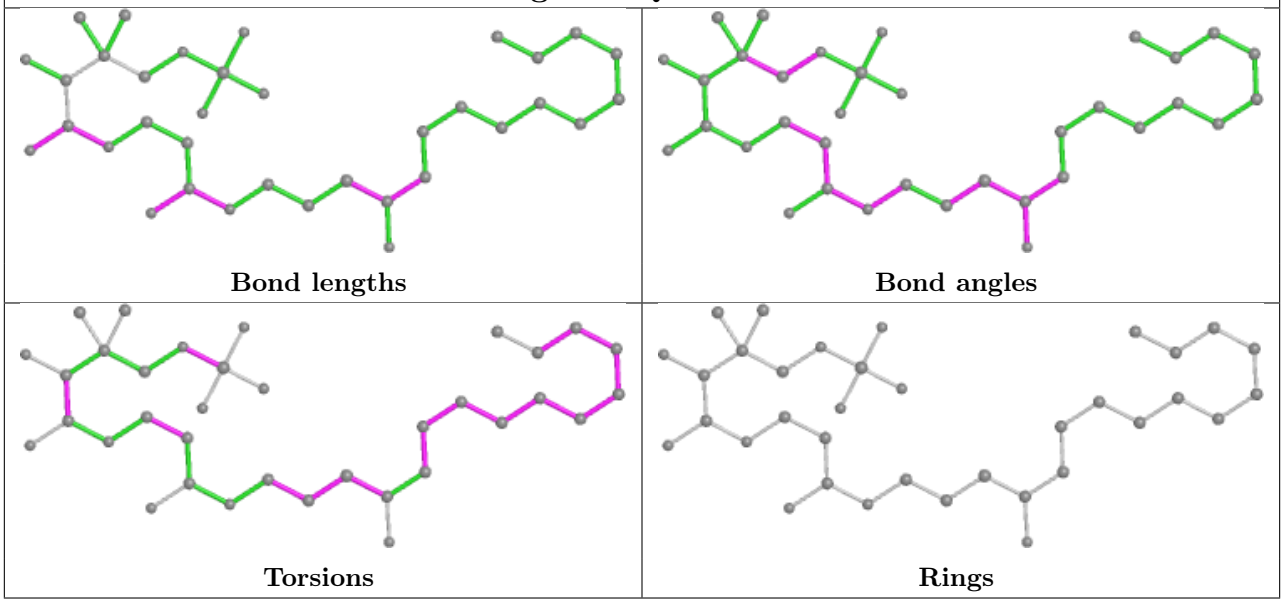


Torsions

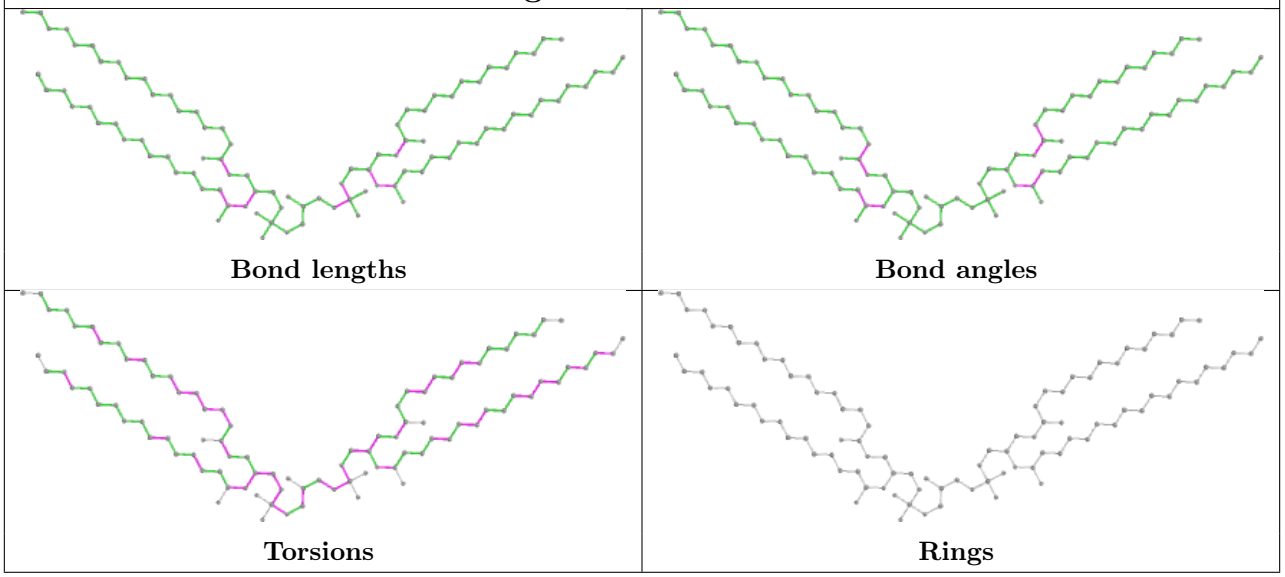


Rings

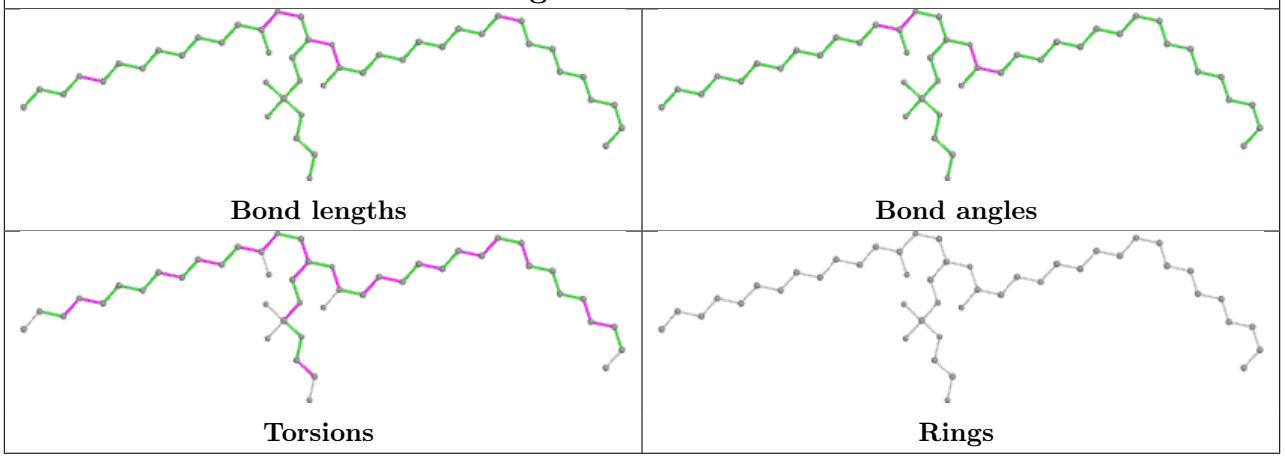
Ligand 8Q1 X 201



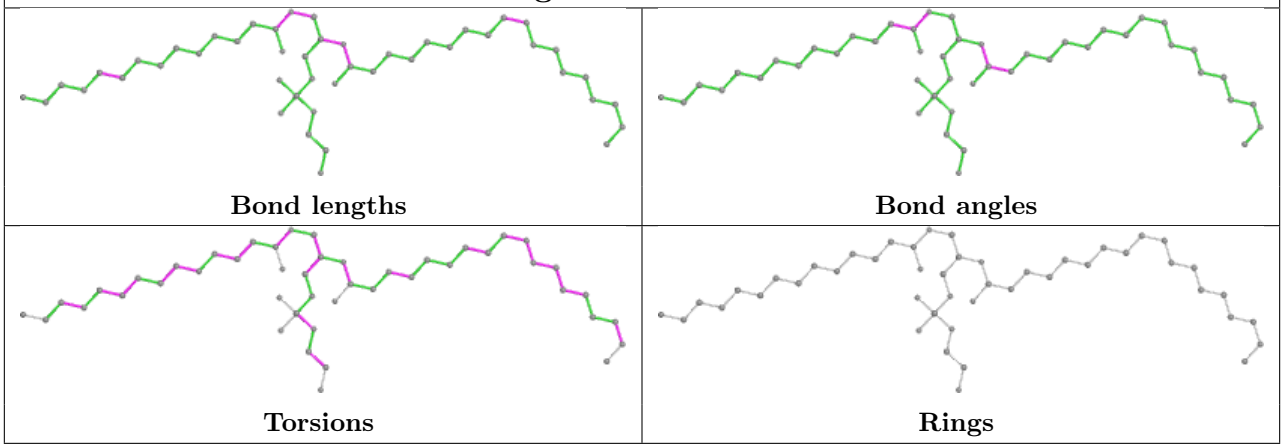
Ligand CDL V 201



Ligand PEE b 201



Ligand PEE i 402



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.

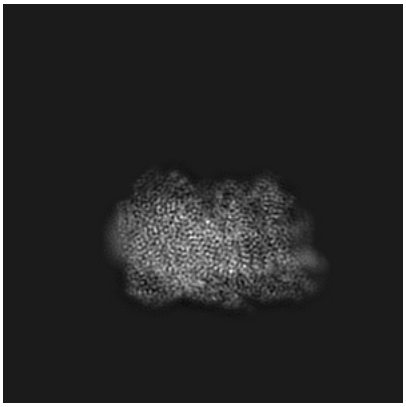
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32187. These allow visual inspection of the internal detail of the map and identification of artifacts.

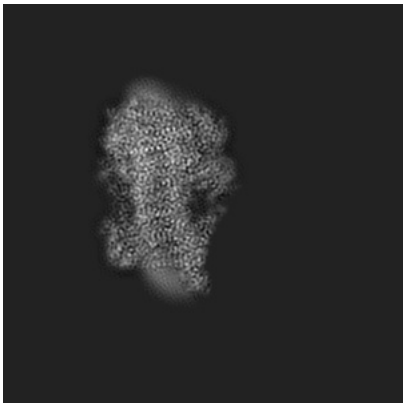
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

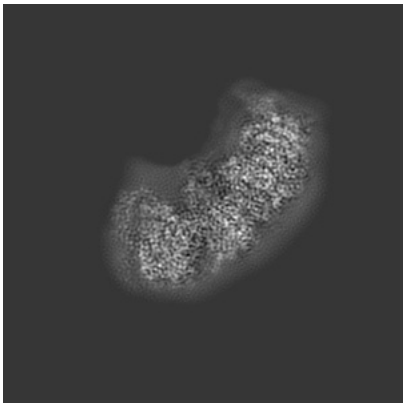
6.1.1 Primary map



X



Y

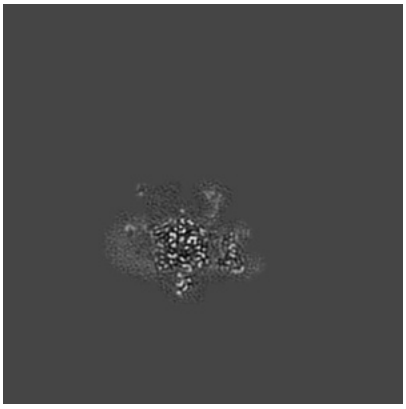


Z

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

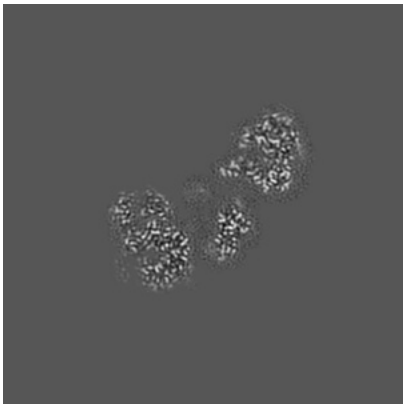
6.2 Central slices

6.2.1 Primary map



X Index: 165

Y Index: 165

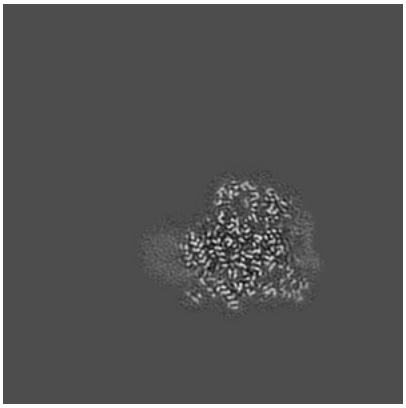


Z Index: 165

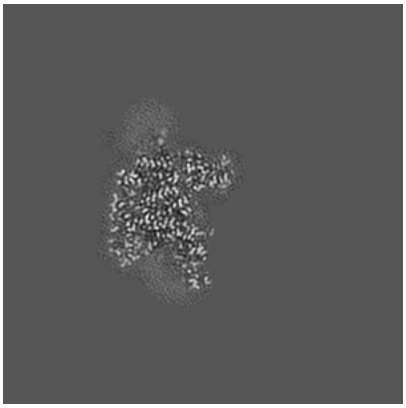
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

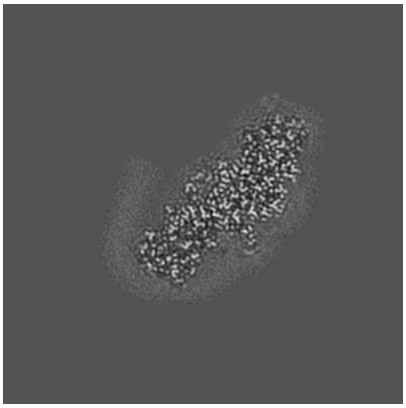
6.3.1 Primary map



X Index: 217



Y Index: 146

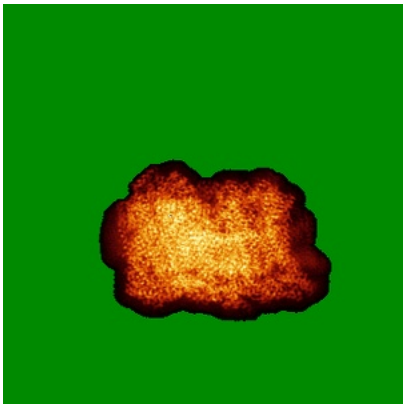


Z Index: 136

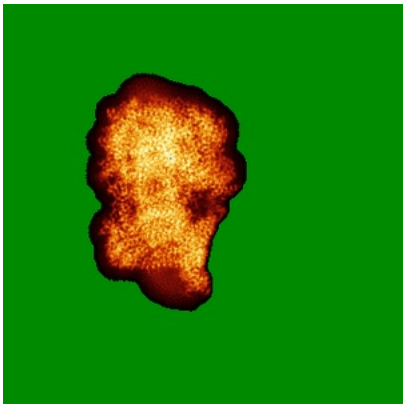
The images above show the largest variance slices of the map in three orthogonal directions.

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

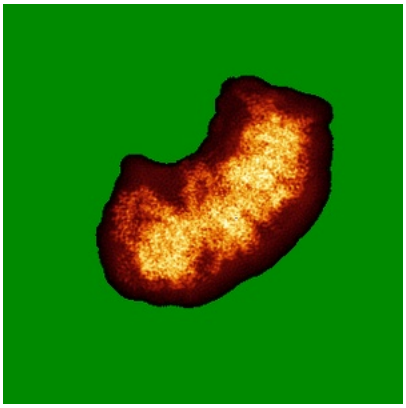
6.4.1 Primary map



X



Y

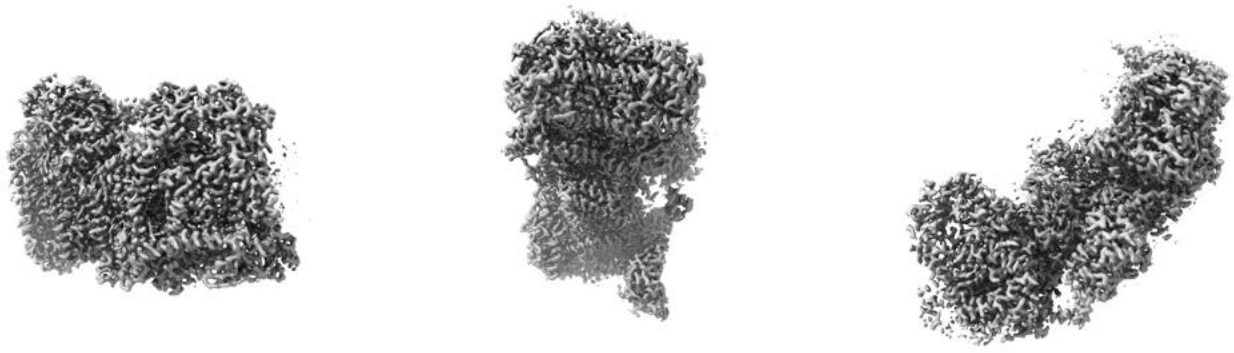


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

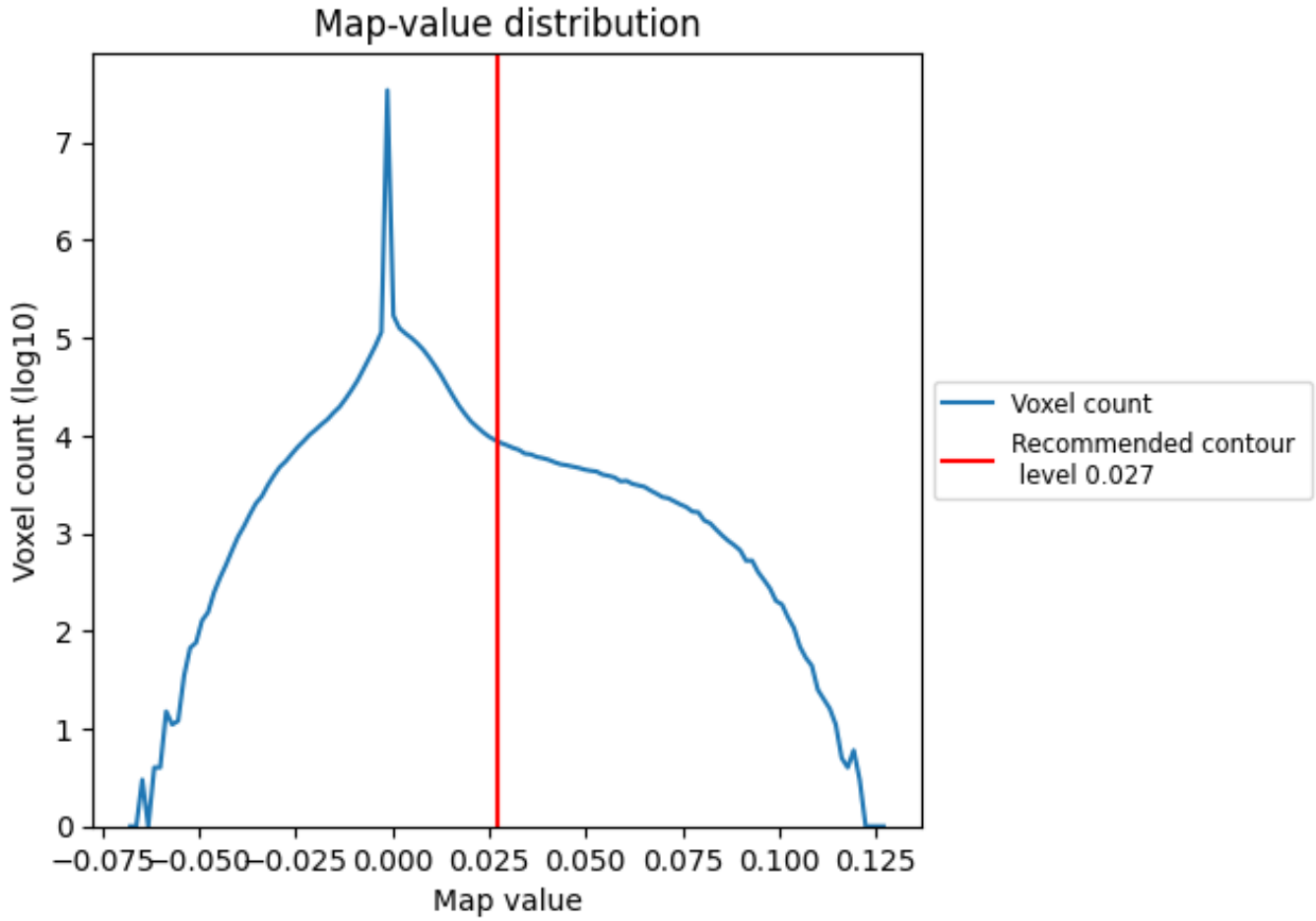
6.6 Mask visualisation (i)

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

7 Map analysis

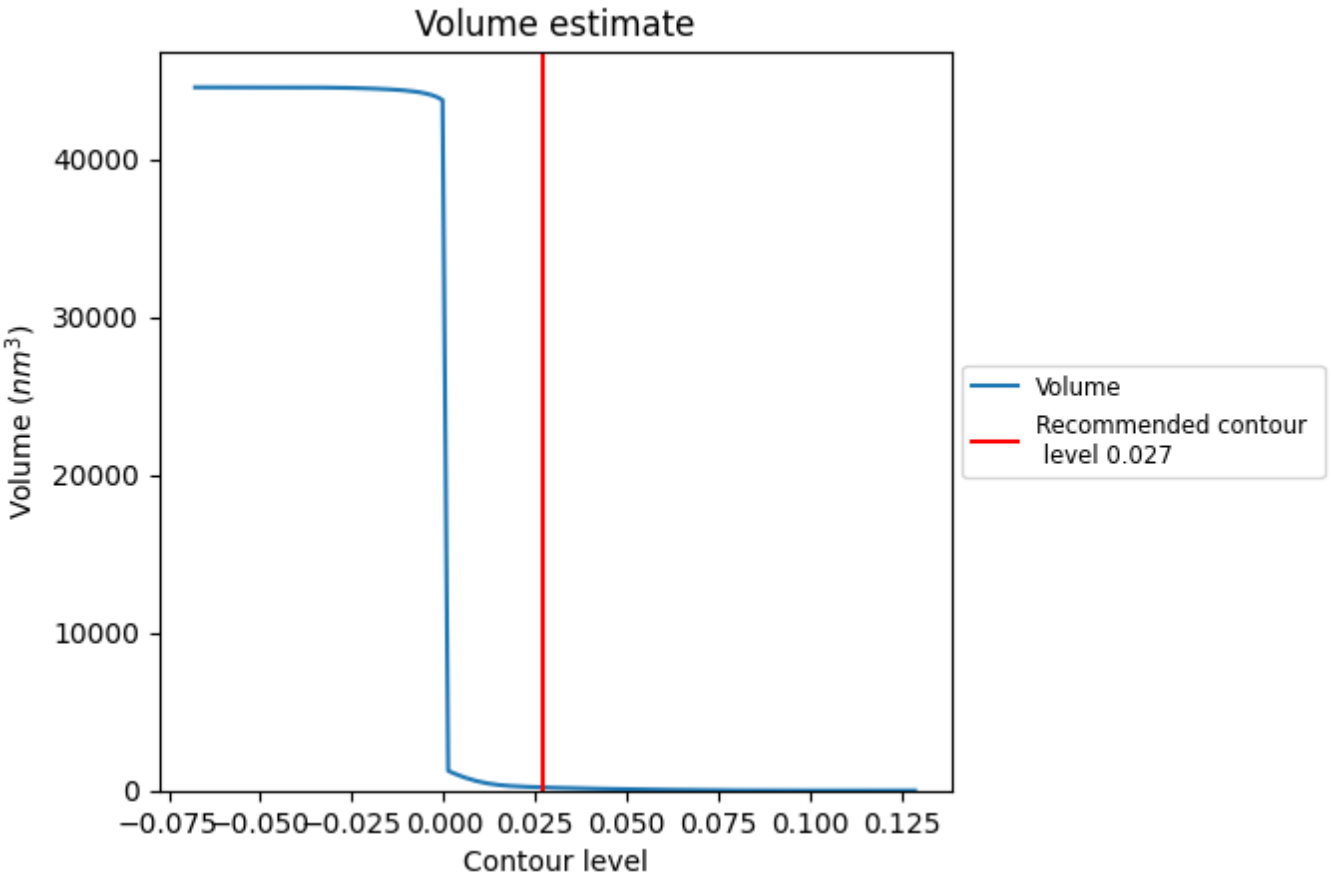
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

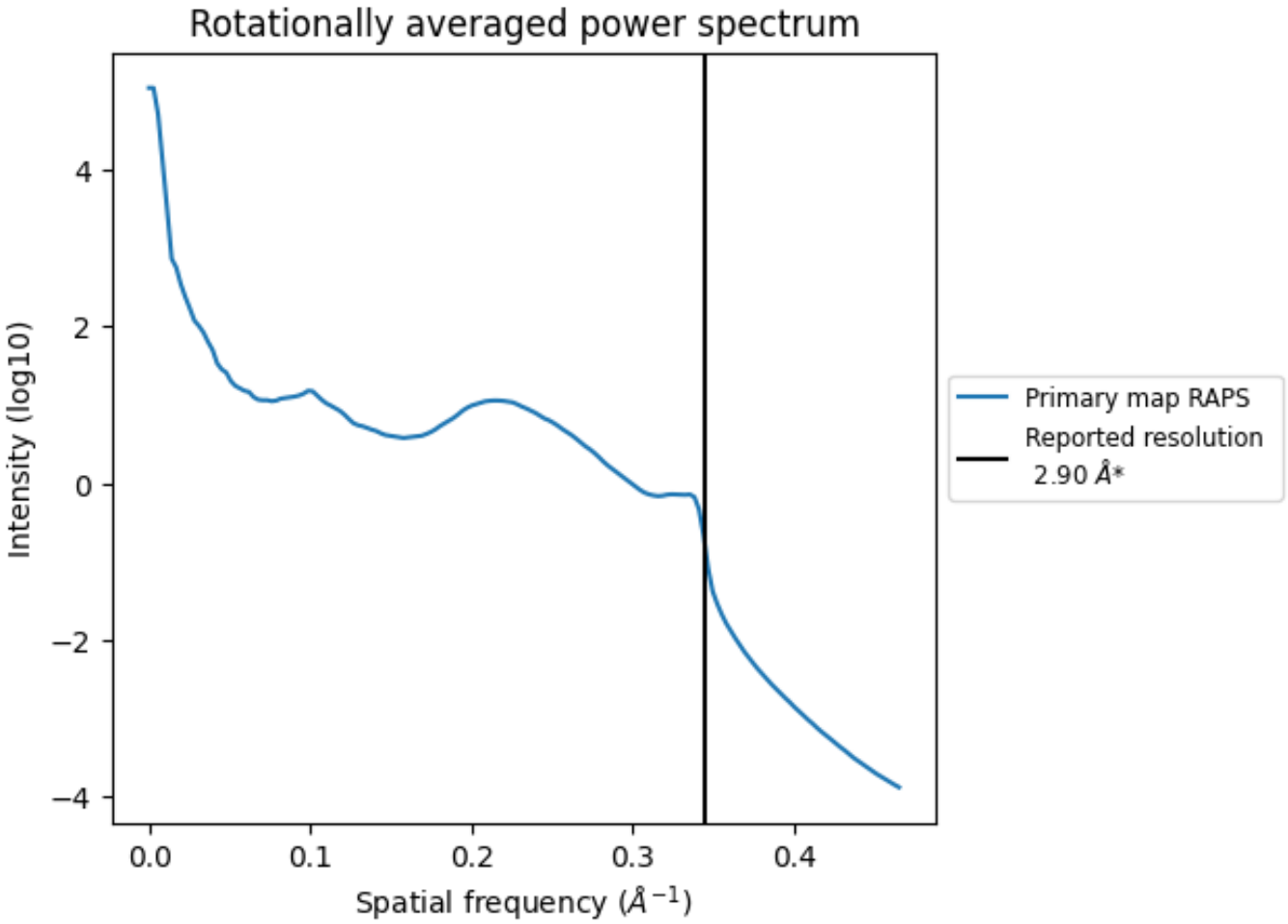
7.2 Volume estimate



The volume at the recommended contour level is 201 nm^3; this corresponds to an approximate mass of 182 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

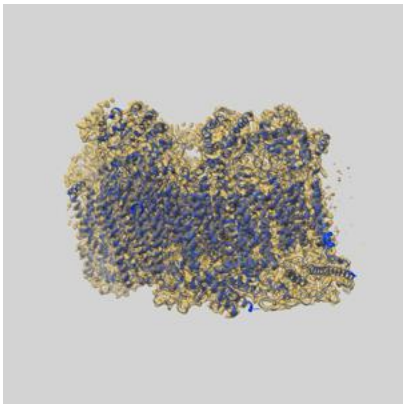
8 Fourier-Shell correlation (i)

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

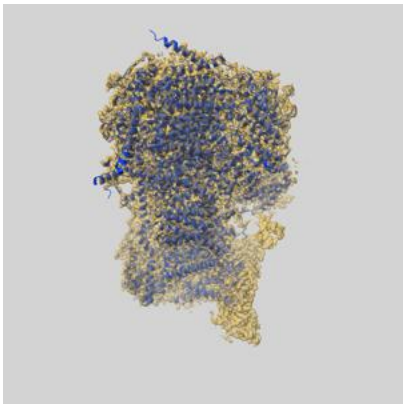
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32187 and PDB model 7VXS. Per-residue inclusion information can be found in section 3 on page 13.

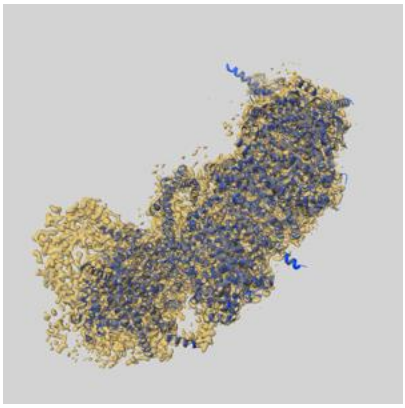
9.1 Map-model overlay



X



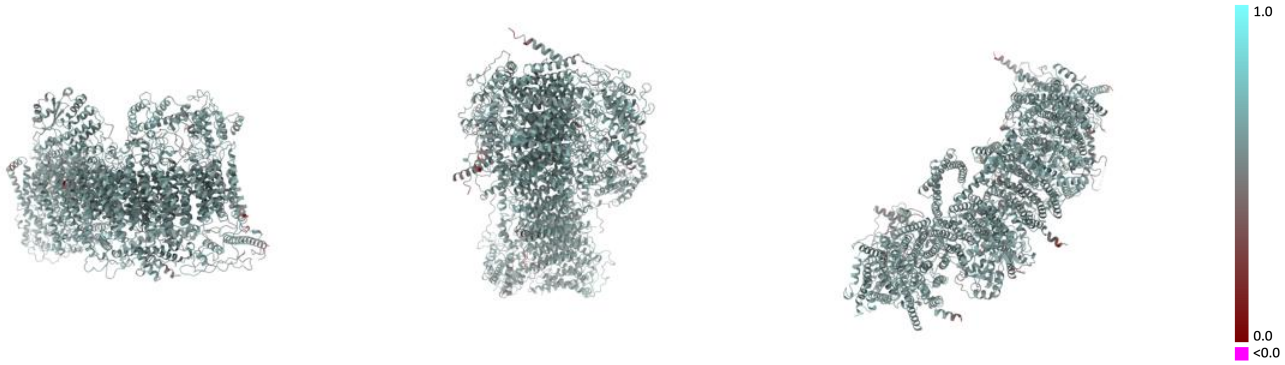
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

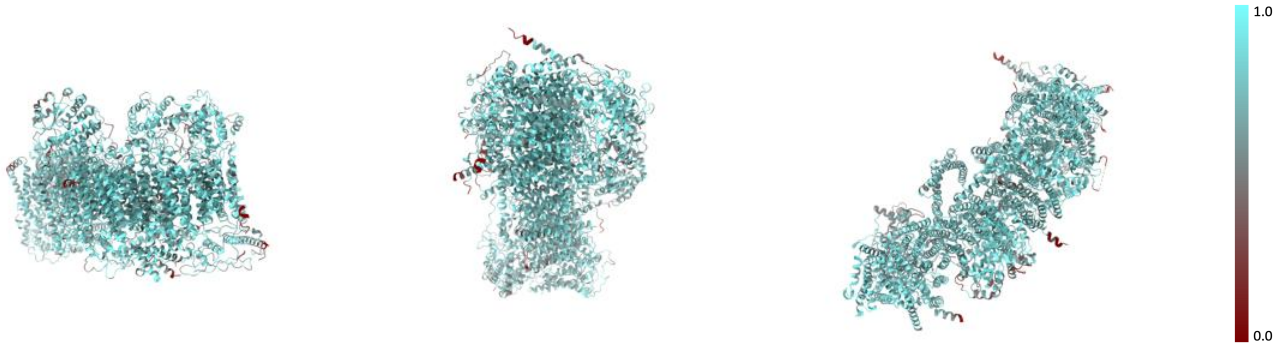
9.2 Q-score mapped to coordinate model (i)



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.

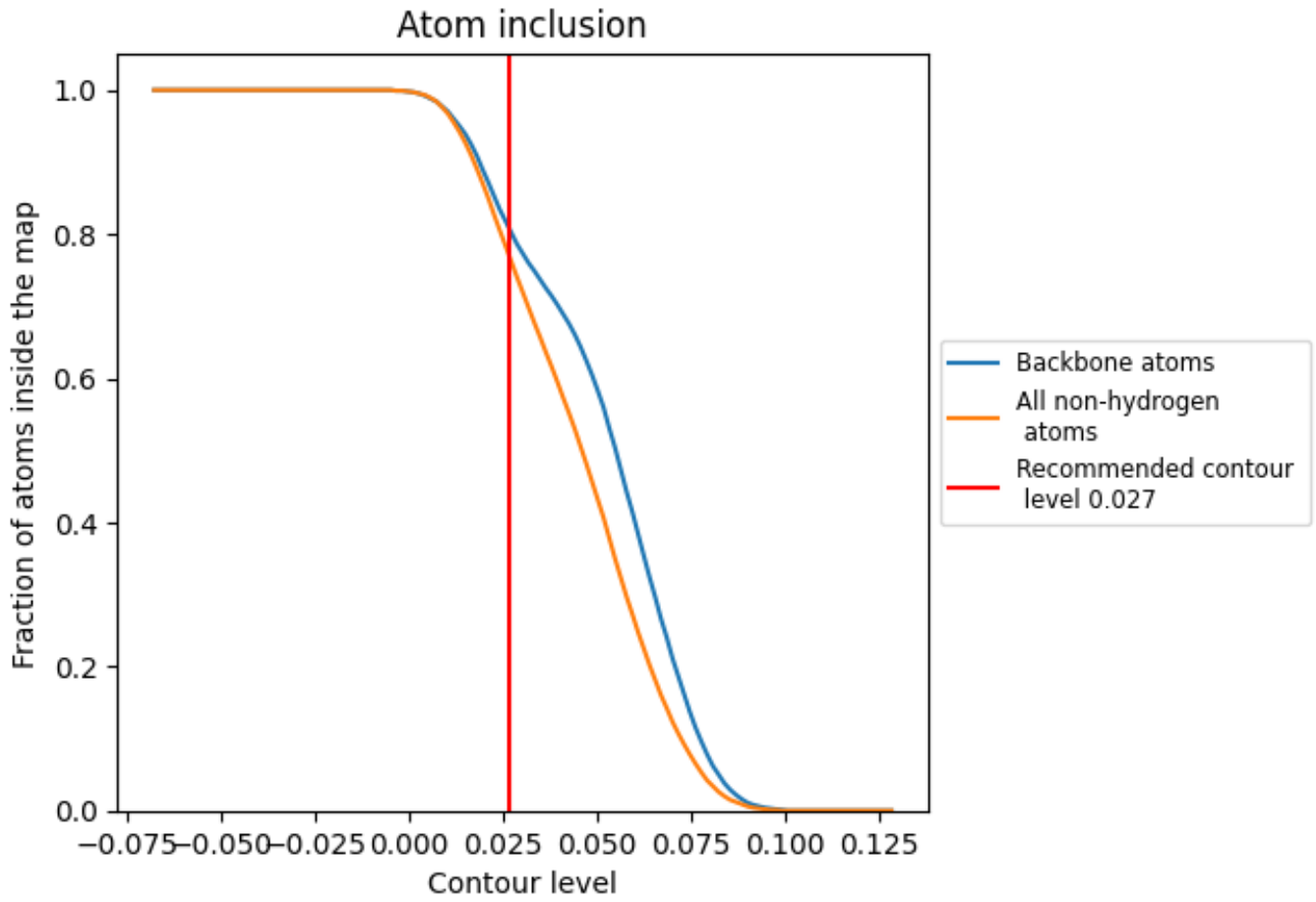
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.5780
Q	0.7360	0.5790
S	0.7990	0.5860
U	0.7420	0.5710
V	0.6630	0.5620
W	0.7810	0.5830
X	0.7460	0.5560
Y	0.7140	0.5520
Z	0.6530	0.5370
a	0.8020	0.5890
b	0.6990	0.5620
c	0.7790	0.5800
d	0.7420	0.5580
e	0.7290	0.5670
f	0.6110	0.5350
g	0.8090	0.5890
h	0.7440	0.5640
i	0.8210	0.5950
j	0.7060	0.5760
k	0.8300	0.5930
l	0.7870	0.5860
m	0.6960	0.5580
n	0.6300	0.5550
o	0.7580	0.5780
p	0.7890	0.5860
r	0.8220	0.5950
s	0.8100	0.5920
u	0.7720	0.5790
v	0.7090	0.5520
w	0.7570	0.5720