Full wwPDB EM Validation Report (i)

Dec 7, 2022 – 01:54 PM JST

PDB ID	:	7V2C
EMDB ID	:	EMD-31640
Title	:	Active state complex I from Q10 dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-08
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 (i) symbol.

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

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

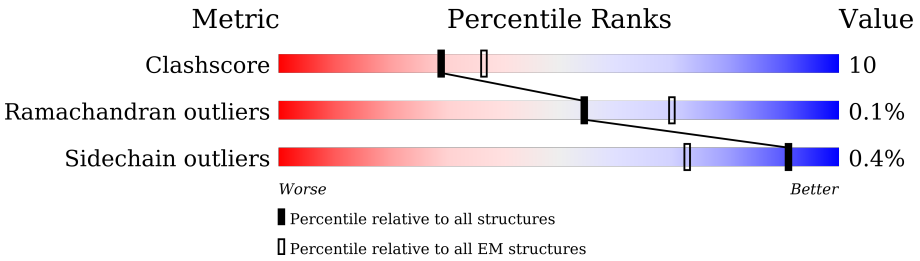
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	433	76% 24%
2	B	176	86% 14%
3	C	156	90% 10%
4	E	115	78% 21%
5	F	86	5% 74% 26%
6	G	88	8% 73% 23% 5%
6	X	88	86% 14%
7	H	112	82% 16%

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Mol	Chain	Length	Quality of chain
8	I	112	69% 18% 13%
9	J	342	84% 16%
10	K	43	77% 21%
11	L	125	5% 86% 14%
12	M	690	79% 21%
13	N	144	85% 15%
14	O	217	81% 19%
15	P	208	81% 19%
16	Q	430	80% 20%
17	S	70	86% 14%
18	T	96	88% 12%
19	U	83	94% 6%
20	V	140	87% 13%
21	W	142	89% 11%
22	Y	67	91% 9%
23	Z	80	9% 95% 5%
24	a	138	100%
25	b	126	77% 22%
26	c	156	100%
27	d	175	99%
28	e	104	99%
29	f	49	16% 100%
30	g	121	100%
31	h	105	98%
32	i	347	99%

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Mol	Chain	Length	Quality of chain
33	j	115	100%
34	k	98	99%
35	l	606	99%
36	m	175	99%
37	n	56	11% 98%
38	o	128	98%
39	p	178	100%
40	r	459	100%
41	s	318	99%
42	u	171	99%
43	v	125	99%
44	w	320	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
45	SF4	M	802	-	-	X	-
46	FMN	A	502	-	-	X	-

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 68315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	433	3330	2103	593	614	20	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	687	432	129	124	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	690	446	102	137	5	0	0
6	X	88	694	447	103	139	5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	342	2751	1783	481	478	9	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	43	366	228	68	69	1	0	0

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	430	3459	2212	594	629	24	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	53	ARG	CYS	conflict	UNP K7GR43

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

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

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

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

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

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1161	749	197	206	9	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4.

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

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

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

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

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

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

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

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

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

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

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

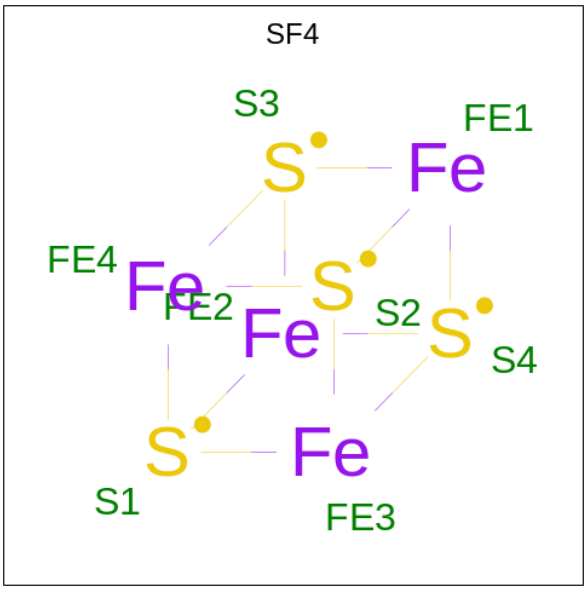
There is a discrepancy between the modelled and reference sequences:

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

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

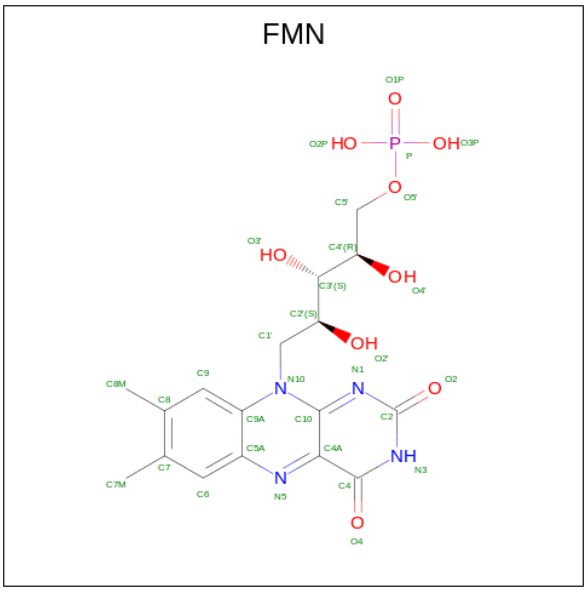
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2590	1649	440	491	10	0	0

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



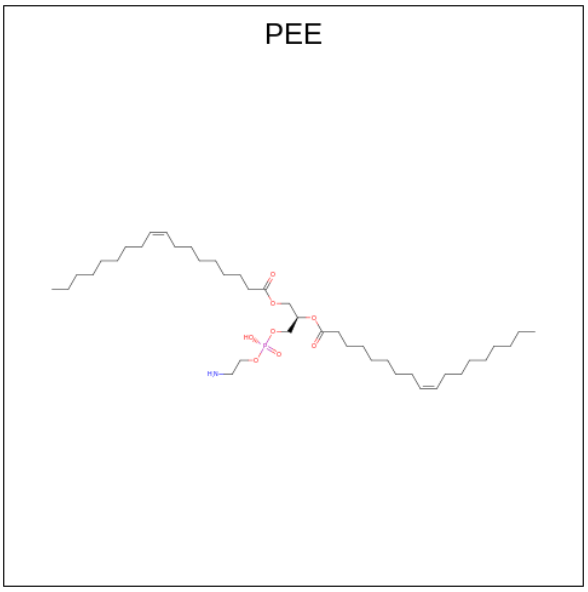
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

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



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	B	1	51	41	1	8	1	0
			Total	C	N	O	P	
47	C	1	47	37	1	8	1	0

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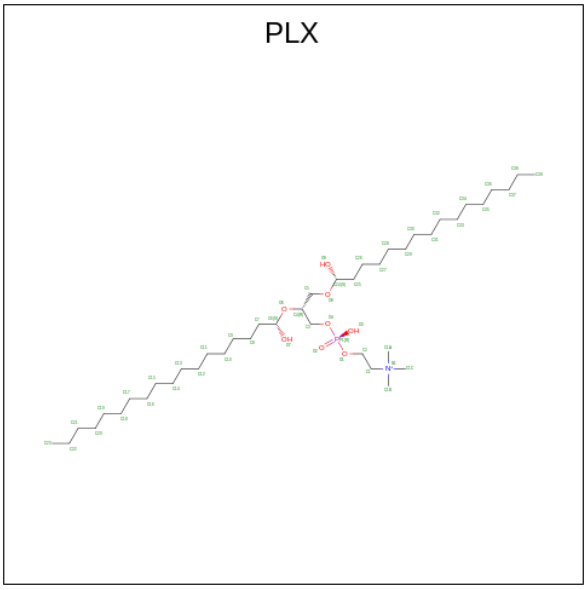
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	Q	1	47	37	1	8	1	0
			Total	C	N	O	P	
47	W	1	41	31	1	8	1	0
			Total	C	N	O	P	
47	b	1	46	36	1	8	1	0
			Total	C	N	O	P	
47	j	1	92	72	2	16	2	0
			Total	C	N	O	P	
47	j	1	92	72	2	16	2	0
			Total	C	N	O	P	
47	l	1	91	71	2	16	2	0
			Total	C	N	O	P	
47	l	1	91	71	2	16	2	0
			Total	C	N	O	P	
47	r	1	51	41	1	8	1	0

- Molecule 48 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
			Total	C	N	O	P	
48	C	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	J	1	52	42	1	8	1	0

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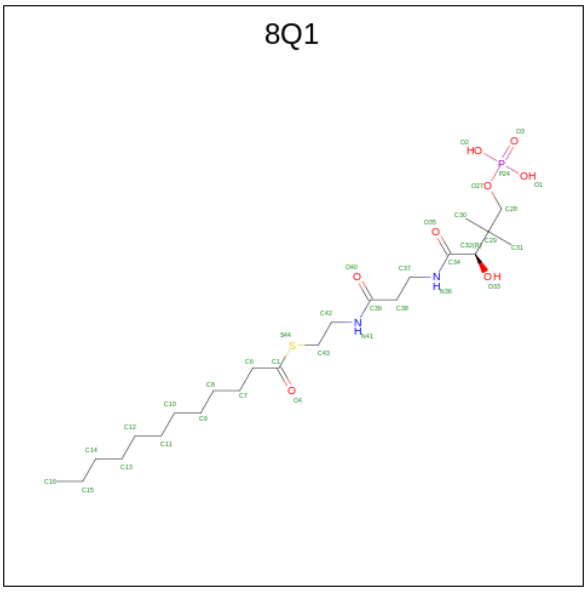
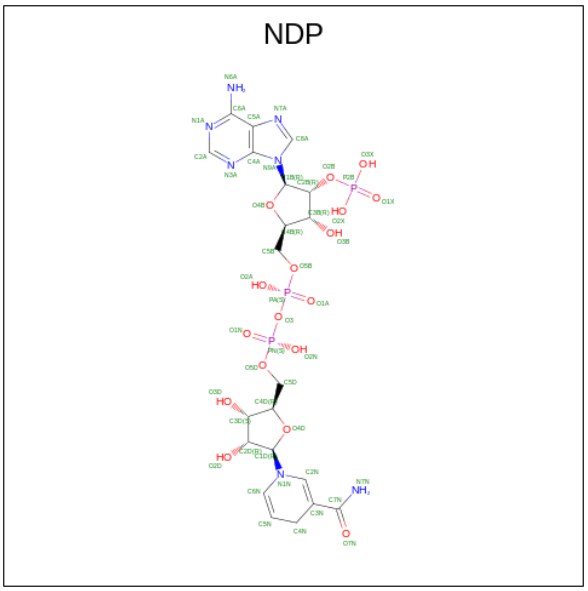
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	N	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	g	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	j	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	n	1	52	42	1	8	1	0
			Total	C	N	O	P	
48	r	1	104	84	2	16	2	0
			Total	C	N	O	P	
48	r	1	104	84	2	16	2	0

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



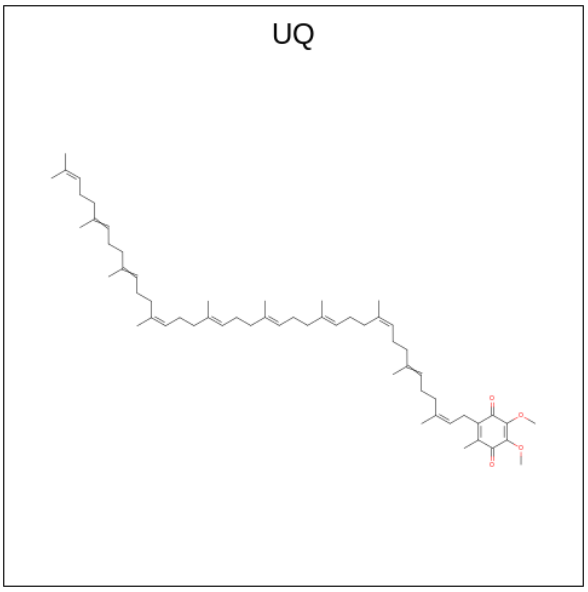
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
49	E	1	35	23	2	8	1	1	0
			Total	C	N	O	P	S	
49	X	1	35	23	2	8	1	1	0

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



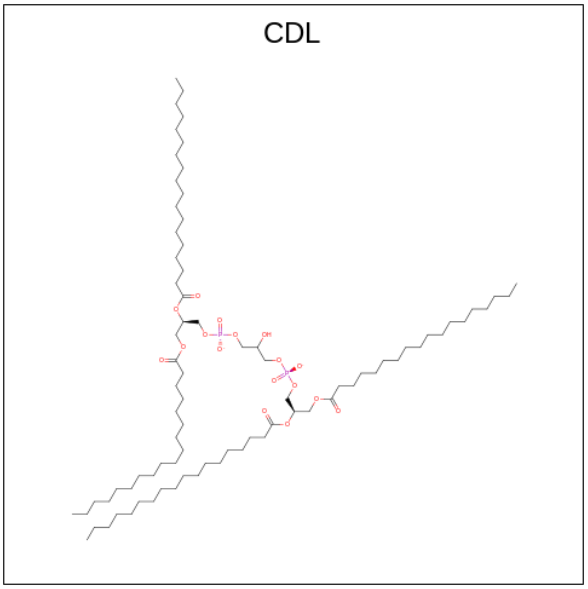
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	J	1	48	21	7	17	3	0

- Molecule 51 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



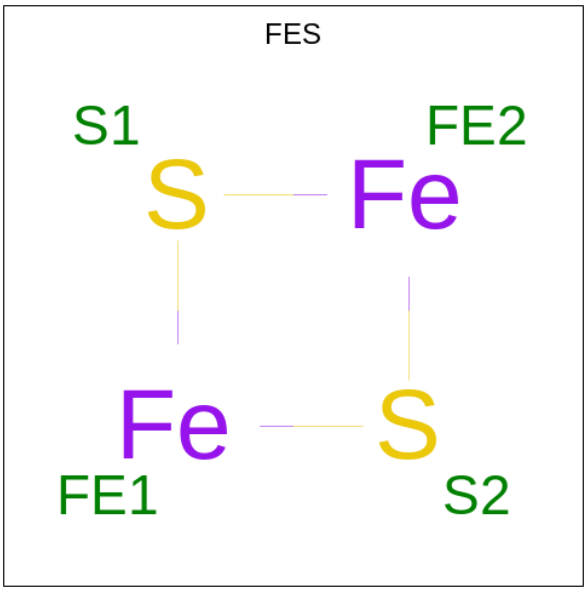
Mol	Chain	Residues	Atoms					AltConf
			Total	C	O			
51	J	1	33	29	4			0
51	s	1	Total	C	O			0
			63	59	4			

- Molecule 52 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
			Total	C	O	P	
52	J	1	89	70	17	2	0
52	N	1	51	32	17	2	0
52	V	1	194	156	34	4	0
52	V	1	194	156	34	4	0
52	a	1	100	81	17	2	0
52	i	1	68	49	17	2	0
52	l	1	199	161	34	4	0
52	l	1	199	161	34	4	0
52	m	1	100	81	17	2	0
52	r	1	100	81	17	2	0
52	u	1	55	36	17	2	0

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

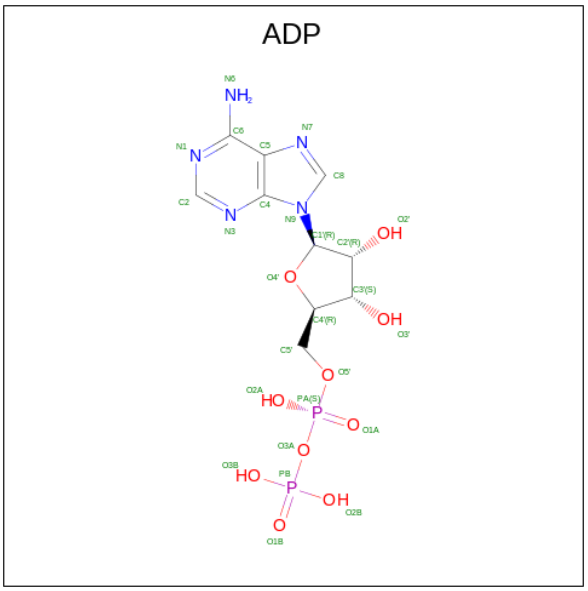
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

3 Residue-property plots (i)

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

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

Chain A: 76% 24%

A26 P27 K28 K29 R48 H49 D50 L53 K54 G55 A56 R59 G60 D61 W62 Y63 E67 K71 I76 K81 G87 R88 G96 L97 K98 P110 N116 E119 D127 R128 I131 R132 H136 G141 G146 M149 G150 A151 R152 I158 R159

G160 E161 E165 Q170 R174 Y191 D192 F193 A201 Y204 P227 A231 C238 P239 T240 T241 V242 A243 N244 V245 V248 A249 V250 S251 P252 T253 I254 C255 R256 F262 A263 N270 S271 G272 T273 H281 P285 V288 N292 P295 L296 K297 E298

H303 V317 P325 L326 D358 D362 I363 E377 S378 C379 G380 C385 R386 E387 G388 V389 D390 W391 M392 R398 D403 E408 S411 E414 I415 S416 E420 G421 H422 T423 I424 C425 A426 D429 W433 Q436 E448 R449 Q452 Q458

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

Chain B: 86% 14%

T37 Y38 K39 S47 R56 W63 L66 Y76 R79 E80 I84 E89 S94 R98 G99 E100 E111 R141 R144 Y145 D146 E160 D165 E169 L184 Y185 N192 E200 Y211 R212

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

Chain C: 90% 10%

S41 R42 V46 L50 D51 D52 L53 V54 N55 W56 E75 R83 L109 L117 Y147 P167 K188 R189 L190 R196

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

Chain E: 78% 21%

G14 T15 S16 V17 S22 E27 R30 R37 A38 W39 E42 V43 F50 D61 K62 V63 R64 E65 M66 F67 M68 L81 K85 L90 I94 N95 V96 W97 K98 T101 R114 L119 Y123 P128

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

Chain F: 5% 74% 26%

L14 R20 C24 Q25 R26 S30 R34 R40 Y41 V42 K46 I53 C58 S59 D60 V61 Q62 P63 W66 F71 A84 T88 L91 E92 L95 S96 G97 K98 A99

• Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 8% 73% 23% 5%

S69 D70 A71 K80 L84 I93 E96 V100 H103 F104 M105 L108 E117 M120 E123 F126 I130 P131 D132 I133 D134 K137 L138 M139 Q142 E143 I144 V145 D146 Y147 I148 Y155 E156

• Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 86% 14%

S69 I93 L98 D111 S112 L113 E117 E123 F128 E129 D132 I133 K151 E156

• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H: 82% 16%

L5 E18 T19 K30 V34 I38 Y44 R45 T48 I51 I77 V80 E101 P102 L103 V104 E105 E106 P107 P108 W114 P115 I116

• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 69% 18% 13%

A2 R6 V7 I8 R12 L20 Q21 A22 K23 L24 Q25 Y28 Q29 P39 K40 V43 G44 P45 S46 S50 N51 N52 R57 R61 P66 K74 VAL LEU ALA SER GLY LYS PRO ALA GLU SER SER ALA VAL ALA GLU T90 E91 K92 K93 A94 L113

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

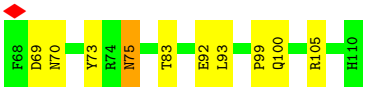
Chain J: 84% 16%

L36 H37 L40 K45 S49 S50 F64 L73 E87 P88 Y89 L100 V119 V120 E135 T136 F139 D140 I167 S168 D173 I174 K175 S176 Y180 E188 R192 A198 T199 I200 I201 K202 P203 S204 F207 G208 D211 R212 F213 L214 F217

M220 I229 Q238 T262 L276 Y279 Y298 R299 R303 L304 V307 E311 D317 E320 R321 V322 H323 P333 E346 P371 A372 I377

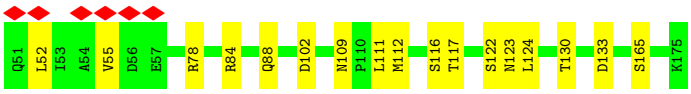
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K: 77% 21%



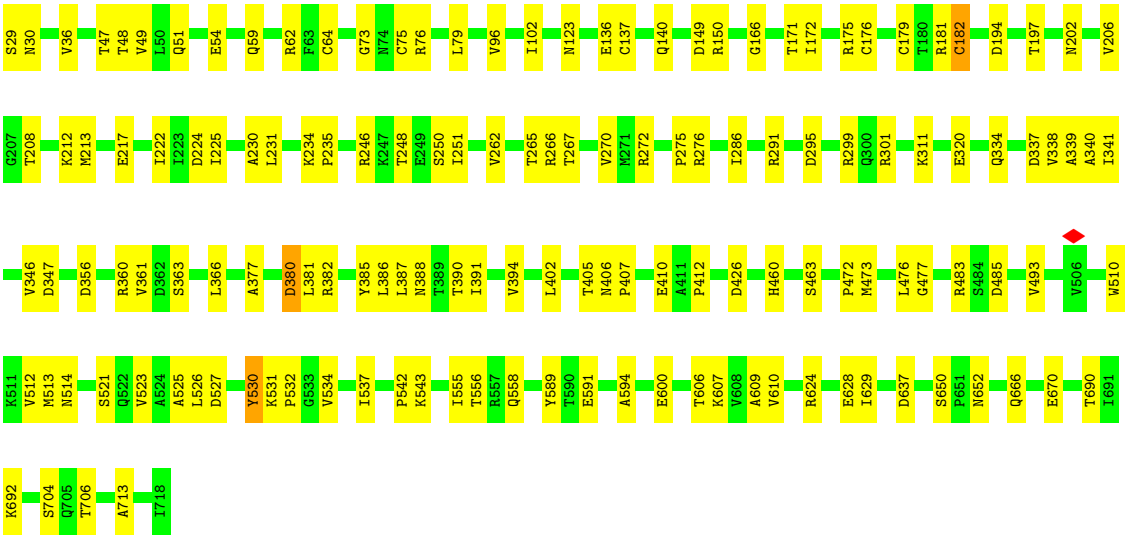
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



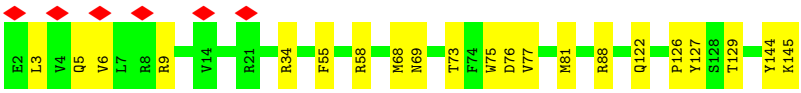
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:



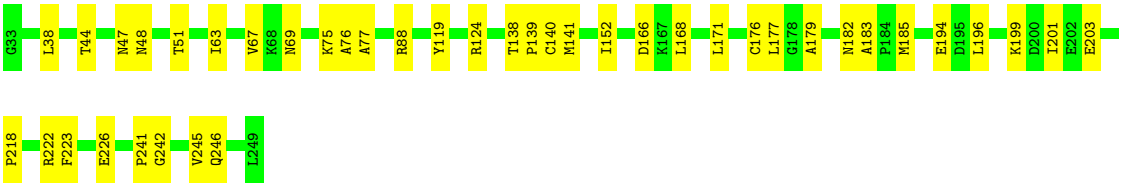
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:



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

Chain O:



• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P: 81% 19%

T43 I47 F61 I68 L69 P70 K71 S79 E83 H89 N105 A106 Q107 F108 L111 D118 V119 P120 T121 R125 L132 F137 R140 I141 R142 V157 N164 M173 F174 H181 P182 L188 H196 P197 F198 R199 K200 D201 Y207

R211 Y212 D213 V219 V224 E225 E229 E250

• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q: 80% 20%

A34 Q38 V41 E45 M52 Y53 D74 F84 H88 A91 V94 L95 R96 L97 V106 L116 H117 R118 E121 K122 L123 K127 M144 Q149 A154 I161 V172 L180 L181 N182 H183 I184 A191 A196 M197 T198 P199 W202

R207 E208 K209 E212 E215 R216 V217 S218 R221 M222 H223 A224 A225 Y226 H233 Q234 D243 I244 F251 S252 F253 E257 L258 E259 E260 M261 L262 T263 R271 D274 G290 R294 L302 D309 V310 R323 E335 E336 H337 R338 L348 K357

V358 D359 D360 A361 K362 V363 S364 R368 K383 E387 Q390 T398 E401 K404 G405 E406 R421 I424 K440 V447 I450 T453 V457 F458 R463

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

Chain S: 86% 14%

M1 A22 I26 N31 K34 V57 Y60 H61 G65 L66 E67 D70

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

Chain T: 88% 12%

G28 T39 Q43 G48 D49 Q59 K60 E61 V62 N63 V76 N101 L102 D103 Q117 H123

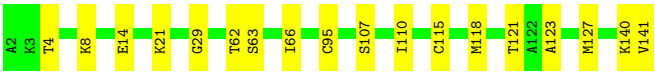
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 94% 6%

A2 Y38 Y41 N46 Y51 P54 L84

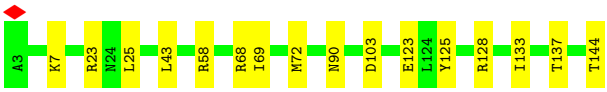
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 87% 13%



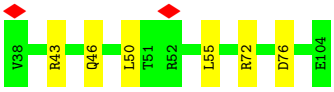
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:



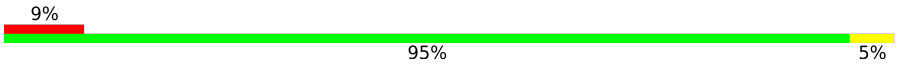
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

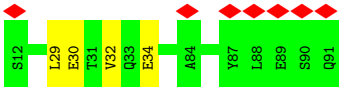
Chain Y:



• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

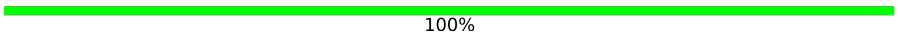
Chain Z:





• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

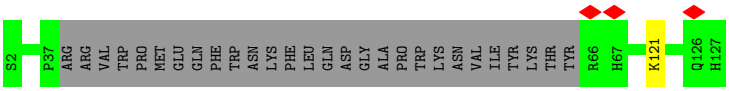
Chain a:



There are no outlier residues recorded for this chain.

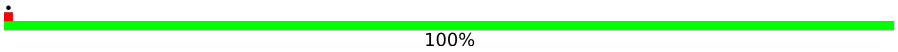
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:

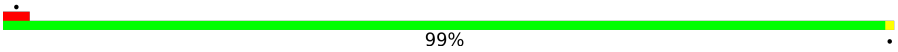


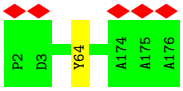
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:

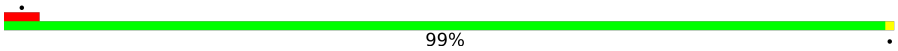


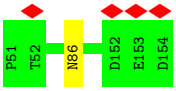
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 

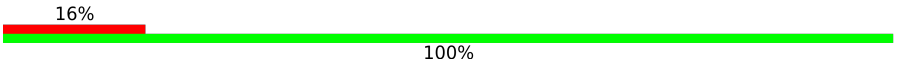


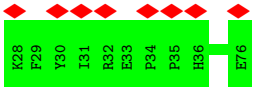
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 

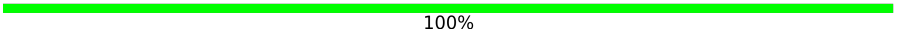


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 

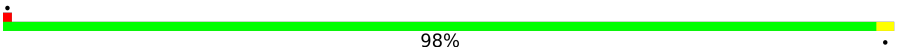


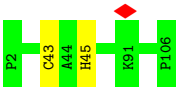
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 

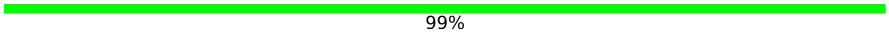
There are no outlier residues recorded for this chain.

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

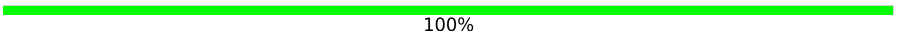
Chain h: 



• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i: 

• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 

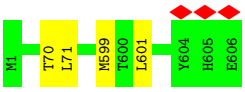
There are no outlier residues recorded for this chain.

• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 99%

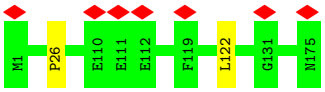
• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l: 99%



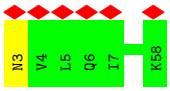
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m: 99%



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

Chain n: 11% 98%



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

Chain o: 98%

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

Chain p: 100%

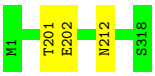
There are no outlier residues recorded for this chain.

• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 100%

• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 99%

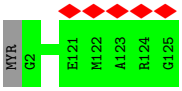


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 99%

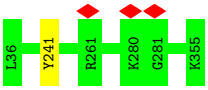
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 99%



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

Chain w: 100%



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	0.211	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	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: FES, 8Q1, 2MR, CDL, FMN, ZN, MG, PEE, PLX, NDP, ADP, SF4, UQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.27	0/3406	0.49	0/4603
2	B	0.31	0/1443	0.50	0/1952
3	C	0.29	0/1279	0.51	0/1730
4	E	0.26	0/995	0.51	0/1340
5	F	0.29	0/698	0.60	0/940
6	G	0.26	0/702	0.60	0/952
6	X	0.27	0/705	0.47	0/954
7	H	0.25	0/929	0.45	0/1258
8	I	0.26	0/798	0.53	0/1079
9	J	0.27	0/2828	0.47	0/3834
10	K	0.25	0/377	0.48	0/509
11	L	0.25	0/1039	0.51	0/1403
12	M	0.26	0/5384	0.51	0/7295
13	N	0.26	0/1245	0.51	0/1694
14	O	0.26	0/1711	0.49	0/2328
15	P	0.29	0/1789	0.51	0/2436
16	Q	0.30	0/3538	0.50	0/4796
17	S	0.25	0/581	0.48	0/781
18	T	0.26	0/755	0.51	0/1018
19	U	0.25	0/664	0.43	0/912
20	V	0.25	0/1042	0.47	0/1411
21	W	0.27	0/1192	0.49	0/1610
22	Y	0.26	0/610	0.44	0/836
23	Z	0.28	0/660	0.49	0/892
24	a	0.27	0/1184	0.49	0/1603
25	b	0.26	0/844	0.50	0/1149
26	c	0.27	0/1371	0.46	0/1875
27	d	0.26	0/1494	0.51	0/2015
28	e	0.26	0/891	0.49	0/1210
29	f	0.26	0/386	0.44	0/523
30	g	0.28	0/1031	0.49	0/1394
31	h	0.26	0/889	0.54	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.27	0/2773	0.47	0/3768
33	j	0.26	0/938	0.41	0/1281
34	k	0.27	0/759	0.47	0/1029
35	l	0.27	0/4947	0.45	0/6728
36	m	0.30	0/1323	0.48	1/1797 (0.1%)
37	n	0.25	0/491	0.51	0/663
38	o	0.27	0/1092	0.50	0/1481
39	p	0.26	0/1590	0.48	0/2155
40	r	0.27	0/3723	0.47	0/5078
41	s	0.28	0/2581	0.49	0/3529
42	u	0.26	0/1436	0.49	0/1938
43	v	0.25	0/1052	0.51	0/1411
44	w	0.26	0/2650	0.47	0/3588
All	All	0.27	0/67815	0.49	1/91968 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
25	b	0	1
32	i	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	m	122	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	PRO	Peptide
25	b	121	LYS	Peptide
32	i	255	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	92	0
2	B	1412	0	1363	32	0
3	C	1248	0	1254	16	0
4	E	971	0	975	23	0
5	F	687	0	700	16	0
6	G	690	0	669	32	0
6	X	694	0	674	12	0
7	H	910	0	950	14	0
8	I	780	0	808	25	0
9	J	2751	0	2773	48	0
10	K	366	0	338	11	0
11	L	1016	0	1016	17	0
12	M	5296	0	5328	115	0
13	N	1204	0	1162	21	0
14	O	1671	0	1673	34	0
15	P	1738	0	1693	44	0
16	Q	3459	0	3396	74	0
17	S	566	0	561	9	0
18	T	741	0	702	10	0
19	U	643	0	642	4	0
20	V	1021	0	1025	9	0
21	W	1161	0	1144	14	0
22	Y	584	0	529	3	0
23	Z	641	0	620	2	0
24	a	1151	0	1164	0	0
25	b	819	0	835	0	0
26	c	1315	0	1208	0	0
27	d	1461	0	1429	0	0
28	e	867	0	817	0	0
29	f	378	0	356	0	0
30	g	1000	0	994	0	0
31	h	867	0	871	0	0
32	i	2710	0	2874	0	0
33	j	914	0	951	0	0
34	k	748	0	799	0	0
35	l	4816	0	4955	0	0
36	m	1291	0	1265	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	479	0	486	0	0
38	o	1062	0	1072	0	0
39	p	1534	0	1470	0	0
40	r	3631	0	3839	0	0
41	s	2508	0	2607	0	0
42	u	1398	0	1374	0	0
43	v	1028	0	982	0	0
44	w	2590	0	2553	0	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	6	0
46	A	31	0	19	14	0
47	B	51	0	82	2	0
47	C	47	0	71	3	0
47	Q	47	0	71	16	0
47	W	41	0	59	5	0
47	b	46	0	69	0	0
47	j	92	0	141	0	0
47	l	91	0	136	0	0
47	r	51	0	82	0	0
48	C	52	0	88	15	0
48	J	52	0	88	0	0
48	N	52	0	88	0	0
48	g	52	0	88	0	0
48	j	52	0	88	0	0
48	n	52	0	88	0	0
48	r	104	0	176	0	0
49	E	35	0	0	1	0
49	X	35	0	0	6	0
50	J	48	0	26	0	0
51	J	33	0	39	10	0
51	s	63	0	90	0	0
52	J	89	0	125	8	0
52	N	51	0	46	11	0
52	V	194	0	294	6	0
52	a	100	0	156	0	0
52	i	68	0	80	0	0
52	l	199	0	307	0	0
52	m	100	0	156	0	0
52	r	100	0	156	0	0
52	u	55	0	54	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	M	4	0	0	1	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	T	1	0	0	0	0
56	w	27	0	11	0	0
All	All	68315	0	69162	639	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (639) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:112:SER:CB	49:X:201:8Q1:O1	1.66	1.42
4:E:30:ARG:HH21	6:G:133:ILE:HD13	1.12	1.13
17:S:31:ASN:ND2	17:S:60:TYR:OH	1.88	1.07
48:C:303:PLX:H212	48:C:303:PLX:H172	1.36	1.06
2:B:98:ARG:HB3	2:B:169:GLU:OE1	1.53	1.05
14:O:182:ASN:ND2	14:O:194:GLU:OE1	1.87	1.04
15:P:105:ASN:O	15:P:137:PHE:CE2	2.12	1.03
12:M:182:CYS:SG	45:M:802:SF4:FE3	1.53	1.00
47:Q:501:PEE:H37	47:Q:501:PEE:C37	1.91	1.00
51:J:402:UQ:H152	51:J:402:UQ:H112	1.38	0.99
6:X:112:SER:CB	49:X:201:8Q1:P24	2.50	0.99
6:G:137:LYS:O	6:G:139:MET:N	1.97	0.98
10:K:100:GLN:NE2	14:O:69:ASN:O	1.97	0.97
8:I:23:LYS:HD2	16:Q:253:PHE:CD2	2.00	0.96
15:P:125:ARG:NH2	15:P:201:ASP:OD1	1.98	0.96
47:Q:501:PEE:H37	47:Q:501:PEE:H61	1.45	0.95
1:A:56:ALA:O	1:A:61:ASP:HB2	1.66	0.95
52:N:202:CDL:C55	52:N:202:CDL:H322	1.97	0.93
20:V:140:LYS:HD3	20:V:141:VAL:HG23	1.54	0.90
15:P:174:PHE:O	15:P:199:ARG:NH2	2.05	0.89
4:E:30:ARG:NH2	6:G:133:ILE:HD13	1.86	0.89
9:J:208:GLY:H	9:J:211:ASP:CG	1.76	0.87
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.08	0.87
48:C:303:PLX:H352	48:C:303:PLX:H393	1.57	0.86
16:Q:226:TYR:OH	16:Q:234:GLN:O	1.92	0.85
2:B:79:ARG:NH2	8:I:20:LEU:HD22	1.90	0.85
9:J:208:GLY:O	9:J:211:ASP:OD1	1.95	0.84
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Q:501:PEE:H28	47:Q:501:PEE:H36	1.59	0.84
47:Q:501:PEE:H28	47:Q:501:PEE:C22	2.05	0.83
12:M:385:TYR:OH	12:M:527:ASP:OD1	1.97	0.83
16:Q:218:SER:CB	16:Q:224:ALA:HB1	2.08	0.83
12:M:337:ASP:O	12:M:542:PRO:CB	2.27	0.83
1:A:149:MET:HE3	1:A:241:THR:CB	2.09	0.83
8:I:23:LYS:HD2	16:Q:253:PHE:CE2	2.12	0.83
8:I:25:GLN:O	16:Q:209:LYS:NZ	2.12	0.82
12:M:382:ARG:NH2	12:M:527:ASP:OD2	2.11	0.82
1:A:149:MET:HE3	1:A:241:THR:HG21	1.62	0.81
9:J:136:THR:HG23	9:J:139:PHE:H	1.44	0.80
4:E:42:GLU:CD	4:E:94:ILE:HD13	2.01	0.80
9:J:299:ARG:NH2	9:J:320:GLU:OE2	2.15	0.80
47:Q:501:PEE:H42	47:Q:501:PEE:H34	1.62	0.80
1:A:149:MET:HE1	1:A:241:THR:HB	1.63	0.80
13:N:3:LEU:HD13	52:N:202:CDL:OA7	1.83	0.79
47:Q:501:PEE:H37	47:Q:501:PEE:H60	1.64	0.78
5:F:71:PHE:HE1	12:M:334:GLN:HE21	1.31	0.78
1:A:87:GLY:HA3	46:A:502:FMN:O2P	1.84	0.78
47:Q:501:PEE:H34	47:Q:501:PEE:C25	2.13	0.78
2:B:79:ARG:NH1	8:I:25:GLN:OE1	2.17	0.78
17:S:65:GLY:O	17:S:67:GLU:N	2.18	0.77
12:M:182:CYS:HG	45:M:802:SF4:FE3	0.47	0.77
5:F:25:GLN:HG3	5:F:26:ARG:HD3	1.66	0.76
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.68	0.76
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.86	0.76
1:A:149:MET:CE	1:A:241:THR:CB	2.63	0.76
1:A:149:MET:CE	1:A:241:THR:HB	2.15	0.76
12:M:171:THR:HG22	12:M:231:LEU:CD2	2.16	0.76
9:J:50:SER:OG	15:P:225:GLU:OE2	2.04	0.75
16:Q:53:TYR:OH	47:Q:501:PEE:H2	1.87	0.74
51:J:402:UQ:O1	51:J:402:UQ:H102	1.87	0.74
3:C:53:LEU:HD22	48:C:303:PLX:H322	1.68	0.74
52:N:202:CDL:H532	52:N:202:CDL:OA9	1.88	0.74
22:Y:72:ARG:NH1	22:Y:76:ASP:OD2	2.21	0.74
6:G:130:ILE:HD12	6:G:130:ILE:N	2.02	0.73
6:G:103:HIS:NE2	6:G:139:MET:HG2	2.04	0.73
1:A:149:MET:HE3	1:A:241:THR:CG2	2.17	0.73
51:J:402:UQ:H152	51:J:402:UQ:C11	2.18	0.72
15:P:43:THR:HA	15:P:47:ILE:HD13	1.71	0.72
6:X:112:SER:CA	49:X:201:8Q1:O1	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:68:MET:HG3	13:N:69:ASN:H	1.54	0.72
48:C:303:PLX:H172	48:C:303:PLX:C21	2.18	0.72
12:M:295:ASP:OD2	12:M:706:THR:OG1	2.02	0.72
4:E:42:GLU:CD	4:E:94:ILE:CD1	2.59	0.72
12:M:176:CYS:SG	45:M:802:SF4:FE4	1.81	0.72
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.23	0.71
12:M:337:ASP:O	12:M:542:PRO:HB2	1.89	0.71
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.24	0.71
6:G:137:LYS:O	6:G:139:MET:HB2	1.90	0.71
1:A:262:PHE:CE2	1:A:272:GLY:HA3	2.26	0.70
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.70	0.70
6:G:137:LYS:O	6:G:139:MET:CB	2.39	0.70
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.21	0.70
1:A:110:PRO:O	1:A:238:CYS:HB3	1.91	0.69
6:G:104:PHE:HA	6:G:108:LEU:HB2	1.72	0.69
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.25	0.69
3:C:190:LEU:CD2	47:C:302:PEE:H13	2.22	0.69
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.25	0.69
5:F:24:CYS:N	5:F:58:CYS:SG	2.66	0.69
12:M:176:CYS:HG	45:M:802:SF4:FE4	1.07	0.68
47:Q:501:PEE:H42	47:Q:501:PEE:C21	2.23	0.68
1:A:49:HIS:O	1:A:59:ARG:NH1	2.25	0.68
1:A:414:GLU:OE2	8:I:50:SER:O	2.11	0.68
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.26	0.68
6:G:134:ASP:OD1	6:G:147:TYR:CE2	2.47	0.68
12:M:171:THR:HG22	12:M:231:LEU:HD22	1.75	0.68
19:U:46:ASN:OD1	21:W:58:ARG:NH2	2.27	0.68
11:L:124:LEU:HD21	15:P:201:ASP:O	1.93	0.67
15:P:125:ARG:HH22	15:P:201:ASP:CG	1.96	0.67
1:A:390:ASP:OD2	12:M:202:ASN:ND2	2.28	0.67
3:C:190:LEU:HD22	47:C:302:PEE:H13	1.75	0.67
7:H:101:GLU:HB3	7:H:102:PRO:HD2	1.75	0.67
4:E:64:ARG:NH1	6:G:117:GLU:OE2	2.27	0.67
6:G:80:LYS:HE2	6:G:100:VAL:HG21	1.76	0.67
15:P:61:PHE:CZ	15:P:106:ALA:HB2	2.30	0.67
47:W:201:PEE:C1	47:W:201:PEE:H10	2.25	0.67
12:M:248:THR:HG21	12:M:609:ALA:HA	1.77	0.67
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.25	0.67
47:W:201:PEE:H10	47:W:201:PEE:H2	1.77	0.66
14:O:140:CYS:SG	14:O:183:ALA:CB	2.83	0.66
6:X:112:SER:CB	49:X:201:8Q1:O2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASP:HB3	1:A:55:GLY:HA3	1.76	0.66
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.29	0.66
12:M:208:THR:HG21	12:M:212:LYS:HB3	1.78	0.66
2:B:79:ARG:NH2	8:I:20:LEU:CD2	2.59	0.66
9:J:304:LEU:C	9:J:304:LEU:HD23	2.15	0.66
12:M:299:ARG:HG3	12:M:299:ARG:HH11	1.60	0.66
12:M:526:LEU:HD21	12:M:532:PRO:HB3	1.78	0.66
8:I:8:ILE:HD11	52:N:202:CDL:H142	1.76	0.66
6:G:130:ILE:HD12	6:G:130:ILE:H	1.61	0.65
15:P:164:ASN:OD1	15:P:181:HIS:HE1	1.79	0.65
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.29	0.65
7:H:105:GLU:HA	7:H:105:GLU:OE1	1.97	0.65
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.77	0.65
2:B:79:ARG:HH21	8:I:20:LEU:CD2	2.09	0.65
6:G:93:ILE:HG12	6:G:108:LEU:HD13	1.79	0.65
12:M:650:SER:OG	12:M:652:ASN:ND2	2.29	0.65
15:P:164:ASN:OD1	15:P:181:HIS:CE1	2.50	0.65
6:G:104:PHE:HD1	6:G:108:LEU:HD12	1.62	0.65
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.78	0.65
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.79	0.65
1:A:422:HIS:O	12:M:76:ARG:HD2	1.97	0.64
46:A:502:FMN:HO3'	46:A:502:FMN:C2	2.05	0.64
14:O:38:LEU:O	14:O:124:ARG:NH2	2.31	0.64
1:A:244:ASN:HB2	46:A:502:FMN:O1P	1.97	0.64
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.32	0.64
3:C:167:PRO:HD3	16:Q:223:HIS:HD2	1.62	0.64
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.32	0.64
14:O:140:CYS:SG	14:O:183:ALA:HB2	2.38	0.64
4:E:68:MET:SD	49:E:201:8Q1:C30	2.86	0.64
13:N:3:LEU:HD11	52:N:202:CDL:C31	2.28	0.64
3:C:56:TRP:CZ2	48:C:303:PLX:H112	2.33	0.64
52:J:404:CDL:H221	52:J:404:CDL:H552	1.78	0.63
4:E:37:ARG:NH1	6:G:132:ASP:OD1	2.31	0.63
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.32	0.63
1:A:159:ARG:NH2	14:O:176:CYS:O	2.31	0.63
16:Q:218:SER:OG	16:Q:224:ALA:HB1	1.97	0.63
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.33	0.62
15:P:61:PHE:CE1	15:P:106:ALA:HB2	2.34	0.62
1:A:426:ALA:HB3	46:A:502:FMN:HM81	1.81	0.62
12:M:390:THR:HB	12:M:600:GLU:OE2	2.00	0.62
4:E:96:VAL:HG12	4:E:96:VAL:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:57:VAL:O	17:S:57:VAL:HG22	2.00	0.62
52:N:202:CDL:H532	52:N:202:CDL:CA7	2.30	0.62
1:A:127:ASP:HB3	1:A:245:VAL:HG11	1.82	0.62
51:J:402:UQ:H112	51:J:402:UQ:C15	2.18	0.62
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.62
1:A:98:LYS:NZ	46:A:502:FMN:O3P	2.33	0.61
12:M:460:HIS:O	12:M:463:SER:OG	2.18	0.61
18:T:39:THR:HG22	18:T:62:VAL:HG22	1.80	0.61
6:G:134:ASP:HB2	6:G:137:LYS:HE2	1.81	0.61
1:A:285:PRO:O	14:O:222:ARG:NH2	2.33	0.61
16:Q:260:GLU:OE2	21:W:25:LEU:HD22	2.00	0.61
48:C:303:PLX:H212	48:C:303:PLX:C17	2.20	0.61
1:A:88:ARG:NH2	1:A:273:THR:O	2.34	0.61
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.34	0.61
7:H:38:ILE:O	7:H:45:ARG:NH1	2.33	0.61
51:J:402:UQ:HM33	51:J:402:UQ:O2	2.01	0.60
12:M:534:VAL:HG22	12:M:534:VAL:O	2.00	0.60
1:A:116:ASN:ND2	46:A:502:FMN:C2	2.64	0.60
12:M:405:THR:HB	12:M:477:GLY:HA3	1.82	0.60
16:Q:144:MET:HG2	16:Q:222:MET:O	2.00	0.60
1:A:251:SER:N	1:A:252:PRO:HD2	2.16	0.60
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.32	0.60
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.30	0.60
9:J:136:THR:HG22	9:J:139:PHE:O	2.01	0.60
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.34	0.60
2:B:47:SER:O	2:B:56:ARG:NH2	2.34	0.60
12:M:472:PRO:O	12:M:510:TRP:NE1	2.31	0.60
9:J:311:GLU:HG3	9:J:311:GLU:O	2.02	0.60
47:C:302:PEE:O5	47:C:302:PEE:H52	2.00	0.60
9:J:135:GLU:HG3	9:J:140:ASP:HA	1.84	0.60
1:A:152:ARG:NH2	10:K:99:PRO:O	2.35	0.59
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.85	0.59
12:M:531:LYS:O	12:M:531:LYS:HG2	2.00	0.59
3:C:56:TRP:CE2	48:C:303:PLX:H112	2.38	0.59
11:L:109:ASN:ND2	11:L:111:LEU:O	2.34	0.59
4:E:17:VAL:HG21	11:L:55:VAL:HG12	1.84	0.59
47:B:303:PEE:H36	21:W:43:LEU:CD1	2.32	0.59
15:P:211:ARG:NH2	15:P:213:ASP:OD2	2.35	0.59
20:V:123:ALA:O	20:V:127:MET:HG3	2.02	0.59
9:J:303:ARG:O	9:J:303:ARG:HD3	2.03	0.58
16:Q:38:GLN:OE1	16:Q:38:GLN:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:65:GLY:C	17:S:67:GLU:H	2.07	0.58
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.85	0.58
51:J:402:UQ:O1	51:J:402:UQ:HM23	2.03	0.58
12:M:337:ASP:O	12:M:542:PRO:HB3	2.02	0.58
13:N:129:THR:HA	18:T:43:GLN:HG2	1.85	0.58
12:M:690:THR:HG21	12:M:692:LYS:HE3	1.85	0.58
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.27	0.58
2:B:160:GLU:OE2	16:Q:233:HIS:NE2	2.37	0.58
48:C:303:PLX:H352	48:C:303:PLX:C39	2.32	0.58
14:O:140:CYS:SG	14:O:183:ALA:HB1	2.44	0.58
2:B:76:TYR:OH	16:Q:257:GLU:OE1	2.22	0.58
12:M:182:CYS:SG	45:M:802:SF4:S2	3.02	0.57
18:T:76:VAL:HG12	18:T:117:GLN:HB2	1.86	0.57
1:A:170:GLN:HA	1:A:170:GLN:OE1	2.53	0.57
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.45	0.57
9:J:64:PHE:CZ	9:J:211:ASP:HB3	2.39	0.57
9:J:201:ILE:HG22	9:J:203:PRO:HD3	1.86	0.57
5:F:91:LEU:O	5:F:95:LEU:HD12	2.05	0.57
6:G:105:MET:CG	6:G:139:MET:HE2	2.35	0.57
14:O:242:GLY:HA2	14:O:245:VAL:HG23	1.87	0.57
15:P:111:LEU:HD12	15:P:132:LEU:HD23	1.85	0.57
16:Q:294:ARG:NH1	16:Q:336:GLU:OE2	2.38	0.56
20:V:62:THR:O	20:V:66:ILE:HG12	2.04	0.56
8:I:40:LYS:HB3	21:W:7:LYS:H	1.71	0.56
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.86	0.56
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.87	0.56
5:F:61:VAL:HG13	5:F:62:GLN:H	1.71	0.56
6:G:134:ASP:O	6:G:138:LEU:HG	2.06	0.56
1:A:60:GLY:HA2	14:O:241:PRO:HB3	1.88	0.56
5:F:71:PHE:CE1	12:M:334:GLN:NE2	2.73	0.56
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.87	0.56
21:W:68:ARG:O	21:W:72:MET:HG3	2.06	0.56
6:X:112:SER:N	49:X:201:8Q1:O1	2.39	0.56
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.87	0.55
5:F:24:CYS:O	5:F:34:ARG:NH1	2.38	0.55
3:C:147:TYR:CZ	15:P:197:PRO:HB3	2.40	0.55
12:M:171:THR:HG22	12:M:231:LEU:HD23	1.87	0.55
19:U:38:TYR:HD1	19:U:41:TYR:HD2	1.54	0.55
6:G:144:ILE:O	6:G:148:ILE:HG13	2.06	0.55
15:P:105:ASN:O	15:P:137:PHE:CZ	2.59	0.55
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.87	0.55
2:B:76:TYR:HE2	16:Q:202:TRP:CD2	2.24	0.55
12:M:166:GLY:HA2	12:M:213:MET:HE2	1.88	0.55
15:P:61:PHE:CZ	15:P:106:ALA:CB	2.89	0.55
16:Q:218:SER:HB3	16:Q:224:ALA:HB1	1.88	0.55
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.89	0.54
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.89	0.54
15:P:207:TYR:C	15:P:224:VAL:HG23	2.27	0.54
1:A:388:GLY:O	1:A:392:MET:HG3	2.07	0.54
16:Q:202:TRP:CZ3	16:Q:261:MET:HG3	2.43	0.54
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.40	0.54
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.88	0.54
3:C:50:LEU:O	3:C:54:VAL:HG23	2.07	0.54
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.88	0.54
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.40	0.54
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.90	0.54
1:A:98:LYS:NZ	1:A:242:VAL:O	2.28	0.54
3:C:53:LEU:HD22	48:C:303:PLX:C32	2.37	0.54
9:J:174:ILE:HG23	9:J:175:LYS:HD2	1.89	0.54
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.88	0.54
17:S:65:GLY:C	17:S:67:GLU:N	2.60	0.54
12:M:36:VAL:HG22	12:M:102:ILE:HD12	1.89	0.54
16:Q:259:GLU:OE2	21:W:23:ARG:NE	2.39	0.54
52:V:201:CDL:H751	52:V:201:CDL:H381	1.89	0.54
1:A:378:SER:OG	1:A:385:CYS:SG	2.64	0.54
48:C:303:PLX:O4	48:C:303:PLX:O7	2.18	0.54
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.89	0.54
7:H:107:PRO:O	7:H:108:PRO:O	2.26	0.54
9:J:87:GLU:HG3	9:J:89:TYR:H	1.72	0.54
21:W:103:ASP:OD1	21:W:103:ASP:N	2.41	0.54
12:M:250:SER:OG	12:M:251:ILE:N	2.40	0.53
1:A:249:ALA:O	1:A:252:PRO:HD2	2.07	0.53
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.44	0.53
9:J:217:PHE:HD1	9:J:220:MET:HE2	1.72	0.53
14:O:75:LYS:O	14:O:77:ALA:N	2.40	0.53
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.91	0.53
12:M:339:ALA:HB1	12:M:537:ILE:HD12	1.91	0.53
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.91	0.53
6:X:132:ASP:OD1	6:X:133:ILE:N	2.39	0.53
7:H:44:TYR:O	7:H:48:THR:HG22	2.08	0.53
12:M:556:THR:HG23	12:M:558:GLN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:W:201:PEE:H42	47:W:201:PEE:H33	1.90	0.53
1:A:263:ALA:HA	1:A:271:SER:HB3	1.90	0.53
8:I:29:GLN:O	8:I:29:GLN:HG3	2.08	0.53
2:B:144:ARG:NH1	11:L:112:MET:O	2.40	0.53
52:N:202:CDL:CA7	52:N:202:CDL:C34	2.86	0.53
1:A:48:ARG:NH1	10:K:70:ASN:O	2.42	0.53
2:B:100:GLU:OE2	2:B:185:TYR:OH	2.21	0.52
10:K:83:THR:HG23	14:O:88:ARG:HH11	1.75	0.52
22:Y:43:ARG:HB3	22:Y:46:GLN:HB2	1.92	0.52
22:Y:50:LEU:HD13	22:Y:55:LEU:HD21	1.91	0.52
11:L:122:SER:HB2	15:P:229:GLU:OE2	2.10	0.52
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.91	0.52
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.41	0.52
15:P:140:ARG:NH2	16:Q:406:GLU:OE2	2.37	0.52
1:A:116:ASN:ND2	46:A:502:FMN:O3'	2.43	0.52
6:G:123:GLU:HB3	6:G:130:ILE:HD13	1.90	0.52
12:M:382:ARG:HE	12:M:527:ASP:CG	2.13	0.52
12:M:591:GLU:HA	12:M:610:VAL:O	2.09	0.52
16:Q:274:ASP:OD1	16:Q:323:ARG:NH2	2.42	0.52
4:E:114:ARG:HH12	9:J:45:LYS:HD2	1.73	0.52
8:I:90:THR:HG22	8:I:92:LYS:HG2	1.92	0.52
12:M:380:ASP:OD1	12:M:380:ASP:N	2.42	0.52
12:M:666:GLN:NE2	12:M:670:GLU:OE2	2.42	0.52
6:G:105:MET:HG3	6:G:139:MET:HE2	1.91	0.52
1:A:250:VAL:C	1:A:252:PRO:HD2	2.29	0.52
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.92	0.52
47:Q:501:PEE:C22	47:Q:501:PEE:C18	2.86	0.52
52:V:202:CDL:H591	52:V:202:CDL:H192	1.92	0.52
2:B:79:ARG:HE	8:I:20:LEU:HD13	1.75	0.52
6:G:105:MET:HG3	6:G:139:MET:CE	2.40	0.52
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.91	0.51
4:E:39:TRP:O	4:E:43:VAL:HG23	2.10	0.51
6:G:130:ILE:N	6:G:130:ILE:CD1	2.73	0.51
9:J:208:GLY:N	9:J:211:ASP:HB3	2.25	0.51
5:F:59:SER:O	5:F:61:VAL:N	2.43	0.51
9:J:229:ILE:HB	9:J:323:HIS:CD2	2.45	0.51
9:J:304:LEU:O	9:J:307:VAL:HG22	2.10	0.51
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.92	0.51
13:N:6:VAL:HG22	13:N:9:ARG:NH2	2.26	0.51
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.34	0.51
12:M:512:VAL:O	12:M:514:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:37:HIS:O	9:J:40:LEU:N	2.40	0.51
21:W:90:ASN:ND2	21:W:123:GLU:O	2.43	0.51
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.92	0.51
12:M:299:ARG:HH11	12:M:299:ARG:CG	2.22	0.51
12:M:341:ILE:HD11	12:M:555:ILE:HD12	1.91	0.51
1:A:67:GLU:O	1:A:71:LYS:HG2	2.11	0.51
1:A:426:ALA:HB3	46:A:502:FMN:C8M	2.41	0.51
9:J:207:PHE:HB2	9:J:214:LEU:HG	1.93	0.51
12:M:48:THR:OG1	12:M:51:GLN:HG3	2.11	0.51
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.93	0.51
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.92	0.51
19:U:54:PRO:HD3	21:W:69:ILE:HD13	1.92	0.51
8:I:46:SER:O	8:I:52:ASN:ND2	2.41	0.50
5:F:61:VAL:HG13	5:F:62:GLN:N	2.26	0.50
51:J:402:UQ:C11	51:J:402:UQ:C15	2.86	0.50
2:B:111:GLU:O	2:B:141:ARG:NH1	2.44	0.50
9:J:180:TYR:HB2	9:J:317:ASP:OD2	2.12	0.50
12:M:29:SER:OG	12:M:30:ASN:N	2.43	0.50
11:L:124:LEU:CD2	15:P:201:ASP:O	2.60	0.50
12:M:194:ASP:OD2	12:M:212:LYS:NZ	2.44	0.50
19:U:51:TYR:O	21:W:68:ARG:NH1	2.44	0.50
2:B:192:ASN:OD1	18:T:63:ASN:ND2	2.41	0.50
48:C:303:PLX:C21	48:C:303:PLX:C17	2.86	0.50
8:I:43:VAL:HG23	8:I:44:GLY:H	1.76	0.50
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.94	0.50
12:M:73:GLY:HA2	53:M:803:FES:S2	2.52	0.50
6:G:134:ASP:OD1	6:G:147:TYR:HE2	1.93	0.50
14:O:166:ASP:OD2	14:O:168:LEU:HD13	2.12	0.50
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.47	0.50
2:B:84:ILE:HA	13:N:58:ARG:HD3	1.94	0.49
12:M:525:ALA:O	12:M:530:TYR:HB2	2.12	0.49
1:A:387:GLU:OE1	12:M:123:ASN:ND2	2.39	0.49
9:J:213:PHE:HZ	9:J:276:LEU:HD21	1.78	0.49
9:J:304:LEU:HD23	9:J:304:LEU:O	2.12	0.49
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.93	0.49
16:Q:357:LYS:HD3	16:Q:364:SER:HB2	1.95	0.49
1:A:48:ARG:HH11	10:K:70:ASN:HB3	1.77	0.49
1:A:174:ARG:NH1	10:K:92:GLU:OE1	2.46	0.49
1:A:231:ALA:O	1:A:239:PRO:HB3	2.13	0.49
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.45	0.49
4:E:42:GLU:OE1	4:E:94:ILE:CD1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:53:ILE:O	12:M:380:ASP:HB3	2.11	0.49
9:J:208:GLY:H	9:J:211:ASP:CB	2.26	0.49
11:L:109:ASN:HB2	11:L:116:SER:OG	2.13	0.48
12:M:406:ASN:O	12:M:410:GLU:HG3	2.13	0.48
12:M:197:THR:HG22	12:M:206:VAL:HG22	1.95	0.48
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.94	0.48
17:S:34:LYS:NZ	17:S:61:HIS:O	2.37	0.48
18:T:101:ASN:ND2	18:T:103:ASP:OD2	2.43	0.48
1:A:272:GLY:O	1:A:292:MET:HB2	2.12	0.48
7:H:48:THR:HA	7:H:51:ILE:HG12	1.95	0.48
12:M:172:ILE:HD12	12:M:175:ARG:NH1	2.28	0.48
16:Q:52:MET:CE	47:Q:501:PEE:H9	2.44	0.48
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.95	0.48
15:P:61:PHE:HZ	15:P:106:ALA:CB	2.26	0.48
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.95	0.48
4:E:62:LYS:O	4:E:66:MET:HG2	2.13	0.48
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.95	0.48
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.49	0.48
1:A:149:MET:CE	1:A:241:THR:OG1	2.62	0.48
1:A:414:GLU:CD	8:I:50:SER:O	2.51	0.48
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.96	0.47
1:A:67:GLU:OE1	1:A:67:GLU:N	2.44	0.47
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.41	0.47
48:C:303:PLX:H341	48:C:303:PLX:H191	1.96	0.47
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.49	0.47
12:M:382:ARG:NE	12:M:527:ASP:OD2	2.47	0.47
17:S:34:LYS:HZ3	17:S:61:HIS:HB2	1.79	0.47
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.97	0.47
17:S:34:LYS:NZ	17:S:61:HIS:HB2	2.30	0.47
8:I:66:PRO:HB3	15:P:79:SER:HA	1.96	0.47
10:K:100:GLN:NE2	14:O:69:ASN:C	2.65	0.47
15:P:105:ASN:O	15:P:137:PHE:HE2	1.87	0.47
21:W:23:ARG:HD3	21:W:25:LEU:HG	1.96	0.47
1:A:281:HIS:ND1	1:A:358:ASP:OD1	2.48	0.47
4:E:14:GLY:O	11:L:52:LEU:HD11	2.14	0.47
6:G:126:PHE:CD2	6:G:148:ILE:HG21	2.49	0.47
51:J:402:UQ:H201	51:J:402:UQ:H221	1.56	0.47
52:J:404:CDL:H171	52:J:404:CDL:H141	1.67	0.47
52:J:404:CDL:H372	52:J:404:CDL:H401	1.57	0.47
11:L:84:ARG:NH1	11:L:88:GLN:O	2.48	0.47
47:Q:501:PEE:H61	47:Q:501:PEE:C23	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:171:THR:CG2	12:M:231:LEU:CD2	2.92	0.47
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.25	0.47
2:B:39:LYS:NZ	16:Q:335:GLU:OE2	2.41	0.47
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.34	0.47
11:L:78:ARG:HD2	12:M:607:LYS:HE2	1.96	0.47
12:M:299:ARG:CZ	12:M:299:ARG:HB3	2.45	0.47
12:M:377:ALA:CB	12:M:381:LEU:HD12	2.45	0.47
12:M:382:ARG:NH2	12:M:652:ASN:OD1	2.48	0.47
14:O:179:ALA:HB3	14:O:185:MET:SD	2.56	0.47
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.50	0.47
6:G:133:ILE:HD12	6:G:133:ILE:HA	1.74	0.46
9:J:49:SER:HB2	15:P:225:GLU:HG2	1.97	0.46
5:F:42:VAL:HG12	5:F:46:LYS:HE3	1.96	0.46
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.51	0.46
13:N:3:LEU:HD11	52:N:202:CDL:H312	1.96	0.46
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.97	0.46
52:J:404:CDL:H341	52:J:404:CDL:H312	1.73	0.46
12:M:483:ARG:NH1	12:M:485:ASP:OD1	2.49	0.46
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.97	0.46
3:C:109:LEU:HD13	3:C:117:LEU:HD13	1.97	0.46
16:Q:53:TYR:CE1	47:Q:501:PEE:O4P	2.69	0.46
20:V:107:SER:HB3	20:V:110:ILE:HB	1.98	0.46
1:A:204:TYR:HB3	1:A:377:GLU:HB3	1.98	0.46
6:G:123:GLU:HB3	6:G:130:ILE:CD1	2.45	0.46
12:M:476:LEU:HD22	12:M:493:VAL:HG21	1.98	0.46
13:N:127:TYR:OH	18:T:61:GLU:O	2.30	0.46
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.98	0.46
1:A:270:ASN:O	1:A:292:MET:HG2	2.16	0.46
9:J:168:SER:O	9:J:203:PRO:HD2	2.16	0.46
12:M:295:ASP:OD1	12:M:704:SER:OG	2.31	0.46
12:M:394:VAL:HA	12:M:473:MET:HE1	1.98	0.46
15:P:118:ASP:OD1	15:P:125:ARG:HG2	2.16	0.46
1:A:448:GLU:O	1:A:452:GLN:HG2	2.16	0.46
2:B:94:SER:OG	16:Q:215:GLU:OE2	2.23	0.46
7:H:103:LEU:HD12	15:P:71:LYS:O	2.16	0.46
12:M:382:ARG:HG2	12:M:386:LEU:CD1	2.46	0.46
1:A:81:LYS:HG2	1:A:96:GLY:HA3	1.98	0.45
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.67	0.45
47:B:303:PEE:H71	47:B:303:PEE:H77	1.61	0.45
10:K:69:ASP:N	10:K:69:ASP:OD1	2.50	0.45
12:M:171:THR:HA	12:M:230:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:118:MET:HA	20:V:121:THR:HG22	1.97	0.45
9:J:37:HIS:NE2	18:T:48:GLY:O	2.49	0.45
51:J:402:UQ:HM51	51:J:402:UQ:H71	1.63	0.45
11:L:117:THR:HG21	15:P:229:GLU:HG3	1.98	0.45
14:O:138:THR:HG22	14:O:139:PRO:HD3	1.97	0.45
1:A:255:CYS:O	14:O:246:GLN:NE2	2.50	0.45
14:O:75:LYS:C	14:O:77:ALA:N	2.70	0.45
1:A:296:LEU:HD11	1:A:317:VAL:HG11	1.97	0.45
4:E:81:LEU:O	4:E:85:LYS:HG3	2.17	0.45
6:G:117:GLU:HA	6:G:120:MET:CE	2.46	0.45
12:M:391:ILE:HG13	12:M:600:GLU:OE2	2.17	0.45
15:P:157:VAL:HG21	15:P:182:PRO:HD3	1.99	0.45
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.52	0.45
9:J:322:VAL:HG13	9:J:323:HIS:ND1	2.32	0.45
5:F:88:THR:O	5:F:92:GLU:OE1	2.35	0.45
16:Q:259:GLU:HG3	16:Q:263:THR:OG1	2.17	0.45
16:Q:440:LYS:HD3	16:Q:440:LYS:HA	1.69	0.45
3:C:75:GLU:HG3	3:C:167:PRO:HB2	1.98	0.45
16:Q:88:HIS:HB3	16:Q:91:ALA:HB2	1.99	0.45
21:W:133:ILE:O	21:W:137:THR:HG22	2.17	0.45
6:X:111:ASP:OD1	6:X:111:ASP:N	2.43	0.45
8:I:8:ILE:HD11	52:N:202:CDL:H111	1.99	0.44
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.99	0.44
52:J:404:CDL:HB61	52:J:404:CDL:H321	1.99	0.44
12:M:391:ILE:N	12:M:600:GLU:OE2	2.31	0.44
12:M:382:ARG:CZ	12:M:527:ASP:OD2	2.64	0.44
16:Q:95:LEU:HD22	16:Q:458:PHE:HZ	1.82	0.44
52:V:202:CDL:H752	52:V:202:CDL:H721	1.55	0.44
3:C:75:GLU:OE1	16:Q:221:ARG:NH1	2.51	0.44
1:A:411:SER:O	1:A:415:ILE:HG13	2.17	0.44
1:A:119:GLU:O	1:A:159:ARG:NH1	2.50	0.44
3:C:51:ASP:OD2	3:C:188:LYS:HA	2.18	0.44
16:Q:41:VAL:O	16:Q:45:GLU:HG3	2.18	0.44
9:J:119:VAL:HG23	9:J:120:VAL:HG13	2.00	0.44
12:M:47:THR:O	12:M:96:VAL:HG22	2.17	0.44
12:M:76:ARG:HD3	12:M:79:LEU:HD21	1.99	0.44
12:M:301:ARG:HD2	12:M:301:ARG:HA	1.69	0.44
15:P:106:ALA:HB1	15:P:108:PHE:HE2	1.82	0.44
52:V:201:CDL:H322	52:V:201:CDL:H352	1.58	0.44
52:V:201:CDL:H402	52:V:201:CDL:H762	2.00	0.44
12:M:299:ARG:CG	12:M:299:ARG:NH1	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.48	0.44
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.33	0.44
13:N:73:THR:HG23	13:N:76:ASP:O	2.18	0.44
14:O:138:THR:HA	14:O:141:MET:HB3	1.99	0.44
1:A:149:MET:HE3	1:A:241:THR:OG1	2.17	0.43
1:A:201:ALA:O	14:O:119:TYR:HB3	2.18	0.43
2:B:76:TYR:CD2	16:Q:202:TRP:CE2	3.06	0.43
12:M:338:VAL:HG23	12:M:363:SER:CB	2.48	0.43
15:P:173:MET:HE2	15:P:188:LEU:HB2	1.99	0.43
1:A:424:ILE:HG12	12:M:76:ARG:NH2	2.34	0.43
8:I:20:LEU:O	8:I:23:LYS:O	2.35	0.43
1:A:60:GLY:HA2	14:O:241:PRO:HA	2.01	0.43
4:E:90:LEU:O	4:E:94:ILE:HG12	2.18	0.43
52:V:202:CDL:H441	52:V:202:CDL:H242	2.00	0.43
2:B:144:ARG:NH1	2:B:146:ASP:OD2	2.43	0.43
47:W:201:PEE:H14	47:W:201:PEE:H20	1.65	0.43
9:J:303:ARG:HD3	9:J:303:ARG:C	2.38	0.43
14:O:182:ASN:CG	14:O:194:GLU:OE1	2.54	0.43
4:E:119:LEU:HD21	12:M:629:ILE:HD11	1.99	0.43
52:J:404:CDL:H331	52:J:404:CDL:H362	1.81	0.43
12:M:265:THR:HG22	12:M:270:VAL:HA	2.01	0.43
21:W:125:TYR:HA	21:W:128:ARG:HD2	2.01	0.43
48:C:303:PLX:H362	48:C:303:PLX:H331	1.73	0.43
7:H:18:GLU:O	7:H:19:THR:OG1	2.36	0.43
11:L:122:SER:CB	15:P:229:GLU:OE2	2.67	0.43
12:M:388:ASN:ND2	12:M:513:MET:O	2.49	0.43
13:N:122:GLN:HA	18:T:59:GLN:HG2	2.01	0.43
14:O:44:THR:HG23	14:O:47:ASN:H	1.83	0.43
1:A:87:GLY:CA	46:A:502:FMN:O2P	2.60	0.43
9:J:204:SER:OG	9:J:238:GLN:O	2.37	0.43
9:J:208:GLY:N	9:J:211:ASP:CG	2.59	0.43
12:M:137:CYS:HB3	12:M:140:GLN:HB2	2.01	0.43
15:P:198:PHE:N	15:P:198:PHE:CD1	2.87	0.43
16:Q:450:ILE:HA	16:Q:453:THR:HG22	2.00	0.43
1:A:53:LEU:HB2	1:A:136:HIS:CE1	2.54	0.43
1:A:116:ASN:HD21	46:A:502:FMN:C2	2.32	0.43
4:E:42:GLU:OE2	4:E:94:ILE:HD13	2.18	0.43
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.54	0.43
9:J:208:GLY:N	9:J:211:ASP:CB	2.82	0.43
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.42	0.43
21:W:144:THR:CG2	47:W:201:PEE:H2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.59	0.43
23:Z:30:GLU:O	23:Z:34:GLU:OE1	2.37	0.43
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.19	0.42
6:G:137:LYS:O	6:G:139:MET:CA	2.66	0.42
11:L:102:ASP:N	11:L:102:ASP:OD1	2.50	0.42
12:M:311:LYS:HB2	12:M:311:LYS:HE3	1.77	0.42
16:Q:144:MET:HE2	16:Q:222:MET:O	2.19	0.42
16:Q:290:GLY:HA2	16:Q:294:ARG:HH21	1.84	0.42
1:A:131:ILE:HD13	1:A:158:ILE:HD13	2.01	0.42
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.01	0.42
12:M:346:VAL:H	12:M:521:SER:HB3	1.84	0.42
14:O:199:LYS:O	14:O:203:GLU:HG3	2.18	0.42
9:J:304:LEU:C	9:J:304:LEU:CD2	2.85	0.42
16:Q:161:ILE:HD13	16:Q:363:VAL:HG11	2.01	0.42
6:X:93:ILE:HD13	6:X:98:LEU:HD12	2.01	0.42
1:A:416:SER:OG	1:A:436:GLN:NE2	2.52	0.42
12:M:589:TYR:O	12:M:606:THR:HG21	2.19	0.42
14:O:242:GLY:HA2	14:O:245:VAL:CG2	2.49	0.42
16:Q:154:ALA:HA	16:Q:398:THR:HG21	2.00	0.42
16:Q:404:LYS:HE2	16:Q:457:VAL:HG23	2.02	0.42
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.84	0.42
9:J:73:LEU:HD23	9:J:73:LEU:HA	2.16	0.42
51:J:402:UQ:H101	51:J:402:UQ:H121	1.83	0.42
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.02	0.42
11:L:130:THR:OG1	11:L:133:ASP:OD2	2.38	0.42
47:Q:501:PEE:H34	47:Q:501:PEE:H41	2.00	0.42
12:M:49:VAL:HG13	12:M:102:ILE:HD13	2.01	0.42
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.19	0.42
1:A:29:LYS:H	1:A:29:LYS:HG3	1.70	0.42
3:C:42:ARG:O	3:C:46:VAL:HG23	2.20	0.42
9:J:135:GLU:OE2	9:J:140:ASP:HB2	2.20	0.42
12:M:64:CYS:HB3	12:M:75:CYS:HB3	2.01	0.42
13:N:5:GLN:HG2	13:N:9:ARG:NH1	2.35	0.42
1:A:141:GLY:HA3	1:A:248:VAL:O	2.19	0.42
1:A:423:THR:HB	45:A:501:SF4:S4	2.59	0.42
48:C:303:PLX:O2	13:N:75:TRP:HB3	2.20	0.42
4:E:101:THR:OG1	15:P:219:VAL:O	2.26	0.42
9:J:37:HIS:NE2	18:T:49:ASP:HA	2.35	0.42
12:M:59:GLN:HG2	12:M:62:ARG:NH2	2.35	0.42
12:M:182:CYS:SG	45:M:802:SF4:S4	3.18	0.42
52:N:202:CDL:C55	52:N:202:CDL:C32	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:245:VAL:HG12	14:O:246:GLN:O	2.20	0.42
20:V:4:THR:O	20:V:8:LYS:HG2	2.20	0.42
6:X:113:LEU:O	6:X:117:GLU:HG3	2.19	0.42
6:X:128:PHE:CE2	6:X:151:LYS:HD3	2.55	0.42
23:Z:29:LEU:HA	23:Z:32:VAL:HG12	2.01	0.42
12:M:213:MET:HE1	12:M:713:ALA:HB1	2.01	0.41
13:N:73:THR:HG21	13:N:81:MET:CE	2.49	0.41
16:Q:180:LEU:HD23	16:Q:180:LEU:HA	1.92	0.41
16:Q:383:LYS:HA	16:Q:383:LYS:HD2	1.89	0.41
1:A:151:ALA:O	1:A:191:TYR:OH	2.25	0.41
12:M:338:VAL:CG2	12:M:363:SER:HB2	2.49	0.41
20:V:95:CYS:HA	20:V:115:CYS:HA	2.01	0.41
52:J:404:CDL:H831	52:J:404:CDL:H411	2.01	0.41
12:M:179:CYS:SG	12:M:181:ARG:HB2	2.61	0.41
12:M:213:MET:CE	12:M:713:ALA:HB1	2.51	0.41
12:M:338:VAL:HG21	12:M:361:VAL:HG21	2.02	0.41
12:M:386:LEU:HD21	12:M:523:VAL:HG13	2.01	0.41
16:Q:121:GLU:OE1	16:Q:421:ARG:NH1	2.41	0.41
20:V:29:GLY:O	20:V:63:SER:HB3	2.20	0.41
2:B:79:ARG:HH21	8:I:20:LEU:HD22	1.67	0.41
12:M:250:SER:OG	12:M:606:THR:HG23	2.20	0.41
12:M:347:ASP:OD1	12:M:347:ASP:N	2.44	0.41
15:P:106:ALA:HB1	15:P:108:PHE:CE2	2.54	0.41
16:Q:53:TYR:HE1	47:Q:501:PEE:H12	1.86	0.41
13:N:3:LEU:HD11	52:N:202:CDL:H311	2.02	0.41
15:P:174:PHE:CE1	15:P:198:PHE:O	2.73	0.41
16:Q:202:TRP:CH2	16:Q:261:MET:HG3	2.55	0.41
52:J:404:CDL:H382	52:J:404:CDL:H212	2.03	0.41
12:M:356:ASP:O	12:M:360:ARG:HG2	2.21	0.41
12:M:543:LYS:HE3	12:M:543:LYS:HB3	1.88	0.41
15:P:196:HIS:HA	15:P:197:PRO:HD3	1.89	0.41
16:Q:183:HIS:NE2	16:Q:336:GLU:OE1	2.53	0.41
1:A:161:GLU:HG2	14:O:177:LEU:HD22	2.03	0.41
1:A:250:VAL:O	1:A:253:THR:N	2.54	0.41
2:B:80:GLU:OE1	8:I:28:TYR:OH	2.39	0.41
16:Q:144:MET:SD	16:Q:144:MET:N	2.94	0.41
16:Q:198:THR:OG1	16:Q:202:TRP:NE1	2.54	0.41
5:F:40:ARG:NH2	5:F:84:ALA:HB1	2.36	0.41
15:P:68:ILE:HG22	15:P:69:LEU:HG	2.02	0.41
20:V:14:GLU:HA	20:V:21:LYS:HE3	2.03	0.41
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.56	0.41
1:A:380:GLY:O	1:A:386:ARG:HD3	2.21	0.41
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.36	0.41
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	2.01	0.41
4:E:50:PHE:HE2	4:E:98:LYS:O	2.03	0.41
4:E:61:ASP:OD1	4:E:62:LYS:N	2.53	0.41
5:F:30:SER:OG	5:F:63:PRO:HG3	2.21	0.41
6:G:84:LEU:HD21	6:G:100:VAL:HG22	2.03	0.41
6:G:142:GLN:O	6:G:145:VAL:HG22	2.20	0.41
7:H:77:ILE:HA	7:H:80:VAL:HG23	2.03	0.41
9:J:100:LEU:HD23	9:J:100:LEU:HA	1.89	0.41
9:J:262:THR:O	9:J:333:PRO:HD2	2.21	0.41
16:Q:198:THR:HG23	16:Q:199:PRO:HD3	2.02	0.41
17:S:22:ALA:O	17:S:26:ILE:HG12	2.20	0.41
1:A:251:SER:N	1:A:252:PRO:CD	2.84	0.41
1:A:325:PRO:HG3	1:A:433:TRP:HB3	2.03	0.41
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.03	0.41
14:O:63:ILE:O	14:O:67:VAL:HG23	2.21	0.41
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.56	0.40
12:M:402:LEU:HD13	12:M:407:PRO:HG2	2.03	0.40
16:Q:53:TYR:HE1	47:Q:501:PEE:O4P	2.02	0.40
48:C:303:PLX:C39	48:C:303:PLX:C35	2.97	0.40
4:E:22:SER:HB2	4:E:27:GLU:HB2	2.02	0.40
1:A:128:ARG:O	1:A:132:ARG:HG2	2.22	0.40
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.41	0.40
1:A:398:ARG:CG	1:A:403:ASP:HB3	2.51	0.40
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	2.04	0.40
1:A:358:ASP:OD1	1:A:358:ASP:N	2.50	0.40
9:J:204:SER:OG	9:J:204:SER:O	2.36	0.40
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.91	0.40
1:A:63:TYR:O	1:A:256:ARG:HD3	2.22	0.40
2:B:98:ARG:CB	2:B:169:GLU:OE1	2.45	0.40
2:B:200:GLU:HG3	13:N:88:ARG:HB2	2.03	0.40
5:F:25:GLN:HG3	5:F:26:ARG:CD	2.44	0.40
7:H:30:LYS:O	7:H:34:VAL:HG23	2.21	0.40
7:H:105:GLU:HB3	15:P:89:HIS:NE2	2.36	0.40
13:N:144:TYR:CE2	13:N:145:LYS:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	410 (95%)	21 (5%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	2 (2%)	1 (1%)	17	48
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	6	23
6	X	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
7	H	110/112 (98%)	103 (94%)	5 (4%)	2 (2%)	8	29
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	340/342 (99%)	327 (96%)	13 (4%)	0	100	100
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	664 (96%)	24 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	29	61
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	427/430 (99%)	413 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	63 (93%)	4 (6%)	1 (2%)	10	34
18	T	94/96 (98%)	94 (100%)	0	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
23	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	94/126 (75%)	91 (97%)	3 (3%)	0	100	100
26	c	154/156 (99%)	141 (92%)	13 (8%)	0	100	100
27	d	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
28	e	102/104 (98%)	94 (92%)	8 (8%)	0	100	100
29	f	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	330 (96%)	14 (4%)	1 (0%)	41	71
33	j	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	574 (95%)	30 (5%)	0	100	100
36	m	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	25	58
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
42	u	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	25	58
43	v	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	8174/8313 (98%)	7839 (96%)	325 (4%)	10 (0%)	54	82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	138	LEU
7	H	108	PRO
17	S	66	LEU
6	G	133	ILE
14	O	76	ALA
32	i	255	PRO
36	m	26	PRO
4	E	96	VAL
7	H	77	ILE
42	u	152	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	75/81 (93%)	73 (97%)	2 (3%)	44	77
6	X	76/81 (94%)	76 (100%)	0	100	100
7	H	99/99 (100%)	98 (99%)	1 (1%)	76	92
8	I	87/97 (90%)	86 (99%)	1 (1%)	73	92
9	J	296/296 (100%)	294 (99%)	2 (1%)	84	95
10	K	42/42 (100%)	41 (98%)	1 (2%)	49	79
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	93
12	M	580/580 (100%)	577 (100%)	3 (0%)	88	96
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	189 (100%)	1 (0%)	88	96
16	Q	370/370 (100%)	370 (100%)	0	100	100
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	154 (99%)	1 (1%)	86	96
28	e	96/96 (100%)	95 (99%)	1 (1%)	76	92
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	91 (98%)	2 (2%)	52	81
32	i	311/311 (100%)	310 (100%)	1 (0%)	92	98
33	j	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	84 (99%)	1 (1%)	71	91
35	l	540/540 (100%)	536 (99%)	4 (1%)	84	95
36	m	130/141 (92%)	130 (100%)	0	100	100
37	n	53/53 (100%)	52 (98%)	1 (2%)	57	84
38	o	113/113 (100%)	111 (98%)	2 (2%)	59	85
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	408 (100%)	2 (0%)	88	96
41	s	275/275 (100%)	272 (99%)	3 (1%)	73	92
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	283/283 (100%)	282 (100%)	1 (0%)	91	97
All	All	7159/7240 (99%)	7128 (100%)	31 (0%)	91	97

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	G	132	ASP
6	G	134	ASP
7	H	104	VAL
8	I	61	ARG
9	J	298	TYR
9	J	303	ARG
10	K	75	ASN
11	L	165	SER
12	M	182	CYS
12	M	380	ASP
12	M	530	TYR

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Mol	Chain	Res	Type
15	P	201	ASP
27	d	64	TYR
28	e	86	ASN
31	h	43	CYS
31	h	45	HIS
32	i	171	ASN
34	k	53	PHE
35	l	70	THR
35	l	71	LEU
35	l	599	MET
35	l	601	LEU
37	n	3	ASN
38	o	56	ARG
38	o	129	TYR
40	r	248	THR
40	r	251	ASN
41	s	201	THR
41	s	202	GLU
41	s	212	ASN
44	w	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	244	ASN
1	A	436	GLN
7	H	86	ASN
9	J	356	HIS
12	M	39	GLN
12	M	331	GLN
12	M	652	ASN
14	O	74	HIS
15	P	181	HIS
16	Q	36	GLN
17	S	31	ASN
27	d	107	GLN
27	d	149	HIS
31	h	98	HIS
32	i	268	GLN
33	j	10	ASN
35	l	67	HIS

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Mol	Chain	Res	Type
35	l	139	GLN
35	l	524	ASN
35	l	541	ASN
40	r	251	ASN
41	s	212	ASN
42	u	151	ASN
42	u	163	HIS
43	v	50	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	1.97	1 (10%)	5,13,15	5.97	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.58	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	12.23	130.69	119.48
16	Q	118	2MR	CD-NE-CZ	4.08	131.05	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.14	130.81	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	CDL	r	504	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
46	FMN	A	502	-	33,33,33	1.40	5 (15%)	48,50,50	1.28	7 (14%)
45	SF4	M	802	12	0,12,12	-	-	-		
52	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.58	1 (1%)
50	NDP	J	401	-	45,52,52	2.23	4 (8%)	53,80,80	1.75	11 (20%)
53	FES	M	803	12	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
52	CDL	l	703	-	99,99,99	0.91	4 (4%)	105,111,111	1.08	7 (6%)
48	PLX	C	303	-	51,51,51	0.62	0	55,59,59	0.67	0
45	SF4	M	801	12	0,12,12	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
47	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.99	2 (4%)
51	UQ	J	402	-	33,33,63	3.44	9 (27%)	40,43,79	2.80	13 (32%)
52	CDL	V	201	-	93,93,99	1.11	8 (8%)	99,105,111	0.87	4 (4%)
45	SF4	C	301	3	0,12,12	-	-	-		
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
52	CDL	u	201	-	54,54,99	1.23	4 (7%)	60,66,111	1.24	5 (8%)
48	PLX	J	403	-	51,51,51	1.14	3 (5%)	55,59,59	0.59	1 (1%)
52	CDL	i	401	-	67,67,99	1.12	4 (5%)	73,79,111	1.22	6 (8%)
47	PEE	r	501	-	50,50,50	1.16	5 (10%)	53,55,55	0.96	2 (3%)
47	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.98	2 (3%)
49	8Q1	E	201	-	31,34,34	2.06	6 (19%)	40,43,43	1.70	11 (27%)
47	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.99	2 (4%)
47	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.04	2 (4%)
52	CDL	l	702	-	98,98,99	1.09	8 (8%)	104,110,111	0.90	4 (3%)
48	PLX	n	101	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
49	8Q1	X	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.57	6 (15%)
47	PEE	W	201	-	40,40,50	1.13	5 (12%)	43,45,55	1.01	2 (4%)
47	PEE	Q	501	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
52	CDL	N	202	-	50,50,99	1.28	4 (8%)	56,62,111	1.29	5 (8%)
48	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.59	1 (1%)
52	CDL	V	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.88	4 (3%)
52	CDL	m	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
48	PLX	N	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
51	UQ	s	501	-	63,63,63	3.63	15 (23%)	76,79,79	3.21	31 (40%)
53	FES	O	301	14	0,4,4	-	-	-		
48	PLX	j	203	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
56	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.45	5 (17%)
52	CDL	J	404	-	88,88,99	1.13	8 (9%)	94,100,111	0.92	4 (4%)
47	PEE	l	704	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
48	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.65	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
47	PEE	j	202	-	40,40,50	1.15	5 (12%)	43,45,55	1.02	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
52	CDL	r	504	-	-	59/110/110/110	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
45	SF4	M	802	12	-	-	0/6/5/5
52	CDL	a	201	-	-	56/110/110/110	-
48	PLX	r	502	-	-	24/55/55/55	-
50	NDP	J	401	-	-	10/30/77/77	0/5/5/5
53	FES	M	803	12	-	-	0/1/1/1
52	CDL	l	703	-	-	38/110/110/110	-
48	PLX	C	303	-	-	16/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
47	PEE	C	302	-	-	25/50/50/54	-
51	UQ	J	402	-	-	17/27/51/87	0/1/1/1
52	CDL	V	201	-	-	53/104/104/110	-
47	PEE	B	303	-	-	28/54/54/54	-
52	CDL	u	201	-	-	23/65/65/110	-
45	SF4	C	301	3	-	-	0/6/5/5
48	PLX	J	403	-	-	35/55/55/55	-
52	CDL	i	401	-	-	33/78/78/110	-
47	PEE	r	501	-	-	23/54/54/54	-
47	PEE	j	201	-	-	27/54/54/54	-
49	8Q1	E	201	-	-	23/41/41/41	-
47	PEE	b	201	-	-	24/49/49/54	-
47	PEE	l	701	-	-	25/43/43/54	-
52	CDL	l	702	-	-	57/109/109/110	-
48	PLX	n	101	-	-	26/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
49	8Q1	X	201	-	-	14/41/41/41	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	W	201	-	-	24/44/44/54	-
47	PEE	Q	501	-	-	27/50/50/54	-
52	CDL	N	202	-	-	21/61/61/110	-
48	PLX	r	503	-	-	26/55/55/55	-
52	CDL	V	202	-	-	61/110/110/110	-
52	CDL	m	201	-	-	61/110/110/110	-
48	PLX	N	201	-	-	28/55/55/55	-
51	UQ	s	501	-	-	32/63/87/87	0/1/1/1
56	ADP	w	401	-	-	4/12/32/32	0/3/3/3
48	PLX	j	203	-	-	30/55/55/55	-
53	FES	O	301	14	-	-	0/1/1/1
52	CDL	J	404	-	-	48/99/99/110	-
47	PEE	l	704	-	-	29/54/54/54	-
48	PLX	g	201	-	-	29/55/55/55	-
47	PEE	j	202	-	-	25/44/44/54	-

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	P2B-O2B	12.43	1.82	1.59
51	s	501	UQ	C18-C19	9.56	1.55	1.33
51	J	402	UQ	C18-C19	9.55	1.55	1.33
51	s	501	UQ	C13-C14	9.24	1.55	1.33
51	J	402	UQ	C13-C14	9.21	1.55	1.33
51	s	501	UQ	C23-C24	9.10	1.54	1.33
51	J	402	UQ	C8-C9	8.99	1.54	1.33
56	w	401	ADP	C3'-C4'	-8.95	1.30	1.53
51	s	501	UQ	C28-C29	8.90	1.54	1.33
51	s	501	UQ	C8-C9	8.89	1.54	1.33
51	s	501	UQ	C33-C34	8.50	1.53	1.33
51	s	501	UQ	C43-C44	8.25	1.52	1.33
51	s	501	UQ	C38-C39	8.22	1.52	1.33
51	s	501	UQ	C48-C49	7.92	1.52	1.33
51	J	402	UQ	C23-C24	7.80	1.54	1.32
49	E	201	8Q1	P24-O27	7.69	1.85	1.60
56	w	401	ADP	O4'-C4'	7.62	1.62	1.45
51	s	501	UQ	C53-C54	7.36	1.53	1.32
56	w	401	ADP	O4'-C1'	-6.91	1.31	1.41
49	X	201	8Q1	C34-N36	5.43	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	X	201	8Q1	C39-N41	5.35	1.45	1.33
46	A	502	FMN	C9A-C5A	4.71	1.49	1.41
52	i	401	CDL	OB8-CB7	4.30	1.45	1.33
52	i	401	CDL	OA8-CA7	4.28	1.45	1.33
52	u	201	CDL	OA8-CA7	4.26	1.45	1.33
52	N	202	CDL	OB8-CB7	4.25	1.45	1.33
52	l	703	CDL	OA8-CA7	4.25	1.45	1.33
52	u	201	CDL	OB8-CB7	4.23	1.45	1.33
52	N	202	CDL	OA8-CA7	4.23	1.45	1.33
52	u	201	CDL	OB6-CB5	4.18	1.46	1.34
52	i	401	CDL	OB6-CB5	4.17	1.46	1.34
52	l	703	CDL	OB8-CB7	4.16	1.45	1.33
52	N	202	CDL	OB6-CB5	4.12	1.45	1.34
52	N	202	CDL	OA6-CA5	4.11	1.45	1.34
52	l	703	CDL	OA6-CA5	4.09	1.45	1.34
52	i	401	CDL	OA6-CA5	4.04	1.45	1.34
52	l	703	CDL	OB6-CB5	4.02	1.45	1.34
52	u	201	CDL	OA6-CA5	4.01	1.45	1.34
56	w	401	ADP	C6-N6	3.85	1.48	1.34
50	J	401	NDP	PN-O5D	3.83	1.74	1.59
49	E	201	8Q1	C1-S44	3.76	1.85	1.76
47	r	501	PEE	C18-C19	3.75	1.53	1.31
47	j	202	PEE	C18-C19	3.74	1.53	1.31
47	l	704	PEE	C18-C19	3.74	1.53	1.31
47	C	302	PEE	C18-C19	3.73	1.53	1.31
47	l	701	PEE	C18-C19	3.73	1.53	1.31
47	B	303	PEE	C18-C19	3.72	1.53	1.31
47	b	201	PEE	C18-C19	3.72	1.53	1.31
47	j	201	PEE	C18-C19	3.71	1.53	1.31
47	W	201	PEE	C18-C19	3.69	1.53	1.31
47	Q	501	PEE	C18-C19	3.68	1.53	1.31
47	l	701	PEE	C39-C38	3.66	1.53	1.31
47	C	302	PEE	C39-C38	3.65	1.52	1.31
47	r	501	PEE	C39-C38	3.64	1.52	1.31
47	b	201	PEE	C39-C38	3.63	1.52	1.31
47	B	303	PEE	C39-C38	3.63	1.52	1.31
47	j	201	PEE	C39-C38	3.62	1.52	1.31
47	l	704	PEE	C39-C38	3.62	1.52	1.31
47	Q	501	PEE	C39-C38	3.62	1.52	1.31
49	E	201	8Q1	C34-N36	3.58	1.41	1.33
52	V	201	CDL	OA8-CA7	3.45	1.43	1.33
52	J	404	CDL	OA8-CA7	3.42	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	V	202	CDL	OA8-CA7	3.42	1.43	1.33
52	l	702	CDL	OA8-CA7	3.41	1.43	1.33
52	a	201	CDL	OA8-CA7	3.38	1.43	1.33
52	r	504	CDL	OA8-CA7	3.38	1.43	1.33
49	E	201	8Q1	O27-C28	-3.36	1.33	1.43
52	m	201	CDL	OA8-CA7	3.36	1.43	1.33
56	w	401	ADP	O2'-C2'	-3.23	1.35	1.43
56	w	401	ADP	O3'-C3'	3.16	1.50	1.43
52	m	201	CDL	OA6-CA5	3.11	1.43	1.34
52	V	201	CDL	OA6-CA5	3.11	1.43	1.34
46	A	502	FMN	C8-C7	3.09	1.48	1.40
52	a	201	CDL	OB6-CB5	3.06	1.42	1.34
50	J	401	NDP	O2B-C2B	-3.05	1.33	1.44
49	E	201	8Q1	C6-C1	3.03	1.53	1.50
52	r	504	CDL	OB6-CB5	3.03	1.42	1.34
52	V	202	CDL	OB6-CB5	3.01	1.42	1.34
52	m	201	CDL	OB8-CB7	3.00	1.42	1.33
52	l	702	CDL	OB6-CB5	2.99	1.42	1.34
52	J	404	CDL	OA6-CA5	2.98	1.42	1.34
52	J	404	CDL	OB6-CB5	2.98	1.42	1.34
52	a	201	CDL	OB8-CB7	2.97	1.42	1.33
52	r	504	CDL	OB8-CB7	2.97	1.42	1.33
52	l	702	CDL	OB8-CB7	2.97	1.42	1.33
49	E	201	8Q1	C39-N41	2.96	1.40	1.33
52	V	201	CDL	OB6-CB5	2.95	1.42	1.34
52	m	201	CDL	OB6-CB5	2.95	1.42	1.34
52	a	201	CDL	OA6-CA5	2.95	1.42	1.34
52	J	404	CDL	OB8-CB7	2.92	1.41	1.33
52	V	201	CDL	OB8-CB7	2.91	1.41	1.33
52	V	202	CDL	OB8-CB7	2.91	1.41	1.33
52	V	202	CDL	OA6-CA5	2.90	1.42	1.34
52	l	702	CDL	OA6-CA5	2.90	1.42	1.34
52	r	504	CDL	OA6-CA5	2.86	1.42	1.34
46	A	502	FMN	C4-N3	-2.83	1.33	1.38
48	n	101	PLX	O6-C4	-2.75	1.40	1.44
48	r	502	PLX	O6-C4	-2.69	1.41	1.44
48	g	201	PLX	O6-C4	-2.68	1.41	1.44
51	s	501	UQ	C6-C1	2.65	1.54	1.46
51	J	402	UQ	C6-C1	2.63	1.54	1.46
48	N	201	PLX	O6-C4	-2.63	1.41	1.44
47	B	303	PEE	O2-C2	-2.63	1.40	1.46
48	j	203	PLX	O6-C4	-2.61	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	r	503	PLX	O6-C4	-2.58	1.41	1.44
47	C	302	PEE	O3-C30	2.56	1.40	1.33
47	r	501	PEE	O3-C30	2.54	1.40	1.33
47	Q	501	PEE	O2-C2	-2.52	1.40	1.46
47	l	704	PEE	O2-C2	-2.50	1.40	1.46
48	j	203	PLX	C7-C6	2.49	1.56	1.50
52	a	201	CDL	OA6-CA4	-2.49	1.40	1.46
47	C	302	PEE	O2-C2	-2.49	1.40	1.46
52	r	504	CDL	OA6-CA4	-2.49	1.40	1.46
47	l	701	PEE	O3-C30	2.46	1.40	1.33
47	r	501	PEE	O2-C2	-2.44	1.40	1.46
47	b	201	PEE	O3-C30	2.44	1.40	1.33
51	J	402	UQ	C7-C8	2.43	1.54	1.50
47	B	303	PEE	O3-C30	2.43	1.40	1.33
52	V	202	CDL	OA6-CA4	-2.43	1.40	1.46
47	j	202	PEE	O3-C30	2.42	1.40	1.33
47	W	201	PEE	O3-C30	2.42	1.40	1.33
48	J	403	PLX	O6-C4	-2.42	1.41	1.44
47	j	202	PEE	O2-C2	-2.40	1.40	1.46
47	W	201	PEE	O2-C2	-2.39	1.40	1.46
47	j	201	PEE	O2-C2	-2.39	1.40	1.46
47	l	701	PEE	O2-C2	-2.39	1.40	1.46
52	J	404	CDL	OA6-CA4	-2.39	1.40	1.46
51	s	501	UQ	C7-C8	2.38	1.54	1.50
52	l	702	CDL	OA6-CA4	-2.38	1.40	1.46
47	j	201	PEE	O3-C30	2.38	1.40	1.33
48	r	503	PLX	C7-C6	2.37	1.55	1.50
47	b	201	PEE	O2-C2	-2.35	1.40	1.46
49	X	201	8Q1	C1-S44	2.35	1.81	1.76
47	Q	501	PEE	O3-C30	2.35	1.40	1.33
48	J	403	PLX	C7-C6	2.35	1.55	1.50
48	r	502	PLX	C7-C6	2.32	1.55	1.50
47	l	704	PEE	O3-C30	2.32	1.40	1.33
48	g	201	PLX	C7-C6	2.30	1.55	1.50
48	N	201	PLX	C7-C6	2.29	1.55	1.50
51	s	501	UQ	O4-C4	-2.29	1.18	1.23
52	V	201	CDL	OB6-CB4	-2.29	1.40	1.46
49	X	201	8Q1	C6-C1	2.28	1.53	1.50
48	n	101	PLX	C7-C6	2.27	1.55	1.50
49	X	201	8Q1	O35-C34	-2.27	1.18	1.23
47	l	701	PEE	O2-C10	2.26	1.40	1.34
47	j	201	PEE	O2-C10	2.25	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	b	201	PEE	O2-C10	2.25	1.40	1.34
52	V	201	CDL	PB2-OB2	2.24	1.68	1.59
47	l	704	PEE	O2-C10	2.24	1.40	1.34
49	X	201	8Q1	O40-C39	-2.23	1.18	1.23
52	m	201	CDL	OB6-CB4	-2.23	1.41	1.46
47	C	302	PEE	O2-C10	2.22	1.40	1.34
46	A	502	FMN	C4A-N5	2.22	1.35	1.30
47	j	202	PEE	O2-C10	2.22	1.40	1.34
52	V	202	CDL	PB2-OB2	2.22	1.68	1.59
51	J	402	UQ	O4-C4	-2.21	1.18	1.23
47	W	201	PEE	O2-C10	2.20	1.40	1.34
52	l	702	CDL	OB6-CB4	-2.20	1.41	1.46
47	r	501	PEE	O2-C10	2.20	1.40	1.34
52	V	202	CDL	PB2-OB5	2.20	1.68	1.59
52	J	404	CDL	OB6-CB4	-2.19	1.41	1.46
46	A	502	FMN	C5A-N5	-2.18	1.35	1.39
52	r	504	CDL	PB2-OB2	2.18	1.68	1.59
47	j	201	PEE	O3-C3	-2.18	1.40	1.45
52	V	202	CDL	OB6-CB4	-2.18	1.41	1.46
52	J	404	CDL	PB2-OB2	2.17	1.68	1.59
52	m	201	CDL	PB2-OB2	2.16	1.68	1.59
52	m	201	CDL	OA6-CA4	-2.16	1.41	1.46
52	V	201	CDL	PB2-OB5	2.16	1.68	1.59
48	N	201	PLX	P1-O4	2.16	1.68	1.59
52	a	201	CDL	PB2-OB2	2.16	1.68	1.59
47	Q	501	PEE	O3-C3	-2.16	1.40	1.45
52	l	702	CDL	PB2-OB2	2.15	1.68	1.59
47	l	704	PEE	O3-C3	-2.15	1.40	1.45
47	Q	501	PEE	O2-C10	2.15	1.40	1.34
52	a	201	CDL	PB2-OB5	2.15	1.68	1.59
47	b	201	PEE	O3-C3	-2.14	1.40	1.45
52	r	504	CDL	OB6-CB4	-2.14	1.41	1.46
48	r	502	PLX	P1-O4	2.14	1.68	1.59
52	l	702	CDL	PB2-OB5	2.13	1.67	1.59
52	m	201	CDL	PB2-OB5	2.13	1.67	1.59
47	j	202	PEE	O3-C3	-2.13	1.40	1.45
48	n	101	PLX	P1-O4	2.13	1.67	1.59
51	J	402	UQ	O1-C1	-2.12	1.18	1.23
48	J	403	PLX	P1-O4	2.12	1.67	1.59
48	j	203	PLX	P1-O4	2.12	1.67	1.59
47	W	201	PEE	O3-C3	-2.11	1.40	1.45
47	B	303	PEE	O2-C10	2.11	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	g	201	PLX	P1-O4	2.10	1.67	1.59
52	r	504	CDL	PB2-OB5	2.09	1.67	1.59
52	J	404	CDL	PB2-OB5	2.09	1.67	1.59
52	a	201	CDL	OB6-CB4	-2.08	1.41	1.46
52	V	201	CDL	OA6-CA4	-2.08	1.41	1.46
47	l	701	PEE	O3-C3	-2.07	1.40	1.45
50	J	401	NDP	O5D-C5D	-2.07	1.36	1.44
48	r	503	PLX	P1-O4	2.06	1.67	1.59
51	s	501	UQ	O1-C1	-2.06	1.18	1.23
48	N	201	PLX	P1-O1	2.06	1.67	1.59
48	r	502	PLX	P1-O1	2.05	1.67	1.59
48	j	203	PLX	P1-O1	2.05	1.67	1.59
47	B	303	PEE	O3-C3	-2.04	1.40	1.45
51	J	402	UQ	C21-C19	2.02	1.55	1.51
48	n	101	PLX	P1-O1	2.02	1.67	1.59
51	s	501	UQ	O3-CM3	-2.02	1.40	1.45
47	C	302	PEE	O3-C3	-2.01	1.40	1.45
48	r	503	PLX	P1-O1	2.01	1.67	1.59

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	J	402	UQ	C7-C8-C9	-8.04	113.41	126.79
51	s	501	UQ	C7-C8-C9	-7.84	113.75	126.79
50	J	401	NDP	PN-O3-PA	-7.11	108.43	132.83
51	s	501	UQ	C42-C43-C44	-6.49	112.04	127.66
51	s	501	UQ	C12-C13-C14	-6.39	112.27	127.66
51	s	501	UQ	C47-C48-C49	-6.19	112.77	127.66
51	s	501	UQ	C32-C33-C34	-6.19	112.77	127.66
51	J	402	UQ	C17-C18-C19	-6.14	112.88	127.66
51	s	501	UQ	C37-C38-C39	-6.11	112.94	127.66
51	s	501	UQ	C17-C18-C19	-6.06	113.07	127.66
51	J	402	UQ	C12-C13-C14	-6.06	113.08	127.66
51	s	501	UQ	C22-C23-C24	-6.02	113.16	127.66
51	s	501	UQ	C27-C28-C29	-5.99	113.25	127.66
49	X	201	8Q1	C6-C1-S44	5.86	120.28	113.46
49	E	201	8Q1	C6-C1-S44	4.62	118.84	113.46
52	i	401	CDL	OA6-CA5-C11	4.52	121.25	111.50
56	w	401	ADP	N3-C2-N1	-4.48	121.68	128.68
51	s	501	UQ	C30-C29-C28	-4.47	112.21	123.68
51	s	501	UQ	C45-C44-C43	-4.37	112.46	123.68
51	s	501	UQ	C15-C14-C13	-4.37	112.47	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	J	402	UQ	C22-C23-C24	-4.36	112.85	127.75
51	s	501	UQ	C52-C53-C54	-4.35	112.89	127.75
51	s	501	UQ	C11-C9-C8	-4.34	112.34	121.12
51	s	501	UQ	C20-C19-C18	-4.33	112.58	123.68
52	a	201	CDL	OB6-CB5-C51	4.30	120.78	111.50
51	s	501	UQ	C35-C34-C33	-4.29	112.67	123.68
51	s	501	UQ	C31-C29-C28	-4.26	112.50	121.12
51	s	501	UQ	C10-C9-C8	-4.24	112.80	123.68
51	s	501	UQ	C21-C19-C18	-4.24	112.53	121.12
51	J	402	UQ	C20-C19-C18	-4.24	112.80	123.68
51	s	501	UQ	C50-C49-C48	-4.22	112.85	123.68
51	s	501	UQ	C51-C49-C48	-4.21	112.59	121.12
51	s	501	UQ	C25-C24-C23	-4.19	112.92	123.68
51	J	402	UQ	C10-C9-C8	-4.19	112.94	123.68
52	l	703	CDL	OB6-CB5-C51	4.18	120.50	111.50
51	J	402	UQ	C11-C9-C8	-4.18	112.67	121.12
51	J	402	UQ	C15-C14-C13	-4.17	112.97	123.68
47	l	704	PEE	O2-C10-C11	4.17	120.48	111.50
47	j	202	PEE	O2-C10-C11	4.15	120.45	111.50
47	j	201	PEE	O2-C10-C11	4.13	120.40	111.50
51	s	501	UQ	C46-C44-C43	-4.12	112.77	121.12
52	l	702	CDL	OA6-CA5-C11	4.12	120.39	111.50
52	l	703	CDL	OA6-CA5-C11	4.10	120.34	111.50
51	J	402	UQ	C16-C14-C13	-4.10	112.82	121.12
47	C	302	PEE	O2-C10-C11	4.08	120.29	111.50
52	J	404	CDL	OB6-CB5-C51	4.08	120.29	111.50
52	V	201	CDL	OA6-CA5-C11	4.08	120.28	111.50
52	N	202	CDL	OA6-CA5-C11	4.06	120.26	111.50
52	N	202	CDL	OB6-CB5-C51	4.06	120.26	111.50
47	B	303	PEE	O2-C10-C11	4.06	120.25	111.50
51	s	501	UQ	C40-C39-C38	-4.06	113.27	123.68
47	l	701	PEE	O2-C10-C11	4.05	120.22	111.50
52	i	401	CDL	OB6-CB5-C51	4.04	120.22	111.50
52	J	404	CDL	OA6-CA5-C11	4.04	120.20	111.50
51	J	402	UQ	C21-C19-C18	-4.03	112.96	121.12
47	r	501	PEE	O2-C10-C11	4.03	120.18	111.50
51	s	501	UQ	C41-C39-C38	-4.01	113.01	121.12
47	b	201	PEE	O2-C10-C11	4.00	120.12	111.50
52	l	702	CDL	OB6-CB5-C51	3.98	120.08	111.50
52	r	504	CDL	OA6-CA5-C11	3.98	120.08	111.50
52	V	202	CDL	OB6-CB5-C51	3.97	120.06	111.50
51	s	501	UQ	C36-C34-C33	-3.96	113.11	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	u	201	CDL	OB6-CB5-C51	3.95	120.01	111.50
52	m	201	CDL	OB6-CB5-C51	3.95	120.01	111.50
47	Q	501	PEE	O2-C10-C11	3.94	120.00	111.50
47	W	201	PEE	O2-C10-C11	3.93	119.97	111.50
52	V	202	CDL	OA6-CA5-C11	3.92	119.95	111.50
52	V	201	CDL	OB6-CB5-C51	3.90	119.91	111.50
51	s	501	UQ	C16-C14-C13	-3.90	113.22	121.12
52	u	201	CDL	OA6-CA5-C11	3.87	119.85	111.50
49	E	201	8Q1	C43-S44-C1	3.81	113.74	101.87
52	a	201	CDL	OA6-CA5-C11	3.77	119.62	111.50
52	r	504	CDL	OB6-CB5-C51	3.76	119.61	111.50
51	s	501	UQ	C26-C24-C23	-3.73	113.57	121.12
52	m	201	CDL	OA6-CA5-C11	3.66	119.38	111.50
49	X	201	8Q1	O4-C1-C6	-3.50	119.86	123.99
51	s	501	UQ	C56-C54-C53	-3.40	112.83	122.65
51	J	402	UQ	C26-C24-C23	-3.39	112.84	122.65
51	s	501	UQ	C55-C54-C53	-3.39	112.85	122.65
51	J	402	UQ	C25-C24-C23	-3.31	113.07	122.65
52	u	201	CDL	OA8-CA7-C31	3.30	120.04	111.38
50	J	401	NDP	O2B-P2B-O1X	-3.26	96.81	109.39
49	E	201	8Q1	O35-C34-N36	-3.16	116.21	122.99
49	X	201	8Q1	C37-C38-C39	3.13	117.58	112.36
52	i	401	CDL	CA4-OA6-CA5	-3.09	110.17	117.79
50	J	401	NDP	PA-O5B-C5B	-3.00	104.09	121.68
52	u	201	CDL	OB8-CB7-C71	2.98	121.24	111.91
46	A	502	FMN	C4A-C10-N1	-2.92	117.95	124.73
50	J	401	NDP	PN-O5D-C5D	-2.87	104.87	121.68
56	w	401	ADP	PA-O3A-PB	-2.85	123.05	132.83
49	E	201	8Q1	O2-P24-O27	-2.82	99.23	106.73
47	B	303	PEE	O3-C30-C31	2.79	120.66	111.91
52	a	201	CDL	OB8-CB7-C71	2.78	120.63	111.91
52	l	703	CDL	OB8-CB7-C71	2.77	120.62	111.91
52	m	201	CDL	OB8-CB7-C71	2.77	120.59	111.91
47	l	704	PEE	O3-C30-C31	2.77	120.59	111.91
52	l	703	CDL	CB4-OB6-CB5	-2.75	111.02	117.79
52	V	202	CDL	OB8-CB7-C71	2.74	120.52	111.91
52	m	201	CDL	OA8-CA7-C31	2.74	120.51	111.91
52	N	202	CDL	OB8-CB7-C71	2.73	120.47	111.91
47	r	501	PEE	O3-C30-C31	2.73	120.47	111.91
52	r	504	CDL	OB8-CB7-C71	2.72	120.46	111.91
52	l	702	CDL	OA8-CA7-C31	2.72	120.45	111.91
49	E	201	8Q1	C32-C34-N36	2.72	121.99	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	N	202	CDL	OA8-CA7-C31	2.70	120.38	111.91
51	s	501	UQ	CM5-C5-C6	-2.69	120.01	124.40
47	Q	501	PEE	O3-C30-C31	2.68	120.32	111.91
52	l	703	CDL	OA8-CA7-C31	2.68	120.31	111.91
52	J	404	CDL	OA8-CA7-C31	2.67	120.28	111.91
52	l	702	CDL	OB8-CB7-C71	2.65	120.22	111.91
47	W	201	PEE	O3-C30-C31	2.63	120.17	111.91
48	g	201	PLX	C1A-N1-C1	2.63	120.68	109.92
47	j	201	PEE	O3-C30-C31	2.63	120.16	111.91
52	V	201	CDL	OB8-CB7-C71	2.62	120.14	111.91
52	V	202	CDL	OA8-CA7-C31	2.60	120.08	111.91
52	i	401	CDL	OB8-CB7-C71	2.59	120.05	111.91
52	a	201	CDL	OA8-CA7-C31	2.58	120.00	111.91
47	b	201	PEE	O3-C30-C31	2.58	120.00	111.91
47	l	701	PEE	O3-C30-C31	2.57	119.99	111.91
49	E	201	8Q1	O40-C39-N41	-2.56	118.19	123.01
52	i	401	CDL	OA8-CA7-C31	2.55	119.92	111.91
50	J	401	NDP	O3X-P2B-O2X	2.55	117.37	107.64
51	J	402	UQ	CM5-C5-C6	-2.54	120.26	124.40
47	j	202	PEE	O3-C30-C31	2.53	119.85	111.91
52	r	504	CDL	OA8-CA7-C31	2.53	119.84	111.91
47	C	302	PEE	O3-C30-C31	2.50	119.77	111.91
49	X	201	8Q1	C43-S44-C1	2.50	109.65	101.87
50	J	401	NDP	O5D-PN-O1N	-2.49	99.32	109.07
52	V	201	CDL	OA8-CA7-C31	2.47	119.67	111.91
50	J	401	NDP	O4B-C4B-C3B	2.45	109.96	105.11
48	j	203	PLX	C1A-N1-C1	2.42	119.82	109.92
50	J	401	NDP	C2A-N1A-C6A	-2.40	114.66	118.75
49	E	201	8Q1	O1-P24-O2	2.39	116.78	107.64
52	N	202	CDL	CB4-OB6-CB5	-2.39	111.91	117.79
48	n	101	PLX	C1A-N1-C1	2.38	119.66	109.92
48	r	503	PLX	C1A-N1-C1	2.36	119.56	109.92
52	J	404	CDL	OB8-CB7-C71	2.35	119.29	111.91
50	J	401	NDP	O2N-PN-O1N	2.35	123.86	112.24
48	N	201	PLX	C1A-N1-C1	2.35	119.52	109.92
56	w	401	ADP	C3'-C2'-C1'	2.34	104.50	100.98
48	J	403	PLX	C1A-N1-C1	2.34	119.48	109.92
48	r	502	PLX	C1A-N1-C1	2.33	119.45	109.92
46	A	502	FMN	O4-C4-C4A	-2.28	120.54	126.60
50	J	401	NDP	C5B-C4B-C3B	-2.25	106.76	115.18
49	X	201	8Q1	C38-C39-N41	2.24	120.20	116.42
49	E	201	8Q1	O4-C1-C6	-2.23	121.35	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	A	502	FMN	C10-N1-C2	2.19	121.28	116.90
56	w	401	ADP	C4-C5-N7	-2.18	107.13	109.40
46	A	502	FMN	C4A-C4-N3	2.16	118.68	113.19
49	E	201	8Q1	O4-C1-S44	-2.16	119.81	122.61
49	E	201	8Q1	C38-C39-N41	2.16	120.06	116.42
56	w	401	ADP	O4'-C1'-C2'	-2.13	103.81	106.93
46	A	502	FMN	C4-N3-C2	-2.12	121.73	125.64
49	X	201	8Q1	O4-C1-S44	-2.11	119.87	122.61
46	A	502	FMN	C4-C4A-N5	2.11	121.24	118.23
46	A	502	FMN	O2-C2-N1	-2.10	118.34	121.83
52	i	401	CDL	OA6-CA5-OA7	-2.10	118.63	123.70
49	E	201	8Q1	C37-C38-C39	2.04	115.75	112.36
50	J	401	NDP	O7N-C7N-C3N	2.02	124.69	120.90
52	l	703	CDL	CA4-OA6-CA5	-2.01	112.84	117.79
52	u	201	CDL	OB8-CB7-OB9	-2.01	118.52	123.59
52	l	703	CDL	OB6-CB5-OB7	-2.00	118.87	123.70

There are no chirality outliers.

All (1088) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
47	B	303	PEE	C11-C10-O2-C2
47	C	302	PEE	C4-O4P-P-O1P
47	Q	501	PEE	C11-C10-O2-C2
47	Q	501	PEE	C4-O4P-P-O1P
47	Q	501	PEE	O4P-C4-C5-N
47	W	201	PEE	O4P-C4-C5-N
47	b	201	PEE	C37-C38-C39-C40
47	j	201	PEE	C17-C18-C19-C20
47	j	201	PEE	C1-O3P-P-O1P
47	j	202	PEE	C11-C10-O2-C2
47	j	202	PEE	C1-O3P-P-O2P
47	j	202	PEE	C1-O3P-P-O1P
47	j	202	PEE	C1-O3P-P-O4P
47	l	701	PEE	C11-C10-O2-C2
47	l	701	PEE	C1-O3P-P-O2P
47	l	701	PEE	C1-O3P-P-O1P
47	l	701	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
47	l	701	PEE	C4-O4P-P-O2P
47	l	701	PEE	C4-O4P-P-O1P
47	l	704	PEE	C11-C10-O2-C2
47	l	704	PEE	C4-O4P-P-O2P
47	r	501	PEE	C11-C10-O2-C2
48	C	303	PLX	C2-O1-P1-O2
48	C	303	PLX	C2-O1-P1-O3
48	J	403	PLX	O7-C6-O6-C4
48	J	403	PLX	C2-O1-P1-O2
48	N	201	PLX	O7-C6-O6-C4
48	N	201	PLX	C2-O1-P1-O2
48	N	201	PLX	C2-O1-P1-O3
48	N	201	PLX	O9-C24-O8-C5
48	g	201	PLX	C2-O1-P1-O4
48	j	203	PLX	O7-C6-C7-C8
48	j	203	PLX	C2-O1-P1-O2
48	n	101	PLX	O7-C6-C7-C8
48	n	101	PLX	O7-C6-O6-C4
48	n	101	PLX	C3-O4-P1-O3
48	n	101	PLX	C2-O1-P1-O2
48	r	502	PLX	O6-C6-C7-C8
48	r	502	PLX	O9-C24-C25-C26
49	E	201	8Q1	C1-C6-C7-C8
49	E	201	8Q1	O27-C28-C29-C32
49	E	201	8Q1	C28-C29-C32-C34
49	E	201	8Q1	C28-C29-C32-O33
49	E	201	8Q1	C30-C29-C32-C34
49	E	201	8Q1	C30-C29-C32-O33
49	E	201	8Q1	C31-C29-C32-C34
49	E	201	8Q1	C31-C29-C32-O33
49	E	201	8Q1	C42-C43-S44-C1
49	E	201	8Q1	C28-O27-P24-O3
49	E	201	8Q1	C28-O27-P24-O2
49	E	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	N41-C42-C43-S44
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	J	401	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
50	J	401	NDP	C5B-O5B-PA-O2A
50	J	401	NDP	O4B-C4B-C5B-O5B
50	J	401	NDP	C3B-C4B-C5B-O5B
50	J	401	NDP	C2B-O2B-P2B-O3X
50	J	401	NDP	O4D-C4D-C5D-O5D
51	J	402	UQ	C7-C8-C9-C10
51	J	402	UQ	C7-C8-C9-C11
51	J	402	UQ	C12-C11-C9-C10
51	J	402	UQ	C11-C12-C13-C14
51	J	402	UQ	C12-C13-C14-C15
51	J	402	UQ	C15-C14-C16-C17
51	J	402	UQ	C14-C16-C17-C18
51	J	402	UQ	C17-C18-C19-C20
51	J	402	UQ	C17-C18-C19-C21
51	J	402	UQ	C18-C19-C21-C22
51	J	402	UQ	C19-C21-C22-C23
51	s	501	UQ	C7-C8-C9-C10
51	s	501	UQ	C16-C17-C18-C19
51	s	501	UQ	C17-C18-C19-C20
51	s	501	UQ	C20-C19-C21-C22
51	s	501	UQ	C25-C24-C26-C27
51	s	501	UQ	C27-C28-C29-C31
51	s	501	UQ	C28-C29-C31-C32
51	s	501	UQ	C32-C33-C34-C36
51	s	501	UQ	C42-C43-C44-C45
51	s	501	UQ	C42-C43-C44-C46
51	s	501	UQ	C47-C48-C49-C51
52	J	404	CDL	O1-C1-CA2-OA2
52	J	404	CDL	CB2-C1-CA2-OA2
52	J	404	CDL	CA2-OA2-PA1-OA3
52	J	404	CDL	CA2-OA2-PA1-OA4
52	J	404	CDL	CB3-OB5-PB2-OB2
52	J	404	CDL	OB6-CB4-CB6-OB8
52	N	202	CDL	CA2-OA2-PA1-OA4
52	N	202	CDL	CA3-OA5-PA1-OA4
52	N	202	CDL	CB2-OB2-PB2-OB4
52	N	202	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CA2-OA2-PA1-OA5
52	V	201	CDL	C11-CA5-OA6-CA4
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB4
52	V	202	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
52	V	202	CDL	C51-CB5-OB6-CB4
52	a	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CA2-OA2-PA1-OA3
52	a	201	CDL	CB2-OB2-PB2-OB3
52	a	201	CDL	CB3-OB5-PB2-OB3
52	a	201	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	OB7-CB5-OB6-CB4
52	i	401	CDL	CA2-OA2-PA1-OA4
52	i	401	CDL	CB2-OB2-PB2-OB3
52	i	401	CDL	CB2-OB2-PB2-OB4
52	i	401	CDL	CB2-OB2-PB2-OB5
52	i	401	CDL	CB3-OB5-PB2-OB3
52	l	702	CDL	O1-C1-CB2-OB2
52	l	702	CDL	CA2-OA2-PA1-OA4
52	l	702	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CB2-OB2-PB2-OB4
52	l	702	CDL	CB3-OB5-PB2-OB3
52	l	703	CDL	CA2-OA2-PA1-OA4
52	l	703	CDL	CA3-OA5-PA1-OA4
52	l	703	CDL	CB2-OB2-PB2-OB3
52	l	703	CDL	CB2-OB2-PB2-OB4
52	m	201	CDL	CA2-OA2-PA1-OA3
52	m	201	CDL	CA2-OA2-PA1-OA4
52	m	201	CDL	CA2-OA2-PA1-OA5
52	m	201	CDL	CA3-OA5-PA1-OA3
52	m	201	CDL	CB3-OB5-PB2-OB2
52	m	201	CDL	CB3-OB5-PB2-OB3
52	m	201	CDL	CB3-OB5-PB2-OB4
52	r	504	CDL	CA2-OA2-PA1-OA3
52	r	504	CDL	CA3-OA5-PA1-OA2
52	r	504	CDL	CA3-OA5-PA1-OA3
52	r	504	CDL	CB2-OB2-PB2-OB3
52	r	504	CDL	CB2-OB2-PB2-OB4
52	r	504	CDL	CB2-OB2-PB2-OB5
52	r	504	CDL	CB3-OB5-PB2-OB3
52	r	504	CDL	C51-CB5-OB6-CB4
52	u	201	CDL	CA2-OA2-PA1-OA3
52	u	201	CDL	CA2-OA2-PA1-OA4
52	u	201	CDL	CA2-OA2-PA1-OA5
52	u	201	CDL	CA3-OA5-PA1-OA3
52	u	201	CDL	CA3-OA5-PA1-OA4
52	u	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
52	u	201	CDL	CB3-OB5-PB2-OB3
52	u	201	CDL	CB3-OB5-PB2-OB4
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A
52	J	404	CDL	OA9-CA7-OA8-CA6
52	J	404	CDL	C31-CA7-OA8-CA6
52	i	401	CDL	OA9-CA7-OA8-CA6
52	l	702	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	O4-C10-O2-C2
47	j	202	PEE	O4-C10-O2-C2
47	l	701	PEE	O4-C10-O2-C2
47	l	704	PEE	O4-C10-O2-C2
47	r	501	PEE	O4-C10-O2-C2
52	V	201	CDL	OA7-CA5-OA6-CA4
52	V	202	CDL	OB7-CB5-OB6-CB4
52	r	504	CDL	OB7-CB5-OB6-CB4
52	l	702	CDL	C31-CA7-OA8-CA6
52	a	201	CDL	C51-CB5-OB6-CB4
51	s	501	UQ	C52-C53-C54-C55
51	s	501	UQ	C43-C44-C46-C47
47	Q	501	PEE	O5-C30-O3-C3
48	r	502	PLX	C11-C12-C13-C14
47	Q	501	PEE	C31-C30-O3-C3
47	j	201	PEE	C31-C30-O3-C3
52	i	401	CDL	C31-CA7-OA8-CA6
47	B	303	PEE	C17-C18-C19-C20
47	l	704	PEE	C37-C38-C39-C40
51	s	501	UQ	C27-C28-C29-C30
51	s	501	UQ	C37-C38-C39-C40
51	s	501	UQ	C47-C48-C49-C50
47	Q	501	PEE	O4-C10-O2-C2
51	s	501	UQ	C12-C13-C14-C16
51	s	501	UQ	C17-C18-C19-C21
51	s	501	UQ	C22-C23-C24-C26
48	g	201	PLX	C2-C1-N1-C1A
52	a	201	CDL	O1-C1-CA2-OA2
52	a	201	CDL	O1-C1-CB2-OB2
52	l	702	CDL	O1-C1-CA2-OA2
52	r	504	CDL	O1-C1-CA2-OA2
52	V	201	CDL	C71-CB7-OB8-CB6
47	C	302	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
52	N	202	CDL	C11-CA5-OA6-CA4
51	J	402	UQ	C22-C23-C24-C26
52	r	504	CDL	C74-C75-C76-C77
47	l	704	PEE	C33-C34-C35-C36
48	g	201	PLX	C9-C10-C11-C12
48	g	201	PLX	C7-C8-C9-C10
52	J	404	CDL	C37-C38-C39-C40
52	V	201	CDL	C62-C63-C64-C65
52	V	202	CDL	C11-C12-C13-C14
52	m	201	CDL	C73-C74-C75-C76
47	B	303	PEE	C42-C43-C44-C45
48	r	502	PLX	C9-C10-C11-C12
48	j	203	PLX	C13-C14-C15-C16
52	V	202	CDL	C32-C33-C34-C35
52	l	702	CDL	C81-C82-C83-C84
47	j	201	PEE	O5-C30-O3-C3
52	V	201	CDL	OB9-CB7-OB8-CB6
51	s	501	UQ	C48-C49-C51-C52
47	j	201	PEE	C30-C31-C32-C33
52	m	201	CDL	C62-C63-C64-C65
51	s	501	UQ	C14-C16-C17-C18
51	s	501	UQ	C34-C36-C37-C38
48	r	502	PLX	C7-C8-C9-C10
52	V	201	CDL	C32-C33-C34-C35
52	l	702	CDL	C32-C33-C34-C35
51	s	501	UQ	C22-C23-C24-C25
47	b	201	PEE	C10-C11-C12-C13
52	a	201	CDL	CA2-C1-CB2-OB2
52	l	702	CDL	CA2-C1-CB2-OB2
47	C	302	PEE	O4-C10-O2-C2
52	l	702	CDL	CB5-C51-C52-C53
52	m	201	CDL	C36-C37-C38-C39
52	V	201	CDL	C59-C60-C61-C62
52	l	702	CDL	C58-C59-C60-C61
52	r	504	CDL	C60-C61-C62-C63
52	N	202	CDL	O1-C1-CB2-OB2
52	i	401	CDL	O1-C1-CB2-OB2
52	l	703	CDL	O1-C1-CA2-OA2
52	u	201	CDL	O1-C1-CB2-OB2
52	a	201	CDL	CA7-C31-C32-C33
48	g	201	PLX	O6-C4-C5-O8
52	J	404	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
47	r	501	PEE	C41-C42-C43-C44
52	l	702	CDL	C34-C35-C36-C37
47	l	701	PEE	C31-C30-O3-C3
52	V	201	CDL	C31-CA7-OA8-CA6
52	J	404	CDL	CA7-C31-C32-C33
52	J	404	CDL	CB5-C51-C52-C53
52	V	202	CDL	C72-C73-C74-C75
46	A	502	FMN	O2'-C2'-C3'-O3'
47	Q	501	PEE	C30-C31-C32-C33
52	J	404	CDL	CB7-C71-C72-C73
52	V	202	CDL	CB7-C71-C72-C73
52	i	401	CDL	CA7-C31-C32-C33
52	m	201	CDL	CA5-C11-C12-C13
52	r	504	CDL	CA5-C11-C12-C13
50	J	401	NDP	C3D-C4D-C5D-O5D
52	N	202	CDL	OA7-CA5-OA6-CA4
47	l	704	PEE	C30-C31-C32-C33
52	a	201	CDL	CA5-C11-C12-C13
52	l	702	CDL	CA7-C31-C32-C33
52	J	404	CDL	C14-C15-C16-C17
52	l	703	CDL	C51-C52-C53-C54
52	m	201	CDL	C13-C14-C15-C16
52	a	201	CDL	CB5-C51-C52-C53
47	l	701	PEE	O5-C30-O3-C3
47	l	701	PEE	C17-C18-C19-C20
47	b	201	PEE	C11-C10-O2-C2
47	j	201	PEE	C11-C10-O2-C2
52	m	201	CDL	C11-CA5-OA6-CA4
47	C	302	PEE	C4-O4P-P-O3P
47	Q	501	PEE	C4-O4P-P-O3P
47	W	201	PEE	C4-O4P-P-O3P
47	l	701	PEE	C4-O4P-P-O3P
47	l	704	PEE	C4-O4P-P-O3P
48	C	303	PLX	C2-O1-P1-O4
48	J	403	PLX	C3-O4-P1-O1
48	J	403	PLX	C2-O1-P1-O4
48	N	201	PLX	C2-O1-P1-O4
48	n	101	PLX	C3-O4-P1-O1
52	J	404	CDL	CA2-OA2-PA1-OA5
52	J	404	CDL	CA3-OA5-PA1-OA2
52	N	202	CDL	CA2-OA2-PA1-OA5
52	N	202	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
52	N	202	CDL	CB2-OB2-PB2-OB5
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	202	CDL	CB3-OB5-PB2-OB2
52	a	201	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	CB3-OB5-PB2-OB2
52	i	401	CDL	CA2-OA2-PA1-OA5
52	i	401	CDL	CA3-OA5-PA1-OA2
52	i	401	CDL	CB3-OB5-PB2-OB2
52	l	702	CDL	CA2-OA2-PA1-OA5
52	l	702	CDL	CB2-OB2-PB2-OB5
52	l	702	CDL	CB3-OB5-PB2-OB2
52	l	703	CDL	CA2-OA2-PA1-OA5
52	l	703	CDL	CA3-OA5-PA1-OA2
52	l	703	CDL	CB2-OB2-PB2-OB5
52	m	201	CDL	CA3-OA5-PA1-OA2
52	r	504	CDL	CA2-OA2-PA1-OA5
52	r	504	CDL	CB3-OB5-PB2-OB2
52	u	201	CDL	CA3-OA5-PA1-OA2
52	u	201	CDL	CB2-OB2-PB2-OB5
47	W	201	PEE	C10-C11-C12-C13
48	J	403	PLX	C11-C10-C9-C8
52	r	504	CDL	CB2-C1-CA2-OA2
47	b	201	PEE	O4-C10-O2-C2
47	j	201	PEE	O4-C10-O2-C2
52	m	201	CDL	OA7-CA5-OA6-CA4
47	j	201	PEE	C32-C33-C34-C35
48	g	201	PLX	C2-C1-N1-C1C
47	b	201	PEE	C31-C30-O3-C3
47	j	201	PEE	C19-C20-C21-C22
48	J	403	PLX	C7-C8-C9-C10
48	N	201	PLX	C14-C15-C16-C17
48	r	502	PLX	C11-C10-C9-C8
52	V	201	CDL	C37-C38-C39-C40
52	l	702	CDL	C56-C57-C58-C59
52	J	404	CDL	C51-CB5-OB6-CB4
52	V	201	CDL	C51-CB5-OB6-CB4
52	l	702	CDL	C51-CB5-OB6-CB4
47	r	501	PEE	C12-C13-C14-C15
48	N	201	PLX	C29-C30-C31-C32
48	g	201	PLX	C25-C26-C27-C28
48	g	201	PLX	C32-C33-C34-C35
48	j	203	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
48	n	101	PLX	C25-C26-C27-C28
48	n	101	PLX	C31-C32-C33-C34
48	r	502	PLX	C30-C31-C32-C33
52	J	404	CDL	C71-C72-C73-C74
52	V	201	CDL	C74-C75-C76-C77
52	V	202	CDL	C59-C60-C61-C62
52	a	201	CDL	C75-C76-C77-C78
52	l	702	CDL	C75-C76-C77-C78
49	E	201	8Q1	O27-C28-C29-C30
49	E	201	8Q1	O27-C28-C29-C31
52	l	702	CDL	C71-CB7-OB8-CB6
52	l	703	CDL	C71-CB7-OB8-CB6
47	W	201	PEE	C11-C12-C13-C14
47	b	201	PEE	C31-C32-C33-C34
47	j	202	PEE	C11-C12-C13-C14
48	j	203	PLX	C14-C15-C16-C17
48	r	503	PLX	C13-C14-C15-C16
48	r	503	PLX	C10-C11-C12-C13
49	E	201	8Q1	C10-C11-C12-C13
52	V	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C37-C38-C39-C40
52	m	201	CDL	C59-C60-C61-C62
52	N	202	CDL	CA6-CA4-OA6-CA5
52	J	404	CDL	OB7-CB5-OB6-CB4
52	V	201	CDL	OB7-CB5-OB6-CB4
46	A	502	FMN	O2'-C2'-C3'-C4'
48	J	403	PLX	C31-C32-C33-C34
48	N	201	PLX	C33-C34-C35-C36
52	V	201	CDL	C58-C59-C60-C61
52	V	202	CDL	C33-C34-C35-C36
52	a	201	CDL	C17-C18-C19-C20
52	a	201	CDL	C62-C63-C64-C65
52	r	504	CDL	C32-C33-C34-C35
48	N	201	PLX	C12-C13-C14-C15
48	j	203	PLX	C16-C17-C18-C19
52	V	201	CDL	C33-C34-C35-C36
52	a	201	CDL	C73-C74-C75-C76
52	m	201	CDL	C32-C33-C34-C35
52	r	504	CDL	C35-C36-C37-C38
52	l	703	CDL	O1-C1-CB2-OB2
52	J	404	CDL	C33-C34-C35-C36
52	V	202	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
52	V	202	CDL	C37-C38-C39-C40
52	l	702	CDL	CB7-C71-C72-C73
47	W	201	PEE	C31-C30-O3-C3
52	a	201	CDL	C71-CB7-OB8-CB6
48	g	201	PLX	C11-C12-C13-C14
48	g	201	PLX	C27-C28-C29-C30
52	m	201	CDL	C55-C56-C57-C58
52	r	504	CDL	C14-C15-C16-C17
47	j	202	PEE	C33-C34-C35-C36
47	l	704	PEE	C40-C41-C42-C43
52	V	201	CDL	C31-C32-C33-C34
52	a	201	CDL	C60-C61-C62-C63
52	l	702	CDL	C14-C15-C16-C17
52	m	201	CDL	C75-C76-C77-C78
47	l	704	PEE	C22-C23-C24-C25
48	N	201	PLX	C27-C28-C29-C30
48	g	201	PLX	C14-C15-C16-C17
48	j	203	PLX	C9-C10-C11-C12
48	j	203	PLX	C7-C8-C9-C10
48	n	101	PLX	C27-C28-C29-C30
48	r	503	PLX	C35-C36-C37-C38
49	X	201	8Q1	C11-C12-C13-C14
52	J	404	CDL	C59-C60-C61-C62
52	J	404	CDL	C73-C74-C75-C76
52	V	201	CDL	C11-C12-C13-C14
52	V	202	CDL	C13-C14-C15-C16
52	V	202	CDL	C42-C43-C44-C45
52	m	201	CDL	C71-C72-C73-C74
52	V	201	CDL	OA9-CA7-OA8-CA6
47	C	302	PEE	C42-C43-C44-C45
47	W	201	PEE	C12-C13-C14-C15
48	J	403	PLX	C9-C10-C11-C12
48	n	101	PLX	C10-C11-C12-C13
52	J	404	CDL	C75-C76-C77-C78
52	V	202	CDL	C74-C75-C76-C77
52	l	702	CDL	C11-C12-C13-C14
52	l	702	CDL	C36-C37-C38-C39
52	l	702	CDL	C39-C40-C41-C42
52	l	702	CDL	C74-C75-C76-C77
52	r	504	CDL	C57-C58-C59-C60
52	l	702	CDL	OB7-CB5-OB6-CB4
48	J	403	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
48	r	502	PLX	C28-C29-C30-C31
48	r	503	PLX	C25-C26-C27-C28
52	J	404	CDL	C36-C37-C38-C39
47	l	704	PEE	C19-C20-C21-C22
47	l	701	PEE	C10-C11-C12-C13
47	B	303	PEE	C12-C13-C14-C15
47	b	201	PEE	C33-C34-C35-C36
47	l	704	PEE	C21-C22-C23-C24
47	r	501	PEE	C40-C41-C42-C43
48	J	403	PLX	C14-C15-C16-C17
48	j	203	PLX	C12-C13-C14-C15
48	j	203	PLX	C28-C29-C30-C31
48	j	203	PLX	C33-C34-C35-C36
48	r	502	PLX	C25-C26-C27-C28
52	J	404	CDL	C55-C56-C57-C58
52	V	202	CDL	C34-C35-C36-C37
52	a	201	CDL	C33-C34-C35-C36
52	l	702	CDL	C71-C72-C73-C74
52	r	504	CDL	C37-C38-C39-C40
48	g	201	PLX	C2-C1-N1-C1B
48	N	201	PLX	C25-C26-C27-C28
52	J	404	CDL	C52-C53-C54-C55
52	m	201	CDL	C79-C80-C81-C82
47	B	303	PEE	O4P-C4-C5-N
48	g	201	PLX	C13-C14-C15-C16
52	V	201	CDL	C71-C72-C73-C74
52	V	202	CDL	C14-C15-C16-C17
52	V	202	CDL	C75-C76-C77-C78
47	Q	501	PEE	C33-C34-C35-C36
48	g	201	PLX	C12-C13-C14-C15
48	r	502	PLX	C13-C14-C15-C16
48	r	502	PLX	C27-C28-C29-C30
49	E	201	8Q1	C11-C10-C9-C8
52	r	504	CDL	C73-C74-C75-C76
48	J	403	PLX	C13-C14-C15-C16
48	n	101	PLX	C14-C15-C16-C17
52	V	202	CDL	C82-C83-C84-C85
52	r	504	CDL	C11-C12-C13-C14
48	J	403	PLX	C30-C31-C32-C33
48	r	503	PLX	C29-C30-C31-C32
52	V	201	CDL	C72-C73-C74-C75
52	r	504	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
48	J	403	PLX	C33-C34-C35-C36
48	n	101	PLX	C13-C14-C15-C16
52	V	202	CDL	C15-C16-C17-C18
52	l	702	CDL	C52-C53-C54-C55
52	r	504	CDL	C62-C63-C64-C65
47	W	201	PEE	C17-C18-C19-C20
47	l	701	PEE	C37-C38-C39-C40
48	r	503	PLX	C14-C15-C16-C17
52	r	504	CDL	C75-C76-C77-C78
52	r	504	CDL	C77-C78-C79-C80
52	r	504	CDL	CB7-C71-C72-C73
52	V	202	CDL	C52-C53-C54-C55
52	l	702	CDL	C55-C56-C57-C58
52	l	702	CDL	C62-C63-C64-C65
47	l	704	PEE	C31-C30-O3-C3
47	l	704	PEE	C32-C33-C34-C35
48	C	303	PLX	O7-C6-C7-C8
48	J	403	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-C7-C8
47	l	704	PEE	C20-C21-C22-C23
48	g	201	PLX	C28-C29-C30-C31
48	r	503	PLX	C11-C10-C9-C8
52	J	404	CDL	C35-C36-C37-C38
52	r	504	CDL	C83-C84-C85-C86
52	u	201	CDL	C73-C74-C75-C76
47	b	201	PEE	O5-C30-O3-C3
47	l	704	PEE	C44-C45-C46-C47
48	C	303	PLX	C10-C11-C12-C13
48	N	201	PLX	C10-C11-C12-C13
52	J	404	CDL	C34-C35-C36-C37
52	a	201	CDL	C11-C12-C13-C14
52	m	201	CDL	C61-C62-C63-C64
52	l	702	CDL	OB9-CB7-OB8-CB6
52	J	404	CDL	CA2-C1-CB2-OB2
52	l	702	CDL	CB2-C1-CA2-OA2
47	B	303	PEE	C13-C14-C15-C16
52	V	202	CDL	C73-C74-C75-C76
52	m	201	CDL	C18-C19-C20-C21
52	m	201	CDL	C41-C42-C43-C44
52	r	504	CDL	C41-C42-C43-C44
52	r	504	CDL	C71-C72-C73-C74
47	W	201	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
47	W	201	PEE	C13-C14-C15-C16
47	j	201	PEE	C23-C24-C25-C26
47	j	202	PEE	C22-C23-C24-C25
47	r	501	PEE	C13-C14-C15-C16
48	g	201	PLX	C30-C31-C32-C33
52	J	404	CDL	C82-C83-C84-C85
52	a	201	CDL	C15-C16-C17-C18
47	W	201	PEE	O5-C30-O3-C3
47	Q	501	PEE	C31-C32-C33-C34
47	B	303	PEE	C23-C24-C25-C26
52	J	404	CDL	C17-C18-C19-C20
52	l	703	CDL	C15-C16-C17-C18
52	l	703	CDL	C73-C74-C75-C76
52	m	201	CDL	C20-C21-C22-C23
52	i	401	CDL	C11-CA5-OA6-CA4
47	l	704	PEE	C34-C35-C36-C37
48	j	203	PLX	C29-C30-C31-C32
52	J	404	CDL	C51-C52-C53-C54
52	V	201	CDL	C55-C56-C57-C58
52	l	702	CDL	C16-C17-C18-C19
52	m	201	CDL	C11-C12-C13-C14
52	r	504	CDL	C43-C44-C45-C46
52	a	201	CDL	OB9-CB7-OB8-CB6
52	l	703	CDL	OB9-CB7-OB8-CB6
47	W	201	PEE	C24-C25-C26-C27
49	E	201	8Q1	C12-C13-C14-C15
51	J	402	UQ	C20-C19-C21-C22
47	l	704	PEE	O5-C30-O3-C3
47	r	501	PEE	C20-C21-C22-C23
52	V	202	CDL	C35-C36-C37-C38
52	a	201	CDL	C71-C72-C73-C74
47	Q	501	PEE	C35-C36-C37-C38
52	u	201	CDL	CB7-C71-C72-C73
52	V	202	CDL	C71-CB7-OB8-CB6
52	r	504	CDL	C71-CB7-OB8-CB6
47	l	704	PEE	C13-C14-C15-C16
48	N	201	PLX	C7-C8-C9-C10
48	r	503	PLX	C30-C31-C32-C33
48	r	503	PLX	C31-C32-C33-C34
52	m	201	CDL	C16-C17-C18-C19
48	J	403	PLX	C32-C33-C34-C35
52	a	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C31-C32-C33-C34
47	l	701	PEE	C11-C12-C13-C14
47	l	701	PEE	C32-C33-C34-C35
48	r	503	PLX	C11-C12-C13-C14
49	E	201	8Q1	N36-C37-C38-C39
48	g	201	PLX	C10-C11-C12-C13
48	r	502	PLX	C33-C34-C35-C36
52	V	201	CDL	C14-C15-C16-C17
52	a	201	CDL	C31-C32-C33-C34
52	m	201	CDL	C60-C61-C62-C63
52	V	201	CDL	OB5-CB3-CB4-OB6
52	m	201	CDL	OA5-CA3-CA4-OA6
48	J	403	PLX	C11-C12-C13-C14
48	r	503	PLX	C18-C19-C20-C21
48	r	503	PLX	C28-C29-C30-C31
48	r	503	PLX	C26-C27-C28-C29
52	u	201	CDL	O1-C1-CA2-OA2
52	i	401	CDL	OA7-CA5-OA6-CA4
52	i	401	CDL	OB6-CB4-CB6-OB8
48	r	503	PLX	C27-C28-C29-C30
47	C	302	PEE	C13-C14-C15-C16
52	a	201	CDL	C21-C22-C23-C24
52	m	201	CDL	C34-C35-C36-C37
47	B	303	PEE	C35-C36-C37-C38
47	j	202	PEE	C15-C16-C17-C18
47	r	501	PEE	C39-C40-C41-C42
48	j	203	PLX	C11-C12-C13-C14
47	b	201	PEE	C13-C14-C15-C16
47	r	501	PEE	C37-C38-C39-C40
52	l	702	CDL	C35-C36-C37-C38
52	V	202	CDL	CA7-C31-C32-C33
47	j	201	PEE	C34-C35-C36-C37
47	Q	501	PEE	C18-C19-C20-C21
48	j	203	PLX	C2-O1-P1-O4
48	n	101	PLX	C2-O1-P1-O4
47	C	302	PEE	C11-C12-C13-C14
47	Q	501	PEE	C34-C35-C36-C37
48	n	101	PLX	C28-C29-C30-C31
52	u	201	CDL	CB5-C51-C52-C53
52	r	504	CDL	OB9-CB7-OB8-CB6
52	V	201	CDL	OB5-CB3-CB4-CB6
52	a	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
52	l	703	CDL	OB5-CB3-CB4-CB6
47	b	201	PEE	C22-C23-C24-C25
52	l	702	CDL	C59-C60-C61-C62
47	j	202	PEE	C12-C13-C14-C15
48	j	203	PLX	C25-C26-C27-C28
48	n	101	PLX	C16-C17-C18-C19
52	V	201	CDL	C54-C55-C56-C57
48	J	403	PLX	C34-C35-C36-C37
48	r	502	PLX	C14-C15-C16-C17
48	n	101	PLX	C15-C16-C17-C18
52	V	202	CDL	C60-C61-C62-C63
52	V	202	CDL	C62-C63-C64-C65
52	a	201	CDL	C52-C53-C54-C55
52	i	401	CDL	C37-C38-C39-C40
47	C	302	PEE	C15-C16-C17-C18
48	J	403	PLX	C25-C26-C27-C28
52	a	201	CDL	C35-C36-C37-C38
52	V	202	CDL	CA2-C1-CB2-OB2
48	n	101	PLX	C30-C31-C32-C33
52	m	201	CDL	C33-C34-C35-C36
47	r	501	PEE	C36-C37-C38-C39
52	V	202	CDL	C84-C85-C86-C87
52	V	202	CDL	O1-C1-CB2-OB2
52	m	201	CDL	O1-C1-CA2-OA2
47	Q	501	PEE	C20-C21-C22-C23
49	X	201	8Q1	C6-C7-C8-C9
52	V	202	CDL	C40-C41-C42-C43
47	C	302	PEE	C1-C2-C3-O3
47	b	201	PEE	C1-C2-C3-O3
48	g	201	PLX	C3-C4-C5-O8
48	j	203	PLX	C3-C4-C5-O8
49	X	201	8Q1	C10-C11-C12-C13
52	m	201	CDL	CA3-CA4-CA6-OA8
52	m	201	CDL	CB3-CB4-CB6-OB8
47	Q	501	PEE	C24-C25-C26-C27
47	j	202	PEE	C24-C25-C26-C27
52	m	201	CDL	C84-C85-C86-C87
47	B	303	PEE	C36-C37-C38-C39
52	V	202	CDL	C64-C65-C66-C67
47	W	201	PEE	C15-C16-C17-C18
47	l	701	PEE	C35-C36-C37-C38
47	l	704	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
52	V	202	CDL	OB9-CB7-OB8-CB6
52	l	702	CDL	C21-C22-C23-C24
52	l	703	CDL	C51-CB5-OB6-CB4
47	l	701	PEE	C33-C34-C35-C36
47	j	201	PEE	C40-C41-C42-C43
52	V	202	CDL	C12-C13-C14-C15
52	l	702	CDL	C63-C64-C65-C66
52	V	202	CDL	CB5-C51-C52-C53
52	r	504	CDL	CA7-C31-C32-C33
49	X	201	8Q1	C13-C14-C15-C16
48	N	201	PLX	C31-C32-C33-C34
52	V	202	CDL	C41-C42-C43-C44
52	r	504	CDL	C42-C43-C44-C45
52	r	504	CDL	C59-C60-C61-C62
47	j	201	PEE	C38-C39-C40-C41
49	X	201	8Q1	C28-O27-P24-O3
52	l	703	CDL	C21-C22-C23-C24
47	j	202	PEE	C31-C30-O3-C3
52	J	404	CDL	C71-CB7-OB8-CB6
52	l	702	CDL	OB5-CB3-CB4-OB6
48	g	201	PLX	C11-C10-C9-C8
52	J	404	CDL	C54-C55-C56-C57
52	r	504	CDL	C64-C65-C66-C67
47	l	704	PEE	O2-C2-C3-O3
52	V	202	CDL	OA6-CA4-CA6-OA8
48	J	403	PLX	C27-C28-C29-C30
48	n	101	PLX	C29-C30-C31-C32
52	m	201	CDL	C14-C15-C16-C17
49	X	201	8Q1	C12-C13-C14-C15
52	r	504	CDL	C33-C34-C35-C36
52	r	504	CDL	C56-C57-C58-C59
51	J	402	UQ	C3-C2-O2-CM2
51	s	501	UQ	C3-C2-O2-CM2
52	V	201	CDL	CA7-C31-C32-C33
47	j	202	PEE	C23-C24-C25-C26
48	r	502	PLX	C12-C13-C14-C15
52	N	202	CDL	C31-CA7-OA8-CA6
52	r	504	CDL	C84-C85-C86-C87
47	l	704	PEE	C17-C18-C19-C20
47	C	302	PEE	C44-C45-C46-C47
48	g	201	PLX	C31-C32-C33-C34
52	a	201	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
47	Q	501	PEE	O3P-C1-C2-C3
52	m	201	CDL	OA5-CA3-CA4-CA6
52	m	201	CDL	C19-C20-C21-C22
47	l	701	PEE	O4P-C4-C5-N
47	l	704	PEE	C14-C15-C16-C17
47	r	501	PEE	C14-C15-C16-C17
51	s	501	UQ	C45-C44-C46-C47
51	s	501	UQ	C13-C14-C16-C17
52	l	703	CDL	CB7-C71-C72-C73
52	V	201	CDL	C75-C76-C77-C78
52	J	404	CDL	OB9-CB7-OB8-CB6
47	B	303	PEE	C41-C42-C43-C44
47	r	501	PEE	C21-C22-C23-C24
49	E	201	8Q1	C6-C7-C8-C9
52	m	201	CDL	C71-CB7-OB8-CB6
52	V	201	CDL	C1-CB2-OB2-PB2
52	r	504	CDL	C1-CB2-OB2-PB2
47	B	303	PEE	C44-C45-C46-C47
48	N	201	PLX	C28-C29-C30-C31
52	a	201	CDL	C36-C37-C38-C39
46	A	502	FMN	C2'-C1'-N10-C10
48	n	101	PLX	C26-C27-C28-C29
52	m	201	CDL	C58-C59-C60-C61
52	r	504	CDL	C39-C40-C41-C42
47	Q	501	PEE	C1-C2-C3-O3
47	W	201	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
48	N	201	PLX	C3-C4-C5-O8
48	r	502	PLX	C3-C4-C5-O8
52	J	404	CDL	CB3-CB4-CB6-OB8
52	N	202	CDL	CA3-CA4-CA6-OA8
52	i	401	CDL	CB3-CB4-CB6-OB8
47	r	501	PEE	C17-C18-C19-C20
52	l	702	CDL	C73-C74-C75-C76
52	m	201	CDL	C31-C32-C33-C34
49	E	201	8Q1	C29-C32-C34-N36
52	l	702	CDL	C31-C32-C33-C34
48	n	101	PLX	C9-C10-C11-C12
52	m	201	CDL	C82-C83-C84-C85
47	j	201	PEE	C1-O3P-P-O4P
48	J	403	PLX	C5-C4-O6-C6
48	r	502	PLX	C3-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	CB3-OB5-PB2-OB2
52	V	202	CDL	CA3-OA5-PA1-OA2
52	a	201	CDL	CA2-OA2-PA1-OA5
48	n	101	PLX	C11-C12-C13-C14
52	J	404	CDL	C40-C41-C42-C43
48	N	201	PLX	O9-C24-C25-C26
48	r	503	PLX	O7-C6-C7-C8
48	r	503	PLX	O9-C24-C25-C26
47	Q	501	PEE	O3P-C1-C2-O2
47	b	201	PEE	O3P-C1-C2-O2
48	N	201	PLX	O4-C3-C4-O6
48	r	502	PLX	O4-C3-C4-O6
52	V	201	CDL	OA5-CA3-CA4-OA6
52	u	201	CDL	OB5-CB3-CB4-OB6
47	j	202	PEE	O5-C30-O3-C3
47	C	302	PEE	O2-C2-C3-O3
47	W	201	PEE	O2-C2-C3-O3
47	r	501	PEE	O2-C2-C3-O3
48	N	201	PLX	O6-C4-C5-O8
48	n	101	PLX	O6-C4-C5-O8
52	m	201	CDL	OB6-CB4-CB6-OB8
48	r	503	PLX	C36-C37-C38-C39
51	J	402	UQ	C9-C11-C12-C13
48	r	502	PLX	C16-C17-C18-C19
52	V	202	CDL	C31-C32-C33-C34
52	u	201	CDL	C72-C73-C74-C75
52	l	703	CDL	OB7-CB5-OB6-CB4
52	r	504	CDL	C13-C14-C15-C16
52	N	202	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	C21-C22-C23-C24
52	J	404	CDL	C84-C85-C86-C87
52	m	201	CDL	C64-C65-C66-C67
47	W	201	PEE	C11-C10-O2-C2
52	l	703	CDL	C56-C57-C58-C59
47	j	202	PEE	C10-C11-C12-C13
47	r	501	PEE	C10-C11-C12-C13
47	W	201	PEE	C20-C21-C22-C23
52	l	702	CDL	C54-C55-C56-C57
48	j	203	PLX	O6-C6-C7-C8
48	r	502	PLX	O4-C3-C4-C5
47	C	302	PEE	C33-C34-C35-C36
48	C	303	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C11-C12-C13-C14
52	l	702	CDL	C18-C19-C20-C21
52	l	703	CDL	CA6-CA4-OA6-CA5
52	m	201	CDL	CA6-CA4-OA6-CA5
47	W	201	PEE	O4-C10-O2-C2
47	j	202	PEE	C13-C14-C15-C16
47	l	704	PEE	C41-C42-C43-C44
48	n	101	PLX	C12-C13-C14-C15
47	B	303	PEE	C32-C33-C34-C35
52	V	202	CDL	C54-C55-C56-C57
52	l	703	CDL	C79-C80-C81-C82
52	i	401	CDL	C71-C72-C73-C74
52	l	703	CDL	C71-C72-C73-C74
47	W	201	PEE	C19-C20-C21-C22
47	l	704	PEE	C1-C2-C3-O3
48	J	403	PLX	C3-C4-C5-O8
48	r	503	PLX	C3-C4-C5-O8
52	r	504	CDL	C15-C16-C17-C18
52	r	504	CDL	C51-C52-C53-C54
48	r	503	PLX	O4-C3-C4-O6
52	V	202	CDL	C32-C31-CA7-OA8
52	V	201	CDL	C21-C22-C23-C24
52	l	703	CDL	C31-CA7-OA8-CA6
47	r	501	PEE	C38-C39-C40-C41
52	V	202	CDL	CB2-C1-CA2-OA2
52	m	201	CDL	OB9-CB7-OB8-CB6
52	l	702	CDL	C84-C85-C86-C87
47	Q	501	PEE	O2-C2-C3-O3
47	b	201	PEE	O2-C2-C3-O3
48	r	502	PLX	O6-C4-C5-O8
52	V	201	CDL	OB6-CB4-CB6-OB8
52	m	201	CDL	OA6-CA4-CA6-OA8
48	r	503	PLX	C7-C8-C9-C10
48	j	203	PLX	C32-C33-C34-C35
52	V	202	CDL	C71-C72-C73-C74
52	m	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C13-C14-C15-C16
47	Q	501	PEE	C11-C12-C13-C14
52	m	201	CDL	C15-C16-C17-C18
47	Q	501	PEE	C39-C40-C41-C42
47	j	202	PEE	C19-C20-C21-C22
47	C	302	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	C3-O4-P1-O1
50	J	401	NDP	O4D-C1D-N1N-C6N
52	V	202	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	C22-C23-C24-C25
52	m	201	CDL	C17-C18-C19-C20
52	u	201	CDL	C71-C72-C73-C74
47	B	303	PEE	C4-O4P-P-O1P
47	C	302	PEE	C1-O3P-P-O2P
47	C	302	PEE	C4-O4P-P-O2P
47	Q	501	PEE	C4-O4P-P-O2P
47	W	201	PEE	C4-O4P-P-O2P
47	W	201	PEE	C4-O4P-P-O1P
47	j	201	PEE	C1-O3P-P-O2P
47	r	501	PEE	C1-O3P-P-O2P
48	J	403	PLX	C3-O4-P1-O2
48	J	403	PLX	C3-O4-P1-O3
48	J	403	PLX	C2-O1-P1-O3
48	N	201	PLX	C3-O4-P1-O3
48	j	203	PLX	C2-O1-P1-O3
48	n	101	PLX	C3-O4-P1-O2
48	n	101	PLX	C2-O1-P1-O3
48	r	503	PLX	C3-O4-P1-O2
48	r	503	PLX	C3-O4-P1-O3
52	J	404	CDL	CA3-OA5-PA1-OA3
52	J	404	CDL	CA3-OA5-PA1-OA4
52	N	202	CDL	CB3-OB5-PB2-OB4
52	V	201	CDL	CA3-OA5-PA1-OA3
52	V	201	CDL	CB2-OB2-PB2-OB4
52	V	201	CDL	CB3-OB5-PB2-OB3
52	V	202	CDL	CB2-OB2-PB2-OB3
52	V	202	CDL	CB2-OB2-PB2-OB4
52	V	202	CDL	CB3-OB5-PB2-OB3
52	V	202	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	CB2-OB2-PB2-OB4
52	i	401	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CA2-OA2-PA1-OA3
52	l	702	CDL	CB3-OB5-PB2-OB4
52	m	201	CDL	CA3-OA5-PA1-OA4
52	r	504	CDL	CA2-OA2-PA1-OA4
52	r	504	CDL	CB3-OB5-PB2-OB4
52	u	201	CDL	CB2-OB2-PB2-OB4
47	b	201	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
48	N	201	PLX	O4-C3-C4-C5
48	r	503	PLX	O4-C3-C4-C5
52	V	201	CDL	OA5-CA3-CA4-CA6
52	l	702	CDL	OB5-CB3-CB4-CB6
52	u	201	CDL	OB5-CB3-CB4-CB6
48	g	201	PLX	C33-C34-C35-C36
52	r	504	CDL	C54-C55-C56-C57
52	a	201	CDL	C43-C44-C45-C46
47	B	303	PEE	C5-C4-O4P-P
47	W	201	PEE	C5-C4-O4P-P
48	g	201	PLX	C25-C24-O8-C5
48	j	203	PLX	C25-C24-O8-C5
48	N	201	PLX	C13-C14-C15-C16
52	l	703	CDL	OA9-CA7-OA8-CA6
48	J	403	PLX	C26-C27-C28-C29
47	l	704	PEE	C39-C40-C41-C42
48	C	303	PLX	C33-C34-C35-C36
48	N	201	PLX	C26-C27-C28-C29
52	i	401	CDL	C35-C36-C37-C38
52	V	201	CDL	CB2-C1-CA2-OA2
47	b	201	PEE	C34-C35-C36-C37
47	l	701	PEE	O3P-C1-C2-O2
52	a	201	CDL	OA5-CA3-CA4-OA6
52	l	703	CDL	OB5-CB3-CB4-OB6
52	l	703	CDL	CB5-C51-C52-C53
47	B	303	PEE	C38-C39-C40-C41
52	J	404	CDL	O1-C1-CB2-OB2
52	V	201	CDL	O1-C1-CA2-OA2
52	V	201	CDL	C40-C41-C42-C43
52	r	504	CDL	CB5-C51-C52-C53
48	C	303	PLX	N1-C1-C2-O1
48	J	403	PLX	N1-C1-C2-O1
48	r	503	PLX	O6-C4-C5-O8
52	N	202	CDL	OA6-CA4-CA6-OA8
47	C	302	PEE	C12-C13-C14-C15
52	i	401	CDL	C75-C76-C77-C78
52	l	703	CDL	C77-C78-C79-C80
48	J	403	PLX	C12-C13-C14-C15
48	J	403	PLX	C10-C11-C12-C13
52	V	201	CDL	CA4-CA3-OA5-PA1
52	m	201	CDL	CA4-CA3-OA5-PA1
52	V	201	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C31-C30-O3-C3
47	W	201	PEE	C23-C24-C25-C26
48	g	201	PLX	O6-C6-C7-C8
52	V	202	CDL	C63-C64-C65-C66
51	s	501	UQ	C9-C11-C12-C13
47	B	303	PEE	O5-C30-O3-C3
48	g	201	PLX	O7-C6-C7-C8
47	b	201	PEE	C14-C15-C16-C17
47	b	201	PEE	C30-C31-C32-C33
47	W	201	PEE	C22-C23-C24-C25
47	Q	501	PEE	C17-C18-C19-C20
52	V	202	CDL	C57-C58-C59-C60
52	a	201	CDL	C84-C85-C86-C87
52	i	401	CDL	C73-C74-C75-C76
52	m	201	CDL	C42-C43-C44-C45
48	g	201	PLX	C36-C37-C38-C39
52	l	702	CDL	C22-C23-C24-C25
47	r	501	PEE	C33-C34-C35-C36
48	j	203	PLX	C30-C31-C32-C33
52	V	201	CDL	CA6-CA4-OA6-CA5
47	l	701	PEE	O3P-C1-C2-C3
52	a	201	CDL	OA5-CA3-CA4-CA6
52	l	703	CDL	OA7-CA5-OA6-CA4
52	V	202	CDL	C58-C59-C60-C61
47	C	302	PEE	C34-C35-C36-C37
47	l	701	PEE	C2-C1-O3P-P
47	B	303	PEE	C22-C23-C24-C25
47	j	201	PEE	O3P-C1-C2-O2
52	V	202	CDL	OB5-CB3-CB4-OB6
52	a	201	CDL	OB5-CB3-CB4-OB6
51	s	501	UQ	C52-C53-C54-C56
48	C	303	PLX	C11-C12-C13-C14
52	a	201	CDL	C12-C13-C14-C15
52	u	201	CDL	C57-C58-C59-C60
47	j	201	PEE	C12-C13-C14-C15
52	r	504	CDL	C20-C21-C22-C23
52	l	703	CDL	C11-CA5-OA6-CA4
47	b	201	PEE	C16-C17-C18-C19
48	J	403	PLX	O6-C4-C5-O8
48	j	203	PLX	O6-C4-C5-O8
48	C	303	PLX	C7-C8-C9-C10
52	V	201	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
47	b	201	PEE	C4-O4P-P-O3P
47	r	501	PEE	C1-O3P-P-O4P
48	C	303	PLX	C3-O4-P1-O1
52	V	202	CDL	CA2-OA2-PA1-OA5
48	n	101	PLX	C3-C4-C5-O8
52	V	202	CDL	CA3-CA4-CA6-OA8
48	g	201	PLX	C15-C16-C17-C18
52	a	201	CDL	C18-C19-C20-C21
51	J	402	UQ	C4-C3-O3-CM3
48	j	203	PLX	C27-C28-C29-C30
47	l	704	PEE	C42-C43-C44-C45
52	l	703	CDL	C82-C83-C84-C85
48	N	201	PLX	C4-C3-O4-P1
48	J	403	PLX	C35-C36-C37-C38
47	b	201	PEE	C18-C19-C20-C21
47	j	201	PEE	C36-C37-C38-C39
48	j	203	PLX	C24-C25-C26-C27
52	m	201	CDL	CB2-C1-CA2-OA2
52	u	201	CDL	CA2-C1-CB2-OB2
47	B	303	PEE	C39-C40-C41-C42
47	Q	501	PEE	C15-C16-C17-C18
52	J	404	CDL	C72-C71-CB7-OB8
52	m	201	CDL	OB5-CB3-CB4-OB6
52	a	201	CDL	C74-C75-C76-C77
52	l	702	CDL	C42-C43-C44-C45
47	C	302	PEE	C41-C42-C43-C44
49	E	201	8Q1	C9-C10-C11-C12
52	N	202	CDL	O1-C1-CA2-OA2
47	l	701	PEE	C39-C40-C41-C42
48	N	201	PLX	O8-C24-C25-C26
51	s	501	UQ	C4-C3-O3-CM3
48	j	203	PLX	C15-C16-C17-C18
52	l	703	CDL	C17-C18-C19-C20
52	N	202	CDL	CA2-C1-CB2-OB2
52	V	201	CDL	CA3-CA4-CA6-OA8
52	a	201	CDL	C64-C65-C66-C67
48	r	503	PLX	C16-C17-C18-C19
52	a	201	CDL	C55-C56-C57-C58
52	i	401	CDL	CA6-CA4-OA6-CA5
47	Q	501	PEE	C10-C11-C12-C13
47	C	302	PEE	C20-C21-C22-C23
47	j	201	PEE	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
48	j	203	PLX	C3-C4-O6-C6
48	C	303	PLX	O4-C3-C4-O6
48	r	502	PLX	C18-C19-C20-C21
52	V	202	CDL	OB5-CB3-CB4-CB6
47	C	302	PEE	C18-C19-C20-C21
48	J	403	PLX	C29-C30-C31-C32
48	g	201	PLX	C18-C19-C20-C21
52	J	404	CDL	C15-C16-C17-C18
47	j	202	PEE	C32-C33-C34-C35
52	l	703	CDL	OB6-CB4-CB6-OB8
52	r	504	CDL	OA6-CA4-CA6-OA8
52	l	702	CDL	C76-C77-C78-C79
52	u	201	CDL	C75-C76-C77-C78
52	V	202	CDL	C23-C24-C25-C26
47	B	303	PEE	C37-C38-C39-C40
47	j	201	PEE	C41-C42-C43-C44
52	l	703	CDL	CB2-C1-CA2-OA2
48	N	201	PLX	C16-C17-C18-C19
52	l	702	CDL	C51-C52-C53-C54
51	s	501	UQ	C12-C11-C9-C8
52	V	201	CDL	C64-C65-C66-C67
47	j	201	PEE	C16-C17-C18-C19
51	s	501	UQ	C40-C39-C41-C42
47	l	704	PEE	C12-C13-C14-C15
47	C	302	PEE	C36-C37-C38-C39
47	W	201	PEE	C16-C17-C18-C19
47	B	303	PEE	O3P-C1-C2-O2
47	j	202	PEE	O3P-C1-C2-O2
47	C	302	PEE	C30-C31-C32-C33
52	V	201	CDL	C60-C61-C62-C63
52	l	702	CDL	C12-C11-CA5-OA6
52	V	202	CDL	C44-C45-C46-C47
52	i	401	CDL	OB9-CB7-OB8-CB6
48	r	502	PLX	O8-C24-C25-C26
49	X	201	8Q1	C1-C6-C7-C8
52	J	404	CDL	C74-C75-C76-C77
52	r	504	CDL	C17-C18-C19-C20
52	a	201	CDL	C12-C11-CA5-OA6
52	l	702	CDL	C72-C71-CB7-OB8
52	m	201	CDL	C77-C78-C79-C80
47	B	303	PEE	C16-C17-C18-C19
47	r	501	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
52	r	504	CDL	C21-C22-C23-C24
47	j	202	PEE	O3-C30-C31-C32
47	b	201	PEE	C2-C3-O3-C30
48	r	502	PLX	C26-C27-C28-C29
47	B	303	PEE	C34-C35-C36-C37
47	j	202	PEE	C14-C15-C16-C17
48	J	403	PLX	C36-C37-C38-C39
52	m	201	CDL	C12-C11-CA5-OA6
52	i	401	CDL	C15-C16-C17-C18
52	J	404	CDL	C12-C11-CA5-OA6
52	a	201	CDL	C32-C31-CA7-OA8
52	a	201	CDL	C39-C40-C41-C42
48	j	203	PLX	C7-C6-O6-C4
47	Q	501	PEE	C37-C38-C39-C40
48	j	203	PLX	C18-C19-C20-C21
52	V	202	CDL	C22-C23-C24-C25
48	C	303	PLX	C6-C7-C8-C9
52	l	703	CDL	C58-C59-C60-C61
47	b	201	PEE	C38-C39-C40-C41
51	J	402	UQ	C12-C13-C14-C16
52	N	202	CDL	C51-C52-C53-C54
52	l	703	CDL	C55-C56-C57-C58
47	B	303	PEE	O3P-C1-C2-C3
47	j	201	PEE	O3P-C1-C2-C3
52	i	401	CDL	OA5-CA3-CA4-CA6
47	j	201	PEE	C24-C25-C26-C27
47	j	201	PEE	O2-C10-C11-C12
47	l	701	PEE	O2-C10-C11-C12
52	i	401	CDL	C12-C11-CA5-OA6
52	r	504	CDL	C12-C13-C14-C15
48	C	303	PLX	O6-C4-C5-O8
52	N	202	CDL	OB6-CB4-CB6-OB8
48	g	201	PLX	C6-C7-C8-C9
48	g	201	PLX	O9-C24-C25-C26
50	J	401	NDP	C5B-O5B-PA-O3
52	i	401	CDL	C71-CB7-OB8-CB6
52	a	201	CDL	C16-C17-C18-C19
52	l	703	CDL	C59-C60-C61-C62
47	C	302	PEE	C38-C39-C40-C41
47	j	202	PEE	C16-C17-C18-C19
47	j	201	PEE	O3-C30-C31-C32
52	V	201	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
52	r	504	CDL	C72-C71-CB7-OB8
47	j	202	PEE	O5-C30-C31-C32
48	C	303	PLX	C35-C36-C37-C38
51	s	501	UQ	C2-C3-O3-CM3
56	w	401	ADP	PB-O3A-PA-O2A
47	C	302	PEE	C16-C17-C18-C19
47	j	202	PEE	C30-C31-C32-C33
52	a	201	CDL	C12-C11-CA5-OA7
47	Q	501	PEE	C40-C41-C42-C43
52	r	504	CDL	C44-C45-C46-C47
52	a	201	CDL	C32-C31-CA7-OA9
52	J	404	CDL	C12-C11-CA5-OA7
52	l	702	CDL	C72-C71-CB7-OB9
48	j	203	PLX	C10-C11-C12-C13
52	V	201	CDL	CB3-CB4-CB6-OB8
52	V	201	CDL	CA3-OA5-PA1-OA2
52	V	202	CDL	O1-C1-CA2-OA2
52	m	201	CDL	C12-C11-CA5-OA7
49	E	201	8Q1	C11-C12-C13-C14
47	b	201	PEE	C24-C25-C26-C27
47	C	302	PEE	C1-O3P-P-O1P
47	b	201	PEE	C1-O3P-P-O1P
50	J	401	NDP	C2N-C3N-C7N-N7N
52	i	401	CDL	CB3-OB5-PB2-OB4
52	m	201	CDL	CB2-OB2-PB2-OB4
47	l	701	PEE	O4-C10-C11-C12
48	n	101	PLX	O4-C3-C4-C5
47	r	501	PEE	C31-C32-C33-C34
48	j	203	PLX	C35-C36-C37-C38
48	C	303	PLX	C25-C26-C27-C28
52	r	504	CDL	C82-C83-C84-C85
47	j	201	PEE	O4-C10-C11-C12
52	m	201	CDL	C74-C75-C76-C77
52	V	202	CDL	C32-C31-CA7-OA9
47	r	501	PEE	C42-C43-C44-C45
48	N	201	PLX	C1-C2-O1-P1
48	N	201	PLX	C25-C24-O8-C5
49	E	201	8Q1	C29-C32-C34-O35
52	i	401	CDL	CA3-CA4-OA6-CA5
47	j	202	PEE	C20-C21-C22-C23
52	l	703	CDL	C57-C58-C59-C60
52	J	404	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
47	l	704	PEE	C31-C32-C33-C34
52	i	401	CDL	CA5-C11-C12-C13
52	i	401	CDL	C12-C11-CA5-OA7
47	l	704	PEE	C24-C25-C26-C27
52	N	202	CDL	C52-C51-CB5-OB6
52	a	201	CDL	C82-C83-C84-C85
48	J	403	PLX	C6-C7-C8-C9
48	J	403	PLX	O4-C3-C4-O6
52	i	401	CDL	OA5-CA3-CA4-OA6
47	j	201	PEE	O5-C30-C31-C32
47	l	701	PEE	O3-C30-C31-C32
52	J	404	CDL	C57-C58-C59-C60
52	l	702	CDL	C44-C45-C46-C47
52	V	202	CDL	C55-C56-C57-C58
48	J	403	PLX	C17-C18-C19-C20
52	m	201	CDL	C43-C44-C45-C46
52	r	504	CDL	C32-C31-CA7-OA8

There are no ring outliers.

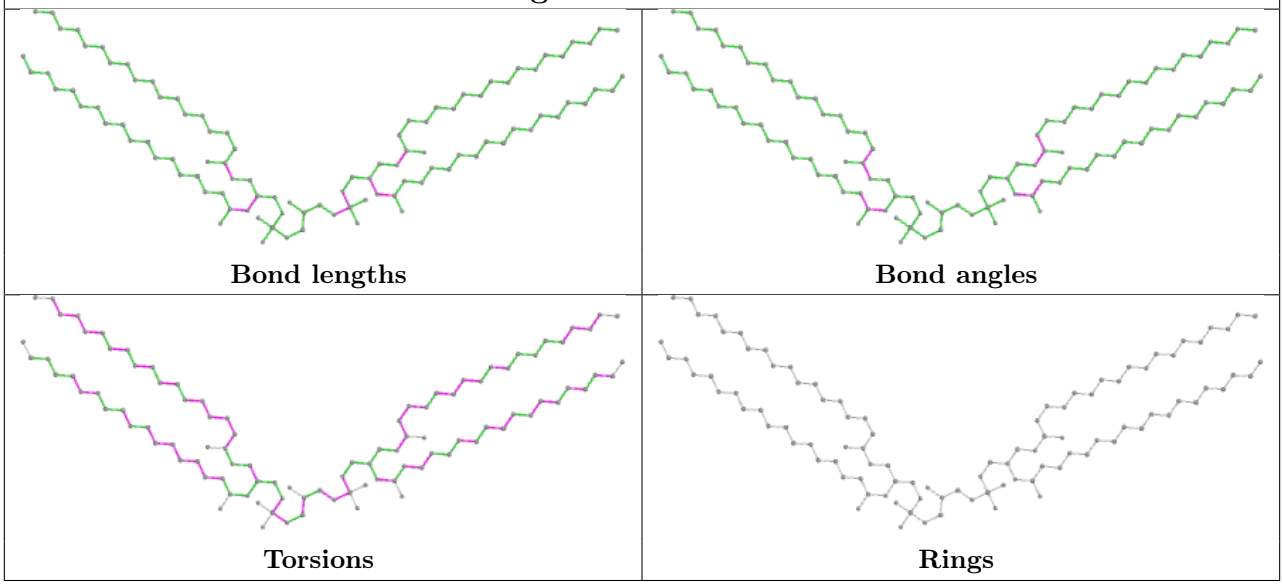
16 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	14	0
45	M	802	SF4	6	0
53	M	803	FES	1	0
48	C	303	PLX	15	0
47	C	302	PEE	3	0
51	J	402	UQ	10	0
52	V	201	CDL	3	0
47	B	303	PEE	2	0
49	E	201	8Q1	1	0
45	A	501	SF4	2	0
49	X	201	8Q1	6	0
47	W	201	PEE	5	0
47	Q	501	PEE	16	0
52	N	202	CDL	11	0
52	V	202	CDL	3	0
52	J	404	CDL	8	0

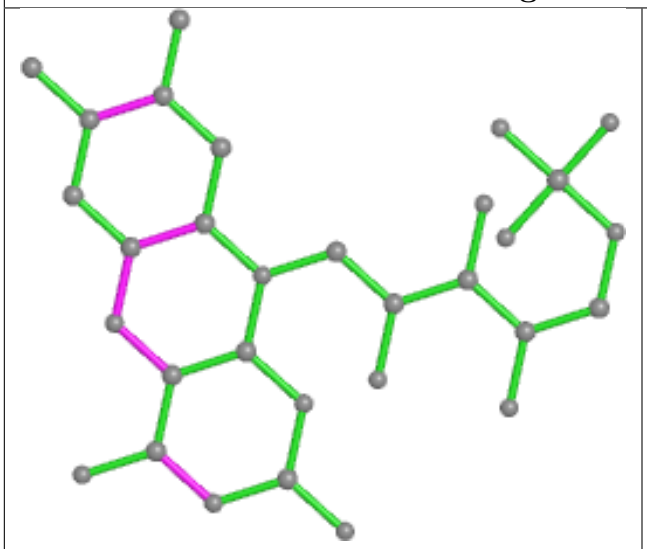
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

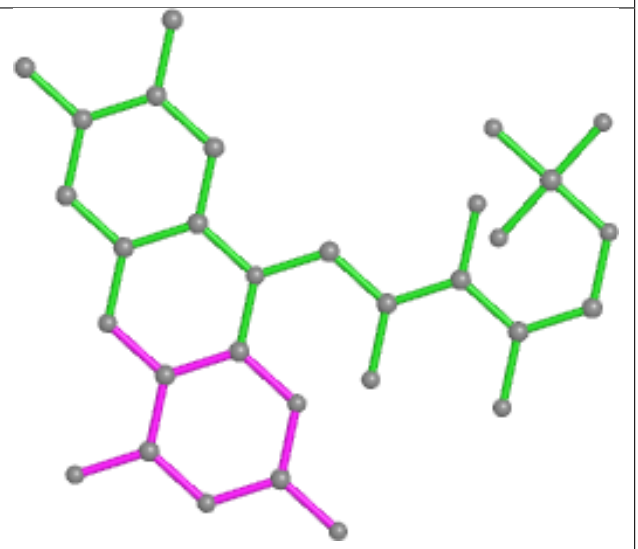
Ligand CDL r 504



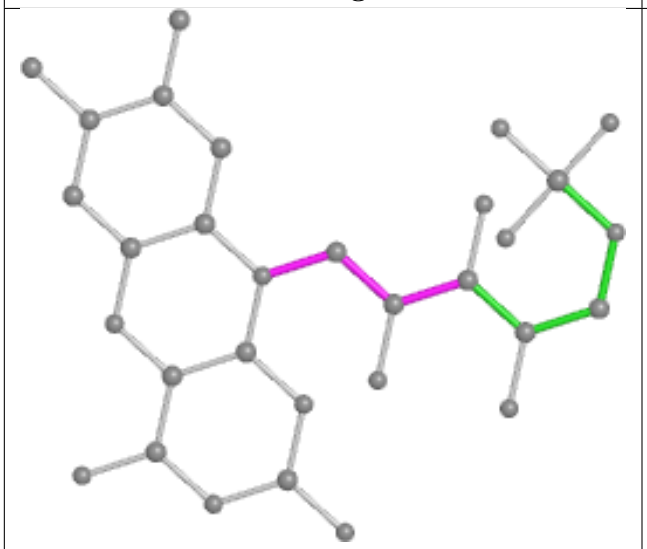
Ligand FMN A 502



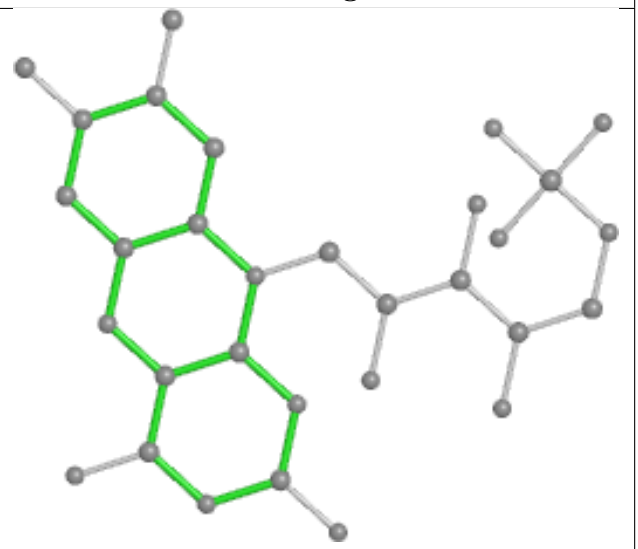
Bond lengths



Bond angles

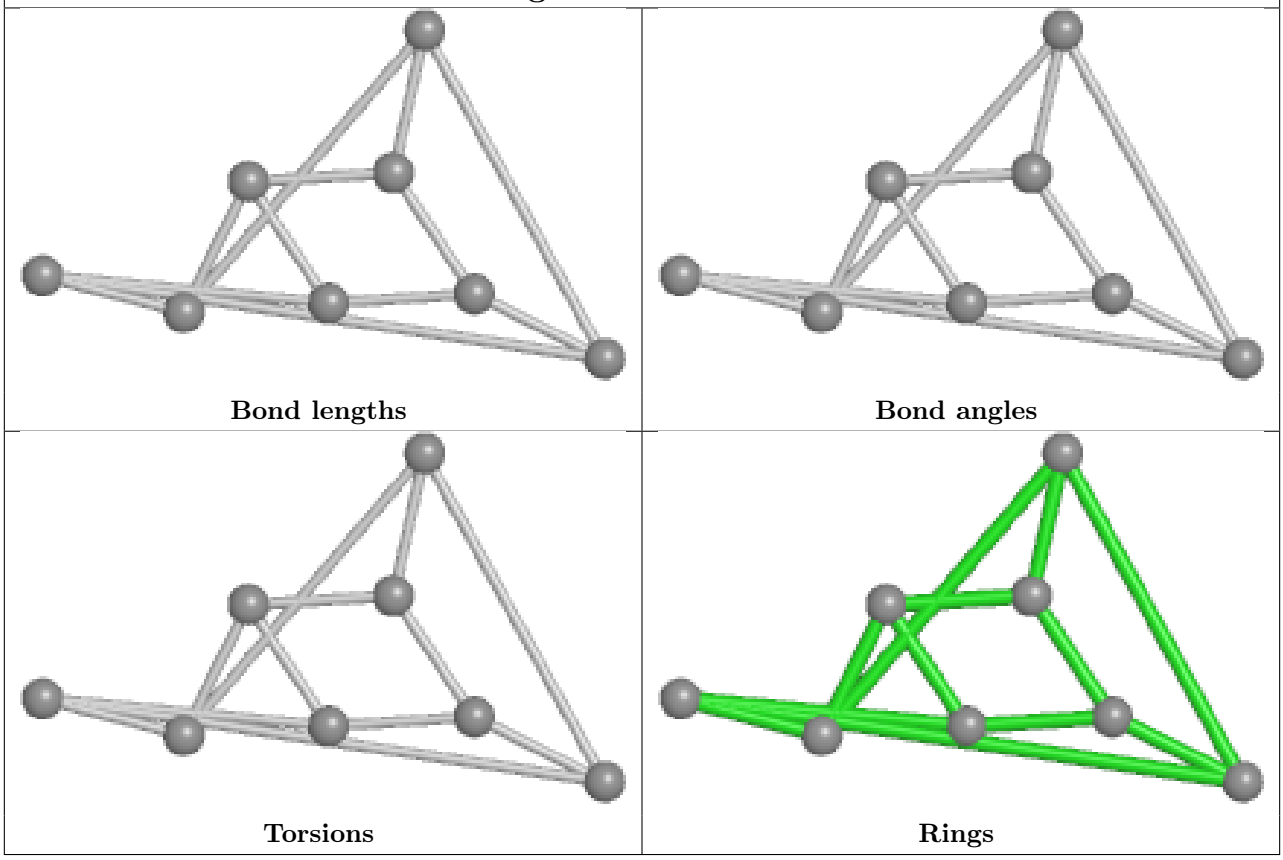


Torsions

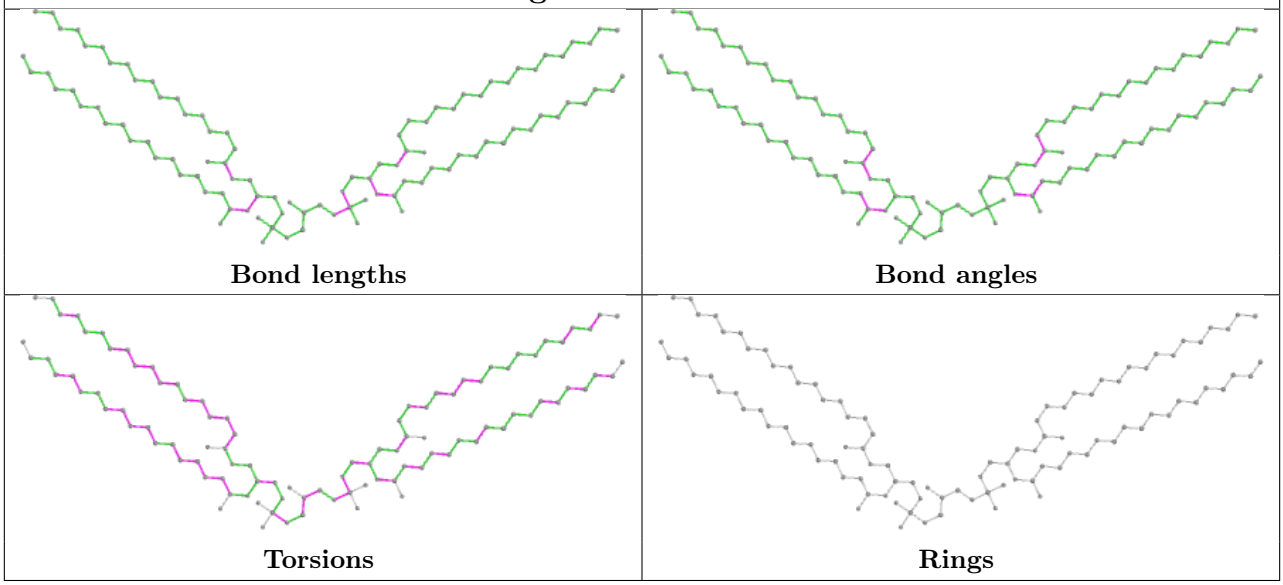


Rings

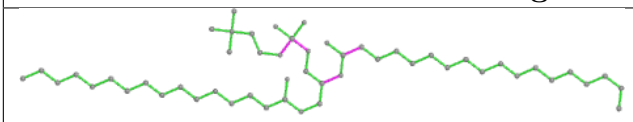
Ligand SF4 M 802



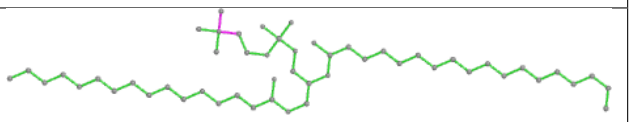
Ligand CDL a 201



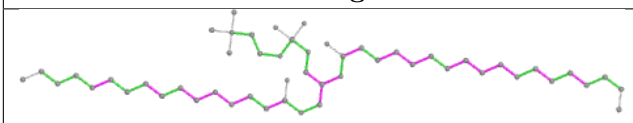
Ligand PLX r 502



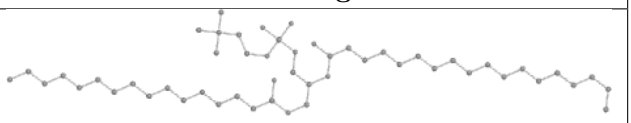
Bond lengths



Bond angles

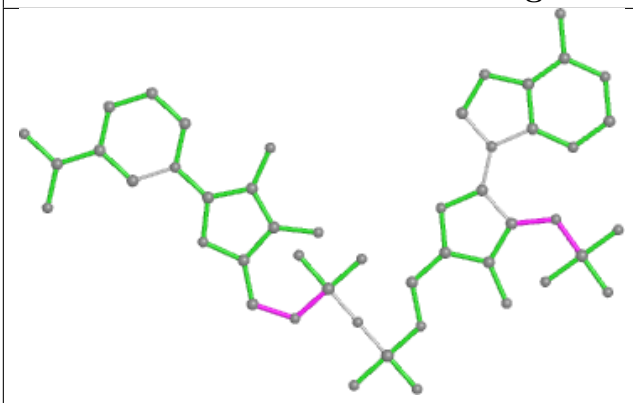


Torsions

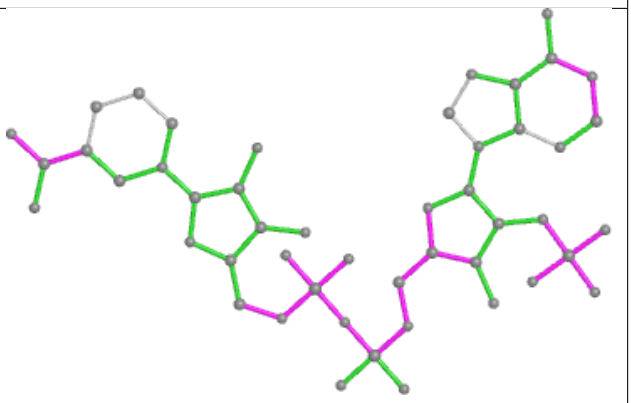


Rings

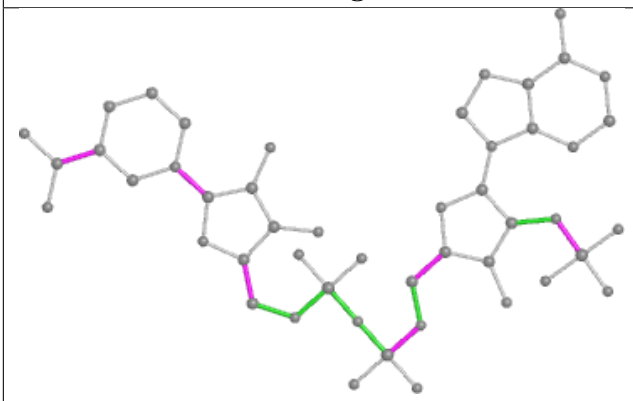
Ligand NDP J 401



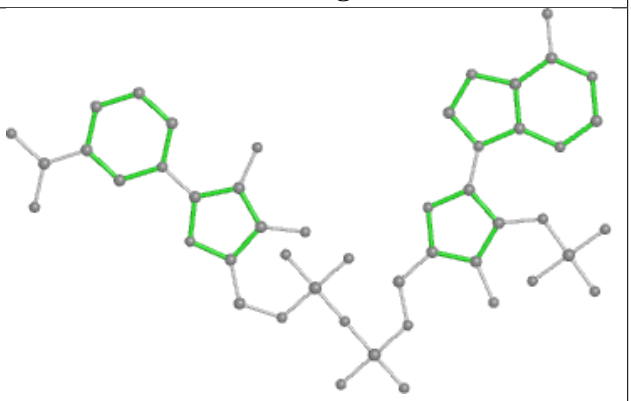
Bond lengths



Bond angles

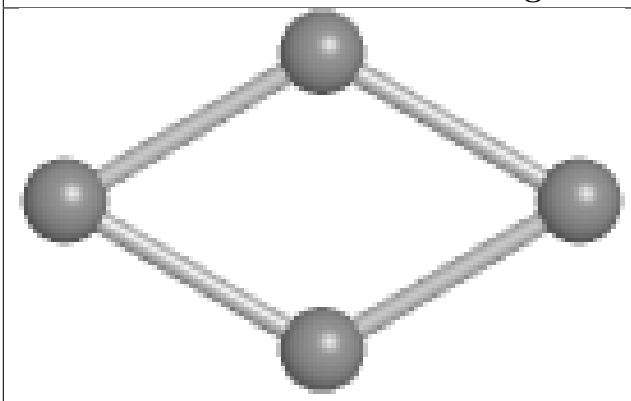


Torsions

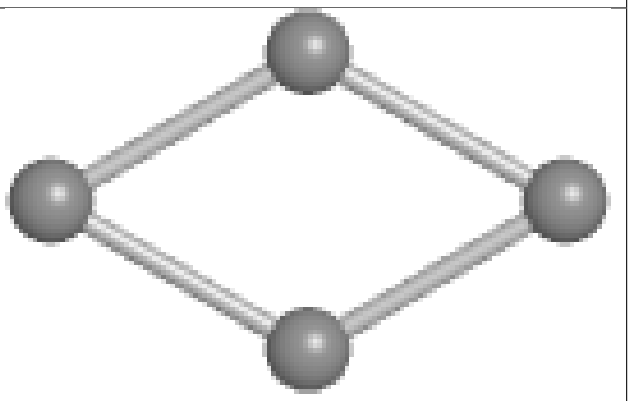


Rings

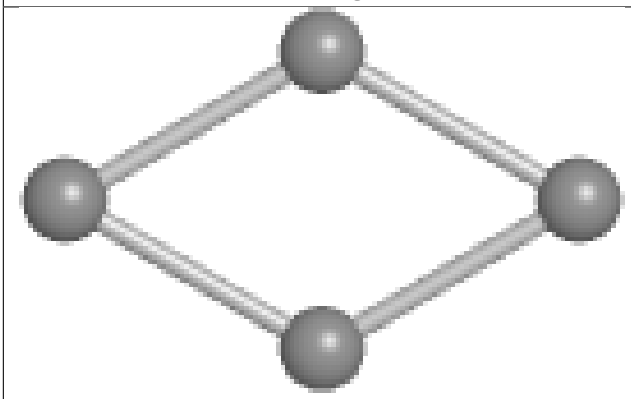
Ligand FES M 803



Bond lengths



Bond angles



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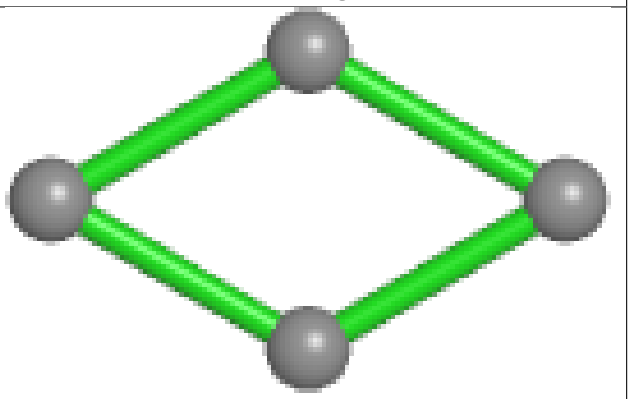
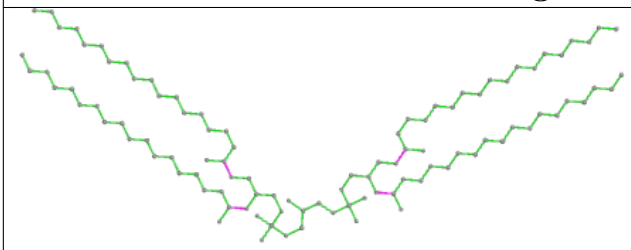


Rings

Ligand CDL l 703



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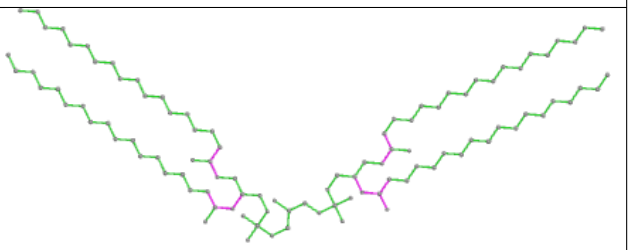
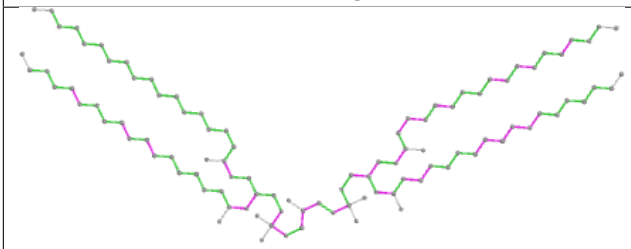


Bond angles



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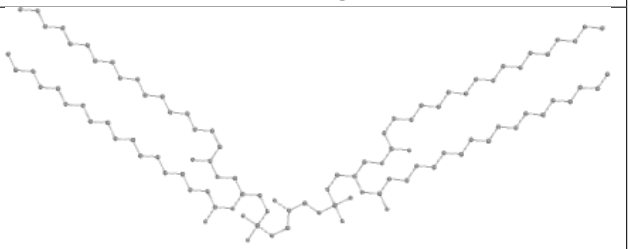
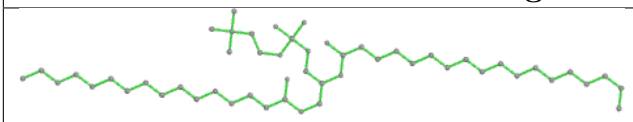
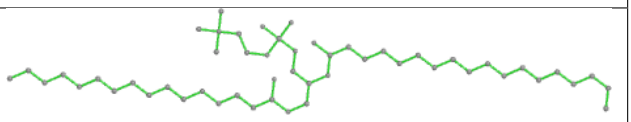


Rings

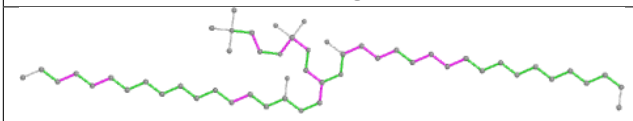
Ligand PLX C 303



Bond lengths



Bond angles



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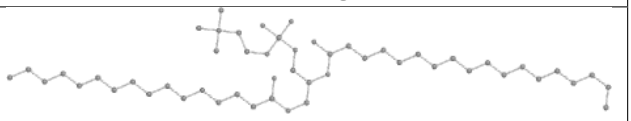
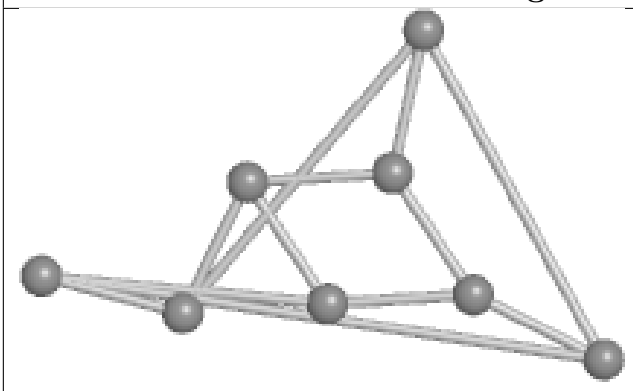
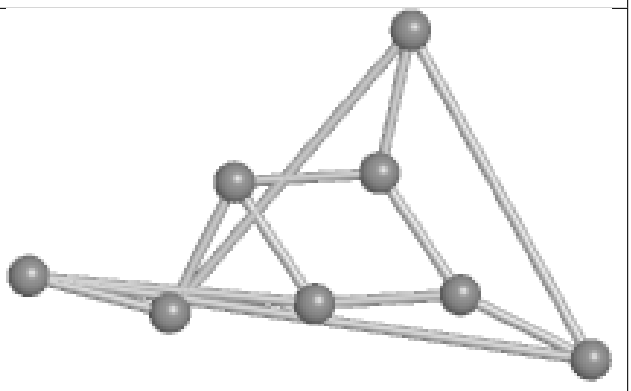


Rings

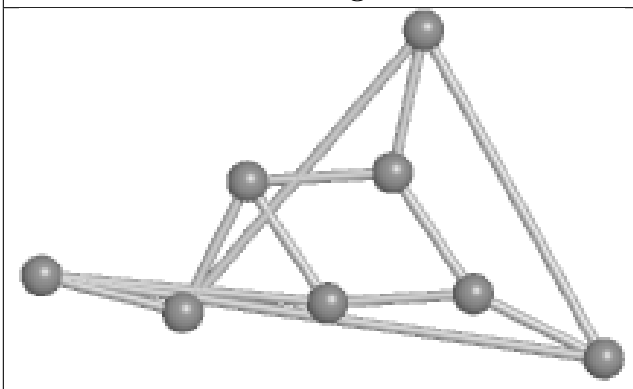
Ligand SF4 M 801



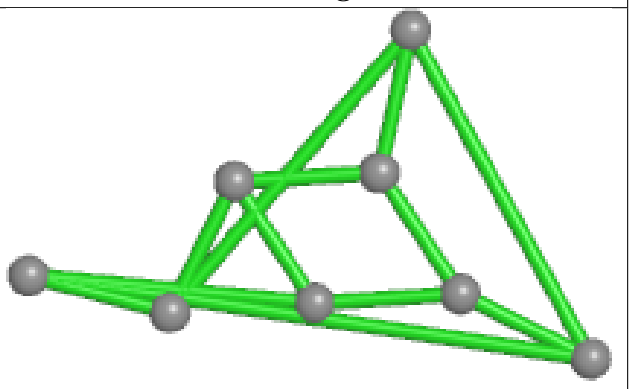
Bond lengths



Bond angles

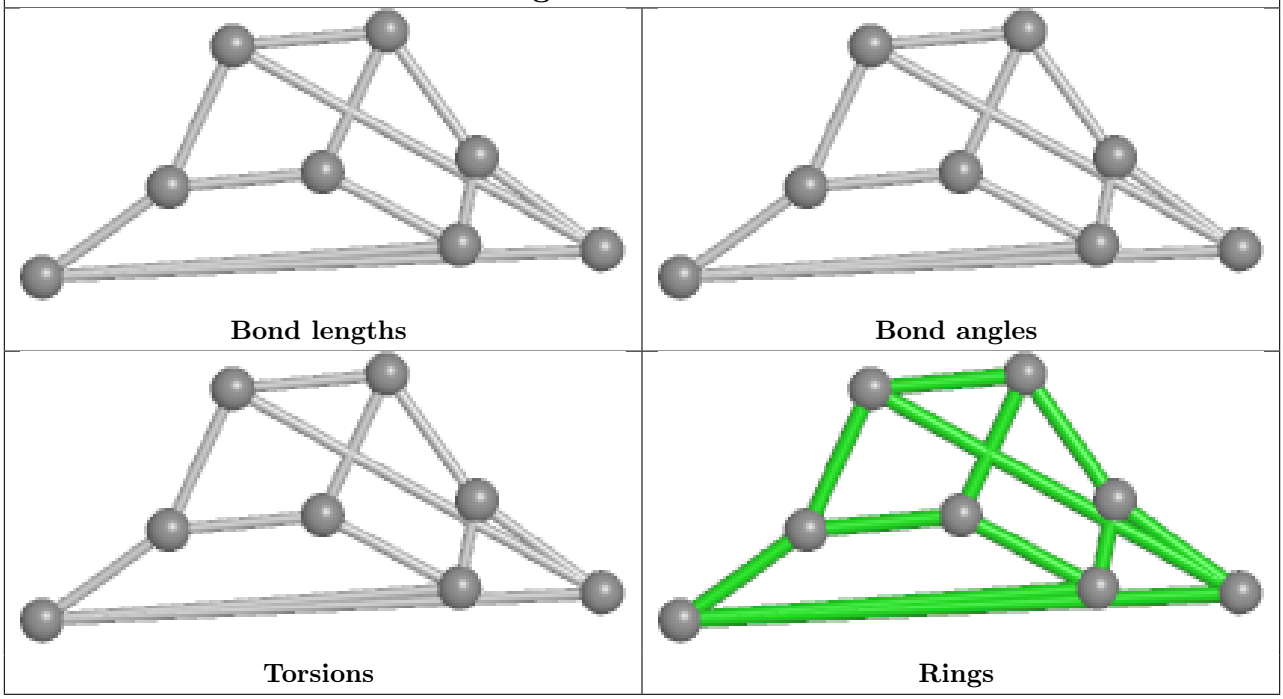


Torsions

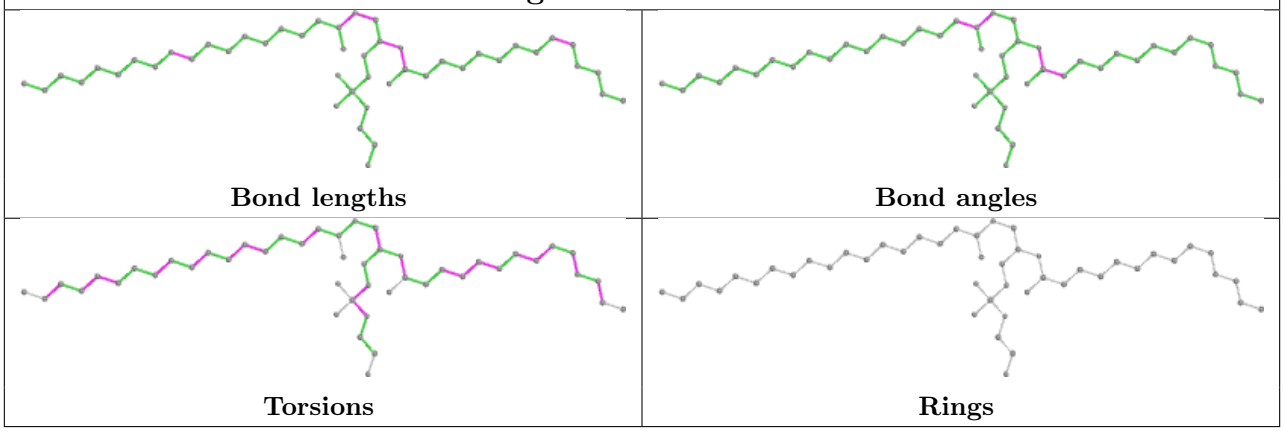


Rings

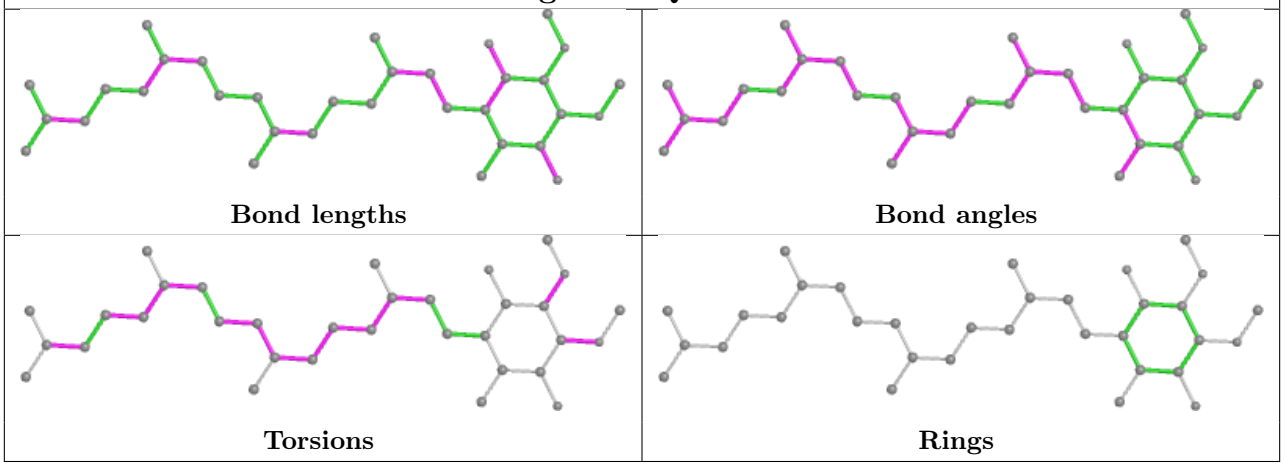
Ligand SF4 B 302



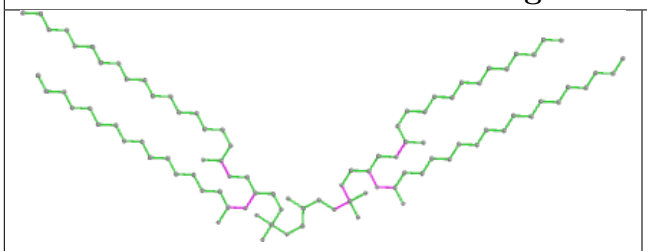
Ligand PEE C 302



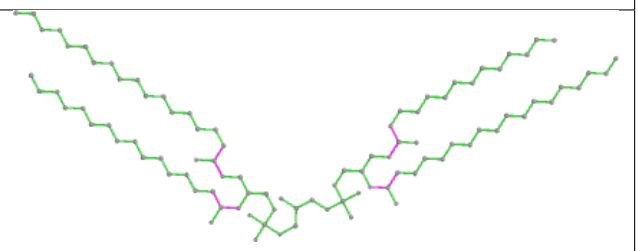
Ligand UQ J 402



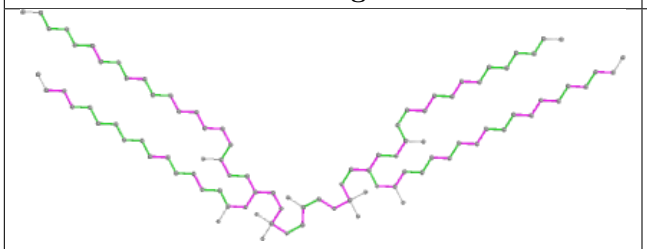
Ligand CDL V 201



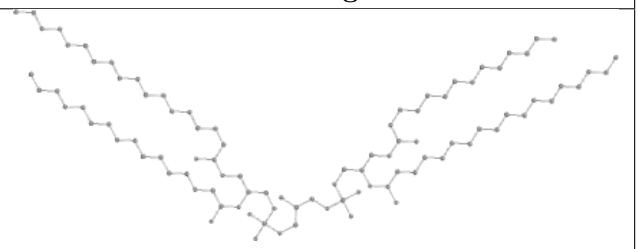
Bond lengths



Bond angles

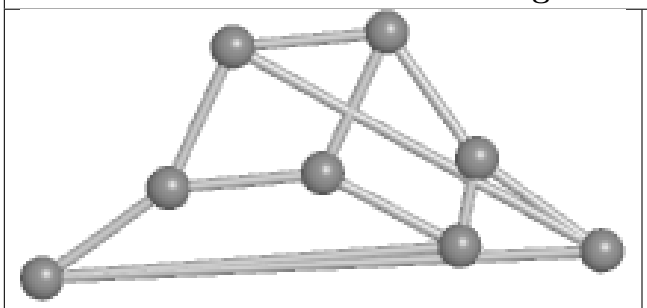


Torsions



Rings

Ligand SF4 C 301



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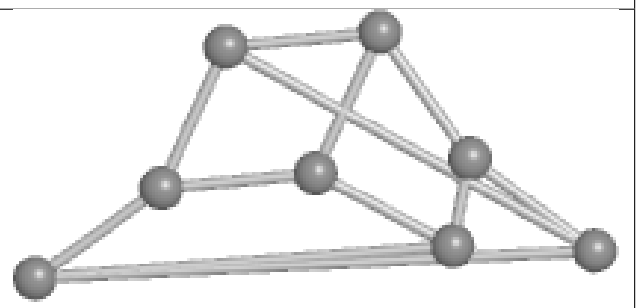
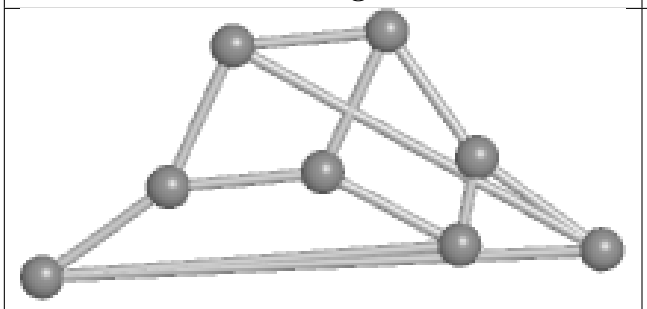
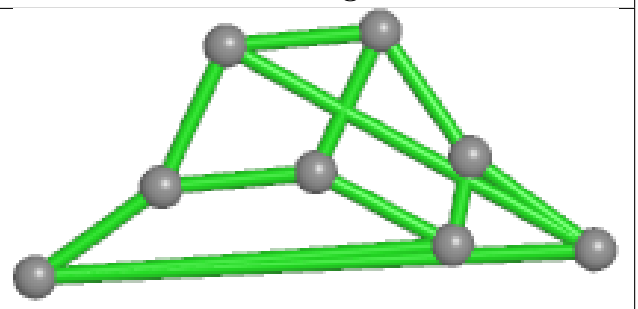


Bond angles

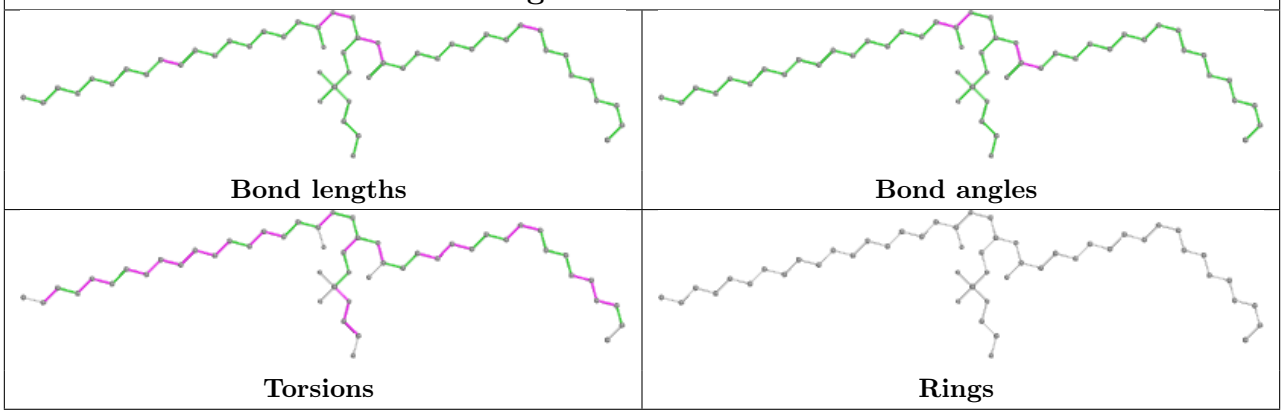


Torsions

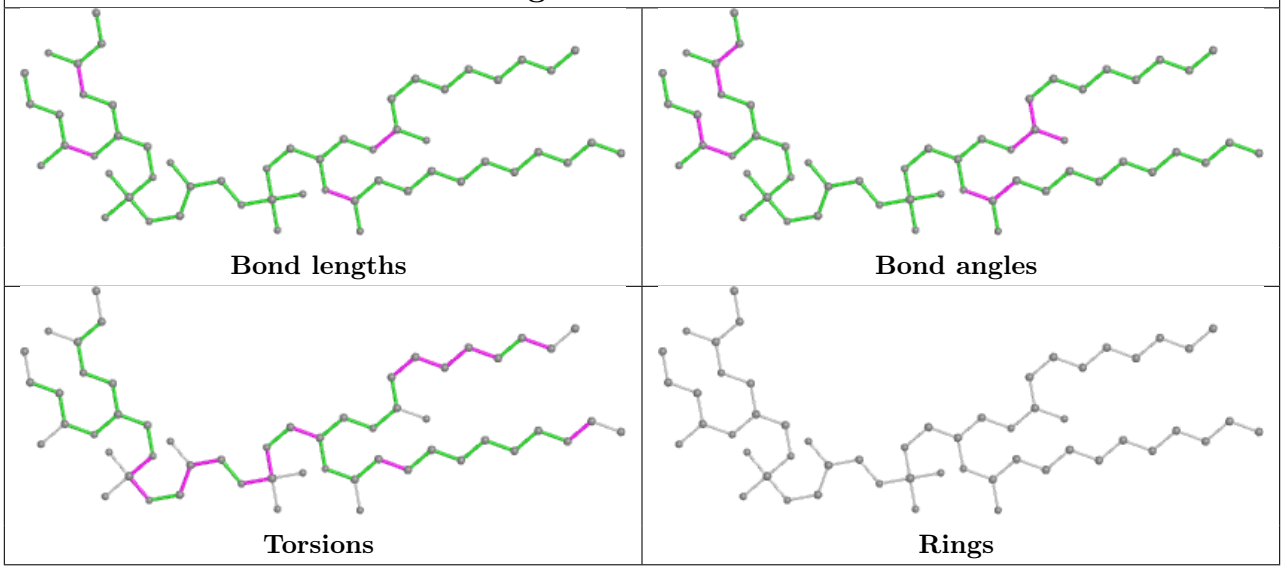


Rings

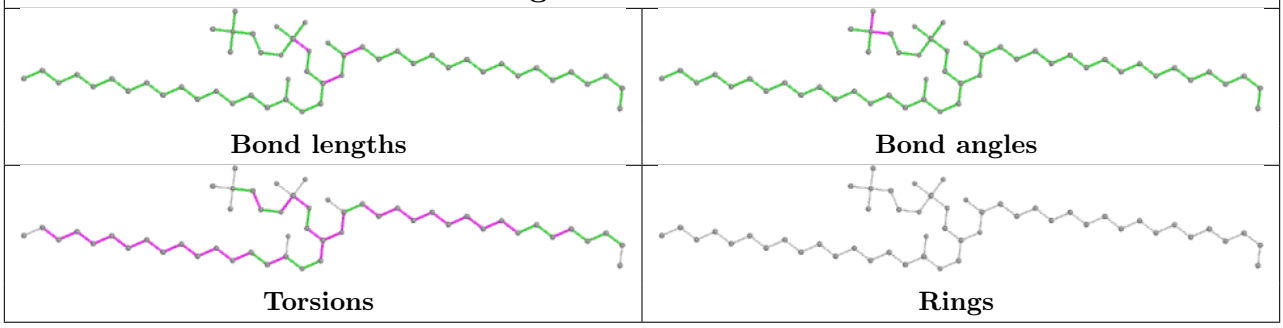
Ligand PEE B 303



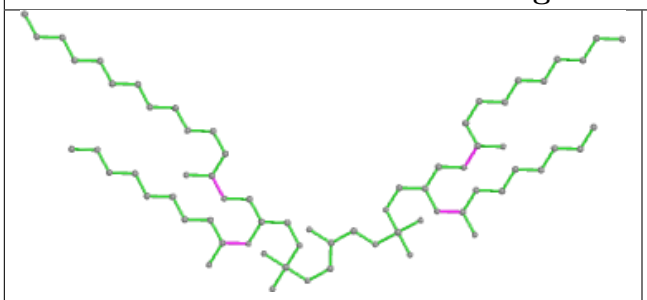
Ligand CDL u 201



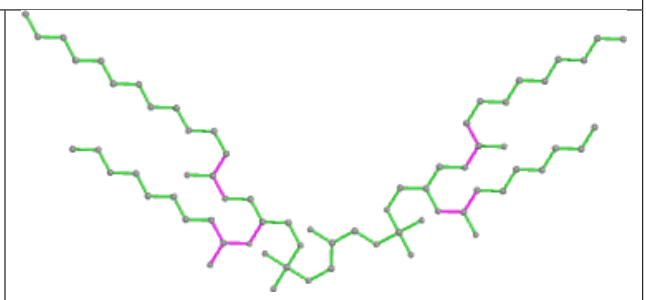
Ligand PLX J 403



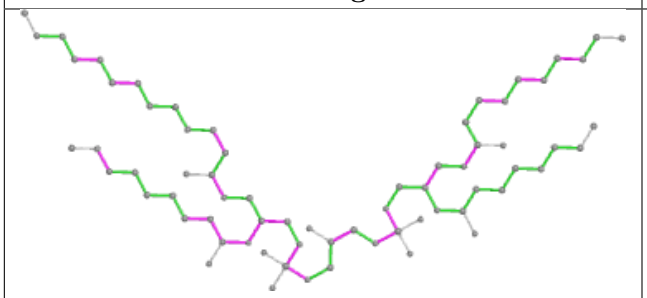
Ligand CDL i 401



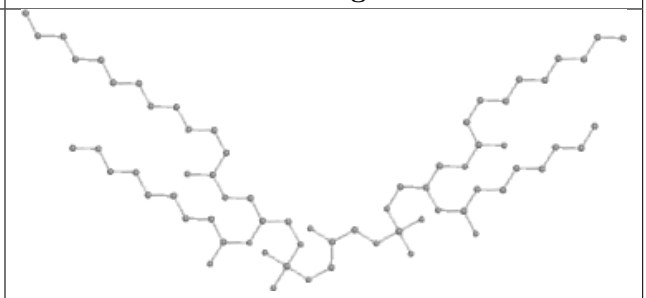
Bond lengths



Bond angles

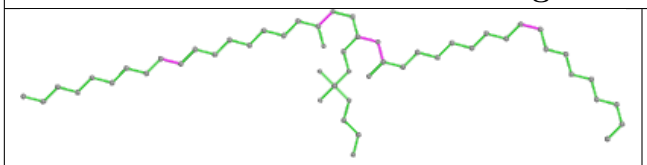


Torsions

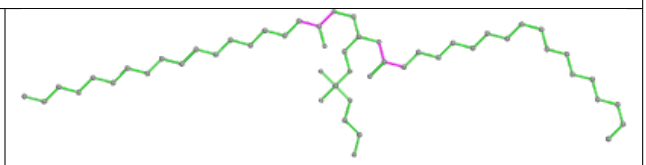


Rings

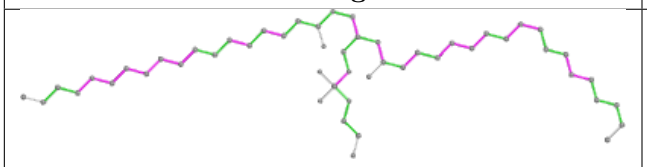
Ligand PEE r 501



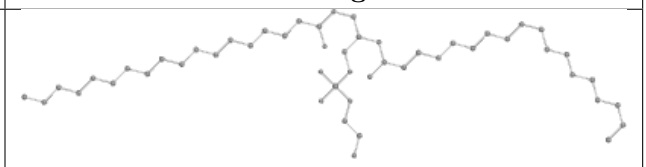
Bond lengths



Bond angles

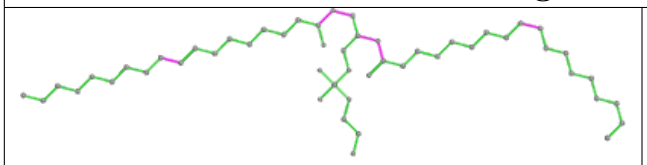


Torsions



Rings

Ligand PEE j 201



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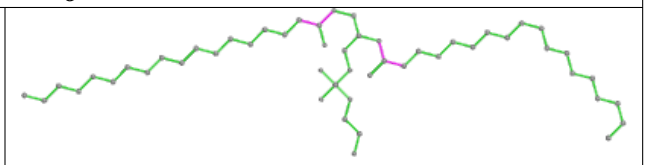
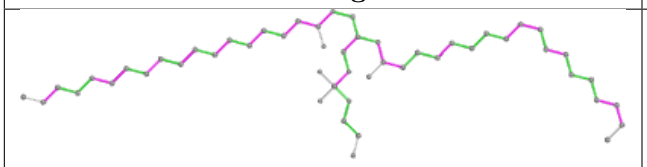
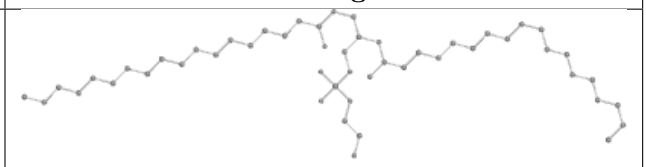


Bond angles

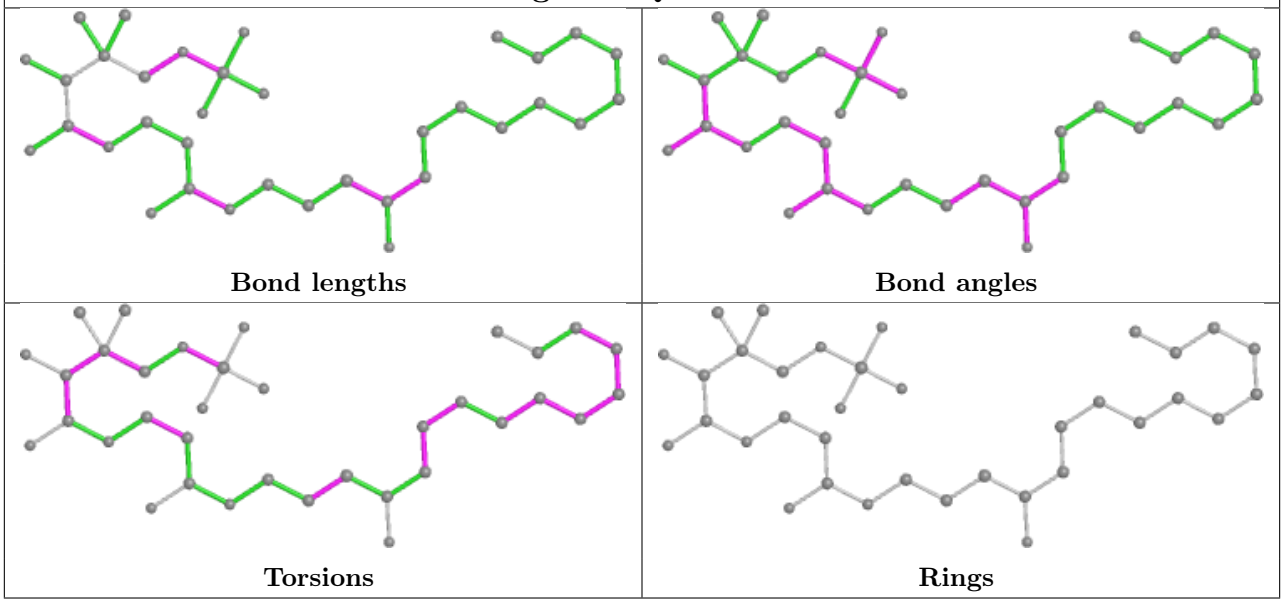


Torsions

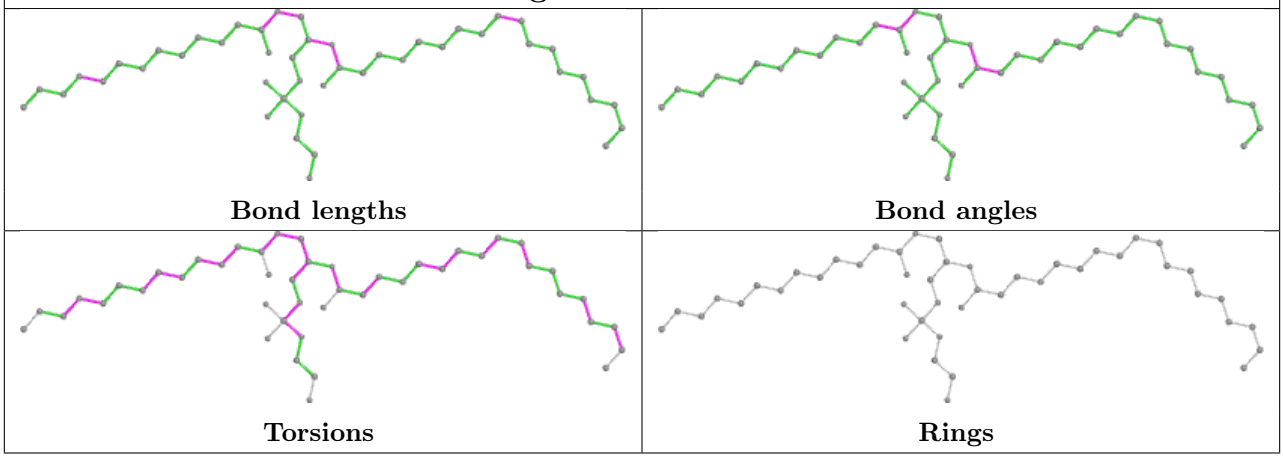


Rings

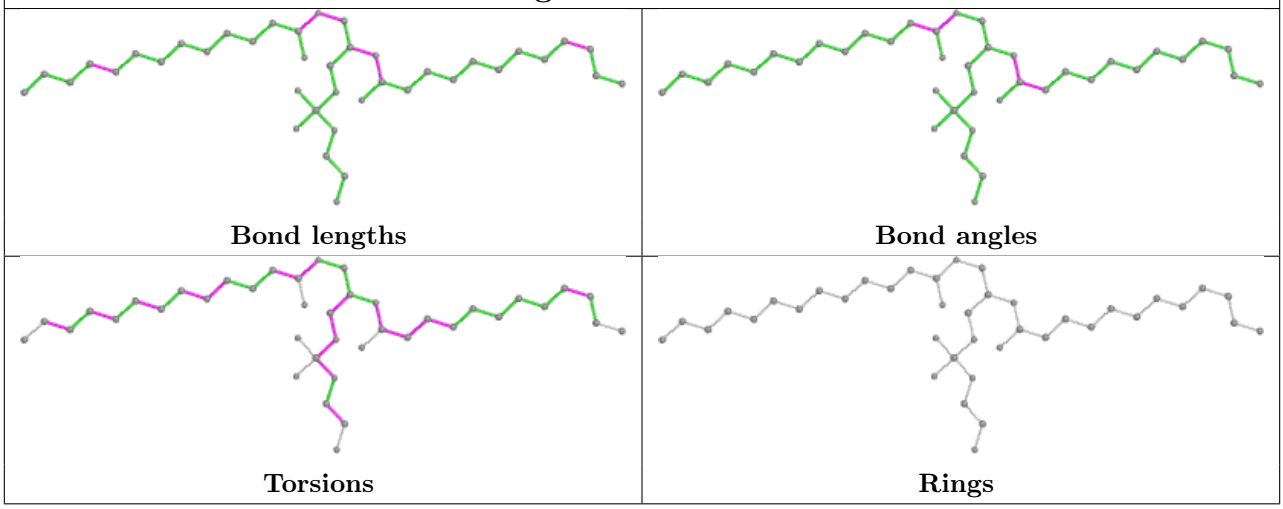
Ligand 8Q1 E 201



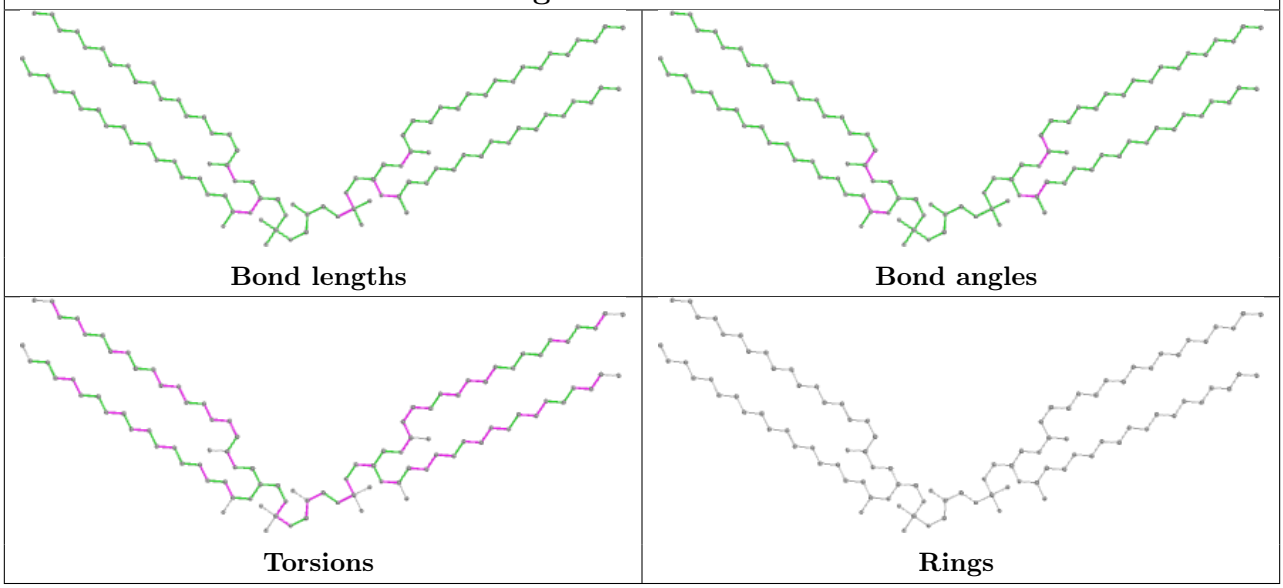
Ligand PEE b 201



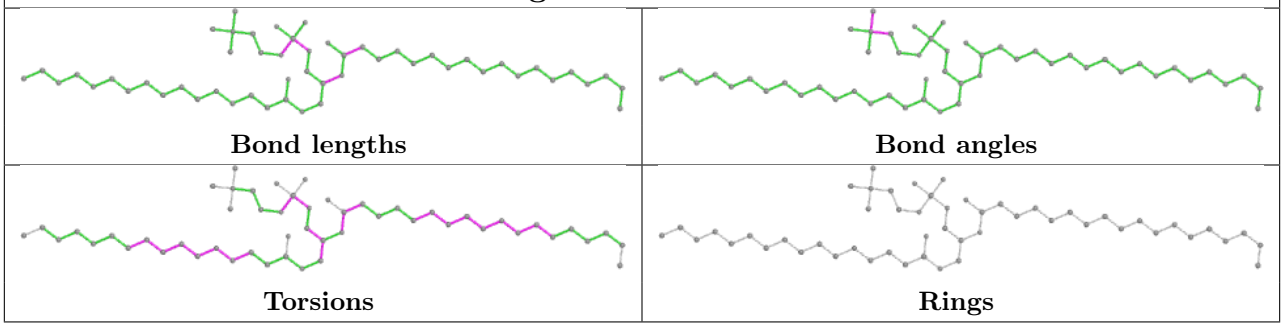
Ligand PEE l 701



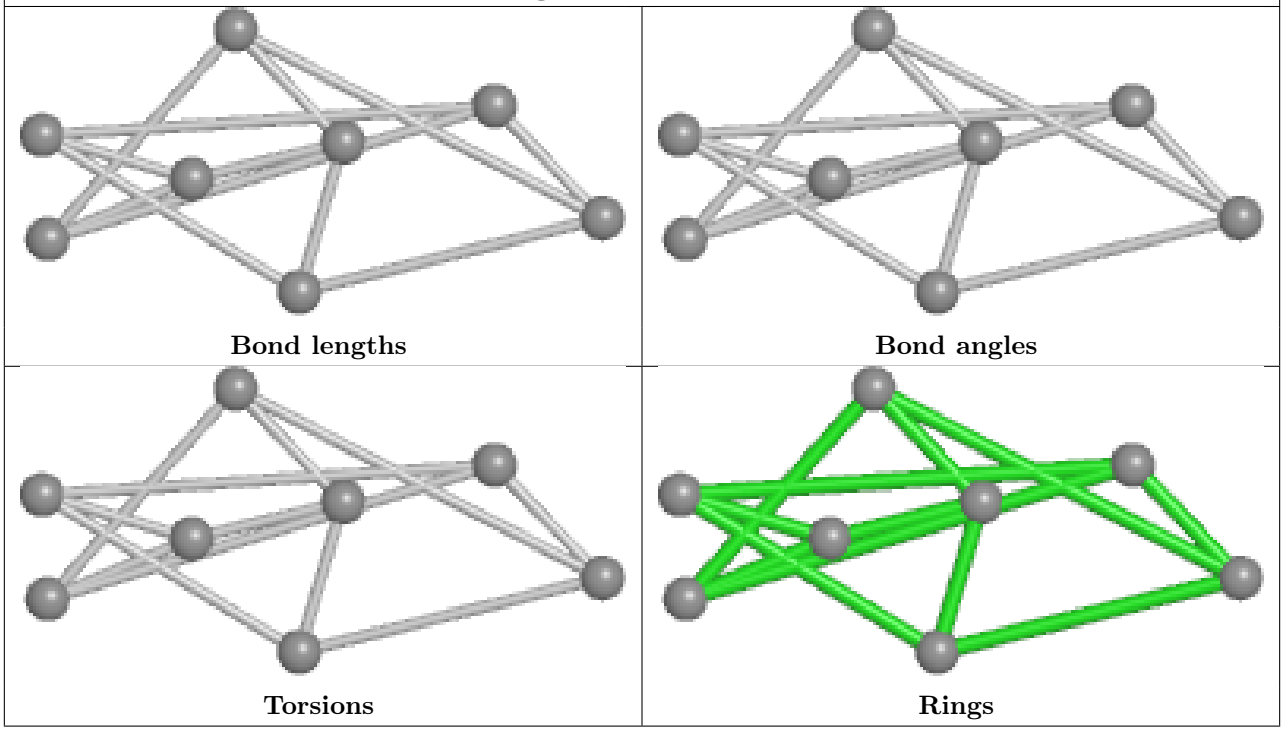
Ligand CDL l 702



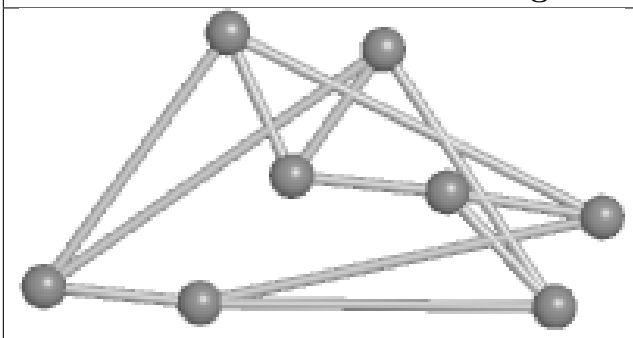
Ligand PLX n 101



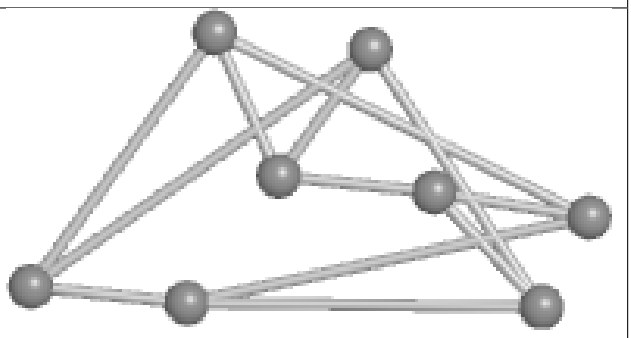
Ligand SF4 B 301



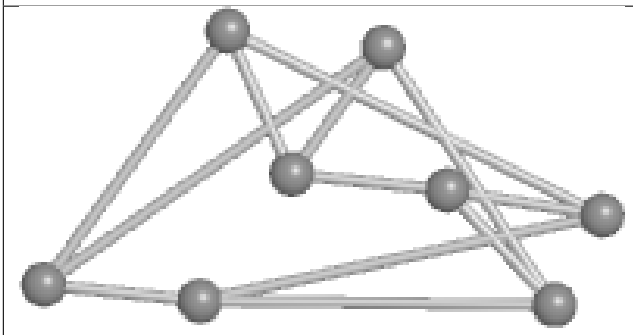
Ligand SF4 A 501



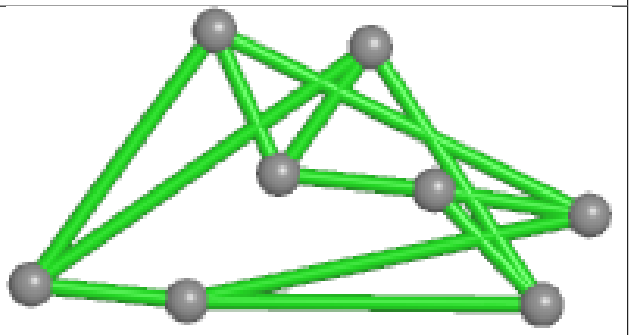
Bond lengths



Bond angles

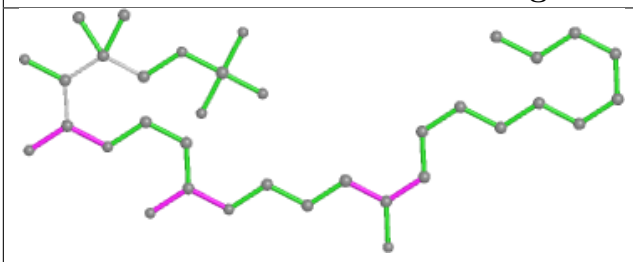


Torsions

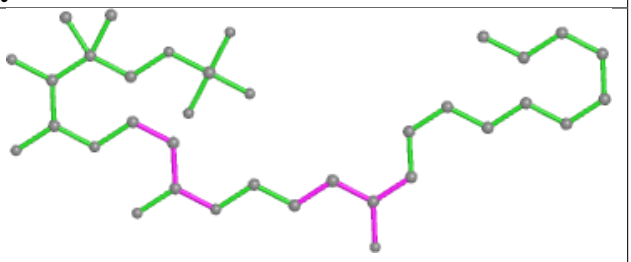


Rings

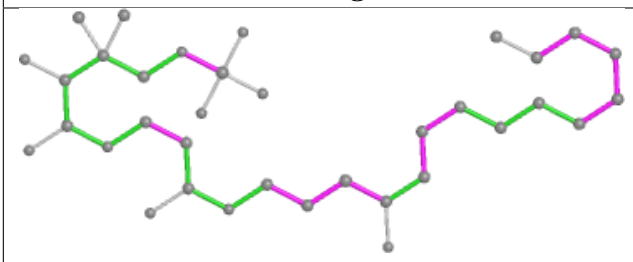
Ligand 8Q1 X 201



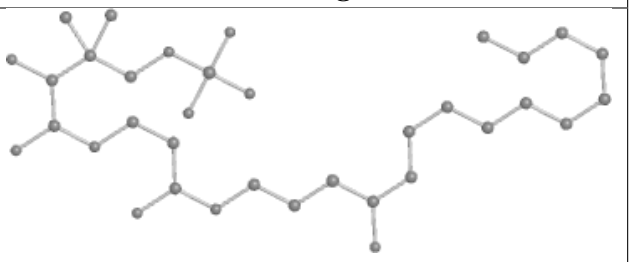
Bond lengths



Bond angles

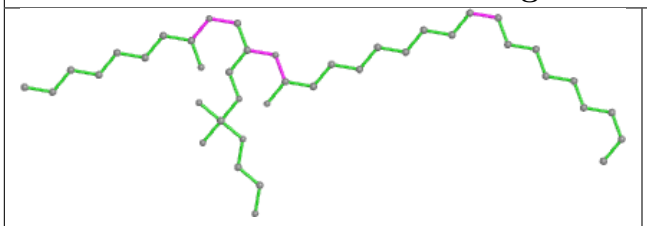


Torsions

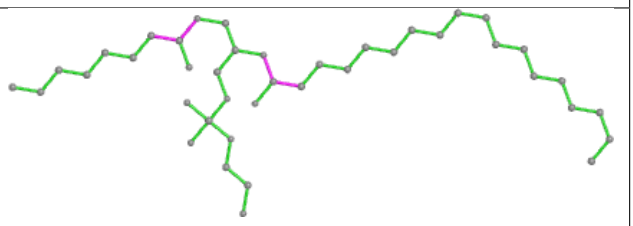


Rings

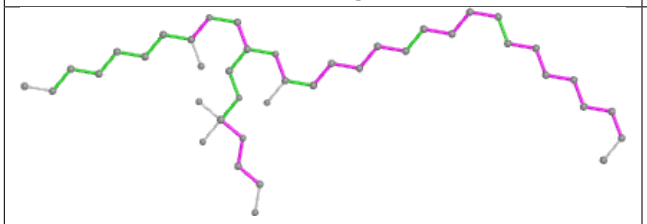
Ligand PEE W 201



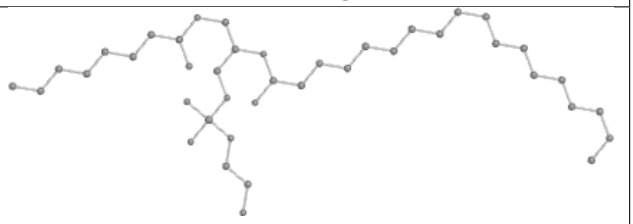
Bond lengths



Bond angles

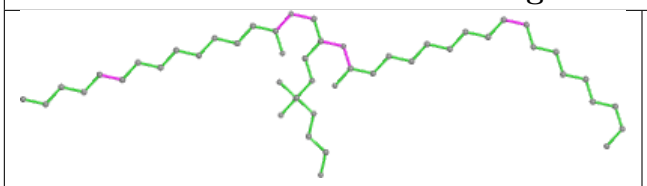


Torsions

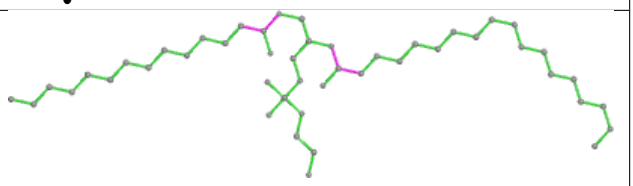


Rings

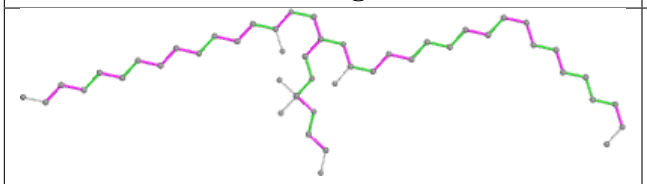
Ligand PEE Q 501



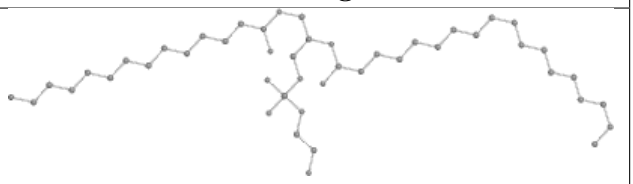
Bond lengths



Bond angles

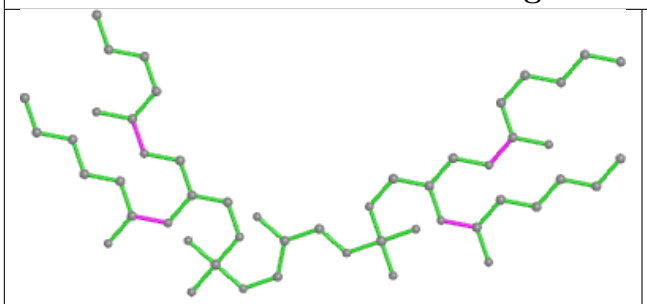


Torsions



Rings

Ligand CDL N 202



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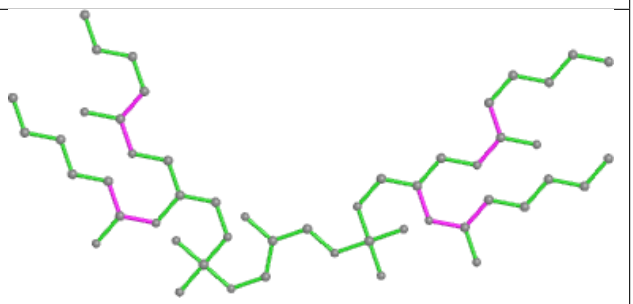
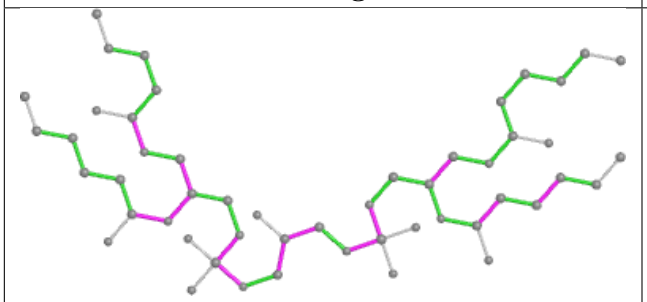
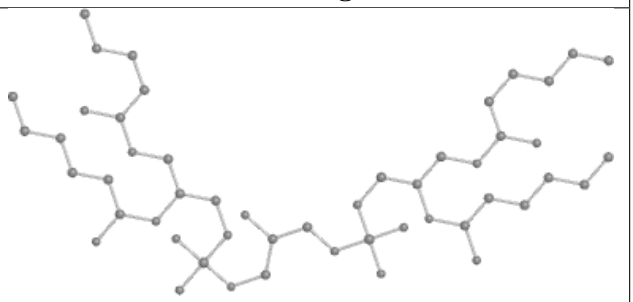


Bond angles

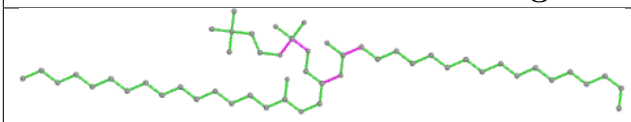


Torsions



Rings

Ligand PLX r 503



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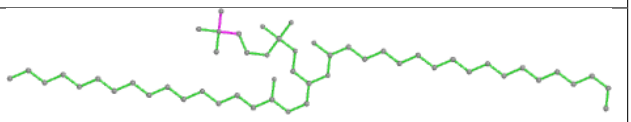
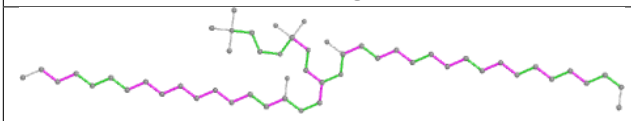


Bond angles



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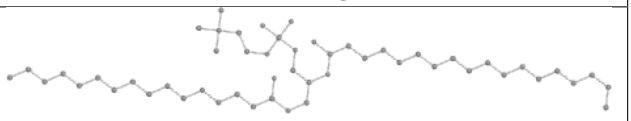
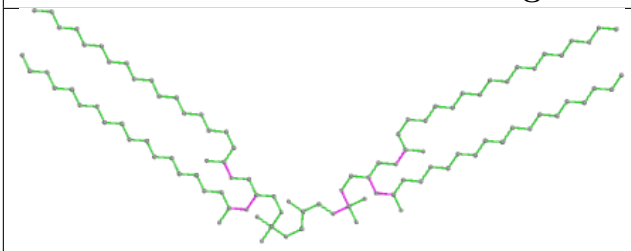


Rings

Ligand CDL V 202



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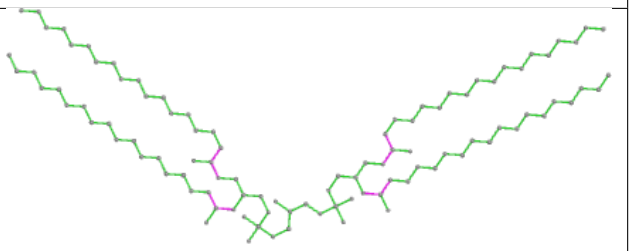

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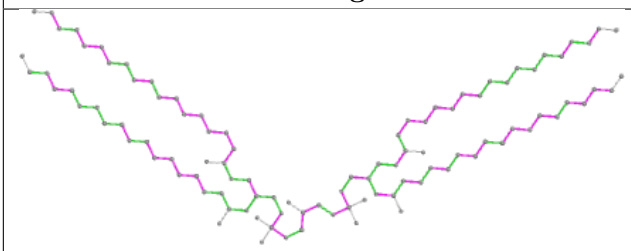

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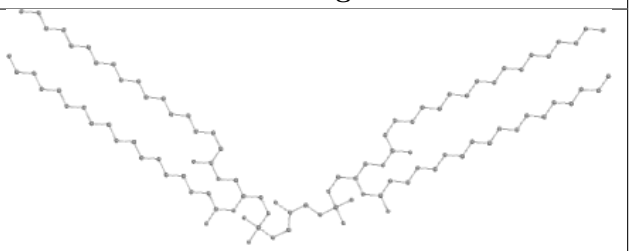
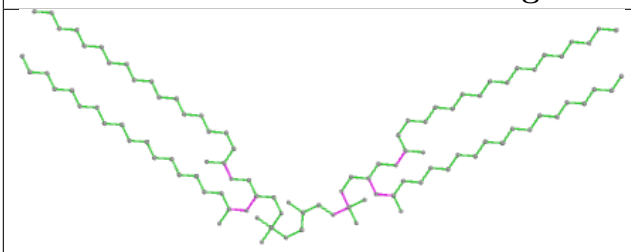


Rings

Ligand CDL m 201



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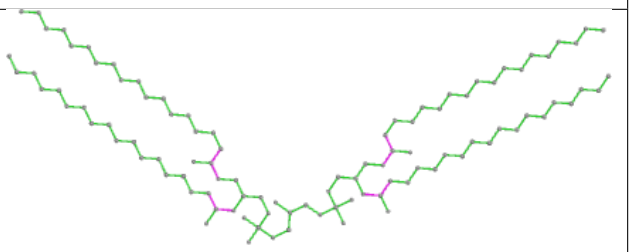

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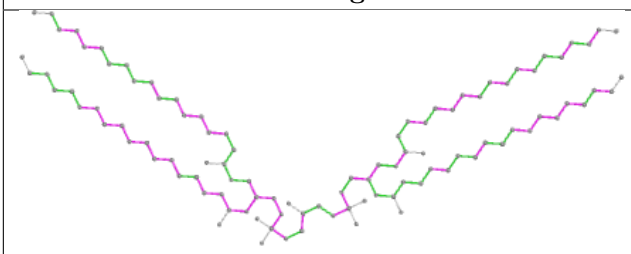

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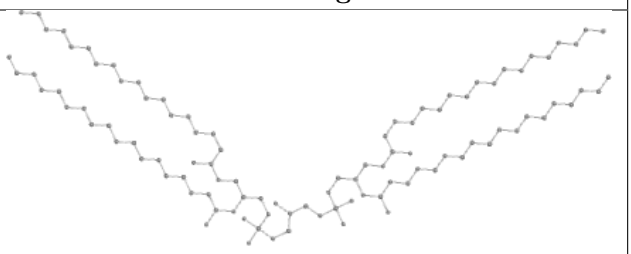
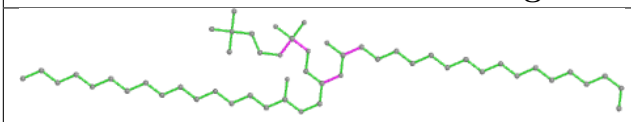


Rings

Ligand PLX N 201



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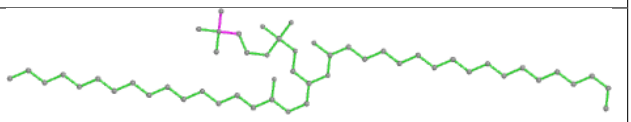

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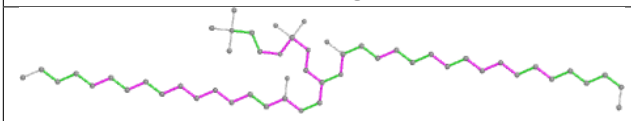

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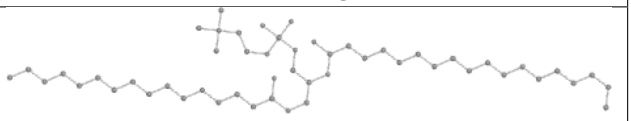
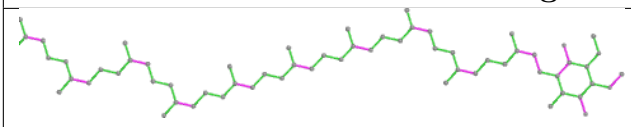


Rings

Ligand UQ s 501



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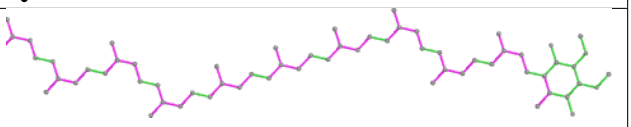
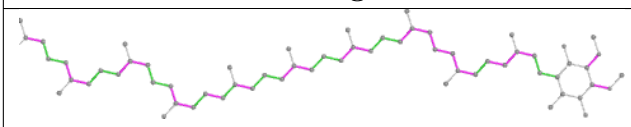


Bond angles



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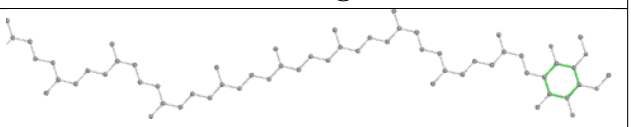
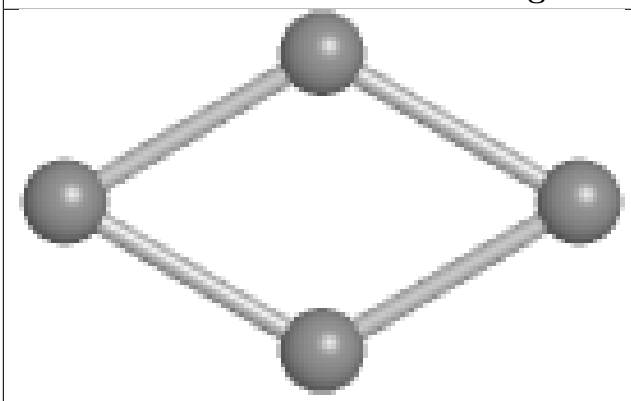


Rings

Ligand FES O 301



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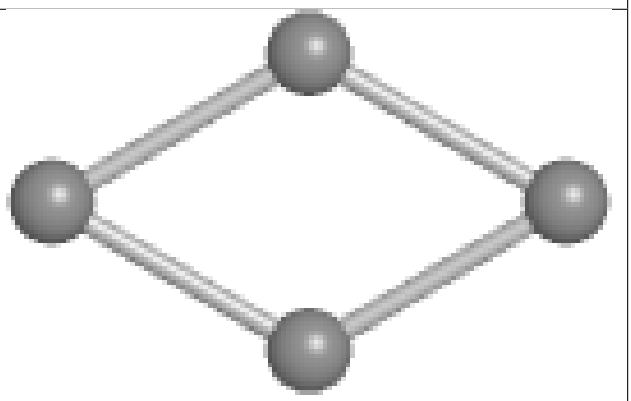

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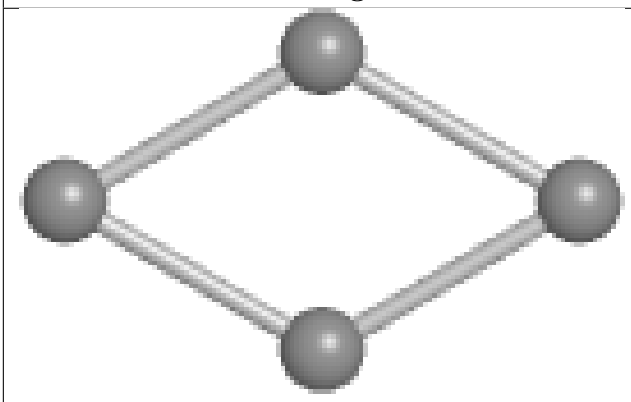

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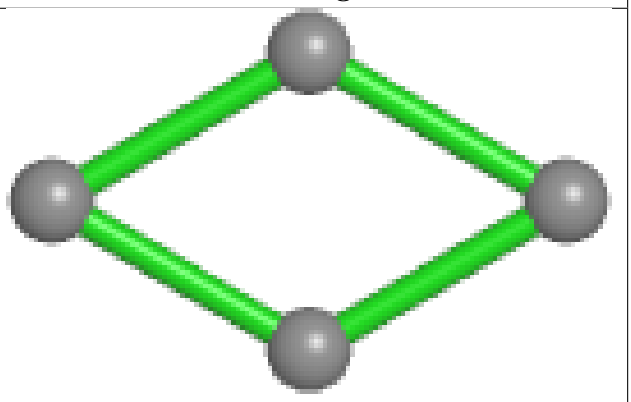
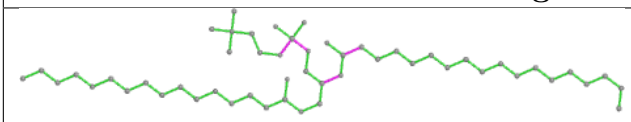


Rings

Ligand PLX j 203



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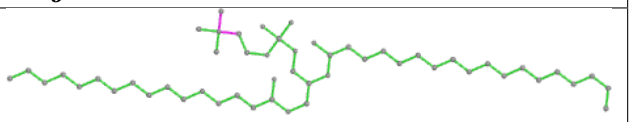

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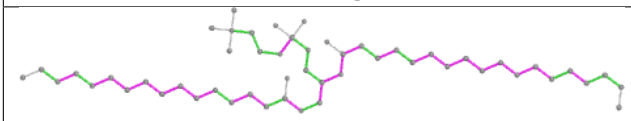

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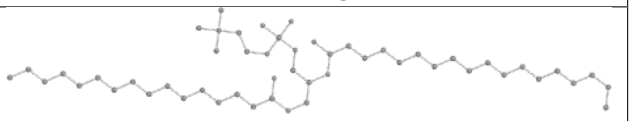
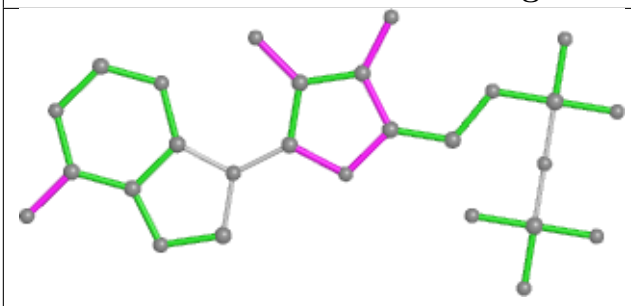
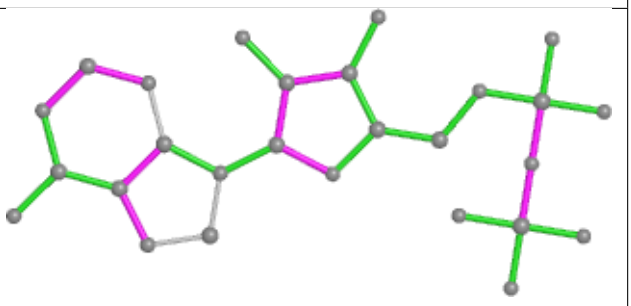


Rings

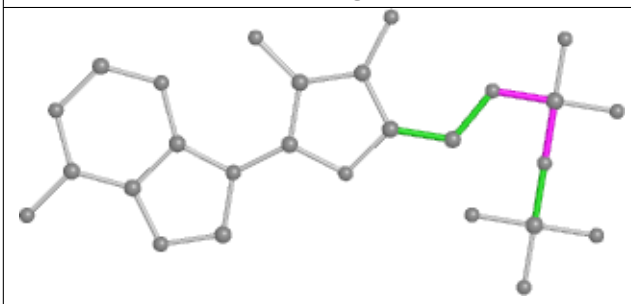
Ligand ADP w 401



Bond lengths



Bond angles



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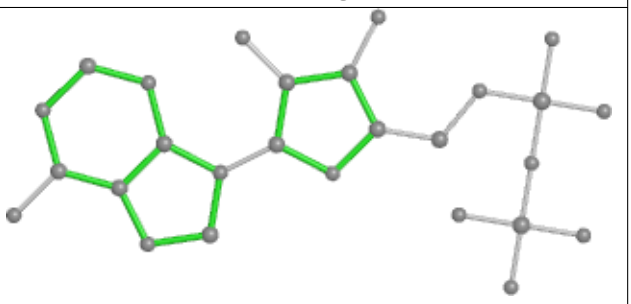
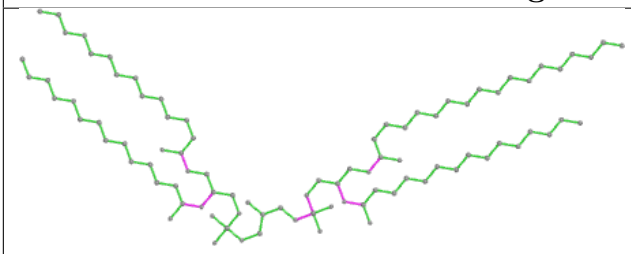


Rings

Ligand CDL J 404



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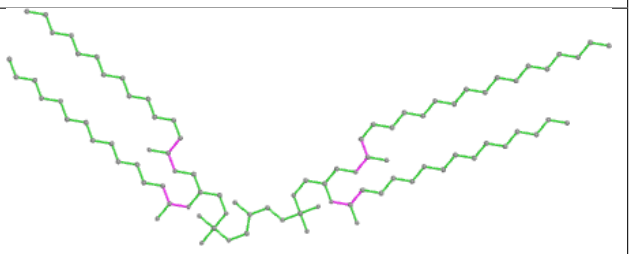
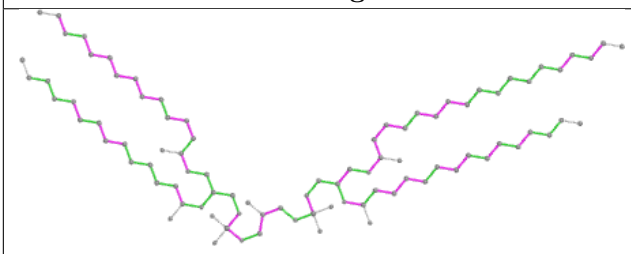


Bond angles



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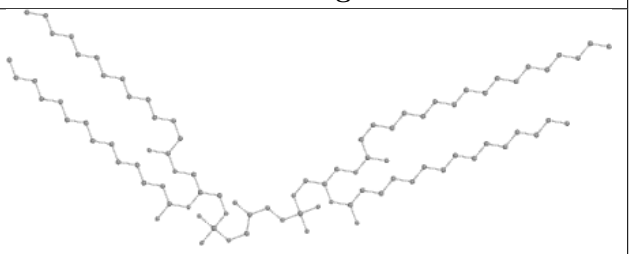
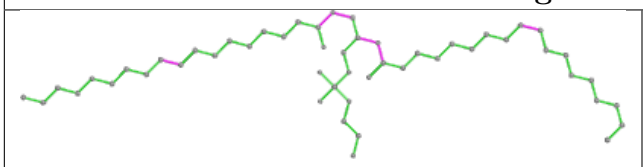
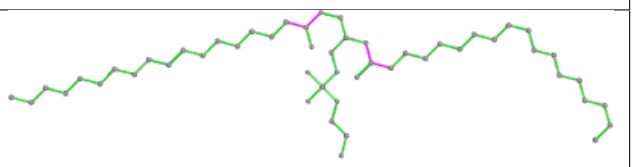
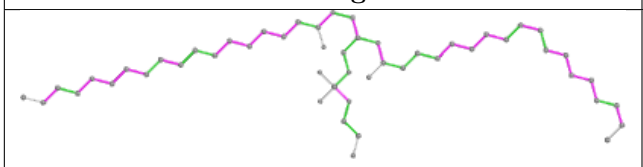
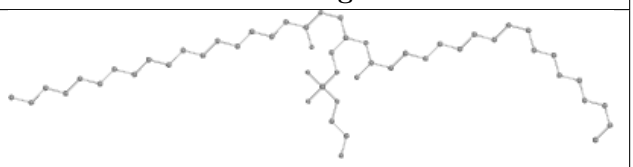
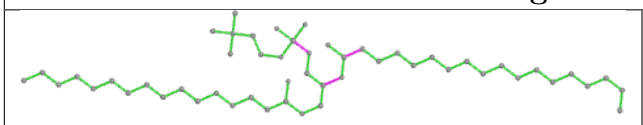
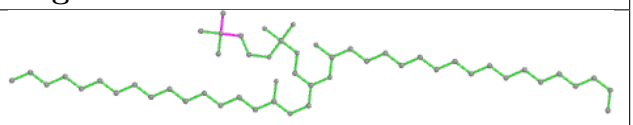
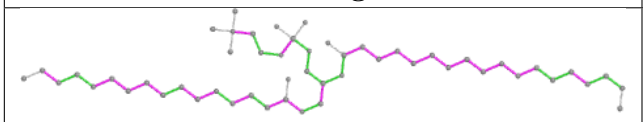
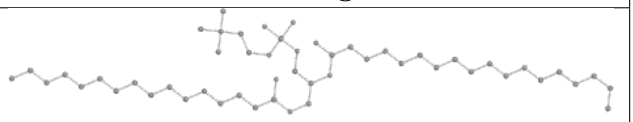
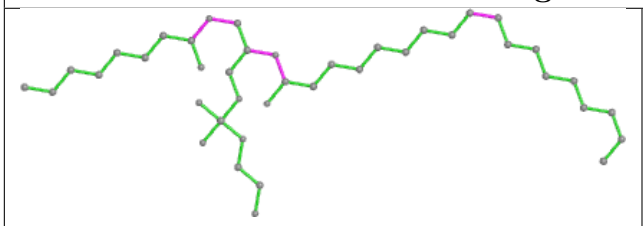
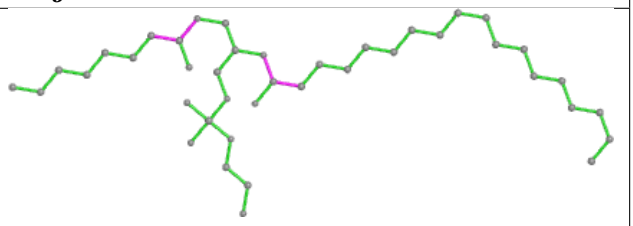
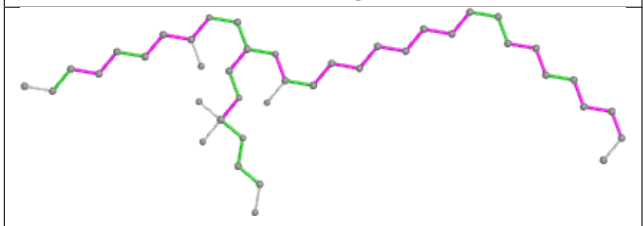
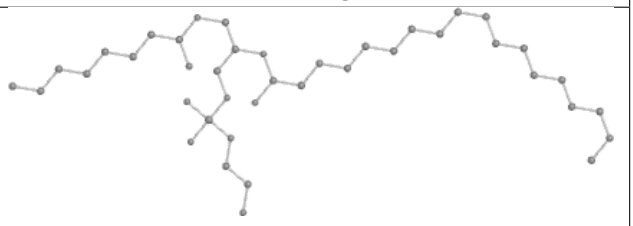


Rings

Ligand PEE l 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX g 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE j 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

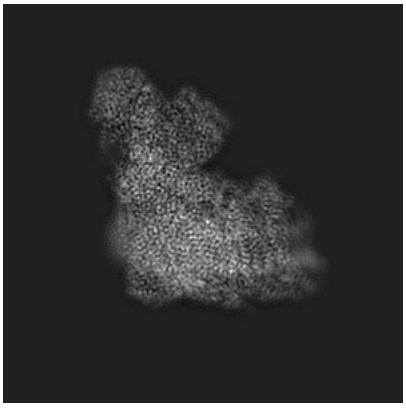
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31640. These allow visual inspection of the internal detail of the map and identification of artifacts.

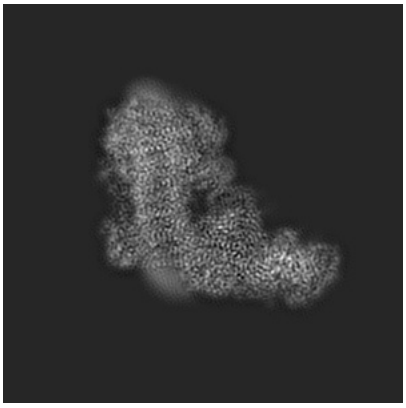
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

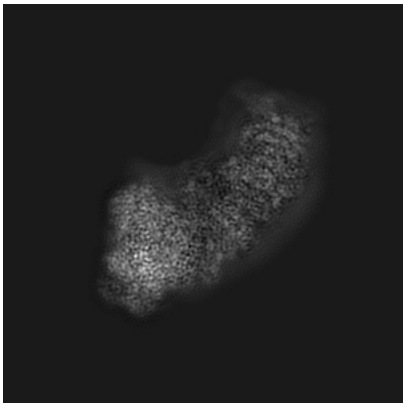
6.1.1 Primary map



X



Y

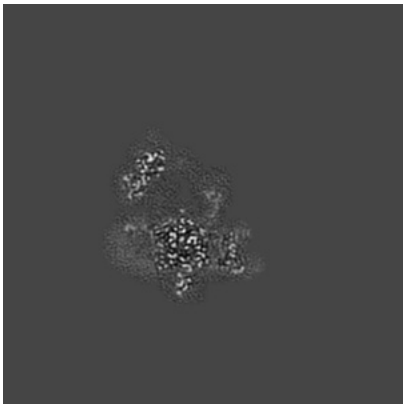


Z

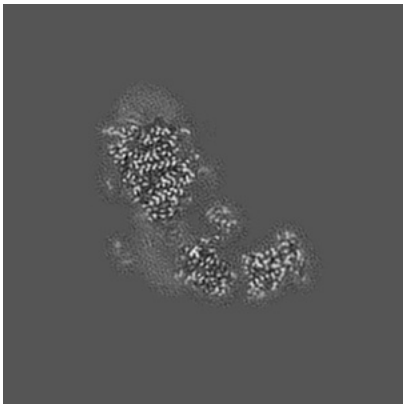
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

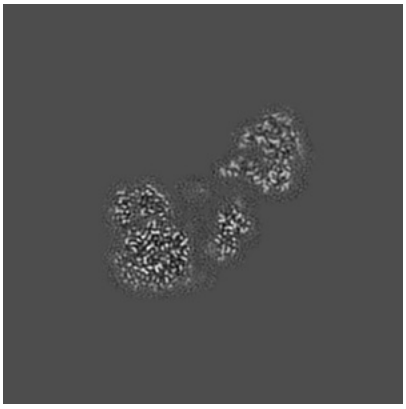
6.2.1 Primary map



X Index: 165



Y Index: 165

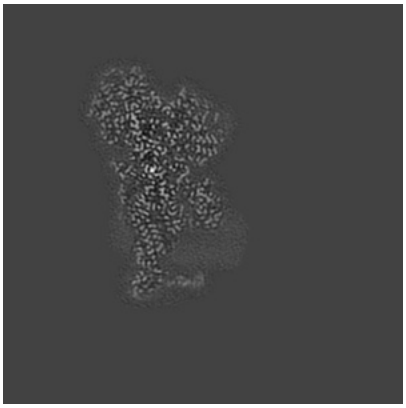


Z Index: 165

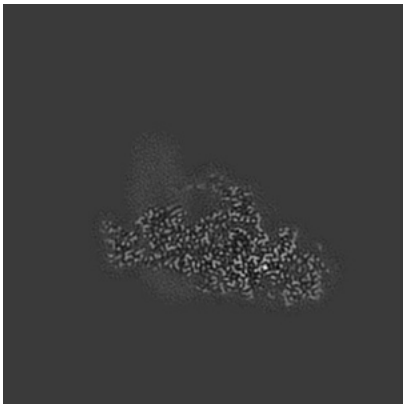
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

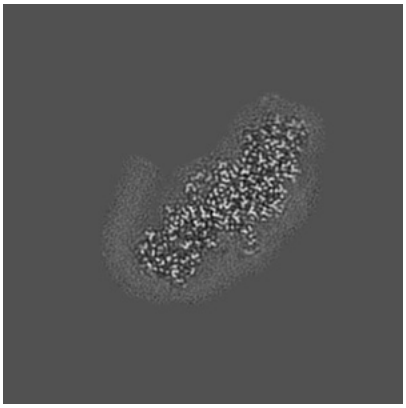
6.3.1 Primary map



X Index: 116



Y Index: 118

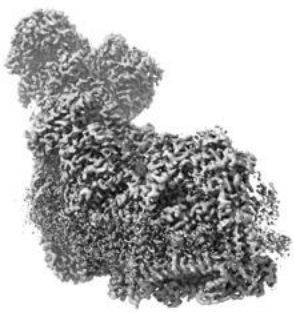


Z Index: 136

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

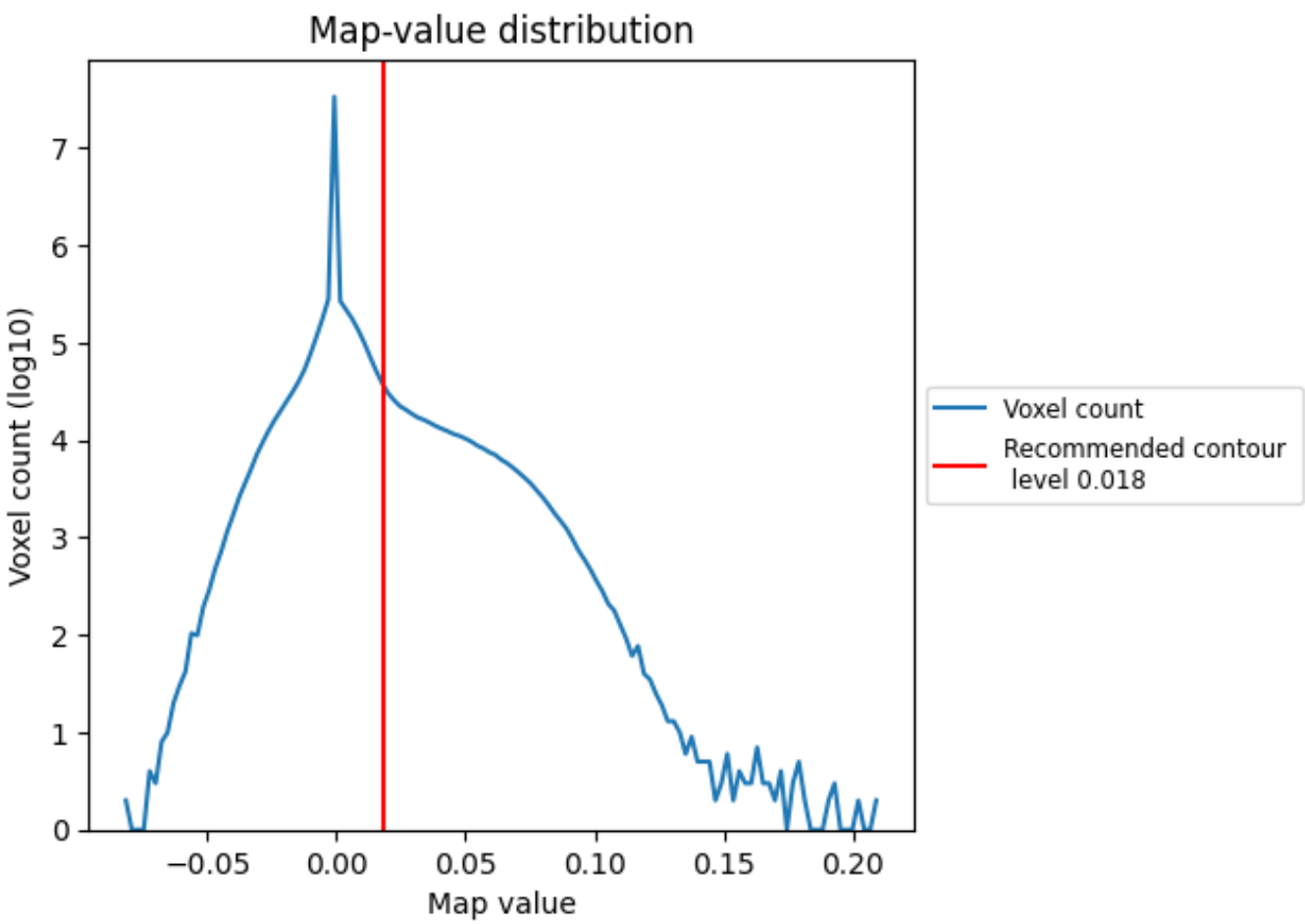
6.5 Mask visualisation (i)

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

7 Map analysis (i)

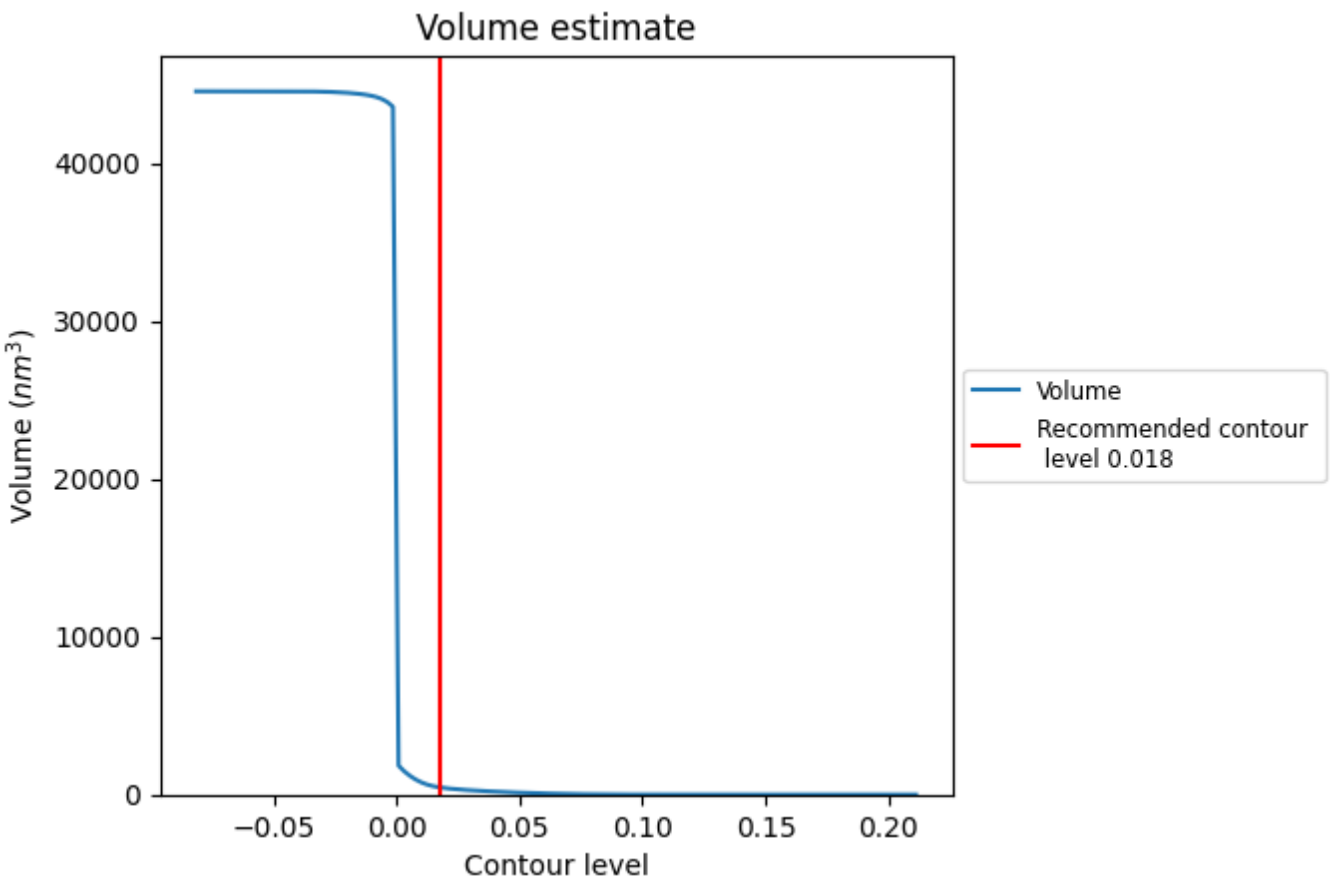
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

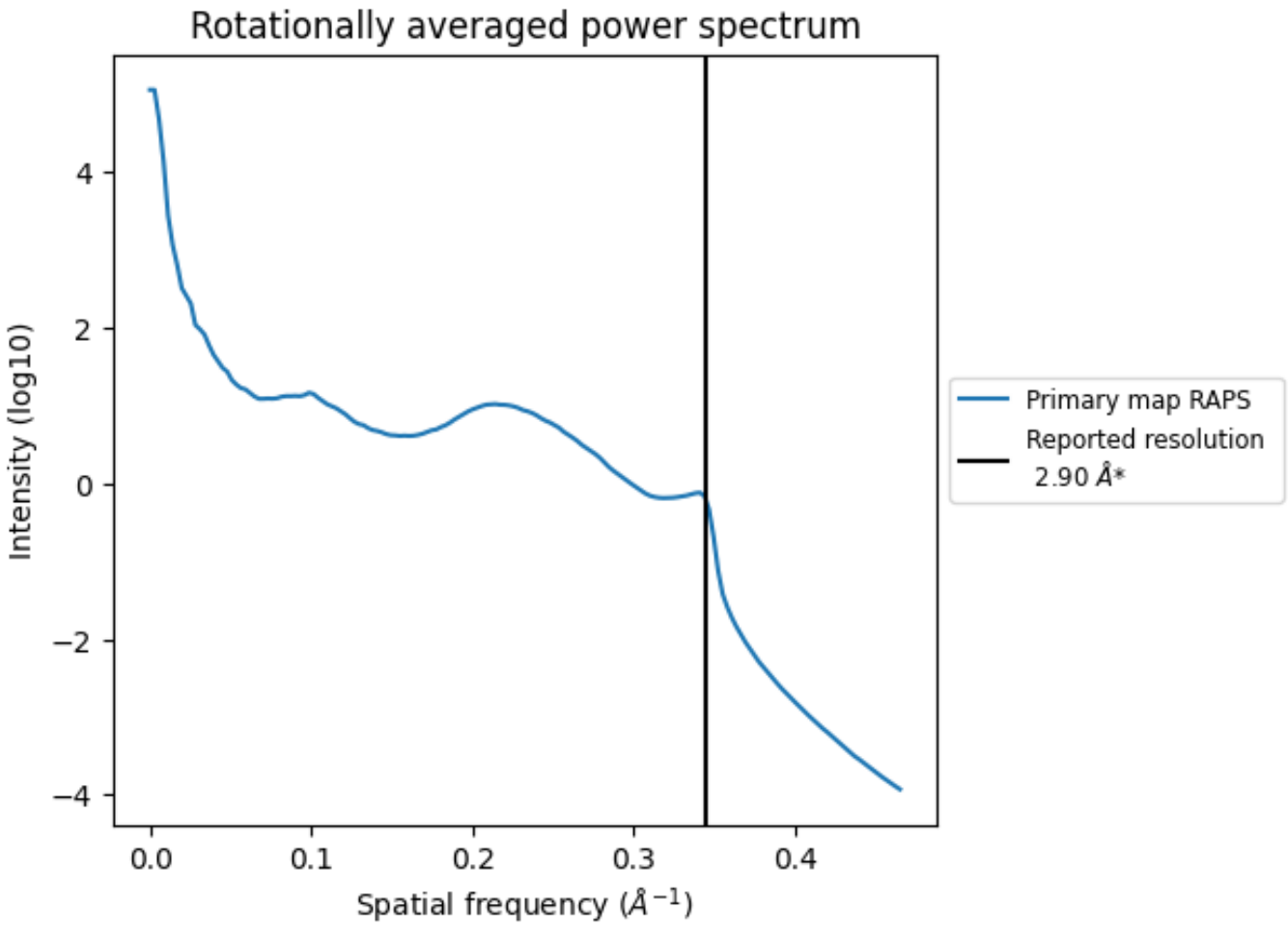
7.2 Volume estimate (i)



The volume at the recommended contour level is 447 nm^3; this corresponds to an approximate mass of 404 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}

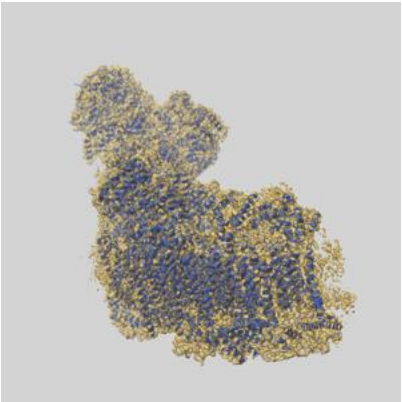
8 Fourier-Shell correlation (i)

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

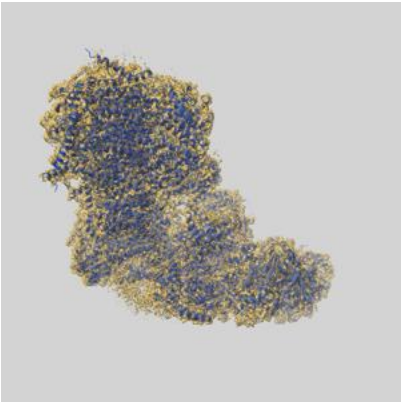
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31640 and PDB model 7V2C. Per-residue inclusion information can be found in section 3 on page 20.

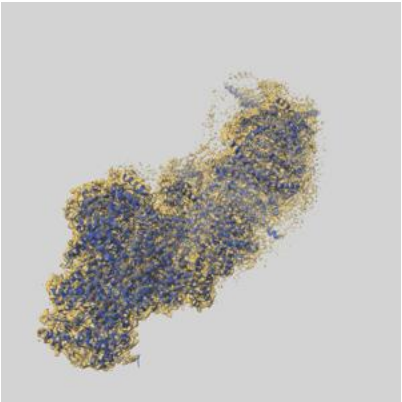
9.1 Map-model overlay (i)



X



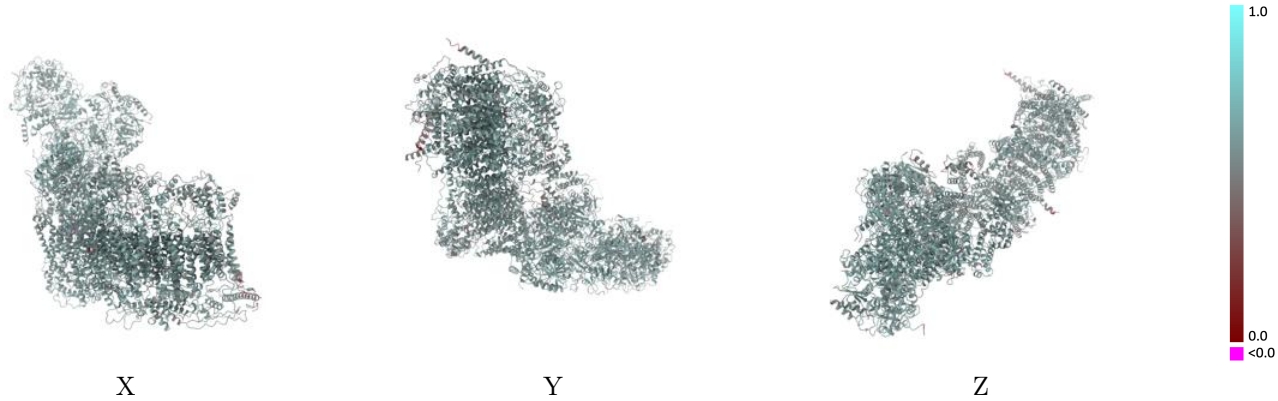
Y



Z

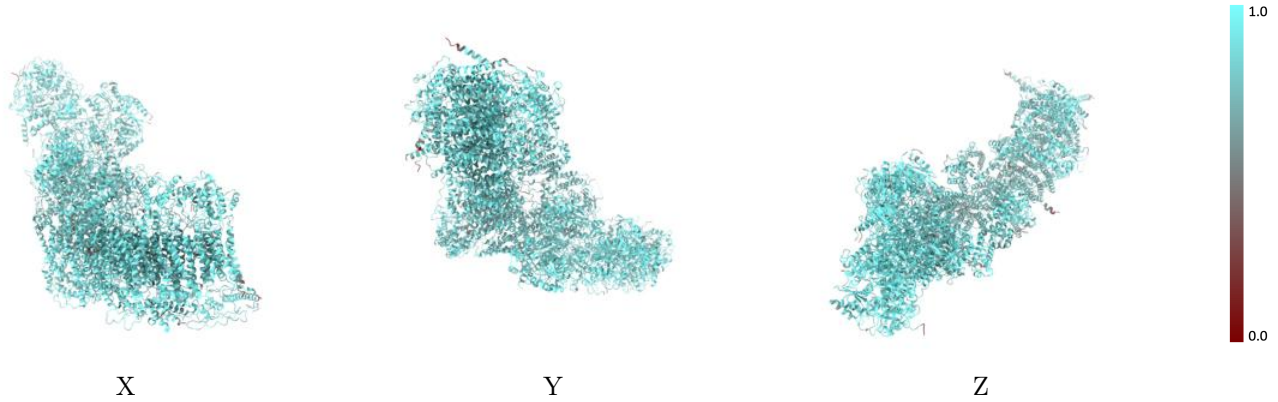
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



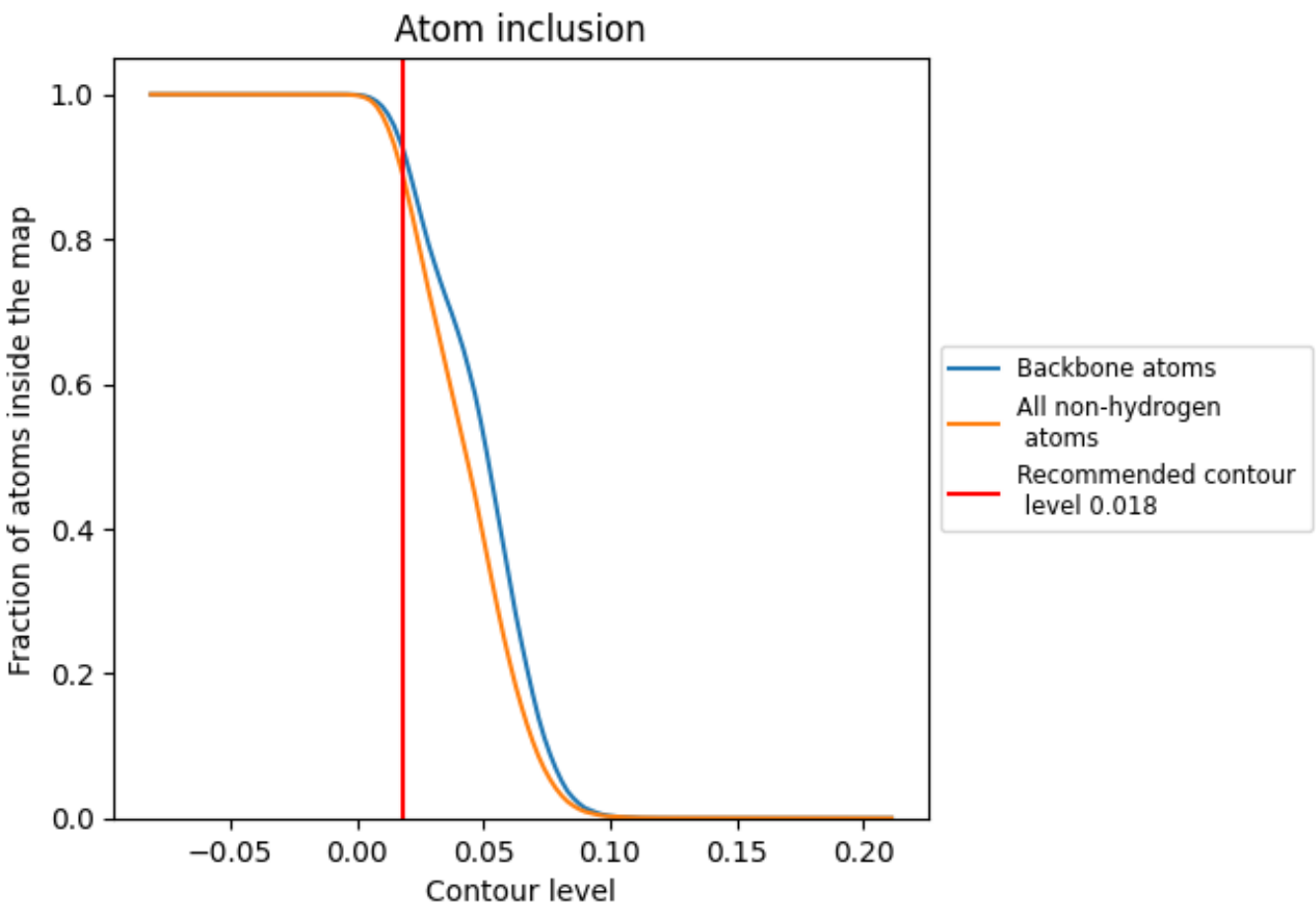
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8903	0.5780
A	0.9132	0.5780
B	0.9528	0.6110
C	0.9441	0.6120
E	0.8936	0.5840
F	0.8578	0.5310
G	0.7427	0.4670
H	0.8983	0.5710
I	0.8294	0.5600
J	0.9065	0.5930
K	0.8873	0.5600
L	0.9034	0.5970
M	0.9220	0.5900
N	0.8241	0.5740
O	0.8945	0.5680
P	0.9450	0.6160
Q	0.9387	0.6080
S	0.9312	0.5880
T	0.8947	0.5910
U	0.8998	0.5730
V	0.8050	0.5580
W	0.8964	0.5690
X	0.8382	0.5260
Y	0.8401	0.5310
Z	0.7792	0.5190
a	0.8875	0.5860
b	0.8476	0.5440
c	0.8726	0.5660
d	0.8481	0.5480
e	0.8322	0.5510
f	0.7838	0.5260
g	0.8952	0.5820
h	0.8759	0.5600
i	0.9212	0.5940
j	0.8770	0.5950

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Chain	Atom inclusion	Q-score
k	0.9164	0.5940
l	0.8797	0.5790
m	0.8401	0.5590
n	0.7868	0.5380
o	0.8678	0.5650
p	0.8835	0.5660
r	0.9049	0.5940
s	0.9187	0.5960
u	0.9015	0.5790
v	0.8338	0.5210
w	0.8766	0.5640