



Full wwPDB EM Validation Report ⓘ

Jan 25, 2023 – 12:34 PM JST

PDB ID : 7W4E
EMDB ID : EMD-32302
Title : Active state CI from Q1-NADH dataset, Subclass 3
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-27
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

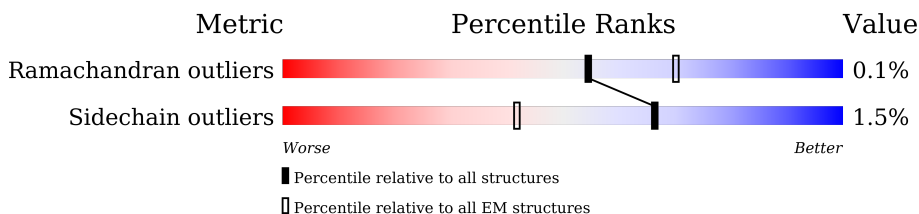
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



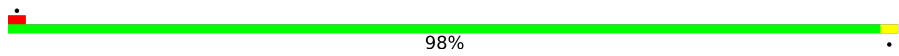
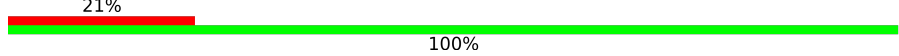
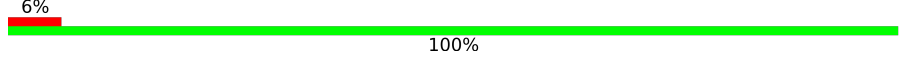
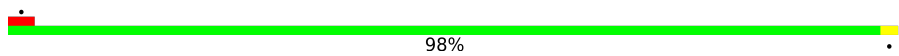
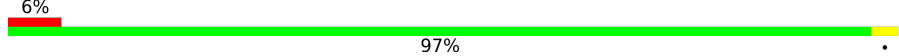
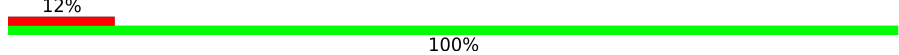

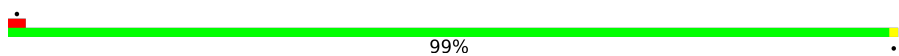


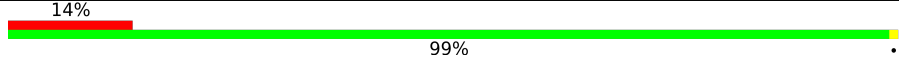
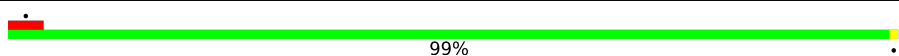
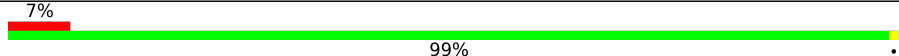
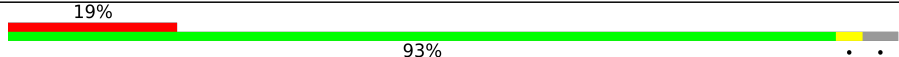
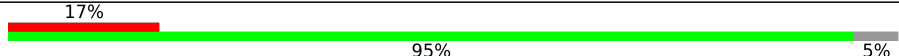
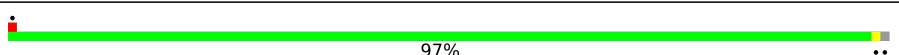
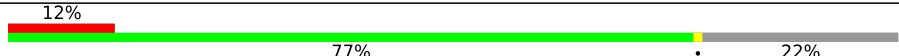
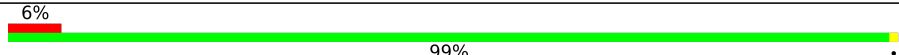
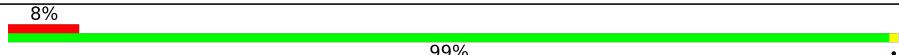
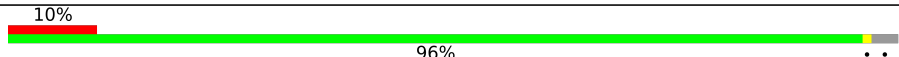
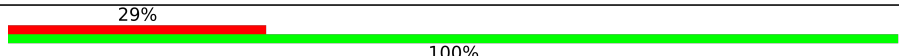
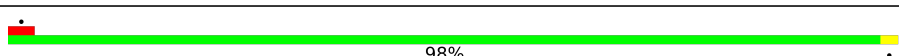
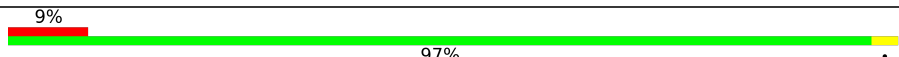
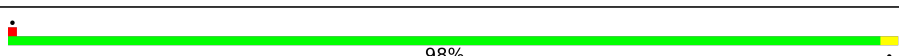
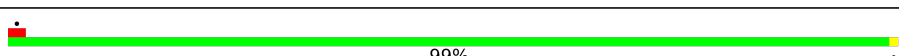
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	

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Mol	Chain	Length	Quality of chain
9	J	342	 98%
10	K	43	 21% 100%
11	L	125	 6% 100%
12	M	690	 98%
13	N	144	 6% 97%
14	O	217	 12% 100%
15	P	208	 100%
16	Q	430	 99%
17	S	70	 100%
18	T	96	 7% 100%
19	U	83	 14% 99%
20	V	140	 99%
21	W	142	 7% 99%
22	Y	70	 19% 93%
23	Z	84	 17% 95% 5%
24	a	140	 97%
25	b	126	 12% 77% 22%
26	c	156	 6% 99%
27	d	175	 8% 99%
28	e	107	 10% 96%
29	f	49	 29% 100%
30	g	122	 98%
31	h	105	 9% 97%
32	i	347	 98%
33	j	115	 99%

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Mol	Chain	Length	Quality of chain
34	k	98	 97%
35	l	606	 98%
36	m	175	 99%
37	n	56	 100%
38	o	128	 100%
39	p	178	 98%
40	r	459	 98%
41	s	318	 99%
42	u	171	 98%
43	v	125	 99%
44	w	320	 99%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68197 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	3327	2102	593	612	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	967	616	178	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	676	427	125	122	2	0	0

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			703	453	104	141	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	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

- 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
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1156	747	199	201	9		

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

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

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

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

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

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

- Molecule 25 is a protein called Complex I-B17.

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

- 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	122	1005	653	174	172	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	851	540	159	146	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
33	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1292	863	188	228	13		

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

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

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

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

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

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

- 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	2582	1643	438	491	10	0	0

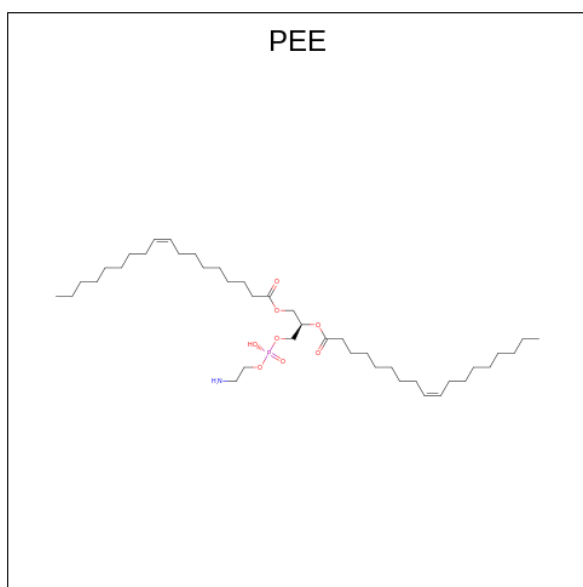
- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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: C₁₇H₂₁N₄O₉P).





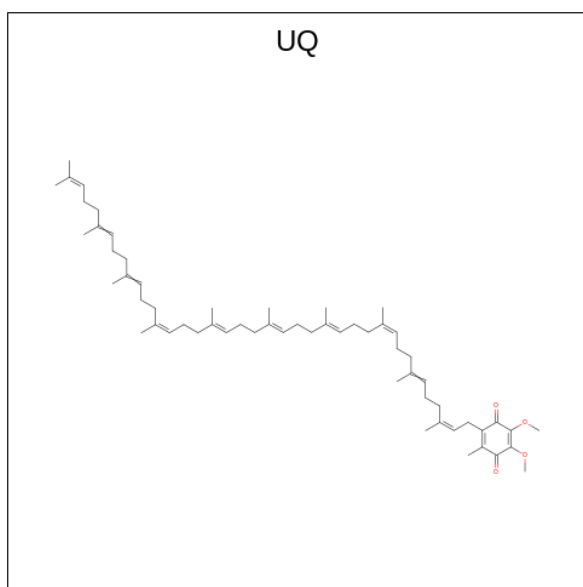
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	51	41	1	8	1	0
48	Q	1	47	37	1	8	1	0
48	V	1	40	30	1	8	1	0
48	W	1	41	31	1	8	1	0
48	j	1	47	37	1	8	1	0
48	l	1	97	77	2	16	2	0
48	l	1	97	77	2	16	2	0
48	r	1	51	41	1	8	1	0
48	s	1	92	72	2	16	2	0
48	s	1	92	72	2	16	2	0

- Molecule 49 is (9R,11S)-9-((1S)-1-HYDROXYHEXADECYL)OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOX (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P).



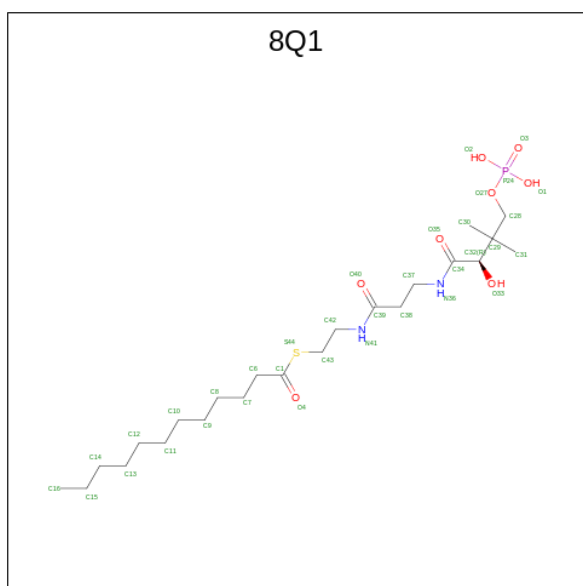
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	52	42	1	8	1	0
49	a	1	52	42	1	8	1	0
49	g	1	52	42	1	8	1	0
49	j	1	52	42	1	8	1	0
49	m	1	52	42	1	8	1	0
49	r	1	104	84	2	16	2	0
49	r	1	104	84	2	16	2	0

- Molecule 50 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	C	1	38	34	4	0
50	J	1	33	29	4	0

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



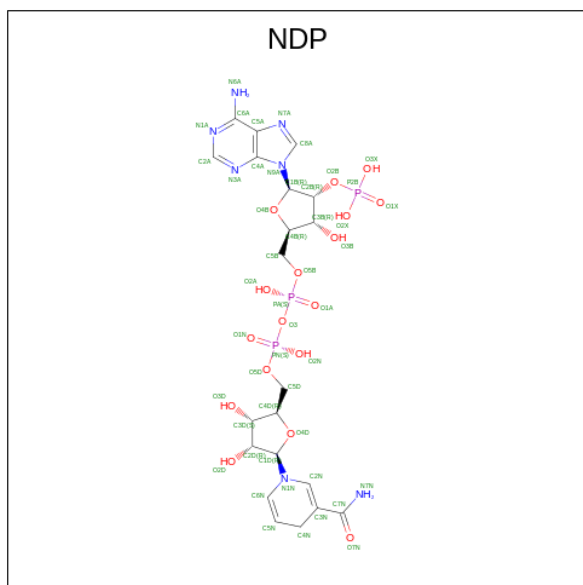
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
51	G	1	35	23	2	8	1	1	0

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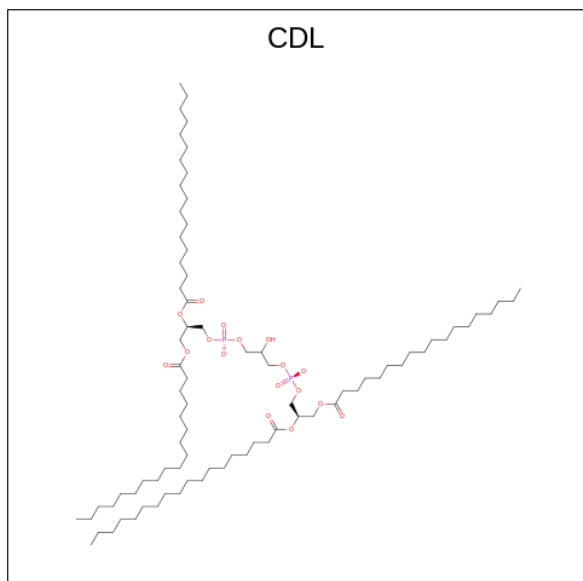
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
51	X	1	35	23	2	8	1	1	0

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



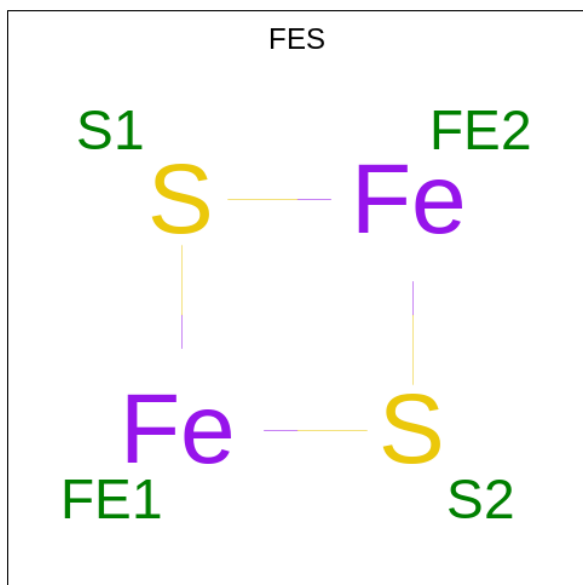
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	J	1	48	21	7	17	3	0

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	J	1	Total 89	C 70	O 17	P 2	0
53	S	1	Total 51	C 32	O 17	P 2	0
53	V	1	Total 288	C 231	O 51	P 6	0
53	V	1	Total 288	C 231	O 51	P 6	0
53	V	1	Total 288	C 231	O 51	P 6	0
53	a	1	Total 100	C 81	O 17	P 2	0
53	l	1	Total 199	C 161	O 34	P 4	0
53	l	1	Total 199	C 161	O 34	P 4	0
53	r	1	Total 100	C 81	O 17	P 2	0
53	u	1	Total 55	C 36	O 17	P 2	0

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

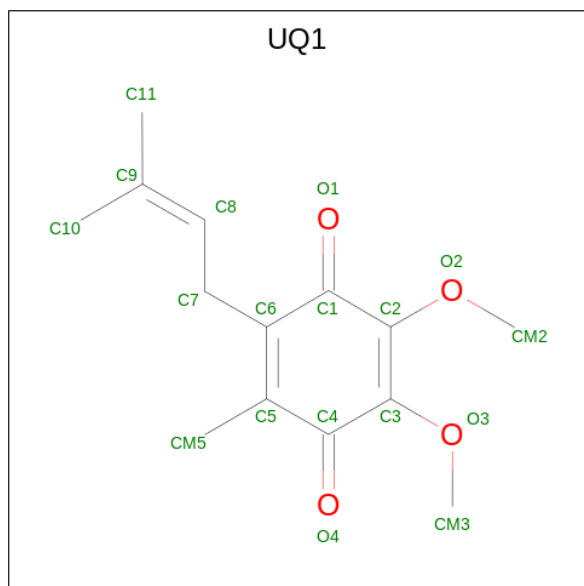


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
54	M	1	Total 4	Fe 2	S 2	0
54	O	1	Total 4	Fe 2	S 2	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 56 is UBIQUINONE-1 (three-letter code: UQ1) (formula: C₁₄H₁₈O₄).



Mol	Chain	Residues	Atoms			AltConf
56	Q	1	Total	C	O	0
			18	14	4	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

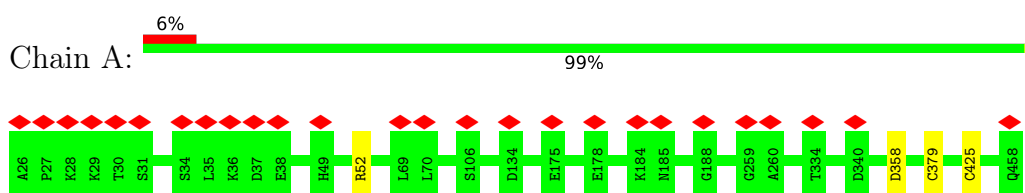
Mol	Chain	Residues	Atoms		AltConf
57	T	1	Total	Zn	0
			1	1	

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

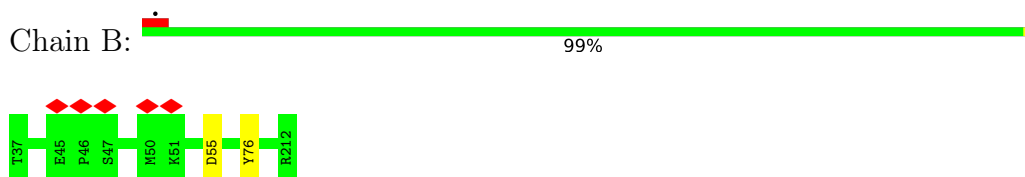
3 Residue-property plots [i](#)

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.

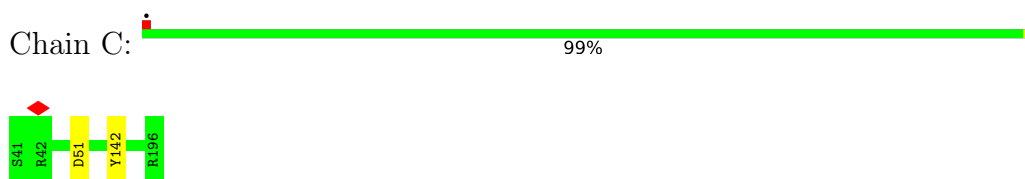
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



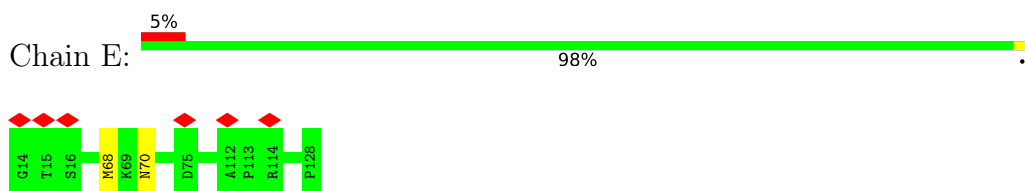
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



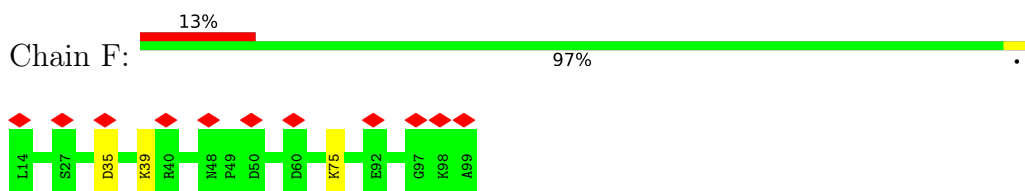
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



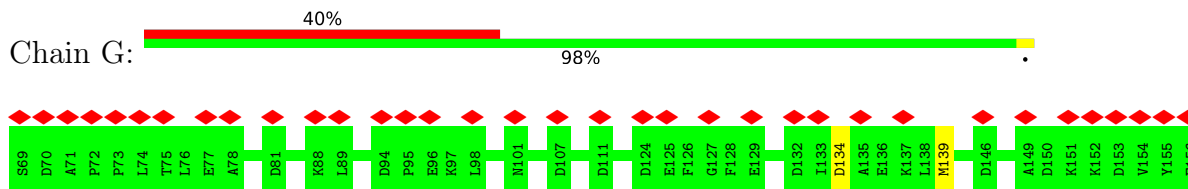
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



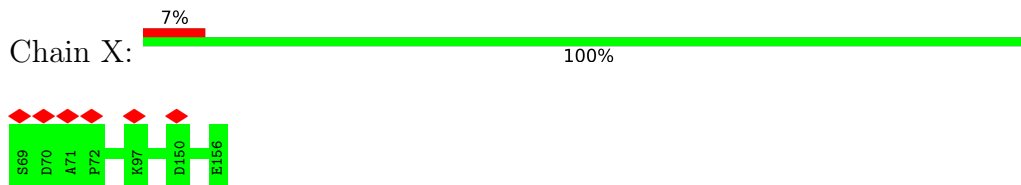
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



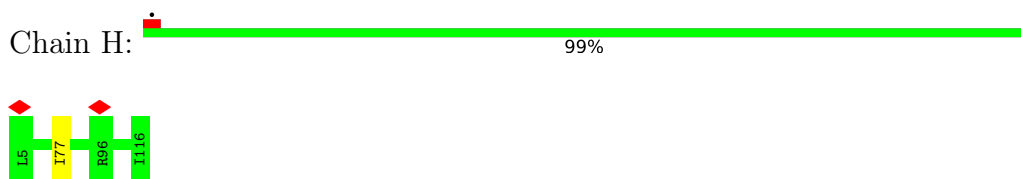
- Molecule 6: Acyl carrier protein



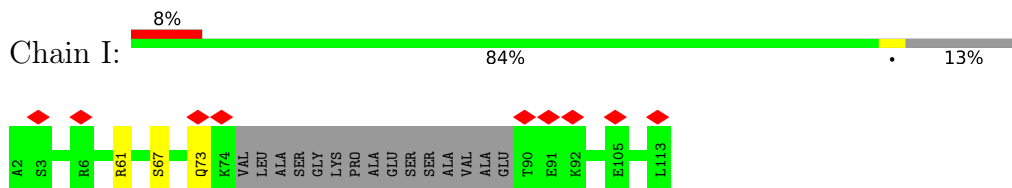
- Molecule 6: Acyl carrier protein



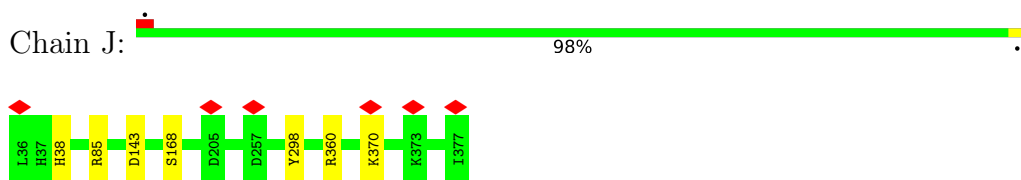
- Molecule 7: Complex I subunit B13



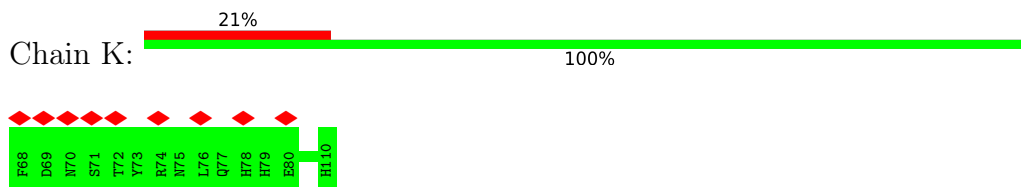
- Molecule 8: Complex I-B14.5a



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

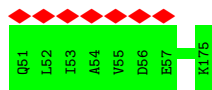


- Molecule 10: Complex I-9kD



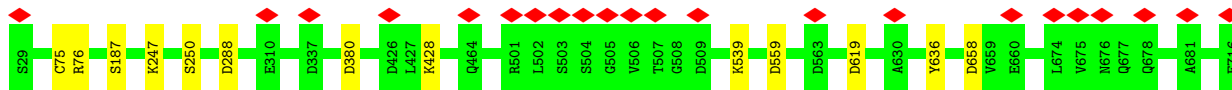
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





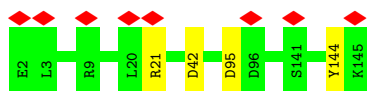
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M: 98%



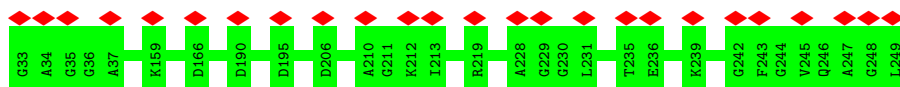
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N: 97%



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

Chain O: 100%



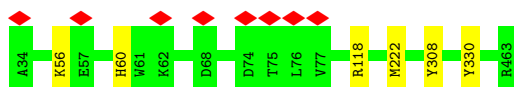
- Molecule 15: Complex I-30kD

Chain P: 100%



- Molecule 16: Complex I-49kD

Chain Q: 99%

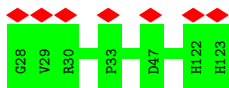


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

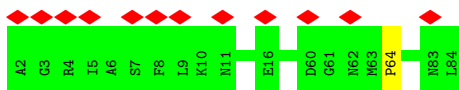
Chain S: 100%



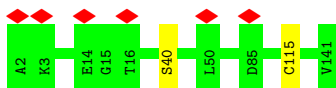
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



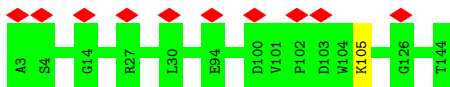
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



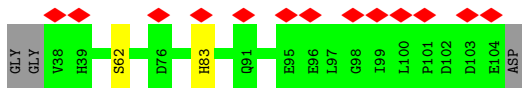
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



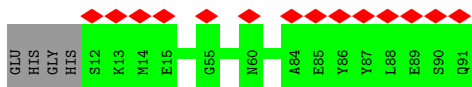
- Molecule 21: Complex I-B16.6



- Molecule 22: Complex I-AGGG

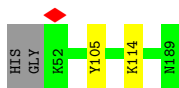


- Molecule 23: Complex I-B12




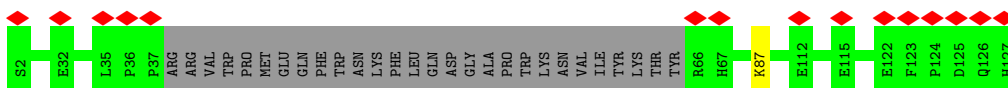
- Molecule 24: Complex I-SGDH

Chain a:  97%



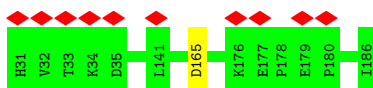
- Molecule 25: Complex I-B17

Chain b:  12% 77% 22%



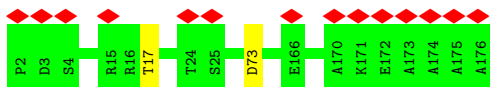
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  6% 99%



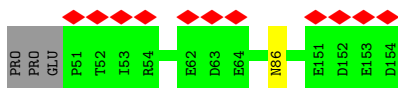
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  8% 99%



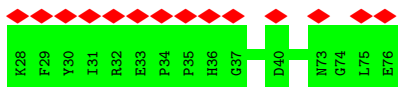
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  10% 96%



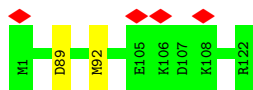
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  29% 100%

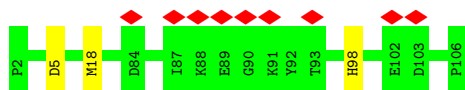


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  98%



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



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



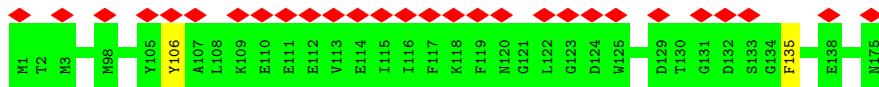
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



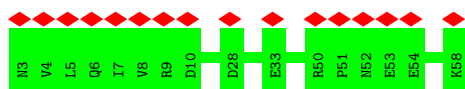
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



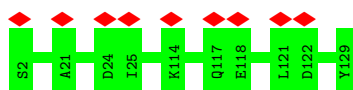
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



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



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



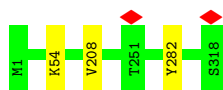
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



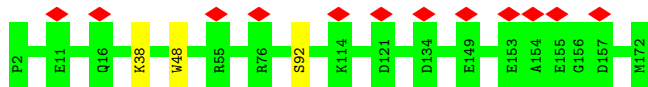
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

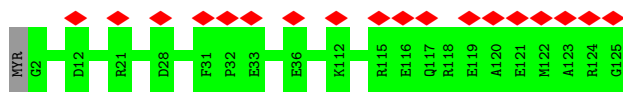


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

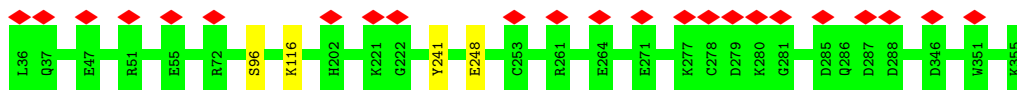


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.226	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0308	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, UQ, 2MR, UQ1, NDP, FES, NAI, SF4, ADP, ZN, FMN, PEE, PLX, 8Q1, MG

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	0/3403	0.50	0/4599
2	B	0.29	0/1443	0.52	0/1952
3	C	0.29	0/1279	0.52	0/1730
4	E	0.27	0/991	0.50	0/1336
5	F	0.25	0/687	0.55	0/927
6	G	0.27	0/705	0.44	0/956
6	X	0.27	0/715	0.40	0/967
7	H	0.26	0/929	0.47	0/1258
8	I	0.27	0/798	0.54	0/1079
9	J	0.27	0/2828	0.49	0/3834
10	K	0.26	0/377	0.52	0/509
11	L	0.26	0/1039	0.51	0/1403
12	M	0.27	0/5384	0.51	0/7295
13	N	0.28	0/1245	0.51	0/1694
14	O	0.27	0/1711	0.47	0/2328
15	P	0.29	0/1789	0.51	0/2436
16	Q	0.29	0/3538	0.50	0/4796
17	S	0.26	0/581	0.50	0/781
18	T	0.27	0/755	0.53	0/1018
19	U	0.26	0/664	0.46	0/912
20	V	0.26	0/1042	0.45	0/1411
21	W	0.28	0/1187	0.50	0/1603
22	Y	0.26	0/610	0.44	0/836
23	Z	0.28	0/660	0.56	0/892
24	a	0.28	0/1184	0.49	0/1603
25	b	0.28	0/844	0.50	0/1149
26	c	0.27	0/1371	0.49	0/1875
27	d	0.27	0/1494	0.49	0/2015
28	e	0.27	0/891	0.49	0/1210
29	f	0.25	0/386	0.42	0/523
30	g	0.28	0/1036	0.49	0/1401
31	h	0.26	0/873	0.53	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.27	0/2773	0.46	0/3768
33	j	0.27	0/938	0.45	0/1281
34	k	0.28	0/759	0.44	0/1029
35	l	0.27	0/4947	0.46	0/6728
36	m	0.29	0/1325	0.46	0/1800
37	n	0.24	0/491	0.50	0/663
38	o	0.28	0/1092	0.50	0/1481
39	p	0.27	0/1590	0.50	0/2155
40	r	0.27	0/3723	0.45	0/5078
41	s	0.28	0/2581	0.48	0/3529
42	u	0.27	0/1436	0.51	0/1938
43	v	0.26	0/1052	0.54	0/1411
44	w	0.28	0/2642	0.49	0/3580
All	All	0.27	0/67788	0.49	0/91941

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	416 (96%)	15 (4%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	151 (98%)	3 (2%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	48
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	100 (91%)	9 (8%)	1 (1%)	17	55
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	340/342 (99%)	331 (97%)	8 (2%)	1 (0%)	41	76
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%)	661 (96%)	27 (4%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	200 (93%)	15 (7%)	0	100	100
15	P	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
16	Q	427/430 (99%)	418 (98%)	9 (2%)	0	100	100
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
21	W	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
22	Y	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
24	a	136/140 (97%)	132 (97%)	4 (3%)	0	100	100
25	b	94/126 (75%)	85 (90%)	9 (10%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/107 (95%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	g	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	329 (95%)	16 (5%)	0	100	100
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	604/606 (100%)	576 (95%)	28 (5%)	0	100	100
36	m	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
39	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	25	64
40	r	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
41	s	316/318 (99%)	306 (97%)	9 (3%)	1 (0%)	41	76
42	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
43	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	309 (97%)	9 (3%)	0	100	100
All	All	8175/8326 (98%)	7865 (96%)	305 (4%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	134	ASP
41	s	208	VAL
9	J	38	HIS
7	H	77	ILE
39	p	174	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/346 (100%)	341 (99%)	4 (1%)	71	90
2	B	151/151 (100%)	149 (99%)	2 (1%)	69	89
3	C	132/132 (100%)	130 (98%)	2 (2%)	65	87
4	E	106/107 (99%)	104 (98%)	2 (2%)	57	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	72/76 (95%)	69 (96%)	3 (4%)	30	66
6	G	76/81 (94%)	75 (99%)	1 (1%)	69	89
6	X	79/81 (98%)	79 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	84 (97%)	3 (3%)	37	72
9	J	296/296 (100%)	290 (98%)	6 (2%)	55	83
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	567 (98%)	13 (2%)	52	81
13	N	130/130 (100%)	126 (97%)	4 (3%)	40	75
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%)	365 (99%)	5 (1%)	67	88
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%)	68 (99%)	1 (1%)	67	88
20	V	101/101 (100%)	99 (98%)	2 (2%)	55	83
21	W	119/123 (97%)	118 (99%)	1 (1%)	81	93
22	Y	62/63 (98%)	60 (97%)	2 (3%)	39	74
23	Z	62/65 (95%)	62 (100%)	0	100	100
24	a	121/122 (99%)	119 (98%)	2 (2%)	60	85
25	b	90/119 (76%)	89 (99%)	1 (1%)	73	90
26	c	141/141 (100%)	140 (99%)	1 (1%)	84	94
27	d	155/155 (100%)	153 (99%)	2 (1%)	69	89
28	e	96/99 (97%)	95 (99%)	1 (1%)	76	91
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/109 (99%)	106 (98%)	2 (2%)	57	84
31	h	89/93 (96%)	86 (97%)	3 (3%)	37	72
32	i	311/311 (100%)	304 (98%)	7 (2%)	50	80
33	j	100/100 (100%)	99 (99%)	1 (1%)	76	91
34	k	85/85 (100%)	82 (96%)	3 (4%)	36	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	l	540/540 (100%)	528 (98%)	12 (2%)	52	81
36	m	129/141 (92%)	127 (98%)	2 (2%)	62	86
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	156 (98%)	3 (2%)	57	84
40	r	410/410 (100%)	403 (98%)	7 (2%)	60	85
41	s	275/275 (100%)	273 (99%)	2 (1%)	84	94
42	u	153/153 (100%)	150 (98%)	3 (2%)	55	83
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	281/283 (99%)	277 (99%)	4 (1%)	67	88
All	All	7149/7249 (99%)	7041 (98%)	108 (2%)	66	87

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	358	ASP
1	A	379	CYS
1	A	425	CYS
2	B	55	ASP
2	B	76	TYR
3	C	51	ASP
3	C	142	TYR
4	E	68	MET
4	E	70	ASN
5	F	35	ASP
5	F	39	LYS
5	F	75	LYS
6	G	139	MET
8	I	61	ARG
8	I	67	SER
8	I	73	GLN
9	J	85	ARG
9	J	143	ASP
9	J	168	SER
9	J	298	TYR
9	J	360	ARG
9	J	370	LYS

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Mol	Chain	Res	Type
12	M	75	CYS
12	M	76	ARG
12	M	187	SER
12	M	247	LYS
12	M	250	SER
12	M	288	ASP
12	M	380	ASP
12	M	428	LYS
12	M	539	LYS
12	M	559	ASP
12	M	619	ASP
12	M	636	TYR
12	M	658	ASP
13	N	21	ARG
13	N	42	ASP
13	N	95	ASP
13	N	144	TYR
15	P	56	LYS
16	Q	56	LYS
16	Q	60	HIS
16	Q	222	MET
16	Q	308	TYR
16	Q	330	TYR
19	U	64	PRO
20	V	40	SER
20	V	115	CYS
21	W	105	LYS
22	Y	62	SER
22	Y	83	HIS
24	a	105	TYR
24	a	114	LYS
25	b	87	LYS
26	c	165	ASP
27	d	17	THR
27	d	73	ASP
28	e	86	ASN
30	g	89	ASP
30	g	92	MET
31	h	5	ASP
31	h	18	MET
31	h	98	HIS
32	i	67	SER

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Mol	Chain	Res	Type
32	i	97	MET
32	i	104	MET
32	i	215	MET
32	i	244	MET
32	i	299	SER
32	i	319	HIS
33	j	87	MET
34	k	24	SER
34	k	53	PHE
34	k	59	MET
35	l	20	MET
35	l	23	ASN
35	l	176	ARG
35	l	207	GLU
35	l	234	PRO
35	l	308	SER
35	l	340	PHE
35	l	349	SER
35	l	498	PHE
35	l	504	LEU
35	l	543	SER
35	l	579	ASN
36	m	106	TYR
36	m	135	PHE
39	p	29	SER
39	p	38	ARG
39	p	55	LYS
40	r	1	MET
40	r	17	MET
40	r	152	TYR
40	r	183	SER
40	r	187	SER
40	r	243	MET
40	r	304	GLN
41	s	54	LYS
41	s	282	TYR
42	u	38	LYS
42	u	48	TRP
42	u	92	SER
44	w	96	SER
44	w	116	LYS
44	w	241	TYR

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Mol	Chain	Res	Type
44	w	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
5	F	31	GLN
5	F	76	ASN
10	K	78	HIS
10	K	79	HIS
15	P	51	ASN
16	Q	92	HIS
21	W	61	GLN
27	d	104	ASN
35	l	72	GLN
42	u	77	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	6.19	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	5.61	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.70	131.12	119.48
16	Q	118	2MR	CD-NE-CZ	4.33	131.52	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.19	130.91	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
49	PLX	g	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.64	1 (1%)
49	PLX	r	502	-	51,51,51	1.13	4 (7%)	55,59,59	0.63	1 (1%)
53	CDL	V	201	-	93,93,99	1.11	8 (8%)	99,105,111	0.82	4 (4%)
48	PEE	V	203	-	39,39,50	1.32	6 (15%)	41,44,55	1.05	2 (4%)
51	8Q1	G	201	6	31,34,34	1.66	5 (16%)	40,43,43	1.84	7 (17%)
46	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.24	8 (16%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
53	CDL	V	204	-	93,93,99	1.11	7 (7%)	99,105,111	0.87	4 (4%)
48	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	0.99	2 (4%)
49	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.54	0
45	SF4	C	301	3	0,12,12	-	-	-	-	-
51	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.60	7 (17%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
53	CDL	r	504	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
48	PEE	j	201	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
50	UQ	J	402	-	33,33,63	3.47	9 (27%)	40,43,79	2.68	13 (32%)
53	CDL	V	202	-	99,99,99	1.07	8 (8%)	105,111,111	0.91	4 (3%)
49	PLX	j	202	-	51,51,51	1.13	4 (7%)	55,59,59	0.61	1 (1%)
53	CDL	J	403	-	88,88,99	1.12	8 (9%)	94,100,111	0.93	4 (4%)
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
48	PEE	Q	502	-	46,46,50	1.19	6 (13%)	49,51,55	1.02	2 (4%)
48	PEE	s	402	-	40,40,50	1.15	5 (12%)	43,45,55	1.02	3 (6%)
58	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.46	4 (13%)
48	PEE	l	703	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	1.01	2 (4%)
48	PEE	s	401	-	50,50,50	1.14	6 (12%)	53,55,55	0.95	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.02	2 (3%)
49	PLX	m	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
47	NAI	A	503	-	42,48,48	4.94	18 (42%)	47,73,73	1.34	7 (14%)
54	FES	O	301	14	0,4,4	-	-	-	-	-
56	UQ1	Q	501	-	18,18,18	2.38	6 (33%)	22,25,25	1.86	6 (27%)
53	CDL	l	701	-	98,98,99	0.93	4 (4%)	104,110,111	1.09	8 (7%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
53	CDL	a	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	u	201	-	54,54,99	1.36	8 (14%)	60,66,111	1.12	4 (6%)
54	FES	M	803	12	0,4,4	-	-	-	-	-
50	UQ	C	303	-	38,38,63	3.52	8 (21%)	46,49,79	2.83	17 (36%)
53	CDL	S	101	-	50,50,99	1.40	9 (18%)	56,62,111	1.14	4 (7%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
53	CDL	l	702	-	99,99,99	1.08	9 (9%)	105,111,111	0.90	4 (3%)
52	NDP	J	401	-	45,52,52	4.56	20 (44%)	53,80,80	1.95	6 (11%)
49	PLX	C	302	-	51,51,51	1.12	3 (5%)	55,59,59	0.64	1 (1%)

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
49	PLX	g	201	-	-	26/55/55/55	-
49	PLX	r	502	-	-	34/55/55/55	-
53	CDL	V	201	-	-	57/104/104/110	-
48	PEE	V	203	-	-	16/43/43/54	-
51	8Q1	G	201	6	-	18/41/41/41	-
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
53	CDL	V	204	-	-	51/104/104/110	-
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	W	201	-	-	17/44/44/54	-
49	PLX	r	503	-	-	32/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5
51	8Q1	X	201	-	-	10/41/41/41	-
45	SF4	B	302	2	-	-	0/6/5/5
53	CDL	r	504	-	-	62/110/110/110	-
48	PEE	j	201	-	-	26/50/50/54	-
50	UQ	J	402	-	-	11/27/51/87	0/1/1/1
53	CDL	V	202	-	-	51/110/110/110	-
49	PLX	j	202	-	-	30/55/55/55	-
53	CDL	J	403	-	-	40/99/99/110	-
49	PLX	a	202	-	-	27/55/55/55	-
48	PEE	Q	502	-	-	23/50/50/54	-
48	PEE	s	402	-	-	25/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ADP	w	401	-	-	3/12/32/32	0/3/3/3
48	PEE	l	703	-	-	29/54/54/54	-
48	PEE	l	704	-	-	21/49/49/54	-
48	PEE	s	401	-	-	19/54/54/54	-
48	PEE	B	303	-	-	27/54/54/54	-
49	PLX	m	201	-	-	22/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
47	NAI	A	503	-	-	4/25/72/72	0/5/5/5
56	UQ1	Q	501	-	-	5/9/33/33	0/1/1/1
45	SF4	M	801	12	-	-	0/6/5/5
54	FES	O	301	14	-	-	0/1/1/1
53	CDL	l	701	-	-	39/109/109/110	-
53	CDL	a	201	-	-	61/110/110/110	-
45	SF4	A	501	1	-	-	0/6/5/5
53	CDL	u	201	-	-	33/65/65/110	-
54	FES	M	803	12	-	-	0/1/1/1
50	UQ	C	303	-	-	11/33/57/87	0/1/1/1
53	CDL	S	101	-	-	28/61/61/110	-
48	PEE	r	501	-	-	30/54/54/54	-
53	CDL	l	702	-	-	52/110/110/110	-
52	NDP	J	401	-	-	8/30/77/77	0/4/5/5
49	PLX	C	302	-	-	26/55/55/55	-

All (242) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.23	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.41	1.30	1.53
52	J	401	NDP	C3B-C2B	-13.01	1.23	1.52
52	J	401	NDP	C6N-C5N	12.39	1.55	1.33
52	J	401	NDP	O4D-C4D	10.68	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.32	1.26	1.53
52	J	401	NDP	C3D-C4D	-9.95	1.27	1.53
50	J	402	UQ	C18-C19	9.59	1.56	1.33
50	C	303	UQ	C18-C19	9.58	1.56	1.33
50	C	303	UQ	C13-C14	9.21	1.55	1.33
50	J	402	UQ	C13-C14	9.21	1.55	1.33
50	J	402	UQ	C8-C9	9.16	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	303	UQ	C23-C24	9.04	1.54	1.33
50	C	303	UQ	C8-C9	8.91	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.89	1.30	1.53
52	J	401	NDP	O4B-C1B	8.40	1.52	1.41
47	A	503	NAI	O4B-C4B	-8.25	1.26	1.45
52	J	401	NDP	O4B-C4B	-7.96	1.27	1.45
50	J	402	UQ	C23-C24	7.81	1.54	1.32
58	w	401	ADP	O4'-C4'	7.74	1.62	1.45
50	C	303	UQ	C28-C29	7.64	1.54	1.32
47	A	503	NAI	C2D-C1D	-7.62	1.29	1.53
52	J	401	NDP	C2N-C3N	7.36	1.55	1.34
56	Q	501	UQ1	C8-C9	7.34	1.53	1.32
58	w	401	ADP	O4'-C1'	-6.85	1.31	1.41
47	A	503	NAI	O4D-C4D	6.83	1.60	1.45
47	A	503	NAI	C2D-C3D	5.95	1.69	1.53
47	A	503	NAI	C7N-N7N	5.76	1.48	1.33
52	J	401	NDP	P2B-O2B	5.55	1.69	1.59
51	X	201	8Q1	C34-N36	5.46	1.45	1.33
47	A	503	NAI	O4D-C1D	5.39	1.54	1.42
51	G	201	8Q1	C34-N36	5.31	1.45	1.33
51	X	201	8Q1	C39-N41	5.25	1.45	1.33
52	J	401	NDP	C3B-C4B	5.23	1.66	1.53
51	G	201	8Q1	C39-N41	5.11	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.11	1.39	1.49
52	J	401	NDP	O4D-C1D	-4.95	1.30	1.42
52	J	401	NDP	C6N-N1N	4.79	1.49	1.37
47	A	503	NAI	O2B-C2B	4.47	1.53	1.43
52	J	401	NDP	O2D-C2D	-4.27	1.32	1.43
53	l	701	CDL	OB8-CB7	4.25	1.45	1.33
53	l	701	CDL	OB6-CB5	4.20	1.46	1.34
53	l	701	CDL	OA8-CA7	4.19	1.45	1.33
52	J	401	NDP	C7N-N7N	4.09	1.44	1.33
52	J	401	NDP	C6A-N6A	4.06	1.48	1.34
53	l	701	CDL	OA6-CA5	4.03	1.45	1.34
47	A	503	NAI	C6N-C5N	3.97	1.40	1.33
58	w	401	ADP	C6-N6	3.83	1.48	1.34
48	V	203	PEE	C18-C19	3.77	1.53	1.31
46	A	502	FMN	C4A-N5	3.77	1.38	1.30
48	j	201	PEE	C18-C19	3.76	1.53	1.31
48	l	704	PEE	C18-C19	3.75	1.53	1.31
48	r	501	PEE	C18-C19	3.75	1.53	1.31
48	B	303	PEE	C18-C19	3.74	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	W	201	PEE	C18-C19	3.73	1.53	1.31
48	l	703	PEE	C18-C19	3.73	1.53	1.31
48	s	401	PEE	C18-C19	3.72	1.53	1.31
48	s	402	PEE	C18-C19	3.71	1.53	1.31
48	Q	502	PEE	C18-C19	3.69	1.53	1.31
48	B	303	PEE	C39-C38	3.67	1.53	1.31
48	V	203	PEE	C39-C38	3.65	1.52	1.31
48	Q	502	PEE	C39-C38	3.65	1.52	1.31
48	r	501	PEE	C39-C38	3.64	1.52	1.31
48	l	704	PEE	C39-C38	3.64	1.52	1.31
48	j	201	PEE	C39-C38	3.63	1.52	1.31
47	A	503	NAI	C6A-N6A	3.62	1.47	1.34
48	s	401	PEE	C39-C38	3.62	1.52	1.31
48	l	703	PEE	C39-C38	3.60	1.52	1.31
47	A	503	NAI	C7N-C3N	3.55	1.56	1.48
53	u	201	CDL	OA8-CA7	3.48	1.43	1.33
53	V	201	CDL	OA8-CA7	3.48	1.43	1.33
53	a	201	CDL	OA8-CA7	3.42	1.43	1.33
53	r	504	CDL	OA8-CA7	3.41	1.43	1.33
53	V	204	CDL	OA8-CA7	3.40	1.43	1.33
53	S	101	CDL	OA8-CA7	3.40	1.43	1.33
53	l	702	CDL	OA8-CA7	3.40	1.43	1.33
58	w	401	ADP	O2'-C2'	-3.39	1.35	1.43
53	V	202	CDL	OA8-CA7	3.37	1.43	1.33
53	J	403	CDL	OA8-CA7	3.36	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.36	1.40	1.48
53	V	204	CDL	OA6-CA5	3.28	1.43	1.34
53	r	504	CDL	OB6-CB5	3.12	1.43	1.34
53	J	403	CDL	OA6-CA5	3.08	1.43	1.34
53	V	201	CDL	OB8-CB7	3.08	1.42	1.33
53	a	201	CDL	OB6-CB5	3.06	1.42	1.34
52	J	401	NDP	O3D-C3D	3.06	1.50	1.43
53	V	201	CDL	OA6-CA5	3.05	1.42	1.34
58	w	401	ADP	O3'-C3'	3.05	1.50	1.43
53	S	101	CDL	OB8-CB7	3.02	1.42	1.33
53	S	101	CDL	OA6-CA5	3.02	1.42	1.34
53	l	702	CDL	OA6-CA5	3.02	1.42	1.34
53	S	101	CDL	OB6-CB5	3.02	1.42	1.34
53	a	201	CDL	OB8-CB7	3.01	1.42	1.33
53	l	702	CDL	OB8-CB7	3.01	1.42	1.33
53	V	204	CDL	OB6-CB5	2.98	1.42	1.34
53	u	201	CDL	OB8-CB7	2.98	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	V	202	CDL	OA6-CA5	2.98	1.42	1.34
53	V	204	CDL	OB8-CB7	2.96	1.42	1.33
53	r	504	CDL	OB8-CB7	2.96	1.42	1.33
53	r	504	CDL	OA6-CA5	2.96	1.42	1.34
53	V	202	CDL	OB6-CB5	2.95	1.42	1.34
53	J	403	CDL	OB6-CB5	2.95	1.42	1.34
53	u	201	CDL	OA6-CA5	2.95	1.42	1.34
53	l	702	CDL	OB6-CB5	2.94	1.42	1.34
53	a	201	CDL	OA6-CA5	2.92	1.42	1.34
53	V	201	CDL	OB6-CB5	2.92	1.42	1.34
53	u	201	CDL	OB6-CB5	2.90	1.42	1.34
53	V	202	CDL	OB8-CB7	2.88	1.41	1.33
53	J	403	CDL	OB8-CB7	2.87	1.41	1.33
52	J	401	NDP	C7N-C3N	2.86	1.54	1.48
49	g	201	PLX	O6-C4	-2.83	1.40	1.44
50	J	402	UQ	C6-C1	2.82	1.54	1.46
49	a	202	PLX	O6-C4	-2.72	1.41	1.44
50	C	303	UQ	C6-C1	2.70	1.54	1.46
56	Q	501	UQ1	C6-C1	2.62	1.54	1.46
49	m	201	PLX	O6-C4	-2.60	1.41	1.44
49	C	302	PLX	O6-C4	-2.59	1.41	1.44
48	j	201	PEE	O2-C2	-2.59	1.40	1.46
49	r	503	PLX	O6-C4	-2.56	1.41	1.44
51	G	201	8Q1	O35-C34	-2.53	1.18	1.23
48	r	501	PEE	O2-C2	-2.52	1.40	1.46
48	l	704	PEE	O3-C30	2.52	1.40	1.33
48	s	402	PEE	O2-C2	-2.51	1.40	1.46
53	a	201	CDL	OA6-CA4	-2.50	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.49	1.37	1.43
50	C	303	UQ	C7-C8	2.49	1.54	1.50
48	s	401	PEE	O2-C2	-2.48	1.40	1.46
48	s	402	PEE	O3-C30	2.47	1.40	1.33
53	r	504	CDL	OA6-CA4	-2.47	1.40	1.46
48	j	201	PEE	O3-C30	2.47	1.40	1.33
48	V	203	PEE	O3-C30	2.47	1.40	1.33
48	B	303	PEE	O2-C2	-2.46	1.40	1.46
51	G	201	8Q1	O40-C39	-2.46	1.18	1.23
48	W	201	PEE	O3-C30	2.45	1.40	1.33
49	r	502	PLX	O6-C4	-2.45	1.41	1.44
48	l	703	PEE	O3-C30	2.44	1.40	1.33
48	Q	502	PEE	O2-C2	-2.44	1.40	1.46
48	W	201	PEE	O2-C2	-2.44	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	703	PEE	O2-C2	-2.43	1.40	1.46
53	u	201	CDL	OA6-CA4	-2.42	1.40	1.46
48	s	401	PEE	O3-C30	2.41	1.40	1.33
47	A	503	NAI	PN-O5D	2.40	1.69	1.59
50	J	402	UQ	C7-C8	2.40	1.54	1.50
48	Q	502	PEE	O3-C30	2.40	1.40	1.33
53	J	403	CDL	OA6-CA4	-2.39	1.40	1.46
53	V	202	CDL	OA6-CA4	-2.39	1.40	1.46
52	J	401	NDP	O2B-C2B	2.39	1.52	1.44
48	l	704	PEE	O2-C10	2.38	1.41	1.34
49	m	201	PLX	C7-C6	2.37	1.55	1.50
49	j	202	PLX	O6-C4	-2.37	1.41	1.44
48	l	703	PEE	O2-C10	2.34	1.40	1.34
51	X	201	8Q1	O35-C34	-2.34	1.18	1.23
56	Q	501	UQ1	O2-CM2	-2.34	1.39	1.45
51	X	201	8Q1	C1-S44	2.34	1.81	1.76
48	V	203	PEE	O2-C2	-2.34	1.40	1.46
48	V	203	PEE	O2-C10	2.33	1.40	1.34
53	S	101	CDL	OA6-CA4	-2.33	1.40	1.46
53	V	202	CDL	OB6-CB4	-2.32	1.40	1.46
48	r	501	PEE	O3-C30	2.31	1.40	1.33
53	l	702	CDL	OA6-CA4	-2.31	1.40	1.46
49	C	302	PLX	C7-C6	2.30	1.55	1.50
46	A	502	FMN	C10-N1	2.30	1.37	1.33
48	B	303	PEE	O3-C30	2.30	1.40	1.33
49	r	503	PLX	C7-C6	2.30	1.55	1.50
48	l	704	PEE	O2-C2	-2.29	1.40	1.46
53	V	201	CDL	OB6-CB4	-2.29	1.40	1.46
49	a	202	PLX	C7-C6	2.29	1.55	1.50
49	j	202	PLX	C7-C6	2.29	1.55	1.50
49	g	201	PLX	C7-C6	2.28	1.55	1.50
51	G	201	8Q1	C1-S44	2.28	1.81	1.76
51	X	201	8Q1	O40-C39	-2.27	1.18	1.23
48	B	303	PEE	O3-C3	-2.27	1.40	1.45
53	V	204	CDL	OB6-CB4	-2.24	1.41	1.46
53	u	201	CDL	OB6-CB4	-2.24	1.41	1.46
49	r	502	PLX	C7-C6	2.23	1.55	1.50
53	a	201	CDL	OB6-CB4	-2.23	1.41	1.46
47	A	503	NAI	C5B-C4B	2.23	1.58	1.51
48	Q	502	PEE	O2-C10	2.23	1.40	1.34
53	V	202	CDL	PB2-OB2	2.22	1.68	1.59
52	J	401	NDP	C2D-C3D	2.21	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	402	UQ	O4-C4	-2.21	1.18	1.23
53	V	201	CDL	PB2-OB2	2.21	1.68	1.59
53	l	702	CDL	OB6-CB4	-2.21	1.41	1.46
53	r	504	CDL	PB2-OB2	2.20	1.68	1.59
53	J	403	CDL	OB6-CB4	-2.20	1.41	1.46
50	J	402	UQ	C21-C19	2.19	1.55	1.51
48	B	303	PEE	O2-C10	2.19	1.40	1.34
48	r	501	PEE	O3-C3	-2.18	1.40	1.45
53	u	201	CDL	PB2-OB5	2.18	1.68	1.59
48	s	401	PEE	O2-C10	2.18	1.40	1.34
53	r	504	CDL	PB2-OB5	2.18	1.68	1.59
48	W	201	PEE	O2-C10	2.18	1.40	1.34
53	V	201	CDL	OA6-CA4	-2.17	1.41	1.46
53	S	101	CDL	PB2-OB2	2.17	1.68	1.59
53	V	201	CDL	PB2-OB5	2.17	1.68	1.59
48	s	402	PEE	O2-C10	2.17	1.40	1.34
48	Q	502	PEE	O3-C3	-2.17	1.40	1.45
49	m	201	PLX	P1-O4	2.17	1.68	1.59
53	u	201	CDL	PB2-OB2	2.16	1.68	1.59
52	J	401	NDP	O7N-C7N	-2.16	1.19	1.24
49	a	202	PLX	P1-O4	2.15	1.68	1.59
48	V	203	PEE	O3-C3	-2.15	1.40	1.45
48	r	501	PEE	O2-C10	2.15	1.40	1.34
53	J	403	CDL	PB2-OB2	2.14	1.68	1.59
50	C	303	UQ	O4-C4	-2.14	1.18	1.23
56	Q	501	UQ1	O4-C4	-2.14	1.18	1.23
49	r	502	PLX	P1-O4	2.14	1.68	1.59
53	l	702	CDL	PB2-OB2	2.14	1.67	1.59
53	a	201	CDL	PB2-OB5	2.13	1.67	1.59
53	l	702	CDL	PB2-OB5	2.13	1.67	1.59
48	j	201	PEE	O2-C10	2.12	1.40	1.34
53	r	504	CDL	OB6-CB4	-2.12	1.41	1.46
48	l	703	PEE	O3-C3	-2.12	1.40	1.45
56	Q	501	UQ1	O1-C1	-2.12	1.18	1.23
48	j	201	PEE	O3-C3	-2.11	1.40	1.45
53	V	204	CDL	PB2-OB2	2.11	1.67	1.59
53	V	204	CDL	PB2-OB5	2.11	1.67	1.59
53	a	201	CDL	PB2-OB2	2.11	1.67	1.59
53	S	101	CDL	PB2-OB5	2.11	1.67	1.59
53	S	101	CDL	OB6-CB4	-2.11	1.41	1.46
48	s	401	PEE	O3-C3	-2.10	1.40	1.45
50	J	402	UQ	O1-C1	-2.09	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	m	201	PLX	P1-O1	2.09	1.67	1.59
56	Q	501	UQ1	O3-CM3	-2.08	1.40	1.45
49	g	201	PLX	P1-O1	2.07	1.67	1.59
48	s	402	PEE	O3-C3	-2.07	1.40	1.45
49	g	201	PLX	P1-O4	2.07	1.67	1.59
49	r	503	PLX	P1-O4	2.07	1.67	1.59
53	V	202	CDL	PB2-OB5	2.06	1.67	1.59
48	W	201	PEE	O3-C3	-2.05	1.40	1.45
51	X	201	8Q1	C6-C1	2.05	1.52	1.50
49	r	502	PLX	P1-O1	2.05	1.67	1.59
49	j	202	PLX	P1-O4	2.05	1.67	1.59
49	j	202	PLX	P1-O1	2.04	1.67	1.59
53	S	101	CDL	C11-CA5	2.03	1.56	1.50
48	l	704	PEE	O3-C3	-2.02	1.40	1.45
53	l	702	CDL	C11-CA5	2.02	1.56	1.50
49	C	302	PLX	P1-O4	2.02	1.67	1.59
49	a	202	PLX	P1-O1	2.01	1.67	1.59
53	J	403	CDL	PB2-OB5	2.01	1.67	1.59
52	J	401	NDP	PA-O5B	2.00	1.67	1.59
49	r	503	PLX	P1-O1	2.00	1.67	1.59

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	C3N-C2N-N1N	-7.92	111.80	123.10
50	C	303	UQ	C7-C8-C9	-7.80	113.80	126.79
51	G	201	8Q1	C6-C1-S44	7.51	122.20	113.46
50	J	402	UQ	C7-C8-C9	-7.15	114.89	126.79
52	J	401	NDP	C1D-N1N-C2N	-6.93	109.57	121.11
51	X	201	8Q1	C6-C1-S44	5.94	120.37	113.46
50	C	303	UQ	C17-C18-C19	-5.93	113.37	127.66
50	J	402	UQ	C17-C18-C19	-5.84	113.59	127.66
50	C	303	UQ	C12-C13-C14	-5.82	113.64	127.66
50	J	402	UQ	C12-C13-C14	-5.76	113.78	127.66
50	C	303	UQ	C22-C23-C24	-5.54	114.31	127.66
52	J	401	NDP	C1D-N1N-C6N	-5.07	109.90	120.83
56	Q	501	UQ1	C7-C6-C1	4.76	124.20	118.48
50	J	402	UQ	C20-C19-C18	-4.55	112.01	123.68
58	w	401	ADP	N3-C2-N1	-4.55	121.57	128.68
50	C	303	UQ	C10-C9-C8	-4.51	112.11	123.68
53	l	701	CDL	OA6-CA5-C11	4.49	121.17	111.50
50	J	402	UQ	C10-C9-C8	-4.47	112.22	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	G	201	8Q1	O4-C1-C6	-4.40	118.79	123.99
50	J	402	UQ	C22-C23-C24	-4.36	112.84	127.75
50	C	303	UQ	C27-C28-C29	-4.35	112.87	127.75
53	l	702	CDL	OA6-CA5-C11	4.32	120.82	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.31	121.95	128.68
50	J	402	UQ	C16-C14-C13	-4.30	112.42	121.12
48	B	303	PEE	O2-C10-C11	4.26	120.69	111.50
50	J	402	UQ	C15-C14-C13	-4.23	112.82	123.68
50	C	303	UQ	C11-C9-C8	-4.23	112.56	121.12
50	C	303	UQ	C25-C24-C23	-4.22	112.85	123.68
53	V	202	CDL	OA6-CA5-C11	4.20	120.55	111.50
48	l	704	PEE	O2-C10-C11	4.19	120.53	111.50
50	J	402	UQ	C21-C19-C18	-4.18	112.66	121.12
53	J	403	CDL	OB6-CB5-C51	4.09	120.31	111.50
48	s	402	PEE	O2-C10-C11	4.08	120.29	111.50
50	C	303	UQ	C16-C14-C13	-4.07	112.87	121.12
53	S	101	CDL	OB6-CB5-C51	4.06	120.25	111.50
53	u	201	CDL	OB6-CB5-C51	4.06	120.24	111.50
53	a	201	CDL	OB6-CB5-C51	4.04	120.21	111.50
53	r	504	CDL	OB6-CB5-C51	4.03	120.19	111.50
48	r	501	PEE	O2-C10-C11	4.02	120.17	111.50
53	l	701	CDL	OB6-CB5-C51	4.02	120.16	111.50
48	l	703	PEE	O2-C10-C11	4.00	120.12	111.50
53	S	101	CDL	OA6-CA5-C11	4.00	120.11	111.50
50	C	303	UQ	C21-C19-C18	-3.99	113.04	121.12
48	V	203	PEE	O2-C10-C11	3.99	120.10	111.50
50	C	303	UQ	C20-C19-C18	-3.98	113.46	123.68
52	J	401	NDP	N3A-C2A-N1A	-3.96	122.49	128.68
50	C	303	UQ	C15-C14-C13	-3.94	113.57	123.68
53	J	403	CDL	OA6-CA5-C11	3.93	119.96	111.50
53	V	204	CDL	OB6-CB5-C51	3.91	119.92	111.50
53	u	201	CDL	OA6-CA5-C11	3.90	119.91	111.50
53	r	504	CDL	OA6-CA5-C11	3.89	119.88	111.50
48	W	201	PEE	O2-C10-C11	3.88	119.86	111.50
53	l	702	CDL	OB6-CB5-C51	3.86	119.83	111.50
48	s	401	PEE	O2-C10-C11	3.79	119.66	111.50
53	V	201	CDL	OB6-CB5-C51	3.76	119.60	111.50
50	C	303	UQ	C26-C24-C23	-3.76	113.52	121.12
48	j	201	PEE	O2-C10-C11	3.74	119.56	111.50
53	V	202	CDL	OB6-CB5-C51	3.72	119.52	111.50
48	Q	502	PEE	O2-C10-C11	3.70	119.47	111.50
53	a	201	CDL	OA6-CA5-C11	3.67	119.41	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	X	201	8Q1	O4-C1-C6	-3.58	119.76	123.99
53	V	201	CDL	OA6-CA5-C11	3.56	119.17	111.50
56	Q	501	UQ1	C7-C8-C9	-3.51	116.25	127.26
50	J	402	UQ	C26-C24-C23	-3.39	112.84	122.65
53	V	204	CDL	OA6-CA5-C11	3.38	118.79	111.50
50	C	303	UQ	C31-C29-C28	-3.38	112.89	122.65
50	J	402	UQ	C25-C24-C23	-3.36	112.93	122.65
50	C	303	UQ	C30-C29-C28	-3.34	113.01	122.65
47	A	503	NAI	C3D-C2D-C1D	3.31	107.72	101.43
46	A	502	FMN	C4-N3-C2	-3.25	119.63	125.64
53	u	201	CDL	OA8-CA7-C31	3.15	119.65	111.38
56	Q	501	UQ1	C10-C9-C8	-3.12	113.64	122.65
51	X	201	8Q1	C37-C38-C39	3.02	117.38	112.36
50	J	402	UQ	C11-C9-C8	-3.01	115.02	121.12
53	l	701	CDL	OA8-CA7-C31	2.96	121.20	111.91
53	l	701	CDL	CA4-OA6-CA5	-2.96	110.50	117.79
58	w	401	ADP	O4'-C1'-C2'	-2.91	102.67	106.93
48	Q	502	PEE	O3-C30-C31	2.87	120.91	111.91
53	V	202	CDL	OB8-CB7-C71	2.81	120.73	111.91
51	G	201	8Q1	C37-C38-C39	2.80	117.03	112.36
51	G	201	8Q1	O4-C1-S44	-2.79	118.99	122.61
53	V	204	CDL	OB8-CB7-C71	2.79	120.65	111.91
53	V	204	CDL	OA8-CA7-C31	2.76	120.56	111.91
53	l	701	CDL	OB8-CB7-C71	2.76	120.56	111.91
47	A	503	NAI	C4A-C5A-N7A	-2.75	106.54	109.40
53	l	702	CDL	OB8-CB7-C71	2.72	120.44	111.91
46	A	502	FMN	C4A-C4-N3	2.71	120.08	113.19
48	B	303	PEE	O3-C30-C31	2.71	120.41	111.91
53	a	201	CDL	OB8-CB7-C71	2.71	120.41	111.91
48	l	703	PEE	O3-C30-C31	2.71	120.40	111.91
53	S	101	CDL	OB8-CB7-C71	2.70	120.37	111.91
47	A	503	NAI	PN-O3-PA	-2.69	123.58	132.83
47	A	503	NAI	C2D-C3D-C4D	2.67	107.82	102.64
48	V	203	PEE	O3-C30-C31	2.66	120.25	111.91
53	u	201	CDL	OB8-CB7-C71	2.66	120.24	111.91
48	r	501	PEE	O3-C30-C31	2.65	120.23	111.91
53	r	504	CDL	OB8-CB7-C71	2.65	120.23	111.91
53	S	101	CDL	OA8-CA7-C31	2.64	120.21	111.91
53	V	201	CDL	OB8-CB7-C71	2.62	120.12	111.91
48	j	201	PEE	O3-C30-C31	2.61	120.10	111.91
48	l	704	PEE	O3-C30-C31	2.60	120.08	111.91
53	l	702	CDL	OA8-CA7-C31	2.59	120.05	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	r	504	CDL	OA8-CA7-C31	2.59	120.05	111.91
53	V	202	CDL	OA8-CA7-C31	2.59	120.04	111.91
48	W	201	PEE	O3-C30-C31	2.59	120.04	111.91
48	s	402	PEE	O3-C30-C31	2.58	120.00	111.91
47	A	503	NAI	C4D-O4D-C1D	-2.58	103.79	109.47
53	a	201	CDL	OA8-CA7-C31	2.56	119.95	111.91
47	A	503	NAI	C3B-C2B-C1B	2.56	104.83	100.98
58	w	401	ADP	PA-O3A-PB	-2.56	124.06	132.83
56	Q	501	UQ1	C11-C9-C8	-2.56	115.26	122.65
56	Q	501	UQ1	C6-C5-C4	2.55	121.19	119.18
52	J	401	NDP	PN-O3-PA	-2.52	124.18	132.83
53	J	403	CDL	OA8-CA7-C31	2.49	119.74	111.91
46	A	502	FMN	O4-C4-C4A	-2.49	119.98	126.60
51	G	201	8Q1	C38-C39-N41	2.49	120.62	116.42
53	V	201	CDL	OA8-CA7-C31	2.49	119.71	111.91
46	A	502	FMN	C4A-C10-N10	2.48	120.10	116.48
53	J	403	CDL	OB8-CB7-C71	2.48	119.68	111.91
51	X	201	8Q1	C38-C39-N41	2.44	120.53	116.42
52	J	401	NDP	C4A-C5A-N7A	-2.42	106.87	109.40
49	g	201	PLX	C1A-N1-C1	2.42	119.81	109.92
49	r	502	PLX	C1A-N1-C1	2.40	119.75	109.92
46	A	502	FMN	C4A-C10-N1	-2.35	119.28	124.73
49	m	201	PLX	C1A-N1-C1	2.34	119.47	109.92
48	s	401	PEE	O3-C30-C31	2.32	119.19	111.91
51	X	201	8Q1	C42-N41-C39	-2.31	118.54	122.84
56	Q	501	UQ1	CM5-C5-C6	-2.31	120.63	124.40
50	J	402	UQ	CM5-C5-C6	-2.28	120.68	124.40
49	a	202	PLX	C1A-N1-C1	2.28	119.25	109.92
49	j	202	PLX	C1A-N1-C1	2.28	119.24	109.92
51	G	201	8Q1	C32-C34-N36	2.26	121.07	116.58
50	C	303	UQ	C10-C9-C11	-2.24	111.50	115.27
49	C	302	PLX	C1A-N1-C1	2.24	119.08	109.92
46	A	502	FMN	C9A-C5A-N5	-2.21	120.03	122.43
46	A	502	FMN	C10-C4A-N5	-2.18	120.23	124.86
58	w	401	ADP	C4-C5-N7	-2.18	107.13	109.40
51	G	201	8Q1	C42-N41-C39	-2.17	118.81	122.84
53	l	701	CDL	OA8-CA7-OA9	-2.12	118.25	123.59
51	X	201	8Q1	O4-C1-S44	-2.12	119.86	122.61
46	A	502	FMN	C5A-C9A-N10	2.11	120.14	117.95
51	X	201	8Q1	C43-S44-C1	2.09	108.38	101.87
53	l	701	CDL	CB4-OB6-CB5	-2.08	112.66	117.79
48	s	402	PEE	C2-O2-C10	-2.08	112.68	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	l	701	CDL	OA6-CA5-OA7	-2.05	118.74	123.70
50	C	303	UQ	CM5-C5-C6	-2.03	121.09	124.40

There are no chirality outliers.

All (980) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C5'-O5'-P-O2P
46	A	502	FMN	C5'-O5'-P-O3P
47	A	503	NAI	PN-O3-PA-O5B
48	B	303	PEE	C1-O3P-P-O1P
48	Q	502	PEE	O4-C10-O2-C2
48	Q	502	PEE	C1-O3P-P-O2P
48	Q	502	PEE	C1-O3P-P-O1P
48	Q	502	PEE	C4-O4P-P-O2P
48	Q	502	PEE	C4-O4P-P-O1P
48	V	203	PEE	C18-C19-C20-C21
48	W	201	PEE	C4-O4P-P-O1P
48	j	201	PEE	C1-O3P-P-O1P
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	C4-O4P-P-O1P
48	l	704	PEE	C4-O4P-P-O3P
48	r	501	PEE	C5-C4-O4P-P
48	s	401	PEE	O5-C30-O3-C3
48	s	402	PEE	C1-O3P-P-O2P
48	s	402	PEE	C4-O4P-P-O2P
48	s	402	PEE	C4-O4P-P-O1P
48	s	402	PEE	O4P-C4-C5-N
49	C	302	PLX	O7-C6-C7-C8
49	C	302	PLX	O6-C4-C5-O8
49	C	302	PLX	C2-O1-P1-O2
49	C	302	PLX	N1-C1-C2-O1
49	C	302	PLX	O9-C24-O8-C5
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O3
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	N1-C1-C2-O1
49	a	202	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C2-O1-P1-O2
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O7-C6-O6-C4
49	m	201	PLX	O7-C6-C7-C8
49	m	201	PLX	O9-C24-O8-C5
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	O9-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C5-C4-O6-C6
49	r	503	PLX	O9-C24-O8-C5
50	C	303	UQ	C7-C8-C9-C10
50	C	303	UQ	C7-C8-C9-C11
50	C	303	UQ	C14-C16-C17-C18
50	C	303	UQ	C17-C18-C19-C21
50	J	402	UQ	C7-C8-C9-C10
50	J	402	UQ	C15-C14-C16-C17
50	J	402	UQ	C17-C18-C19-C21
50	J	402	UQ	C18-C19-C21-C22
50	J	402	UQ	C20-C19-C21-C22
51	G	201	8Q1	O27-C28-C29-C32
51	G	201	8Q1	C28-C29-C32-C34
51	G	201	8Q1	C28-C29-C32-O33
51	G	201	8Q1	C30-C29-C32-C34
51	G	201	8Q1	C30-C29-C32-O33
51	G	201	8Q1	C31-C29-C32-C34
51	G	201	8Q1	C31-C29-C32-O33
51	G	201	8Q1	O33-C32-C34-N36
51	G	201	8Q1	C42-C43-S44-C1
51	G	201	8Q1	C28-O27-P24-O2
51	X	201	8Q1	C1-C6-C7-C8
51	X	201	8Q1	C28-O27-P24-O3
51	X	201	8Q1	C28-O27-P24-O2
51	X	201	8Q1	C28-O27-P24-O1
53	J	403	CDL	OA5-CA3-CA4-OA6
53	J	403	CDL	OA9-CA7-OA8-CA6
53	J	403	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
53	S	101	CDL	CB2-C1-CA2-OA2
53	S	101	CDL	CA2-OA2-PA1-OA4
53	S	101	CDL	CB2-OB2-PB2-OB3
53	S	101	CDL	CB2-OB2-PB2-OB4
53	V	201	CDL	CA2-C1-CB2-OB2
53	V	201	CDL	CB2-OB2-PB2-OB3
53	V	201	CDL	CB2-OB2-PB2-OB4
53	V	201	CDL	CB2-OB2-PB2-OB5
53	V	201	CDL	CB3-OB5-PB2-OB3
53	V	201	CDL	CB3-OB5-PB2-OB4
53	V	202	CDL	CA3-OA5-PA1-OA2
53	V	202	CDL	CA3-OA5-PA1-OA3
53	V	202	CDL	CA3-OA5-PA1-OA4
53	V	202	CDL	CB3-OB5-PB2-OB2
53	V	202	CDL	CB3-OB5-PB2-OB3
53	V	202	CDL	CB3-OB5-PB2-OB4
53	V	202	CDL	OB6-CB4-CB6-OB8
53	V	204	CDL	CA2-OA2-PA1-OA3
53	V	204	CDL	CA3-OA5-PA1-OA2
53	V	204	CDL	CA3-OA5-PA1-OA3
53	V	204	CDL	CA3-OA5-PA1-OA4
53	V	204	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB2-C1-CA2-OA2
53	a	201	CDL	CA2-C1-CB2-OB2
53	a	201	CDL	CA2-OA2-PA1-OA3
53	a	201	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB2-OB2-PB2-OB4
53	a	201	CDL	CB3-OB5-PB2-OB3
53	a	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	C51-CB5-OB6-CB4
53	l	701	CDL	CA2-OA2-PA1-OA3
53	l	701	CDL	CA2-OA2-PA1-OA4
53	l	701	CDL	CA2-OA2-PA1-OA5
53	l	701	CDL	CA3-OA5-PA1-OA3
53	l	701	CDL	CB2-OB2-PB2-OB4
53	l	701	CDL	CB3-OB5-PB2-OB4
53	l	702	CDL	CB2-C1-CA2-OA2
53	l	702	CDL	O1-C1-CB2-OB2
53	l	702	CDL	CA2-C1-CB2-OB2
53	l	702	CDL	CA3-OA5-PA1-OA4
53	l	702	CDL	CB2-OB2-PB2-OB4
53	r	504	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
53	r	504	CDL	CA3-OA5-PA1-OA2
53	r	504	CDL	CA3-OA5-PA1-OA3
53	r	504	CDL	CB2-OB2-PB2-OB3
53	r	504	CDL	CB2-OB2-PB2-OB4
53	r	504	CDL	CB2-OB2-PB2-OB5
53	r	504	CDL	C51-CB5-OB6-CB4
53	u	201	CDL	CA3-OA5-PA1-OA3
53	u	201	CDL	CA3-OA5-PA1-OA4
53	u	201	CDL	CB2-OB2-PB2-OB3
53	u	201	CDL	CB2-OB2-PB2-OB4
53	u	201	CDL	CB3-OB5-PB2-OB4
56	Q	501	UQ1	C1-C6-C7-C8
56	Q	501	UQ1	C5-C6-C7-C8
58	w	401	ADP	O4'-C4'-C5'-O5'
58	w	401	ADP	C3'-C4'-C5'-O5'
48	Q	502	PEE	O5-C30-O3-C3
48	Q	502	PEE	C31-C30-O3-C3
48	s	401	PEE	C31-C30-O3-C3
56	Q	501	UQ1	C7-C8-C9-C10
48	B	303	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
53	a	201	CDL	OB7-CB5-OB6-CB4
53	r	504	CDL	OB7-CB5-OB6-CB4
53	l	702	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	C11-C10-O2-C2
48	Q	502	PEE	C11-C10-O2-C2
50	J	402	UQ	C22-C23-C24-C26
50	C	303	UQ	C18-C19-C21-C22
53	l	701	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C17-C18-C19-C20
48	B	303	PEE	C37-C38-C39-C40
48	l	704	PEE	C37-C38-C39-C40
48	s	401	PEE	C17-C18-C19-C20
50	C	303	UQ	C22-C23-C24-C25
50	J	402	UQ	C12-C13-C14-C15
50	C	303	UQ	C12-C13-C14-C16
53	l	702	CDL	OB9-CB7-OB8-CB6
53	J	403	CDL	O1-C1-CB2-OB2
53	S	101	CDL	O1-C1-CA2-OA2
53	S	101	CDL	O1-C1-CB2-OB2
53	V	201	CDL	O1-C1-CB2-OB2
53	V	202	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	O1-C1-CA2-OA2
53	l	701	CDL	O1-C1-CA2-OA2
53	l	702	CDL	O1-C1-CA2-OA2
53	r	504	CDL	O1-C1-CA2-OA2
53	u	201	CDL	O1-C1-CA2-OA2
48	j	201	PEE	C11-C10-O2-C2
53	V	201	CDL	C11-CA5-OA6-CA4
49	j	202	PLX	C25-C26-C27-C28
49	m	201	PLX	C13-C14-C15-C16
49	r	502	PLX	C9-C10-C11-C12
53	V	201	CDL	C11-C12-C13-C14
53	V	201	CDL	C62-C63-C64-C65
48	B	303	PEE	C11-C12-C13-C14
53	l	702	CDL	C37-C38-C39-C40
49	r	502	PLX	C11-C12-C13-C14
53	l	701	CDL	OA9-CA7-OA8-CA6
50	J	402	UQ	C12-C11-C9-C8
50	J	402	UQ	C14-C16-C17-C18
49	C	302	PLX	C25-C26-C27-C28
50	C	303	UQ	C27-C28-C29-C31
48	l	704	PEE	C34-C35-C36-C37
53	J	403	CDL	CA2-C1-CB2-OB2
53	V	201	CDL	CB2-C1-CA2-OA2
53	V	202	CDL	CB2-C1-CA2-OA2
53	V	202	CDL	CA2-C1-CB2-OB2
53	l	701	CDL	CB2-C1-CA2-OA2
53	u	201	CDL	CB2-C1-CA2-OA2
50	C	303	UQ	C22-C23-C24-C26
49	r	502	PLX	C7-C8-C9-C10
53	l	702	CDL	C33-C34-C35-C36
48	V	203	PEE	C31-C30-O3-C3
53	V	202	CDL	C31-CA7-OA8-CA6
53	V	202	CDL	C39-C40-C41-C42
53	S	101	CDL	OA5-CA3-CA4-OA6
53	J	403	CDL	C14-C15-C16-C17
53	a	201	CDL	O1-C1-CB2-OB2
53	V	201	CDL	OB6-CB4-CB6-OB8
48	l	704	PEE	C11-C10-O2-C2
48	s	402	PEE	C11-C10-O2-C2
53	V	202	CDL	CB7-C71-C72-C73
53	V	202	CDL	OA9-CA7-OA8-CA6
53	V	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C10-C11-C12-C13
53	J	403	CDL	CB7-C71-C72-C73
53	S	101	CDL	CA7-C31-C32-C33
53	J	403	CDL	CA7-C31-C32-C33
53	V	201	CDL	CB7-C71-C72-C73
53	l	701	CDL	CB7-C71-C72-C73
53	l	702	CDL	CB7-C71-C72-C73
53	a	201	CDL	C71-CB7-OB8-CB6
53	V	204	CDL	C43-C44-C45-C46
53	a	201	CDL	C34-C35-C36-C37
53	r	504	CDL	C74-C75-C76-C77
48	j	201	PEE	O4-C10-O2-C2
53	V	201	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C2-C1-N1-C1A
53	J	403	CDL	CB5-C51-C52-C53
53	V	204	CDL	CA7-C31-C32-C33
53	r	504	CDL	CB5-C51-C52-C53
49	j	202	PLX	C11-C10-C9-C8
49	m	201	PLX	C32-C33-C34-C35
48	V	203	PEE	O5-C30-O3-C3
53	l	702	CDL	C51-C52-C53-C54
53	V	201	CDL	O1-C1-CA2-OA2
48	s	401	PEE	C37-C38-C39-C40
53	V	201	CDL	OA9-CA7-OA8-CA6
53	a	201	CDL	OB9-CB7-OB8-CB6
48	Q	502	PEE	C1-O3P-P-O4P
48	Q	502	PEE	C4-O4P-P-O3P
48	j	201	PEE	C1-O3P-P-O4P
48	l	703	PEE	C4-O4P-P-O3P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
48	s	402	PEE	C1-O3P-P-O4P
48	s	402	PEE	C4-O4P-P-O3P
49	a	202	PLX	C3-O4-P1-O1
49	g	201	PLX	C3-O4-P1-O1
49	g	201	PLX	C2-O1-P1-O4
49	j	202	PLX	C3-O4-P1-O1
49	r	502	PLX	C2-O1-P1-O4
49	r	503	PLX	C3-O4-P1-O1
49	r	503	PLX	C2-O1-P1-O4
53	S	101	CDL	CA2-OA2-PA1-OA5
53	S	101	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
53	V	201	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CB3-OB5-PB2-OB2
53	l	701	CDL	CB2-OB2-PB2-OB5
53	l	701	CDL	CB3-OB5-PB2-OB2
53	l	702	CDL	CA2-OA2-PA1-OA5
53	l	702	CDL	CA3-OA5-PA1-OA2
53	u	201	CDL	CA3-OA5-PA1-OA2
53	u	201	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CB5-C51-C52-C53
52	J	401	NDP	C2D-C1D-N1N-C6N
53	r	504	CDL	C71-CB7-OB8-CB6
53	r	504	CDL	CB2-C1-CA2-OA2
48	l	704	PEE	O4-C10-O2-C2
48	s	402	PEE	O4-C10-O2-C2
49	g	201	PLX	C2-C1-N1-C1B
49	C	302	PLX	O6-C6-C7-C8
49	j	202	PLX	O8-C24-C25-C26
49	r	502	PLX	O6-C6-C7-C8
49	r	503	PLX	O8-C24-C25-C26
49	a	202	PLX	C25-C26-C27-C28
53	J	403	CDL	C51-CB5-OB6-CB4
53	l	702	CDL	C51-CB5-OB6-CB4
49	m	201	PLX	C12-C13-C14-C15
53	V	201	CDL	C52-C53-C54-C55
53	V	202	CDL	C14-C15-C16-C17
53	V	202	CDL	C42-C43-C44-C45
53	V	204	CDL	C15-C16-C17-C18
53	l	702	CDL	C11-C12-C13-C14
53	l	702	CDL	C14-C15-C16-C17
53	r	504	CDL	C62-C63-C64-C65
53	r	504	CDL	C75-C76-C77-C78
51	G	201	8Q1	O27-C28-C29-C30
51	G	201	8Q1	O27-C28-C29-C31
48	B	303	PEE	C31-C30-O3-C3
53	V	201	CDL	C71-CB7-OB8-CB6
53	V	204	CDL	C71-CB7-OB8-CB6
48	s	401	PEE	C22-C23-C24-C25
48	s	402	PEE	C12-C13-C14-C15
49	a	202	PLX	C9-C10-C11-C12
49	g	201	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C33-C34-C35-C36
49	r	503	PLX	C25-C26-C27-C28
53	J	403	CDL	C71-C72-C73-C74
53	S	101	CDL	C11-C12-C13-C14
53	a	201	CDL	C35-C36-C37-C38
53	u	201	CDL	C71-C72-C73-C74
53	J	403	CDL	OB7-CB5-OB6-CB4
53	l	702	CDL	OB7-CB5-OB6-CB4
49	j	202	PLX	C7-C8-C9-C10
53	V	204	CDL	C73-C74-C75-C76
53	a	201	CDL	C62-C63-C64-C65
53	u	201	CDL	C52-C53-C54-C55
53	V	201	CDL	C1-CB2-OB2-PB2
48	l	703	PEE	O3P-C1-C2-O2
48	Q	502	PEE	C37-C38-C39-C40
49	m	201	PLX	C33-C34-C35-C36
53	V	201	CDL	C31-C32-C33-C34
53	r	504	CDL	C41-C42-C43-C44
53	r	504	CDL	C57-C58-C59-C60
53	V	202	CDL	O1-C1-CB2-OB2
53	V	204	CDL	O1-C1-CB2-OB2
48	Q	502	PEE	C21-C22-C23-C24
49	g	201	PLX	C28-C29-C30-C31
53	V	202	CDL	C74-C75-C76-C77
53	V	204	CDL	C20-C21-C22-C23
49	m	201	PLX	C7-C8-C9-C10
53	V	204	CDL	C11-C12-C13-C14
53	a	201	CDL	C20-C21-C22-C23
49	a	202	PLX	C31-C32-C33-C34
49	j	202	PLX	C14-C15-C16-C17
49	j	202	PLX	C13-C14-C15-C16
49	r	502	PLX	C11-C10-C9-C8
49	r	502	PLX	C27-C28-C29-C30
49	r	502	PLX	C30-C31-C32-C33
53	V	201	CDL	C73-C74-C75-C76
53	V	202	CDL	C12-C13-C14-C15
53	u	201	CDL	CB7-C71-C72-C73
48	s	401	PEE	C21-C22-C23-C24
49	C	302	PLX	C11-C12-C13-C14
49	m	201	PLX	C14-C15-C16-C17
49	m	201	PLX	C10-C11-C12-C13
49	r	503	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
51	X	201	8Q1	C11-C12-C13-C14
53	V	201	CDL	C55-C56-C57-C58
53	V	204	CDL	C21-C22-C23-C24
53	a	201	CDL	C71-C72-C73-C74
53	r	504	CDL	C71-C72-C73-C74
48	l	704	PEE	C21-C22-C23-C24
49	C	302	PLX	C10-C11-C12-C13
49	C	302	PLX	C9-C10-C11-C12
49	g	201	PLX	C30-C31-C32-C33
49	j	202	PLX	C33-C34-C35-C36
53	J	403	CDL	C73-C74-C75-C76
53	V	204	CDL	C36-C37-C38-C39
48	V	203	PEE	O4-C10-O2-C2
48	V	203	PEE	C11-C10-O2-C2
49	g	201	PLX	C32-C33-C34-C35
49	r	502	PLX	C28-C29-C30-C31
49	r	503	PLX	C10-C11-C12-C13
53	r	504	CDL	C37-C38-C39-C40
53	u	201	CDL	C55-C56-C57-C58
53	l	701	CDL	CA5-C11-C12-C13
48	W	201	PEE	C12-C13-C14-C15
49	C	302	PLX	C33-C34-C35-C36
49	a	202	PLX	C7-C8-C9-C10
49	r	502	PLX	C13-C14-C15-C16
49	r	503	PLX	C27-C28-C29-C30
51	X	201	8Q1	C12-C13-C14-C15
53	J	403	CDL	C52-C53-C54-C55
53	V	202	CDL	C32-C33-C34-C35
53	V	204	CDL	C37-C38-C39-C40
53	r	504	CDL	C34-C35-C36-C37
53	u	201	CDL	C73-C74-C75-C76
48	l	704	PEE	C11-C12-C13-C14
49	C	302	PLX	C28-C29-C30-C31
49	m	201	PLX	C25-C26-C27-C28
53	J	403	CDL	C34-C35-C36-C37
53	V	202	CDL	C55-C56-C57-C58
53	V	204	CDL	C34-C35-C36-C37
53	V	204	CDL	C52-C53-C54-C55
53	a	201	CDL	C11-C12-C13-C14
48	r	501	PEE	C21-C22-C23-C24
49	C	302	PLX	C14-C15-C16-C17
49	j	202	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
49	m	201	PLX	C11-C12-C13-C14
49	r	502	PLX	C12-C13-C14-C15
49	r	503	PLX	C14-C15-C16-C17
53	V	204	CDL	C75-C76-C77-C78
53	r	504	CDL	C43-C44-C45-C46
49	g	201	PLX	C14-C15-C16-C17
49	g	201	PLX	C10-C11-C12-C13
49	g	201	PLX	C9-C10-C11-C12
49	r	502	PLX	C16-C17-C18-C19
53	V	202	CDL	C34-C35-C36-C37
53	V	202	CDL	C37-C38-C39-C40
53	l	702	CDL	C62-C63-C64-C65
48	Q	502	PEE	C12-C13-C14-C15
49	g	201	PLX	C33-C34-C35-C36
48	B	303	PEE	C23-C24-C25-C26
48	s	401	PEE	C13-C14-C15-C16
48	s	402	PEE	C11-C12-C13-C14
49	C	302	PLX	C11-C10-C9-C8
49	j	202	PLX	C31-C32-C33-C34
53	J	403	CDL	C75-C76-C77-C78
53	u	201	CDL	C74-C75-C76-C77
53	r	504	CDL	OB9-CB7-OB8-CB6
49	j	202	PLX	C35-C36-C37-C38
51	X	201	8Q1	C10-C11-C12-C13
53	J	403	CDL	C35-C36-C37-C38
53	V	202	CDL	C59-C60-C61-C62
53	l	702	CDL	C72-C73-C74-C75
48	r	501	PEE	C1-C2-C3-O3
49	m	201	PLX	C30-C31-C32-C33
53	V	201	CDL	C75-C76-C77-C78
53	a	201	CDL	C21-C22-C23-C24
53	a	201	CDL	C31-C32-C33-C34
49	a	202	PLX	C13-C14-C15-C16
53	V	202	CDL	C51-CB5-OB6-CB4
49	m	201	PLX	O9-C24-C25-C26
49	r	503	PLX	O9-C24-C25-C26
49	j	202	PLX	C27-C28-C29-C30
53	J	403	CDL	C32-C33-C34-C35
53	V	201	CDL	C32-C33-C34-C35
53	V	201	CDL	C37-C38-C39-C40
53	V	202	CDL	C75-C76-C77-C78
53	a	201	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C40-C41-C42-C43
53	l	702	CDL	C73-C74-C75-C76
48	l	703	PEE	C33-C34-C35-C36
49	j	202	PLX	C34-C35-C36-C37
53	V	204	CDL	C71-C72-C73-C74
48	s	402	PEE	C13-C14-C15-C16
53	l	701	CDL	C16-C17-C18-C19
53	V	201	CDL	OB9-CB7-OB8-CB6
53	V	204	CDL	OB9-CB7-OB8-CB6
48	l	703	PEE	C11-C12-C13-C14
48	r	501	PEE	C31-C32-C33-C34
53	l	702	CDL	C55-C56-C57-C58
53	V	202	CDL	OB7-CB5-OB6-CB4
49	a	202	PLX	C14-C15-C16-C17
53	J	403	CDL	C82-C83-C84-C85
53	l	702	CDL	C32-C33-C34-C35
53	a	201	CDL	C54-C55-C56-C57
53	l	701	CDL	C75-C76-C77-C78
53	u	201	CDL	C56-C57-C58-C59
49	g	201	PLX	C2-C1-N1-C1C
48	l	703	PEE	C31-C30-O3-C3
53	J	403	CDL	C59-C60-C61-C62
53	r	504	CDL	C17-C18-C19-C20
53	u	201	CDL	CB5-C51-C52-C53
53	V	202	CDL	C40-C41-C42-C43
48	s	401	PEE	C34-C35-C36-C37
48	B	303	PEE	O5-C30-O3-C3
48	W	201	PEE	C11-C12-C13-C14
48	B	303	PEE	C35-C36-C37-C38
48	j	201	PEE	C15-C16-C17-C18
48	l	703	PEE	C19-C20-C21-C22
48	W	201	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
53	J	403	CDL	OA7-CA5-OA6-CA4
48	s	402	PEE	C31-C30-O3-C3
53	u	201	CDL	C54-C55-C56-C57
53	u	201	CDL	C75-C76-C77-C78
49	r	503	PLX	C13-C14-C15-C16
53	V	201	CDL	C74-C75-C76-C77
53	r	504	CDL	C52-C53-C54-C55
49	a	202	PLX	C11-C12-C13-C14
49	r	503	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
53	V	202	CDL	C17-C18-C19-C20
48	r	501	PEE	C14-C15-C16-C17
49	g	201	PLX	C11-C10-C9-C8
53	V	204	CDL	C42-C43-C44-C45
53	V	204	CDL	C82-C83-C84-C85
53	l	701	CDL	C71-C72-C73-C74
48	r	501	PEE	C20-C21-C22-C23
48	s	401	PEE	C40-C41-C42-C43
49	g	201	PLX	C11-C12-C13-C14
49	r	503	PLX	C11-C10-C9-C8
53	V	202	CDL	C11-C12-C13-C14
53	a	201	CDL	C51-C52-C53-C54
48	Q	502	PEE	C11-C12-C13-C14
49	C	302	PLX	C27-C28-C29-C30
49	a	202	PLX	C12-C13-C14-C15
49	r	502	PLX	C31-C32-C33-C34
53	V	202	CDL	C83-C84-C85-C86
53	a	201	CDL	C32-C33-C34-C35
53	V	204	CDL	CA5-C11-C12-C13
48	W	201	PEE	C11-C10-O2-C2
48	r	501	PEE	C11-C10-O2-C2
53	J	403	CDL	C11-CA5-OA6-CA4
53	l	701	CDL	C11-CA5-OA6-CA4
53	V	202	CDL	OB5-CB3-CB4-OB6
53	J	403	CDL	C36-C37-C38-C39
53	r	504	CDL	C63-C64-C65-C66
48	B	303	PEE	C38-C39-C40-C41
53	a	201	CDL	C42-C43-C44-C45
48	V	203	PEE	O2-C2-C3-O3
53	V	204	CDL	OB6-CB4-CB6-OB8
53	l	702	CDL	OA6-CA4-CA6-OA8
48	W	201	PEE	C21-C22-C23-C24
49	r	503	PLX	C11-C12-C13-C14
53	J	403	CDL	C37-C38-C39-C40
53	r	504	CDL	C14-C15-C16-C17
48	j	201	PEE	C11-C12-C13-C14
48	s	401	PEE	C14-C15-C16-C17
53	V	201	CDL	C14-C15-C16-C17
48	Q	502	PEE	C19-C20-C21-C22
48	j	201	PEE	C19-C20-C21-C22
50	C	303	UQ	C13-C14-C16-C17
49	j	202	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C61-C62-C63-C64
48	l	703	PEE	O5-C30-O3-C3
48	r	501	PEE	C41-C42-C43-C44
53	J	403	CDL	C51-C52-C53-C54
53	l	702	CDL	C35-C36-C37-C38
48	V	203	PEE	C17-C18-C19-C20
53	J	403	CDL	C55-C56-C57-C58
53	V	204	CDL	C35-C36-C37-C38
48	j	201	PEE	C41-C42-C43-C44
53	V	201	CDL	C71-C72-C73-C74
53	a	201	CDL	C52-C53-C54-C55
53	r	504	CDL	C83-C84-C85-C86
49	C	302	PLX	C2-O1-P1-O4
53	r	504	CDL	CA2-OA2-PA1-OA5
53	u	201	CDL	CB3-OB5-PB2-OB2
53	r	504	CDL	C1-CB2-OB2-PB2
53	J	403	CDL	C31-C32-C33-C34
53	J	403	CDL	OA5-CA3-CA4-CA6
53	S	101	CDL	OA5-CA3-CA4-CA6
53	V	204	CDL	C33-C34-C35-C36
49	r	502	PLX	C14-C15-C16-C17
49	a	202	PLX	C27-C28-C29-C30
48	l	703	PEE	C21-C22-C23-C24
49	m	201	PLX	C31-C32-C33-C34
48	s	402	PEE	O5-C30-O3-C3
48	W	201	PEE	C23-C24-C25-C26
48	j	201	PEE	C1-C2-C3-O3
48	l	704	PEE	C1-C2-C3-O3
48	s	402	PEE	C1-C2-C3-O3
49	C	302	PLX	C3-C4-C5-O8
49	r	503	PLX	C28-C29-C30-C31
53	V	201	CDL	CA3-CA4-CA6-OA8
53	V	201	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	CA3-CA4-CA6-OA8
53	r	504	CDL	C64-C65-C66-C67
53	l	702	CDL	C17-C18-C19-C20
49	a	202	PLX	O6-C6-C7-C8
50	C	303	UQ	C9-C11-C12-C13
51	G	201	8Q1	O33-C32-C34-O35
53	V	204	CDL	C78-C79-C80-C81
53	a	201	CDL	C37-C38-C39-C40
48	W	201	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C15-C16-C17-C18
48	r	501	PEE	C15-C16-C17-C18
53	V	204	CDL	C14-C15-C16-C17
53	r	504	CDL	CA5-C11-C12-C13
53	r	504	CDL	CA7-C31-C32-C33
53	S	101	CDL	C31-CA7-OA8-CA6
48	W	201	PEE	C22-C23-C24-C25
46	A	502	FMN	C5'-O5'-P-O1P
49	r	503	PLX	C29-C30-C31-C32
53	r	504	CDL	C32-C33-C34-C35
48	B	303	PEE	O3P-C1-C2-O2
53	S	101	CDL	OB5-CB3-CB4-OB6
53	V	201	CDL	OA5-CA3-CA4-OA6
53	V	204	CDL	OA5-CA3-CA4-OA6
53	a	201	CDL	OA5-CA3-CA4-OA6
48	r	501	PEE	C17-C18-C19-C20
49	g	201	PLX	C15-C16-C17-C18
53	a	201	CDL	C17-C18-C19-C20
48	j	201	PEE	C33-C34-C35-C36
48	j	201	PEE	O2-C2-C3-O3
48	l	703	PEE	O2-C2-C3-O3
48	r	501	PEE	C13-C14-C15-C16
53	l	701	CDL	OA7-CA5-OA6-CA4
53	V	202	CDL	C54-C55-C56-C57
48	W	201	PEE	C13-C14-C15-C16
48	s	402	PEE	C23-C24-C25-C26
48	V	203	PEE	C36-C37-C38-C39
48	j	201	PEE	C34-C35-C36-C37
49	r	503	PLX	C26-C27-C28-C29
48	r	501	PEE	C33-C34-C35-C36
48	s	401	PEE	C31-C32-C33-C34
53	a	201	CDL	C58-C59-C60-C61
53	l	701	CDL	CB5-C51-C52-C53
48	l	703	PEE	C44-C45-C46-C47
48	r	501	PEE	C36-C37-C38-C39
48	s	402	PEE	C24-C25-C26-C27
53	V	202	CDL	C60-C61-C62-C63
48	l	703	PEE	O3P-C1-C2-C3
49	j	202	PLX	O4-C3-C4-C5
53	S	101	CDL	OB5-CB3-CB4-CB6
53	V	202	CDL	OB5-CB3-CB4-CB6
53	a	201	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	OB5-CB3-CB4-CB6
53	a	201	CDL	CA5-C11-C12-C13
48	r	501	PEE	C11-C12-C13-C14
49	j	202	PLX	C11-C12-C13-C14
53	a	201	CDL	C81-C82-C83-C84
48	W	201	PEE	C31-C30-O3-C3
53	J	403	CDL	C11-C12-C13-C14
53	u	201	CDL	C72-C73-C74-C75
56	Q	501	UQ1	C7-C8-C9-C11
53	V	202	CDL	CA5-C11-C12-C13
49	g	201	PLX	C25-C26-C27-C28
48	r	501	PEE	C40-C41-C42-C43
48	j	201	PEE	C42-C43-C44-C45
53	a	201	CDL	C36-C37-C38-C39
53	V	204	CDL	C32-C33-C34-C35
49	r	503	PLX	C12-C13-C14-C15
53	S	101	CDL	C51-C52-C53-C54
53	S	101	CDL	C71-C72-C73-C74
53	V	202	CDL	C31-C32-C33-C34
53	V	202	CDL	C33-C34-C35-C36
53	l	702	CDL	C41-C42-C43-C44
53	r	504	CDL	C54-C55-C56-C57
48	j	201	PEE	C31-C30-O3-C3
48	V	203	PEE	C1-C2-C3-O3
48	W	201	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
49	r	503	PLX	C3-C4-C5-O8
53	V	202	CDL	CB3-CB4-CB6-OB8
53	V	204	CDL	CB3-CB4-CB6-OB8
53	l	701	CDL	C72-C73-C74-C75
49	a	202	PLX	C28-C29-C30-C31
49	r	503	PLX	C16-C17-C18-C19
51	G	201	8Q1	C11-C10-C9-C8
53	r	504	CDL	C55-C56-C57-C58
48	Q	502	PEE	C24-C25-C26-C27
53	V	201	CDL	C57-C58-C59-C60
49	j	202	PLX	C3-C4-O6-C6
49	r	502	PLX	C3-C4-O6-C6
53	l	702	CDL	CB2-OB2-PB2-OB5
53	V	201	CDL	C44-C45-C46-C47
49	j	202	PLX	O4-C3-C4-O6
48	r	501	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
53	S	101	CDL	OA9-CA7-OA8-CA6
48	l	703	PEE	C42-C43-C44-C45
53	V	202	CDL	C84-C85-C86-C87
53	V	204	CDL	C84-C85-C86-C87
53	J	403	CDL	OB6-CB4-CB6-OB8
53	r	504	CDL	OA6-CA4-CA6-OA8
48	j	201	PEE	C32-C33-C34-C35
53	l	702	CDL	C15-C16-C17-C18
53	S	101	CDL	CA2-C1-CB2-OB2
53	a	201	CDL	C84-C85-C86-C87
53	r	504	CDL	C12-C13-C14-C15
53	J	403	CDL	C74-C75-C76-C77
53	r	504	CDL	C59-C60-C61-C62
53	l	702	CDL	C59-C60-C61-C62
49	a	202	PLX	C16-C17-C18-C19
53	V	202	CDL	C1-CB2-OB2-PB2
53	l	701	CDL	CA4-CA3-OA5-PA1
53	J	403	CDL	C12-C13-C14-C15
53	V	201	CDL	C54-C55-C56-C57
53	a	201	CDL	C53-C54-C55-C56
48	l	704	PEE	C18-C19-C20-C21
51	G	201	8Q1	O4-C1-S44-C43
49	C	302	PLX	C26-C27-C28-C29
53	r	504	CDL	C15-C16-C17-C18
53	V	201	CDL	C43-C44-C45-C46
49	r	502	PLX	O8-C24-C25-C26
53	r	504	CDL	C77-C78-C79-C80
48	Q	502	PEE	C18-C19-C20-C21
48	s	402	PEE	C34-C35-C36-C37
51	G	201	8Q1	C6-C7-C8-C9
48	V	203	PEE	C11-C12-C13-C14
49	m	201	PLX	C9-C10-C11-C12
53	a	201	CDL	C64-C65-C66-C67
48	B	303	PEE	C34-C35-C36-C37
53	V	204	CDL	C38-C39-C40-C41
53	V	204	CDL	C53-C54-C55-C56
53	r	504	CDL	C60-C61-C62-C63
53	r	504	CDL	C73-C74-C75-C76
51	G	201	8Q1	C6-C1-S44-C43
53	V	201	CDL	CA6-CA4-OA6-CA5
53	l	702	CDL	C44-C45-C46-C47
48	l	703	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C3-C4-C5-O8
53	J	403	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	CB3-CB4-CB6-OB8
53	r	504	CDL	CA3-CA4-CA6-OA8
53	u	201	CDL	CA3-CA4-CA6-OA8
48	W	201	PEE	O5-C30-O3-C3
53	l	702	CDL	C11-CA5-OA6-CA4
53	a	201	CDL	OB5-CB3-CB4-OB6
53	l	702	CDL	OA5-CA3-CA4-OA6
49	g	201	PLX	C12-C13-C14-C15
49	C	302	PLX	C13-C14-C15-C16
52	J	401	NDP	O4D-C1D-N1N-C6N
48	j	201	PEE	O5-C30-O3-C3
48	s	402	PEE	C21-C22-C23-C24
49	m	201	PLX	O6-C4-C5-O8
53	u	201	CDL	OA6-CA4-CA6-OA8
53	l	702	CDL	C74-C75-C76-C77
53	r	504	CDL	C35-C36-C37-C38
58	w	401	ADP	C5'-O5'-PA-O3A
53	V	204	CDL	C23-C24-C25-C26
53	r	504	CDL	C33-C34-C35-C36
48	l	703	PEE	C30-C31-C32-C33
53	V	204	CDL	C54-C55-C56-C57
53	l	702	CDL	OA7-CA5-OA6-CA4
53	V	201	CDL	C72-C73-C74-C75
53	a	201	CDL	C76-C77-C78-C79
53	V	201	CDL	C53-C54-C55-C56
53	V	204	CDL	C58-C59-C60-C61
48	l	704	PEE	C15-C16-C17-C18
48	V	203	PEE	C1-O3P-P-O4P
49	a	202	PLX	C2-O1-P1-O4
53	S	101	CDL	CB3-OB5-PB2-OB2
53	V	201	CDL	CA3-OA5-PA1-OA2
53	r	504	CDL	CB3-OB5-PB2-OB2
53	u	201	CDL	CA2-OA2-PA1-OA5
53	l	701	CDL	C18-C19-C20-C21
48	l	704	PEE	C2-C1-O3P-P
49	g	201	PLX	C13-C14-C15-C16
53	r	504	CDL	C39-C40-C41-C42
48	j	201	PEE	C1-O3P-P-O2P
48	l	704	PEE	C4-O4P-P-O2P
48	r	501	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O2P
48	s	402	PEE	C1-O3P-P-O1P
49	C	302	PLX	C2-O1-P1-O3
49	g	201	PLX	C3-O4-P1-O3
49	g	201	PLX	C2-O1-P1-O3
49	j	202	PLX	C3-O4-P1-O3
49	j	202	PLX	C2-O1-P1-O3
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O3
53	S	101	CDL	CB3-OB5-PB2-OB3
53	S	101	CDL	CB3-OB5-PB2-OB4
53	V	201	CDL	CA3-OA5-PA1-OA3
53	V	201	CDL	CA3-OA5-PA1-OA4
53	V	204	CDL	CB2-OB2-PB2-OB4
53	l	702	CDL	CA2-OA2-PA1-OA4
53	l	702	CDL	CB2-OB2-PB2-OB3
53	r	504	CDL	CA2-OA2-PA1-OA4
53	r	504	CDL	CB3-OB5-PB2-OB4
53	u	201	CDL	CB3-OB5-PB2-OB3
56	Q	501	UQ1	C6-C7-C8-C9
53	a	201	CDL	CB7-C71-C72-C73
48	B	303	PEE	O3P-C1-C2-C3
53	V	201	CDL	OA5-CA3-CA4-CA6
53	V	204	CDL	OA5-CA3-CA4-CA6
53	l	702	CDL	OA5-CA3-CA4-CA6
53	J	403	CDL	C39-C40-C41-C42
48	r	501	PEE	C24-C25-C26-C27
53	a	201	CDL	C44-C45-C46-C47
53	a	201	CDL	C82-C83-C84-C85
49	C	302	PLX	C25-C24-O8-C5
49	g	201	PLX	C25-C24-O8-C5
49	j	202	PLX	C1-C2-O1-P1
53	V	201	CDL	CA7-C31-C32-C33
53	V	202	CDL	C64-C65-C66-C67
48	r	501	PEE	C10-C11-C12-C13
51	X	201	8Q1	C9-C10-C11-C12
48	s	401	PEE	C36-C37-C38-C39
48	s	401	PEE	C38-C39-C40-C41
53	l	702	CDL	C82-C83-C84-C85
48	B	303	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
53	J	403	CDL	C17-C18-C19-C20
53	l	701	CDL	C56-C57-C58-C59
53	r	504	CDL	C84-C85-C86-C87
49	j	202	PLX	N1-C1-C2-O1
49	r	502	PLX	C3-C4-C5-O8
48	W	201	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	j	202	PLX	O6-C4-C5-O8
49	r	502	PLX	O6-C4-C5-O8
53	l	702	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C13-C14-C15-C16
53	l	701	CDL	C34-C35-C36-C37
53	S	101	CDL	C51-CB5-OB6-CB4
53	l	702	CDL	C71-C72-C73-C74
48	V	203	PEE	C32-C33-C34-C35
49	C	302	PLX	C7-C8-C9-C10
53	S	101	CDL	OB7-CB5-OB6-CB4
53	l	702	CDL	C38-C39-C40-C41
50	J	402	UQ	C13-C14-C16-C17
49	j	202	PLX	C16-C17-C18-C19
53	J	403	CDL	C16-C17-C18-C19
53	r	504	CDL	C13-C14-C15-C16
53	u	201	CDL	C51-C52-C53-C54
53	a	201	CDL	C38-C39-C40-C41
53	a	201	CDL	C14-C15-C16-C17
53	a	201	CDL	C22-C23-C24-C25
48	l	703	PEE	C3-C2-O2-C10
53	V	202	CDL	CA7-C31-C32-C33
53	V	204	CDL	C12-C13-C14-C15
53	V	202	CDL	C32-C31-CA7-OA8
48	l	703	PEE	C13-C14-C15-C16
53	V	201	CDL	CB5-C51-C52-C53
48	B	303	PEE	C20-C21-C22-C23
53	V	201	CDL	C64-C65-C66-C67
48	j	201	PEE	C36-C37-C38-C39
48	s	402	PEE	O2-C2-C3-O3
53	V	201	CDL	OA6-CA4-CA6-OA8
48	l	703	PEE	C24-C25-C26-C27
48	V	203	PEE	C4-O4P-P-O3P
48	s	401	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
48	s	401	PEE	C4-O4P-P-O3P
49	C	302	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O1
53	J	403	CDL	CB3-OB5-PB2-OB2
53	V	201	CDL	CA2-OA2-PA1-OA5
53	V	202	CDL	CA2-OA2-PA1-OA5
48	B	303	PEE	C24-C25-C26-C27
48	j	201	PEE	C13-C14-C15-C16
52	J	401	NDP	O4D-C4D-C5D-O5D
49	r	503	PLX	C36-C37-C38-C39
47	A	503	NAI	O4D-C1D-N1N-C2N
53	V	201	CDL	C32-C31-CA7-OA8
48	l	703	PEE	C10-C11-C12-C13
53	V	202	CDL	C82-C83-C84-C85
53	V	201	CDL	CA4-CA3-OA5-PA1
53	V	204	CDL	CA4-CA3-OA5-PA1
48	l	704	PEE	O5-C30-O3-C3
49	g	201	PLX	C7-C8-C9-C10
48	l	704	PEE	C31-C30-O3-C3
53	u	201	CDL	CA5-C11-C12-C13
48	l	704	PEE	C17-C18-C19-C20
48	s	402	PEE	C33-C34-C35-C36
53	l	702	CDL	C52-C53-C54-C55
48	r	501	PEE	C38-C39-C40-C41
53	r	504	CDL	C16-C17-C18-C19
53	V	201	CDL	OB5-CB3-CB4-OB6
53	l	701	CDL	OA5-CA3-CA4-OA6
53	l	702	CDL	C39-C40-C41-C42
49	r	503	PLX	C30-C31-C32-C33
53	l	701	CDL	C31-C32-C33-C34
53	r	504	CDL	C44-C45-C46-C47
49	r	503	PLX	C24-C25-C26-C27
49	m	201	PLX	O6-C6-C7-C8
48	l	703	PEE	C20-C21-C22-C23
48	j	201	PEE	C44-C45-C46-C47
48	Q	502	PEE	C16-C17-C18-C19
48	V	203	PEE	C38-C39-C40-C41
47	A	503	NAI	C2D-C1D-N1N-C2N
53	r	504	CDL	C72-C71-CB7-OB8
49	C	302	PLX	C16-C17-C18-C19
49	j	202	PLX	C28-C29-C30-C31
53	V	204	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
53	V	204	CDL	C80-C81-C82-C83
53	J	403	CDL	C15-C16-C17-C18
53	V	204	CDL	C83-C84-C85-C86
49	m	201	PLX	C28-C29-C30-C31
48	W	201	PEE	C24-C25-C26-C27
49	r	502	PLX	C18-C19-C20-C21
49	j	202	PLX	C24-C25-C26-C27
48	s	402	PEE	C32-C33-C34-C35
48	s	402	PEE	C16-C17-C18-C19
53	V	201	CDL	C60-C61-C62-C63
49	g	201	PLX	C29-C30-C31-C32
53	r	504	CDL	C58-C59-C60-C61
49	r	502	PLX	C34-C35-C36-C37
48	r	501	PEE	C16-C17-C18-C19
48	s	401	PEE	C16-C17-C18-C19
53	l	701	CDL	C58-C59-C60-C61
48	l	704	PEE	C13-C14-C15-C16
49	r	502	PLX	C19-C20-C21-C22
51	X	201	8Q1	C42-C43-S44-C1
53	r	504	CDL	C51-C52-C53-C54
48	B	303	PEE	O2-C2-C3-O3
48	l	704	PEE	C2-C3-O3-C30
53	V	202	CDL	C53-C54-C55-C56
48	j	201	PEE	C12-C13-C14-C15
49	m	201	PLX	C34-C35-C36-C37
49	r	503	PLX	C31-C32-C33-C34
53	V	204	CDL	C13-C14-C15-C16
48	l	704	PEE	C16-C17-C18-C19
48	s	401	PEE	O2-C10-C11-C12
48	B	303	PEE	C44-C45-C46-C47
48	l	703	PEE	C16-C17-C18-C19
53	V	202	CDL	C78-C79-C80-C81
48	l	703	PEE	C37-C38-C39-C40
49	r	502	PLX	C4-C5-O8-C24
53	l	701	CDL	C74-C75-C76-C77
53	l	702	CDL	C32-C31-CA7-OA8
48	l	703	PEE	C40-C41-C42-C43
48	Q	502	PEE	C36-C37-C38-C39
48	W	201	PEE	C16-C17-C18-C19
48	l	703	PEE	C36-C37-C38-C39
48	s	402	PEE	C18-C19-C20-C21
53	l	701	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	r	504	CDL	C80-C81-C82-C83
53	J	403	CDL	C77-C78-C79-C80
49	a	202	PLX	C30-C31-C32-C33
48	r	501	PEE	C44-C45-C46-C47
53	a	201	CDL	C24-C25-C26-C27
49	a	202	PLX	C29-C30-C31-C32
48	W	201	PEE	O4P-C4-C5-N
48	j	201	PEE	O4P-C4-C5-N
53	V	202	CDL	C71-C72-C73-C74
48	j	201	PEE	C16-C17-C18-C19
48	Q	502	PEE	C23-C24-C25-C26
48	Q	502	PEE	C2-C1-O3P-P
49	r	503	PLX	O6-C4-C5-O8
53	a	201	CDL	C32-C31-CA7-OA8
52	J	401	NDP	C2B-O2B-P2B-O1X
51	G	201	8Q1	C7-C8-C9-C10
51	X	201	8Q1	C13-C14-C15-C16
53	a	201	CDL	C41-C42-C43-C44
50	J	402	UQ	C1-C6-C7-C8
48	l	703	PEE	C38-C39-C40-C41
53	V	204	CDL	CA3-CA4-OA6-CA5
46	A	502	FMN	O4'-C4'-C5'-O5'
53	V	201	CDL	C36-C37-C38-C39
53	S	101	CDL	C72-C71-CB7-OB8
53	a	201	CDL	C12-C11-CA5-OA6
53	u	201	CDL	C57-C58-C59-C60
48	j	201	PEE	O3-C30-C31-C32
48	s	402	PEE	O3-C30-C31-C32
53	S	101	CDL	C12-C11-CA5-OA6
48	B	303	PEE	C18-C19-C20-C21
48	Q	502	PEE	C38-C39-C40-C41
48	j	201	PEE	C18-C19-C20-C21
48	l	704	PEE	C38-C39-C40-C41
53	V	201	CDL	C56-C57-C58-C59
49	m	201	PLX	C7-C6-O6-C4
49	m	201	PLX	C3-C4-C5-O8
48	B	303	PEE	C31-C32-C33-C34
53	l	701	CDL	C71-CB7-OB8-CB6
53	r	504	CDL	C72-C73-C74-C75
53	l	702	CDL	C76-C77-C78-C79
53	l	701	CDL	C12-C11-CA5-OA6
53	V	204	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
49	m	201	PLX	C24-C25-C26-C27
53	l	702	CDL	C72-C71-CB7-OB8
53	a	201	CDL	C61-C62-C63-C64
49	C	302	PLX	O9-C24-C25-C26
52	J	401	NDP	C2B-O2B-P2B-O2X
48	r	501	PEE	C23-C24-C25-C26
49	C	302	PLX	C19-C20-C21-C22
48	V	203	PEE	O3-C30-C31-C32
52	J	401	NDP	O4B-C4B-C5B-O5B
53	a	201	CDL	C72-C73-C74-C75
53	r	504	CDL	C52-C51-CB5-OB6
49	j	202	PLX	C18-C19-C20-C21
48	V	203	PEE	C16-C17-C18-C19
53	l	701	CDL	C39-C40-C41-C42
53	a	201	CDL	C32-C31-CA7-OA9
48	B	303	PEE	C21-C22-C23-C24
53	l	701	CDL	C62-C63-C64-C65
53	u	201	CDL	C72-C71-CB7-OB8
53	r	504	CDL	C52-C51-CB5-OB7
53	S	101	CDL	C72-C71-CB7-OB9
53	S	101	CDL	C12-C11-CA5-OA7
53	a	201	CDL	C12-C11-CA5-OA7
48	j	201	PEE	O5-C30-C31-C32
48	s	401	PEE	C33-C34-C35-C36
53	V	202	CDL	C52-C51-CB5-OB6
47	A	503	NAI	C2N-C3N-C7N-N7N
48	l	704	PEE	C1-O3P-P-O1P
49	r	503	PLX	C3-O4-P1-O3
52	J	401	NDP	C5B-O5B-PA-O1A
53	J	403	CDL	CA2-OA2-PA1-OA3
52	J	401	NDP	C3D-C4D-C5D-O5D
48	B	303	PEE	C40-C41-C42-C43
53	l	701	CDL	C12-C11-CA5-OA7
53	l	701	CDL	C59-C60-C61-C62
48	Q	502	PEE	C34-C35-C36-C37
53	l	702	CDL	C72-C71-CB7-OB9
53	r	504	CDL	C23-C24-C25-C26
49	r	502	PLX	C25-C26-C27-C28
53	V	201	CDL	C34-C35-C36-C37
49	a	202	PLX	C1-C2-O1-P1
49	a	202	PLX	C25-C24-O8-C5
49	r	502	PLX	C25-C24-O8-C5

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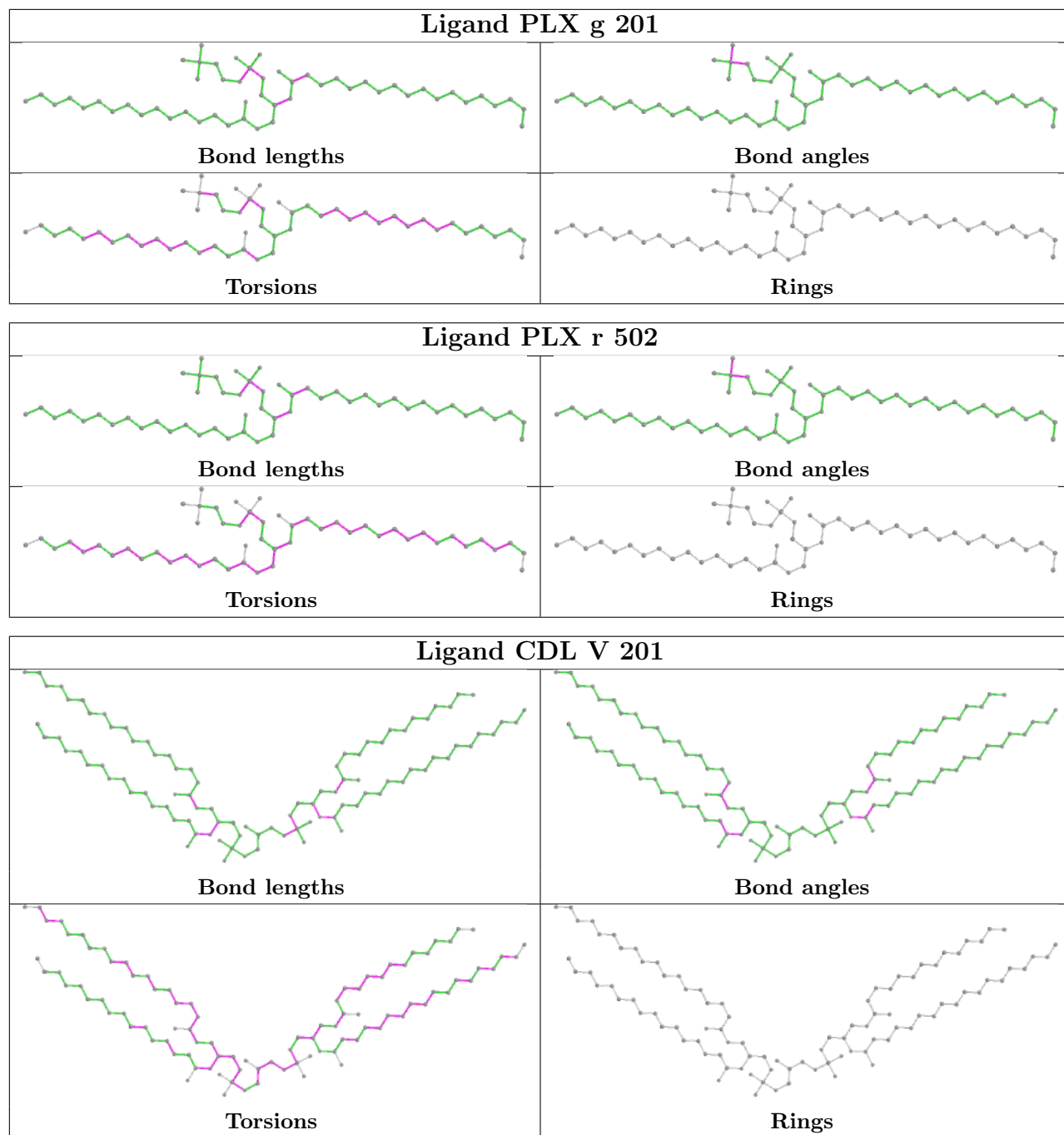
Continued from previous page...

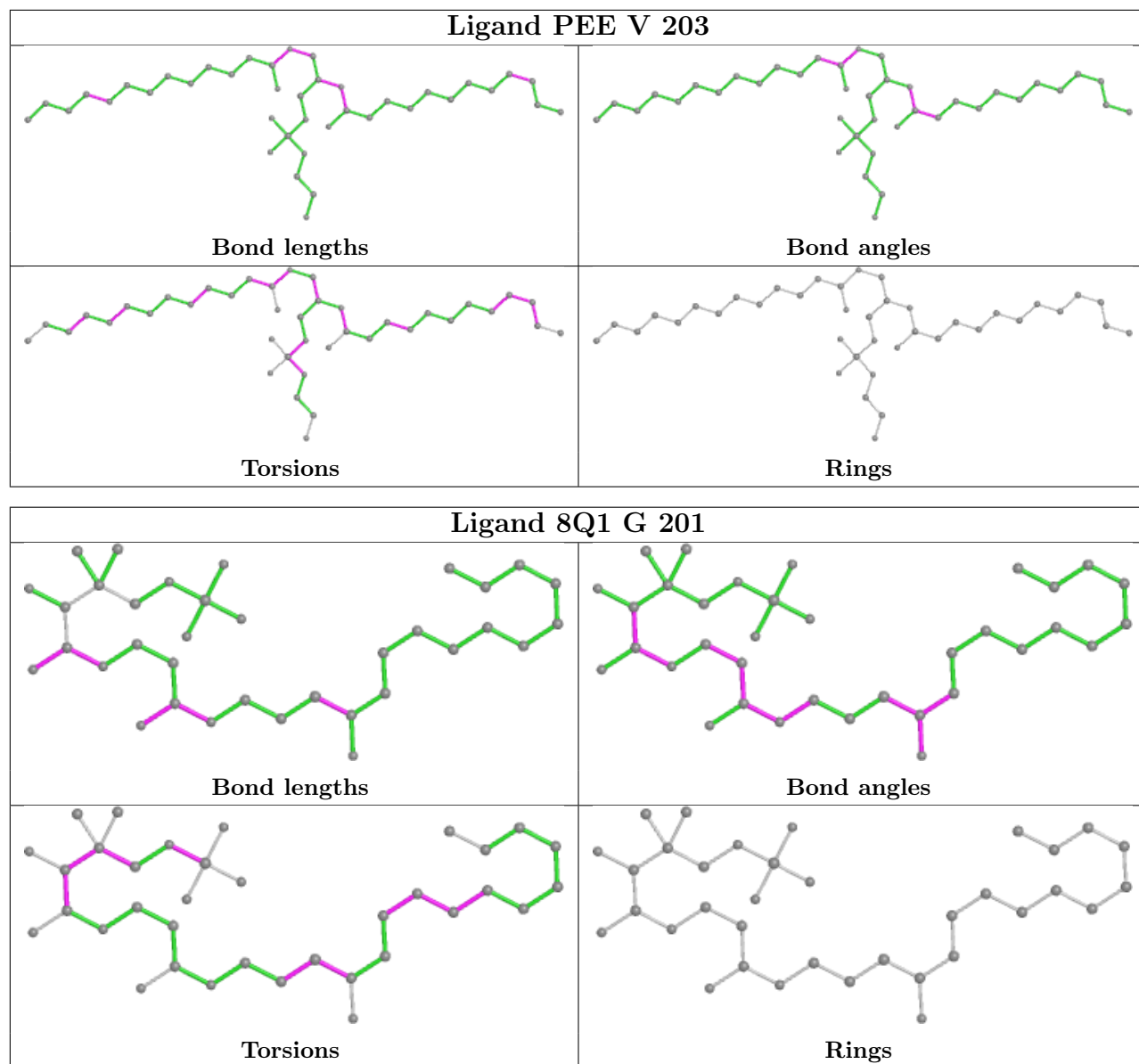
Mol	Chain	Res	Type	Atoms
53	V	204	CDL	CA6-CA4-OA6-CA5
53	u	201	CDL	OB9-CB7-OB8-CB6
53	a	201	CDL	C57-C58-C59-C60
48	B	303	PEE	O3-C30-C31-C32
48	r	501	PEE	O2-C10-C11-C12
53	u	201	CDL	C52-C51-CB5-OB6
53	l	701	CDL	C37-C38-C39-C40
49	r	502	PLX	C26-C27-C28-C29
53	r	504	CDL	C12-C11-CA5-OA6
48	s	401	PEE	C30-C31-C32-C33
53	l	701	CDL	C52-C53-C54-C55
48	B	303	PEE	O5-C30-C31-C32
53	V	204	CDL	C32-C31-CA7-OA8
53	V	202	CDL	C52-C51-CB5-OB7
53	u	201	CDL	C72-C71-CB7-OB9
53	a	201	CDL	C40-C41-C42-C43
53	a	201	CDL	C78-C79-C80-C81
53	u	201	CDL	C52-C51-CB5-OB7
53	l	701	CDL	C72-C71-CB7-OB8
49	r	503	PLX	C2-C1-N1-C1C
49	r	503	PLX	C2-C1-N1-C1B

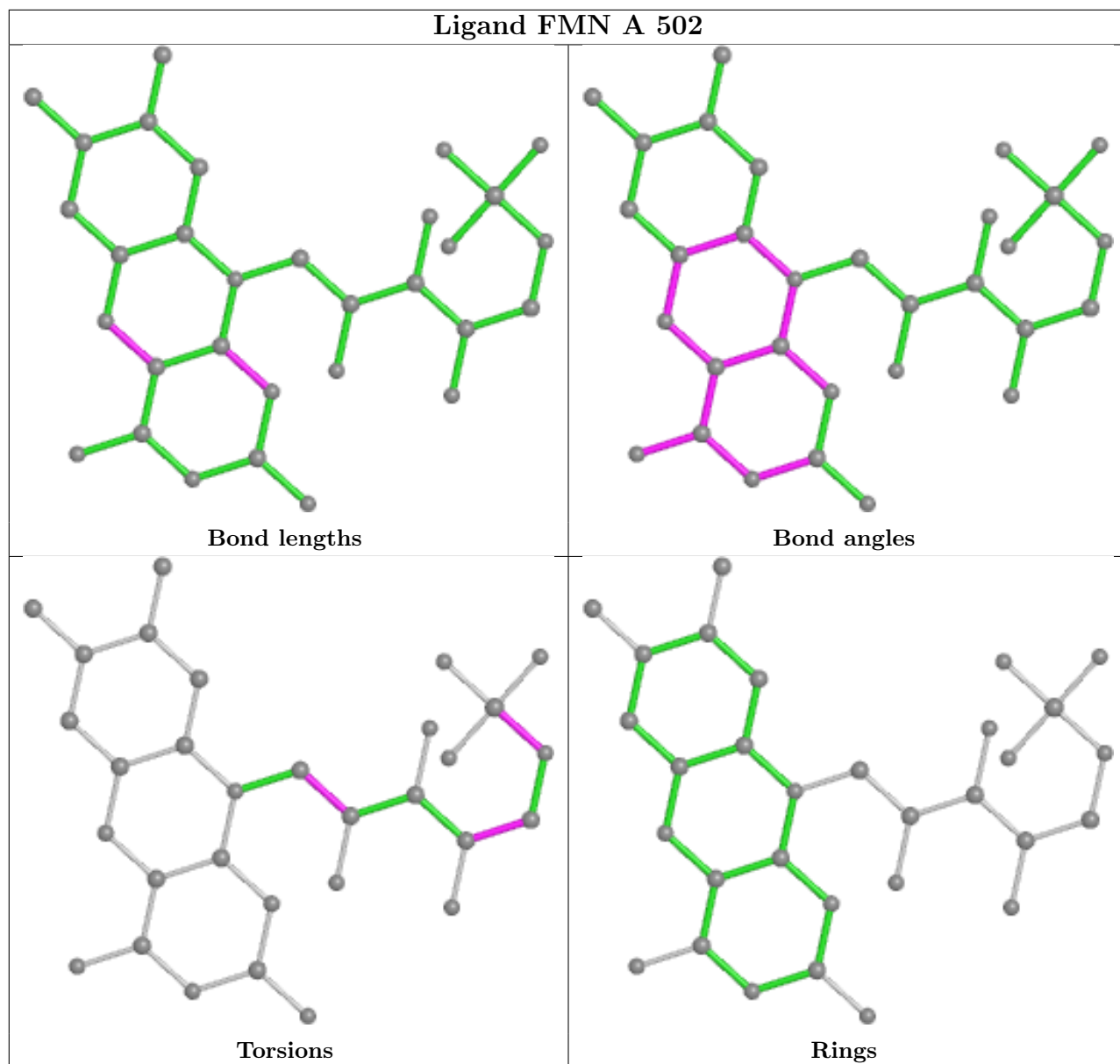
There are no ring outliers.

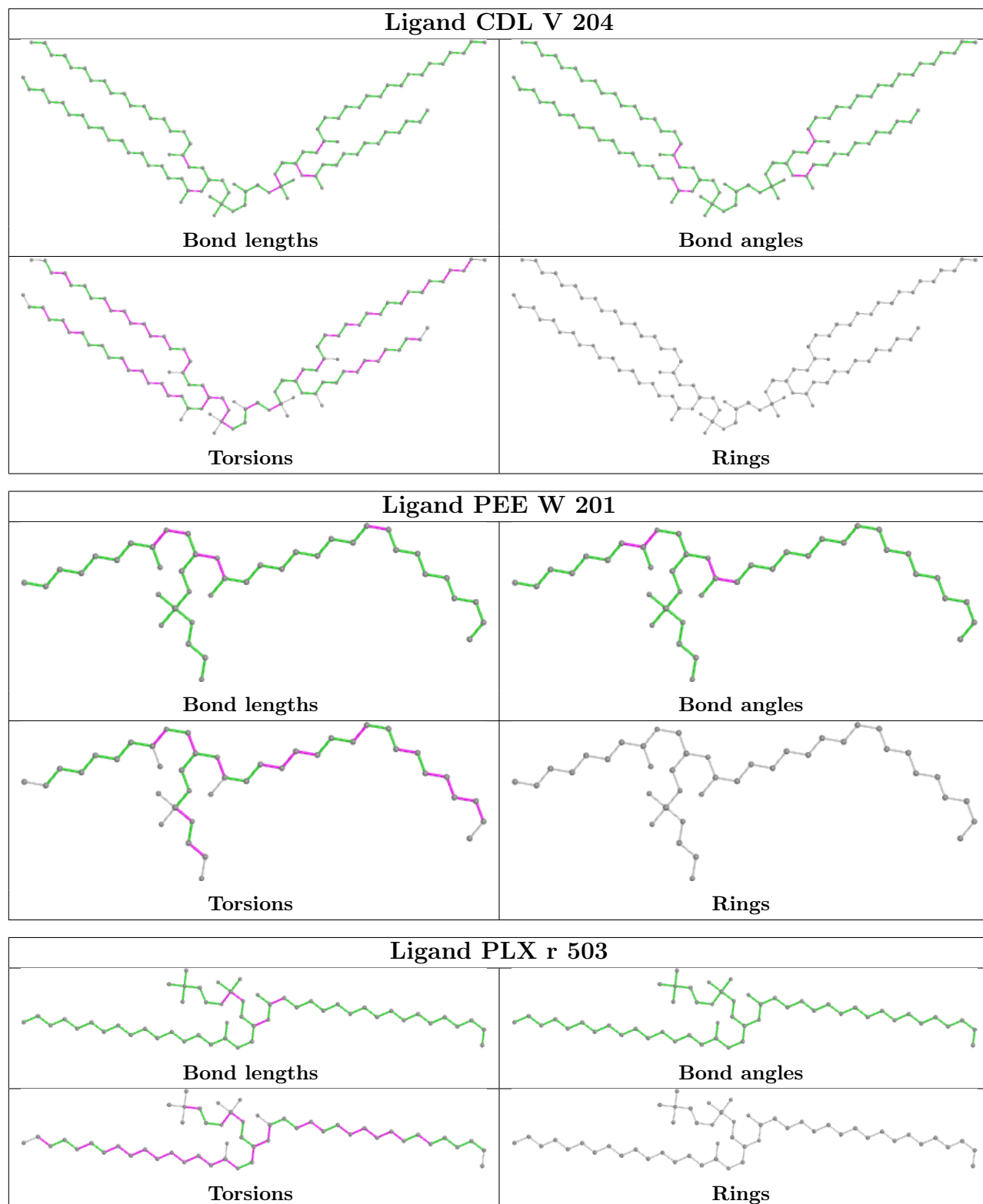
No monomer is involved in short contacts.

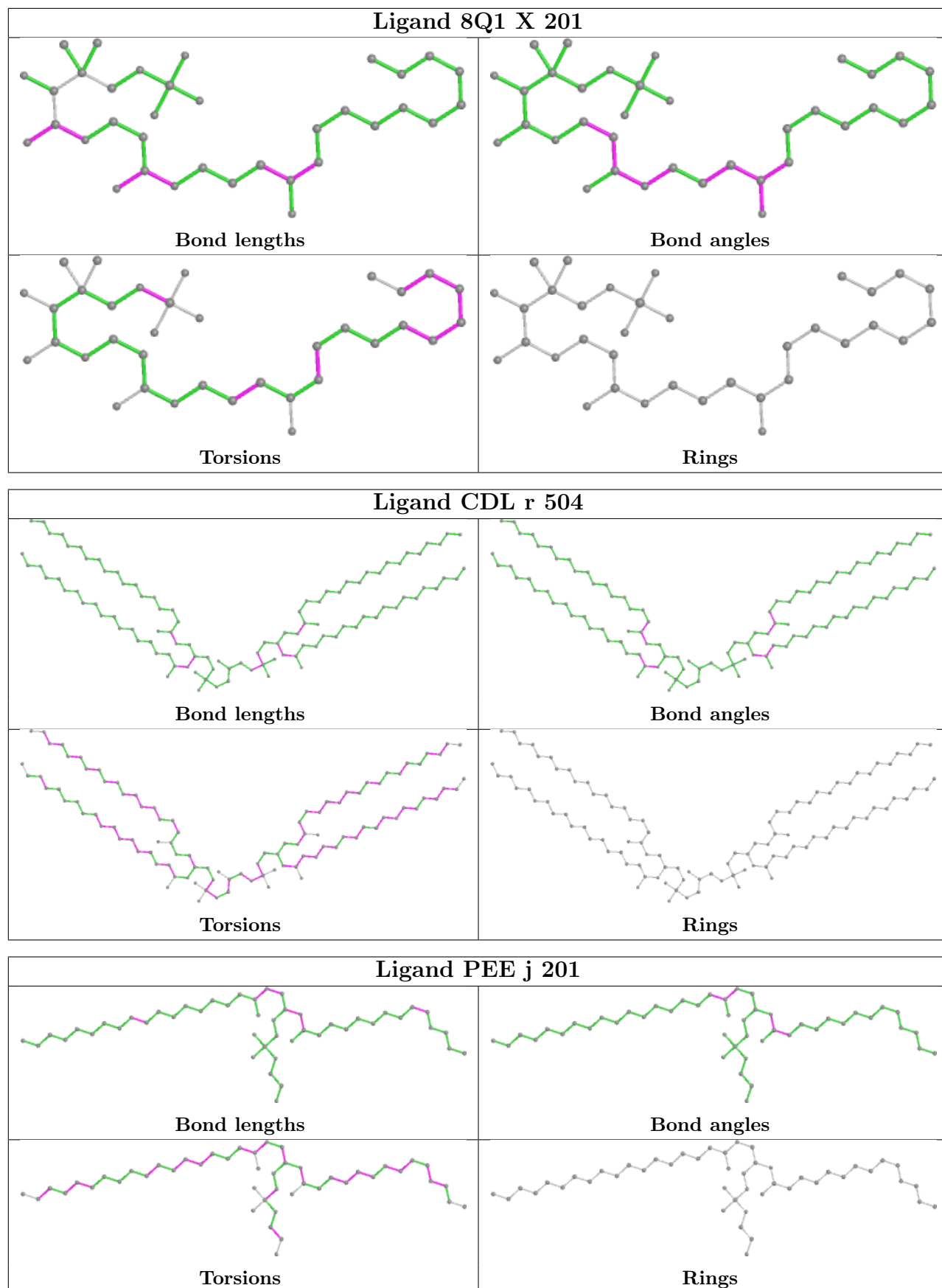
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

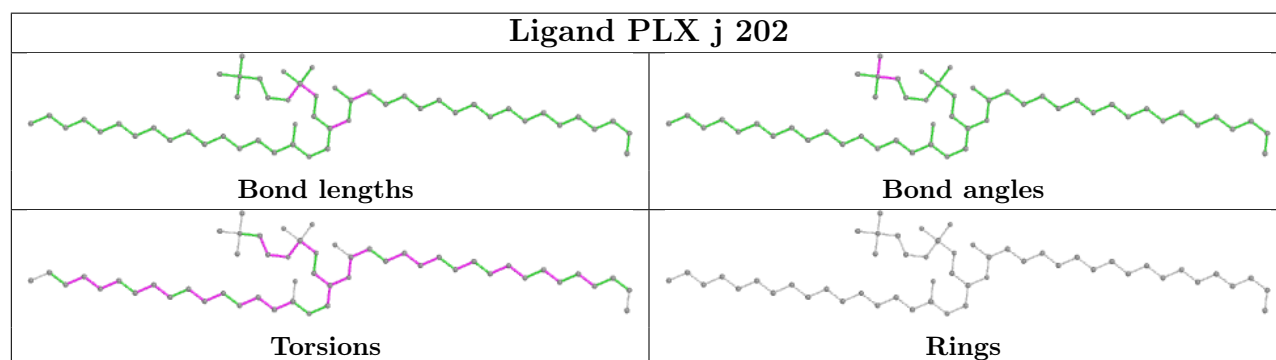
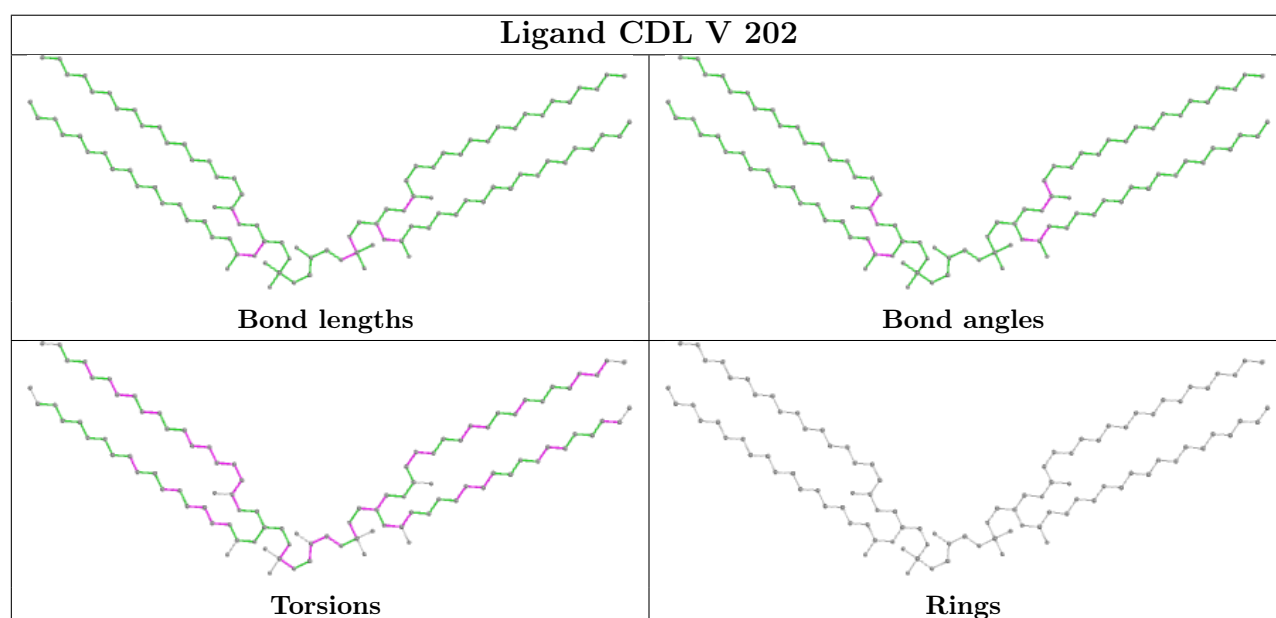
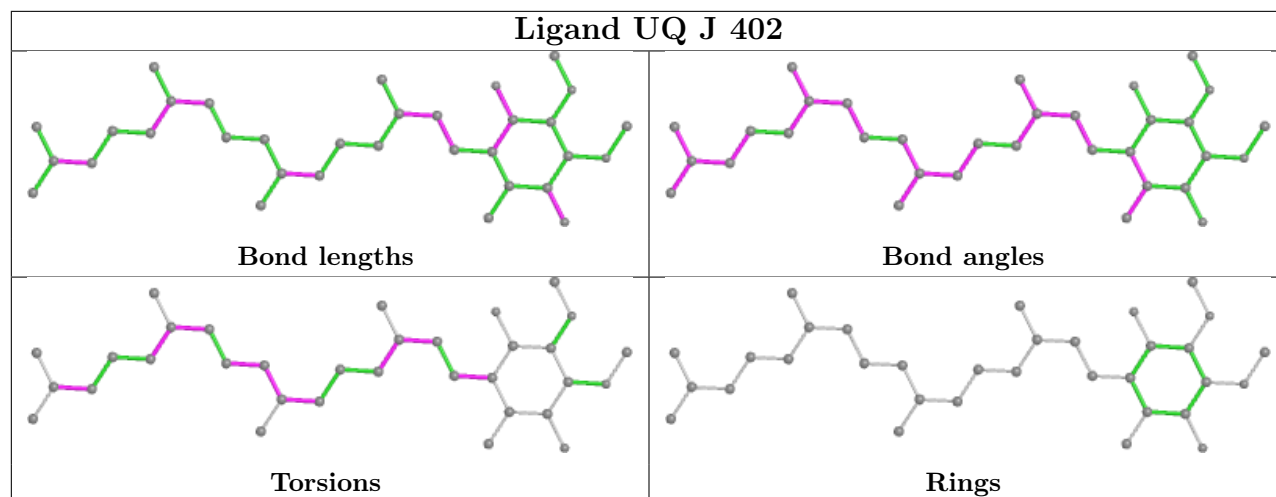


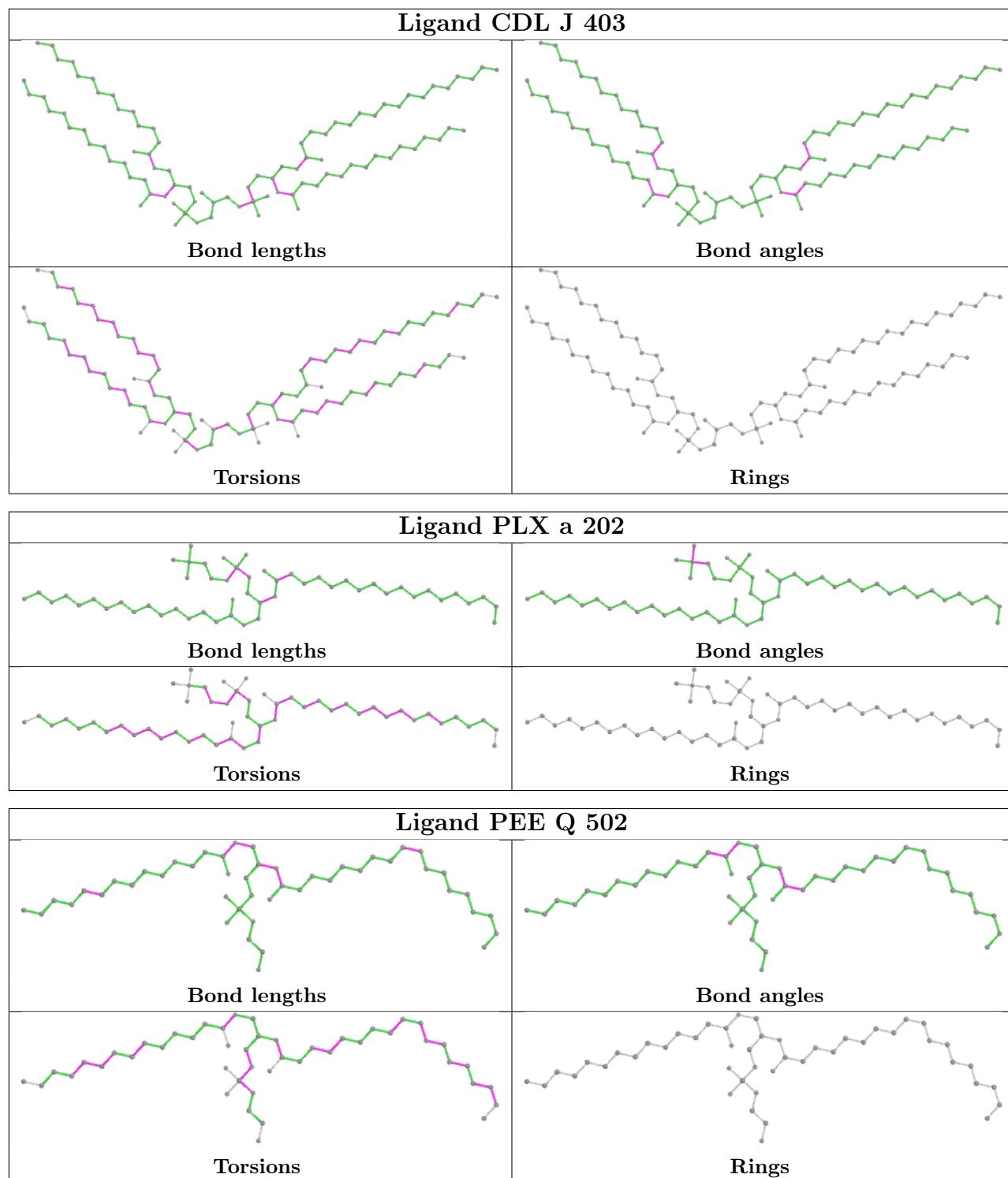


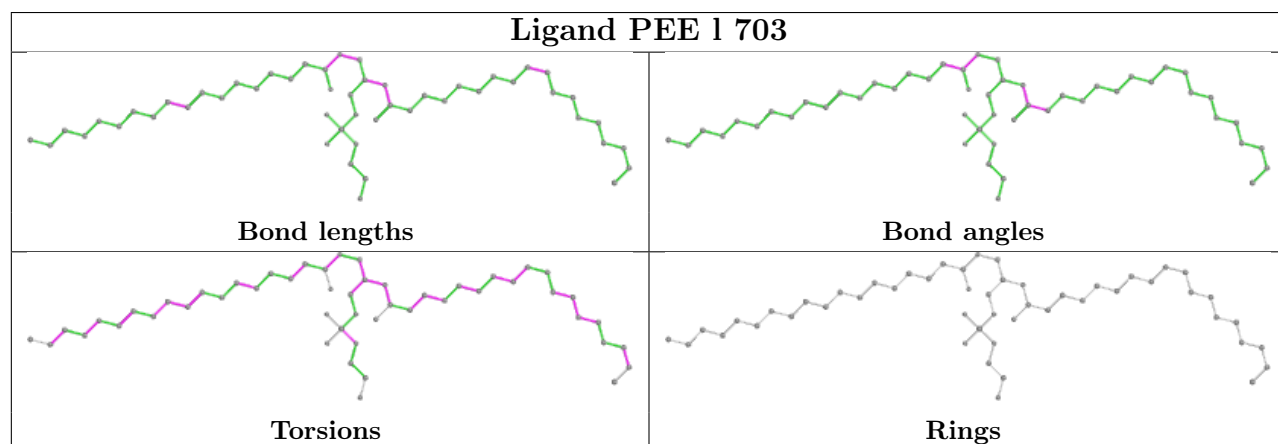
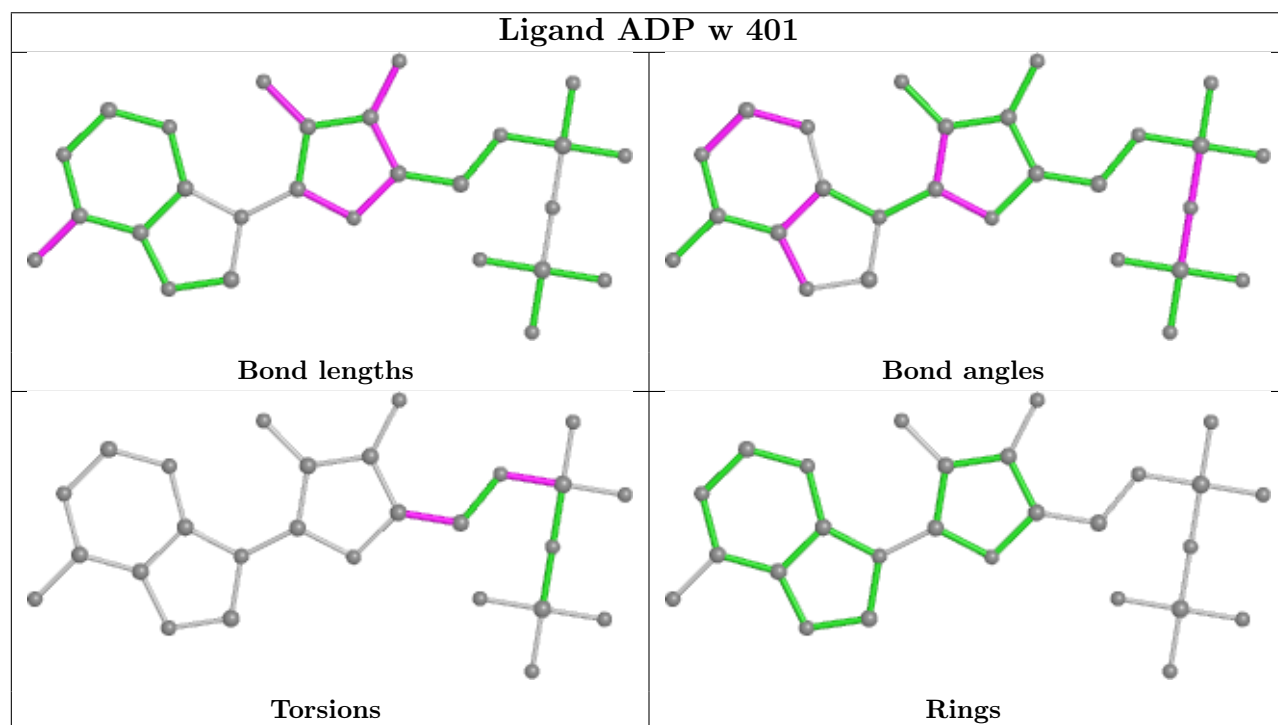
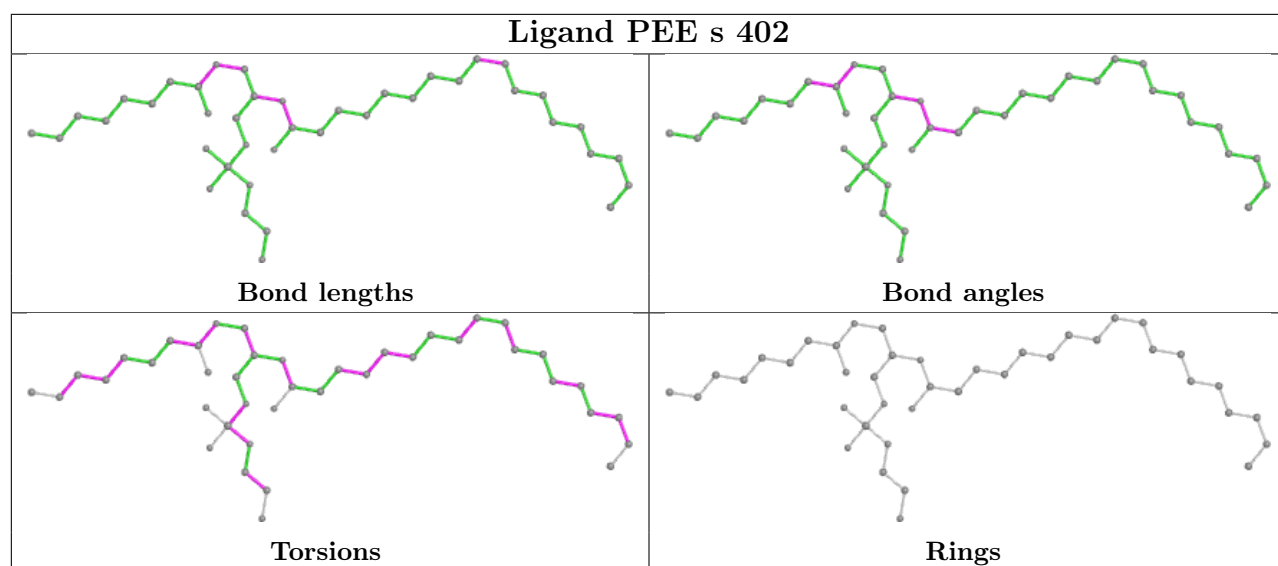


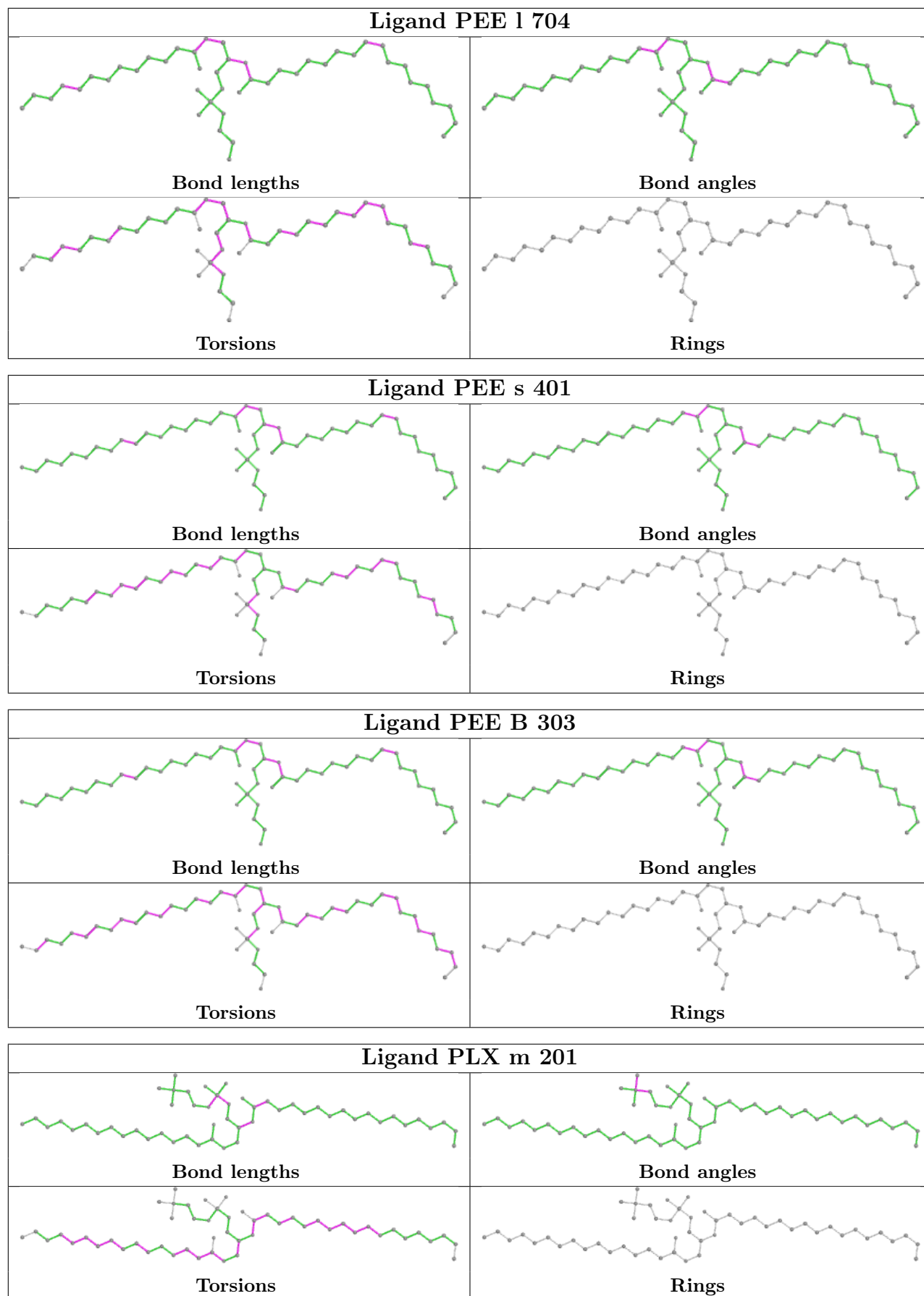


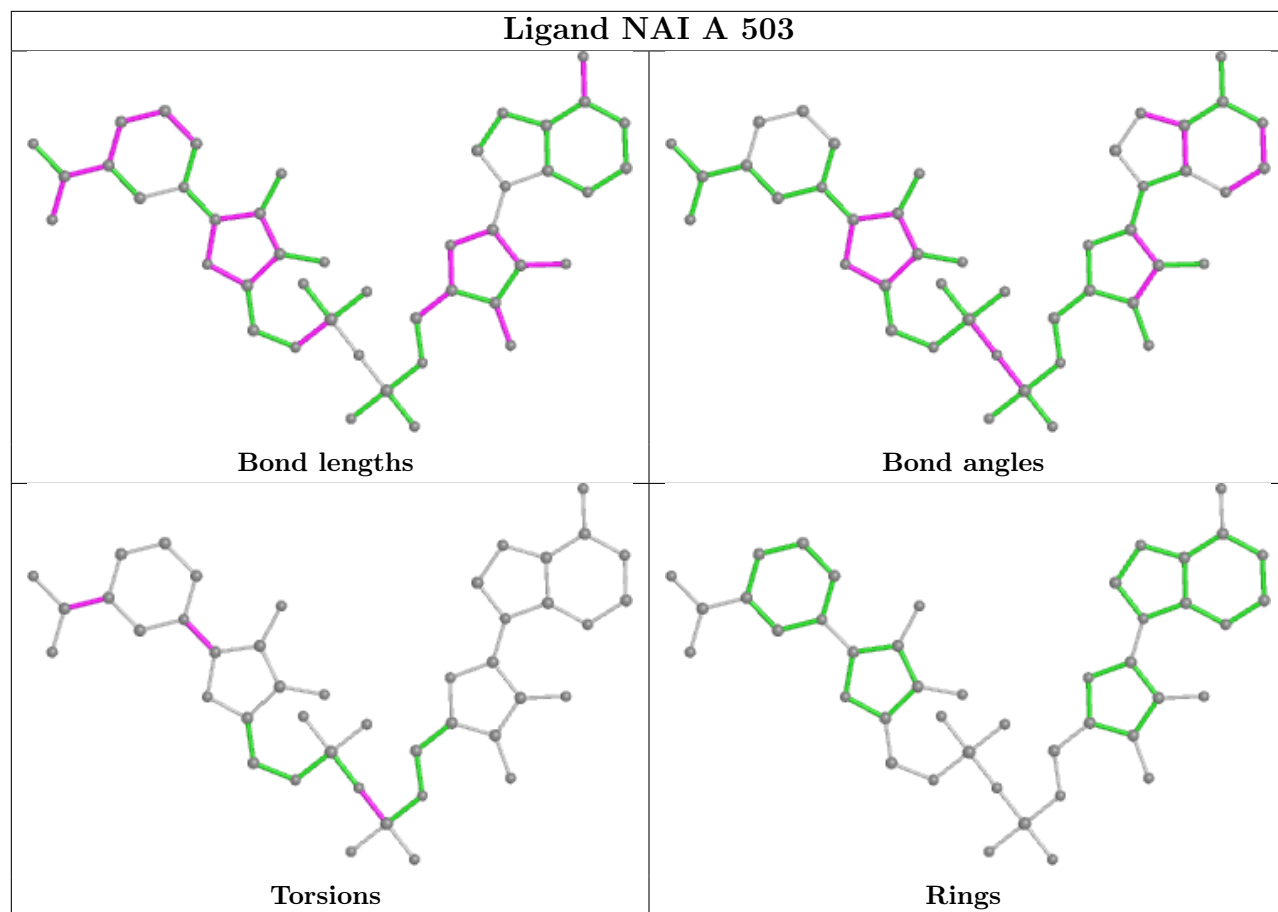


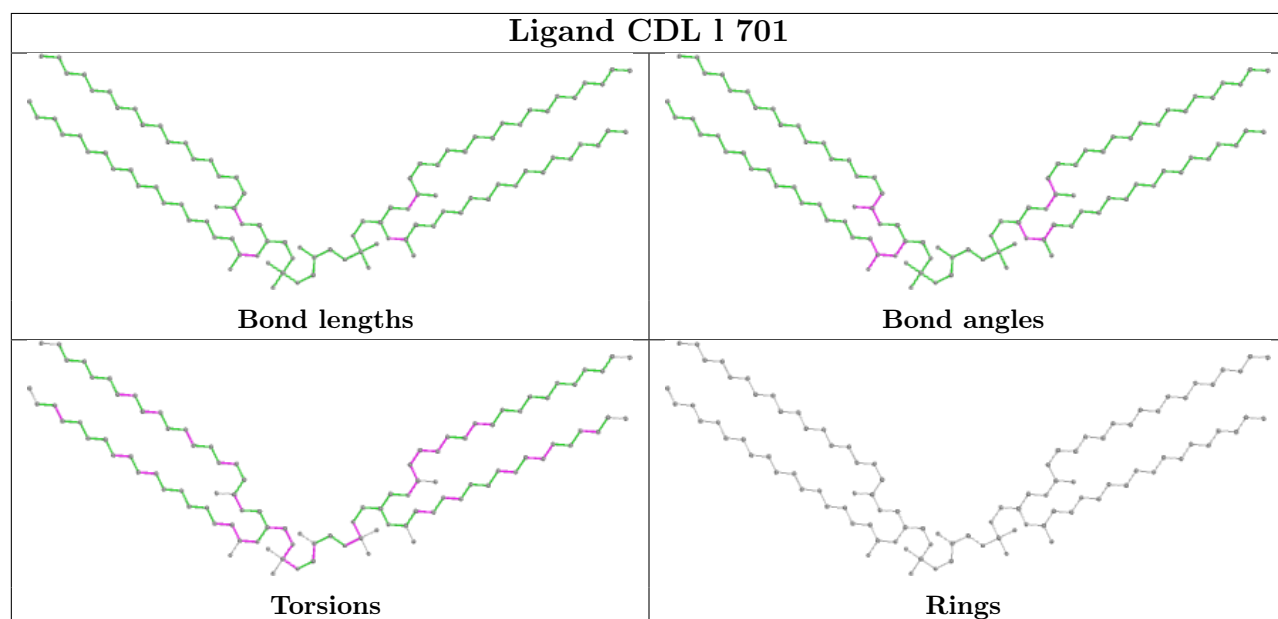
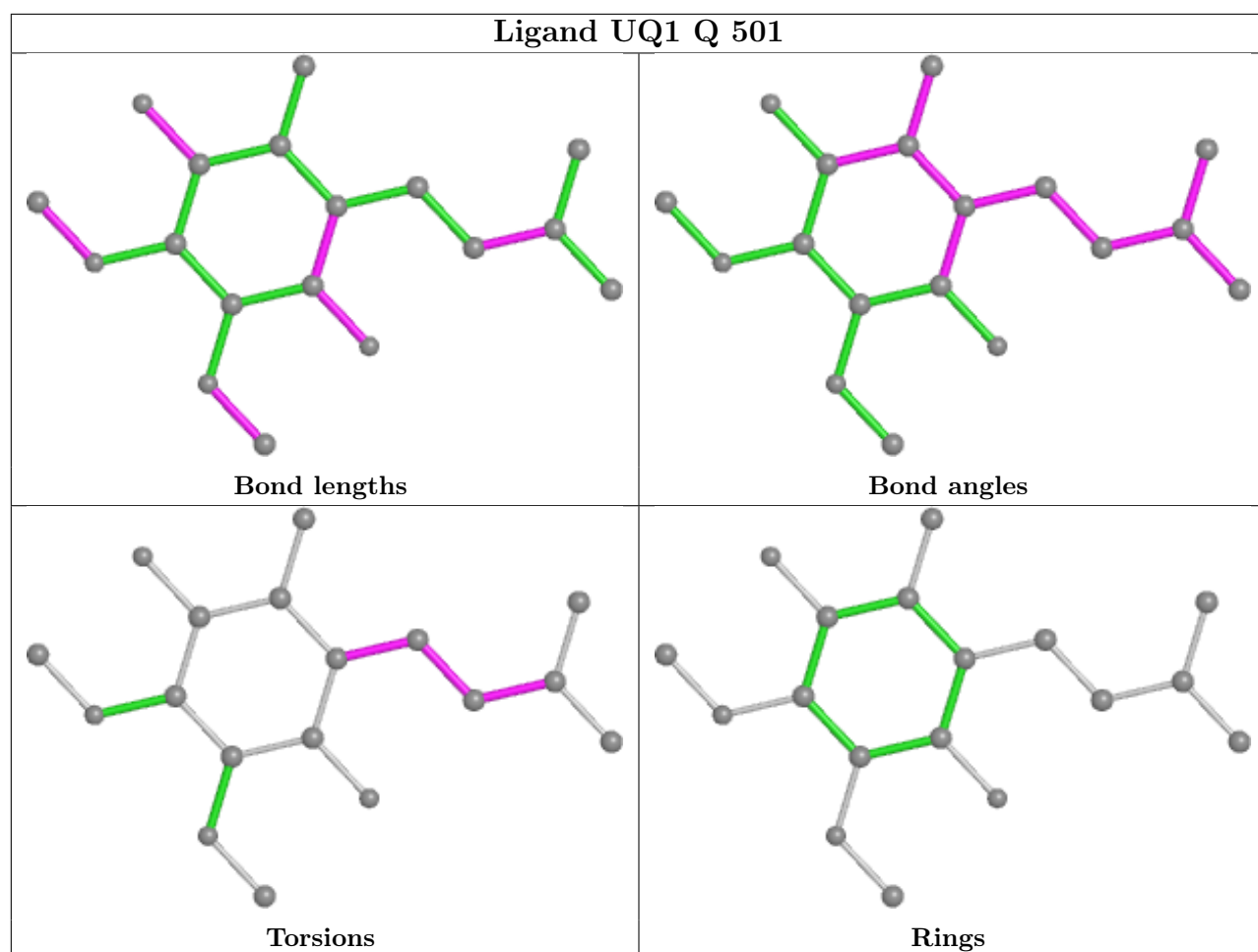


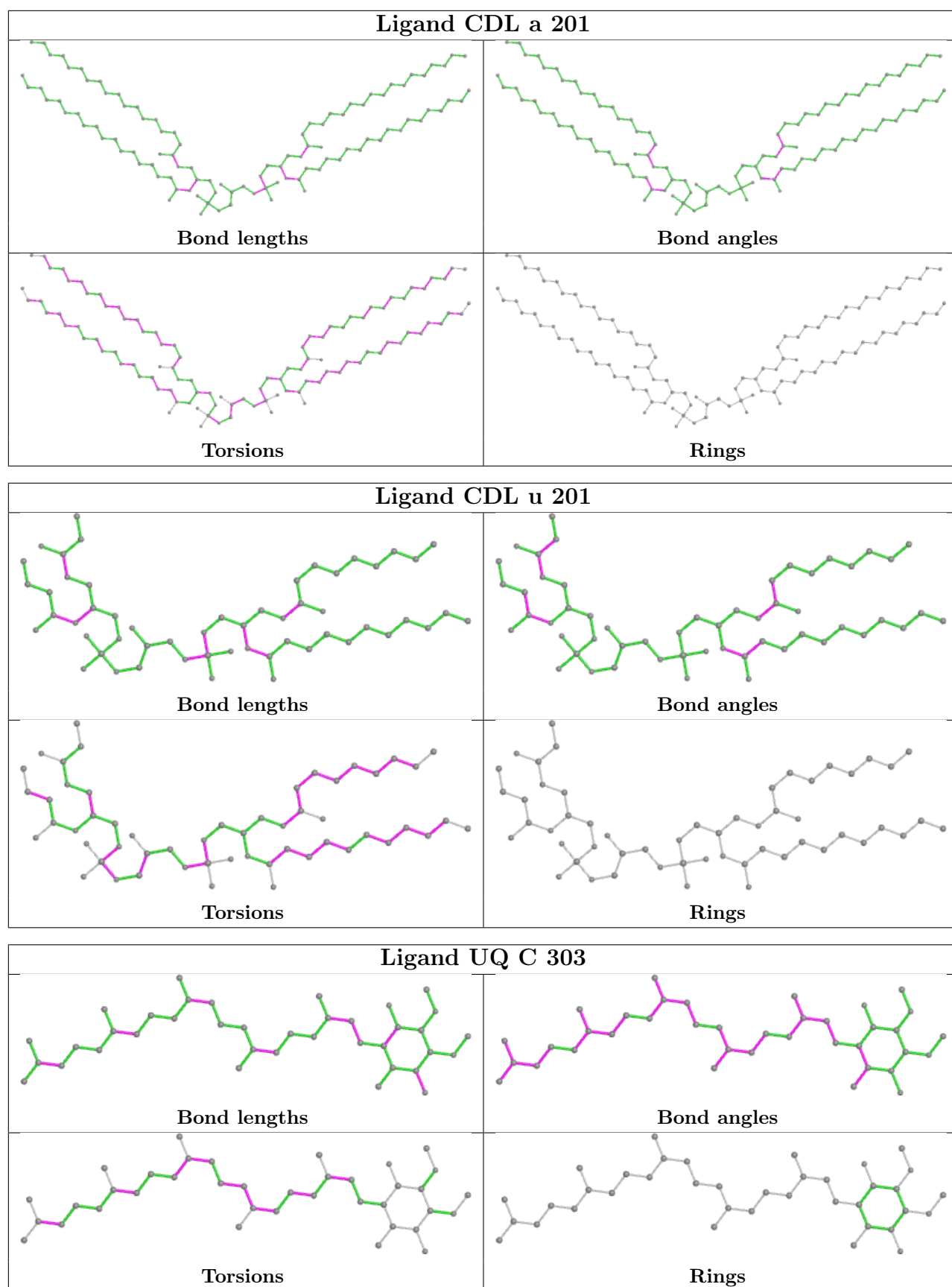


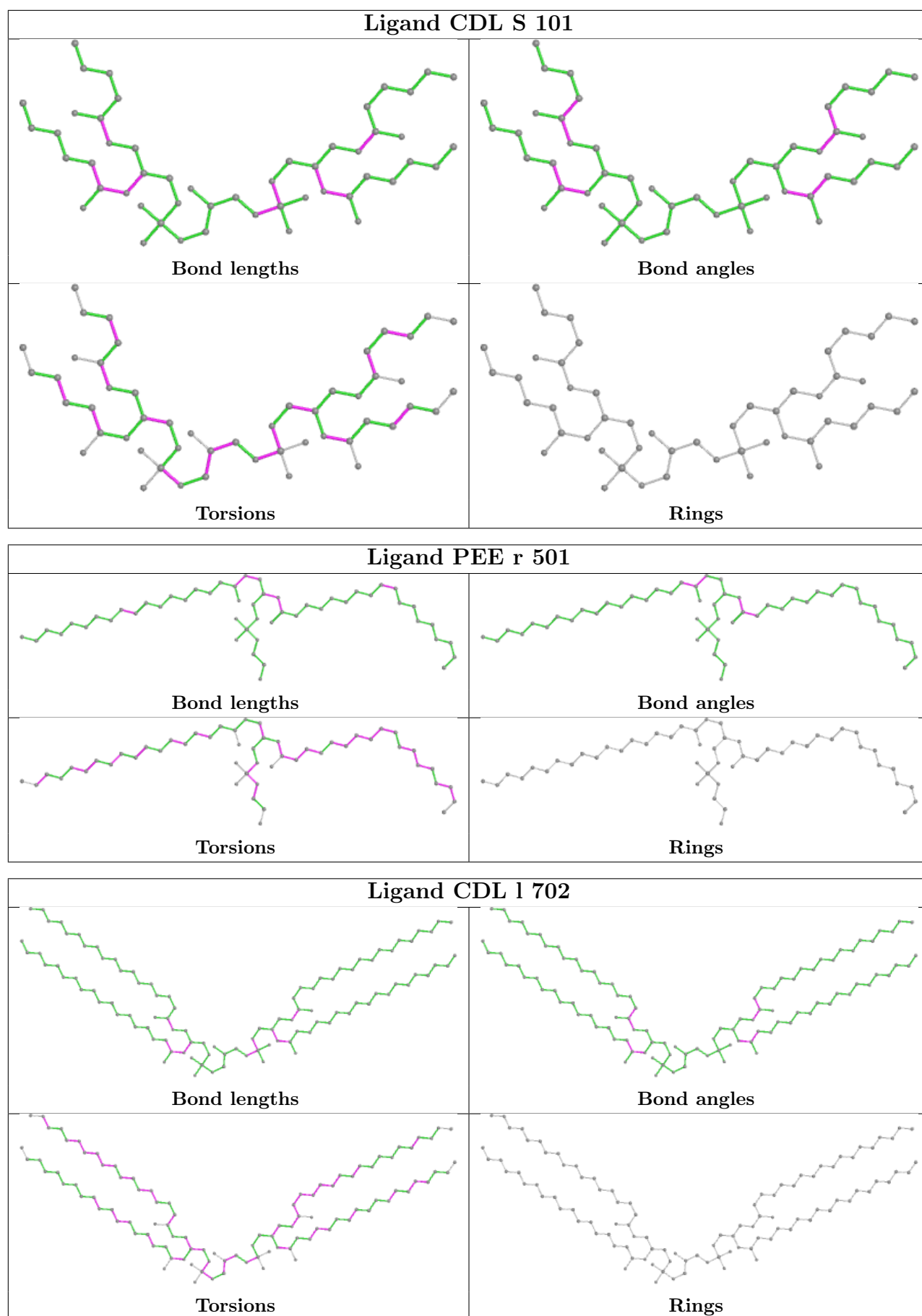


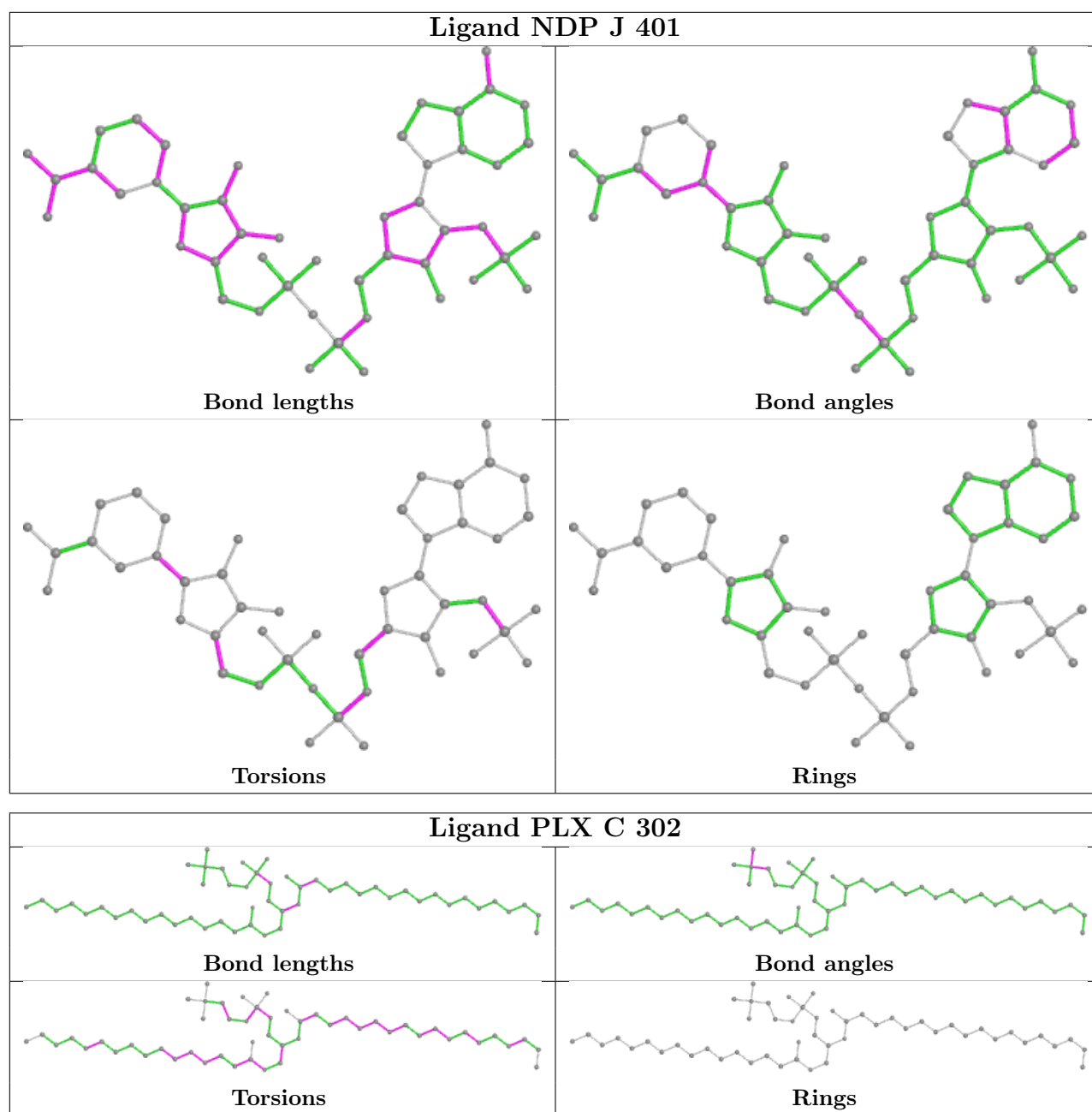












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

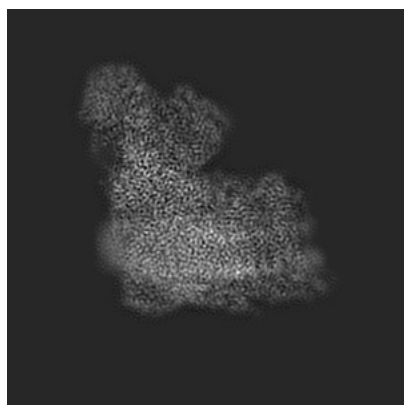
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32302. These allow visual inspection of the internal detail of the map and identification of artifacts.

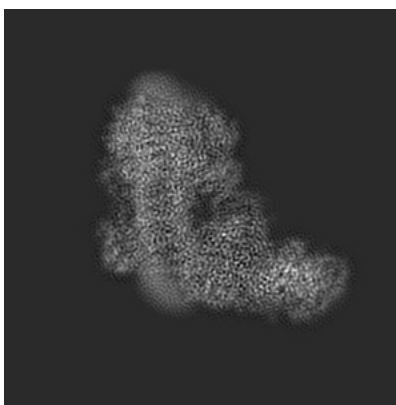
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

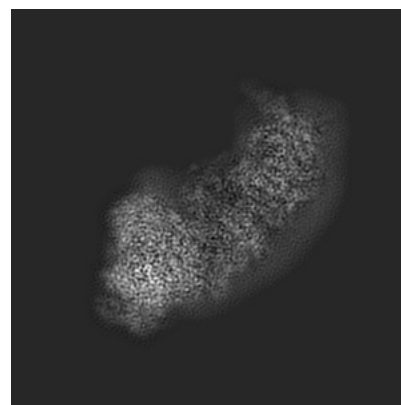
6.1.1 Primary map



X



Y

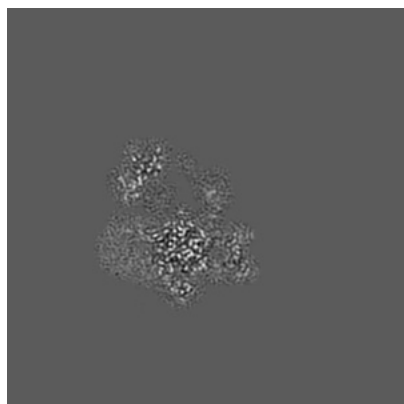


Z

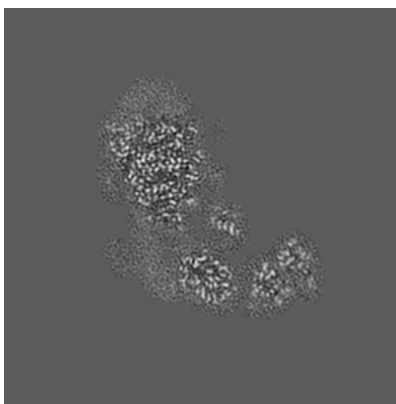
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

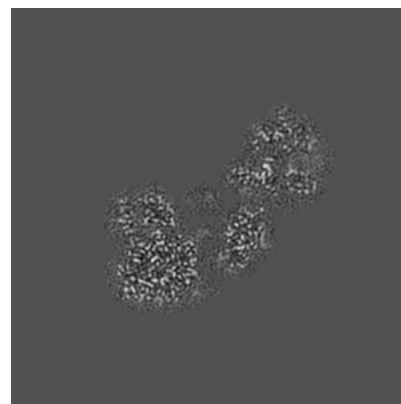
6.2.1 Primary map



X Index: 152



Y Index: 152

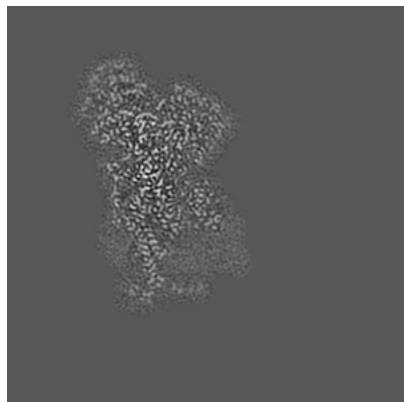


Z Index: 152

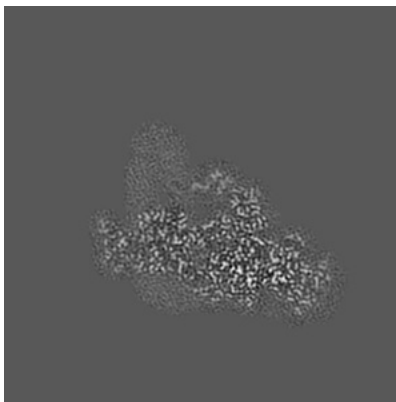
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

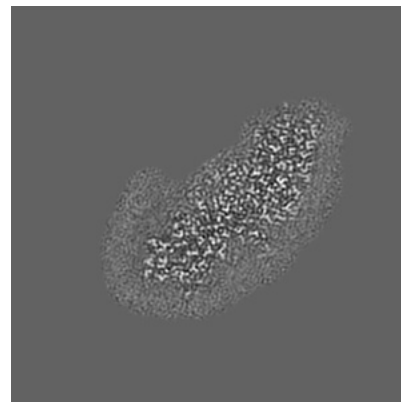
6.3.1 Primary map



X Index: 104



Y Index: 105

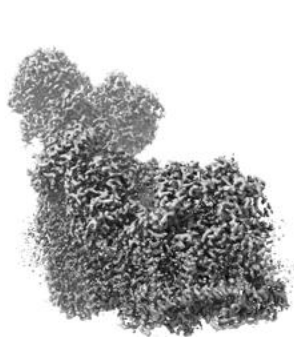


Z Index: 129

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 0.0308. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

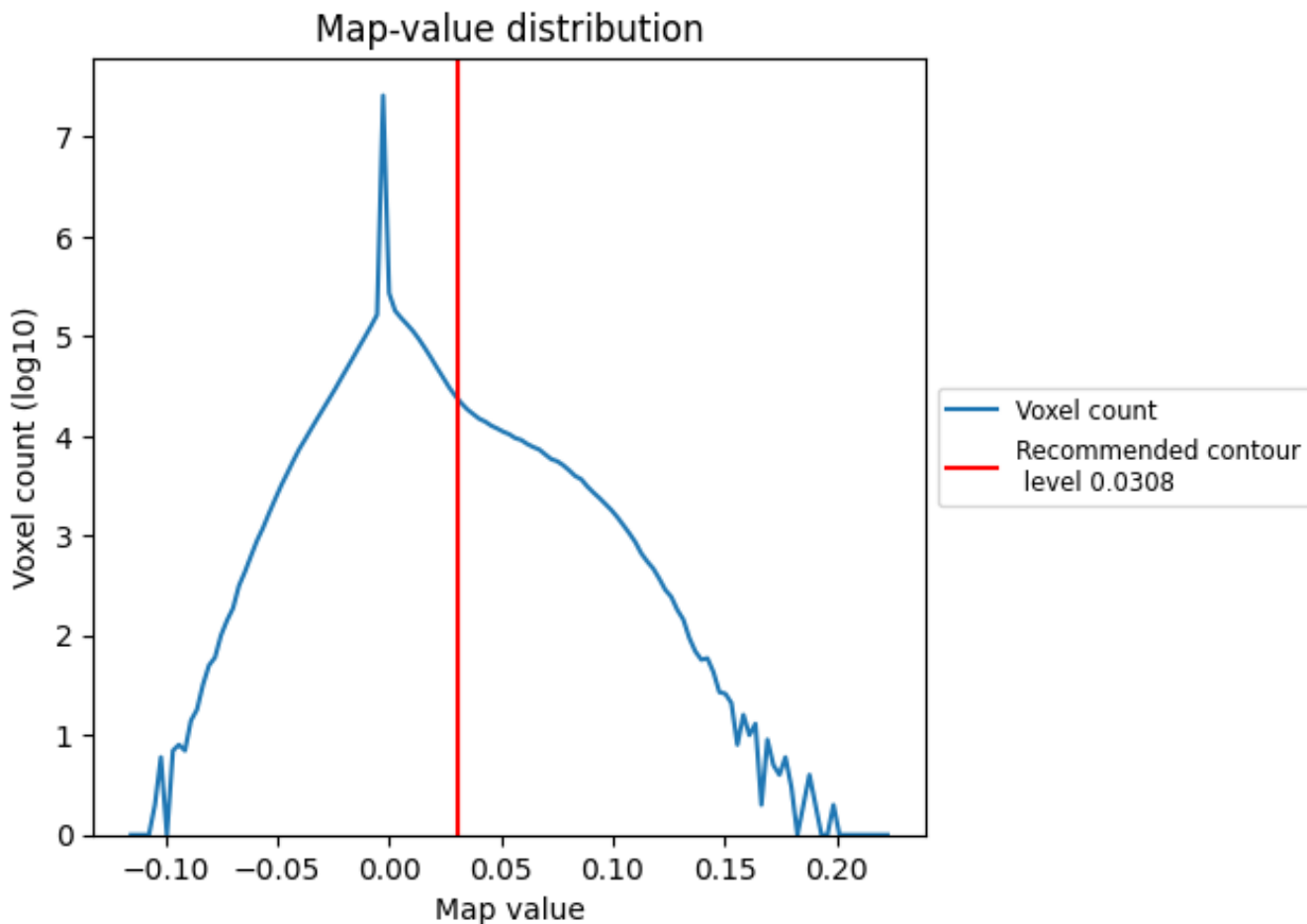
6.5 Mask visualisation

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

7 Map analysis [i](#)

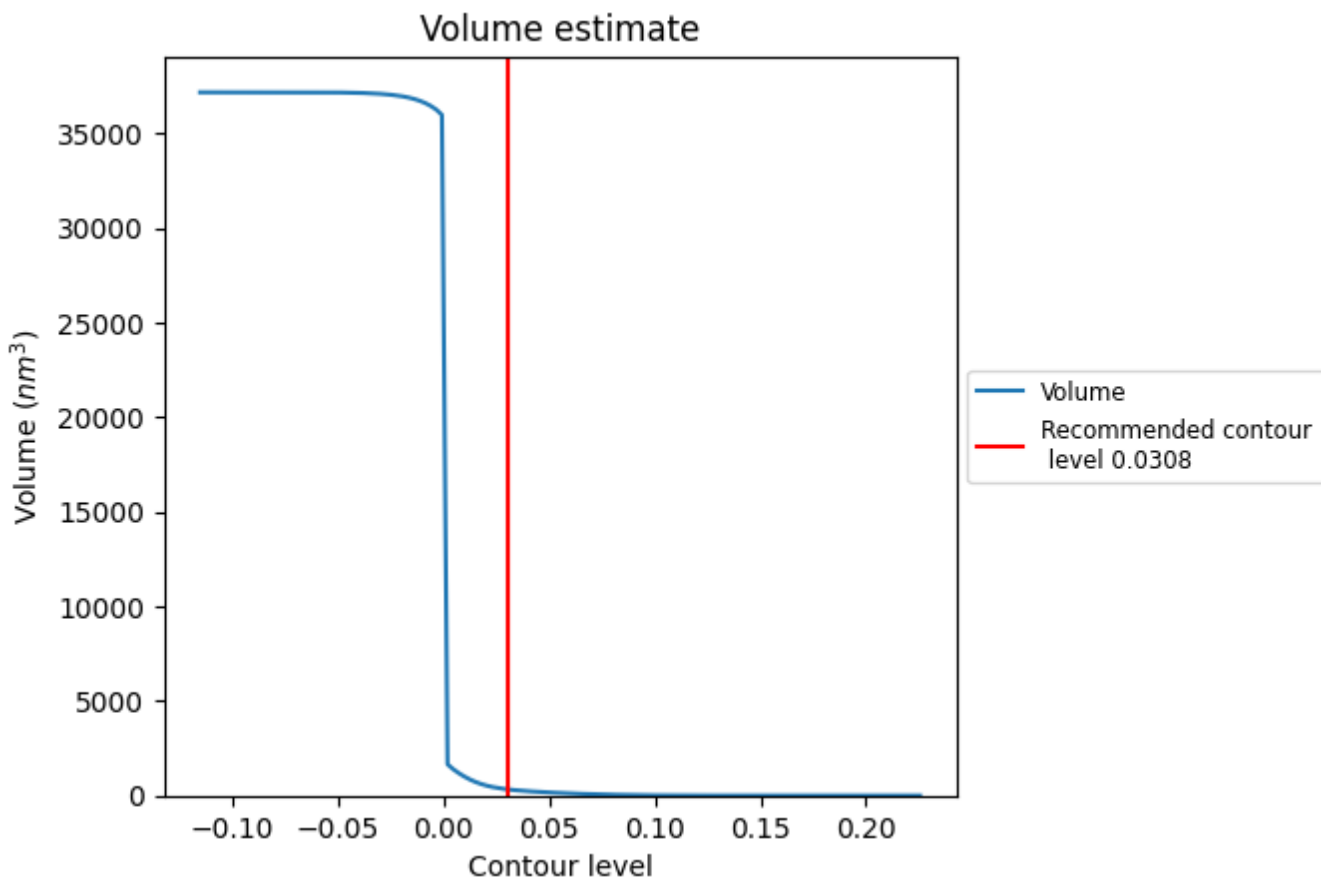
This section contains the results of statistical analysis of the map.

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.

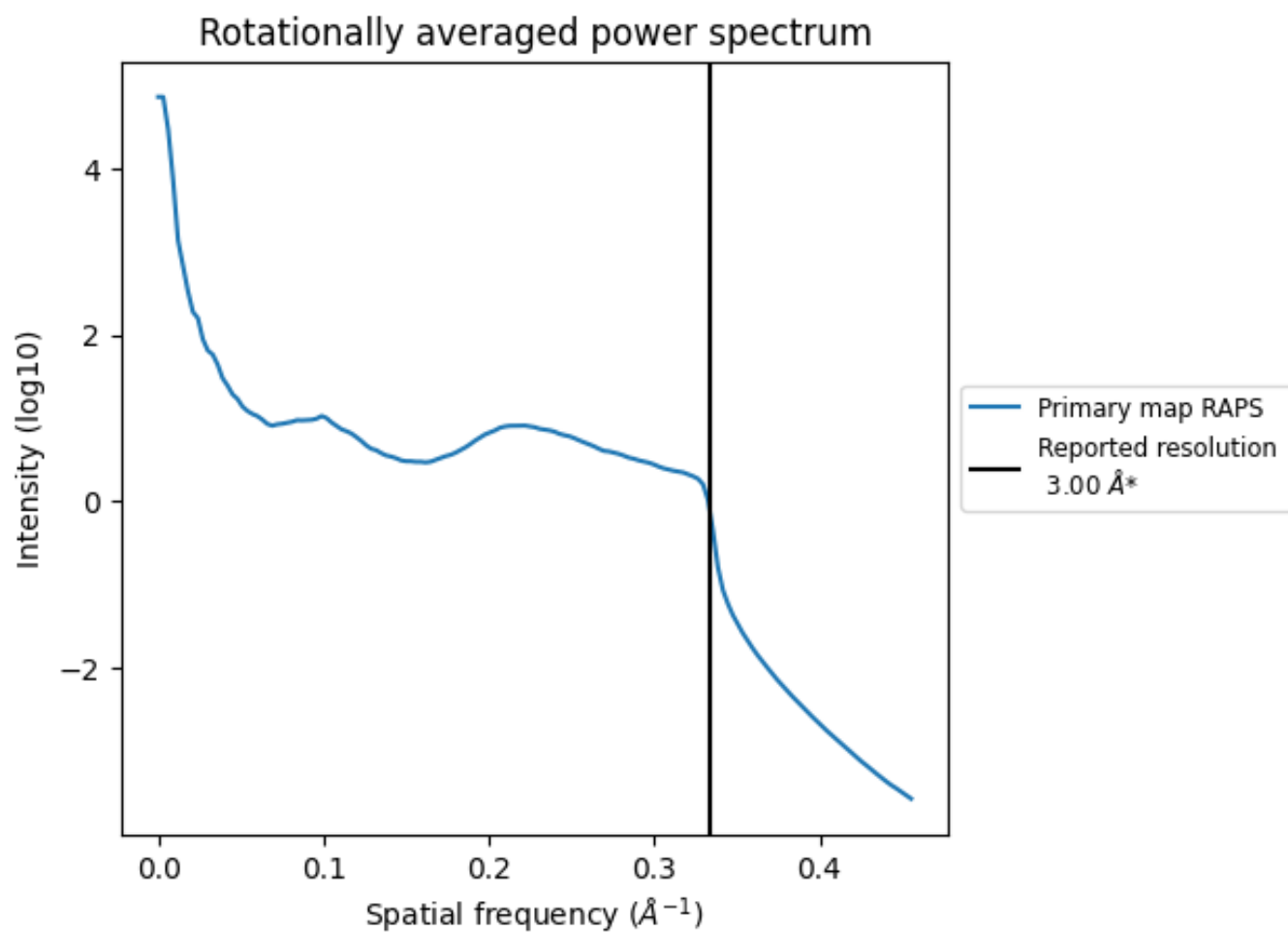
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 321 nm³; this corresponds to an approximate mass of 290 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

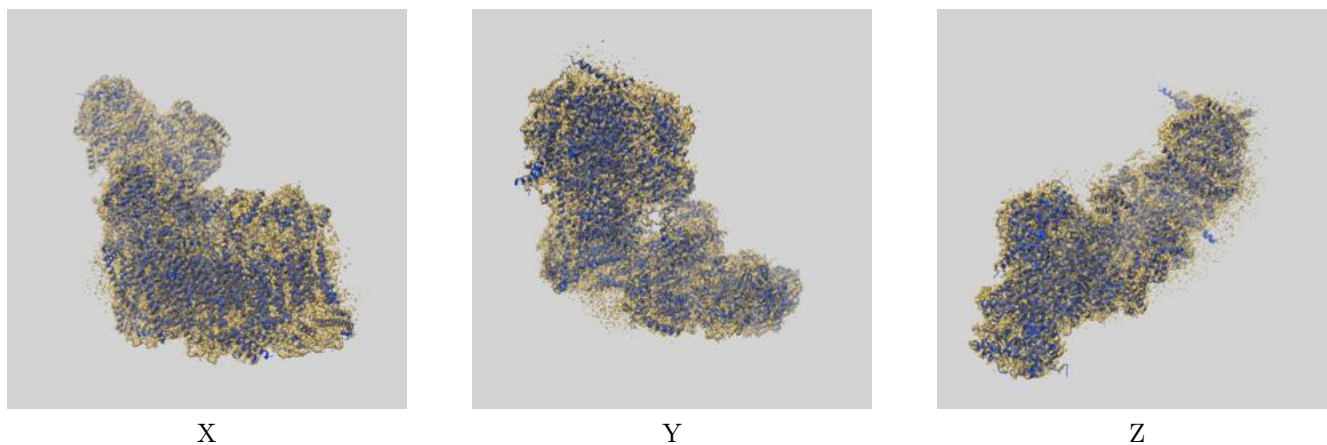
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

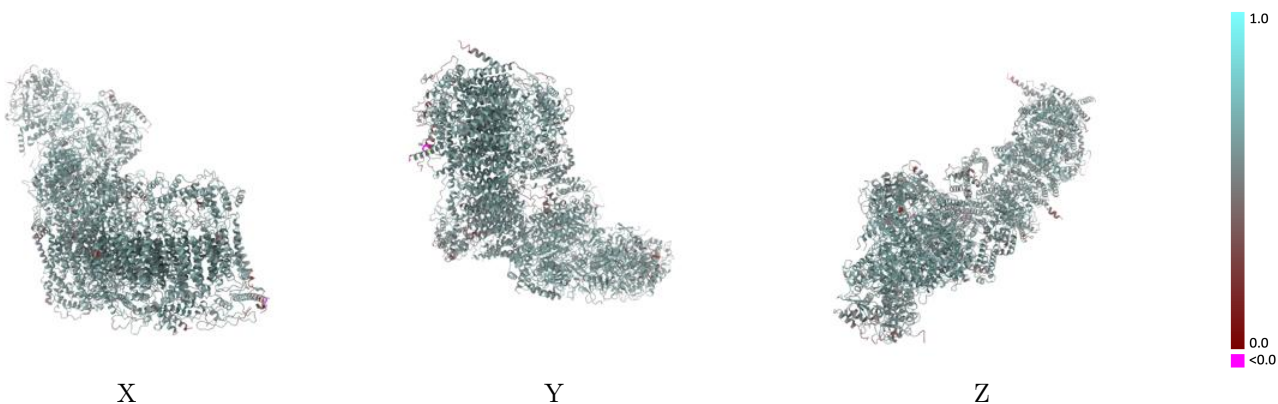
This section contains information regarding the fit between EMDB map EMD-32302 and PDB model 7W4E. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



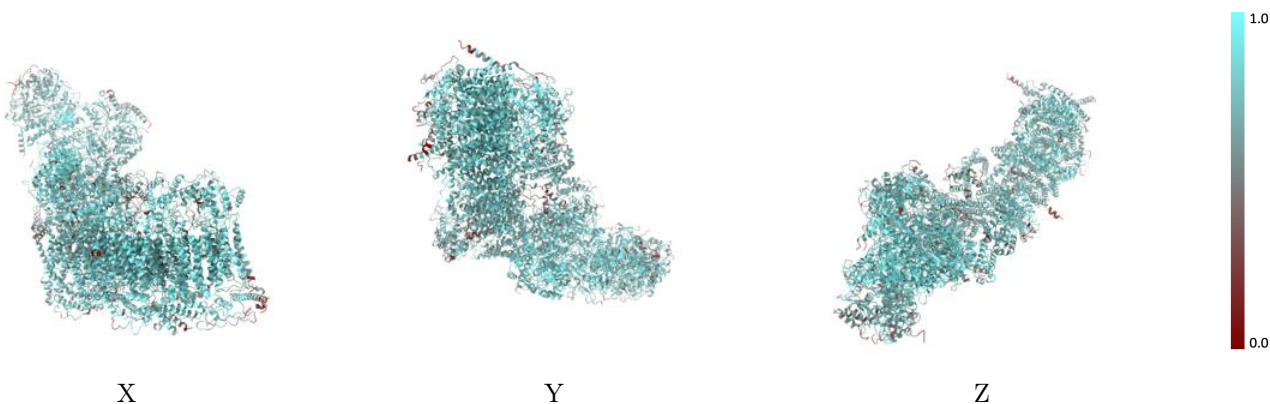
The images above show the 3D surface view of the map at the recommended contour level 0.0308 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



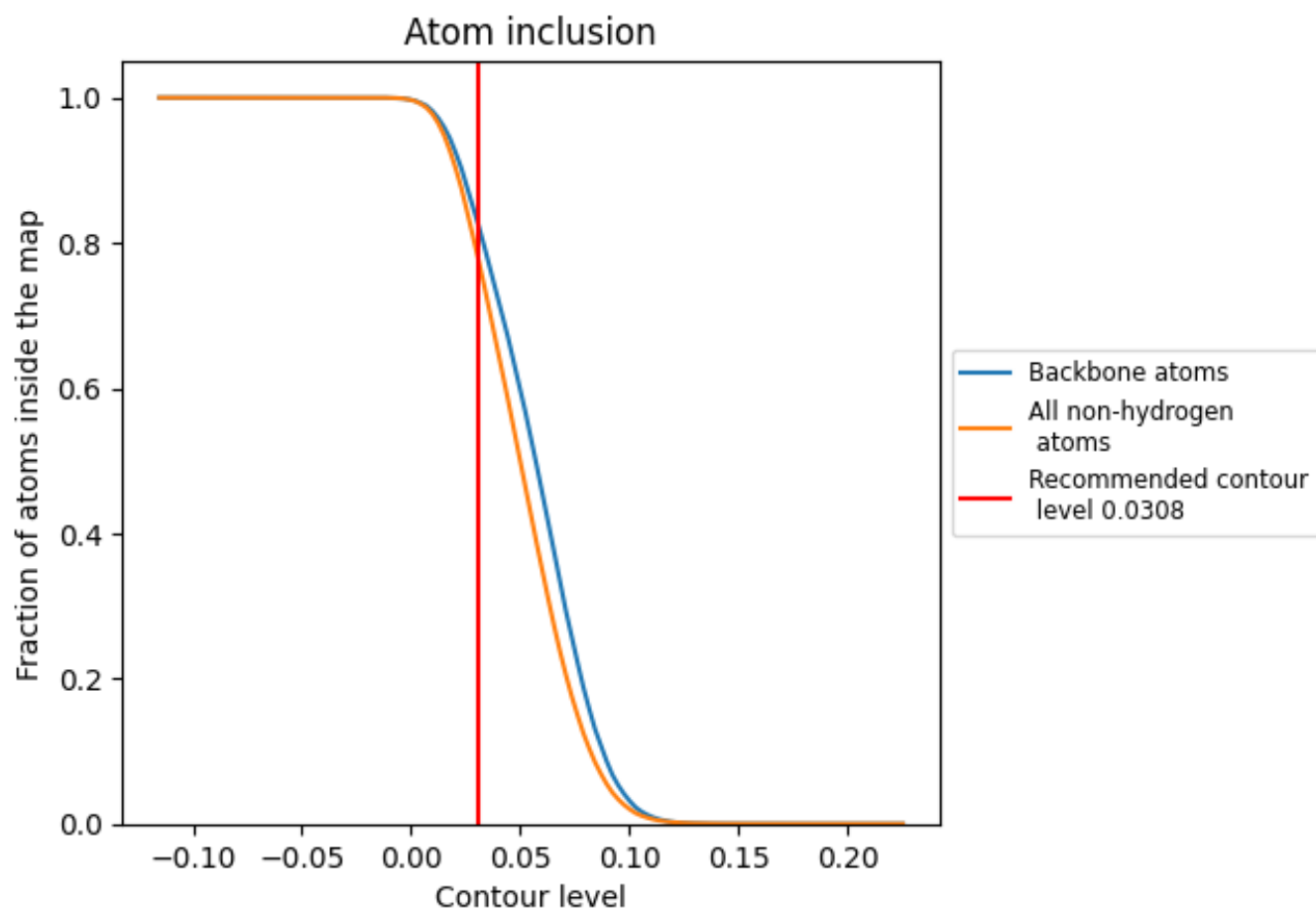
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0308).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.0308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7788	 0.5790
A	 0.7246	 0.5560
B	 0.8875	 0.6180
C	 0.8837	 0.6180
E	 0.8038	 0.5980
F	 0.6510	 0.5170
G	 0.5139	 0.4670
H	 0.7609	 0.5720
I	 0.7460	 0.5660
J	 0.8029	 0.5910
K	 0.6254	 0.5240
L	 0.8099	 0.6010
M	 0.8096	 0.5880
N	 0.7888	 0.5930
O	 0.6939	 0.5460
P	 0.9024	 0.6230
Q	 0.8751	 0.6160
S	 0.7828	 0.5860
T	 0.7839	 0.5910
U	 0.7170	 0.5360
V	 0.6275	 0.5500
W	 0.7373	 0.5620
X	 0.7172	 0.5610
Y	 0.6608	 0.5160
Z	 0.6272	 0.5080
a	 0.7598	 0.5810
b	 0.6977	 0.5360
c	 0.7795	 0.5810
d	 0.7406	 0.5610
e	 0.7222	 0.5520
f	 0.5892	 0.5060
g	 0.7768	 0.5810
h	 0.7422	 0.5590
i	 0.8637	 0.6080
j	 0.7689	 0.5910



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Chain	Atom inclusion	Q-score
k	 0.8329	 0.6050
l	 0.8088	 0.5920
m	 0.7041	 0.5440
n	 0.6034	 0.5130
o	 0.7707	 0.5820
p	 0.7779	 0.5780
r	 0.8327	 0.6020
s	 0.8357	 0.6030
u	 0.7291	 0.5450
v	 0.6788	 0.5220
w	 0.7547	 0.5630