



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:07 AM UTC

PDB ID : 8Q47 / pdb_00008q47
EMDB ID : EMD-18140
Title : Inward-facing, open1 proteoliposome complex I at 2.9 Å. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-05
Resolution : 2.90 Å(reported)
Based on initial model : 7QSN

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:

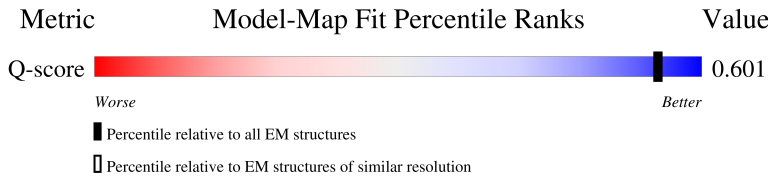
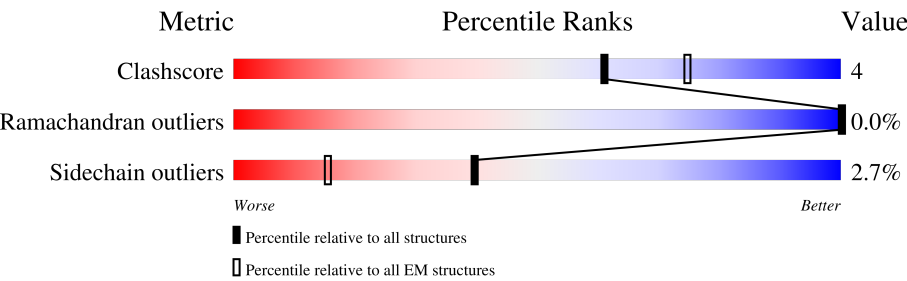
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



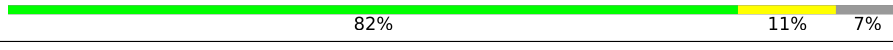
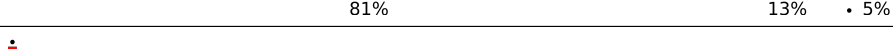
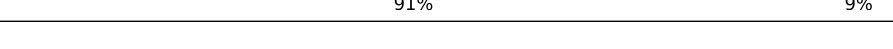
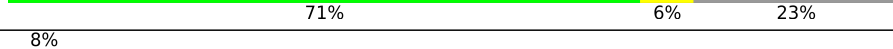
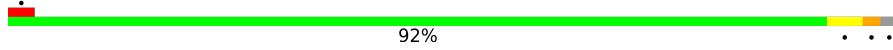
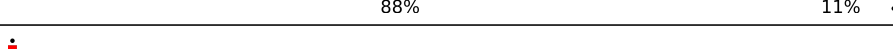
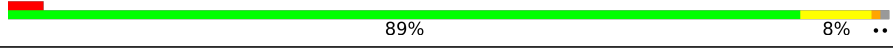
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	115	
2	B	216	
3	C	266	
4	D	463	

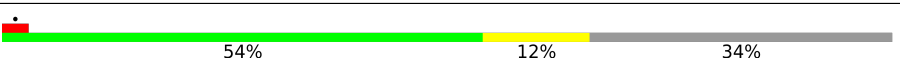
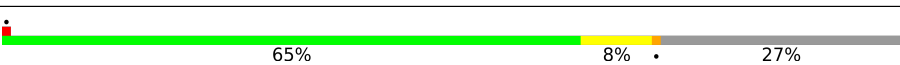
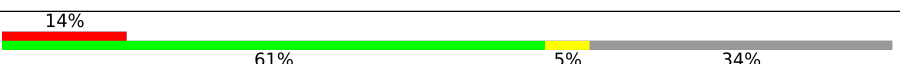
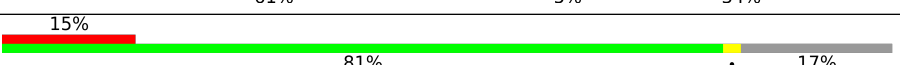
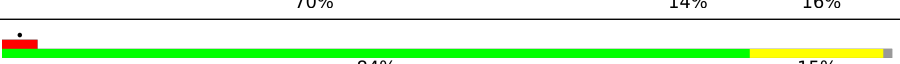
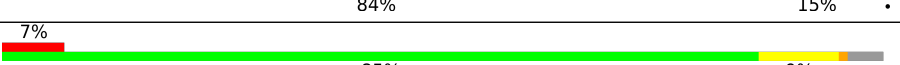
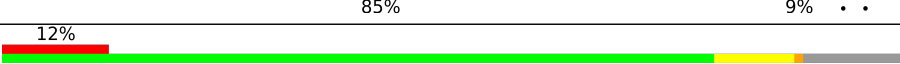
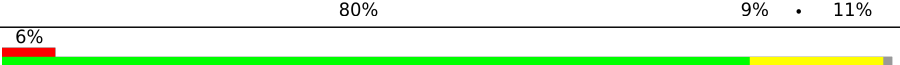
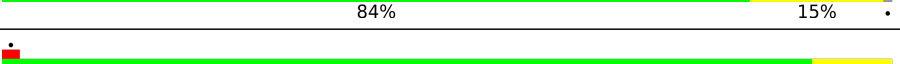
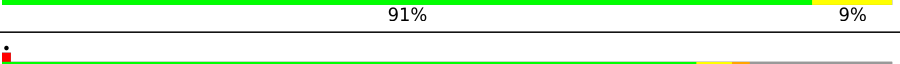
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 69237 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	421	Total	C	N	O	S	0	0
			3392	2168	584	615	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	0	0
			3326	2096	594	616	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	691	Total	C	N	O	S	0	0
			5298	3318	925	1016	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	339	Total	C	N	O	S	0	0
			2728	1765	484	474	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

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

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			707	454	104	144	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total	C	N	O	S	0	0
			923	597	156	167	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	116	Total	C	N	O	S	0	0
			982	628	182	168	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	142	Total	C	N	O	S	0	0
			1157	743	202	203	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			654	427	109	116	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	98	Total	C	N	O	S	0	0
			825	521	157	141	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			846	544	140	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	127	Total	C	N	O	S	0	0
			1097	722	191	183	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	128	Total	C	N	O	S	0	0
			1070	686	188	196			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	174	Total	C	N	O	S	0	0
			1458	913	269	268	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1212	780	216	211	5		

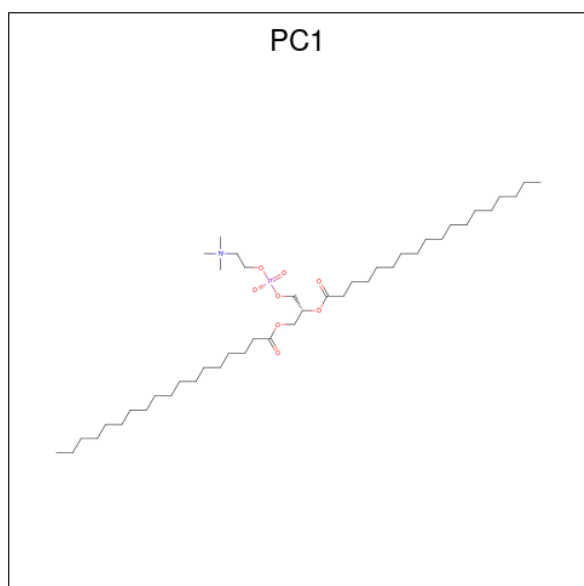
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			776	490	144	139	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



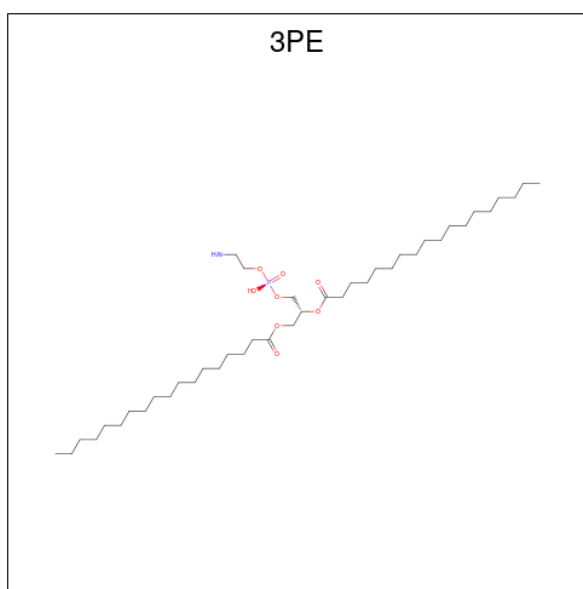
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	H	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	I	1	Total	C	N	O	P	0
			37	27	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
45	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	M	1	Total	C	N	O	P	0
			26	16	1	8	1	
45	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	h	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	m	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	q	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	I	1	Total	C	N	O	P	0
			36	26	1	8	1	

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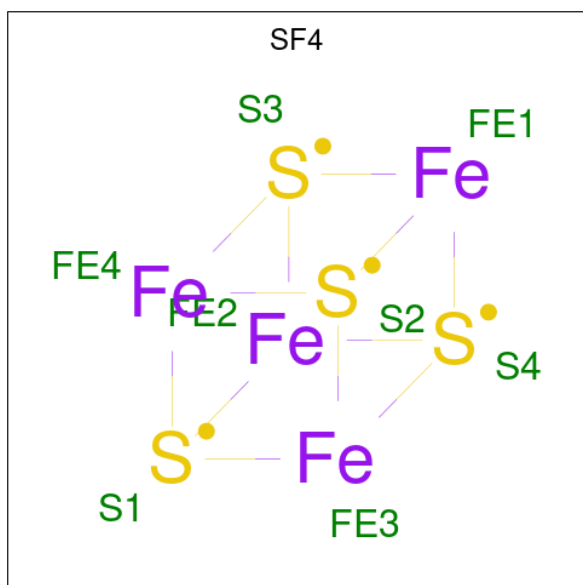
Mol	Chain	Residues	Atoms					AltConf
46	J	1	Total 33	C 23	N 1	O 8	P 1	0
46	J	1	Total 44	C 34	N 1	O 8	P 1	0
46	L	1	Total 35	C 25	N 1	O 8	P 1	0
46	L	1	Total 45	C 35	N 1	O 8	P 1	0
46	L	1	Total 46	C 36	N 1	O 8	P 1	0
46	L	1	Total 37	C 27	N 1	O 8	P 1	0
46	M	1	Total 50	C 40	N 1	O 8	P 1	0
46	N	1	Total 49	C 39	N 1	O 8	P 1	0
46	N	1	Total 36	C 26	N 1	O 8	P 1	0
46	Y	1	Total 45	C 35	N 1	O 8	P 1	0
46	Y	1	Total 27	C 17	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 45	C 35	N 1	O 8	P 1	0
46	Z	1	Total 45	C 35	N 1	O 8	P 1	0
46	b	1	Total 47	C 37	N 1	O 8	P 1	0
46	d	1	Total 49	C 39	N 1	O 8	P 1	0
46	f	1	Total 29	C 19	N 1	O 8	P 1	0
46	f	1	Total 51	C 41	N 1	O 8	P 1	0
46	j	1	Total 44	C 34	N 1	O 8	P 1	0
46	m	1	Total 41	C 31	N 1	O 8	P 1	0

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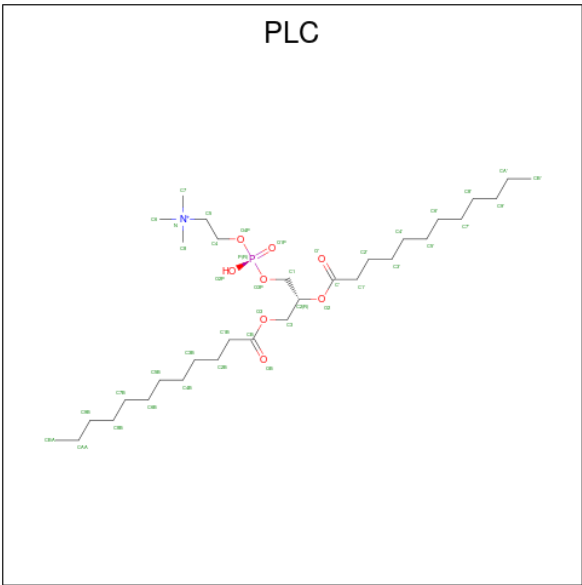
Mol	Chain	Residues	Atoms					AltConf
46	m	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	o	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



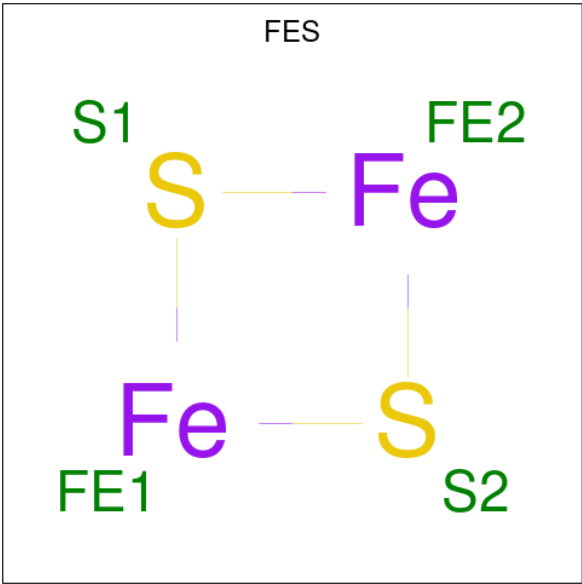
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $\text{C}_{32}\text{H}_{65}\text{NO}_8\text{P}$).



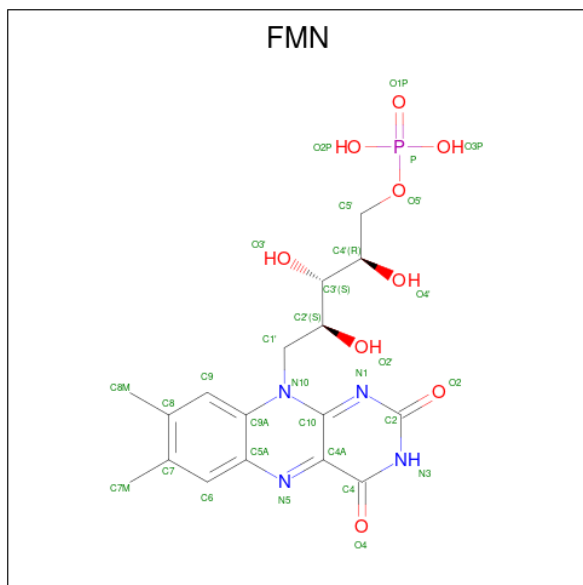
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
48	L	1	Total	C	N	O	P	0
			27	17	1	8	1	
48	O	1	Total	C	N	O	P	0
			26	16	1	8	1	
48	b	1	Total	C	N	O	P	0
			32	22	1	8	1	
48	g	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
49	E	1	Total	Fe	S	0
			4	2	2	
49	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

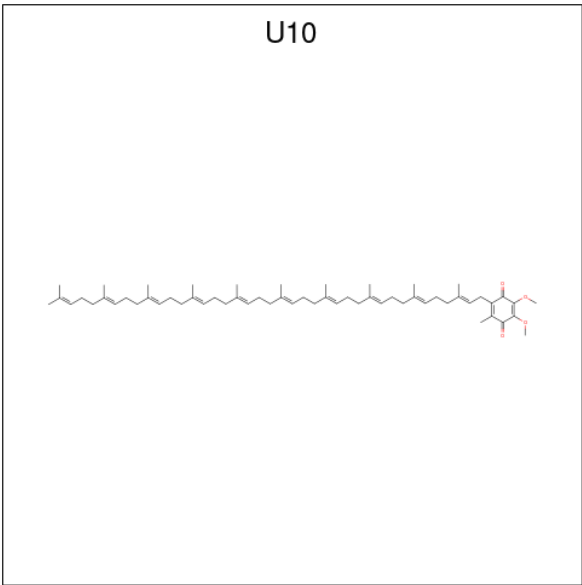


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

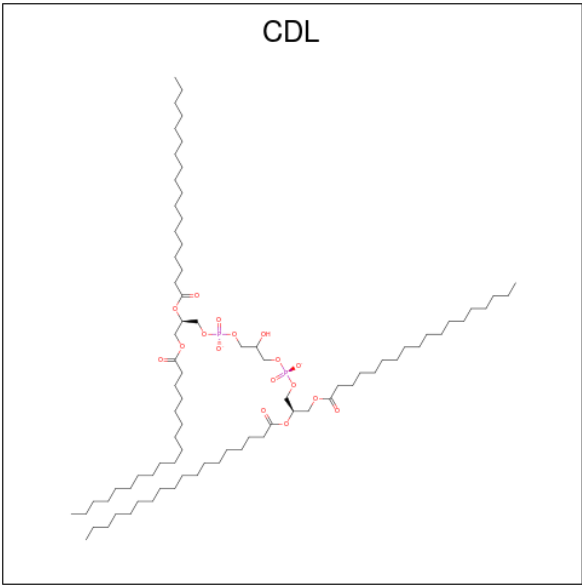
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	K	0
			1	1	

- Molecule 52 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
52	H	1	28	24	4	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	J	1	36	17	17	2	0
53	L	1	87	68	17	2	0
53	M	1	91	72	17	2	0

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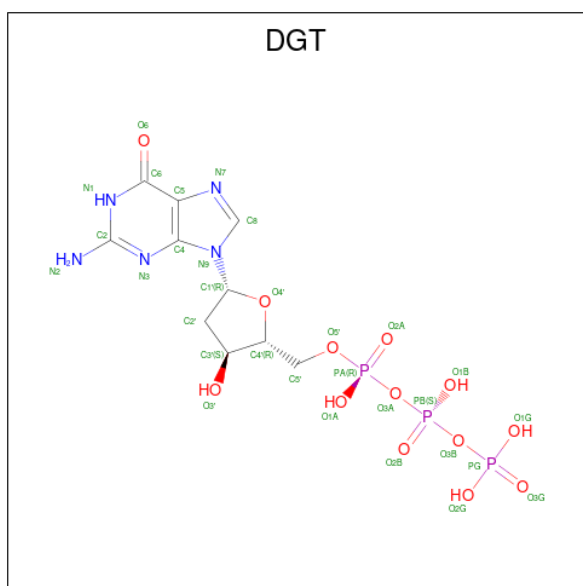
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Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			74	55	17	2	
53	X	1	Total	C	O	P	0
			87	68	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			80	61	17	2	
53	q	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	M	1	Total	Zn	0
			1	1	
54	R	1	Total	Zn	0
			1	1	

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



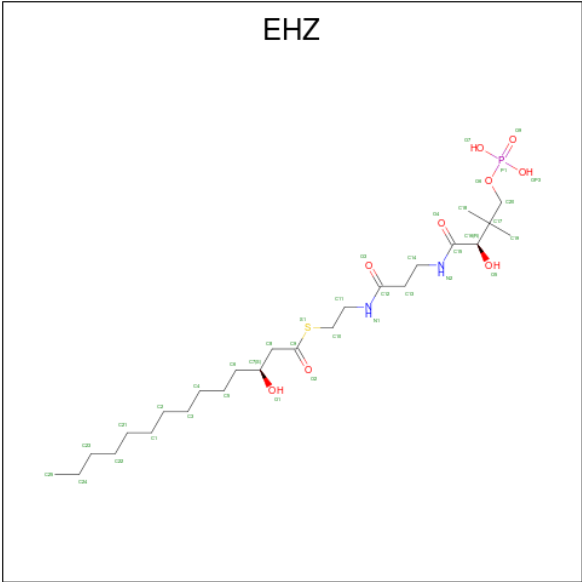
Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- | Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 56 | O | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- # NDP

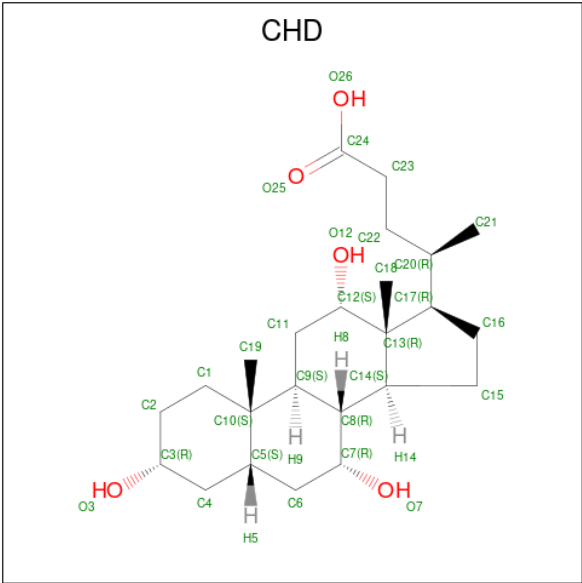
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EH2) (formula: C₂₅H₄₉N₂O₉PS).



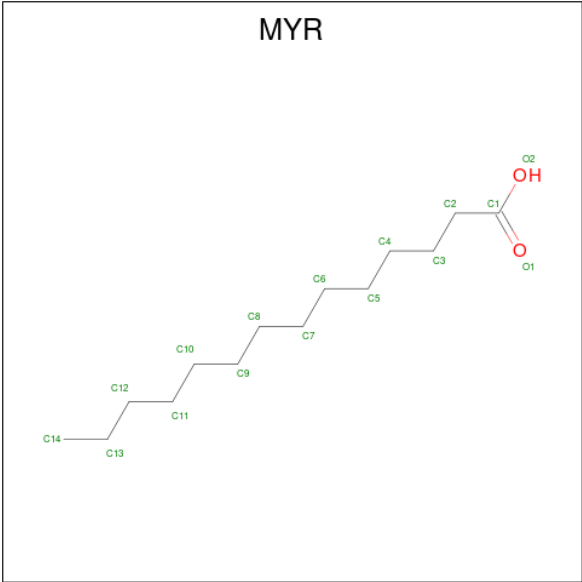
Mol	Chain	Residues	Atoms					AltConf
58	T	1	Total	C	N	O	P	S
			37	25	2	8	1	1
58	U	1	Total	C	N	O	P	S
			37	25	2	8	1	1

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
59	i	1	Total	C	O	0
			29	24	5	

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



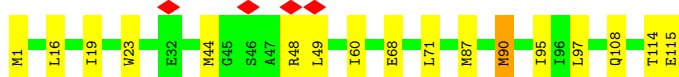
Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

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.

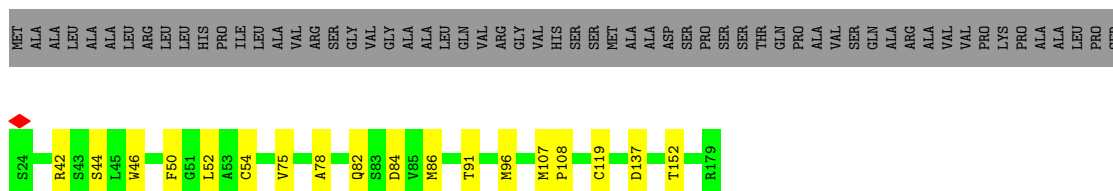
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



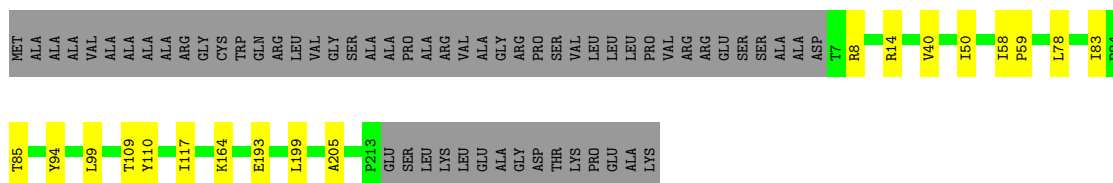
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



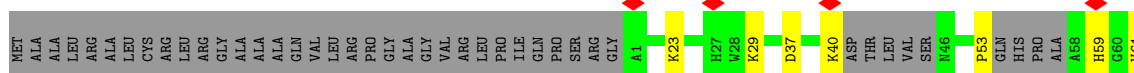
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

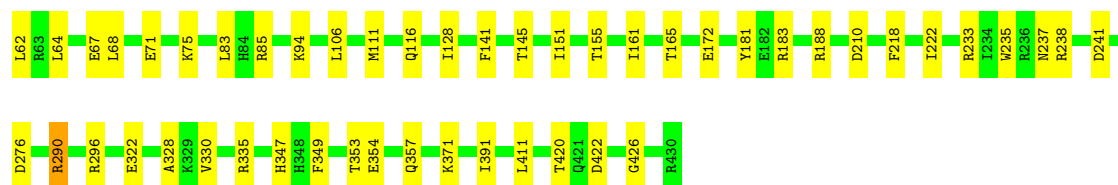
Chain C: 



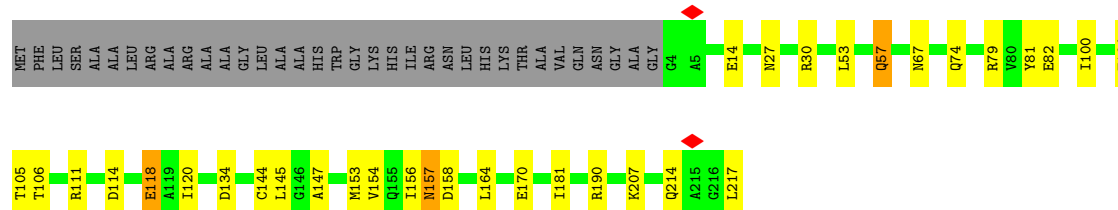
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 

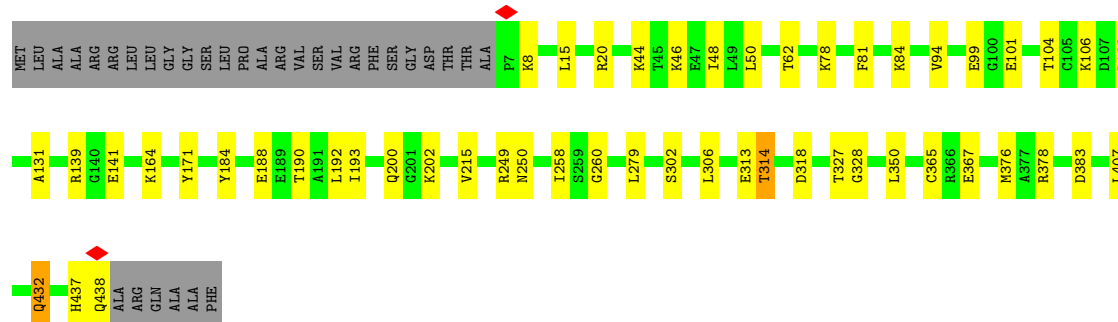
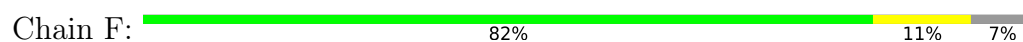




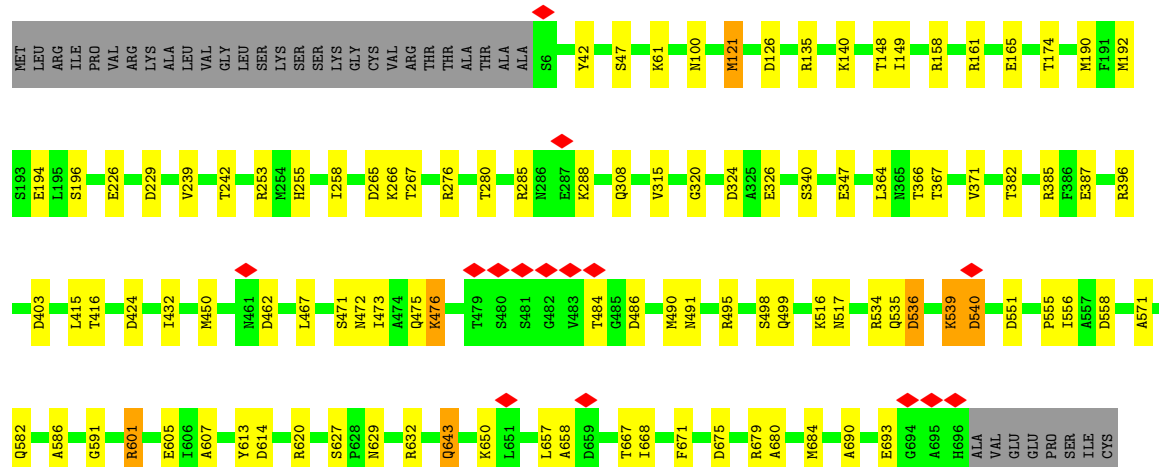
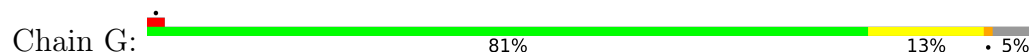
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



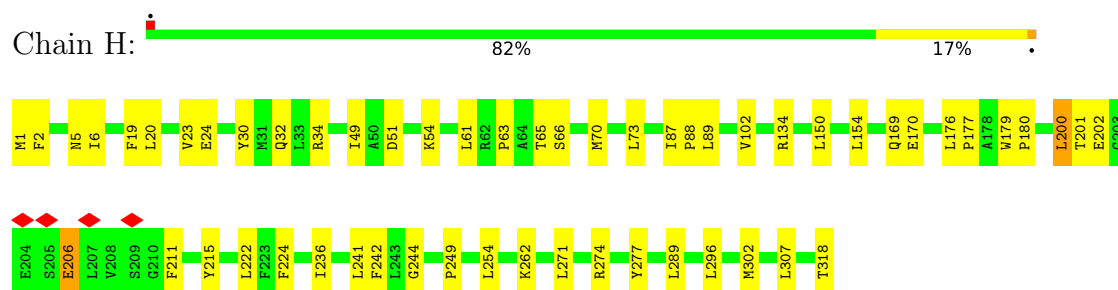
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



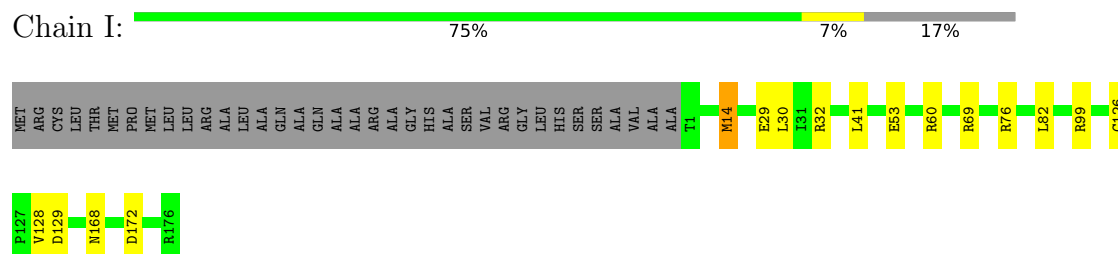
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



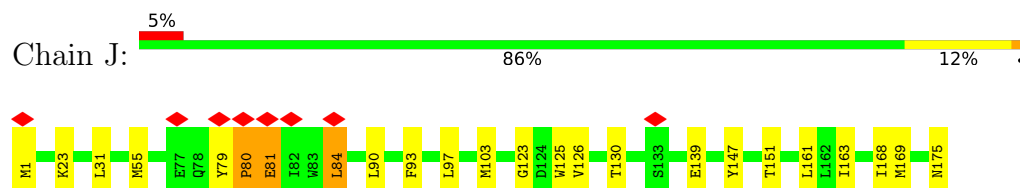
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



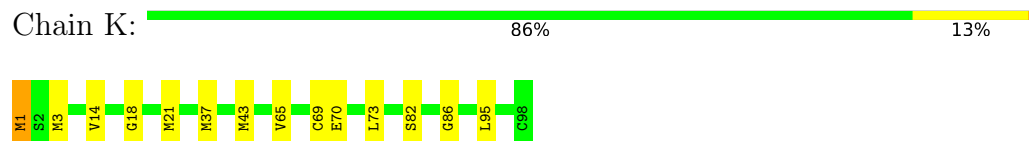
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



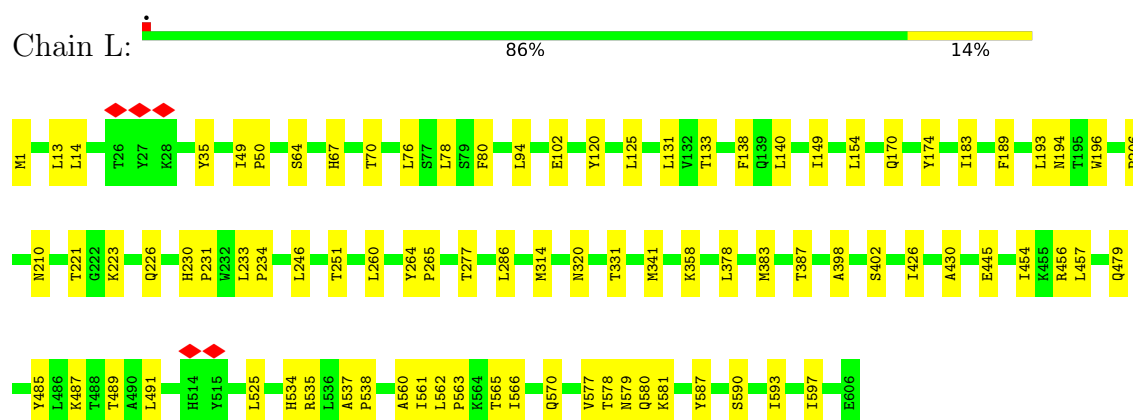
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

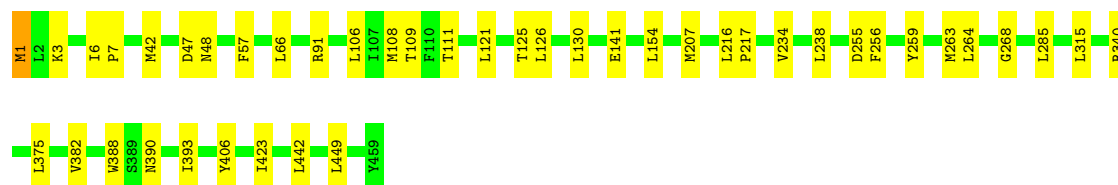


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



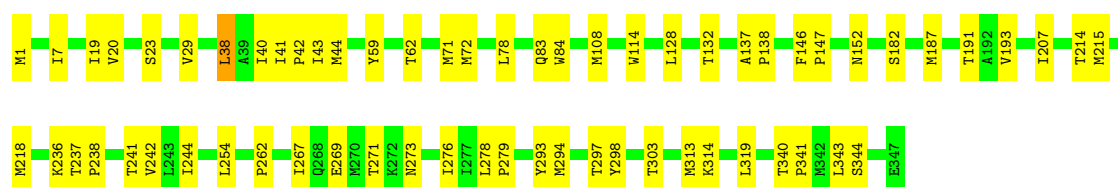
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  91% 9%



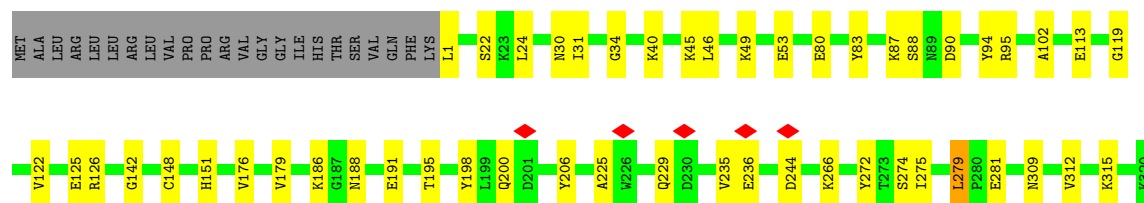
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  82% 18%



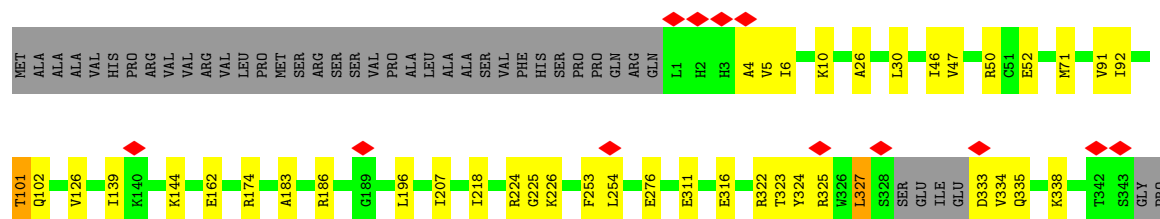
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  79% 14% 7%



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

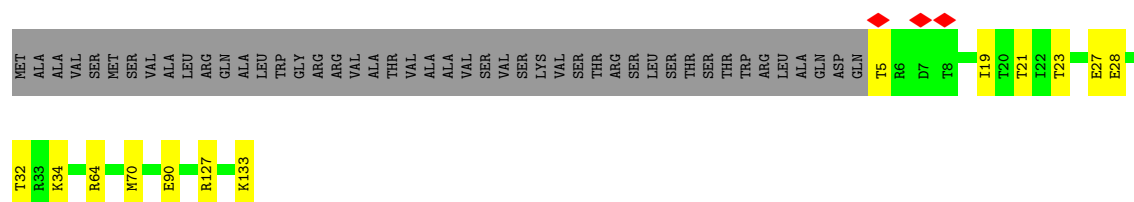
Chain P:  78% 11% 11%



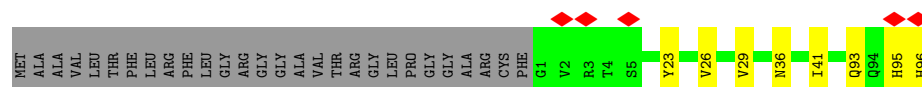
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  66% 7% 26%





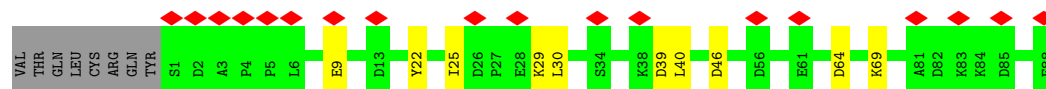
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



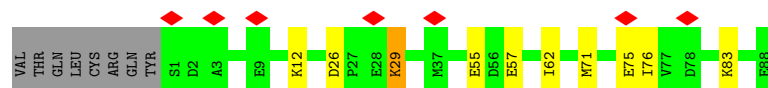
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



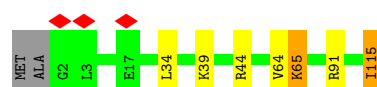
- Molecule 20: Acyl carrier protein, mitochondrial



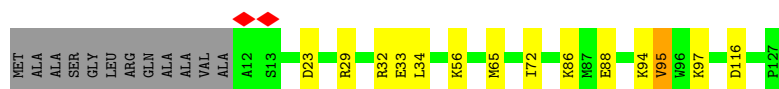
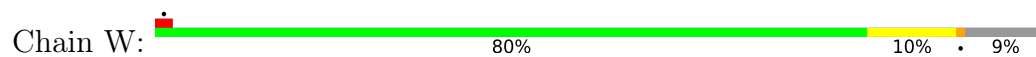
- Molecule 20: Acyl carrier protein, mitochondrial



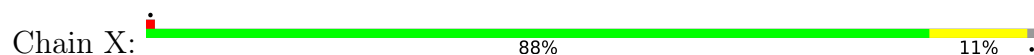
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



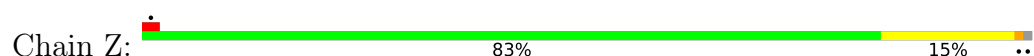
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



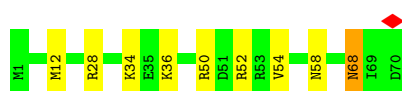
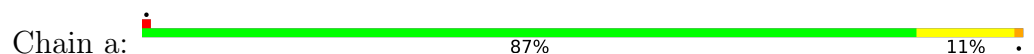
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



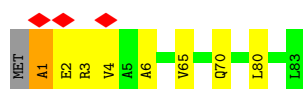
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

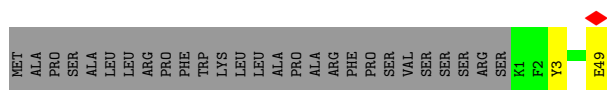


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

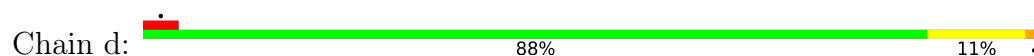


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

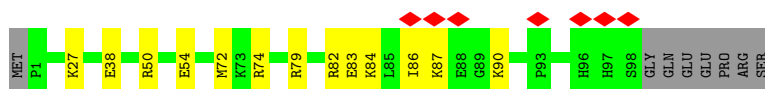
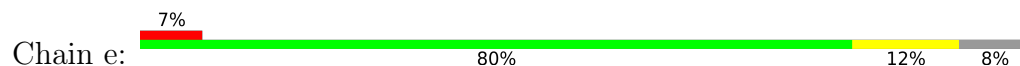




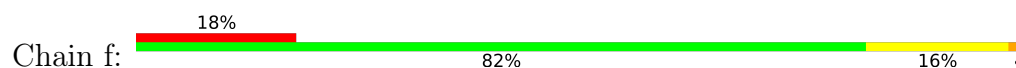
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



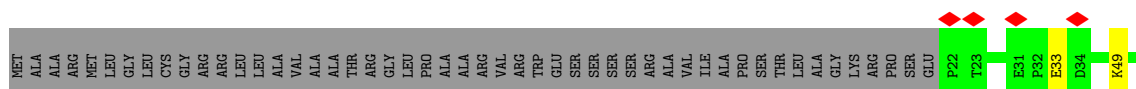
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



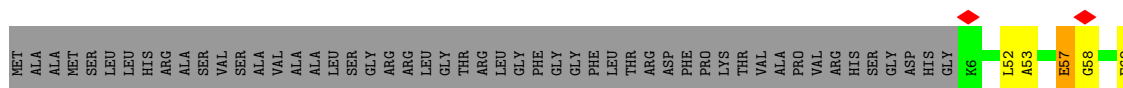
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



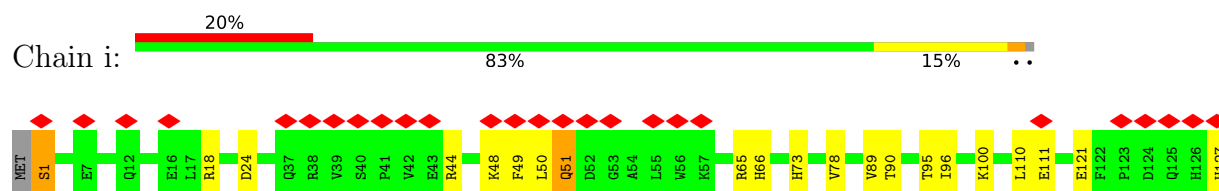
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



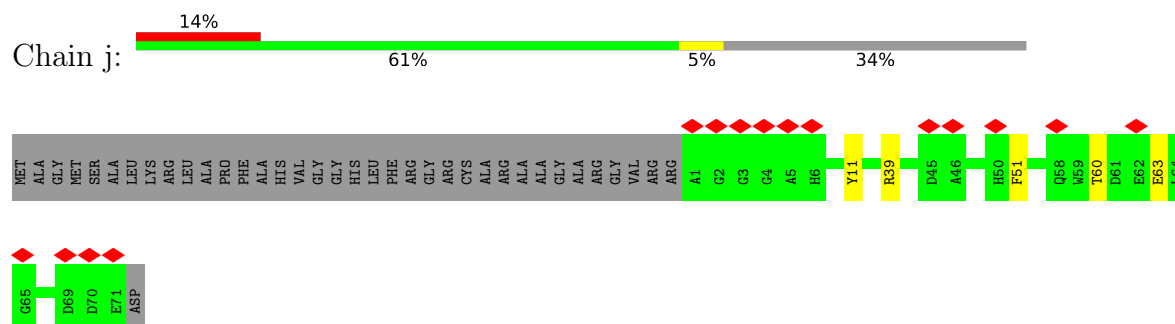
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



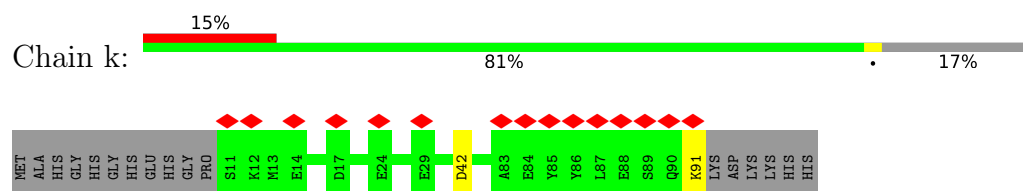
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



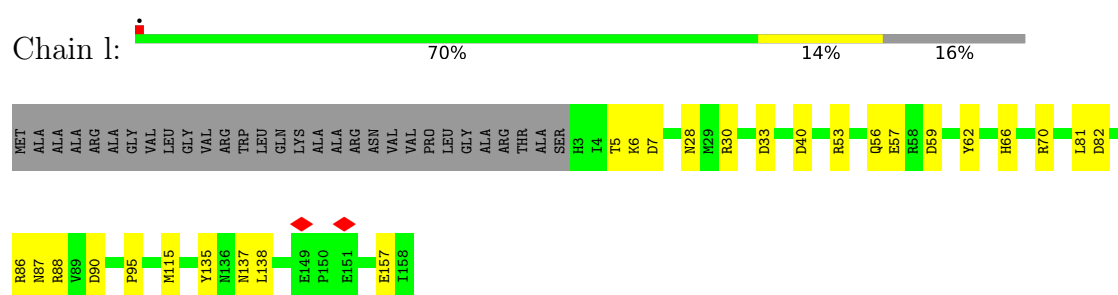
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



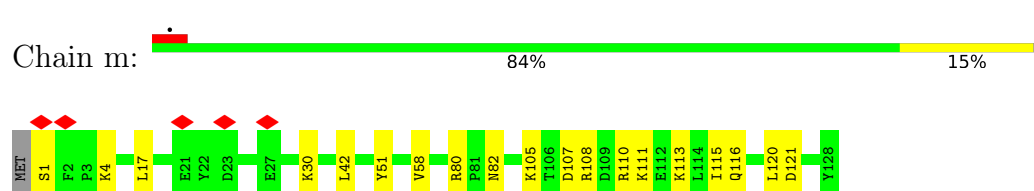
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



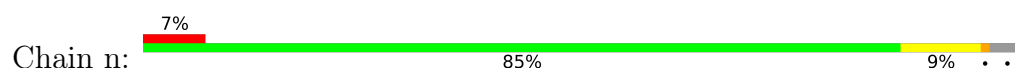
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

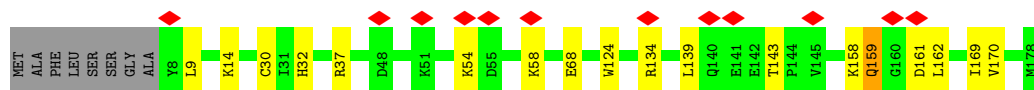


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

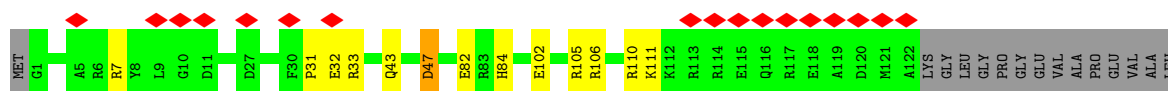
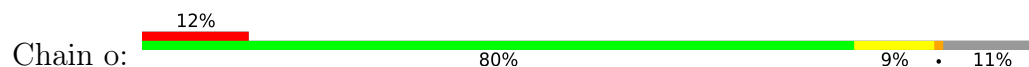


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

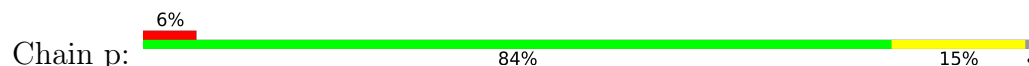




- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



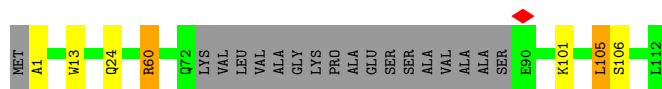
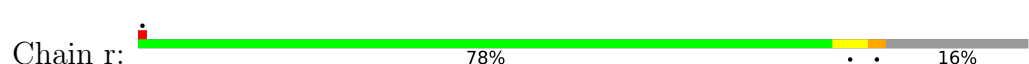
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



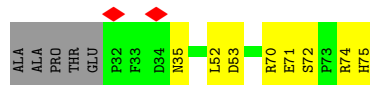
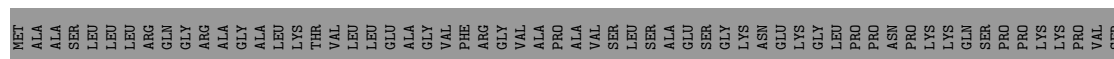
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30701	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 ($e^-/\text{\AA}^2$)	45.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.364	Depositor
Minimum map value	-0.007	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	479.69998, 479.69998, 479.69998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, PLC, PC1, MYR, SF4, FME, CHD, SAC, DGT, 2MR, K, ZN, AME, U10, MG, NDP, EHZ, CDL, FMN, 3PE, FES

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	0.13	0/936	0.23	0/1281
2	B	0.19	0/1278	0.25	0/1728
3	C	0.18	0/1772	0.25	0/2413
4	D	0.18	0/3466	0.24	0/4692
5	E	0.14	0/1699	0.26	0/2312
6	F	0.15	0/3401	0.25	0/4595
7	G	0.16	0/5387	0.25	0/7301
8	H	0.16	0/2571	0.27	0/3513
9	I	0.20	0/1445	0.28	0/1956
10	J	0.14	0/1370	0.24	0/1859
11	K	0.14	0/745	0.23	0/1008
12	L	0.14	0/4920	0.25	0/6694
13	M	0.16	0/3738	0.24	0/5097
14	N	0.17	0/2792	0.25	0/3800
15	O	0.12	0/2651	0.23	0/3587
16	P	0.14	0/2804	0.25	0/3803
17	Q	0.16	0/1072	0.24	0/1449
18	R	0.17	0/753	0.23	0/1014
19	S	0.11	0/702	0.24	0/945
20	T	0.12	0/719	0.24	0/971
20	U	0.12	0/719	0.25	0/971
21	V	0.13	0/943	0.22	0/1277
22	W	0.13	0/1006	0.22	0/1352
23	X	0.14	0/1439	0.22	0/1942
24	Y	0.11	0/1042	0.20	0/1414
25	Z	0.13	0/1186	0.20	0/1599
26	a	0.16	0/584	0.24	0/786
27	b	0.12	0/667	0.24	0/916
28	c	0.13	0/427	0.20	0/579
29	d	0.15	0/1018	0.22	0/1375
30	e	0.13	0/846	0.23	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.14	0/505	0.25	0/681
32	g	0.13	0/873	0.25	0/1186
33	h	0.14	0/1188	0.23	0/1607
34	i	0.11	0/1127	0.23	0/1534
35	j	0.13	0/624	0.25	0/855
36	k	0.09	0/672	0.20	0/906
37	l	0.12	0/1369	0.24	0/1873
38	m	0.12	0/1088	0.22	0/1472
39	n	0.11	0/1540	0.22	0/2085
40	o	0.13	0/1073	0.22	0/1437
41	p	0.12	0/1491	0.21	0/2011
42	q	0.16	0/1242	0.23	0/1688
43	r	0.15	0/789	0.23	0/1068
44	s	0.12	0/383	0.22	0/518
All	All	0.15	0/68062	0.24	0/92281

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	12	0
2	B	1247	0	1256	16	0
3	C	1721	0	1675	11	0
4	D	3392	0	3339	34	0
5	E	1659	0	1664	31	0
6	F	3326	0	3282	37	0
7	G	5298	0	5316	64	0
8	H	2509	0	2621	44	0
9	I	1414	0	1370	14	0
10	J	1345	0	1352	20	0
11	K	745	0	785	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	58	0
13	M	3654	0	3852	30	0
14	N	2733	0	2912	39	0
15	O	2589	0	2566	31	0
16	P	2728	0	2749	27	0
17	Q	1049	0	1045	8	0
18	R	740	0	714	5	0
19	S	691	0	706	12	0
20	T	707	0	700	3	0
20	U	707	0	700	5	0
21	V	923	0	964	5	0
22	W	982	0	999	10	0
23	X	1402	0	1383	14	0
24	Y	1030	0	1039	5	0
25	Z	1157	0	1156	16	0
26	a	569	0	568	7	0
27	b	654	0	663	5	0
28	c	414	0	415	2	0
29	d	999	0	988	11	0
30	e	825	0	826	10	0
31	f	492	0	501	3	0
32	g	846	0	798	14	0
33	h	1154	0	1168	9	0
34	i	1097	0	1108	18	0
35	j	597	0	536	3	0
36	k	653	0	639	1	0
37	l	1314	0	1210	15	0
38	m	1070	0	1068	13	0
39	n	1487	0	1433	12	0
40	o	1048	0	1018	8	0
41	p	1458	0	1430	16	0
42	q	1212	0	1183	8	0
43	r	776	0	782	3	0
44	s	371	0	344	7	0
45	A	35	0	44	2	0
45	B	94	0	136	1	0
45	H	87	0	128	2	0
45	I	91	0	136	0	0
45	J	35	0	44	0	0
45	L	47	0	71	1	0
45	M	70	0	91	2	0
45	d	39	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	h	31	0	36	0	0
45	m	40	0	54	1	0
45	q	30	0	34	2	0
46	A	75	0	101	0	0
46	I	36	0	49	0	0
46	J	77	0	102	1	0
46	L	163	0	231	3	0
46	M	50	0	77	0	0
46	N	85	0	124	1	0
46	Y	219	0	323	4	0
46	Z	45	0	67	0	0
46	b	47	0	71	0	0
46	d	49	0	75	0	0
46	f	80	0	114	0	0
46	j	44	0	65	0	0
46	m	74	0	99	0	0
46	o	35	0	47	0	0
47	B	8	0	0	0	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	B	38	0	53	0	0
48	L	27	0	28	0	0
48	O	26	0	26	1	0
48	b	32	0	38	0	0
48	g	32	0	41	1	0
49	E	4	0	0	0	0
49	G	4	0	0	1	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	H	28	0	31	14	0
53	J	36	0	16	0	0
53	L	87	0	127	2	0
53	M	91	0	135	4	0
53	N	74	0	92	0	0
53	X	87	0	127	0	0
53	d	65	0	77	2	0
53	h	80	0	104	0	0
53	q	61	0	66	1	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	O	1	0	0	0	0
57	P	48	0	26	2	0
58	T	37	0	0	1	0
58	U	37	0	0	1	0
59	i	29	0	38	8	0
60	o	15	0	27	0	0
All	All	69237	0	70189	616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (616) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:H:401:U10:H101	52:H:401:U10:H13	1.43	1.00
2:B:42:ARG:NH1	45:B:204:PC1:O14	2.01	0.93
41:p:72:ASP:OD1	41:p:74:THR:OG1	1.91	0.85
14:N:298:TYR:O	14:N:303:THR:OG1	1.95	0.83
39:n:134:ARG:NH1	39:n:161:ASP:OD2	2.14	0.81
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.63	0.81
2:B:84:ASP:OD2	8:H:54:LYS:NZ	2.14	0.79
15:O:236:GLU:OE2	21:V:91:ARG:NH1	2.14	0.79
7:G:627:SER:OG	7:G:629:ASN:OD1	1.99	0.79
7:G:140:LYS:O	7:G:148:THR:OG1	2.00	0.79
4:D:151:ILE:O	4:D:155:THR:OG1	2.01	0.79
14:N:182:SER:OG	14:N:293:TYR:OH	2.00	0.78
33:h:57:GLU:OE1	33:h:58:GLY:N	2.16	0.78
15:O:83:TYR:HH	55:O:401:DGT:HO3'	1.24	0.78
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.17	0.77
7:G:415:LEU:O	7:G:416:THR:OG1	2.02	0.77
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.01	0.76
40:o:43:GLN:NE2	40:o:47:ASP:OD1	2.18	0.76
30:e:27:LYS:NZ	33:h:134:ASP:OD2	2.19	0.76
13:M:141:GLU:N	13:M:141:GLU:OE1	2.18	0.76
10:J:23:LYS:NZ	11:K:21:MET:O	2.16	0.76
25:Z:92:GLU:N	25:Z:92:GLU:OE1	2.19	0.76
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.19	0.75
37:l:5:THR:OG1	37:l:7:ASP:OD1	2.05	0.75
23:X:143:SER:OG	30:e:38:GLU:OE2	2.02	0.75
20:T:64:ASP:OD2	22:W:32:ARG:NH1	2.20	0.75
23:X:129:LYS:NZ	27:b:65:VAL:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:83:TYR:OH	55:O:401:DGT:O3'	2.02	0.74
10:J:23:LYS:NZ	11:K:18:GLY:O	2.16	0.74
6:F:99:GLU:OE2	6:F:104:THR:HG22	1.87	0.74
7:G:366:THR:O	7:G:367:THR:OG1	2.06	0.73
8:H:277:TYR:OH	9:I:30:LEU:O	2.06	0.73
34:i:121:GLU:N	34:i:121:GLU:OE1	2.22	0.73
34:i:18:ARG:NH1	39:n:170:VAL:O	2.22	0.73
2:B:44:SER:OG	8:H:51:ASP:OD1	2.05	0.73
7:G:266:LYS:NZ	7:G:671:PHE:O	2.21	0.72
42:q:25:ARG:NH1	45:q:202:PC1:O12	2.22	0.72
14:N:314:LYS:NZ	15:O:274:SER:OG	2.22	0.72
15:O:88:SER:OG	15:O:90:ASP:OD1	2.05	0.72
4:D:67:GLU:OE1	4:D:75:LYS:NZ	2.23	0.72
4:D:145:THR:HG1	4:D:181:TYR:HH	1.34	0.72
15:O:95:ARG:NH1	15:O:281:GLU:O	2.21	0.72
57:P:501:NDP:N7N	57:P:501:NDP:O2N	2.23	0.72
59:i:201:CHD:H212	59:i:201:CHD:H12	1.70	0.72
44:s:35:ASN:O	44:s:35:ASN:ND2	2.22	0.72
7:G:535:GLN:N	7:G:535:GLN:OE1	2.23	0.71
6:F:202:LYS:O	17:Q:133:LYS:NZ	2.22	0.71
15:O:53:GLU:OE2	15:O:126:ARG:NH1	2.23	0.71
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.24	0.71
15:O:30:ASN:OD1	15:O:31:ILE:N	2.23	0.71
8:H:51:ASP:HB2	52:H:401:U10:H152	1.73	0.71
15:O:125:GLU:N	15:O:125:GLU:OE1	2.24	0.71
6:F:131:ALA:O	6:F:171:TYR:OH	2.04	0.70
7:G:347:GLU:OE2	7:G:495:ARG:NH1	2.25	0.69
44:s:71:GLU:OE1	44:s:71:GLU:N	2.26	0.69
8:H:170:GLU:OE2	23:X:97:ARG:NH2	2.26	0.69
14:N:182:SER:HG	14:N:293:TYR:HH	1.30	0.69
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.25	0.68
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.26	0.68
2:B:46:TRP:CZ2	52:H:401:U10:H1M2	2.28	0.68
9:I:29:GLU:N	9:I:29:GLU:OE1	2.25	0.68
5:E:170:GLU:N	5:E:170:GLU:OE1	2.27	0.68
8:H:224:PHE:CE2	52:H:401:U10:H121	2.28	0.68
37:l:53:ARG:NE	37:l:57:GLU:OE1	2.27	0.68
5:E:111:ARG:NH1	6:F:260:GLY:O	2.26	0.67
16:P:102:GLN:OE1	16:P:102:GLN:N	2.27	0.67
15:O:24:LEU:HD13	15:O:122:VAL:HG23	1.76	0.67
12:L:561:ILE:O	12:L:565:THR:OG1	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:84:LEU:HA	10:J:90:LEU:HD21	1.74	0.67
12:L:246:LEU:O	12:L:251:THR:OG1	2.12	0.67
34:i:127:HIS:O	40:o:84:HIS:ND1	2.26	0.67
7:G:432:ILE:O	7:G:476:LYS:NZ	2.27	0.67
24:Y:6:ARG:NH1	24:Y:10:ASP:OD1	2.28	0.67
35:j:60:THR:O	40:o:106:ARG:NH1	2.28	0.66
5:E:144:CYS:O	6:F:139:ARG:NH2	2.28	0.66
14:N:294:MET:O	14:N:297:THR:OG1	2.14	0.66
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.13	0.66
7:G:276:ARG:NH1	7:G:680:ALA:O	2.29	0.65
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.30	0.65
26:a:54:VAL:HG12	26:a:54:VAL:O	1.95	0.64
33:h:87:TYR:OH	41:p:86:GLU:OE1	2.05	0.64
17:Q:27:GLU:N	17:Q:27:GLU:OE1	2.30	0.64
25:Z:88:GLU:OE1	25:Z:127:ARG:NH2	2.30	0.64
7:G:326:GLU:N	7:G:326:GLU:OE1	2.31	0.64
37:l:30:ARG:NH1	37:l:33:ASP:OD2	2.31	0.64
6:F:81:PHE:O	6:F:84:LYS:NZ	2.30	0.64
7:G:190:MET:HE1	7:G:690:ALA:O	1.97	0.64
15:O:272:TYR:O	15:O:275:ILE:HG23	1.97	0.64
8:H:65:THR:HG21	16:P:325:ARG:HG3	1.80	0.64
14:N:237:THR:HG21	14:N:319:LEU:HD11	1.80	0.64
1:A:16:LEU:HD13	1:A:19:ILE:HD11	1.79	0.63
29:d:63:LEU:HD23	53:d:201:CDL:HA62	1.80	0.63
12:L:64:SER:O	34:i:95:THR:HG23	1.97	0.63
15:O:80:GLU:N	15:O:80:GLU:OE1	2.31	0.63
8:H:63:PRO:O	8:H:66:SER:OG	2.12	0.63
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.81	0.63
52:H:401:U10:C8	52:H:401:U10:H1M1	2.29	0.62
12:L:260:LEU:CD1	12:L:314:MET:HE1	2.28	0.62
37:l:137:ASN:O	37:l:137:ASN:ND2	2.32	0.62
4:D:233:ARG:O	4:D:237:ASN:ND2	2.31	0.62
52:H:401:U10:H101	52:H:401:U10:C13	2.24	0.62
20:U:26:ASP:OD2	20:U:29:LYS:N	2.33	0.62
8:H:249:PRO:O	26:a:28:ARG:NH2	2.32	0.62
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.25	0.62
15:O:34:GLY:N	55:O:401:DGT:O3G	2.33	0.62
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.81	0.62
41:p:171:GLU:N	41:p:171:GLU:OE1	2.33	0.61
58:T:101:EHZ:O1	58:T:101:EHZ:O2	2.13	0.61
30:e:50:ARG:NH1	30:e:54:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:53:LEU:HD13	44:s:52:LEU:HD22	1.82	0.61
29:d:1:AME:HT22	29:d:3:THR:HG23	1.83	0.61
32:g:121:PRO:HD2	41:p:163:LEU:HD21	1.81	0.61
25:Z:107:GLU:O	30:e:74:ARG:NH1	2.34	0.61
32:g:33:GLU:N	32:g:33:GLU:OE1	2.31	0.61
7:G:47:SER:OG	7:G:165:GLU:OE2	2.14	0.60
7:G:536:ASP:OD1	7:G:536:ASP:N	2.33	0.60
34:i:44:ARG:O	34:i:48:LYS:N	2.34	0.60
7:G:475:GLN:NE2	7:G:643:GLN:OE1	2.34	0.60
14:N:19:ILE:O	14:N:23:SER:OG	2.15	0.60
2:B:108:PRO:HB3	8:H:61:LEU:HD23	1.84	0.60
10:J:123:GLY:HA2	11:K:3:MET:HE2	1.82	0.59
16:P:174:ARG:NH1	16:P:316:GLU:OE2	2.35	0.59
1:A:71:LEU:O	10:J:147:TYR:OH	2.13	0.59
7:G:192:MET:HE2	7:G:192:MET:HA	1.84	0.59
16:P:335:GLN:N	16:P:335:GLN:OE1	2.36	0.59
39:n:139:LEU:O	39:n:143:THR:OG1	2.07	0.59
41:p:129:GLU:OE2	41:p:133:GLN:NE2	2.35	0.59
5:E:14:GLU:N	5:E:14:GLU:OE1	2.35	0.59
12:L:341:MET:HE3	12:L:454:ILE:HD13	1.84	0.59
39:n:9:LEU:O	39:n:14:LYS:NZ	2.34	0.59
7:G:601:ARG:NH1	7:G:605:GLU:OE2	2.36	0.58
15:O:225:ALA:O	15:O:229:GLN:NE2	2.36	0.58
12:L:170:GLN:NE2	45:L:707:PC1:O22	2.35	0.58
37:l:157:GLU:O	40:o:33:ARG:NH2	2.36	0.58
5:E:105:THR:HG22	5:E:106:THR:H	1.68	0.58
52:H:401:U10:H13	52:H:401:U10:C10	2.28	0.58
15:O:22:SER:OG	15:O:119:GLY:O	2.18	0.58
29:d:17:GLU:OE2	29:d:81:TYR:OH	2.14	0.58
4:D:218:PHE:CE2	4:D:222:ILE:HD11	2.38	0.58
35:j:60:THR:HG21	35:j:63:GLU:HB3	1.85	0.58
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.36	0.58
32:g:90:ARG:NH2	41:p:107:GLU:OE2	2.37	0.58
34:i:111:GLU:OE1	34:i:111:GLU:N	2.36	0.58
8:H:32:GLN:OE1	8:H:34:ARG:NH1	2.36	0.58
46:L:706:3PE:N	46:Y:203:3PE:O14	2.35	0.58
13:M:423:ILE:HD12	38:m:58:VAL:HG22	1.85	0.58
13:M:1:FME:O1	13:M:3:LYS:NZ	2.37	0.57
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.40	0.57
4:D:322:GLU:OE1	4:D:322:GLU:N	2.35	0.57
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1:AME:HT22	29:d:3:THR:CG2	2.34	0.57
34:i:51:GLN:OE1	34:i:51:GLN:N	2.37	0.57
1:A:48:ARG:NH1	1:A:49:LEU:O	2.38	0.57
29:d:82:MET:HE2	29:d:82:MET:HA	1.85	0.57
6:F:432:GLN:N	6:F:432:GLN:OE1	2.38	0.56
19:S:50:LEU:O	19:S:52:ILE:HD12	2.04	0.56
41:p:127:GLU:N	41:p:127:GLU:OE1	2.37	0.56
5:E:156:ILE:O	5:E:158:ASP:N	2.38	0.56
12:L:560:ALA:O	12:L:565:THR:HG23	2.05	0.56
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.88	0.56
5:E:104:THR:HG22	5:E:104:THR:O	2.04	0.56
7:G:684:MET:HA	7:G:684:MET:HE2	1.88	0.56
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.37	0.56
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.34	0.56
13:M:259:TYR:O	13:M:263:MET:HE2	2.05	0.56
33:h:143:ASN:O	33:h:143:ASN:ND2	2.38	0.56
7:G:693:GLU:OE1	7:G:693:GLU:N	2.39	0.56
8:H:51:ASP:CB	52:H:401:U10:H152	2.36	0.56
10:J:79:TYR:O	10:J:80:PRO:C	2.49	0.56
8:H:169:GLN:OE1	8:H:244:GLY:N	2.39	0.56
12:L:398:ALA:O	12:L:402:SER:OG	2.19	0.56
13:M:42:MET:HE1	32:g:77:VAL:HG22	1.87	0.56
5:E:67:ASN:OD1	5:E:81:TYR:OH	2.17	0.56
12:L:320:ASN:O	12:L:320:ASN:ND2	2.39	0.56
5:E:154:VAL:HG22	5:E:164:LEU:HD11	1.88	0.55
10:J:93:PHE:HE2	10:J:97:LEU:HD11	1.71	0.55
14:N:214:THR:HG22	14:N:218:MET:HE2	1.87	0.55
7:G:308:GLN:NE2	7:G:607:ALA:O	2.38	0.55
13:M:255:ASP:OD1	13:M:256:PHE:N	2.40	0.55
3:C:205:ALA:O	43:r:60:ARG:NH1	2.33	0.55
4:D:111:MET:SD	4:D:111:MET:N	2.78	0.55
12:L:260:LEU:HD12	12:L:314:MET:HE1	1.88	0.55
23:X:97:ARG:HD2	25:Z:59:LEU:HD13	1.89	0.55
12:L:341:MET:CE	12:L:457:LEU:HD12	2.33	0.55
16:P:333:ASP:OD1	16:P:334:VAL:N	2.40	0.55
2:B:46:TRP:CH2	52:H:401:U10:H1M2	2.42	0.55
5:E:156:ILE:HG22	5:E:157:ASN:ND2	2.22	0.55
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.88	0.55
31:f:46:ARG:NH2	31:f:52:GLU:OE1	2.36	0.55
7:G:675:ASP:N	7:G:675:ASP:OD1	2.39	0.55
22:W:29:ARG:NH1	22:W:33:GLU:OE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:ILE:HD13	4:D:330:VAL:HG11	1.89	0.54
9:I:32:ARG:NH2	25:Z:25:PRO:O	2.39	0.54
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.88	0.54
5:E:217:LEU:HD11	6:F:48:ILE:HG13	1.89	0.54
33:h:52:LEU:HD23	33:h:53:ALA:N	2.22	0.54
34:i:65:ARG:HB3	59:i:201:CHD:H213	1.88	0.54
12:L:183:ILE:HG21	13:M:382:VAL:HG11	1.90	0.54
53:M:602:CDL:H231	53:M:602:CDL:H872	1.90	0.54
4:D:371:LYS:NZ	4:D:422:ASP:OD1	2.40	0.54
6:F:15:LEU:O	6:F:20:ARG:NH1	2.40	0.54
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.90	0.54
5:E:217:LEU:HD11	6:F:48:ILE:CG1	2.38	0.54
7:G:403:ASP:OD2	44:s:70:ARG:NH2	2.40	0.54
7:G:516:LYS:O	7:G:517:ASN:ND2	2.40	0.54
26:a:68:ASN:O	26:a:68:ASN:ND2	2.41	0.54
37:l:82:ASP:OD1	37:l:82:ASP:N	2.40	0.54
29:d:109:TYR:HA	29:d:112:VAL:HG22	1.89	0.54
10:J:123:GLY:O	10:J:126:VAL:HG22	2.08	0.54
1:A:23:TRP:NE1	45:A:201:PC1:O22	2.38	0.53
22:W:34:LEU:HD13	22:W:86:LYS:HG2	1.90	0.53
38:m:120:LEU:HD23	38:m:121:ASP:N	2.23	0.53
3:C:85:THR:HG21	21:V:115:ILE:HG13	1.91	0.53
29:d:119:VAL:O	29:d:119:VAL:HG12	2.09	0.53
8:H:262:LYS:NZ	45:H:403:PC1:O12	2.35	0.53
7:G:467:LEU:O	7:G:471:SER:OG	2.16	0.53
8:H:201:THR:HG21	8:H:211:PHE:CE1	2.43	0.53
13:M:449:LEU:HD13	45:M:603:PC1:O32	2.09	0.53
25:Z:130:GLU:OE1	25:Z:130:GLU:N	2.40	0.53
5:E:30:ARG:NH1	44:s:53:ASP:OD1	2.41	0.53
4:D:71:GLU:OE2	8:H:134:ARG:NH2	2.42	0.52
4:D:347:HIS:CD2	7:G:121:MET:HE3	2.43	0.52
7:G:490:MET:HE3	7:G:491:ASN:H	1.74	0.52
16:P:91:VAL:HG23	16:P:126:VAL:HG11	1.92	0.52
23:X:6:LEU:O	25:Z:87:ARG:NH2	2.42	0.52
7:G:196:SER:OG	7:G:265:ASP:OD2	2.27	0.52
10:J:93:PHE:CE2	10:J:97:LEU:HD11	2.44	0.52
15:O:87:LYS:NZ	15:O:142:GLY:O	2.41	0.52
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.40	0.52
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.92	0.52
3:C:85:THR:HG21	21:V:115:ILE:CG1	2.39	0.52
5:E:79:ARG:NH1	5:E:82:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:40:ASP:O	38:m:82:ASN:ND2	2.43	0.52
25:Z:85:MET:HE1	25:Z:124:TYR:CE2	2.44	0.52
1:A:19:ILE:HD12	45:A:201:PC1:H291	1.92	0.51
5:E:217:LEU:HD13	5:E:217:LEU:O	2.11	0.51
6:F:318:ASP:N	6:F:318:ASP:OD1	2.44	0.51
13:M:423:ILE:CD1	38:m:58:VAL:HG22	2.41	0.51
15:O:186:LYS:NZ	15:O:191:GLU:OE1	2.28	0.51
34:i:89:VAL:CG1	34:i:95:THR:HG21	2.40	0.51
4:D:183:ARG:NH1	4:D:210:ASP:OD2	2.38	0.51
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.40	0.51
12:L:577:VAL:HG13	12:L:578:THR:HG23	1.92	0.51
5:E:100:ILE:HG12	5:E:156:ILE:HD12	1.92	0.51
16:P:218:ILE:HG22	16:P:218:ILE:O	2.10	0.51
59:i:201:CHD:O7	59:i:201:CHD:H41	2.10	0.51
7:G:424:ASP:OD1	7:G:424:ASP:N	2.43	0.51
15:O:31:ILE:O	15:O:179:VAL:HG13	2.10	0.51
13:M:108:MET:HB3	13:M:121:LEU:HD13	1.93	0.51
8:H:202:GLU:N	8:H:202:GLU:OE1	2.43	0.51
10:J:175:ASN:O	10:J:175:ASN:ND2	2.43	0.51
12:L:138:PHE:HD2	46:L:703:3PE:H3I2	1.74	0.51
18:R:93:GLN:OE1	18:R:96:HIS:ND1	2.43	0.51
29:d:5:ARG:NH1	29:d:89:ASP:OD1	2.44	0.50
59:i:201:CHD:H212	59:i:201:CHD:C12	2.39	0.50
4:D:68:LEU:HD21	4:D:411:LEU:HD22	1.93	0.50
5:E:217:LEU:HD12	6:F:44:LYS:HG2	1.92	0.50
14:N:152:ASN:OD1	46:N:403:3PE:N	2.28	0.50
7:G:255:HIS:CD2	7:G:258:ILE:HD12	2.46	0.50
7:G:315:VAL:O	7:G:340:SER:OG	2.22	0.50
4:D:145:THR:OG1	4:D:181:TYR:OH	2.08	0.50
22:W:88:GLU:OE2	22:W:97:LYS:NZ	2.39	0.50
34:i:90:THR:HG22	34:i:96:ILE:HD12	1.93	0.50
14:N:269:GLU:O	14:N:273:ASN:ND2	2.42	0.50
29:d:120:ARG:HD3	38:m:115:ILE:HD13	1.92	0.50
37:l:59:ASP:OD2	37:l:62:TYR:N	2.42	0.50
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.45	0.50
7:G:280:THR:HG21	42:q:136:GLU:CD	2.37	0.50
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.41	0.50
10:J:81:GLU:N	16:P:324:TYR:OH	2.45	0.50
5:E:217:LEU:HD13	5:E:217:LEU:C	2.37	0.50
7:G:285:ARG:NH2	7:G:555:PRO:O	2.45	0.50
12:L:562:LEU:HB2	12:L:563:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:79:GLU:N	23:X:79:GLU:OE1	2.45	0.50
5:E:118:GLU:N	5:E:118:GLU:OE1	2.45	0.49
11:K:1:FME:O	30:e:72:MET:HE1	2.12	0.49
16:P:162:GLU:O	16:P:225:GLY:N	2.42	0.49
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.93	0.49
8:H:19:PHE:O	8:H:23:VAL:HG23	2.11	0.49
12:L:264:TYR:N	12:L:265:PRO:CD	2.76	0.49
32:g:113:PHE:CE1	41:p:73:ILE:HG22	2.46	0.49
4:D:241:ASP:OD1	4:D:290:ARG:NH1	2.41	0.49
52:H:401:U10:C18	52:H:401:U10:H151	2.42	0.49
5:E:214:GLN:OE1	5:E:214:GLN:N	2.44	0.49
37:l:81:LEU:HD13	37:l:81:LEU:C	2.37	0.49
14:N:313:MET:HE1	15:O:102:ALA:HB3	1.93	0.49
22:W:65:MET:HA	22:W:65:MET:HE2	1.94	0.49
6:F:407:LEU:HD23	6:F:407:LEU:O	2.13	0.49
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.42	0.49
53:M:602:CDL:H872	53:M:602:CDL:C23	2.43	0.49
12:L:49:ILE:HB	12:L:50:PRO:HD3	1.95	0.49
12:L:194:ASN:OD1	41:p:106:GLN:NE2	2.45	0.49
3:C:83:ILE:HG22	3:C:85:THR:HG22	1.95	0.49
7:G:582:GLN:OE1	7:G:620:ARG:NH1	2.41	0.49
17:Q:90:GLU:OE1	17:Q:90:GLU:N	2.41	0.49
3:C:40:VAL:HG13	3:C:50:ILE:HD13	1.95	0.49
8:H:65:THR:HG23	16:P:323:THR:O	2.13	0.49
53:M:602:CDL:H1O1	53:M:602:CDL:PA1	2.36	0.49
19:S:57:CYS:SG	19:S:58:SER:N	2.80	0.49
5:E:100:ILE:HG21	5:E:120:ILE:HD13	1.94	0.48
7:G:534:ARG:NH2	7:G:558:ASP:OD1	2.46	0.48
53:M:602:CDL:H541	14:N:242:VAL:HG11	1.94	0.48
22:W:23:ASP:N	22:W:23:ASP:OD1	2.46	0.48
1:A:44:MET:HE3	22:W:94:LYS:O	2.14	0.48
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.94	0.48
2:B:44:SER:O	8:H:54:LYS:NZ	2.44	0.48
6:F:46:LYS:O	6:F:50:LEU:HD13	2.13	0.48
20:T:22:TYR:OH	20:T:46:ASP:OD1	2.30	0.48
14:N:276:ILE:HG21	46:Y:201:3PE:H251	1.96	0.48
7:G:324:ASP:OD1	7:G:324:ASP:N	2.45	0.48
12:L:593:ILE:HG22	12:L:597:ILE:HD12	1.95	0.48
19:S:47:ASN:OD1	19:S:47:ASN:N	2.46	0.48
7:G:551:ASP:OD2	7:G:679:ARG:NH2	2.44	0.48
12:L:331:THR:HB	12:L:387:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:311:GLU:OE1	16:P:311:GLU:N	2.41	0.48
19:S:43:LEU:HD23	19:S:43:LEU:O	2.14	0.48
37:l:28:ASN:HB3	38:m:42:LEU:HD11	1.95	0.48
2:B:82:GLN:NE2	8:H:215:TYR:O	2.47	0.48
39:n:30:CYS:O	39:n:32:HIS:N	2.45	0.48
12:L:193:LEU:HD11	12:L:206:PRO:CG	2.44	0.47
14:N:238:PRO:O	14:N:241:THR:OG1	2.31	0.47
15:O:45:LYS:HB2	15:O:235:VAL:HG21	1.95	0.47
13:M:130:LEU:HD21	14:N:294:MET:HE1	1.94	0.47
14:N:40:ILE:HD12	14:N:43:ILE:HD11	1.96	0.47
40:o:31:PRO:O	40:o:32:GLU:C	2.57	0.47
6:F:378:ARG:NH1	6:F:383:ASP:O	2.45	0.47
7:G:229:ASP:OD1	7:G:267:THR:HG23	2.15	0.47
7:G:382:THR:OG1	7:G:387:GLU:OE1	2.28	0.47
52:H:401:U10:C8	52:H:401:U10:C1M	2.93	0.47
14:N:20:VAL:HG13	14:N:29:VAL:HG13	1.96	0.47
16:P:26:ALA:HB3	16:P:47:VAL:HG13	1.95	0.47
16:P:253:PHE:C	16:P:254:LEU:HD12	2.39	0.47
24:Y:27:ILE:HG21	46:Y:203:3PE:H3E2	1.97	0.47
7:G:47:SER:O	7:G:161:ARG:NH1	2.47	0.47
7:G:371:VAL:HG22	7:G:450:MET:HE1	1.96	0.47
8:H:224:PHE:CZ	52:H:401:U10:H72	2.50	0.47
12:L:76:LEU:HD21	12:L:196:TRP:HE3	1.78	0.47
19:S:18:ILE:HG22	19:S:52:ILE:HG23	1.97	0.47
33:h:114:MET:O	33:h:118:GLY:N	2.42	0.47
7:G:667:THR:HG22	7:G:668:ILE:H	1.79	0.47
17:Q:21:THR:HG21	22:W:72:ILE:HD11	1.96	0.47
19:S:63:LYS:NZ	19:S:75:ASN:OD1	2.37	0.47
33:h:62:GLU:OE1	33:h:64:TRP:NE1	2.48	0.47
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.96	0.47
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.97	0.47
37:l:66:HIS:O	37:l:70:ARG:N	2.47	0.47
37:l:135:TYR:O	37:l:138:LEU:N	2.47	0.47
4:D:62:LEU:HD21	4:D:64:LEU:HD21	1.96	0.46
7:G:632:ARG:NH2	19:S:58:SER:O	2.46	0.46
8:H:289:LEU:C	8:H:289:LEU:HD13	2.41	0.46
1:A:108:GLN:HB2	10:J:169:MET:HE1	1.98	0.46
14:N:343:LEU:C	14:N:343:LEU:HD12	2.40	0.46
21:V:64:VAL:HG13	21:V:65:LYS:HD3	1.97	0.46
40:o:102:GLU:OE2	40:o:105:ARG:NH1	2.45	0.46
2:B:137:ASP:N	2:B:137:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:87:ILE:N	8:H:88:PRO:CD	2.79	0.46
12:L:13:LEU:O	12:L:13:LEU:HD23	2.15	0.46
4:D:238:ARG:NH1	8:H:206:GLU:OE2	2.46	0.46
14:N:193:VAL:O	14:N:193:VAL:HG22	2.16	0.46
16:P:4:ALA:O	16:P:5:VAL:C	2.59	0.46
26:a:50:ARG:O	26:a:54:VAL:HG23	2.15	0.46
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.98	0.46
19:S:18:ILE:HD11	19:S:64:LEU:HD21	1.96	0.46
22:W:95:VAL:HG12	22:W:95:VAL:O	2.16	0.46
39:n:159:GLN:N	39:n:159:GLN:OE1	2.49	0.46
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.49	0.46
11:K:43:MET:HE1	14:N:72:MET:SD	2.56	0.46
15:O:94:TYR:OH	15:O:151:HIS:ND1	2.30	0.46
39:n:162:LEU:HD12	39:n:162:LEU:N	2.31	0.46
5:E:145:LEU:HD12	5:E:153:MET:HE2	1.97	0.46
8:H:241:LEU:HD23	8:H:242:PHE:CE2	2.51	0.46
10:J:125:TRP:HB2	25:Z:136:THR:HG21	1.96	0.46
12:L:131:LEU:HD23	12:L:131:LEU:C	2.41	0.46
12:L:193:LEU:HD11	12:L:206:PRO:HG3	1.97	0.46
15:O:188:ASN:OD1	15:O:191:GLU:N	2.40	0.46
12:L:140:LEU:O	12:L:140:LEU:HD23	2.16	0.46
14:N:215:MET:HE1	14:N:244:ILE:HG23	1.98	0.46
23:X:165:ARG:NH1	29:d:87:ASP:OD2	2.46	0.46
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.51	0.46
6:F:306:LEU:C	6:F:306:LEU:HD12	2.41	0.46
23:X:79:GLU:HB2	23:X:80:PRO:HD3	1.97	0.46
32:g:109:GLU:O	41:p:141:ARG:NH2	2.45	0.46
32:g:118:ILE:HG21	41:p:162:MET:HE1	1.97	0.46
59:i:201:CHD:H112	59:i:201:CHD:H12A	1.77	0.46
2:B:96:MET:HE1	4:D:53:PRO:HG3	1.98	0.45
13:M:108:MET:CB	13:M:121:LEU:HD13	2.46	0.45
13:M:216:LEU:HB3	13:M:217:PRO:HD3	1.98	0.45
34:i:1:SAC:O	34:i:1:SAC:OG	2.21	0.45
1:A:60:ILE:HG21	10:J:168:ILE:HD13	1.97	0.45
6:F:139:ARG:NH1	6:F:141:GLU:OE1	2.49	0.45
12:L:174:TYR:OH	12:L:534:HIS:NE2	2.45	0.45
42:q:21:ARG:NH1	45:q:202:PC1:O14	2.49	0.45
6:F:313:GLU:O	6:F:314:THR:HG22	2.16	0.45
12:L:13:LEU:HD23	12:L:13:LEU:C	2.41	0.45
12:L:120:TYR:HB3	12:L:154:LEU:HD21	1.98	0.45
45:M:603:PC1:O13	45:M:603:PC1:H132	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:286:LEU:C	12:L:286:LEU:HD13	2.42	0.45
16:P:183:ALA:O	16:P:186:ARG:NH1	2.50	0.45
22:W:116:ASP:OD1	22:W:116:ASP:N	2.50	0.45
34:i:110:LEU:HD21	41:p:18:ALA:HB2	1.99	0.45
5:E:217:LEU:HD12	6:F:44:LYS:CD	2.47	0.45
8:H:179:TRP:N	8:H:180:PRO:CD	2.80	0.45
12:L:378:LEU:HD22	12:L:383:MET:HE2	1.99	0.45
14:N:41:ILE:HD13	14:N:44:MET:HE2	1.97	0.45
2:B:52:LEU:HD23	4:D:61:VAL:HG11	1.98	0.45
12:L:587:TYR:O	12:L:590:SER:OG	2.31	0.45
16:P:50:ARG:NH2	57:P:501:NDP:O2X	2.45	0.45
19:S:43:LEU:HD23	19:S:43:LEU:C	2.41	0.45
13:M:388:TRP:O	38:m:111:LYS:NZ	2.45	0.45
15:O:125:GLU:O	15:O:126:ARG:C	2.58	0.45
5:E:147:ALA:HB2	6:F:108:ARG:NH1	2.31	0.45
5:E:114:ASP:OD1	5:E:114:ASP:N	2.49	0.44
6:F:99:GLU:OE2	6:F:106:LYS:N	2.50	0.44
6:F:200:GLN:NE2	7:G:174:THR:O	2.50	0.44
8:H:307:LEU:HD21	25:Z:46:TYR:CD1	2.52	0.44
12:L:138:PHE:CD2	46:L:703:3PE:H3I2	2.52	0.44
12:L:579:ASN:O	24:Y:43:LYS:NZ	2.48	0.44
16:P:324:TYR:O	16:P:327:LEU:HD11	2.17	0.44
16:P:254:LEU:HD12	16:P:254:LEU:N	2.33	0.44
7:G:149:ILE:HD12	7:G:149:ILE:N	2.33	0.44
53:L:701:CDL:H771	13:M:442:LEU:HD22	2.00	0.44
19:S:64:LEU:HD23	19:S:64:LEU:C	2.42	0.44
20:U:62:ILE:HD12	20:U:62:ILE:N	2.33	0.44
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.99	0.44
14:N:236:LYS:HG3	14:N:237:THR:HG23	1.99	0.44
6:F:101:GLU:OE1	6:F:184:TYR:OH	2.23	0.44
8:H:49:ILE:N	8:H:49:ILE:HD12	2.32	0.44
8:H:61:LEU:N	8:H:61:LEU:HD22	2.33	0.44
9:I:76:ARG:O	9:I:128:VAL:HG21	2.18	0.44
14:N:108:MET:SD	14:N:191:THR:HG21	2.58	0.44
30:e:79:ARG:NH1	30:e:83:GLU:OE2	2.51	0.44
33:h:86:ASN:O	33:h:90:THR:OG1	2.22	0.44
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.52	0.44
7:G:280:THR:HG21	42:q:136:GLU:OE1	2.18	0.44
34:i:90:THR:CG2	34:i:96:ILE:HD12	2.47	0.44
5:E:134:ASP:OD1	5:E:134:ASP:N	2.51	0.44
9:I:99:ARG:HG2	18:R:41:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:314:MET:HE3	12:L:314:MET:HA	1.99	0.44
59:i:201:CHD:H213	59:i:201:CHD:H231	1.62	0.44
3:C:109:THR:OG1	3:C:110:TYR:N	2.51	0.43
12:L:230:HIS:N	12:L:231:PRO:CD	2.80	0.43
14:N:146:PHE:N	14:N:147:PRO:CD	2.81	0.43
19:S:24:GLN:NE2	19:S:56:GLU:O	2.51	0.43
32:g:58:MET:HE1	48:g:201:PLC:H83	2.00	0.43
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.00	0.43
7:G:320:GLY:O	7:G:498:SER:OG	2.33	0.43
7:G:657:LEU:HD23	7:G:658:ALA:N	2.33	0.43
26:a:54:VAL:O	26:a:54:VAL:CG1	2.66	0.43
8:H:73:LEU:O	8:H:73:LEU:HD23	2.17	0.43
13:M:154:LEU:HD11	14:N:254:LEU:HD21	2.01	0.43
8:H:20:LEU:HD13	26:a:12:MET:HE1	2.01	0.43
13:M:390:ASN:O	13:M:393:ILE:HG22	2.19	0.43
16:P:30:LEU:HD12	16:P:207:ILE:HD11	1.99	0.43
23:X:25:LYS:NZ	23:X:94:GLN:O	2.41	0.43
32:g:81:PRO:O	32:g:82:ASP:C	2.60	0.43
8:H:30:TYR:HB3	9:I:41:LEU:HD12	2.00	0.43
16:P:322:ARG:NE	16:P:327:LEU:HD13	2.34	0.43
16:P:322:ARG:HE	16:P:327:LEU:HD13	1.84	0.43
58:U:101:EHZ:O2	58:U:101:EHZ:O1	2.34	0.43
7:G:366:THR:HB	7:G:450:MET:HE3	2.01	0.43
8:H:200:LEU:HD12	8:H:201:THR:N	2.33	0.43
12:L:535:ARG:NH2	37:l:90:ASP:OD2	2.52	0.43
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.99	0.43
37:l:56:GLN:OE1	37:l:86:ARG:NE	2.49	0.43
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.00	0.43
7:G:591:GLY:HA2	16:P:6:ILE:HD13	2.00	0.43
12:L:78:LEU:HD11	53:L:701:CDL:H472	2.01	0.43
12:L:277:THR:HB	12:L:314:MET:HE2	2.00	0.43
13:M:375:LEU:C	13:M:375:LEU:HD13	2.44	0.43
17:Q:5:THR:HG22	17:Q:5:THR:O	2.19	0.43
10:J:79:TYR:O	10:J:81:GLU:N	2.52	0.43
13:M:125:THR:O	13:M:126:LEU:HD12	2.18	0.43
13:M:423:ILE:CD1	38:m:58:VAL:HG13	2.49	0.43
15:O:309:ASN:HB2	15:O:312:VAL:HG22	2.01	0.43
15:O:309:ASN:ND2	28:c:3:TYR:OH	2.50	0.43
7:G:194:GLU:OE1	7:G:194:GLU:N	2.41	0.43
12:L:566:ILE:O	12:L:570:GLN:HG2	2.19	0.43
13:M:109:THR:HG21	13:M:238:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:148:CYS:HA	15:O:279:LEU:HD21	2.00	0.43
19:S:43:LEU:HD11	19:S:90:LEU:HD13	2.01	0.43
34:i:89:VAL:HG12	34:i:95:THR:HG21	1.99	0.43
40:o:102:GLU:CD	40:o:105:ARG:HH12	2.27	0.43
43:r:105:LEU:HD23	43:r:106:SER:H	1.84	0.43
4:D:106:LEU:HD13	4:D:391:ILE:HG21	2.01	0.42
4:D:349:PHE:CE2	9:I:82:LEU:HD11	2.54	0.42
12:L:183:ILE:CG2	13:M:382:VAL:HG11	2.49	0.42
13:M:6:ILE:HB	13:M:7:PRO:HD3	2.01	0.42
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.49	0.42
23:X:117:VAL:O	27:b:70:GLN:NE2	2.50	0.42
32:g:121:PRO:O	41:p:166:ARG:NH2	2.45	0.42
1:A:114:THR:O	1:A:115:GLU:C	2.62	0.42
12:L:565:THR:HG21	45:m:203:PC1:H222	2.01	0.42
15:O:176:VAL:HG21	15:O:200:GLN:OE1	2.18	0.42
18:R:23:TYR:O	18:R:26:VAL:HG12	2.18	0.42
21:V:34:LEU:O	21:V:44:ARG:NE	2.52	0.42
25:Z:27:ARG:NH2	43:r:13:TRP:O	2.40	0.42
36:k:42:ASP:OD1	39:n:37:ARG:NE	2.48	0.42
7:G:472:ASN:OD1	7:G:473:ILE:N	2.52	0.42
12:L:221:THR:HG23	12:L:226:GLN:HB2	2.00	0.42
14:N:40:ILE:HG21	14:N:59:TYR:HE2	1.84	0.42
30:e:83:GLU:HA	30:e:86:ILE:HD12	2.01	0.42
5:E:217:LEU:HD12	6:F:44:LYS:CG	2.50	0.42
6:F:367:GLU:OE2	7:G:135:ARG:NH2	2.52	0.42
10:J:90:LEU:HD22	10:J:90:LEU:H	1.84	0.42
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.19	0.42
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.50	0.42
59:i:201:CHD:O3	59:i:201:CHD:H9	2.19	0.42
2:B:78:ALA:HB1	52:H:401:U10:H3M3	2.00	0.42
5:E:156:ILE:HG22	5:E:157:ASN:HD22	1.83	0.42
6:F:188:GLU:OE1	6:F:190:THR:N	2.51	0.42
6:F:327:THR:OG1	6:F:328:GLY:N	2.51	0.42
7:G:556:ILE:HD12	7:G:556:ILE:O	2.19	0.42
16:P:71:MET:HE2	18:R:29:VAL:HB	2.02	0.42
6:F:314:THR:O	6:F:314:THR:HG23	2.20	0.42
29:d:63:LEU:HD23	53:d:201:CDL:CA6	2.46	0.42
32:g:66:PHE:HD1	32:g:70:LEU:HD12	1.84	0.42
40:o:82:GLU:OE1	40:o:82:GLU:N	2.49	0.42
7:G:484:THR:HG23	7:G:486:ASP:OD1	2.20	0.42
25:Z:126:LEU:HD12	30:e:82:ARG:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:72:SER:OG	44:s:75:HIS:ND1	2.48	0.42
4:D:141:PHE:O	4:D:145:THR:OG1	2.37	0.42
23:X:7:PRO:HG2	23:X:56:LEU:HD11	2.01	0.42
39:n:169:ILE:H	39:n:169:ILE:HD12	1.85	0.42
6:F:306:LEU:HD12	6:F:306:LEU:O	2.20	0.42
7:G:385:ARG:HD2	7:G:416:THR:HG23	2.01	0.42
8:H:89:LEU:HD13	8:H:236:ILE:HG21	2.02	0.42
27:b:2:GLU:O	27:b:6:ALA:N	2.53	0.42
31:f:41:SER:O	31:f:45:LYS:HB2	2.20	0.42
31:f:48:LEU:HD22	31:f:52:GLU:O	2.18	0.42
34:i:89:VAL:HG13	34:i:95:THR:HG21	2.02	0.42
10:J:31:LEU:HD13	10:J:31:LEU:C	2.45	0.42
12:L:14:LEU:HD23	12:L:14:LEU:O	2.20	0.42
13:M:285:LEU:HD23	13:M:285:LEU:C	2.44	0.42
16:P:46:ILE:N	16:P:46:ILE:HD12	2.35	0.42
23:X:148:GLU:O	30:e:50:ARG:NH2	2.51	0.42
3:C:78:LEU:HD13	3:C:94:TYR:CD2	2.55	0.41
4:D:37:ASP:OD2	11:K:95:LEU:HD13	2.19	0.41
7:G:42:TYR:N	49:G:803:FES:S1	2.93	0.41
11:K:69:CYS:SG	14:N:38:LEU:HD21	2.60	0.41
15:O:195:THR:HG23	15:O:198:TYR:H	1.84	0.41
28:c:49:GLU:OE1	28:c:49:GLU:N	2.40	0.41
38:m:107:ASP:OD1	38:m:110:ARG:NH2	2.53	0.41
1:A:90:MET:SD	10:J:151:THR:HG23	2.59	0.41
12:L:485:TYR:O	12:L:489:THR:OG1	2.38	0.41
32:g:103:HIS:O	32:g:105:LEU:HD12	2.20	0.41
2:B:91:THR:HA	2:B:119:CYS:HB3	2.02	0.41
4:D:83:LEU:HD23	4:D:426:GLY:HA2	2.02	0.41
20:T:39:ASP:OD1	20:T:40:LEU:N	2.54	0.41
5:E:74:GLN:O	44:s:74:ARG:NH2	2.53	0.41
6:F:258:ILE:HD11	6:F:279:LEU:HG	2.03	0.41
8:H:318:THR:HG22	25:Z:60:GLN:OE1	2.20	0.41
10:J:130:THR:HG23	25:Z:118:PRO:O	2.19	0.41
12:L:80:PHE:HB3	12:L:133:THR:HG22	2.02	0.41
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.40	0.41
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.03	0.41
38:m:51:TYR:OH	39:n:169:ILE:HD11	2.19	0.41
9:I:14:MET:HE2	9:I:14:MET:HA	2.03	0.41
14:N:7:ILE:HD11	48:O:403:PLC:H1'1	2.02	0.41
15:O:244:ASP:OD1	15:O:244:ASP:N	2.51	0.41
20:U:76:ILE:O	20:U:76:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:1:AYA:HB2	27:b:4:VAL:HG23	2.02	0.41
6:F:302:SER:HB2	6:F:350:LEU:HD13	2.03	0.41
12:L:189:PHE:HD1	12:L:193:LEU:HD12	1.86	0.41
12:L:491:LEU:H	12:L:491:LEU:HD22	1.85	0.41
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.56	0.41
24:Y:68:ILE:HG13	24:Y:99:ILE:HG13	2.02	0.41
3:C:99:LEU:N	3:C:99:LEU:HD12	2.35	0.41
3:C:193:GLU:OE1	17:Q:64:ARG:NE	2.43	0.41
7:G:239:VAL:HG23	7:G:253:ARG:HB2	2.01	0.41
8:H:65:THR:HG21	16:P:325:ARG:CG	2.50	0.41
38:m:80:ARG:O	38:m:82:ASN:N	2.49	0.41
4:D:296:ARG:HH21	4:D:420:THR:HG21	1.85	0.41
46:J:204:3PE:H371	11:K:14:VAL:HG13	2.03	0.41
13:M:388:TRP:O	38:m:108:ARG:NH1	2.53	0.41
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.55	0.41
34:i:66:HIS:HD2	59:i:201:CHD:H211	1.85	0.41
2:B:86:MET:HB2	2:B:107:MET:HE1	2.02	0.41
3:C:199:LEU:HD22	4:D:353:THR:O	2.20	0.41
7:G:539:LYS:O	7:G:540:ASP:OD1	2.38	0.41
8:H:176:LEU:HB3	8:H:177:PRO:HD3	2.01	0.41
9:I:60:ARG:NH1	9:I:172:ASP:OD1	2.54	0.41
9:I:168:ASN:HD21	42:q:93:MET:HE1	1.85	0.41
11:K:82:SER:O	11:K:86:GLY:N	2.48	0.41
12:L:525:LEU:HD11	37:l:95:PRO:HG2	2.03	0.41
13:M:47:ASP:OD1	13:M:48:ASN:N	2.53	0.41
14:N:128:LEU:O	14:N:132:THR:OG1	2.30	0.41
14:N:207:ILE:HD12	14:N:262:PRO:HG3	2.03	0.41
14:N:340:THR:N	14:N:341:PRO:HD2	2.36	0.41
15:O:46:LEU:HD21	15:O:235:VAL:HG13	2.01	0.41
15:O:113:GLU:OE1	15:O:266:LYS:NZ	2.52	0.41
16:P:101:THR:HG22	16:P:102:GLN:H	1.86	0.41
20:U:71:MET:N	20:U:75:GLU:OE1	2.54	0.41
14:N:343:LEU:HD12	14:N:344:SER:N	2.36	0.41
24:Y:124:VAL:HG11	46:Y:203:3PE:H3I1	2.02	0.41
25:Z:58:ARG:NH1	27:b:80:LEU:O	2.53	0.41
38:m:17:LEU:HD22	39:n:68:GLU:OE1	2.21	0.41
14:N:41:ILE:N	14:N:42:PRO:HD2	2.35	0.40
41:p:42:ARG:HB3	41:p:43:PRO:HD3	2.02	0.40
41:p:109:LEU:C	41:p:109:LEU:HD23	2.46	0.40
42:q:3:LEU:HD13	42:q:3:LEU:C	2.45	0.40
6:F:62:THR:O	6:F:62:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:437:HIS:O	6:F:438:GLN:C	2.64	0.40
7:G:462:ASP:OD1	7:G:462:ASP:N	2.53	0.40
45:H:402:PC1:O13	45:H:402:PC1:H133	2.21	0.40
32:g:66:PHE:O	32:g:71:VAL:HG23	2.21	0.40
42:q:3:LEU:HD23	53:q:201:CDL:OB6	2.20	0.40
2:B:75:VAL:HG11	52:H:401:U10:H1M3	2.03	0.40
4:D:335:ARG:NH2	9:I:126:CYS:O	2.42	0.40
12:L:76:LEU:HD21	12:L:196:TRP:CE3	2.55	0.40
12:L:426:ILE:O	12:L:430:ALA:HB3	2.21	0.40
13:M:264:LEU:O	13:M:268:GLY:N	2.51	0.40
14:N:267:ILE:O	14:N:271:THR:HG23	2.21	0.40
14:N:278:LEU:HB3	14:N:279:PRO:HD3	2.04	0.40
25:Z:126:LEU:HD12	30:e:82:ARG:CD	2.51	0.40
13:M:406:TYR:CD1	13:M:406:TYR:C	2.99	0.40
7:G:242:THR:HG21	7:G:586:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	B	154/216 (71%)	150 (97%)	4 (3%)	0	100	100
3	C	205/266 (77%)	202 (98%)	3 (2%)	0	100	100
4	D	414/463 (89%)	402 (97%)	12 (3%)	0	100	100
5	E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	24	54
6	F	430/464 (93%)	413 (96%)	17 (4%)	0	100	100
7	G	689/727 (95%)	662 (96%)	27 (4%)	0	100	100
8	H	316/318 (99%)	305 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	174/212 (82%)	168 (97%)	6 (3%)	0	100	100
10	J	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	21	51
11	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
12	L	604/606 (100%)	581 (96%)	23 (4%)	0	100	100
13	M	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
14	N	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
15	O	318/343 (93%)	307 (96%)	11 (4%)	0	100	100
16	P	335/380 (88%)	322 (96%)	13 (4%)	0	100	100
17	Q	127/175 (73%)	126 (99%)	1 (1%)	0	100	100
18	R	94/124 (76%)	91 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	83 (99%)	1 (1%)	0	100	100
20	T	86/156 (55%)	80 (93%)	6 (7%)	0	100	100
20	U	86/156 (55%)	81 (94%)	5 (6%)	0	100	100
21	V	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
22	W	114/128 (89%)	110 (96%)	3 (3%)	1 (1%)	14	41
23	X	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
24	Y	138/141 (98%)	138 (100%)	0	0	100	100
25	Z	140/144 (97%)	136 (97%)	4 (3%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
30	e	96/106 (91%)	93 (97%)	3 (3%)	0	100	100
31	f	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	6	25
32	g	99/154 (64%)	91 (92%)	8 (8%)	0	100	100
33	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	64 (93%)	5 (7%)	0	100	100
36	k	79/98 (81%)	77 (98%)	2 (2%)	0	100	100
37	l	154/186 (83%)	143 (93%)	11 (7%)	0	100	100
38	m	126/129 (98%)	124 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	n	169/179 (94%)	164 (97%)	5 (3%)	0	100	100
40	o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	p	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
42	q	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
43	r	91/113 (80%)	88 (97%)	3 (3%)	0	100	100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8175/9213 (89%)	7893 (97%)	278 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	157	ASN
10	J	80	PRO
31	f	3	LEU
22	W	95	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	97 (97%)	3 (3%)	36	70
2	B	132/175 (75%)	130 (98%)	2 (2%)	57	84
3	C	188/228 (82%)	184 (98%)	4 (2%)	47	77
4	D	362/392 (92%)	354 (98%)	8 (2%)	45	77
5	E	183/205 (89%)	178 (97%)	5 (3%)	39	73
6	F	346/368 (94%)	337 (97%)	9 (3%)	40	73
7	G	579/608 (95%)	563 (97%)	16 (3%)	38	72
8	H	274/274 (100%)	267 (97%)	7 (3%)	40	73
9	I	151/175 (86%)	150 (99%)	1 (1%)	76	92
10	J	141/141 (100%)	135 (96%)	6 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	85/85 (100%)	81 (95%)	4 (5%)	23	56
12	L	533/533 (100%)	524 (98%)	9 (2%)	53	82
13	M	412/412 (100%)	407 (99%)	5 (1%)	63	86
14	N	315/315 (100%)	311 (99%)	4 (1%)	61	86
15	O	283/303 (93%)	277 (98%)	6 (2%)	47	77
16	P	293/327 (90%)	282 (96%)	11 (4%)	29	64
17	Q	116/153 (76%)	113 (97%)	3 (3%)	40	73
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	86
19	S	76/82 (93%)	70 (92%)	6 (8%)	11	34
20	T	81/135 (60%)	76 (94%)	5 (6%)	16	46
20	U	81/135 (60%)	77 (95%)	4 (5%)	22	54
21	V	101/102 (99%)	98 (97%)	3 (3%)	36	70
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	90
23	X	154/155 (99%)	151 (98%)	3 (2%)	50	79
24	Y	101/102 (99%)	97 (96%)	4 (4%)	28	62
25	Z	120/121 (99%)	114 (95%)	6 (5%)	22	53
26	a	59/59 (100%)	56 (95%)	3 (5%)	21	53
27	b	71/72 (99%)	70 (99%)	1 (1%)	59	85
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	71
30	e	89/96 (93%)	86 (97%)	3 (3%)	32	66
31	f	54/54 (100%)	49 (91%)	5 (9%)	8	27
32	g	92/131 (70%)	90 (98%)	2 (2%)	45	77
33	h	121/158 (77%)	118 (98%)	3 (2%)	42	74
34	i	120/121 (99%)	115 (96%)	5 (4%)	26	60
35	j	61/84 (73%)	59 (97%)	2 (3%)	33	67
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	83
37	l	140/159 (88%)	136 (97%)	4 (3%)	37	71
38	m	113/114 (99%)	108 (96%)	5 (4%)	25	59
39	n	156/161 (97%)	152 (97%)	4 (3%)	40	73
40	o	110/120 (92%)	106 (96%)	4 (4%)	31	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	p	155/157 (99%)	148 (96%)	7 (4%)	24	58
42	q	130/130 (100%)	124 (95%)	6 (5%)	24	57
43	r	85/97 (88%)	81 (95%)	4 (5%)	23	56
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7206/7891 (91%)	7008 (97%)	198 (3%)	40	73

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	MET
1	A	90	MET
1	A	97	LEU
2	B	50	PHE
2	B	54	CYS
3	C	8	ARG
3	C	14	ARG
3	C	117	ILE
3	C	164	LYS
4	D	23	LYS
4	D	29	LYS
4	D	40	LYS
4	D	59	HIS
4	D	94	LYS
4	D	165	THR
4	D	172	GLU
4	D	290	ARG
5	E	57	GLN
5	E	118	GLU
5	E	181	ILE
5	E	190	ARG
5	E	207	LYS
6	F	8	LYS
6	F	78	LYS
6	F	164	LYS
6	F	249	ARG
6	F	250	ASN
6	F	314	THR
6	F	365	CYS
6	F	376	MET
6	F	432	GLN
7	G	61	LYS

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Mol	Chain	Res	Type
7	G	121	MET
7	G	158	ARG
7	G	226	GLU
7	G	288	LYS
7	G	364	LEU
7	G	396	ARG
7	G	476	LYS
7	G	499	GLN
7	G	536	ASP
7	G	539	LYS
7	G	540	ASP
7	G	601	ARG
7	G	613	TYR
7	G	643	GLN
7	G	650	LYS
8	H	5	ASN
8	H	70	MET
8	H	200	LEU
8	H	206	GLU
8	H	222	LEU
8	H	254	LEU
8	H	296	LEU
9	I	14	MET
10	J	55	MET
10	J	81	GLU
10	J	84	LEU
10	J	103	MET
10	J	139	GLU
10	J	163	ILE
11	K	37	MET
11	K	65	VAL
11	K	70	GLU
11	K	73	LEU
12	L	149	ILE
12	L	210	ASN
12	L	223	LYS
12	L	358	LYS
12	L	445	GLU
12	L	479	GLN
12	L	487	LYS
12	L	580	GLN
12	L	581	LYS

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Mol	Chain	Res	Type
13	M	57	PHE
13	M	91	ARG
13	M	207	MET
13	M	315	LEU
13	M	340	ARG
14	N	38	LEU
14	N	71	MET
14	N	83	GLN
14	N	187	MET
15	O	1	LEU
15	O	40	LYS
15	O	49	LYS
15	O	206	TYR
15	O	279	LEU
15	O	315	LYS
16	P	10	LYS
16	P	52	GLU
16	P	101	THR
16	P	139	ILE
16	P	144	LYS
16	P	196	LEU
16	P	224	ARG
16	P	226	LYS
16	P	276	GLU
16	P	327	LEU
16	P	338	LYS
17	Q	34	LYS
17	Q	70	MET
17	Q	127	ARG
18	R	95	HIS
19	S	18	ILE
19	S	25	ARG
19	S	38	LYS
19	S	61	GLN
19	S	74	LYS
19	S	97	LYS
20	T	9	GLU
20	T	25	ILE
20	T	29	LYS
20	T	30	LEU
20	T	69	LYS
20	U	12	LYS

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Mol	Chain	Res	Type
20	U	29	LYS
20	U	55	GLU
20	U	83	LYS
21	V	39	LYS
21	V	65	LYS
21	V	115	ILE
22	W	56	LYS
23	X	10	GLU
23	X	146	ARG
23	X	158	LYS
24	Y	43	LYS
24	Y	50	GLU
24	Y	90	LEU
24	Y	119	LEU
25	Z	4	LYS
25	Z	21	LYS
25	Z	51	LYS
25	Z	65	GLU
25	Z	98	LYS
25	Z	126	LEU
26	a	34	LYS
26	a	36	LYS
26	a	68	ASN
27	b	3	ARG
29	d	5	ARG
29	d	6	GLN
29	d	104	LYS
30	e	84	LYS
30	e	87	LYS
30	e	90	LYS
31	f	38	ARG
31	f	40	LYS
31	f	48	LEU
31	f	49	LYS
31	f	57	LYS
32	g	49	LYS
32	g	57	ASN
33	h	57	GLU
33	h	106	LYS
33	h	130	LYS
34	i	49	PHE
34	i	50	LEU

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Mol	Chain	Res	Type
34	i	51	GLN
34	i	78	VAL
34	i	100	LYS
35	j	39	ARG
35	j	51	PHE
36	k	91	LYS
37	l	6	LYS
37	l	87	ASN
37	l	88	ARG
37	l	115	MET
38	m	4	LYS
38	m	30	LYS
38	m	105	LYS
38	m	113	LYS
38	m	116	GLN
39	n	54	LYS
39	n	58	LYS
39	n	158	LYS
39	n	159	GLN
40	o	7	ARG
40	o	47	ASP
40	o	110	ARG
40	o	111	LYS
41	p	34	LYS
41	p	57	LYS
41	p	66	GLU
41	p	69	ARG
41	p	88	GLU
41	p	116	GLU
41	p	136	LYS
42	q	53	LYS
42	q	59	HIS
42	q	60	ARG
42	q	107	LYS
42	q	138	VAL
42	q	144	TYR
43	r	24	GLN
43	r	60	ARG
43	r	101	LYS
43	r	105	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
3	C	95	ASN
3	C	160	HIS
4	D	217	ASN
4	D	231	ASN
6	F	29	HIS
6	F	421	HIS
7	G	119	GLN
7	G	336	ASN
7	G	401	HIS
7	G	402	ASN
7	G	517	ASN
7	G	653	ASN
8	H	47	GLN
8	H	250	HIS
8	H	292	ASN
12	L	541	ASN
12	L	603	ASN
13	M	44	GLN
13	M	48	ASN
13	M	51	ASN
13	M	251	ASN
13	M	279	GLN
13	M	293	HIS
13	M	304	GLN
13	M	331	ASN
13	M	415	GLN
14	N	91	ASN
14	N	150	ASN
15	O	89	ASN
16	P	2	HIS
17	Q	29	HIS
18	R	90	GLN
19	S	79	ASN
21	V	40	ASN
22	W	25	ASN
22	W	69	ASN
23	X	29	HIS
23	X	103	GLN
25	Z	53	ASN
28	c	9	HIS
28	c	34	GLN
29	d	6	GLN

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Mol	Chain	Res	Type
29	d	117	HIS
30	e	69	GLN
33	h	135	HIS
34	i	12	GLN
34	i	58	ASN
35	j	24	GLN
35	j	50	HIS
36	k	20	GLN
39	n	72	HIS
40	o	46	ASN
41	p	123	ASN
42	q	91	HIS
42	q	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	AME	q	1	42	9,10,11	1.54	1 (11%)	9,11,13	1.44	2 (22%)
27	AYA	b	1	27	6,7,8	1.87	1 (16%)	6,8,10	1.34	1 (16%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	8,9,11	1.35	1 (12%)
4	2MR	D	85	4	10,12,13	2.45	2 (20%)	5,13,15	1.30	1 (20%)
10	FME	J	1	10	8,9,10	1.49	1 (12%)	8,9,11	1.42	2 (25%)
8	FME	H	1	8	8,9,10	1.50	1 (12%)	8,9,11	1.42	2 (25%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	8,9,11	1.43	1 (12%)
34	SAC	i	1	34	7,8,9	1.75	1 (14%)	7,9,11	1.74	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	AYA	r	1	43	6,7,8	1.87	2 (33%)	6,8,10	1.37	1 (16%)
12	FME	L	1	12	8,9,10	1.51	1 (12%)	8,9,11	1.31	0
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.38	1 (11%)
1	FME	A	1	1	8,9,10	1.50	1 (12%)	8,9,11	1.42	2 (25%)
24	AYA	Y	1	24	6,7,8	1.89	2 (33%)	6,8,10	1.38	1 (16%)
38	SAC	m	1	38	7,8,9	1.73	1 (14%)	7,9,11	1.25	1 (14%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	8,9,11	1.28	0

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
42	AME	q	1	42	-	2/9/10/12	-
27	AYA	b	1	27	-	2/5/6/8	-
11	FME	K	1	11	-	2/7/9/11	-
4	2MR	D	85	4	-	1/10/13/15	-
10	FME	J	1	10	-	2/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
13	FME	M	1	13	-	3/7/9/11	-
34	SAC	i	1	34	-	4/7/8/10	-
43	AYA	r	1	43	-	1/5/6/8	-
12	FME	L	1	12	-	2/7/9/11	-
29	AME	d	1	29	-	5/9/10/12	-
1	FME	A	1	1	-	0/7/9/11	-
24	AYA	Y	1	24	-	0/5/6/8	-
38	SAC	m	1	38	-	2/7/8/10	-
14	FME	N	1	14	-	2/7/9/11	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.40	1.44	1.33
4	D	85	2MR	CZ-NE	5.14	1.45	1.34
14	N	1	FME	CN-N	3.75	1.45	1.33
12	L	1	FME	CN-N	3.74	1.45	1.33
11	K	1	FME	CN-N	3.72	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1	FME	CN-N	3.72	1.45	1.33
8	H	1	FME	CN-N	3.69	1.45	1.33
1	A	1	FME	CN-N	3.69	1.45	1.33
10	J	1	FME	CN-N	3.68	1.45	1.33
34	i	1	SAC	C1A-N	3.62	1.46	1.34
27	b	1	AYA	CT-N	3.54	1.45	1.34
42	q	1	AME	CT1-N	3.51	1.45	1.34
38	m	1	SAC	C1A-N	3.51	1.45	1.34
29	d	1	AME	CT1-N	3.47	1.45	1.34
43	r	1	AYA	CT-N	3.43	1.45	1.34
24	Y	1	AYA	CT-N	3.42	1.45	1.34
24	Y	1	AYA	OT-CT	-2.10	1.18	1.23
43	r	1	AYA	OT-CT	-2.06	1.18	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	3.45	121.84	116.12
42	q	1	AME	CE-SD-CG	2.48	113.16	100.32
42	q	1	AME	CT2-CT1-N	2.46	120.19	116.12
27	b	1	AYA	CM-CT-N	2.36	120.04	116.12
24	Y	1	AYA	CM-CT-N	2.34	120.00	116.12
43	r	1	AYA	CM-CT-N	2.34	119.99	116.12
38	m	1	SAC	C2A-C1A-N	2.31	119.95	116.12
29	d	1	AME	CT2-CT1-N	2.23	119.81	116.12
1	A	1	FME	O1-CN-N	-2.18	119.70	125.32
4	D	85	2MR	CD-NE-CZ	-2.17	119.28	123.36
10	J	1	FME	O1-CN-N	-2.15	119.75	125.32
8	H	1	FME	O1-CN-N	-2.14	119.78	125.32
1	A	1	FME	CA-N-CN	-2.09	119.60	122.82
13	M	1	FME	O1-CN-N	-2.05	120.01	125.32
11	K	1	FME	O1-CN-N	-2.01	120.12	125.32
10	J	1	FME	CA-N-CN	-2.01	119.73	122.82
8	H	1	FME	CA-N-CN	-2.00	119.74	122.82

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	85	2MR	O-C-CA-CB
8	H	1	FME	C-CA-CB-CG
8	H	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
11	K	1	FME	O-C-CA-CB
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
27	b	1	AYA	O-C-CA-CB
29	d	1	AME	N-CA-CB-CG
34	i	1	SAC	C-CA-CB-OG
38	m	1	SAC	N-CA-CB-OG
38	m	1	SAC	C-CA-CB-OG
43	r	1	AYA	O-C-CA-CB
42	q	1	AME	CB-CG-SD-CE
10	J	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
34	i	1	SAC	N-CA-CB-OG
8	H	1	FME	N-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
13	M	1	FME	N-CA-CB-CG
29	d	1	AME	CB-CA-N-CT1
29	d	1	AME	C-CA-CB-CG
13	M	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
27	b	1	AYA	C-CA-N-CT
29	d	1	AME	C-CA-N-CT1
29	d	1	AME	CA-CB-CG-SD
42	q	1	AME	CA-CB-CG-SD
11	K	1	FME	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	1	AYA	1	0
11	K	1	FME	1	0
13	M	1	FME	1	0
34	i	1	SAC	1	0
29	d	1	AME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 4 are monoatomic - leaving 70 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
45	PC1	B	204	45	47,47,53	1.01	4 (8%)	53,55,61	1.06	2 (3%)
46	3PE	I	205	-	35,35,50	1.02	4 (11%)	38,40,55	1.13	2 (5%)
53	CDL	N	401	-	73,73,99	1.02	8 (10%)	79,85,111	1.09	4 (5%)
48	PLC	b	102	-	31,31,41	0.58	0	37,39,49	0.58	0
46	3PE	f	102	-	50,50,50	0.88	4 (8%)	53,55,55	1.08	2 (3%)
45	PC1	I	204	-	36,36,53	1.14	4 (11%)	42,44,61	1.01	2 (4%)
45	PC1	q	202	-	29,29,53	1.27	4 (13%)	35,37,61	1.14	2 (5%)
46	3PE	d	202	-	48,48,50	0.89	4 (8%)	51,53,55	1.08	2 (3%)
53	CDL	q	201	-	60,60,99	1.12	7 (11%)	66,72,111	1.15	4 (6%)
46	3PE	L	704	-	45,45,50	0.92	3 (6%)	48,50,55	1.09	2 (4%)
45	PC1	H	403	-	38,38,53	1.12	4 (10%)	44,46,61	0.94	2 (4%)
45	PC1	I	203	-	53,53,53	0.94	4 (7%)	59,61,61	1.01	2 (3%)
46	3PE	A	203	-	40,40,50	0.97	4 (10%)	43,45,55	1.10	2 (4%)
52	U10	H	401	-	28,28,63	2.04	15 (53%)	36,37,79	2.09	9 (25%)
46	3PE	J	204	-	43,43,50	0.94	4 (9%)	46,48,55	1.10	2 (4%)
45	PC1	H	402	-	47,47,53	1.02	4 (8%)	53,55,61	1.00	2 (3%)
46	3PE	f	101	-	28,28,50	1.14	4 (14%)	31,33,55	1.31	3 (9%)
46	3PE	j	101	-	43,43,50	0.94	4 (9%)	46,48,55	1.06	2 (4%)
46	3PE	N	403	-	35,35,50	1.02	4 (11%)	38,40,55	1.17	2 (5%)
46	3PE	o	202	-	34,34,50	0.98	3 (8%)	37,39,55	1.09	1 (2%)
45	PC1	M	603	-	43,43,53	1.05	4 (9%)	49,51,61	1.06	2 (4%)
46	3PE	b	101	-	46,46,50	0.90	4 (8%)	49,51,55	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	I	201	9	0,12,12	-	-	-		
46	3PE	A	202	-	33,33,50	1.06	4 (12%)	36,38,55	1.17	2 (5%)
46	3PE	L	706	-	36,36,50	1.00	4 (11%)	39,41,55	1.13	2 (5%)
47	SF4	G	802	7	0,12,12	-	-	-		
53	CDL	h	201	-	79,79,99	0.99	7 (8%)	85,91,111	1.10	4 (4%)
48	PLC	B	203	-	37,37,41	0.53	0	43,45,49	0.56	0
57	NDP	P	501	-	51,52,52	4.01	27 (52%)	71,80,80	1.90	14 (19%)
59	CHD	i	201	-	32,32,32	3.26	10 (31%)	51,51,51	2.31	16 (31%)
46	3PE	J	203	-	32,32,50	1.08	4 (12%)	35,37,55	1.11	2 (5%)
45	PC1	d	203	-	38,38,53	1.13	4 (10%)	44,46,61	1.02	2 (4%)
46	3PE	M	604	-	49,49,50	0.88	4 (8%)	52,54,55	0.99	2 (3%)
46	3PE	Y	202	-	26,26,50	1.19	4 (15%)	29,31,55	1.22	2 (6%)
45	PC1	A	201	-	34,34,53	1.17	4 (11%)	40,42,61	1.05	2 (5%)
45	PC1	J	202	-	34,34,53	1.16	4 (11%)	40,42,61	1.02	2 (5%)
45	PC1	M	605	-	25,25,53	1.35	4 (16%)	31,33,61	1.00	2 (6%)
46	3PE	Y	205	-	44,44,50	0.93	4 (9%)	47,49,55	1.10	2 (4%)
48	PLC	O	403	-	25,25,41	0.63	0	31,33,49	0.66	0
48	PLC	L	705	-	26,26,41	0.62	0	32,34,49	0.60	0
47	SF4	I	202	9	0,12,12	-	-	-		
58	EHZ	U	101	20	31,36,37	1.58	5 (16%)	36,44,47	1.65	6 (16%)
60	MYR	o	201	40	13,14,15	0.43	0	12,13,15	0.79	0
55	DGT	O	401	56	32,33,33	3.33	14 (43%)	48,52,52	1.95	13 (27%)
46	3PE	L	702	-	34,34,50	0.98	3 (8%)	37,39,55	1.10	1 (2%)
50	FMN	F	501	-	33,33,33	2.72	10 (30%)	48,50,50	1.76	15 (31%)
46	3PE	Y	204	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
46	3PE	N	402	-	48,48,50	0.89	4 (8%)	51,53,55	1.10	2 (3%)
58	EHZ	T	101	20	31,36,37	1.59	5 (16%)	36,44,47	1.63	7 (19%)
46	3PE	Z	201	-	44,44,50	0.93	4 (9%)	47,49,55	1.06	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-		
46	3PE	Y	201	-	44,44,50	0.91	4 (9%)	47,49,55	1.07	2 (4%)
53	CDL	M	602	-	90,90,99	0.92	7 (7%)	96,102,111	1.10	4 (4%)
47	SF4	B	201	2	0,12,12	-	-	-		
46	3PE	m	202	-	32,32,50	1.07	4 (12%)	35,37,55	1.22	2 (5%)
45	PC1	m	203	-	39,39,53	1.10	4 (10%)	45,47,61	1.06	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-		
53	CDL	L	701	-	86,86,99	0.95	8 (9%)	92,98,111	1.10	4 (4%)
53	CDL	X	201	-	86,86,99	0.94	7 (8%)	92,98,111	1.11	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PC1	L	707	-	46,46,53	1.01	3 (6%)	52,54,61	1.03	2 (3%)
45	PC1	B	202	45	45,45,53	1.02	3 (6%)	51,53,61	1.00	2 (3%)
46	3PE	L	703	-	44,44,50	0.92	4 (9%)	47,49,55	1.08	2 (4%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
46	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.11	2 (4%)
53	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.06	4 (5%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
46	3PE	Y	203	-	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
45	PC1	h	202	-	30,30,53	1.24	4 (13%)	36,38,61	1.10	2 (5%)
48	PLC	g	201	-	31,31,41	0.58	0	37,39,49	0.53	0
53	CDL	J	201	-	35,35,99	1.35	6 (17%)	41,47,111	1.47	3 (7%)

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
45	PC1	B	204	45	-	22/51/51/57	-
46	3PE	I	205	-	-	18/39/39/54	-
53	CDL	N	401	-	-	39/84/84/110	-
48	PLC	b	102	-	-	8/35/35/45	-
46	3PE	f	102	-	-	22/54/54/54	-
45	PC1	I	204	-	-	11/40/40/57	-
45	PC1	q	202	-	-	8/33/33/57	-
46	3PE	d	202	-	-	21/52/52/54	-
53	CDL	q	201	-	-	31/71/71/110	-
46	3PE	L	704	-	-	25/49/49/54	-
45	PC1	H	403	-	-	18/42/42/57	-
45	PC1	I	203	-	-	21/57/57/57	-
46	3PE	A	203	-	-	16/44/44/54	-
52	U10	H	401	-	-	5/21/45/87	0/1/1/1
46	3PE	J	204	-	-	19/47/47/54	-
45	PC1	H	402	-	-	23/51/51/57	-
46	3PE	f	101	-	-	13/31/31/54	-
46	3PE	j	101	-	-	18/47/47/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	N	403	-	-	21/39/39/54	-
46	3PE	o	202	-	-	14/37/37/54	-
45	PC1	M	603	-	-	18/47/47/57	-
46	3PE	b	101	-	-	17/50/50/54	-
47	SF4	I	201	9	-	-	0/6/5/5
46	3PE	A	202	-	-	15/37/37/54	-
46	3PE	L	706	-	-	13/40/40/54	-
57	NDP	P	501	-	-	10/34/77/77	0/5/5/5
53	CDL	h	201	-	-	32/90/90/110	-
48	PLC	B	203	-	-	21/41/41/45	-
47	SF4	G	802	7	-	-	0/6/5/5
59	CHD	i	201	-	-	5/9/74/74	0/4/4/4
46	3PE	J	203	-	-	17/36/36/54	-
45	PC1	d	203	-	-	17/42/42/57	-
46	3PE	M	604	-	-	19/53/53/54	-
46	3PE	Y	202	-	-	11/30/30/54	-
45	PC1	A	201	-	-	12/38/38/57	-
45	PC1	J	202	-	-	12/38/38/57	-
45	PC1	M	605	-	-	17/29/29/57	-
46	3PE	Y	205	-	-	18/48/48/54	-
48	PLC	O	403	-	-	9/28/28/45	-
48	PLC	L	705	-	-	8/30/30/45	-
47	SF4	I	202	9	-	-	0/6/5/5
58	EHZ	U	101	20	-	10/42/44/45	-
60	MYR	o	201	40	-	6/12/12/13	-
55	DGT	O	401	56	-	4/22/34/34	0/3/3/3
46	3PE	L	702	-	-	15/37/37/54	-
50	FMN	F	501	-	-	6/18/18/18	0/3/3/3
46	3PE	Y	204	-	-	24/54/54/54	-
46	3PE	N	402	-	-	26/52/52/54	-
58	EHZ	T	101	20	-	14/42/44/45	-
46	3PE	Z	201	-	-	25/48/48/54	-
47	SF4	F	502	6	-	-	0/6/5/5
46	3PE	Y	201	-	-	29/48/48/54	-
53	CDL	M	602	-	-	42/101/101/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	B	201	2	-	-	0/6/5/5
46	3PE	m	202	-	-	15/36/36/54	-
45	PC1	m	203	-	-	16/43/43/57	-
53	CDL	L	701	-	-	27/97/97/110	-
53	CDL	X	201	-	-	46/97/97/110	-
47	SF4	G	801	7	-	-	0/6/5/5
45	PC1	L	707	-	-	26/50/50/57	-
45	PC1	B	202	45	-	14/49/49/57	-
46	3PE	L	703	-	-	24/48/48/54	-
49	FES	G	803	7	-	-	0/1/1/1
46	3PE	m	201	-	-	23/44/44/54	-
53	CDL	d	201	-	-	37/75/75/110	-
49	FES	E	301	5	-	-	0/1/1/1
46	3PE	Y	203	-	-	29/54/54/54	-
45	PC1	h	202	-	-	15/34/34/57	-
48	PLC	g	201	-	-	10/34/34/45	-
53	CDL	J	201	-	-	21/42/42/110	-

All (303) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	10.13	1.70	1.59
57	P	501	NDP	C2B-C1B	-8.98	1.31	1.53
59	i	201	CHD	C11-C12	8.88	1.67	1.53
55	O	401	DGT	O6-C6	8.81	1.40	1.23
57	P	501	NDP	O4B-C1B	8.61	1.61	1.42
57	P	501	NDP	O4D-C1D	8.42	1.61	1.42
57	P	501	NDP	C7N-N7N	7.65	1.55	1.33
57	P	501	NDP	C2D-C1D	-7.42	1.30	1.53
59	i	201	CHD	C16-C15	7.22	1.73	1.54
57	P	501	NDP	C6N-C5N	7.04	1.54	1.33
55	O	401	DGT	C5-N7	6.72	1.52	1.39
57	P	501	NDP	O4D-C4D	-6.56	1.30	1.45
50	F	501	FMN	C10-N1	6.50	1.46	1.33
50	F	501	FMN	C4A-N5	6.34	1.44	1.30
59	i	201	CHD	C20-C17	-6.29	1.43	1.54
57	P	501	NDP	P2B-O2B	5.70	1.69	1.59
55	O	401	DGT	PA-O3A	5.37	1.65	1.59
59	i	201	CHD	C8-C9	5.37	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	F	501	FMN	C5A-N5	5.35	1.49	1.39
57	P	501	NDP	C6A-N6A	5.33	1.47	1.34
59	i	201	CHD	O12-C12	-5.26	1.35	1.43
58	T	101	EHZ	C12-N1	5.26	1.45	1.33
55	O	401	DGT	PB-O3A	5.17	1.65	1.59
59	i	201	CHD	C13-C17	5.14	1.64	1.55
57	P	501	NDP	O4B-C4B	-5.13	1.33	1.45
58	U	101	EHZ	C12-N1	5.10	1.45	1.33
58	U	101	EHZ	C15-N2	5.03	1.45	1.33
55	O	401	DGT	PB-O3B	4.98	1.64	1.59
50	F	501	FMN	C2-N1	4.93	1.47	1.36
58	T	101	EHZ	C15-N2	4.93	1.45	1.33
50	F	501	FMN	C9A-N10	4.87	1.49	1.41
55	O	401	DGT	C2-N2	4.86	1.45	1.34
55	O	401	DGT	C2-N1	4.76	1.49	1.37
57	P	501	NDP	C2N-C3N	4.70	1.48	1.35
59	i	201	CHD	C6-C5	4.60	1.61	1.53
57	P	501	NDP	PN-O3	4.59	1.64	1.59
50	F	501	FMN	C2-N3	4.43	1.48	1.39
55	O	401	DGT	C2-N3	4.38	1.43	1.33
55	O	401	DGT	C8-N9	-4.28	1.27	1.37
59	i	201	CHD	C15-C14	4.27	1.63	1.54
57	P	501	NDP	C5A-C4A	-4.25	1.31	1.39
57	P	501	NDP	O7N-C7N	-4.11	1.14	1.24
57	P	501	NDP	C8A-N9A	-3.95	1.30	1.37
55	O	401	DGT	C4-N9	-3.90	1.28	1.38
50	F	501	FMN	C10-N10	3.79	1.45	1.37
57	P	501	NDP	O2D-C2D	3.79	1.52	1.43
50	F	501	FMN	C4-N3	3.65	1.45	1.38
59	i	201	CHD	C6-C7	3.58	1.59	1.52
57	P	501	NDP	C4N-C3N	3.34	1.56	1.50
52	H	401	U10	C4-C5	-3.25	1.39	1.48
52	H	401	U10	C3-C2	-3.06	1.40	1.48
50	F	501	FMN	O2-C2	-3.01	1.18	1.24
53	M	602	CDL	OB6-CB4	-2.91	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.88	1.39	1.46
52	H	401	U10	C7-C8	2.86	1.55	1.50
45	L	707	PC1	O21-C2	-2.86	1.39	1.46
52	H	401	U10	C6-C1	2.85	1.40	1.35
53	L	701	CDL	OB6-CB4	-2.83	1.40	1.46
45	B	202	PC1	O21-C2	-2.82	1.40	1.46
53	X	201	CDL	OB6-CB4	-2.81	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	h	201	CDL	OB6-CB4	-2.81	1.40	1.46
52	H	401	U10	C21-C19	2.81	1.57	1.50
50	F	501	FMN	O4-C4	-2.79	1.18	1.23
57	P	501	NDP	C5A-N7A	-2.78	1.34	1.39
53	h	201	CDL	OA6-CA4	-2.77	1.40	1.46
45	B	204	PC1	O21-C2	-2.75	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.75	1.40	1.46
45	q	202	PC1	O21-C2	-2.75	1.40	1.46
46	j	101	3PE	O21-C2	-2.75	1.40	1.46
57	P	501	NDP	C4N-C5N	2.74	1.56	1.49
46	L	704	3PE	O21-C2	-2.74	1.40	1.46
46	b	101	3PE	O21-C2	-2.73	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.72	1.40	1.46
53	L	701	CDL	OA6-CA4	-2.72	1.40	1.46
53	N	401	CDL	OB6-CB4	-2.71	1.40	1.46
46	f	101	3PE	O21-C2	-2.71	1.40	1.46
45	d	203	PC1	O21-C2	-2.70	1.40	1.46
45	H	402	PC1	O21-C2	-2.69	1.40	1.46
45	h	202	PC1	O21-C2	-2.69	1.40	1.46
45	M	603	PC1	O21-C2	-2.69	1.40	1.46
45	I	204	PC1	O21-C2	-2.69	1.40	1.46
46	Y	201	3PE	O21-C2	-2.68	1.40	1.46
53	J	201	CDL	OA6-CA4	-2.67	1.40	1.46
46	Y	202	3PE	O21-C2	-2.67	1.40	1.46
45	I	203	PC1	O21-C2	-2.67	1.40	1.46
46	m	201	3PE	O21-C2	-2.67	1.40	1.46
46	A	202	3PE	O21-C2	-2.66	1.40	1.46
53	J	201	CDL	OB6-CB4	-2.66	1.40	1.46
53	d	201	CDL	OB6-CB4	-2.66	1.40	1.46
46	I	205	3PE	O21-C2	-2.66	1.40	1.46
45	M	605	PC1	O21-C2	-2.65	1.40	1.46
46	J	204	3PE	O21-C2	-2.65	1.40	1.46
55	O	401	DGT	C1'-N9	-2.65	1.41	1.48
46	L	702	3PE	O21-C2	-2.64	1.40	1.46
46	Y	203	3PE	O21-C2	-2.64	1.40	1.46
46	d	202	3PE	O21-C2	-2.64	1.40	1.46
45	J	202	PC1	O21-C2	-2.63	1.40	1.46
46	A	203	3PE	O21-C2	-2.63	1.40	1.46
45	H	403	PC1	O21-C2	-2.63	1.40	1.46
46	Z	201	3PE	O21-C2	-2.63	1.40	1.46
46	Y	205	3PE	O21-C2	-2.63	1.40	1.46
53	M	602	CDL	OA6-CA4	-2.63	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	J	203	3PE	O21-C2	-2.63	1.40	1.46
46	N	402	3PE	O21-C2	-2.63	1.40	1.46
45	m	203	PC1	O21-C2	-2.62	1.40	1.46
46	f	102	3PE	O21-C2	-2.62	1.40	1.46
46	N	403	3PE	O21-C2	-2.59	1.40	1.46
46	M	604	3PE	O21-C2	-2.59	1.40	1.46
46	m	202	3PE	O21-C2	-2.58	1.40	1.46
59	i	201	CHD	C13-C12	-2.57	1.50	1.54
53	X	201	CDL	OA6-CA4	-2.55	1.40	1.46
53	q	201	CDL	OB8-CB7	2.54	1.40	1.33
46	o	202	3PE	O21-C2	-2.53	1.40	1.46
52	H	401	U10	C15-C14	2.52	1.56	1.50
53	N	401	CDL	OA6-CA4	-2.50	1.40	1.46
58	T	101	EHZ	C9-S1	2.50	1.82	1.76
53	d	201	CDL	OB8-CB7	2.48	1.40	1.33
52	H	401	U10	C7-C6	2.46	1.56	1.51
57	P	501	NDP	O3D-C3D	-2.45	1.36	1.43
53	N	401	CDL	OB8-CB7	2.45	1.40	1.33
53	N	401	CDL	OA8-CA7	2.45	1.40	1.33
57	P	501	NDP	O3B-C3B	-2.44	1.36	1.43
45	I	204	PC1	O31-C31	2.43	1.40	1.33
53	M	602	CDL	OA8-CA7	2.42	1.40	1.33
58	T	101	EHZ	O4-C15	-2.42	1.18	1.23
57	P	501	NDP	C6N-N1N	2.42	1.43	1.37
46	Z	201	3PE	O31-C31	2.41	1.40	1.33
45	m	203	PC1	O31-C31	2.41	1.40	1.33
53	h	201	CDL	OB8-CB7	2.41	1.40	1.33
45	B	202	PC1	O31-C31	2.40	1.40	1.33
53	X	201	CDL	OA8-CA7	2.40	1.40	1.33
58	U	101	EHZ	O3-C12	-2.40	1.18	1.23
52	H	401	U10	C11-C9	2.40	1.56	1.51
46	L	704	3PE	O31-C31	2.40	1.40	1.33
45	d	203	PC1	O31-C31	2.40	1.40	1.33
53	L	701	CDL	OB8-CB7	2.39	1.40	1.33
46	Y	205	3PE	O31-C31	2.39	1.40	1.33
45	H	402	PC1	O31-C31	2.39	1.40	1.33
45	h	202	PC1	O31-C31	2.39	1.40	1.33
46	f	101	3PE	O31-C31	2.39	1.40	1.33
46	N	403	3PE	O31-C31	2.39	1.40	1.33
45	H	403	PC1	O31-C31	2.39	1.40	1.33
46	L	703	3PE	O21-C2	-2.39	1.41	1.46
45	M	605	PC1	O31-C31	2.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Y	204	3PE	O31-C31	2.38	1.40	1.33
53	X	201	CDL	OB8-CB6	-2.38	1.39	1.45
46	Y	201	3PE	O31-C3	-2.38	1.39	1.45
53	d	201	CDL	OA8-CA7	2.37	1.40	1.33
45	J	202	PC1	O31-C31	2.37	1.40	1.33
46	Y	204	3PE	O21-C2	-2.37	1.41	1.46
46	A	202	3PE	O31-C31	2.37	1.40	1.33
46	I	205	3PE	O31-C31	2.37	1.40	1.33
46	J	203	3PE	O31-C31	2.37	1.40	1.33
46	j	101	3PE	O31-C31	2.36	1.40	1.33
57	P	501	NDP	C7N-C3N	2.36	1.53	1.48
46	m	201	3PE	O31-C31	2.36	1.40	1.33
58	T	101	EHZ	O3-C12	-2.36	1.18	1.23
46	A	203	3PE	O31-C31	2.36	1.40	1.33
46	f	102	3PE	O31-C31	2.36	1.40	1.33
45	B	204	PC1	O31-C31	2.35	1.40	1.33
53	L	701	CDL	OA8-CA7	2.35	1.40	1.33
58	U	101	EHZ	O4-C15	-2.35	1.18	1.23
45	q	202	PC1	O31-C31	2.35	1.40	1.33
58	U	101	EHZ	C9-S1	2.35	1.81	1.76
53	M	602	CDL	OB8-CB7	2.35	1.40	1.33
45	A	201	PC1	O21-C21	2.34	1.40	1.34
45	A	201	PC1	O31-C31	2.34	1.40	1.33
45	I	203	PC1	O31-C31	2.34	1.40	1.33
46	M	604	3PE	O31-C31	2.34	1.40	1.33
53	J	201	CDL	OB6-CB5	2.34	1.40	1.35
57	P	501	NDP	P2B-O1X	2.33	1.57	1.50
46	N	402	3PE	O31-C3	-2.33	1.40	1.45
46	Y	202	3PE	O31-C31	2.33	1.40	1.33
46	d	202	3PE	O31-C31	2.32	1.40	1.33
53	q	201	CDL	OA8-CA7	2.32	1.40	1.33
46	Y	203	3PE	O31-C31	2.32	1.40	1.33
46	b	101	3PE	O31-C31	2.32	1.40	1.33
53	h	201	CDL	OA8-CA7	2.31	1.40	1.33
53	J	201	CDL	OA6-CA5	2.31	1.40	1.35
46	Y	203	3PE	O31-C3	-2.31	1.40	1.45
53	L	701	CDL	OA8-CA6	-2.30	1.40	1.45
46	L	706	3PE	O21-C2	-2.30	1.41	1.46
45	A	201	PC1	O21-C2	-2.30	1.41	1.46
57	P	501	NDP	PA-O5B	2.29	1.68	1.59
46	J	204	3PE	O31-C31	2.29	1.40	1.33
45	M	603	PC1	O31-C31	2.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	707	PC1	O31-C3	-2.29	1.40	1.45
46	f	101	3PE	O21-C21	2.28	1.40	1.35
46	L	706	3PE	O21-C21	2.28	1.40	1.34
46	A	203	3PE	O31-C3	-2.28	1.40	1.45
45	M	603	PC1	O31-C3	-2.28	1.40	1.45
46	L	706	3PE	O31-C31	2.27	1.40	1.33
53	h	201	CDL	OA8-CA6	-2.27	1.40	1.45
46	m	202	3PE	O31-C3	-2.27	1.40	1.45
46	N	402	3PE	O31-C31	2.27	1.40	1.33
55	O	401	DGT	PG-O1G	-2.26	1.46	1.54
46	L	706	3PE	O31-C3	-2.26	1.40	1.45
46	m	202	3PE	O31-C31	2.26	1.39	1.33
46	L	703	3PE	O31-C31	2.26	1.39	1.33
55	O	401	DGT	PG-O2G	-2.26	1.46	1.54
45	L	707	PC1	O31-C31	2.26	1.39	1.33
46	Y	204	3PE	O21-C21	2.25	1.40	1.34
53	h	201	CDL	OB8-CB6	-2.25	1.40	1.45
53	q	201	CDL	OA8-CA6	-2.25	1.40	1.45
46	d	202	3PE	O31-C3	-2.25	1.40	1.45
55	O	401	DGT	C4-N3	2.24	1.39	1.34
46	I	205	3PE	O31-C3	-2.24	1.40	1.45
53	d	201	CDL	OA8-CA6	-2.23	1.40	1.45
46	Y	205	3PE	O31-C3	-2.23	1.40	1.45
45	d	203	PC1	O31-C3	-2.23	1.40	1.45
45	H	403	PC1	O31-C3	-2.23	1.40	1.45
46	j	101	3PE	O31-C3	-2.22	1.40	1.45
46	L	703	3PE	O31-C3	-2.22	1.40	1.45
46	J	204	3PE	O31-C3	-2.22	1.40	1.45
46	Y	202	3PE	O31-C3	-2.22	1.40	1.45
46	Z	201	3PE	O31-C3	-2.22	1.40	1.45
46	M	604	3PE	O21-C21	2.22	1.40	1.34
46	Y	204	3PE	O31-C3	-2.22	1.40	1.45
53	X	201	CDL	OA8-CA6	-2.22	1.40	1.45
46	m	201	3PE	O31-C3	-2.22	1.40	1.45
53	N	401	CDL	OA6-CA5	2.22	1.40	1.34
46	J	203	3PE	O31-C3	-2.21	1.40	1.45
53	M	602	CDL	OA6-CA5	2.21	1.40	1.34
53	L	701	CDL	OB8-CB6	-2.21	1.40	1.45
46	L	703	3PE	O21-C21	2.21	1.40	1.34
45	I	204	PC1	O21-C21	2.21	1.40	1.34
53	M	602	CDL	OB8-CB6	-2.21	1.40	1.45
46	o	202	3PE	O21-C21	2.20	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	L	702	3PE	O31-C3	-2.20	1.40	1.45
45	q	202	PC1	O31-C3	-2.20	1.40	1.45
45	M	605	PC1	O31-C3	-2.20	1.40	1.45
53	N	401	CDL	OB8-CB6	-2.20	1.40	1.45
46	M	604	3PE	O31-C3	-2.20	1.40	1.45
45	I	204	PC1	O31-C3	-2.20	1.40	1.45
46	f	102	3PE	O31-C3	-2.20	1.40	1.45
45	A	201	PC1	O31-C3	-2.20	1.40	1.45
46	m	202	3PE	O21-C21	2.19	1.40	1.34
45	I	203	PC1	O31-C3	-2.19	1.40	1.45
45	B	204	PC1	O31-C3	-2.19	1.40	1.45
46	J	204	3PE	O21-C21	2.19	1.40	1.34
53	d	201	CDL	OB6-CB5	2.18	1.40	1.34
46	J	203	3PE	O21-C21	2.18	1.40	1.34
45	H	402	PC1	O31-C3	-2.18	1.40	1.45
46	Z	201	3PE	O21-C21	2.18	1.40	1.34
45	J	202	PC1	O21-C21	2.18	1.40	1.34
46	f	102	3PE	O21-C21	2.17	1.40	1.34
52	H	401	U10	C1M-C1	2.17	1.55	1.50
46	L	704	3PE	O31-C3	-2.17	1.40	1.45
52	H	401	U10	C16-C14	2.17	1.55	1.51
52	H	401	U10	C1-C2	-2.17	1.39	1.47
57	P	501	NDP	C5B-C4B	2.17	1.58	1.51
45	m	203	PC1	O21-C21	2.17	1.40	1.34
46	N	403	3PE	O31-C3	-2.17	1.40	1.45
53	X	201	CDL	OB8-CB7	2.16	1.39	1.33
53	J	201	CDL	OA8-CA6	-2.16	1.40	1.45
53	J	201	CDL	OB8-CB6	-2.16	1.40	1.45
45	q	202	PC1	O21-C21	2.16	1.40	1.34
46	A	202	3PE	O21-C21	2.16	1.40	1.34
52	H	401	U10	O3-C3	2.16	1.42	1.36
46	o	202	3PE	O31-C3	-2.16	1.40	1.45
45	I	203	PC1	O21-C21	2.16	1.40	1.34
46	f	101	3PE	O31-C3	-2.15	1.40	1.45
46	b	101	3PE	O31-C3	-2.15	1.40	1.45
45	B	202	PC1	O31-C3	-2.15	1.40	1.45
53	M	602	CDL	OA8-CA6	-2.14	1.40	1.45
53	d	201	CDL	OB8-CB6	-2.14	1.40	1.45
45	h	202	PC1	O31-C3	-2.14	1.40	1.45
45	h	202	PC1	O21-C21	2.14	1.40	1.34
45	m	203	PC1	O31-C3	-2.14	1.40	1.45
46	Y	203	3PE	O21-C21	2.13	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	d	202	3PE	O21-C21	2.13	1.40	1.34
46	Y	205	3PE	O21-C21	2.13	1.40	1.34
46	A	203	3PE	O21-C21	2.13	1.40	1.34
46	I	205	3PE	O21-C21	2.13	1.40	1.34
45	M	605	PC1	O21-C21	2.13	1.40	1.34
46	j	101	3PE	O21-C21	2.12	1.40	1.34
52	H	401	U10	C6-C5	-2.12	1.40	1.46
46	A	202	3PE	O31-C3	-2.12	1.40	1.45
46	Y	202	3PE	O21-C21	2.12	1.40	1.34
46	Y	201	3PE	O21-C21	2.11	1.40	1.34
45	d	203	PC1	O21-C21	2.11	1.40	1.34
46	m	201	3PE	O21-C21	2.11	1.40	1.34
53	q	201	CDL	OB8-CB6	-2.11	1.40	1.45
46	N	403	3PE	O21-C21	2.11	1.40	1.34
46	N	402	3PE	O21-C21	2.11	1.40	1.34
45	M	603	PC1	O21-C21	2.11	1.40	1.34
53	L	701	CDL	OA6-CA5	2.11	1.40	1.34
45	H	403	PC1	O21-C21	2.10	1.40	1.34
52	H	401	U10	O4-C4	2.10	1.41	1.36
46	L	702	3PE	O21-C21	2.10	1.40	1.34
53	N	401	CDL	OB6-CB5	2.09	1.40	1.34
45	B	204	PC1	O21-C21	2.09	1.40	1.34
45	H	402	PC1	O21-C21	2.09	1.40	1.34
53	q	201	CDL	OB6-CB5	2.08	1.40	1.34
45	J	202	PC1	O31-C3	-2.08	1.40	1.45
53	N	401	CDL	OA8-CA6	-2.07	1.40	1.45
53	d	201	CDL	OA6-CA5	2.07	1.40	1.34
46	Y	201	3PE	O31-C31	2.07	1.39	1.33
53	h	201	CDL	OA6-CA5	2.06	1.40	1.34
46	b	101	3PE	O21-C21	2.06	1.40	1.34
53	X	201	CDL	OA6-CA5	2.06	1.40	1.34
53	L	701	CDL	OB6-CB5	2.02	1.40	1.34
52	H	401	U10	C10-C9	2.01	1.55	1.50

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	C8-N9-C4	7.47	120.04	106.03
59	i	201	CHD	C13-C17-C20	-6.99	111.02	119.48
52	H	401	U10	C7-C8-C9	-6.26	116.05	126.83
52	H	401	U10	C12-C13-C14	-5.84	114.26	127.62
57	P	501	NDP	N6A-C6A-N1A	-5.72	105.63	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	U	101	EHZ	C8-C9-S1	5.55	120.57	113.56
59	i	201	CHD	C14-C13-C12	5.50	112.44	107.42
57	P	501	NDP	N3A-C2A-N1A	-5.38	120.44	128.58
57	P	501	NDP	C4A-N9A-C1B	-5.31	114.22	126.63
58	T	101	EHZ	C8-C9-S1	5.22	120.15	113.56
57	P	501	NDP	C5A-C4A-N3A	-5.16	119.61	126.72
53	J	201	CDL	OA6-CA5-C11	5.16	120.28	111.09
59	i	201	CHD	C17-C13-C12	5.06	122.22	117.67
59	i	201	CHD	C17-C13-C14	5.06	105.19	100.11
46	f	101	3PE	O21-C21-C22	5.01	120.02	111.09
53	J	201	CDL	OB6-CB5-C51	5.01	120.02	111.09
57	P	501	NDP	C1B-N9A-C8A	4.84	137.83	127.09
50	F	501	FMN	C7M-C7-C6	4.55	127.59	119.57
46	m	202	3PE	O21-C21-C22	4.54	121.31	111.48
50	F	501	FMN	C9-C8-C7	4.52	126.32	119.69
52	H	401	U10	C17-C18-C19	-4.44	112.83	127.64
46	L	703	3PE	O21-C21-C22	4.31	120.81	111.48
46	Y	203	3PE	O21-C21-C22	4.28	120.74	111.48
46	N	403	3PE	O21-C21-C22	4.25	120.67	111.48
57	P	501	NDP	C5A-C6A-N6A	4.21	133.71	123.29
45	q	202	PC1	O21-C21-C22	4.19	120.54	111.48
46	L	706	3PE	O21-C21-C22	4.17	120.51	111.48
46	d	202	3PE	O21-C21-C22	4.15	120.47	111.48
46	o	202	3PE	O21-C21-C22	4.15	120.45	111.48
46	f	102	3PE	O21-C21-C22	4.13	120.41	111.48
46	J	204	3PE	O21-C21-C22	4.12	120.40	111.48
46	L	702	3PE	O21-C21-C22	4.11	120.38	111.48
46	Y	205	3PE	O21-C21-C22	4.11	120.38	111.48
53	X	201	CDL	OB6-CB5-C51	4.09	120.33	111.48
45	B	204	PC1	O21-C21-C22	4.08	120.32	111.48
53	M	602	CDL	OA6-CA5-C11	4.08	120.31	111.48
46	A	202	3PE	O21-C21-C22	4.07	120.29	111.48
45	I	203	PC1	O21-C21-C22	4.07	120.29	111.48
46	Y	202	3PE	O21-C21-C22	4.06	120.25	111.48
45	h	202	PC1	O21-C21-C22	4.03	120.20	111.48
46	A	203	3PE	O21-C21-C22	4.03	120.19	111.48
59	i	201	CHD	C18-C13-C17	-4.01	104.91	111.20
46	Y	204	3PE	O21-C21-C22	4.01	120.15	111.48
46	Z	201	3PE	O21-C21-C22	4.00	120.14	111.48
59	i	201	CHD	C18-C13-C12	-4.00	105.05	109.06
45	H	402	PC1	O21-C21-C22	4.00	120.13	111.48
46	N	402	3PE	O21-C21-C22	4.00	120.13	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	X	201	CDL	OA6-CA5-C11	3.99	120.11	111.48
45	M	603	PC1	O21-C21-C22	3.99	120.10	111.48
53	d	201	CDL	OA6-CA5-C11	3.96	120.04	111.48
57	P	501	NDP	N9A-C8A-N7A	-3.95	108.34	113.94
53	q	201	CDL	OB6-CB5-C51	3.93	119.99	111.48
46	L	704	3PE	O21-C21-C22	3.92	119.96	111.48
53	N	401	CDL	OB6-CB5-C51	3.92	119.96	111.48
53	M	602	CDL	OB6-CB5-C51	3.91	119.95	111.48
46	m	201	3PE	O21-C21-C22	3.91	119.94	111.48
46	I	205	3PE	O21-C21-C22	3.90	119.92	111.48
53	L	701	CDL	OB6-CB5-C51	3.89	119.89	111.48
53	L	701	CDL	OA6-CA5-C11	3.88	119.88	111.48
53	q	201	CDL	OA6-CA5-C11	3.87	119.85	111.48
53	h	201	CDL	OA6-CA5-C11	3.86	119.83	111.48
46	J	203	3PE	O21-C21-C22	3.85	119.80	111.48
45	B	202	PC1	O21-C21-C22	3.84	119.79	111.48
45	J	202	PC1	O21-C21-C22	3.84	119.78	111.48
52	H	401	U10	C8-C7-C6	3.83	121.52	112.08
45	A	201	PC1	O21-C21-C22	3.83	119.76	111.48
53	h	201	CDL	OB6-CB5-C51	3.82	119.75	111.48
45	d	203	PC1	O21-C21-C22	3.81	119.72	111.48
45	m	203	PC1	O21-C21-C22	3.73	119.56	111.48
45	L	707	PC1	O21-C21-C22	3.72	119.53	111.48
55	O	401	DGT	C1'-N9-C8	-3.69	119.64	127.91
45	I	204	PC1	O21-C21-C22	3.66	119.39	111.48
46	M	604	3PE	O21-C21-C22	3.60	119.26	111.48
46	j	101	3PE	O21-C21-C22	3.59	119.25	111.48
46	Y	201	3PE	O21-C21-C22	3.57	119.20	111.48
53	N	401	CDL	OA6-CA5-C11	3.54	119.13	111.48
50	F	501	FMN	C4-N3-C2	-3.52	119.39	125.64
59	i	201	CHD	C18-C13-C14	-3.50	105.71	111.20
46	b	101	3PE	O21-C21-C22	3.46	118.98	111.48
57	P	501	NDP	C2A-N3A-C4A	3.45	120.25	111.83
59	i	201	CHD	C1-C10-C5	3.44	112.68	107.75
50	F	501	FMN	C8M-C8-C7	-3.28	114.06	120.76
55	O	401	DGT	C2-N1-C6	-3.15	119.39	125.11
57	P	501	NDP	N3A-C4A-N9A	3.13	132.49	127.17
55	O	401	DGT	C2'-C3'-C4'	3.12	109.12	102.80
46	N	403	3PE	O31-C31-C32	3.00	120.26	111.15
46	I	205	3PE	O31-C31-C32	2.94	120.09	111.15
46	Y	204	3PE	O31-C31-C32	2.91	120.71	111.83
58	T	101	EHZ	C13-C12-N1	2.90	121.62	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	i	201	CHD	C23-C22-C20	-2.89	109.06	114.46
46	Y	203	3PE	O31-C31-C32	2.88	120.62	111.83
46	L	704	3PE	O31-C31-C32	2.86	120.57	111.83
52	H	401	U10	C10-C9-C11	2.86	120.19	115.23
45	q	202	PC1	O31-C31-C32	2.86	120.56	111.83
46	J	204	3PE	O31-C31-C32	2.86	120.55	111.83
45	A	201	PC1	O31-C31-C32	2.84	120.50	111.83
53	M	602	CDL	OA8-CA7-C31	2.84	120.49	111.83
53	q	201	CDL	OA8-CA7-C31	2.84	120.49	111.83
45	m	203	PC1	O31-C31-C32	2.83	120.46	111.83
59	i	201	CHD	C15-C14-C8	2.82	122.22	118.36
45	M	605	PC1	O31-C31-C32	2.82	120.43	111.83
55	O	401	DGT	O1G-PG-O3B	2.81	114.07	104.64
55	O	401	DGT	O2G-PG-O3B	2.81	114.06	104.64
53	h	201	CDL	OB8-CB7-C71	2.81	120.39	111.83
46	f	102	3PE	O31-C31-C32	2.79	120.36	111.83
46	N	402	3PE	O31-C31-C32	2.79	120.35	111.83
46	Y	201	3PE	O31-C31-C32	2.79	120.34	111.83
46	Y	202	3PE	O31-C31-C32	2.79	120.33	111.83
46	m	201	3PE	O31-C31-C32	2.78	120.30	111.83
53	N	401	CDL	OA8-CA7-C31	2.77	120.29	111.83
50	F	501	FMN	C5A-C9A-N10	2.77	120.47	117.97
50	F	501	FMN	C4A-C10-N10	2.77	120.44	116.48
53	L	701	CDL	OA8-CA7-C31	2.76	120.26	111.83
45	H	403	PC1	O31-C31-C32	2.76	120.24	111.83
46	j	101	3PE	O31-C31-C32	2.75	120.23	111.83
45	L	707	PC1	O31-C31-C32	2.74	120.20	111.83
46	m	202	3PE	O31-C31-C32	2.74	120.19	111.83
53	X	201	CDL	OA8-CA7-C31	2.74	120.18	111.83
45	I	204	PC1	O31-C31-C32	2.73	120.16	111.83
59	i	201	CHD	C9-C11-C12	-2.73	110.73	114.29
53	d	201	CDL	OB6-CB5-C51	2.72	120.91	110.93
45	M	603	PC1	O31-C31-C32	2.72	120.11	111.83
53	d	201	CDL	OB8-CB7-C71	2.71	120.10	111.83
46	A	202	3PE	O31-C31-C32	2.71	120.10	111.83
57	P	501	NDP	C5A-N7A-C8A	2.70	107.69	103.45
53	N	401	CDL	OB8-CB7-C71	2.69	120.05	111.83
46	J	203	3PE	O31-C31-C32	2.68	120.02	111.83
46	Y	205	3PE	O31-C31-C32	2.68	119.99	111.83
46	L	706	3PE	O31-C31-C32	2.67	119.98	111.83
45	J	202	PC1	O31-C31-C32	2.66	119.94	111.83
46	L	703	3PE	O31-C31-C32	2.65	119.92	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	X	201	CDL	OB8-CB7-C71	2.65	119.92	111.83
53	h	201	CDL	OA8-CA7-C31	2.64	119.89	111.83
45	B	204	PC1	O31-C31-C32	2.64	119.88	111.83
53	L	701	CDL	OB8-CB7-C71	2.64	119.87	111.83
52	H	401	U10	C7-C6-C5	-2.63	115.46	118.52
50	F	501	FMN	C6-C7-C8	-2.63	115.83	119.69
45	h	202	PC1	O31-C31-C32	2.62	119.82	111.83
58	T	101	EHZ	O2-C9-C8	-2.61	119.64	123.74
45	B	202	PC1	O31-C31-C32	2.59	119.73	111.83
45	d	203	PC1	O31-C31-C32	2.56	119.64	111.83
50	F	501	FMN	O4-C4-C4A	-2.55	119.81	126.53
46	A	203	3PE	O31-C31-C32	2.54	119.59	111.83
46	f	101	3PE	O31-C31-C32	2.54	119.58	111.83
46	M	604	3PE	O31-C31-C32	2.54	119.58	111.83
45	H	402	PC1	O31-C31-C32	2.53	119.55	111.83
58	U	101	EHZ	O2-C9-C8	-2.52	119.77	123.74
53	q	201	CDL	OB8-CB7-C71	2.52	119.52	111.83
58	T	101	EHZ	C10-S1-C9	2.50	109.24	101.84
46	Z	201	3PE	O31-C31-C32	2.50	119.46	111.83
45	M	605	PC1	O21-C21-C22	2.50	120.10	110.93
57	P	501	NDP	C2B-C1B-N9A	-2.49	109.65	113.75
45	I	203	PC1	O31-C31-C32	2.48	119.40	111.83
53	M	602	CDL	OB8-CB7-C71	2.47	119.37	111.83
55	O	401	DGT	C5-C6-N1	2.47	119.54	113.25
55	O	401	DGT	O1A-PA-O2A	-2.47	100.97	112.44
53	d	201	CDL	OA8-CA7-C31	2.47	119.35	111.83
46	b	101	3PE	O31-C31-C32	2.46	119.33	111.83
55	O	401	DGT	O1B-PB-O2B	-2.46	101.02	112.44
50	F	501	FMN	C4A-C4-N3	2.45	119.48	113.25
59	i	201	CHD	C6-C5-C4	-2.43	108.45	111.23
46	d	202	3PE	O31-C31-C32	2.41	119.17	111.83
55	O	401	DGT	O6-C6-C5	-2.40	120.19	126.53
45	H	403	PC1	O21-C21-C22	2.40	119.75	110.93
58	U	101	EHZ	C13-C12-N1	2.39	120.69	116.34
58	U	101	EHZ	O2-C9-S1	-2.38	119.66	122.68
52	H	401	U10	C10-C9-C8	-2.36	117.58	123.63
53	J	201	CDL	CA4-OA6-CA5	-2.35	113.70	117.85
59	i	201	CHD	C19-C10-C9	-2.33	108.05	111.18
58	T	101	EHZ	C19-C17-C16	2.32	112.72	108.77
58	U	101	EHZ	C14-C13-C12	-2.29	108.58	112.39
52	H	401	U10	C15-C14-C16	2.26	119.16	115.23
50	F	501	FMN	C9A-C5A-N5	-2.26	120.06	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	T	101	EHZ	C11-N1-C12	-2.24	118.65	122.82
55	O	401	DGT	N9-C4-N3	2.23	130.41	125.95
50	F	501	FMN	C4-C4A-C10	2.23	120.75	116.93
55	O	401	DGT	C5-C4-N9	-2.23	101.67	105.66
50	F	501	FMN	C6-C5A-C9A	2.20	122.07	119.05
50	F	501	FMN	C10-C4A-N5	-2.18	120.36	124.81
52	H	401	U10	C21-C19-C20	2.16	119.56	114.59
57	P	501	NDP	C4A-C5A-N7A	-2.16	108.11	110.58
58	T	101	EHZ	C7-C8-C9	-2.16	109.05	113.86
59	i	201	CHD	C21-C20-C17	-2.12	109.71	112.88
57	P	501	NDP	C4A-N9A-C8A	2.11	107.95	105.74
46	f	101	3PE	C2-O21-C21	-2.09	114.15	117.85
58	U	101	EHZ	C7-C8-C9	-2.07	109.24	113.86
59	i	201	CHD	C6-C5-C10	-2.06	110.46	112.66
55	O	401	DGT	N9-C8-N7	-2.06	109.58	113.40
50	F	501	FMN	C7M-C7-C8	-2.05	116.57	120.76
50	F	501	FMN	C4A-C10-N1	-2.03	119.62	124.59
57	P	501	NDP	C6A-C5A-C4A	2.00	119.92	117.18
59	i	201	CHD	C4-C3-C2	2.00	113.06	110.62

There are no chirality outliers.

All (1148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	PC1	C11-O13-P-O14
45	A	201	PC1	C1-O11-P-O14
45	A	201	PC1	C1-O11-P-O13
45	B	202	PC1	C22-C21-O21-C2
45	B	204	PC1	C11-O13-P-O12
45	B	204	PC1	C11-O13-P-O14
45	B	204	PC1	C11-O13-P-O11
45	B	204	PC1	C1-O11-P-O12
45	B	204	PC1	C1-O11-P-O13
45	H	402	PC1	O13-C11-C12-N
45	H	403	PC1	O13-C11-C12-N
45	I	203	PC1	C11-O13-P-O12
45	I	203	PC1	C11-O13-P-O11
45	I	203	PC1	O13-C11-C12-N
45	I	204	PC1	C11-O13-P-O12
45	I	204	PC1	C11-O13-P-O14
45	I	204	PC1	C11-O13-P-O11
45	I	204	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
45	I	204	PC1	C1-O11-P-O14
45	I	204	PC1	C1-O11-P-O13
45	J	202	PC1	C1-O11-P-O12
45	L	707	PC1	C11-O13-P-O12
45	L	707	PC1	C11-O13-P-O14
45	L	707	PC1	C11-O13-P-O11
45	L	707	PC1	O13-C11-C12-N
45	M	603	PC1	C1-O11-P-O12
45	M	603	PC1	C1-O11-P-O14
45	M	603	PC1	C1-O11-P-O13
45	M	603	PC1	O13-C11-C12-N
45	M	605	PC1	C11-O13-P-O12
45	M	605	PC1	C11-O13-P-O14
45	M	605	PC1	C11-O13-P-O11
45	M	605	PC1	O11-C1-C2-O21
45	M	605	PC1	C22-C21-O21-C2
45	d	203	PC1	C11-O13-P-O12
45	d	203	PC1	C11-O13-P-O11
45	h	202	PC1	C22-C21-O21-C2
45	m	203	PC1	C11-O13-P-O12
45	q	202	PC1	C11-O13-P-O11
45	q	202	PC1	O22-C21-O21-C2
46	A	202	3PE	C1-O11-P-O12
46	A	202	3PE	C1-O11-P-O13
46	A	202	3PE	C1-O11-P-O14
46	A	202	3PE	O13-C11-C12-N
46	A	202	3PE	O22-C21-O21-C2
46	A	203	3PE	C11-O13-P-O12
46	A	203	3PE	C11-O13-P-O14
46	A	203	3PE	O22-C21-O21-C2
46	I	205	3PE	C1-O11-P-O12
46	I	205	3PE	C1-O11-P-O13
46	I	205	3PE	C1-O11-P-O14
46	I	205	3PE	O11-C1-C2-O21
46	J	203	3PE	C11-O13-P-O11
46	J	203	3PE	C11-O13-P-O14
46	J	204	3PE	C1-O11-P-O13
46	J	204	3PE	C1-O11-P-O14
46	J	204	3PE	O13-C11-C12-N
46	L	702	3PE	C1-O11-P-O13
46	L	702	3PE	C1-O11-P-O14
46	L	702	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	L	702	3PE	C11-O13-P-O14
46	L	702	3PE	O22-C21-O21-C2
46	L	702	3PE	C22-C21-O21-C2
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13
46	L	704	3PE	C1-O11-P-O12
46	L	704	3PE	C1-O11-P-O13
46	L	704	3PE	C11-O13-P-O14
46	L	704	3PE	O13-C11-C12-N
46	L	704	3PE	O22-C21-O21-C2
46	L	704	3PE	C22-C21-O21-C2
46	L	706	3PE	O13-C11-C12-N
46	L	706	3PE	C22-C21-O21-C2
46	M	604	3PE	C1-O11-P-O13
46	M	604	3PE	C1-O11-P-O14
46	N	402	3PE	C11-O13-P-O11
46	N	402	3PE	C11-O13-P-O12
46	N	403	3PE	C1-O11-P-O12
46	N	403	3PE	C1-O11-P-O13
46	N	403	3PE	O13-C11-C12-N
46	N	403	3PE	O22-C21-O21-C2
46	Y	201	3PE	C1-O11-P-O13
46	Y	201	3PE	C1-O11-P-O14
46	Y	201	3PE	C11-O13-P-O11
46	Y	201	3PE	C11-O13-P-O14
46	Y	201	3PE	C12-C11-O13-P
46	Y	203	3PE	C1-O11-P-O12
46	Y	203	3PE	C1-O11-P-O13
46	Y	203	3PE	C1-O11-P-O14
46	Y	203	3PE	C11-O13-P-O14
46	Y	203	3PE	O22-C21-O21-C2
46	Y	203	3PE	C22-C21-O21-C2
46	Y	204	3PE	C1-O11-P-O12
46	Y	204	3PE	C1-O11-P-O13
46	Y	204	3PE	C1-O11-P-O14
46	Y	204	3PE	C11-O13-P-O11
46	Y	204	3PE	C11-O13-P-O12
46	Y	204	3PE	C22-C21-O21-C2
46	Y	205	3PE	C11-O13-P-O11
46	Y	205	3PE	C11-O13-P-O14
46	Y	205	3PE	C12-C11-O13-P
46	Z	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	Z	201	3PE	C11-O13-P-O11
46	Z	201	3PE	O13-C11-C12-N
46	Z	201	3PE	O21-C2-C3-O31
46	b	101	3PE	C1-O11-P-O13
46	d	202	3PE	C1-O11-P-O12
46	d	202	3PE	C1-O11-P-O13
46	d	202	3PE	C1-O11-P-O14
46	d	202	3PE	C11-O13-P-O11
46	d	202	3PE	C11-O13-P-O12
46	f	101	3PE	C11-O13-P-O11
46	f	101	3PE	C11-O13-P-O12
46	f	101	3PE	C11-O13-P-O14
46	f	101	3PE	O13-C11-C12-N
46	f	102	3PE	C1-O11-P-O12
46	f	102	3PE	C1-O11-P-O13
46	f	102	3PE	C11-O13-P-O11
46	f	102	3PE	C11-O13-P-O12
46	j	101	3PE	C1-O11-P-O12
46	j	101	3PE	C1-O11-P-O13
46	j	101	3PE	C11-O13-P-O11
46	j	101	3PE	C11-O13-P-O12
46	j	101	3PE	C11-O13-P-O14
46	j	101	3PE	C12-C11-O13-P
46	m	201	3PE	C1-O11-P-O13
46	m	201	3PE	C1-O11-P-O14
46	m	201	3PE	O22-C21-O21-C2
46	m	202	3PE	C11-O13-P-O11
46	m	202	3PE	C11-O13-P-O12
46	m	202	3PE	O13-C11-C12-N
46	m	202	3PE	O22-C21-O21-C2
46	o	202	3PE	O22-C21-O21-C2
48	B	203	PLC	O4P-C4-C5-N
48	B	203	PLC	C1'-C'-O2-C2
48	B	203	PLC	O'-C'-O2-C2
48	B	203	PLC	C1-O3P-P-O2P
48	B	203	PLC	C4-O4P-P-O2P
48	B	203	PLC	C4-O4P-P-O3P
48	O	403	PLC	C4-O4P-P-O3P
48	b	102	PLC	C4-O4P-P-O1P
48	g	201	PLC	C1-O3P-P-O2P
48	g	201	PLC	C1-O3P-P-O4P
48	g	201	PLC	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	g	201	PLC	C4-O4P-P-O2P
52	H	401	U10	C1-C6-C7-C8
52	H	401	U10	C5-C6-C7-C8
53	J	201	CDL	CB2-C1-CA2-OA2
53	J	201	CDL	C1-CA2-OA2-PA1
53	J	201	CDL	CA2-OA2-PA1-OA5
53	J	201	CDL	CA3-OA5-PA1-OA2
53	J	201	CDL	CA3-OA5-PA1-OA4
53	L	701	CDL	C11-CA5-OA6-CA4
53	L	701	CDL	CB3-OB5-PB2-OB3
53	M	602	CDL	O1-C1-CA2-OA2
53	M	602	CDL	CA2-OA2-PA1-OA4
53	M	602	CDL	OB7-CB5-OB6-CB4
53	M	602	CDL	C51-CB5-OB6-CB4
53	N	401	CDL	CA3-OA5-PA1-OA3
53	N	401	CDL	CB2-OB2-PB2-OB3
53	N	401	CDL	CB2-OB2-PB2-OB5
53	N	401	CDL	OB6-CB4-CB6-OB8
53	N	401	CDL	C51-CB5-OB6-CB4
53	X	201	CDL	CA2-OA2-PA1-OA3
53	X	201	CDL	CA2-OA2-PA1-OA4
53	X	201	CDL	CA2-OA2-PA1-OA5
53	X	201	CDL	CA3-OA5-PA1-OA2
53	X	201	CDL	CA3-OA5-PA1-OA3
53	X	201	CDL	CA3-OA5-PA1-OA4
53	X	201	CDL	C1-CB2-OB2-PB2
53	X	201	CDL	CB3-OB5-PB2-OB2
53	X	201	CDL	CB3-OB5-PB2-OB3
53	X	201	CDL	CB3-OB5-PB2-OB4
53	X	201	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	C51-CB5-OB6-CB4
53	d	201	CDL	CB2-C1-CA2-OA2
53	d	201	CDL	CB2-OB2-PB2-OB3
53	d	201	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CA3-OA5-PA1-OA2
53	h	201	CDL	CA3-OA5-PA1-OA3
53	h	201	CDL	CA3-OA5-PA1-OA4
53	h	201	CDL	C11-CA5-OA6-CA4
53	h	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	CB2-C1-CA2-OA2
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CA3-OA5-PA1-OA4
53	q	201	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CB2-OB2-PB2-OB5
53	q	201	CDL	CB3-OB5-PB2-OB2
53	q	201	CDL	CB3-OB5-PB2-OB3
53	q	201	CDL	CB3-OB5-PB2-OB4
53	q	201	CDL	C51-CB5-OB6-CB4
55	O	401	DGT	C5'-O5'-PA-O1A
55	O	401	DGT	C5'-O5'-PA-O2A
57	P	501	NDP	C5B-O5B-PA-O1A
57	P	501	NDP	C5D-O5D-PN-O3
57	P	501	NDP	C5D-O5D-PN-O1N
57	P	501	NDP	C5D-O5D-PN-O2N
58	T	101	EHZ	S1-C10-C11-N1
58	T	101	EHZ	O2-C9-S1-C10
58	T	101	EHZ	C8-C9-S1-C10
58	U	101	EHZ	S1-C10-C11-N1
58	U	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
60	o	201	MYR	O1-C1-C2-C3
53	J	201	CDL	C11-CA5-OA6-CA4
45	m	203	PC1	O32-C31-O31-C3
46	Y	203	3PE	O32-C31-O31-C3
46	f	102	3PE	O32-C31-O31-C3
53	X	201	CDL	OA9-CA7-OA8-CA6
53	d	201	CDL	OB9-CB7-OB8-CB6
53	J	201	CDL	C51-CB5-OB6-CB4
45	d	203	PC1	C32-C31-O31-C3
45	m	203	PC1	C32-C31-O31-C3
46	Y	203	3PE	C32-C31-O31-C3
46	f	102	3PE	C32-C31-O31-C3
53	M	602	CDL	C31-CA7-OA8-CA6
53	X	201	CDL	C31-CA7-OA8-CA6
53	d	201	CDL	C71-CB7-OB8-CB6
45	A	201	PC1	O32-C31-O31-C3
45	M	603	PC1	O32-C31-O31-C3
45	M	605	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	d	203	PC1	O32-C31-O31-C3
45	q	202	PC1	O32-C31-O31-C3
46	L	704	3PE	O32-C31-O31-C3
46	Y	204	3PE	O32-C31-O31-C3
53	L	701	CDL	OA9-CA7-OA8-CA6
53	M	602	CDL	OA9-CA7-OA8-CA6
53	d	201	CDL	OA9-CA7-OA8-CA6
45	H	403	PC1	O32-C31-O31-C3
45	B	202	PC1	O22-C21-O21-C2
45	M	605	PC1	O22-C21-O21-C2
45	h	202	PC1	O22-C21-O21-C2
45	m	203	PC1	O22-C21-O21-C2
46	L	706	3PE	O22-C21-O21-C2
46	Y	204	3PE	O22-C21-O21-C2
53	L	701	CDL	OA7-CA5-OA6-CA4
53	N	401	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	OA7-CA5-OA6-CA4
53	q	201	CDL	OA7-CA5-OA6-CA4
53	q	201	CDL	OB7-CB5-OB6-CB4
45	q	202	PC1	C32-C31-O31-C3
46	N	403	3PE	C32-C31-O31-C3
46	Y	204	3PE	C32-C31-O31-C3
53	L	701	CDL	C31-CA7-OA8-CA6
53	M	602	CDL	C71-CB7-OB8-CB6
53	d	201	CDL	C31-CA7-OA8-CA6
53	J	201	CDL	C71-CB7-OB8-CB6
45	m	203	PC1	C22-C21-O21-C2
45	q	202	PC1	C22-C21-O21-C2
46	A	202	3PE	C22-C21-O21-C2
46	A	203	3PE	C22-C21-O21-C2
46	N	403	3PE	C22-C21-O21-C2
46	m	201	3PE	C22-C21-O21-C2
46	m	202	3PE	C22-C21-O21-C2
46	o	202	3PE	C22-C21-O21-C2
53	d	201	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	C51-CB5-OB6-CB4
52	H	401	U10	C15-C14-C16-C17
46	L	702	3PE	O32-C31-O31-C3
45	A	201	PC1	C32-C31-O31-C3
45	H	403	PC1	C32-C31-O31-C3
45	M	603	PC1	C32-C31-O31-C3
45	M	605	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	I	205	3PE	C32-C31-O31-C3
46	L	704	3PE	C32-C31-O31-C3
46	Y	205	3PE	C32-C31-O31-C3
46	j	101	3PE	C32-C31-O31-C3
53	J	201	CDL	OA7-CA5-OA6-CA4
53	J	201	CDL	OB7-CB5-OB6-CB4
59	i	201	CHD	C21-C20-C22-C23
46	I	205	3PE	O32-C31-O31-C3
46	J	203	3PE	O32-C31-O31-C3
46	N	402	3PE	O32-C31-O31-C3
46	N	403	3PE	O32-C31-O31-C3
46	Y	205	3PE	O32-C31-O31-C3
46	L	702	3PE	C32-C31-O31-C3
53	J	201	CDL	O1-C1-CA2-OA2
53	N	401	CDL	O1-C1-CB2-OB2
53	d	201	CDL	O1-C1-CA2-OA2
53	q	201	CDL	O1-C1-CA2-OA2
46	J	203	3PE	C32-C31-O31-C3
46	N	402	3PE	C32-C31-O31-C3
53	N	401	CDL	C71-CB7-OB8-CB6
53	M	602	CDL	OB9-CB7-OB8-CB6
53	X	201	CDL	C11-CA5-OA6-CA4
53	q	201	CDL	C11-CA5-OA6-CA4
53	N	401	CDL	OB9-CB7-OB8-CB6
57	P	501	NDP	O4D-C4D-C5D-O5D
57	P	501	NDP	C3D-C4D-C5D-O5D
53	J	201	CDL	OA9-CA7-OA8-CA6
46	j	101	3PE	O32-C31-O31-C3
46	o	202	3PE	O32-C31-O31-C3
46	A	202	3PE	C32-C31-O31-C3
53	N	401	CDL	C31-CA7-OA8-CA6
53	h	201	CDL	C71-CB7-OB8-CB6
53	J	201	CDL	C31-CA7-OA8-CA6
59	i	201	CHD	C17-C20-C22-C23
46	L	703	3PE	C22-C21-O21-C2
46	f	102	3PE	C22-C21-O21-C2
53	J	201	CDL	OB9-CB7-OB8-CB6
46	o	202	3PE	C32-C31-O31-C3
53	h	201	CDL	OB9-CB7-OB8-CB6
53	N	401	CDL	CA2-C1-CB2-OB2
45	L	707	PC1	C32-C31-O31-C3
46	Y	201	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	d	202	3PE	C32-C31-O31-C3
52	H	401	U10	C13-C14-C16-C17
57	P	501	NDP	O4D-C1D-N1N-C6N
46	Y	202	3PE	C21-C22-C23-C24
46	Y	201	3PE	O32-C31-O31-C3
53	X	201	CDL	OA7-CA5-OA6-CA4
46	M	604	3PE	O11-C1-C2-O21
53	M	602	CDL	C11-CA5-OA6-CA4
46	Y	201	3PE	O21-C2-C3-O31
45	L	707	PC1	O32-C31-O31-C3
46	f	101	3PE	C22-C21-O21-C2
46	Y	201	3PE	C31-C32-C33-C34
46	L	703	3PE	O22-C21-O21-C2
46	f	102	3PE	O22-C21-O21-C2
50	F	501	FMN	O3'-C3'-C4'-C5'
46	J	204	3PE	C21-C22-C23-C24
46	Y	201	3PE	C21-C22-C23-C24
46	d	202	3PE	C31-C32-C33-C34
46	f	101	3PE	C31-C32-C33-C34
53	X	201	CDL	CA5-C11-C12-C13
53	d	201	CDL	CA7-C31-C32-C33
46	d	202	3PE	O32-C31-O31-C3
45	d	203	PC1	C21-C22-C23-C24
46	J	204	3PE	C31-C32-C33-C34
46	L	703	3PE	C21-C22-C23-C24
46	L	704	3PE	C31-C32-C33-C34
53	M	602	CDL	CA5-C11-C12-C13
46	A	202	3PE	O32-C31-O31-C3
53	N	401	CDL	OA9-CA7-OA8-CA6
46	Y	204	3PE	C31-C32-C33-C34
48	B	203	PLC	C'-C1'-C2'-C3'
45	h	202	PC1	C32-C31-O31-C3
45	L	707	PC1	C22-C21-O21-C2
45	q	202	PC1	C21-C22-C23-C24
53	d	201	CDL	CB7-C71-C72-C73
45	B	202	PC1	C31-C32-C33-C34
53	M	602	CDL	CB5-C51-C52-C53
45	L	707	PC1	O22-C21-O21-C2
53	M	602	CDL	OA7-CA5-OA6-CA4
53	M	602	CDL	CB2-C1-CA2-OA2
46	Y	202	3PE	C22-C21-O21-C2
53	L	701	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
46	Y	202	3PE	O22-C21-O21-C2
46	j	101	3PE	C31-C32-C33-C34
53	d	201	CDL	C1-CB2-OB2-PB2
45	h	202	PC1	O32-C31-O31-C3
45	I	204	PC1	C21-C22-C23-C24
46	Y	204	3PE	C3-C2-O21-C21
46	I	205	3PE	C22-C21-O21-C2
46	Z	201	3PE	C22-C21-O21-C2
53	d	201	CDL	CA5-C11-C12-C13
45	B	202	PC1	C3D-C3E-C3F-C3G
45	H	403	PC1	C36-C37-C38-C39
53	h	201	CDL	C33-C34-C35-C36
45	L	707	PC1	C3E-C3F-C3G-C3H
46	N	403	3PE	C28-C29-C2A-C2B
53	L	701	CDL	C81-C82-C83-C84
53	N	401	CDL	C16-C17-C18-C19
46	Y	203	3PE	C35-C36-C37-C38
46	Y	204	3PE	C26-C27-C28-C29
46	m	202	3PE	C32-C31-O31-C3
48	B	203	PLC	C1B-CB-O3-C3
46	L	702	3PE	C27-C28-C29-C2A
53	h	201	CDL	C74-C75-C76-C77
53	L	701	CDL	OB7-CB5-OB6-CB4
45	J	202	PC1	C23-C24-C25-C26
46	A	203	3PE	C36-C37-C38-C39
46	j	101	3PE	C2E-C2F-C2G-C2H
46	m	202	3PE	C33-C34-C35-C36
45	H	403	PC1	C31-C32-C33-C34
45	H	402	PC1	C32-C33-C34-C35
46	J	204	3PE	C33-C34-C35-C36
46	Y	205	3PE	C26-C27-C28-C29
46	b	101	3PE	C29-C2A-C2B-C2C
46	d	202	3PE	C26-C27-C28-C29
53	h	201	CDL	C58-C59-C60-C61
53	N	401	CDL	C11-CA5-OA6-CA4
45	L	707	PC1	C22-C23-C24-C25
46	I	205	3PE	C2C-C2D-C2E-C2F
46	M	604	3PE	C32-C33-C34-C35
46	Z	201	3PE	C37-C38-C39-C3A
53	h	201	CDL	C71-C72-C73-C74
53	N	401	CDL	CB5-C51-C52-C53
46	I	205	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
46	Y	201	3PE	C34-C35-C36-C37
46	Y	201	3PE	C24-C25-C26-C27
46	b	101	3PE	C23-C24-C25-C26
46	b	101	3PE	C2D-C2E-C2F-C2G
46	d	202	3PE	C34-C35-C36-C37
46	m	201	3PE	C25-C26-C27-C28
53	N	401	CDL	C18-C19-C20-C21
53	X	201	CDL	C57-C58-C59-C60
45	B	202	PC1	C37-C38-C39-C3A
45	L	707	PC1	C37-C38-C39-C3A
45	M	603	PC1	C32-C33-C34-C35
53	L	701	CDL	CB5-C51-C52-C53
53	q	201	CDL	CA5-C11-C12-C13
46	f	101	3PE	C35-C36-C37-C38
53	N	401	CDL	C54-C55-C56-C57
53	d	201	CDL	C36-C37-C38-C39
45	B	202	PC1	C25-C26-C27-C28
45	J	202	PC1	C33-C34-C35-C36
46	J	204	3PE	C35-C36-C37-C38
46	L	703	3PE	C35-C36-C37-C38
46	b	101	3PE	C36-C37-C38-C39
48	b	102	PLC	C1B-C2B-C3B-C4B
53	L	701	CDL	C78-C79-C80-C81
53	X	201	CDL	C78-C79-C80-C81
45	B	204	PC1	C38-C39-C3A-C3B
46	d	202	3PE	C22-C23-C24-C25
48	B	203	PLC	C7B-C8B-C9B-CAA
53	N	401	CDL	C74-C75-C76-C77
60	o	201	MYR	C5-C6-C7-C8
45	d	203	PC1	C3A-C3B-C3C-C3D
45	h	202	PC1	C22-C23-C24-C25
46	Y	201	3PE	C39-C3A-C3B-C3C
48	L	705	PLC	C4-C5-N-C6
48	L	705	PLC	C4-C5-N-C7
48	L	705	PLC	C4-C5-N-C8
46	J	203	3PE	C33-C34-C35-C36
46	Y	201	3PE	C2C-C2D-C2E-C2F
46	b	101	3PE	C2C-C2D-C2E-C2F
53	L	701	CDL	C37-C38-C39-C40
53	L	701	CDL	C61-C62-C63-C64
53	M	602	CDL	C78-C79-C80-C81
53	h	201	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
46	o	202	3PE	C2B-C2C-C2D-C2E
50	F	501	FMN	C2'-C3'-C4'-O4'
46	Y	205	3PE	C2C-C2D-C2E-C2F
53	d	201	CDL	C72-C73-C74-C75
46	Y	204	3PE	C21-C22-C23-C24
46	J	204	3PE	C32-C33-C34-C35
53	X	201	CDL	C60-C61-C62-C63
48	B	203	PLC	OB-CB-O3-C3
46	L	703	3PE	C3E-C3F-C3G-C3H
46	I	205	3PE	O22-C21-O21-C2
46	Z	201	3PE	O22-C21-O21-C2
45	d	203	PC1	C33-C34-C35-C36
46	Z	201	3PE	C21-C22-C23-C24
46	M	604	3PE	C32-C31-O31-C3
46	A	203	3PE	C33-C34-C35-C36
45	L	707	PC1	C39-C3A-C3B-C3C
45	L	707	PC1	C3B-C3C-C3D-C3E
46	L	704	3PE	C27-C28-C29-C2A
46	d	202	3PE	C28-C29-C2A-C2B
53	X	201	CDL	CB7-C71-C72-C73
53	M	602	CDL	C83-C84-C85-C86
45	d	203	PC1	C36-C37-C38-C39
46	L	706	3PE	C25-C26-C27-C28
46	M	604	3PE	C2D-C2E-C2F-C2G
53	M	602	CDL	C32-C33-C34-C35
45	B	204	PC1	C22-C21-O21-C2
45	I	203	PC1	C22-C21-O21-C2
46	J	203	3PE	C22-C21-O21-C2
46	J	204	3PE	C22-C21-O21-C2
48	O	403	PLC	C1'-C'-O2-C2
53	d	201	CDL	C11-CA5-OA6-CA4
53	N	401	CDL	CA5-C11-C12-C13
53	q	201	CDL	CA7-C31-C32-C33
46	A	203	3PE	C3C-C3D-C3E-C3F
45	B	204	PC1	O22-C21-O21-C2
46	J	204	3PE	O22-C21-O21-C2
48	O	403	PLC	O'-C'-O2-C2
53	N	401	CDL	OA7-CA5-OA6-CA4
58	U	101	EHZ	C1-C2-C3-C4
46	m	202	3PE	O32-C31-O31-C3
46	Y	205	3PE	C34-C35-C36-C37
46	m	201	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
46	Y	203	3PE	C31-C32-C33-C34
53	d	201	CDL	OA7-CA5-OA6-CA4
45	B	202	PC1	O11-C1-C2-O21
46	N	402	3PE	O11-C1-C2-O21
46	o	202	3PE	C27-C28-C29-C2A
58	U	101	EHZ	C22-C23-C24-C25
53	L	701	CDL	C59-C60-C61-C62
53	X	201	CDL	C36-C37-C38-C39
45	d	203	PC1	C39-C3A-C3B-C3C
46	Y	205	3PE	C2A-C2B-C2C-C2D
53	M	602	CDL	C75-C76-C77-C78
46	d	202	3PE	O21-C2-C3-O31
48	g	201	PLC	O2-C2-C3-O3
46	M	604	3PE	C35-C36-C37-C38
46	M	604	3PE	C39-C3A-C3B-C3C
53	q	201	CDL	C71-C72-C73-C74
53	M	602	CDL	C1-CA2-OA2-PA1
46	Y	205	3PE	C23-C24-C25-C26
45	I	203	PC1	O22-C21-O21-C2
46	N	402	3PE	C22-C23-C24-C25
46	N	403	3PE	C2C-C2D-C2E-C2F
46	Y	201	3PE	C22-C21-O21-C2
46	m	202	3PE	C22-C23-C24-C25
48	g	201	PLC	C2'-C3'-C4'-C5'
53	L	701	CDL	C39-C40-C41-C42
46	L	704	3PE	C2A-C2B-C2C-C2D
45	d	203	PC1	C34-C35-C36-C37
53	X	201	CDL	C37-C38-C39-C40
53	L	701	CDL	C76-C77-C78-C79
53	N	401	CDL	C72-C73-C74-C75
45	M	605	PC1	O11-C1-C2-C3
46	A	203	3PE	O11-C1-C2-C3
46	I	205	3PE	O11-C1-C2-C3
46	L	704	3PE	O11-C1-C2-C3
46	j	101	3PE	O11-C1-C2-C3
53	N	401	CDL	OA5-CA3-CA4-CA6
53	d	201	CDL	OA5-CA3-CA4-CA6
46	J	203	3PE	O22-C21-O21-C2
46	j	101	3PE	C35-C36-C37-C38
46	Y	201	3PE	C36-C37-C38-C39
46	L	702	3PE	C29-C2A-C2B-C2C
46	L	704	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
46	M	604	3PE	O32-C31-O31-C3
46	m	201	3PE	C23-C24-C25-C26
53	M	602	CDL	C12-C13-C14-C15
46	Z	201	3PE	C2D-C2E-C2F-C2G
46	f	101	3PE	C33-C34-C35-C36
46	d	202	3PE	C39-C3A-C3B-C3C
53	L	701	CDL	CB7-C71-C72-C73
45	d	203	PC1	C1-C2-C3-O31
45	h	202	PC1	C1-C2-C3-O31
46	L	703	3PE	C1-C2-C3-O31
48	g	201	PLC	C1-C2-C3-O3
58	T	101	EHZ	C22-C23-C24-C25
45	L	707	PC1	C23-C24-C25-C26
46	M	604	3PE	C37-C38-C39-C3A
46	Y	204	3PE	C32-C33-C34-C35
46	f	101	3PE	O22-C21-O21-C2
53	L	701	CDL	C35-C36-C37-C38
53	h	201	CDL	C54-C55-C56-C57
46	f	102	3PE	C23-C24-C25-C26
53	X	201	CDL	C54-C55-C56-C57
46	Z	201	3PE	C34-C35-C36-C37
45	B	204	PC1	O11-C1-C2-O21
45	H	402	PC1	O11-C1-C2-O21
45	H	403	PC1	O11-C1-C2-O21
46	N	403	3PE	O11-C1-C2-O21
48	b	102	PLC	O3P-C1-C2-O2
53	M	602	CDL	OB5-CB3-CB4-OB6
46	L	703	3PE	C32-C31-O31-C3
53	M	602	CDL	C71-C72-C73-C74
46	Y	201	3PE	C27-C28-C29-C2A
53	L	701	CDL	C74-C75-C76-C77
53	X	201	CDL	C64-C65-C66-C67
46	f	102	3PE	O21-C2-C3-O31
45	I	203	PC1	C3A-C3B-C3C-C3D
45	M	603	PC1	C26-C27-C28-C29
45	m	203	PC1	C39-C3A-C3B-C3C
46	N	402	3PE	C2F-C2G-C2H-C2I
53	M	602	CDL	C20-C21-C22-C23
53	X	201	CDL	C81-C82-C83-C84
46	N	402	3PE	C38-C39-C3A-C3B
53	d	201	CDL	C40-C41-C42-C43
45	H	403	PC1	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
60	o	201	MYR	C4-C5-C6-C7
53	L	701	CDL	C84-C85-C86-C87
53	N	401	CDL	C51-C52-C53-C54
45	H	402	PC1	C28-C29-C2A-C2B
45	I	204	PC1	C31-C32-C33-C34
45	h	202	PC1	C31-C32-C33-C34
53	d	201	CDL	C42-C43-C44-C45
46	Y	201	3PE	C2E-C2F-C2G-C2H
46	Z	201	3PE	C27-C28-C29-C2A
53	X	201	CDL	C52-C53-C54-C55
53	M	602	CDL	C58-C59-C60-C61
45	H	403	PC1	C2-C1-O11-P
46	Y	203	3PE	C2-C1-O11-P
50	F	501	FMN	C4'-C5'-O5'-P
46	Y	203	3PE	C2C-C2D-C2E-C2F
53	h	201	CDL	C56-C57-C58-C59
45	A	201	PC1	C23-C24-C25-C26
46	L	704	3PE	C23-C24-C25-C26
46	Y	203	3PE	C22-C23-C24-C25
46	f	102	3PE	C34-C35-C36-C37
53	d	201	CDL	C37-C38-C39-C40
45	B	202	PC1	O11-C1-C2-C3
45	B	204	PC1	O11-C1-C2-C3
45	H	402	PC1	O11-C1-C2-C3
45	H	403	PC1	O11-C1-C2-C3
46	M	604	3PE	O11-C1-C2-C3
46	N	402	3PE	O11-C1-C2-C3
48	L	705	PLC	O3P-C1-C2-C3
48	b	102	PLC	O3P-C1-C2-C3
46	Y	204	3PE	C2C-C2D-C2E-C2F
48	O	403	PLC	C2'-C3'-C4'-C5'
48	O	403	PLC	O2-C'-C1'-C2'
45	I	203	PC1	C28-C29-C2A-C2B
45	d	203	PC1	C31-C32-C33-C34
53	X	201	CDL	C31-C32-C33-C34
46	N	402	3PE	O21-C21-C22-C23
53	X	201	CDL	C38-C39-C40-C41
53	d	201	CDL	C38-C39-C40-C41
53	X	201	CDL	C33-C34-C35-C36
45	H	403	PC1	C1-C2-C3-O31
45	L	707	PC1	C1-C2-C3-O31
45	M	605	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	A	202	3PE	C1-C2-C3-O31
46	Y	201	3PE	C1-C2-C3-O31
46	Z	201	3PE	C1-C2-C3-O31
46	d	202	3PE	C1-C2-C3-O31
46	f	102	3PE	C1-C2-C3-O31
46	m	202	3PE	C1-C2-C3-O31
46	o	202	3PE	C1-C2-C3-O31
48	B	203	PLC	C1-C2-C3-O3
53	M	602	CDL	CA3-CA4-CA6-OA8
53	N	401	CDL	C78-C79-C80-C81
50	F	501	FMN	O3'-C3'-C4'-O4'
58	U	101	EHZ	C5-C6-C7-O1
50	F	501	FMN	C2'-C3'-C4'-C5'
46	f	102	3PE	C2E-C2F-C2G-C2H
46	Z	201	3PE	C29-C2A-C2B-C2C
46	Y	203	3PE	C27-C28-C29-C2A
46	N	402	3PE	C23-C24-C25-C26
46	A	202	3PE	C26-C27-C28-C29
58	U	101	EHZ	C3-C4-C5-C6
46	m	201	3PE	O11-C1-C2-O21
53	J	201	CDL	OB5-CB3-CB4-OB6
53	M	602	CDL	OA5-CA3-CA4-OA6
53	d	201	CDL	OA5-CA3-CA4-OA6
46	L	704	3PE	C3A-C3B-C3C-C3D
46	m	201	3PE	C2C-C2D-C2E-C2F
60	o	201	MYR	C3-C4-C5-C6
53	L	701	CDL	C11-C12-C13-C14
46	Y	203	3PE	C2D-C2E-C2F-C2G
53	h	201	CDL	CB4-CB3-OB5-PB2
58	T	101	EHZ	O1-C7-C8-C9
46	b	101	3PE	C2B-C2C-C2D-C2E
46	J	203	3PE	C22-C23-C24-C25
46	Y	203	3PE	C26-C27-C28-C29
45	L	707	PC1	O21-C2-C3-O31
46	A	202	3PE	O21-C2-C3-O31
46	o	202	3PE	O21-C2-C3-O31
48	O	403	PLC	O2-C2-C3-O3
53	J	201	CDL	OA6-CA4-CA6-OA8
46	M	604	3PE	C2A-C2B-C2C-C2D
48	B	203	PLC	C6B-C7B-C8B-C9B
45	H	402	PC1	C21-C22-C23-C24
46	Y	205	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
46	d	202	3PE	C29-C2A-C2B-C2C
53	N	401	CDL	C35-C36-C37-C38
46	L	703	3PE	C3B-C3C-C3D-C3E
48	B	203	PLC	C3B-C4B-C5B-C6B
58	T	101	EHZ	C6-C7-C8-C9
46	L	703	3PE	O32-C31-O31-C3
60	o	201	MYR	C9-C10-C11-C12
46	b	101	3PE	O21-C21-C22-C23
46	N	402	3PE	C33-C34-C35-C36
45	B	202	PC1	C3B-C3C-C3D-C3E
46	L	703	3PE	C28-C29-C2A-C2B
53	M	602	CDL	C56-C57-C58-C59
46	N	403	3PE	O11-C1-C2-C3
46	Z	201	3PE	O11-C1-C2-C3
46	f	101	3PE	O11-C1-C2-C3
53	J	201	CDL	OB5-CB3-CB4-CB6
46	Z	201	3PE	C24-C25-C26-C27
46	Y	204	3PE	C36-C37-C38-C39
46	L	704	3PE	C34-C35-C36-C37
46	L	704	3PE	C36-C37-C38-C39
46	Y	201	3PE	O22-C21-O21-C2
46	d	202	3PE	C35-C36-C37-C38
45	I	203	PC1	C36-C37-C38-C39
46	N	403	3PE	C3-C2-O21-C21
53	N	401	CDL	CA6-CA4-OA6-CA5
53	X	201	CDL	CA3-CA4-OA6-CA5
46	L	704	3PE	C32-C33-C34-C35
45	J	202	PC1	C21-C22-C23-C24
53	h	201	CDL	C40-C41-C42-C43
45	m	203	PC1	C37-C38-C39-C3A
46	o	202	3PE	C2E-C2F-C2G-C2H
46	L	704	3PE	O11-C1-C2-O21
46	Y	203	3PE	O11-C1-C2-O21
46	Y	205	3PE	O11-C1-C2-O21
46	Z	201	3PE	O11-C1-C2-O21
46	f	101	3PE	O11-C1-C2-O21
48	L	705	PLC	O3P-C1-C2-O2
53	N	401	CDL	OA5-CA3-CA4-OA6
53	X	201	CDL	OB5-CB3-CB4-OB6
53	d	201	CDL	OB5-CB3-CB4-OB6
45	B	204	PC1	C1-C2-C3-O31
46	Y	202	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
48	O	403	PLC	C1-C2-C3-O3
53	N	401	CDL	CB3-CB4-CB6-OB8
45	L	707	PC1	C21-C22-C23-C24
46	M	604	3PE	C21-C22-C23-C24
53	h	201	CDL	C37-C38-C39-C40
45	H	403	PC1	C12-C11-O13-P
45	L	707	PC1	C12-C11-O13-P
45	M	605	PC1	C12-C11-O13-P
46	I	205	3PE	C12-C11-O13-P
46	J	204	3PE	C12-C11-O13-P
46	L	702	3PE	C12-C11-O13-P
46	M	604	3PE	C12-C11-O13-P
46	Y	203	3PE	C12-C11-O13-P
46	Z	201	3PE	C12-C11-O13-P
46	m	202	3PE	C12-C11-O13-P
46	A	202	3PE	C35-C36-C37-C38
45	H	403	PC1	O21-C2-C3-O31
45	M	605	PC1	O21-C2-C3-O31
45	h	202	PC1	O21-C2-C3-O31
53	M	602	CDL	OA6-CA4-CA6-OA8
46	Y	205	3PE	C32-C33-C34-C35
45	M	603	PC1	C28-C29-C2A-C2B
45	h	202	PC1	C24-C25-C26-C27
46	d	202	3PE	C24-C25-C26-C27
53	N	401	CDL	C17-C18-C19-C20
45	A	201	PC1	O13-C11-C12-N
45	J	202	PC1	O13-C11-C12-N
45	M	605	PC1	O13-C11-C12-N
48	b	102	PLC	O4P-C4-C5-N
45	B	204	PC1	C23-C24-C25-C26
46	A	202	3PE	C32-C33-C34-C35
45	H	402	PC1	C22-C23-C24-C25
46	b	101	3PE	C38-C39-C3A-C3B
53	q	201	CDL	CB5-C51-C52-C53
45	H	403	PC1	C3C-C3D-C3E-C3F
53	L	701	CDL	C79-C80-C81-C82
60	o	201	MYR	C1-C2-C3-C4
45	H	402	PC1	C25-C26-C27-C28
53	X	201	CDL	C71-CB7-OB8-CB6
48	g	201	PLC	C1B-CB-O3-C3
53	q	201	CDL	C31-CA7-OA8-CA6
46	L	703	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	L	704	3PE	C24-C25-C26-C27
46	o	202	3PE	C24-C25-C26-C27
45	J	202	PC1	O11-C1-C2-C3
45	M	603	PC1	O11-C1-C2-C3
46	Y	201	3PE	O11-C1-C2-C3
46	Y	203	3PE	O11-C1-C2-C3
53	M	602	CDL	OA5-CA3-CA4-CA6
53	M	602	CDL	OB5-CB3-CB4-CB6
46	L	706	3PE	C37-C38-C39-C3A
58	T	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
45	I	203	PC1	C32-C33-C34-C35
53	h	201	CDL	C14-C15-C16-C17
53	M	602	CDL	C72-C73-C74-C75
45	H	403	PC1	C35-C36-C37-C38
53	h	201	CDL	C31-CA7-OA8-CA6
46	Y	204	3PE	C37-C38-C39-C3A
53	h	201	CDL	C59-C60-C61-C62
46	M	604	3PE	C2-C1-O11-P
46	Y	201	3PE	C2-C1-O11-P
46	L	703	3PE	C3A-C3B-C3C-C3D
57	P	501	NDP	C2B-O2B-P2B-O1X
53	N	401	CDL	C11-C12-C13-C14
45	J	202	PC1	O11-C1-C2-O21
45	M	603	PC1	O11-C1-C2-O21
46	Y	201	3PE	O11-C1-C2-O21
46	j	101	3PE	O11-C1-C2-O21
53	N	401	CDL	OB5-CB3-CB4-OB6
46	b	101	3PE	C22-C21-O21-C2
46	Y	201	3PE	C2A-C2B-C2C-C2D
53	X	201	CDL	OB9-CB7-OB8-CB6
53	q	201	CDL	OA9-CA7-OA8-CA6
45	H	402	PC1	O21-C2-C3-O31
45	d	203	PC1	O21-C2-C3-O31
46	m	202	3PE	O21-C2-C3-O31
48	B	203	PLC	O2-C2-C3-O3
46	N	402	3PE	C34-C35-C36-C37
45	L	707	PC1	C31-C32-C33-C34
45	H	402	PC1	C1-C2-C3-O31
46	A	203	3PE	C1-C2-C3-O31
48	b	102	PLC	C1-C2-C3-O3
58	T	101	EHZ	C10-C11-N1-C12

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	OA9-CA7-OA8-CA6
45	A	201	PC1	C22-C21-O21-C2
58	T	101	EHZ	C16-C17-C20-O6
53	N	401	CDL	C36-C37-C38-C39
48	B	203	PLC	C5B-C6B-C7B-C8B
45	I	203	PC1	C34-C35-C36-C37
45	A	201	PC1	C1-O11-P-O12
45	B	202	PC1	C11-C12-N-C15
45	H	402	PC1	C11-O13-P-O12
45	H	402	PC1	C11-O13-P-O14
45	H	402	PC1	C11-O13-P-O11
45	H	403	PC1	C11-O13-P-O11
45	J	202	PC1	C1-O11-P-O14
45	J	202	PC1	C1-O11-P-O13
45	L	707	PC1	C1-O11-P-O12
45	L	707	PC1	C1-O11-P-O14
45	L	707	PC1	C1-O11-P-O13
45	M	605	PC1	C1-O11-P-O12
45	M	605	PC1	C1-O11-P-O14
45	M	605	PC1	C1-O11-P-O13
45	d	203	PC1	C11-O13-P-O14
45	h	202	PC1	C11-O13-P-O14
45	m	203	PC1	C11-O13-P-O14
45	m	203	PC1	C11-O13-P-O11
45	m	203	PC1	C1-O11-P-O12
45	m	203	PC1	C1-O11-P-O13
45	q	202	PC1	C11-O13-P-O14
46	A	203	3PE	C1-O11-P-O14
46	A	203	3PE	C11-O13-P-O11
46	I	205	3PE	C11-O13-P-O11
46	I	205	3PE	C11-O13-P-O12
46	I	205	3PE	C11-O13-P-O14
46	J	203	3PE	C1-O11-P-O14
46	J	203	3PE	O13-C11-C12-N
46	L	702	3PE	C11-O13-P-O12
46	L	703	3PE	O13-C11-C12-N
46	L	704	3PE	C1-O11-P-O14
46	N	403	3PE	C11-O13-P-O11
46	N	403	3PE	C11-O13-P-O12
46	N	403	3PE	C11-O13-P-O14
46	Y	201	3PE	O13-C11-C12-N
46	Y	203	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	Y	203	3PE	C11-O13-P-O12
46	Y	203	3PE	O13-C11-C12-N
46	Y	204	3PE	C11-O13-P-O14
46	Y	205	3PE	C1-O11-P-O14
46	Y	205	3PE	O13-C11-C12-N
46	Z	201	3PE	C11-O13-P-O12
46	Z	201	3PE	C11-O13-P-O14
46	b	101	3PE	O13-C11-C12-N
46	f	101	3PE	C1-O11-P-O14
46	f	102	3PE	C11-O13-P-O14
46	f	102	3PE	O13-C11-C12-N
46	m	201	3PE	C1-O11-P-O12
46	m	201	3PE	C11-O13-P-O14
46	m	202	3PE	C1-O11-P-O14
46	o	202	3PE	C11-O13-P-O14
48	O	403	PLC	C4-O4P-P-O1P
48	b	102	PLC	C1-O3P-P-O1P
48	g	201	PLC	C4-O4P-P-O3P
53	J	201	CDL	CA2-OA2-PA1-OA3
53	L	701	CDL	CA3-OA5-PA1-OA3
53	M	602	CDL	CA2-OA2-PA1-OA5
53	q	201	CDL	CB2-OB2-PB2-OB3
55	O	401	DGT	C5'-O5'-PA-O3A
53	M	602	CDL	C63-C64-C65-C66
46	N	403	3PE	O31-C31-C32-C33
45	M	603	PC1	C33-C34-C35-C36
45	M	605	PC1	C2-C1-O11-P
45	h	202	PC1	C2-C1-O11-P
46	L	706	3PE	C2-C1-O11-P
53	M	602	CDL	C1-CB2-OB2-PB2
53	h	201	CDL	C11-C12-C13-C14
46	N	402	3PE	C36-C37-C38-C39
45	I	203	PC1	C35-C36-C37-C38
45	B	204	PC1	C31-C32-C33-C34
45	A	201	PC1	C3-C2-O21-C21
45	h	202	PC1	C1-C2-O21-C21
46	L	703	3PE	C3-C2-O21-C21
46	Y	202	3PE	C3-C2-O21-C21
53	q	201	CDL	CB3-CB4-OB6-CB5
46	N	402	3PE	C2A-C2B-C2C-C2D
46	J	204	3PE	C25-C26-C27-C28
46	N	403	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	B	202	PC1	C11-C12-N-C13
45	M	603	PC1	C11-C12-N-C13
48	B	203	PLC	C4-C5-N-C8
46	L	706	3PE	O11-C1-C2-C3
46	Y	205	3PE	O11-C1-C2-C3
53	X	201	CDL	OB5-CB3-CB4-CB6
53	h	201	CDL	OB5-CB3-CB4-CB6
45	I	203	PC1	C3B-C3C-C3D-C3E
46	A	203	3PE	O11-C1-C2-O21
45	I	203	PC1	C23-C24-C25-C26
46	Y	204	3PE	C3A-C3B-C3C-C3D
53	h	201	CDL	C16-C17-C18-C19
45	H	402	PC1	C33-C34-C35-C36
46	L	703	3PE	C33-C34-C35-C36
53	N	401	CDL	C76-C77-C78-C79
53	X	201	CDL	C71-C72-C73-C74
46	b	101	3PE	O22-C21-O21-C2
46	I	205	3PE	C2B-C2C-C2D-C2E
45	B	204	PC1	O21-C2-C3-O31
46	L	703	3PE	O21-C2-C3-O31
48	L	705	PLC	O2-C2-C3-O3
53	X	201	CDL	C44-C45-C46-C47
46	N	402	3PE	C32-C33-C34-C35
46	N	402	3PE	C24-C25-C26-C27
46	Y	203	3PE	C24-C25-C26-C27
46	N	402	3PE	C22-C21-O21-C2
46	Y	203	3PE	C23-C24-C25-C26
46	Y	201	3PE	C22-C23-C24-C25
45	A	201	PC1	O22-C21-O21-C2
46	N	402	3PE	O22-C21-O21-C2
45	H	403	PC1	C39-C3A-C3B-C3C
45	I	204	PC1	C24-C25-C26-C27
46	N	403	3PE	C2E-C2F-C2G-C2H
55	O	401	DGT	PG-O3B-PB-O1B
57	P	501	NDP	PN-O3-PA-O2A
48	B	203	PLC	C2-C3-O3-CB
45	H	403	PC1	C3E-C3F-C3G-C3H
45	m	203	PC1	C24-C25-C26-C27
46	L	702	3PE	C2C-C2D-C2E-C2F
46	Z	201	3PE	C2F-C2G-C2H-C2I
46	Y	205	3PE	C36-C37-C38-C39
45	M	603	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
45	L	707	PC1	C24-C25-C26-C27
48	L	705	PLC	C2B-C1B-CB-O3
46	Y	204	3PE	C3F-C3G-C3H-C3I
46	j	101	3PE	C33-C34-C35-C36
45	H	402	PC1	C32-C31-O31-C3
53	q	201	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	OB9-CB7-OB8-CB6
53	q	201	CDL	C52-C53-C54-C55
46	N	402	3PE	C2E-C2F-C2G-C2H
45	H	402	PC1	O32-C31-O31-C3
45	M	603	PC1	C2B-C2C-C2D-C2E
46	m	201	3PE	C29-C2A-C2B-C2C
45	I	203	PC1	C24-C25-C26-C27
58	T	101	EHZ	N2-C15-C16-C17
53	q	201	CDL	C18-C19-C20-C21
46	f	102	3PE	C33-C34-C35-C36
46	L	703	3PE	C3D-C3E-C3F-C3G
46	Z	201	3PE	C35-C36-C37-C38
53	L	701	CDL	C54-C55-C56-C57
46	L	703	3PE	C3F-C3G-C3H-C3I
53	L	701	CDL	C43-C44-C45-C46
46	L	702	3PE	C2-C1-O11-P
53	J	201	CDL	CA4-CA3-OA5-PA1
45	I	203	PC1	C2C-C2D-C2E-C2F
46	f	102	3PE	C32-C33-C34-C35
53	q	201	CDL	C13-C14-C15-C16
46	J	203	3PE	C32-C33-C34-C35
45	M	603	PC1	C2A-C2B-C2C-C2D
45	B	202	PC1	C11-C12-N-C14
45	B	204	PC1	C33-C34-C35-C36
46	L	703	3PE	C25-C26-C27-C28
48	B	203	PLC	C4B-C5B-C6B-C7B
53	N	401	CDL	C52-C53-C54-C55
46	N	403	3PE	C1-C2-C3-O31
45	m	203	PC1	C35-C36-C37-C38
45	B	204	PC1	C1-C2-O21-C21
45	B	204	PC1	C3-C2-O21-C21
46	L	706	3PE	C3-C2-O21-C21
46	Y	202	3PE	C1-C2-O21-C21
46	M	604	3PE	C3D-C3E-C3F-C3G
53	d	201	CDL	C33-C34-C35-C36
46	m	201	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
46	A	203	3PE	C38-C39-C3A-C3B
53	X	201	CDL	C72-C73-C74-C75
45	M	603	PC1	C11-C12-N-C14
46	L	703	3PE	C26-C27-C28-C29
45	B	204	PC1	C2B-C2C-C2D-C2E
46	d	202	3PE	C2F-C2G-C2H-C2I
45	H	402	PC1	C24-C25-C26-C27
45	d	203	PC1	C32-C33-C34-C35
46	j	101	3PE	C29-C2A-C2B-C2C
53	M	602	CDL	C80-C81-C82-C83
46	L	706	3PE	C34-C35-C36-C37
46	m	201	3PE	C2E-C2F-C2G-C2H
46	Z	201	3PE	C28-C29-C2A-C2B
53	M	602	CDL	C76-C77-C78-C79
53	h	201	CDL	C52-C53-C54-C55
46	J	203	3PE	C31-C32-C33-C34
46	A	203	3PE	O21-C2-C3-O31
46	N	402	3PE	C25-C26-C27-C28
46	N	402	3PE	C28-C29-C2A-C2B
46	f	102	3PE	C25-C26-C27-C28
53	N	401	CDL	C13-C14-C15-C16
53	L	701	CDL	C57-C58-C59-C60
46	A	203	3PE	C3E-C3F-C3G-C3H
46	j	101	3PE	C2B-C2C-C2D-C2E
45	M	603	PC1	C29-C2A-C2B-C2C
46	Y	205	3PE	C38-C39-C3A-C3B
53	M	602	CDL	C16-C17-C18-C19
45	m	203	PC1	C26-C27-C28-C29
45	J	202	PC1	C36-C37-C38-C39
53	X	201	CDL	C80-C81-C82-C83
46	N	403	3PE	C25-C26-C27-C28
53	N	401	CDL	C14-C15-C16-C17
45	B	204	PC1	C27-C28-C29-C2A
53	L	701	CDL	C40-C41-C42-C43
46	L	704	3PE	C2-C1-O11-P
45	I	203	PC1	C25-C26-C27-C28
45	H	402	PC1	C27-C28-C29-C2A
48	O	403	PLC	O'-C'-C1'-C2'
45	I	203	PC1	C26-C27-C28-C29
53	N	401	CDL	C75-C76-C77-C78
46	Y	203	3PE	O21-C21-C22-C23
45	A	201	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	m	201	3PE	C1-C2-C3-O31
46	d	202	3PE	C36-C37-C38-C39
46	Y	204	3PE	O11-C1-C2-O21
46	N	403	3PE	C2A-C2B-C2C-C2D
45	J	202	PC1	C22-C23-C24-C25
46	b	101	3PE	C26-C27-C28-C29
46	L	704	3PE	C33-C34-C35-C36
46	N	402	3PE	O22-C21-C22-C23
46	J	203	3PE	C23-C24-C25-C26
46	J	204	3PE	C3D-C3E-C3F-C3G
53	q	201	CDL	C51-C52-C53-C54
46	J	204	3PE	C29-C2A-C2B-C2C
53	X	201	CDL	C75-C76-C77-C78
46	A	202	3PE	C23-C24-C25-C26
53	M	602	CDL	C81-C82-C83-C84
46	Y	202	3PE	C25-C26-C27-C28
46	M	604	3PE	C23-C24-C25-C26
46	m	201	3PE	O11-C1-C2-C3
53	N	401	CDL	OB5-CB3-CB4-CB6
53	M	602	CDL	C33-C34-C35-C36
46	Y	202	3PE	O21-C2-C3-O31
53	d	201	CDL	OB6-CB4-CB6-OB8
46	m	201	3PE	C21-C22-C23-C24
53	L	701	CDL	C72-C71-CB7-OB8
53	q	201	CDL	C52-C51-CB5-OB6
53	q	201	CDL	C1-CA2-OA2-PA1
46	N	402	3PE	C27-C28-C29-C2A
46	J	203	3PE	C24-C25-C26-C27
48	L	705	PLC	C2B-C1B-CB-OB
46	L	706	3PE	C22-C23-C24-C25
46	Y	203	3PE	C3D-C3E-C3F-C3G
45	h	202	PC1	C3-C2-O21-C21
48	b	102	PLC	C1-C2-O2-C'
45	I	203	PC1	C2D-C2E-C2F-C2G
46	m	201	3PE	C22-C23-C24-C25
45	B	204	PC1	C22-C23-C24-C25
53	X	201	CDL	C72-C71-CB7-OB8
45	B	202	PC1	C23-C24-C25-C26
46	L	706	3PE	C36-C37-C38-C39
46	A	203	3PE	C3F-C3G-C3H-C3I
46	b	101	3PE	C22-C23-C24-C25
53	J	201	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
59	i	201	CHD	C20-C22-C23-C24
46	Y	202	3PE	O31-C31-C32-C33
46	L	704	3PE	C12-C11-O13-P
46	N	402	3PE	C12-C11-O13-P
46	m	201	3PE	C12-C11-O13-P
46	Z	201	3PE	C33-C34-C35-C36
53	d	201	CDL	C76-C77-C78-C79
48	g	201	PLC	OB-CB-O3-C3
46	Y	204	3PE	C23-C24-C25-C26
46	d	202	3PE	C33-C34-C35-C36
46	m	202	3PE	C36-C37-C38-C39
45	H	402	PC1	O21-C21-C22-C23
46	j	101	3PE	O31-C31-C32-C33
53	M	602	CDL	C62-C63-C64-C65
46	m	201	3PE	O31-C31-C32-C33
53	X	201	CDL	C12-C11-CA5-OA6
46	L	706	3PE	C32-C31-O31-C3
46	o	202	3PE	O11-C1-C2-C3
53	d	201	CDL	OB5-CB3-CB4-CB6
45	L	707	PC1	C32-C33-C34-C35
59	i	201	CHD	C22-C23-C24-O26
58	T	101	EHZ	C5-C6-C7-C8
46	f	101	3PE	C36-C37-C38-C39
46	o	202	3PE	C26-C27-C28-C29
45	I	203	PC1	O31-C31-C32-C33
46	Y	201	3PE	O31-C31-C32-C33
45	m	203	PC1	C38-C39-C3A-C3B
46	f	102	3PE	C27-C28-C29-C2A
58	T	101	EHZ	C5-C6-C7-O1
46	J	204	3PE	C39-C3A-C3B-C3C
45	B	204	PC1	C26-C27-C28-C29
45	H	402	PC1	C23-C24-C25-C26
46	L	706	3PE	O32-C31-O31-C3
46	I	205	3PE	O21-C21-C22-C23
46	b	101	3PE	O22-C21-C22-C23
46	J	203	3PE	O21-C21-C22-C23
46	Z	201	3PE	O31-C31-C32-C33
45	J	202	PC1	C35-C36-C37-C38
58	T	101	EHZ	O4-C15-C16-C17
53	M	602	CDL	C51-C52-C53-C54
53	d	201	CDL	C73-C74-C75-C76
45	B	204	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	C72-C71-CB7-OB8
46	L	704	3PE	C2B-C2C-C2D-C2E
45	m	203	PC1	C22-C23-C24-C25
46	m	201	3PE	C34-C35-C36-C37
45	B	202	PC1	C36-C37-C38-C39
45	d	203	PC1	C3B-C3C-C3D-C3E
45	h	202	PC1	O21-C21-C22-C23
45	L	707	PC1	C36-C37-C38-C39
45	d	203	PC1	C38-C39-C3A-C3B
53	d	201	CDL	C12-C11-CA5-OA6
46	Y	203	3PE	C29-C2A-C2B-C2C
58	U	101	EHZ	C2-C3-C4-C5
45	H	402	PC1	C11-C12-N-C15
46	o	202	3PE	C2C-C2D-C2E-C2F
46	L	703	3PE	O31-C31-C32-C33
46	Y	202	3PE	C24-C25-C26-C27
45	q	202	PC1	O31-C31-C32-C33
46	J	203	3PE	O31-C31-C32-C33
46	J	204	3PE	O31-C31-C32-C33
53	M	602	CDL	C79-C80-C81-C82
45	H	403	PC1	C3F-C3G-C3H-C3I
46	M	604	3PE	C28-C29-C2A-C2B
53	d	201	CDL	C44-C45-C46-C47
46	Y	204	3PE	O11-C1-C2-C3
46	f	102	3PE	O21-C21-C22-C23
46	N	402	3PE	C3C-C3D-C3E-C3F
59	i	201	CHD	C22-C23-C24-O25
50	F	501	FMN	N10-C1'-C2'-O2'
58	T	101	EHZ	C19-C17-C20-O6
46	J	204	3PE	C37-C38-C39-C3A
46	Y	203	3PE	O31-C31-C32-C33
53	h	201	CDL	CB5-C51-C52-C53
53	J	201	CDL	CA6-CA4-OA6-CA5
45	H	402	PC1	C11-C12-N-C13
45	H	402	PC1	C11-C12-N-C14
46	b	101	3PE	C37-C38-C39-C3A
45	I	204	PC1	C27-C28-C29-C2A
46	b	101	3PE	C2A-C2B-C2C-C2D
46	m	201	3PE	C2F-C2G-C2H-C2I
53	d	201	CDL	C52-C51-CB5-OB6
46	M	604	3PE	C22-C23-C24-C25
46	J	204	3PE	O21-C21-C22-C23

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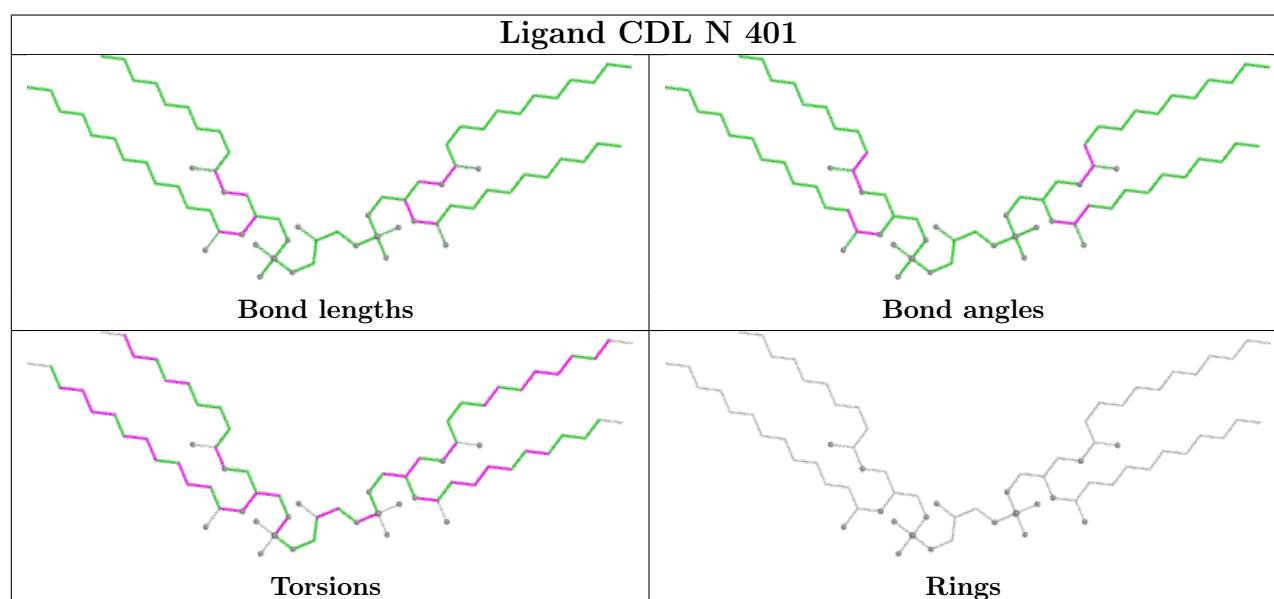
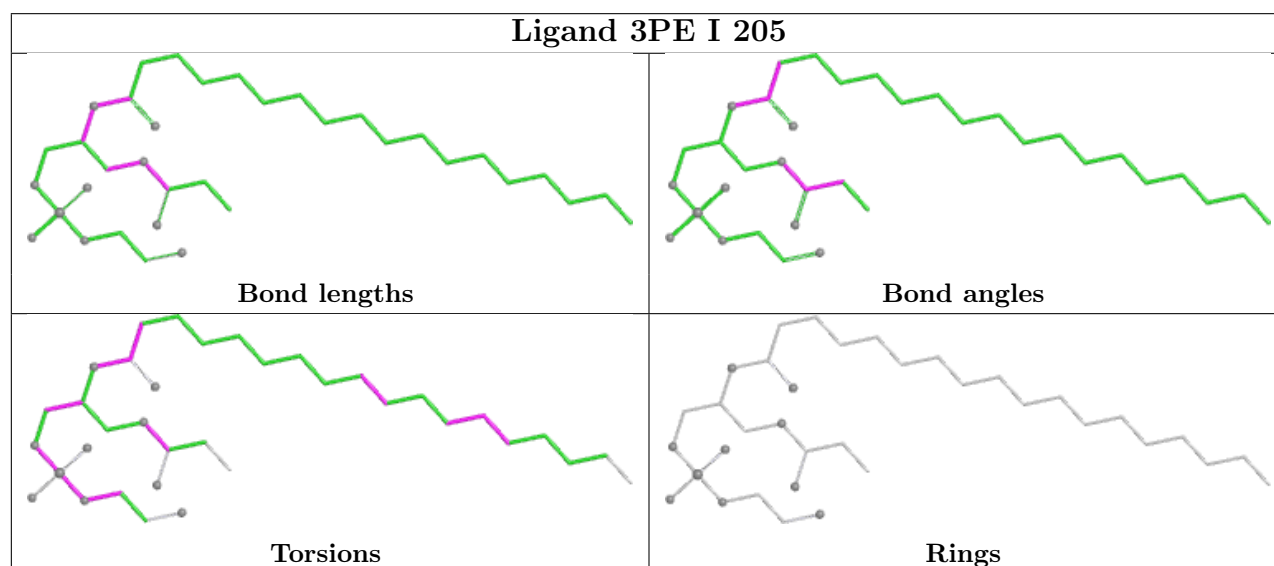
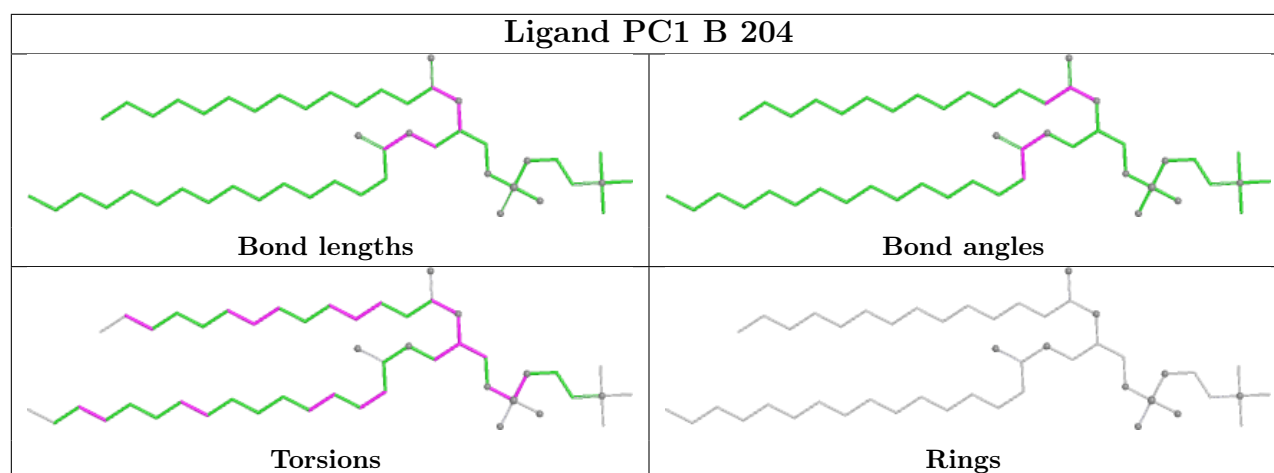
Mol	Chain	Res	Type	Atoms
52	H	401	U10	C6-C7-C8-C9
46	A	202	3PE	C2-C1-O11-P
53	q	201	CDL	CB4-CB3-OB5-PB2
45	I	203	PC1	C22-C23-C24-C25
46	Y	201	3PE	C32-C33-C34-C35
45	L	707	PC1	C33-C34-C35-C36
46	I	205	3PE	O22-C21-C22-C23
53	d	201	CDL	C72-C71-CB7-OB9
53	N	401	CDL	C33-C34-C35-C36
45	h	202	PC1	O22-C21-C22-C23
53	X	201	CDL	C42-C43-C44-C45
53	d	201	CDL	C39-C40-C41-C42
46	J	203	3PE	O22-C21-C22-C23
46	j	101	3PE	O32-C31-C32-C33
46	f	102	3PE	C2B-C2C-C2D-C2E
46	L	702	3PE	C2E-C2F-C2G-C2H
46	Y	202	3PE	O32-C31-C32-C33
53	d	201	CDL	C75-C76-C77-C78
46	Y	201	3PE	O32-C31-C32-C33
46	f	102	3PE	O22-C21-C22-C23
46	m	201	3PE	O32-C31-C32-C33
53	X	201	CDL	C12-C11-CA5-OA7
53	d	201	CDL	C12-C11-CA5-OA7
46	m	202	3PE	C21-C22-C23-C24
53	X	201	CDL	C32-C33-C34-C35
46	Y	204	3PE	C3B-C3C-C3D-C3E
46	Z	201	3PE	O32-C31-C32-C33
45	I	204	PC1	C33-C34-C35-C36
48	B	203	PLC	C2B-C3B-C4B-C5B
46	J	204	3PE	O32-C31-C32-C33
46	Y	203	3PE	O32-C31-C32-C33
48	B	203	PLC	C4-C5-N-C6
48	B	203	PLC	C4-C5-N-C7
53	X	201	CDL	C39-C40-C41-C42
45	I	203	PC1	O32-C31-C32-C33
53	M	602	CDL	C12-C11-CA5-OA6
57	P	501	NDP	PN-O3-PA-O1A
46	L	703	3PE	O32-C31-C32-C33

There are no ring outliers.

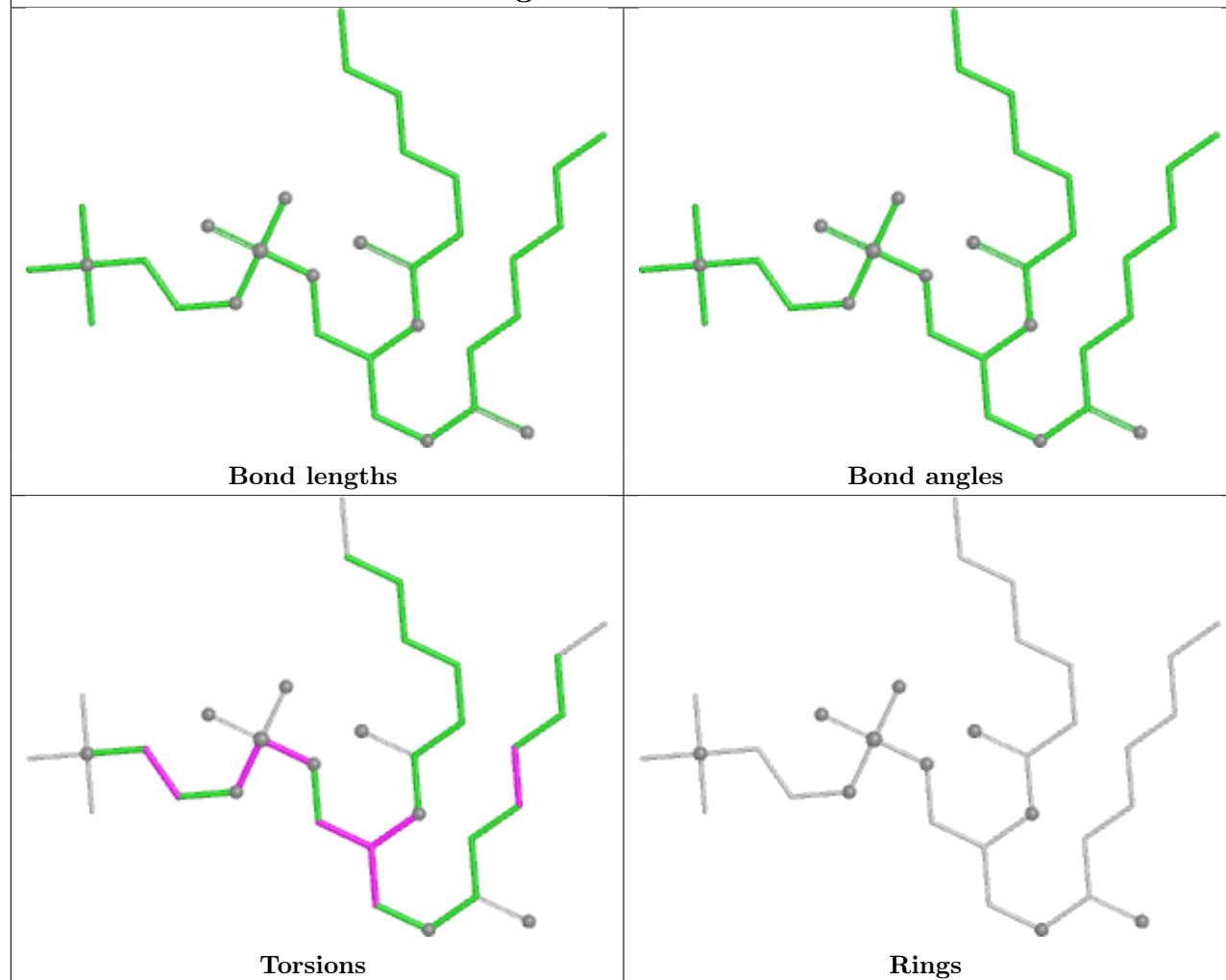
27 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	B	204	PC1	1	0
45	q	202	PC1	2	0
53	q	201	CDL	1	0
45	H	403	PC1	1	0
52	H	401	U10	14	0
46	J	204	3PE	1	0
45	H	402	PC1	1	0
46	N	403	3PE	1	0
45	M	603	PC1	2	0
46	L	706	3PE	1	0
57	P	501	NDP	2	0
59	i	201	CHD	8	0
45	A	201	PC1	2	0
48	O	403	PLC	1	0
58	U	101	EHZ	1	0
55	O	401	DGT	3	0
58	T	101	EHZ	1	0
46	Y	201	3PE	1	0
53	M	602	CDL	4	0
45	m	203	PC1	1	0
53	L	701	CDL	2	0
45	L	707	PC1	1	0
46	L	703	3PE	2	0
49	G	803	FES	1	0
53	d	201	CDL	2	0
46	Y	203	3PE	3	0
48	g	201	PLC	1	0

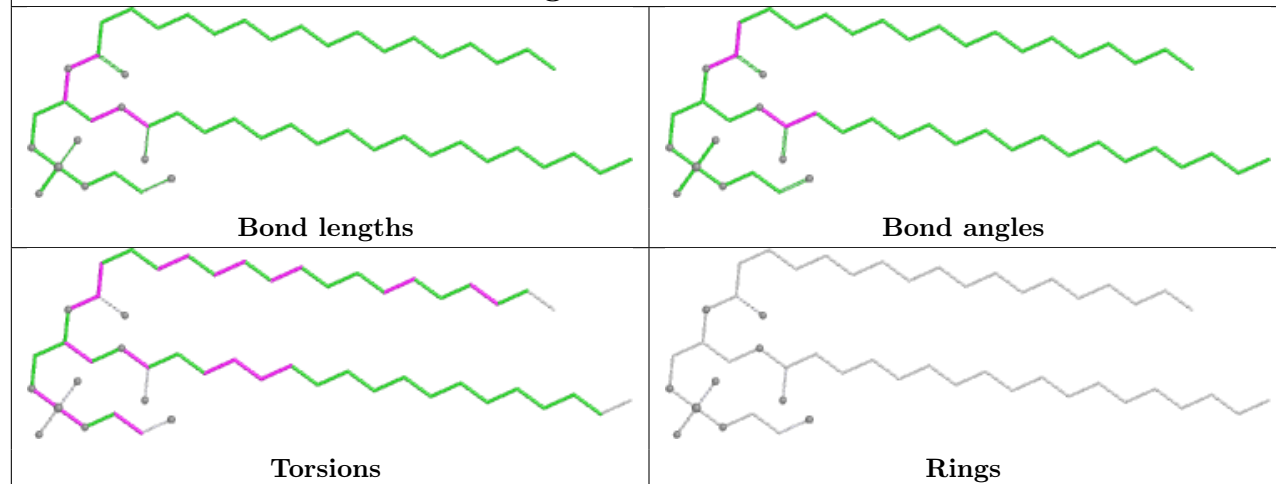
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

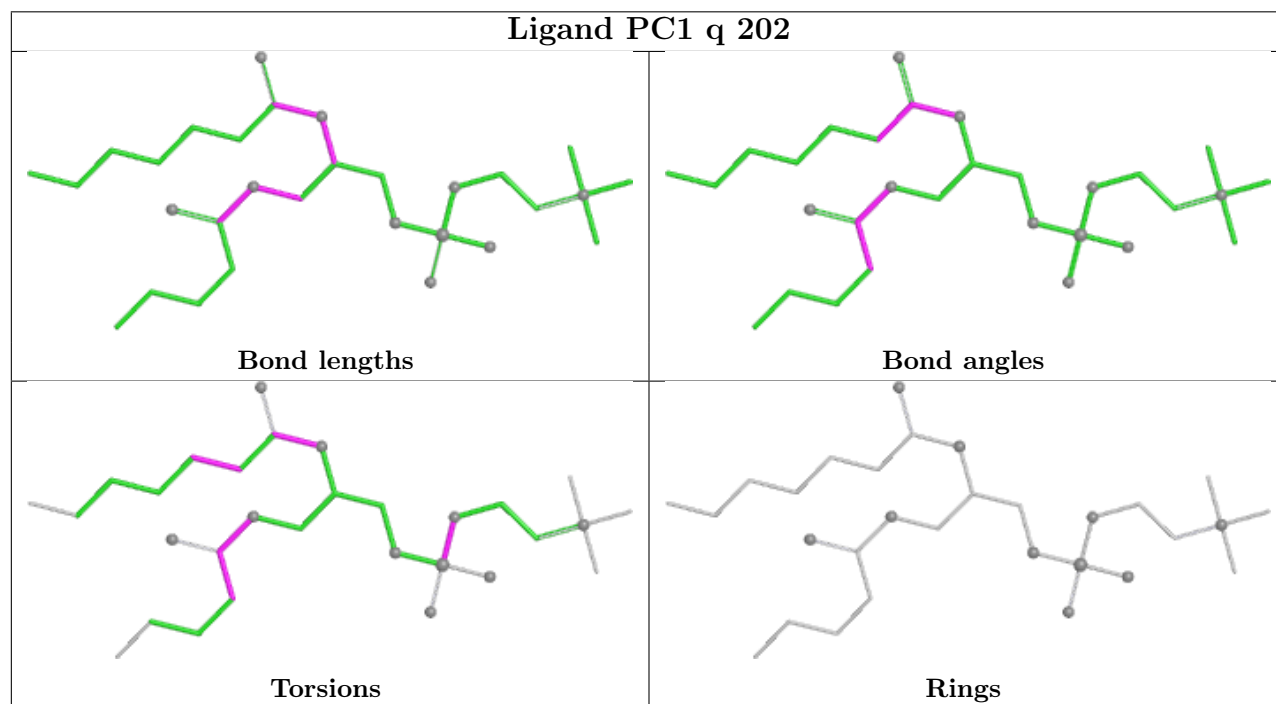
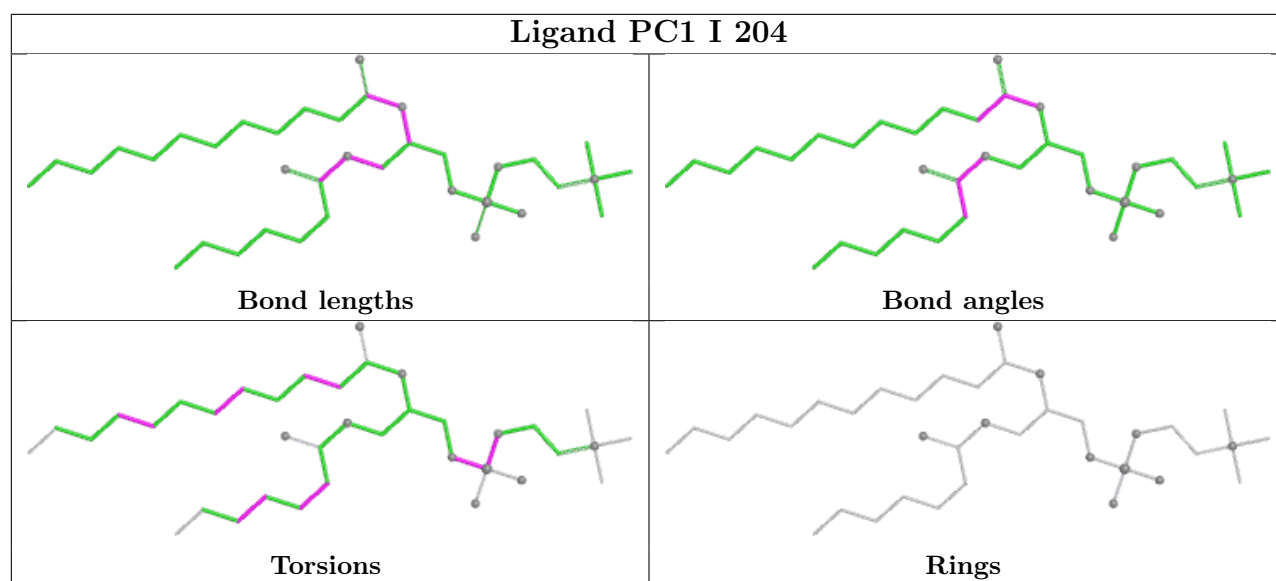


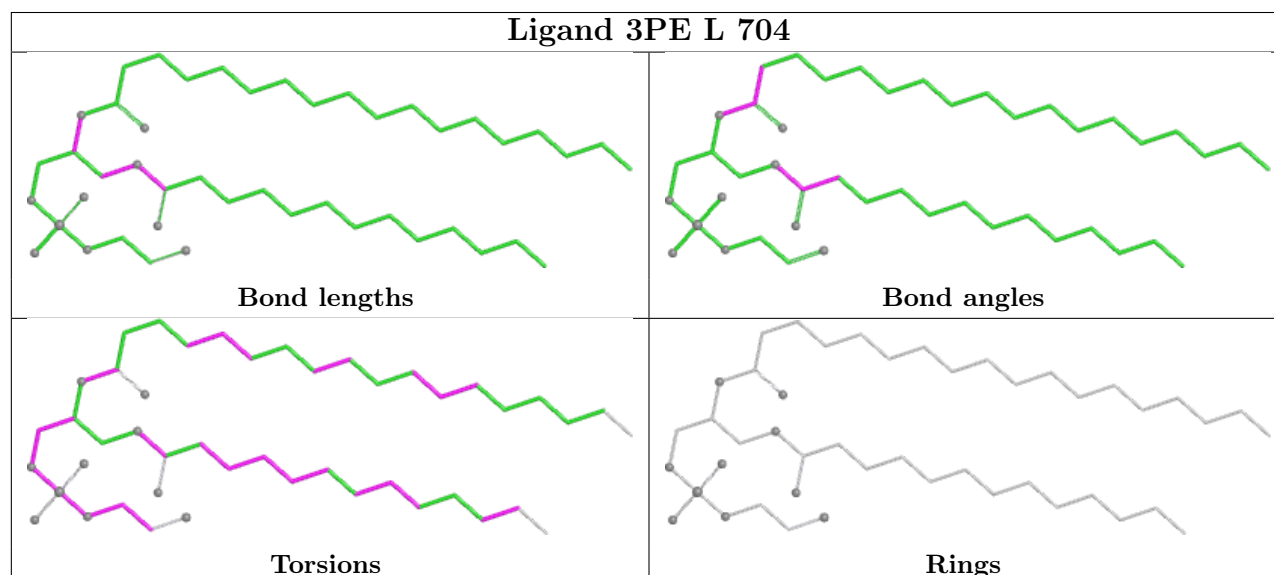
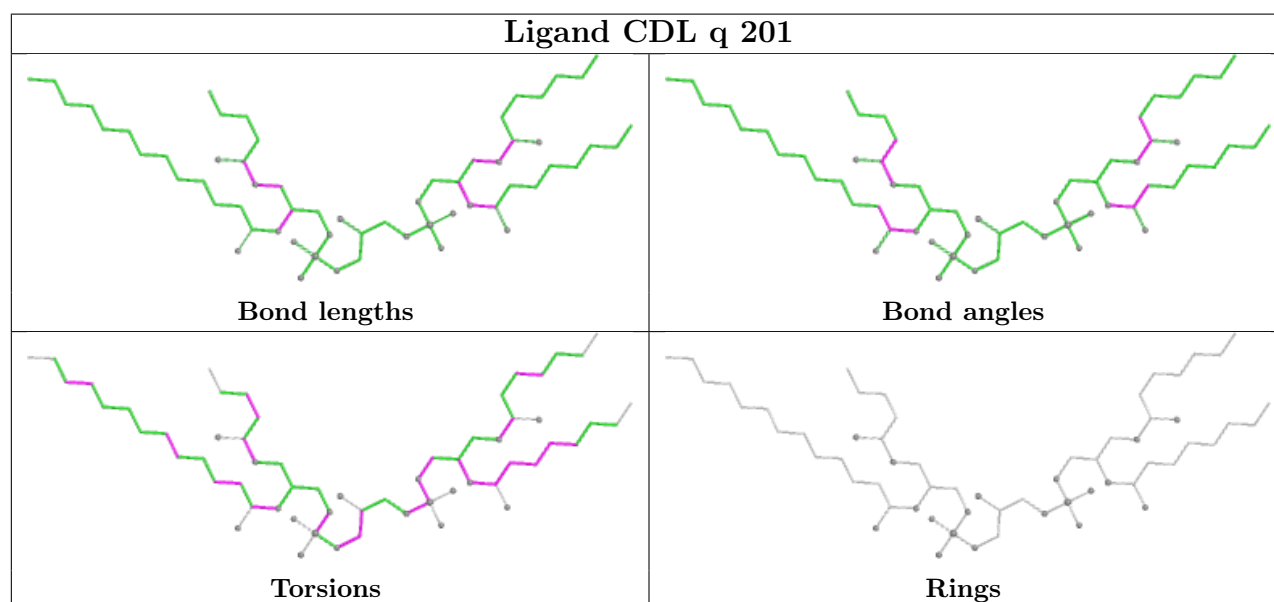
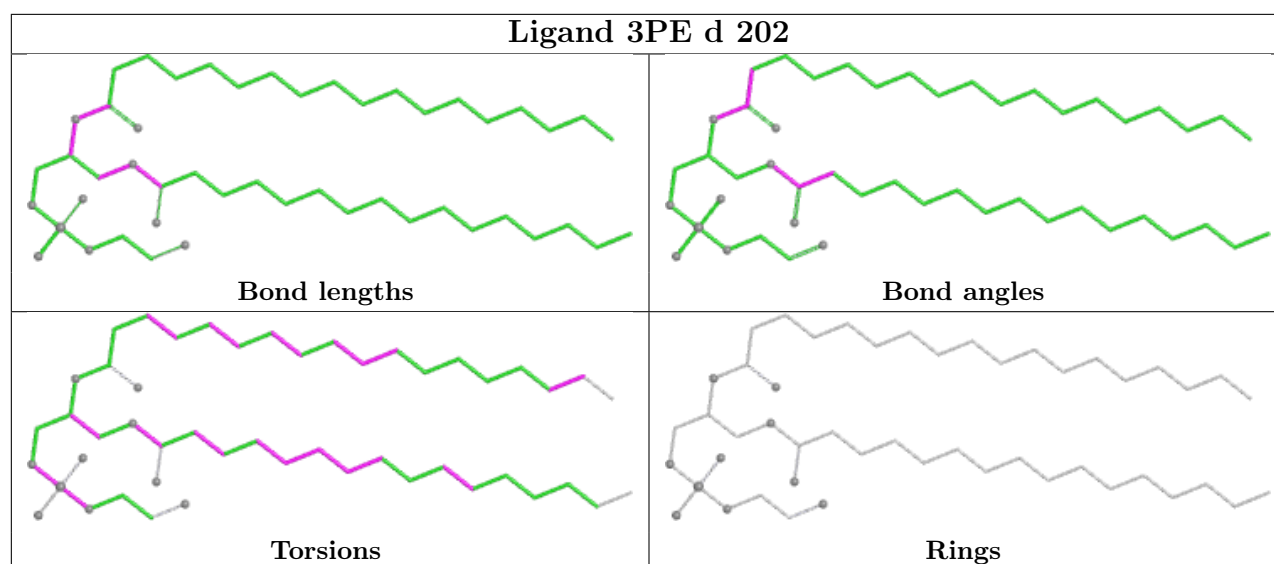
Ligand PLC b 102

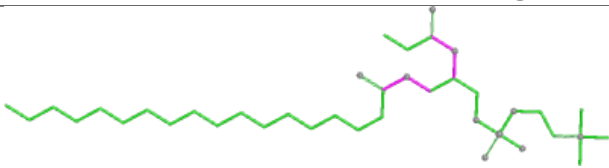
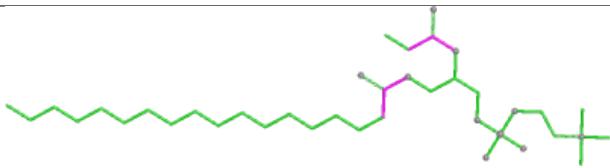
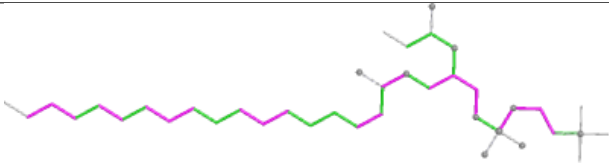
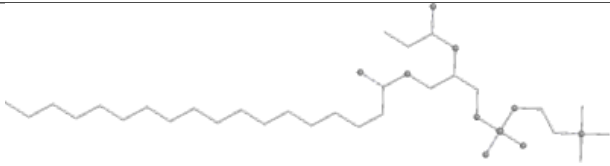
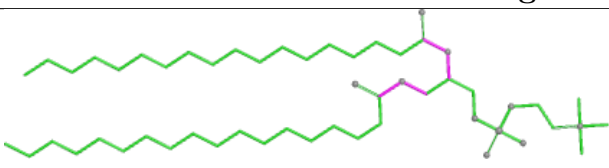
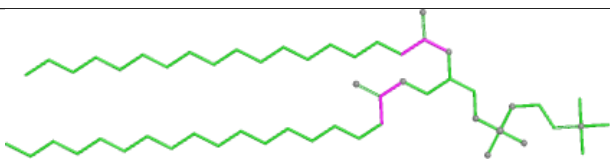
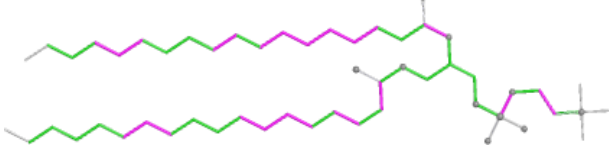
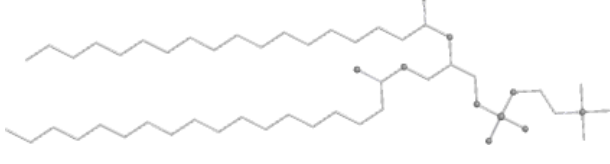
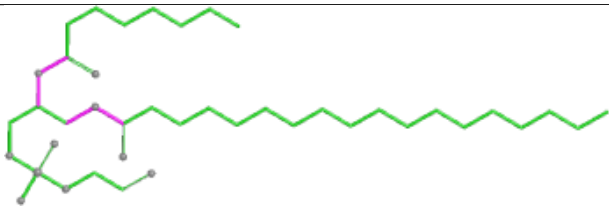
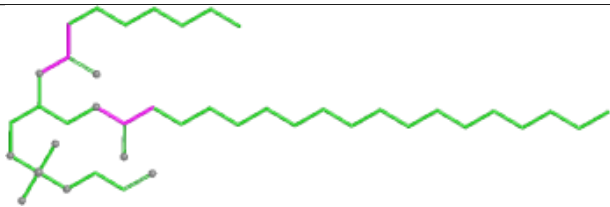
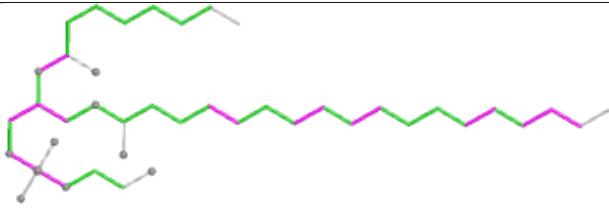
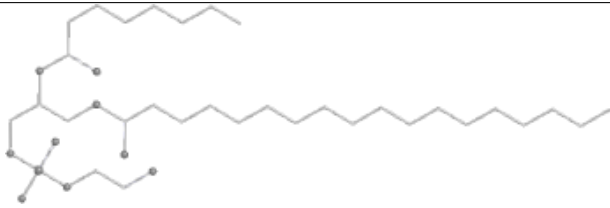


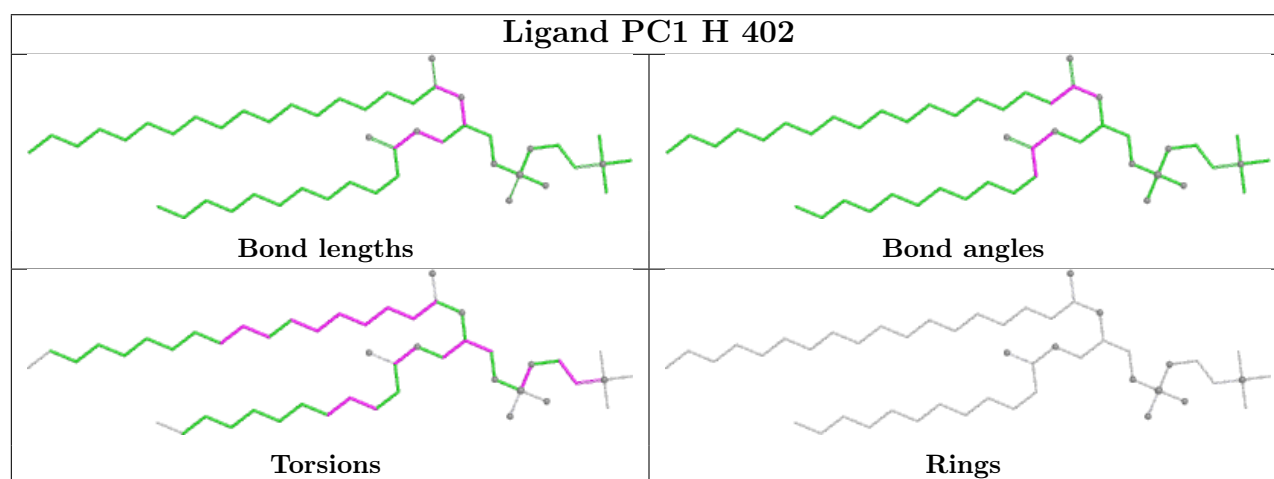
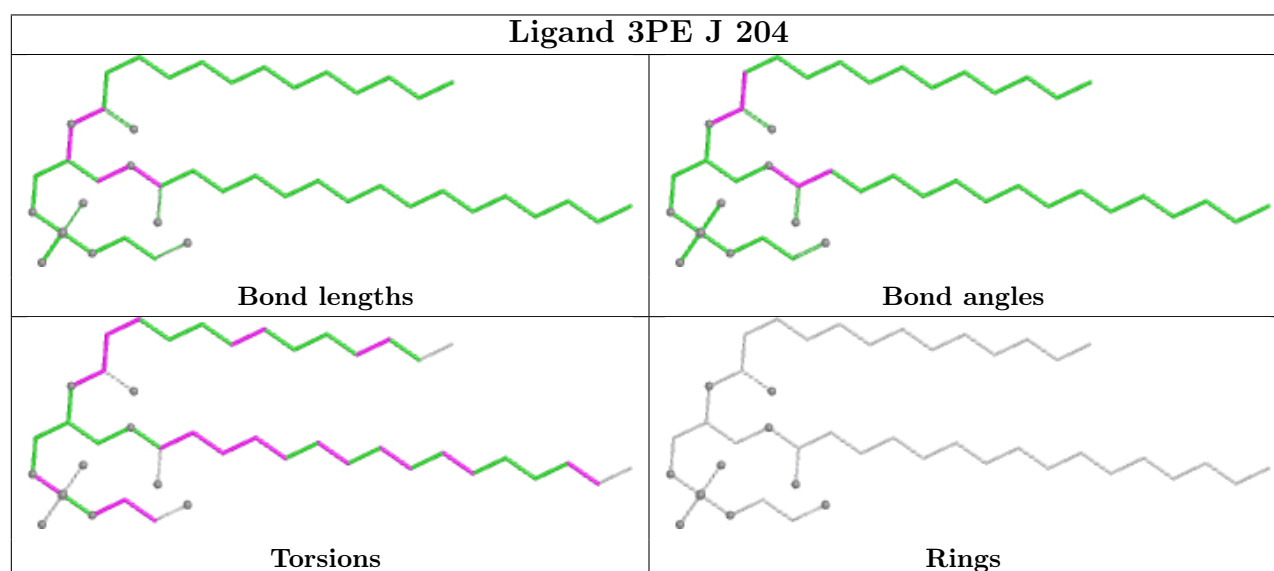
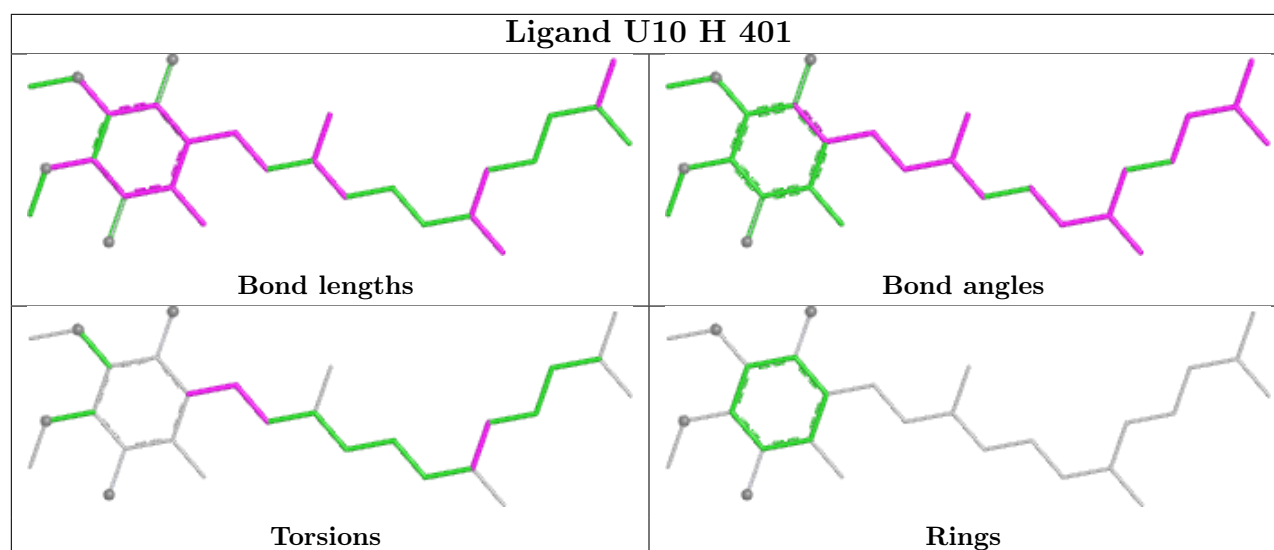
Ligand 3PE f 102

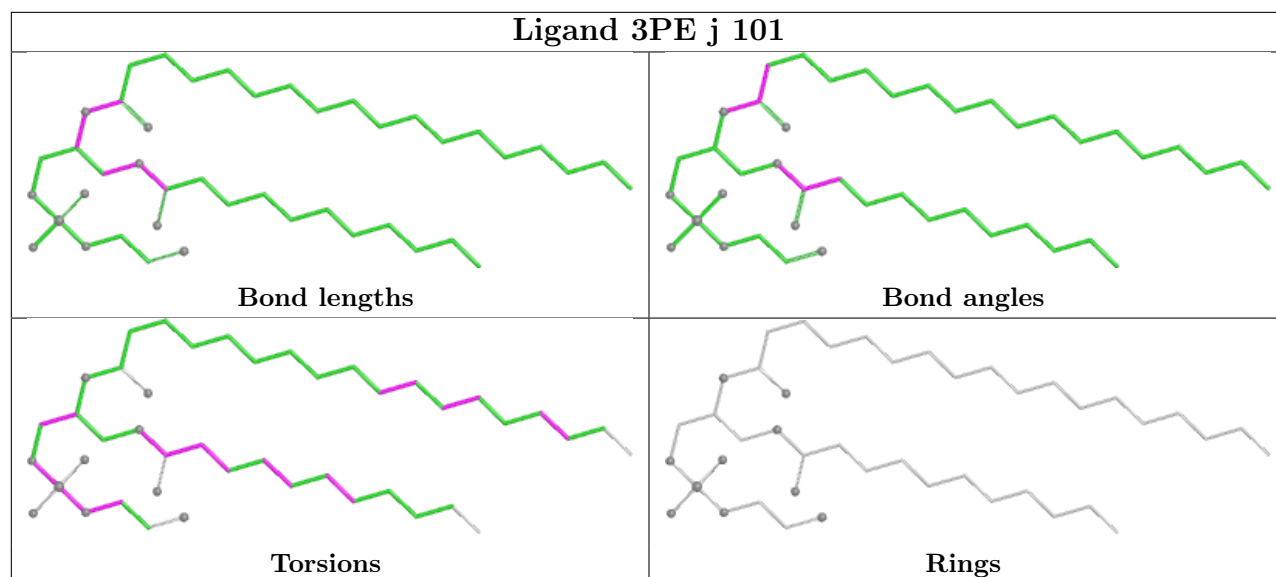
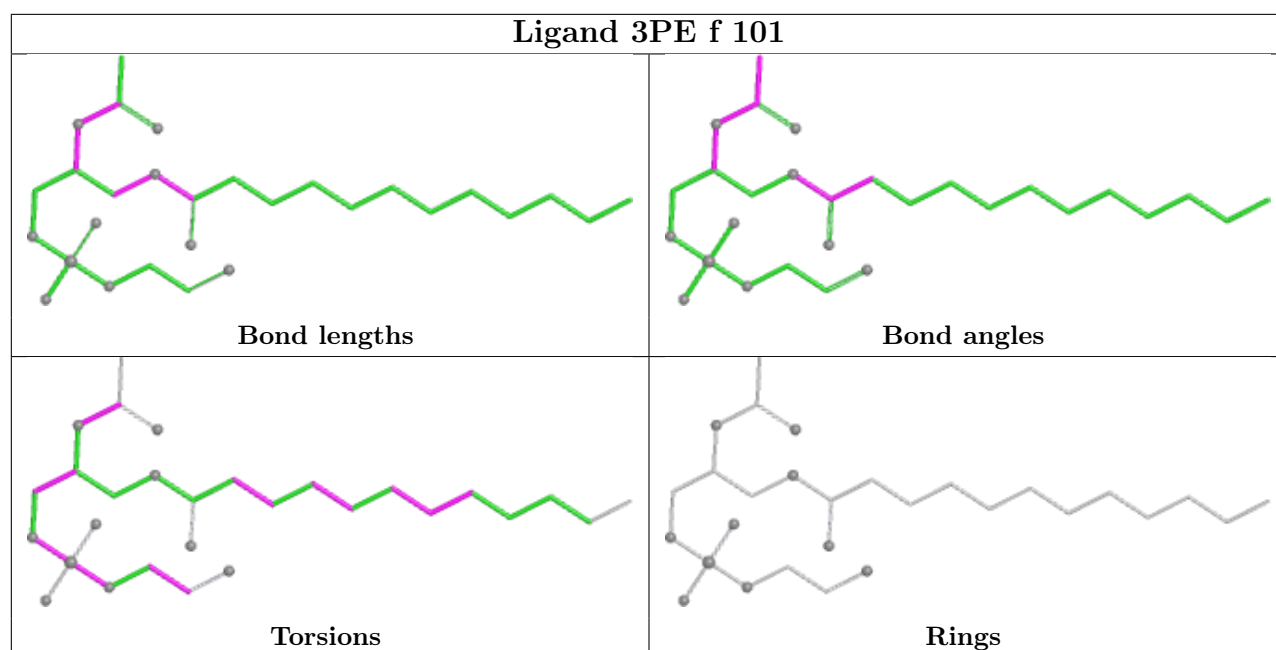


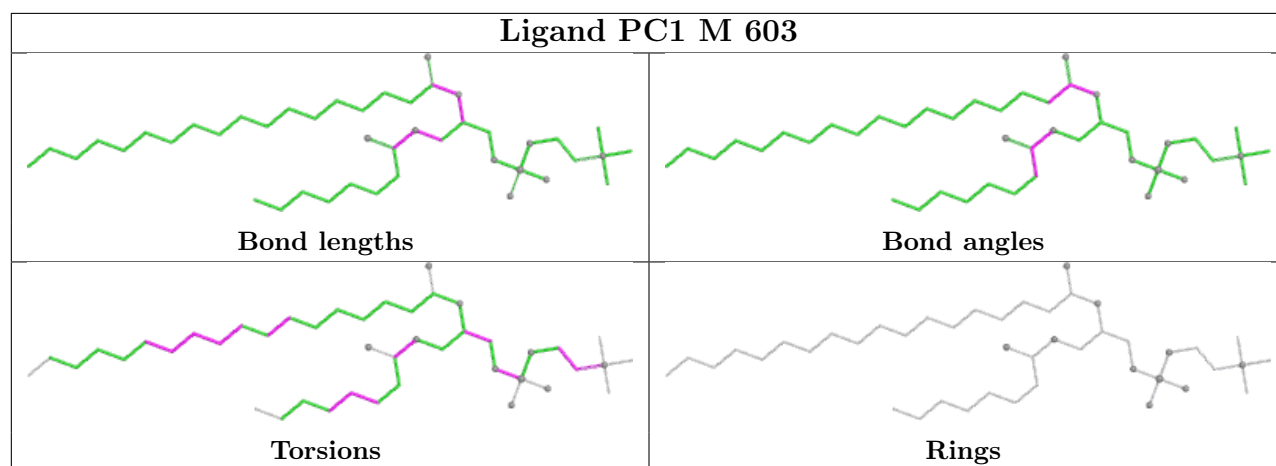
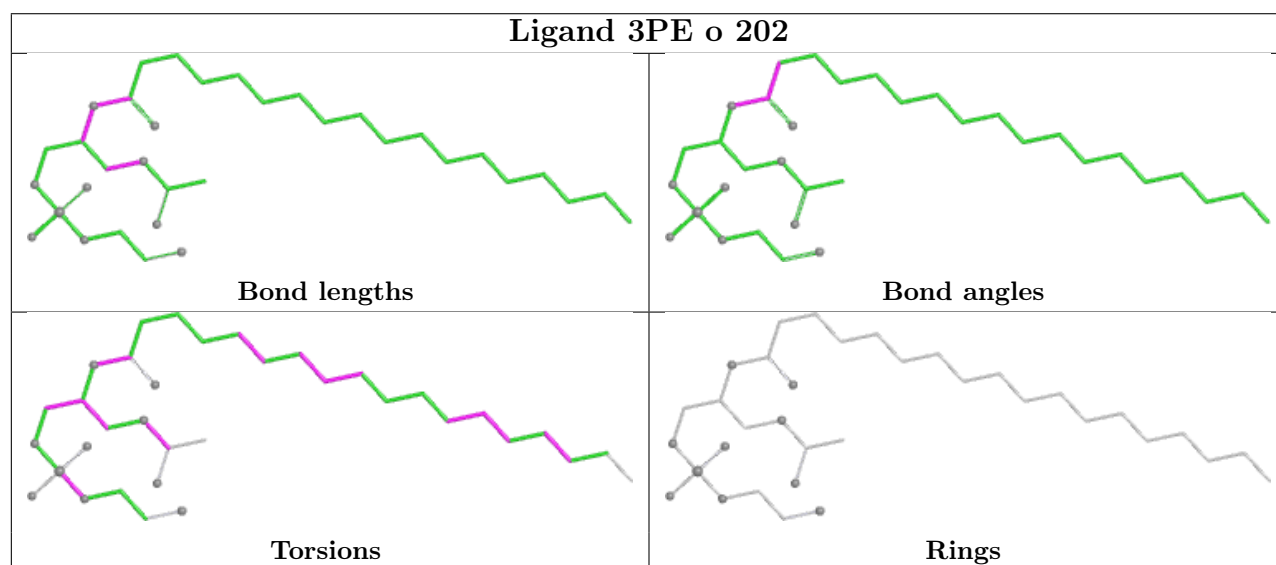
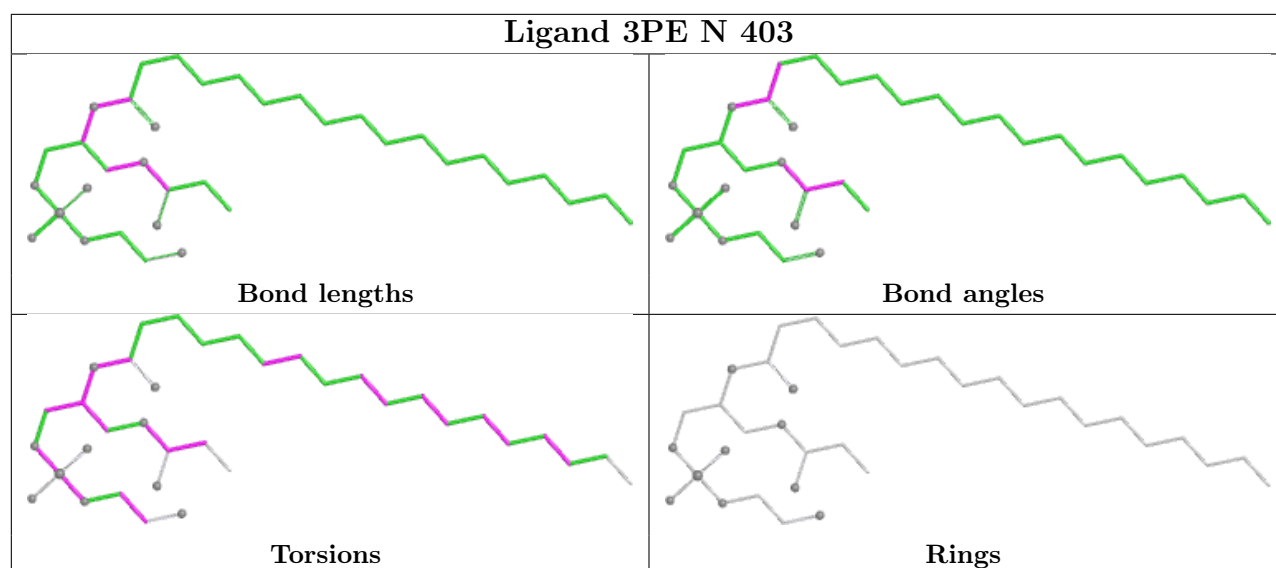


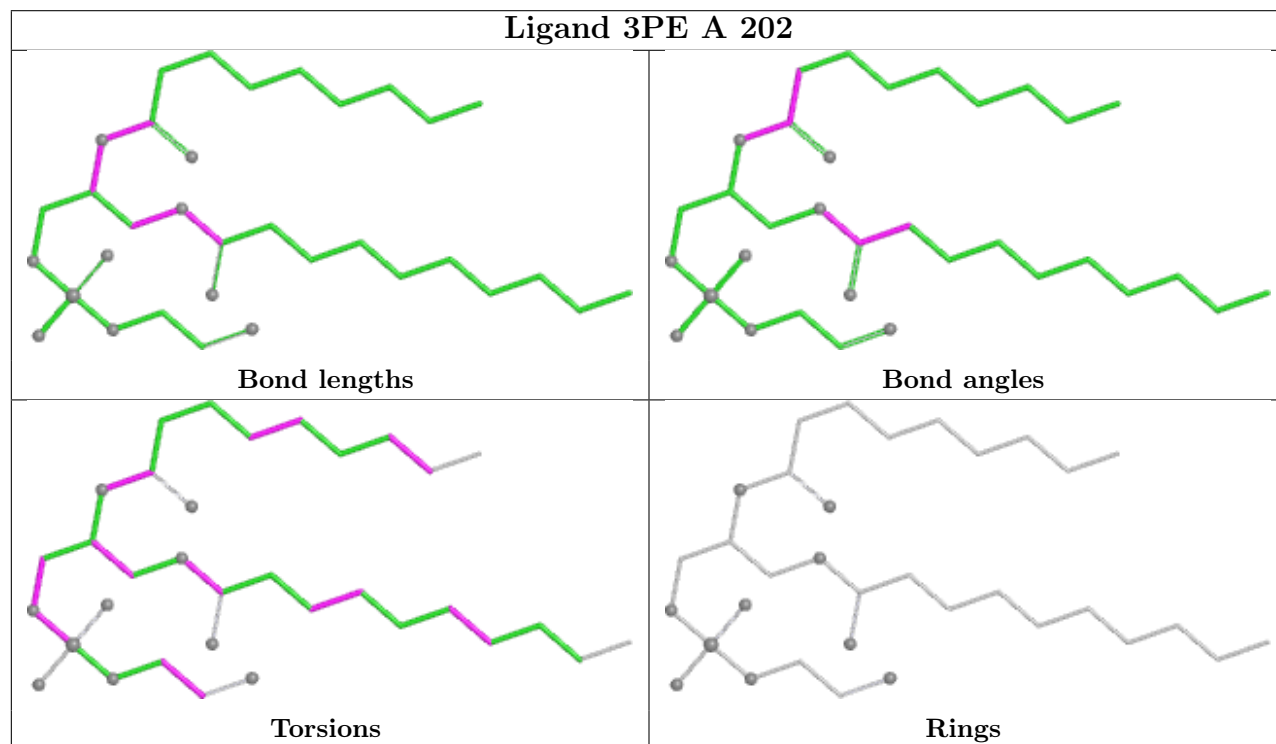
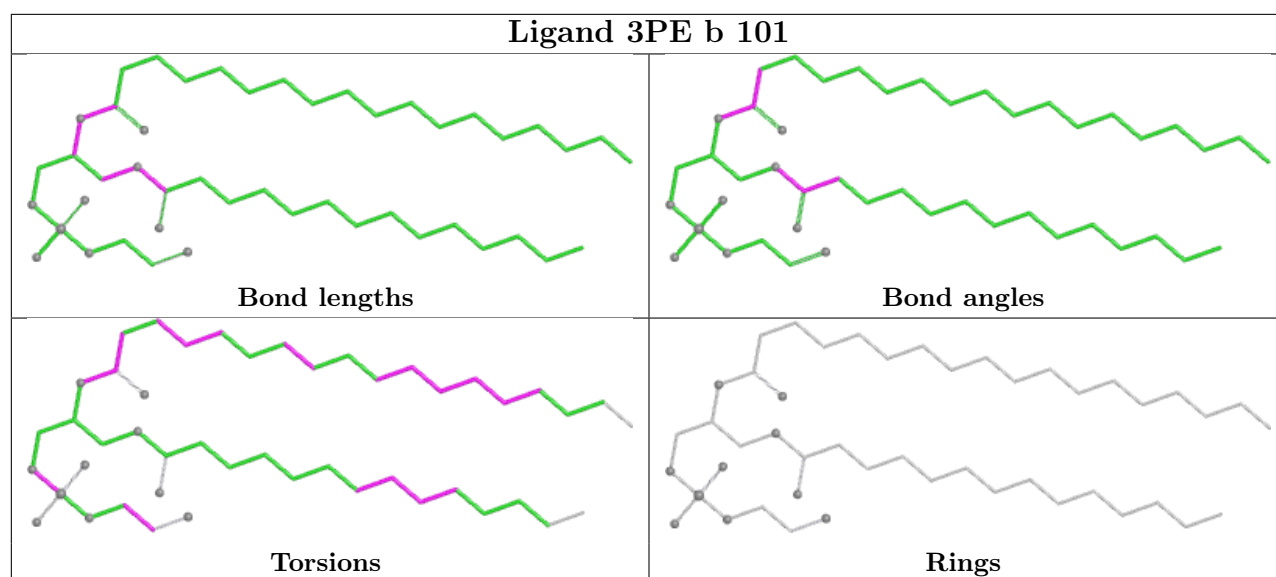


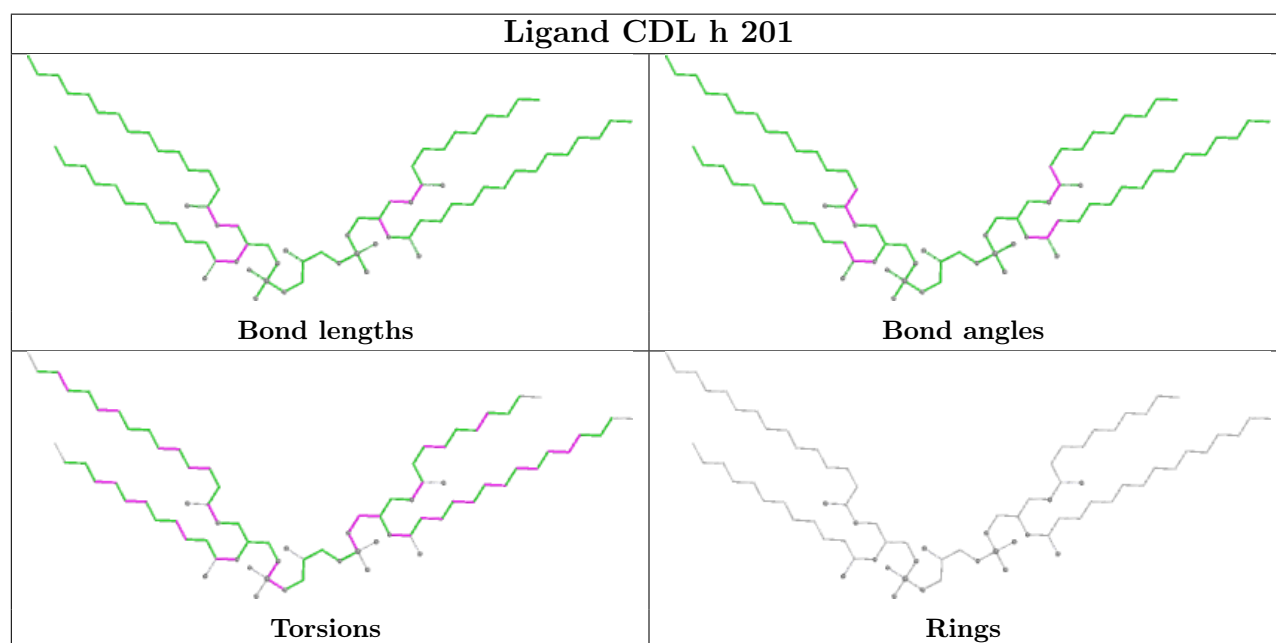
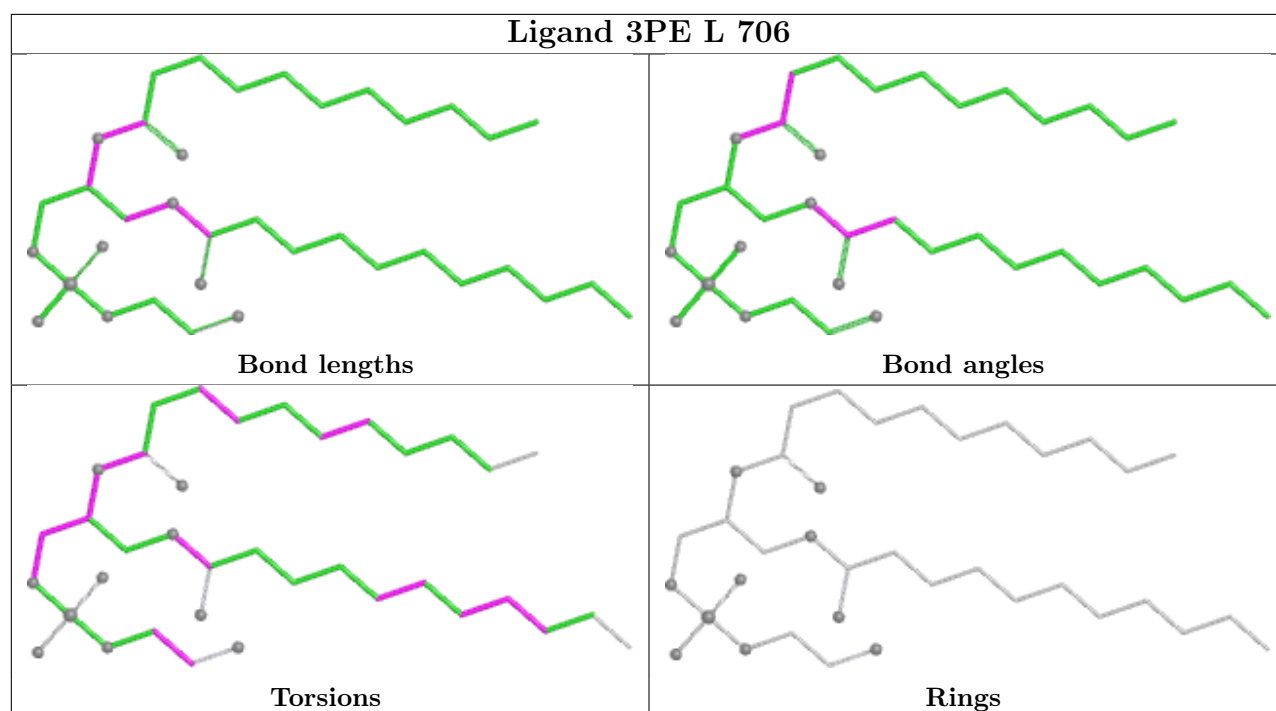
Ligand PC1 H 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 I 203	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 3PE A 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

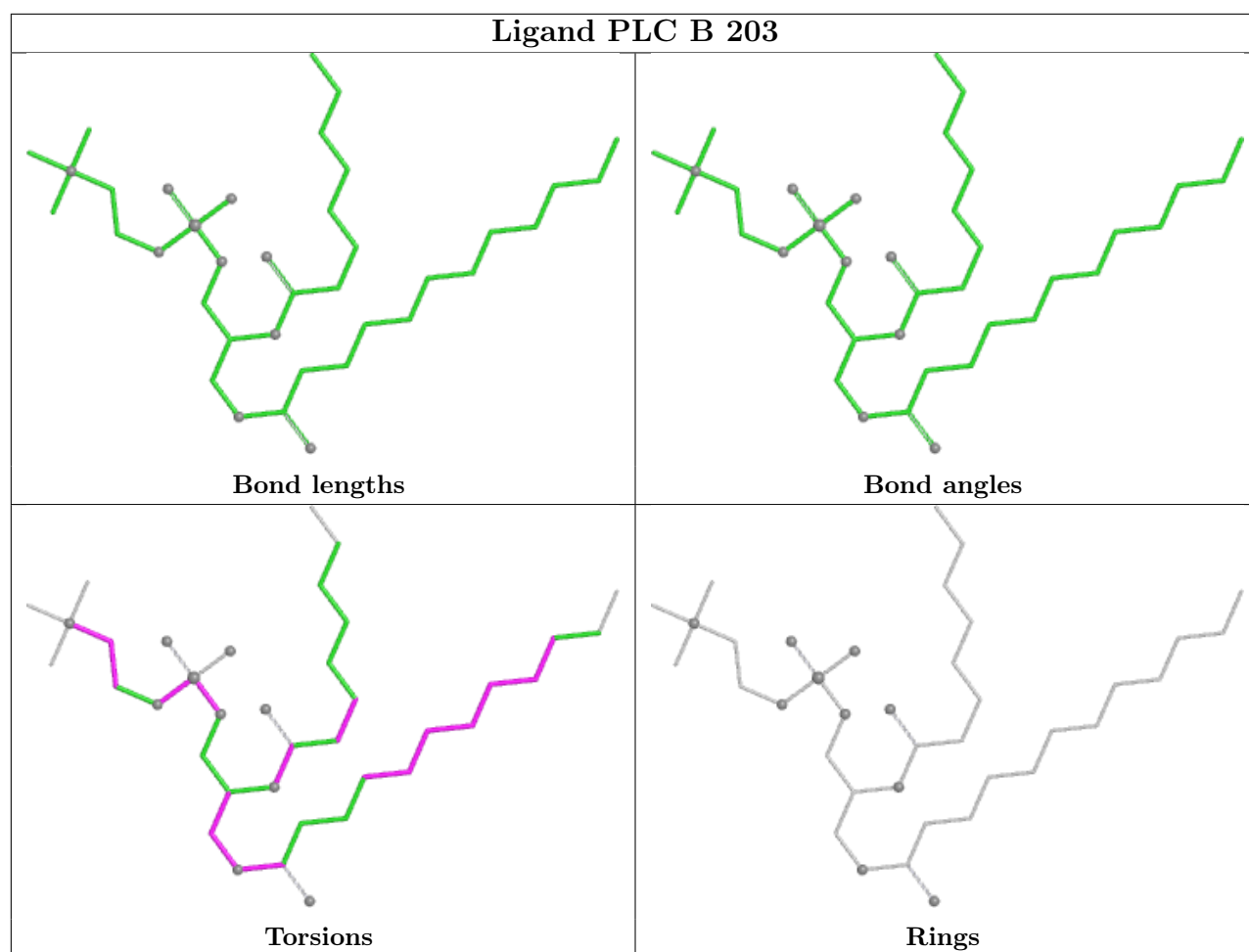


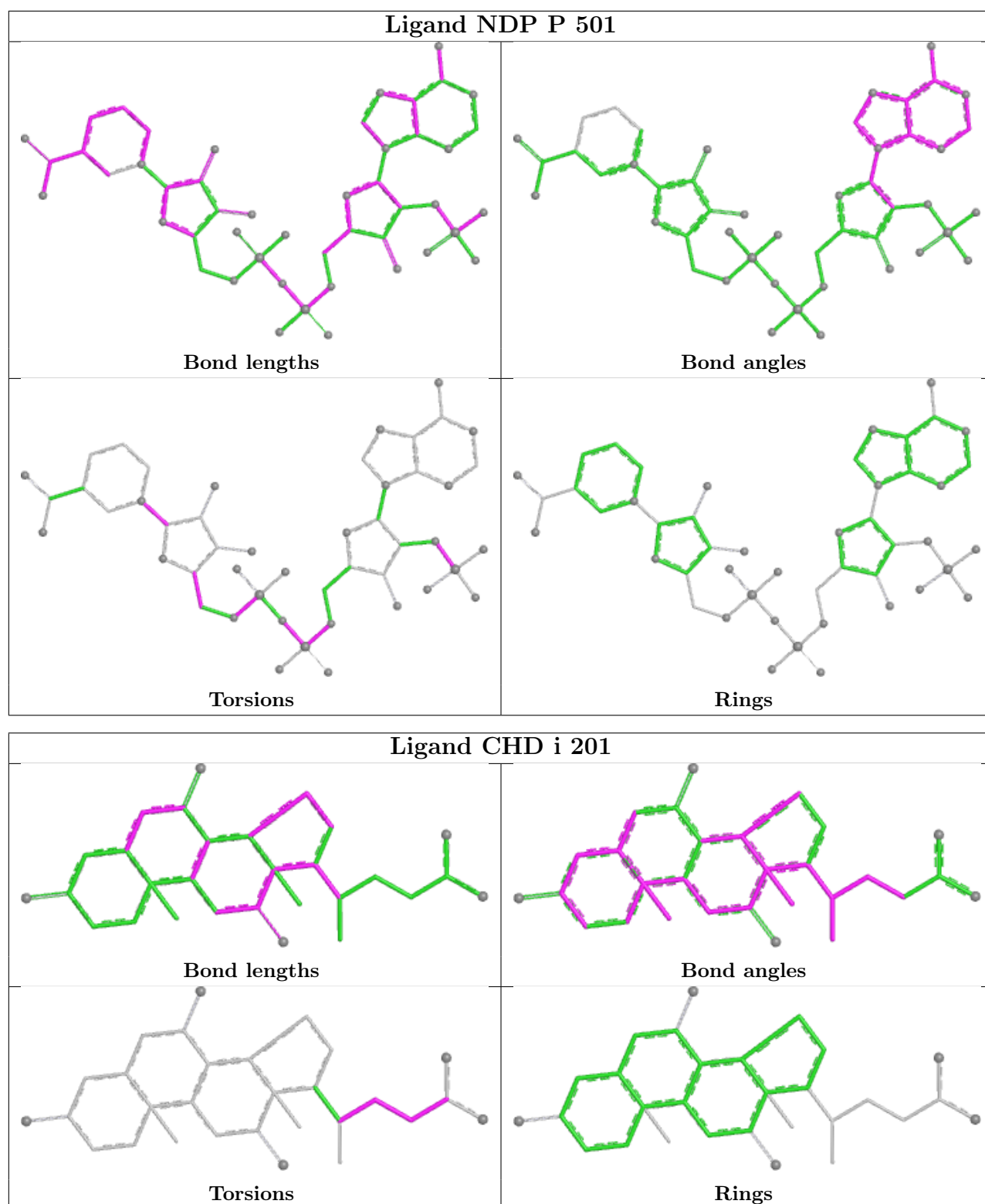


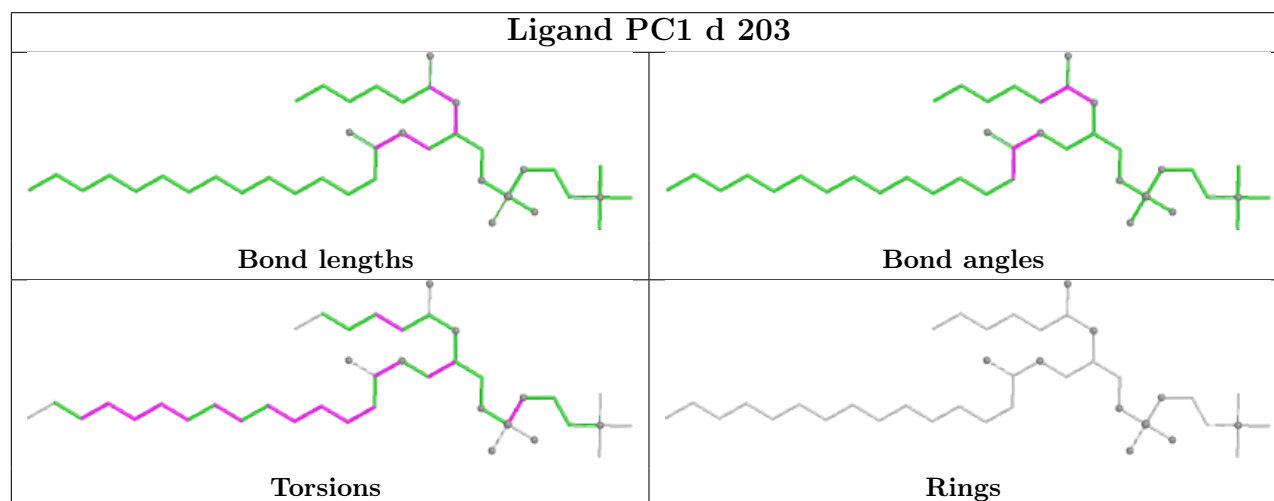
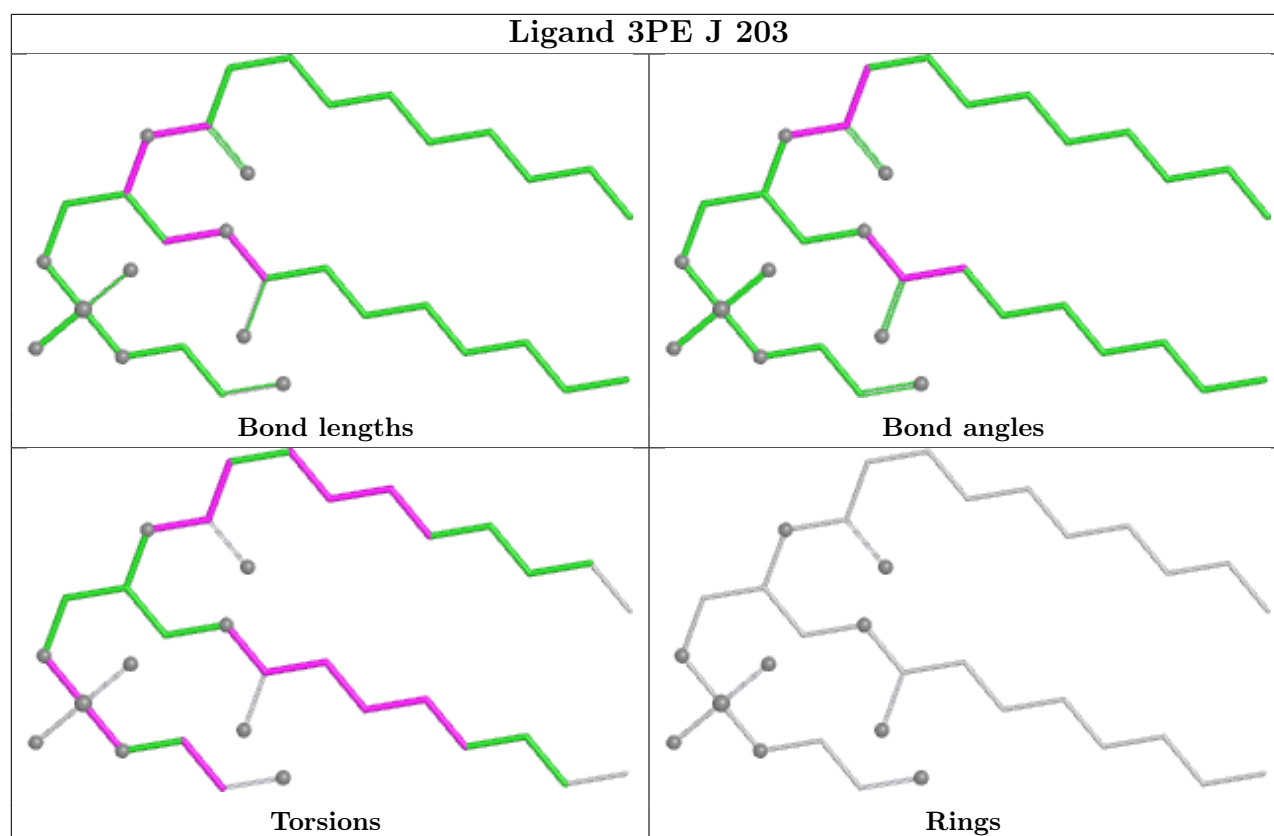


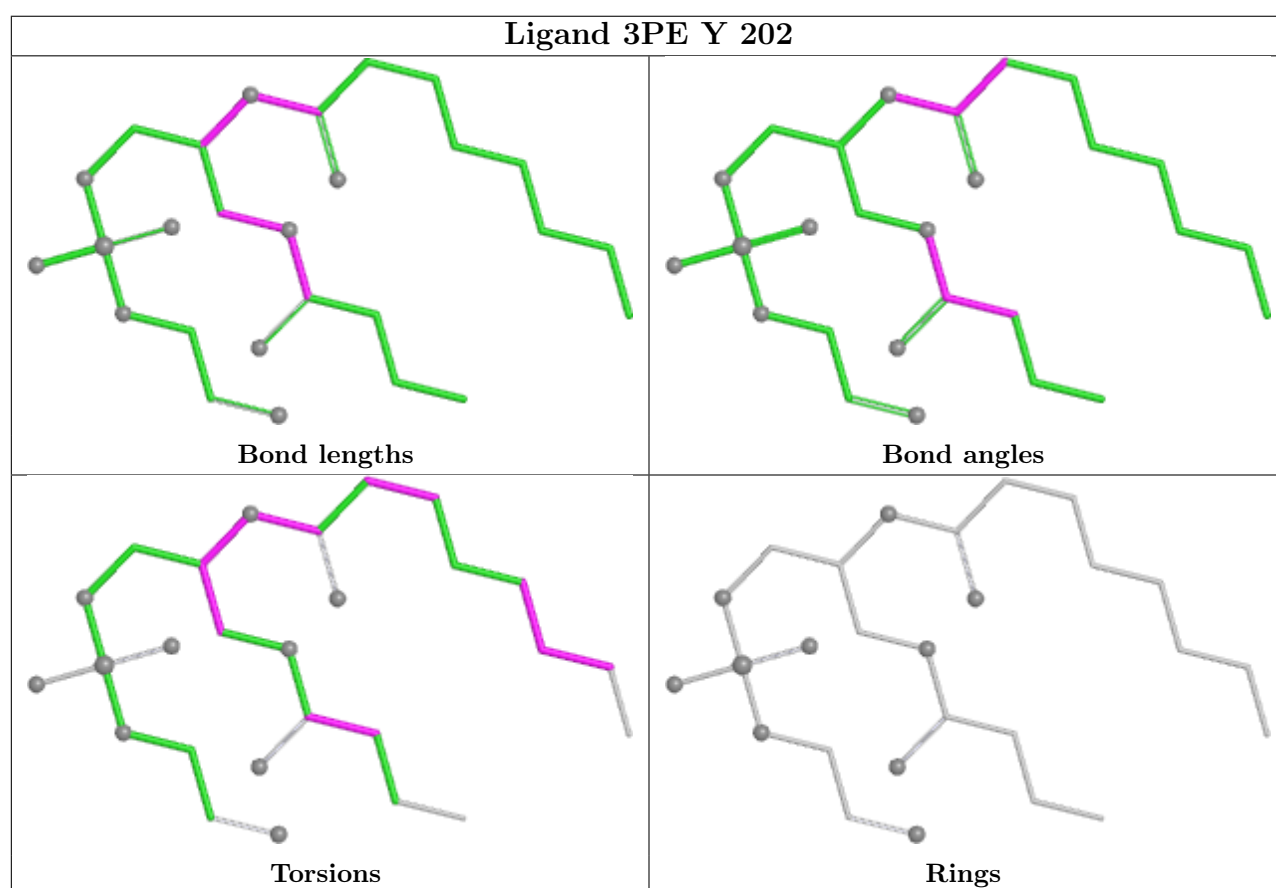
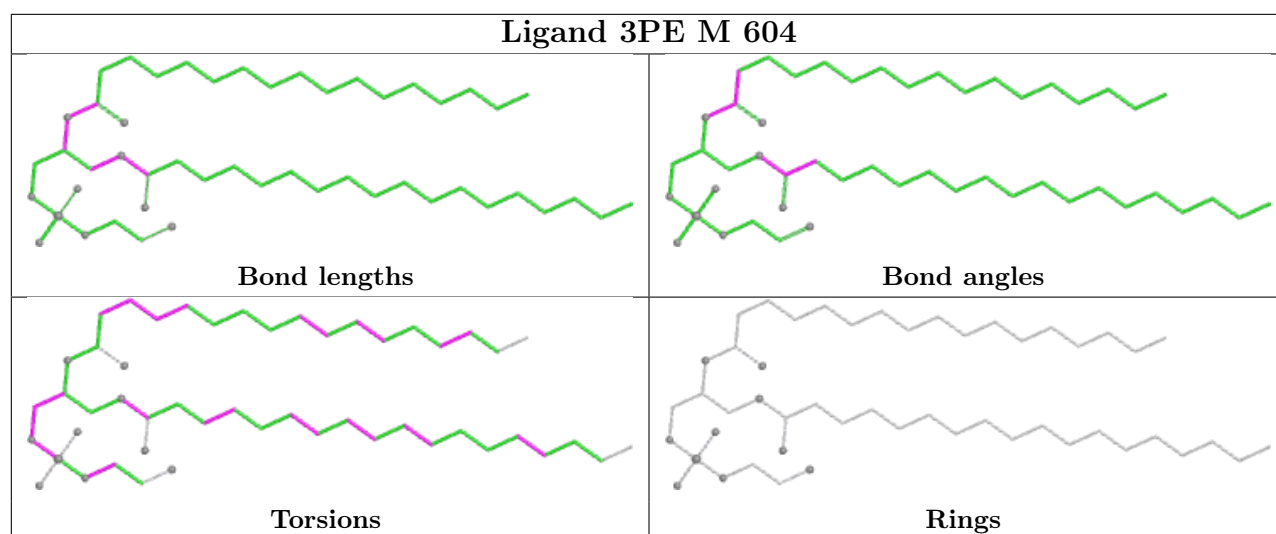


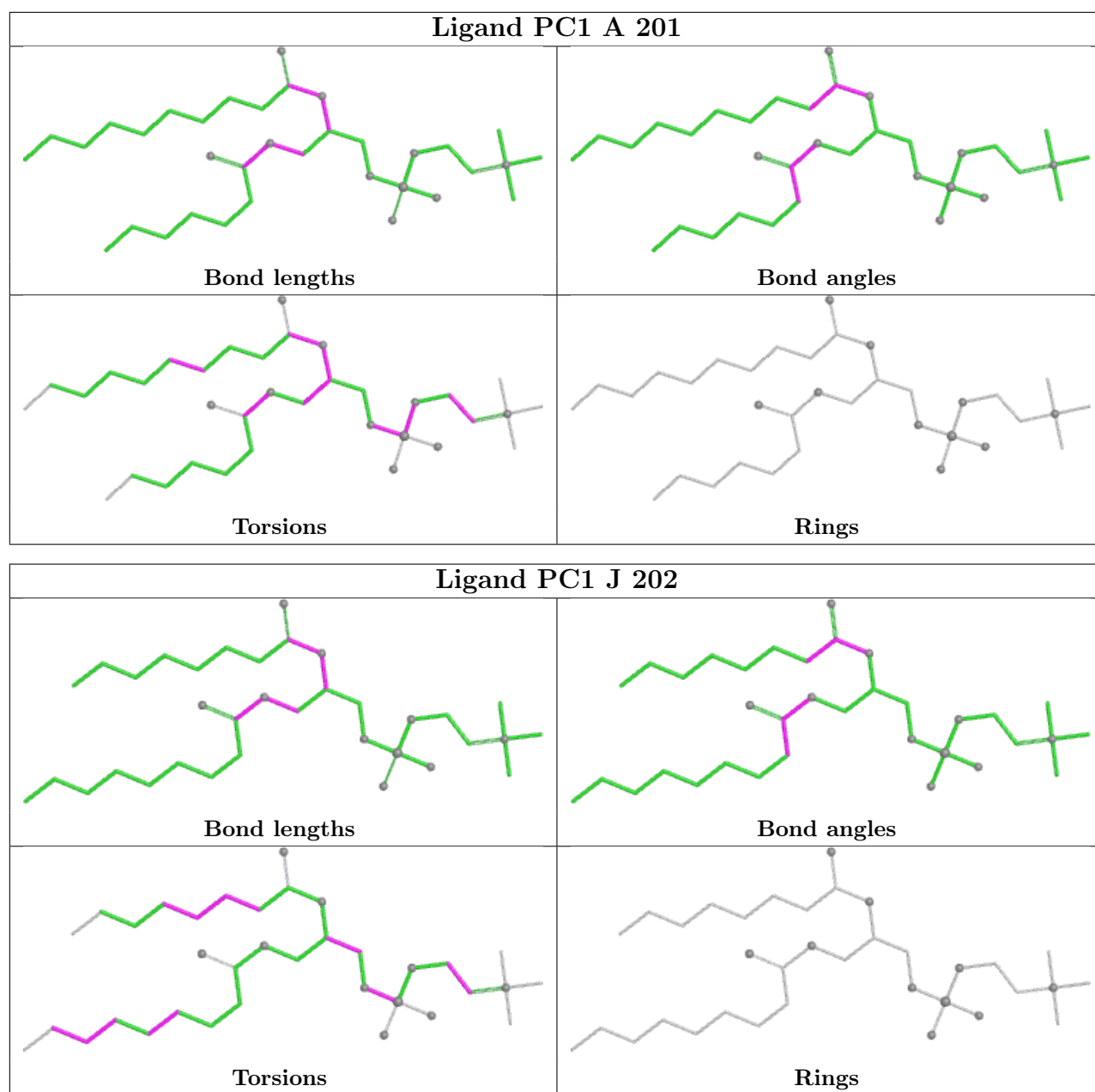


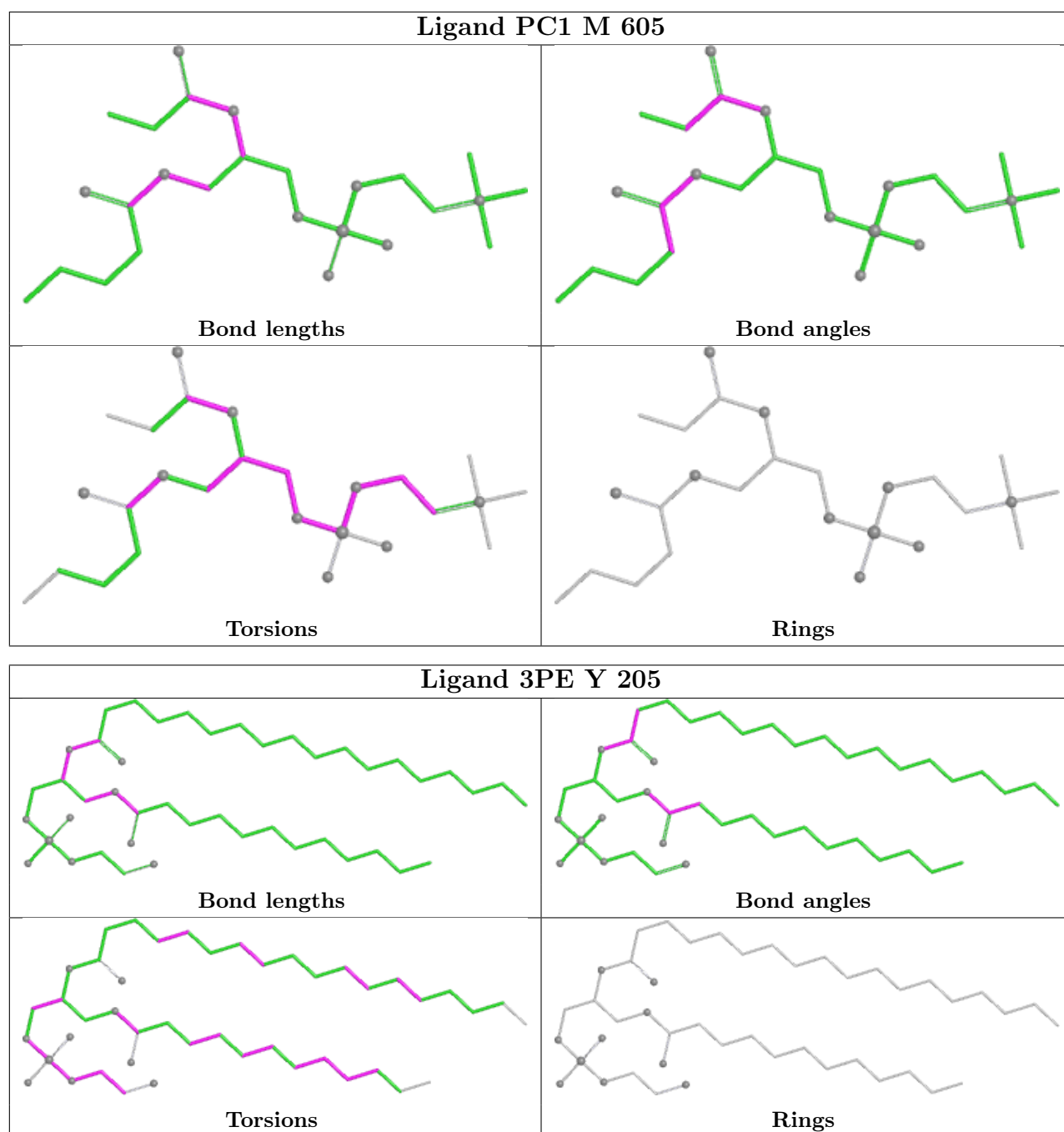


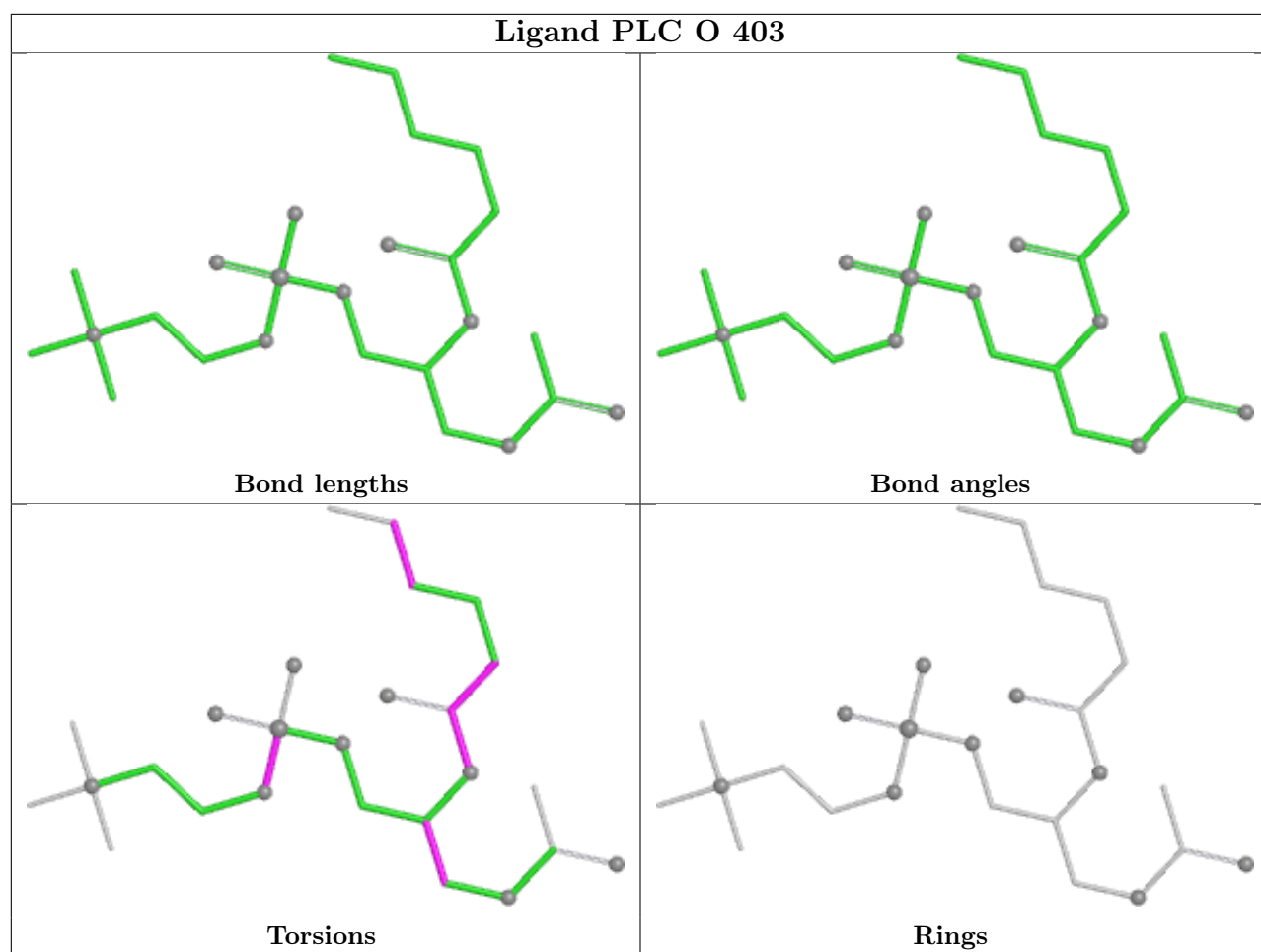


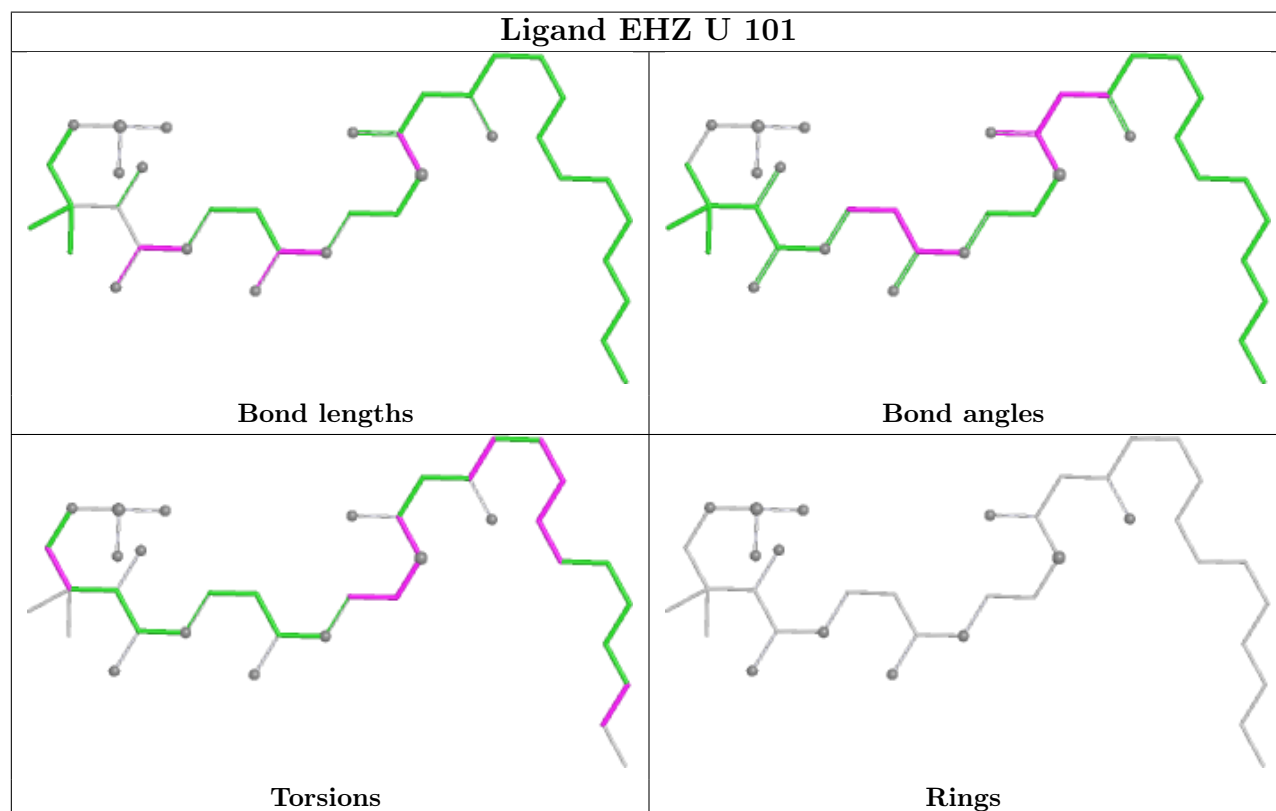
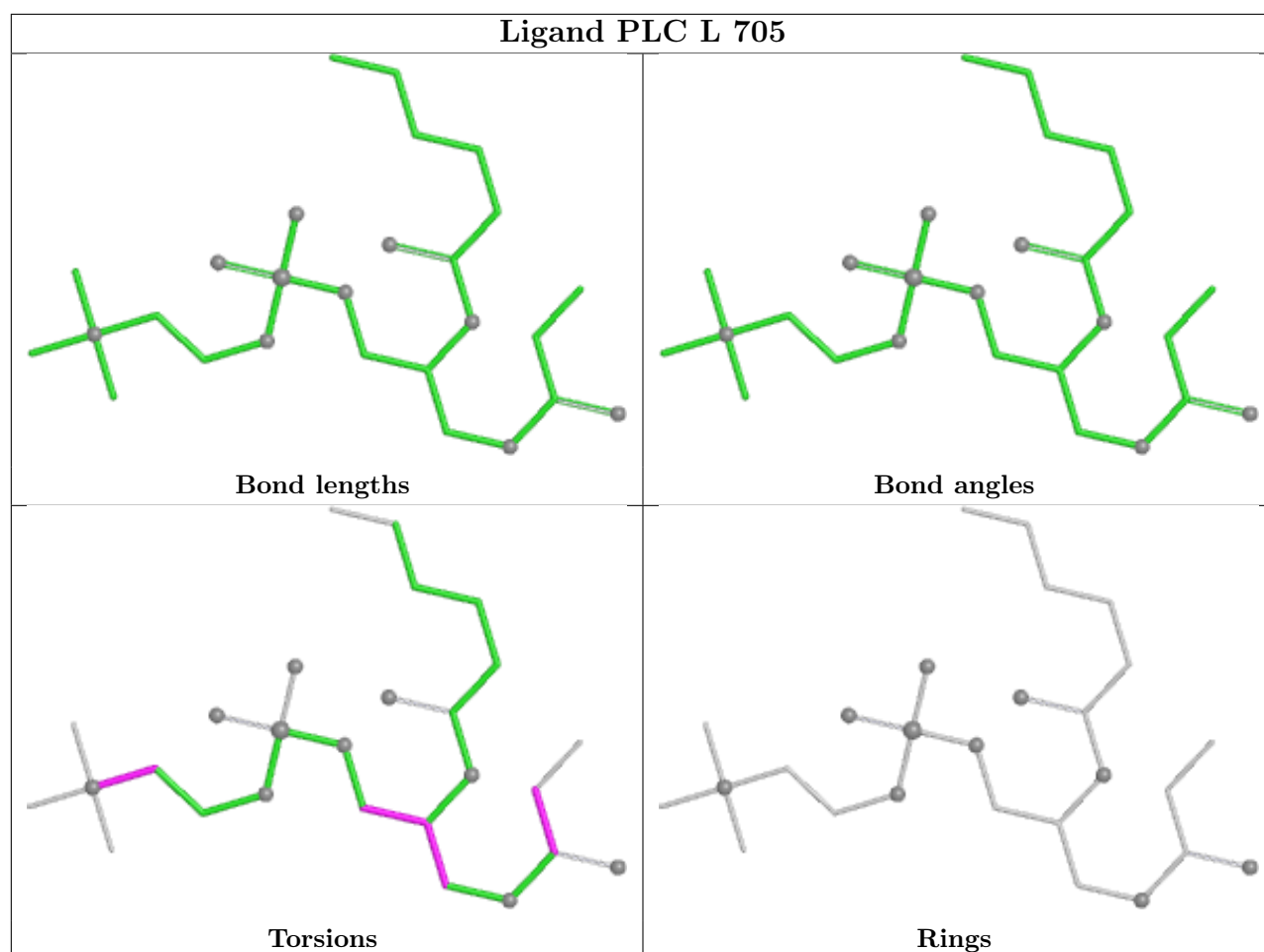


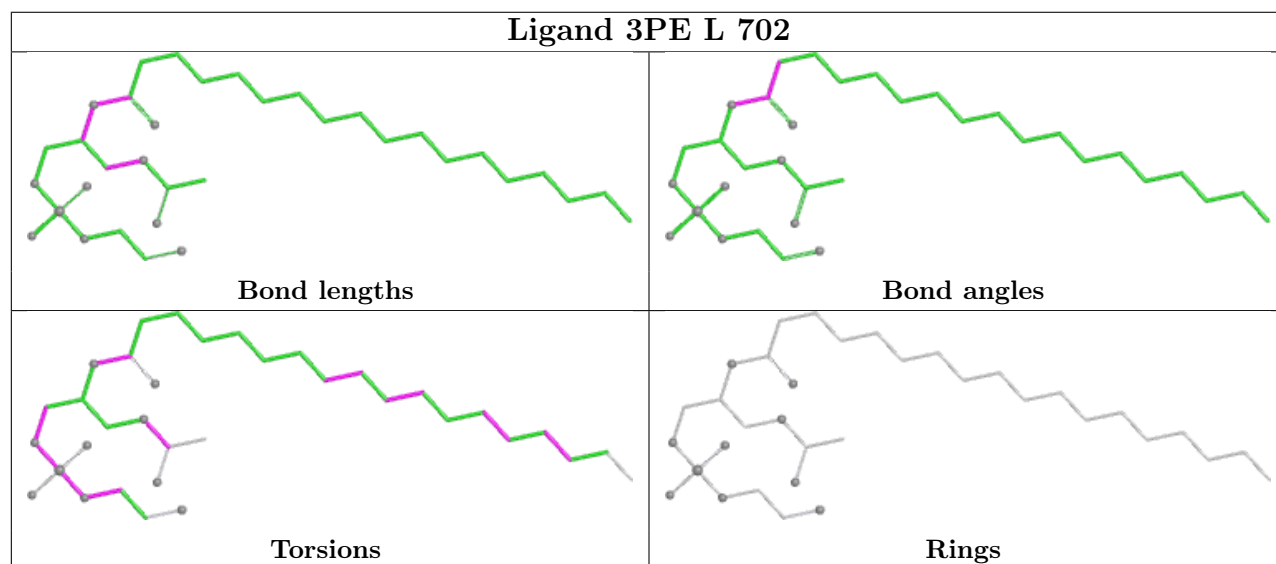
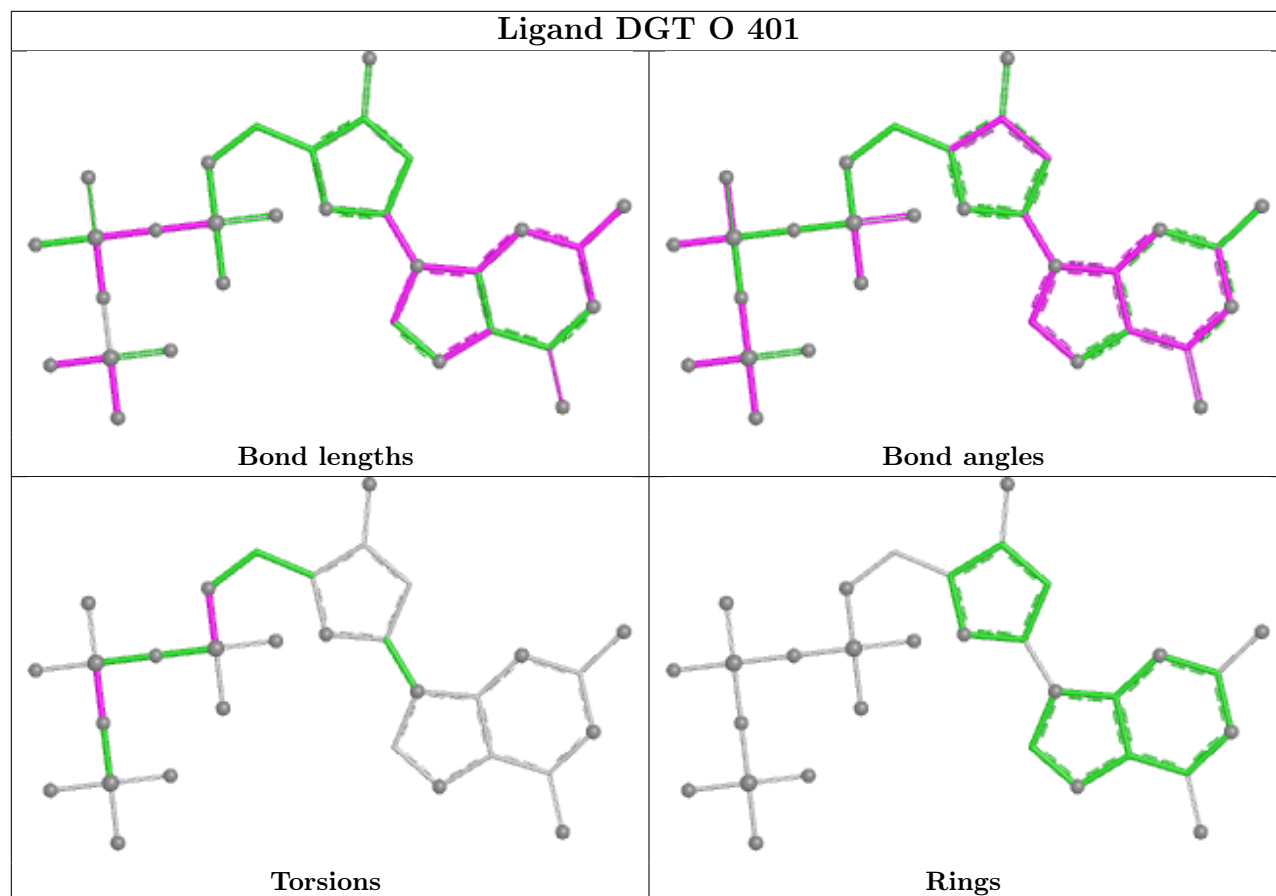


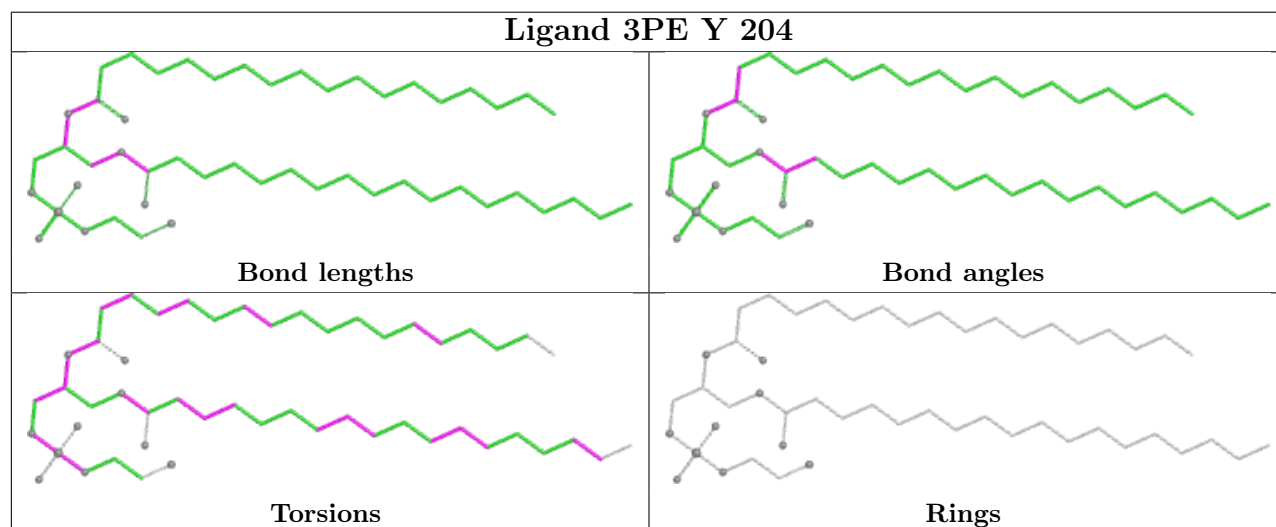
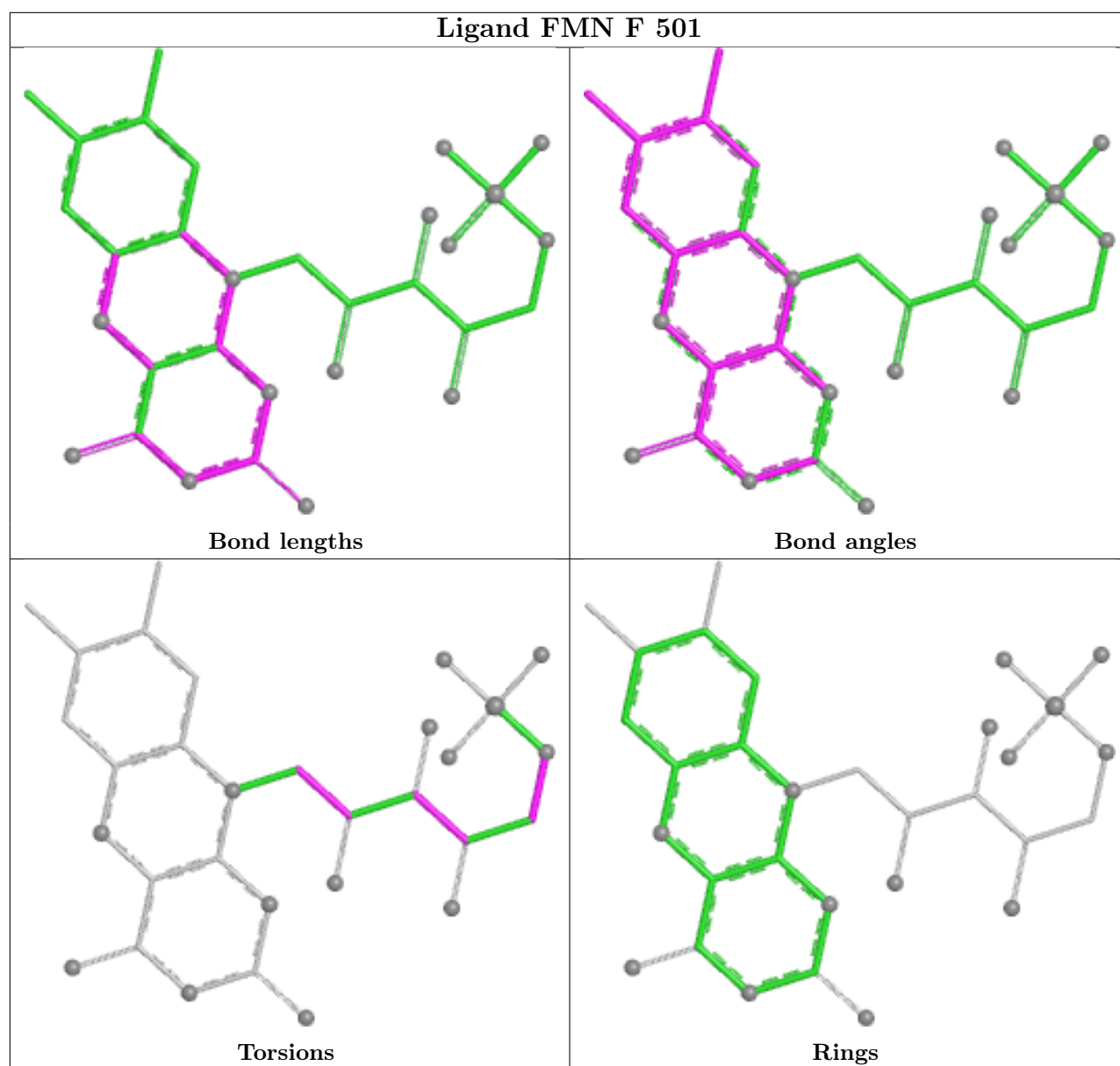


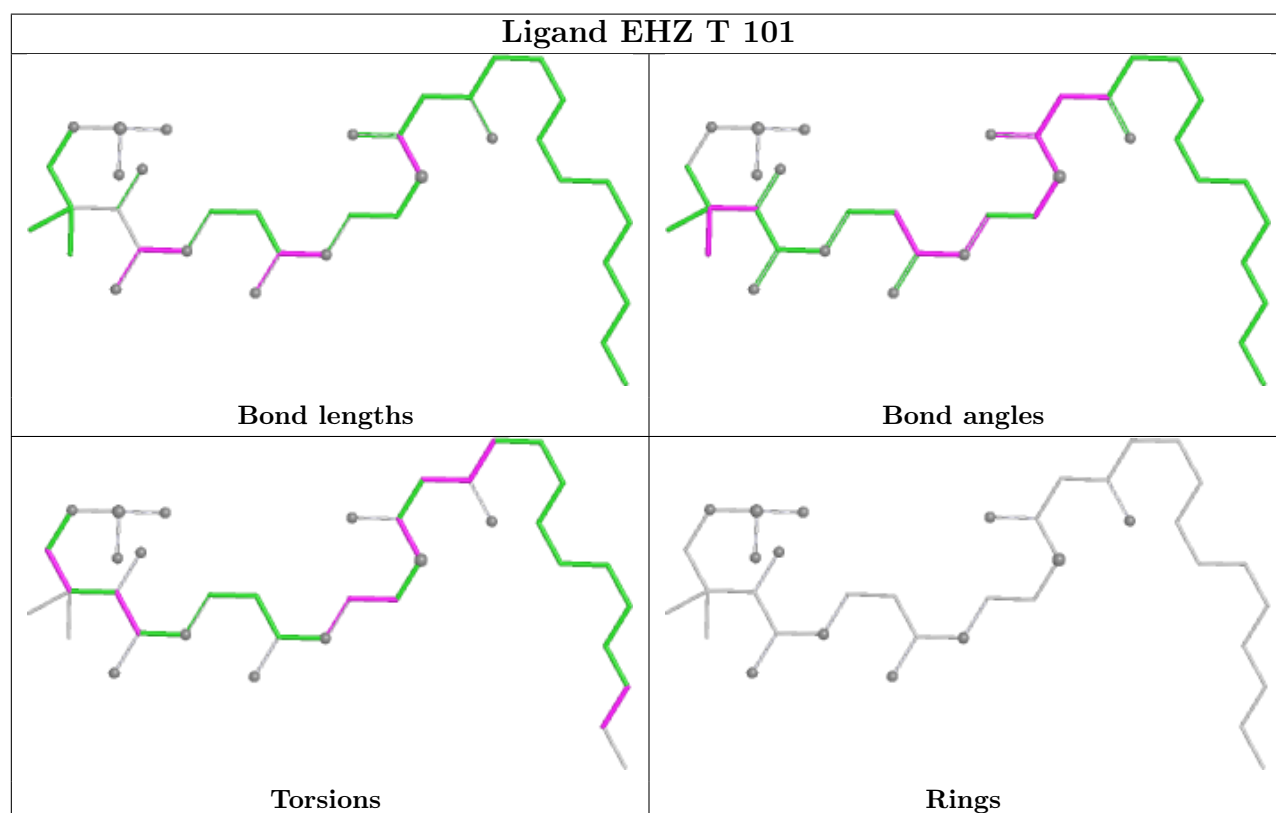
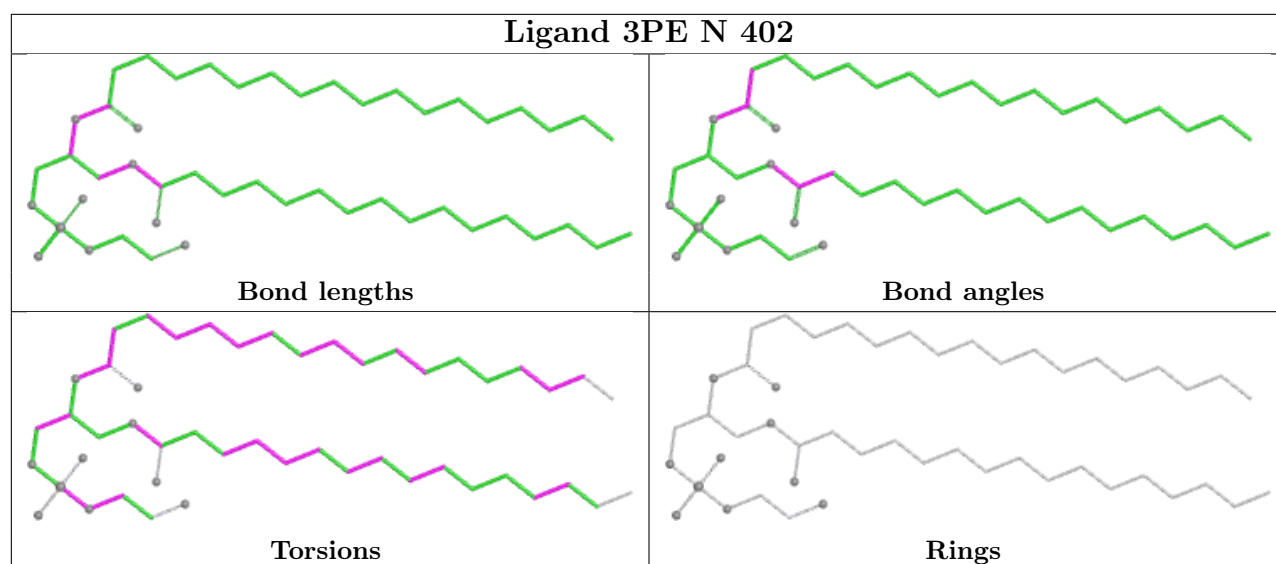


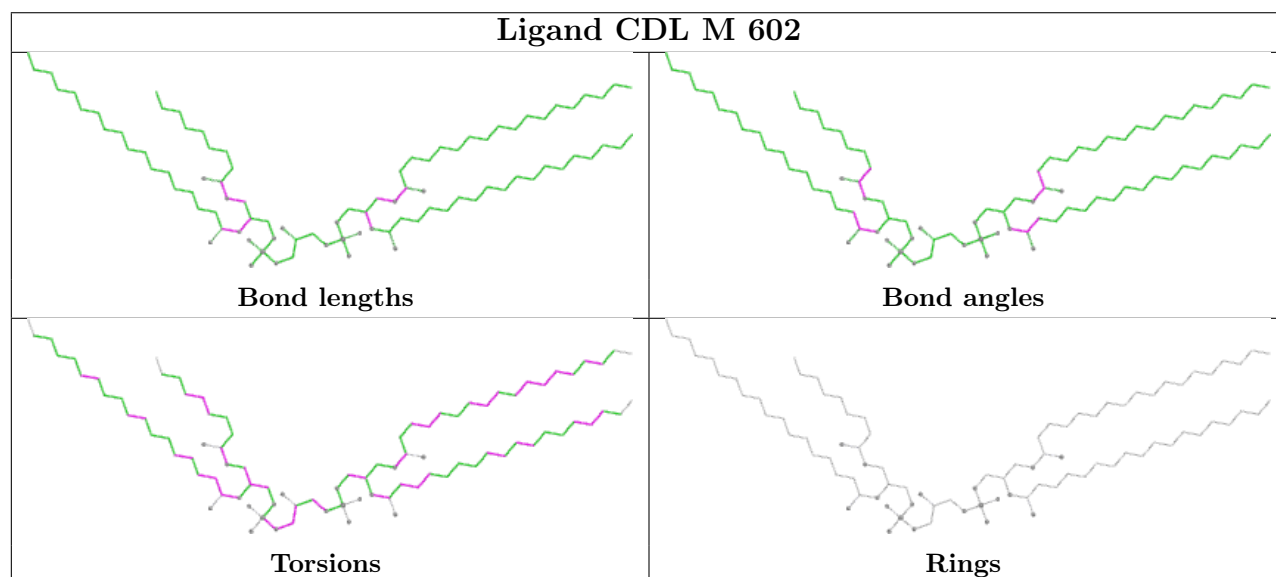
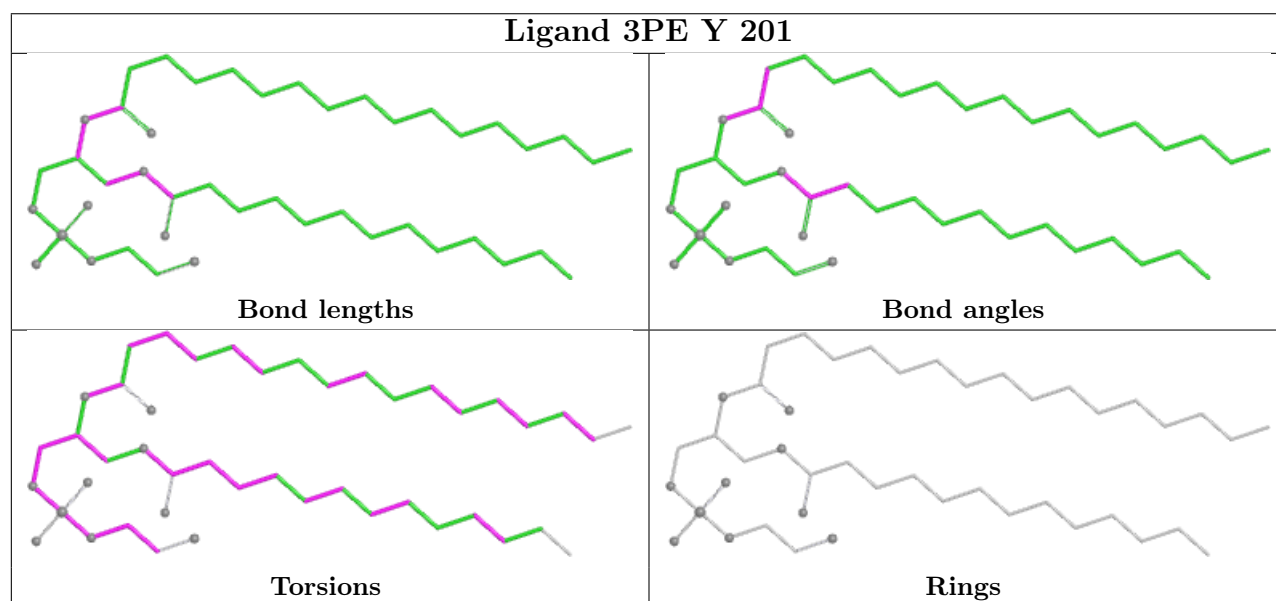
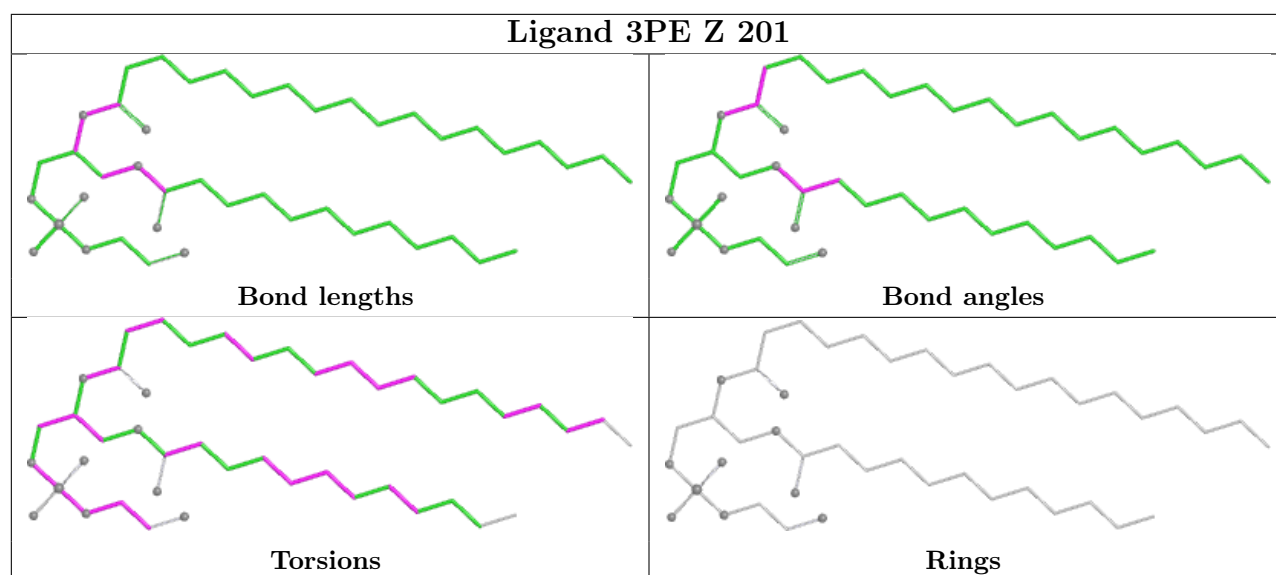


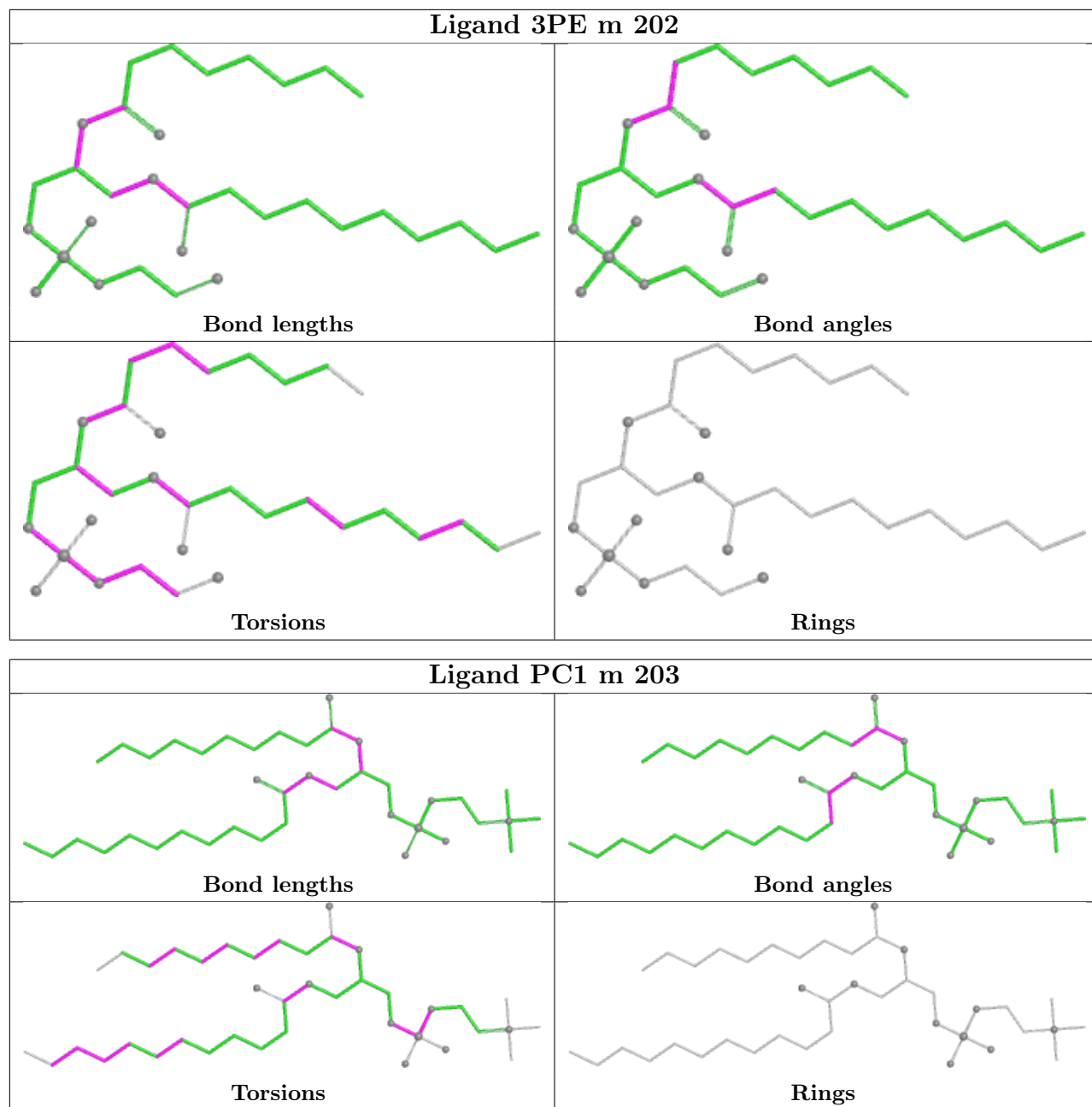


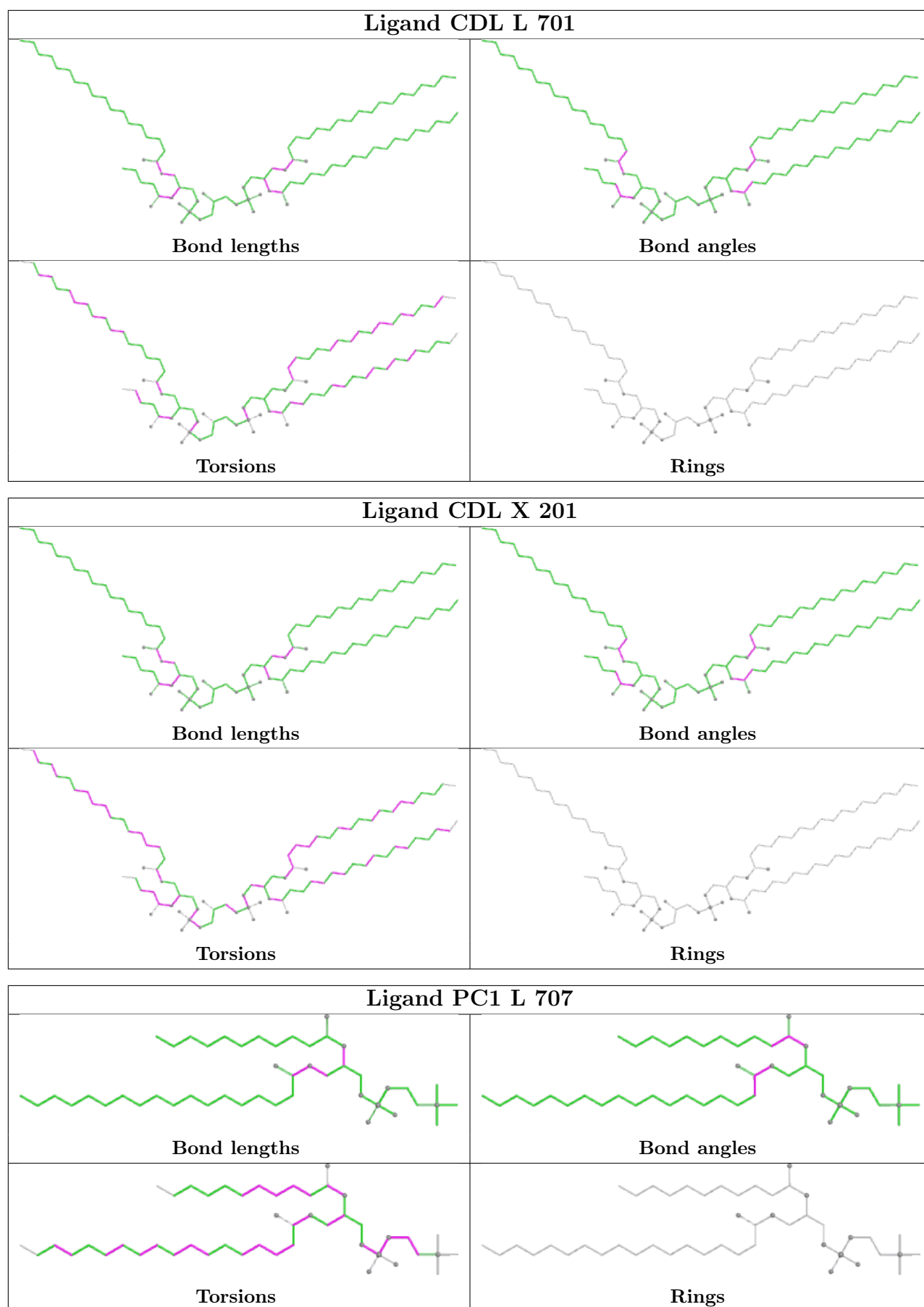


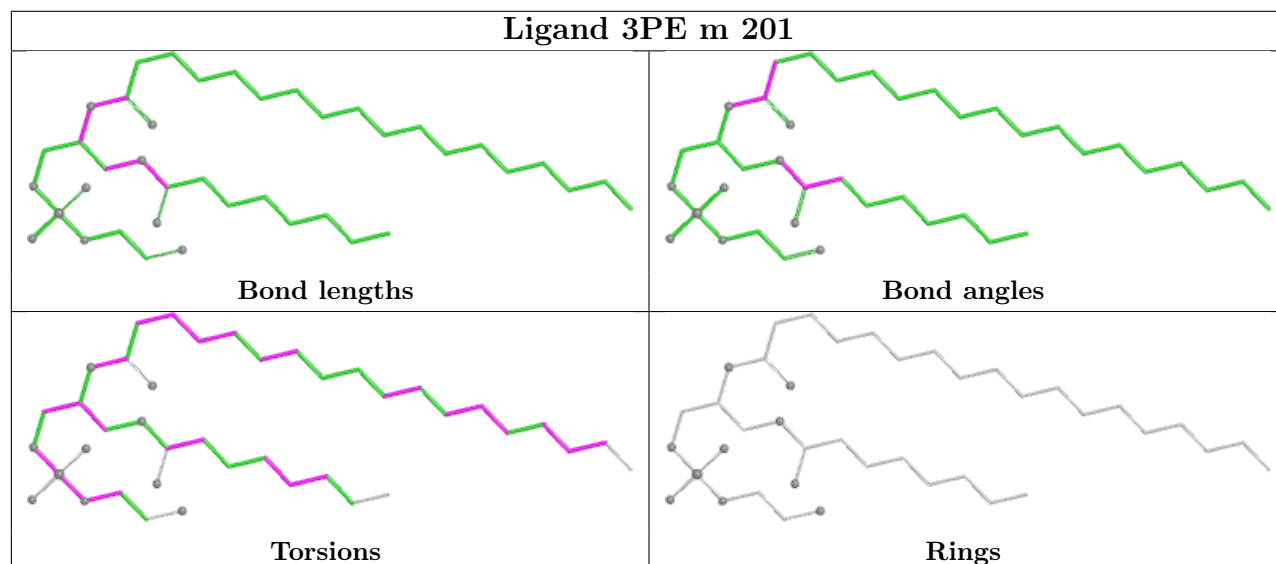
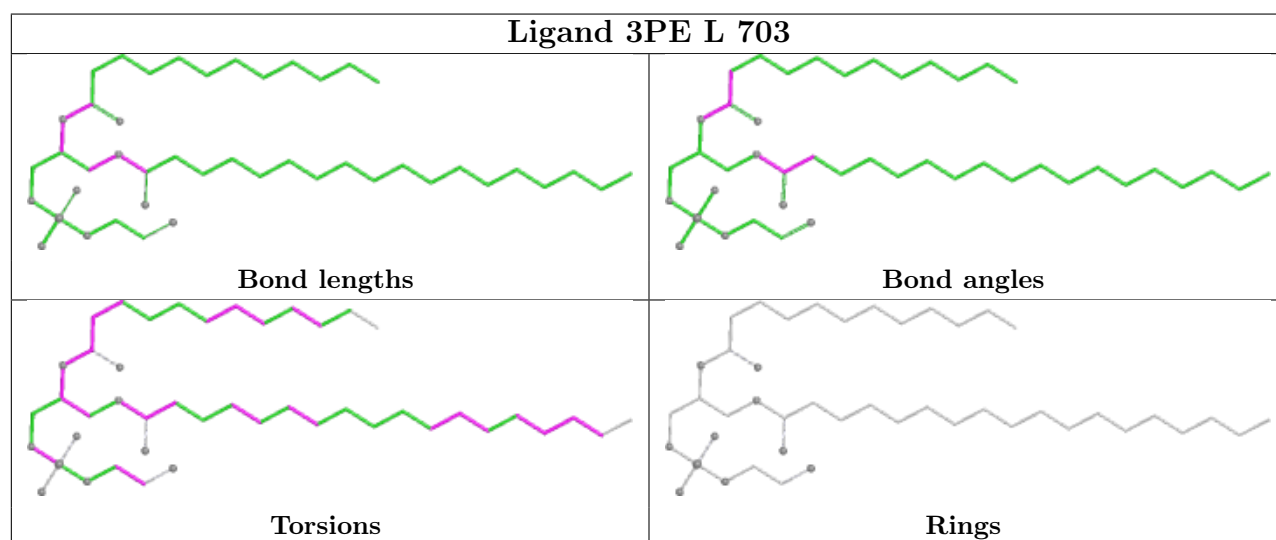
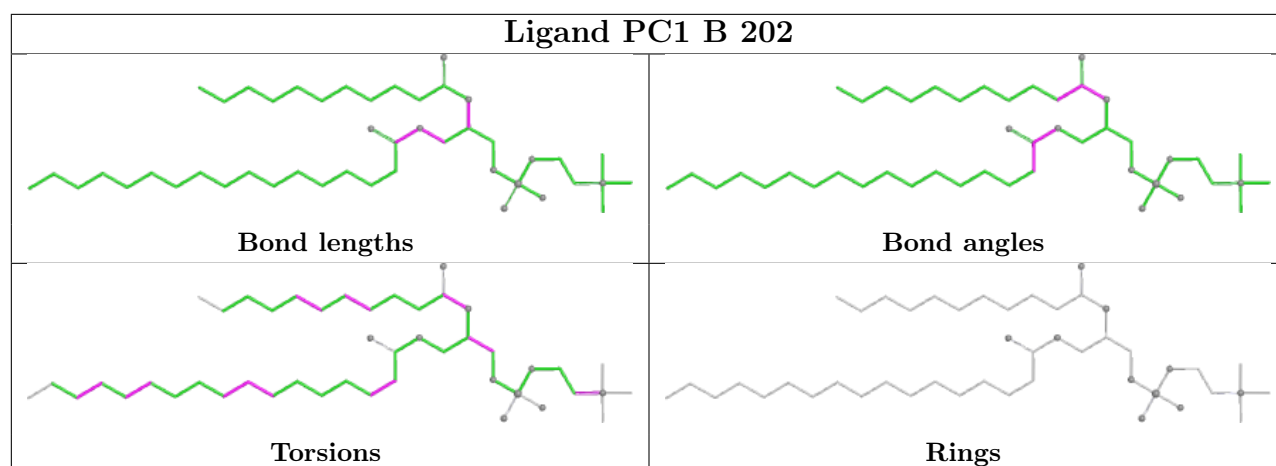


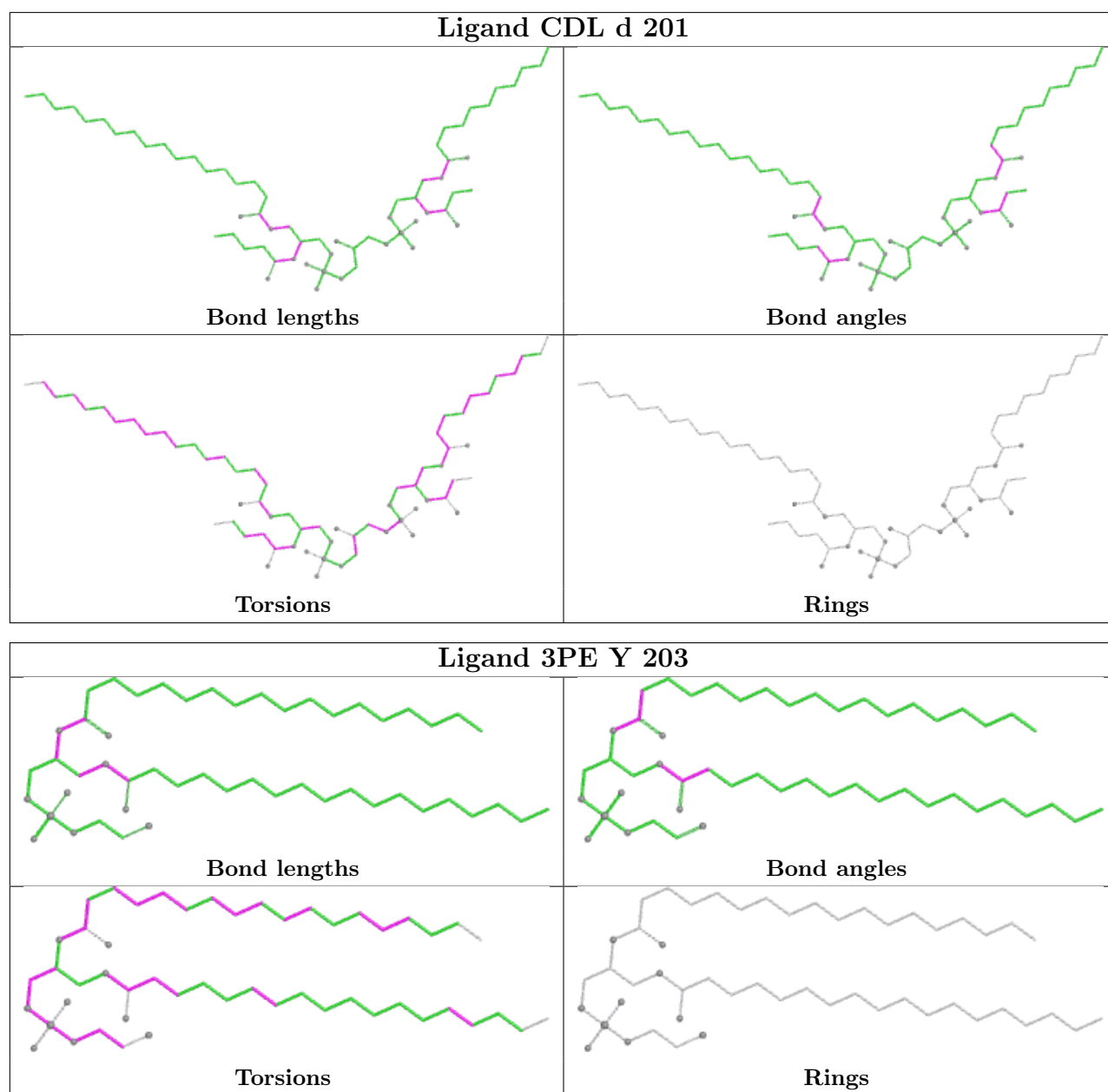




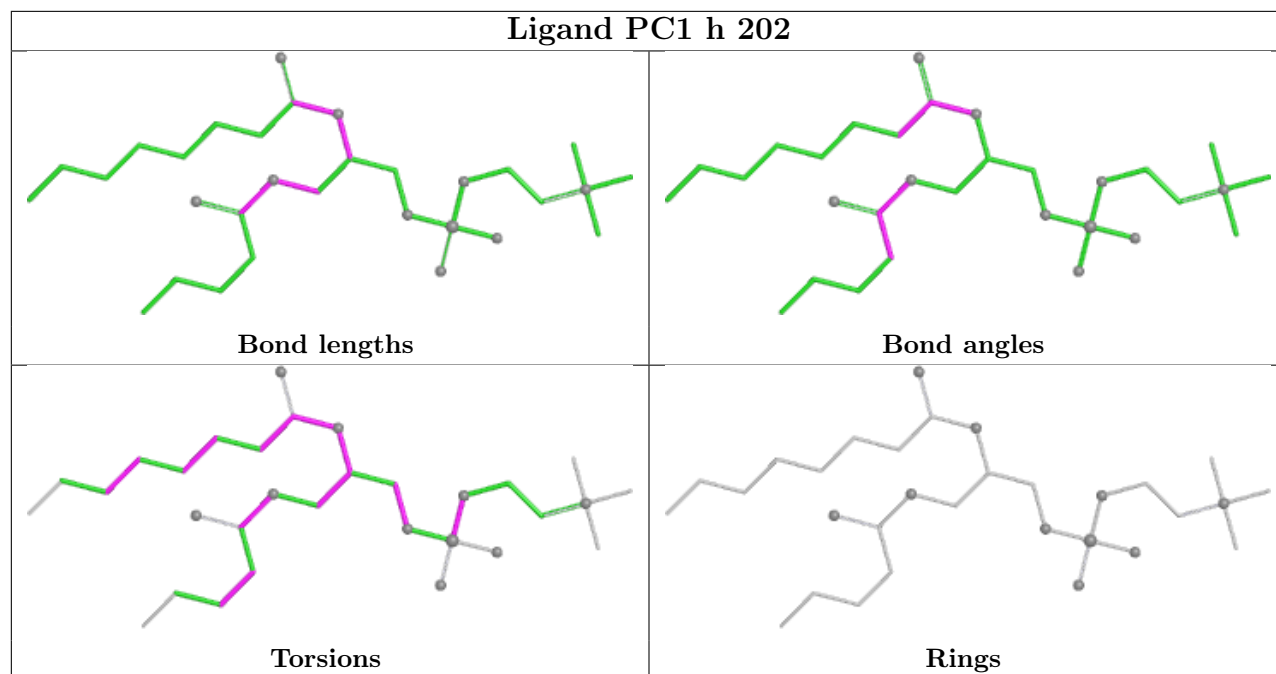




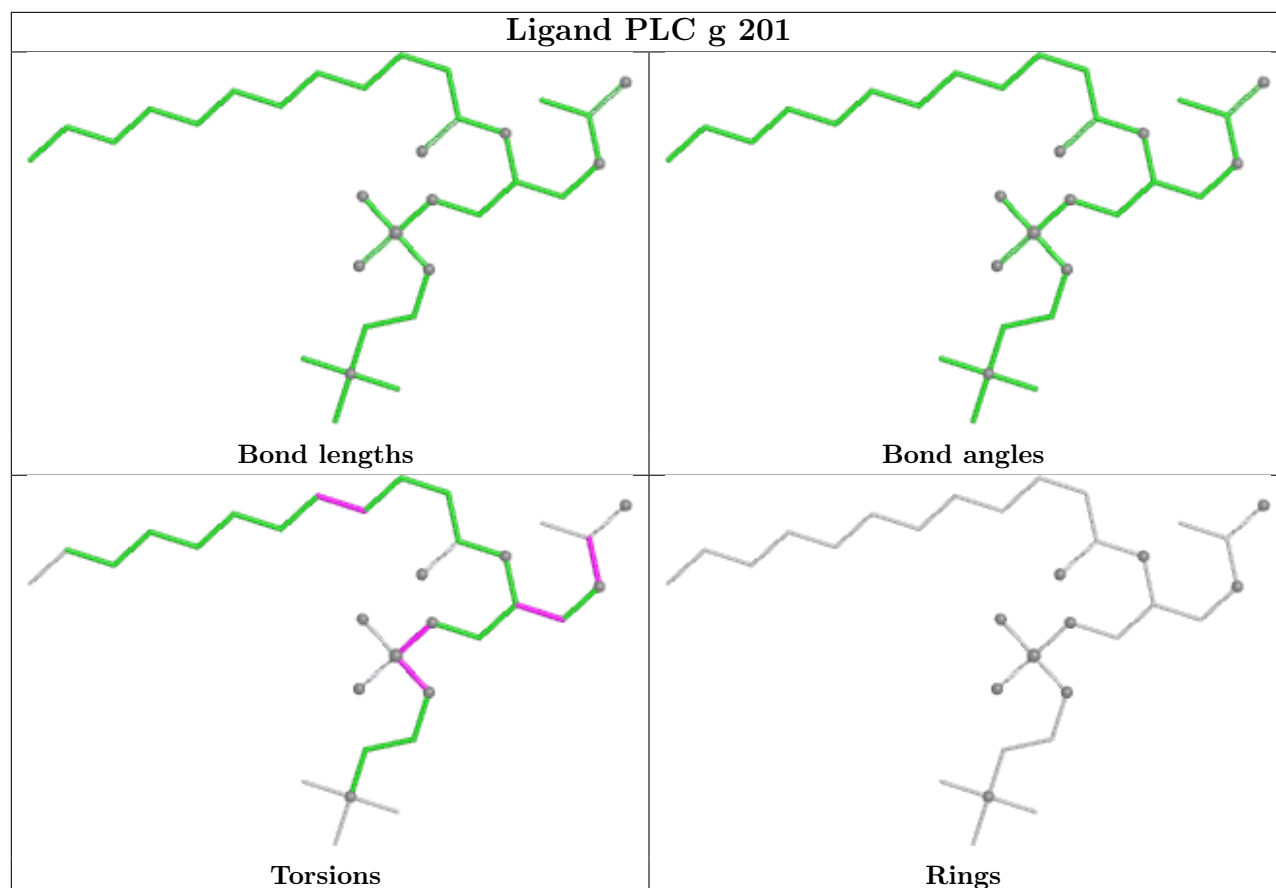


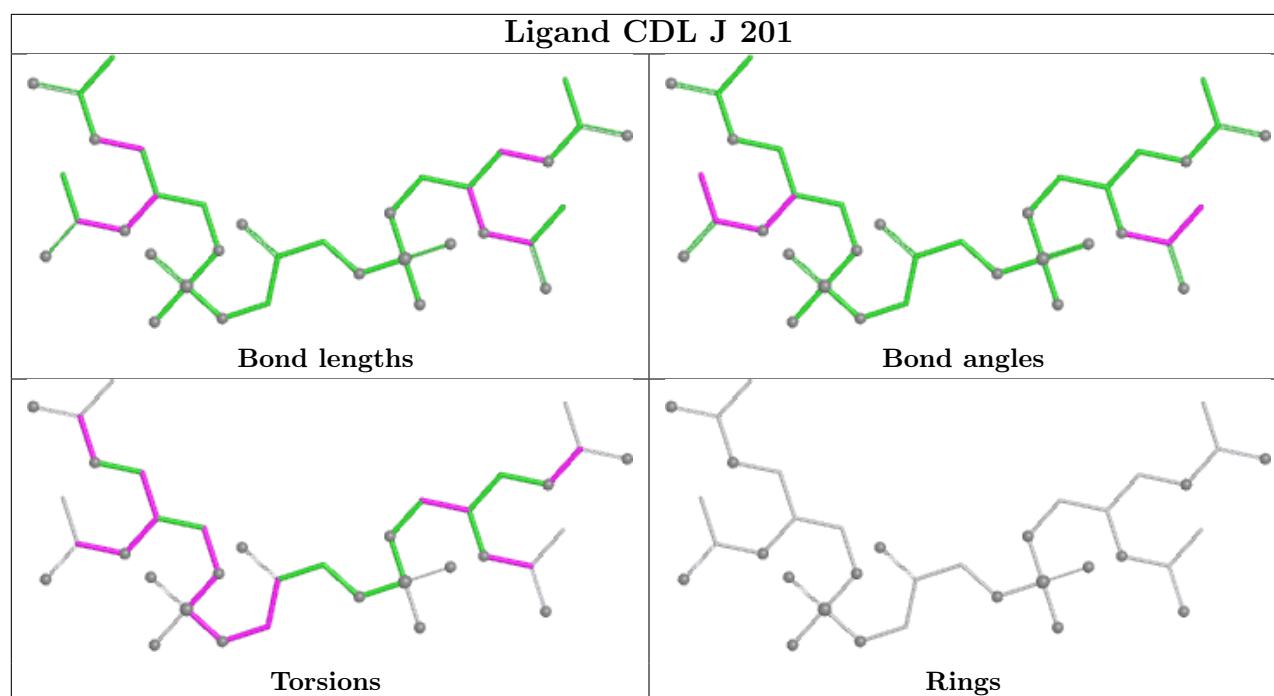


Ligand PC1 h 202



Ligand PLC g 201





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.

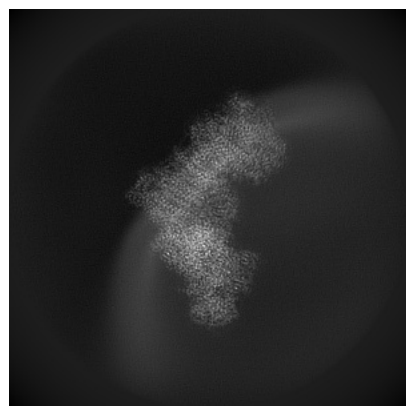
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18140. These allow visual inspection of the internal detail of the map and identification of artifacts.

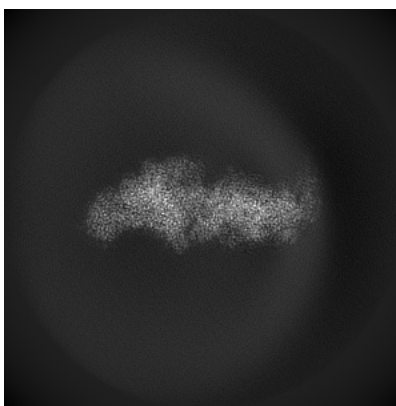
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

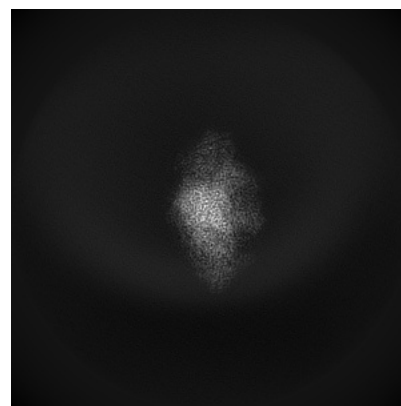
6.1.1 Primary map



X

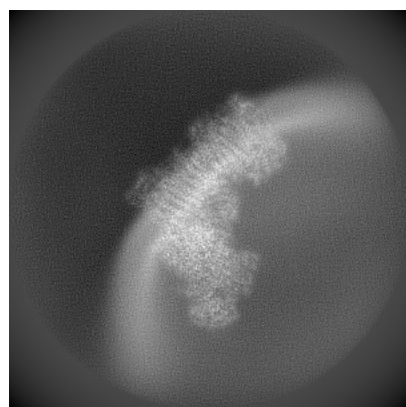


Y

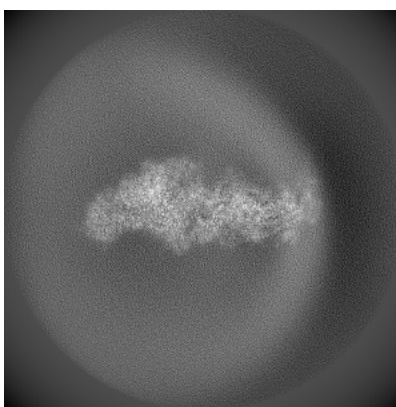


Z

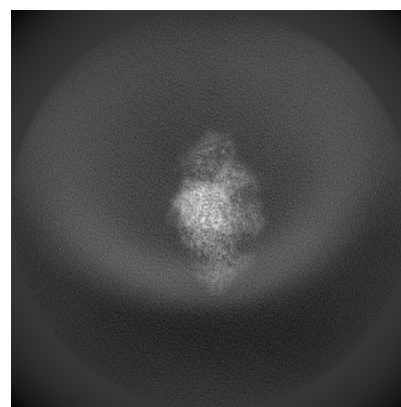
6.1.2 Raw map



X



Y



Z

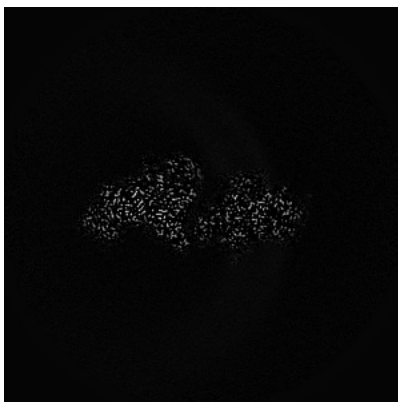
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225

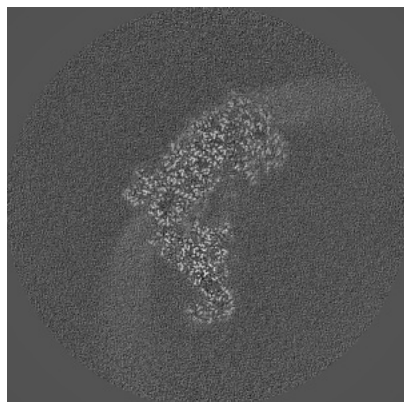


Y Index: 225

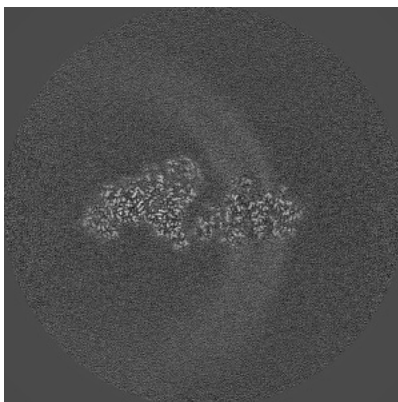


Z Index: 225

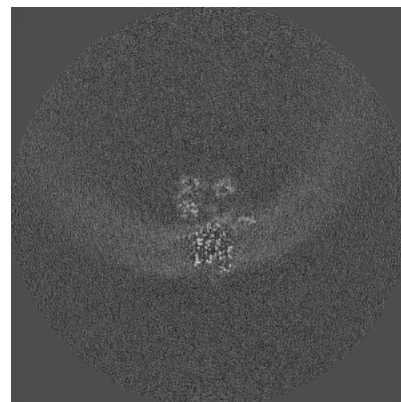
6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

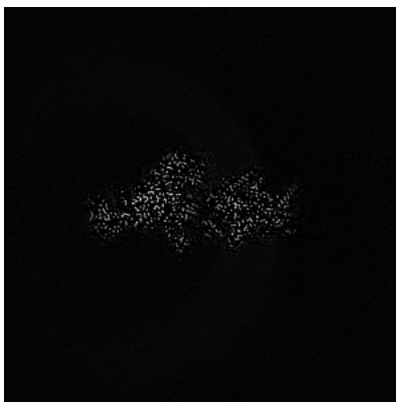
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

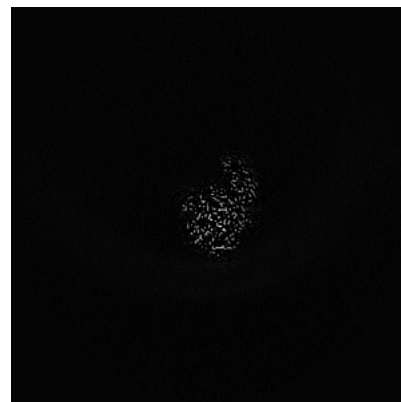
6.3.1 Primary map



X Index: 227

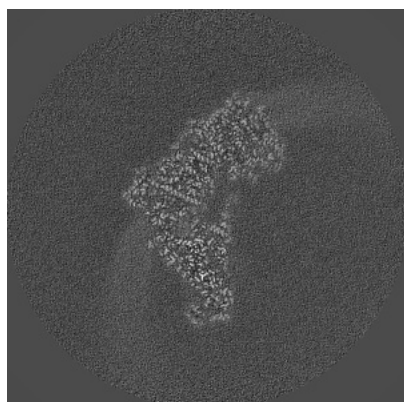


Y Index: 214

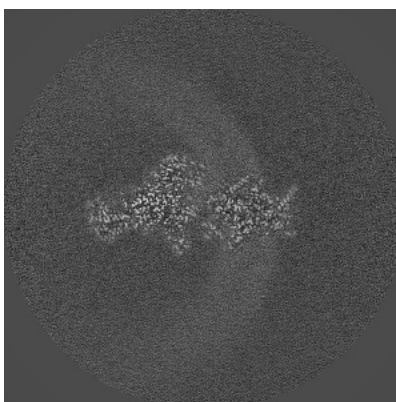


Z Index: 174

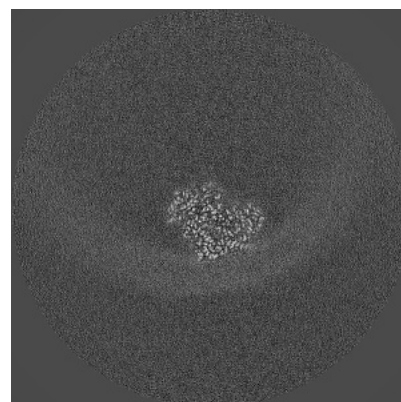
6.3.2 Raw map



X Index: 228



Y Index: 214

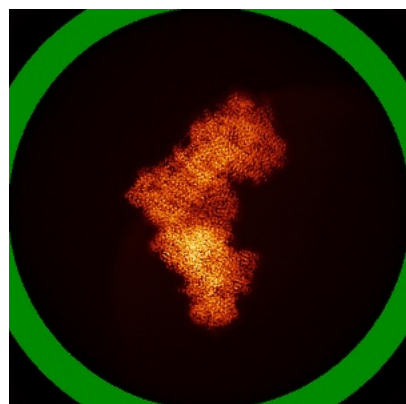


Z Index: 193

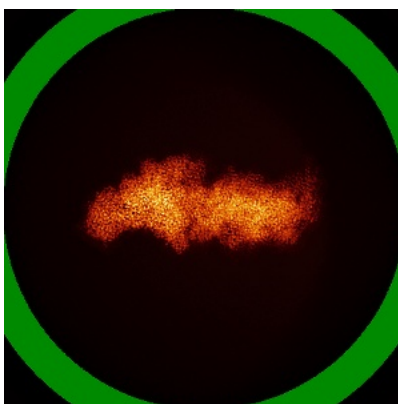
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

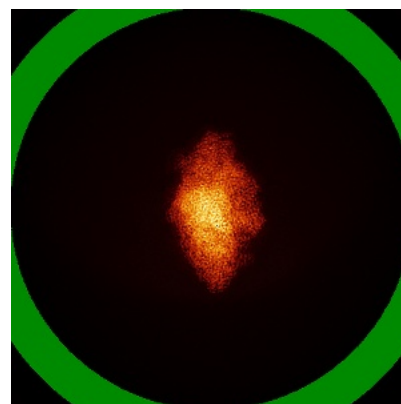
6.4.1 Primary map



X

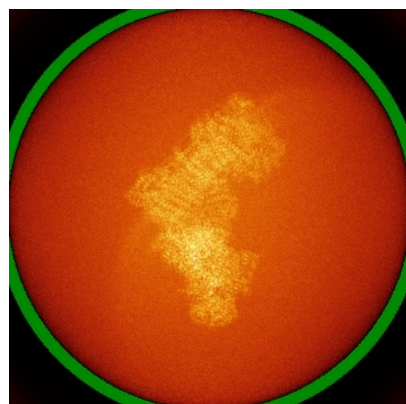


Y

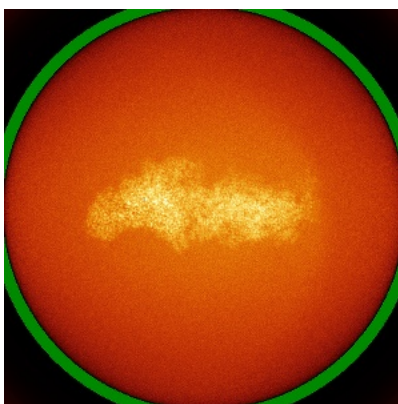


Z

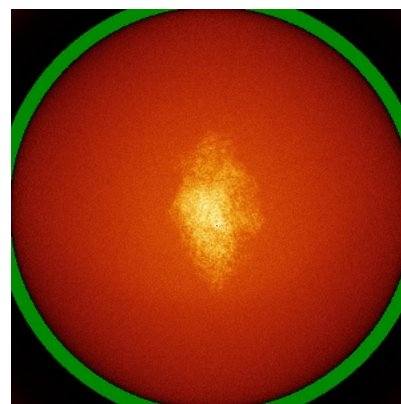
6.4.2 Raw map



X



Y

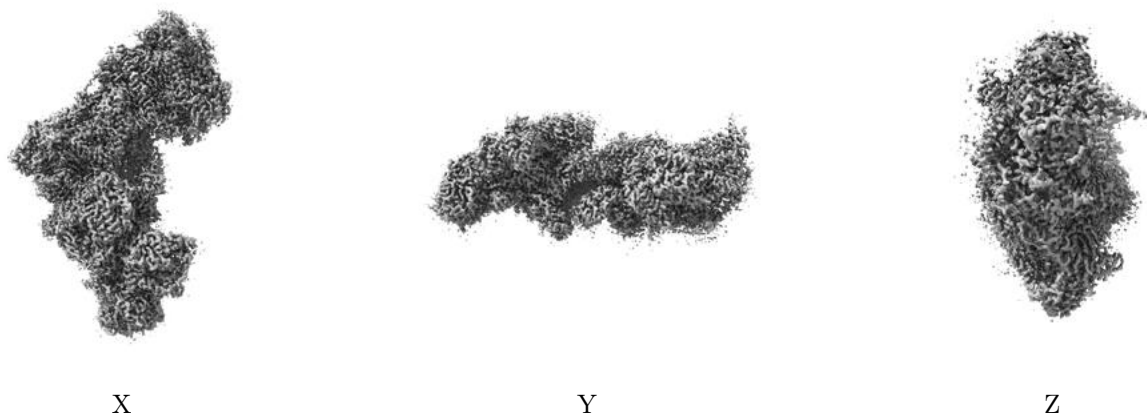


Z

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

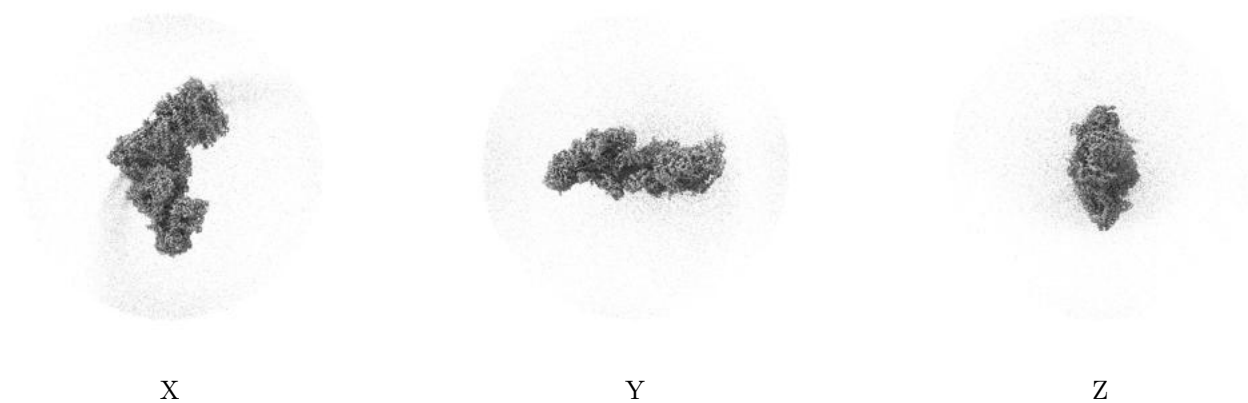
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

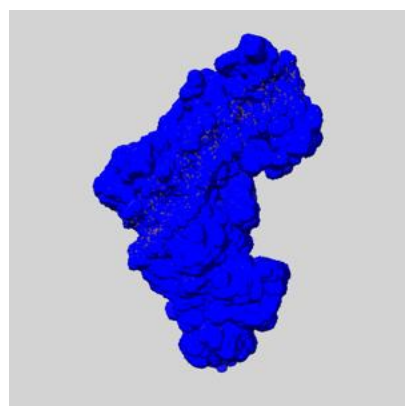
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

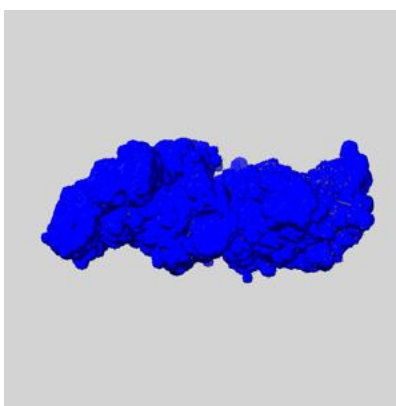
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

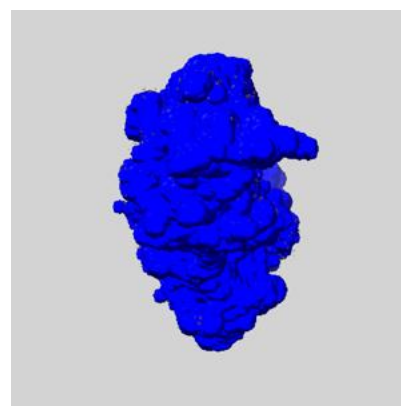
6.6.1 emd_18140_msk_1.map [i](#)



X



Y

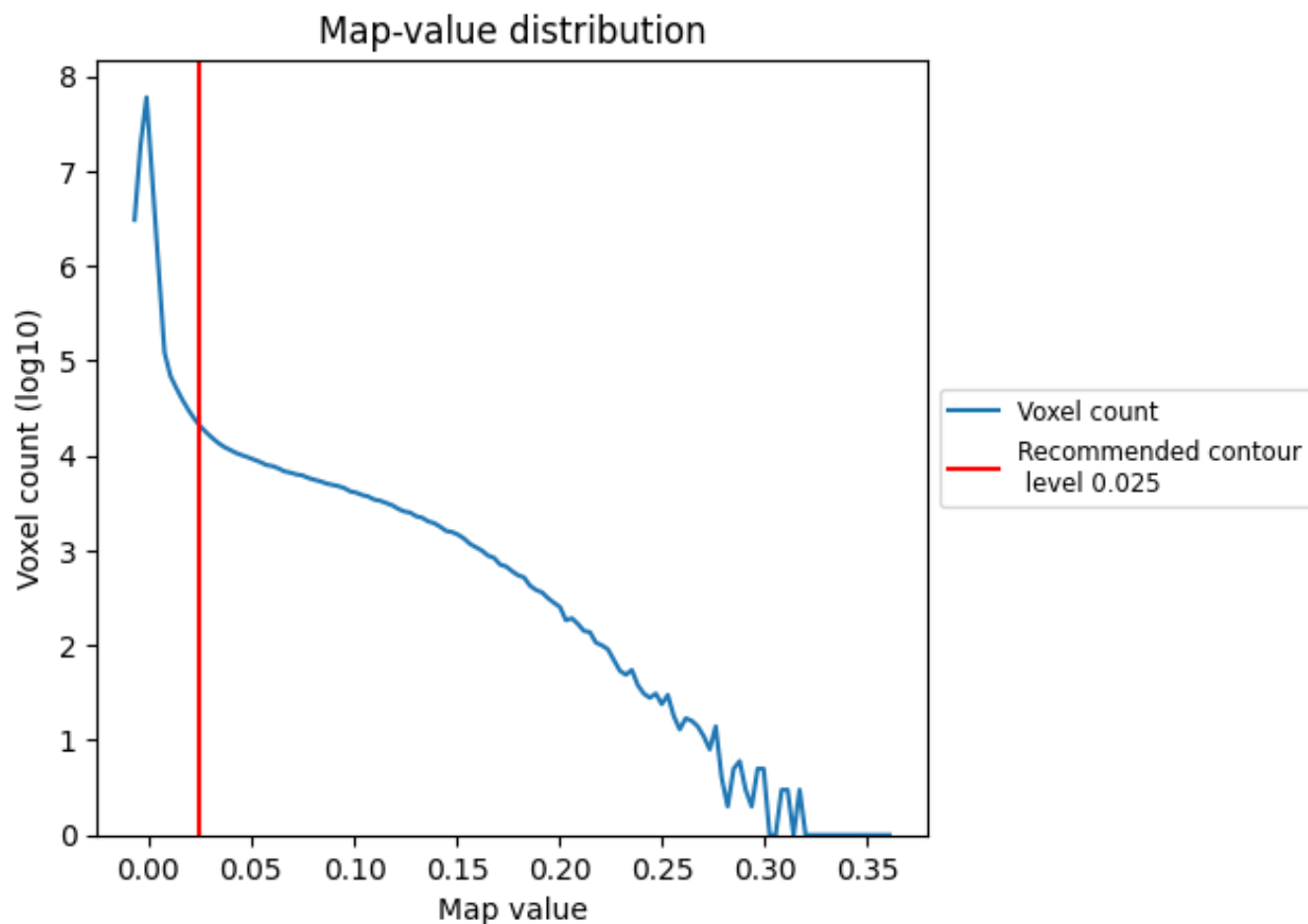


Z

7 Map analysis [i](#)

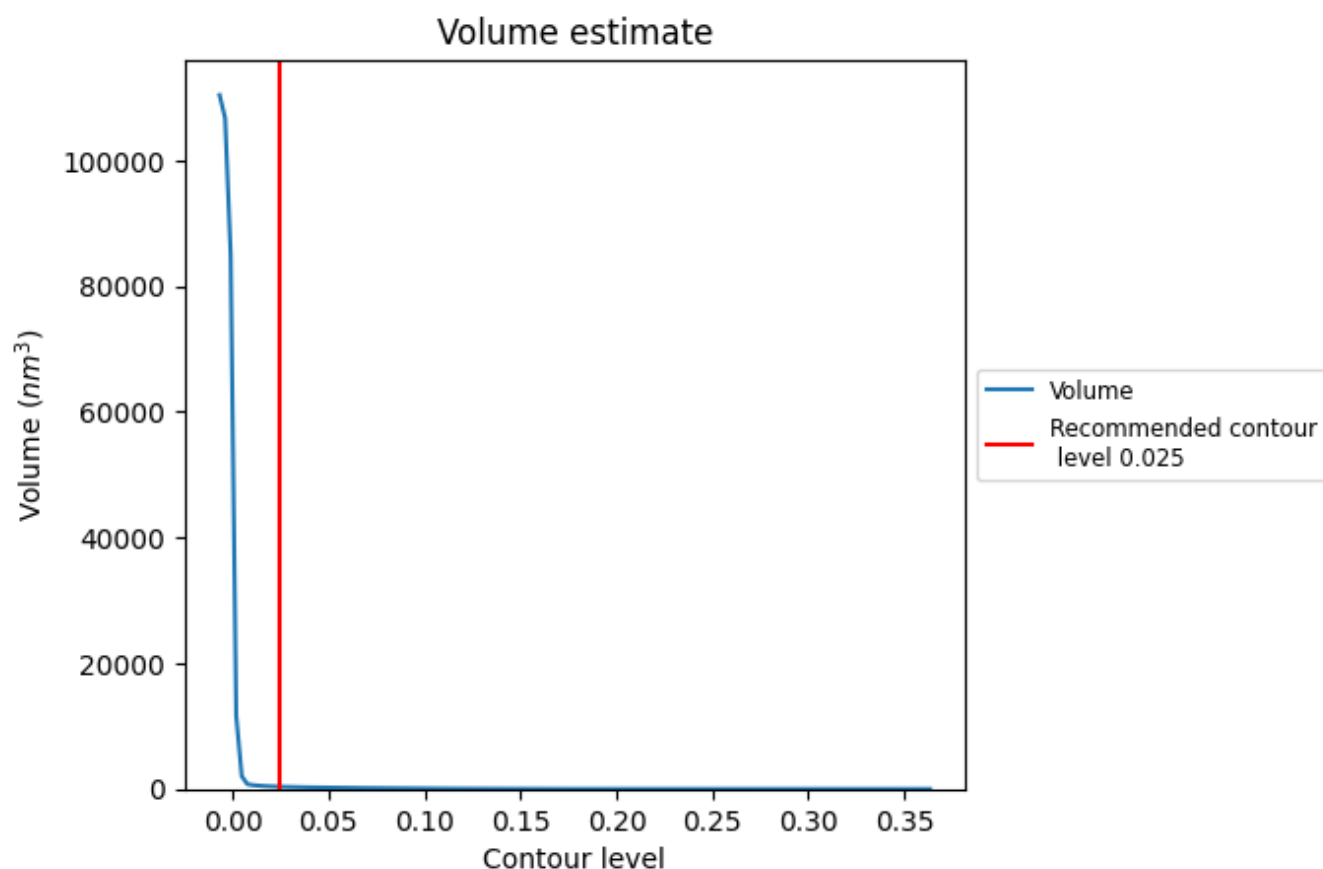
This section contains the results of statistical analysis of the map.

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.

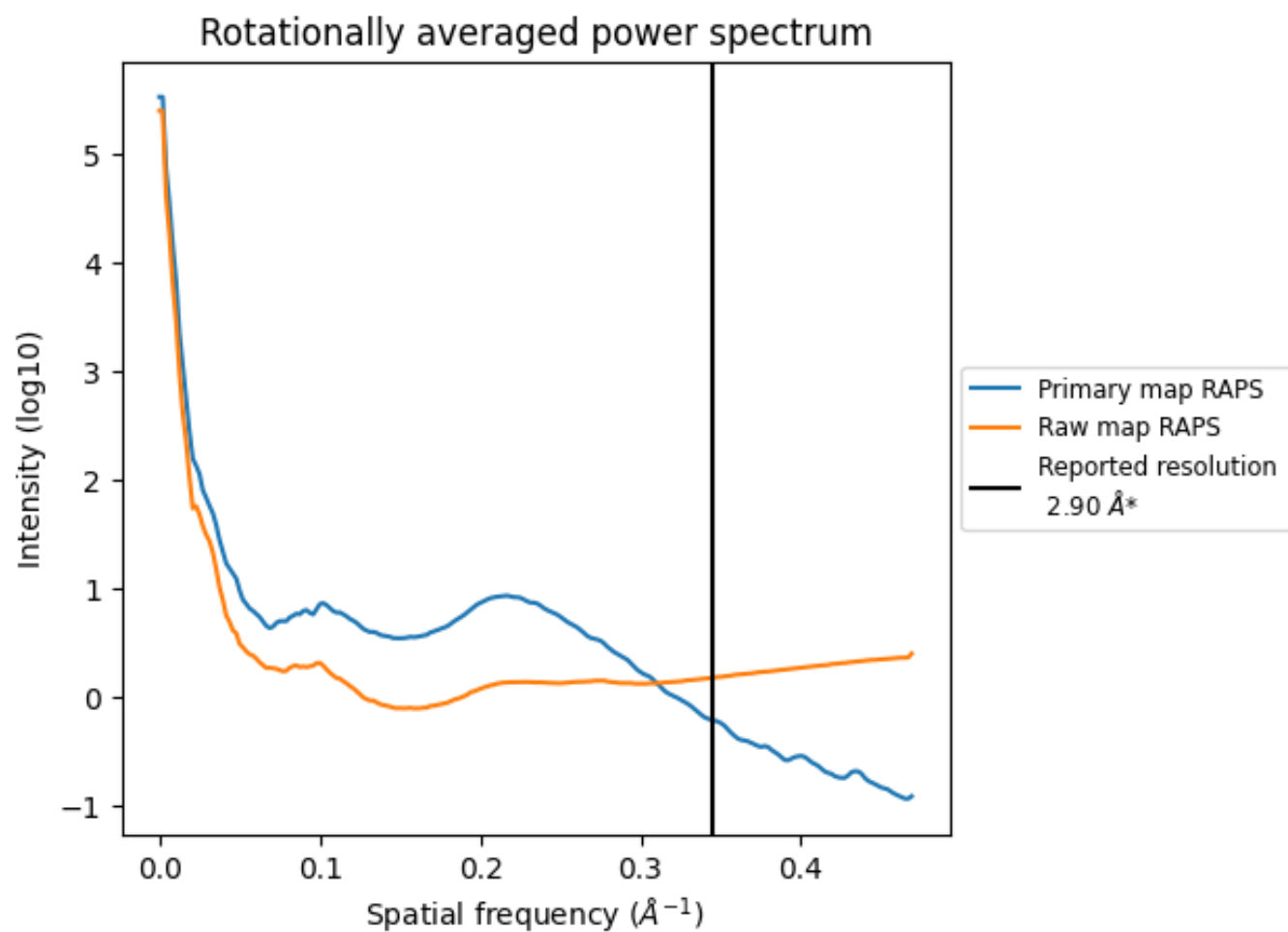
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm^3 ; this corresponds to an approximate mass of 318 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 ⓘ

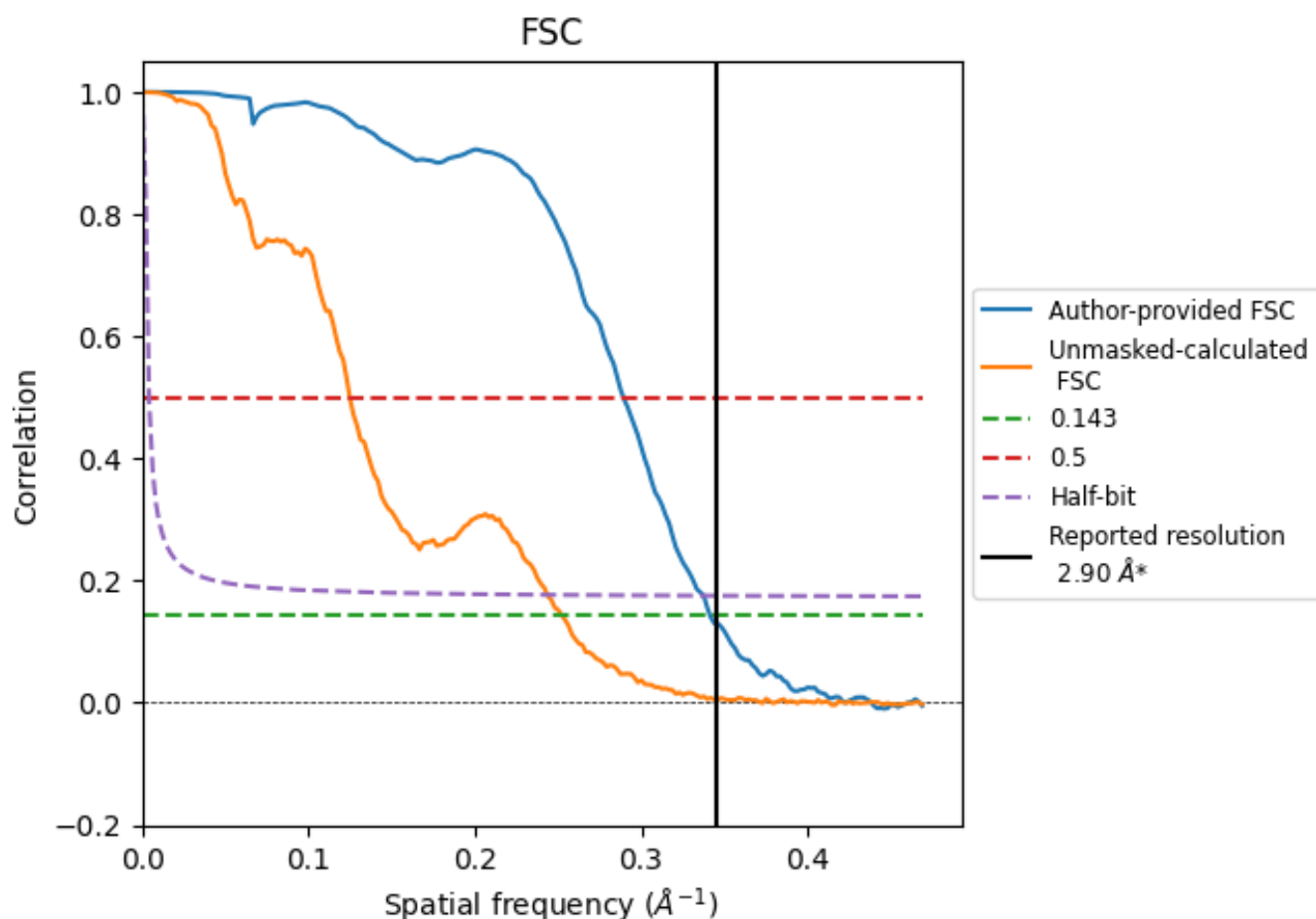


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

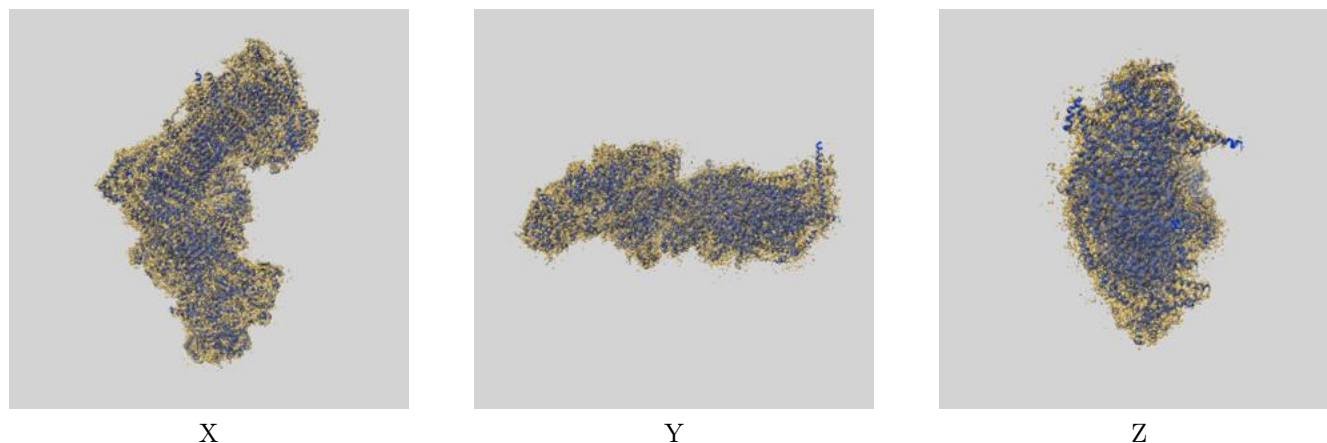
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.46	2.96
Unmasked-calculated*	3.96	8.01	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

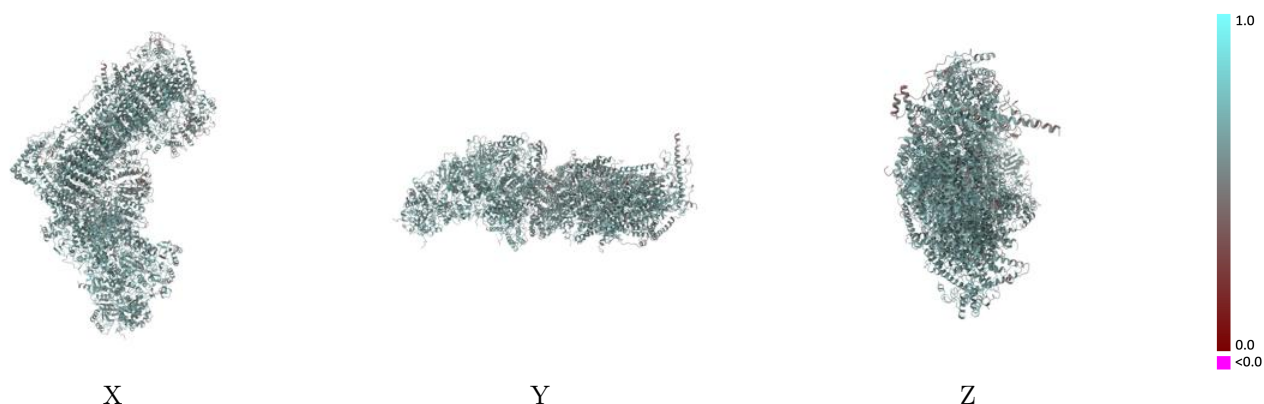
This section contains information regarding the fit between EMDB map EMD-18140 and PDB model 8Q47. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



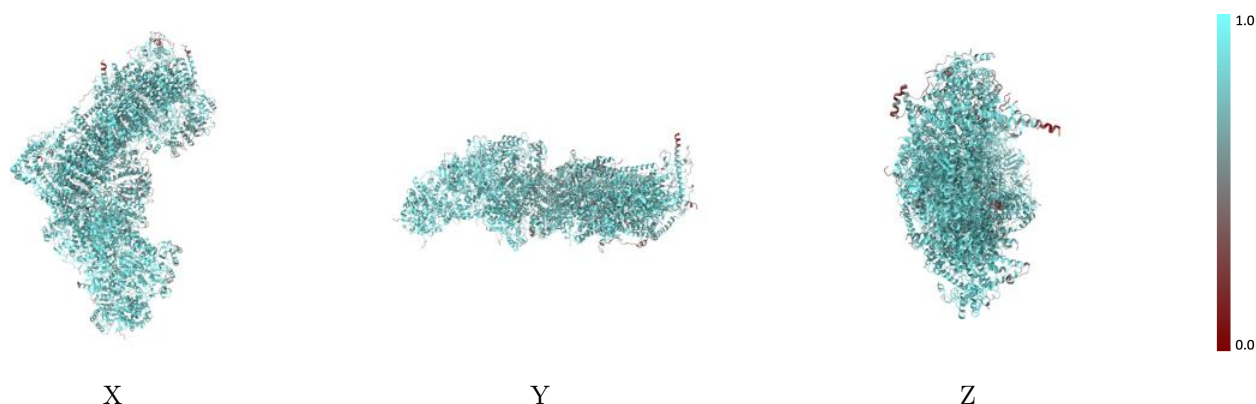
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



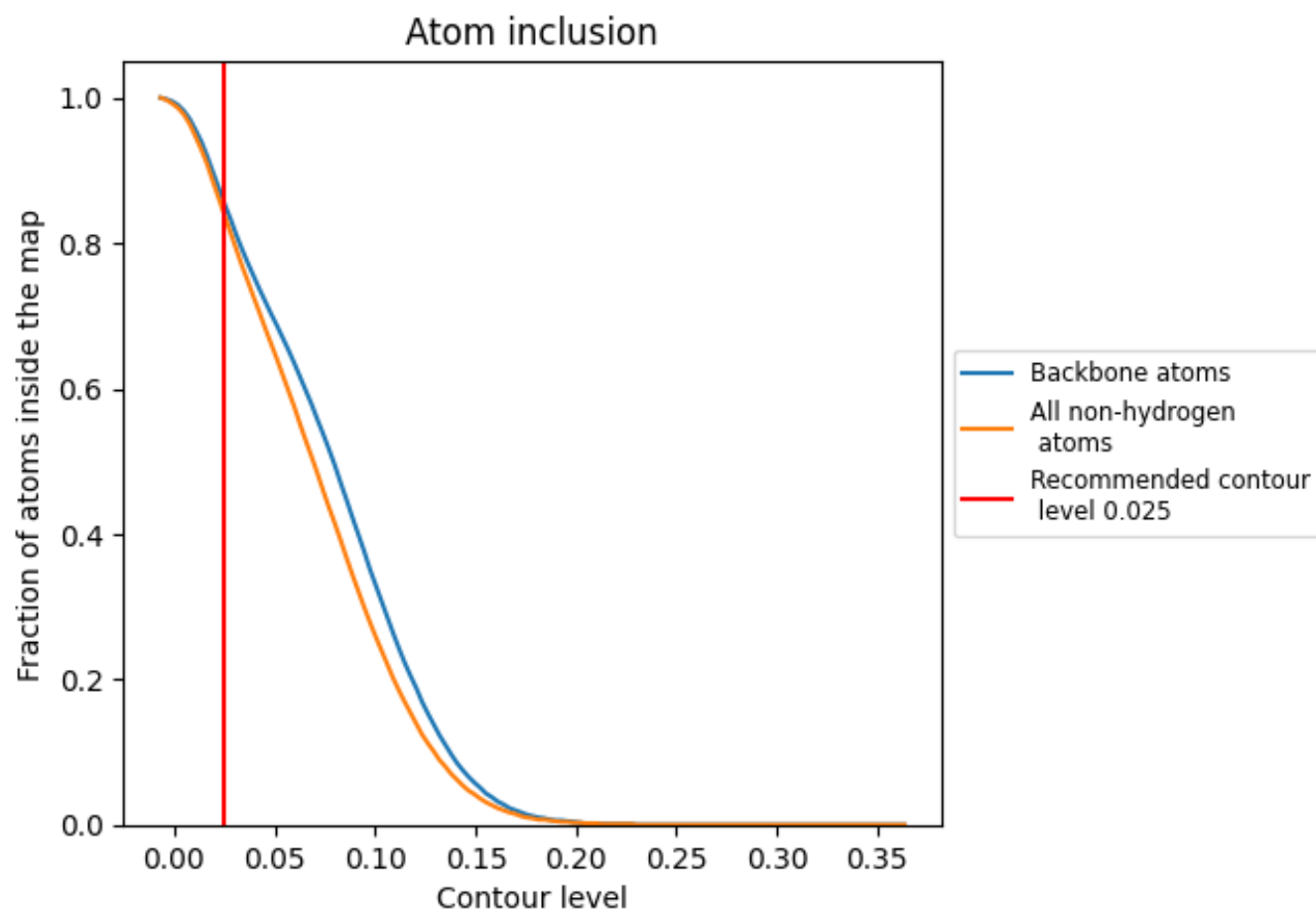
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.6010
A	 0.8080	 0.5990
B	 0.9040	 0.6330
C	 0.9290	 0.6410
D	 0.9070	 0.6380
E	 0.8250	 0.5850
F	 0.8670	 0.6100
G	 0.8720	 0.6160
H	 0.8800	 0.6150
I	 0.9290	 0.6450
J	 0.8020	 0.5870
K	 0.9040	 0.6230
L	 0.8430	 0.5990
M	 0.9040	 0.6320
N	 0.9160	 0.6380
O	 0.7950	 0.5800
P	 0.8140	 0.5810
Q	 0.8610	 0.6190
R	 0.8580	 0.6220
S	 0.7560	 0.5620
T	 0.6270	 0.5080
U	 0.7200	 0.5410
V	 0.8410	 0.6000
W	 0.8250	 0.6050
X	 0.8380	 0.6010
Y	 0.8060	 0.5880
Z	 0.8350	 0.5940
a	 0.8820	 0.6140
b	 0.7980	 0.5930
c	 0.8100	 0.5930
d	 0.8510	 0.6090
e	 0.8020	 0.5760
f	 0.7160	 0.5680
g	 0.8100	 0.5860
h	 0.8520	 0.6110



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Chain	Atom inclusion	Q-score
i	 0.6570	 0.5250
j	 0.6910	 0.5390
k	 0.6620	 0.5320
l	 0.8160	 0.5780
m	 0.7890	 0.5780
n	 0.7680	 0.5610
o	 0.6900	 0.5420
p	 0.7810	 0.5740
q	 0.8680	 0.6150
r	 0.8840	 0.6280
s	 0.8290	 0.5650