



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:18 PM UTC

PDB ID : 8Q1U / pdb_00008q1u
EMDB ID : EMD-18067
Title : Inward-facing, open1 proteoliposome complex I at 3.3 Å, after deactivation treatment. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-01
Resolution : 3.30 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:

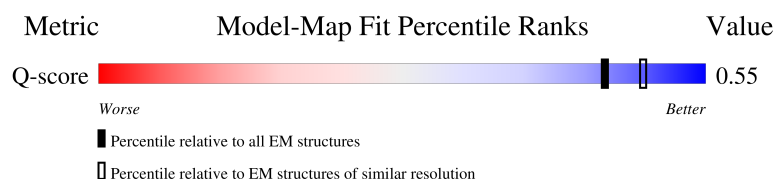
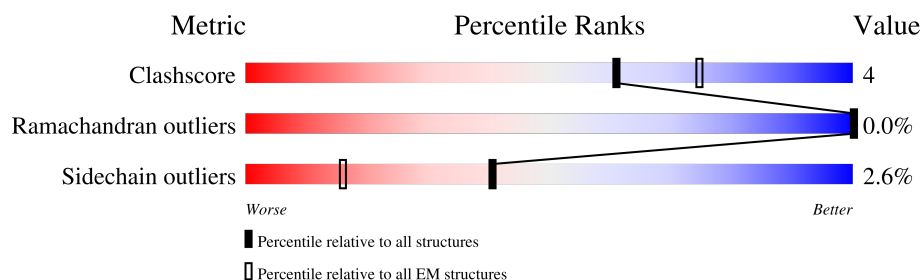
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 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	15087 (2.80 - 3.80)

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	

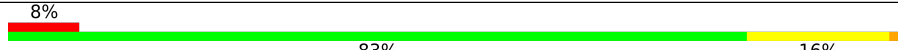
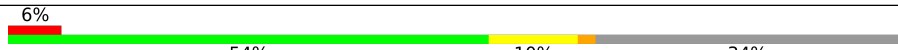
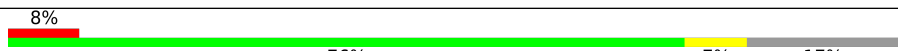
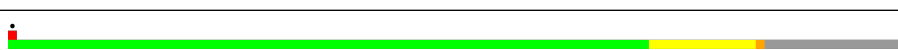
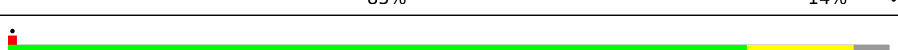
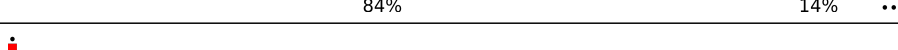
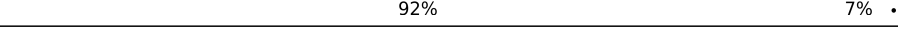
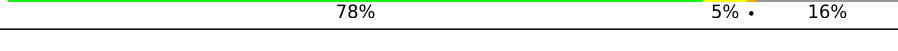
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	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 69145 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		

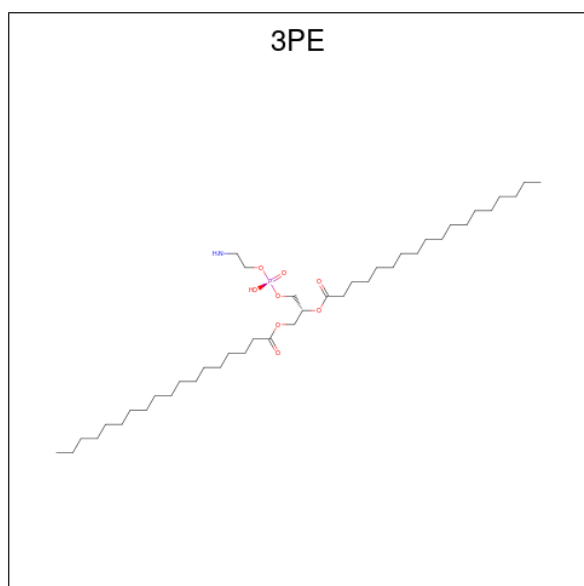
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



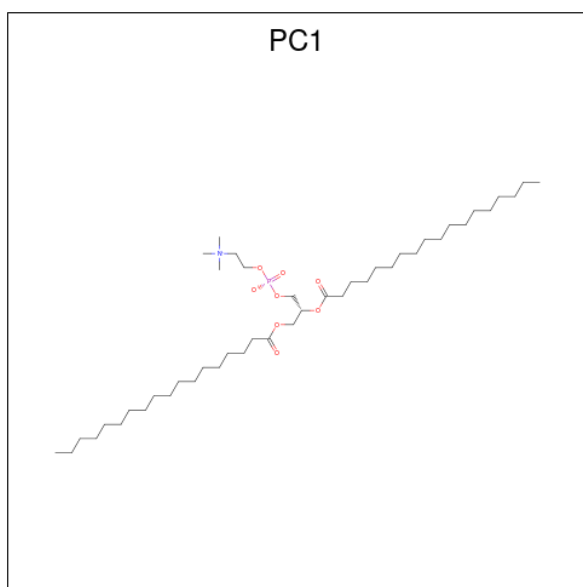
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
45	I	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	J	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	K	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			46	36	1	8	1	

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

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



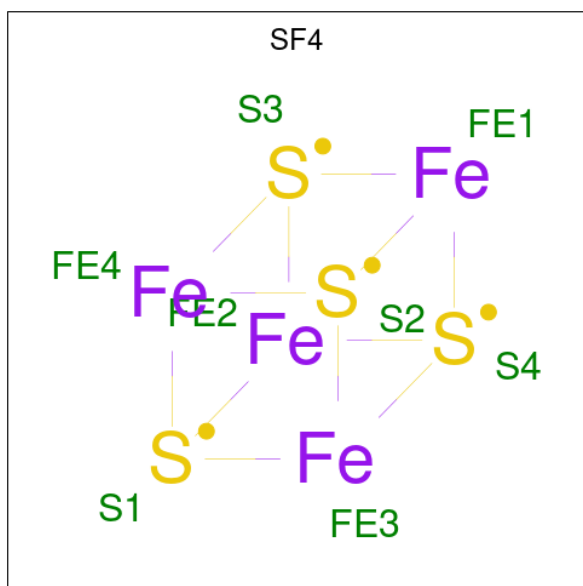
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	I	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	M	1	Total	C	N	O	P	0
			26	16	1	8	1	
46	P	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	h	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	q	1	Total	C	N	O	P	0
			48	38	1	8	1	

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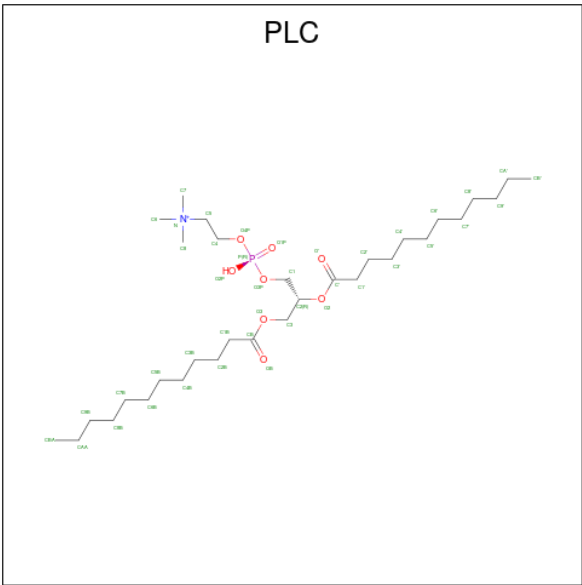
Mol	Chain	Residues	Atoms					AltConf
46	q	1	Total	C	N	O	P	0
			30	20	1	8	1	

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



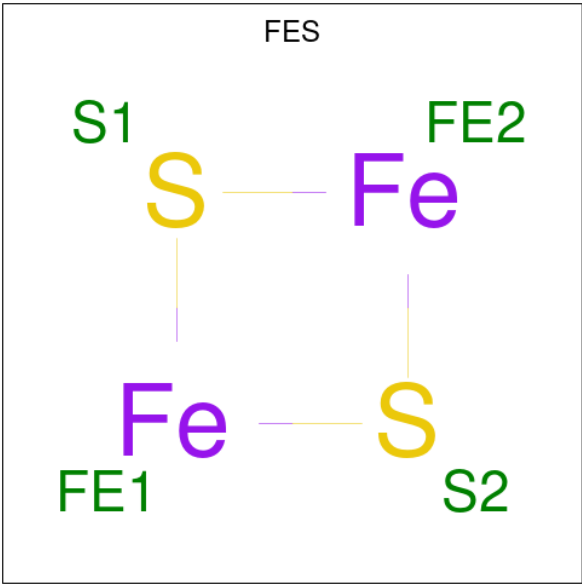
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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



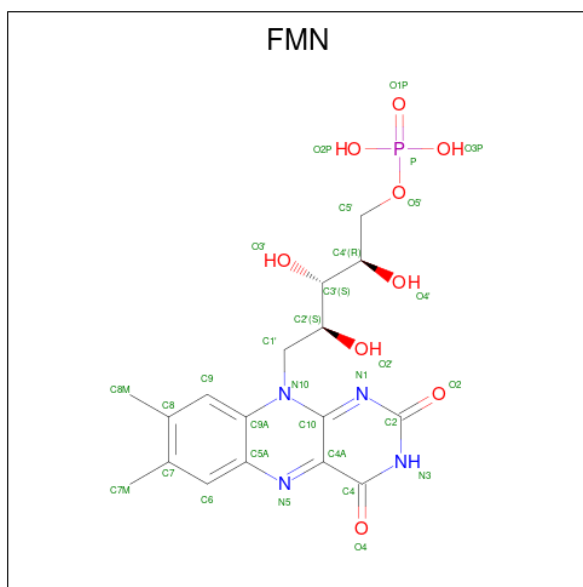
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
48	L	1	Total	C	N	O	P	0
			27	17	1	8	1	
48	N	1	Total	C	N	O	P	0
			26	16	1	8	1	
48	b	1	Total	C	N	O	P	0
			32	22	1	8	1	
48	g	1	Total	C	N	O	P	0
			32	22	1	8	1	

- 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: $C_{17}H_{21}N_4O_9P$).

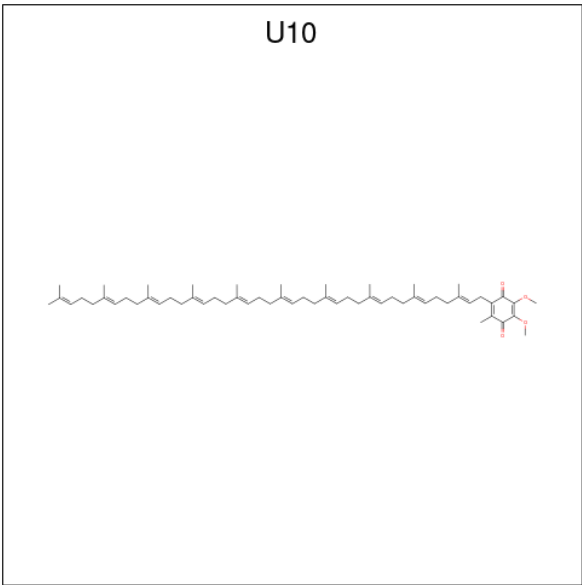


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

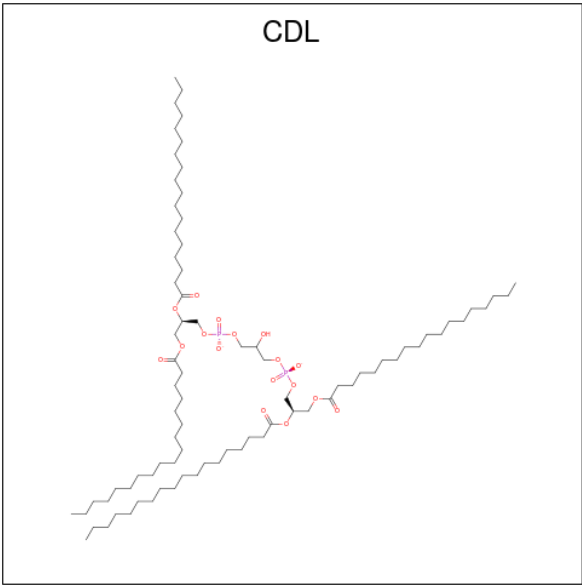
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	K	0
			1	1	

- 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

Continued on next page...

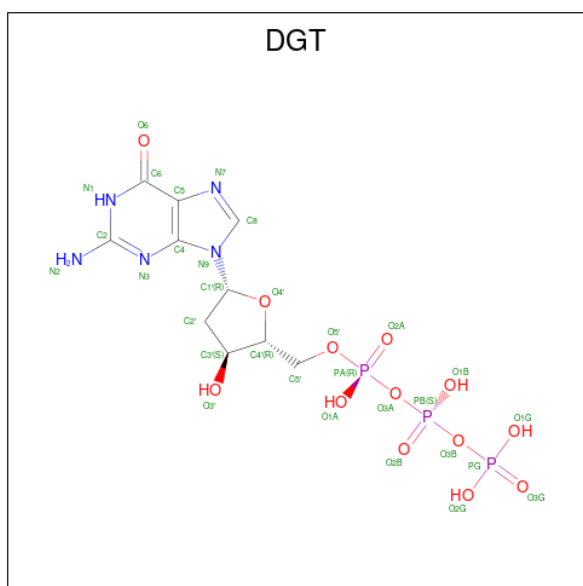
Continued from previous page...

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).

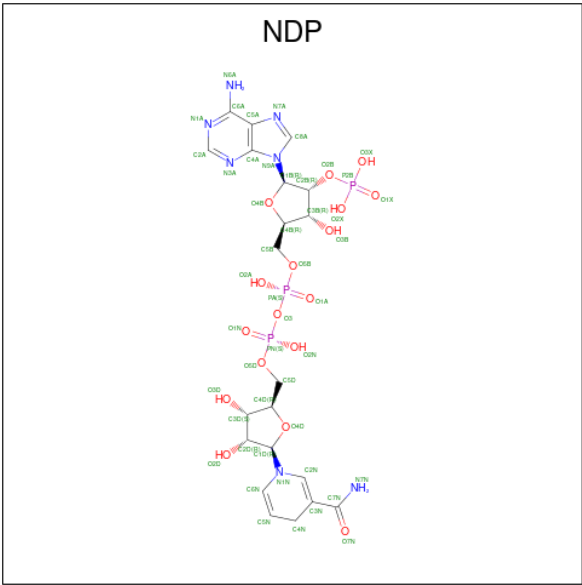


Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

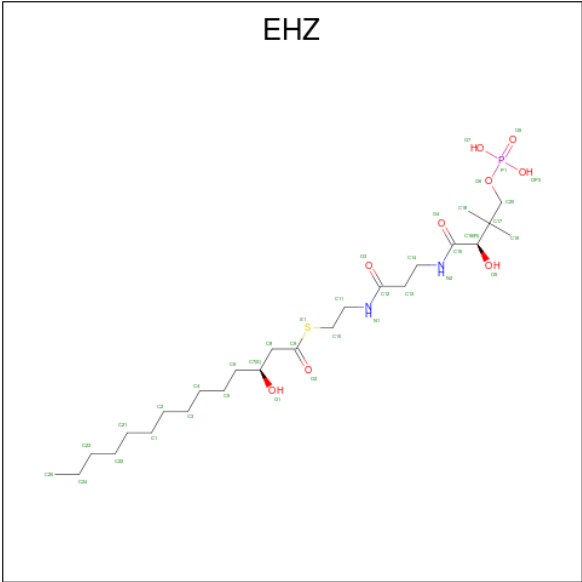
Mol	Chain	Residues	Atoms		AltConf
56	O	1	Total	Mg	0
			1	1	

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



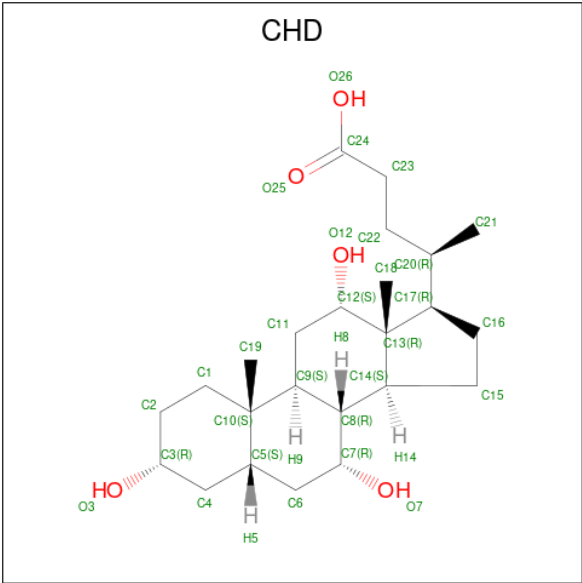
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- 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: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



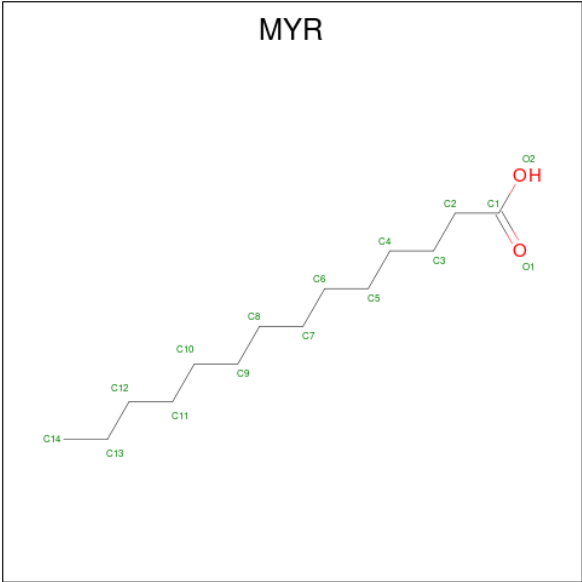
Mol	Chain	Residues	Atoms					AltConf
58	T	1	Total	C	N	O	P	S
			37	25	2	8	1	1
58	U	1	Total	C	N	O	P	S
			37	25	2	8	1	1

- 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).



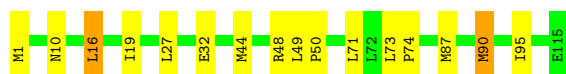
Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

3 Residue-property plots

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.

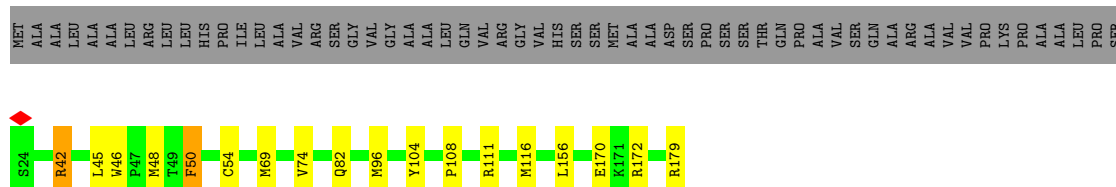
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



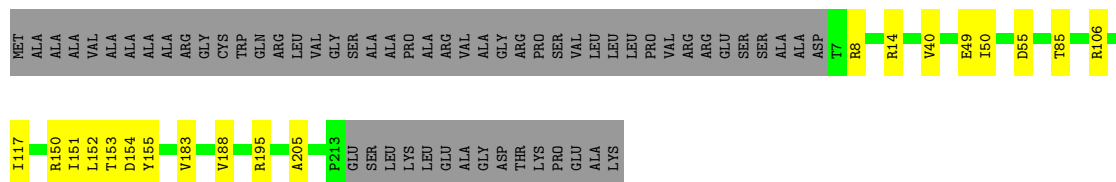
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



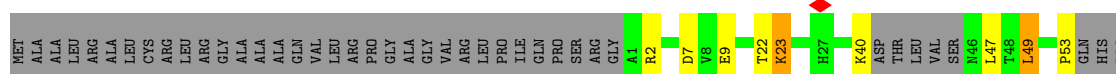
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

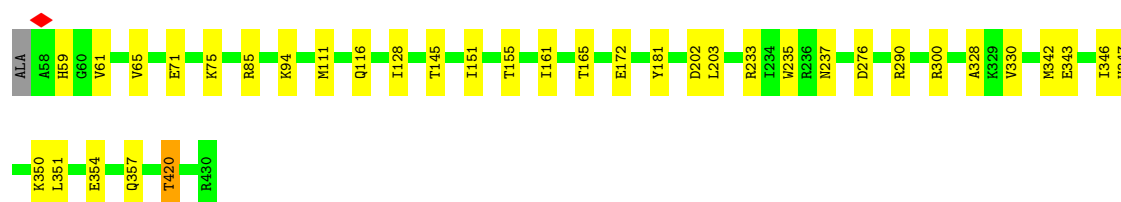
Chain C: 



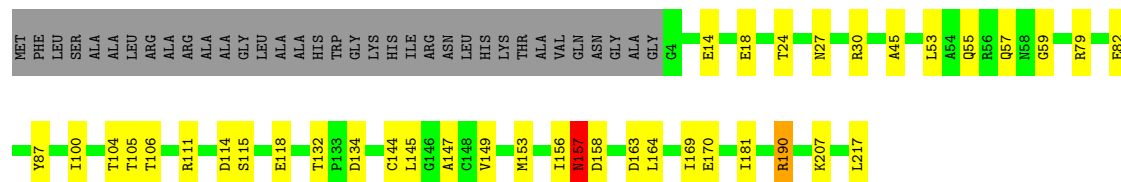
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 

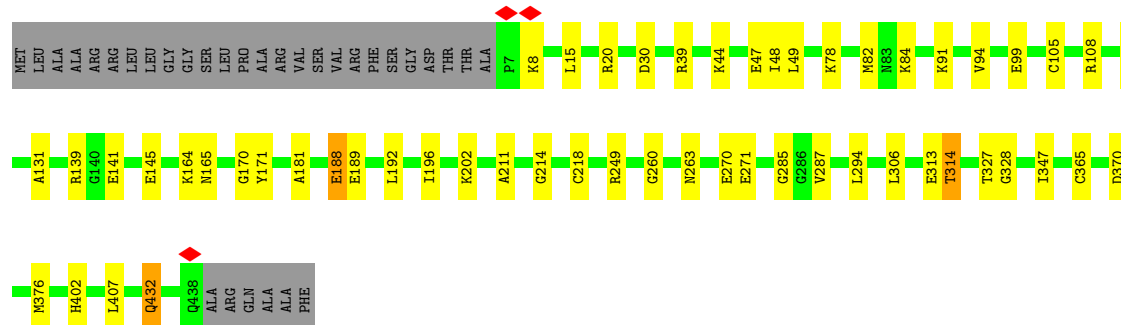
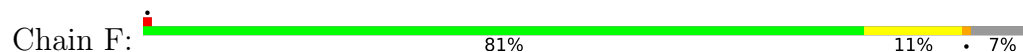




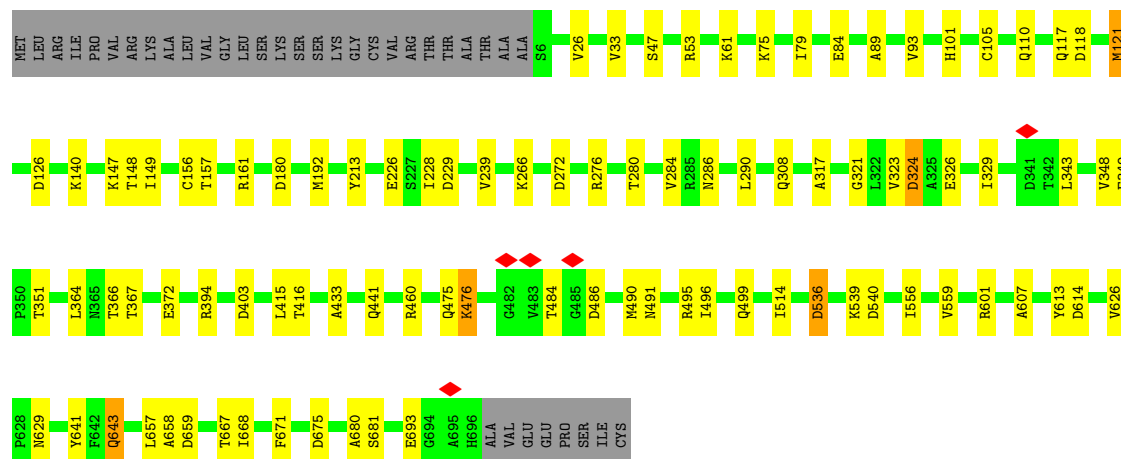
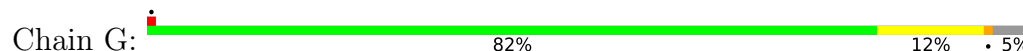
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



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

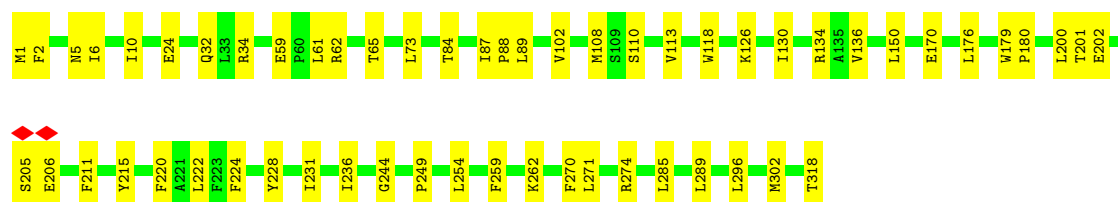


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



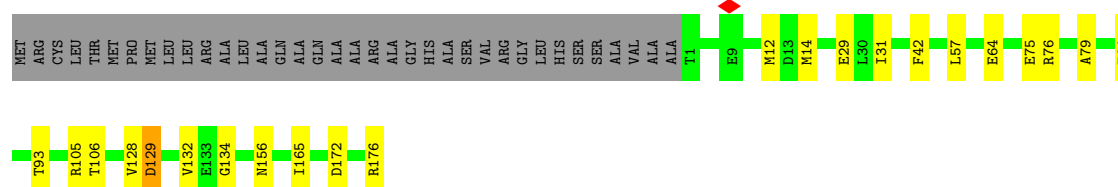
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  82% 18%



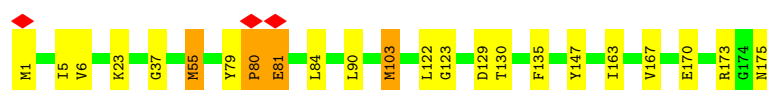
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  73% 10% 17%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  87% 11%



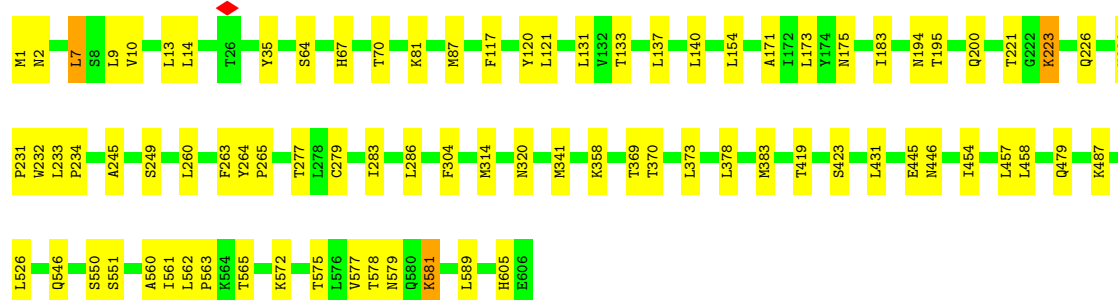
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  87% 11%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  86% 13%



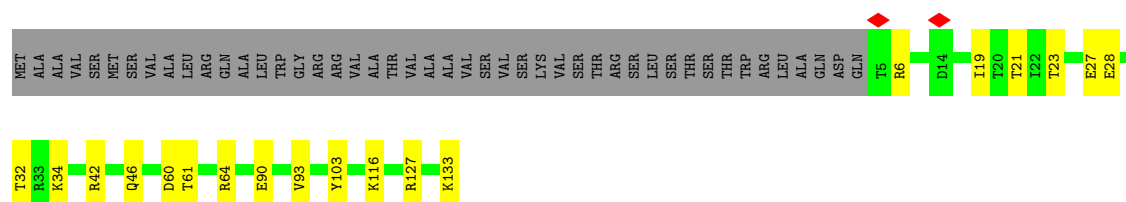
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

R278	M1
L285	R20
L315	D47
R340	M48
T350	L65
L375	M71
V382	L106
S397	T109 F110
I391	M113
M413	I120
K418	T125 L126
I423	L130
L442 P443	E141 R142
Y459	L143
	I167
	M175
	M201
	M207
	L216 P217
	V234
	L239
	T249
	D255 F256
	Y259
	M263 L264
	G268 M269
	I270 M271
	T275

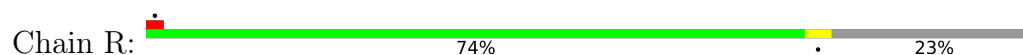
M1	M294
I19	Y298
S23	T303
T31	K314
I41	P318
M44	L319
M68	M320
M71	L343
M72	S344
L78	E347
M84	
K88	
M93	
T99	
F146	
P147	
L153	
T156	
L157	
S158	
T191	
A192	
V193	
L194	
P195	
M215	
K236	
T237	
V242	
L243	
I244	
V264	
E269	
K272	
M273	
L290	

RET	ALA	LEU	ARG	LEU	ARG	LEU	VAL	PRO	ARG	VAL	GLY	GLY	ILE	HIS	THR	SER	VAL	GLN	PHE	LYS	L1	T15	S22	L24	L25	N30	K40	K45	F51	Y58	S61	Q72	Y83	R104	L116	G119	V122	L124	E125	P126
V133	F134	L135	K146	Y152	Y163	V179	K186	E232	V235	E236	N252	D253	L259	R260	V263	V269	Y272	T273	S274	L275	L279	P280	E281	K315	K320															

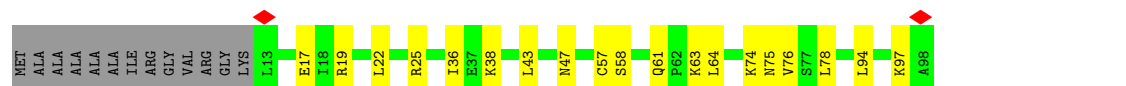
Diagram illustrating a protein-protein interaction network. The network is composed of various proteins represented by colored nodes (yellow, green, grey) and their interactions represented by lines. The proteins are organized into three main horizontal sections. The top section contains a large grey block of proteins (MET, ALA, VAL, HIS, PRO, ARG, VAL, VAL, ARG, VAL, LEU, MET, SER, ARG, SER, SER, VAL, PRO, GLN, ARG, GLN, L1, H2, H3, A4, V5, L30, Q44, V45, I46, E52, I69, D72, V91, I92, E98, T101) with several yellow nodes (K122, V126, Y136, I139, K140, S141, K144, R147, K154, E158, E162, A163, T164, I165, I166, K167, P168, A169, E170, R174, I185, S195, L196, I207, T218, K223, R224, G225, K226, F230, F253, L254, E276, R286, G299, D302, E311) and a few green nodes (L327, D333, V334, Q335, K338, S343, GLY, PRO). The middle section contains a large grey block of proteins (MET, ALA, VAL, HIS, PRO, ARG, VAL, VAL, ARG, VAL, LEU, MET, SER, ARG, SER, SER, VAL, PRO, GLN, ARG, GLN, L1, H2, H3, A4, V5, L30, Q44, V45, I46, E52, I69, D72, V91, I92, E98, T101) with several yellow nodes (K122, V126, Y136, I139, K140, S141, K144, R147, K154, E158, E162, A163, T164, I165, I166, K167, P168, A169, E170, R174, I185, S195, L196, I207, T218, K223, R224, G225, K226, F230, F253, L254, E276, R286, G299, D302, E311) and a few green nodes (L327, D333, V334, Q335, K338, S343, GLY, PRO). The bottom section contains a large grey block of proteins (MET, ALA, VAL, HIS, PRO, ARG, VAL, VAL, ARG, VAL, LEU, MET, SER, ARG, SER, SER, VAL, PRO, GLN, ARG, GLN, L1, H2, H3, A4, V5, L30, Q44, V45, I46, E52, I69, D72, V91, I92, E98, T101) with several yellow nodes (K122, V126, Y136, I139, K140, S141, K144, R147, K154, E158, E162, A163, T164, I165, I166, K167, P168, A169, E170, R174, I185, S195, L196, I207, T218, K223, R224, G225, K226, F230, F253, L254, E276, R286, G299, D302, E311) and a few green nodes (L327, D333, V334, Q335, K338, S343, GLY, PRO).



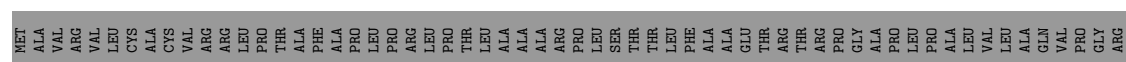
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



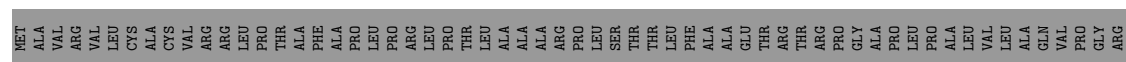
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



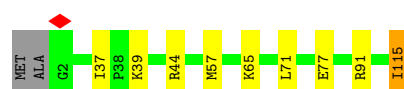
- Molecule 20: Acyl carrier protein, mitochondrial



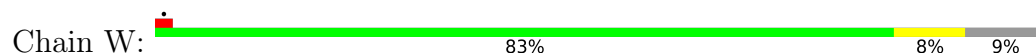
- Molecule 20: Acyl carrier protein, mitochondrial



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



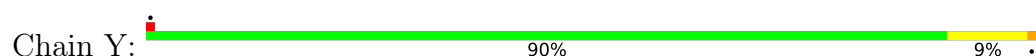
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



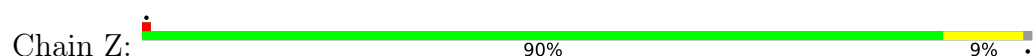
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



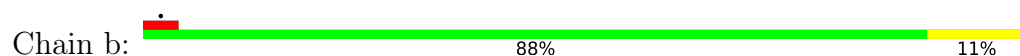
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



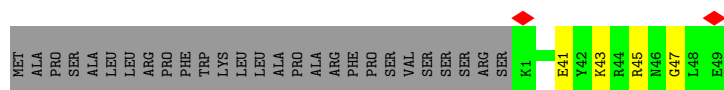
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

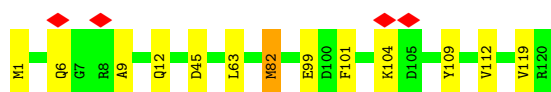


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



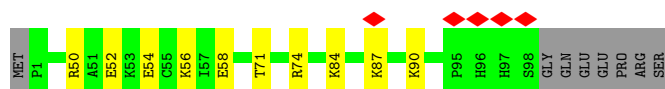
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  89% 10%



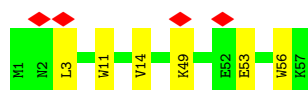
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  5% 83% 9% 8%



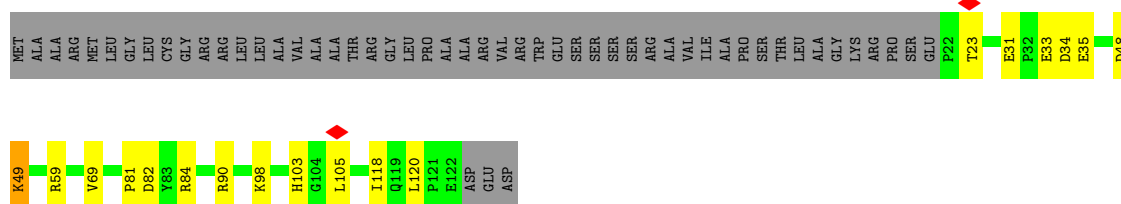
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  7% 89% 11%



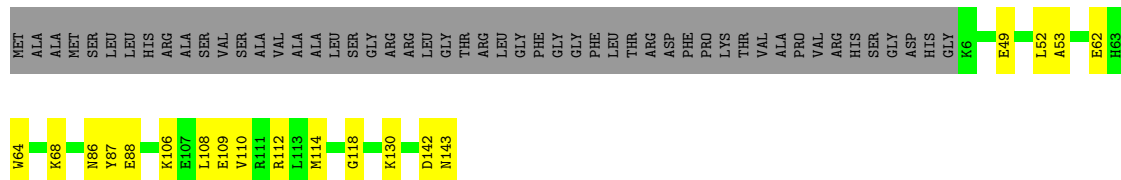
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:  54% 11% 34%



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

Chain h:  63% 10% 27%



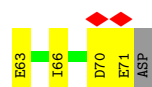
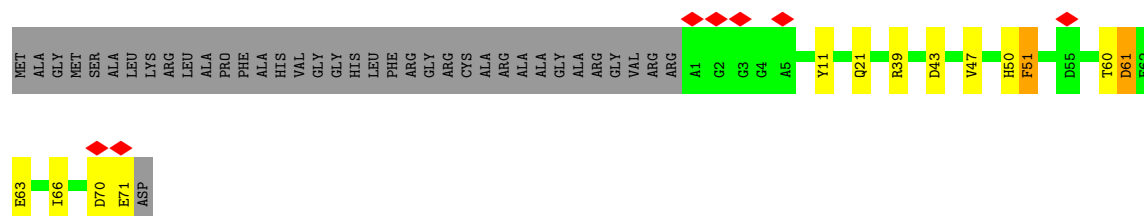
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:  8% 83% 16%

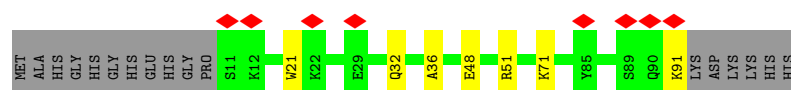
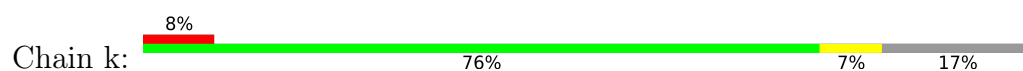




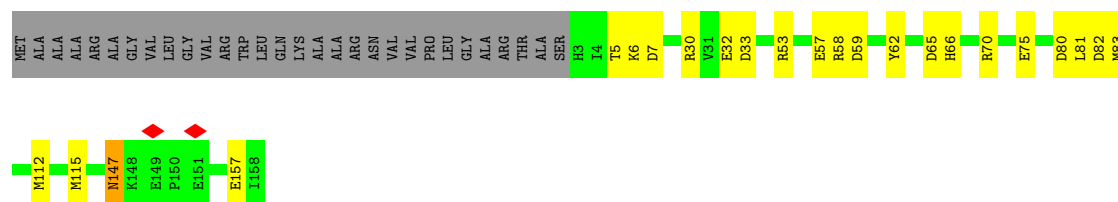
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



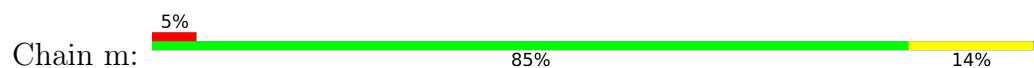
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



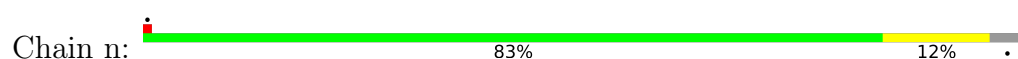
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



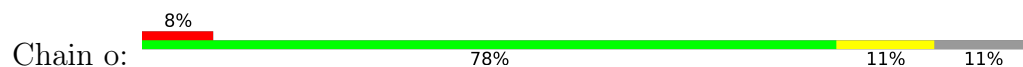
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



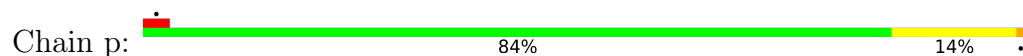
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



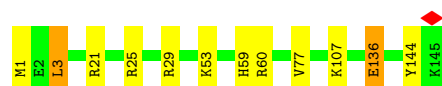
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



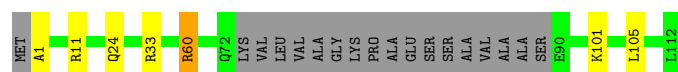
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



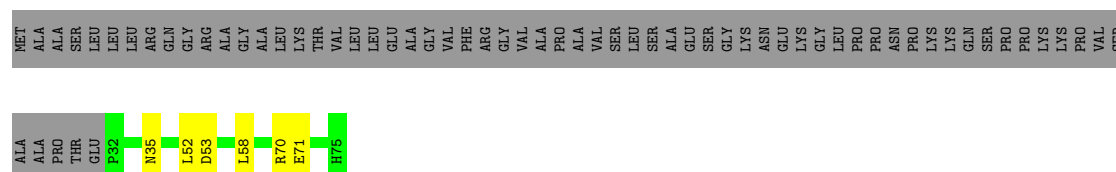
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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, C1	Depositor
Number of particles used	14905	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 ($e^-/\text{\AA}^2$)	40, 40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/936	0.24	0/1281
2	B	0.22	0/1278	0.25	0/1728
3	C	0.21	0/1772	0.27	0/2413
4	D	0.21	0/3466	0.26	0/4692
5	E	0.16	0/1699	0.27	0/2312
6	F	0.17	0/3401	0.25	0/4595
7	G	0.18	0/5387	0.26	0/7301
8	H	0.20	0/2571	0.27	0/3513
9	I	0.23	0/1445	0.27	0/1956
10	J	0.17	0/1370	0.26	0/1859
11	K	0.18	0/745	0.24	0/1008
12	L	0.16	0/4920	0.25	0/6694
13	M	0.19	0/3738	0.25	0/5097
14	N	0.20	0/2792	0.27	0/3800
15	O	0.14	0/2651	0.23	0/3587
16	P	0.15	0/2804	0.24	0/3803
17	Q	0.19	0/1072	0.25	0/1449
18	R	0.19	0/753	0.24	0/1014
19	S	0.11	0/702	0.24	0/945
20	T	0.12	0/719	0.23	0/971
20	U	0.12	0/719	0.23	0/971
21	V	0.15	0/943	0.23	0/1277
22	W	0.17	0/1006	0.25	0/1352
23	X	0.16	0/1439	0.23	0/1942
24	Y	0.13	0/1042	0.20	0/1414
25	Z	0.16	0/1186	0.22	0/1599
26	a	0.18	0/584	0.24	0/786
27	b	0.14	0/667	0.24	0/916
28	c	0.15	0/427	0.20	0/579
29	d	0.17	0/1018	0.24	0/1375
30	e	0.16	0/846	0.24	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.15	0/505	0.26	0/681
32	g	0.15	0/873	0.25	0/1186
33	h	0.16	0/1188	0.23	0/1607
34	i	0.12	0/1127	0.23	0/1534
35	j	0.13	0/624	0.24	0/855
36	k	0.09	0/672	0.20	0/906
37	l	0.13	0/1369	0.24	0/1873
38	m	0.14	0/1088	0.23	0/1472
39	n	0.12	0/1540	0.22	0/2085
40	o	0.13	0/1073	0.21	0/1437
41	p	0.14	0/1491	0.22	0/2011
42	q	0.18	0/1242	0.24	0/1688
43	r	0.18	0/789	0.22	0/1068
44	s	0.13	0/383	0.23	0/518
All	All	0.17	0/68062	0.25	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	12	0
2	B	1247	0	1256	14	0
3	C	1721	0	1675	12	0
4	D	3392	0	3339	32	0
5	E	1659	0	1664	30	0
6	F	3326	0	3282	35	0
7	G	5298	0	5316	59	0
8	H	2509	0	2621	46	0
9	I	1414	0	1370	16	0
10	J	1345	0	1352	16	0
11	K	745	0	785	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	62	0
13	M	3654	0	3852	33	0
14	N	2733	0	2912	32	0
15	O	2589	0	2566	26	0
16	P	2728	0	2749	27	0
17	Q	1049	0	1045	10	0
18	R	740	0	714	2	0
19	S	691	0	706	10	0
20	T	707	0	700	6	0
20	U	707	0	700	7	0
21	V	923	0	964	7	0
22	W	982	0	999	8	0
23	X	1402	0	1383	11	0
24	Y	1030	0	1039	7	0
25	Z	1157	0	1156	9	0
26	a	569	0	568	5	0
27	b	654	0	663	6	0
28	c	414	0	415	2	0
29	d	999	0	988	8	0
30	e	825	0	826	5	0
31	f	492	0	501	3	0
32	g	846	0	798	13	0
33	h	1154	0	1168	12	0
34	i	1097	0	1108	18	0
35	j	597	0	536	10	0
36	k	653	0	639	3	0
37	l	1314	0	1210	15	0
38	m	1070	0	1068	9	0
39	n	1487	0	1433	13	0
40	o	1048	0	1018	12	0
41	p	1458	0	1430	17	0
42	q	1212	0	1183	8	0
43	r	776	0	782	3	0
44	s	371	0	344	5	0
45	A	34	0	42	0	0
45	I	36	0	49	1	0
45	J	33	0	40	0	0
45	K	44	0	62	0	0
45	L	162	0	229	3	0
45	M	50	0	77	0	0
45	N	139	0	206	0	0
45	Y	165	0	241	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	45	0	67	1	0
45	b	47	0	71	0	0
45	d	49	0	75	0	0
45	g	29	0	32	0	0
45	i	45	0	67	2	0
45	m	74	0	99	0	0
45	o	35	0	47	1	0
46	A	70	0	88	1	0
46	H	87	0	128	1	0
46	I	91	0	136	2	0
46	L	47	0	71	0	0
46	M	70	0	91	2	0
46	P	46	0	66	0	0
46	Y	40	0	54	0	0
46	d	39	0	52	1	0
46	h	31	0	36	0	0
46	q	78	0	104	5	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	N	26	0	26	0	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	0	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	H	28	0	31	9	0
53	J	36	0	16	0	0
53	L	87	0	127	0	0
53	M	91	0	135	1	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	1	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	25	0	0
58	T	37	0	0	2	0
58	U	37	0	0	1	0
59	i	29	0	38	7	0
60	o	15	0	27	0	0
All	All	69145	0	70047	607	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 (607) 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)
5:E:30:ARG:NH1	44:s:53:ASP:OD1	2.06	0.88
24:Y:6:ARG:NH1	24:Y:10:ASP:OD1	2.09	0.85
41:p:72:ASP:OD1	41:p:74:THR:OG1	1.94	0.85
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.59	0.84
16:P:98:GLU:OE1	16:P:286:ARG:NH2	2.10	0.83
33:h:87:TYR:OH	41:p:86:GLU:OE1	1.96	0.83
20:U:46:ASP:OD1	39:n:44:ARG:NH2	2.13	0.82
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.13	0.81
5:E:132:THR:OG1	5:E:134:ASP:OD1	1.96	0.81
12:L:579:ASN:O	24:Y:43:LYS:NZ	2.13	0.81
52:H:401:U10:H101	52:H:401:U10:H13	1.62	0.81
42:q:25:ARG:NH1	46:q:203:PC1:O12	2.14	0.80
15:O:83:TYR:HH	55:O:401:DGT:HO3'	0.82	0.80
10:J:23:LYS:NZ	11:K:18:GLY:O	2.14	0.80
32:g:90:ARG:NH2	41:p:107:GLU:OE2	2.15	0.79
4:D:71:GLU:OE1	8:H:134:ARG:NH2	2.15	0.79
10:J:170:GLU:OE1	10:J:173:ARG:NH2	2.15	0.79
25:Z:92:GLU:N	25:Z:92:GLU:OE1	2.17	0.78
14:N:314:LYS:NZ	15:O:274:SER:OG	2.17	0.78
40:o:102:GLU:OE2	40:o:105:ARG:NH1	2.18	0.77
7:G:140:LYS:O	7:G:148:THR:OG1	2.03	0.77
14:N:298:TYR:O	14:N:303:THR:OG1	2.02	0.77
37:l:30:ARG:NE	38:m:34:GLU:OE2	2.18	0.77
15:O:58:TYR:O	15:O:61:SER:OG	2.03	0.77
14:N:269:GLU:O	14:N:273:ASN:ND2	2.17	0.77
20:T:68:GLU:OE2	22:W:32:ARG:NH2	2.18	0.76
16:P:154:LYS:NZ	16:P:158:GLU:OE2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:263:ASN:ND2	6:F:285:GLY:O	2.19	0.75
15:O:236:GLU:OE2	21:V:91:ARG:NH1	2.20	0.75
22:W:29:ARG:NH1	22:W:33:GLU:OE2	2.18	0.75
23:X:90:TYR:OH	26:a:28:ARG:NH2	2.20	0.74
40:o:75:ASN:ND2	45:o:202:3PE:O14	2.19	0.74
6:F:131:ALA:O	6:F:171:TYR:OH	2.06	0.74
9:I:156:ASN:ND2	18:R:34:GLU:OE2	2.21	0.74
16:P:276:GLU:N	16:P:276:GLU:OE1	2.20	0.74
52:H:401:U10:H101	52:H:401:U10:C13	2.18	0.73
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.20	0.73
41:p:129:GLU:OE2	41:p:133:GLN:NE2	2.22	0.73
46:A:202:PC1:O12	8:H:62:ARG:NH1	2.21	0.73
6:F:270:GLU:OE1	6:F:271:GLU:N	2.22	0.73
15:O:125:GLU:N	15:O:125:GLU:OE1	2.21	0.73
59:i:201:CHD:H212	59:i:201:CHD:H12	1.71	0.73
25:Z:130:GLU:N	25:Z:130:GLU:OE1	2.21	0.72
7:G:366:THR:O	7:G:367:THR:OG1	2.05	0.72
15:O:83:TYR:OH	55:O:401:DGT:O3'	1.87	0.72
12:L:175:ASN:OD1	12:L:223:LYS:NZ	2.23	0.71
34:i:121:GLU:N	34:i:121:GLU:OE1	2.23	0.71
5:E:24:THR:OG1	5:E:27:ASN:OD1	2.07	0.71
21:V:57:MET:HE3	21:V:71:LEU:HD23	1.73	0.71
17:Q:90:GLU:OE1	17:Q:90:GLU:N	2.24	0.71
32:g:33:GLU:N	32:g:33:GLU:OE1	2.22	0.71
7:G:627:SER:OG	7:G:629:ASN:OD1	2.09	0.70
30:e:58:GLU:N	30:e:58:GLU:OE1	2.24	0.70
5:E:14:GLU:N	5:E:14:GLU:OE1	2.25	0.69
58:T:101:EHZ:O1	58:T:101:EHZ:O2	2.01	0.69
34:i:66:HIS:CD2	59:i:201:CHD:H231	2.27	0.69
37:l:5:THR:OG1	37:l:7:ASP:OD1	2.08	0.69
42:q:29:ARG:O	46:q:202:PC1:H131	1.92	0.69
2:B:82:GLN:NE2	8:H:215:TYR:O	2.25	0.69
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.75	0.69
6:F:82:MET:O	6:F:91:LYS:NZ	2.25	0.69
8:H:224:PHE:CE2	52:H:401:U10:H111	2.28	0.69
12:L:64:SER:O	34:i:95:THR:HG23	1.93	0.69
15:O:232:GLU:OE1	15:O:232:GLU:N	2.26	0.69
23:X:112:ASP:OD1	23:X:113:LYS:N	2.26	0.69
37:l:58:ARG:NH2	37:l:75:GLU:OE2	2.25	0.69
34:i:51:GLN:OE1	34:i:51:GLN:N	2.26	0.69
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD13	1:A:19:ILE:HD11	1.73	0.68
6:F:202:LYS:O	17:Q:133:LYS:NZ	2.25	0.68
14:N:236:LYS:HG3	14:N:237:THR:HG23	1.75	0.68
12:L:260:LEU:CD1	12:L:314:MET:HE1	2.24	0.68
8:H:206:GLU:N	8:H:206:GLU:OE1	2.26	0.68
30:e:50:ARG:NH1	30:e:54:GLU:OE1	2.27	0.68
41:p:11:GLU:OE1	41:p:115:ARG:NH2	2.27	0.68
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.20	0.68
12:L:446:ASN:ND2	35:j:21:GLN:OE1	2.27	0.68
13:M:141:GLU:N	13:M:141:GLU:OE1	2.25	0.67
25:Z:107:GLU:O	30:e:74:ARG:NH1	2.27	0.67
7:G:475:GLN:NE2	7:G:643:GLN:OE1	2.28	0.67
6:F:139:ARG:NH1	6:F:141:GLU:OE2	2.27	0.67
39:n:167:TRP:O	39:n:171:THR:OG1	2.11	0.67
7:G:272:ASP:OD1	7:G:681:SER:OG	2.05	0.67
14:N:19:ILE:O	14:N:23:SER:OG	2.05	0.67
7:G:53:ARG:O	7:G:93:VAL:HG21	1.94	0.66
7:G:441:GLN:N	7:G:441:GLN:OE1	2.28	0.66
15:O:186:LYS:NZ	55:O:401:DGT:O2B	2.28	0.66
23:X:129:LYS:NZ	27:b:65:VAL:O	2.27	0.66
10:J:84:LEU:HA	10:J:90:LEU:HD21	1.78	0.66
4:D:343:GLU:N	4:D:343:GLU:OE1	2.28	0.66
20:U:49:GLU:OE2	39:n:19:TYR:OH	2.12	0.66
32:g:48:ASP:OD1	32:g:49:LYS:N	2.28	0.66
12:L:577:VAL:HG13	12:L:578:THR:HG23	1.76	0.66
45:I:203:3PE:O22	45:I:203:3PE:N	2.23	0.66
4:D:233:ARG:O	4:D:237:ASN:ND2	2.29	0.65
7:G:286:ASN:OD1	7:G:290:LEU:N	2.29	0.65
45:L:705:3PE:N	45:Y:202:3PE:O14	2.17	0.65
5:E:118:GLU:N	5:E:118:GLU:OE1	2.30	0.65
9:I:12:MET:O	27:b:9:LYS:NZ	2.30	0.65
46:M:604:PC1:O14	45:i:202:3PE:N	2.22	0.65
12:L:561:ILE:O	12:L:565:THR:OG1	2.14	0.65
10:J:23:LYS:NZ	11:K:21:MET:O	2.20	0.65
12:L:81:LYS:O	12:L:133:THR:HG23	1.96	0.65
3:C:55:ASP:OD2	17:Q:6:ARG:NE	2.30	0.64
53:h:201:CDL:OB3	34:i:88:HIS:NE2	2.28	0.64
5:E:105:THR:HG22	5:E:106:THR:H	1.62	0.64
19:S:17:GLU:OE2	19:S:19:ARG:NH1	2.31	0.64
4:D:2:ARG:N	32:g:31:GLU:OE2	2.31	0.64
6:F:432:GLN:N	6:F:432:GLN:OE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:276:ARG:NH1	7:G:680:ALA:O	2.30	0.64
7:G:372:GLU:OE2	7:G:394:ARG:NH1	2.30	0.63
11:K:43:MET:HE1	14:N:72:MET:SD	2.37	0.63
35:j:71:GLU:O	40:o:110:ARG:NH2	2.32	0.63
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.81	0.63
8:H:249:PRO:O	26:a:28:ARG:NH2	2.32	0.63
12:L:320:ASN:O	12:L:320:ASN:ND2	2.32	0.63
41:p:116:GLU:OE1	41:p:116:GLU:N	2.32	0.63
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.32	0.62
15:O:272:TYR:O	15:O:275:ILE:HG23	1.99	0.62
17:Q:27:GLU:N	17:Q:27:GLU:OE1	2.32	0.62
13:M:259:TYR:O	13:M:263:MET:HE2	2.00	0.62
8:H:220:PHE:CZ	52:H:401:U10:H1M2	2.34	0.62
2:B:42:ARG:NH1	46:q:202:PC1:O14	2.32	0.62
7:G:415:LEU:O	7:G:416:THR:OG1	2.05	0.62
41:p:171:GLU:N	41:p:171:GLU:OE1	2.33	0.61
7:G:326:GLU:N	7:G:326:GLU:OE1	2.33	0.61
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.32	0.61
4:D:145:THR:OG1	4:D:181:TYR:OH	2.08	0.61
29:d:45:ASP:OD2	53:d:201:CDL:O1	2.18	0.61
34:i:89:VAL:HG12	34:i:95:THR:HG21	1.82	0.61
7:G:433:ALA:O	7:G:476:LYS:NZ	2.34	0.60
14:N:88:LYS:NZ	30:e:52:GLU:OE2	2.32	0.60
27:b:2:GLU:O	27:b:6:ALA:N	2.34	0.60
5:E:156:ILE:HG22	5:E:157:ASN:ND2	2.16	0.60
40:o:43:GLN:NE2	40:o:47:ASP:OD1	2.34	0.60
4:D:346:ILE:HG23	7:G:117:GLN:HG2	1.83	0.60
7:G:536:ASP:OD1	7:G:536:ASP:N	2.34	0.60
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.01	0.60
20:T:64:ASP:OD2	22:W:32:ARG:NH1	2.35	0.60
59:i:201:CHD:O3	59:i:201:CHD:H9	2.01	0.60
5:E:18:GLU:N	5:E:18:GLU:OE1	2.35	0.60
9:I:29:GLU:N	9:I:29:GLU:OE1	2.30	0.60
59:i:201:CHD:H212	59:i:201:CHD:C12	2.31	0.60
37:l:59:ASP:OD2	37:l:62:TYR:N	2.33	0.60
8:H:65:THR:HG21	16:P:325:ARG:HG3	1.82	0.60
12:L:581:LYS:NZ	24:Y:42:LEU:O	2.32	0.60
31:f:53:GLU:N	31:f:53:GLU:OE1	2.35	0.60
13:M:48:ASN:OD1	33:h:86:ASN:ND2	2.35	0.59
10:J:79:TYR:O	10:J:81:GLU:N	2.35	0.59
1:A:71:LEU:O	10:J:147:TYR:OH	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:350:LYS:NZ	7:G:118:ASP:OD1	2.31	0.59
6:F:141:GLU:OE1	6:F:141:GLU:N	2.35	0.59
16:P:311:GLU:OE1	16:P:311:GLU:N	2.36	0.59
5:E:145:LEU:HD12	5:E:153:MET:HE2	1.85	0.58
5:E:170:GLU:N	5:E:170:GLU:OE1	2.37	0.58
40:o:82:GLU:N	40:o:82:GLU:OE1	2.35	0.58
4:D:151:ILE:O	4:D:155:THR:OG1	2.17	0.58
16:P:162:GLU:O	16:P:224:ARG:NH1	2.36	0.58
34:i:37:GLN:N	34:i:37:GLN:OE1	2.36	0.58
13:M:387:SER:O	38:m:111:LYS:NZ	2.36	0.58
15:O:281:GLU:N	15:O:281:GLU:OE1	2.35	0.58
35:j:60:THR:O	40:o:106:ARG:NH1	2.37	0.58
12:L:9:LEU:HD12	34:i:85:LEU:HD11	1.85	0.58
12:L:171:ALA:O	12:L:175:ASN:ND2	2.37	0.58
34:i:89:VAL:CG1	34:i:95:THR:HG21	2.34	0.58
5:E:53:LEU:HD13	44:s:52:LEU:HD22	1.86	0.58
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.36	0.58
34:i:18:ARG:NH1	39:n:170:VAL:O	2.36	0.57
13:M:47:ASP:OD1	13:M:48:ASN:N	2.38	0.57
40:o:77:LEU:O	40:o:80:LYS:NZ	2.36	0.57
6:F:15:LEU:O	6:F:20:ARG:NH1	2.37	0.57
8:H:244:GLY:O	8:H:262:LYS:NZ	2.38	0.57
37:l:157:GLU:O	40:o:33:ARG:NH2	2.38	0.57
12:L:378:LEU:HD22	12:L:383:MET:CE	2.34	0.57
33:h:62:GLU:OE1	33:h:64:TRP:NE1	2.38	0.57
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.37	0.57
8:H:220:PHE:CE2	52:H:401:U10:H1M2	2.39	0.57
52:H:401:U10:C18	52:H:401:U10:H151	2.35	0.57
4:D:202:ASP:OD1	4:D:203:LEU:N	2.38	0.57
7:G:693:GLU:OE1	7:G:693:GLU:N	2.38	0.56
4:D:342:MET:HE2	7:G:101:HIS:HD2	1.70	0.56
13:M:271:MET:HE2	13:M:271:MET:HA	1.88	0.56
10:J:79:TYR:O	10:J:80:PRO:C	2.47	0.56
12:L:314:MET:HE3	12:L:314:MET:HA	1.88	0.56
31:f:56:TRP:NE1	33:h:88:GLU:OE1	2.36	0.56
3:C:183:VAL:O	22:W:100:THR:OG1	2.22	0.56
5:E:217:LEU:HD12	6:F:44:LYS:CD	2.36	0.56
12:L:575:THR:O	12:L:579:ASN:ND2	2.38	0.56
19:S:57:CYS:SG	19:S:58:SER:N	2.73	0.56
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.86	0.56
7:G:675:ASP:N	7:G:675:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.41	0.55
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.06	0.55
5:E:217:LEU:HD13	5:E:217:LEU:O	2.05	0.55
7:G:192:MET:HE2	7:G:192:MET:HA	1.88	0.55
7:G:460:ARG:NH1	7:G:659:ASP:OD1	2.39	0.55
38:m:29:ARG:NH2	39:n:8:TYR:OH	2.39	0.55
29:d:63:LEU:HD23	53:d:201:CDL:HA62	1.88	0.55
8:H:32:GLN:OE1	8:H:34:ARG:NH1	2.40	0.55
6:F:108:ARG:NH2	6:F:145:GLU:OE2	2.35	0.55
2:B:96:MET:HE1	4:D:53:PRO:HG3	1.89	0.55
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.41	0.55
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.42	0.55
3:C:85:THR:HG21	21:V:115:ILE:HG13	1.89	0.54
8:H:73:LEU:O	8:H:73:LEU:HD23	2.06	0.54
9:I:42:PHE:O	43:r:11:ARG:NH2	2.41	0.54
14:N:158:SER:OG	14:N:191:THR:OG1	2.21	0.54
23:X:48:GLU:OE1	27:b:57:ARG:NH2	2.40	0.54
24:Y:80:ARG:NH2	24:Y:85:ASP:OD2	2.39	0.54
44:s:35:ASN:O	44:s:35:ASN:ND2	2.40	0.54
7:G:147:LYS:HD3	7:G:149:ILE:HD11	1.88	0.54
14:N:237:THR:HG21	14:N:319:LEU:HD11	1.88	0.54
33:h:143:ASN:O	33:h:143:ASN:ND2	2.40	0.54
35:j:60:THR:HG21	35:j:63:GLU:HB3	1.87	0.54
8:H:318:THR:HG22	25:Z:60:GLN:OE1	2.07	0.54
5:E:79:ARG:NH1	5:E:82:GLU:OE2	2.41	0.54
15:O:24:LEU:HD13	15:O:122:VAL:HG23	1.90	0.54
20:T:47:GLN:NE2	20:T:67:ALA:O	2.41	0.54
58:U:101:EHZ:O2	58:U:101:EHZ:O1	2.26	0.54
7:G:266:LYS:NZ	7:G:671:PHE:O	2.39	0.54
21:V:77:GLU:OE1	21:V:77:GLU:N	2.41	0.54
2:B:108:PRO:HB3	8:H:61:LEU:HD23	1.89	0.54
12:L:194:ASN:O	12:L:194:ASN:ND2	2.40	0.54
32:g:118:ILE:HG21	41:p:162:MET:HE1	1.89	0.54
44:s:71:GLU:OE1	44:s:71:GLU:N	2.41	0.54
6:F:313:GLU:O	6:F:314:THR:HG22	2.08	0.53
7:G:556:ILE:HD12	7:G:556:ILE:O	2.08	0.53
13:M:143:LEU:HD21	14:N:303:THR:HG21	1.90	0.53
13:M:255:ASP:OD1	13:M:256:PHE:N	2.42	0.53
19:S:47:ASN:OD1	19:S:47:ASN:N	2.41	0.53
12:L:589:LEU:HD21	45:Y:201:3PE:H321	1.90	0.53
4:D:71:GLU:OE2	8:H:134:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.89	0.53
40:o:102:GLU:CD	40:o:105:ARG:HH12	2.16	0.53
42:q:21:ARG:NH1	46:q:203:PC1:O14	2.42	0.53
12:L:140:LEU:O	12:L:140:LEU:HD23	2.09	0.53
16:P:46:ILE:N	16:P:46:ILE:HD12	2.23	0.53
12:L:87:MET:HA	12:L:87:MET:HE2	1.90	0.53
2:B:50:PHE:HE1	2:B:96:MET:HE3	1.74	0.53
5:E:163:ASP:OD2	5:E:190:ARG:NH1	2.39	0.53
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.42	0.52
24:Y:80:ARG:NH1	24:Y:88:ASN:OD1	2.41	0.52
10:J:90:LEU:HD22	10:J:90:LEU:H	1.73	0.52
12:L:183:ILE:HG21	13:M:382:VAL:HG11	1.91	0.52
41:p:109:LEU:C	41:p:109:LEU:HD23	2.35	0.52
5:E:156:ILE:O	5:E:158:ASP:N	2.41	0.52
6:F:407:LEU:HD23	6:F:407:LEU:O	2.08	0.52
13:M:125:THR:O	13:M:126:LEU:HD12	2.08	0.52
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.43	0.52
7:G:156:CYS:O	7:G:157:THR:OG1	2.21	0.52
16:P:335:GLN:N	16:P:335:GLN:OE1	2.43	0.52
14:N:215:MET:HE1	14:N:244:ILE:HG23	1.90	0.52
5:E:100:ILE:HG12	5:E:156:ILE:HD12	1.91	0.52
42:q:3:LEU:HD22	42:q:3:LEU:O	2.10	0.52
7:G:84:GLU:OE1	7:G:84:GLU:N	2.39	0.52
2:B:104:TYR:O	2:B:111:ARG:NH1	2.43	0.52
6:F:30:ASP:O	6:F:39:ARG:NH2	2.41	0.52
46:I:205:PC1:H142	25:Z:29:LEU:O	2.10	0.52
12:L:378:LEU:HD22	12:L:383:MET:HE2	1.91	0.52
12:L:13:LEU:O	12:L:13:LEU:HD23	2.09	0.52
20:T:21:LEU:HD12	20:T:21:LEU:O	2.09	0.52
23:X:46:ARG:NH2	33:h:142:ASP:OD1	2.40	0.52
2:B:116:MET:SD	2:B:156:LEU:HD22	2.50	0.51
3:C:150:ARG:NH1	3:C:153:THR:OG1	2.43	0.51
36:k:32:GLN:O	36:k:36:ALA:N	2.41	0.51
6:F:47:GLU:N	6:F:47:GLU:OE1	2.43	0.51
39:n:34:ASP:OD1	39:n:35:LYS:N	2.44	0.51
1:A:49:LEU:HD11	8:H:130:ILE:HD11	1.92	0.51
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.91	0.51
9:I:105:ARG:NH2	18:R:86:TYR:O	2.40	0.51
16:P:299:GLY:N	16:P:302:ASP:OD2	2.39	0.51
46:d:203:PC1:H322	46:d:203:PC1:H143	1.91	0.51
12:L:277:THR:HB	12:L:314:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:T:101:EHZ:O2	22:W:69:ASN:ND2	2.41	0.51
59:i:201:CHD:O7	59:i:201:CHD:H41	2.10	0.51
38:m:82:ASN:OD1	38:m:84:LYS:N	2.39	0.51
5:E:144:CYS:O	6:F:139:ARG:NH2	2.44	0.51
20:U:55:GLU:O	20:U:59:GLY:N	2.37	0.51
42:q:3:LEU:HD23	53:q:201:CDL:OB7	2.11	0.51
15:O:51:PHE:HB2	15:O:124:LEU:HD23	1.92	0.51
33:h:52:LEU:HD23	33:h:53:ALA:N	2.26	0.51
37:l:53:ARG:NE	37:l:57:GLU:OE1	2.44	0.51
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.76	0.51
6:F:99:GLU:O	6:F:139:ARG:NE	2.39	0.50
6:F:165:ASN:OD1	6:F:170:GLY:N	2.35	0.50
3:C:40:VAL:HG13	3:C:50:ILE:HD13	1.92	0.50
13:M:413:MET:HE3	13:M:413:MET:HA	1.92	0.50
25:Z:85:MET:HE3	25:Z:127:ARG:NH1	2.25	0.50
7:G:147:LYS:CD	7:G:149:ILE:HD11	2.41	0.50
32:g:34:ASP:OD1	32:g:35:GLU:N	2.45	0.50
27:b:68:HIS:N	27:b:71:ASP:OD2	2.44	0.50
8:H:231:ILE:HG23	8:H:270:PHE:CD2	2.46	0.50
6:F:314:THR:O	6:F:314:THR:HG23	2.12	0.50
15:O:116:LEU:HD11	15:O:259:LEU:HD23	1.94	0.50
29:d:82:MET:HE2	29:d:82:MET:HA	1.93	0.50
3:C:195:ARG:NH1	9:I:84:GLU:OE2	2.44	0.50
9:I:75:GLU:O	9:I:105:ARG:NH1	2.45	0.50
9:I:172:ASP:OD2	9:I:176:ARG:NH2	2.41	0.50
22:W:65:MET:HA	22:W:65:MET:HE2	1.93	0.50
34:i:90:THR:CG2	34:i:96:ILE:HD12	2.41	0.50
13:M:350:THR:HG22	13:M:350:THR:O	2.12	0.50
14:N:99:THR:HG21	14:N:153:LEU:HD23	1.94	0.49
12:L:341:MET:HE3	12:L:454:ILE:HD13	1.94	0.49
23:X:58:GLU:N	23:X:58:GLU:OE1	2.43	0.49
12:L:14:LEU:HD23	12:L:14:LEU:O	2.12	0.49
12:L:373:LEU:HD23	12:L:431:LEU:HD11	1.94	0.49
13:M:20:ASN:OD1	13:M:20:ASN:N	2.45	0.49
38:m:120:LEU:HD23	38:m:121:ASP:N	2.27	0.49
7:G:148:THR:C	7:G:149:ILE:HD12	2.36	0.49
5:E:164:LEU:HD13	5:E:169:ILE:HD11	1.93	0.49
12:L:560:ALA:O	12:L:565:THR:HG23	2.12	0.49
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.31	0.49
7:G:657:LEU:HD23	7:G:658:ALA:N	2.28	0.49
12:L:546:GLN:OE1	12:L:551:SER:OG	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:260:LEU:HD13	12:L:314:MET:HE1	1.94	0.49
26:a:68:ASN:O	26:a:68:ASN:ND2	2.46	0.49
4:D:342:MET:HE3	4:D:346:ILE:HD11	1.95	0.49
8:H:102:VAL:CG1	8:H:150:LEU:HD21	2.43	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.77	0.48
15:O:104:ARG:NH1	15:O:126:ARG:O	2.46	0.48
3:C:85:THR:HG21	21:V:115:ILE:CG1	2.43	0.48
4:D:47:LEU:HD11	8:H:126:LYS:NZ	2.28	0.48
5:E:111:ARG:NH1	6:F:260:GLY:O	2.46	0.48
12:L:264:TYR:N	12:L:265:PRO:CD	2.76	0.48
13:M:65:LEU:HD13	13:M:110:PHE:CE1	2.49	0.48
19:S:63:LYS:NZ	19:S:75:ASN:OD1	2.41	0.48
35:j:61:ASP:OD1	40:o:106:ARG:NH1	2.46	0.48
16:P:44:GLN:OE1	16:P:69:ILE:HD12	2.14	0.48
3:C:151:ILE:HG23	3:C:152:LEU:HG	1.94	0.48
12:L:195:THR:HG21	12:L:200:GLN:HB3	1.96	0.48
15:O:30:ASN:OD1	15:O:31:ILE:N	2.38	0.48
16:P:170:GLU:OE1	16:P:170:GLU:N	2.41	0.48
16:P:253:PHE:C	16:P:254:LEU:HD12	2.39	0.48
16:P:254:LEU:HD12	16:P:254:LEU:N	2.29	0.48
37:l:147:ASN:OD1	37:l:147:ASN:N	2.46	0.48
16:P:141:SER:O	16:P:147:ARG:NH1	2.40	0.48
19:S:22:LEU:HD23	19:S:22:LEU:N	2.29	0.48
29:d:109:TYR:HA	29:d:112:VAL:HG22	1.95	0.48
1:A:32:GLU:N	1:A:32:GLU:OE1	2.47	0.48
5:E:45:ALA:HB1	6:F:196:ILE:O	2.14	0.48
16:P:174:ARG:NH2	16:P:316:GLU:OE2	2.47	0.48
26:a:49:GLU:OE1	26:a:52:ARG:NH2	2.42	0.48
7:G:324:ASP:OD1	7:G:324:ASP:N	2.47	0.47
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.21	0.47
15:O:45:LYS:HB2	15:O:235:VAL:HG21	1.96	0.47
34:i:103:ILE:HD13	41:p:17:PRO:HG3	1.96	0.47
41:p:27:ASN:OD1	41:p:30:THR:N	2.41	0.47
12:L:13:LEU:HD23	12:L:13:LEU:C	2.39	0.47
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.50	0.47
13:M:113:MET:SD	13:M:175:ASN:ND2	2.81	0.47
39:n:30:CYS:O	39:n:32:HIS:N	2.45	0.47
39:n:49:GLU:O	39:n:50:HIS:ND1	2.47	0.47
1:A:10:ASN:OD1	8:H:10:ILE:HD11	2.14	0.47
7:G:329:ILE:CD1	7:G:626:VAL:HG21	2.44	0.47
8:H:84:THR:HG22	8:H:84:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:205:SER:OG	8:H:206:GLU:OE1	2.33	0.47
37:l:81:LEU:HD13	37:l:81:LEU:C	2.39	0.47
2:B:46:TRP:CZ3	52:H:401:U10:H1M1	2.50	0.47
4:D:233:ARG:NE	9:I:29:GLU:OE2	2.41	0.47
9:I:79:ALA:HB2	9:I:106:THR:HG23	1.97	0.47
16:P:91:VAL:HG23	16:P:126:VAL:HG11	1.97	0.47
23:X:79:GLU:N	23:X:79:GLU:OE1	2.47	0.47
4:D:47:LEU:HG	4:D:49:LEU:HD11	1.96	0.47
13:M:143:LEU:HD21	14:N:303:THR:CG2	2.45	0.47
28:c:43:LYS:O	28:c:47:GLY:N	2.48	0.47
59:i:201:CHD:H112	59:i:201:CHD:H12A	1.71	0.47
5:E:217:LEU:HD13	5:E:217:LEU:C	2.40	0.47
12:L:245:ALA:O	12:L:249:SER:OG	2.32	0.47
23:X:79:GLU:HB2	23:X:80:PRO:HD3	1.96	0.47
14:N:343:LEU:C	14:N:343:LEU:HD12	2.39	0.47
37:l:30:ARG:NH1	37:l:33:ASP:OD2	2.48	0.47
7:G:495:ARG:C	7:G:496:ILE:HD12	2.40	0.46
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.96	0.46
15:O:260:ARG:HA	15:O:263:VAL:HG22	1.96	0.46
25:Z:85:MET:HE1	25:Z:124:TYR:CE2	2.50	0.46
6:F:327:THR:OG1	6:F:328:GLY:N	2.48	0.46
7:G:484:THR:HG23	7:G:486:ASP:OD1	2.16	0.46
10:J:129:ASP:OD1	10:J:130:THR:N	2.48	0.46
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.97	0.46
16:P:166:ILE:HG21	16:P:230:PHE:CE2	2.50	0.46
35:j:70:ASP:OD1	35:j:70:ASP:N	2.48	0.46
37:l:80:ASP:HB3	37:l:83:MET:HE2	1.97	0.46
13:M:285:LEU:HD23	13:M:285:LEU:C	2.39	0.46
13:M:423:ILE:CD1	38:m:58:VAL:HG13	2.45	0.46
16:P:164:THR:OG1	16:P:223:ALA:O	2.31	0.46
4:D:22:THR:OG1	4:D:23:LYS:N	2.49	0.46
14:N:343:LEU:HD12	14:N:344:SER:N	2.31	0.46
1:A:48:ARG:NH1	1:A:49:LEU:O	2.49	0.46
7:G:280:THR:HG21	42:q:136:GLU:OE1	2.16	0.46
8:H:87:ILE:N	8:H:88:PRO:CD	2.79	0.46
8:H:201:THR:HG21	8:H:211:PHE:CE2	2.50	0.46
8:H:289:LEU:C	8:H:289:LEU:HD13	2.41	0.46
12:L:260:LEU:HD12	12:L:314:MET:HE1	1.98	0.46
13:M:375:LEU:C	13:M:375:LEU:HD13	2.41	0.46
15:O:125:GLU:O	15:O:126:ARG:C	2.59	0.46
32:g:120:LEU:HD21	41:p:162:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:ILE:HD13	4:D:330:VAL:HG11	1.98	0.46
5:E:149:VAL:HG13	6:F:105:CYS:SG	2.56	0.46
7:G:514:ILE:HG22	7:G:514:ILE:O	2.16	0.46
11:K:40:LEU:HD21	14:N:72:MET:HE2	1.98	0.46
1:A:90:MET:SD	1:A:90:MET:N	2.89	0.46
9:I:57:LEU:O	43:r:33:ARG:NH2	2.49	0.46
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.40	0.46
2:B:96:MET:HE2	4:D:61:VAL:HG11	1.97	0.46
4:D:328:ALA:O	4:D:351:LEU:HD11	2.15	0.46
5:E:55:GLN:O	5:E:59:GLY:N	2.41	0.46
8:H:73:LEU:HD22	8:H:118:TRP:CZ3	2.50	0.46
10:J:103:MET:HA	10:J:103:MET:HE2	1.98	0.46
10:J:37:GLY:HA2	11:K:38:LEU:HD21	1.97	0.45
12:L:279:CYS:O	12:L:283:ILE:HG22	2.16	0.45
12:L:341:MET:HE2	12:L:457:LEU:CD1	2.36	0.45
36:k:48:GLU:OE1	36:k:51:ARG:NH1	2.49	0.45
1:A:27:LEU:HD23	8:H:59:GLU:HG2	1.98	0.45
8:H:202:GLU:N	8:H:202:GLU:OE1	2.49	0.45
14:N:146:PHE:N	14:N:147:PRO:CD	2.80	0.45
7:G:47:SER:O	7:G:161:ARG:NH1	2.50	0.45
7:G:228:ILE:HG22	7:G:229:ASP:N	2.32	0.45
11:K:62:ILE:HG21	14:N:31:ILE:HD11	1.97	0.45
19:S:43:LEU:HD23	19:S:43:LEU:O	2.16	0.45
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.52	0.45
40:o:31:PRO:O	40:o:32:GLU:C	2.60	0.45
12:L:230:HIS:O	12:L:232:TRP:N	2.49	0.45
16:P:166:ILE:HG22	16:P:168:PRO:HD3	1.98	0.45
4:D:347:HIS:CD2	7:G:121:MET:HE3	2.51	0.45
46:M:604:PC1:O13	46:M:604:PC1:H132	2.17	0.45
14:N:318:PRO:HG2	14:N:320:MET:HE2	1.99	0.45
29:d:99:GLU:OE1	29:d:99:GLU:N	2.42	0.45
39:n:162:LEU:HD12	39:n:162:LEU:N	2.32	0.45
1:A:49:LEU:HD12	1:A:50:PRO:HD2	1.99	0.45
4:D:111:MET:SD	4:D:111:MET:N	2.88	0.45
10:J:163:ILE:O	10:J:167:VAL:HG23	2.16	0.45
12:L:550:SER:OG	13:M:275:ILE:HG23	2.17	0.45
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.32	0.45
33:h:49:GLU:OE1	33:h:68:LYS:NZ	2.26	0.45
7:G:667:THR:HG22	7:G:668:ILE:H	1.82	0.45
8:H:65:THR:O	8:H:65:THR:HG22	2.17	0.45
2:B:48:MET:HE3	2:B:50:PHE:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:284:VAL:HG12	7:G:559:VAL:HG13	1.98	0.45
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.49	0.44
12:L:286:LEU:C	12:L:286:LEU:HD13	2.41	0.44
22:W:123:VAL:HG23	22:W:124:GLY:N	2.32	0.44
6:F:84:LYS:NZ	6:F:211:ALA:O	2.36	0.44
12:L:173:LEU:HD23	12:L:173:LEU:O	2.17	0.44
15:O:22:SER:OG	15:O:119:GLY:O	2.25	0.44
16:P:101:THR:HG22	16:P:102:GLN:N	2.33	0.44
23:X:97:ARG:HD2	25:Z:59:LEU:HD13	1.97	0.44
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.99	0.44
19:S:64:LEU:HB2	19:S:78:LEU:HD11	2.00	0.44
10:J:123:GLY:HA2	11:K:3:MET:HE2	1.98	0.44
12:L:572:LYS:O	12:L:575:THR:OG1	2.27	0.44
34:i:92:LYS:NZ	45:i:202:3PE:O14	2.50	0.44
13:M:278:ARG:NH1	37:l:82:ASP:OD1	2.50	0.44
8:H:285:LEU:HD12	8:H:285:LEU:C	2.43	0.44
14:N:156:THR:HG23	45:Y:204:3PE:H262	1.99	0.44
37:l:65:ASP:OD1	38:m:43:LYS:NZ	2.50	0.44
41:p:8:VAL:O	41:p:108:ARG:NH2	2.48	0.44
13:M:264:LEU:O	13:M:268:GLY:N	2.51	0.44
3:C:205:ALA:O	43:r:60:ARG:NH1	2.50	0.44
5:E:147:ALA:HB2	6:F:108:ARG:NH1	2.32	0.44
7:G:226:GLU:OE1	7:G:239:VAL:HG22	2.17	0.44
9:I:129:ASP:N	9:I:129:ASP:OD1	2.51	0.44
12:L:562:LEU:HB2	12:L:563:PRO:HD3	2.00	0.44
15:O:24:LEU:HD13	15:O:122:VAL:CG2	2.48	0.44
5:E:114:ASP:OD1	5:E:115:SER:N	2.51	0.44
7:G:149:ILE:HD12	7:G:149:ILE:N	2.31	0.44
16:P:30:LEU:HD12	16:P:207:ILE:HD11	1.99	0.44
17:Q:93:VAL:HG13	17:Q:103:TYR:CZ	2.53	0.44
6:F:214:GLY:N	6:F:218:CYS:O	2.47	0.43
7:G:317:ALA:HB3	7:G:343:LEU:HD13	1.99	0.43
13:M:109:THR:HG21	13:M:238:LEU:HD22	2.00	0.43
13:M:167:ILE:HD13	13:M:249:ILE:HD12	2.00	0.43
20:U:62:ILE:HD12	20:U:62:ILE:N	2.33	0.43
23:X:25:LYS:NZ	23:X:94:GLN:O	2.29	0.43
35:j:39:ARG:NH1	35:j:43:ASP:OD1	2.51	0.43
4:D:7:ASP:OD1	4:D:9:GLU:N	2.51	0.43
21:V:57:MET:CE	21:V:71:LEU:HD23	2.47	0.43
4:D:233:ARG:NH1	46:I:204:PC1:O21	2.51	0.43
4:D:342:MET:HE1	7:G:105:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:348:VAL:HG12	7:G:349:PHE:N	2.33	0.43
8:H:110:SER:O	8:H:113:VAL:HG12	2.18	0.43
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.48	0.43
13:M:350:THR:HG22	39:n:98:VAL:HG22	1.99	0.43
35:j:50:HIS:O	35:j:51:PHE:C	2.62	0.43
19:S:94:LEU:HD23	19:S:94:LEU:O	2.18	0.43
32:g:81:PRO:O	32:g:82:ASP:C	2.59	0.43
12:L:283:ILE:CD1	37:l:112:MET:HE2	2.48	0.43
45:L:705:3PE:H2	24:Y:109:ILE:HD11	1.99	0.43
34:i:83:TYR:HD1	41:p:44:VAL:HG13	1.84	0.43
5:E:217:LEU:HD12	6:F:44:LYS:HG2	1.99	0.43
5:E:217:LEU:HD11	6:F:48:ILE:CG1	2.49	0.43
7:G:641:TYR:CE2	19:S:36:ILE:HG21	2.53	0.43
29:d:119:VAL:HG21	41:p:146:GLY:HA3	2.00	0.43
7:G:403:ASP:OD2	44:s:70:ARG:NH2	2.52	0.43
12:L:230:HIS:N	12:L:231:PRO:CD	2.81	0.43
15:O:25:ILE:HD12	15:O:25:ILE:N	2.34	0.43
14:N:272:LYS:HE3	33:h:108:LEU:HD21	2.00	0.42
38:m:80:ARG:O	38:m:82:ASN:N	2.52	0.42
6:F:188:GLU:OE1	6:F:189:GLU:N	2.52	0.42
8:H:224:PHE:CD2	52:H:401:U10:H111	2.53	0.42
13:M:391:ILE:O	13:M:391:ILE:HG22	2.20	0.42
16:P:185:ILE:HG22	16:P:185:ILE:O	2.18	0.42
6:F:306:LEU:C	6:F:306:LEU:HD12	2.44	0.42
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.54	0.42
20:T:39:ASP:OD1	20:T:39:ASP:N	2.52	0.42
9:I:31:ILE:HD12	45:Z:201:3PE:H3A2	2.00	0.42
12:L:458:LEU:HD23	12:L:458:LEU:O	2.19	0.42
13:M:270:ILE:HD12	13:M:270:ILE:H	1.84	0.42
32:g:98:LYS:NZ	41:p:5:ASP:OD1	2.47	0.42
34:i:90:THR:HG22	34:i:96:ILE:HD12	2.02	0.42
7:G:351:THR:HG22	7:G:351:THR:O	2.18	0.42
12:L:369:THR:OG1	12:L:445:GLU:OE1	2.25	0.42
20:T:56:ASP:OD1	20:T:57:GLU:N	2.52	0.42
21:V:37:ILE:O	21:V:44:ARG:NH2	2.52	0.42
2:B:170:GLU:OE1	2:B:172:ARG:NE	2.52	0.42
7:G:321:GLY:HA2	7:G:496:ILE:HG23	2.01	0.42
7:G:329:ILE:HD11	7:G:626:VAL:HG21	2.02	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.00	0.42
41:p:29:ILE:HD12	41:p:29:ILE:N	2.35	0.42
4:D:300:ARG:NH2	4:D:420:THR:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L:702:3PE:H2C2	14:N:93:MET:HE2	2.02	0.42
42:q:3:LEU:HD13	42:q:3:LEU:C	2.45	0.42
8:H:108:MET:HE1	46:H:402:PC1:H361	2.02	0.42
10:J:55:MET:HA	10:J:55:MET:HE2	2.01	0.42
12:L:131:LEU:HD23	12:L:131:LEU:O	2.20	0.42
34:i:111:GLU:OE1	34:i:111:GLU:N	2.52	0.42
3:C:49:GLU:OE2	3:C:106:ARG:NH2	2.39	0.41
7:G:26:VAL:HG13	7:G:79:ILE:HD13	2.02	0.41
7:G:490:MET:HE3	7:G:491:ASN:H	1.85	0.41
11:K:40:LEU:CD2	14:N:72:MET:HE2	2.50	0.41
24:Y:101:GLY:O	24:Y:105:ARG:N	2.53	0.41
2:B:45:LEU:O	2:B:74:VAL:HA	2.20	0.41
11:K:37:MET:HG3	11:K:67:ALA:CB	2.50	0.41
14:N:194:LEU:HB3	14:N:195:PRO:HD3	2.01	0.41
16:P:101:THR:HG22	16:P:102:GLN:H	1.85	0.41
20:U:17:TYR:OH	36:k:21:TRP:NE1	2.37	0.41
27:b:61:ASN:ND2	27:b:61:ASN:O	2.53	0.41
42:q:77:VAL:HG22	46:q:202:PC1:H133	2.03	0.41
1:A:73:LEU:N	1:A:74:PRO:HD2	2.35	0.41
6:F:287:VAL:HG21	6:F:294:LEU:HD13	2.02	0.41
12:L:2:ASN:N	12:L:2:ASN:OD1	2.53	0.41
17:Q:61:THR:HG23	17:Q:64:ARG:HH12	1.84	0.41
5:E:87:TYR:CG	6:F:181:ALA:HB3	2.55	0.41
6:F:306:LEU:HD23	6:F:347:ILE:HD11	2.02	0.41
7:G:89:ALA:O	7:G:93:VAL:HG23	2.20	0.41
7:G:323:VAL:HG12	7:G:324:ASP:N	2.35	0.41
8:H:89:LEU:HD13	8:H:236:ILE:HG21	2.03	0.41
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.56	0.41
16:P:4:ALA:O	16:P:5:VAL:C	2.63	0.41
32:g:103:HIS:HB2	32:g:105:LEU:HD13	2.01	0.41
35:j:66:ILE:N	35:j:66:ILE:HD12	2.36	0.41
4:D:128:ILE:CD1	4:D:330:VAL:HG11	2.50	0.41
9:I:64:GLU:O	9:I:134:GLY:N	2.53	0.41
9:I:132:VAL:HG21	9:I:165:ILE:HG21	2.03	0.41
15:O:31:ILE:O	15:O:179:VAL:HG13	2.21	0.41
22:W:116:ASP:N	22:W:116:ASP:OD1	2.54	0.41
7:G:110:GLN:HG3	7:G:110:GLN:O	2.20	0.41
13:M:442:LEU:HB2	13:M:443:PRO:HD3	2.03	0.41
17:Q:60:ASP:OD1	17:Q:60:ASP:N	2.52	0.41
25:Z:119:MET:HE2	30:e:71:THR:CG2	2.50	0.41
33:h:109:GLU:OE2	33:h:112:ARG:NH2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:213:TYR:O	7:G:213:TYR:CG	2.74	0.41
32:g:59:ARG:HE	48:g:202:PLC:H82	1.84	0.41
38:m:76:TYR:N	38:m:77:PRO:HD2	2.36	0.41
12:L:419:THR:O	12:L:423:SER:OG	2.38	0.41
14:N:193:VAL:O	14:N:193:VAL:HG22	2.20	0.41
33:h:114:MET:O	33:h:118:GLY:N	2.42	0.41
1:A:44:MET:HE1	4:D:65:VAL:HG13	2.03	0.41
3:C:188:VAL:O	3:C:188:VAL:HG13	2.21	0.41
6:F:49:LEU:HD23	6:F:127:ARG:HG2	2.02	0.41
8:H:236:ILE:HG23	8:H:259:PHE:CE1	2.56	0.41
12:L:304:PHE:HZ	12:L:526:LEU:HD22	1.85	0.41
53:M:602:CDL:H792	14:N:242:VAL:HG13	2.01	0.41
15:O:133:VAL:HG23	15:O:134:PHE:N	2.36	0.41
29:d:9:ALA:HB1	29:d:12:GLN:OE1	2.21	0.41
37:l:66:HIS:O	37:l:70:ARG:N	2.47	0.41
39:n:169:ILE:N	39:n:169:ILE:HD12	2.35	0.41
11:K:36:MET:HE2	14:N:68:MET:HB3	2.02	0.41
15:O:15:THR:HG23	15:O:253:ASP:OD1	2.21	0.41
16:P:72:ASP:OD1	16:P:72:ASP:N	2.52	0.41
2:B:179:ARG:O	16:P:101:THR:HG21	2.21	0.40
8:H:87:ILE:CG1	8:H:88:PRO:HD3	2.51	0.40
14:N:41:ILE:HD13	14:N:44:MET:HE2	2.03	0.40
14:N:290:LEU:O	14:N:294:MET:HG2	2.21	0.40
31:f:11:TRP:O	31:f:14:VAL:HG22	2.21	0.40
59:i:201:CHD:H183	59:i:201:CHD:H20	1.91	0.40
2:B:69:MET:HE2	2:B:74:VAL:HG12	2.02	0.40
3:C:154:ASP:OD1	3:C:155:TYR:N	2.55	0.40
8:H:113:VAL:CG2	8:H:136:VAL:HG13	2.52	0.40
52:H:401:U10:H151	52:H:401:U10:H18	2.03	0.40
10:J:5:ILE:HG23	10:J:6:VAL:N	2.36	0.40
11:K:1:FME:O	11:K:2:SER:HB2	2.22	0.40
12:L:561:ILE:HG13	12:L:562:LEU:N	2.36	0.40
19:S:76:VAL:HG13	19:S:76:VAL:O	2.22	0.40
37:l:32:GLU:OE1	37:l:32:GLU:N	2.53	0.40
6:F:94:VAL:HG11	6:F:192:LEU:HD22	2.04	0.40
8:H:61:LEU:HD22	8:H:61:LEU:N	2.36	0.40
12:L:7:LEU:HA	12:L:10:VAL:HG12	2.03	0.40
20:U:56:ASP:OD1	39:n:24:ARG:NH2	2.54	0.40
29:d:101:PHE:CZ	33:h:110:VAL:HG22	2.56	0.40
32:g:23:THR:O	32:g:23:THR:HG22	2.20	0.40
40:o:106:ARG:O	40:o:110:ARG:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:104:THR:O	5:E:104:THR:HG22	2.20	0.40
7:G:308:GLN:NE2	7:G:607:ALA:O	2.55	0.40
9:I:76:ARG:O	9:I:128:VAL:HG21	2.21	0.40
10:J:175:ASN:O	10:J:175:ASN:ND2	2.54	0.40
12:L:120:TYR:CB	12:L:154:LEU:HD21	2.52	0.40
13:M:130:LEU:HD21	14:N:294:MET:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	154/216 (71%)	145 (94%)	9 (6%)	0	100	100
3	C	205/266 (77%)	196 (96%)	9 (4%)	0	100	100
4	D	414/463 (89%)	396 (96%)	18 (4%)	0	100	100
5	E	212/249 (85%)	200 (94%)	11 (5%)	1 (0%)	24	55
6	F	430/464 (93%)	407 (95%)	23 (5%)	0	100	100
7	G	689/727 (95%)	646 (94%)	43 (6%)	0	100	100
8	H	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	163 (94%)	9 (5%)	1 (1%)	21	52
11	K	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	12	40
12	L	604/606 (100%)	572 (95%)	32 (5%)	0	100	100
13	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
14	N	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
15	O	318/343 (93%)	306 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	335/380 (88%)	319 (95%)	16 (5%)	0	100	100
17	Q	127/175 (73%)	122 (96%)	5 (4%)	0	100	100
18	R	94/124 (76%)	88 (94%)	6 (6%)	0	100	100
19	S	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
20	T	86/156 (55%)	81 (94%)	5 (6%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
21	V	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
22	W	114/128 (89%)	109 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	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%)	66 (97%)	2 (3%)	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
30	e	96/106 (91%)	90 (94%)	6 (6%)	0	100	100
31	f	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	6	29
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%)	119 (95%)	6 (5%)	0	100	100
35	j	69/108 (64%)	64 (93%)	5 (7%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	m	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	p	172/176 (98%)	168 (98%)	4 (2%)	0	100	100
42	q	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
43	r	91/113 (80%)	85 (93%)	6 (7%)	0	100	100
44	s	42/109 (38%)	39 (93%)	3 (7%)	0	100	100
All	All	8175/9213 (89%)	7805 (96%)	366 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	157	ASN
10	J	80	PRO
11	K	2	SER
31	f	3	LEU

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	61
2	B	132/175 (75%)	129 (98%)	3 (2%)	44	66
3	C	188/228 (82%)	185 (98%)	3 (2%)	55	72
4	D	362/392 (92%)	352 (97%)	10 (3%)	38	62
5	E	183/205 (89%)	178 (97%)	5 (3%)	39	63
6	F	346/368 (94%)	335 (97%)	11 (3%)	34	60
7	G	579/608 (95%)	565 (98%)	14 (2%)	43	65
8	H	274/274 (100%)	268 (98%)	6 (2%)	45	66
9	I	151/175 (86%)	148 (98%)	3 (2%)	48	68
10	J	141/141 (100%)	136 (96%)	5 (4%)	32	58
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	75
12	L	533/533 (100%)	526 (99%)	7 (1%)	61	74
13	M	412/412 (100%)	405 (98%)	7 (2%)	53	71
14	N	315/315 (100%)	314 (100%)	1 (0%)	86	86
15	O	283/303 (93%)	276 (98%)	7 (2%)	42	64
16	P	293/327 (90%)	281 (96%)	12 (4%)	27	55
17	Q	116/153 (76%)	112 (97%)	4 (3%)	32	59
18	R	79/97 (81%)	77 (98%)	2 (2%)	42	64
19	S	76/82 (93%)	71 (93%)	5 (7%)	15	43
20	T	81/135 (60%)	75 (93%)	6 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	81/135 (60%)	77 (95%)	4 (5%)	22	51
21	V	101/102 (99%)	98 (97%)	3 (3%)	36	61
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	78
23	X	154/155 (99%)	151 (98%)	3 (2%)	50	68
24	Y	101/102 (99%)	98 (97%)	3 (3%)	36	61
25	Z	120/121 (99%)	117 (98%)	3 (2%)	42	64
26	a	59/59 (100%)	57 (97%)	2 (3%)	32	59
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	62
30	e	89/96 (93%)	85 (96%)	4 (4%)	24	53
31	f	54/54 (100%)	53 (98%)	1 (2%)	50	68
32	g	92/131 (70%)	90 (98%)	2 (2%)	45	66
33	h	121/158 (77%)	119 (98%)	2 (2%)	53	71
34	i	120/121 (99%)	116 (97%)	4 (3%)	33	59
35	j	61/84 (73%)	58 (95%)	3 (5%)	22	51
36	k	63/76 (83%)	61 (97%)	2 (3%)	34	60
37	l	140/159 (88%)	137 (98%)	3 (2%)	47	67
38	m	113/114 (99%)	108 (96%)	5 (4%)	25	54
39	n	156/161 (97%)	151 (97%)	5 (3%)	34	60
40	o	110/120 (92%)	108 (98%)	2 (2%)	51	70
41	p	155/157 (99%)	149 (96%)	6 (4%)	28	56
42	q	130/130 (100%)	123 (95%)	7 (5%)	20	49
43	r	85/97 (88%)	81 (95%)	4 (5%)	23	52
44	s	43/92 (47%)	42 (98%)	1 (2%)	44	66
All	All	7206/7891 (91%)	7018 (97%)	188 (3%)	41	64

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	87	MET
1	A	90	MET

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Mol	Chain	Res	Type
2	B	42	ARG
2	B	50	PHE
2	B	54	CYS
3	C	8	ARG
3	C	14	ARG
3	C	117	ILE
4	D	23	LYS
4	D	40	LYS
4	D	49	LEU
4	D	59	HIS
4	D	75	LYS
4	D	94	LYS
4	D	165	THR
4	D	172	GLU
4	D	290	ARG
4	D	420	THR
5	E	57	GLN
5	E	157	ASN
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	188	GLU
6	F	249	ARG
6	F	314	THR
6	F	365	CYS
6	F	370	ASP
6	F	376	MET
6	F	402	HIS
6	F	432	GLN
7	G	33	VAL
7	G	61	LYS
7	G	75	LYS
7	G	121	MET
7	G	180	ASP
7	G	324	ASP
7	G	364	LEU
7	G	476	LYS
7	G	499	GLN
7	G	536	ASP

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Mol	Chain	Res	Type
7	G	539	LYS
7	G	540	ASP
7	G	613	TYR
7	G	643	GLN
8	H	5	ASN
8	H	176	LEU
8	H	200	LEU
8	H	222	LEU
8	H	254	LEU
8	H	296	LEU
9	I	14	MET
9	I	93	THR
9	I	129	ASP
10	J	55	MET
10	J	81	GLU
10	J	103	MET
10	J	122	LEU
10	J	135	PHE
11	K	73	LEU
12	L	7	LEU
12	L	223	LYS
12	L	358	LYS
12	L	479	GLN
12	L	487	LYS
12	L	581	LYS
12	L	605	HIS
13	M	20	ASN
13	M	130	LEU
13	M	201	MET
13	M	207	MET
13	M	315	LEU
13	M	340	ARG
13	M	418	LYS
14	N	71	MET
15	O	40	LYS
15	O	72	GLN
15	O	122	VAL
15	O	146	LYS
15	O	252	ASN
15	O	279	LEU
15	O	315	LYS
16	P	2	HIS

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Mol	Chain	Res	Type
16	P	52	GLU
16	P	122	LYS
16	P	136	ASN
16	P	139	ILE
16	P	144	LYS
16	P	196	LEU
16	P	224	ARG
16	P	226	LYS
16	P	327	LEU
16	P	335	GLN
16	P	338	LYS
17	Q	21	THR
17	Q	34	LYS
17	Q	116	LYS
17	Q	127	ARG
18	R	83	THR
18	R	95	HIS
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	29	LYS
20	T	30	LEU
20	T	69	LYS
20	T	86	VAL
20	T	88	GLU
20	U	12	LYS
20	U	29	LYS
20	U	69	LYS
20	U	83	LYS
21	V	39	LYS
21	V	65	LYS
21	V	115	ILE
22	W	56	LYS
23	X	65	CYS
23	X	146	ARG
23	X	158	LYS
24	Y	43	LYS
24	Y	50	GLU
24	Y	114	CYS

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Mol	Chain	Res	Type
25	Z	4	LYS
25	Z	51	LYS
25	Z	65	GLU
26	a	34	LYS
26	a	68	ASN
29	d	6	GLN
29	d	82	MET
29	d	104	LYS
30	e	56	LYS
30	e	84	LYS
30	e	87	LYS
30	e	90	LYS
31	f	49	LYS
32	g	49	LYS
32	g	84	ARG
33	h	106	LYS
33	h	130	LYS
34	i	49	PHE
34	i	50	LEU
34	i	100	LYS
34	i	121	GLU
35	j	47	VAL
35	j	51	PHE
35	j	61	ASP
36	k	71	LYS
36	k	91	LYS
37	l	6	LYS
37	l	115	MET
37	l	147	ASN
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	95	CYS
39	n	158	LYS
39	n	159	GLN
40	o	7	ARG
40	o	111	LYS
41	p	34	LYS

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Mol	Chain	Res	Type
41	p	57	LYS
41	p	88	GLU
41	p	90	GLN
41	p	116	GLU
41	p	136	LYS
42	q	3	LEU
42	q	53	LYS
42	q	59	HIS
42	q	60	ARG
42	q	107	LYS
42	q	136	GLU
42	q	144	TYR
43	r	24	GLN
43	r	60	ARG
43	r	101	LYS
43	r	105	LEU
44	s	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	41	GLN
4	D	149	ASN
4	D	217	ASN
4	D	306	GLN
5	E	150	ASN
7	G	43	HIS
7	G	255	HIS
7	G	392	ASN
7	G	401	HIS
7	G	475	GLN
8	H	5	ASN
8	H	47	GLN
8	H	250	HIS
8	H	304	HIS
12	L	446	ASN
12	L	447	ASN
12	L	471	ASN
13	M	51	ASN
13	M	293	HIS
13	M	338	HIS
13	M	399	ASN

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Mol	Chain	Res	Type
14	N	49	ASN
14	N	77	ASN
14	N	134	GLN
14	N	268	GLN
15	O	120	GLN
15	O	180	GLN
15	O	251	GLN
16	P	243	GLN
17	Q	29	HIS
17	Q	44	ASN
17	Q	67	ASN
17	Q	99	ASN
22	W	98	GLN
25	Z	111	HIS
26	a	27	HIS
29	d	117	HIS
32	g	27	GLN
33	h	135	HIS
34	i	58	ASN
34	i	82	HIS
35	j	6	HIS
35	j	24	GLN
37	l	99	ASN
37	l	136	ASN
39	n	32	HIS
40	o	43	GLN
42	q	31	ASN
42	q	113	HIS

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$
8	FME	H	1	8	8,9,10	1.49	1 (12%)	8,9,11	1.49	2 (25%)
11	FME	K	1	11	8,9,10	1.50	1 (12%)	8,9,11	1.21	0
34	SAC	i	1	34	7,8,9	1.76	1 (14%)	7,9,11	1.70	1 (14%)
29	AME	d	1	29	9,10,11	1.51	1 (11%)	9,11,13	1.37	1 (11%)
4	2MR	D	85	4	10,12,13	2.46	2 (20%)	5,13,15	1.24	1 (20%)
14	FME	N	1	14	8,9,10	1.49	1 (12%)	8,9,11	1.46	2 (25%)
27	AYA	b	1	27	6,7,8	1.89	1 (16%)	6,8,10	1.44	1 (16%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	8,9,11	1.36	1 (12%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	8,9,11	1.46	2 (25%)
38	SAC	m	1	38	7,8,9	1.73	1 (14%)	7,9,11	1.26	1 (14%)
42	AME	q	1	42	9,10,11	1.52	1 (11%)	9,11,13	1.40	1 (11%)
12	FME	L	1	12	8,9,10	1.50	1 (12%)	8,9,11	1.40	1 (12%)
13	FME	M	1	13	8,9,10	1.52	1 (12%)	8,9,11	1.41	1 (12%)
24	AYA	Y	1	24	6,7,8	1.88	2 (33%)	6,8,10	1.33	1 (16%)
43	AYA	r	1	43	6,7,8	1.90	1 (16%)	6,8,10	1.36	1 (16%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AYA	Y	1	24	-	1/5/6/8	-
43	AYA	r	1	43	-	1/5/6/8	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.43	1.44	1.33
4	D	85	2MR	CZ-NE	5.16	1.45	1.34
11	K	1	FME	CN-N	3.77	1.45	1.33
13	M	1	FME	CN-N	3.76	1.45	1.33
10	J	1	FME	CN-N	3.76	1.45	1.33
12	L	1	FME	CN-N	3.72	1.45	1.33
14	N	1	FME	CN-N	3.71	1.45	1.33
1	A	1	FME	CN-N	3.69	1.45	1.33
8	H	1	FME	CN-N	3.66	1.45	1.33
34	i	1	SAC	C1A-N	3.61	1.46	1.34
38	m	1	SAC	C1A-N	3.50	1.45	1.34
27	b	1	AYA	CT-N	3.50	1.45	1.34
43	r	1	AYA	CT-N	3.48	1.45	1.34
42	q	1	AME	CT1-N	3.45	1.45	1.34
29	d	1	AME	CT1-N	3.45	1.45	1.34
24	Y	1	AYA	CT-N	3.44	1.45	1.34
24	Y	1	AYA	OT-CT	-2.04	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	3.34	121.66	116.12
42	q	1	AME	CT2-CT1-N	2.53	120.31	116.12
29	d	1	AME	CT2-CT1-N	2.48	120.23	116.12
38	m	1	SAC	C2A-C1A-N	2.41	120.12	116.12
43	r	1	AYA	CM-CT-N	2.40	120.11	116.12
27	b	1	AYA	CM-CT-N	2.38	120.06	116.12
8	H	1	FME	CA-N-CN	-2.34	119.23	122.82
14	N	1	FME	CA-N-CN	-2.26	119.35	122.82
8	H	1	FME	O1-CN-N	-2.22	119.57	125.32
24	Y	1	AYA	CM-CT-N	2.20	119.77	116.12
1	A	1	FME	O1-CN-N	-2.17	119.71	125.32
1	A	1	FME	CA-N-CN	-2.16	119.50	122.82
12	L	1	FME	O1-CN-N	-2.14	119.80	125.32
4	D	85	2MR	CD-NE-CZ	-2.13	119.36	123.36
10	J	1	FME	O1-CN-N	-2.08	119.93	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1	FME	O1-CN-N	-2.07	119.98	125.32
14	N	1	FME	O1-CN-N	-2.02	120.09	125.32

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 72 ligands modelled in this entry, 4 are monoatomic - leaving 68 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	3PE	J	202	-	32,32,50	1.07	4 (12%)	35,37,55	1.11	2 (5%)
46	PC1	A	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.07	2 (5%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
53	CDL	J	201	-	35,35,99	1.35	6 (17%)	41,47,111	1.48	3 (7%)
58	EHZ	T	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.75	10 (27%)
46	PC1	q	203	-	29,29,53	1.26	4 (13%)	35,37,61	1.15	2 (5%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
52	U10	H	401	-	28,28,63	2.01	15 (53%)	36,37,79	1.97	8 (22%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
49	FES	E	301	5	0,4,4	-	-	-	-	-
48	PLC	B	202	-	37,37,41	0.53	0	43,45,49	0.55	0
46	PC1	I	205	-	36,36,53	1.14	4 (11%)	42,44,61	1.03	2 (4%)
45	3PE	Z	201	-	44,44,50	0.93	4 (9%)	47,49,55	1.06	2 (4%)
46	PC1	A	202	-	34,34,53	1.18	4 (11%)	40,42,61	1.04	2 (5%)
53	CDL	h	201	-	79,79,99	0.99	8 (10%)	85,91,111	1.12	4 (4%)
55	DGT	O	401	56	32,33,33	3.33	14 (43%)	48,52,52	1.93	14 (29%)
53	CDL	X	201	-	86,86,99	0.94	8 (9%)	92,98,111	1.10	4 (4%)
50	FMN	F	501	-	33,33,33	2.73	10 (30%)	48,50,50	1.73	12 (25%)
45	3PE	Y	201	-	26,26,50	1.17	4 (15%)	29,31,55	1.13	2 (6%)
45	3PE	o	202	-	34,34,50	0.98	3 (8%)	37,39,55	1.09	1 (2%)
45	3PE	i	202	-	44,44,50	0.92	4 (9%)	47,49,55	1.09	2 (4%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
53	CDL	M	602	-	90,90,99	0.92	7 (7%)	96,102,111	1.14	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	L	706	-	46,46,53	1.00	4 (8%)	52,54,61	1.07	2 (3%)
45	3PE	L	702	-	34,34,50	0.98	3 (8%)	37,39,55	1.13	1 (2%)
48	PLC	g	202	-	31,31,41	0.59	0	37,39,49	0.58	0
45	3PE	m	202	-	32,32,50	1.07	4 (12%)	35,37,55	1.15	2 (5%)
46	PC1	q	202	46	47,47,53	1.02	4 (8%)	53,55,61	0.97	2 (3%)
45	3PE	b	101	-	46,46,50	0.91	4 (8%)	49,51,55	1.06	2 (4%)
45	3PE	N	404	-	44,44,50	0.93	4 (9%)	47,49,55	1.04	2 (4%)
45	3PE	M	603	-	49,49,50	0.89	3 (6%)	52,54,55	1.02	2 (3%)
58	EHZ	U	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.63	7 (19%)
48	PLC	b	102	-	31,31,41	0.57	0	37,39,49	0.61	0
46	PC1	H	402	-	47,47,53	1.01	4 (8%)	53,55,61	1.05	2 (3%)
45	3PE	L	703	-	43,43,50	0.94	4 (9%)	46,48,55	1.09	2 (4%)
60	MYR	o	201	40	13,14,15	0.43	0	12,13,15	0.81	0
47	SF4	F	502	6	0,12,12	-	-	-	-	-
48	PLC	L	707	-	26,26,41	0.62	0	32,34,49	0.62	0
48	PLC	N	405	-	25,25,41	0.63	0	31,33,49	0.64	0
53	CDL	N	401	-	73,73,99	1.02	8 (10%)	79,85,111	1.13	4 (5%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
46	PC1	P	502	46	45,45,53	1.04	3 (6%)	51,53,61	1.03	3 (5%)
46	PC1	M	605	-	25,25,53	1.36	4 (16%)	31,33,61	0.99	2 (6%)
46	PC1	Y	205	-	39,39,53	1.10	4 (10%)	45,47,61	1.06	2 (4%)
45	3PE	N	403	-	44,44,50	0.92	4 (9%)	47,49,55	1.05	2 (4%)
45	3PE	L	704	-	45,45,50	0.93	4 (8%)	48,50,55	1.11	2 (4%)
59	CHD	i	201	-	32,32,32	3.25	11 (34%)	51,51,51	2.38	16 (31%)
53	CDL	q	201	-	60,60,99	1.12	7 (11%)	66,72,111	1.16	4 (6%)
45	3PE	L	705	-	36,36,50	1.01	4 (11%)	39,41,55	1.16	2 (5%)
45	3PE	K	101	-	43,43,50	0.93	4 (9%)	46,48,55	1.12	2 (4%)
46	PC1	d	203	-	38,38,53	1.12	4 (10%)	44,46,61	1.02	2 (4%)
45	3PE	A	201	-	33,33,50	1.05	4 (12%)	36,38,55	1.19	2 (5%)
57	NDP	P	501	-	51,52,52	3.98	27 (52%)	71,80,80	1.93	13 (18%)
46	PC1	M	604	-	43,43,53	1.04	4 (9%)	49,51,61	1.05	2 (4%)
45	3PE	Y	203	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
53	CDL	d	201	-	64,64,99	1.09	8 (12%)	70,76,111	1.11	4 (5%)
45	3PE	g	201	-	28,28,50	1.15	4 (14%)	31,33,55	1.36	3 (9%)
45	3PE	d	202	-	48,48,50	0.89	4 (8%)	51,53,55	1.09	2 (3%)
45	3PE	I	203	-	35,35,50	1.03	4 (11%)	38,40,55	1.12	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	Y	202	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
53	CDL	L	701	-	86,86,99	0.95	7 (8%)	92,98,111	1.14	6 (6%)
45	3PE	N	402	-	48,48,50	0.89	4 (8%)	51,53,55	1.08	2 (3%)
45	3PE	m	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.14	2 (4%)
46	PC1	I	204	-	53,53,53	0.96	4 (7%)	59,61,61	0.98	2 (3%)
47	SF4	I	201	9	0,12,12	-	-	-		
46	PC1	h	202	-	30,30,53	1.24	4 (13%)	36,38,61	1.08	2 (5%)
45	3PE	Y	204	-	35,35,50	1.02	4 (11%)	38,40,55	1.19	2 (5%)
46	PC1	H	403	-	38,38,53	1.11	4 (10%)	44,46,61	0.97	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	J	202	-	-	21/36/36/54	-
46	PC1	A	203	-	-	11/38/38/57	-
53	CDL	J	201	-	-	18/42/42/110	-
47	SF4	G	802	7	-	-	0/6/5/5
58	EHZ	T	101	20	-	11/42/44/45	-
46	PC1	q	203	-	-	15/33/33/57	-
47	SF4	I	202	9	-	-	0/6/5/5
52	U10	H	401	-	-	2/21/45/87	0/1/1/1
47	SF4	G	801	7	-	-	0/6/5/5
49	FES	E	301	5	-	-	0/1/1/1
48	PLC	B	202	-	-	14/41/41/45	-
46	PC1	I	205	-	-	14/40/40/57	-
45	3PE	Z	201	-	-	25/48/48/54	-
46	PC1	A	202	-	-	20/38/38/57	-
53	CDL	h	201	-	-	32/90/90/110	-
55	DGT	O	401	56	-	8/22/34/34	0/3/3/3
53	CDL	X	201	-	-	45/97/97/110	-
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
45	3PE	Y	201	-	-	11/30/30/54	-
45	3PE	o	202	-	-	13/37/37/54	-
45	3PE	i	202	-	-	21/48/48/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	FES	G	803	7	-	-	0/1/1/1
53	CDL	M	602	-	-	42/101/101/110	-
46	PC1	L	706	-	-	23/50/50/57	-
45	3PE	L	702	-	-	14/37/37/54	-
48	PLC	g	202	-	-	7/34/34/45	-
45	3PE	m	202	-	-	11/36/36/54	-
46	PC1	q	202	46	-	15/51/51/57	-
45	3PE	b	101	-	-	15/50/50/54	-
45	3PE	N	404	-	-	20/48/48/54	-
45	3PE	M	603	-	-	23/53/53/54	-
58	EHZ	U	101	20	-	9/42/44/45	-
48	PLC	b	102	-	-	12/35/35/45	-
46	PC1	H	402	-	-	18/51/51/57	-
45	3PE	L	703	-	-	19/47/47/54	-
60	MYR	o	201	40	-	3/12/12/13	-
48	PLC	L	707	-	-	11/30/30/45	-
47	SF4	F	502	6	-	-	0/6/5/5
48	PLC	N	405	-	-	9/28/28/45	-
53	CDL	N	401	-	-	31/84/84/110	-
47	SF4	B	201	2	-	-	0/6/5/5
46	PC1	P	502	46	-	14/49/49/57	-
46	PC1	M	605	-	-	18/29/29/57	-
46	PC1	Y	205	-	-	12/43/43/57	-
45	3PE	N	403	-	-	29/48/48/54	-
45	3PE	L	704	-	-	24/49/49/54	-
59	CHD	i	201	-	-	2/9/74/74	0/4/4/4
53	CDL	q	201	-	-	25/71/71/110	-
45	3PE	L	705	-	-	16/40/40/54	-
45	3PE	K	101	-	-	17/47/47/54	-
46	PC1	d	203	-	-	14/42/42/57	-
45	3PE	A	201	-	-	11/37/37/54	-
57	NDP	P	501	-	-	14/34/77/77	0/5/5/5
46	PC1	M	604	-	-	22/47/47/57	-
45	3PE	Y	203	-	-	21/54/54/54	-
53	CDL	d	201	-	-	31/75/75/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	g	201	-	-	10/31/31/54	-
45	3PE	d	202	-	-	17/52/52/54	-
45	3PE	I	203	-	-	19/39/39/54	-
45	3PE	Y	202	-	-	30/54/54/54	-
53	CDL	L	701	-	-	31/97/97/110	-
45	3PE	N	402	-	-	26/52/52/54	-
45	3PE	m	201	-	-	15/44/44/54	-
46	PC1	I	204	-	-	18/57/57/57	-
47	SF4	I	201	9	-	-	0/6/5/5
46	PC1	h	202	-	-	12/34/34/57	-
45	3PE	Y	204	-	-	19/39/39/54	-
46	PC1	H	403	-	-	17/42/42/57	-

All (298) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	9.90	1.70	1.59
57	P	501	NDP	C2B-C1B	-9.13	1.30	1.53
59	i	201	CHD	C11-C12	8.95	1.67	1.53
55	O	401	DGT	O6-C6	8.79	1.40	1.23
57	P	501	NDP	O4B-C1B	8.48	1.61	1.42
57	P	501	NDP	O4D-C1D	8.43	1.61	1.42
57	P	501	NDP	C7N-N7N	7.70	1.55	1.33
57	P	501	NDP	C2D-C1D	-7.38	1.30	1.53
59	i	201	CHD	C16-C15	7.25	1.73	1.54
57	P	501	NDP	C6N-C5N	6.97	1.54	1.33
55	O	401	DGT	C5-N7	6.77	1.52	1.39
50	F	501	FMN	C10-N1	6.53	1.46	1.33
57	P	501	NDP	O4D-C4D	-6.44	1.30	1.45
50	F	501	FMN	C4A-N5	6.43	1.44	1.30
59	i	201	CHD	C20-C17	-6.29	1.43	1.54
50	F	501	FMN	C5A-N5	5.50	1.49	1.39
57	P	501	NDP	P2B-O2B	5.36	1.68	1.59
57	P	501	NDP	C6A-N6A	5.35	1.47	1.34
55	O	401	DGT	PA-O3A	5.33	1.65	1.59
57	P	501	NDP	O4B-C4B	-5.26	1.33	1.45
55	O	401	DGT	PB-O3A	5.24	1.65	1.59
59	i	201	CHD	O12-C12	-5.24	1.35	1.43
59	i	201	CHD	C8-C9	5.18	1.63	1.53
58	T	101	EHZ	C12-N1	5.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	O	401	DGT	PB-O3B	5.12	1.65	1.59
59	i	201	CHD	C13-C17	5.08	1.64	1.55
58	U	101	EHZ	C12-N1	5.08	1.45	1.33
58	U	101	EHZ	C15-N2	5.03	1.45	1.33
50	F	501	FMN	C9A-N10	5.00	1.49	1.41
50	F	501	FMN	C2-N1	4.95	1.47	1.36
58	T	101	EHZ	C15-N2	4.87	1.45	1.33
55	O	401	DGT	C2-N2	4.83	1.45	1.34
55	O	401	DGT	C2-N1	4.72	1.49	1.37
57	P	501	NDP	C2N-C3N	4.61	1.47	1.35
57	P	501	NDP	PN-O3	4.57	1.64	1.59
59	i	201	CHD	C6-C5	4.57	1.61	1.53
50	F	501	FMN	C2-N3	4.44	1.48	1.39
55	O	401	DGT	C2-N3	4.37	1.43	1.33
57	P	501	NDP	C5A-C4A	-4.35	1.31	1.39
55	O	401	DGT	C8-N9	-4.24	1.28	1.37
59	i	201	CHD	C15-C14	4.17	1.62	1.54
57	P	501	NDP	O7N-C7N	-4.11	1.14	1.24
55	O	401	DGT	C4-N9	-3.99	1.27	1.38
57	P	501	NDP	C8A-N9A	-3.81	1.31	1.37
57	P	501	NDP	O2D-C2D	3.80	1.52	1.43
50	F	501	FMN	C10-N10	3.69	1.45	1.37
50	F	501	FMN	C4-N3	3.62	1.45	1.38
59	i	201	CHD	C6-C7	3.50	1.59	1.52
57	P	501	NDP	C4N-C3N	3.31	1.56	1.50
52	H	401	U10	C4-C5	-3.16	1.39	1.48
52	H	401	U10	C3-C2	-3.06	1.40	1.48
46	P	502	PC1	O21-C2	-2.96	1.39	1.46
53	M	602	CDL	OB6-CB4	-2.93	1.39	1.46
53	L	701	CDL	OA6-CA4	-2.89	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.89	1.39	1.46
50	F	501	FMN	O2-C2	-2.86	1.18	1.24
53	h	201	CDL	OA6-CA4	-2.86	1.39	1.46
57	P	501	NDP	C5A-N7A	-2.82	1.33	1.39
46	I	204	PC1	O21-C2	-2.82	1.40	1.46
45	M	603	3PE	O21-C2	-2.81	1.40	1.46
45	K	101	3PE	O21-C2	-2.81	1.40	1.46
50	F	501	FMN	O4-C4	-2.80	1.18	1.23
53	X	201	CDL	OB6-CB4	-2.78	1.40	1.46
52	H	401	U10	C7-C8	2.76	1.54	1.50
53	N	401	CDL	OB6-CB4	-2.74	1.40	1.46
52	H	401	U10	C21-C19	2.74	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	O	401	DGT	C1'-N9	-2.73	1.41	1.48
53	h	201	CDL	OB6-CB4	-2.73	1.40	1.46
53	J	201	CDL	OA6-CA4	-2.73	1.40	1.46
46	h	202	PC1	O21-C2	-2.73	1.40	1.46
46	L	706	PC1	O21-C2	-2.72	1.40	1.46
53	L	701	CDL	OB6-CB4	-2.72	1.40	1.46
46	d	203	PC1	O21-C2	-2.71	1.40	1.46
46	q	203	PC1	O21-C2	-2.71	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.70	1.40	1.46
45	L	702	3PE	O21-C2	-2.69	1.40	1.46
45	A	201	3PE	O21-C2	-2.69	1.40	1.46
46	M	604	PC1	O21-C2	-2.69	1.40	1.46
45	I	203	3PE	O21-C2	-2.69	1.40	1.46
45	J	202	3PE	O21-C2	-2.68	1.40	1.46
53	M	602	CDL	OA6-CA4	-2.68	1.40	1.46
45	m	202	3PE	O21-C2	-2.67	1.40	1.46
46	q	202	PC1	O21-C2	-2.67	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.67	1.40	1.46
45	N	402	3PE	O21-C2	-2.67	1.40	1.46
53	J	201	CDL	OB6-CB4	-2.67	1.40	1.46
45	L	703	3PE	O21-C2	-2.67	1.40	1.46
45	Y	202	3PE	O21-C2	-2.66	1.40	1.46
57	P	501	NDP	C4N-C5N	2.66	1.55	1.49
45	g	201	3PE	O21-C2	-2.66	1.40	1.46
53	d	201	CDL	OB6-CB4	-2.65	1.40	1.46
45	N	404	3PE	O21-C2	-2.65	1.40	1.46
45	d	202	3PE	O21-C2	-2.63	1.40	1.46
53	X	201	CDL	OA6-CA4	-2.62	1.40	1.46
46	M	605	PC1	O21-C2	-2.62	1.40	1.46
45	Z	201	3PE	O21-C2	-2.61	1.40	1.46
46	I	205	PC1	O21-C2	-2.61	1.40	1.46
45	L	704	3PE	O21-C2	-2.61	1.40	1.46
45	b	101	3PE	O21-C2	-2.61	1.40	1.46
45	m	201	3PE	O21-C2	-2.59	1.40	1.46
46	Y	205	PC1	O21-C2	-2.59	1.40	1.46
46	A	203	PC1	O21-C2	-2.58	1.40	1.46
59	i	201	CHD	C13-C12	-2.57	1.50	1.54
46	H	402	PC1	O21-C2	-2.57	1.40	1.46
52	H	401	U10	C15-C14	2.56	1.57	1.50
46	H	403	PC1	O21-C2	-2.55	1.40	1.46
53	X	201	CDL	OB8-CB6	-2.54	1.39	1.45
45	Y	204	3PE	O21-C2	-2.53	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	d	201	CDL	OB8-CB7	2.52	1.40	1.33
53	N	401	CDL	OA6-CA4	-2.52	1.40	1.46
45	o	202	3PE	O21-C2	-2.51	1.40	1.46
45	Y	201	3PE	O21-C2	-2.50	1.40	1.46
46	q	203	PC1	O31-C31	2.49	1.40	1.33
53	q	201	CDL	OB8-CB7	2.49	1.40	1.33
45	L	705	3PE	O21-C2	-2.49	1.40	1.46
53	h	201	CDL	OB8-CB7	2.48	1.40	1.33
57	P	501	NDP	O3B-C3B	-2.48	1.36	1.43
45	L	704	3PE	O31-C31	2.47	1.40	1.33
58	T	101	EHZ	O4-C15	-2.47	1.18	1.23
45	Y	203	3PE	O31-C31	2.46	1.40	1.33
46	A	202	PC1	O31-C31	2.45	1.40	1.33
52	H	401	U10	C11-C9	2.45	1.56	1.51
45	i	202	3PE	O21-C2	-2.44	1.40	1.46
52	H	401	U10	C6-C1	2.43	1.39	1.35
46	I	205	PC1	O31-C31	2.43	1.40	1.33
46	Y	205	PC1	O31-C31	2.43	1.40	1.33
46	M	605	PC1	O31-C31	2.43	1.40	1.33
46	A	202	PC1	O21-C2	-2.43	1.40	1.46
53	M	602	CDL	OA8-CA7	2.42	1.40	1.33
45	N	403	3PE	O21-C21	2.42	1.41	1.34
58	T	101	EHZ	C9-S1	2.41	1.81	1.76
45	M	603	3PE	O31-C31	2.41	1.40	1.33
57	P	501	NDP	O3D-C3D	-2.41	1.37	1.43
45	N	404	3PE	O31-C31	2.41	1.40	1.33
46	q	202	PC1	O31-C31	2.41	1.40	1.33
53	X	201	CDL	OA8-CA7	2.41	1.40	1.33
53	N	401	CDL	OA8-CA7	2.40	1.40	1.33
45	Z	201	3PE	O31-C31	2.40	1.40	1.33
45	L	703	3PE	O31-C31	2.39	1.40	1.33
45	I	203	3PE	O31-C31	2.39	1.40	1.33
53	L	701	CDL	OB8-CB7	2.39	1.40	1.33
45	Y	204	3PE	O31-C31	2.38	1.40	1.33
46	A	203	PC1	O31-C31	2.38	1.40	1.33
46	d	203	PC1	O31-C31	2.38	1.40	1.33
53	N	401	CDL	OB8-CB7	2.37	1.40	1.33
45	A	201	3PE	O31-C31	2.37	1.40	1.33
46	H	403	PC1	O31-C3	-2.37	1.39	1.45
58	U	101	EHZ	C9-S1	2.37	1.81	1.76
45	i	202	3PE	O31-C31	2.37	1.40	1.33
53	d	201	CDL	OA8-CA7	2.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	m	201	3PE	O31-C31	2.37	1.40	1.33
45	J	202	3PE	O31-C31	2.36	1.40	1.33
45	d	202	3PE	O31-C31	2.36	1.40	1.33
46	I	204	PC1	O31-C31	2.36	1.40	1.33
53	h	201	CDL	OA8-CA7	2.36	1.40	1.33
58	T	101	EHZ	O3-C12	-2.36	1.18	1.23
53	L	701	CDL	OA8-CA7	2.36	1.40	1.33
46	M	604	PC1	O31-C31	2.35	1.40	1.33
57	P	501	NDP	PA-O5B	2.35	1.68	1.59
46	H	402	PC1	O31-C31	2.34	1.40	1.33
46	h	202	PC1	O31-C31	2.34	1.40	1.33
58	U	101	EHZ	O3-C12	-2.34	1.18	1.23
53	q	201	CDL	OA8-CA7	2.33	1.40	1.33
57	P	501	NDP	C5B-C4B	2.33	1.58	1.51
45	g	201	3PE	O21-C21	2.33	1.40	1.35
45	Y	201	3PE	O31-C31	2.33	1.40	1.33
45	m	202	3PE	O31-C31	2.33	1.40	1.33
45	b	101	3PE	O31-C31	2.32	1.40	1.33
58	U	101	EHZ	O4-C15	-2.32	1.18	1.23
45	N	402	3PE	O31-C31	2.32	1.40	1.33
46	L	706	PC1	O31-C3	-2.31	1.40	1.45
53	J	201	CDL	OA6-CA5	2.31	1.40	1.35
53	d	201	CDL	OA8-CA6	-2.30	1.40	1.45
45	N	403	3PE	O21-C2	-2.30	1.41	1.46
45	Y	203	3PE	O21-C2	-2.30	1.41	1.46
45	Y	202	3PE	O31-C3	-2.29	1.40	1.45
53	M	602	CDL	OB8-CB6	-2.29	1.40	1.45
57	P	501	NDP	P2B-O1X	2.29	1.57	1.50
53	J	201	CDL	OB6-CB5	2.29	1.40	1.35
45	N	403	3PE	O31-C3	-2.29	1.40	1.45
46	P	502	PC1	O31-C31	2.28	1.40	1.33
45	Y	202	3PE	O31-C31	2.28	1.40	1.33
45	K	101	3PE	O31-C3	-2.28	1.40	1.45
45	g	201	3PE	O31-C31	2.27	1.40	1.33
57	P	501	NDP	C6N-N1N	2.27	1.42	1.37
45	N	402	3PE	O31-C3	-2.27	1.40	1.45
45	b	101	3PE	O31-C3	-2.26	1.40	1.45
45	L	705	3PE	O31-C3	-2.26	1.40	1.45
46	P	502	PC1	O31-C3	-2.26	1.40	1.45
45	d	202	3PE	O31-C3	-2.25	1.40	1.45
53	N	401	CDL	OB8-CB6	-2.25	1.40	1.45
45	m	202	3PE	O31-C3	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	L	701	CDL	OA8-CA6	-2.25	1.40	1.45
45	K	101	3PE	O31-C31	2.24	1.39	1.33
45	g	201	3PE	O31-C3	-2.24	1.40	1.45
53	q	201	CDL	OB8-CB6	-2.24	1.40	1.45
46	H	403	PC1	O31-C31	2.24	1.39	1.33
46	L	706	PC1	O31-C31	2.24	1.39	1.33
45	L	702	3PE	O31-C3	-2.24	1.40	1.45
46	I	205	PC1	O21-C21	2.24	1.40	1.34
52	H	401	U10	C1-C2	-2.24	1.39	1.47
53	L	701	CDL	OB8-CB6	-2.24	1.40	1.45
53	q	201	CDL	OA8-CA6	-2.24	1.40	1.45
46	A	202	PC1	O31-C3	-2.24	1.40	1.45
46	M	604	PC1	O31-C3	-2.23	1.40	1.45
45	L	705	3PE	O21-C21	2.23	1.40	1.34
45	o	202	3PE	O21-C21	2.23	1.40	1.34
45	L	705	3PE	O31-C31	2.23	1.39	1.33
45	o	202	3PE	O31-C3	-2.23	1.40	1.45
45	N	403	3PE	O31-C31	2.23	1.39	1.33
55	O	401	DGT	PG-O2G	-2.23	1.46	1.54
53	M	602	CDL	OB8-CB7	2.23	1.39	1.33
53	d	201	CDL	OB6-CB5	2.22	1.40	1.34
46	H	403	PC1	O21-C21	2.22	1.40	1.34
45	I	203	3PE	O31-C3	-2.22	1.40	1.45
52	H	401	U10	O4-C4	2.22	1.42	1.36
53	N	401	CDL	OA6-CA5	2.22	1.40	1.34
53	h	201	CDL	OA8-CA6	-2.22	1.40	1.45
46	d	203	PC1	O31-C3	-2.22	1.40	1.45
45	m	201	3PE	O21-C21	2.21	1.40	1.34
46	Y	205	PC1	O21-C21	2.21	1.40	1.34
57	P	501	NDP	C7N-C3N	2.21	1.53	1.48
55	O	401	DGT	PG-O1G	-2.21	1.46	1.54
46	A	202	PC1	O21-C21	2.20	1.40	1.34
52	H	401	U10	C6-C5	-2.20	1.40	1.46
53	X	201	CDL	OA8-CA6	-2.20	1.40	1.45
46	H	402	PC1	O21-C21	2.19	1.40	1.34
46	h	202	PC1	O21-C21	2.19	1.40	1.34
53	M	602	CDL	OA8-CA6	-2.19	1.40	1.45
46	H	402	PC1	O31-C3	-2.19	1.40	1.45
46	h	202	PC1	O31-C3	-2.18	1.40	1.45
45	i	202	3PE	O21-C21	2.18	1.40	1.34
46	A	203	PC1	O21-C21	2.18	1.40	1.34
45	N	404	3PE	O21-C21	2.18	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	703	3PE	O31-C3	-2.18	1.40	1.45
45	J	202	3PE	O31-C3	-2.18	1.40	1.45
45	b	101	3PE	O21-C21	2.17	1.40	1.34
46	M	605	PC1	O21-C21	2.17	1.40	1.34
45	Y	203	3PE	O31-C3	-2.17	1.40	1.45
46	q	202	PC1	O21-C21	2.17	1.40	1.34
52	H	401	U10	O3-C3	2.16	1.42	1.36
46	q	202	PC1	O31-C3	-2.16	1.40	1.45
53	N	401	CDL	OB6-CB5	2.16	1.40	1.34
53	d	201	CDL	OA6-CA5	2.16	1.40	1.34
45	L	704	3PE	O31-C3	-2.16	1.40	1.45
46	I	204	PC1	O31-C3	-2.16	1.40	1.45
45	m	201	3PE	O31-C3	-2.16	1.40	1.45
45	i	202	3PE	O31-C3	-2.15	1.40	1.45
45	Y	204	3PE	O21-C21	2.15	1.40	1.34
46	I	205	PC1	O31-C3	-2.15	1.40	1.45
46	M	605	PC1	O31-C3	-2.15	1.40	1.45
53	h	201	CDL	OB8-CB6	-2.15	1.40	1.45
53	M	602	CDL	OA6-CA5	2.15	1.40	1.34
45	Z	201	3PE	O31-C3	-2.15	1.40	1.45
45	J	202	3PE	O21-C21	2.15	1.40	1.34
53	J	201	CDL	OB8-CB6	-2.15	1.40	1.45
55	O	401	DGT	C4-N3	2.14	1.39	1.34
53	L	701	CDL	OB6-CB5	2.14	1.40	1.34
53	N	401	CDL	OA8-CA6	-2.14	1.40	1.45
45	d	202	3PE	O21-C21	2.14	1.40	1.34
53	h	201	CDL	OB6-CB5	2.14	1.40	1.34
45	N	402	3PE	O21-C21	2.13	1.40	1.34
45	Y	203	3PE	O21-C21	2.13	1.40	1.34
45	I	203	3PE	O21-C21	2.13	1.40	1.34
45	N	404	3PE	O31-C3	-2.13	1.40	1.45
46	A	203	PC1	O31-C3	-2.13	1.40	1.45
45	Y	204	3PE	O31-C3	-2.13	1.40	1.45
52	H	401	U10	C16-C14	2.13	1.55	1.51
45	Y	201	3PE	O31-C3	-2.13	1.40	1.45
53	d	201	CDL	OB8-CB6	-2.12	1.40	1.45
46	L	706	PC1	O21-C21	2.12	1.40	1.34
53	J	201	CDL	OA8-CA6	-2.12	1.40	1.45
52	H	401	U10	C1M-C1	2.12	1.55	1.50
45	M	603	3PE	O31-C3	-2.12	1.40	1.45
45	A	201	3PE	O31-C3	-2.11	1.40	1.45
53	X	201	CDL	OA6-CA5	2.11	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	704	3PE	O21-C21	2.11	1.40	1.34
46	Y	205	PC1	O31-C3	-2.11	1.40	1.45
46	I	204	PC1	O21-C21	2.10	1.40	1.34
53	X	201	CDL	OB8-CB7	2.10	1.39	1.33
45	L	703	3PE	O21-C21	2.10	1.40	1.34
46	q	203	PC1	O21-C21	2.10	1.40	1.34
45	m	202	3PE	O21-C21	2.09	1.40	1.34
45	Z	201	3PE	O21-C21	2.09	1.40	1.34
46	q	203	PC1	O31-C3	-2.09	1.40	1.45
45	Y	201	3PE	O21-C21	2.08	1.40	1.34
52	H	401	U10	C10-C9	2.08	1.55	1.50
46	d	203	PC1	O21-C21	2.07	1.40	1.34
45	L	702	3PE	O21-C21	2.07	1.40	1.34
53	q	201	CDL	OB6-CB5	2.07	1.40	1.34
46	M	604	PC1	O21-C21	2.07	1.40	1.34
45	A	201	3PE	O21-C21	2.06	1.40	1.34
53	X	201	CDL	OB6-CB5	2.06	1.40	1.34
45	Y	202	3PE	O21-C21	2.06	1.40	1.34
52	H	401	U10	C7-C6	2.05	1.55	1.51
53	h	201	CDL	OA6-CA5	2.03	1.40	1.34
59	i	201	CHD	C11-C9	-2.01	1.50	1.53
45	K	101	3PE	O21-C21	2.01	1.39	1.34

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	C8-N9-C4	7.58	120.23	106.03
59	i	201	CHD	C14-C13-C12	7.37	114.16	107.42
59	i	201	CHD	C13-C17-C20	-6.89	111.14	119.48
52	H	401	U10	C7-C8-C9	-6.30	115.98	126.83
57	P	501	NDP	N6A-C6A-N1A	-5.62	105.86	118.38
58	T	101	EHZ	C8-C9-S1	5.59	120.61	113.56
58	U	101	EHZ	C8-C9-S1	5.57	120.59	113.56
57	P	501	NDP	N3A-C2A-N1A	-5.41	120.40	128.58
57	P	501	NDP	C4A-N9A-C1B	-5.38	114.04	126.63
45	g	201	3PE	O21-C21-C22	5.14	120.25	111.09
53	J	201	CDL	OA6-CA5-C11	5.11	120.20	111.09
53	J	201	CDL	OB6-CB5-C51	5.10	120.18	111.09
57	P	501	NDP	C5A-C4A-N3A	-5.09	119.71	126.72
52	H	401	U10	C12-C13-C14	-5.08	115.99	127.62
57	P	501	NDP	C1B-N9A-C8A	4.89	137.95	127.09
59	i	201	CHD	C17-C13-C12	4.72	121.91	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	F	501	FMN	C9-C8-C7	4.60	126.44	119.69
52	H	401	U10	C17-C18-C19	-4.57	112.41	127.64
50	F	501	FMN	C7M-C7-C6	4.45	127.41	119.57
45	L	705	3PE	O21-C21-C22	4.43	121.06	111.48
45	Y	204	3PE	O21-C21-C22	4.40	121.01	111.48
46	H	402	PC1	O21-C21-C22	4.37	120.94	111.48
45	i	202	3PE	O21-C21-C22	4.36	120.91	111.48
45	L	704	3PE	O21-C21-C22	4.27	120.71	111.48
53	h	201	CDL	OB6-CB5-C51	4.21	120.58	111.48
53	M	602	CDL	OA6-CA5-C11	4.19	120.55	111.48
45	A	201	3PE	O21-C21-C22	4.18	120.52	111.48
45	m	201	3PE	O21-C21-C22	4.17	120.51	111.48
46	L	706	PC1	O21-C21-C22	4.15	120.46	111.48
45	Y	202	3PE	O21-C21-C22	4.14	120.44	111.48
45	Y	203	3PE	O21-C21-C22	4.14	120.44	111.48
53	N	401	CDL	OB6-CB5-C51	4.14	120.43	111.48
46	q	203	PC1	O21-C21-C22	4.13	120.42	111.48
45	d	202	3PE	O21-C21-C22	4.13	120.41	111.48
45	N	402	3PE	O21-C21-C22	4.12	120.39	111.48
57	P	501	NDP	C5A-C6A-N6A	4.11	133.47	123.29
45	o	202	3PE	O21-C21-C22	4.08	120.31	111.48
53	d	201	CDL	OA6-CA5-C11	4.08	120.30	111.48
53	L	701	CDL	OB6-CB5-C51	4.07	120.29	111.48
59	i	201	CHD	C18-C13-C17	-4.07	104.83	111.20
45	L	702	3PE	O21-C21-C22	4.04	120.21	111.48
53	X	201	CDL	OB6-CB5-C51	4.02	120.17	111.48
45	b	101	3PE	O21-C21-C22	4.02	120.17	111.48
57	P	501	NDP	N9A-C8A-N7A	-4.00	108.26	113.94
45	m	202	3PE	O21-C21-C22	4.00	120.13	111.48
45	K	101	3PE	O21-C21-C22	3.96	120.05	111.48
53	q	201	CDL	OB6-CB5-C51	3.95	120.03	111.48
46	A	203	PC1	O21-C21-C22	3.95	120.02	111.48
46	h	202	PC1	O21-C21-C22	3.93	119.98	111.48
53	M	602	CDL	OB6-CB5-C51	3.93	119.98	111.48
46	P	502	PC1	O21-C21-C22	3.92	119.96	111.48
53	q	201	CDL	OA6-CA5-C11	3.91	119.94	111.48
45	N	403	3PE	O21-C21-C22	3.90	119.92	111.48
45	J	202	3PE	O21-C21-C22	3.90	119.92	111.48
45	Z	201	3PE	O21-C21-C22	3.90	119.91	111.48
46	I	204	PC1	O21-C21-C22	3.88	119.87	111.48
59	i	201	CHD	C18-C13-C12	-3.88	105.18	109.06
53	X	201	CDL	OA6-CA5-C11	3.88	119.86	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	h	201	CDL	OA6-CA5-C11	3.87	119.86	111.48
45	N	404	3PE	O21-C21-C22	3.86	119.83	111.48
46	I	205	PC1	O21-C21-C22	3.86	119.83	111.48
45	M	603	3PE	O21-C21-C22	3.82	119.75	111.48
46	M	604	PC1	O21-C21-C22	3.80	119.71	111.48
46	q	202	PC1	O21-C21-C22	3.80	119.71	111.48
46	d	203	PC1	O21-C21-C22	3.78	119.65	111.48
45	I	203	3PE	O21-C21-C22	3.77	119.65	111.48
45	L	703	3PE	O21-C21-C22	3.75	119.59	111.48
53	L	701	CDL	OA6-CA5-C11	3.71	119.50	111.48
55	O	401	DGT	C1'-N9-C8	-3.68	119.67	127.91
46	Y	205	PC1	O21-C21-C22	3.64	119.36	111.48
53	N	401	CDL	OA6-CA5-C11	3.62	119.30	111.48
46	A	202	PC1	O21-C21-C22	3.61	119.29	111.48
59	i	201	CHD	C1-C10-C5	3.58	112.89	107.75
50	F	501	FMN	C4-N3-C2	-3.47	119.49	125.64
57	P	501	NDP	C2A-N3A-C4A	3.45	120.26	111.83
59	i	201	CHD	C17-C13-C14	3.45	103.58	100.11
45	Y	201	3PE	O21-C21-C22	3.41	118.87	111.48
59	i	201	CHD	C18-C13-C14	-3.40	105.88	111.20
50	F	501	FMN	C8M-C8-C7	-3.33	113.96	120.76
57	P	501	NDP	N3A-C4A-N9A	3.13	132.49	127.17
53	d	201	CDL	OB8-CB7-C71	3.08	121.24	111.83
55	O	401	DGT	C2-N1-C6	-3.08	119.52	125.11
50	F	501	FMN	C4A-C10-N10	3.04	120.83	116.48
45	Y	203	3PE	O31-C31-C32	3.04	121.09	111.83
59	i	201	CHD	C19-C10-C9	-3.00	107.15	111.18
52	H	401	U10	C10-C9-C11	2.99	120.43	115.23
45	I	203	3PE	O31-C31-C32	2.99	120.22	111.15
46	q	203	PC1	O31-C31-C32	2.99	120.94	111.83
53	L	701	CDL	OA8-CA7-C31	2.97	120.90	111.83
45	Y	204	3PE	O31-C31-C32	2.97	120.17	111.15
53	M	602	CDL	OA8-CA7-C31	2.97	120.88	111.83
58	T	101	EHZ	C13-C12-N1	2.97	121.75	116.34
59	i	201	CHD	C6-C5-C4	-2.95	107.86	111.23
45	Y	202	3PE	O31-C31-C32	2.93	120.78	111.83
55	O	401	DGT	O2G-PG-O3B	2.92	114.42	104.64
45	L	704	3PE	O31-C31-C32	2.89	120.65	111.83
59	i	201	CHD	C23-C22-C20	-2.87	109.09	114.46
53	N	401	CDL	OA8-CA7-C31	2.87	120.58	111.83
46	A	202	PC1	O31-C31-C32	2.86	120.56	111.83
55	O	401	DGT	C2'-C3'-C4'	2.85	108.59	102.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	M	604	PC1	O31-C31-C32	2.84	120.50	111.83
45	L	703	3PE	O31-C31-C32	2.84	120.49	111.83
53	h	201	CDL	OB8-CB7-C71	2.83	120.47	111.83
45	N	403	3PE	O31-C31-C32	2.81	120.40	111.83
46	Y	205	PC1	O31-C31-C32	2.81	120.39	111.83
46	M	605	PC1	O31-C31-C32	2.79	120.34	111.83
53	L	701	CDL	OB8-CB7-C71	2.78	120.30	111.83
53	q	201	CDL	OA8-CA7-C31	2.77	120.28	111.83
45	A	201	3PE	O31-C31-C32	2.77	120.28	111.83
46	I	204	PC1	O31-C31-C32	2.76	120.25	111.83
45	Y	201	3PE	O31-C31-C32	2.76	120.25	111.83
46	H	403	PC1	O31-C31-C32	2.76	120.24	111.83
53	X	201	CDL	OA8-CA7-C31	2.74	120.19	111.83
57	P	501	NDP	C2B-C1B-N9A	-2.73	109.26	113.75
45	K	101	3PE	O31-C31-C32	2.72	120.14	111.83
45	m	201	3PE	O31-C31-C32	2.72	120.14	111.83
53	d	201	CDL	OB6-CB5-C51	2.71	120.88	110.93
46	P	502	PC1	O31-C31-C32	2.70	120.06	111.83
55	O	401	DGT	O1G-PG-O3B	2.68	113.63	104.64
46	A	203	PC1	O31-C31-C32	2.68	120.01	111.83
46	H	402	PC1	O31-C31-C32	2.68	120.01	111.83
45	i	202	3PE	O31-C31-C32	2.67	119.98	111.83
57	P	501	NDP	C5A-N7A-C8A	2.66	107.63	103.45
53	N	401	CDL	OB8-CB7-C71	2.66	119.94	111.83
46	d	203	PC1	O31-C31-C32	2.66	119.94	111.83
45	m	202	3PE	O31-C31-C32	2.65	119.93	111.83
46	L	706	PC1	O31-C31-C32	2.65	119.92	111.83
58	T	101	EHZ	C11-N1-C12	-2.65	117.89	122.82
45	L	705	3PE	O31-C31-C32	2.64	119.89	111.83
53	M	602	CDL	OB8-CB7-C71	2.64	119.87	111.83
58	U	101	EHZ	O2-C9-C8	-2.63	119.61	123.74
50	F	501	FMN	C4A-C4-N3	2.62	119.92	113.25
46	I	205	PC1	O31-C31-C32	2.60	119.76	111.83
46	h	202	PC1	O31-C31-C32	2.60	119.75	111.83
45	Z	201	3PE	O31-C31-C32	2.58	119.72	111.83
45	J	202	3PE	O31-C31-C32	2.58	119.69	111.83
53	h	201	CDL	OA8-CA7-C31	2.57	119.68	111.83
45	g	201	3PE	O31-C31-C32	2.57	119.66	111.83
50	F	501	FMN	C6-C7-C8	-2.56	115.92	119.69
58	T	101	EHZ	O2-C9-C8	-2.56	119.71	123.74
45	N	404	3PE	O31-C31-C32	2.55	119.62	111.83
53	q	201	CDL	OB8-CB7-C71	2.54	119.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	F	501	FMN	O4-C4-C4A	-2.54	119.82	126.53
45	N	402	3PE	O31-C31-C32	2.53	119.54	111.83
45	g	201	3PE	C2-O21-C21	-2.52	113.40	117.85
59	i	201	CHD	C9-C11-C12	-2.51	111.01	114.29
53	d	201	CDL	OA8-CA7-C31	2.50	119.46	111.83
59	i	201	CHD	C11-C9-C10	-2.49	111.17	113.70
45	M	603	3PE	O31-C31-C32	2.49	119.43	111.83
46	M	605	PC1	O21-C21-C22	2.48	120.05	110.93
52	H	401	U10	C1M-C1-C6	-2.48	120.38	124.45
53	J	201	CDL	CA4-OA6-CA5	-2.46	113.49	117.85
58	T	101	EHZ	C7-C8-C9	-2.46	108.37	113.86
59	i	201	CHD	C15-C14-C8	2.44	121.71	118.36
52	H	401	U10	C10-C9-C8	-2.44	117.35	123.63
45	b	101	3PE	O31-C31-C32	2.43	119.26	111.83
59	i	201	CHD	C1-C2-C3	2.43	113.71	110.48
55	O	401	DGT	C5-C6-N1	2.42	119.41	113.25
59	i	201	CHD	C4-C3-C2	2.41	113.56	110.62
45	d	202	3PE	O31-C31-C32	2.41	119.19	111.83
55	O	401	DGT	O1A-PA-O2A	-2.41	101.26	112.44
58	T	101	EHZ	C10-S1-C9	2.40	108.94	101.84
53	X	201	CDL	OB8-CB7-C71	2.40	119.15	111.83
52	H	401	U10	C15-C14-C16	2.37	119.34	115.23
55	O	401	DGT	O6-C6-C5	-2.37	120.29	126.53
58	T	101	EHZ	O2-C9-S1	-2.36	119.68	122.68
50	F	501	FMN	C10-C4A-N5	-2.35	120.00	124.81
46	H	403	PC1	O21-C21-C22	2.35	119.58	110.93
55	O	401	DGT	O1B-PB-O2B	-2.35	101.50	112.44
46	q	202	PC1	O31-C31-C32	2.35	118.99	111.83
55	O	401	DGT	C5-C4-N9	-2.33	101.48	105.66
58	T	101	EHZ	C19-C17-C16	2.29	112.68	108.77
58	U	101	EHZ	O2-C9-S1	-2.27	119.80	122.68
57	P	501	NDP	P2B-O2B-C2B	-2.25	117.42	123.43
58	U	101	EHZ	C13-C12-N1	2.24	120.43	116.34
52	H	401	U10	C7-C6-C1	-2.22	121.08	124.89
50	F	501	FMN	C6-C5A-C9A	2.18	122.05	119.05
58	T	101	EHZ	C14-C13-C12	-2.18	108.77	112.39
57	P	501	NDP	C4A-N9A-C8A	2.16	108.00	105.74
58	U	101	EHZ	C14-C13-C12	-2.16	108.80	112.39
55	O	401	DGT	N9-C4-N3	2.15	130.26	125.95
58	U	101	EHZ	C7-C8-C9	-2.15	109.07	113.86
46	P	502	PC1	C2-O21-C21	-2.10	112.78	117.80
58	U	101	EHZ	C10-S1-C9	2.08	107.99	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	N9-C8-N7	-2.06	109.58	113.40
50	F	501	FMN	C5A-C9A-N10	2.06	119.83	117.97
53	L	701	CDL	CA4-OA6-CA5	-2.05	112.89	117.80
58	T	101	EHZ	O3-C12-N1	-2.02	119.06	123.03
53	L	701	CDL	OA6-CA5-OA7	-2.02	118.99	123.70
50	F	501	FMN	C7M-C7-C8	-2.00	116.67	120.76
55	O	401	DGT	C1'-N9-C4	-2.00	120.10	125.50

There are no chirality outliers.

All (1049) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	O22-C21-O21-C2
45	I	203	3PE	C1-O11-P-O12
45	I	203	3PE	C1-O11-P-O13
45	I	203	3PE	C1-O11-P-O14
45	I	203	3PE	O11-C1-C2-O21
45	J	202	3PE	C11-O13-P-O11
45	J	202	3PE	C11-O13-P-O12
45	J	202	3PE	O13-C11-C12-N
45	K	101	3PE	C22-C21-O21-C2
45	L	702	3PE	C1-O11-P-O14
45	L	702	3PE	C11-O13-P-O11
45	L	702	3PE	C11-O13-P-O14
45	L	702	3PE	O13-C11-C12-N
45	L	702	3PE	C22-C21-O21-C2
45	L	703	3PE	C11-O13-P-O11
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	704	3PE	C1-O11-P-O13
45	L	704	3PE	C1-O11-P-O14
45	L	704	3PE	C11-O13-P-O11
45	L	704	3PE	C11-O13-P-O14
45	L	704	3PE	O13-C11-C12-N
45	L	704	3PE	O22-C21-O21-C2
45	L	705	3PE	C22-C21-O21-C2
45	M	603	3PE	C1-O11-P-O13
45	M	603	3PE	C1-O11-P-O14
45	M	603	3PE	O13-C11-C12-N
45	M	603	3PE	O11-C1-C2-O21
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
45	N	402	3PE	C1-O11-P-O14
45	N	402	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C11-O13-P-O14
45	N	403	3PE	C1-O11-P-O13
45	N	403	3PE	C1-O11-P-O14
45	N	403	3PE	C11-O13-P-O11
45	N	403	3PE	C12-C11-O13-P
45	N	403	3PE	O21-C2-C3-O31
45	N	404	3PE	C11-O13-P-O14
45	N	404	3PE	C12-C11-O13-P
45	Y	201	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O14
45	Y	202	3PE	C11-O13-P-O11
45	Y	202	3PE	C11-O13-P-O12
45	Y	202	3PE	C11-O13-P-O14
45	Y	202	3PE	C22-C21-O21-C2
45	Y	203	3PE	C1-O11-P-O12
45	Y	203	3PE	C1-O11-P-O13
45	Y	203	3PE	C1-O11-P-O14
45	Y	203	3PE	C11-O13-P-O11
45	Y	203	3PE	C11-O13-P-O12
45	Y	203	3PE	C11-O13-P-O14
45	Y	203	3PE	C3-C2-O21-C21
45	Y	203	3PE	C22-C21-O21-C2
45	Y	204	3PE	C1-O11-P-O12
45	Y	204	3PE	C1-O11-P-O14
45	Y	204	3PE	C11-O13-P-O11
45	Y	204	3PE	C11-O13-P-O12
45	Y	204	3PE	C11-O13-P-O14
45	Y	204	3PE	O13-C11-C12-N
45	Y	204	3PE	C22-C21-O21-C2
45	Z	201	3PE	C1-O11-P-O12
45	Z	201	3PE	C1-O11-P-O13
45	Z	201	3PE	C1-O11-P-O14
45	Z	201	3PE	C11-O13-P-O11
45	Z	201	3PE	C11-O13-P-O12
45	Z	201	3PE	O13-C11-C12-N
45	Z	201	3PE	O21-C2-C3-O31
45	d	202	3PE	C1-O11-P-O12
45	d	202	3PE	C1-O11-P-O13
45	d	202	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	i	202	3PE	C11-O13-P-O12
45	i	202	3PE	C22-C21-O21-C2
45	m	201	3PE	O22-C21-O21-C2
45	m	202	3PE	C1-O11-P-O13
45	m	202	3PE	C11-O13-P-O11
45	m	202	3PE	C11-O13-P-O12
45	m	202	3PE	O22-C21-O21-C2
45	m	202	3PE	C22-C21-O21-C2
45	o	202	3PE	O22-C21-O21-C2
46	A	202	PC1	C11-O13-P-O14
46	A	202	PC1	C11-O13-P-O11
46	A	202	PC1	C1-O11-P-O12
46	A	202	PC1	C1-O11-P-O14
46	A	202	PC1	C1-O11-P-O13
46	A	202	PC1	O13-C11-C12-N
46	A	202	PC1	C22-C21-O21-C2
46	A	203	PC1	C11-O13-P-O11
46	H	402	PC1	C11-O13-P-O12
46	H	402	PC1	C11-O13-P-O14
46	H	402	PC1	C11-O13-P-O11
46	H	403	PC1	O13-C11-C12-N
46	I	205	PC1	C11-O13-P-O14
46	I	205	PC1	C11-O13-P-O11
46	I	205	PC1	C1-O11-P-O12
46	I	205	PC1	C1-O11-P-O14
46	I	205	PC1	C1-O11-P-O13
46	L	706	PC1	C11-O13-P-O14
46	L	706	PC1	C11-O13-P-O11
46	L	706	PC1	C1-O11-P-O12
46	L	706	PC1	C1-O11-P-O14
46	L	706	PC1	C1-O11-P-O13
46	L	706	PC1	O13-C11-C12-N
46	M	604	PC1	C1-O11-P-O12
46	M	604	PC1	C1-O11-P-O13
46	M	604	PC1	O13-C11-C12-N
46	M	605	PC1	C11-O13-P-O12
46	M	605	PC1	C11-O13-P-O11
46	M	605	PC1	C1-O11-P-O14
46	M	605	PC1	C1-O11-P-O13
46	M	605	PC1	C12-C11-O13-P
46	M	605	PC1	O11-C1-C2-O21
46	M	605	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
46	P	502	PC1	C11-O13-P-O11
46	P	502	PC1	C1-O11-P-O12
46	P	502	PC1	C1-O11-P-O14
46	P	502	PC1	C1-O11-P-O13
46	P	502	PC1	C22-C21-O21-C2
46	Y	205	PC1	C11-O13-P-O12
46	Y	205	PC1	C22-C21-O21-C2
46	h	202	PC1	C11-O13-P-O14
46	q	202	PC1	C11-O13-P-O12
46	q	202	PC1	C11-O13-P-O14
46	q	202	PC1	C11-O13-P-O11
46	q	203	PC1	C11-O13-P-O14
46	q	203	PC1	C11-O13-P-O11
46	q	203	PC1	C1-O11-P-O12
46	q	203	PC1	C1-O11-P-O14
46	q	203	PC1	O22-C21-O21-C2
48	B	202	PLC	C1-O3P-P-O2P
48	B	202	PLC	C1-O3P-P-O4P
48	L	707	PLC	C1-O3P-P-O2P
48	L	707	PLC	C1-O3P-P-O4P
48	N	405	PLC	C4-O4P-P-O1P
48	N	405	PLC	C4-O4P-P-O2P
48	N	405	PLC	C4-O4P-P-O3P
48	b	102	PLC	C4-O4P-P-O1P
48	g	202	PLC	O2-C2-C3-O3
48	g	202	PLC	C1-O3P-P-O2P
48	g	202	PLC	C1-O3P-P-O4P
53	J	201	CDL	C1-CA2-OA2-PA1
53	J	201	CDL	CA2-OA2-PA1-OA3
53	J	201	CDL	CA2-OA2-PA1-OA4
53	J	201	CDL	CA2-OA2-PA1-OA5
53	J	201	CDL	C11-CA5-OA6-CA4
53	L	701	CDL	C11-CA5-OA6-CA4
53	L	701	CDL	OB7-CB5-OB6-CB4
53	L	701	CDL	C51-CB5-OB6-CB4
53	M	602	CDL	C1-CA2-OA2-PA1
53	M	602	CDL	CA3-OA5-PA1-OA2
53	M	602	CDL	CA3-OA5-PA1-OA3
53	M	602	CDL	CA3-OA5-PA1-OA4
53	M	602	CDL	CB2-OB2-PB2-OB5
53	M	602	CDL	C51-CB5-OB6-CB4
53	N	401	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
53	N	401	CDL	CB3-OB5-PB2-OB3
53	N	401	CDL	CB3-OB5-PB2-OB4
53	N	401	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	CA2-OA2-PA1-OA3
53	X	201	CDL	CA2-OA2-PA1-OA5
53	X	201	CDL	C11-CA5-OA6-CA4
53	X	201	CDL	OA9-CA7-OA8-CA6
53	X	201	CDL	CB2-OB2-PB2-OB3
53	X	201	CDL	CB2-OB2-PB2-OB4
53	X	201	CDL	CB2-OB2-PB2-OB5
53	X	201	CDL	CB3-OB5-PB2-OB2
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	CB3-OB5-PB2-OB2
53	d	201	CDL	CB3-OB5-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB4
53	d	201	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CB3-OB5-PB2-OB2
53	h	201	CDL	CB3-OB5-PB2-OB3
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	C11-CA5-OA6-CA4
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	OB7-CB5-OB6-CB4
53	q	201	CDL	C51-CB5-OB6-CB4
55	O	401	DGT	PB-O3B-PG-O1G
55	O	401	DGT	PB-O3B-PG-O2G
57	P	501	NDP	C5B-O5B-PA-O1A
57	P	501	NDP	C5B-O5B-PA-O2A
57	P	501	NDP	C5B-O5B-PA-O3
57	P	501	NDP	C5D-O5D-PN-O3
57	P	501	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
57	P	501	NDP	C5D-O5D-PN-O2N
58	T	101	EHZ	C6-C7-C8-C9
58	T	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	C1-C2-C3-C4
53	J	201	CDL	C51-CB5-OB6-CB4
45	L	703	3PE	O32-C31-O31-C3
46	d	203	PC1	O32-C31-O31-C3
53	d	201	CDL	OB9-CB7-OB8-CB6
45	N	402	3PE	C32-C31-O31-C3
46	d	203	PC1	C32-C31-O31-C3
53	d	201	CDL	C71-CB7-OB8-CB6
45	I	203	3PE	O32-C31-O31-C3
45	L	704	3PE	O32-C31-O31-C3
45	N	402	3PE	O32-C31-O31-C3
45	Y	202	3PE	O32-C31-O31-C3
45	Y	203	3PE	O32-C31-O31-C3
46	A	202	PC1	O32-C31-O31-C3
46	M	604	PC1	O32-C31-O31-C3
46	M	605	PC1	O32-C31-O31-C3
46	q	203	PC1	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
53	J	201	CDL	OA7-CA5-OA6-CA4
45	K	101	3PE	O22-C21-O21-C2
45	L	702	3PE	O22-C21-O21-C2
45	Y	202	3PE	O22-C21-O21-C2
45	Y	203	3PE	O22-C21-O21-C2
45	Y	204	3PE	O22-C21-O21-C2
45	i	202	3PE	O22-C21-O21-C2
46	A	202	PC1	O22-C21-O21-C2
46	P	502	PC1	O22-C21-O21-C2
46	Y	205	PC1	O22-C21-O21-C2
46	h	202	PC1	O22-C21-O21-C2
53	L	701	CDL	OA7-CA5-OA6-CA4
53	M	602	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	OA7-CA5-OA6-CA4
53	q	201	CDL	OA7-CA5-OA6-CA4
53	J	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
48	B	202	PLC	C2-C3-O3-CB
45	I	203	3PE	C32-C31-O31-C3
45	L	703	3PE	C32-C31-O31-C3
45	L	704	3PE	C32-C31-O31-C3
45	Y	202	3PE	C32-C31-O31-C3
45	Y	203	3PE	C32-C31-O31-C3
46	A	202	PC1	C32-C31-O31-C3
46	M	604	PC1	C32-C31-O31-C3
46	q	203	PC1	C32-C31-O31-C3
53	M	602	CDL	C31-CA7-OA8-CA6
53	X	201	CDL	C31-CA7-OA8-CA6
45	g	201	3PE	C22-C21-O21-C2
45	A	201	3PE	C22-C21-O21-C2
45	L	704	3PE	C22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
45	o	202	3PE	C22-C21-O21-C2
46	M	605	PC1	C22-C21-O21-C2
46	h	202	PC1	C22-C21-O21-C2
46	q	203	PC1	C22-C21-O21-C2
53	N	401	CDL	C51-CB5-OB6-CB4
53	d	201	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	C51-CB5-OB6-CB4
45	d	202	3PE	C32-C31-O31-C3
46	H	403	PC1	C32-C31-O31-C3
46	M	605	PC1	C32-C31-O31-C3
46	h	202	PC1	C32-C31-O31-C3
53	L	701	CDL	C31-CA7-OA8-CA6
53	d	201	CDL	C31-CA7-OA8-CA6
45	L	702	3PE	O32-C31-O31-C3
45	o	202	3PE	O32-C31-O31-C3
46	H	403	PC1	O32-C31-O31-C3
46	h	202	PC1	O32-C31-O31-C3
53	N	401	CDL	OB9-CB7-OB8-CB6
45	L	705	3PE	O22-C21-O21-C2
45	L	702	3PE	C32-C31-O31-C3
45	o	202	3PE	C32-C31-O31-C3
45	N	403	3PE	C32-C31-O31-C3
48	B	202	PLC	C1B-CB-O3-C3
53	N	401	CDL	C71-CB7-OB8-CB6
45	d	202	3PE	O32-C31-O31-C3
45	Z	201	3PE	C22-C21-O21-C2
53	h	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
53	J	201	CDL	C71-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
45	N	403	3PE	O32-C31-O31-C3
48	B	202	PLC	OB-CB-O3-C3
45	Z	201	3PE	O22-C21-O21-C2
53	h	201	CDL	C71-CB7-OB8-CB6
59	i	201	CHD	C17-C20-C22-C23
53	M	602	CDL	C11-CA5-OA6-CA4
59	i	201	CHD	C21-C20-C22-C23
53	h	201	CDL	OB9-CB7-OB8-CB6
53	h	201	CDL	OA7-CA5-OA6-CA4
53	X	201	CDL	CB2-C1-CA2-OA2
45	A	201	3PE	C32-C31-O31-C3
46	Y	205	PC1	C32-C31-O31-C3
48	b	102	PLC	C1B-CB-O3-C3
53	M	602	CDL	C71-CB7-OB8-CB6
53	N	401	CDL	C31-CA7-OA8-CA6
53	J	201	CDL	C31-CA7-OA8-CA6
46	L	706	PC1	C32-C31-O31-C3
46	d	203	PC1	C21-C22-C23-C24
53	N	401	CDL	OB6-CB4-CB6-OB8
45	N	404	3PE	C32-C31-O31-C3
45	A	201	3PE	O32-C31-O31-C3
57	P	501	NDP	O4B-C4B-C5B-O5B
45	L	704	3PE	C31-C32-C33-C34
53	M	602	CDL	OA7-CA5-OA6-CA4
45	N	403	3PE	C21-C22-C23-C24
46	q	203	PC1	C21-C22-C23-C24
48	b	102	PLC	OB-CB-O3-C3
53	J	201	CDL	OB9-CB7-OB8-CB6
45	K	101	3PE	C31-C32-C33-C34
45	L	703	3PE	C31-C32-C33-C34
45	M	603	3PE	C21-C22-C23-C24
45	Y	203	3PE	C31-C32-C33-C34
46	I	205	PC1	C21-C22-C23-C24
46	M	604	PC1	C31-C32-C33-C34
48	B	202	PLC	C'-C1'-C2'-C3'
53	M	602	CDL	CA5-C11-C12-C13
53	M	602	CDL	OB9-CB7-OB8-CB6
53	N	401	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	P	501	NDP	O4D-C1D-N1N-C6N
53	q	201	CDL	O1-C1-CA2-OA2
46	Y	205	PC1	O32-C31-O31-C3
45	i	202	3PE	C21-C22-C23-C24
53	L	701	CDL	CA5-C11-C12-C13
53	X	201	CDL	CA5-C11-C12-C13
53	d	201	CDL	CA5-C11-C12-C13
45	N	404	3PE	O32-C31-O31-C3
46	L	706	PC1	O32-C31-O31-C3
45	Y	203	3PE	C21-C22-C23-C24
45	Y	204	3PE	C32-C31-O31-C3
46	I	204	PC1	C22-C21-O21-C2
45	g	201	3PE	O22-C21-O21-C2
46	H	403	PC1	C31-C32-C33-C34
46	I	204	PC1	O22-C21-O21-C2
45	i	202	3PE	C32-C31-O31-C3
57	P	501	NDP	C3B-C4B-C5B-O5B
45	I	203	3PE	C22-C21-O21-C2
45	M	603	3PE	C22-C21-O21-C2
46	L	706	PC1	C22-C21-O21-C2
45	I	203	3PE	O22-C21-O21-C2
48	N	405	PLC	C'-C1'-C2'-C3'
53	N	401	CDL	O1-C1-CB2-OB2
53	X	201	CDL	O1-C1-CA2-OA2
53	N	401	CDL	CB7-C71-C72-C73
53	d	201	CDL	C11-CA5-OA6-CA4
45	M	603	3PE	C32-C31-O31-C3
45	i	202	3PE	O32-C31-O31-C3
53	X	201	CDL	C78-C79-C80-C81
45	N	404	3PE	C2C-C2D-C2E-C2F
46	h	202	PC1	C22-C23-C24-C25
53	L	701	CDL	C37-C38-C39-C40
53	h	201	CDL	C74-C75-C76-C77
53	q	201	CDL	C51-C52-C53-C54
53	q	201	CDL	C71-C72-C73-C74
45	L	704	3PE	C23-C24-C25-C26
46	h	202	PC1	C24-C25-C26-C27
46	q	202	PC1	C38-C39-C3A-C3B
53	M	602	CDL	C32-C33-C34-C35
45	N	402	3PE	C24-C25-C26-C27
53	M	602	CDL	C78-C79-C80-C81
53	M	602	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
60	o	201	MYR	C4-C5-C6-C7
45	M	603	3PE	O22-C21-O21-C2
46	L	706	PC1	O22-C21-O21-C2
53	d	201	CDL	OA7-CA5-OA6-CA4
45	Z	201	3PE	C27-C28-C29-C2A
58	U	101	EHZ	S1-C10-C11-N1
53	M	602	CDL	CB5-C51-C52-C53
45	Y	204	3PE	C2C-C2D-C2E-C2F
46	M	604	PC1	C24-C25-C26-C27
45	L	703	3PE	C2E-C2F-C2G-C2H
53	X	201	CDL	C57-C58-C59-C60
53	h	201	CDL	C71-C72-C73-C74
45	d	202	3PE	C31-C32-C33-C34
46	H	403	PC1	C36-C37-C38-C39
53	X	201	CDL	C37-C38-C39-C40
45	Y	204	3PE	O32-C31-O31-C3
45	L	704	3PE	C36-C37-C38-C39
45	N	404	3PE	C34-C35-C36-C37
46	H	402	PC1	C28-C29-C2A-C2B
53	h	201	CDL	C31-C32-C33-C34
45	d	202	3PE	C39-C3A-C3B-C3C
53	M	602	CDL	C56-C57-C58-C59
45	K	101	3PE	C33-C34-C35-C36
45	L	702	3PE	C27-C28-C29-C2A
45	N	404	3PE	C23-C24-C25-C26
45	m	201	3PE	C25-C26-C27-C28
53	L	701	CDL	C81-C82-C83-C84
53	N	401	CDL	CA2-C1-CB2-OB2
45	L	702	3PE	C2C-C2D-C2E-C2F
45	L	704	3PE	C24-C25-C26-C27
45	Y	203	3PE	C37-C38-C39-C3A
46	L	706	PC1	C37-C38-C39-C3A
46	L	706	PC1	C3E-C3F-C3G-C3H
46	A	202	PC1	C21-C22-C23-C24
46	H	402	PC1	C21-C22-C23-C24
45	N	403	3PE	C39-C3A-C3B-C3C
45	Z	201	3PE	C34-C35-C36-C37
46	I	204	PC1	C36-C37-C38-C39
48	B	202	PLC	C3B-C4B-C5B-C6B
53	N	401	CDL	C18-C19-C20-C21
45	M	603	3PE	O32-C31-O31-C3
45	J	202	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C33-C34-C35-C36
45	M	603	3PE	C32-C33-C34-C35
45	Y	204	3PE	C28-C29-C2A-C2B
45	Y	203	3PE	C3A-C3B-C3C-C3D
46	I	204	PC1	C22-C23-C24-C25
46	I	205	PC1	C24-C25-C26-C27
46	L	706	PC1	C33-C34-C35-C36
46	I	205	PC1	C26-C27-C28-C29
45	N	402	3PE	C28-C29-C2A-C2B
45	N	404	3PE	C26-C27-C28-C29
45	Y	202	3PE	C3B-C3C-C3D-C3E
46	L	706	PC1	C21-C22-C23-C24
45	Y	202	3PE	C32-C33-C34-C35
46	A	203	PC1	C33-C34-C35-C36
45	o	202	3PE	C2E-C2F-C2G-C2H
45	N	402	3PE	C27-C28-C29-C2A
46	H	402	PC1	C32-C33-C34-C35
46	P	502	PC1	C25-C26-C27-C28
46	d	203	PC1	C36-C37-C38-C39
48	g	202	PLC	C2'-C3'-C4'-C5'
46	H	402	PC1	C22-C23-C24-C25
53	X	201	CDL	C60-C61-C62-C63
46	H	402	PC1	C31-C32-C33-C34
45	J	202	3PE	C32-C31-O31-C3
46	q	202	PC1	C32-C31-O31-C3
45	N	403	3PE	C22-C23-C24-C25
45	N	403	3PE	C2C-C2D-C2E-C2F
45	m	201	3PE	C33-C34-C35-C36
53	M	602	CDL	C71-C72-C73-C74
45	I	203	3PE	C28-C29-C2A-C2B
53	N	401	CDL	C16-C17-C18-C19
46	M	604	PC1	C28-C29-C2A-C2B
48	g	202	PLC	C'-C1'-C2'-C3'
53	d	201	CDL	CA7-C31-C32-C33
45	Y	202	3PE	C35-C36-C37-C38
45	g	201	3PE	C35-C36-C37-C38
45	K	101	3PE	C35-C36-C37-C38
53	M	602	CDL	C12-C13-C14-C15
45	J	202	3PE	C22-C21-O21-C2
48	B	202	PLC	C1'-C'-O2-C2
53	N	401	CDL	C11-CA5-OA6-CA4
45	N	403	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
46	h	202	PC1	C21-C22-C23-C24
46	L	706	PC1	C3B-C3C-C3D-C3E
45	K	101	3PE	C27-C28-C29-C2A
45	Y	203	3PE	C32-C33-C34-C35
45	d	202	3PE	C25-C26-C27-C28
46	L	706	PC1	C39-C3A-C3B-C3C
53	M	602	CDL	C75-C76-C77-C78
46	I	204	PC1	C31-C32-C33-C34
46	P	502	PC1	C31-C32-C33-C34
45	o	202	3PE	C2B-C2C-C2D-C2E
53	L	701	CDL	C35-C36-C37-C38
53	X	201	CDL	C71-C72-C73-C74
45	N	403	3PE	C36-C37-C38-C39
53	d	201	CDL	C36-C37-C38-C39
58	U	101	EHZ	C1-C2-C3-C4
46	H	403	PC1	C3C-C3D-C3E-C3F
53	h	201	CDL	C33-C34-C35-C36
45	N	403	3PE	C34-C35-C36-C37
46	I	204	PC1	O11-C1-C2-O21
53	M	602	CDL	OB5-CB3-CB4-OB6
48	B	202	PLC	C1B-C2B-C3B-C4B
45	o	202	3PE	C2C-C2D-C2E-C2F
53	d	201	CDL	C72-C73-C74-C75
53	q	201	CDL	C71-CB7-OB8-CB6
46	P	502	PC1	C3B-C3C-C3D-C3E
53	q	201	CDL	C13-C14-C15-C16
45	N	402	3PE	C21-C22-C23-C24
48	b	102	PLC	C2-C3-O3-CB
45	L	703	3PE	C35-C36-C37-C38
45	d	202	3PE	C29-C2A-C2B-C2C
45	Y	202	3PE	C22-C23-C24-C25
45	b	101	3PE	C36-C37-C38-C39
46	I	204	PC1	C32-C33-C34-C35
45	J	202	3PE	O22-C21-O21-C2
48	B	202	PLC	O'-C'-O2-C2
53	M	602	CDL	O1-C1-CA2-OA2
45	I	203	3PE	C2B-C2C-C2D-C2E
46	Y	205	PC1	C24-C25-C26-C27
45	A	201	3PE	C32-C33-C34-C35
45	N	404	3PE	C2A-C2B-C2C-C2D
45	m	202	3PE	C33-C34-C35-C36
46	I	204	PC1	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
46	L	706	PC1	C22-C23-C24-C25
46	q	202	PC1	O32-C31-O31-C3
45	L	702	3PE	C29-C2A-C2B-C2C
45	i	202	3PE	C3E-C3F-C3G-C3H
53	N	401	CDL	C72-C73-C74-C75
45	L	704	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
53	N	401	CDL	OA5-CA3-CA4-CA6
53	N	401	CDL	OA7-CA5-OA6-CA4
45	J	202	3PE	O32-C31-O31-C3
53	h	201	CDL	C58-C59-C60-C61
53	N	401	CDL	CA5-C11-C12-C13
45	I	203	3PE	C2C-C2D-C2E-C2F
45	b	101	3PE	C2D-C2E-C2F-C2G
45	m	201	3PE	C29-C2A-C2B-C2C
58	T	101	EHZ	C22-C23-C24-C25
45	Y	202	3PE	C2C-C2D-C2E-C2F
58	U	101	EHZ	C22-C23-C24-C25
45	b	101	3PE	C23-C24-C25-C26
53	L	701	CDL	C59-C60-C61-C62
45	J	202	3PE	C1-C2-C3-O31
45	N	403	3PE	C1-C2-C3-O31
45	Y	201	3PE	C1-C2-C3-O31
45	g	201	3PE	C1-C2-C3-O31
45	m	201	3PE	C1-C2-C3-O31
46	h	202	PC1	C1-C2-C3-O31
48	b	102	PLC	C1-C2-C3-O3
48	g	202	PLC	C1-C2-C3-O3
53	N	401	CDL	CB3-CB4-CB6-OB8
45	N	402	3PE	C38-C39-C3A-C3B
45	o	202	3PE	C27-C28-C29-C2A
45	K	101	3PE	C32-C33-C34-C35
45	L	705	3PE	C32-C33-C34-C35
53	q	201	CDL	OB9-CB7-OB8-CB6
45	N	402	3PE	C22-C23-C24-C25
46	I	205	PC1	C33-C34-C35-C36
45	Y	201	3PE	C21-C22-C23-C24
45	N	402	3PE	C36-C37-C38-C39
53	q	201	CDL	C31-CA7-OA8-CA6
45	M	603	3PE	C2B-C2C-C2D-C2E
45	m	201	3PE	C2E-C2F-C2G-C2H
45	M	603	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
45	N	404	3PE	O11-C1-C2-O21
45	Y	202	3PE	O11-C1-C2-O21
45	Y	201	3PE	C25-C26-C27-C28
53	X	201	CDL	C64-C65-C66-C67
45	b	101	3PE	C2A-C2B-C2C-C2D
45	N	402	3PE	C32-C33-C34-C35
53	L	701	CDL	C84-C85-C86-C87
46	M	605	PC1	O21-C2-C3-O31
53	M	602	CDL	OB6-CB4-CB6-OB8
48	N	405	PLC	C2'-C3'-C4'-C5'
45	L	705	3PE	C32-C31-O31-C3
53	d	201	CDL	C40-C41-C42-C43
53	N	401	CDL	C36-C37-C38-C39
46	I	204	PC1	C26-C27-C28-C29
46	L	706	PC1	C24-C25-C26-C27
53	M	602	CDL	C34-C35-C36-C37
45	N	402	3PE	C2F-C2G-C2H-C2I
45	N	403	3PE	C29-C2A-C2B-C2C
45	o	202	3PE	C26-C27-C28-C29
45	Z	201	3PE	C37-C38-C39-C3A
45	M	603	3PE	C35-C36-C37-C38
45	i	202	3PE	C35-C36-C37-C38
46	I	204	PC1	C23-C24-C25-C26
45	L	705	3PE	C25-C26-C27-C28
45	M	603	3PE	O11-C1-C2-C3
45	N	403	3PE	O11-C1-C2-C3
45	g	201	3PE	O11-C1-C2-C3
46	I	204	PC1	O11-C1-C2-C3
46	M	605	PC1	O11-C1-C2-C3
48	L	707	PLC	O3P-C1-C2-C3
53	M	602	CDL	OB5-CB3-CB4-CB6
58	T	101	EHZ	N2-C15-C16-C17
45	N	404	3PE	C36-C37-C38-C39
58	U	101	EHZ	C3-C4-C5-C6
53	q	201	CDL	OA9-CA7-OA8-CA6
45	L	704	3PE	C2A-C2B-C2C-C2D
45	A	201	3PE	C26-C27-C28-C29
45	Z	201	3PE	C1-C2-C3-O31
46	A	202	PC1	C1-C2-C3-O31
46	H	403	PC1	C1-C2-C3-O31
46	q	203	PC1	C1-C2-C3-O31
48	B	202	PLC	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
45	d	202	3PE	C24-C25-C26-C27
53	X	201	CDL	C44-C45-C46-C47
46	M	604	PC1	C2A-C2B-C2C-C2D
45	M	603	3PE	C2E-C2F-C2G-C2H
45	Y	204	3PE	O11-C1-C2-O21
46	H	402	PC1	O11-C1-C2-O21
48	b	102	PLC	O3P-C1-C2-O2
53	N	401	CDL	OA5-CA3-CA4-OA6
53	d	201	CDL	C76-C77-C78-C79
58	T	101	EHZ	O1-C7-C8-C9
58	T	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	O1-C7-C8-C9
45	Z	201	3PE	C28-C29-C2A-C2B
45	b	101	3PE	C2C-C2D-C2E-C2F
45	J	202	3PE	O21-C2-C3-O31
45	d	202	3PE	O21-C2-C3-O31
45	o	202	3PE	O21-C2-C3-O31
46	A	202	PC1	O21-C2-C3-O31
46	q	203	PC1	O21-C2-C3-O31
48	L	707	PLC	O2-C2-C3-O3
48	N	405	PLC	O2-C2-C3-O3
53	X	201	CDL	OA6-CA4-CA6-OA8
53	d	201	CDL	OB6-CB4-CB6-OB8
46	d	203	PC1	C34-C35-C36-C37
53	M	602	CDL	C20-C21-C22-C23
45	d	202	3PE	C21-C22-C23-C24
45	L	703	3PE	C37-C38-C39-C3A
53	h	201	CDL	C37-C38-C39-C40
53	N	401	CDL	C74-C75-C76-C77
46	q	202	PC1	C31-C32-C33-C34
53	h	201	CDL	C31-CA7-OA8-CA6
45	J	202	3PE	C23-C24-C25-C26
45	J	202	3PE	C24-C25-C26-C27
53	X	201	CDL	C31-C32-C33-C34
45	L	704	3PE	C27-C28-C29-C2A
53	N	401	CDL	C56-C57-C58-C59
45	N	404	3PE	C25-C26-C27-C28
58	T	101	EHZ	C8-C9-S1-C10
45	g	201	3PE	C31-C32-C33-C34
45	M	603	3PE	C2D-C2E-C2F-C2G
45	I	203	3PE	O11-C1-C2-C3
45	L	703	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
45	N	404	3PE	O11-C1-C2-C3
53	L	701	CDL	OB5-CB3-CB4-CB6
53	d	201	CDL	OA5-CA3-CA4-CA6
45	N	403	3PE	C2-C1-O11-P
45	Y	203	3PE	C36-C37-C38-C39
53	L	701	CDL	C11-C12-C13-C14
45	L	705	3PE	O32-C31-O31-C3
46	A	203	PC1	C32-C33-C34-C35
53	M	602	CDL	C73-C74-C75-C76
46	A	203	PC1	C23-C24-C25-C26
45	d	202	3PE	C22-C23-C24-C25
53	q	201	CDL	CB3-CB4-OB6-CB5
53	M	602	CDL	C58-C59-C60-C61
45	Y	202	3PE	C23-C24-C25-C26
53	h	201	CDL	OA9-CA7-OA8-CA6
45	N	402	3PE	C2E-C2F-C2G-C2H
45	A	201	3PE	O11-C1-C2-O21
45	N	403	3PE	O11-C1-C2-O21
45	g	201	3PE	O11-C1-C2-O21
53	L	701	CDL	OB5-CB3-CB4-OB6
53	X	201	CDL	OA5-CA3-CA4-OA6
45	N	404	3PE	C33-C34-C35-C36
48	B	202	PLC	C7B-C8B-C9B-CAA
45	Y	202	3PE	C1-C2-C3-O31
45	Y	204	3PE	C1-C2-C3-O31
45	i	202	3PE	C1-C2-C3-O31
46	d	203	PC1	C1-C2-C3-O31
53	M	602	CDL	CA3-CA4-CA6-OA8
53	X	201	CDL	CA3-CA4-CA6-OA8
45	N	403	3PE	C26-C27-C28-C29
53	M	602	CDL	C72-C73-C74-C75
45	I	203	3PE	C12-C11-O13-P
45	L	702	3PE	C12-C11-O13-P
45	L	703	3PE	C12-C11-O13-P
45	L	704	3PE	C12-C11-O13-P
45	M	603	3PE	C12-C11-O13-P
45	Y	202	3PE	C12-C11-O13-P
45	Z	201	3PE	C12-C11-O13-P
45	o	202	3PE	C12-C11-O13-P
46	A	202	PC1	C12-C11-O13-P
46	L	706	PC1	C12-C11-O13-P
45	Z	201	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
45	d	202	3PE	C37-C38-C39-C3A
45	Y	201	3PE	O21-C2-C3-O31
45	Y	202	3PE	O21-C2-C3-O31
45	g	201	3PE	O21-C2-C3-O31
45	m	201	3PE	O21-C2-C3-O31
46	H	403	PC1	O21-C2-C3-O31
46	M	604	PC1	O21-C2-C3-O31
46	h	202	PC1	O21-C2-C3-O31
48	b	102	PLC	O2-C2-C3-O3
53	M	602	CDL	OA6-CA4-CA6-OA8
45	I	203	3PE	C2E-C2F-C2G-C2H
45	M	603	3PE	C34-C35-C36-C37
45	o	202	3PE	C24-C25-C26-C27
46	A	202	PC1	C31-C32-C33-C34
45	N	402	3PE	C2C-C2D-C2E-C2F
46	M	604	PC1	C2B-C2C-C2D-C2E
46	A	203	PC1	O13-C11-C12-N
46	M	605	PC1	O13-C11-C12-N
48	b	102	PLC	O4P-C4-C5-N
57	P	501	NDP	PN-O3-PA-O2A
46	I	204	PC1	C35-C36-C37-C38
45	d	202	3PE	C28-C29-C2A-C2B
48	g	202	PLC	C7'-C8'-C9'-CA'
45	L	704	3PE	C37-C38-C39-C3A
45	L	704	3PE	C33-C34-C35-C36
45	N	403	3PE	C2E-C2F-C2G-C2H
45	L	703	3PE	C29-C2A-C2B-C2C
53	q	201	CDL	CA5-C11-C12-C13
53	M	602	CDL	C62-C63-C64-C65
53	L	701	CDL	C78-C79-C80-C81
48	N	405	PLC	C1B-CB-O3-C3
53	L	701	CDL	C62-C63-C64-C65
53	X	201	CDL	CA7-C31-C32-C33
46	H	402	PC1	O11-C1-C2-C3
46	H	403	PC1	O11-C1-C2-C3
45	b	101	3PE	C37-C38-C39-C3A
45	d	202	3PE	C2F-C2G-C2H-C2I
58	T	101	EHZ	C18-C17-C20-O6
45	m	201	3PE	C23-C24-C25-C26
53	N	401	CDL	C31-C32-C33-C34
53	q	201	CDL	O1-C1-CB2-OB2
45	Y	203	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C51-C52-C53-C54
46	H	403	PC1	C2-C1-O11-P
53	h	201	CDL	C1-CA2-OA2-PA1
57	P	501	NDP	C2B-O2B-P2B-O1X
46	I	205	PC1	C29-C2A-C2B-C2C
46	A	202	PC1	C23-C24-C25-C26
53	L	701	CDL	C72-C73-C74-C75
45	L	703	3PE	O11-C1-C2-O21
45	L	704	3PE	O11-C1-C2-O21
45	b	101	3PE	O11-C1-C2-O21
48	L	707	PLC	O3P-C1-C2-O2
53	J	201	CDL	OB5-CB3-CB4-OB6
53	d	201	CDL	OA5-CA3-CA4-OA6
45	M	603	3PE	C37-C38-C39-C3A
46	H	402	PC1	C33-C34-C35-C36
45	Y	201	3PE	C22-C21-O21-C2
53	L	701	CDL	C64-C65-C66-C67
45	L	704	3PE	C32-C33-C34-C35
53	X	201	CDL	C81-C82-C83-C84
45	i	202	3PE	O21-C2-C3-O31
46	d	203	PC1	O21-C2-C3-O31
48	B	202	PLC	O2-C2-C3-O3
45	L	705	3PE	C36-C37-C38-C39
46	M	604	PC1	C1-C2-C3-O31
48	N	405	PLC	C1-C2-C3-O3
53	M	602	CDL	CB3-CB4-CB6-OB8
58	T	101	EHZ	C10-C11-N1-C12
53	d	201	CDL	C37-C38-C39-C40
53	h	201	CDL	C36-C37-C38-C39
46	q	203	PC1	C32-C33-C34-C35
58	T	101	EHZ	C16-C17-C20-O6
45	Y	202	3PE	C29-C2A-C2B-C2C
53	X	201	CDL	C75-C76-C77-C78
45	b	101	3PE	C29-C2A-C2B-C2C
46	H	403	PC1	C3A-C3B-C3C-C3D
45	I	203	3PE	C11-O13-P-O11
45	I	203	3PE	C11-O13-P-O12
45	I	203	3PE	C11-O13-P-O14
45	J	202	3PE	C11-O13-P-O14
45	K	101	3PE	C1-O11-P-O12
45	K	101	3PE	C1-O11-P-O13
45	K	101	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	L	702	3PE	C11-O13-P-O12
45	L	705	3PE	O13-C11-C12-N
45	N	403	3PE	C11-O13-P-O14
45	N	403	3PE	O13-C11-C12-N
45	N	404	3PE	C11-O13-P-O11
45	N	404	3PE	O13-C11-C12-N
45	Y	202	3PE	C1-O11-P-O12
45	Y	202	3PE	C1-O11-P-O13
45	Y	204	3PE	C1-O11-P-O13
45	Z	201	3PE	C11-O13-P-O14
45	b	101	3PE	C1-O11-P-O12
45	b	101	3PE	C1-O11-P-O13
45	g	201	3PE	C11-O13-P-O12
45	g	201	3PE	O13-C11-C12-N
45	i	202	3PE	C1-O11-P-O13
45	i	202	3PE	C11-O13-P-O11
45	m	201	3PE	C1-O11-P-O12
45	m	202	3PE	C1-O11-P-O14
45	m	202	3PE	O13-C11-C12-N
46	I	204	PC1	C1-O11-P-O12
46	I	204	PC1	C1-O11-P-O14
46	I	204	PC1	C1-O11-P-O13
46	I	205	PC1	C11-O13-P-O12
46	L	706	PC1	C11-O13-P-O12
46	M	604	PC1	C1-O11-P-O14
46	M	605	PC1	C11-O13-P-O14
46	M	605	PC1	C1-O11-P-O12
46	Y	205	PC1	C11-O13-P-O14
46	Y	205	PC1	C11-O13-P-O11
46	d	203	PC1	C11-O13-P-O14
46	q	203	PC1	C1-O11-P-O13
53	L	701	CDL	CB3-OB5-PB2-OB2
53	L	701	CDL	CB3-OB5-PB2-OB3
53	L	701	CDL	CB3-OB5-PB2-OB4
53	M	602	CDL	CB2-OB2-PB2-OB3
53	X	201	CDL	CA3-OA5-PA1-OA2
53	X	201	CDL	CA3-OA5-PA1-OA3
53	d	201	CDL	CB2-OB2-PB2-OB3
53	q	201	CDL	CB2-OB2-PB2-OB3
46	I	205	PC1	C22-C23-C24-C25
45	Z	201	3PE	C29-C2A-C2B-C2C
45	I	203	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	L	707	PLC	C2B-C1B-CB-O3
45	b	101	3PE	O21-C21-C22-C23
45	L	705	3PE	C2-C1-O11-P
46	M	604	PC1	C2-C1-O11-P
46	M	605	PC1	C2-C1-O11-P
53	X	201	CDL	C1-CB2-OB2-PB2
45	Y	201	3PE	O22-C21-O21-C2
45	Y	202	3PE	C2D-C2E-C2F-C2G
45	J	202	3PE	C35-C36-C37-C38
46	P	502	PC1	C37-C38-C39-C3A
45	Y	202	3PE	O21-C21-C22-C23
48	b	102	PLC	CB-C1B-C2B-C3B
45	Y	203	3PE	C26-C27-C28-C29
45	Y	201	3PE	C3-C2-O21-C21
45	Y	204	3PE	C3-C2-O21-C21
45	i	202	3PE	C1-C2-O21-C21
46	A	202	PC1	C3-C2-O21-C21
53	N	401	CDL	CA6-CA4-OA6-CA5
45	Z	201	3PE	C2F-C2G-C2H-C2I
45	Y	202	3PE	O11-C1-C2-C3
48	b	102	PLC	O3P-C1-C2-C3
53	X	201	CDL	OA5-CA3-CA4-CA6
53	M	602	CDL	C79-C80-C81-C82
53	h	201	CDL	C17-C18-C19-C20
45	Y	202	3PE	C3F-C3G-C3H-C3I
45	J	202	3PE	C22-C23-C24-C25
45	Z	201	3PE	C2E-C2F-C2G-C2H
53	X	201	CDL	CB7-C71-C72-C73
45	N	404	3PE	C39-C3A-C3B-C3C
46	H	403	PC1	O11-C1-C2-O21
46	d	203	PC1	C39-C3A-C3B-C3C
46	A	202	PC1	C24-C25-C26-C27
53	L	701	CDL	C39-C40-C41-C42
45	Z	201	3PE	C31-C32-C33-C34
53	d	201	CDL	C38-C39-C40-C41
53	X	201	CDL	C54-C55-C56-C57
45	Y	204	3PE	O21-C2-C3-O31
46	A	203	PC1	O21-C2-C3-O31
53	N	401	CDL	OA6-CA4-CA6-OA8
45	N	402	3PE	O21-C21-C22-C23
53	h	201	CDL	C76-C77-C78-C79
46	H	403	PC1	C3F-C3G-C3H-C3I

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Mol	Chain	Res	Type	Atoms
46	L	706	PC1	C23-C24-C25-C26
46	M	605	PC1	C1-C2-C3-O31
46	d	203	PC1	C31-C32-C33-C34
53	L	701	CDL	C73-C74-C75-C76
55	O	401	DGT	PA-O3A-PB-O1B
46	H	402	PC1	C22-C21-O21-C2
53	h	201	CDL	C55-C56-C57-C58
45	I	203	3PE	O32-C31-C32-C33
53	L	701	CDL	C72-C71-CB7-OB8
45	b	101	3PE	C24-C25-C26-C27
46	q	202	PC1	C27-C28-C29-C2A
58	T	101	EHZ	O4-C15-C16-C17
48	b	102	PLC	C3B-C4B-C5B-C6B
46	Y	205	PC1	C37-C38-C39-C3A
46	H	403	PC1	C39-C3A-C3B-C3C
46	M	604	PC1	C11-C12-N-C13
45	K	101	3PE	C29-C2A-C2B-C2C
45	i	202	3PE	C39-C3A-C3B-C3C
53	J	201	CDL	CB2-C1-CA2-OA2
45	N	403	3PE	C2A-C2B-C2C-C2D
53	X	201	CDL	C34-C35-C36-C37
45	m	201	3PE	C34-C35-C36-C37
46	d	203	PC1	C32-C33-C34-C35
45	M	603	3PE	C3D-C3E-C3F-C3G
48	L	707	PLC	C2B-C1B-CB-OB
45	N	404	3PE	C35-C36-C37-C38
46	H	402	PC1	O22-C21-O21-C2
45	L	705	3PE	C22-C23-C24-C25
53	N	401	CDL	C1-CA2-OA2-PA1
53	d	201	CDL	C1-CA2-OA2-PA1
45	L	704	3PE	C26-C27-C28-C29
46	d	203	PC1	C3B-C3C-C3D-C3E
46	P	502	PC1	C32-C33-C34-C35
45	d	202	3PE	C1-C2-C3-O31
45	o	202	3PE	C1-C2-C3-O31
45	A	201	3PE	C35-C36-C37-C38
45	L	703	3PE	C2B-C2C-C2D-C2E
46	H	403	PC1	C3E-C3F-C3G-C3H
55	O	401	DGT	O4'-C4'-C5'-O5'
45	L	705	3PE	C3-C2-O21-C21
46	Y	205	PC1	C1-C2-O21-C21
46	Y	205	PC1	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
48	L	707	PLC	C1-C2-O2-C'
48	b	102	PLC	C1-C2-O2-C'
53	X	201	CDL	CA3-CA4-OA6-CA5
46	I	204	PC1	C25-C26-C27-C28
45	K	101	3PE	O21-C21-C22-C23
46	M	604	PC1	C11-C12-N-C14
53	h	201	CDL	C32-C33-C34-C35
45	N	402	3PE	O11-C1-C2-O21
50	F	501	FMN	C4'-C5'-O5'-P
53	J	201	CDL	CA4-CA3-OA5-PA1
46	Y	205	PC1	C38-C39-C3A-C3B
53	h	201	CDL	C73-C74-C75-C76
53	J	201	CDL	OB5-CB3-CB4-CB6
46	M	604	PC1	C26-C27-C28-C29
53	h	201	CDL	C54-C55-C56-C57
58	U	101	EHZ	C2-C3-C4-C5
46	L	706	PC1	O21-C2-C3-O31
57	P	501	NDP	C2N-C3N-C7N-N7N
45	L	705	3PE	C34-C35-C36-C37
46	q	202	PC1	C3A-C3B-C3C-C3D
52	H	401	U10	C12-C11-C9-C10
45	L	705	3PE	C33-C34-C35-C36
46	A	202	PC1	C22-C23-C24-C25
53	h	201	CDL	C52-C53-C54-C55
45	N	402	3PE	C3C-C3D-C3E-C3F
53	L	701	CDL	C74-C75-C76-C77
45	N	402	3PE	C26-C27-C28-C29
45	m	202	3PE	C36-C37-C38-C39
48	L	707	PLC	C'-C1'-C2'-C3'
46	d	203	PC1	C33-C34-C35-C36
45	L	704	3PE	C34-C35-C36-C37
45	M	603	3PE	C2-C1-O11-P
46	h	202	PC1	C2-C1-O11-P
53	M	602	CDL	C76-C77-C78-C79
45	i	202	3PE	O21-C21-C22-C23
45	M	603	3PE	C27-C28-C29-C2A
45	b	101	3PE	C1-C2-C3-O31
53	d	201	CDL	CB3-CB4-CB6-OB8
53	N	401	CDL	C57-C58-C59-C60
45	J	202	3PE	C32-C33-C34-C35
45	N	403	3PE	C32-C33-C34-C35
46	A	203	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
60	o	201	MYR	C5-C6-C7-C8
53	M	602	CDL	OA5-CA3-CA4-OA6
45	m	202	3PE	C22-C23-C24-C25
46	h	202	PC1	O31-C31-C32-C33
45	i	202	3PE	C33-C34-C35-C36
46	M	604	PC1	C11-C12-N-C15
46	q	203	PC1	C23-C24-C25-C26
46	q	202	PC1	C37-C38-C39-C3A
45	Y	204	3PE	O11-C1-C2-C3
45	Y	202	3PE	C31-C32-C33-C34
45	i	202	3PE	C25-C26-C27-C28
46	I	205	PC1	C27-C28-C29-C2A
45	L	705	3PE	C23-C24-C25-C26
53	M	602	CDL	C81-C82-C83-C84
55	O	401	DGT	PB-O3B-PG-O3G
45	Y	202	3PE	C37-C38-C39-C3A
53	X	201	CDL	C72-C71-CB7-OB8
45	Y	203	3PE	C3F-C3G-C3H-C3I
45	i	202	3PE	C28-C29-C2A-C2B
45	N	403	3PE	C24-C25-C26-C27
46	q	202	PC1	C33-C34-C35-C36
53	N	401	CDL	C76-C77-C78-C79
45	L	703	3PE	C28-C29-C2A-C2B
45	N	403	3PE	C33-C34-C35-C36
45	m	202	3PE	C34-C35-C36-C37
45	m	201	3PE	C31-C32-C33-C34
46	I	204	PC1	C3B-C3C-C3D-C3E
45	Z	201	3PE	C33-C34-C35-C36
46	A	203	PC1	C1-C2-C3-O31
46	q	202	PC1	C29-C2A-C2B-C2C
45	N	402	3PE	C23-C24-C25-C26
46	A	202	PC1	C34-C35-C36-C37
45	Y	202	3PE	C27-C28-C29-C2A
45	N	402	3PE	C12-C11-O13-P
46	H	403	PC1	C12-C11-O13-P
53	d	201	CDL	C42-C43-C44-C45
45	N	404	3PE	C32-C33-C34-C35
53	L	701	CDL	C57-C58-C59-C60
48	N	405	PLC	OB-CB-O3-C3
45	J	202	3PE	C26-C27-C28-C29
45	N	403	3PE	C23-C24-C25-C26
46	M	604	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	O11-C1-C2-C3
53	X	201	CDL	C51-C52-C53-C54
46	I	204	PC1	C2D-C2E-C2F-C2G
46	M	605	PC1	C32-C33-C34-C35
45	Y	203	3PE	C35-C36-C37-C38
46	M	604	PC1	C22-C21-O21-C2
46	P	502	PC1	C3A-C3B-C3C-C3D
45	L	703	3PE	O31-C31-C32-C33
46	H	402	PC1	O13-C11-C12-N
55	O	401	DGT	PB-O3A-PA-O1A
55	O	401	DGT	PB-O3A-PA-O2A
45	i	202	3PE	C3B-C3C-C3D-C3E
45	L	705	3PE	O31-C31-C32-C33
46	P	502	PC1	C26-C27-C28-C29
46	P	502	PC1	C33-C34-C35-C36
45	m	201	3PE	O31-C31-C32-C33
45	J	202	3PE	O21-C21-C22-C23
45	K	101	3PE	C3D-C3E-C3F-C3G
46	d	203	PC1	O11-C1-C2-O21
52	H	401	U10	C12-C11-C9-C8
53	L	701	CDL	C54-C55-C56-C57
53	X	201	CDL	C36-C37-C38-C39
45	M	603	3PE	C25-C26-C27-C28
45	Y	202	3PE	C26-C27-C28-C29
53	h	201	CDL	CB4-CB3-OB5-PB2
48	L	707	PLC	O2-C'-C1'-C2'
46	H	403	PC1	C35-C36-C37-C38
53	L	701	CDL	C61-C62-C63-C64
53	h	201	CDL	C75-C76-C77-C78
45	A	201	3PE	C1-C2-C3-O31
53	J	201	CDL	CB3-CB4-CB6-OB8
45	J	202	3PE	O31-C31-C32-C33
45	Y	202	3PE	O31-C31-C32-C33
45	i	202	3PE	O31-C31-C32-C33
53	X	201	CDL	C32-C31-CA7-OA8
46	I	205	PC1	O21-C2-C3-O31
45	N	404	3PE	C38-C39-C3A-C3B
53	L	701	CDL	C32-C33-C34-C35
53	M	602	CDL	C21-C22-C23-C24
45	K	101	3PE	O31-C31-C32-C33
45	Y	201	3PE	O31-C31-C32-C33
46	A	203	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	H	402	PC1	O31-C31-C32-C33
45	Y	204	3PE	C2D-C2E-C2F-C2G
50	F	501	FMN	N10-C1'-C2'-O2'
53	d	201	CDL	C33-C34-C35-C36
53	X	201	CDL	CA6-CA4-OA6-CA5
53	d	201	CDL	C74-C75-C76-C77
55	O	401	DGT	C3'-C4'-C5'-O5'
45	L	702	3PE	C2-C1-O11-P
45	L	703	3PE	C2-C1-O11-P
45	L	704	3PE	C2-C1-O11-P
53	d	201	CDL	C72-C71-CB7-OB8
45	N	402	3PE	C31-C32-C33-C34
53	d	201	CDL	CB7-C71-C72-C73
45	K	101	3PE	C37-C38-C39-C3A
45	b	101	3PE	C2E-C2F-C2G-C2H
53	X	201	CDL	C80-C81-C82-C83
45	L	703	3PE	O32-C31-C32-C33
53	h	201	CDL	C56-C57-C58-C59
53	M	602	CDL	C80-C81-C82-C83
45	J	202	3PE	O22-C21-C22-C23
45	L	705	3PE	O32-C31-C32-C33
45	Y	202	3PE	O32-C31-C32-C33
53	d	201	CDL	C39-C40-C41-C42
45	K	101	3PE	O32-C31-C32-C33
53	X	201	CDL	C32-C31-CA7-OA9
48	L	707	PLC	O'-C'-C1'-C2'
45	K	101	3PE	C24-C25-C26-C27
53	h	201	CDL	C11-C12-C13-C14
45	A	201	3PE	O21-C2-C3-O31
53	J	201	CDL	OB6-CB4-CB6-OB8
45	Z	201	3PE	C25-C26-C27-C28
45	m	201	3PE	O32-C31-C32-C33
45	m	201	3PE	C22-C23-C24-C25
53	L	701	CDL	C58-C59-C60-C61
46	q	202	PC1	C36-C37-C38-C39
46	H	402	PC1	O21-C21-C22-C23
46	q	202	PC1	O31-C31-C32-C33
46	A	203	PC1	O22-C21-C22-C23
46	H	402	PC1	C24-C25-C26-C27
46	q	202	PC1	C2B-C2C-C2D-C2E
45	Y	201	3PE	C24-C25-C26-C27
46	M	604	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
46	H	402	PC1	O32-C31-O31-C3
46	M	604	PC1	C29-C2A-C2B-C2C
46	A	203	PC1	C22-C23-C24-C25
48	B	202	PLC	C4B-C5B-C6B-C7B
45	i	202	3PE	O32-C31-C32-C33
45	Z	201	3PE	O21-C21-C22-C23
45	N	403	3PE	O21-C21-C22-C23
46	L	706	PC1	O31-C31-C32-C33
46	q	203	PC1	O31-C31-C32-C33
45	J	202	3PE	O32-C31-C32-C33
45	Z	201	3PE	C38-C39-C3A-C3B

There are no ring outliers.

27 monomers are involved in 49 short contacts:

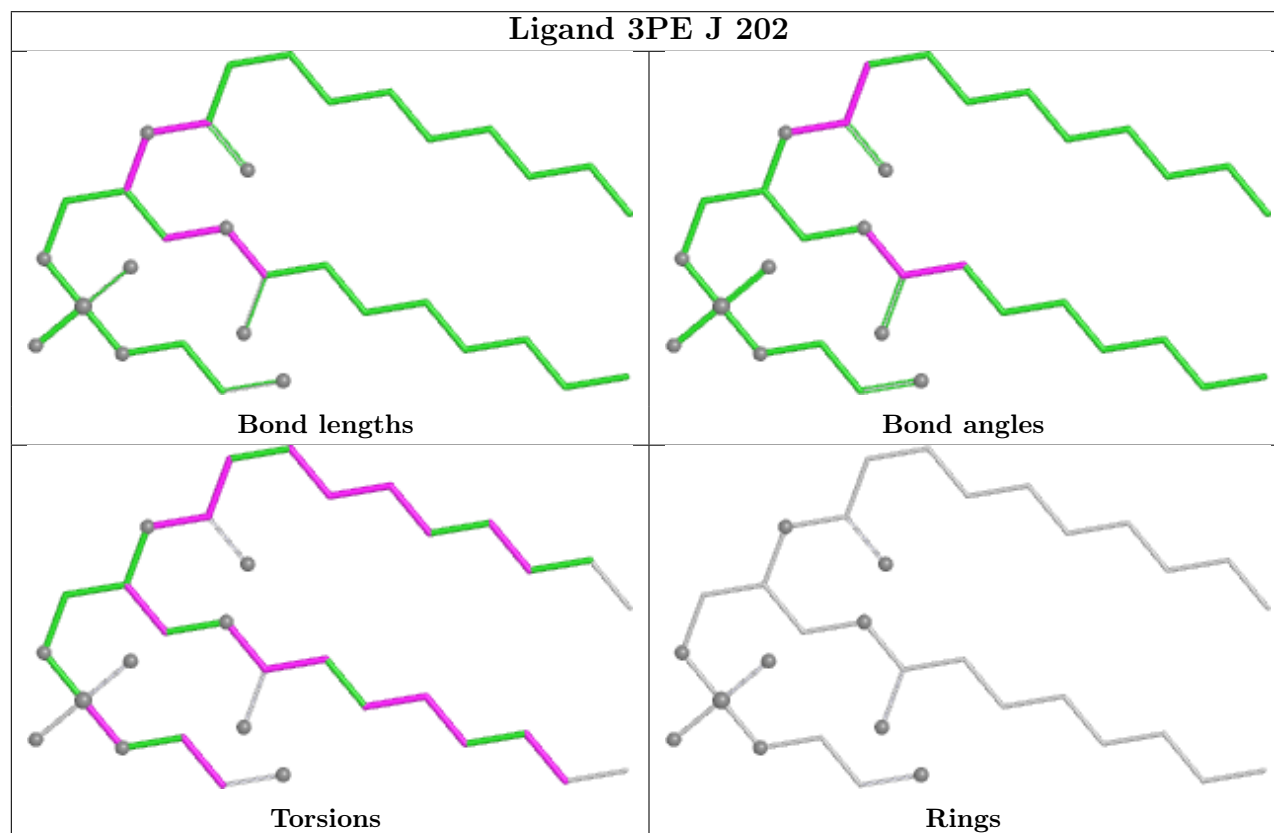
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	T	101	EHZ	2	0
46	q	203	PC1	2	0
52	H	401	U10	9	0
46	I	205	PC1	1	0
45	Z	201	3PE	1	0
46	A	202	PC1	1	0
53	h	201	CDL	1	0
55	O	401	DGT	3	0
45	Y	201	3PE	1	0
45	o	202	3PE	1	0
45	i	202	3PE	2	0
53	M	602	CDL	1	0
45	L	702	3PE	1	0
48	g	202	PLC	1	0
46	q	202	PC1	3	0
58	U	101	EHZ	1	0
46	H	402	PC1	1	0
59	i	201	CHD	7	0
53	q	201	CDL	1	0
45	L	705	3PE	2	0
46	d	203	PC1	1	0
46	M	604	PC1	2	0
53	d	201	CDL	2	0
45	I	203	3PE	1	0
45	Y	202	3PE	1	0
46	I	204	PC1	1	0

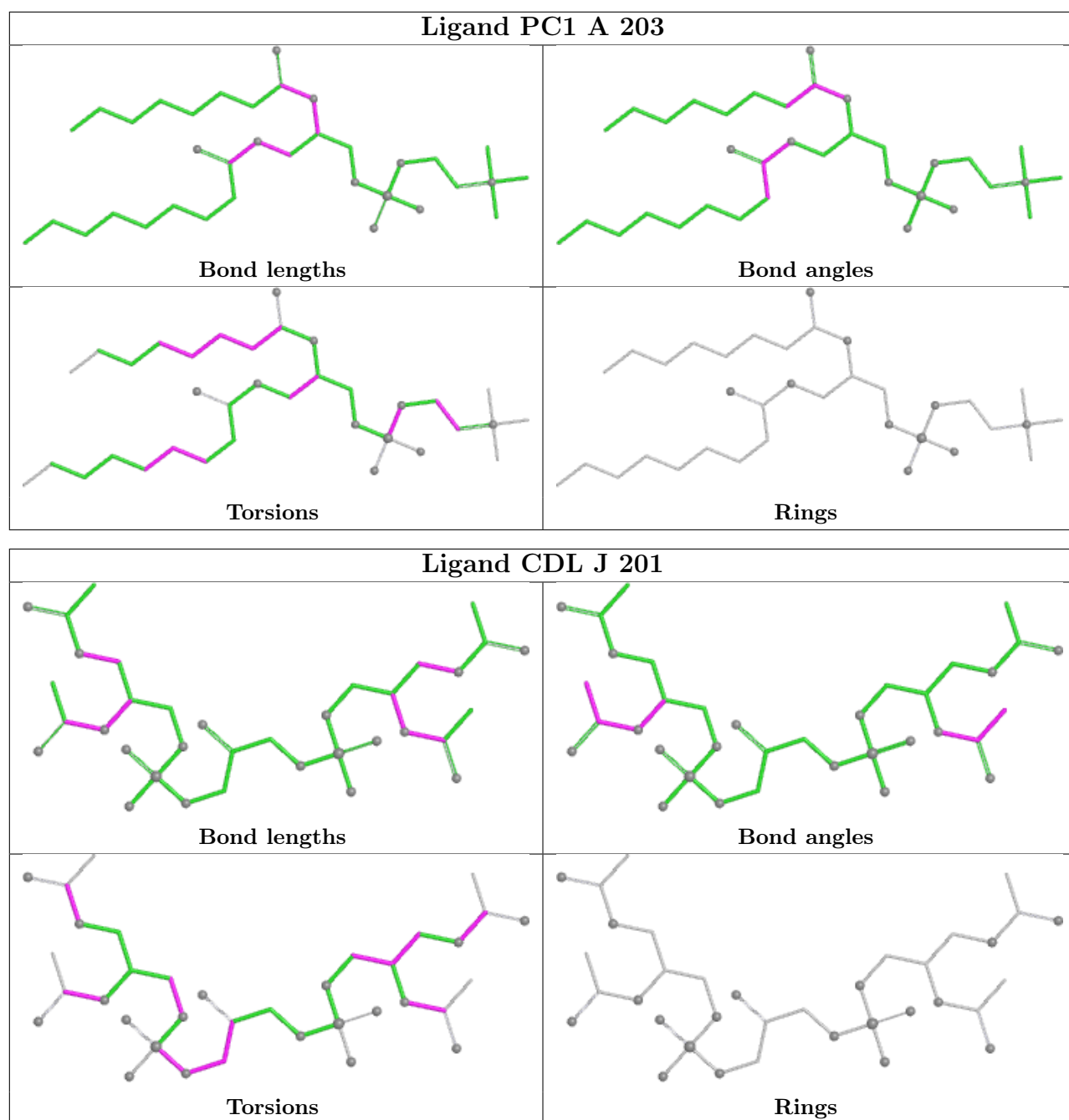
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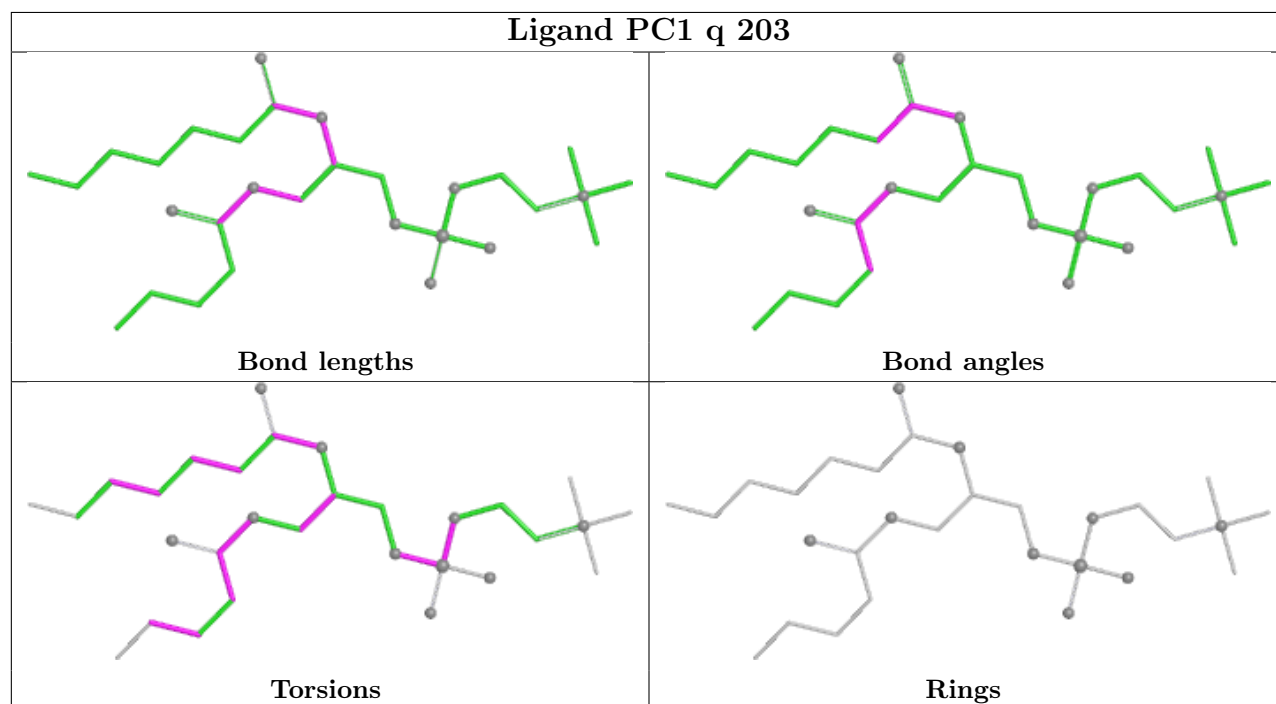
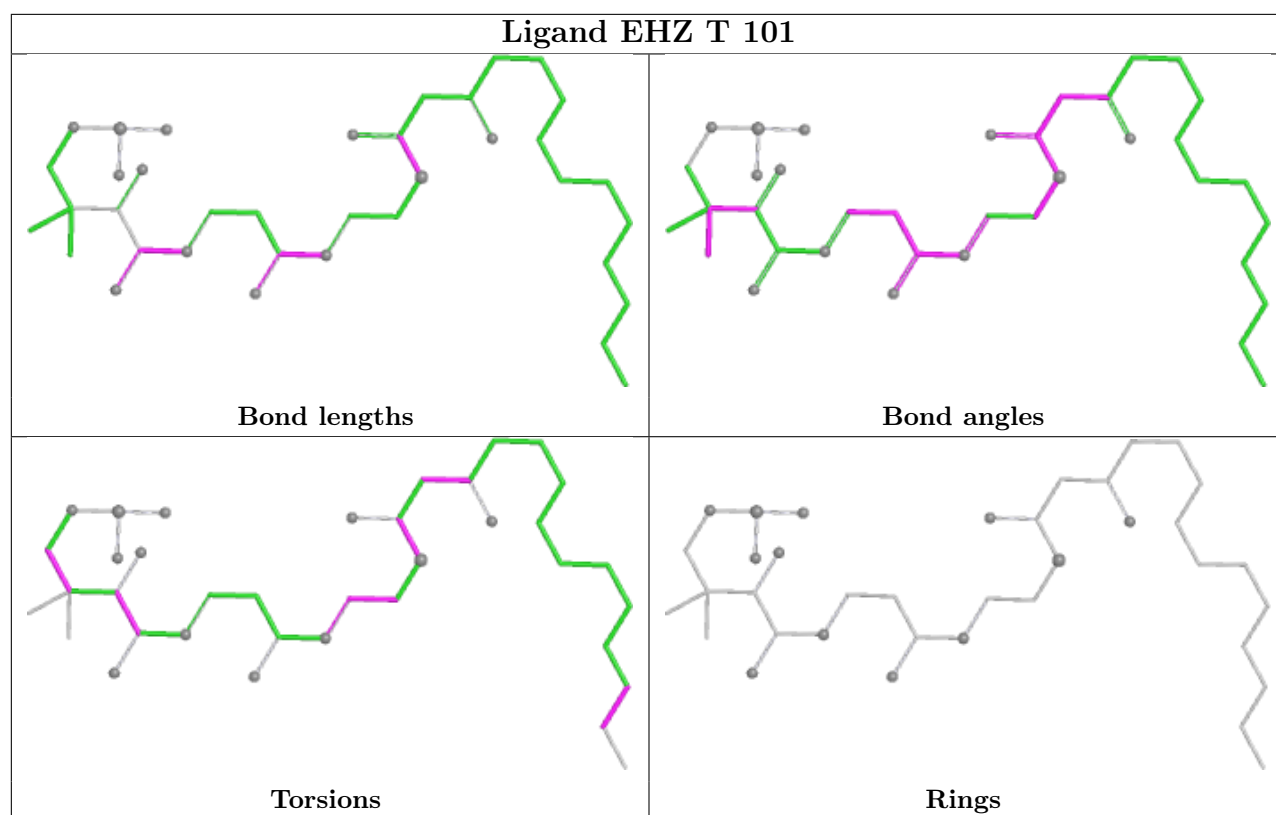
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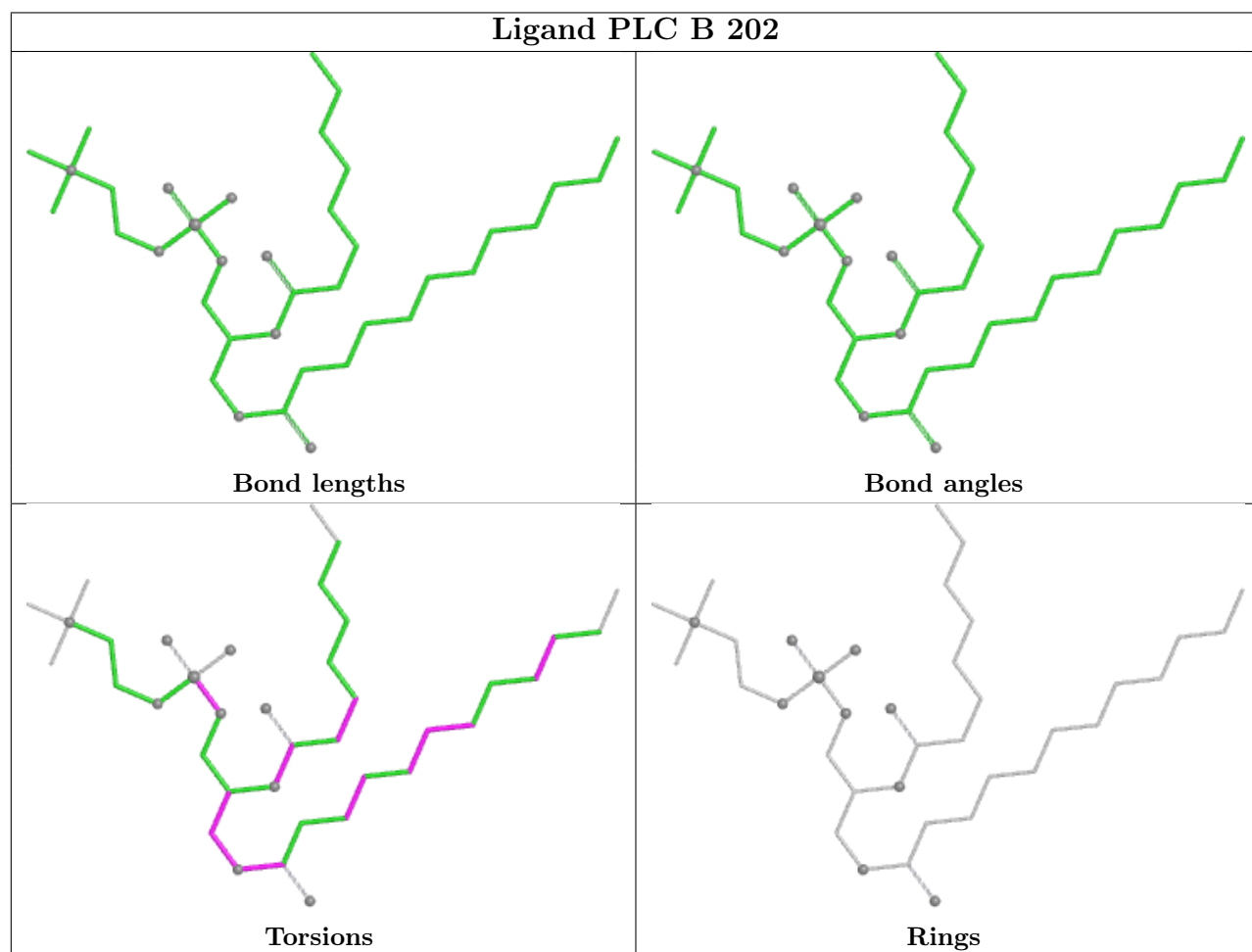
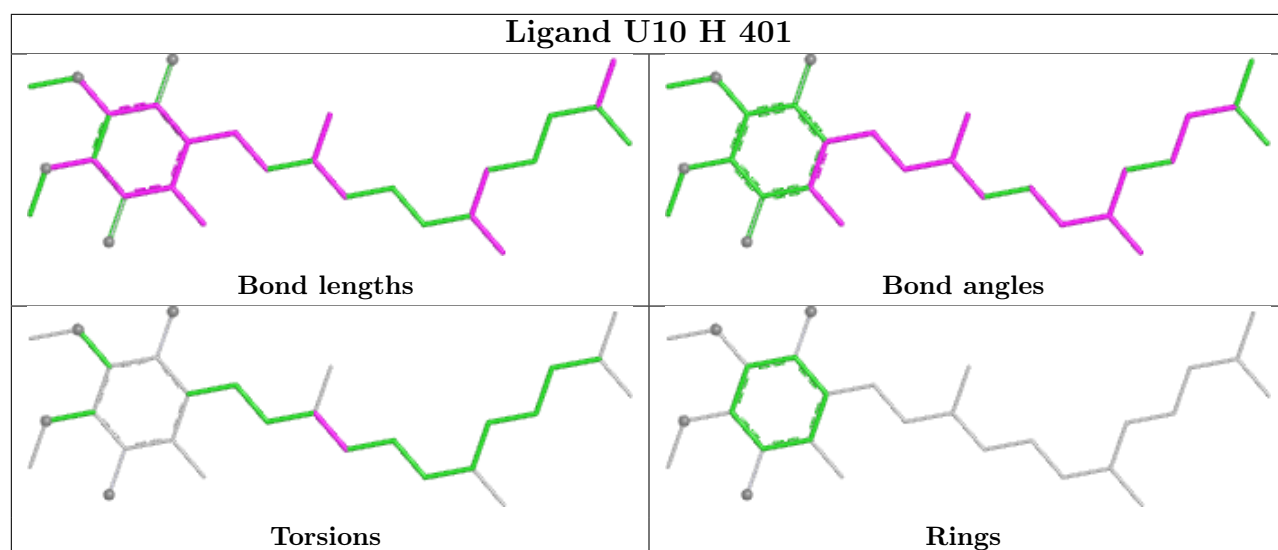
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	Y	204	3PE	1	0

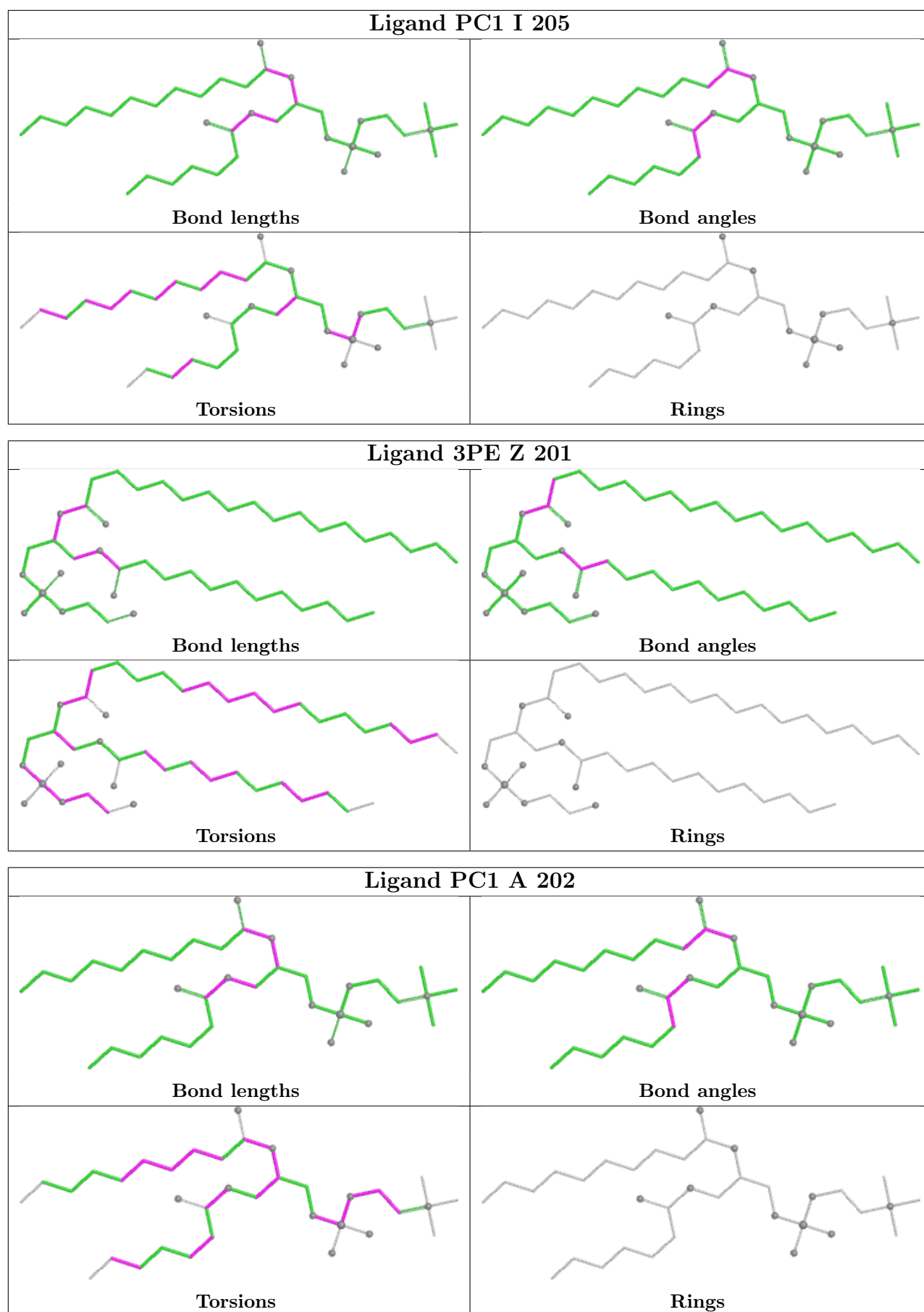
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

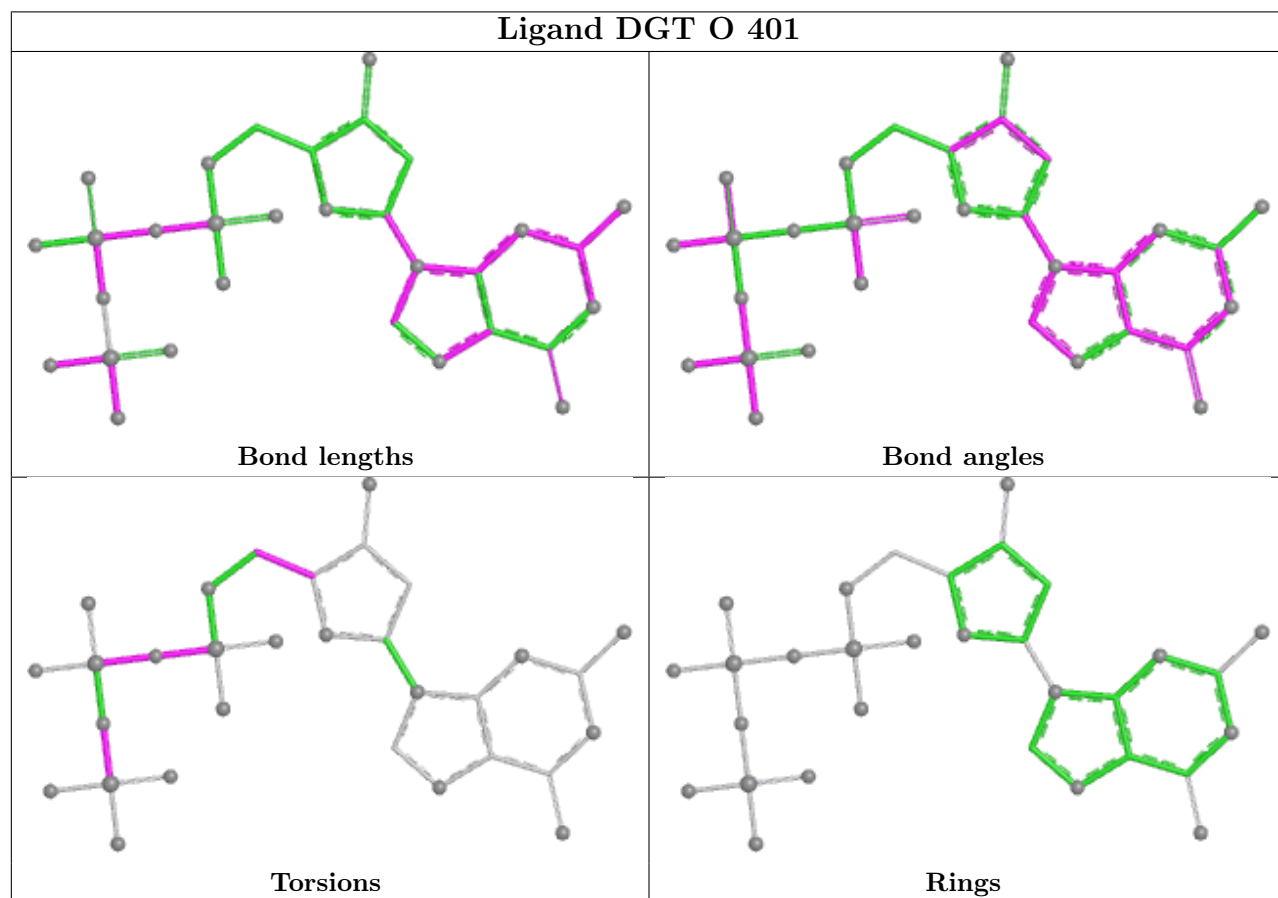
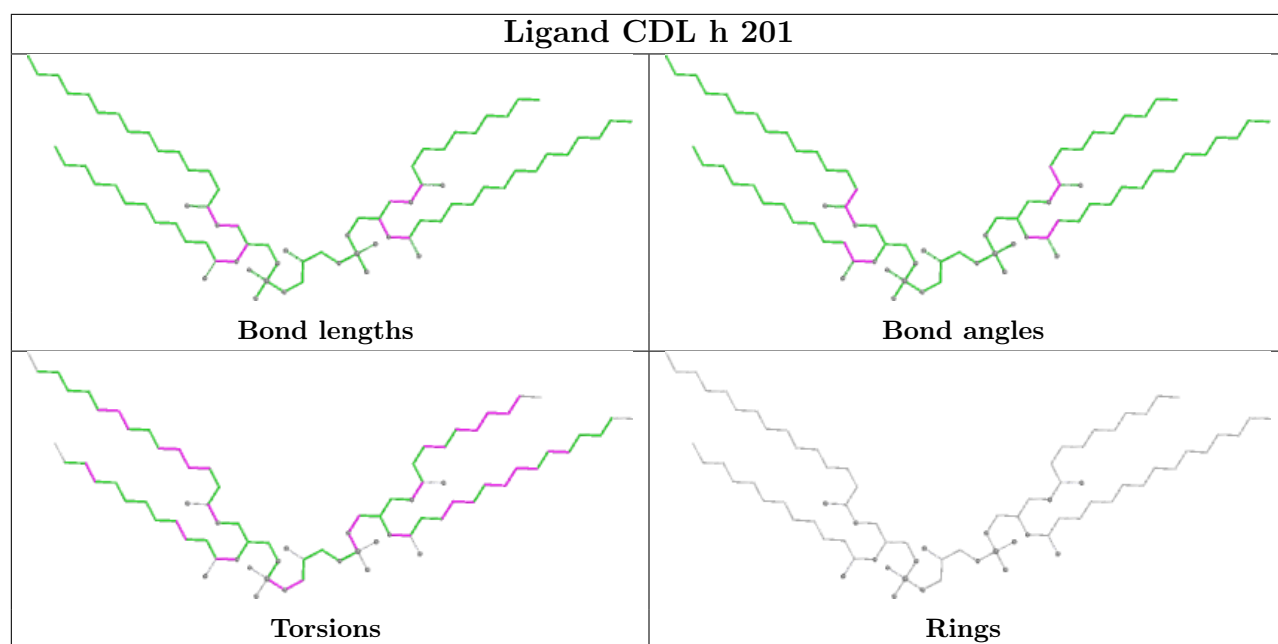


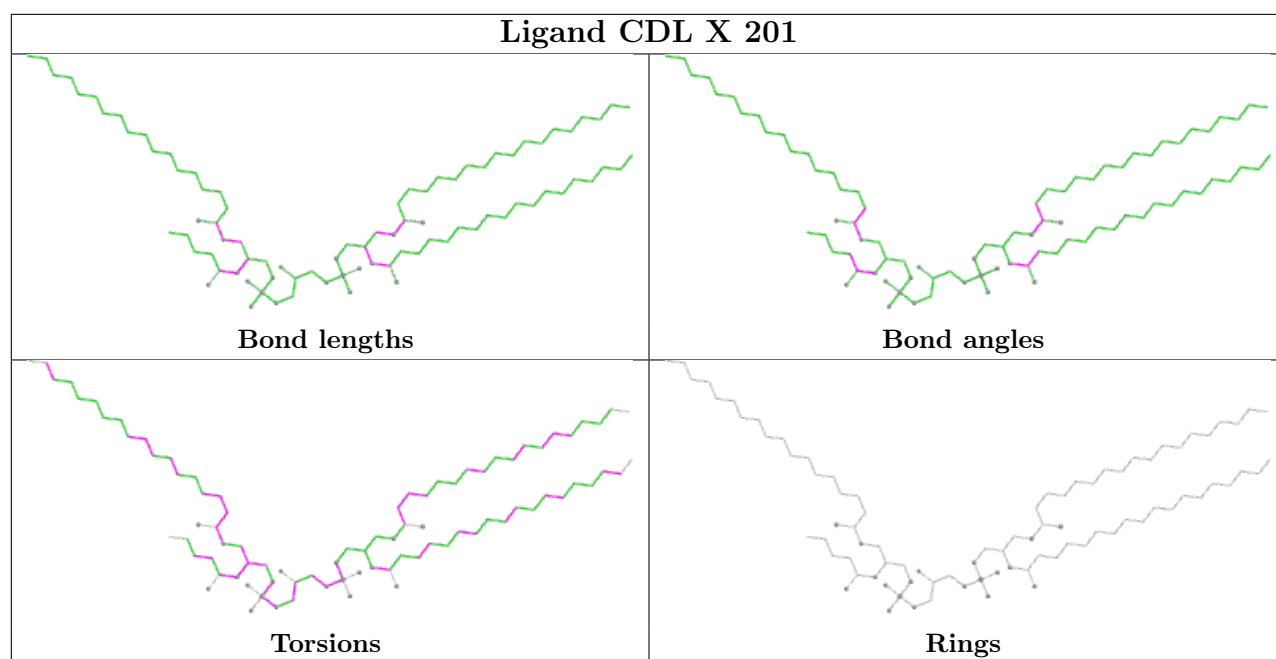


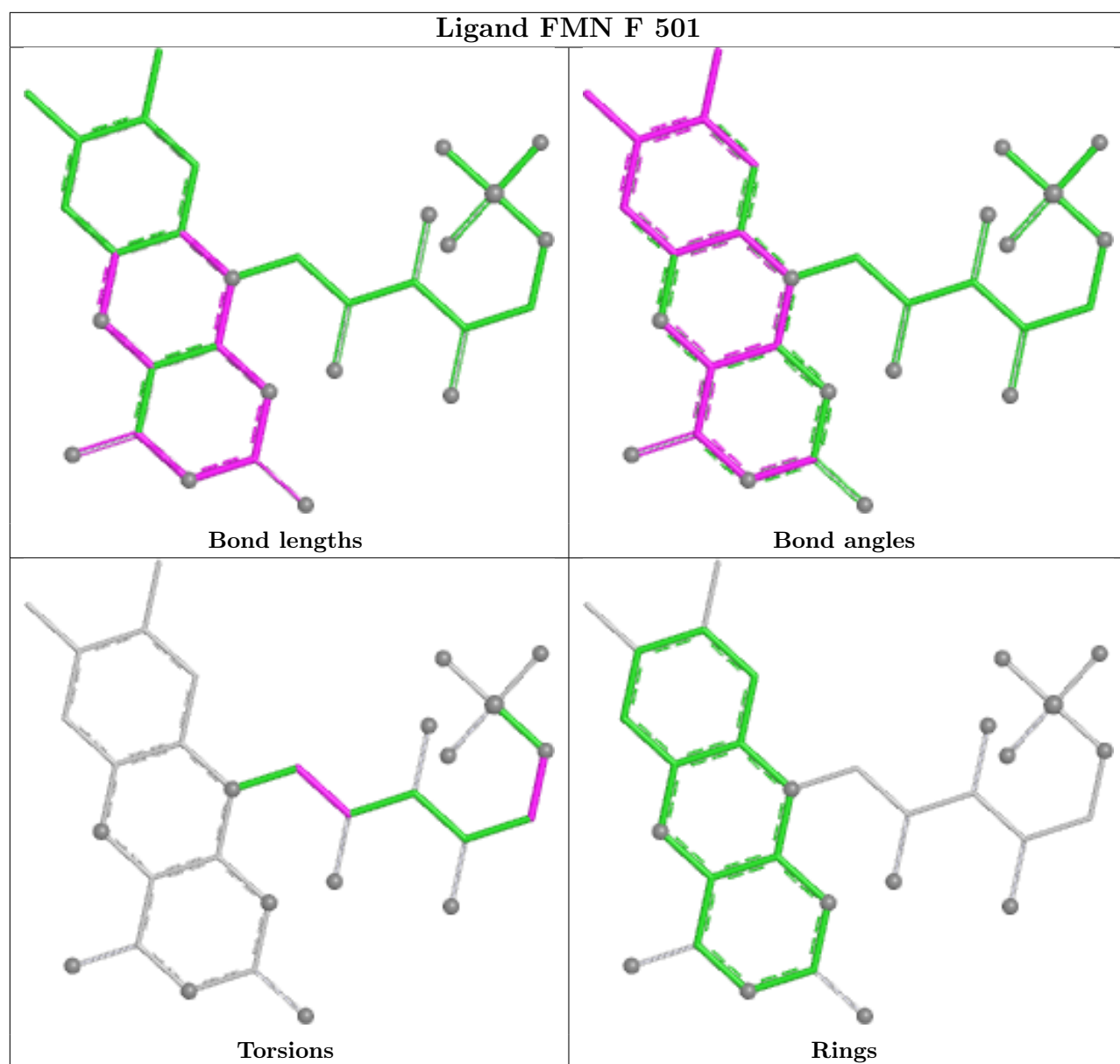




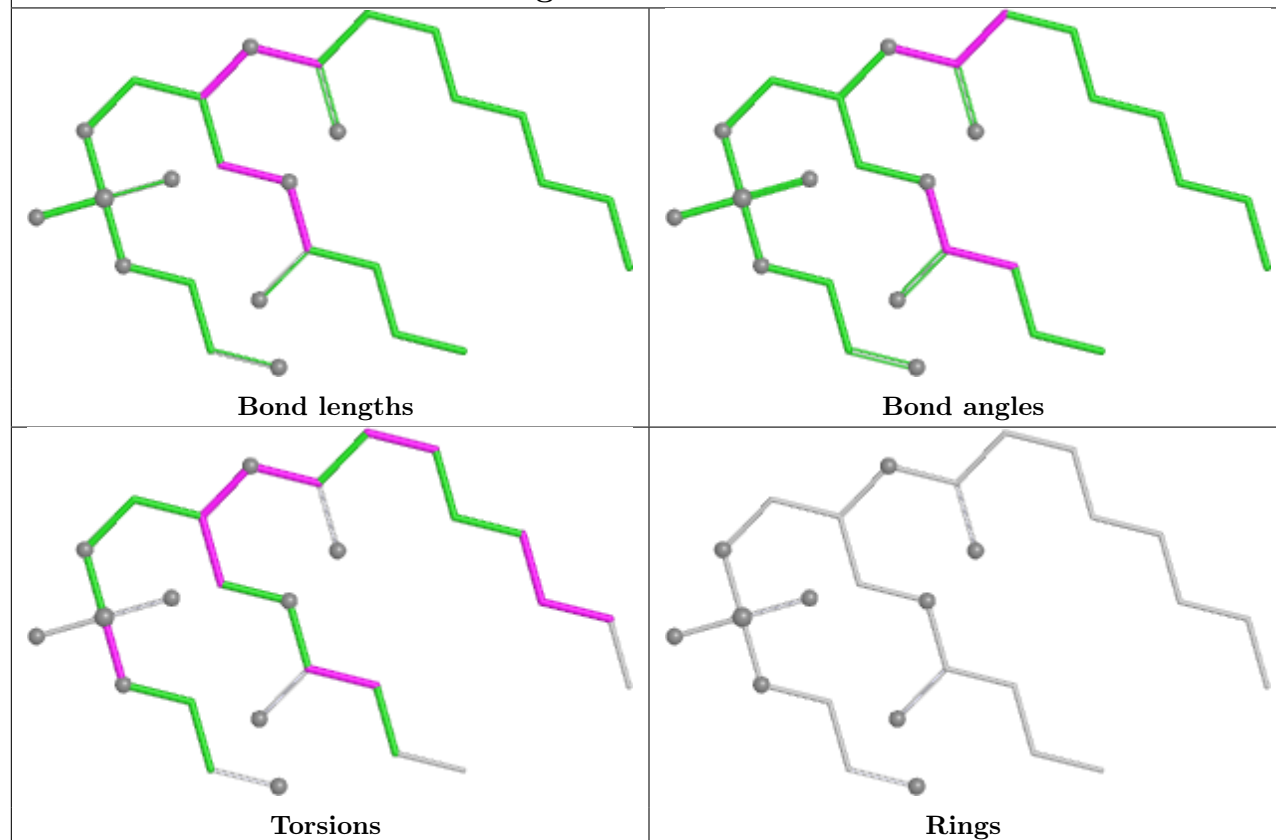




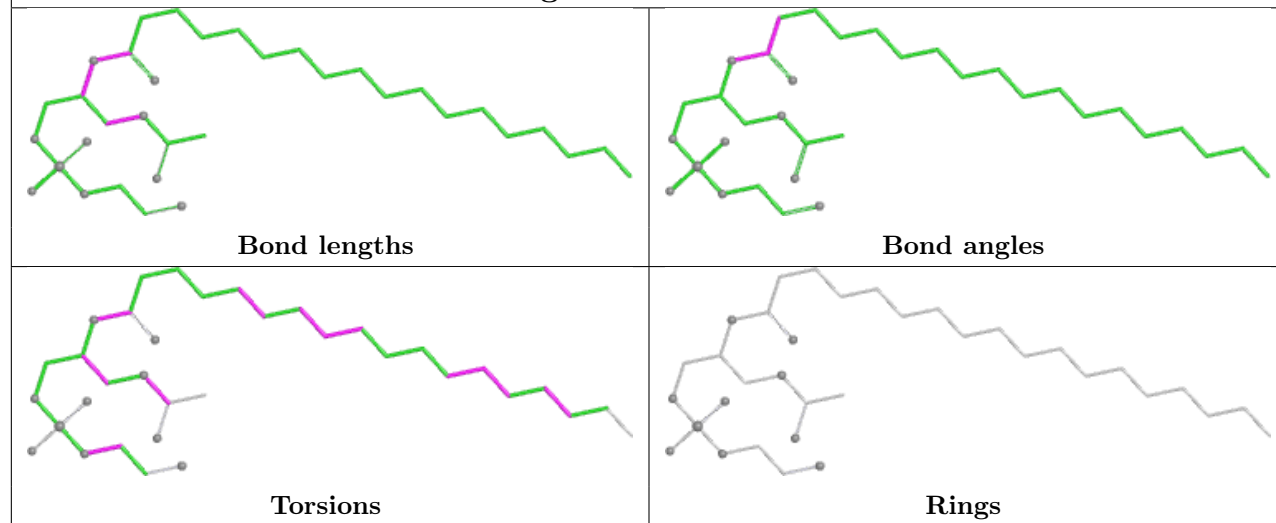


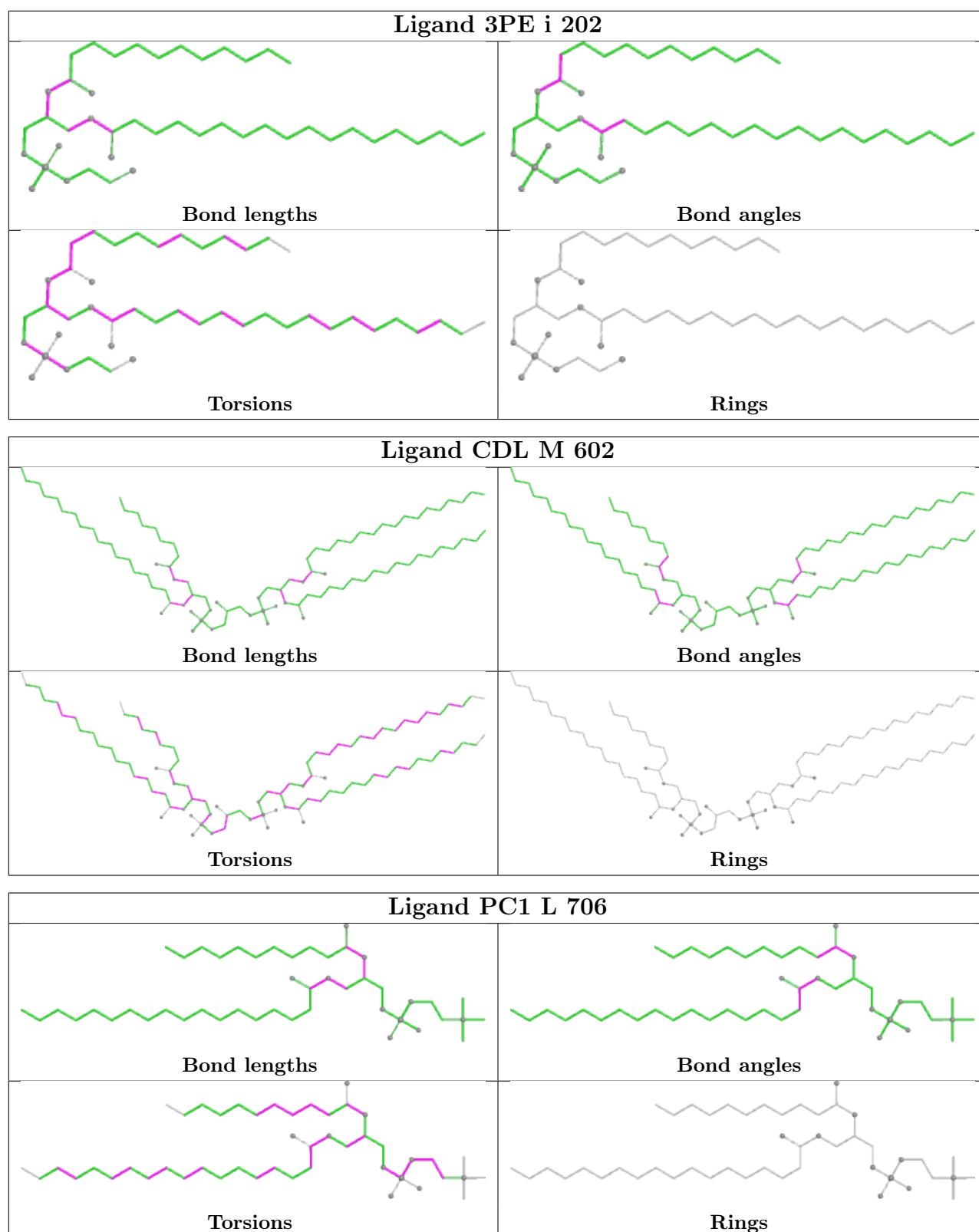


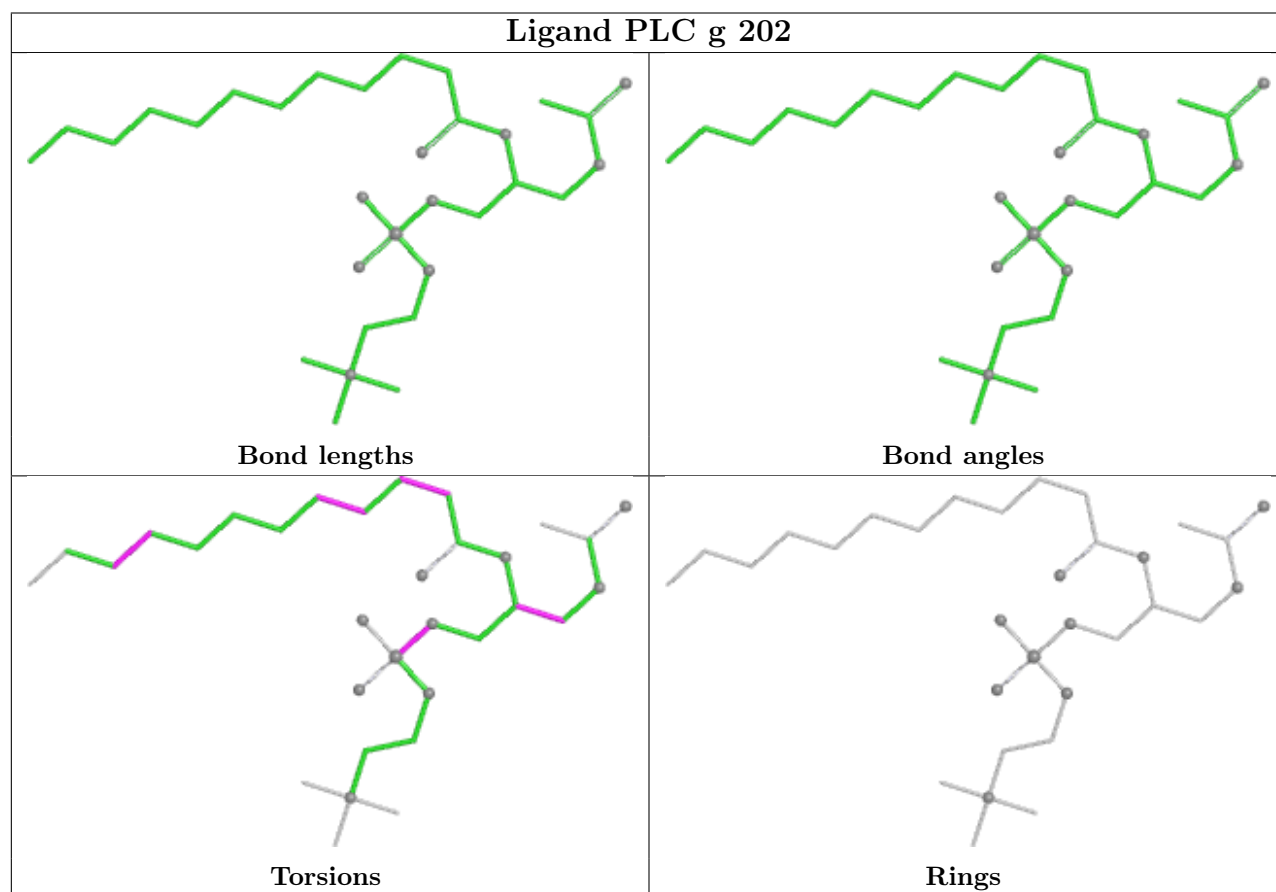
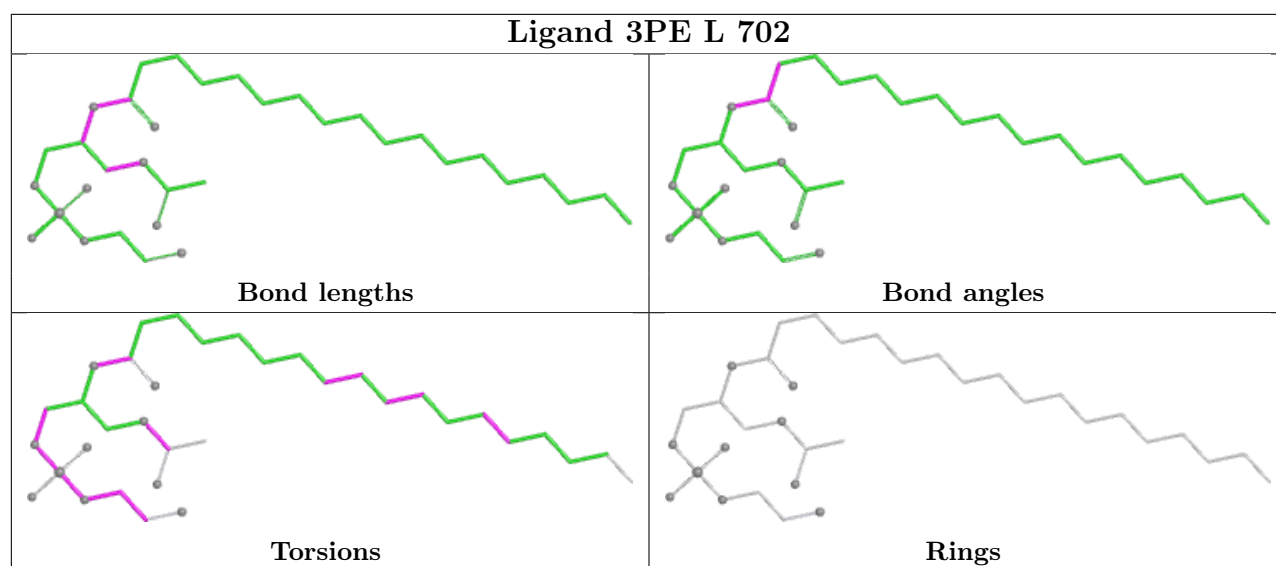
Ligand 3PE Y 201

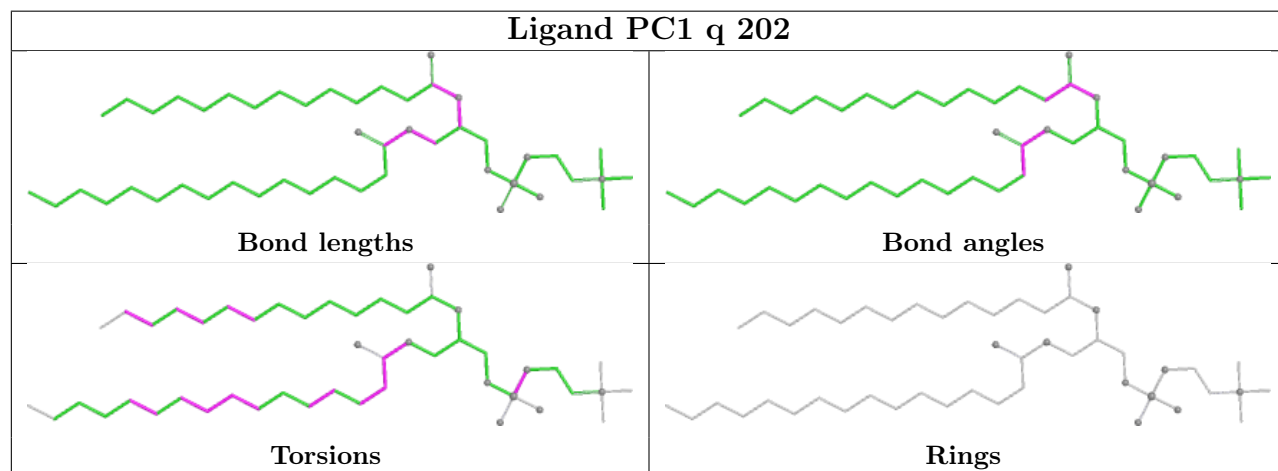
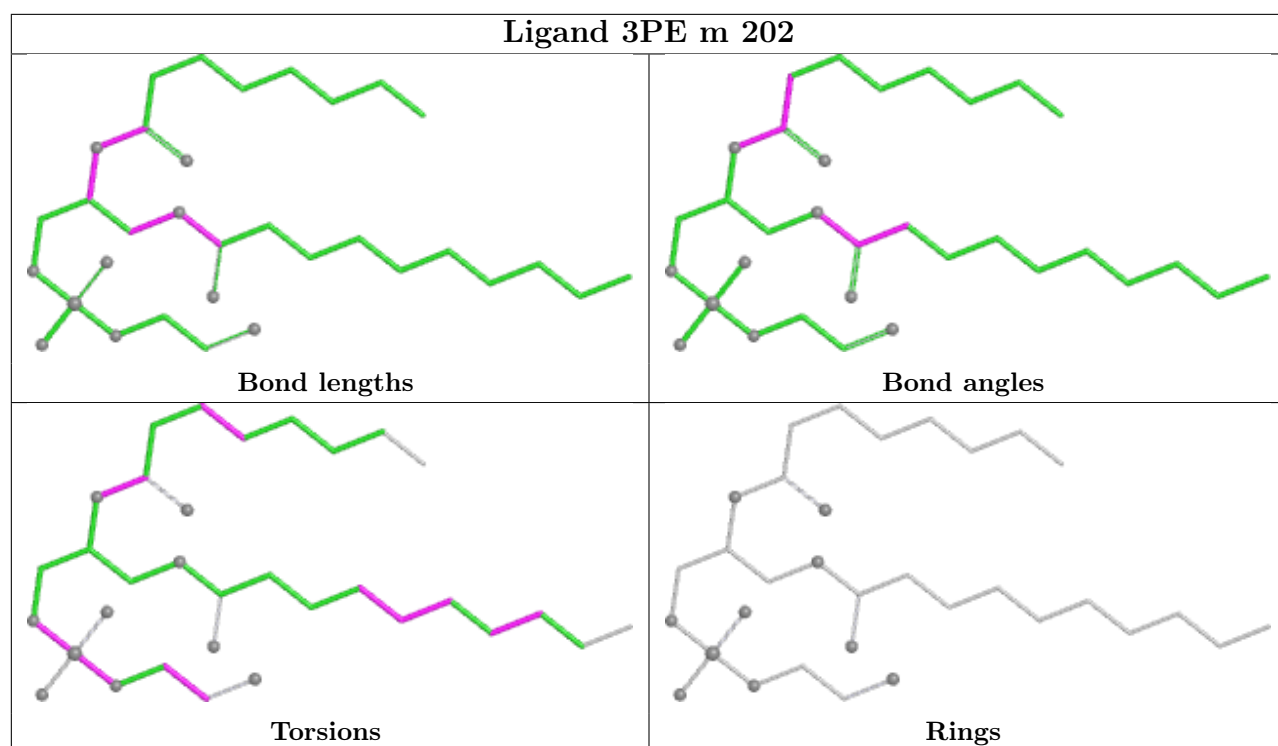


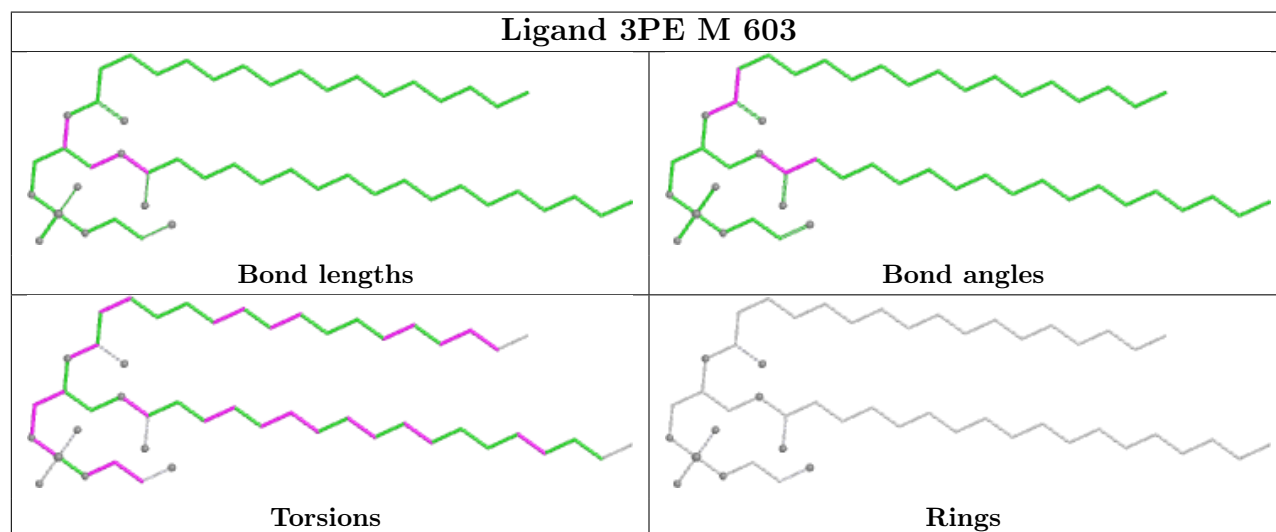
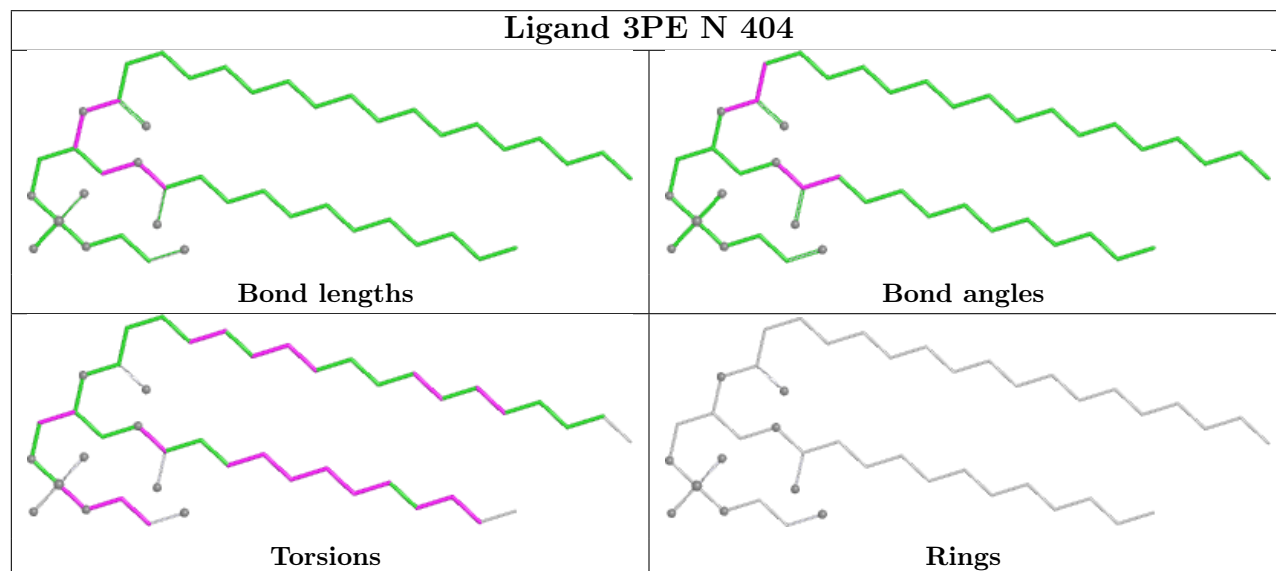
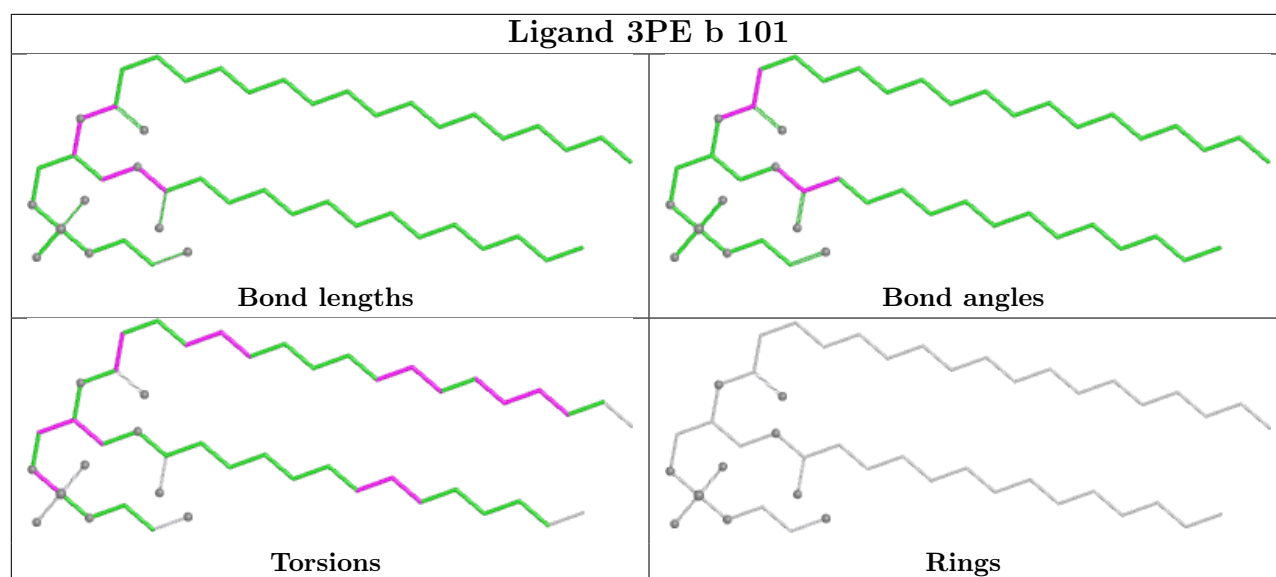
Ligand 3PE o 202

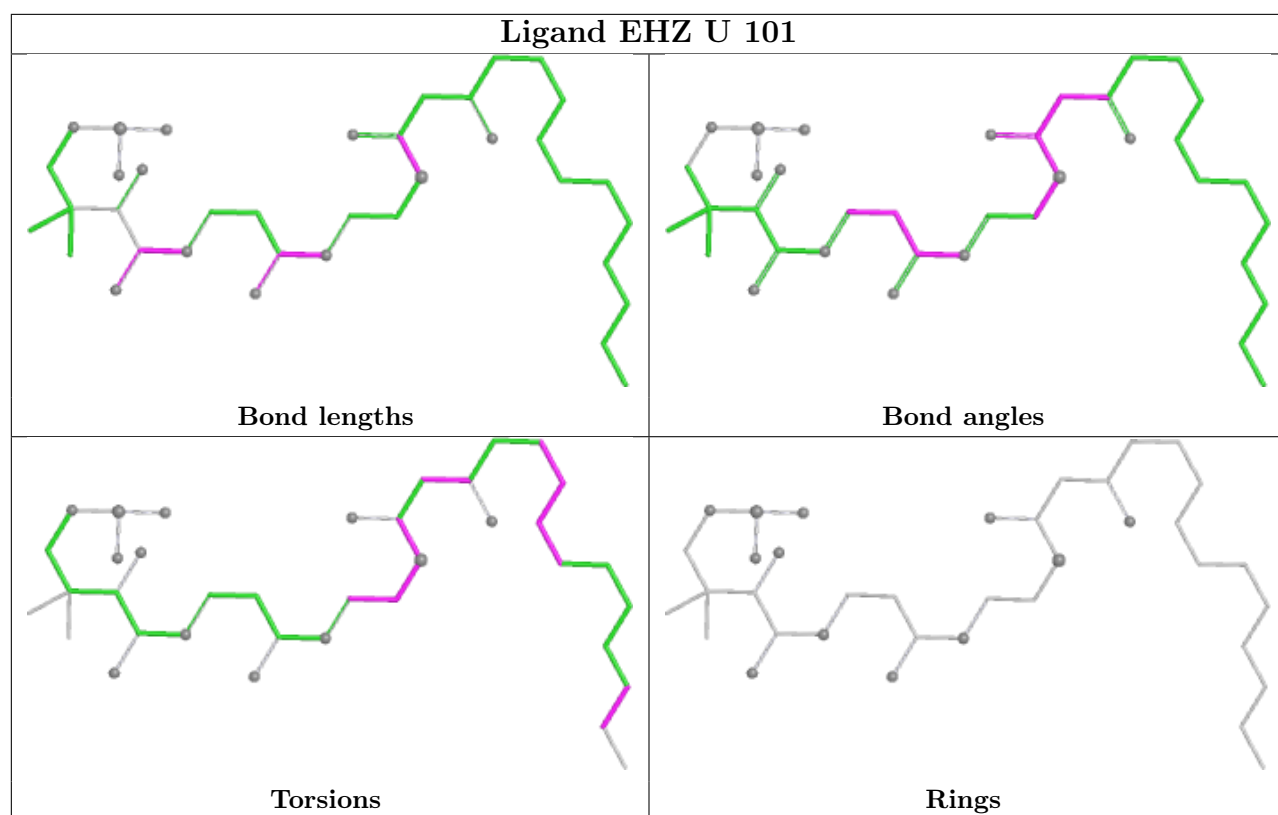




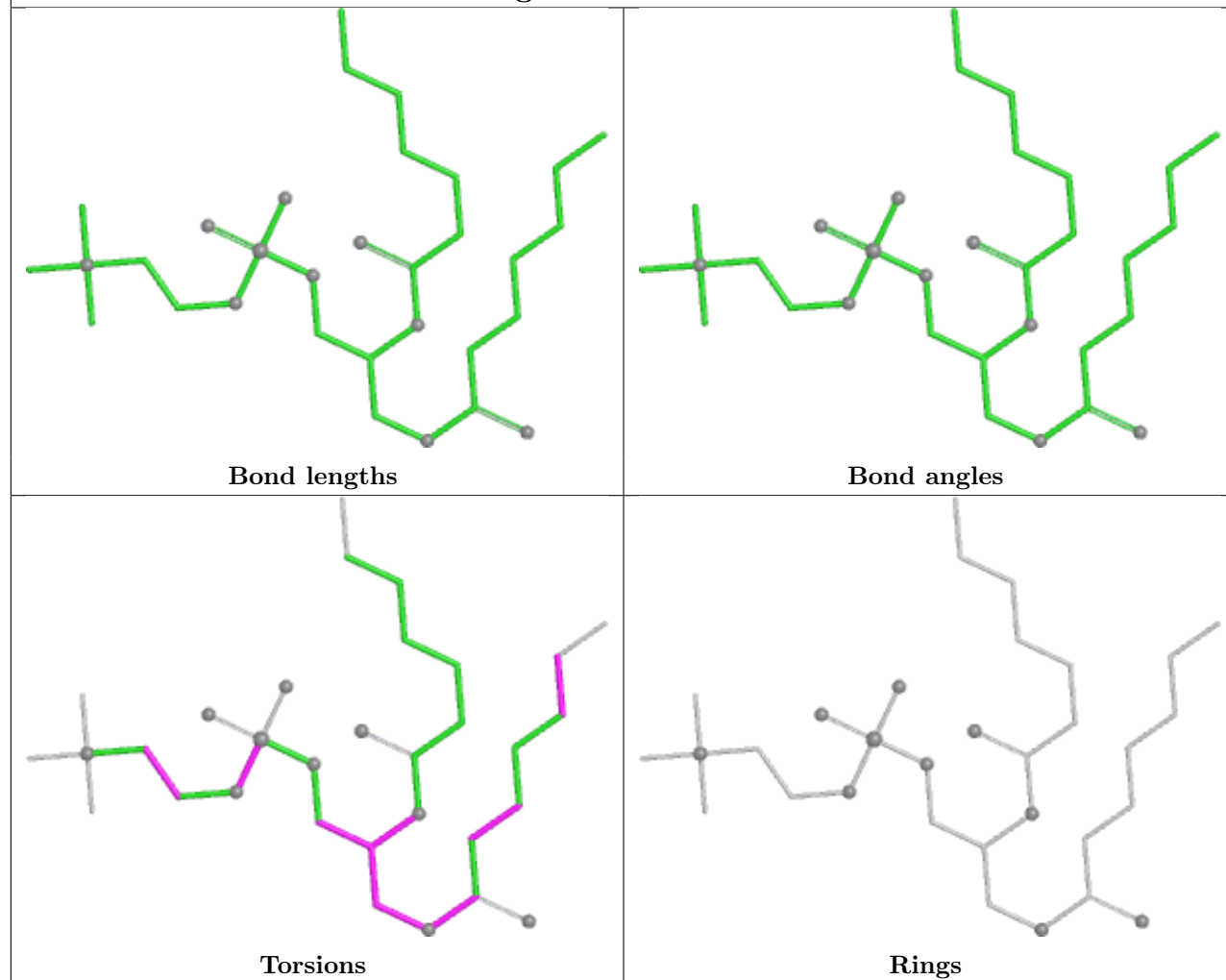




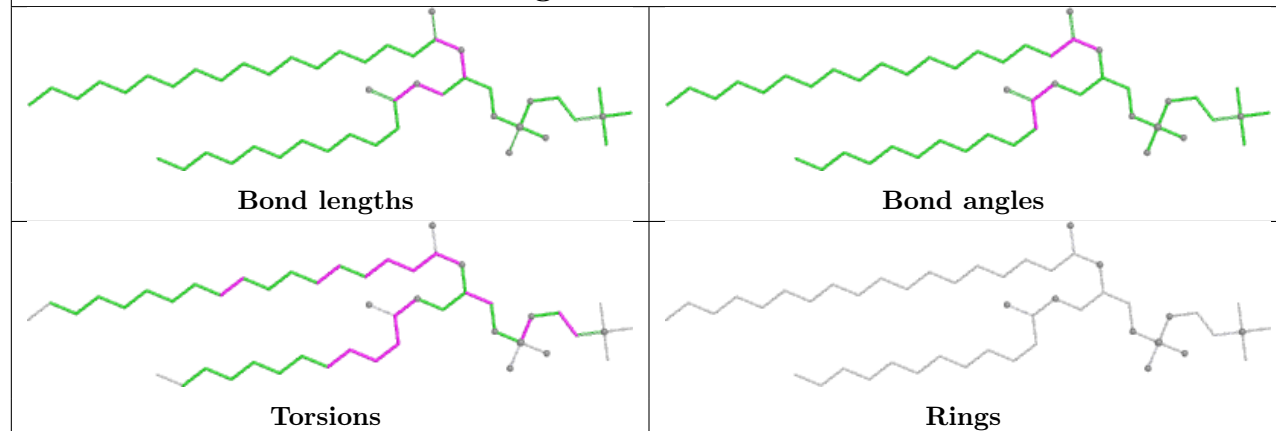


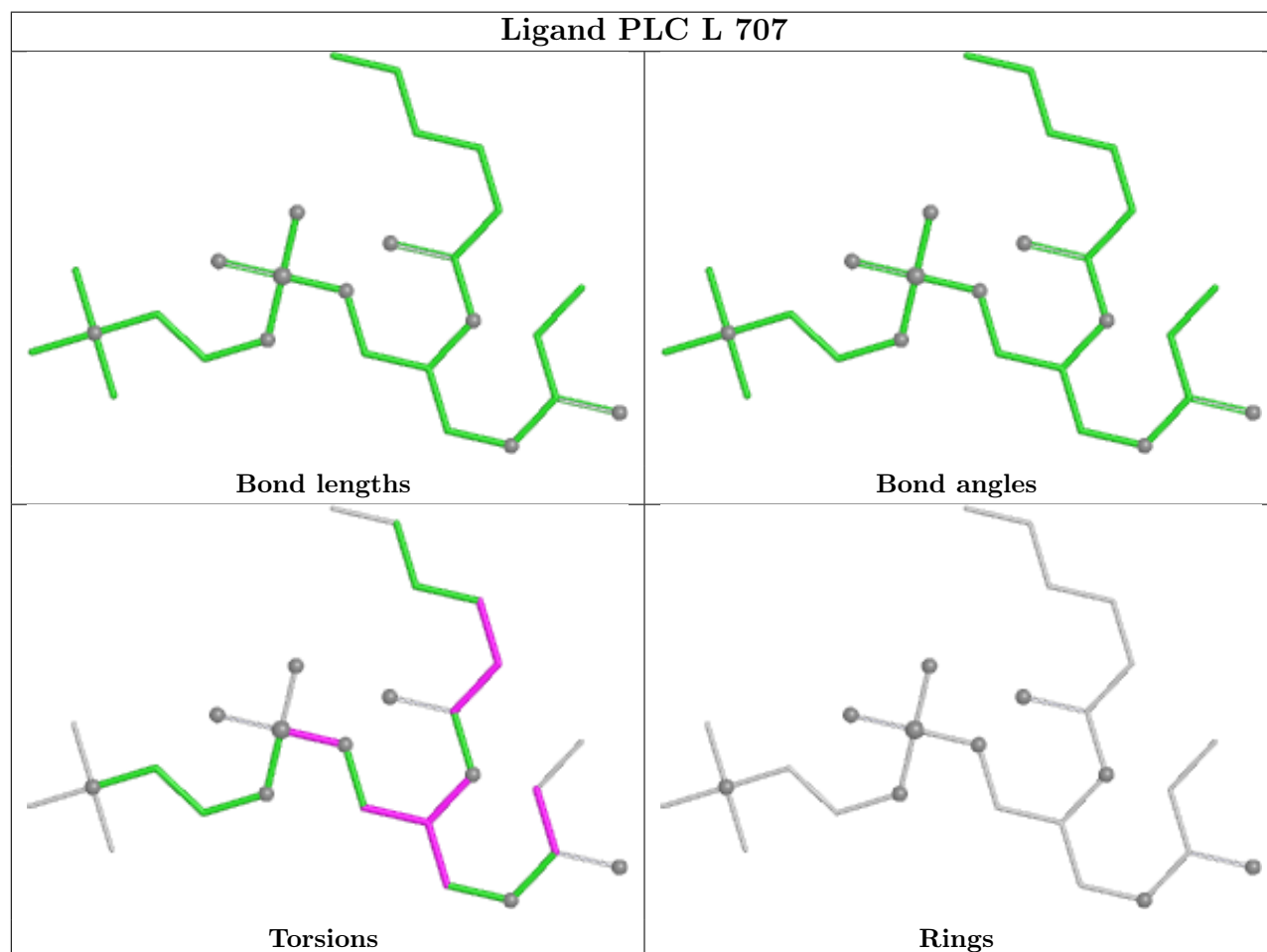
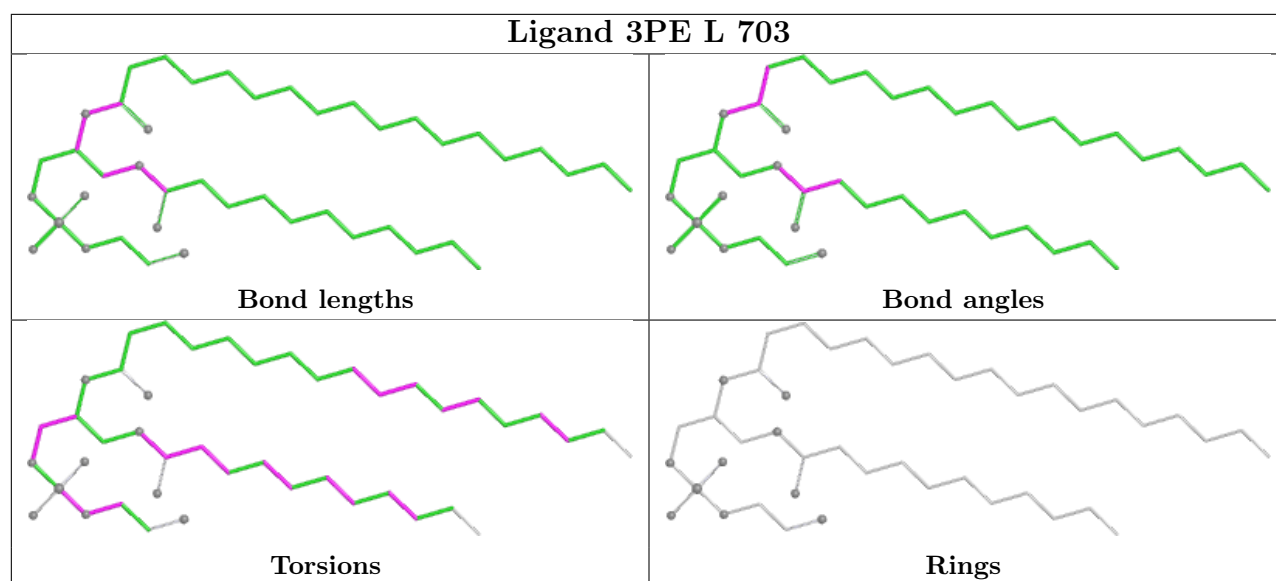


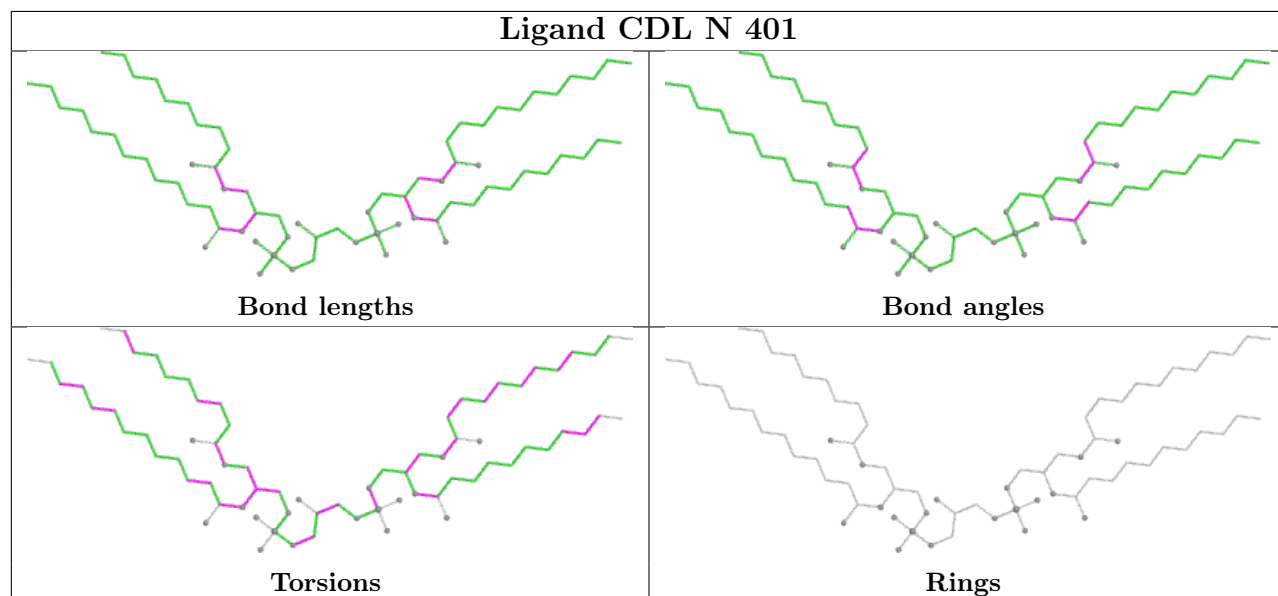
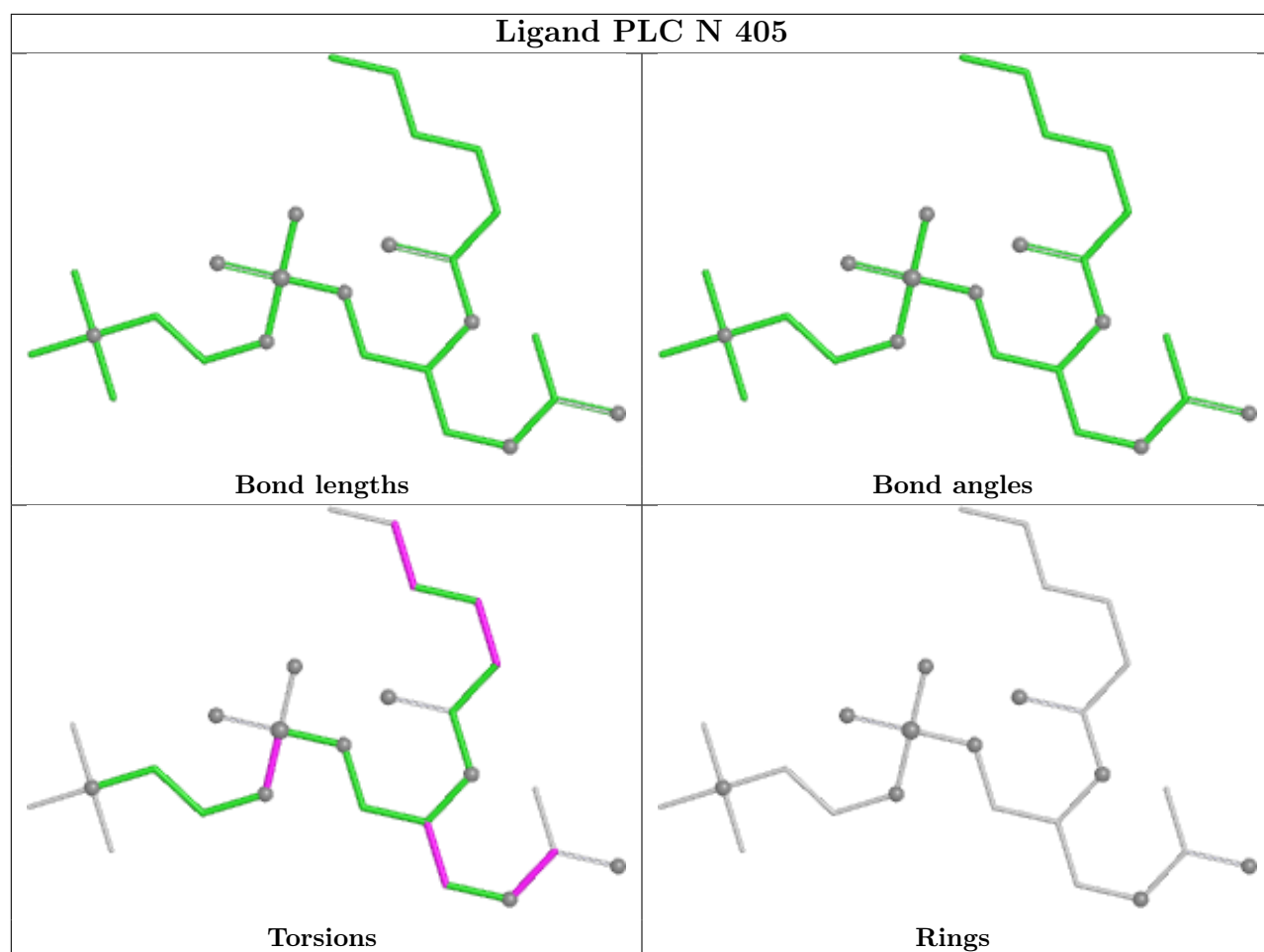
Ligand PLC b 102



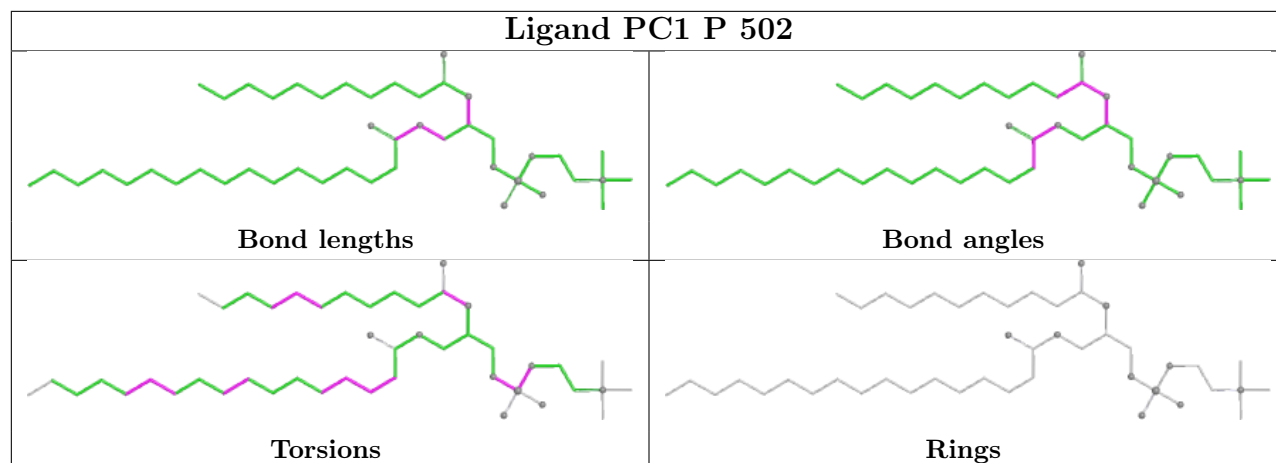
Ligand PC1 H 402



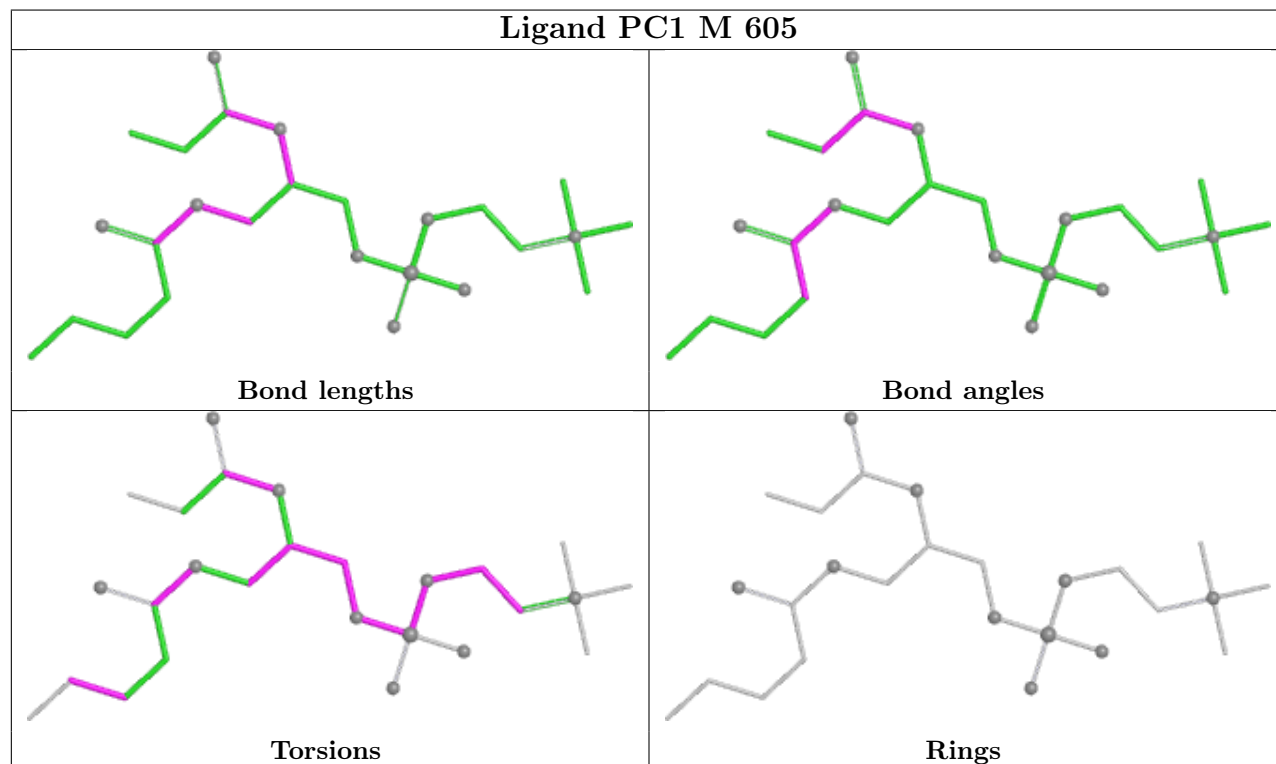




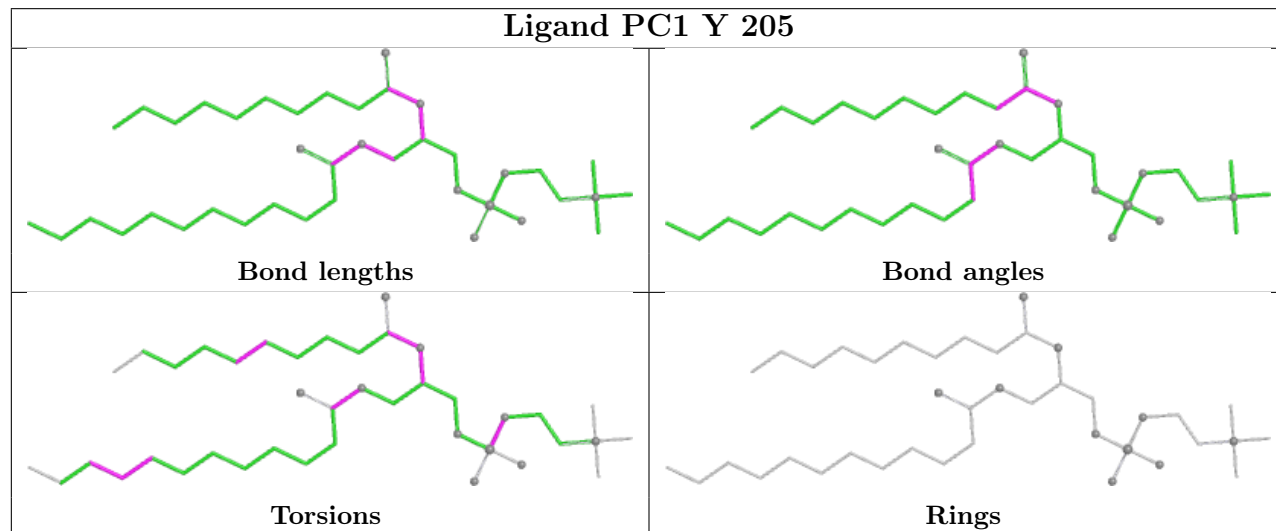
Ligand PC1 P 502

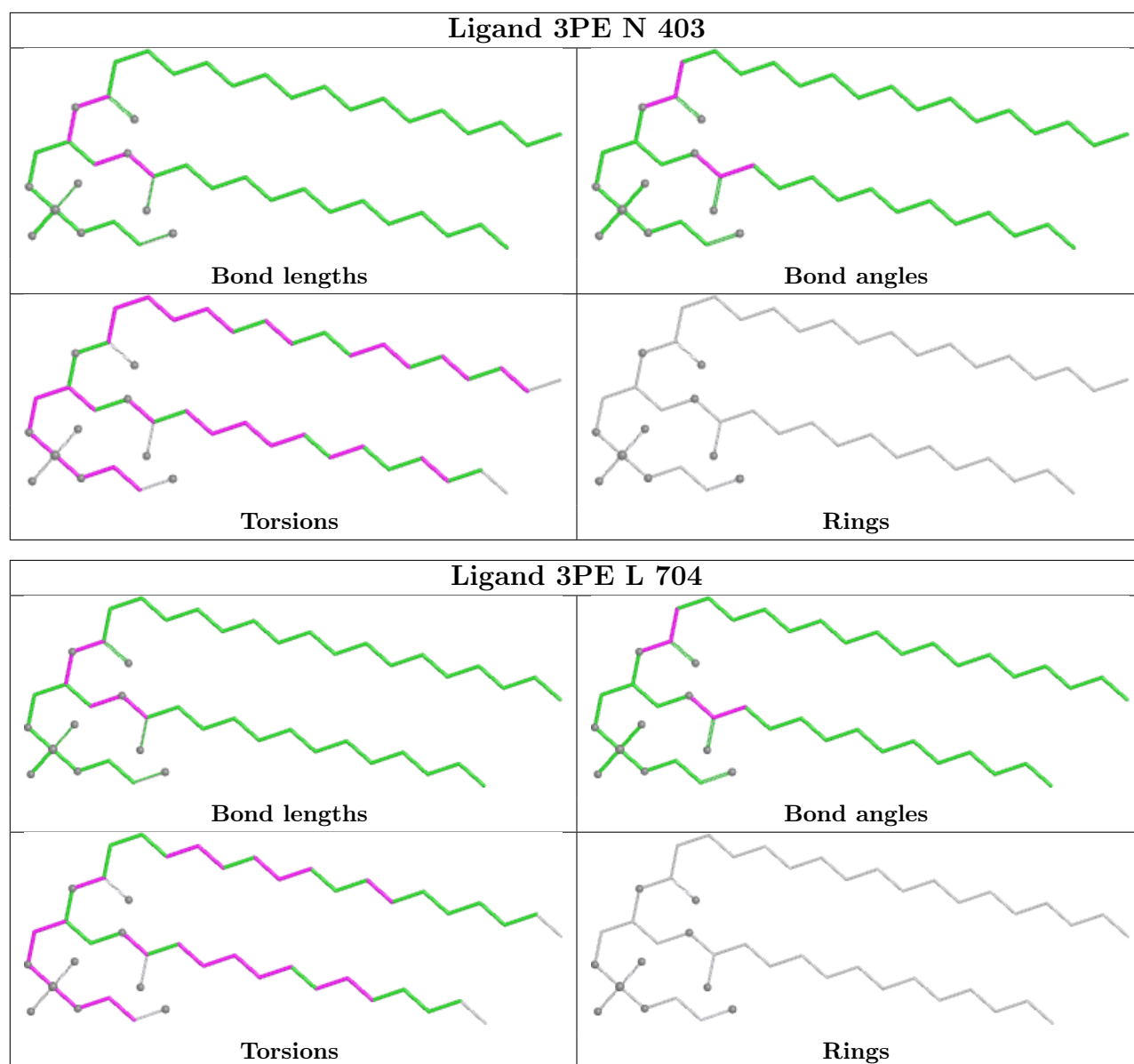


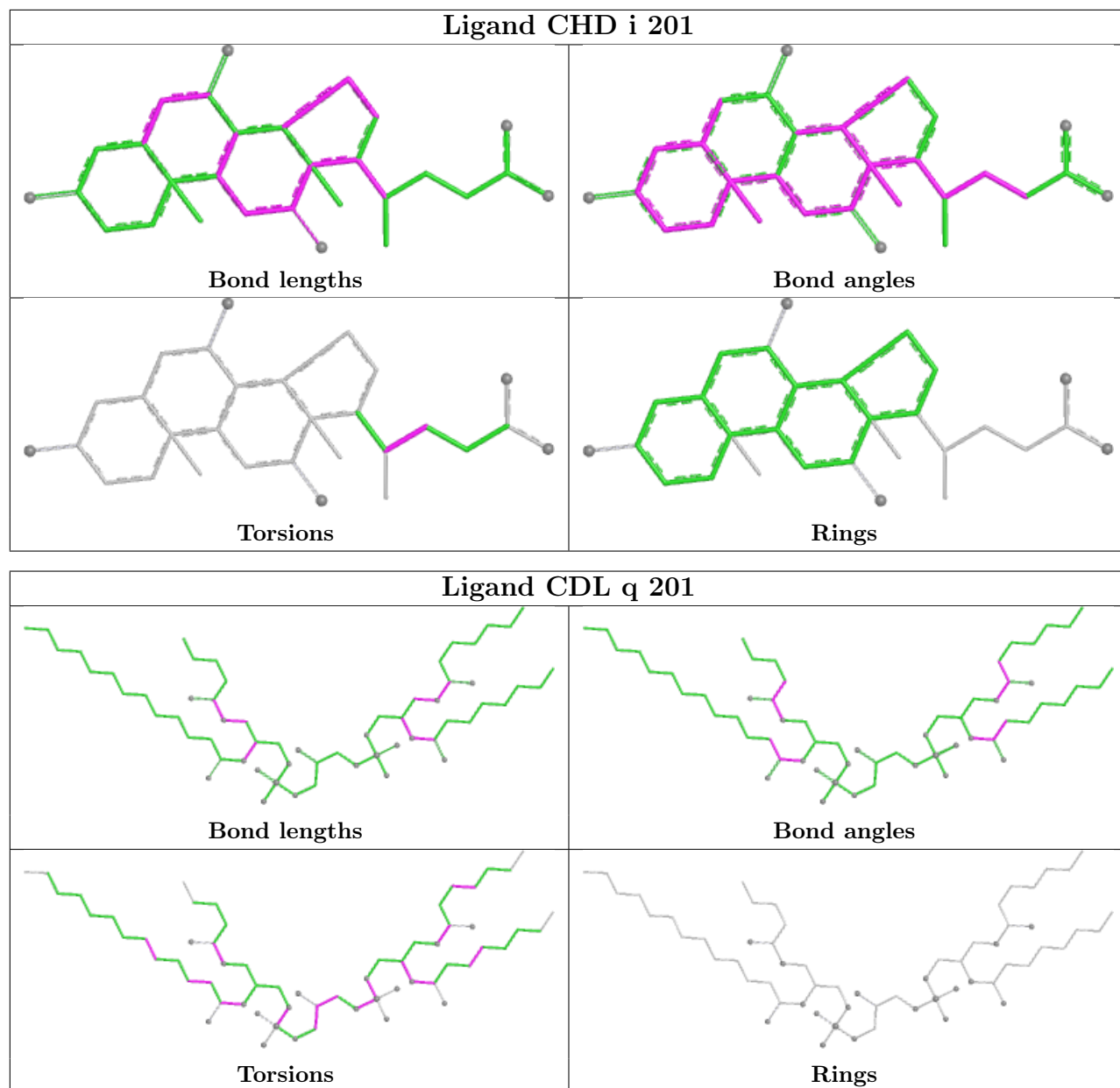
Ligand PC1 M 605

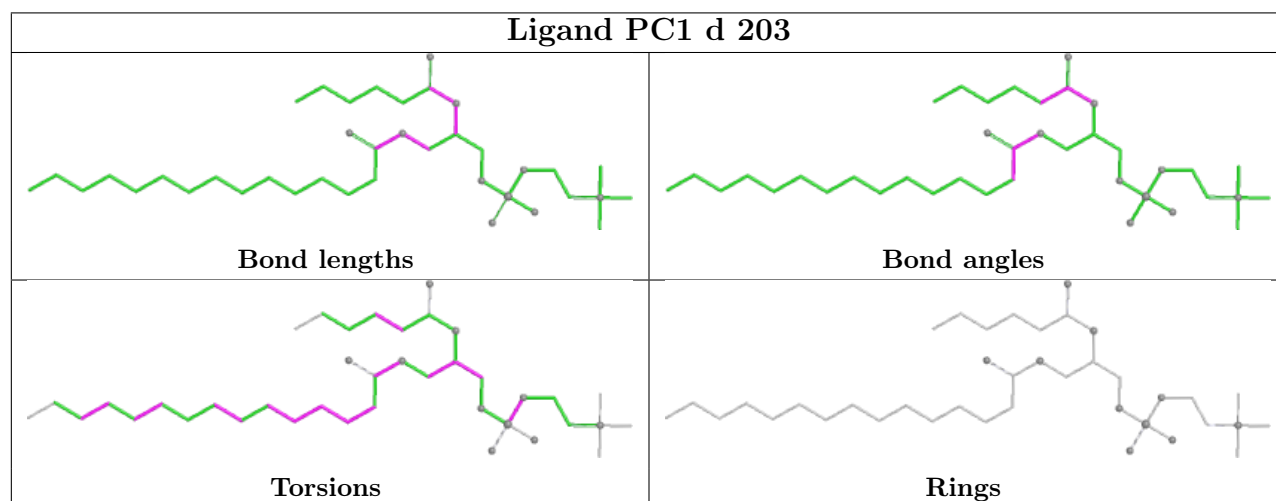
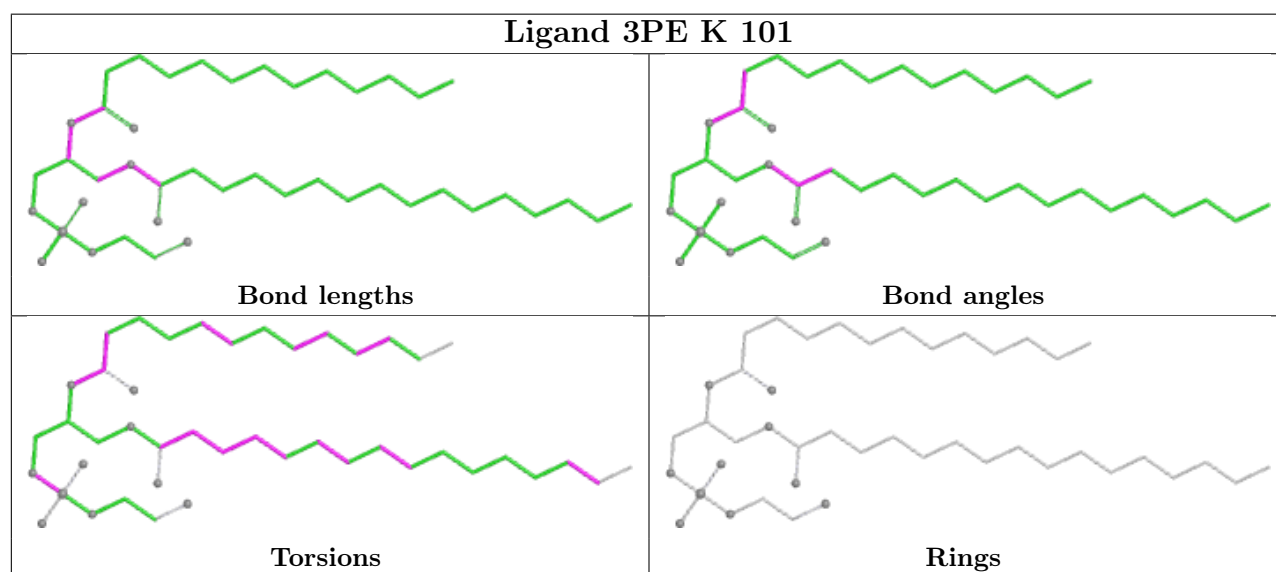
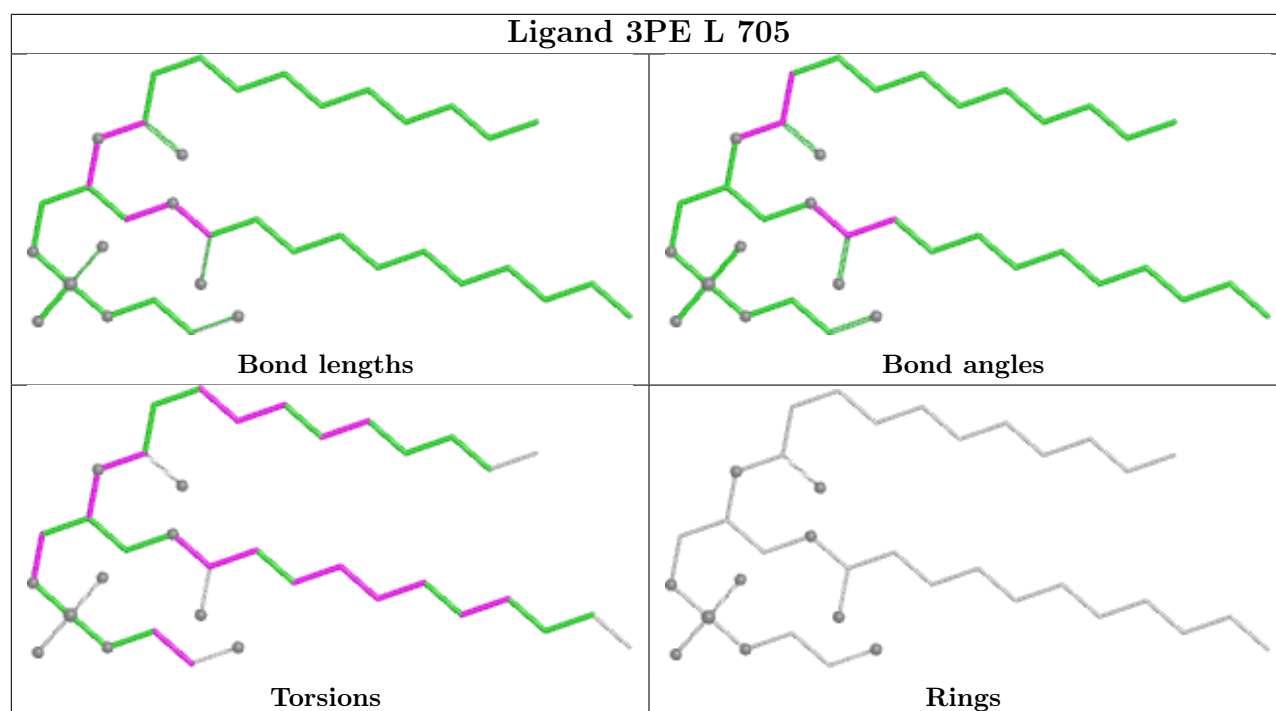


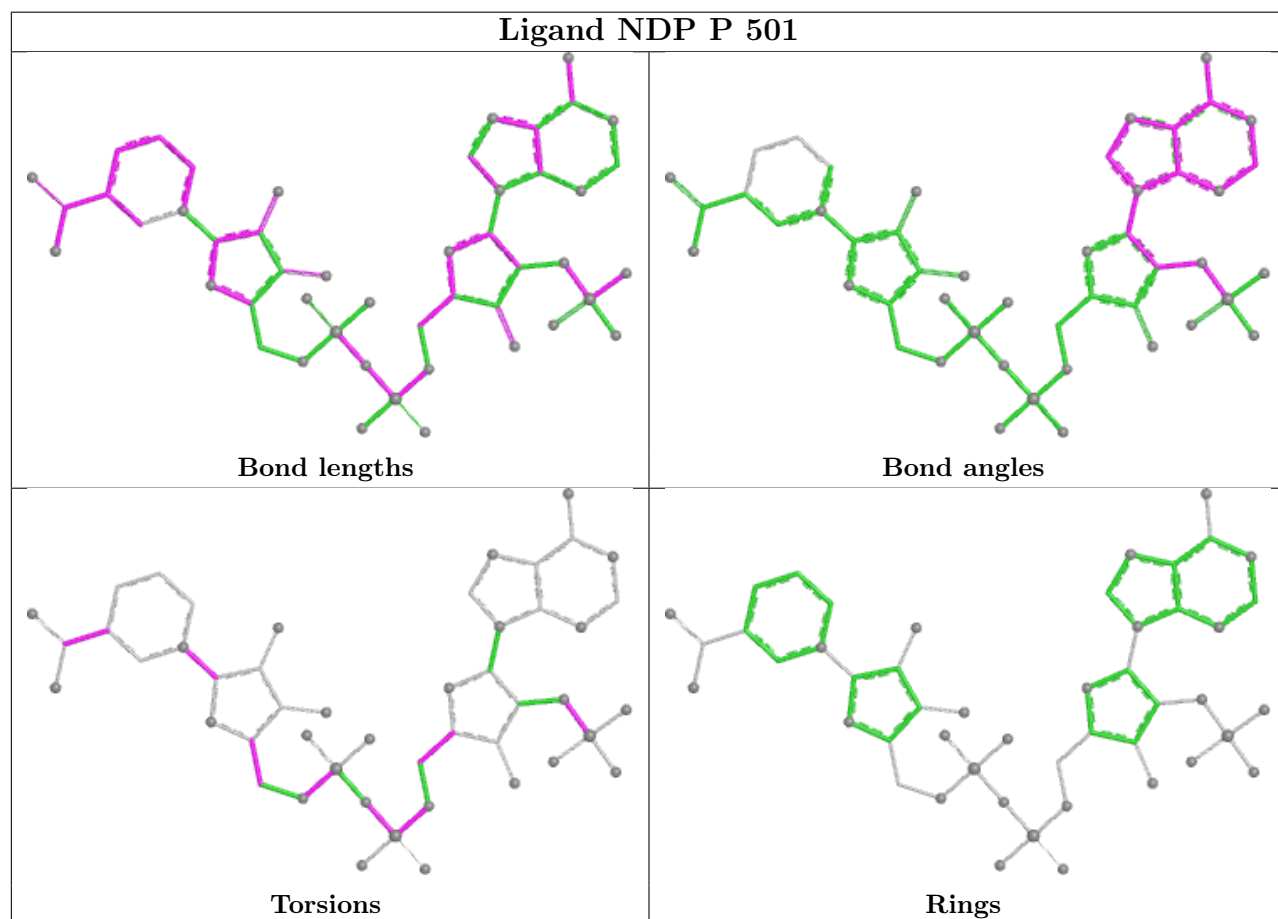
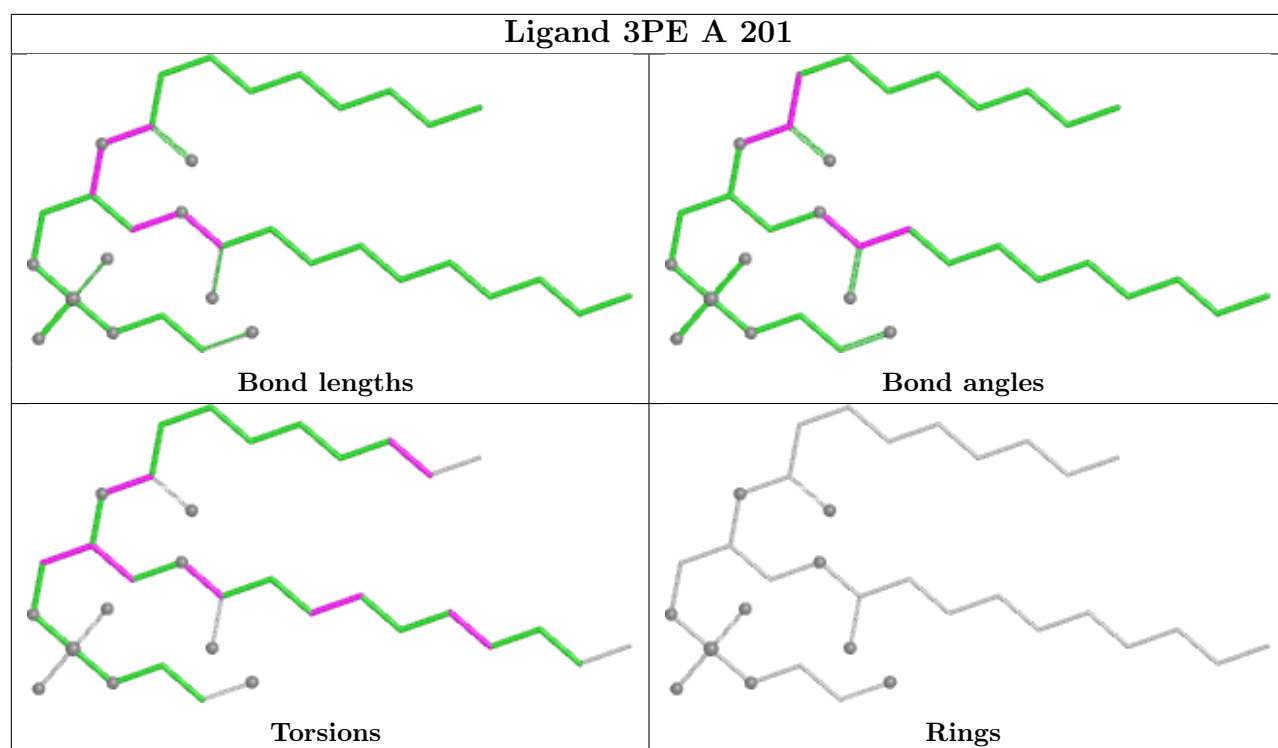
Ligand PC1 Y 205

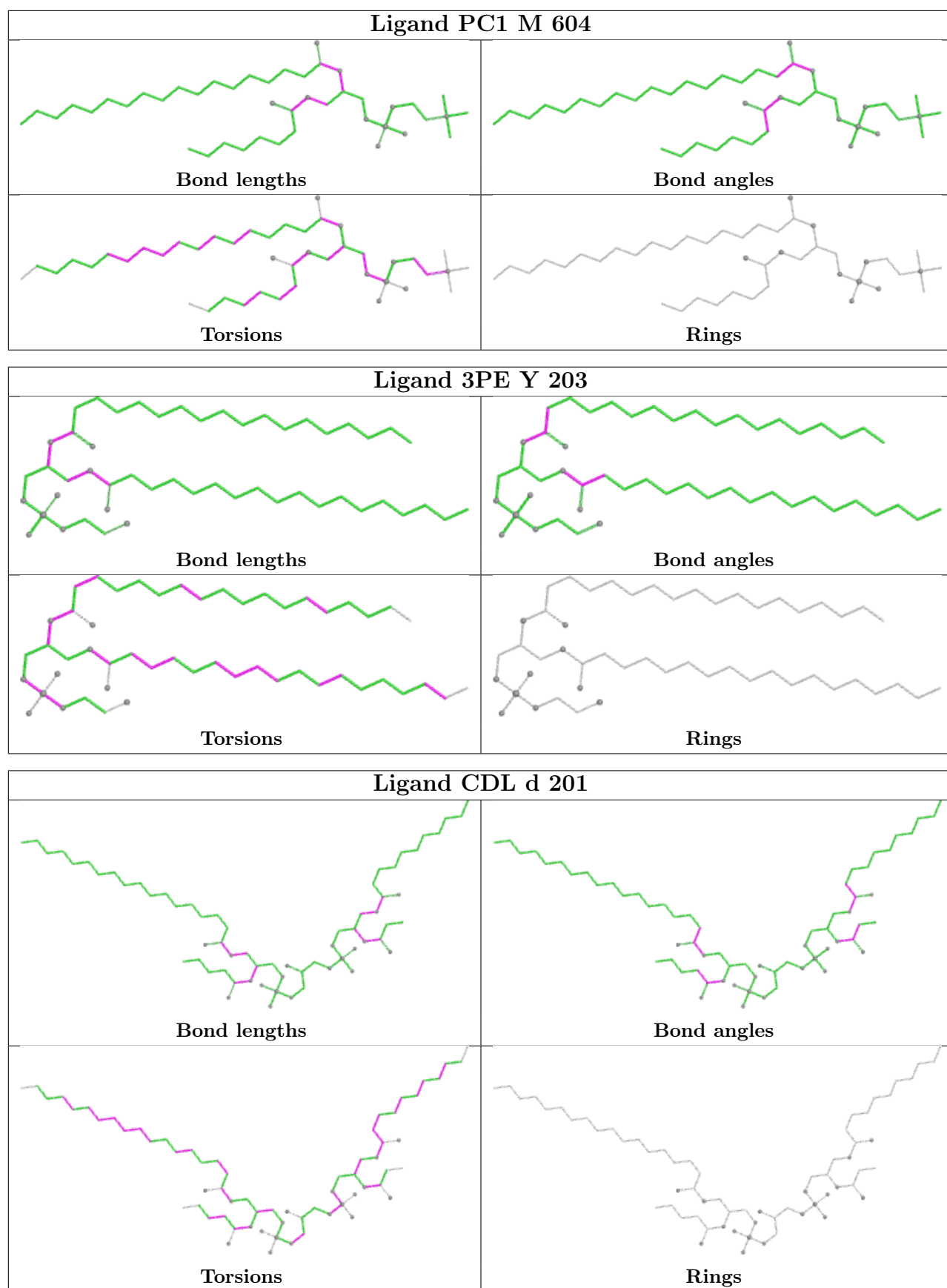


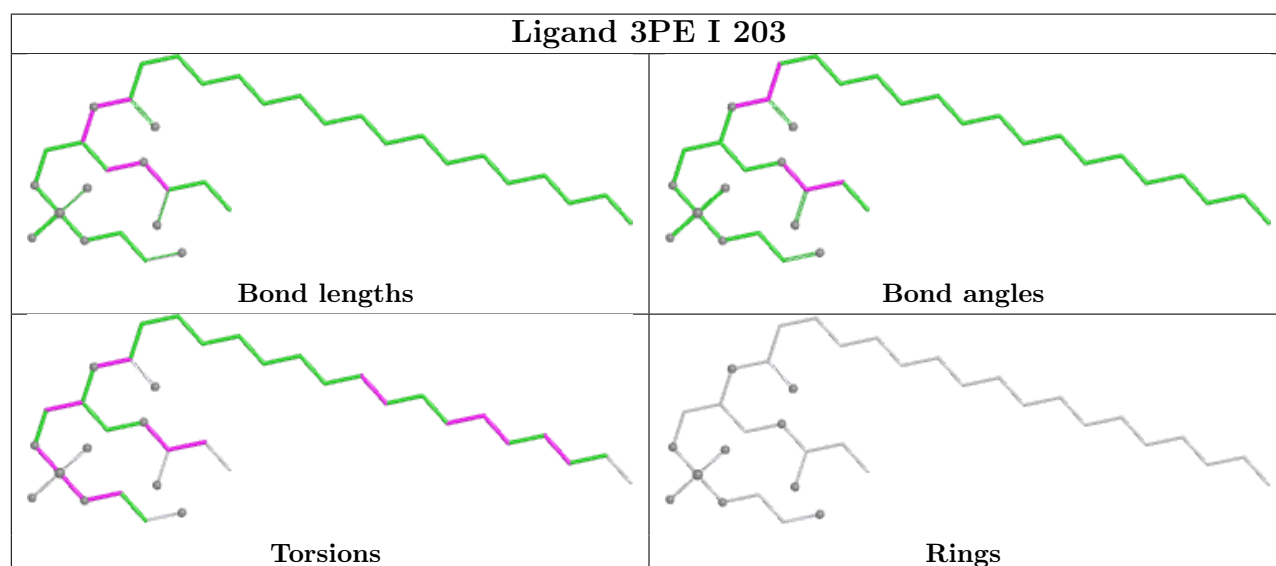
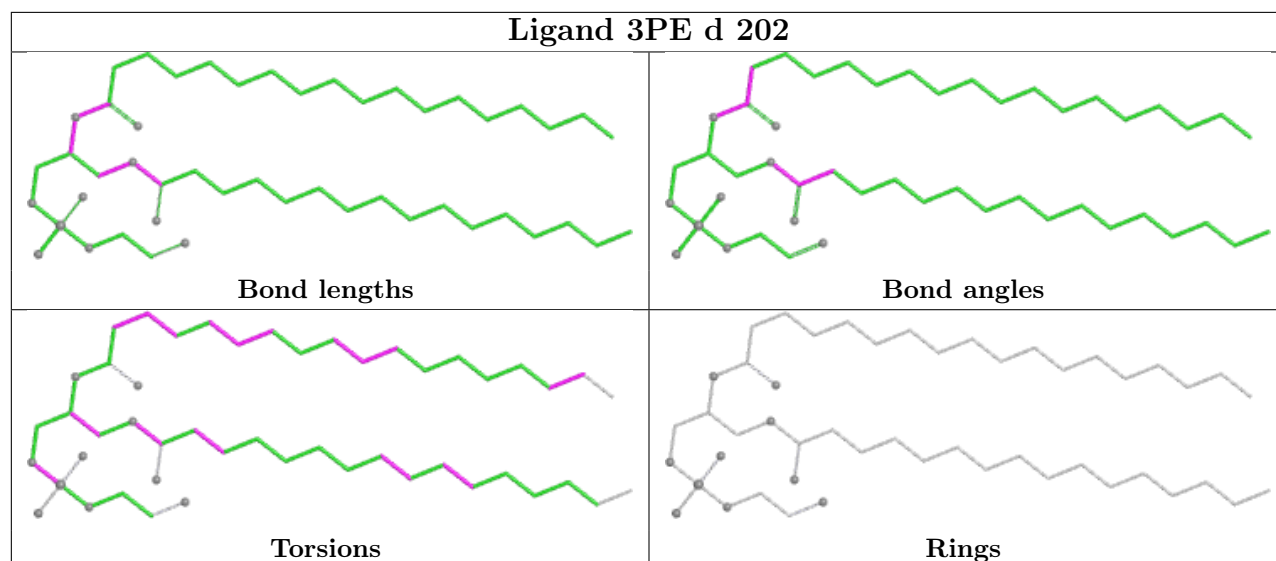
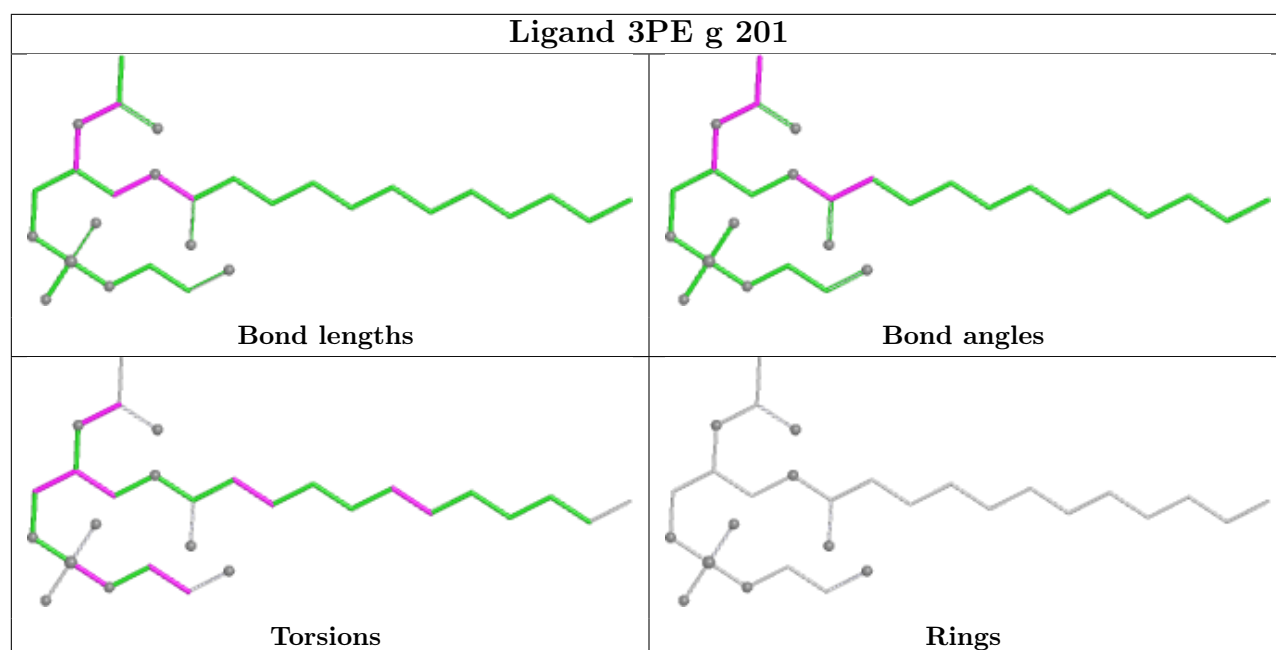


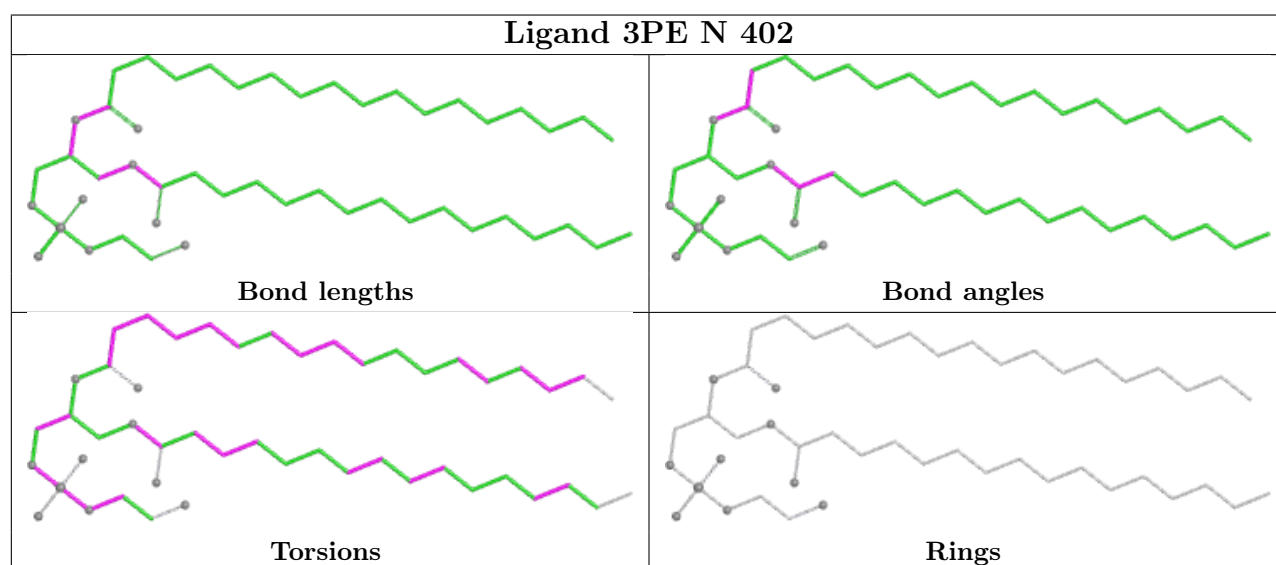
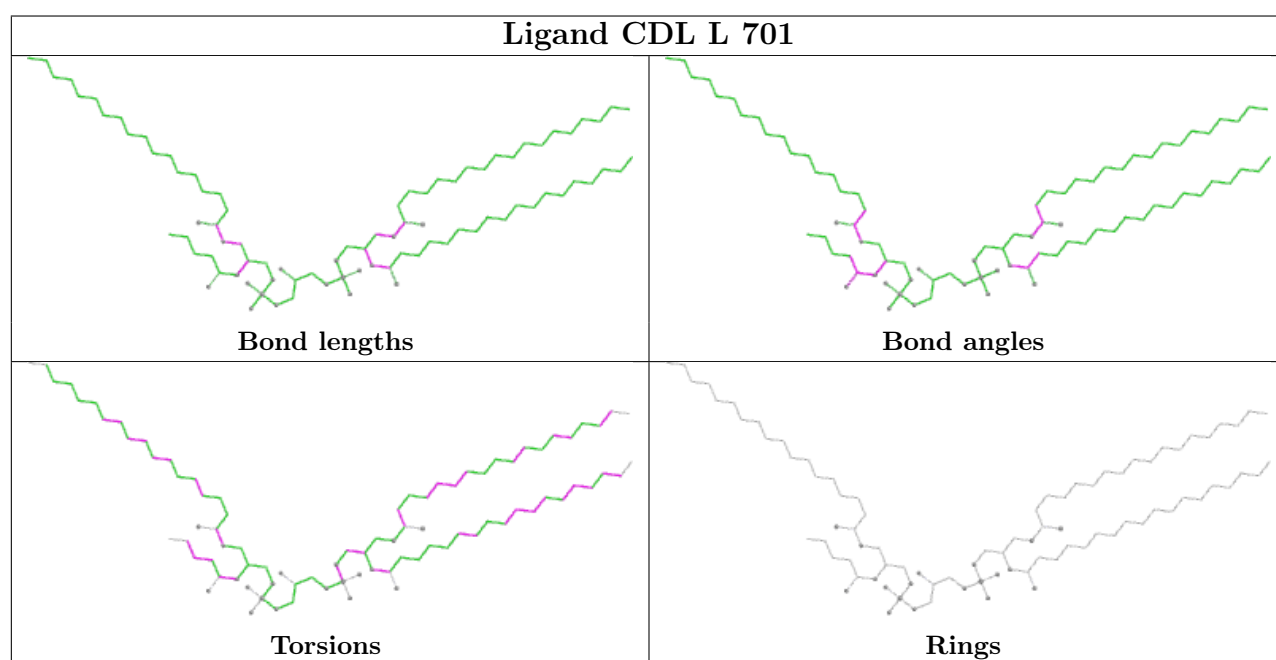
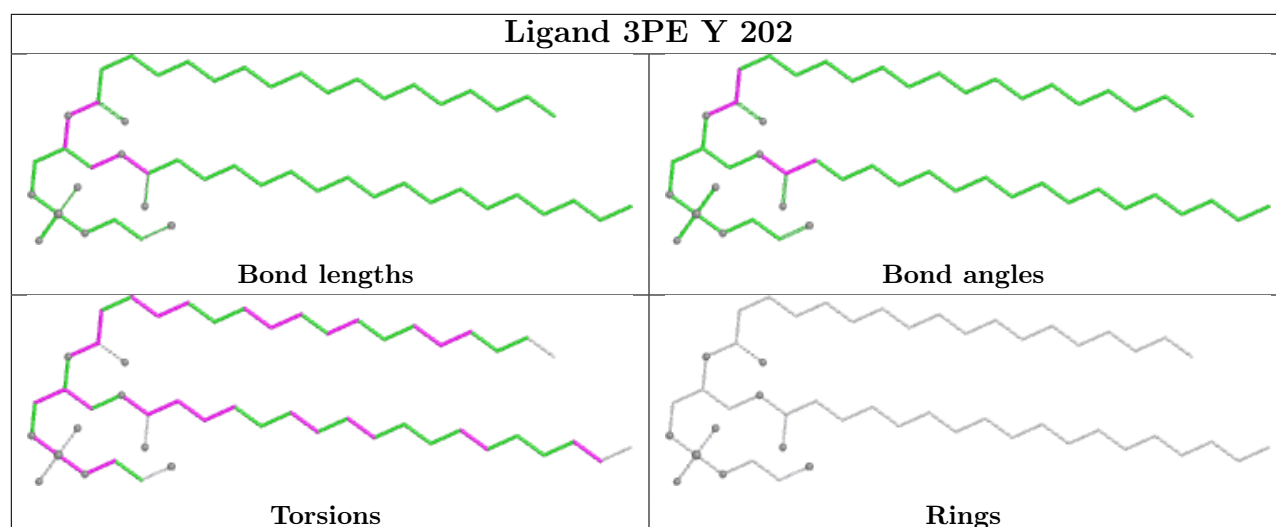


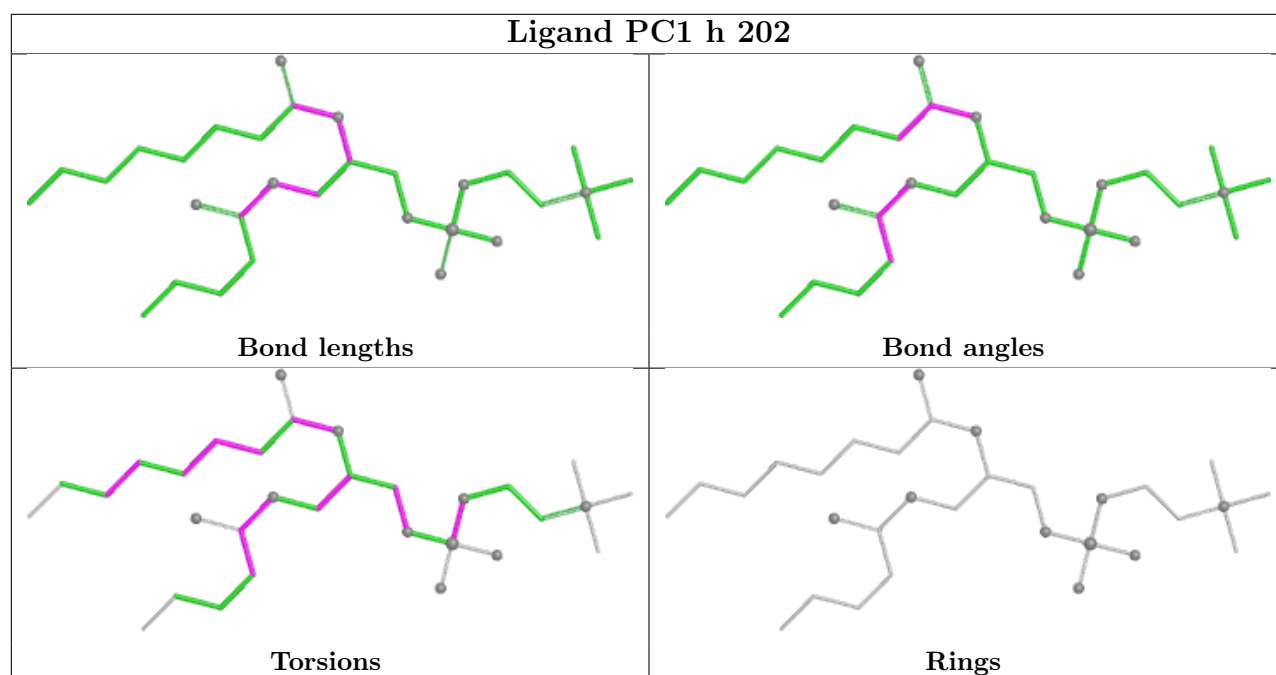
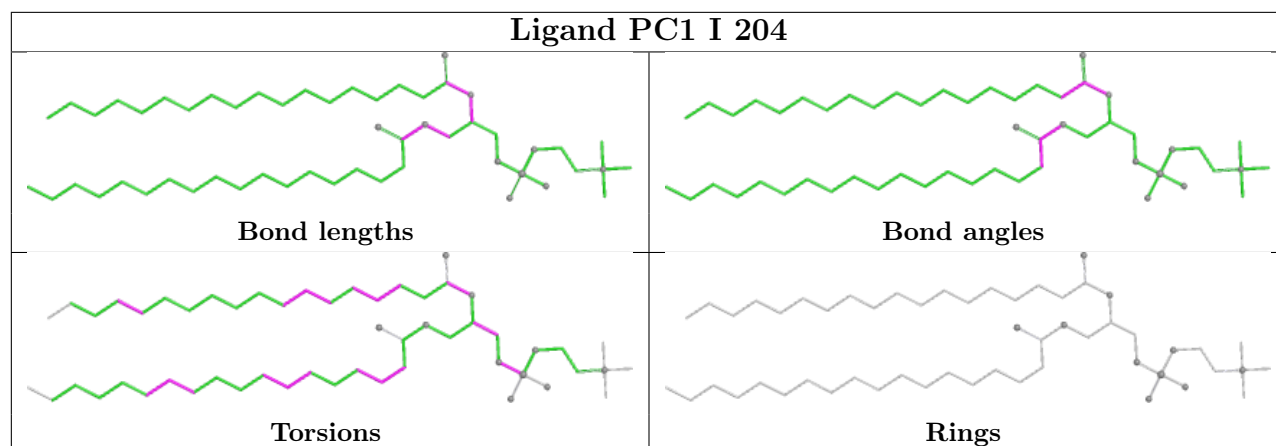
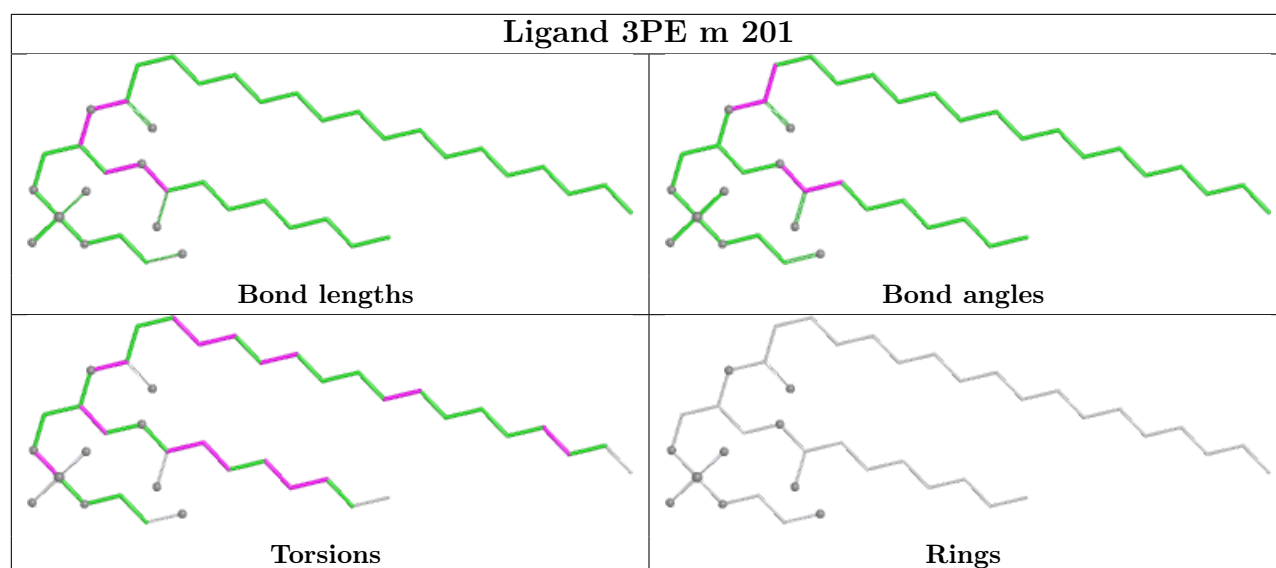


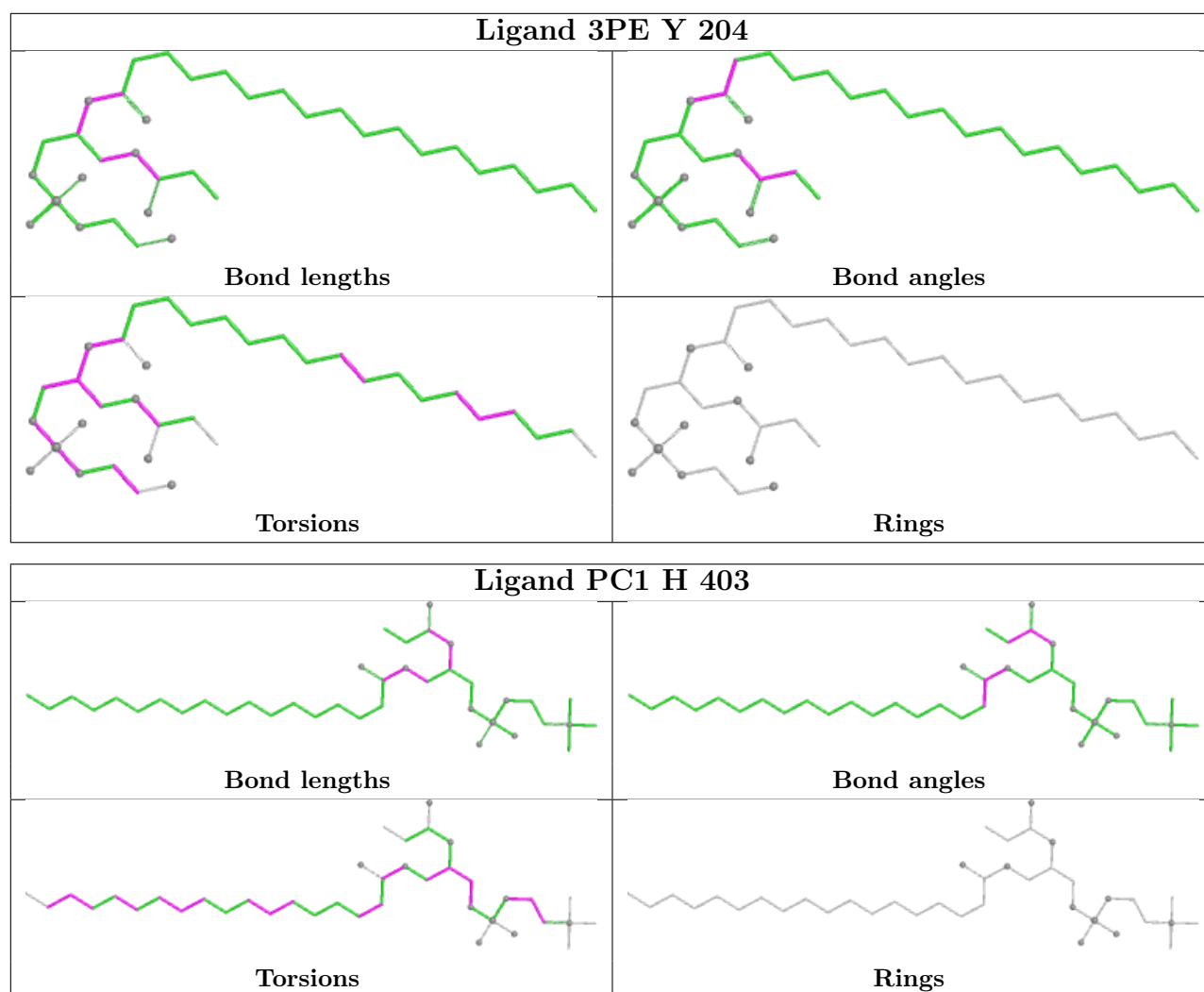












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

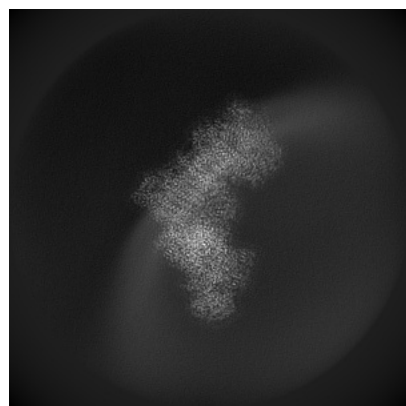
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18067. These allow visual inspection of the internal detail of the map and identification of artifacts.

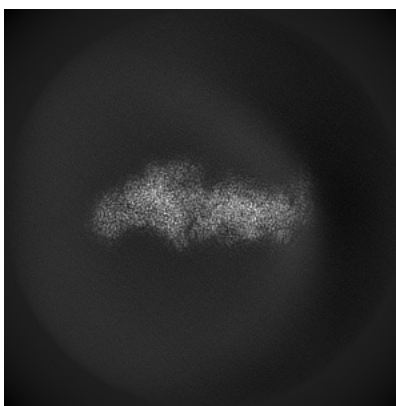
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

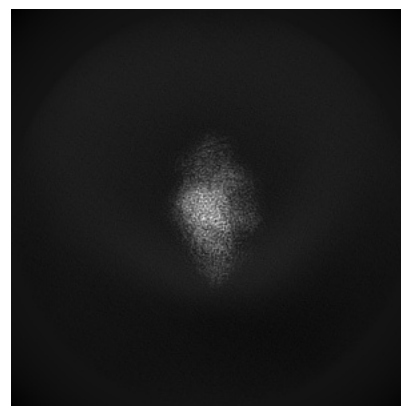
6.1.1 Primary map



X

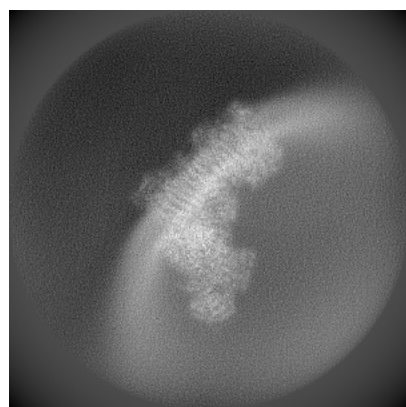


Y

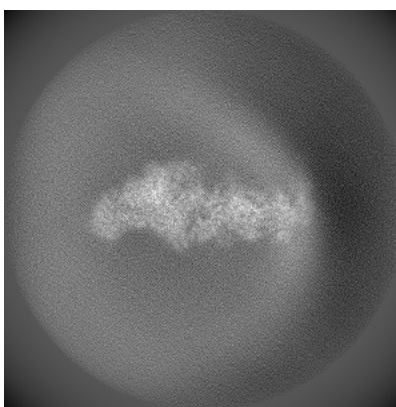


Z

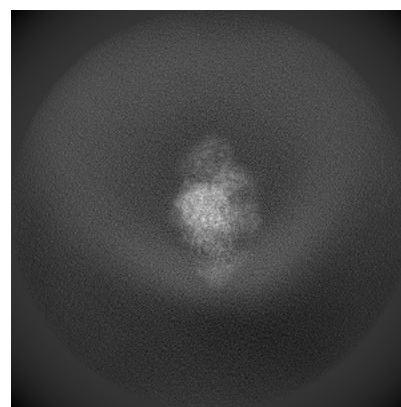
6.1.2 Raw map



X



Y



Z

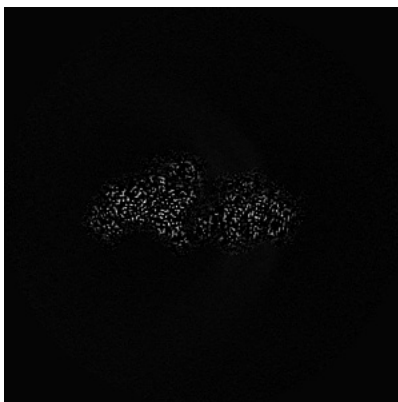
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

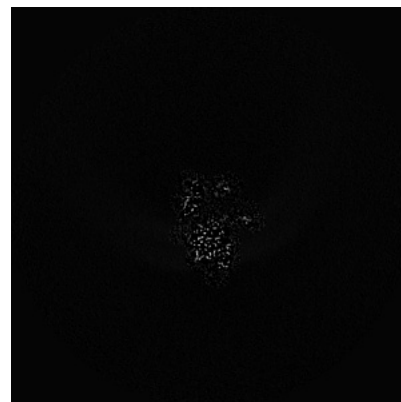
6.2.1 Primary map



X Index: 240

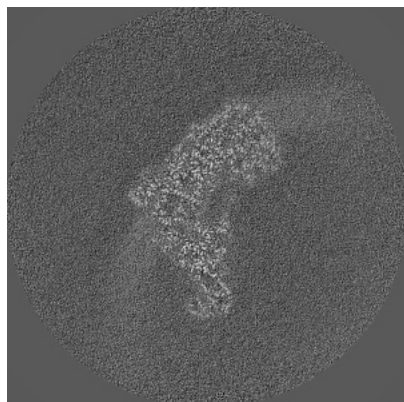


Y Index: 240

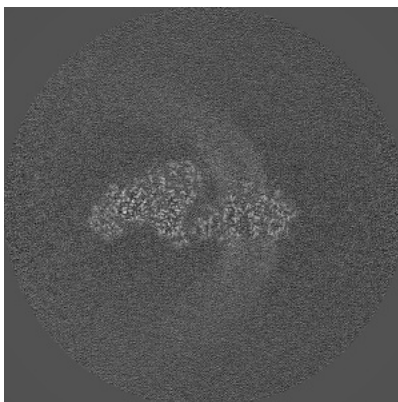


Z Index: 240

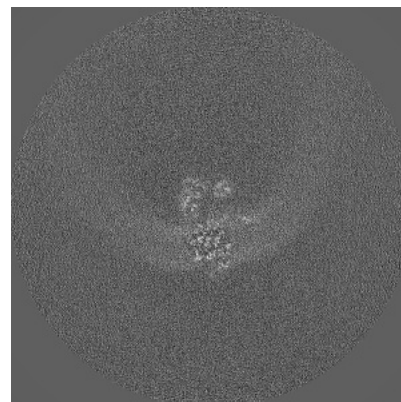
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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: 243

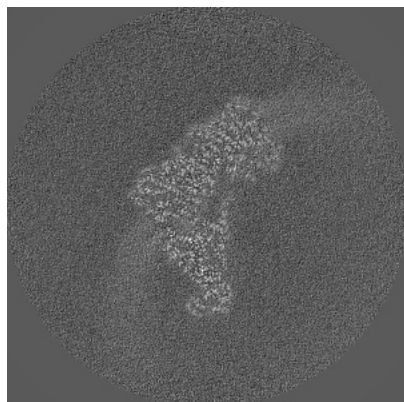


Y Index: 230

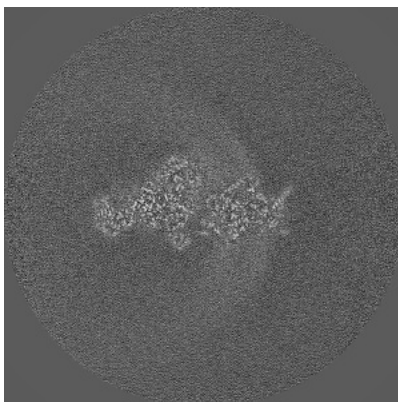


Z Index: 202

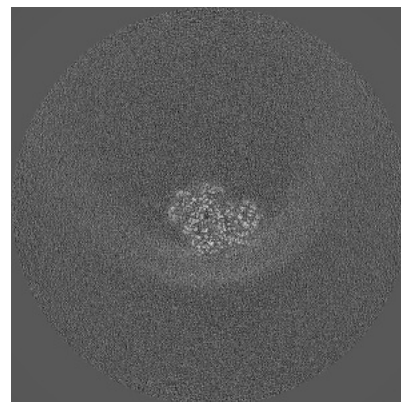
6.3.2 Raw map



X Index: 243



Y Index: 230

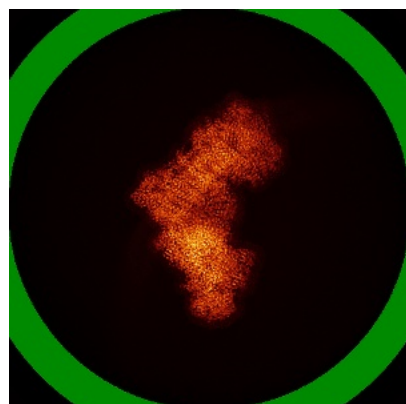


Z Index: 209

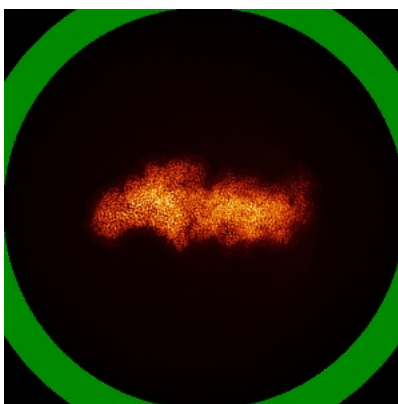
The images above show the largest variance slices of the map in three orthogonal directions.

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

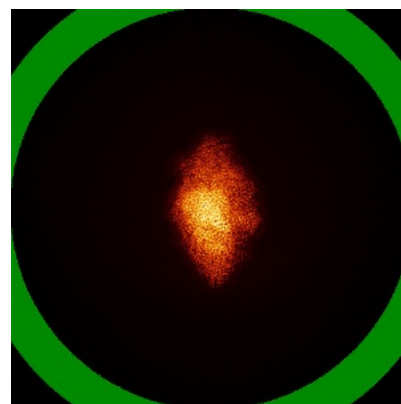
6.4.1 Primary map



X

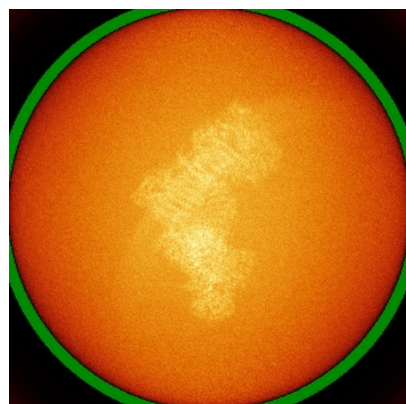


Y

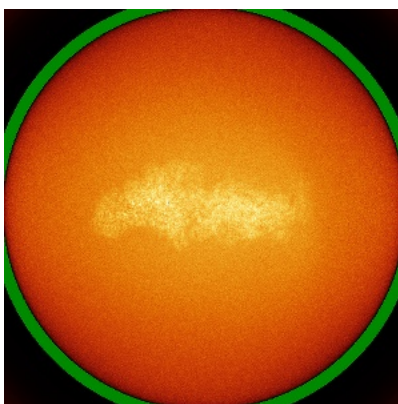


Z

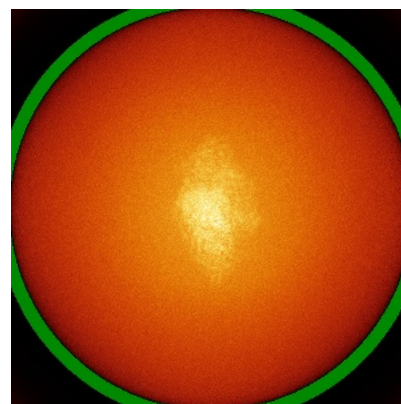
6.4.2 Raw map



X



Y

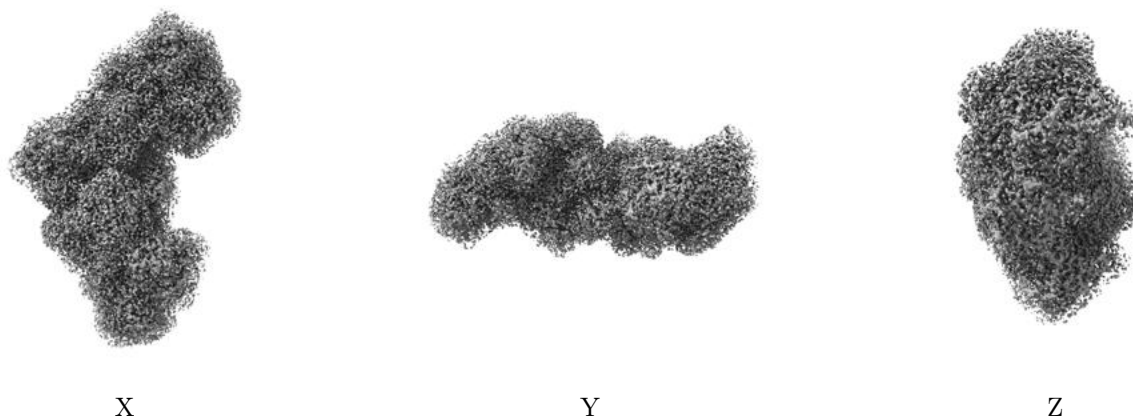


Z

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.

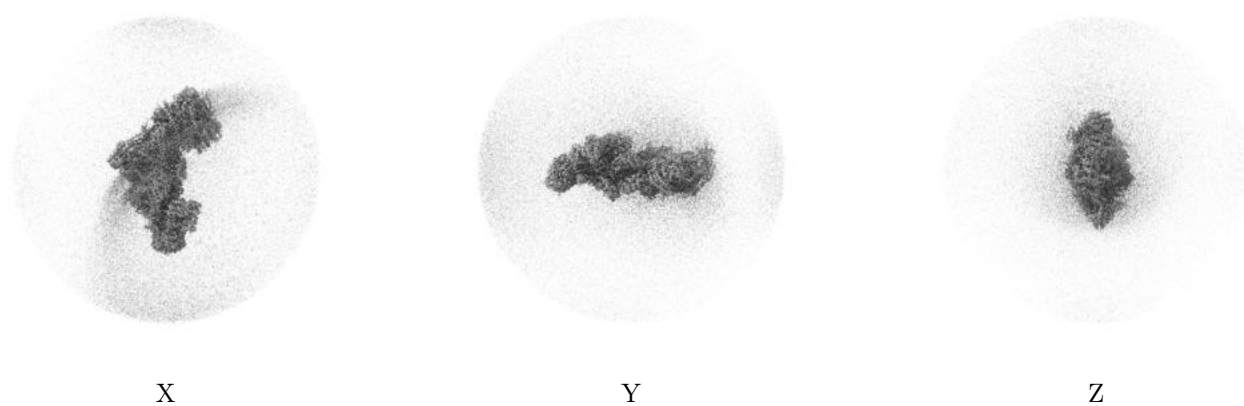
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. 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.

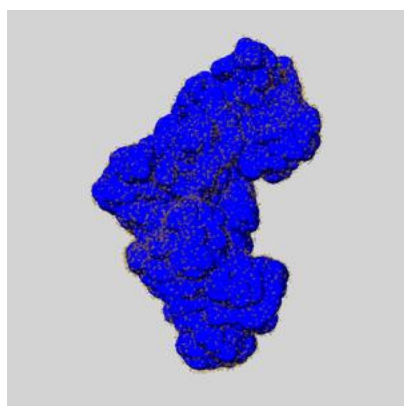
6.6 Mask visualisation [i](#)

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

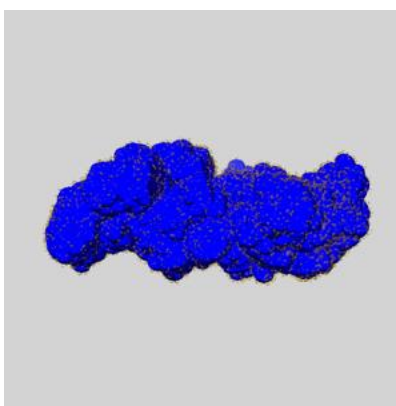
A mask typically either:

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

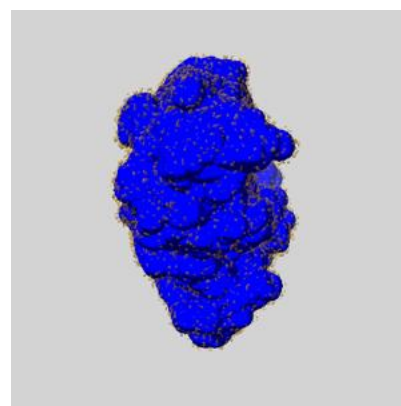
6.6.1 emd_18067_msk_1.map [i](#)



X



Y

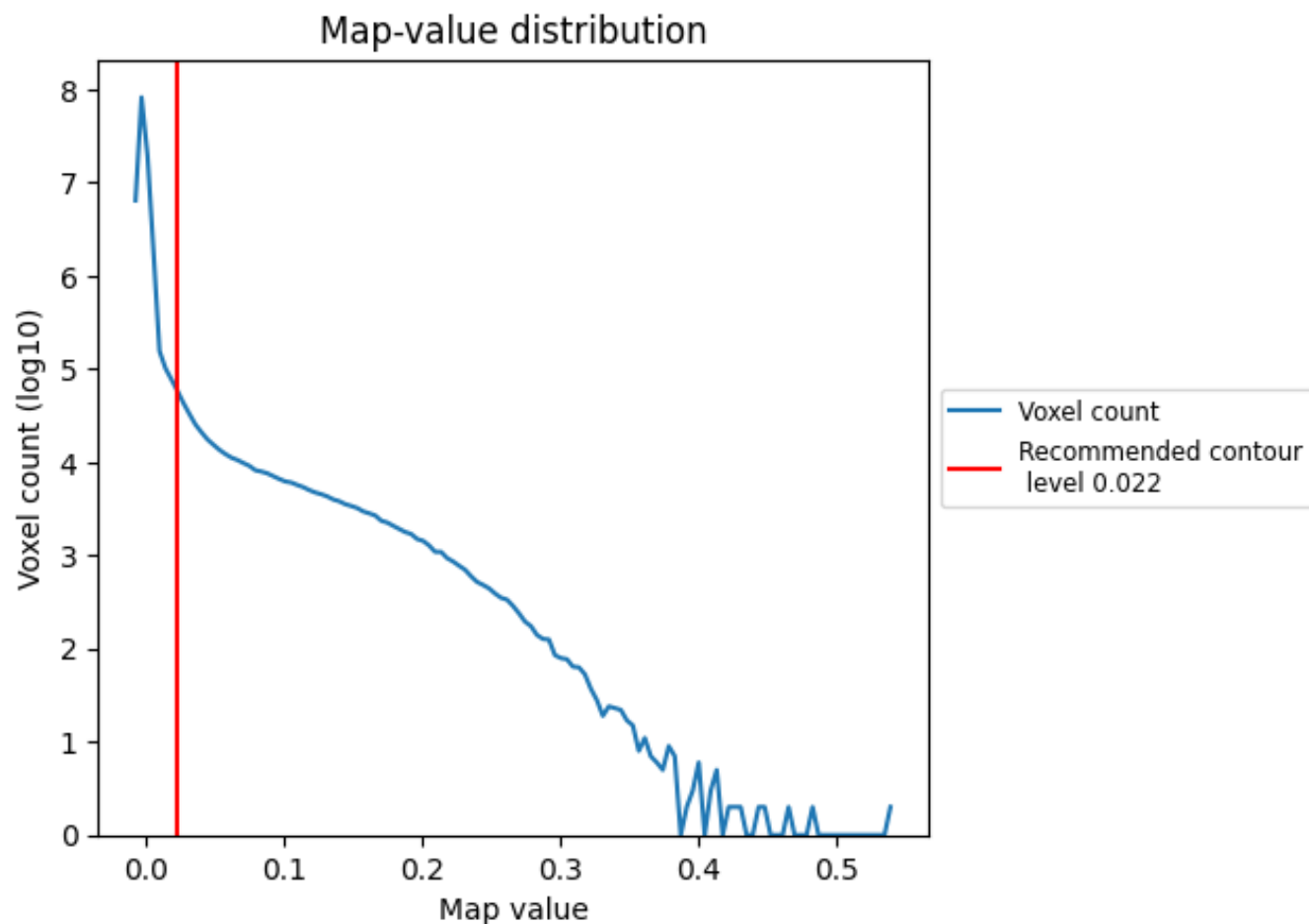


Z

7 Map analysis [i](#)

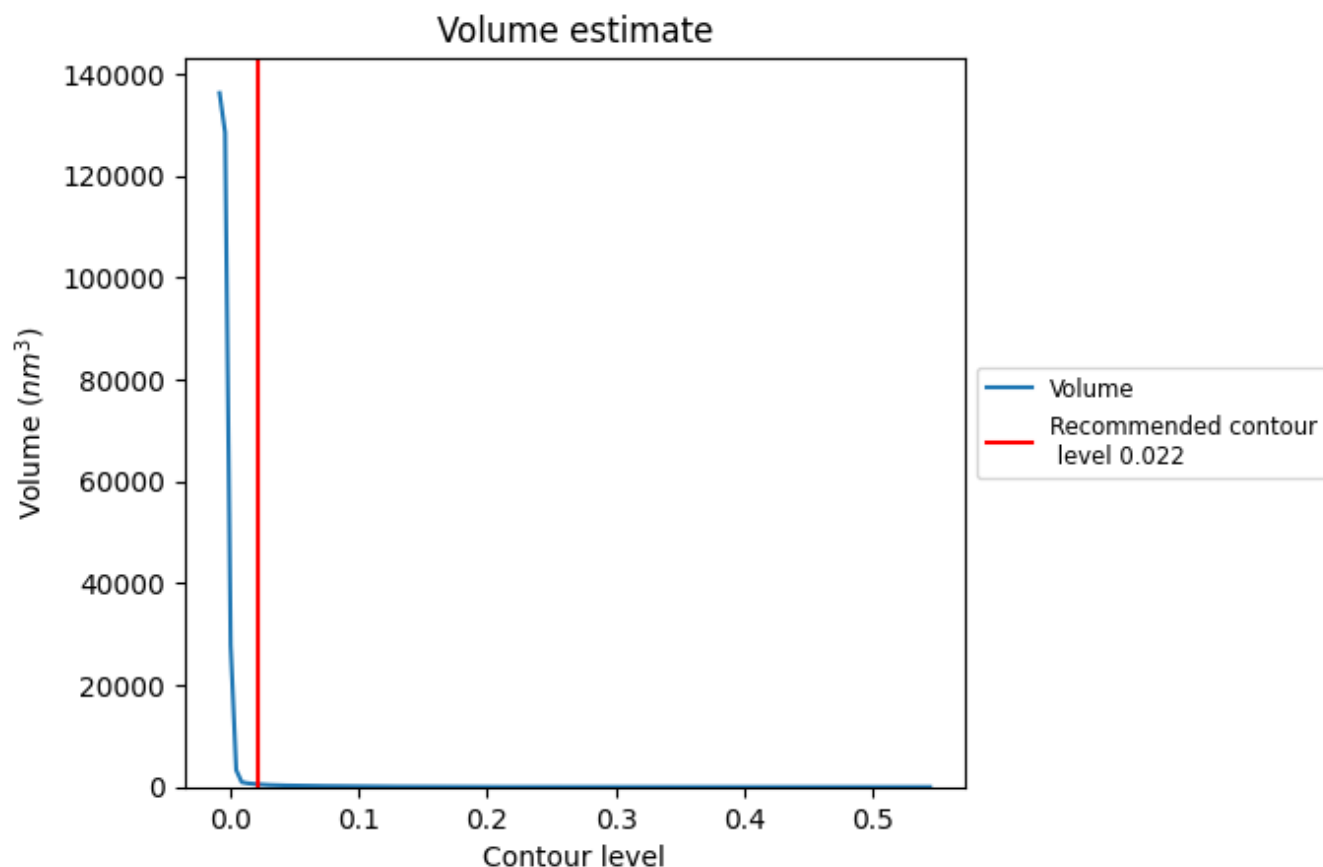
This section contains the results of statistical analysis of the map.

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.

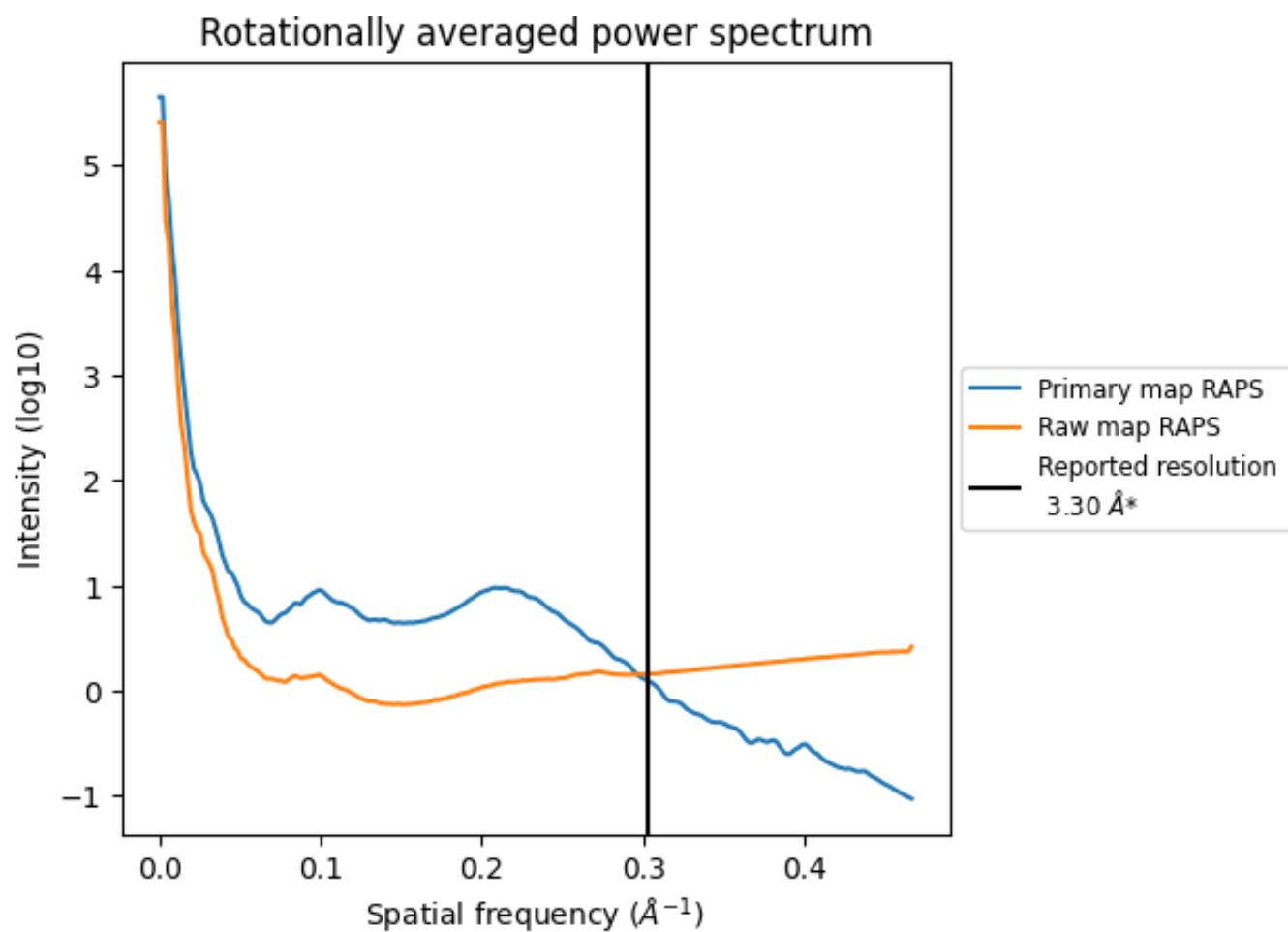
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm^3 ; this corresponds to an approximate mass of 468 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 ⓘ

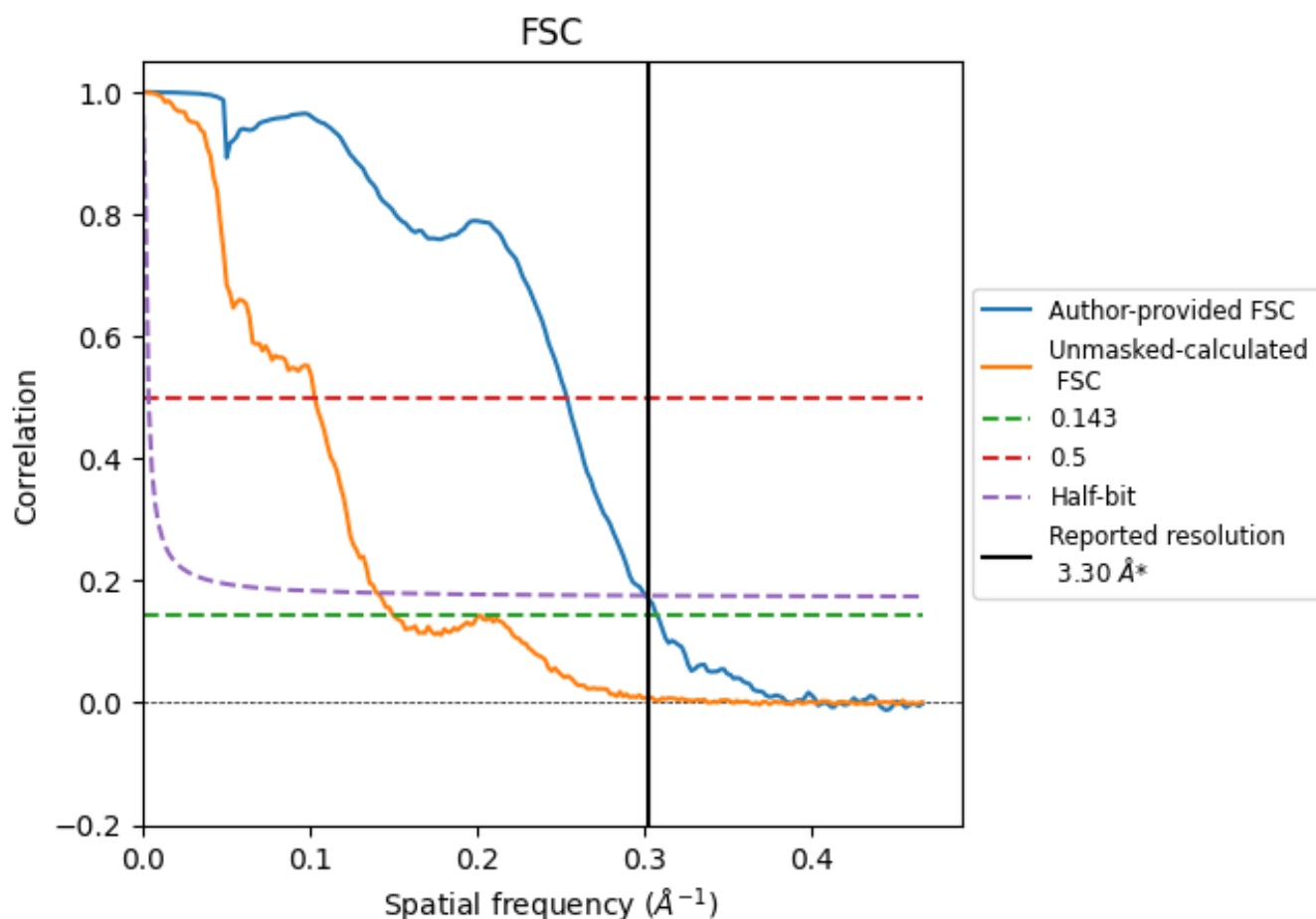


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

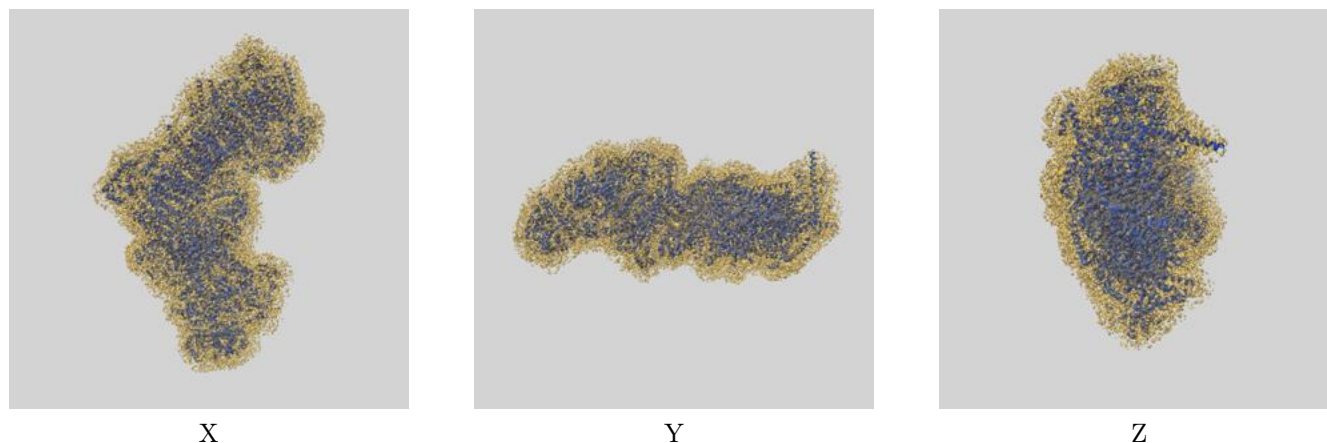
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.94	3.32
Unmasked-calculated*	6.65	9.69	7.13

*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 6.65 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

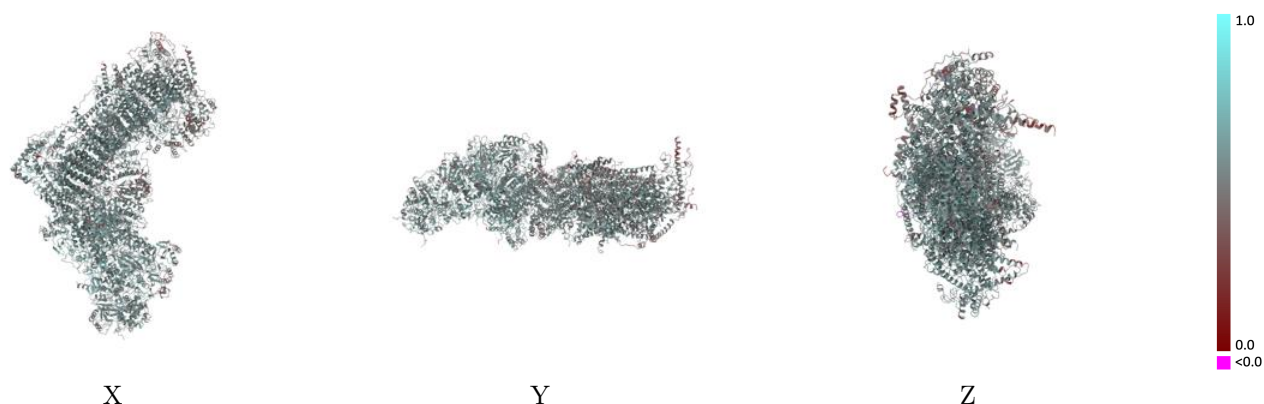
This section contains information regarding the fit between EMDB map EMD-18067 and PDB model 8Q1U. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



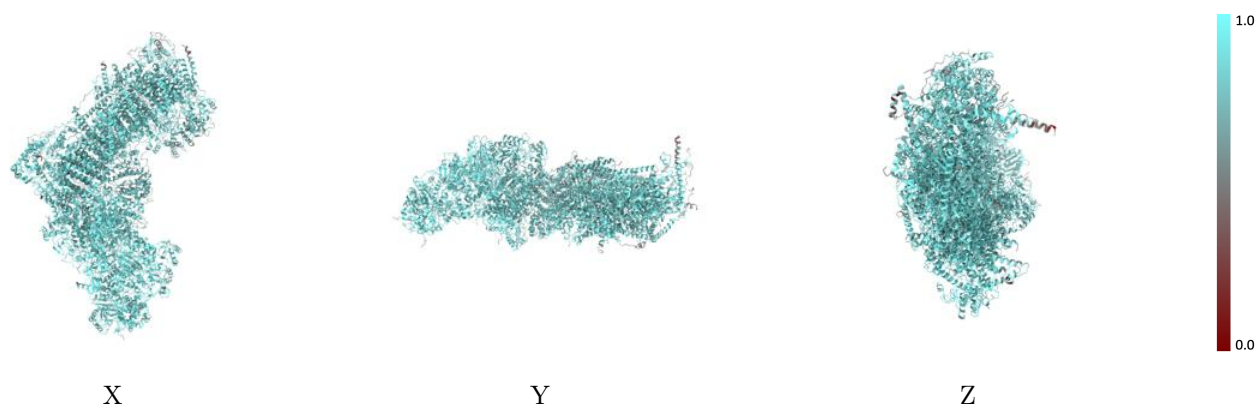
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



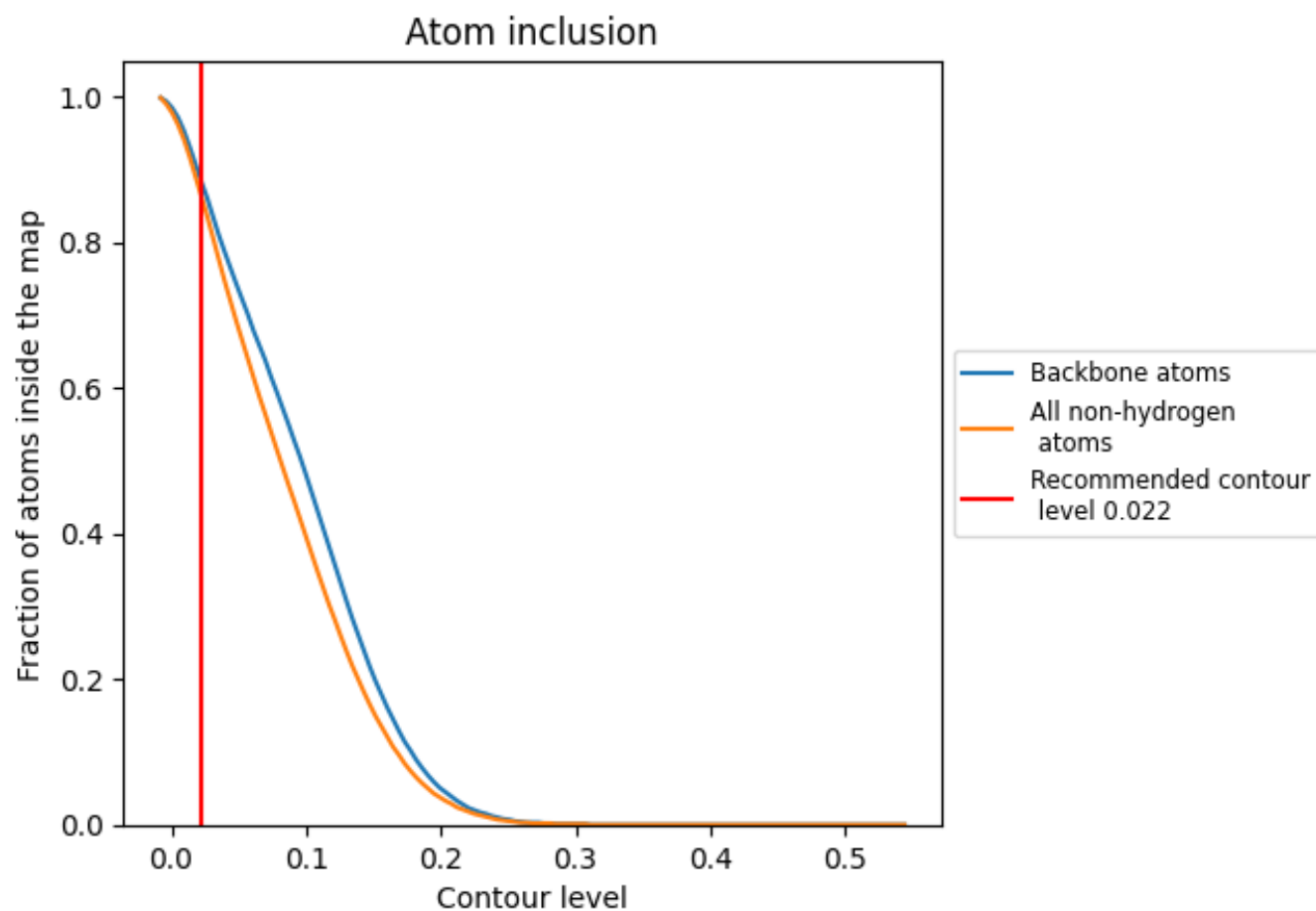
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8650	 0.5500
A	 0.8740	 0.5630
B	 0.9090	 0.5860
C	 0.9350	 0.6060
D	 0.9190	 0.5940
E	 0.8600	 0.5330
F	 0.8740	 0.5550
G	 0.8880	 0.5680
H	 0.8970	 0.5740
I	 0.9340	 0.6080
J	 0.8480	 0.5390
K	 0.9160	 0.5740
L	 0.8620	 0.5480
M	 0.9120	 0.5880
N	 0.9230	 0.5910
O	 0.8440	 0.5240
P	 0.8500	 0.5360
Q	 0.8950	 0.5770
R	 0.8850	 0.5660
S	 0.8120	 0.5220
T	 0.6980	 0.4290
U	 0.7670	 0.4670
V	 0.8570	 0.5510
W	 0.8730	 0.5510
X	 0.8610	 0.5490
Y	 0.8380	 0.5220
Z	 0.8520	 0.5440
a	 0.9020	 0.5790
b	 0.8440	 0.5400
c	 0.8300	 0.5350
d	 0.8630	 0.5530
e	 0.8140	 0.5330
f	 0.7540	 0.4710
g	 0.8280	 0.5210
h	 0.8720	 0.5570



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Chain	Atom inclusion	Q-score
i	 0.7400	 0.4540
j	 0.7700	 0.4540
k	 0.7170	 0.4460
l	 0.8370	 0.5200
m	 0.8200	 0.5180
n	 0.8200	 0.5040
o	 0.7420	 0.4610
p	 0.8170	 0.5160
q	 0.8880	 0.5710
r	 0.8920	 0.5770
s	 0.8540	 0.5330