



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 12:25 AM UTC

PDB ID : 8Q0F / pdb_00008q0f
EMDB ID : EMD-18052
Title : Inward-facing, open2 proteoliposome complex I at 3.1 Å. Initially purified in DDM.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-07-28
Resolution : 3.10 Å(reported)
Based on initial model : 7QSK

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

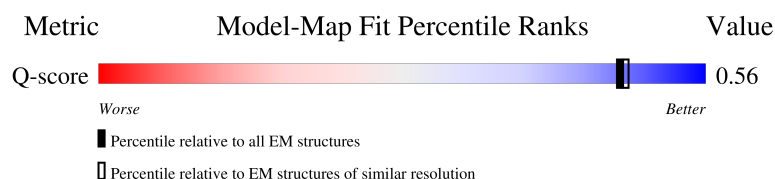
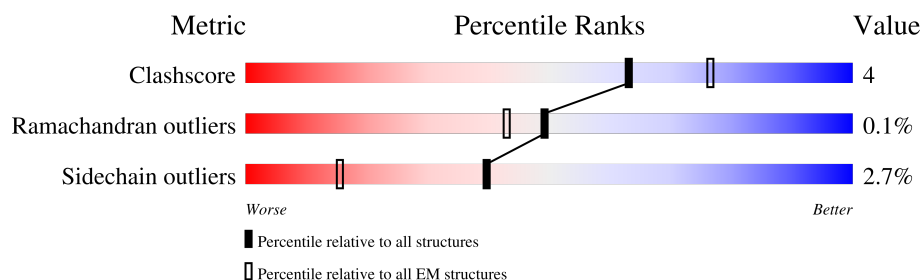
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



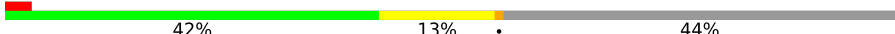
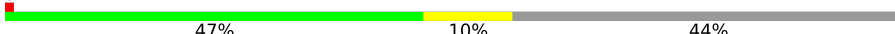
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	SF4	F	502	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 68888 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	102	Total	C	N	O	S	0	0
			823	561	117	140	5		

- 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	418	Total	C	N	O	S	0	0
			3373	2157	579	612	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	315	Total	C	N	O	S	0	0
			2488	1667	382	416	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	168	Total	C	N	O	S	0	0
			1281	861	183	225	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	334	Total	C	N	O	S	0	0
			2677	1730	475	467	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		

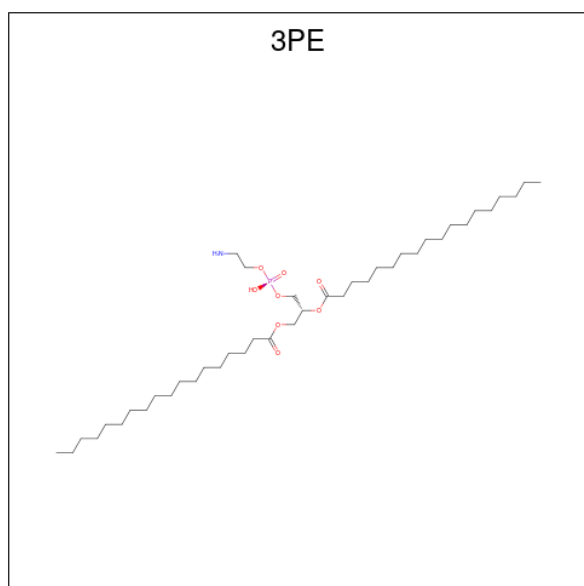
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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).



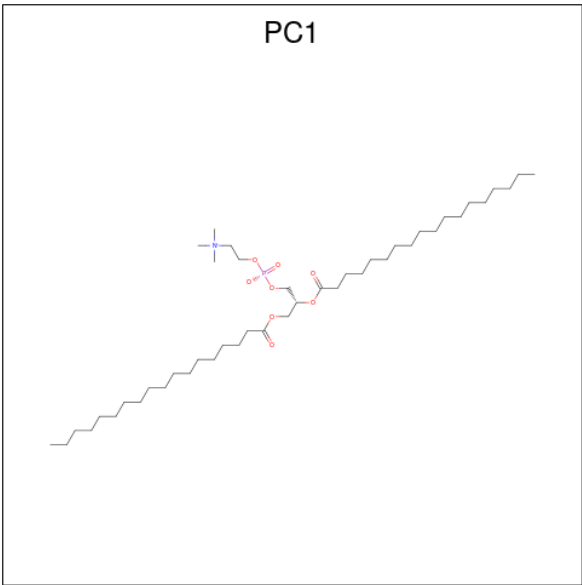
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	I	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	K	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			35	25	1	8	1	

Continued on next page...

Continued from previous page...

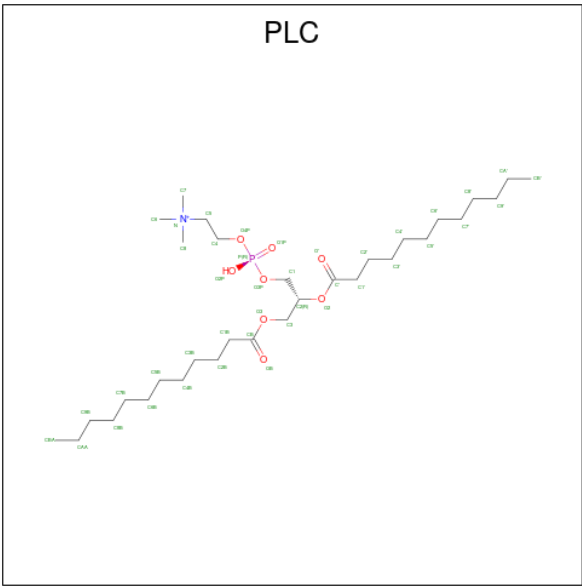
Mol	Chain	Residues	Atoms					AltConf
45	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	N	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	Y	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	Z	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	b	1	Total	C	N	O	P	0
			35	25	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
			30	20	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
			41	31	1	8	1	

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



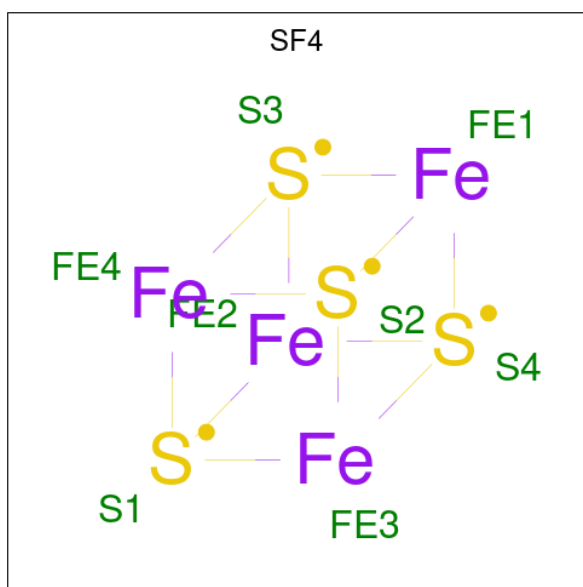
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	L	1	Total	C	N	O	P	0
			54	44	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
			35	25	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
			36	26	1	8	1	
46	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	q	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	q	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 47 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



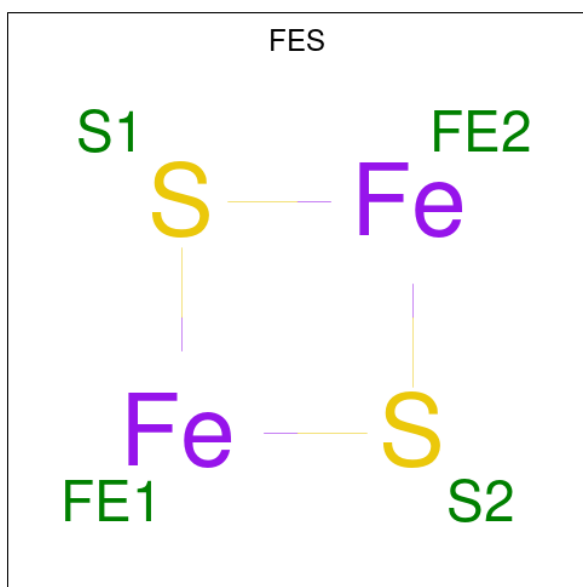
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	M	1	Total	C	N	O	P	0
			34	24	1	8	1	
47	Y	1	Total	C	N	O	P	0
			32	22	1	8	1	
47	Z	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	g	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



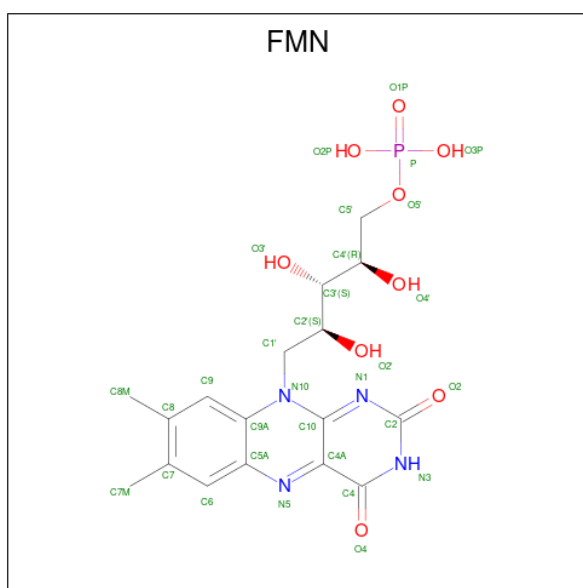
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

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

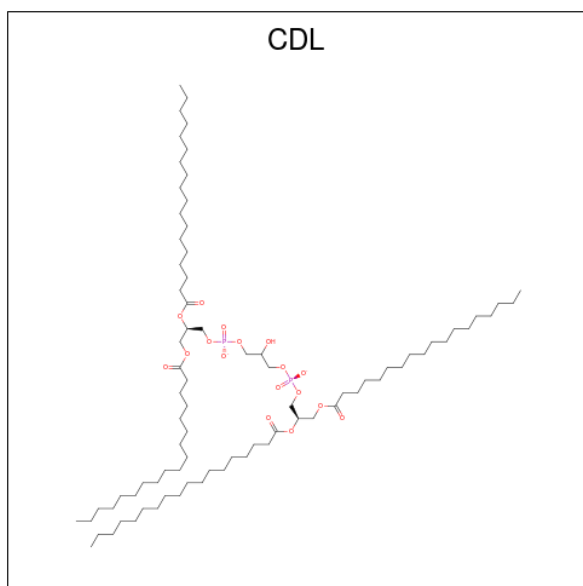


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

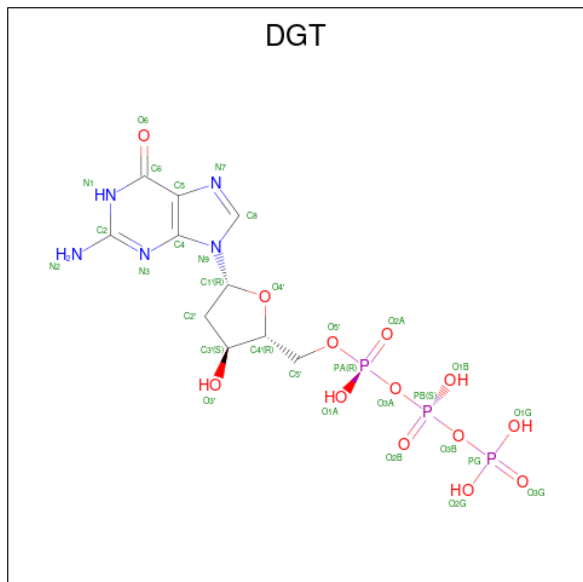


Mol	Chain	Residues	Atoms				AltConf
52	L	1	Total	C	O	P	0
			100	81	17	2	
52	M	1	Total	C	O	P	0
			100	81	17	2	
52	N	1	Total	C	O	P	0
			85	66	17	2	
52	X	1	Total	C	O	P	0
			100	81	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	i	1	Total	C	O	P	0
			80	61	17	2	
52	q	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 54 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

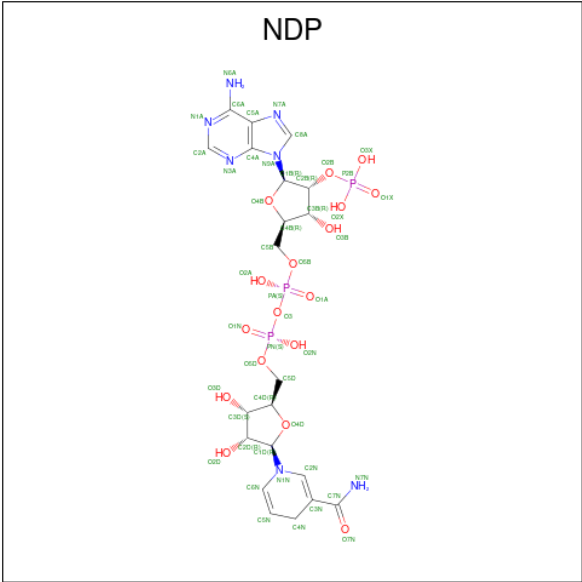


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

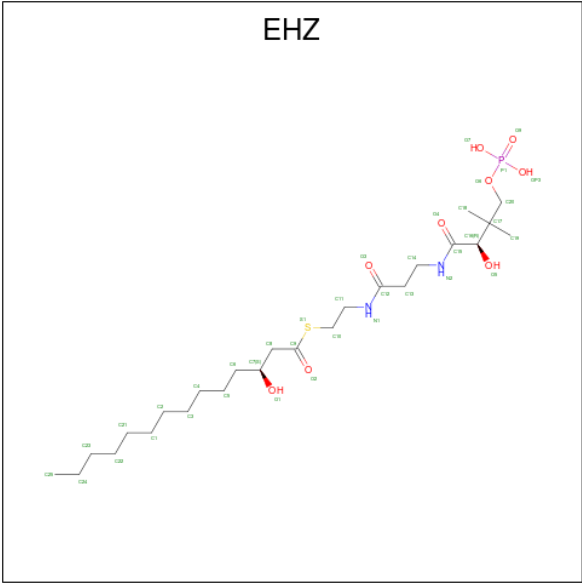
Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



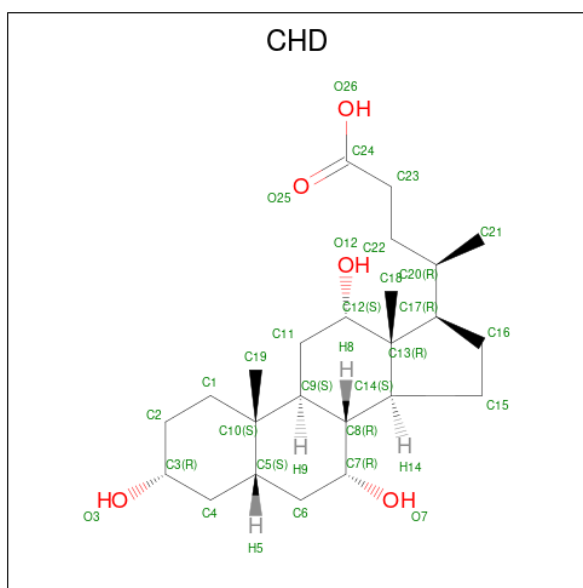
Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 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).



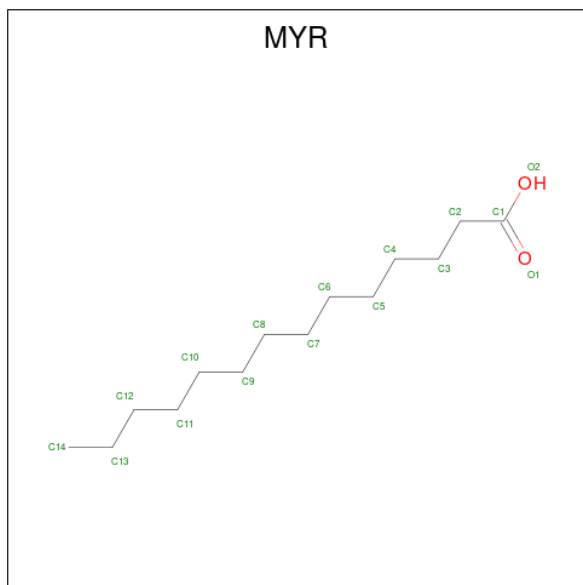
Mol	Chain	Residues	Atoms						AltConf
57	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
57	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 58 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

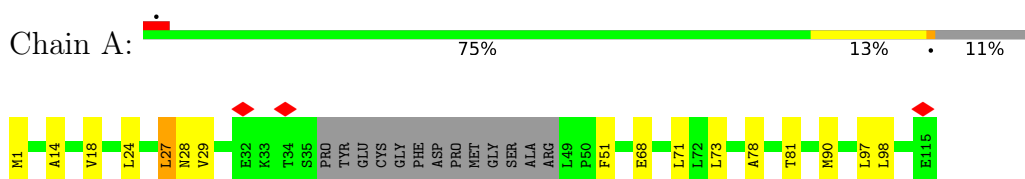


Mol	Chain	Residues	Atoms			AltConf
59	o	1	Total	C	O	0
			15	14	1	

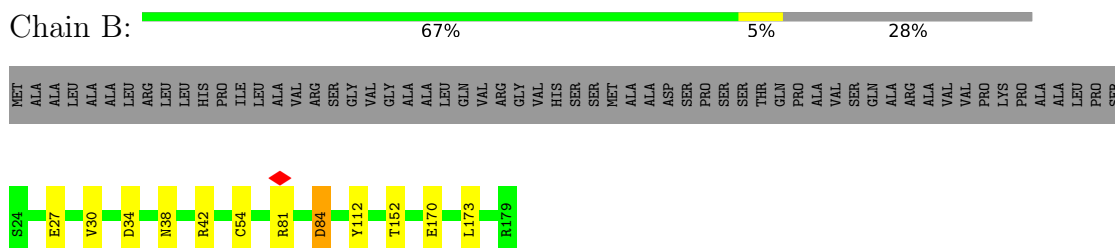
3 Residue-property plots [i](#)

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

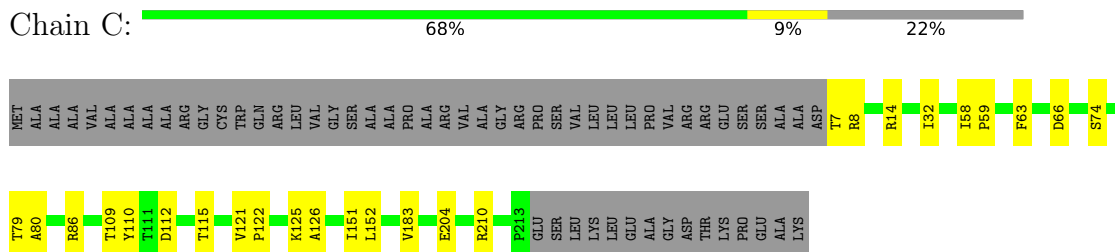
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



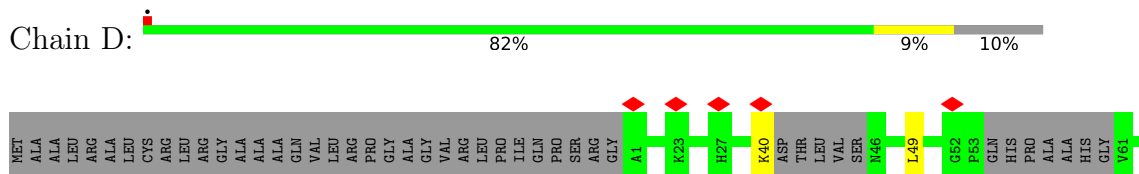
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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



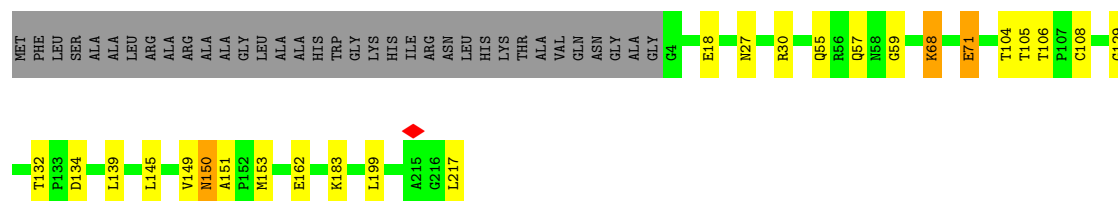
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





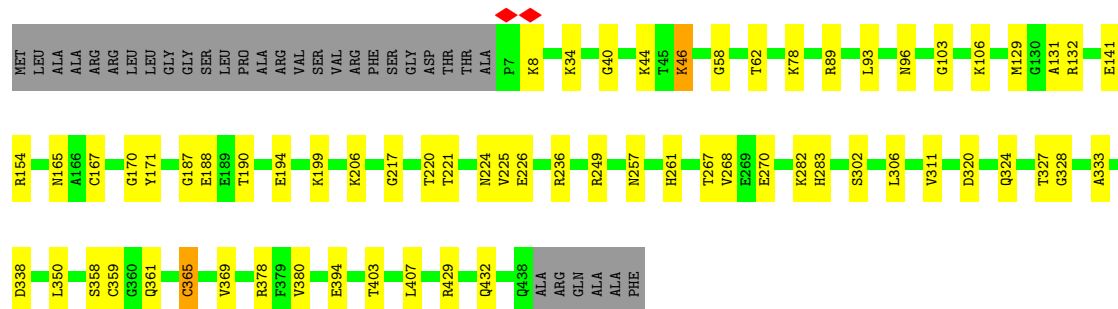
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 76% 9% 14%



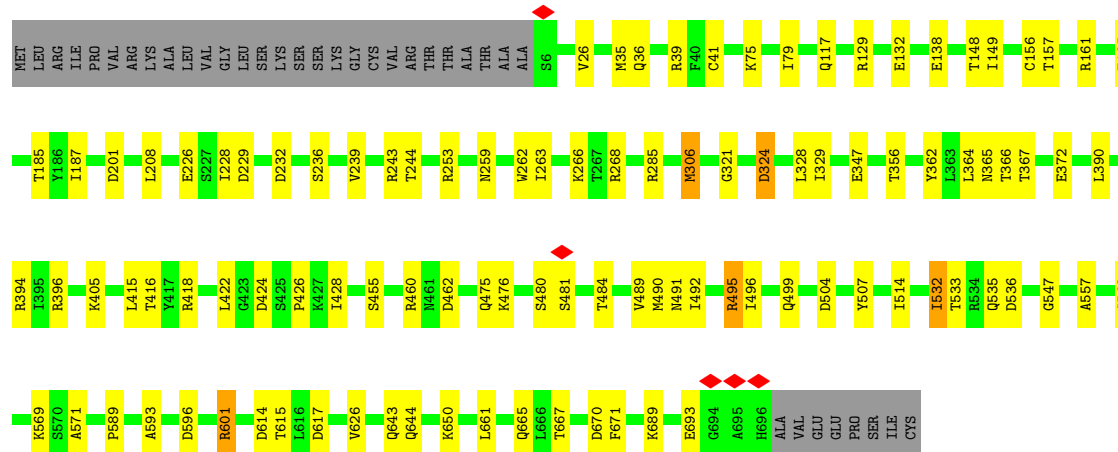
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 79% 14% 7%



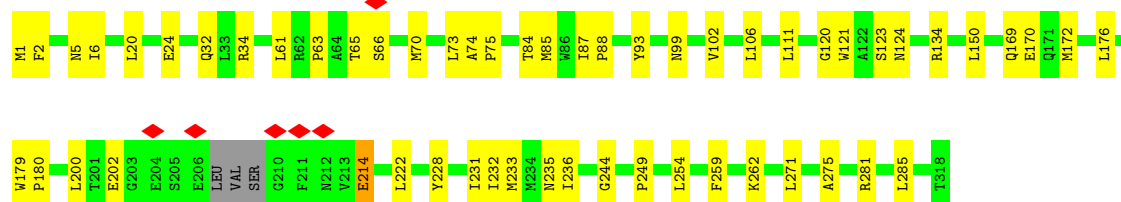
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 81% 14% 5%



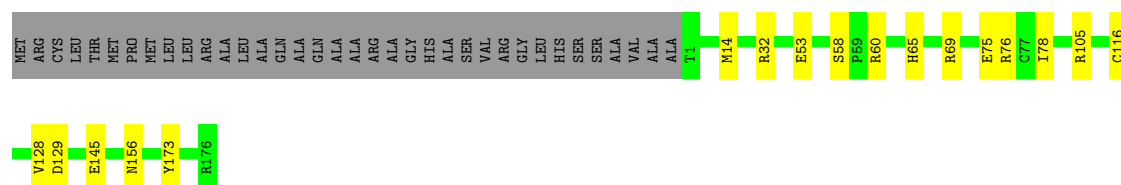
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  81% 17%



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

Chain I:  75% 8% 17%



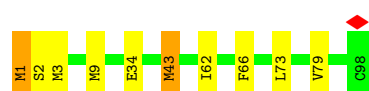
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  81% 14%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  90% 8%



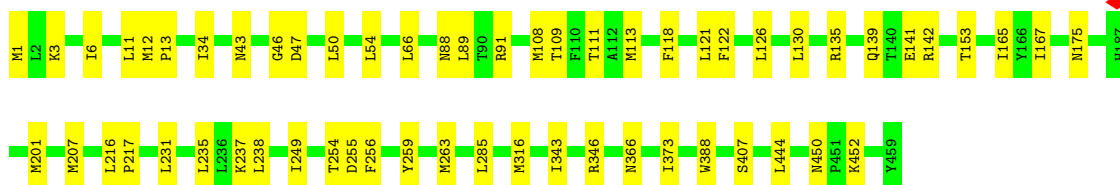
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  86% 14%



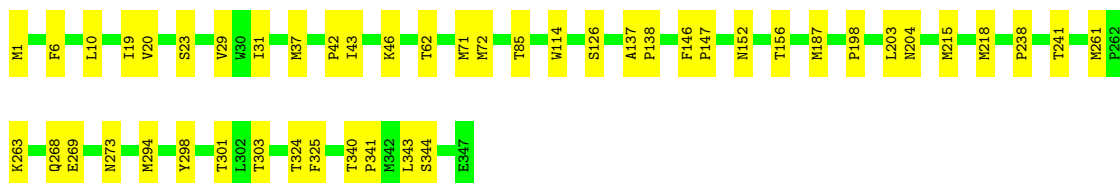
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  87% 13%



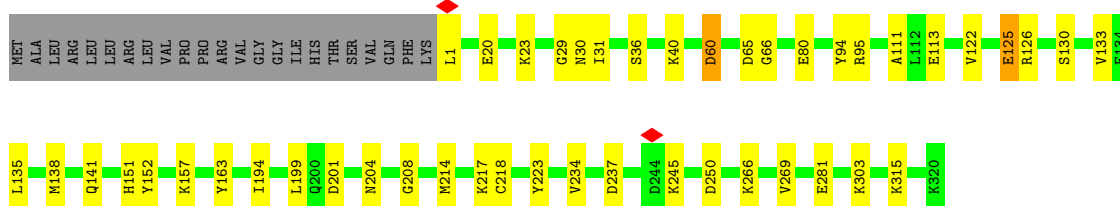
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  86% 14%



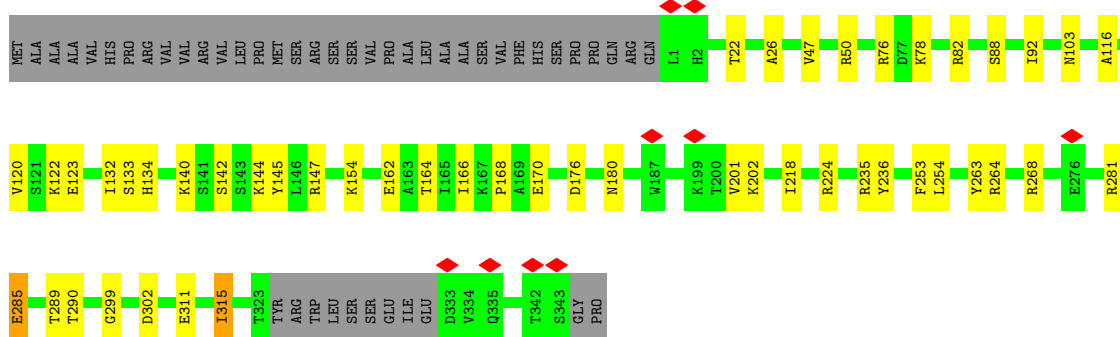
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  80% 13% 7%



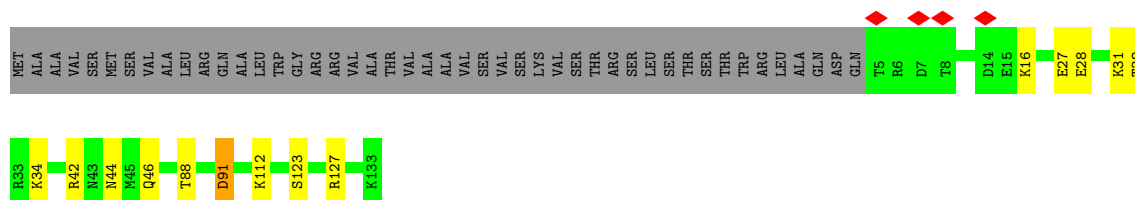
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  75% 12% 12%

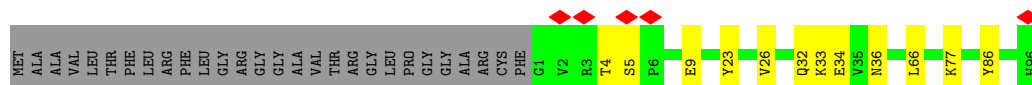


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

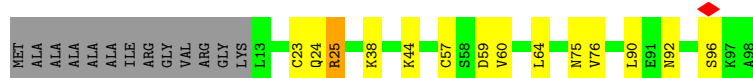
Chain Q:  66% 7% 26%



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



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



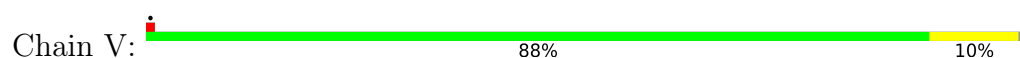
- Molecule 20: Acyl carrier protein, mitochondrial



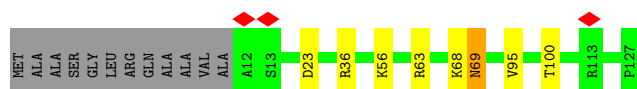
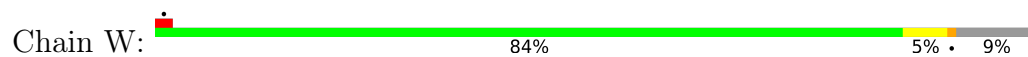
- Molecule 20: Acyl carrier protein, mitochondrial



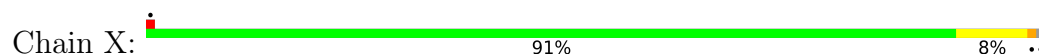
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



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



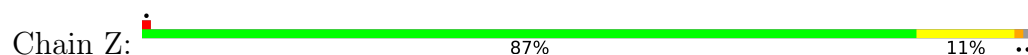
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



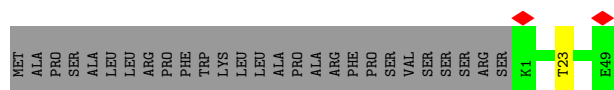
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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



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



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

Chain d:  86% 12% .



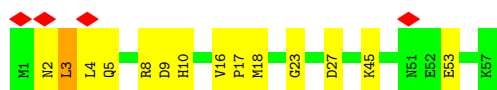
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  86% 7% 8%



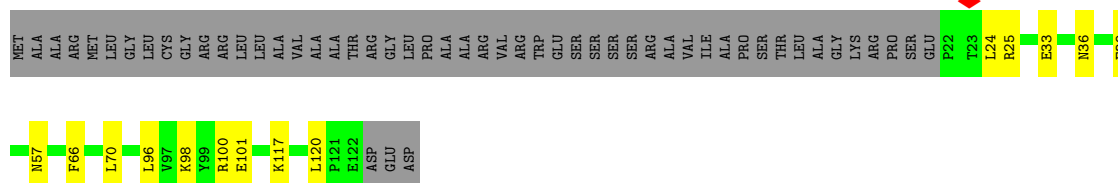
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  7% 75% 23% .



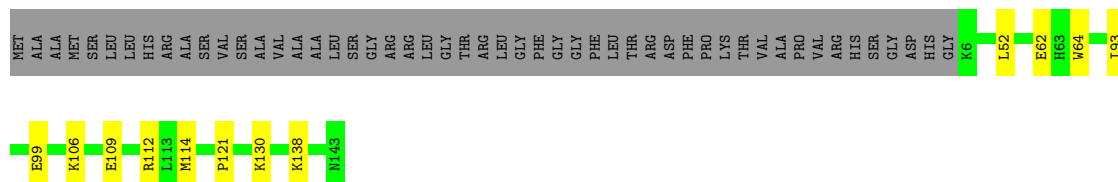
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:  56% 9% 34%



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

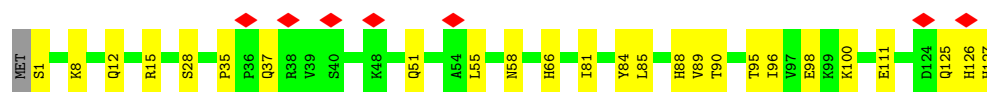
Chain h:  67% 6% 27%



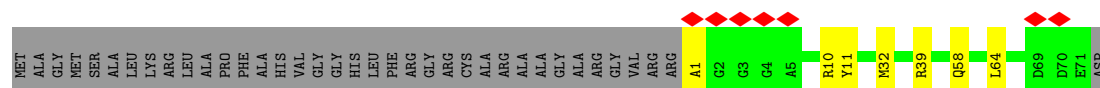
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:  5% 80% 20% .

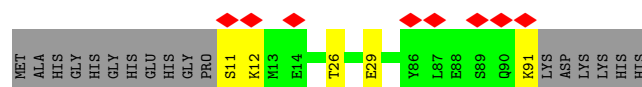
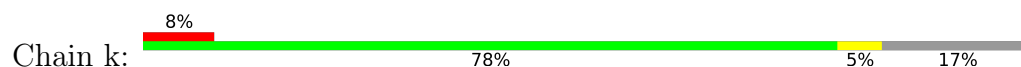




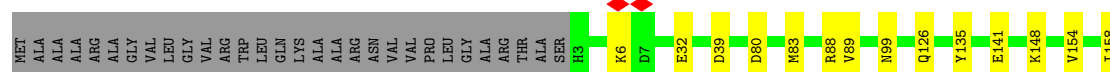
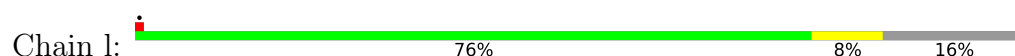
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



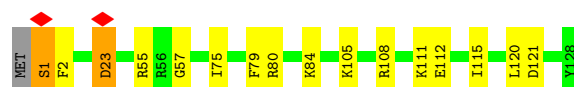
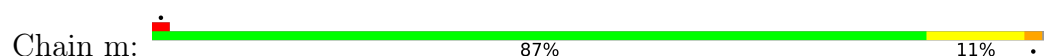
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



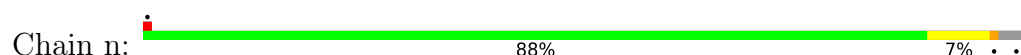
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



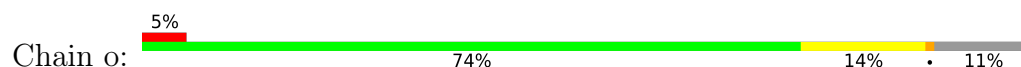
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



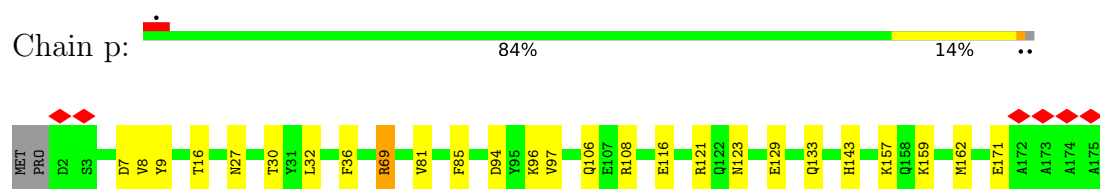
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



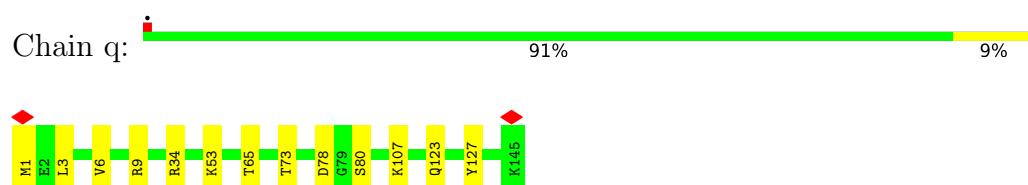
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



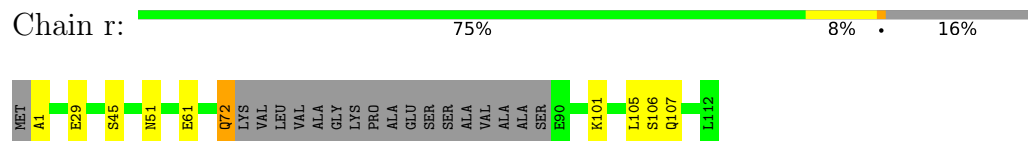
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



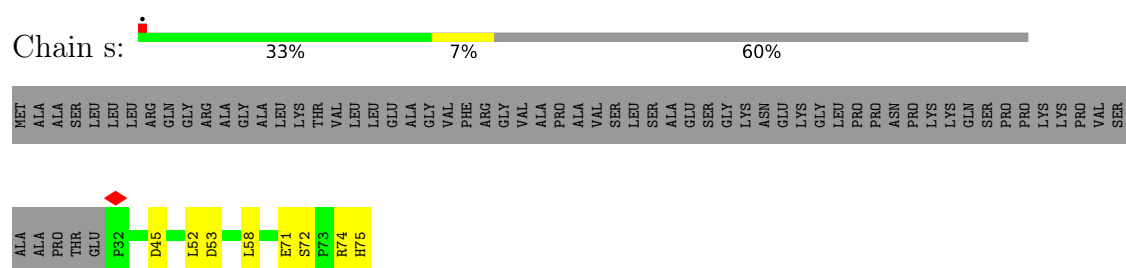
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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	116474	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 ($e^-/\text{\AA}^2$)	39.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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, AME, CHD, MG, FMN, 3PE, NDP, K, 2MR, AYA, CDL, MYR, PLC, ZN, SAC, SF4, DGT, FES, FME, EHZ

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	0.15	0/833	0.24	0/1140
2	B	0.19	0/1278	0.26	0/1728
3	C	0.18	0/1772	0.25	0/2413
4	D	0.19	0/3446	0.24	0/4665
5	E	0.13	0/1699	0.26	0/2312
6	F	0.14	0/3401	0.25	0/4595
7	G	0.16	0/5387	0.26	0/7301
8	H	0.17	0/2549	0.26	0/3481
9	I	0.21	0/1445	0.28	0/1956
10	J	0.14	0/1301	0.24	0/1761
11	K	0.15	0/745	0.22	0/1008
12	L	0.14	0/4920	0.24	0/6694
13	M	0.16	0/3738	0.23	0/5097
14	N	0.16	0/2792	0.25	0/3800
15	O	0.12	0/2651	0.21	0/3587
16	P	0.13	0/2750	0.24	0/3729
17	Q	0.16	0/1072	0.24	0/1449
18	R	0.17	0/753	0.22	0/1014
19	S	0.11	0/702	0.23	0/945
20	T	0.12	0/719	0.24	0/971
20	U	0.12	0/719	0.24	0/971
21	V	0.14	0/943	0.22	0/1277
22	W	0.13	0/1006	0.23	0/1352
23	X	0.13	0/1439	0.23	0/1942
24	Y	0.11	0/1042	0.19	0/1414
25	Z	0.14	0/1186	0.21	0/1599
26	a	0.17	0/584	0.24	0/786
27	b	0.13	0/667	0.23	0/916
28	c	0.14	0/427	0.20	0/579
29	d	0.15	0/1018	0.24	0/1375
30	e	0.14	0/846	0.23	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.15	0/505	0.30	0/681
32	g	0.13	0/873	0.25	0/1186
33	h	0.14	0/1188	0.21	0/1607
34	i	0.11	0/1127	0.22	0/1534
35	j	0.12	0/624	0.20	0/855
36	k	0.09	0/672	0.19	0/906
37	l	0.12	0/1369	0.24	0/1873
38	m	0.12	0/1088	0.22	0/1472
39	n	0.12	0/1540	0.22	0/2085
40	o	0.12	0/1073	0.21	0/1437
41	p	0.12	0/1491	0.22	0/2011
42	q	0.15	0/1242	0.24	0/1688
43	r	0.15	0/789	0.23	0/1068
44	s	0.10	0/383	0.21	0/518
All	All	0.15	0/67794	0.24	0/91909

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	823	0	866	15	0
2	B	1247	0	1256	8	0
3	C	1721	0	1675	15	0
4	D	3373	0	3324	25	0
5	E	1659	0	1664	18	0
6	F	3326	0	3282	35	0
7	G	5298	0	5316	62	0
8	H	2488	0	2595	39	0
9	I	1414	0	1370	15	0
10	J	1281	0	1292	19	0
11	K	745	0	785	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	58	0
13	M	3654	0	3852	35	0
14	N	2733	0	2912	27	0
15	O	2589	0	2566	25	0
16	P	2677	0	2701	26	0
17	Q	1049	0	1045	4	0
18	R	740	0	714	11	0
19	S	691	0	706	7	0
20	T	707	0	700	10	0
20	U	707	0	700	11	0
21	V	923	0	964	8	0
22	W	982	0	999	5	0
23	X	1402	0	1381	10	0
24	Y	1030	0	1039	9	0
25	Z	1157	0	1156	11	0
26	a	569	0	568	5	0
27	b	654	0	663	4	0
28	c	414	0	415	0	0
29	d	999	0	988	16	0
30	e	825	0	826	6	0
31	f	492	0	501	8	0
32	g	846	0	798	7	0
33	h	1154	0	1168	7	0
34	i	1097	0	1108	17	0
35	j	597	0	536	5	0
36	k	653	0	639	2	0
37	l	1314	0	1210	7	0
38	m	1070	0	1068	14	0
39	n	1487	0	1433	9	0
40	o	1048	0	1018	13	0
41	p	1458	0	1430	17	0
42	q	1212	0	1183	8	0
43	r	776	0	782	4	0
44	s	371	0	344	8	0
45	A	47	0	71	0	0
45	D	49	0	75	0	0
45	I	36	0	49	0	0
45	K	44	0	62	1	0
45	L	131	0	196	2	0
45	M	95	0	141	0	0
45	N	44	0	65	0	0
45	Y	213	0	314	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	41	0	59	1	0
45	b	35	0	44	3	0
45	d	49	0	75	1	0
45	g	30	0	34	0	0
45	m	82	0	118	2	0
46	A	81	0	110	4	0
46	H	90	0	134	2	0
46	I	98	0	150	1	0
46	L	54	0	88	1	0
46	M	79	0	109	0	0
46	d	39	0	52	1	0
46	h	36	0	46	0	0
46	m	54	0	88	1	0
46	q	82	0	112	1	0
47	A	42	0	64	0	0
47	B	42	0	64	0	0
47	L	31	0	36	0	0
47	M	34	0	45	0	0
47	Y	32	0	41	0	0
47	Z	36	0	49	0	0
47	g	29	0	32	0	0
48	B	8	0	0	0	0
48	F	8	0	0	2	0
48	G	16	0	0	0	0
48	I	16	0	0	1	0
49	E	4	0	0	0	0
49	G	4	0	0	1	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	L	100	0	156	1	0
52	M	100	0	156	3	0
52	N	85	0	117	0	0
52	X	100	0	156	2	0
52	d	65	0	77	2	0
52	i	80	0	104	1	0
52	q	61	0	66	2	0
53	M	1	0	0	0	0
53	R	1	0	0	0	0
54	O	31	0	12	2	0
55	O	1	0	0	0	0
56	P	48	0	26	4	0
57	T	37	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	U	37	0	0	1	0
58	i	29	0	38	6	0
59	o	15	0	27	0	0
All	All	68888	0	69975	585	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 (585) 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)
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.08	0.87
42:q:78:ASP:OD2	42:q:80:SER:OG	1.93	0.86
20:U:57:GLU:OE2	35:j:11:TYR:OH	1.94	0.86
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.09	0.85
15:O:113:GLU:OE1	15:O:266:LYS:NZ	2.11	0.84
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.09	0.84
5:E:30:ARG:NH1	44:s:53:ASP:OD1	2.10	0.83
6:F:320:ASP:O	6:F:324:GLN:NE2	2.12	0.83
7:G:569:LYS:NZ	7:G:596:ASP:OD2	2.14	0.81
12:L:175:ASN:OD1	12:L:223:LYS:NZ	2.14	0.81
19:S:92:ASN:O	19:S:96:SER:OG	1.98	0.81
24:Y:13:GLU:OE2	24:Y:89:TYR:OH	1.98	0.79
7:G:644:GLN:N	7:G:644:GLN:OE1	2.16	0.79
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.15	0.79
6:F:131:ALA:O	6:F:171:TYR:OH	2.01	0.78
29:d:120:ARG:O	38:m:108:ARG:NH2	2.16	0.77
5:E:150:ASN:ND2	5:E:162:GLU:OE1	2.18	0.77
7:G:615:THR:OG1	7:G:617:ASP:OD1	2.01	0.77
19:S:23:CYS:SG	19:S:25:ARG:NH2	2.57	0.77
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.15	0.77
29:d:112:VAL:O	41:p:159:LYS:NZ	2.17	0.77
10:J:170:GLU:OE1	10:J:173:ARG:NH2	2.18	0.77
6:F:261:HIS:ND1	6:F:338:ASP:OD1	2.18	0.77
32:g:98:LYS:NZ	41:p:7:ASP:OD2	2.18	0.77
5:E:68:LYS:NZ	5:E:71:GLU:OE2	2.17	0.76
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.02	0.75
7:G:533:THR:OG1	7:G:535:GLN:OE1	2.03	0.75
14:N:19:ILE:O	14:N:23:SER:OG	2.02	0.74
41:p:171:GLU:N	41:p:171:GLU:OE1	2.19	0.74
25:Z:130:GLU:N	25:Z:130:GLU:OE1	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:69:ARG:NH2	41:p:94:ASP:OD2	2.20	0.74
16:P:162:GLU:O	16:P:224:ARG:NH1	2.20	0.74
13:M:43:ASN:O	13:M:50:LEU:HD11	1.87	0.74
8:H:66:SER:N	8:H:124:ASN:OD1	2.20	0.74
40:o:35:GLU:OE1	40:o:35:GLU:N	2.21	0.74
7:G:366:THR:O	7:G:367:THR:OG1	2.04	0.73
23:X:6:LEU:O	25:Z:87:ARG:NH1	2.20	0.73
7:G:266:LYS:NZ	7:G:671:PHE:O	2.22	0.73
8:H:61:LEU:O	8:H:61:LEU:HD13	1.88	0.73
2:B:81:ARG:CZ	8:H:61:LEU:HD11	2.19	0.73
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.22	0.73
57:T:101:EHZ:O1	57:T:101:EHZ:O2	2.01	0.72
9:I:75:GLU:O	9:I:105:ARG:NH1	2.21	0.72
16:P:164:THR:OG1	16:P:224:ARG:NH2	2.22	0.72
13:M:46:GLY:O	41:p:96:LYS:NZ	2.21	0.72
12:L:161:ARG:NH1	12:L:238:GLU:OE1	2.23	0.71
15:O:20:GLU:O	15:O:23:LYS:NZ	2.17	0.71
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.24	0.71
9:I:145:GLU:OE1	9:I:145:GLU:N	2.21	0.71
58:i:201:CHD:H212	58:i:201:CHD:H12	1.71	0.71
23:X:150:ASN:OD1	30:e:50:ARG:NH1	2.24	0.71
7:G:415:LEU:O	7:G:416:THR:OG1	2.09	0.71
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.08	0.71
31:f:2:ASN:C	31:f:3:LEU:HD13	2.15	0.70
1:A:24:LEU:O	1:A:27:LEU:HD22	1.91	0.70
12:L:245:ALA:O	12:L:249:SER:OG	2.08	0.70
52:M:602:CDL:OA4	52:M:602:CDL:O1	2.08	0.70
34:i:51:GLN:OE1	34:i:51:GLN:N	2.25	0.70
40:o:32:GLU:N	40:o:32:GLU:OE1	2.25	0.69
6:F:141:GLU:OE1	6:F:141:GLU:N	2.25	0.69
7:G:165:GLU:O	7:G:396:ARG:NH1	2.25	0.69
1:A:18:VAL:HG22	8:H:222:LEU:HD23	1.73	0.69
15:O:281:GLU:N	15:O:281:GLU:OE1	2.26	0.69
21:V:17:GLU:OE1	21:V:17:GLU:N	2.25	0.69
39:n:94:GLU:OE1	39:n:97:LYS:NZ	2.26	0.68
40:o:11:ASP:OD1	40:o:12:ALA:N	2.26	0.68
7:G:475:GLN:NE2	7:G:643:GLN:OE1	2.26	0.68
13:M:343:ILE:O	13:M:346:ARG:NH1	2.27	0.68
34:i:88:HIS:NE2	52:i:202:CDL:OB3	2.22	0.68
41:p:129:GLU:OE2	41:p:133:GLN:NE2	2.26	0.68
7:G:148:THR:HG22	7:G:208:LEU:CD2	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.27	0.67
12:L:508:THR:O	39:n:35:LYS:NZ	2.23	0.67
16:P:162:GLU:OE1	16:P:162:GLU:N	2.26	0.67
16:P:82:ARG:NH1	16:P:123:GLU:OE2	2.27	0.67
9:I:156:ASN:ND2	18:R:34:GLU:OE2	2.28	0.67
20:T:22:TYR:O	20:T:24:LYS:N	2.28	0.66
45:m:201:3PE:O22	45:m:201:3PE:N	2.16	0.66
12:L:467:ILE:O	12:L:471:ASN:ND2	2.28	0.66
13:M:135:ARG:NH1	14:N:301:THR:O	2.28	0.66
19:S:23:CYS:SG	19:S:59:ASP:N	2.68	0.66
11:K:43:MET:HE1	14:N:72:MET:SD	2.36	0.66
13:M:139:GLN:O	13:M:142:ARG:NH1	2.27	0.65
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.29	0.65
7:G:285:ARG:NH1	7:G:557:ALA:O	2.29	0.65
13:M:237:LYS:NZ	13:M:316:MET:O	2.30	0.65
4:D:71:GLU:OE2	8:H:134:ARG:NH1	2.30	0.65
6:F:188:GLU:OE1	6:F:190:THR:N	2.28	0.65
43:r:72:GLN:N	43:r:72:GLN:OE1	2.29	0.65
9:I:65:HIS:CE1	9:I:116:CYS:SG	2.89	0.65
16:P:176:ASP:O	16:P:180:ASN:ND2	2.29	0.65
57:U:101:EHZ:O2	57:U:101:EHZ:O1	2.14	0.65
1:A:28:ASN:ND2	46:A:203:PC1:O32	2.30	0.64
1:A:14:ALA:O	1:A:18:VAL:HG23	1.98	0.64
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.31	0.64
38:m:79:PHE:O	46:m:203:PC1:H132	1.97	0.64
44:s:72:SER:HG	44:s:75:HIS:HD1	1.43	0.64
8:H:231:ILE:O	8:H:235:ASN:ND2	2.30	0.64
9:I:65:HIS:CD2	48:I:201:SF4:S1	2.90	0.64
16:P:285:GLU:N	16:P:285:GLU:OE1	2.31	0.64
1:A:71:LEU:O	10:J:147:TYR:OH	2.15	0.64
13:M:141:GLU:N	13:M:141:GLU:OE1	2.31	0.64
23:X:5:GLU:N	23:X:5:GLU:OE1	2.30	0.64
7:G:263:ILE:HA	7:G:390:LEU:HD11	1.79	0.64
12:L:445:GLU:O	12:L:451:ILE:HD11	1.98	0.64
12:L:534:HIS:ND1	46:L:705:PC1:O12	2.30	0.63
10:J:123:GLY:HA2	11:K:3:MET:HE2	1.80	0.63
8:H:61:LEU:HD12	8:H:214:GLU:O	1.99	0.62
33:h:62:GLU:OE1	33:h:64:TRP:NE1	2.32	0.62
34:i:90:THR:HG22	34:i:96:ILE:HD12	1.81	0.62
9:I:156:ASN:OD1	18:R:36:ASN:ND2	2.32	0.62
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.27	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:601:ARG:NH1	7:G:614:ASP:OD1	2.33	0.62
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.11	0.62
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.34	0.62
6:F:257:ASN:ND2	6:F:267:THR:OG1	2.33	0.62
12:L:102:GLU:OE1	12:L:456:ARG:NH1	2.32	0.61
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.82	0.61
6:F:394:GLU:OE1	7:G:129:ARG:NH2	2.33	0.61
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.81	0.61
12:L:603:ASN:ND2	12:L:606:GLU:OE2	2.32	0.61
14:N:324:THR:HG23	52:d:201:CDL:HB32	1.81	0.61
4:D:413:ASP:OD1	8:H:281:ARG:NH1	2.33	0.61
6:F:40:GLY:O	6:F:236:ARG:NH2	2.32	0.61
41:p:143:HIS:O	41:p:157:LYS:NZ	2.25	0.61
39:n:34:ASP:OD1	39:n:35:LYS:N	2.33	0.61
7:G:138:GLU:OE2	18:R:77:LYS:NZ	2.23	0.61
5:E:149:VAL:HG23	5:E:150:ASN:OD1	2.01	0.61
7:G:328:LEU:O	7:G:507:TYR:OH	2.13	0.61
23:X:71:ARG:NE	26:a:70:ASP:OD2	2.34	0.61
27:b:1:AYA:O	27:b:5:ALA:N	2.34	0.60
41:p:8:VAL:HG23	41:p:9:TYR:CD2	2.36	0.60
7:G:480:SER:O	7:G:481:SER:OG	2.13	0.60
17:Q:88:THR:OG1	17:Q:91:ASP:OD2	2.17	0.60
31:f:5:GLN:OE1	31:f:8:ARG:NH2	2.32	0.60
29:d:5:ARG:NH1	29:d:89:ASP:OD1	2.35	0.60
2:B:42:ARG:NH1	46:q:202:PC1:O14	2.31	0.59
2:B:27:GLU:N	2:B:27:GLU:OE1	2.35	0.59
29:d:13:PHE:N	45:d:202:3PE:O14	2.35	0.59
2:B:34:ASP:OD1	2:B:38:ASN:ND2	2.35	0.59
12:L:560:ALA:O	12:L:565:THR:HG23	2.03	0.59
13:M:450:ASN:OD1	13:M:452:LYS:NZ	2.35	0.59
29:d:82:MET:HE2	29:d:82:MET:HA	1.83	0.59
5:E:132:THR:OG1	5:E:134:ASP:OD1	2.04	0.59
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.36	0.59
12:L:194:ASN:ND2	41:p:106:GLN:OE1	2.37	0.58
13:M:231:LEU:HD23	13:M:235:LEU:HD12	1.85	0.58
18:R:32:GLN:NE2	42:q:123:GLN:O	2.35	0.58
20:U:28:GLU:N	20:U:28:GLU:OE1	2.37	0.58
32:g:33:GLU:N	32:g:33:GLU:OE1	2.35	0.58
7:G:547:GLY:O	7:G:563:GLY:N	2.32	0.58
16:P:145:TYR:HH	56:P:501:NDP:HO2N	1.52	0.58
35:j:58:GLN:N	35:j:58:GLN:OE1	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:75:GLU:OE2	34:i:8:LYS:NZ	2.31	0.58
6:F:380:VAL:O	6:F:429:ARG:NH1	2.37	0.58
14:N:198:PRO:HG2	29:d:1:AME:HT21	1.86	0.58
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.39	0.57
16:P:22:THR:OG1	16:P:88:SER:OG	2.07	0.57
17:Q:27:GLU:N	17:Q:27:GLU:OE1	2.35	0.57
25:Z:89:ASN:ND2	25:Z:122:GLU:O	2.37	0.57
32:g:36:ASN:ND2	32:g:39:GLU:OE2	2.37	0.57
1:A:73:LEU:CD1	10:J:55:MET:HE1	2.35	0.57
15:O:36:SER:OG	54:O:401:DGT:O1G	2.21	0.57
6:F:96:ASN:ND2	6:F:187:GLY:O	2.35	0.57
7:G:489:VAL:O	7:G:491:ASN:ND2	2.37	0.57
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.87	0.57
20:T:35:HIS:N	20:T:39:ASP:OD2	2.38	0.56
5:E:145:LEU:HD12	5:E:153:MET:SD	2.45	0.56
6:F:194:GLU:OE1	6:F:199:LYS:NZ	2.33	0.56
4:D:227:GLU:OE2	9:I:32:ARG:NH2	2.39	0.56
6:F:407:LEU:HD23	6:F:407:LEU:O	2.05	0.56
42:q:3:LEU:HD13	42:q:3:LEU:O	2.06	0.56
8:H:169:GLN:OE1	8:H:244:GLY:N	2.31	0.55
8:H:102:VAL:CG1	8:H:150:LEU:HD21	2.37	0.55
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.37	0.55
1:A:73:LEU:HD13	10:J:55:MET:HE1	1.89	0.55
7:G:324:ASP:OD1	7:G:324:ASP:N	2.38	0.55
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.13	0.55
3:C:66:ASP:O	21:V:82:GLN:NE2	2.37	0.55
7:G:156:CYS:O	7:G:157:THR:OG1	2.18	0.55
40:o:6:ARG:NE	40:o:15:GLU:OE2	2.37	0.55
3:C:8:ARG:NH2	43:r:61:GLU:OE2	2.35	0.55
34:i:66:HIS:NE2	58:i:201:CHD:O25	2.40	0.55
9:I:173:TYR:CG	18:R:66:LEU:HD21	2.41	0.54
13:M:259:TYR:O	13:M:263:MET:HE2	2.06	0.54
7:G:41:CYS:O	7:G:161:ARG:NH2	2.37	0.54
9:I:105:ARG:NH2	18:R:86:TYR:O	2.37	0.54
3:C:204:GLU:OE1	3:C:210:ARG:NH2	2.38	0.54
12:L:375:VAL:HG22	35:j:32:MET:SD	2.47	0.54
16:P:253:PHE:C	16:P:254:LEU:HD22	2.32	0.54
3:C:112:ASP:OD1	3:C:115:THR:OG1	2.22	0.54
7:G:239:VAL:HG23	7:G:253:ARG:HB2	1.89	0.54
14:N:269:GLU:O	14:N:273:ASN:ND2	2.40	0.54
1:A:18:VAL:HG22	8:H:222:LEU:CD2	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:193:LEU:HD11	12:L:206:PRO:CG	2.38	0.54
12:L:466:TYR:O	12:L:470:ASN:ND2	2.40	0.54
12:L:87:MET:HA	12:L:87:MET:HE2	1.89	0.53
4:D:88:GLU:OE2	4:D:430:ARG:NH1	2.41	0.53
20:U:22:TYR:CD2	20:U:50:ILE:HD11	2.44	0.53
40:o:23:THR:N	40:o:104:GLU:OE2	2.37	0.53
5:E:104:THR:HG22	5:E:104:THR:O	2.09	0.53
7:G:226:GLU:HG2	7:G:239:VAL:HG22	1.89	0.53
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.91	0.53
16:P:202:LYS:NZ	16:P:289:THR:O	2.41	0.53
40:o:43:GLN:NE2	40:o:47:ASP:OD1	2.41	0.53
45:L:703:3PE:H3I1	24:Y:123:LEU:HD12	1.91	0.53
24:Y:80:ARG:NH1	24:Y:88:ASN:OD1	2.41	0.53
7:G:259:ASN:HB3	7:G:390:LEU:HD13	1.90	0.53
10:J:124:ASP:N	10:J:124:ASP:OD1	2.41	0.53
20:U:74:GLN:NE2	20:U:78:ASP:OD1	2.41	0.53
4:D:107:ASP:OD2	4:D:110:SER:OG	2.22	0.53
15:O:303:LYS:O	29:d:50:ARG:NH1	2.41	0.53
7:G:693:GLU:OE1	7:G:693:GLU:N	2.41	0.53
12:L:65:ASN:O	34:i:84:TYR:OH	2.26	0.53
12:L:371:THR:O	12:L:375:VAL:HG23	2.09	0.53
15:O:125:GLU:N	15:O:125:GLU:OE1	2.42	0.53
15:O:130:SER:O	15:O:133:VAL:HG22	2.09	0.53
6:F:270:GLU:OE2	6:F:283:HIS:NE2	2.40	0.53
8:H:120:GLY:O	8:H:123:SER:OG	2.27	0.53
21:V:77:GLU:OE1	21:V:77:GLU:N	2.40	0.53
4:D:343:GLU:N	4:D:343:GLU:OE1	2.38	0.52
3:C:151:ILE:HG23	3:C:152:LEU:HG	1.92	0.52
8:H:285:LEU:HD12	8:H:285:LEU:C	2.35	0.52
15:O:30:ASN:OD1	15:O:31:ILE:N	2.38	0.52
8:H:200:LEU:HD23	8:H:285:LEU:HD21	1.92	0.52
13:M:113:MET:SD	13:M:175:ASN:ND2	2.82	0.52
13:M:366:ASN:OD1	13:M:407:SER:OG	2.26	0.52
25:Z:96:VAL:O	25:Z:96:VAL:HG12	2.08	0.52
44:s:71:GLU:OE1	44:s:71:GLU:N	2.37	0.52
34:i:28:SER:OG	39:n:116:ASP:OD2	2.21	0.52
16:P:315:ILE:HD13	16:P:315:ILE:O	2.10	0.52
4:D:165:THR:OG1	8:H:275:ALA:O	2.15	0.51
7:G:148:THR:C	7:G:149:ILE:HD12	2.35	0.51
7:G:422:LEU:O	7:G:428:ILE:HD13	2.10	0.51
26:a:67:GLU:N	26:a:67:GLU:OE1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:63:LEU:HD23	52:d:201:CDL:OA9	2.09	0.51
40:o:5:ALA:O	40:o:9:LEU:N	2.38	0.51
6:F:46:LYS:NZ	6:F:167:CYS:O	2.36	0.51
29:d:6:GLN:N	29:d:6:GLN:OE1	2.43	0.51
34:i:12:GLN:OE1	34:i:15:ARG:NH2	2.42	0.51
34:i:111:GLU:OE1	41:p:16:THR:N	2.41	0.51
34:i:125:GLN:O	34:i:127:HIS:N	2.43	0.51
15:O:65:ASP:OD1	15:O:66:GLY:N	2.43	0.51
6:F:361:GLN:N	48:F:502:SF4:S3	2.84	0.51
12:L:586:LEU:HD22	24:Y:41:ALA:O	2.10	0.51
42:q:65:THR:O	42:q:73:THR:OG1	2.29	0.51
6:F:268:VAL:HG21	6:F:283:HIS:ND1	2.26	0.51
6:F:365:CYS:O	6:F:369:VAL:HG22	2.11	0.51
20:U:11:ILE:O	20:U:15:VAL:HG23	2.11	0.51
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.20	0.50
35:j:64:LEU:HD12	40:o:106:ARG:NH1	2.25	0.50
37:l:39:ASP:OD1	38:m:80:ARG:NH1	2.43	0.50
14:N:324:THR:HG22	14:N:325:PHE:CD2	2.46	0.50
7:G:35:MET:SD	7:G:36:GLN:N	2.85	0.50
15:O:60:ASP:OD1	15:O:60:ASP:N	2.41	0.50
16:P:76:ARG:NH2	16:P:103:ASN:O	2.41	0.50
6:F:306:LEU:C	6:F:306:LEU:HD12	2.37	0.50
13:M:126:LEU:HD11	13:M:153:THR:HG21	1.94	0.50
20:T:55:GLU:OE2	22:W:36:ARG:NH2	2.44	0.50
32:g:66:PHE:HD1	32:g:70:LEU:HD12	1.77	0.50
13:M:255:ASP:OD1	13:M:256:PHE:N	2.45	0.50
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.47	0.50
7:G:347:GLU:OE2	7:G:495:ARG:NE	2.44	0.49
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.15	0.49
8:H:99:ASN:N	46:H:401:PC1:O12	2.44	0.49
10:J:101:PHE:O	10:J:105:TYR:N	2.41	0.49
3:C:183:VAL:O	22:W:100:THR:OG1	2.29	0.49
5:E:108:CYS:HA	5:E:151:ALA:HB1	1.94	0.49
12:L:193:LEU:HD11	12:L:206:PRO:HG3	1.93	0.49
38:m:1:SAC:OAC	38:m:2:PHE:N	2.45	0.49
12:L:556:ILE:HD12	38:m:79:PHE:CB	2.42	0.49
13:M:54:LEU:HD23	33:h:93:ILE:HG23	1.95	0.49
23:X:122:GLY:N	25:Z:65:GLU:OE2	2.43	0.49
12:L:264:TYR:N	12:L:265:PRO:CD	2.76	0.49
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.93	0.49
8:H:63:PRO:O	8:H:65:THR:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.94	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
29:d:94:ILE:HD13	33:h:106:LYS:HD3	1.95	0.49
18:R:9:GLU:OE2	18:R:33:LYS:NZ	2.46	0.48
4:D:184:VAL:O	9:I:60:ARG:NH1	2.41	0.48
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.95	0.48
2:B:30:VAL:HG22	2:B:173:LEU:HB3	1.95	0.48
6:F:224:ASN:OD1	6:F:225:VAL:N	2.46	0.48
12:L:120:TYR:HB3	12:L:154:LEU:HD21	1.96	0.48
12:L:562:LEU:CB	12:L:563:PRO:HD3	2.44	0.48
4:D:182:GLU:OE1	9:I:58:SER:OG	2.30	0.48
8:H:32:GLN:OE1	8:H:34:ARG:NH1	2.45	0.48
13:M:47:ASP:OD1	13:M:47:ASP:N	2.47	0.48
13:M:167:ILE:HD13	13:M:249:ILE:HD12	1.95	0.48
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.95	0.48
20:U:49:GLU:OE2	39:n:19:TYR:OH	2.32	0.48
25:Z:50:MET:HE1	45:b:101:3PE:H2	1.94	0.48
31:f:9:ASP:O	31:f:10:HIS:ND1	2.42	0.48
7:G:329:ILE:HD11	7:G:626:VAL:HG21	1.96	0.48
13:M:109:THR:HG21	13:M:238:LEU:HD22	1.96	0.48
20:U:22:TYR:CE2	20:U:50:ILE:HD11	2.49	0.48
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.43	0.48
25:Z:126:LEU:N	25:Z:126:LEU:HD23	2.29	0.48
5:E:105:THR:HG22	5:E:106:THR:H	1.79	0.47
12:L:227:PHE:N	12:L:284:THR:OG1	2.47	0.47
16:P:142:SER:O	16:P:147:ARG:NH1	2.47	0.47
12:L:64:SER:O	34:i:95:THR:HG23	2.14	0.47
12:L:562:LEU:HB2	12:L:563:PRO:HD3	1.96	0.47
25:Z:126:LEU:HD23	25:Z:126:LEU:H	1.79	0.47
34:i:84:TYR:O	34:i:89:VAL:HG23	2.15	0.47
8:H:262:LYS:NZ	46:H:402:PC1:O12	2.43	0.47
7:G:259:ASN:CB	7:G:390:LEU:HD13	2.44	0.47
11:K:62:ILE:HG21	14:N:31:ILE:HD11	1.96	0.47
42:q:6:VAL:HG22	42:q:9:ARG:NH2	2.29	0.47
44:s:72:SER:OG	44:s:75:HIS:ND1	2.34	0.47
2:B:152:THR:HG22	4:D:188:ARG:HD3	1.96	0.47
7:G:228:ILE:HG22	7:G:229:ASP:N	2.29	0.47
46:I:205:PC1:O13	46:I:205:PC1:H132	2.14	0.47
12:L:119:LYS:NZ	52:L:701:CDL:OA4	2.44	0.47
1:A:29:VAL:O	1:A:29:VAL:HG22	2.14	0.47
3:C:126:ALA:HB2	4:D:253:TYR:C	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:MET:SD	4:D:111:MET:N	2.83	0.47
4:D:291:GLY:O	4:D:296:ARG:NH1	2.48	0.47
5:E:150:ASN:OD1	5:E:150:ASN:N	2.47	0.47
8:H:202:GLU:N	8:H:202:GLU:OE1	2.48	0.47
14:N:343:LEU:C	14:N:343:LEU:HD12	2.40	0.47
58:i:201:CHD:H112	58:i:201:CHD:H12A	1.74	0.47
38:m:55:ARG:NH1	38:m:57:GLY:O	2.48	0.47
7:G:460:ARG:NH2	7:G:462:ASP:OD2	2.48	0.47
10:J:123:GLY:O	10:J:126:VAL:HG22	2.15	0.47
15:O:80:GLU:OE1	15:O:80:GLU:N	2.42	0.47
20:U:45:LEU:HD12	39:n:16:LEU:CD2	2.45	0.47
3:C:14:ARG:NH1	4:D:127:ASN:OD1	2.47	0.47
7:G:418:ARG:NH1	44:s:74:ARG:O	2.48	0.47
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.47
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.49	0.47
29:d:10:THR:OG1	30:e:7:LYS:NZ	2.47	0.47
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.96	0.47
23:X:48:GLU:OE1	27:b:57:ARG:NH2	2.48	0.47
27:b:42:LEU:HD22	27:b:46:ARG:NH1	2.31	0.46
43:r:45:SER:O	43:r:51:ASN:ND2	2.48	0.46
7:G:460:ARG:NE	7:G:462:ASP:OD1	2.43	0.46
6:F:358:SER:OG	6:F:365:CYS:SG	2.54	0.46
14:N:261:MET:HG3	14:N:340:THR:HG23	1.97	0.46
19:S:75:ASN:N	19:S:75:ASN:OD1	2.46	0.46
25:Z:50:MET:HE1	45:b:101:3PE:C2	2.46	0.46
14:N:43:ILE:O	14:N:126:SER:OG	2.25	0.46
16:P:26:ALA:HB3	16:P:47:VAL:HG13	1.97	0.46
40:o:11:ASP:OD2	40:o:14:VAL:HG22	2.15	0.46
40:o:82:GLU:OE1	40:o:82:GLU:N	2.42	0.46
41:p:32:LEU:O	41:p:36:PHE:N	2.42	0.46
1:A:68:GLU:CB	1:A:98:LEU:HD13	2.46	0.46
12:L:120:TYR:CB	12:L:154:LEU:HD21	2.45	0.46
16:P:299:GLY:N	16:P:302:ASP:OD2	2.49	0.46
7:G:514:ILE:HG21	7:G:532:ILE:HD13	1.97	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.46
13:M:6:ILE:HD12	31:f:23:GLY:HA2	1.96	0.46
20:U:46:ASP:OD1	39:n:44:ARG:NH1	2.48	0.46
22:W:23:ASP:N	22:W:23:ASP:OD1	2.47	0.46
6:F:58:GLY:O	6:F:62:THR:HG22	2.16	0.46
10:J:110:ASP:OD1	10:J:110:ASP:N	2.48	0.46
13:M:216:LEU:HB3	13:M:217:PRO:HD3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:378:ARG:NE	7:G:132:GLU:OE2	2.43	0.46
7:G:201:ASP:OD2	7:G:268:ARG:NH2	2.46	0.46
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.51	0.46
33:h:109:GLU:OE2	33:h:112:ARG:NH2	2.44	0.46
6:F:302:SER:CB	6:F:350:LEU:HD22	2.46	0.45
6:F:220:THR:HG22	6:F:221:THR:N	2.31	0.45
12:L:140:LEU:O	12:L:140:LEU:HD23	2.16	0.45
13:M:216:LEU:HD23	13:M:216:LEU:C	2.41	0.45
33:h:114:MET:HE2	33:h:121:PRO:HD2	1.98	0.45
58:i:201:CHD:O7	58:i:201:CHD:H41	2.16	0.45
37:l:32:GLU:N	37:l:32:GLU:OE1	2.47	0.45
16:P:289:THR:HG22	16:P:290:THR:N	2.30	0.45
18:R:23:TYR:O	18:R:26:VAL:HG12	2.16	0.45
3:C:86:ARG:NH2	21:V:112:LYS:O	2.46	0.45
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.51	0.45
13:M:130:LEU:HD21	14:N:294:MET:HE2	1.99	0.45
16:P:201:VAL:HG11	16:P:235:ARG:HE	1.81	0.45
20:U:46:ASP:OD1	39:n:44:ARG:NH2	2.49	0.45
9:I:76:ARG:NH1	9:I:128:VAL:O	2.45	0.45
7:G:306:MET:HE2	7:G:306:MET:HA	1.97	0.45
7:G:661:LEU:HD12	7:G:661:LEU:H	1.80	0.45
4:D:49:LEU:CD1	4:D:68:LEU:HD13	2.46	0.45
14:N:203:LEU:HD22	14:N:343:LEU:HD22	1.97	0.45
56:P:501:NDP:O2N	56:P:501:NDP:N7N	2.50	0.45
24:Y:28:GLY:O	24:Y:62:ALA:HB1	2.17	0.45
5:E:105:THR:HG22	5:E:106:THR:N	2.32	0.45
10:J:7:PHE:HB2	11:K:3:MET:HE3	1.98	0.45
24:Y:81:GLU:OE1	24:Y:81:GLU:N	2.50	0.45
30:e:64:GLU:O	30:e:68:ARG:N	2.46	0.45
58:i:201:CHD:H213	58:i:201:CHD:H231	1.75	0.45
41:p:27:ASN:OD1	41:p:30:THR:N	2.41	0.45
19:S:57:CYS:O	19:S:60:VAL:HG22	2.16	0.45
36:k:11:SER:OG	36:k:12:LYS:N	2.41	0.45
10:J:92:ALA:HB1	45:K:101:3PE:H352	1.98	0.45
14:N:152:ASN:O	14:N:156:THR:OG1	2.23	0.45
7:G:366:THR:C	7:G:367:THR:HG1	2.12	0.44
32:g:96:LEU:HD12	41:p:97:VAL:HG11	1.99	0.44
8:H:106:LEU:HD11	8:H:150:LEU:HD23	1.99	0.44
13:M:3:LYS:NZ	31:f:27:ASP:OD2	2.47	0.44
19:S:57:CYS:HB3	19:S:60:VAL:HG11	1.99	0.44
3:C:7:THR:OG1	3:C:8:ARG:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:407:LEU:HD23	6:F:407:LEU:C	2.43	0.44
3:C:79:THR:OG1	3:C:80:ALA:N	2.50	0.44
3:C:109:THR:OG1	3:C:110:TYR:N	2.50	0.44
5:E:55:GLN:O	5:E:59:GLY:N	2.39	0.44
20:T:55:GLU:O	20:T:59:GLY:N	2.49	0.44
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	2.00	0.44
58:i:201:CHD:O3	58:i:201:CHD:H9	2.16	0.44
15:O:204:ASN:O	15:O:208:GLY:N	2.41	0.44
34:i:55:LEU:HD13	34:i:55:LEU:C	2.42	0.44
7:G:185:THR:O	7:G:187:ILE:N	2.49	0.44
12:L:234:PRO:O	12:L:300:LYS:NZ	2.50	0.44
13:M:388:TRP:O	38:m:111:LYS:NZ	2.50	0.44
16:P:166:ILE:HG22	16:P:168:PRO:HD3	1.99	0.44
2:B:84:ASP:OD1	2:B:84:ASP:N	2.49	0.44
6:F:403:THR:HB	48:F:502:SF4:S1	2.58	0.44
12:L:194:ASN:ND2	12:L:194:ASN:O	2.51	0.44
6:F:89:ARG:NH1	6:F:217:GLY:O	2.46	0.44
15:O:138:MET:CE	54:O:401:DGT:HN2	2.31	0.44
29:d:120:ARG:NH1	38:m:112:GLU:OE2	2.49	0.44
37:l:158:ILE:HG21	40:o:99:LYS:HE2	1.98	0.44
6:F:165:ASN:OD1	6:F:170:GLY:N	2.42	0.44
6:F:327:THR:OG1	6:F:328:GLY:N	2.49	0.44
7:G:236:SER:OG	7:G:390:LEU:HD12	2.17	0.44
12:L:203:MET:HE3	12:L:203:MET:O	2.17	0.44
13:M:88:ASN:OD1	13:M:89:LEU:N	2.50	0.44
15:O:214:MET:O	15:O:218:CYS:N	2.51	0.44
23:X:102:GLN:OE1	23:X:102:GLN:N	2.51	0.44
10:J:141:MET:SD	30:e:26:HIS:NE2	2.91	0.43
29:d:13:PHE:N	46:d:203:PC1:O22	2.50	0.43
4:D:346:ILE:HG23	7:G:117:GLN:HG2	1.99	0.43
10:J:35:VAL:O	10:J:39:VAL:HG23	2.18	0.43
14:N:238:PRO:O	14:N:241:THR:OG1	2.33	0.43
15:O:95:ARG:NH1	15:O:281:GLU:O	2.49	0.43
21:V:8:THR:OG1	21:V:13:LEU:O	2.30	0.43
7:G:149:ILE:HD12	7:G:149:ILE:N	2.33	0.43
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.99	0.43
12:L:286:LEU:C	12:L:286:LEU:HD13	2.44	0.43
15:O:29:GLY:O	15:O:126:ARG:NH2	2.46	0.43
24:Y:43:LYS:O	24:Y:54:ARG:NH1	2.48	0.43
41:p:81:VAL:O	41:p:85:PHE:N	2.47	0.43
7:G:365:ASN:ND2	7:G:490:MET:O	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:55:MET:HE2	10:J:55:MET:HA	2.00	0.43
13:M:254:THR:HG22	13:M:254:THR:O	2.18	0.43
24:Y:79:VAL:HG23	24:Y:80:ARG:HG3	2.00	0.43
5:E:129:GLY:N	5:E:139:LEU:O	2.43	0.43
7:G:321:GLY:HA2	7:G:496:ILE:HG23	2.00	0.43
12:L:398:ALA:O	12:L:402:SER:OG	2.27	0.43
12:L:514:HIS:O	12:L:514:HIS:ND1	2.52	0.43
15:O:194:ILE:HG21	15:O:199:LEU:HD21	2.01	0.43
18:R:34:GLU:O	42:q:127:TYR:OH	2.21	0.43
27:b:37:TYR:OH	45:b:101:3PE:O14	2.26	0.43
5:E:217:LEU:HD13	5:E:217:LEU:O	2.18	0.43
29:d:120:ARG:HD3	38:m:115:ILE:HD13	2.00	0.43
31:f:4:LEU:O	31:f:5:GLN:HB2	2.19	0.43
5:E:18:GLU:N	5:E:18:GLU:OE1	2.51	0.43
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.49	0.43
7:G:589:PRO:HB2	7:G:593:ALA:HB3	2.01	0.43
12:L:230:HIS:N	12:L:231:PRO:HD3	2.33	0.43
12:L:526:LEU:HD12	12:L:530:PRO:HG2	1.99	0.43
16:P:116:ALA:O	16:P:120:VAL:HG23	2.18	0.43
12:L:458:LEU:HD23	12:L:458:LEU:O	2.18	0.43
7:G:372:GLU:OE2	7:G:394:ARG:NH1	2.46	0.43
13:M:11:LEU:HD11	13:M:34:ILE:HD12	1.99	0.43
20:T:76:ILE:HG22	20:T:80:ILE:HD12	2.00	0.43
57:T:101:EHZ:O2	22:W:69:ASN:ND2	2.49	0.43
13:M:165:ILE:HG21	14:N:268:GLN:HA	2.01	0.43
7:G:535:GLN:OE1	7:G:535:GLN:N	2.49	0.42
8:H:249:PRO:O	26:a:28:ARG:NH2	2.52	0.42
10:J:110:ASP:O	30:e:80:ARG:NH2	2.52	0.42
12:L:556:ILE:HD11	38:m:75:ILE:HG22	2.00	0.42
16:P:132:ILE:HG21	56:P:501:NDP:O4D	2.19	0.42
21:V:97:LYS:N	21:V:98:PRO:HD3	2.34	0.42
32:g:101:GLU:OE2	41:p:108:ARG:NH1	2.49	0.42
37:l:99:ASN:OD1	45:m:202:3PE:N	2.52	0.42
1:A:29:VAL:O	46:A:203:PC1:H141	2.19	0.42
1:A:51:PHE:CZ	11:K:79:VAL:HG13	2.53	0.42
5:E:199:LEU:HD12	5:E:199:LEU:N	2.34	0.42
7:G:426:PRO:HB3	7:G:661:LEU:HD11	2.00	0.42
10:J:136:PHE:CE1	30:e:28:ILE:HD11	2.54	0.42
12:L:465:GLY:O	12:L:469:SER:OG	2.10	0.42
20:T:22:TYR:O	20:T:23:ASP:C	2.62	0.42
37:l:88:ARG:O	37:l:89:VAL:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:MET:SD	8:H:233:MET:HE2	2.60	0.42
8:H:200:LEU:CD2	8:H:285:LEU:HD21	2.49	0.42
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.85	0.42
52:M:602:CDL:H401	52:X:201:CDL:H673	2.01	0.42
26:a:2:TRP:NE1	52:q:201:CDL:OB4	2.42	0.42
31:f:53:GLU:N	31:f:53:GLU:OE1	2.53	0.42
32:g:120:LEU:HD21	41:p:162:MET:HE3	2.01	0.42
1:A:27:LEU:HD21	46:A:203:PC1:H342	2.00	0.42
2:B:112:TYR:OH	2:B:170:GLU:OE2	2.33	0.42
4:D:284:ASP:OD2	43:r:106:SER:OG	2.14	0.42
6:F:103:GLY:O	6:F:333:ALA:HB1	2.19	0.42
6:F:106:LYS:NZ	6:F:226:GLU:OE1	2.51	0.42
12:L:97:THR:HG21	12:L:125:LEU:HD22	2.00	0.42
1:A:27:LEU:HD21	46:A:203:PC1:C34	2.50	0.42
14:N:146:PHE:N	14:N:147:PRO:CD	2.83	0.42
15:O:223:TYR:CE2	15:O:234:VAL:HG22	2.55	0.42
7:G:243:ARG:O	7:G:244:THR:OG1	2.34	0.42
12:L:13:LEU:HD22	34:i:81:ILE:HD11	2.02	0.42
7:G:490:MET:HE3	7:G:492:ILE:HD11	2.02	0.42
11:K:1:FME:HE1	11:K:9:MET:HE1	2.01	0.42
52:M:602:CDL:H272	52:X:201:CDL:H671	2.02	0.42
23:X:25:LYS:NZ	23:X:94:GLN:O	2.29	0.42
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.20	0.41
18:R:4:THR:HG22	18:R:5:SER:O	2.19	0.41
7:G:26:VAL:HG13	7:G:79:ILE:HD13	2.01	0.41
7:G:39:ARG:HB2	49:G:803:FES:S1	2.60	0.41
7:G:262:TRP:O	7:G:263:ILE:HG23	2.20	0.41
10:J:5:ILE:HG23	10:J:6:VAL:N	2.36	0.41
13:M:66:LEU:HD11	13:M:111:THR:HG23	2.01	0.41
34:i:90:THR:CG2	34:i:96:ILE:HD12	2.47	0.41
6:F:93:LEU:HD13	6:F:129:MET:SD	2.59	0.41
8:H:111:LEU:HD11	10:J:57:PHE:CD2	2.54	0.41
40:o:11:ASP:OD2	40:o:14:VAL:HG13	2.21	0.41
5:E:217:LEU:HD13	5:E:217:LEU:C	2.45	0.41
8:H:20:LEU:HD22	8:H:232:ILE:HD11	2.03	0.41
11:K:66:PHE:CZ	14:N:31:ILE:HG23	2.55	0.41
12:L:106:TRP:CD1	35:j:1:ALA:H3	2.38	0.41
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.85	0.41
3:C:32:ILE:HG21	3:C:63:PHE:CE1	2.56	0.41
4:D:151:ILE:O	4:D:155:THR:OG1	2.32	0.41
14:N:340:THR:N	14:N:341:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:64:LEU:HD22	19:S:90:LEU:HD22	2.02	0.41
29:d:109:TYR:HA	29:d:112:VAL:HG22	2.01	0.41
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.02	0.41
37:l:141:GLU:OE1	37:l:141:GLU:N	2.50	0.41
7:G:424:ASP:OD1	7:G:424:ASP:N	2.53	0.41
7:G:661:LEU:HD12	7:G:661:LEU:N	2.36	0.41
13:M:108:MET:CB	13:M:121:LEU:HD13	2.51	0.41
15:O:94:TYR:HH	15:O:151:HIS:CE1	2.33	0.41
33:h:52:LEU:C	33:h:52:LEU:HD13	2.45	0.41
34:i:85:LEU:HD22	34:i:96:ILE:HD11	2.02	0.41
4:D:148:LEU:O	4:D:174:ARG:NH1	2.53	0.41
6:F:154:ARG:HB2	44:s:58:LEU:HD21	2.02	0.41
36:k:26:THR:O	36:k:29:GLU:N	2.48	0.41
39:n:8:TYR:C	39:n:9:LEU:HD12	2.46	0.41
44:s:52:LEU:N	44:s:52:LEU:HD12	2.35	0.41
6:F:311:VAL:HG12	6:F:311:VAL:O	2.19	0.41
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.03	0.41
20:T:61:GLU:OE1	20:T:61:GLU:N	2.52	0.41
37:l:80:ASP:HB3	37:l:83:MET:HE2	2.03	0.41
41:p:123:ASN:OD1	41:p:123:ASN:N	2.53	0.41
44:s:45:ASP:OD1	44:s:45:ASP:N	2.53	0.41
3:C:121:VAL:N	3:C:122:PRO:CD	2.84	0.41
7:G:665:GLN:NE2	7:G:670:ASP:O	2.46	0.41
8:H:84:THR:O	8:H:84:THR:HG22	2.21	0.41
12:L:193:LEU:HD11	12:L:206:PRO:HG2	2.03	0.41
12:L:417:SER:OG	12:L:493:VAL:HG13	2.20	0.41
12:L:577:VAL:HG22	12:L:577:VAL:O	2.20	0.41
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.51	0.41
14:N:20:VAL:HG13	14:N:29:VAL:HG13	2.03	0.41
14:N:298:TYR:O	14:N:303:THR:OG1	2.23	0.41
14:N:343:LEU:HD12	14:N:344:SER:N	2.36	0.41
40:o:11:ASP:HB3	40:o:14:VAL:HG22	2.03	0.41
42:q:6:VAL:HG11	52:q:201:CDL:HB62	2.02	0.41
8:H:74:ALA:HB3	8:H:75:PRO:HD3	2.03	0.41
13:M:118:PHE:O	13:M:122:PHE:HB3	2.20	0.41
34:i:35:PRO:O	34:i:37:GLN:NE2	2.54	0.41
38:m:120:LEU:HD23	38:m:121:ASP:N	2.35	0.41
15:O:223:TYR:HE2	15:O:234:VAL:HG13	1.86	0.40
16:P:50:ARG:NH2	56:P:501:NDP:O2X	2.48	0.40
16:P:133:SER:O	16:P:168:PRO:HD2	2.21	0.40
20:T:7:THR:OG1	20:T:10:GLY:N	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:32:VAL:HG22	20:T:32:VAL:O	2.21	0.40
21:V:37:ILE:HG23	21:V:38:PRO:HD2	2.03	0.40
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.02	0.40
12:L:131:LEU:HD23	12:L:131:LEU:C	2.47	0.40
12:L:556:ILE:HD12	38:m:79:PHE:HB2	2.02	0.40
45:L:703:3PE:H3I1	24:Y:123:LEU:CD1	2.52	0.40
14:N:6:PHE:CE2	14:N:10:LEU:HD11	2.56	0.40
16:P:133:SER:OG	16:P:134:HIS:N	2.53	0.40
25:Z:28:GLY:N	45:Z:201:3PE:O14	2.53	0.40
38:m:23:ASP:N	38:m:23:ASP:OD1	2.54	0.40
4:D:77:ASP:OD2	4:D:79:HIS:NE2	2.55	0.40
13:M:285:LEU:HD23	13:M:285:LEU:C	2.45	0.40
29:d:9:ALA:HB1	29:d:12:GLN:CD	2.46	0.40
38:m:120:LEU:HD23	38:m:120:LEU:C	2.46	0.40
1:A:78:ALA:O	1:A:81:THR:HG22	2.21	0.40
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.04	0.40
13:M:373:ILE:HD11	13:M:444:LEU:HD12	2.03	0.40
21:V:3:LEU:H	21:V:3:LEU:HD23	1.86	0.40
4:D:100:LEU:HB3	4:D:101:PRO:HD3	2.03	0.40
8:H:172:MET:SD	8:H:176:LEU:HD23	2.62	0.40
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.04	0.40
14:N:215:MET:HE3	14:N:218:MET:HE3	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	98/115 (85%)	94 (96%)	4 (4%)	0	100	100
2	B	154/216 (71%)	147 (96%)	7 (4%)	0	100	100
3	C	205/266 (77%)	199 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	411/463 (89%)	399 (97%)	12 (3%)	0	100	100
5	E	212/249 (85%)	204 (96%)	8 (4%)	0	100	100
6	F	430/464 (93%)	412 (96%)	18 (4%)	0	100	100
7	G	689/727 (95%)	658 (96%)	31 (4%)	0	100	100
8	H	311/318 (98%)	299 (96%)	12 (4%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	164/175 (94%)	155 (94%)	9 (6%)	0	100	100
11	K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	41
12	L	604/606 (100%)	579 (96%)	24 (4%)	1 (0%)	43	73
13	M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
15	O	318/343 (93%)	309 (97%)	9 (3%)	0	100	100
16	P	330/380 (87%)	310 (94%)	20 (6%)	0	100	100
17	Q	127/175 (73%)	123 (97%)	4 (3%)	0	100	100
18	R	94/124 (76%)	88 (94%)	6 (6%)	0	100	100
19	S	84/99 (85%)	80 (95%)	4 (5%)	0	100	100
20	T	86/156 (55%)	81 (94%)	4 (5%)	1 (1%)	10	37
20	U	86/156 (55%)	81 (94%)	5 (6%)	0	100	100
21	V	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
22	W	114/128 (89%)	108 (95%)	5 (4%)	1 (1%)	14	44
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	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%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
30	e	96/106 (91%)	93 (97%)	3 (3%)	0	100	100
31	f	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
32	g	99/154 (64%)	92 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	68 (99%)	1 (1%)	0	100	100
36	k	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
37	l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	m	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
39	n	169/179 (94%)	164 (97%)	4 (2%)	1 (1%)	21	52
40	o	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
41	p	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	r	91/113 (80%)	86 (94%)	5 (6%)	0	100	100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8138/9213 (88%)	7844 (96%)	289 (4%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	T	23	ASP
11	K	2	SER
12	L	562	LEU
22	W	95	VAL
39	n	31	ILE

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	90/100 (90%)	87 (97%)	3 (3%)	33	63
2	B	132/175 (75%)	130 (98%)	2 (2%)	57	75
3	C	188/228 (82%)	186 (99%)	2 (1%)	65	78
4	D	361/392 (92%)	358 (99%)	3 (1%)	73	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	183/205 (89%)	179 (98%)	4 (2%)	45	71
6	F	346/368 (94%)	334 (96%)	12 (4%)	32	62
7	G	579/608 (95%)	561 (97%)	18 (3%)	35	64
8	H	271/274 (99%)	265 (98%)	6 (2%)	45	71
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	77
10	J	134/141 (95%)	127 (95%)	7 (5%)	21	51
11	K	85/85 (100%)	82 (96%)	3 (4%)	32	62
12	L	533/533 (100%)	526 (99%)	7 (1%)	61	77
13	M	412/412 (100%)	409 (99%)	3 (1%)	76	82
14	N	315/315 (100%)	308 (98%)	7 (2%)	45	71
15	O	283/303 (93%)	274 (97%)	9 (3%)	34	64
16	P	288/327 (88%)	276 (96%)	12 (4%)	26	58
17	Q	116/153 (76%)	108 (93%)	8 (7%)	14	41
18	R	79/97 (81%)	79 (100%)	0	100	100
19	S	76/82 (93%)	71 (93%)	5 (7%)	15	43
20	T	81/135 (60%)	72 (89%)	9 (11%)	6	24
20	U	81/135 (60%)	78 (96%)	3 (4%)	30	61
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	79
22	W	108/114 (95%)	105 (97%)	3 (3%)	38	66
23	X	154/155 (99%)	150 (97%)	4 (3%)	40	68
24	Y	101/102 (99%)	98 (97%)	3 (3%)	36	65
25	Z	120/121 (99%)	113 (94%)	7 (6%)	18	48
26	a	59/59 (100%)	57 (97%)	2 (3%)	32	63
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	44 (98%)	1 (2%)	45	71
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	66
30	e	89/96 (93%)	89 (100%)	0	100	100
31	f	54/54 (100%)	51 (94%)	3 (6%)	19	49
32	g	92/131 (70%)	87 (95%)	5 (5%)	20	50
33	h	121/158 (77%)	119 (98%)	2 (2%)	53	74
34	i	120/121 (99%)	116 (97%)	4 (3%)	33	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	j	61/84 (73%)	59 (97%)	2 (3%)	33	63
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	75
37	l	140/159 (88%)	135 (96%)	5 (4%)	31	62
38	m	113/114 (99%)	110 (97%)	3 (3%)	39	67
39	n	156/161 (97%)	152 (97%)	4 (3%)	40	68
40	o	110/120 (92%)	105 (96%)	5 (4%)	24	56
41	p	155/157 (99%)	152 (98%)	3 (2%)	50	73
42	q	130/130 (100%)	128 (98%)	2 (2%)	57	75
43	r	85/97 (88%)	80 (94%)	5 (6%)	18	48
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7180/7891 (91%)	6987 (97%)	193 (3%)	40	67

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	90	MET
1	A	97	LEU
2	B	54	CYS
2	B	84	ASP
3	C	74	SER
3	C	125	LYS
4	D	40	LYS
4	D	75	LYS
4	D	216	LYS
5	E	68	LYS
5	E	71	GLU
5	E	150	ASN
5	E	183	LYS
6	F	8	LYS
6	F	34	LYS
6	F	44	LYS
6	F	46	LYS
6	F	78	LYS
6	F	132	ARG
6	F	206	LYS
6	F	249	ARG
6	F	282	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	359	CYS
6	F	365	CYS
6	F	432	GLN
7	G	75	LYS
7	G	232	ASP
7	G	306	MET
7	G	324	ASP
7	G	356	THR
7	G	364	LEU
7	G	405	LYS
7	G	455	SER
7	G	476	LYS
7	G	484	THR
7	G	495	ARG
7	G	499	GLN
7	G	532	ILE
7	G	536	ASP
7	G	601	ARG
7	G	650	LYS
7	G	667	THR
7	G	689	LYS
8	H	5	ASN
8	H	70	MET
8	H	73	LEU
8	H	121	TRP
8	H	214	GLU
8	H	254	LEU
9	I	14	MET
9	I	78	ILE
10	J	23	LYS
10	J	87	LYS
10	J	103	MET
10	J	109	LYS
10	J	110	ASP
10	J	111	LYS
10	J	124	ASP
11	K	34	GLU
11	K	43	MET
11	K	73	LEU
12	L	223	LYS
12	L	336	LYS
12	L	364	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	487	LYS
12	L	512	LYS
12	L	580	GLN
12	L	581	LYS
13	M	91	ARG
13	M	201	MET
13	M	207	MET
14	N	37	MET
14	N	46	LYS
14	N	71	MET
14	N	85	THR
14	N	187	MET
14	N	204	ASN
14	N	263	LYS
15	O	1	LEU
15	O	40	LYS
15	O	60	ASP
15	O	125	GLU
15	O	157	LYS
15	O	217	LYS
15	O	245	LYS
15	O	250	ASP
15	O	315	LYS
16	P	78	LYS
16	P	122	LYS
16	P	140	LYS
16	P	144	LYS
16	P	154	LYS
16	P	170	GLU
16	P	263	TYR
16	P	264	ARG
16	P	268	ARG
16	P	281	ARG
16	P	285	GLU
16	P	315	ILE
17	Q	16	LYS
17	Q	31	LYS
17	Q	34	LYS
17	Q	44	ASN
17	Q	91	ASP
17	Q	112	LYS
17	Q	123	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	127	ARG
19	S	24	GLN
19	S	25	ARG
19	S	38	LYS
19	S	44	LYS
19	S	76	VAL
20	T	12	LYS
20	T	16	LEU
20	T	24	LYS
20	T	25	ILE
20	T	69	LYS
20	T	71	MET
20	T	72	CYS
20	T	83	LYS
20	T	86	VAL
20	U	20	LYS
20	U	71	MET
20	U	83	LYS
21	V	65	LYS
22	W	56	LYS
22	W	68	LYS
22	W	69	ASN
23	X	5	GLU
23	X	13	LYS
23	X	87	CYS
23	X	101	LYS
24	Y	90	LEU
24	Y	114	CYS
24	Y	119	LEU
25	Z	4	LYS
25	Z	51	LYS
25	Z	98	LYS
25	Z	120	MET
25	Z	130	GLU
25	Z	133	LEU
25	Z	143	THR
26	a	25	ARG
26	a	34	LYS
28	c	23	THR
29	d	77	LYS
29	d	104	LYS
29	d	112	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	f	3	LEU
31	f	18	MET
31	f	45	LYS
32	g	24	LEU
32	g	25	ARG
32	g	57	ASN
32	g	100	ARG
32	g	117	LYS
33	h	130	LYS
33	h	138	LYS
34	i	58	ASN
34	i	98	GLU
34	i	100	LYS
34	i	126	HIS
35	j	10	ARG
35	j	39	ARG
36	k	91	LYS
37	l	6	LYS
37	l	126	GLN
37	l	135	TYR
37	l	148	LYS
37	l	154	VAL
38	m	23	ASP
38	m	84	LYS
38	m	105	LYS
39	n	8	TYR
39	n	54	LYS
39	n	120	LYS
39	n	126	LYS
40	o	27	ASP
40	o	35	GLU
40	o	83	ARG
40	o	110	ARG
40	o	112	LYS
41	p	69	ARG
41	p	116	GLU
41	p	121	ARG
42	q	53	LYS
42	q	107	LYS
43	r	29	GLU
43	r	72	GLN
43	r	101	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	r	105	LEU
43	r	107	GLN

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

Mol	Chain	Res	Type
1	A	83	ASN
2	B	94	ASN
3	C	88	ASN
3	C	160	HIS
4	D	157	HIS
4	D	190	HIS
4	D	200	HIS
4	D	201	GLN
4	D	316	ASN
5	E	121	GLN
5	E	155	GLN
6	F	257	ASN
6	F	324	GLN
6	F	356	HIS
6	F	435	GLN
7	G	402	ASN
7	G	546	GLN
7	G	581	GLN
8	H	47	GLN
11	K	83	ASN
12	L	135	ASN
12	L	194	ASN
12	L	199	GLN
12	L	205	ASN
12	L	348	HIS
13	M	30	HIS
13	M	293	HIS
13	M	331	ASN
14	N	48	HIS
14	N	63	GLN
14	N	274	ASN
16	P	8	HIS
16	P	321	HIS
17	Q	29	HIS
18	R	93	GLN
22	W	44	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	X	29	HIS
23	X	30	HIS
29	d	59	HIS
29	d	79	GLN
29	d	97	HIS
32	g	27	GLN
32	g	57	ASN
33	h	143	ASN
35	j	50	HIS
37	l	97	ASN
41	p	106	GLN
42	q	31	ASN
42	q	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	FME	N	1	14	8,9,10	1.52	1 (12%)	8,9,11	1.20	0
27	AYA	b	1	27	6,7,8	1.87	1 (16%)	6,8,10	1.19	1 (16%)
43	AYA	r	1	43	6,7,8	1.87	2 (33%)	6,8,10	1.32	1 (16%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	8,9,11	1.30	0
38	SAC	m	1	38	7,8,9	1.73	1 (14%)	7,9,11	1.27	1 (14%)
42	AME	q	1	42	9,10,11	1.53	1 (11%)	9,11,13	1.35	1 (11%)
24	AYA	Y	1	24	6,7,8	1.88	2 (33%)	6,8,10	1.15	1 (16%)
34	SAC	i	1	34	7,8,9	1.73	1 (14%)	7,9,11	1.47	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	FME	M	1	13	8,9,10	1.52	1 (12%)	8,9,11	1.36	0
1	FME	A	1	1	8,9,10	1.51	1 (12%)	8,9,11	1.44	2 (25%)
29	AME	d	1	29	9,10,11	1.51	2 (22%)	9,11,13	1.31	2 (22%)
4	2MR	D	85	4	10,12,13	2.42	2 (20%)	5,13,15	1.53	2 (40%)
8	FME	H	1	8	8,9,10	1.52	1 (12%)	8,9,11	1.39	1 (12%)
11	FME	K	1	11	8,9,10	1.52	1 (12%)	8,9,11	1.29	0
12	FME	L	1	12	8,9,10	1.50	1 (12%)	8,9,11	1.35	1 (12%)

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.38	1.44	1.33
4	D	85	2MR	CZ-NE	5.03	1.45	1.34
14	N	1	FME	CN-N	3.81	1.45	1.33
11	K	1	FME	CN-N	3.78	1.45	1.33
10	J	1	FME	CN-N	3.76	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	FME	CN-N	3.75	1.45	1.33
13	M	1	FME	CN-N	3.75	1.45	1.33
12	L	1	FME	CN-N	3.72	1.45	1.33
1	A	1	FME	CN-N	3.71	1.45	1.33
38	m	1	SAC	C1A-N	3.53	1.45	1.34
34	i	1	SAC	C1A-N	3.53	1.45	1.34
27	b	1	AYA	CT-N	3.52	1.45	1.34
24	Y	1	AYA	CT-N	3.47	1.45	1.34
42	q	1	AME	CT1-N	3.43	1.45	1.34
29	d	1	AME	CT1-N	3.41	1.45	1.34
43	r	1	AYA	CT-N	3.41	1.45	1.34
29	d	1	AME	OT-CT1	-2.03	1.18	1.23
24	Y	1	AYA	OT-CT	-2.01	1.18	1.23
43	r	1	AYA	OT-CT	-2.01	1.18	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	2.89	120.91	116.12
4	D	85	2MR	CD-NE-CZ	-2.46	118.74	123.36
29	d	1	AME	CT2-CT1-N	2.32	119.97	116.12
42	q	1	AME	CT2-CT1-N	2.28	119.91	116.12
43	r	1	AYA	CM-CT-N	2.25	119.84	116.12
38	m	1	SAC	C2A-C1A-N	2.20	119.77	116.12
8	H	1	FME	O1-CN-N	-2.12	119.84	125.32
4	D	85	2MR	CQ2-NH2-CZ	-2.11	119.11	123.65
1	A	1	FME	O1-CN-N	-2.11	119.88	125.32
1	A	1	FME	CA-N-CN	-2.07	119.63	122.82
27	b	1	AYA	CM-CT-N	2.07	119.56	116.12
12	L	1	FME	O1-CN-N	-2.06	120.00	125.32
29	d	1	AME	CE-SD-CG	2.02	110.75	100.32
24	Y	1	AYA	CM-CT-N	2.01	119.44	116.12

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
13	M	1	FME	O-C-CA-CB
14	N	1	FME	N-CA-CB-CG

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	1	AYA	1	0
38	m	1	SAC	1	0
29	d	1	AME	1	0
11	K	1	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 68 ligands modelled in this entry, 4 are monoatomic - leaving 64 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	M	604	-	44,44,50	0.93	4 (9%)	47,49,55	1.07	2 (4%)
47	PLC	M	607	-	33,33,41	0.57	0	39,41,49	0.52	0
47	PLC	B	202	-	41,41,41	0.51	0	47,49,49	0.52	0
49	FES	G	803	7	0,4,4	-	-	-		
47	PLC	Z	202	-	35,35,41	0.54	0	41,43,49	0.57	0
45	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.10	2 (4%)
45	3PE	N	402	-	43,43,50	0.94	4 (9%)	46,48,55	1.09	2 (4%)
52	CDL	i	202	-	79,79,99	0.99	8 (10%)	85,91,111	1.11	4 (4%)
47	PLC	L	706	-	30,30,41	0.59	0	36,38,49	0.57	0
46	PC1	M	606	-	34,34,53	1.17	4 (11%)	40,42,61	1.08	2 (5%)
52	CDL	q	201	-	60,60,99	1.12	8 (13%)	66,72,111	1.13	4 (6%)
45	3PE	Y	202	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
45	3PE	I	203	-	35,35,50	1.03	4 (11%)	38,40,55	1.14	2 (5%)
46	PC1	I	205	-	43,43,53	1.05	4 (9%)	49,51,61	1.00	2 (4%)
46	PC1	A	203	-	45,45,53	1.04	4 (8%)	51,53,61	1.07	2 (3%)
46	PC1	d	203	-	38,38,53	1.13	4 (10%)	44,46,61	1.09	2 (4%)
46	PC1	H	402	-	41,41,53	1.08	4 (9%)	47,49,61	1.10	2 (4%)
45	3PE	L	703	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
46	PC1	A	202	-	34,34,53	1.17	4 (11%)	40,42,61	1.07	2 (5%)
45	3PE	g	201	-	29,29,50	1.13	4 (13%)	32,34,55	1.28	2 (6%)
45	3PE	b	101	-	34,34,50	1.02	4 (11%)	37,39,55	1.15	2 (5%)
45	3PE	L	704	-	34,34,50	0.98	3 (8%)	37,39,55	1.10	1 (2%)
59	MYR	o	201	40	13,14,15	0.42	0	12,13,15	0.84	0
48	SF4	B	201	2	0,12,12	-	-	-		
52	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.11	4 (5%)
52	CDL	N	401	-	84,84,99	0.95	8 (9%)	90,96,111	1.10	4 (4%)
47	PLC	g	202	-	28,28,41	0.60	0	34,36,49	0.68	0
47	PLC	Y	206	-	31,31,41	0.57	0	37,39,49	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	M	605	-	43,43,53	1.05	4 (9%)	49,51,61	1.07	2 (4%)
54	DGT	O	401	55	32,33,33	3.32	14 (43%)	48,52,52	1.94	13 (27%)
52	CDL	M	602	-	99,99,99	0.89	8 (8%)	105,111,111	1.12	4 (3%)
46	PC1	q	203	-	33,33,53	1.18	4 (12%)	39,41,61	0.99	2 (5%)
46	PC1	m	203	-	53,53,53	0.94	4 (7%)	59,61,61	1.00	2 (3%)
52	CDL	X	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)
45	3PE	D	501	-	48,48,50	0.89	4 (8%)	51,53,55	1.03	2 (3%)
46	PC1	q	202	-	47,47,53	1.01	3 (6%)	53,55,61	1.00	2 (3%)
48	SF4	I	201	9	0,12,12	-	-	-	-	-
57	EHZ	U	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.71	9 (25%)
58	CHD	i	201	-	32,32,32	3.25	11 (34%)	51,51,51	2.46	18 (35%)
46	PC1	h	201	-	35,35,53	1.15	4 (11%)	41,43,61	1.10	2 (4%)
45	3PE	Y	205	-	36,36,50	1.02	4 (11%)	39,41,55	1.12	2 (5%)
48	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	Y	203	-	50,50,50	0.88	4 (8%)	53,55,55	1.03	2 (3%)
45	3PE	d	202	-	48,48,50	0.89	4 (8%)	51,53,55	1.08	2 (3%)
45	3PE	K	101	-	43,43,50	0.94	4 (9%)	46,48,55	1.11	2 (4%)
52	CDL	L	701	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
46	PC1	I	204	-	53,53,53	0.94	4 (7%)	59,61,61	1.05	2 (3%)
45	3PE	M	603	-	49,49,50	0.88	4 (8%)	52,54,55	1.05	2 (3%)
45	3PE	Y	204	-	46,46,50	0.90	4 (8%)	49,51,55	1.02	2 (4%)
46	PC1	L	705	-	53,53,53	0.95	4 (7%)	59,61,61	1.02	2 (3%)
45	3PE	Z	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.07	2 (4%)
45	3PE	m	202	-	40,40,50	0.97	4 (10%)	43,45,55	1.12	2 (4%)
47	PLC	A	204	-	41,41,41	0.52	0	47,49,49	0.54	0
45	3PE	A	201	-	46,46,50	0.91	4 (8%)	49,51,55	1.07	2 (4%)
57	EHZ	T	101	20	31,36,37	1.60	5 (16%)	36,44,47	1.68	8 (22%)
50	FMN	F	501	-	33,33,33	2.76	10 (30%)	48,50,50	1.76	13 (27%)
45	3PE	Y	201	-	26,26,50	1.18	4 (15%)	29,31,55	1.18	2 (6%)
48	SF4	G	802	7	0,12,12	-	-	-	-	-
48	SF4	I	202	9	0,12,12	-	-	-	-	-
46	PC1	H	401	-	47,47,53	1.02	4 (8%)	53,55,61	1.03	2 (3%)
56	NDP	P	501	-	51,52,52	3.98	27 (52%)	71,80,80	1.91	14 (19%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
45	3PE	L	702	-	44,44,50	0.92	4 (9%)	47,49,55	1.15	2 (4%)
48	SF4	F	502	6	0,12,12	-	-	-	-	-

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	M	604	-	-	29/48/48/54	-
47	PLC	M	607	-	-	8/37/37/45	-
47	PLC	B	202	-	-	18/45/45/45	-
49	FES	G	803	7	-	-	0/1/1/1
47	PLC	Z	202	-	-	16/39/39/45	-
45	3PE	m	201	-	-	23/44/44/54	-
45	3PE	N	402	-	-	19/47/47/54	-
52	CDL	i	202	-	-	29/90/90/110	-
47	PLC	L	706	-	-	10/34/34/45	-
46	PC1	M	606	-	-	11/38/38/57	-
52	CDL	q	201	-	-	36/71/71/110	-
45	3PE	Y	202	-	-	21/54/54/54	-
45	3PE	I	203	-	-	18/39/39/54	-
46	PC1	I	205	-	-	18/47/47/57	-
46	PC1	A	203	-	-	16/49/49/57	-
46	PC1	d	203	-	-	25/42/42/57	-
46	PC1	H	402	-	-	19/45/45/57	-
45	3PE	L	703	-	-	25/54/54/54	-
46	PC1	A	202	-	-	14/38/38/57	-
45	3PE	g	201	-	-	13/32/32/54	-
45	3PE	b	101	-	-	13/38/38/54	-
45	3PE	L	704	-	-	20/37/37/54	-
59	MYR	o	201	40	-	4/12/12/13	-
48	SF4	B	201	2	-	-	0/6/5/5
52	CDL	d	201	-	-	38/75/75/110	-
52	CDL	N	401	-	-	43/95/95/110	-
47	PLC	g	202	-	-	9/31/31/45	-
47	PLC	Y	206	-	-	9/34/34/45	-
46	PC1	M	605	-	-	23/47/47/57	-
54	DGT	O	401	55	-	5/22/34/34	0/3/3/3
52	CDL	M	602	-	-	43/110/110/110	-
46	PC1	q	203	-	-	13/37/37/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	m	203	-	-	24/57/57/57	-
52	CDL	X	201	-	-	51/110/110/110	-
45	3PE	D	501	-	-	26/52/52/54	-
46	PC1	q	202	-	-	22/51/51/57	-
58	CHD	i	201	-	-	4/9/74/74	0/4/4/4
57	EHZ	U	101	20	-	11/42/44/45	-
48	SF4	I	201	9	-	-	0/6/5/5
46	PC1	h	201	-	-	19/39/39/57	-
45	3PE	Y	205	-	-	11/40/40/54	-
48	SF4	G	801	7	-	-	0/6/5/5
45	3PE	Y	203	-	-	25/54/54/54	-
45	3PE	d	202	-	-	17/52/52/54	-
45	3PE	K	101	-	-	14/47/47/54	-
52	CDL	L	701	-	-	35/110/110/110	-
46	PC1	I	204	-	-	17/57/57/57	-
45	3PE	M	603	-	-	20/53/53/54	-
45	3PE	Y	204	-	-	23/50/50/54	-
46	PC1	L	705	-	-	24/57/57/57	-
45	3PE	Z	201	-	-	18/44/44/54	-
45	3PE	m	202	-	-	25/44/44/54	-
47	PLC	A	204	-	-	21/45/45/45	-
45	3PE	A	201	-	-	24/50/50/54	-
57	EHZ	T	101	20	-	14/42/44/45	-
50	FMN	F	501	-	-	9/18/18/18	0/3/3/3
45	3PE	Y	201	-	-	14/30/30/54	-
48	SF4	G	802	7	-	-	0/6/5/5
48	SF4	I	202	9	-	-	0/6/5/5
46	PC1	H	401	-	-	27/51/51/57	-
56	NDP	P	501	-	-	4/34/77/77	0/5/5/5
49	FES	E	301	5	-	-	0/1/1/1
45	3PE	L	702	-	-	18/48/48/54	-
48	SF4	F	502	6	-	-	0/6/5/5

All (266) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	PA-O3	10.08	1.70	1.59
56	P	501	NDP	C2B-C1B	-9.05	1.30	1.53
54	O	401	DGT	O6-C6	8.78	1.40	1.23
58	i	201	CHD	C11-C12	8.77	1.67	1.53
56	P	501	NDP	O4B-C1B	8.54	1.61	1.42
56	P	501	NDP	O4D-C1D	8.27	1.61	1.42
56	P	501	NDP	C7N-N7N	7.62	1.55	1.33
56	P	501	NDP	C2D-C1D	-7.20	1.30	1.53
58	i	201	CHD	C16-C15	7.10	1.73	1.54
56	P	501	NDP	C6N-C5N	7.06	1.54	1.33
54	O	401	DGT	C5-N7	6.75	1.52	1.39
56	P	501	NDP	O4D-C4D	-6.64	1.30	1.45
50	F	501	FMN	C10-N1	6.60	1.46	1.33
50	F	501	FMN	C4A-N5	6.51	1.44	1.30
58	i	201	CHD	C20-C17	-6.29	1.43	1.54
56	P	501	NDP	P2B-O2B	5.61	1.69	1.59
50	F	501	FMN	C5A-N5	5.56	1.49	1.39
58	i	201	CHD	C8-C9	5.38	1.64	1.53
56	P	501	NDP	C6A-N6A	5.38	1.47	1.34
58	i	201	CHD	O12-C12	-5.35	1.34	1.43
57	T	101	EHZ	C12-N1	5.29	1.45	1.33
58	i	201	CHD	C13-C17	5.27	1.64	1.55
56	P	501	NDP	O4B-C4B	-5.26	1.33	1.45
54	O	401	DGT	PB-O3A	5.18	1.65	1.59
54	O	401	DGT	PA-O3A	5.18	1.65	1.59
57	U	101	EHZ	C12-N1	5.12	1.45	1.33
54	O	401	DGT	PB-O3B	5.06	1.65	1.59
50	F	501	FMN	C2-N1	5.03	1.48	1.36
57	T	101	EHZ	C15-N2	4.95	1.45	1.33
50	F	501	FMN	C9A-N10	4.94	1.49	1.41
57	U	101	EHZ	C15-N2	4.93	1.45	1.33
54	O	401	DGT	C2-N2	4.84	1.45	1.34
54	O	401	DGT	C2-N1	4.79	1.49	1.37
56	P	501	NDP	C2N-C3N	4.61	1.47	1.35
58	i	201	CHD	C6-C5	4.60	1.61	1.53
50	F	501	FMN	C2-N3	4.55	1.49	1.39
56	P	501	NDP	PN-O3	4.43	1.64	1.59
54	O	401	DGT	C2-N3	4.36	1.43	1.33
54	O	401	DGT	C8-N9	-4.31	1.27	1.37
56	P	501	NDP	C5A-C4A	-4.27	1.31	1.39
58	i	201	CHD	C15-C14	4.16	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	O7N-C7N	-4.08	1.14	1.24
54	O	401	DGT	C4-N9	-3.86	1.28	1.38
56	P	501	NDP	C8A-N9A	-3.83	1.31	1.37
56	P	501	NDP	O2D-C2D	3.79	1.52	1.43
50	F	501	FMN	C4-N3	3.75	1.45	1.38
50	F	501	FMN	C10-N10	3.72	1.45	1.37
58	i	201	CHD	C6-C7	3.48	1.59	1.52
56	P	501	NDP	C4N-C3N	3.26	1.56	1.50
50	F	501	FMN	O2-C2	-2.96	1.18	1.24
52	q	201	CDL	OB6-CB4	-2.83	1.39	1.46
52	M	602	CDL	OB6-CB4	-2.81	1.40	1.46
58	i	201	CHD	C13-C12	-2.81	1.50	1.54
46	L	705	PC1	O21-C2	-2.80	1.40	1.46
52	q	201	CDL	OA6-CA4	-2.78	1.40	1.46
46	A	203	PC1	O21-C2	-2.78	1.40	1.46
45	M	604	3PE	O21-C2	-2.77	1.40	1.46
46	d	203	PC1	O21-C2	-2.76	1.40	1.46
52	i	202	CDL	OA6-CA4	-2.76	1.40	1.46
45	I	203	3PE	O21-C2	-2.75	1.40	1.46
46	H	401	PC1	O21-C2	-2.75	1.40	1.46
45	K	101	3PE	O21-C2	-2.74	1.40	1.46
56	P	501	NDP	C4N-C5N	2.73	1.56	1.49
45	d	202	3PE	O21-C2	-2.73	1.40	1.46
52	L	701	CDL	OA6-CA4	-2.72	1.40	1.46
46	H	402	PC1	O21-C2	-2.72	1.40	1.46
46	q	203	PC1	O21-C2	-2.72	1.40	1.46
45	D	501	3PE	O21-C2	-2.71	1.40	1.46
52	i	202	CDL	OB6-CB4	-2.71	1.40	1.46
52	N	401	CDL	OB6-CB4	-2.70	1.40	1.46
46	A	202	PC1	O21-C2	-2.70	1.40	1.46
52	d	201	CDL	OA6-CA4	-2.69	1.40	1.46
52	L	701	CDL	OB6-CB4	-2.69	1.40	1.46
52	X	201	CDL	OB6-CB4	-2.69	1.40	1.46
50	F	501	FMN	O4-C4	-2.68	1.18	1.23
45	A	201	3PE	O21-C2	-2.68	1.40	1.46
46	h	201	PC1	O21-C2	-2.68	1.40	1.46
54	O	401	DGT	C17-N9	-2.68	1.41	1.48
46	M	606	PC1	O21-C2	-2.68	1.40	1.46
45	L	704	3PE	O21-C2	-2.67	1.40	1.46
46	M	605	PC1	O21-C2	-2.66	1.40	1.46
45	Y	205	3PE	O21-C2	-2.66	1.40	1.46
45	g	201	3PE	O21-C2	-2.66	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	202	3PE	O21-C2	-2.65	1.40	1.46
45	m	201	3PE	O21-C2	-2.64	1.40	1.46
46	q	202	PC1	O21-C2	-2.64	1.40	1.46
52	M	602	CDL	OA6-CA4	-2.63	1.40	1.46
56	P	501	NDP	C5A-N7A	-2.63	1.34	1.39
46	I	205	PC1	O21-C2	-2.63	1.40	1.46
45	Y	201	3PE	O21-C2	-2.62	1.40	1.46
52	d	201	CDL	OB6-CB4	-2.62	1.40	1.46
46	I	204	PC1	O21-C2	-2.62	1.40	1.46
45	m	202	3PE	O21-C2	-2.60	1.40	1.46
46	m	203	PC1	O21-C2	-2.58	1.40	1.46
45	N	402	3PE	O21-C2	-2.57	1.40	1.46
52	N	401	CDL	OA6-CA4	-2.56	1.40	1.46
45	M	603	3PE	O21-C2	-2.55	1.40	1.46
45	Z	201	3PE	O21-C2	-2.54	1.40	1.46
46	q	202	PC1	O31-C31	2.53	1.40	1.33
56	P	501	NDP	C6N-N1N	2.52	1.43	1.37
45	L	702	3PE	O21-C2	-2.51	1.40	1.46
45	L	703	3PE	O21-C2	-2.50	1.40	1.46
57	T	101	EHZ	C9-S1	2.47	1.82	1.76
52	q	201	CDL	OB8-CB7	2.47	1.40	1.33
45	Y	203	3PE	O21-C2	-2.46	1.40	1.46
46	d	203	PC1	O31-C31	2.46	1.40	1.33
46	M	606	PC1	O31-C31	2.44	1.40	1.33
52	d	201	CDL	OB8-CB7	2.44	1.40	1.33
56	P	501	NDP	O3B-C3B	-2.44	1.36	1.43
45	Y	204	3PE	O21-C2	-2.43	1.40	1.46
46	h	201	PC1	O31-C31	2.43	1.40	1.33
45	d	202	3PE	O31-C31	2.43	1.40	1.33
52	M	602	CDL	OA8-CA7	2.42	1.40	1.33
45	L	702	3PE	O31-C31	2.42	1.40	1.33
52	N	401	CDL	OA8-CA7	2.42	1.40	1.33
56	P	501	NDP	O3D-C3D	-2.41	1.37	1.43
52	X	201	CDL	OA8-CA7	2.39	1.40	1.33
45	Z	201	3PE	O31-C31	2.39	1.40	1.33
45	M	603	3PE	O31-C31	2.39	1.40	1.33
45	A	201	3PE	O31-C31	2.39	1.40	1.33
52	L	701	CDL	OB8-CB7	2.39	1.40	1.33
45	m	202	3PE	O31-C31	2.39	1.40	1.33
52	L	701	CDL	OA8-CA6	-2.38	1.39	1.45
52	N	401	CDL	OB8-CB7	2.38	1.40	1.33
57	U	101	EHZ	C9-S1	2.38	1.81	1.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	I	203	3PE	O31-C31	2.37	1.40	1.33
45	M	604	3PE	O31-C3	-2.37	1.39	1.45
57	T	101	EHZ	O4-C15	-2.37	1.18	1.23
46	H	401	PC1	O31-C31	2.37	1.40	1.33
46	q	203	PC1	O31-C31	2.37	1.40	1.33
52	M	602	CDL	OB8-CB7	2.37	1.40	1.33
45	b	101	3PE	O31-C31	2.36	1.40	1.33
52	i	202	CDL	OA8-CA7	2.36	1.40	1.33
57	T	101	EHZ	O3-C12	-2.36	1.18	1.23
46	A	203	PC1	O31-C31	2.36	1.40	1.33
52	i	202	CDL	OB8-CB7	2.35	1.40	1.33
52	X	201	CDL	OB8-CB6	-2.35	1.39	1.45
45	Y	201	3PE	O31-C31	2.34	1.40	1.33
45	Y	203	3PE	O31-C3	-2.34	1.39	1.45
45	Y	205	3PE	O31-C31	2.34	1.40	1.33
52	X	201	CDL	OA6-CA4	-2.33	1.41	1.46
45	m	201	3PE	O31-C31	2.33	1.40	1.33
45	N	402	3PE	O31-C31	2.33	1.40	1.33
46	m	203	PC1	O31-C31	2.33	1.40	1.33
46	I	204	PC1	O31-C31	2.33	1.40	1.33
45	L	703	3PE	O31-C31	2.33	1.40	1.33
45	g	201	3PE	O31-C31	2.33	1.40	1.33
57	U	101	EHZ	O4-C15	-2.33	1.18	1.23
46	I	205	PC1	O31-C31	2.32	1.40	1.33
45	Y	202	3PE	O31-C31	2.32	1.40	1.33
46	A	202	PC1	O31-C31	2.32	1.40	1.33
45	Y	204	3PE	O31-C31	2.32	1.40	1.33
46	H	402	PC1	O31-C31	2.32	1.40	1.33
45	b	101	3PE	O21-C2	-2.31	1.41	1.46
45	D	501	3PE	O31-C31	2.31	1.40	1.33
45	Y	203	3PE	O31-C31	2.31	1.40	1.33
52	q	201	CDL	OA8-CA6	-2.30	1.40	1.45
52	q	201	CDL	OA8-CA7	2.30	1.40	1.33
52	X	201	CDL	OA6-CA5	2.30	1.40	1.34
46	M	605	PC1	O31-C31	2.30	1.40	1.33
46	L	705	PC1	O31-C31	2.30	1.40	1.33
45	K	101	3PE	O31-C31	2.29	1.40	1.33
45	Y	202	3PE	O31-C3	-2.29	1.40	1.45
57	U	101	EHZ	O3-C12	-2.28	1.18	1.23
56	P	501	NDP	P2B-O1X	2.28	1.57	1.50
45	K	101	3PE	O31-C3	-2.28	1.40	1.45
52	L	701	CDL	OA8-CA7	2.27	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	D	501	3PE	O31-C3	-2.27	1.40	1.45
52	M	602	CDL	OB8-CB6	-2.27	1.40	1.45
45	Y	201	3PE	O31-C3	-2.27	1.40	1.45
45	g	201	3PE	O31-C3	-2.27	1.40	1.45
46	I	205	PC1	O31-C3	-2.27	1.40	1.45
52	i	202	CDL	OA8-CA6	-2.27	1.40	1.45
52	i	202	CDL	OB8-CB6	-2.26	1.40	1.45
52	d	201	CDL	OA8-CA6	-2.26	1.40	1.45
52	d	201	CDL	OA8-CA7	2.26	1.39	1.33
54	O	401	DGT	PG-O1G	-2.26	1.46	1.54
45	g	201	3PE	O21-C21	2.26	1.40	1.35
45	I	203	3PE	O31-C3	-2.26	1.40	1.45
56	P	501	NDP	PA-O5B	2.25	1.68	1.59
45	Y	205	3PE	O31-C3	-2.25	1.40	1.45
45	Y	204	3PE	O31-C3	-2.24	1.40	1.45
52	X	201	CDL	OB8-CB7	2.24	1.39	1.33
52	L	701	CDL	OB8-CB6	-2.24	1.40	1.45
46	H	401	PC1	O31-C3	-2.23	1.40	1.45
46	M	605	PC1	O31-C3	-2.23	1.40	1.45
45	Z	201	3PE	O31-C3	-2.23	1.40	1.45
54	O	401	DGT	PG-O2G	-2.23	1.46	1.54
54	O	401	DGT	C4-N3	2.22	1.39	1.34
45	L	703	3PE	O31-C3	-2.22	1.40	1.45
52	N	401	CDL	OB8-CB6	-2.22	1.40	1.45
45	m	201	3PE	O31-C3	-2.22	1.40	1.45
45	m	202	3PE	O31-C3	-2.22	1.40	1.45
45	Y	204	3PE	O21-C21	2.22	1.40	1.34
46	q	202	PC1	O21-C21	2.22	1.40	1.34
46	A	202	PC1	O31-C3	-2.21	1.40	1.45
45	L	702	3PE	O21-C21	2.21	1.40	1.34
45	M	603	3PE	O21-C21	2.21	1.40	1.34
46	I	205	PC1	O21-C21	2.21	1.40	1.34
45	N	402	3PE	O31-C3	-2.21	1.40	1.45
46	L	705	PC1	O31-C3	-2.21	1.40	1.45
45	M	604	3PE	O31-C31	2.21	1.39	1.33
52	N	401	CDL	OA6-CA5	2.21	1.40	1.34
46	q	203	PC1	O21-C21	2.21	1.40	1.34
52	d	201	CDL	OB6-CB5	2.20	1.40	1.34
46	A	203	PC1	O31-C3	-2.20	1.40	1.45
45	A	201	3PE	O31-C3	-2.20	1.40	1.45
46	m	203	PC1	O21-C21	2.20	1.40	1.34
46	m	203	PC1	O31-C3	-2.20	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	402	PC1	O31-C3	-2.19	1.40	1.45
45	b	101	3PE	O21-C21	2.19	1.40	1.34
45	L	703	3PE	O21-C21	2.19	1.40	1.34
52	d	201	CDL	OA6-CA5	2.18	1.40	1.34
46	h	201	PC1	O31-C3	-2.18	1.40	1.45
52	X	201	CDL	OA8-CA6	-2.18	1.40	1.45
45	m	202	3PE	O21-C21	2.18	1.40	1.34
56	P	501	NDP	C7N-C3N	2.18	1.53	1.48
45	M	603	3PE	O31-C3	-2.17	1.40	1.45
46	I	204	PC1	O21-C21	2.17	1.40	1.34
45	d	202	3PE	O31-C3	-2.17	1.40	1.45
46	H	401	PC1	O21-C21	2.17	1.40	1.34
45	Z	201	3PE	O21-C21	2.16	1.40	1.34
45	Y	203	3PE	O21-C21	2.16	1.40	1.34
52	L	701	CDL	OB6-CB5	2.15	1.40	1.34
46	A	202	PC1	O21-C21	2.15	1.40	1.34
45	Y	202	3PE	O21-C21	2.15	1.40	1.34
45	L	702	3PE	O31-C3	-2.14	1.40	1.45
52	M	602	CDL	OA6-CA5	2.14	1.40	1.34
46	q	203	PC1	O31-C3	-2.14	1.40	1.45
45	N	402	3PE	O21-C21	2.14	1.40	1.34
52	i	202	CDL	OB6-CB5	2.14	1.40	1.34
45	m	201	3PE	O21-C21	2.14	1.40	1.34
46	M	606	PC1	O31-C3	-2.14	1.40	1.45
52	q	201	CDL	OB8-CB6	-2.14	1.40	1.45
45	Y	201	3PE	O21-C21	2.14	1.40	1.34
46	H	402	PC1	O21-C21	2.13	1.40	1.34
46	M	605	PC1	O21-C21	2.13	1.40	1.34
52	N	401	CDL	OA8-CA6	-2.13	1.40	1.45
52	X	201	CDL	OB6-CB5	2.12	1.40	1.34
46	M	606	PC1	O21-C21	2.12	1.40	1.34
52	M	602	CDL	OB6-CB5	2.12	1.40	1.34
45	b	101	3PE	O31-C3	-2.11	1.40	1.45
52	L	701	CDL	OA6-CA5	2.11	1.40	1.34
52	M	602	CDL	OA8-CA6	-2.11	1.40	1.45
46	A	203	PC1	O21-C21	2.11	1.40	1.34
46	d	203	PC1	O21-C21	2.10	1.40	1.34
46	h	201	PC1	O21-C21	2.10	1.40	1.34
45	L	704	3PE	O21-C21	2.10	1.40	1.34
45	Y	205	3PE	O21-C21	2.10	1.40	1.34
46	I	204	PC1	O31-C3	-2.10	1.40	1.45
52	N	401	CDL	OB6-CB5	2.10	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	704	3PE	O31-C3	-2.09	1.40	1.45
56	P	501	NDP	C5B-C4B	2.09	1.57	1.51
45	D	501	3PE	O21-C21	2.09	1.40	1.34
52	d	201	CDL	OB8-CB6	-2.09	1.40	1.45
45	A	201	3PE	O21-C21	2.09	1.40	1.34
52	i	202	CDL	OA6-CA5	2.09	1.40	1.34
46	L	705	PC1	O21-C21	2.07	1.40	1.34
46	d	203	PC1	O31-C3	-2.06	1.40	1.45
58	i	201	CHD	O7-C7	-2.05	1.39	1.43
45	d	202	3PE	O21-C21	2.05	1.40	1.34
45	I	203	3PE	O21-C21	2.05	1.40	1.34
52	q	201	CDL	OA6-CA5	2.03	1.40	1.34
52	q	201	CDL	OB6-CB5	2.02	1.40	1.34
45	M	604	3PE	O21-C21	2.01	1.40	1.34
45	K	101	3PE	O21-C21	2.00	1.39	1.34

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	401	DGT	C8-N9-C4	7.44	119.97	106.03
58	i	201	CHD	C13-C17-C20	-7.41	110.51	119.48
58	i	201	CHD	C17-C13-C14	7.00	107.14	100.11
57	T	101	EHZ	C8-C9-S1	5.94	121.06	113.56
57	U	101	EHZ	C8-C9-S1	5.67	120.72	113.56
56	P	501	NDP	N6A-C6A-N1A	-5.63	105.84	118.38
56	P	501	NDP	C4A-N9A-C1B	-5.49	113.79	126.63
56	P	501	NDP	N3A-C2A-N1A	-5.46	120.31	128.58
56	P	501	NDP	C5A-C4A-N3A	-5.04	119.77	126.72
45	g	201	3PE	O21-C21-C22	4.95	119.91	111.09
58	i	201	CHD	C17-C13-C12	4.93	122.11	117.67
56	P	501	NDP	C1B-N9A-C8A	4.92	138.02	127.09
50	F	501	FMN	C7M-C7-C6	4.69	127.84	119.57
50	F	501	FMN	C9-C8-C7	4.57	126.40	119.69
45	L	702	3PE	O21-C21-C22	4.52	121.26	111.48
58	i	201	CHD	C18-C13-C12	-4.34	104.71	109.06
52	M	602	CDL	OA6-CA5-C11	4.32	120.83	111.48
45	K	101	3PE	O21-C21-C22	4.31	120.80	111.48
45	N	402	3PE	O21-C21-C22	4.24	120.64	111.48
46	I	204	PC1	O21-C21-C22	4.23	120.64	111.48
45	m	202	3PE	O21-C21-C22	4.22	120.62	111.48
45	L	704	3PE	O21-C21-C22	4.19	120.54	111.48
52	X	201	CDL	OB6-CB5-C51	4.18	120.52	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	402	PC1	O21-C21-C22	4.15	120.46	111.48
56	P	501	NDP	N9A-C8A-N7A	-4.15	108.05	113.94
46	d	203	PC1	O21-C21-C22	4.14	120.43	111.48
46	M	605	PC1	O21-C21-C22	4.13	120.41	111.48
56	P	501	NDP	C5A-C6A-N6A	4.10	133.45	123.29
46	h	201	PC1	O21-C21-C22	4.10	120.36	111.48
52	M	602	CDL	OB6-CB5-C51	4.10	120.35	111.48
52	N	401	CDL	OB6-CB5-C51	4.09	120.32	111.48
45	Y	205	3PE	O21-C21-C22	4.07	120.29	111.48
46	A	203	PC1	O21-C21-C22	4.06	120.26	111.48
45	m	201	3PE	O21-C21-C22	4.05	120.24	111.48
45	Y	202	3PE	O21-C21-C22	4.03	120.21	111.48
45	d	202	3PE	O21-C21-C22	4.01	120.15	111.48
45	M	603	3PE	O21-C21-C22	3.98	120.09	111.48
45	b	101	3PE	O21-C21-C22	3.98	120.09	111.48
45	Y	203	3PE	O21-C21-C22	3.95	120.03	111.48
45	L	703	3PE	O21-C21-C22	3.95	120.02	111.48
52	d	201	CDL	OA6-CA5-C11	3.95	120.02	111.48
46	A	202	PC1	O21-C21-C22	3.94	120.00	111.48
45	Y	201	3PE	O21-C21-C22	3.93	119.99	111.48
52	q	201	CDL	OB6-CB5-C51	3.93	119.98	111.48
52	i	202	CDL	OB6-CB5-C51	3.93	119.97	111.48
46	H	401	PC1	O21-C21-C22	3.91	119.94	111.48
46	M	606	PC1	O21-C21-C22	3.91	119.93	111.48
45	A	201	3PE	O21-C21-C22	3.89	119.90	111.48
45	I	203	3PE	O21-C21-C22	3.89	119.90	111.48
45	M	604	3PE	O21-C21-C22	3.88	119.87	111.48
52	i	202	CDL	OA6-CA5-C11	3.87	119.85	111.48
46	m	203	PC1	O21-C21-C22	3.85	119.81	111.48
45	Z	201	3PE	O21-C21-C22	3.84	119.78	111.48
46	L	705	PC1	O21-C21-C22	3.83	119.77	111.48
52	L	701	CDL	OB6-CB5-C51	3.83	119.77	111.48
58	i	201	CHD	C1-C10-C5	3.82	113.23	107.75
52	X	201	CDL	OA6-CA5-C11	3.82	119.74	111.48
52	L	701	CDL	OA6-CA5-C11	3.81	119.72	111.48
45	Y	204	3PE	O21-C21-C22	3.79	119.67	111.48
46	q	202	PC1	O21-C21-C22	3.78	119.66	111.48
46	I	205	PC1	O21-C21-C22	3.75	119.59	111.48
52	q	201	CDL	OA6-CA5-C11	3.70	119.48	111.48
45	D	501	3PE	O21-C21-C22	3.68	119.45	111.48
54	O	401	DGT	C1'-N9-C8	-3.67	119.68	127.91
58	i	201	CHD	C18-C13-C17	-3.66	105.47	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	N	401	CDL	OA6-CA5-C11	3.66	119.39	111.48
58	i	201	CHD	C18-C13-C14	-3.59	105.58	111.20
50	F	501	FMN	C4-N3-C2	-3.50	119.43	125.64
58	i	201	CHD	C14-C13-C12	3.45	110.57	107.42
56	P	501	NDP	C2A-N3A-C4A	3.44	120.24	111.83
50	F	501	FMN	C8M-C8-C7	-3.36	113.90	120.76
58	i	201	CHD	C9-C11-C12	-3.25	110.04	114.29
54	O	401	DGT	C2-N1-C6	-3.17	119.36	125.11
57	U	101	EHZ	C14-C13-C12	-3.13	107.17	112.39
54	O	401	DGT	C2'-C3'-C4'	3.13	109.15	102.80
58	i	201	CHD	C23-C22-C20	-3.08	108.72	114.46
56	P	501	NDP	N3A-C4A-N9A	3.07	132.39	127.17
52	d	201	CDL	OB8-CB7-C71	3.06	121.15	111.83
58	i	201	CHD	C16-C17-C13	2.99	106.44	103.54
45	L	703	3PE	O31-C31-C32	2.97	120.90	111.83
54	O	401	DGT	O2G-PG-O3B	2.92	114.44	104.64
52	M	602	CDL	OA8-CA7-C31	2.91	120.70	111.83
46	d	203	PC1	O31-C31-C32	2.91	120.69	111.83
52	M	602	CDL	OB8-CB7-C71	2.89	120.65	111.83
50	F	501	FMN	C4A-C10-N10	2.87	120.59	116.48
45	I	203	3PE	O31-C31-C32	2.87	119.85	111.15
46	H	402	PC1	O31-C31-C32	2.86	120.55	111.83
46	L	705	PC1	O31-C31-C32	2.85	120.53	111.83
45	Y	203	3PE	O31-C31-C32	2.84	120.50	111.83
45	Y	204	3PE	O31-C31-C32	2.83	120.47	111.83
52	i	202	CDL	OA8-CA7-C31	2.82	120.43	111.83
56	P	501	NDP	C5A-N7A-C8A	2.82	107.88	103.45
52	X	201	CDL	OA8-CA7-C31	2.81	120.39	111.83
57	T	101	EHZ	O2-C9-C8	-2.80	119.33	123.74
46	M	605	PC1	O31-C31-C32	2.80	120.37	111.83
45	L	702	3PE	O31-C31-C32	2.79	120.35	111.83
52	L	701	CDL	OB8-CB7-C71	2.78	120.32	111.83
46	m	203	PC1	O31-C31-C32	2.78	120.32	111.83
46	I	204	PC1	O31-C31-C32	2.75	120.23	111.83
45	A	201	3PE	O31-C31-C32	2.75	120.23	111.83
58	i	201	CHD	C15-C14-C8	2.74	122.12	118.36
58	i	201	CHD	C19-C10-C9	-2.74	107.49	111.18
46	H	401	PC1	O31-C31-C32	2.74	120.19	111.83
45	m	201	3PE	O31-C31-C32	2.74	120.17	111.83
46	M	606	PC1	O31-C31-C32	2.73	120.17	111.83
45	M	604	3PE	O31-C31-C32	2.73	120.15	111.83
52	L	701	CDL	OA8-CA7-C31	2.73	120.15	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	q	203	PC1	O31-C31-C32	2.72	120.14	111.83
58	i	201	CHD	C6-C5-C4	-2.72	108.12	111.23
52	i	202	CDL	OB8-CB7-C71	2.72	120.12	111.83
45	M	603	3PE	O31-C31-C32	2.70	120.06	111.83
57	U	101	EHZ	C13-C14-N2	-2.69	106.27	112.00
46	q	202	PC1	O31-C31-C32	2.69	120.04	111.83
52	N	401	CDL	OB8-CB7-C71	2.69	120.03	111.83
46	I	205	PC1	O31-C31-C32	2.69	120.03	111.83
45	Y	202	3PE	O31-C31-C32	2.68	120.02	111.83
50	F	501	FMN	C6-C7-C8	-2.67	115.77	119.69
46	A	203	PC1	O31-C31-C32	2.67	119.97	111.83
54	O	401	DGT	O1G-PG-O3B	2.66	113.57	104.64
45	K	101	3PE	O31-C31-C32	2.66	119.96	111.83
45	b	101	3PE	O31-C31-C32	2.66	119.95	111.83
45	m	202	3PE	O31-C31-C32	2.66	119.94	111.83
46	h	201	PC1	O31-C31-C32	2.64	119.89	111.83
52	N	401	CDL	OA8-CA7-C31	2.62	119.83	111.83
45	N	402	3PE	O31-C31-C32	2.62	119.83	111.83
52	d	201	CDL	OB6-CB5-C51	2.62	120.56	110.93
45	Y	205	3PE	O31-C31-C32	2.61	119.79	111.83
57	T	101	EHZ	C13-C12-N1	2.61	121.10	116.34
45	Z	201	3PE	O31-C31-C32	2.59	119.74	111.83
52	q	201	CDL	OA8-CA7-C31	2.59	119.74	111.83
46	A	202	PC1	O31-C31-C32	2.59	119.73	111.83
52	d	201	CDL	OA8-CA7-C31	2.59	119.72	111.83
45	Y	201	3PE	O31-C31-C32	2.58	119.72	111.83
45	g	201	3PE	O31-C31-C32	2.58	119.71	111.83
50	F	501	FMN	C4A-C4-N3	2.57	119.80	113.25
45	D	501	3PE	O31-C31-C32	2.57	119.68	111.83
52	q	201	CDL	OB8-CB7-C71	2.56	119.64	111.83
46	q	203	PC1	O21-C21-C22	2.56	120.32	110.93
57	U	101	EHZ	O2-C9-S1	-2.54	119.45	122.68
50	F	501	FMN	O4-C4-C4A	-2.54	119.83	126.53
56	P	501	NDP	C2B-C1B-N9A	-2.52	109.60	113.75
52	X	201	CDL	OB8-CB7-C71	2.50	119.46	111.83
57	U	101	EHZ	O2-C9-C8	-2.48	119.83	123.74
50	F	501	FMN	C5A-C9A-N10	2.48	120.21	117.97
54	O	401	DGT	C5-C6-N1	2.45	119.50	113.25
57	T	101	EHZ	O2-C9-S1	-2.42	119.61	122.68
45	d	202	3PE	O31-C31-C32	2.40	119.16	111.83
54	O	401	DGT	O1A-PA-O2A	-2.39	101.31	112.44
57	U	101	EHZ	C7-C8-C9	-2.39	108.53	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	401	DGT	O1B-PB-O2B	-2.39	101.34	112.44
58	i	201	CHD	C11-C9-C10	-2.37	111.30	113.70
54	O	401	DGT	O6-C6-C5	-2.37	120.28	126.53
58	i	201	CHD	C13-C14-C8	-2.35	111.73	114.72
57	T	101	EHZ	C7-C8-C9	-2.33	108.65	113.86
56	P	501	NDP	C4A-N9A-C8A	2.33	108.19	105.74
50	F	501	FMN	C9A-C5A-N5	-2.31	120.00	122.45
50	F	501	FMN	C10-C4A-N5	-2.28	120.14	124.81
57	T	101	EHZ	C11-N1-C12	-2.27	118.59	122.82
56	P	501	NDP	P2B-O2B-C2B	-2.24	117.46	123.43
54	O	401	DGT	C5-C4-N9	-2.22	101.68	105.66
50	F	501	FMN	C6-C5A-C9A	2.22	122.10	119.05
56	P	501	NDP	C4A-C5A-N7A	-2.22	108.05	110.58
57	T	101	EHZ	C10-S1-C9	2.21	108.38	101.84
54	O	401	DGT	N9-C4-N3	2.20	130.36	125.95
57	U	101	EHZ	C13-C12-N1	2.18	120.31	116.34
58	i	201	CHD	C4-C3-C2	2.16	113.25	110.62
58	i	201	CHD	C15-C14-C13	2.15	105.62	103.54
50	F	501	FMN	C7M-C7-C8	-2.14	116.39	120.76
57	U	101	EHZ	C10-S1-C9	2.10	108.05	101.84
57	T	101	EHZ	C14-C13-C12	-2.07	108.95	112.39
57	U	101	EHZ	C18-C17-C16	2.02	112.22	108.77
54	O	401	DGT	N9-C8-N7	-2.00	109.69	113.40

There are no chirality outliers.

All (1105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O12
45	A	201	3PE	C11-O13-P-O14
45	D	501	3PE	C1-O11-P-O13
45	D	501	3PE	C1-O11-P-O14
45	D	501	3PE	C11-O13-P-O11
45	D	501	3PE	C11-O13-P-O12
45	D	501	3PE	C11-O13-P-O14
45	I	203	3PE	C1-O11-P-O12
45	I	203	3PE	C1-O11-P-O13
45	I	203	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	I	203	3PE	C11-O13-P-O14
45	I	203	3PE	O13-C11-C12-N
45	I	203	3PE	C22-C21-O21-C2
45	K	101	3PE	C1-O11-P-O12
45	K	101	3PE	C1-O11-P-O13
45	K	101	3PE	O11-C1-C2-O21
45	L	702	3PE	C11-O13-P-O11
45	L	702	3PE	C11-O13-P-O12
45	L	702	3PE	O22-C21-O21-C2
45	L	703	3PE	C1-O11-P-O12
45	L	703	3PE	C1-O11-P-O13
45	L	703	3PE	O13-C11-C12-N
45	L	703	3PE	C22-C21-O21-C2
45	L	704	3PE	C1-O11-P-O12
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-O12
45	L	704	3PE	O22-C21-O21-C2
45	M	603	3PE	C1-O11-P-O12
45	M	603	3PE	C1-O11-P-O13
45	M	603	3PE	C12-C11-O13-P
45	M	604	3PE	C1-O11-P-O12
45	M	604	3PE	C1-O11-P-O13
45	M	604	3PE	C11-O13-P-O11
45	M	604	3PE	C12-C11-O13-P
45	N	402	3PE	C11-O13-P-O11
45	N	402	3PE	O22-C21-O21-C2
45	Y	201	3PE	C1-O11-P-O13
45	Y	201	3PE	C1-O11-P-O14
45	Y	201	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O14
45	Y	202	3PE	C1-O11-P-O12
45	Y	202	3PE	C1-O11-P-O13
45	Y	202	3PE	O13-C11-C12-N
45	Y	202	3PE	C22-C21-O21-C2
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	204	3PE	C1-O11-P-O12
45	Y	204	3PE	C1-O11-P-O13
45	Y	204	3PE	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	205	3PE	C11-O13-P-O11
45	Y	205	3PE	C12-C11-O13-P
45	Y	205	3PE	O22-C21-O21-C2
45	Z	201	3PE	C11-O13-P-O14
45	Z	201	3PE	C12-C11-O13-P
45	Z	201	3PE	O13-C11-C12-N
45	Z	201	3PE	O21-C2-C3-O31
45	b	101	3PE	O11-C1-C2-O21
45	b	101	3PE	C22-C21-O21-C2
45	d	202	3PE	C1-O11-P-O12
45	d	202	3PE	C1-O11-P-O13
45	d	202	3PE	C1-O11-P-O14
45	d	202	3PE	O21-C2-C3-O31
45	g	201	3PE	O21-C2-C3-O31
45	m	201	3PE	C22-C21-O21-C2
45	m	202	3PE	C1-O11-P-O13
45	m	202	3PE	C1-O11-P-O14
45	m	202	3PE	O13-C11-C12-N
45	m	202	3PE	O22-C21-O21-C2
46	A	202	PC1	C1-O11-P-O14
46	A	202	PC1	C1-O11-P-O13
46	H	401	PC1	C11-O13-P-O12
46	H	401	PC1	C11-O13-P-O11
46	H	401	PC1	C1-O11-P-O12
46	H	401	PC1	C1-O11-P-O14
46	H	401	PC1	C1-O11-P-O13
46	H	401	PC1	O13-C11-C12-N
46	H	402	PC1	C1-O11-P-O14
46	H	402	PC1	C1-O11-P-O13
46	I	204	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O14
46	I	204	PC1	C11-O13-P-O11
46	I	204	PC1	O13-C11-C12-N
46	I	205	PC1	O13-C11-C12-N
46	L	705	PC1	C11-O13-P-O14
46	L	705	PC1	C11-O13-P-O11
46	M	605	PC1	C1-O11-P-O12
46	M	605	PC1	C1-O11-P-O14
46	M	605	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	M	606	PC1	C1-O11-P-O12
46	M	606	PC1	C1-O11-P-O14
46	M	606	PC1	C1-O11-P-O13
46	M	606	PC1	O13-C11-C12-N
46	M	606	PC1	O21-C2-C3-O31
46	M	606	PC1	O22-C21-O21-C2
46	M	606	PC1	C22-C21-O21-C2
46	d	203	PC1	C11-O13-P-O12
46	d	203	PC1	C11-O13-P-O14
46	d	203	PC1	C11-O13-P-O11
46	d	203	PC1	C22-C21-O21-C2
46	h	201	PC1	C11-O13-P-O11
46	h	201	PC1	C1-O11-P-O12
46	h	201	PC1	C1-O11-P-O14
46	h	201	PC1	C22-C21-O21-C2
46	m	203	PC1	C11-O13-P-O12
46	m	203	PC1	C1-O11-P-O12
46	m	203	PC1	C1-O11-P-O13
46	q	202	PC1	C1-O11-P-O12
46	q	202	PC1	C1-O11-P-O14
46	q	202	PC1	C1-O11-P-O13
46	q	203	PC1	O13-C11-C12-N
46	q	203	PC1	O22-C21-O21-C2
46	q	203	PC1	C22-C21-O21-C2
47	A	204	PLC	C1-O3P-P-O1P
47	A	204	PLC	C1-O3P-P-O2P
47	A	204	PLC	C1-O3P-P-O4P
47	A	204	PLC	C4-O4P-P-O1P
47	A	204	PLC	C4-O4P-P-O2P
47	A	204	PLC	C4-O4P-P-O3P
47	B	202	PLC	C1'-C'-O2-C2
47	B	202	PLC	C1-O3P-P-O2P
47	B	202	PLC	C4-O4P-P-O1P
47	L	706	PLC	C1'-C'-O2-C2
47	L	706	PLC	C4-O4P-P-O2P
47	M	607	PLC	O4P-C4-C5-N
47	M	607	PLC	C4-O4P-P-O3P
47	Y	206	PLC	C5-C4-O4P-P
47	Y	206	PLC	C4-O4P-P-O1P
47	Z	202	PLC	O4P-C4-C5-N
47	Z	202	PLC	C4-O4P-P-O1P
47	Z	202	PLC	C4-O4P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	Z	202	PLC	C4-O4P-P-O3P
47	g	202	PLC	O2-C2-C3-O3
47	g	202	PLC	C1-O3P-P-O1P
47	g	202	PLC	C1-O3P-P-O2P
47	g	202	PLC	C1-O3P-P-O4P
50	F	501	FMN	C5'-O5'-P-O2P
50	F	501	FMN	C5'-O5'-P-O3P
52	L	701	CDL	C11-CA5-OA6-CA4
52	L	701	CDL	CB2-OB2-PB2-OB3
52	L	701	CDL	CB2-OB2-PB2-OB4
52	L	701	CDL	CB2-OB2-PB2-OB5
52	M	602	CDL	C1-CA2-OA2-PA1
52	M	602	CDL	CB3-OB5-PB2-OB3
52	M	602	CDL	OB5-CB3-CB4-OB6
52	M	602	CDL	OB7-CB5-OB6-CB4
52	N	401	CDL	CA2-OA2-PA1-OA3
52	N	401	CDL	CA2-OA2-PA1-OA5
52	N	401	CDL	CA3-OA5-PA1-OA3
52	N	401	CDL	CB2-OB2-PB2-OB3
52	N	401	CDL	C51-CB5-OB6-CB4
52	X	201	CDL	C1-CA2-OA2-PA1
52	X	201	CDL	CA3-OA5-PA1-OA2
52	X	201	CDL	CA3-OA5-PA1-OA3
52	X	201	CDL	OA7-CA5-OA6-CA4
52	X	201	CDL	C51-CB5-OB6-CB4
52	d	201	CDL	CB2-OB2-PB2-OB4
52	d	201	CDL	CB2-OB2-PB2-OB5
52	d	201	CDL	CB3-OB5-PB2-OB2
52	d	201	CDL	OB7-CB5-OB6-CB4
52	i	202	CDL	OB7-CB5-OB6-CB4
52	q	201	CDL	O1-C1-CB2-OB2
52	q	201	CDL	CA2-C1-CB2-OB2
52	q	201	CDL	CA2-OA2-PA1-OA3
52	q	201	CDL	CA2-OA2-PA1-OA5
52	q	201	CDL	CA3-OA5-PA1-OA2
52	q	201	CDL	CA3-OA5-PA1-OA3
52	q	201	CDL	CA3-OA5-PA1-OA4
52	q	201	CDL	OA7-CA5-OA6-CA4
52	q	201	CDL	C11-CA5-OA6-CA4
52	q	201	CDL	CB2-OB2-PB2-OB4
52	q	201	CDL	CB3-OB5-PB2-OB2
52	q	201	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	q	201	CDL	CB3-OB5-PB2-OB4
54	O	401	DGT	C5'-O5'-PA-O1A
56	P	501	NDP	C5B-O5B-PA-O1A
57	T	101	EHZ	C6-C7-C8-C9
57	T	101	EHZ	S1-C10-C11-N1
57	T	101	EHZ	C16-C17-C20-O6
57	T	101	EHZ	O2-C9-S1-C10
57	T	101	EHZ	C8-C9-S1-C10
57	U	101	EHZ	C6-C7-C8-C9
57	U	101	EHZ	S1-C10-C11-N1
57	U	101	EHZ	C11-C10-S1-C9
57	U	101	EHZ	O2-C9-S1-C10
57	U	101	EHZ	C8-C9-S1-C10
59	o	201	MYR	O1-C1-C2-C3
45	g	201	3PE	C22-C21-O21-C2
45	m	201	3PE	O32-C31-O31-C3
46	m	203	PC1	O32-C31-O31-C3
52	d	201	CDL	OB9-CB7-OB8-CB6
52	i	202	CDL	OA9-CA7-OA8-CA6
52	X	201	CDL	C31-CA7-OA8-CA6
52	d	201	CDL	C71-CB7-OB8-CB6
45	Y	202	3PE	O32-C31-O31-C3
45	Y	204	3PE	O32-C31-O31-C3
46	H	401	PC1	O32-C31-O31-C3
46	H	402	PC1	O32-C31-O31-C3
46	M	605	PC1	O32-C31-O31-C3
46	d	203	PC1	O32-C31-O31-C3
46	q	203	PC1	O32-C31-O31-C3
52	M	602	CDL	OA9-CA7-OA8-CA6
52	M	602	CDL	OB9-CB7-OB8-CB6
52	X	201	CDL	OA9-CA7-OA8-CA6
52	i	202	CDL	OB9-CB7-OB8-CB6
45	I	203	3PE	O22-C21-O21-C2
45	K	101	3PE	O22-C21-O21-C2
45	L	703	3PE	O22-C21-O21-C2
45	Y	202	3PE	O22-C21-O21-C2
45	b	101	3PE	O22-C21-O21-C2
45	m	201	3PE	O22-C21-O21-C2
46	d	203	PC1	O22-C21-O21-C2
46	h	201	PC1	O22-C21-O21-C2
47	B	202	PLC	O'-C'-O2-C2
47	L	706	PLC	O'-C'-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	L	701	CDL	OA7-CA5-OA6-CA4
52	X	201	CDL	OB7-CB5-OB6-CB4
45	Y	202	3PE	C32-C31-O31-C3
45	Y	204	3PE	C32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
46	H	401	PC1	C32-C31-O31-C3
46	H	402	PC1	C32-C31-O31-C3
46	M	605	PC1	C32-C31-O31-C3
46	d	203	PC1	C32-C31-O31-C3
46	m	203	PC1	C32-C31-O31-C3
46	q	203	PC1	C32-C31-O31-C3
47	Z	202	PLC	C1B-CB-O3-C3
52	M	602	CDL	C31-CA7-OA8-CA6
52	M	602	CDL	C71-CB7-OB8-CB6
52	i	202	CDL	C31-CA7-OA8-CA6
45	K	101	3PE	C22-C21-O21-C2
45	L	702	3PE	C22-C21-O21-C2
45	L	704	3PE	C22-C21-O21-C2
45	N	402	3PE	C22-C21-O21-C2
45	Y	205	3PE	C22-C21-O21-C2
45	m	202	3PE	C22-C21-O21-C2
52	M	602	CDL	C51-CB5-OB6-CB4
52	X	201	CDL	C11-CA5-OA6-CA4
52	d	201	CDL	C51-CB5-OB6-CB4
52	i	202	CDL	C51-CB5-OB6-CB4
45	N	402	3PE	O32-C31-O31-C3
52	i	202	CDL	C71-CB7-OB8-CB6
45	g	201	3PE	O22-C21-O21-C2
45	M	604	3PE	O32-C31-O31-C3
47	Z	202	PLC	OB-CB-O3-C3
52	N	401	CDL	OB7-CB5-OB6-CB4
45	Y	203	3PE	C32-C31-O31-C3
46	L	705	PC1	C32-C31-O31-C3
52	N	401	CDL	C71-CB7-OB8-CB6
45	Y	203	3PE	O32-C31-O31-C3
47	A	204	PLC	OB-CB-O3-C3
47	M	607	PLC	C1'-C'-O2-C2
52	M	602	CDL	C11-CA5-OA6-CA4
45	M	604	3PE	C32-C31-O31-C3
45	N	402	3PE	C32-C31-O31-C3
46	A	203	PC1	C32-C31-O31-C3
47	A	204	PLC	C1B-CB-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	M	602	CDL	OA7-CA5-OA6-CA4
45	M	604	3PE	C2-C1-O11-P
46	A	203	PC1	O32-C31-O31-C3
45	d	202	3PE	C32-C31-O31-C3
46	L	705	PC1	O32-C31-O31-C3
52	N	401	CDL	OB9-CB7-OB8-CB6
45	d	202	3PE	O32-C31-O31-C3
46	I	205	PC1	C32-C31-O31-C3
52	L	701	CDL	C31-CA7-OA8-CA6
52	d	201	CDL	O1-C1-CA2-OA2
46	I	205	PC1	O32-C31-O31-C3
47	M	607	PLC	O'-C'-O2-C2
46	d	203	PC1	O11-C1-C2-O21
52	i	202	CDL	CA7-C31-C32-C33
52	L	701	CDL	OA9-CA7-OA8-CA6
45	M	604	3PE	C31-C32-C33-C34
47	g	202	PLC	C'-C1'-C2'-C3'
45	K	101	3PE	C21-C22-C23-C24
45	m	202	3PE	C21-C22-C23-C24
52	N	401	CDL	CB7-C71-C72-C73
45	Y	204	3PE	C21-C22-C23-C24
45	Z	201	3PE	C21-C22-C23-C24
46	A	202	PC1	C21-C22-C23-C24
52	M	602	CDL	CA5-C11-C12-C13
45	L	702	3PE	C31-C32-C33-C34
46	m	203	PC1	C31-C32-C33-C34
52	q	201	CDL	CA5-C11-C12-C13
45	b	101	3PE	C21-C22-C23-C24
47	Z	202	PLC	C2-C3-O3-CB
45	L	703	3PE	C31-C32-C33-C34
45	m	202	3PE	C32-C31-O31-C3
52	N	401	CDL	C31-CA7-OA8-CA6
52	d	201	CDL	C11-CA5-OA6-CA4
52	d	201	CDL	OA7-CA5-OA6-CA4
47	g	202	PLC	C1B-CB-O3-C3
46	h	201	PC1	C2-C1-O11-P
52	N	401	CDL	OA9-CA7-OA8-CA6
45	b	101	3PE	C3-C2-O21-C21
57	U	101	EHZ	C5-C6-C7-O1
45	I	203	3PE	O11-C1-C2-O21
45	Y	201	3PE	C22-C21-O21-C2
46	m	203	PC1	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	A	204	PLC	CB-C1B-C2B-C3B
45	Y	204	3PE	C33-C34-C35-C36
57	U	101	EHZ	C3-C4-C5-C6
45	L	703	3PE	C35-C36-C37-C38
45	L	703	3PE	C3E-C3F-C3G-C3H
46	M	605	PC1	C2A-C2B-C2C-C2D
52	M	602	CDL	C74-C75-C76-C77
47	B	202	PLC	CB-C1B-C2B-C3B
52	N	401	CDL	CA5-C11-C12-C13
46	H	402	PC1	C36-C37-C38-C39
46	m	203	PC1	C3B-C3C-C3D-C3E
52	L	701	CDL	C57-C58-C59-C60
52	d	201	CDL	C38-C39-C40-C41
45	I	203	3PE	C32-C31-O31-C3
45	A	201	3PE	C2C-C2D-C2E-C2F
45	g	201	3PE	C37-C38-C39-C3A
46	H	402	PC1	C3A-C3B-C3C-C3D
46	L	705	PC1	C23-C24-C25-C26
52	N	401	CDL	C58-C59-C60-C61
52	X	201	CDL	C13-C14-C15-C16
45	Y	201	3PE	O22-C21-O21-C2
52	N	401	CDL	C36-C37-C38-C39
52	i	202	CDL	CB5-C51-C52-C53
52	q	201	CDL	CA7-C31-C32-C33
45	A	201	3PE	C2B-C2C-C2D-C2E
46	L	705	PC1	C2B-C2C-C2D-C2E
46	q	202	PC1	C27-C28-C29-C2A
52	X	201	CDL	C37-C38-C39-C40
45	D	501	3PE	C2A-C2B-C2C-C2D
59	o	201	MYR	C9-C10-C11-C12
46	A	202	PC1	C22-C21-O21-C2
52	L	701	CDL	C51-CB5-OB6-CB4
52	N	401	CDL	C11-CA5-OA6-CA4
45	Y	202	3PE	C2E-C2F-C2G-C2H
45	b	101	3PE	C34-C35-C36-C37
46	L	705	PC1	C2E-C2F-C2G-C2H
47	Y	206	PLC	C1'-C2'-C3'-C4'
45	m	202	3PE	O32-C31-O31-C3
45	A	201	3PE	C36-C37-C38-C39
52	X	201	CDL	C78-C79-C80-C81
45	m	202	3PE	C3A-C3B-C3C-C3D
46	H	401	PC1	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	N	401	CDL	C59-C60-C61-C62
45	L	702	3PE	C32-C33-C34-C35
45	M	603	3PE	C35-C36-C37-C38
45	Y	203	3PE	C26-C27-C28-C29
46	I	205	PC1	C22-C23-C24-C25
46	q	203	PC1	C36-C37-C38-C39
52	M	602	CDL	C83-C84-C85-C86
45	L	703	3PE	C33-C34-C35-C36
52	q	201	CDL	C53-C54-C55-C56
46	L	705	PC1	C1-C2-C3-O31
45	Y	203	3PE	C32-C33-C34-C35
45	m	201	3PE	C2B-C2C-C2D-C2E
46	H	401	PC1	C25-C26-C27-C28
46	L	705	PC1	C3E-C3F-C3G-C3H
46	q	202	PC1	C32-C33-C34-C35
46	q	202	PC1	C34-C35-C36-C37
46	q	202	PC1	C3C-C3D-C3E-C3F
45	M	603	3PE	C33-C34-C35-C36
45	N	402	3PE	C36-C37-C38-C39
45	Y	204	3PE	C2C-C2D-C2E-C2F
47	A	204	PLC	C3'-C4'-C5'-C6'
47	Z	202	PLC	C1B-C2B-C3B-C4B
59	o	201	MYR	C4-C5-C6-C7
46	H	401	PC1	C23-C24-C25-C26
46	L	705	PC1	C3B-C3C-C3D-C3E
52	L	701	CDL	C83-C84-C85-C86
52	X	201	CDL	C35-C36-C37-C38
52	M	602	CDL	C63-C64-C65-C66
46	L	705	PC1	C39-C3A-C3B-C3C
46	m	203	PC1	C37-C38-C39-C3A
52	X	201	CDL	C16-C17-C18-C19
52	X	201	CDL	C58-C59-C60-C61
45	Y	201	3PE	C21-C22-C23-C24
52	N	401	CDL	C18-C19-C20-C21
52	N	401	CDL	C51-C52-C53-C54
52	L	701	CDL	C71-CB7-OB8-CB6
45	L	702	3PE	C21-C22-C23-C24
45	D	501	3PE	C24-C25-C26-C27
45	I	203	3PE	O32-C31-O31-C3
46	m	203	PC1	O22-C21-O21-C2
52	L	701	CDL	OB7-CB5-OB6-CB4
45	Z	201	3PE	C27-C28-C29-C2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	d	203	PC1	C32-C33-C34-C35
52	M	602	CDL	C14-C15-C16-C17
52	d	201	CDL	C72-C73-C74-C75
45	A	201	3PE	C32-C33-C34-C35
45	M	603	3PE	C3C-C3D-C3E-C3F
46	M	605	PC1	C28-C29-C2A-C2B
52	d	201	CDL	C40-C41-C42-C43
45	L	702	3PE	C3C-C3D-C3E-C3F
52	N	401	CDL	C22-C23-C24-C25
52	X	201	CDL	C32-C33-C34-C35
45	M	604	3PE	C22-C21-O21-C2
45	Y	203	3PE	C22-C21-O21-C2
46	A	203	PC1	C22-C21-O21-C2
46	H	402	PC1	C22-C21-O21-C2
46	I	204	PC1	C22-C21-O21-C2
46	I	205	PC1	C22-C21-O21-C2
46	L	705	PC1	C22-C21-O21-C2
45	N	402	3PE	C26-C27-C28-C29
52	i	202	CDL	C15-C16-C17-C18
45	Y	203	3PE	O22-C21-O21-C2
46	A	202	PC1	O22-C21-O21-C2
46	I	204	PC1	O22-C21-O21-C2
46	L	705	PC1	O22-C21-O21-C2
52	N	401	CDL	OA7-CA5-OA6-CA4
45	Y	204	3PE	C35-C36-C37-C38
52	d	201	CDL	C42-C43-C44-C45
46	H	401	PC1	C37-C38-C39-C3A
52	M	602	CDL	CB5-C51-C52-C53
52	d	201	CDL	CB7-C71-C72-C73
45	D	501	3PE	C38-C39-C3A-C3B
45	D	501	3PE	C29-C2A-C2B-C2C
45	L	702	3PE	C39-C3A-C3B-C3C
47	M	607	PLC	C7B-C8B-C9B-CAA
45	L	703	3PE	C25-C26-C27-C28
45	Y	202	3PE	C29-C2A-C2B-C2C
52	L	701	CDL	C33-C34-C35-C36
45	Y	203	3PE	C31-C32-C33-C34
52	M	602	CDL	CB7-C71-C72-C73
46	I	204	PC1	C36-C37-C38-C39
52	M	602	CDL	C41-C42-C43-C44
45	D	501	3PE	O11-C1-C2-O21
45	M	603	3PE	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	q	202	PC1	O11-C1-C2-O21
46	L	705	PC1	C37-C38-C39-C3A
52	q	201	CDL	C17-C18-C19-C20
47	L	706	PLC	C1B-C2B-C3B-C4B
45	L	704	3PE	C27-C28-C29-C2A
47	A	204	PLC	C6'-C7'-C8'-C9'
52	N	401	CDL	C17-C18-C19-C20
46	L	705	PC1	O21-C2-C3-O31
52	N	401	CDL	OB6-CB4-CB6-OB8
52	L	701	CDL	OB9-CB7-OB8-CB6
45	K	101	3PE	C33-C34-C35-C36
52	L	701	CDL	C54-C55-C56-C57
46	I	204	PC1	C2D-C2E-C2F-C2G
52	X	201	CDL	C52-C53-C54-C55
45	Y	203	3PE	C38-C39-C3A-C3B
45	M	604	3PE	O22-C21-O21-C2
46	I	205	PC1	C25-C26-C27-C28
46	I	205	PC1	C34-C35-C36-C37
52	N	401	CDL	C20-C21-C22-C23
45	K	101	3PE	C26-C27-C28-C29
45	M	603	3PE	C38-C39-C3A-C3B
57	T	101	EHZ	C22-C23-C24-C25
47	L	706	PLC	C'-C1'-C2'-C3'
45	L	704	3PE	C28-C29-C2A-C2B
45	Y	201	3PE	C22-C23-C24-C25
47	A	204	PLC	C4B-C5B-C6B-C7B
47	g	202	PLC	OB-CB-O3-C3
45	K	101	3PE	C38-C39-C3A-C3B
52	L	701	CDL	C16-C17-C18-C19
45	I	203	3PE	O11-C1-C2-C3
45	K	101	3PE	O11-C1-C2-C3
45	M	603	3PE	O11-C1-C2-C3
45	M	604	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
46	H	402	PC1	O11-C1-C2-C3
46	d	203	PC1	O11-C1-C2-C3
47	L	706	PLC	O3P-C1-C2-C3
52	M	602	CDL	OB5-CB3-CB4-CB6
52	q	201	CDL	OB5-CB3-CB4-CB6
46	H	402	PC1	O22-C21-O21-C2
46	I	205	PC1	O22-C21-O21-C2
45	Z	201	3PE	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	B	202	PLC	C4B-C5B-C6B-C7B
57	U	101	EHZ	C5-C6-C7-C8
45	A	201	3PE	C24-C25-C26-C27
45	m	202	3PE	C33-C34-C35-C36
52	M	602	CDL	C79-C80-C81-C82
46	I	205	PC1	C24-C25-C26-C27
52	q	201	CDL	C72-C73-C74-C75
52	M	602	CDL	C40-C41-C42-C43
45	M	604	3PE	C32-C33-C34-C35
46	A	203	PC1	C23-C24-C25-C26
52	X	201	CDL	C22-C23-C24-C25
45	D	501	3PE	C2E-C2F-C2G-C2H
52	i	202	CDL	C72-C73-C74-C75
46	H	402	PC1	C21-C22-C23-C24
45	Y	201	3PE	C1-C2-C3-O31
45	Z	201	3PE	C1-C2-C3-O31
45	d	202	3PE	C1-C2-C3-O31
45	g	201	3PE	C1-C2-C3-O31
45	m	201	3PE	C1-C2-C3-O31
45	m	202	3PE	C1-C2-C3-O31
46	M	606	PC1	C1-C2-C3-O31
46	q	202	PC1	C1-C2-C3-O31
47	g	202	PLC	C1-C2-C3-O3
45	Y	204	3PE	C2B-C2C-C2D-C2E
46	M	605	PC1	C32-C33-C34-C35
46	q	202	PC1	C3A-C3B-C3C-C3D
47	B	202	PLC	C7B-C8B-C9B-CAA
52	i	202	CDL	C34-C35-C36-C37
57	T	101	EHZ	C2-C1-C21-C22
45	Y	203	3PE	C29-C2A-C2B-C2C
46	M	605	PC1	C26-C27-C28-C29
45	M	604	3PE	C33-C34-C35-C36
45	m	201	3PE	C2A-C2B-C2C-C2D
52	i	202	CDL	C56-C57-C58-C59
46	h	201	PC1	C26-C27-C28-C29
46	m	203	PC1	C28-C29-C2A-C2B
52	d	201	CDL	OB5-CB3-CB4-OB6
52	i	202	CDL	C11-CA5-OA6-CA4
47	A	204	PLC	C3B-C4B-C5B-C6B
45	I	203	3PE	C22-C23-C24-C25
45	L	704	3PE	C23-C24-C25-C26
45	Z	201	3PE	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	H	402	PC1	C32-C33-C34-C35
46	H	401	PC1	C34-C35-C36-C37
47	Z	202	PLC	C6B-C7B-C8B-C9B
52	d	201	CDL	C31-C32-C33-C34
45	A	201	3PE	O21-C2-C3-O31
46	d	203	PC1	O21-C2-C3-O31
52	M	602	CDL	C13-C14-C15-C16
52	d	201	CDL	C34-C35-C36-C37
45	L	703	3PE	C3A-C3B-C3C-C3D
47	B	202	PLC	C2B-C3B-C4B-C5B
45	Z	201	3PE	C35-C36-C37-C38
45	d	202	3PE	C31-C32-C33-C34
52	N	401	CDL	CB5-C51-C52-C53
52	i	202	CDL	C58-C59-C60-C61
47	Y	206	PLC	C5'-C6'-C7'-C8'
57	U	101	EHZ	C1-C2-C3-C4
52	N	401	CDL	C19-C20-C21-C22
46	A	203	PC1	O22-C21-O21-C2
58	i	201	CHD	C17-C20-C22-C23
52	X	201	CDL	C1-CB2-OB2-PB2
52	M	602	CDL	C76-C77-C78-C79
45	L	702	3PE	C3F-C3G-C3H-C3I
47	B	202	PLC	C4'-C5'-C6'-C7'
57	U	101	EHZ	C2-C1-C21-C22
45	A	201	3PE	O11-C1-C2-C3
45	D	501	3PE	O11-C1-C2-C3
45	N	402	3PE	O11-C1-C2-C3
45	Y	202	3PE	O11-C1-C2-C3
46	q	202	PC1	O11-C1-C2-C3
47	Z	202	PLC	O3P-C1-C2-C3
52	X	201	CDL	OA5-CA3-CA4-CA6
46	M	605	PC1	C22-C21-O21-C2
45	A	201	3PE	C33-C34-C35-C36
52	X	201	CDL	C44-C45-C46-C47
45	g	201	3PE	C34-C35-C36-C37
46	m	203	PC1	C2B-C2C-C2D-C2E
45	I	203	3PE	C27-C28-C29-C2A
45	M	604	3PE	C28-C29-C2A-C2B
45	Y	204	3PE	C38-C39-C3A-C3B
45	Y	202	3PE	C31-C32-C33-C34
52	X	201	CDL	C19-C20-C21-C22
45	A	201	3PE	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	L	704	3PE	C1-C2-C3-O31
45	Y	205	3PE	C1-C2-C3-O31
46	H	401	PC1	C1-C2-C3-O31
52	M	602	CDL	CA3-CA4-CA6-OA8
52	N	401	CDL	CB3-CB4-CB6-OB8
52	X	201	CDL	CB3-CB4-CB6-OB8
52	q	201	CDL	CA3-CA4-CA6-OA8
46	h	201	PC1	C2B-C2C-C2D-C2E
46	d	203	PC1	C39-C3A-C3B-C3C
52	M	602	CDL	C15-C16-C17-C18
52	X	201	CDL	C11-C12-C13-C14
46	H	402	PC1	C2-C3-O31-C31
52	X	201	CDL	CB7-C71-C72-C73
46	h	201	PC1	C25-C26-C27-C28
46	H	402	PC1	O11-C1-C2-O21
47	L	706	PLC	O3P-C1-C2-O2
52	q	201	CDL	OB5-CB3-CB4-OB6
52	M	602	CDL	C16-C17-C18-C19
50	F	501	FMN	C4'-C5'-O5'-P
52	d	201	CDL	C1-CB2-OB2-PB2
47	Y	206	PLC	C8'-C9'-CA'-CB'
57	T	101	EHZ	O1-C7-C8-C9
57	U	101	EHZ	O1-C7-C8-C9
45	I	203	3PE	C24-C25-C26-C27
45	m	202	3PE	C3D-C3E-C3F-C3G
52	X	201	CDL	C71-C72-C73-C74
45	Y	202	3PE	C33-C34-C35-C36
45	d	202	3PE	C24-C25-C26-C27
52	X	201	CDL	C64-C65-C66-C67
45	L	704	3PE	O21-C2-C3-O31
45	m	202	3PE	O21-C2-C3-O31
47	A	204	PLC	O2-C2-C3-O3
45	m	202	3PE	C37-C38-C39-C3A
52	X	201	CDL	C17-C18-C19-C20
52	L	701	CDL	C24-C25-C26-C27
45	L	703	3PE	C3C-C3D-C3E-C3F
45	m	201	3PE	C32-C33-C34-C35
52	L	701	CDL	C63-C64-C65-C66
45	L	704	3PE	C26-C27-C28-C29
45	d	202	3PE	C22-C23-C24-C25
45	I	203	3PE	C26-C27-C28-C29
46	H	402	PC1	C3E-C3F-C3G-C3H

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	L	701	CDL	C76-C77-C78-C79
45	Z	201	3PE	C31-C32-C33-C34
46	A	203	PC1	C21-C22-C23-C24
45	g	201	3PE	C32-C31-O31-C3
45	m	201	3PE	C27-C28-C29-C2A
52	L	701	CDL	C81-C82-C83-C84
45	b	101	3PE	C32-C33-C34-C35
45	m	202	3PE	C3E-C3F-C3G-C3H
45	D	501	3PE	C2C-C2D-C2E-C2F
47	B	202	PLC	C8B-C9B-CAA-CBA
45	m	201	3PE	O21-C21-C22-C23
46	m	203	PC1	C2A-C2B-C2C-C2D
52	q	201	CDL	C51-CB5-OB6-CB4
45	L	704	3PE	C2D-C2E-C2F-C2G
52	L	701	CDL	C79-C80-C81-C82
52	X	201	CDL	CB2-C1-CA2-OA2
47	B	202	PLC	C6B-C7B-C8B-C9B
52	q	201	CDL	C16-C17-C18-C19
52	d	201	CDL	C31-CA7-OA8-CA6
45	Y	202	3PE	C35-C36-C37-C38
45	Y	202	3PE	C27-C28-C29-C2A
46	A	203	PC1	C34-C35-C36-C37
47	B	202	PLC	C1'-C2'-C3'-C4'
45	Y	203	3PE	C36-C37-C38-C39
46	I	204	PC1	C22-C23-C24-C25
52	L	701	CDL	C39-C40-C41-C42
52	i	202	CDL	OA7-CA5-OA6-CA4
52	M	602	CDL	C11-C12-C13-C14
46	I	204	PC1	C35-C36-C37-C38
52	X	201	CDL	C55-C56-C57-C58
52	N	401	CDL	CA6-CA4-OA6-CA5
52	X	201	CDL	CA6-CA4-OA6-CA5
45	D	501	3PE	C33-C34-C35-C36
45	D	501	3PE	C35-C36-C37-C38
46	M	605	PC1	O22-C21-O21-C2
45	A	201	3PE	O11-C1-C2-O21
45	M	604	3PE	O11-C1-C2-O21
45	N	402	3PE	O11-C1-C2-O21
45	Y	202	3PE	O11-C1-C2-O21
45	Y	204	3PE	O11-C1-C2-O21
46	L	705	PC1	O11-C1-C2-O21
46	M	605	PC1	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	Z	202	PLC	O3P-C1-C2-O2
50	F	501	FMN	O3'-C3'-C4'-C5'
47	A	204	PLC	C1-C2-C3-O3
47	B	202	PLC	C7'-C8'-C9'-CA'
46	H	401	PC1	C33-C34-C35-C36
45	D	501	3PE	C12-C11-O13-P
45	I	203	3PE	C12-C11-O13-P
45	Y	202	3PE	C12-C11-O13-P
45	m	201	3PE	C12-C11-O13-P
45	m	202	3PE	C12-C11-O13-P
46	H	402	PC1	C12-C11-O13-P
46	M	606	PC1	C12-C11-O13-P
46	m	203	PC1	C3E-C3F-C3G-C3H
45	Y	201	3PE	O21-C2-C3-O31
46	H	401	PC1	O21-C2-C3-O31
52	M	602	CDL	OA6-CA4-CA6-OA8
52	q	201	CDL	OA6-CA4-CA6-OA8
52	N	401	CDL	C31-C32-C33-C34
45	g	201	3PE	O32-C31-O31-C3
45	A	201	3PE	C25-C26-C27-C28
45	Y	204	3PE	C28-C29-C2A-C2B
46	A	202	PC1	C23-C24-C25-C26
52	M	602	CDL	C37-C38-C39-C40
46	H	401	PC1	C35-C36-C37-C38
46	h	201	PC1	C24-C25-C26-C27
45	L	703	3PE	C26-C27-C28-C29
45	L	702	3PE	C24-C25-C26-C27
46	q	203	PC1	C35-C36-C37-C38
52	N	401	CDL	C16-C17-C18-C19
46	H	402	PC1	O13-C11-C12-N
47	A	204	PLC	O4P-C4-C5-N
47	Y	206	PLC	O4P-C4-C5-N
54	O	401	DGT	PB-O3A-PA-O2A
56	P	501	NDP	PN-O3-PA-O2A
46	A	202	PC1	C31-C32-C33-C34
52	L	701	CDL	C14-C15-C16-C17
52	X	201	CDL	O1-C1-CA2-OA2
52	L	701	CDL	C31-C32-C33-C34
52	X	201	CDL	C81-C82-C83-C84
52	d	201	CDL	OA9-CA7-OA8-CA6
52	L	701	CDL	C23-C24-C25-C26
47	A	204	PLC	C2'-C3'-C4'-C5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	B	202	PLC	C3'-C4'-C5'-C6'
46	m	203	PC1	C38-C39-C3A-C3B
45	m	201	3PE	C33-C34-C35-C36
45	Y	203	3PE	O11-C1-C2-C3
45	Y	204	3PE	O11-C1-C2-C3
46	L	705	PC1	O11-C1-C2-C3
46	M	605	PC1	O11-C1-C2-C3
52	N	401	CDL	OA5-CA3-CA4-CA6
52	d	201	CDL	OB5-CB3-CB4-CB6
46	m	203	PC1	C3D-C3E-C3F-C3G
57	T	101	EHZ	C18-C17-C20-O6
57	T	101	EHZ	C19-C17-C20-O6
57	T	101	EHZ	C5-C6-C7-O1
45	Y	203	3PE	C39-C3A-C3B-C3C
52	d	201	CDL	C44-C45-C46-C47
52	d	201	CDL	C77-C78-C79-C80
46	d	203	PC1	C37-C38-C39-C3A
52	L	701	CDL	C19-C20-C21-C22
45	b	101	3PE	C2-C1-O11-P
45	N	402	3PE	C28-C29-C2A-C2B
45	N	402	3PE	C22-C23-C24-C25
52	L	701	CDL	C61-C62-C63-C64
59	o	201	MYR	C6-C7-C8-C9
52	q	201	CDL	OB7-CB5-OB6-CB4
45	L	703	3PE	O11-C1-C2-O21
45	Y	203	3PE	O11-C1-C2-O21
46	A	202	PC1	O11-C1-C2-O21
52	X	201	CDL	OA5-CA3-CA4-OA6
46	M	606	PC1	C35-C36-C37-C38
50	F	501	FMN	C2'-C3'-C4'-O4'
46	L	705	PC1	C2F-C2G-C2H-C2I
45	m	201	3PE	C34-C35-C36-C37
45	D	501	3PE	C37-C38-C39-C3A
45	Y	205	3PE	O21-C2-C3-O31
45	m	201	3PE	O21-C2-C3-O31
52	X	201	CDL	OB6-CB4-CB6-OB8
52	L	701	CDL	C75-C76-C77-C78
46	d	203	PC1	C1-C2-C3-O31
52	i	202	CDL	CA3-CA4-CA6-OA8
52	L	701	CDL	O1-C1-CB2-OB2
45	N	402	3PE	C2F-C2G-C2H-C2I
45	L	703	3PE	C2B-C2C-C2D-C2E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	m	203	PC1	C32-C33-C34-C35
46	q	202	PC1	C36-C37-C38-C39
45	D	501	3PE	C1-O11-P-O12
45	D	501	3PE	O13-C11-C12-N
45	I	203	3PE	C1-O11-P-O14
45	L	702	3PE	C1-O11-P-O14
45	L	702	3PE	O13-C11-C12-N
45	M	603	3PE	C1-O11-P-O14
45	M	603	3PE	C11-O13-P-O11
45	M	603	3PE	O13-C11-C12-N
45	M	604	3PE	C1-O11-P-O14
45	M	604	3PE	C11-O13-P-O14
45	M	604	3PE	O13-C11-C12-N
45	N	402	3PE	C11-O13-P-O14
45	Y	201	3PE	C1-O11-P-O12
45	Y	203	3PE	C11-O13-P-O14
45	Y	205	3PE	C1-O11-P-O14
45	Y	205	3PE	C11-O13-P-O14
45	Y	205	3PE	O13-C11-C12-N
45	d	202	3PE	C11-O13-P-O14
45	m	201	3PE	C1-O11-P-O12
45	m	201	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O12
45	m	201	3PE	C11-O13-P-O14
45	m	201	3PE	O13-C11-C12-N
45	m	202	3PE	C1-O11-P-O12
45	m	202	3PE	C11-O13-P-O11
45	m	202	3PE	C11-O13-P-O12
45	m	202	3PE	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O14
46	H	402	PC1	C1-O11-P-O12
46	I	205	PC1	C11-O13-P-O12
46	I	205	PC1	C11-O13-P-O14
46	I	205	PC1	C11-O13-P-O11
46	d	203	PC1	C1-O11-P-O12
46	d	203	PC1	C1-O11-P-O14
46	d	203	PC1	C1-O11-P-O13
46	h	201	PC1	C11-O13-P-O14
46	h	201	PC1	C1-O11-P-O13
46	m	203	PC1	C11-O13-P-O14
46	m	203	PC1	C11-O13-P-O11
46	q	203	PC1	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	q	203	PC1	C11-O13-P-O14
46	q	203	PC1	C11-O13-P-O11
47	L	706	PLC	C4-O4P-P-O1P
47	L	706	PLC	C4-O4P-P-O3P
47	M	607	PLC	C4-O4P-P-O1P
52	N	401	CDL	CA2-OA2-PA1-OA4
52	N	401	CDL	CB2-OB2-PB2-OB5
52	d	201	CDL	CA3-OA5-PA1-OA2
52	d	201	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	CA3-OA5-PA1-OA4
52	d	201	CDL	CB2-OB2-PB2-OB3
52	i	202	CDL	CB3-OB5-PB2-OB2
52	i	202	CDL	CB3-OB5-PB2-OB3
52	i	202	CDL	CB3-OB5-PB2-OB4
52	q	201	CDL	CA2-OA2-PA1-OA4
52	q	201	CDL	CB2-OB2-PB2-OB3
52	q	201	CDL	CB2-OB2-PB2-OB5
54	O	401	DGT	C5'-O5'-PA-O3A
45	m	201	3PE	C2F-C2G-C2H-C2I
46	m	203	PC1	C35-C36-C37-C38
46	A	203	PC1	C32-C33-C34-C35
46	H	401	PC1	C22-C21-O21-C2
58	i	201	CHD	C21-C20-C22-C23
45	Y	201	3PE	C23-C24-C25-C26
45	Y	204	3PE	C2-C1-O11-P
45	m	202	3PE	C2-C1-O11-P
46	M	606	PC1	C2-C1-O11-P
47	Z	202	PLC	C2-C1-O3P-P
52	L	701	CDL	CB4-CB3-OB5-PB2
52	i	202	CDL	CB4-CB3-OB5-PB2
45	N	402	3PE	C32-C33-C34-C35
47	B	202	PLC	C'-C1'-C2'-C3'
46	M	605	PC1	C23-C24-C25-C26
46	q	202	PC1	C29-C2A-C2B-C2C
45	d	202	3PE	C28-C29-C2A-C2B
47	L	706	PLC	C3'-C4'-C5'-C6'
45	Y	203	3PE	C3-C2-O21-C21
47	Z	202	PLC	C1-C2-O2-C'
52	L	701	CDL	CA6-CA4-OA6-CA5
52	q	201	CDL	C13-C14-C15-C16
52	N	401	CDL	C55-C56-C57-C58
46	M	605	PC1	C11-C12-N-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	A	202	PC1	O11-C1-C2-C3
45	M	603	3PE	C39-C3A-C3B-C3C
46	L	705	PC1	C3A-C3B-C3C-C3D
45	D	501	3PE	C31-C32-C33-C34
47	M	607	PLC	CB-C1B-C2B-C3B
52	M	602	CDL	CA7-C31-C32-C33
52	X	201	CDL	CA2-C1-CB2-OB2
45	D	501	3PE	C34-C35-C36-C37
52	N	401	CDL	C56-C57-C58-C59
52	d	201	CDL	C36-C37-C38-C39
45	Z	201	3PE	O32-C31-O31-C3
45	Z	201	3PE	C2F-C2G-C2H-C2I
52	X	201	CDL	C36-C37-C38-C39
46	H	401	PC1	O22-C21-O21-C2
45	d	202	3PE	C34-C35-C36-C37
45	L	703	3PE	O21-C2-C3-O31
46	q	202	PC1	O21-C2-C3-O31
45	Y	203	3PE	C37-C38-C39-C3A
45	b	101	3PE	C25-C26-C27-C28
46	A	203	PC1	C3A-C3B-C3C-C3D
52	X	201	CDL	C84-C85-C86-C87
47	Y	206	PLC	C1'-C'-O2-C2
45	D	501	3PE	C39-C3A-C3B-C3C
45	L	704	3PE	C2C-C2D-C2E-C2F
47	Y	206	PLC	O'-C'-O2-C2
45	g	201	3PE	C36-C37-C38-C39
52	N	401	CDL	C21-C22-C23-C24
46	A	203	PC1	C22-C23-C24-C25
46	I	204	PC1	C29-C2A-C2B-C2C
46	M	605	PC1	C33-C34-C35-C36
45	A	201	3PE	C37-C38-C39-C3A
45	Z	201	3PE	C32-C31-O31-C3
46	M	605	PC1	C11-C12-N-C15
45	Y	203	3PE	C3B-C3C-C3D-C3E
52	d	201	CDL	CB2-C1-CA2-OA2
52	N	401	CDL	C11-C12-C13-C14
46	I	204	PC1	C3B-C3C-C3D-C3E
52	q	201	CDL	C71-CB7-OB8-CB6
56	P	501	NDP	O4D-C1D-N1N-C6N
46	A	203	PC1	O11-C1-C2-O21
45	g	201	3PE	C32-C33-C34-C35
46	I	205	PC1	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	H	402	PC1	C3B-C3C-C3D-C3E
46	d	203	PC1	C23-C24-C25-C26
46	d	203	PC1	C34-C35-C36-C37
47	g	202	PLC	C1'-C2'-C3'-C4'
52	M	602	CDL	C44-C45-C46-C47
45	g	201	3PE	C33-C34-C35-C36
52	M	602	CDL	C81-C82-C83-C84
46	I	205	PC1	C21-C22-C23-C24
46	M	605	PC1	C2D-C2E-C2F-C2G
45	M	604	3PE	C2B-C2C-C2D-C2E
46	L	705	PC1	C34-C35-C36-C37
46	L	705	PC1	C33-C34-C35-C36
46	m	203	PC1	C22-C23-C24-C25
45	b	101	3PE	C33-C34-C35-C36
46	I	204	PC1	C37-C38-C39-C3A
45	M	604	3PE	C25-C26-C27-C28
52	N	401	CDL	CA2-C1-CB2-OB2
45	L	702	3PE	C2-C3-O31-C31
45	N	402	3PE	C2D-C2E-C2F-C2G
46	m	203	PC1	C24-C25-C26-C27
47	A	204	PLC	C7'-C8'-C9'-CA'
46	L	705	PC1	C27-C28-C29-C2A
46	h	201	PC1	C23-C24-C25-C26
46	d	203	PC1	C3A-C3B-C3C-C3D
45	L	702	3PE	C1-C2-O21-C21
45	L	702	3PE	C3-C2-O21-C21
45	L	703	3PE	C3-C2-O21-C21
47	Z	202	PLC	C3-C2-O2-C'
52	X	201	CDL	CB6-CB4-OB6-CB5
46	I	205	PC1	C3A-C3B-C3C-C3D
46	L	705	PC1	C32-C33-C34-C35
52	q	201	CDL	C52-C51-CB5-OB6
45	M	603	3PE	C3A-C3B-C3C-C3D
46	M	605	PC1	C35-C36-C37-C38
52	q	201	CDL	C31-C32-C33-C34
52	q	201	CDL	OB9-CB7-OB8-CB6
45	D	501	3PE	C36-C37-C38-C39
46	M	605	PC1	C11-C12-N-C14
52	L	701	CDL	C78-C79-C80-C81
46	d	203	PC1	C3B-C3C-C3D-C3E
46	h	201	PC1	C32-C31-O31-C3
45	K	101	3PE	C29-C2A-C2B-C2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	604	3PE	C2D-C2E-C2F-C2G
45	M	603	3PE	C2-C1-O11-P
45	Y	202	3PE	C2-C1-O11-P
52	q	201	CDL	C19-C20-C21-C22
45	g	201	3PE	C39-C3A-C3B-C3C
52	d	201	CDL	OA5-CA3-CA4-CA6
46	H	401	PC1	C2D-C2E-C2F-C2G
46	A	203	PC1	C38-C39-C3A-C3B
52	i	202	CDL	OA6-CA4-CA6-OA8
45	Y	203	3PE	C35-C36-C37-C38
52	X	201	CDL	C62-C63-C64-C65
45	Y	205	3PE	C2C-C2D-C2E-C2F
52	d	201	CDL	C41-C42-C43-C44
45	A	201	3PE	C3B-C3C-C3D-C3E
45	D	501	3PE	C2D-C2E-C2F-C2G
45	N	402	3PE	C34-C35-C36-C37
52	N	401	CDL	C71-C72-C73-C74
52	L	701	CDL	CA2-C1-CB2-OB2
50	F	501	FMN	C2'-C3'-C4'-C5'
45	M	603	3PE	C23-C24-C25-C26
52	q	201	CDL	C15-C16-C17-C18
45	Y	204	3PE	C2F-C2G-C2H-C2I
45	K	101	3PE	O21-C21-C22-C23
45	L	704	3PE	C2B-C2C-C2D-C2E
52	i	202	CDL	C54-C55-C56-C57
46	q	203	PC1	C37-C38-C39-C3A
52	M	602	CDL	C19-C20-C21-C22
46	M	605	PC1	C2C-C2D-C2E-C2F
52	M	602	CDL	C51-C52-C53-C54
52	N	401	CDL	C34-C35-C36-C37
50	F	501	FMN	O3'-C3'-C4'-O4'
45	A	201	3PE	C23-C24-C25-C26
45	L	703	3PE	C24-C25-C26-C27
45	d	202	3PE	C39-C3A-C3B-C3C
46	H	401	PC1	C36-C37-C38-C39
52	X	201	CDL	C72-C73-C74-C75
46	h	201	PC1	O32-C31-O31-C3
46	A	202	PC1	C1-C2-C3-O31
46	I	205	PC1	C1-C2-C3-O31
46	q	202	PC1	O32-C31-O31-C3
45	L	704	3PE	C21-C22-C23-C24
47	A	204	PLC	C5'-C6'-C7'-C8'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	i	202	CDL	C14-C15-C16-C17
52	N	401	CDL	OA5-CA3-CA4-OA6
46	q	202	PC1	C2A-C2B-C2C-C2D
46	A	203	PC1	C3D-C3E-C3F-C3G
45	M	604	3PE	C23-C24-C25-C26
52	X	201	CDL	C72-C71-CB7-OB8
46	A	202	PC1	C22-C23-C24-C25
45	L	703	3PE	O11-C1-C2-C3
47	Y	206	PLC	O3P-C1-C2-C3
45	N	402	3PE	C2A-C2B-C2C-C2D
45	Y	203	3PE	C28-C29-C2A-C2B
45	Y	204	3PE	C2A-C2B-C2C-C2D
46	h	201	PC1	C22-C23-C24-C25
45	D	501	3PE	C2-C1-O11-P
45	d	202	3PE	C3A-C3B-C3C-C3D
45	Y	203	3PE	C25-C26-C27-C28
52	X	201	CDL	C61-C62-C63-C64
52	i	202	CDL	C52-C53-C54-C55
50	F	501	FMN	C5'-O5'-P-O1P
52	d	201	CDL	C74-C75-C76-C77
46	d	203	PC1	C3C-C3D-C3E-C3F
46	A	202	PC1	C36-C37-C38-C39
45	d	202	3PE	C21-C22-C23-C24
52	X	201	CDL	C54-C55-C56-C57
52	X	201	CDL	C83-C84-C85-C86
46	q	202	PC1	C11-C12-N-C15
45	m	202	3PE	C32-C33-C34-C35
46	q	202	PC1	C32-C31-O31-C3
45	Y	205	3PE	O31-C31-C32-C33
45	L	704	3PE	C1-C2-O21-C21
45	L	704	3PE	C3-C2-O21-C21
47	M	607	PLC	C'-C1'-C2'-C3'
52	i	202	CDL	C31-C32-C33-C34
52	X	201	CDL	C80-C81-C82-C83
52	d	201	CDL	C1-CA2-OA2-PA1
45	m	201	3PE	O11-C1-C2-O21
52	i	202	CDL	CB7-C71-C72-C73
45	A	201	3PE	C26-C27-C28-C29
52	d	201	CDL	C35-C36-C37-C38
45	L	703	3PE	C39-C3A-C3B-C3C
45	L	704	3PE	C12-C11-O13-P
46	H	402	PC1	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	604	3PE	C2A-C2B-C2C-C2D
46	H	401	PC1	C29-C2A-C2B-C2C
52	X	201	CDL	C60-C61-C62-C63
46	q	202	PC1	C38-C39-C3A-C3B
45	M	603	3PE	C2D-C2E-C2F-C2G
52	X	201	CDL	C75-C76-C77-C78
47	B	202	PLC	C2-C3-O3-CB
45	M	604	3PE	C26-C27-C28-C29
46	q	202	PC1	C11-C12-N-C14
45	Y	202	3PE	C32-C33-C34-C35
52	M	602	CDL	C12-C11-CA5-OA6
45	Z	201	3PE	O22-C21-O21-C2
45	Y	202	3PE	C2A-C2B-C2C-C2D
45	I	203	3PE	C28-C29-C2A-C2B
45	L	702	3PE	C22-C23-C24-C25
47	B	202	PLC	C2B-C1B-CB-O3
46	M	605	PC1	O13-C11-C12-N
54	O	401	DGT	PA-O3A-PB-O1B
54	O	401	DGT	PA-O3A-PB-O2B
45	L	703	3PE	C2A-C2B-C2C-C2D
45	A	201	3PE	O31-C31-C32-C33
45	D	501	3PE	C3C-C3D-C3E-C3F
52	i	202	CDL	C73-C74-C75-C76
47	A	204	PLC	C2B-C1B-CB-O3
45	L	703	3PE	C29-C2A-C2B-C2C
46	I	204	PC1	C39-C3A-C3B-C3C
52	M	602	CDL	C32-C33-C34-C35
45	Y	202	3PE	O21-C21-C22-C23
46	h	201	PC1	O31-C31-C32-C33
52	d	201	CDL	C72-C71-CB7-OB8
45	L	703	3PE	C22-C23-C24-C25
45	Y	204	3PE	C27-C28-C29-C2A
46	m	203	PC1	C2D-C2E-C2F-C2G
52	N	401	CDL	C61-C62-C63-C64
47	Z	202	PLC	O2-C'-C1'-C2'
45	m	201	3PE	O22-C21-C22-C23
45	L	703	3PE	C2-C1-O11-P
45	N	402	3PE	O21-C21-C22-C23
46	q	203	PC1	O31-C31-C32-C33
45	d	202	3PE	C27-C28-C29-C2A
52	X	201	CDL	C63-C64-C65-C66
45	L	702	3PE	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	d	203	PC1	C36-C37-C38-C39
46	H	401	PC1	C11-C12-N-C15
46	q	202	PC1	C11-C12-N-C13
45	b	101	3PE	C27-C28-C29-C2A
52	N	401	CDL	OA6-CA4-CA6-OA8
46	I	204	PC1	C33-C34-C35-C36
52	M	602	CDL	C64-C65-C66-C67
45	m	202	3PE	C36-C37-C38-C39
45	M	604	3PE	O31-C31-C32-C33
45	Z	201	3PE	O21-C21-C22-C23
46	A	202	PC1	O21-C21-C22-C23
46	I	205	PC1	O31-C31-C32-C33
46	H	401	PC1	C32-C33-C34-C35
52	X	201	CDL	C33-C34-C35-C36
46	L	705	PC1	C31-C32-C33-C34
52	M	602	CDL	C20-C21-C22-C23
45	M	603	3PE	C3B-C3C-C3D-C3E
58	i	201	CHD	C22-C23-C24-O26
46	A	203	PC1	O11-C1-C2-C3
45	M	604	3PE	O21-C21-C22-C23
45	Y	201	3PE	O31-C31-C32-C33
50	F	501	FMN	N10-C1'-C2'-O2'
45	K	101	3PE	C28-C29-C2A-C2B
45	M	603	3PE	O21-C21-C22-C23
45	Y	204	3PE	O31-C31-C32-C33
52	q	201	CDL	C71-C72-C73-C74
57	T	101	EHZ	C5-C6-C7-C8
45	L	703	3PE	C1-C2-O21-C21
46	H	401	PC1	C11-C12-N-C13
46	H	401	PC1	C11-C12-N-C14
52	N	401	CDL	O1-C1-CB2-OB2
46	q	202	PC1	O31-C31-C32-C33
57	T	101	EHZ	C1-C2-C3-C4
45	m	201	3PE	C29-C2A-C2B-C2C
46	d	203	PC1	C35-C36-C37-C38
46	H	401	PC1	O21-C21-C22-C23
57	T	101	EHZ	C12-C13-C14-N2
46	m	203	PC1	C2-C1-O11-P
56	P	501	NDP	C2B-O2B-P2B-O1X
46	q	203	PC1	O32-C31-C32-C33
45	b	101	3PE	O31-C31-C32-C33
45	m	202	3PE	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

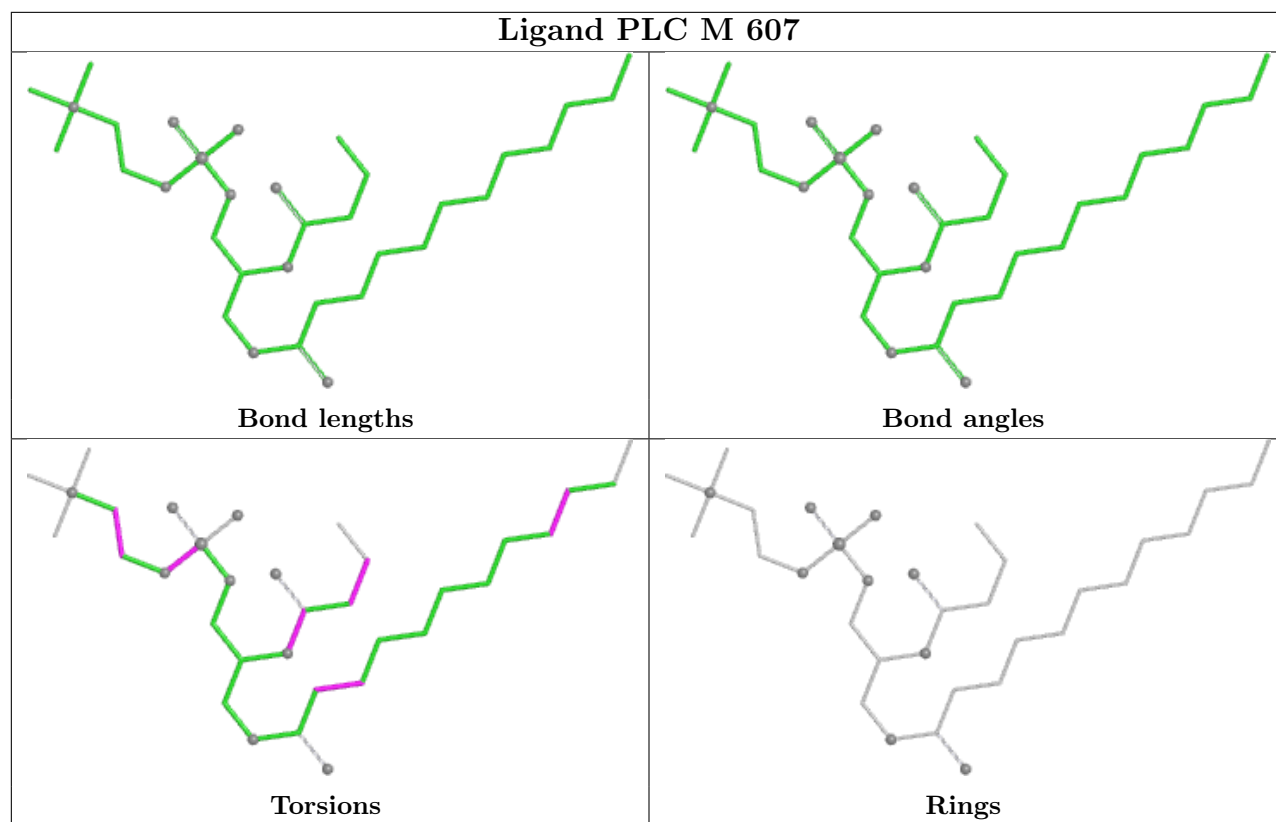
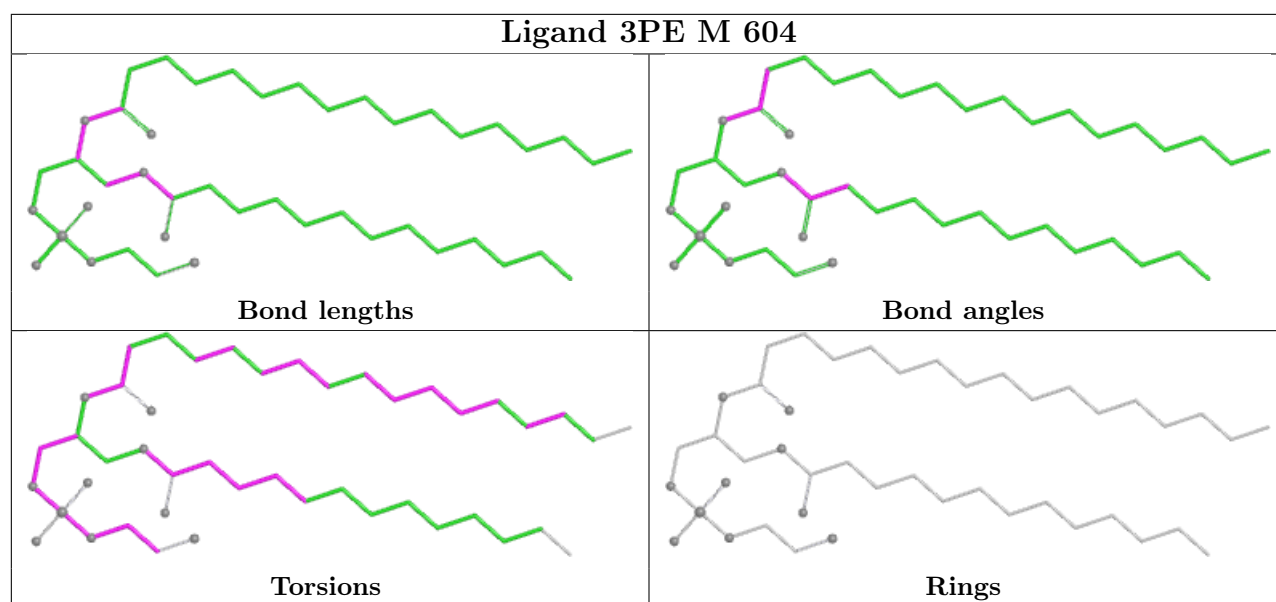
Mol	Chain	Res	Type	Atoms
52	L	701	CDL	C43-C44-C45-C46
45	N	402	3PE	O22-C21-C22-C23
52	M	602	CDL	C72-C73-C74-C75
52	i	202	CDL	C33-C34-C35-C36
47	B	202	PLC	C2B-C1B-CB-OB
52	M	602	CDL	C77-C78-C79-C80
45	Z	201	3PE	C22-C21-O21-C2
46	I	204	PC1	C11-C12-N-C15
45	Y	202	3PE	O22-C21-C22-C23
46	h	201	PC1	O32-C31-C32-C33
47	Z	202	PLC	O'-C'-C1'-C2'
45	M	604	3PE	O22-C21-C22-C23
52	d	201	CDL	C72-C71-CB7-OB9
46	M	605	PC1	C2E-C2F-C2G-C2H
45	Y	203	3PE	C24-C25-C26-C27
45	A	201	3PE	O32-C31-C32-C33
46	A	202	PC1	O22-C21-C22-C23
46	A	203	PC1	C35-C36-C37-C38
45	K	101	3PE	C39-C3A-C3B-C3C
46	h	201	PC1	O21-C21-C22-C23
52	i	202	CDL	C32-C31-CA7-OA8
45	M	604	3PE	C29-C2A-C2B-C2C
46	d	203	PC1	C22-C23-C24-C25
46	I	205	PC1	O32-C31-C32-C33
46	I	204	PC1	C11-C12-N-C13
45	M	603	3PE	O22-C21-C22-C23
45	Y	204	3PE	O32-C31-C32-C33
47	A	204	PLC	C2B-C1B-CB-OB
58	i	201	CHD	C22-C23-C24-O25
45	Z	201	3PE	O22-C21-C22-C23
45	g	201	3PE	C35-C36-C37-C38
52	M	602	CDL	C52-C53-C54-C55
52	L	701	CDL	C71-C72-C73-C74
45	M	604	3PE	O32-C31-C32-C33
52	d	201	CDL	CA5-C11-C12-C13
52	M	602	CDL	C34-C35-C36-C37
45	m	202	3PE	O31-C31-C32-C33
45	Y	201	3PE	O32-C31-C32-C33
45	A	201	3PE	C3A-C3B-C3C-C3D
52	X	201	CDL	C52-C51-CB5-OB6
45	Y	203	3PE	C2E-C2F-C2G-C2H

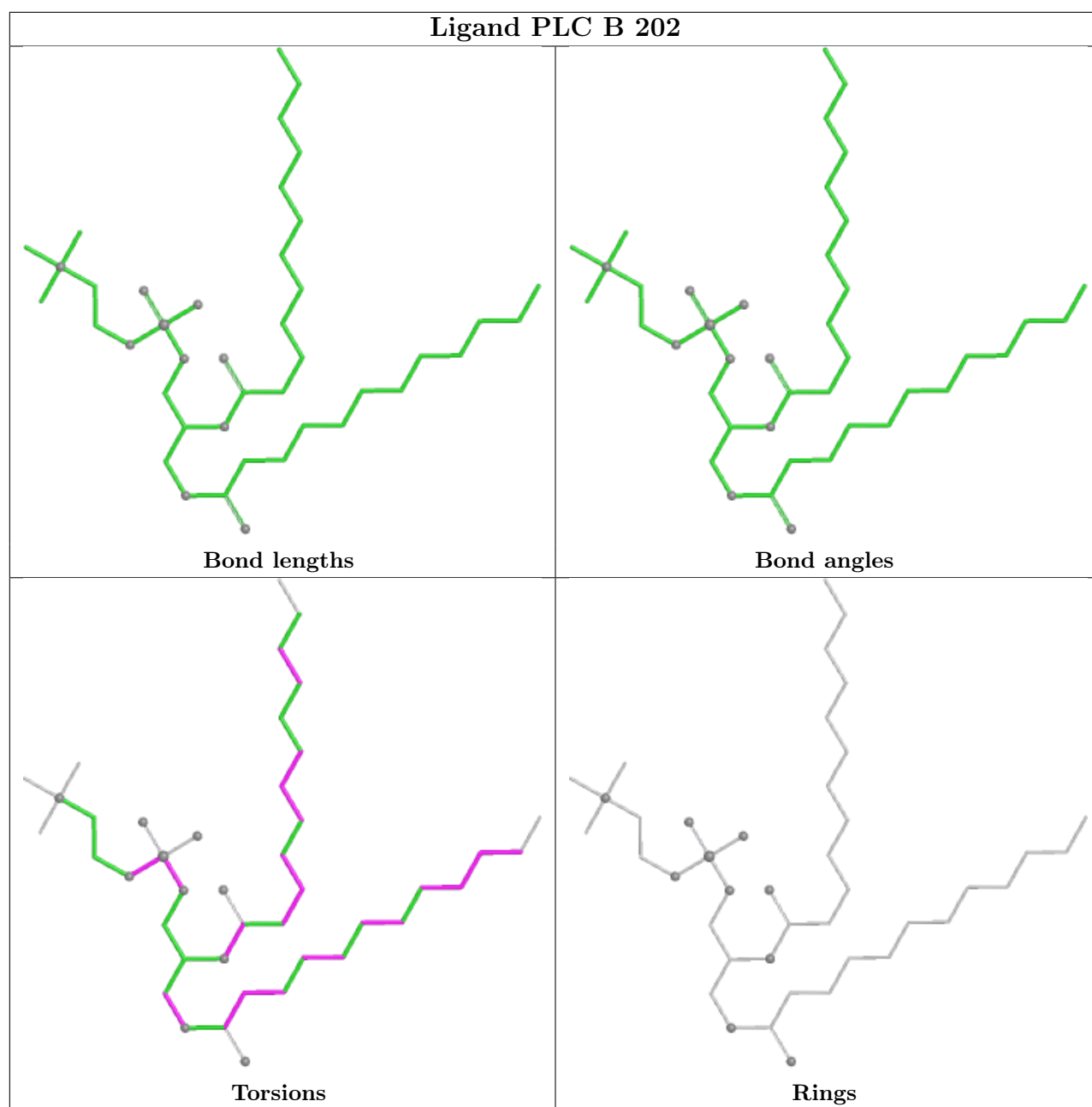
There are no ring outliers.

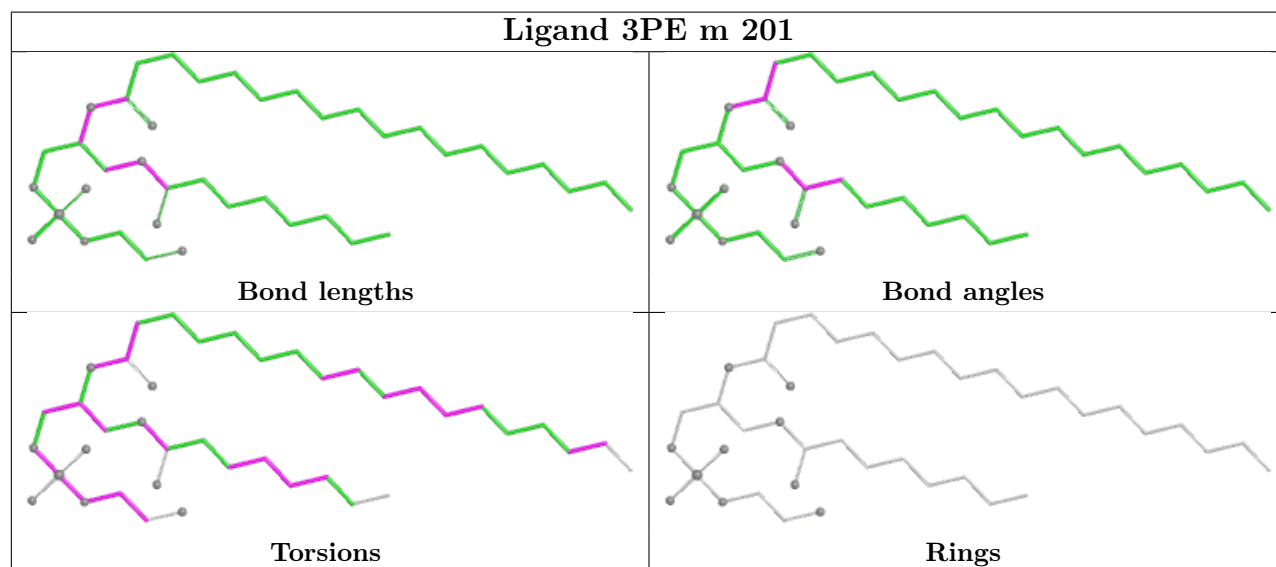
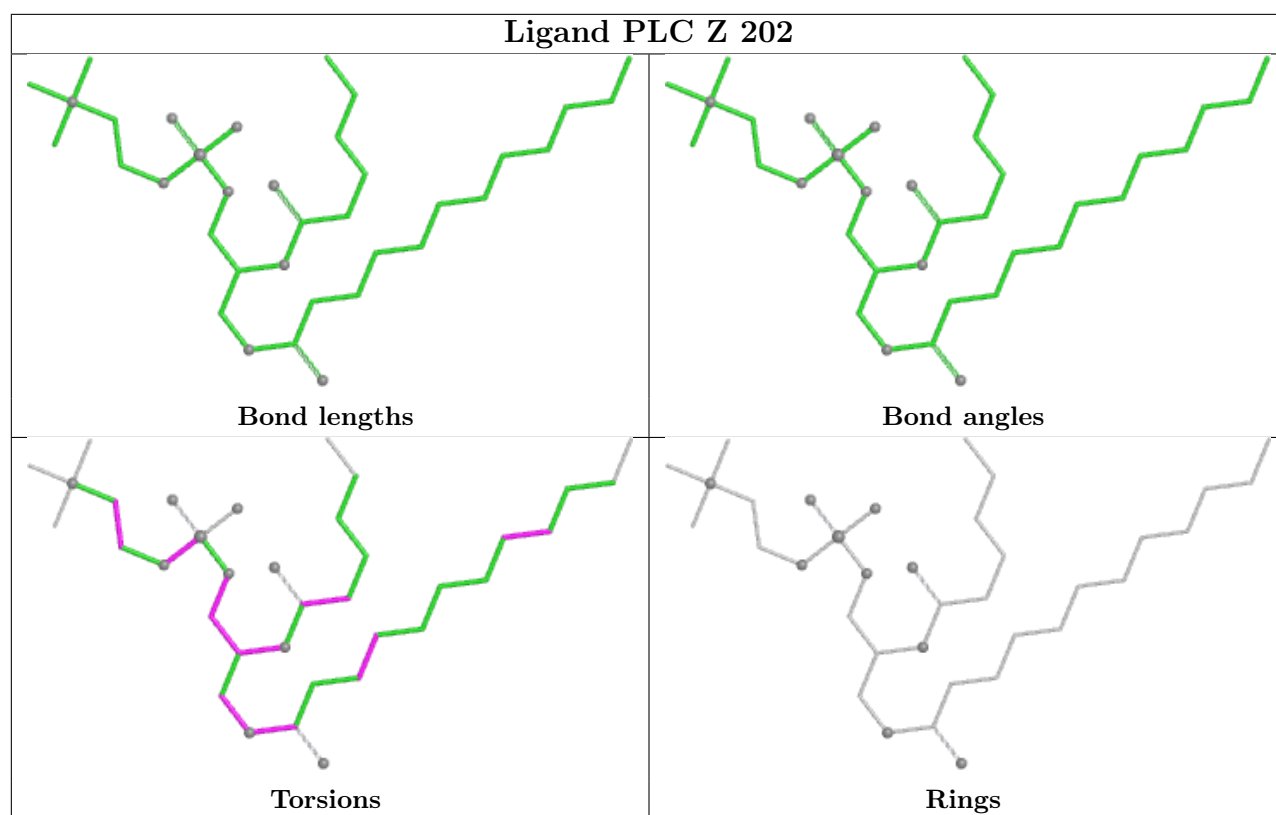
29 monomers are involved in 49 short contacts:

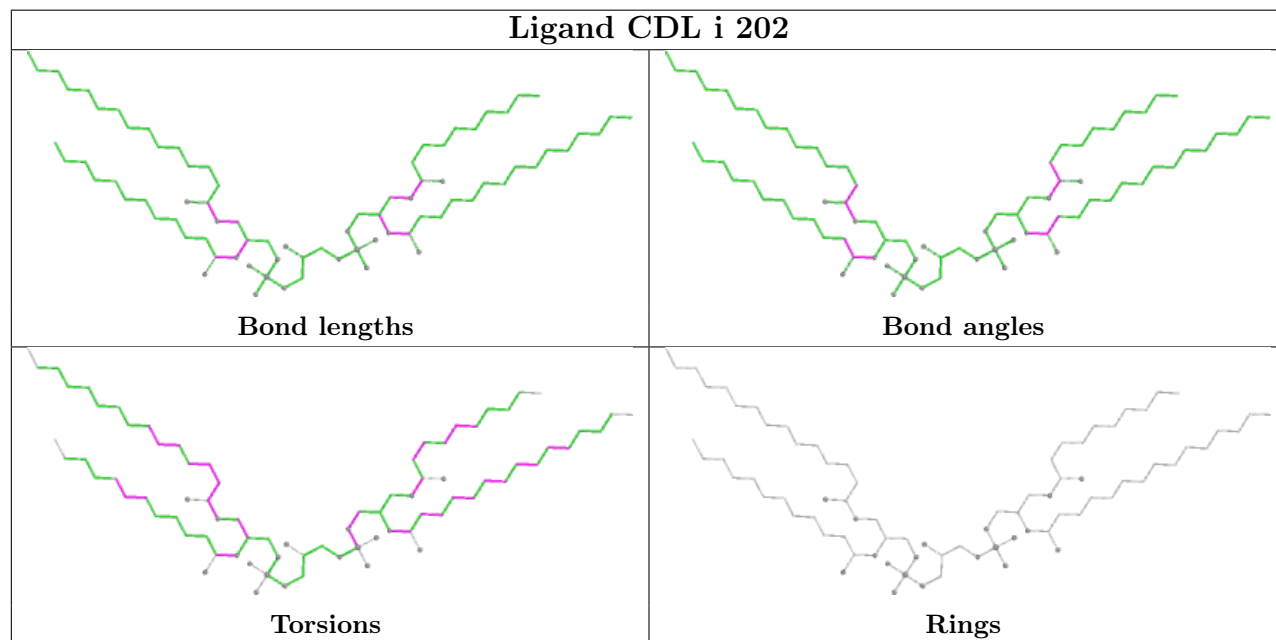
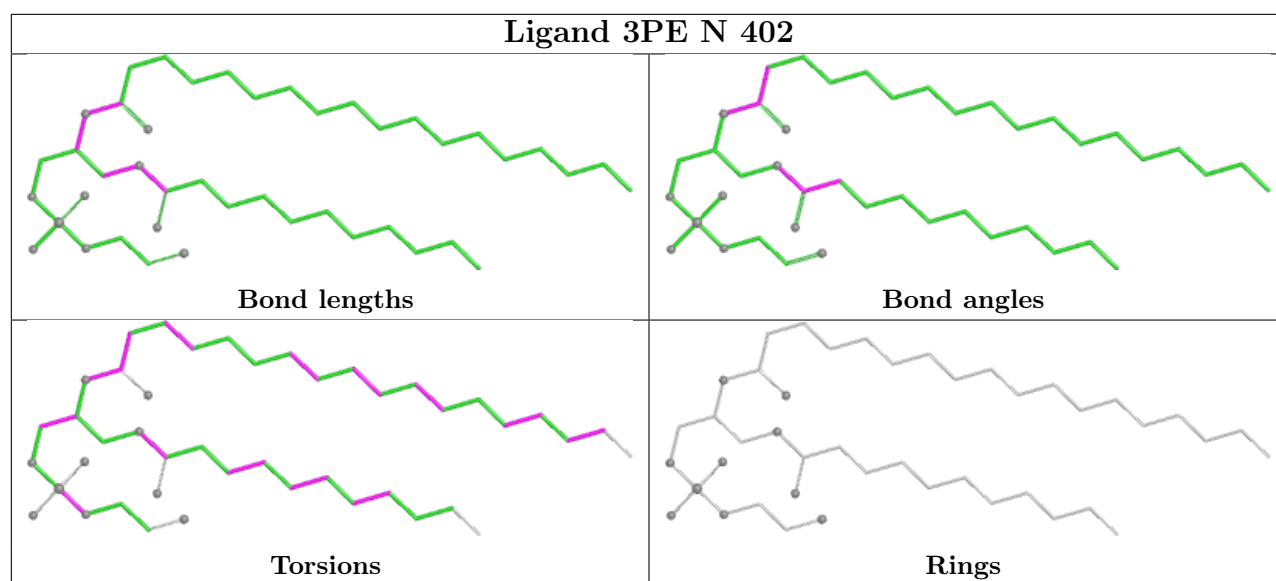
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	G	803	FES	1	0
45	m	201	3PE	1	0
52	i	202	CDL	1	0
52	q	201	CDL	2	0
46	I	205	PC1	1	0
46	A	203	PC1	4	0
46	d	203	PC1	1	0
46	H	402	PC1	1	0
45	L	703	3PE	2	0
45	b	101	3PE	3	0
52	d	201	CDL	2	0
54	O	401	DGT	2	0
52	M	602	CDL	3	0
46	m	203	PC1	1	0
52	X	201	CDL	2	0
46	q	202	PC1	1	0
48	I	201	SF4	1	0
57	U	101	EHZ	1	0
58	i	201	CHD	6	0
45	d	202	3PE	1	0
45	K	101	3PE	1	0
52	L	701	CDL	1	0
46	L	705	PC1	1	0
45	Z	201	3PE	1	0
45	m	202	3PE	1	0
57	T	101	EHZ	2	0
46	H	401	PC1	1	0
56	P	501	NDP	4	0
48	F	502	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

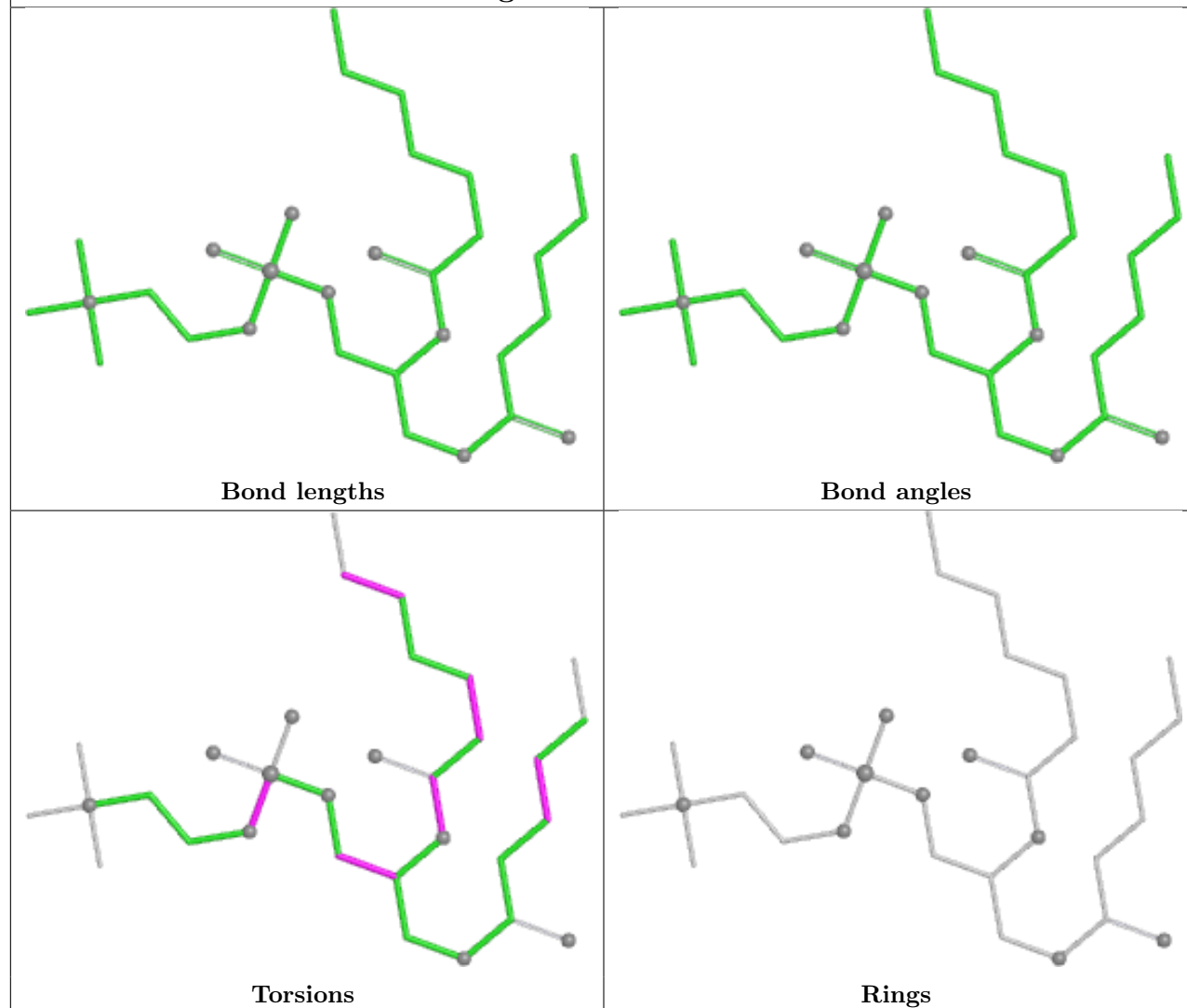




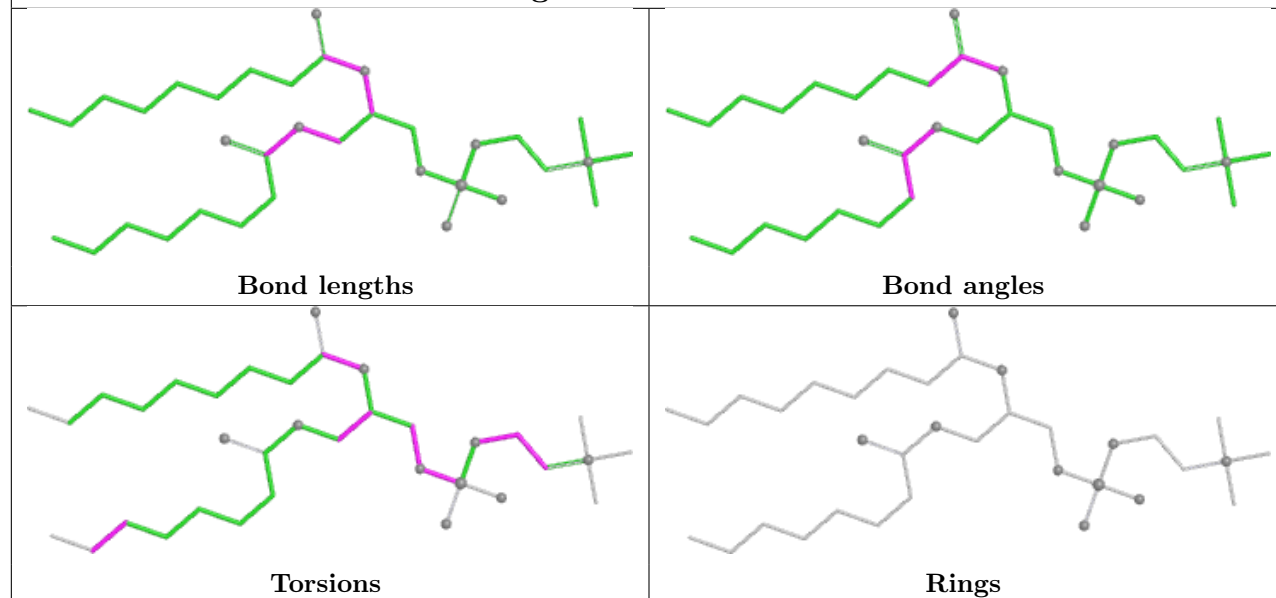


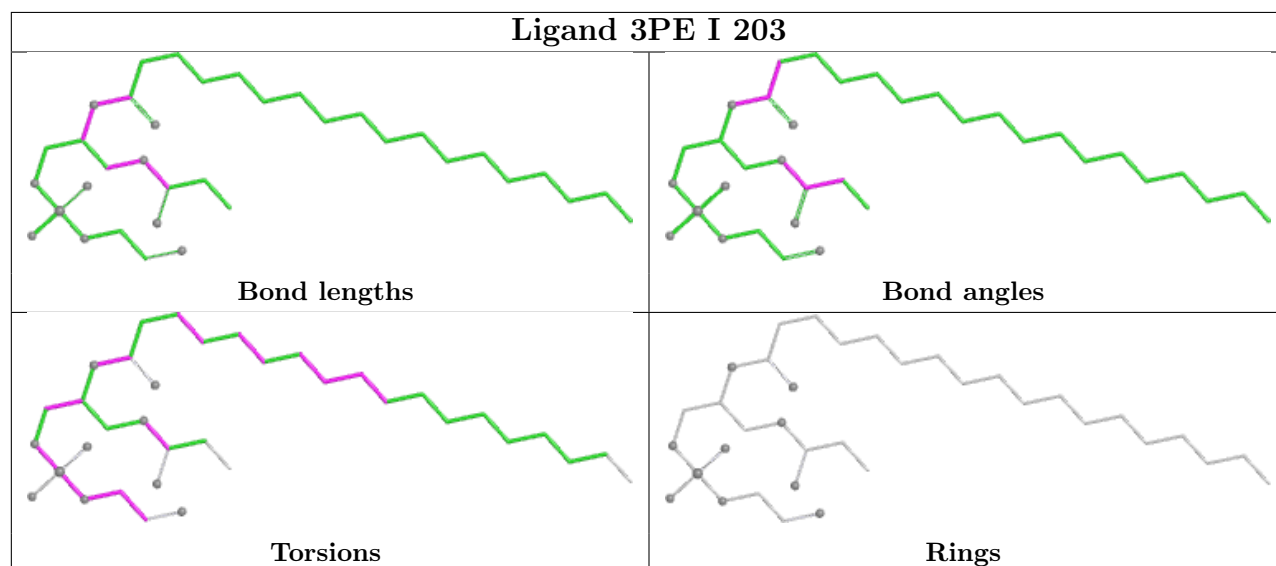
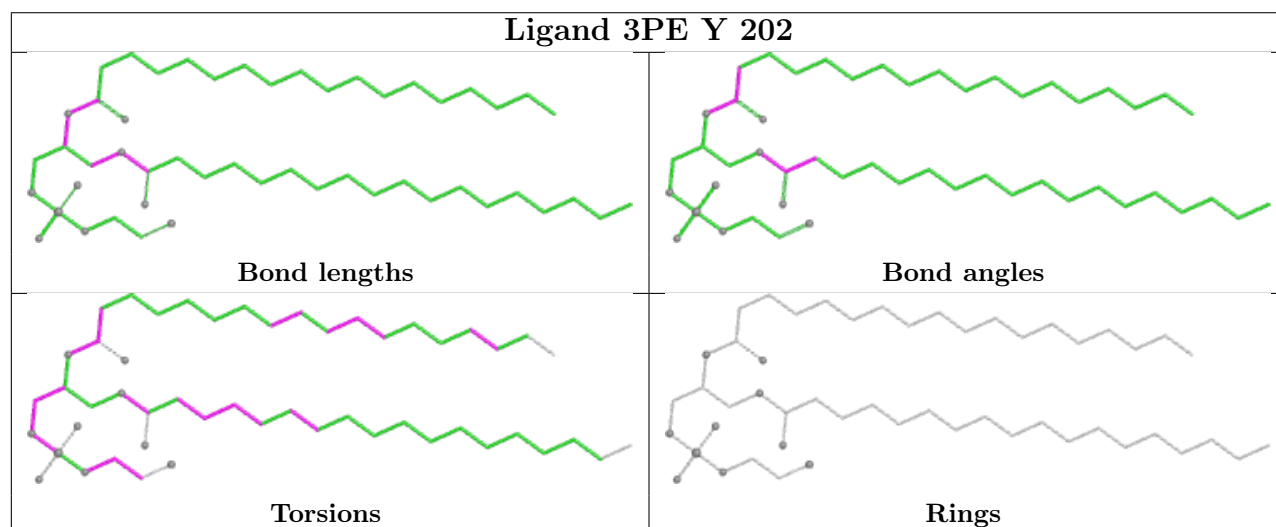
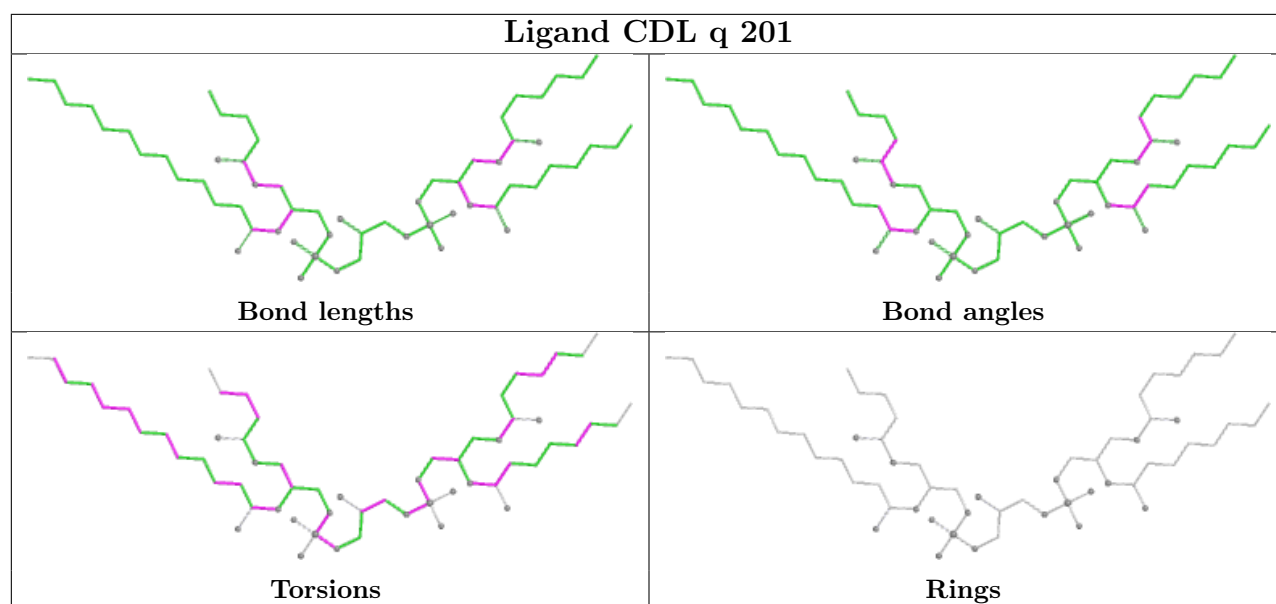


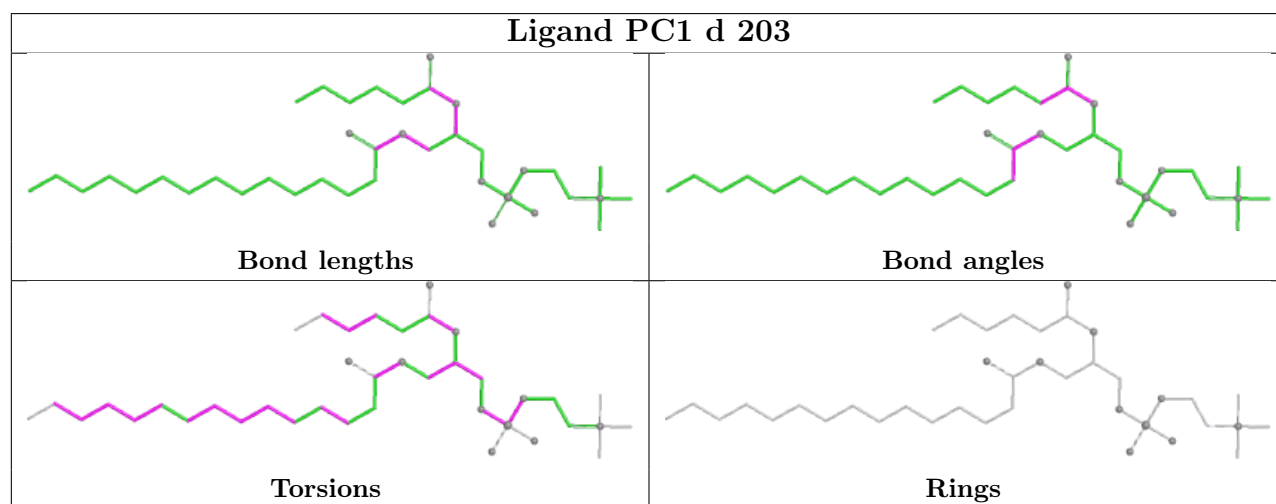
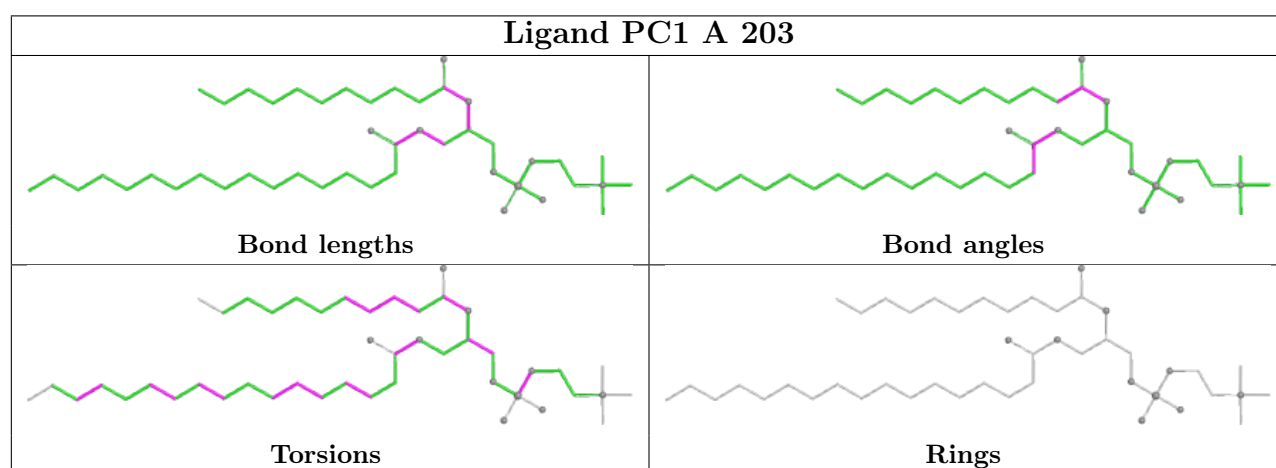
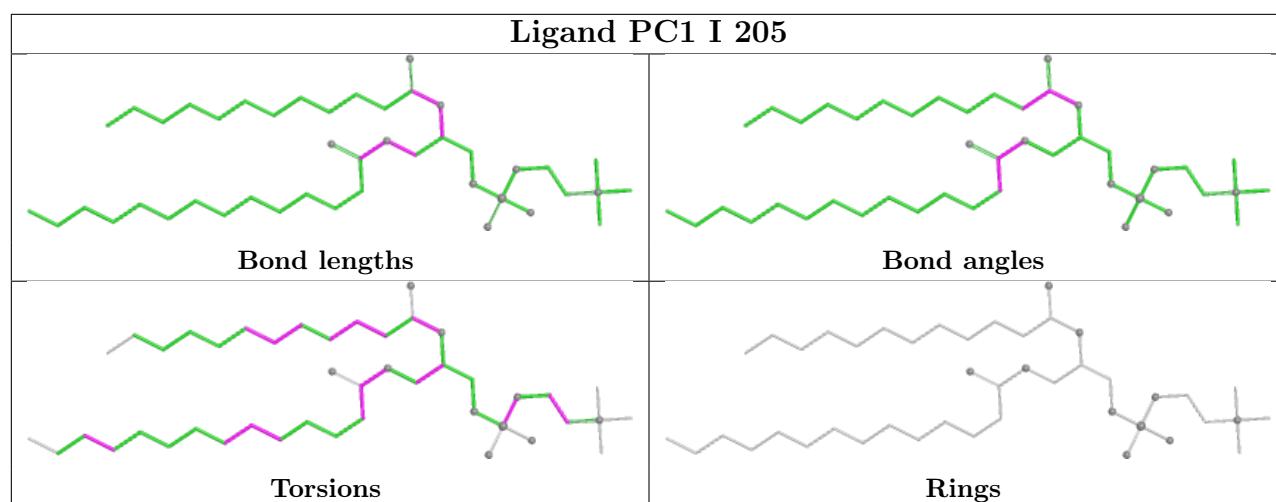
Ligand PLC L 706

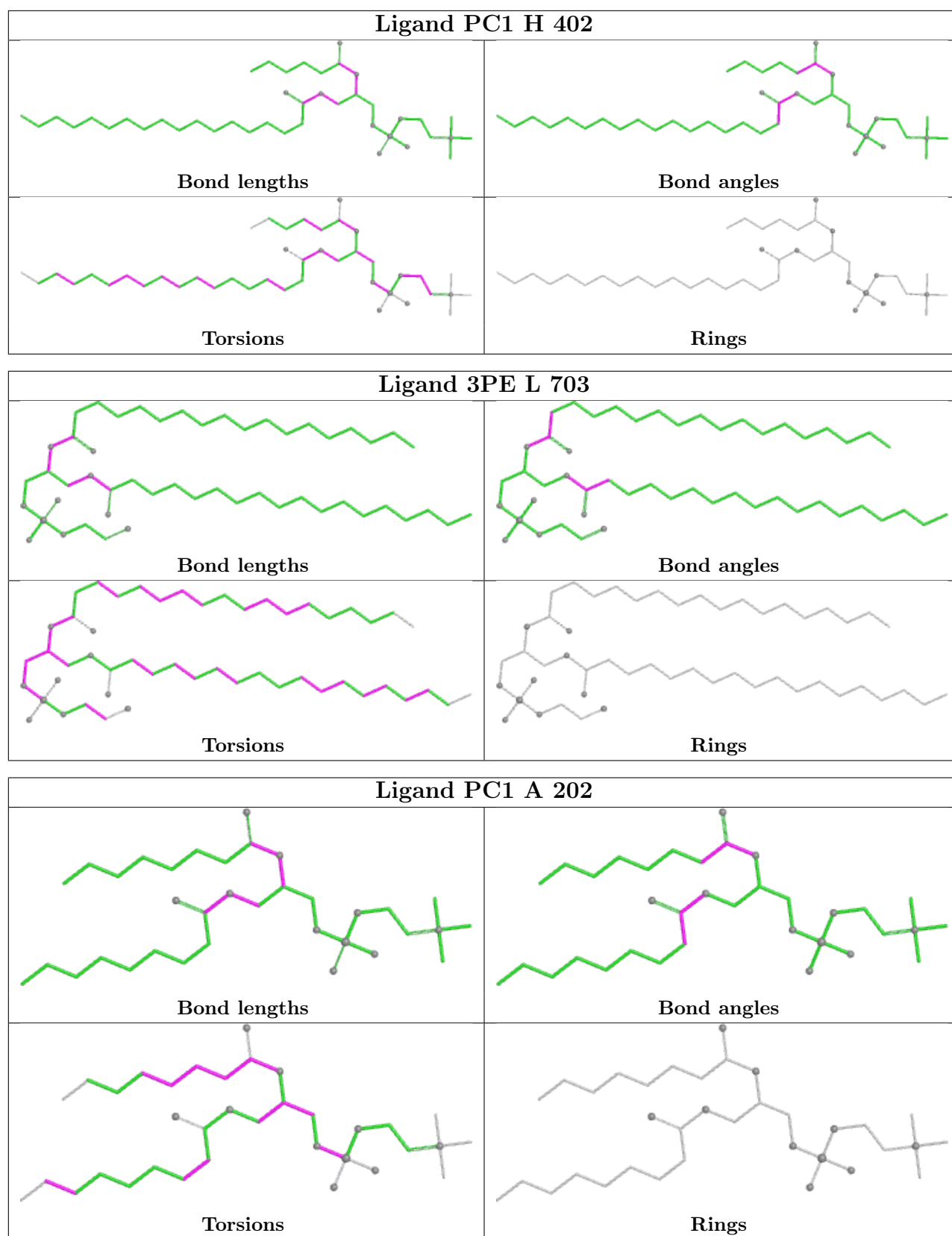


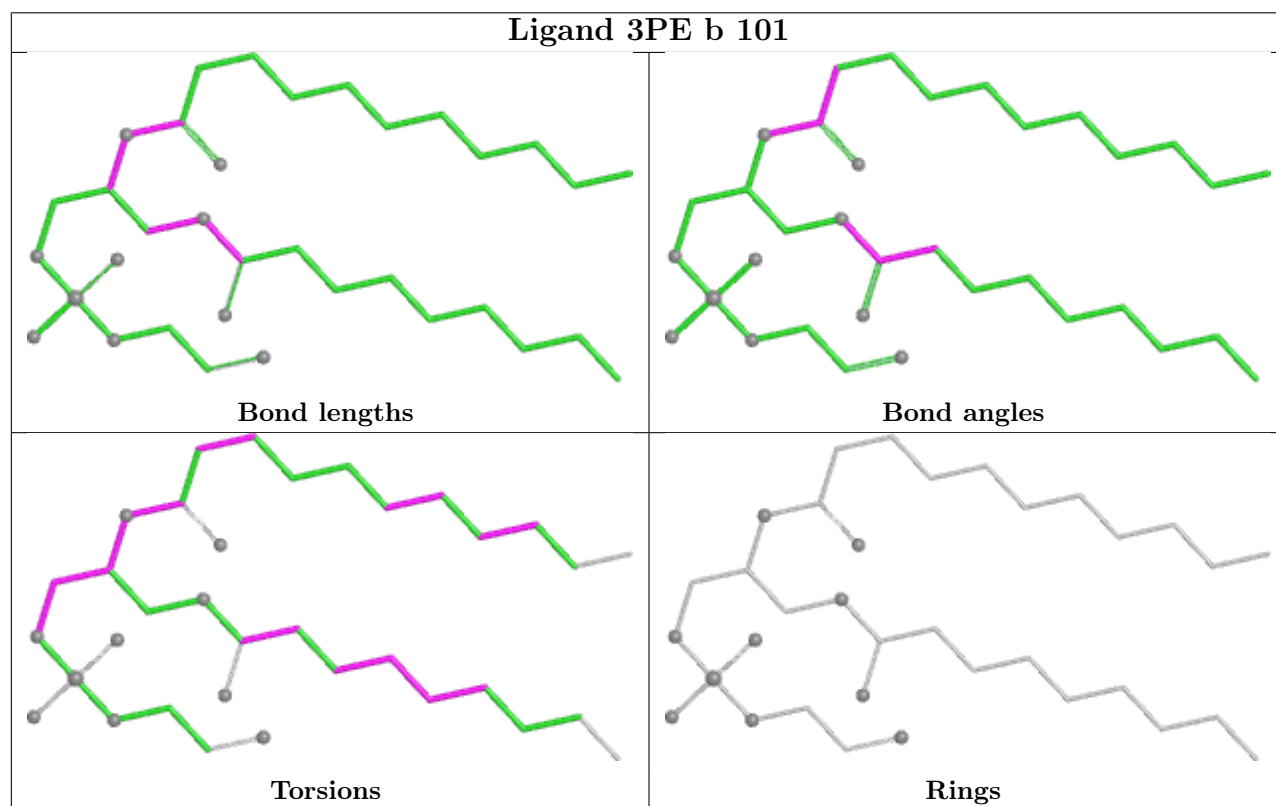
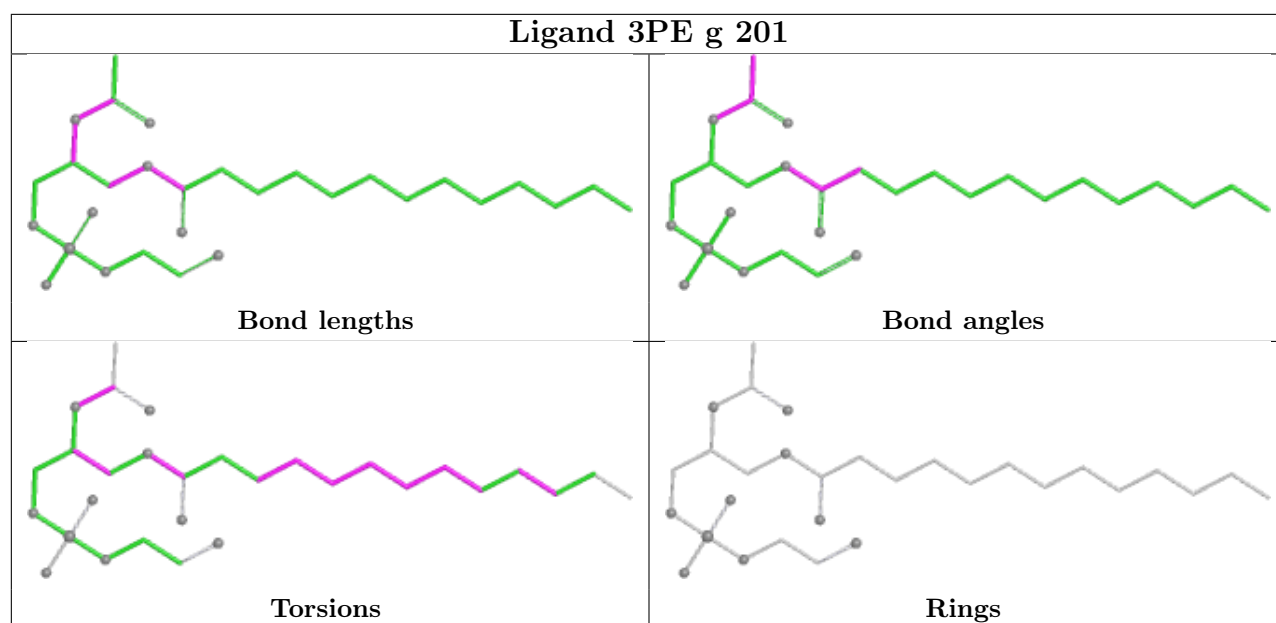
Ligand PC1 M 606

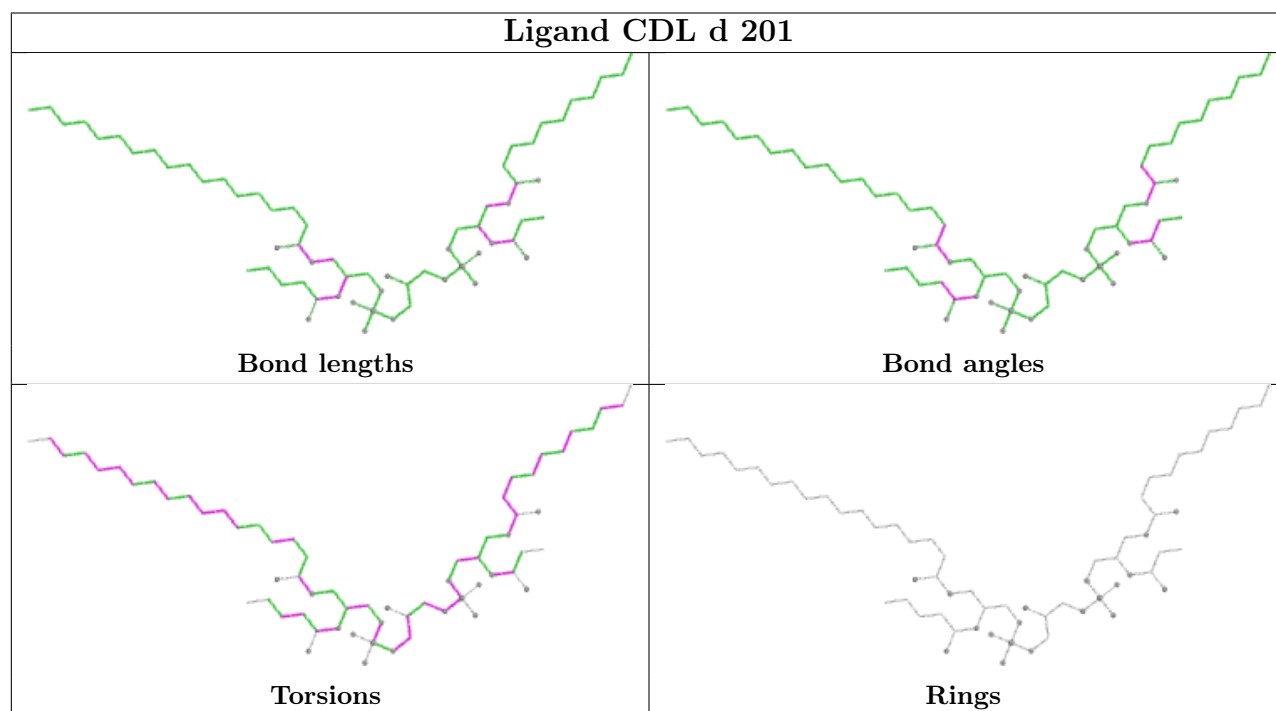
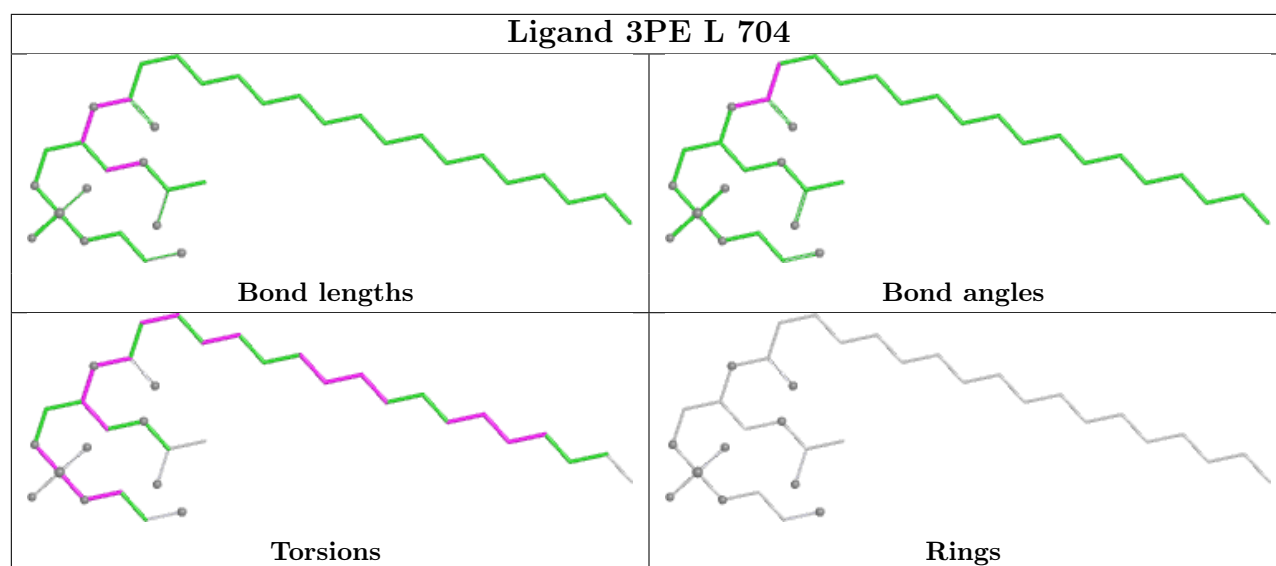


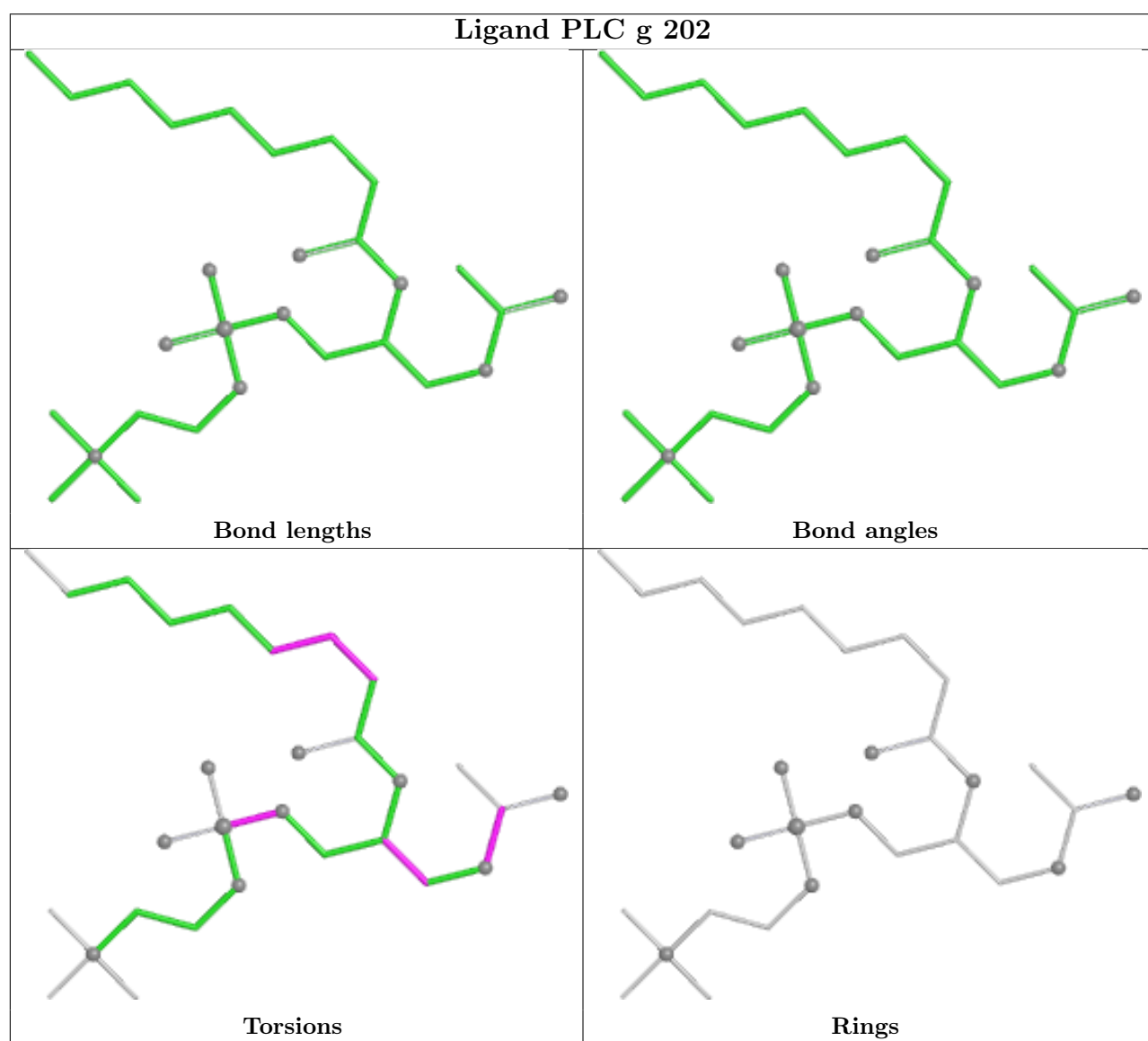
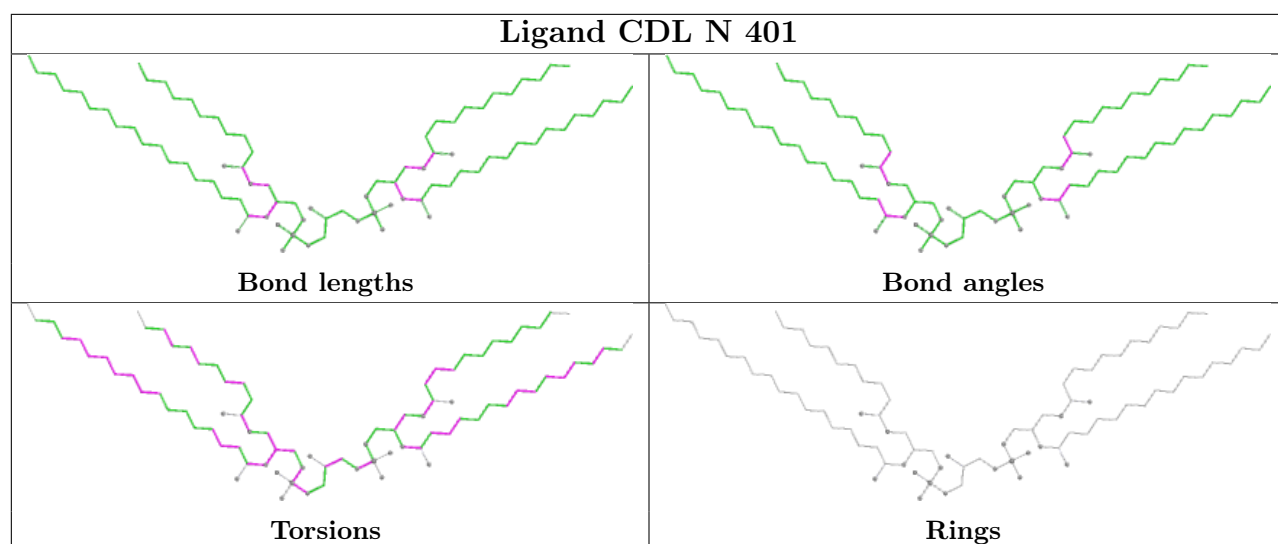


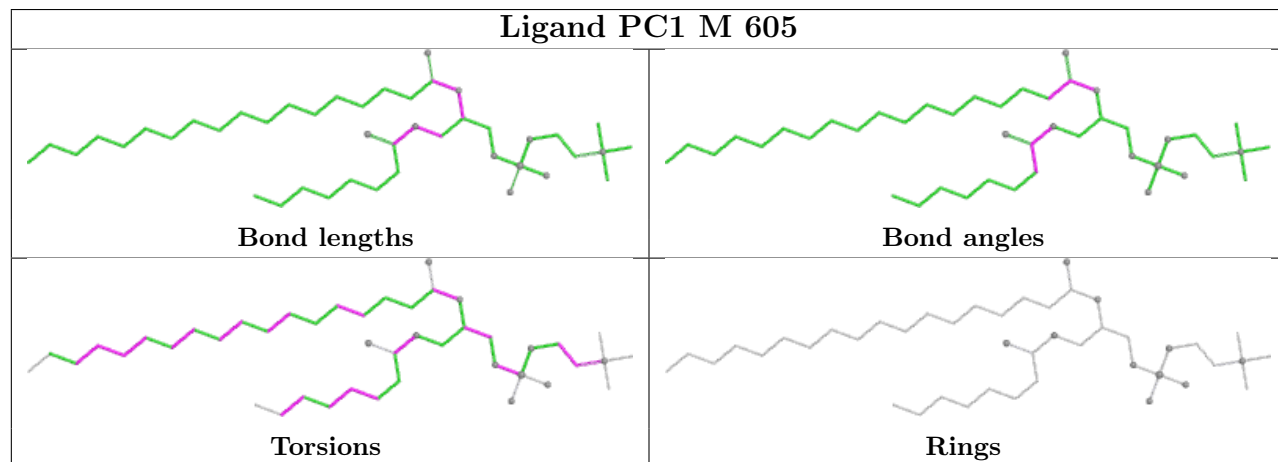
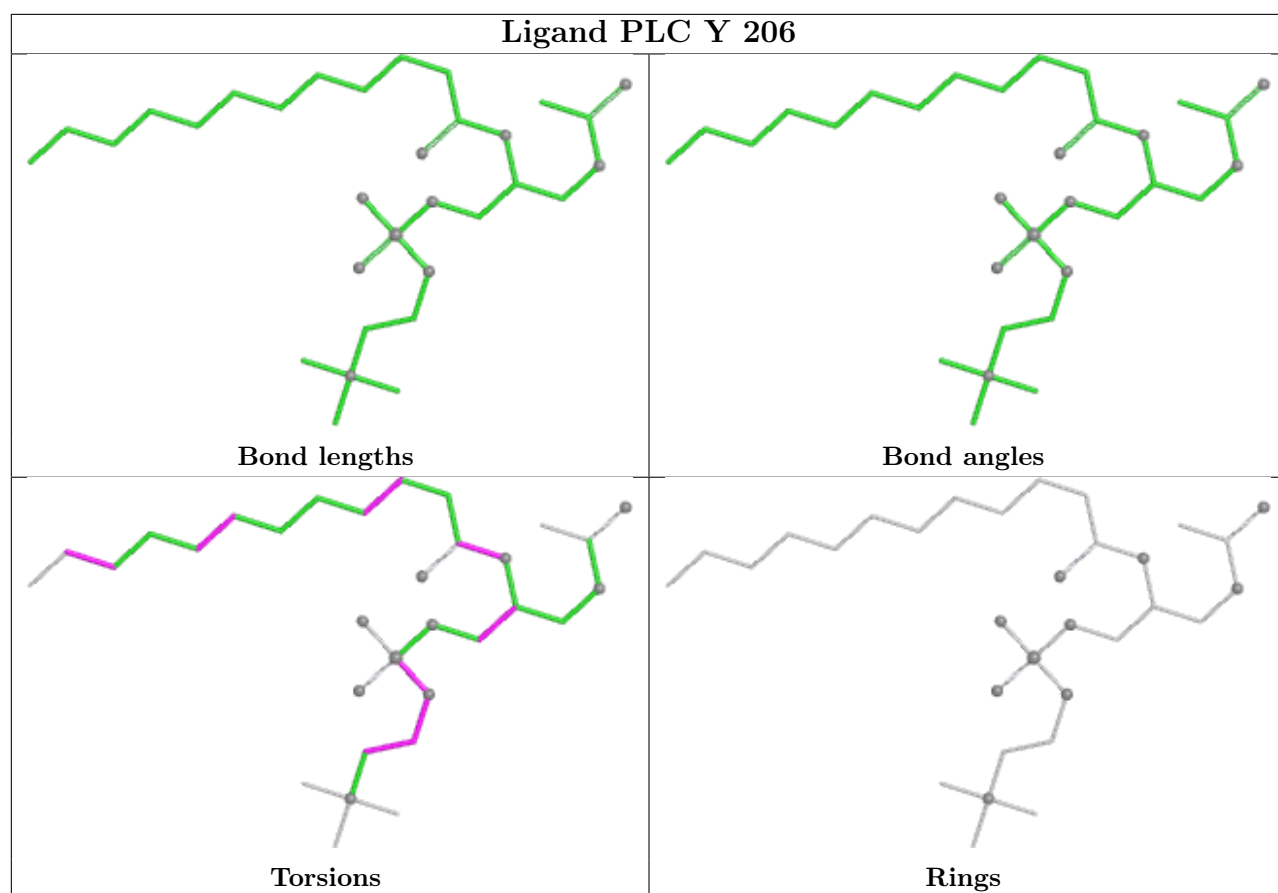


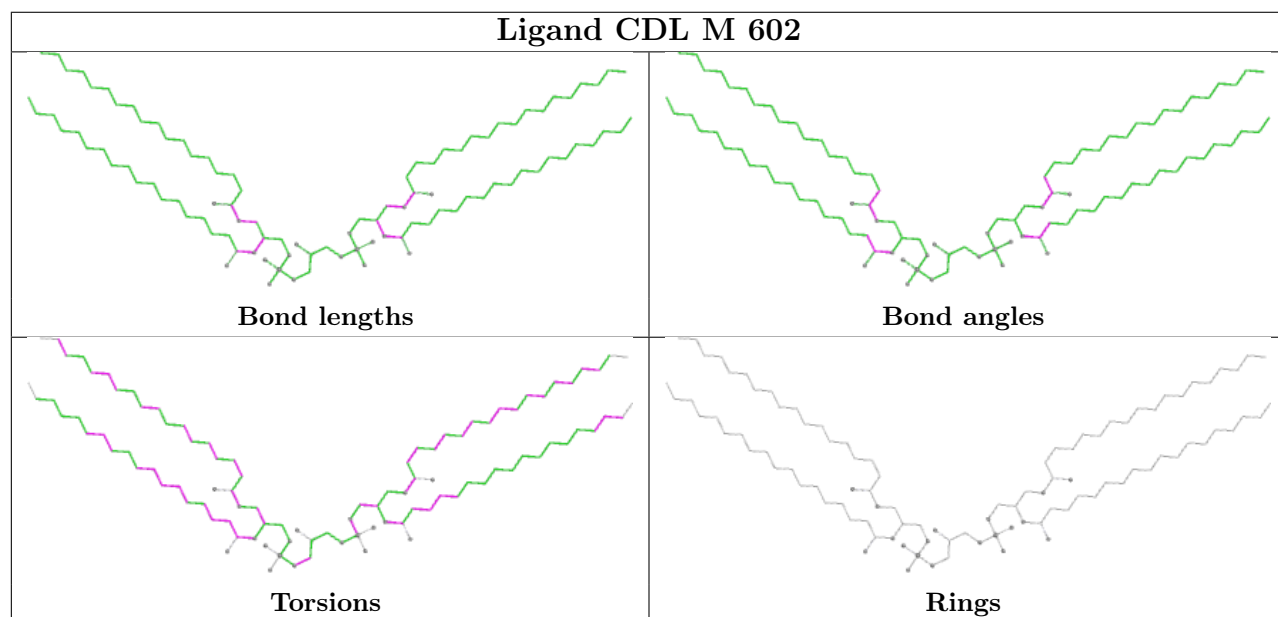
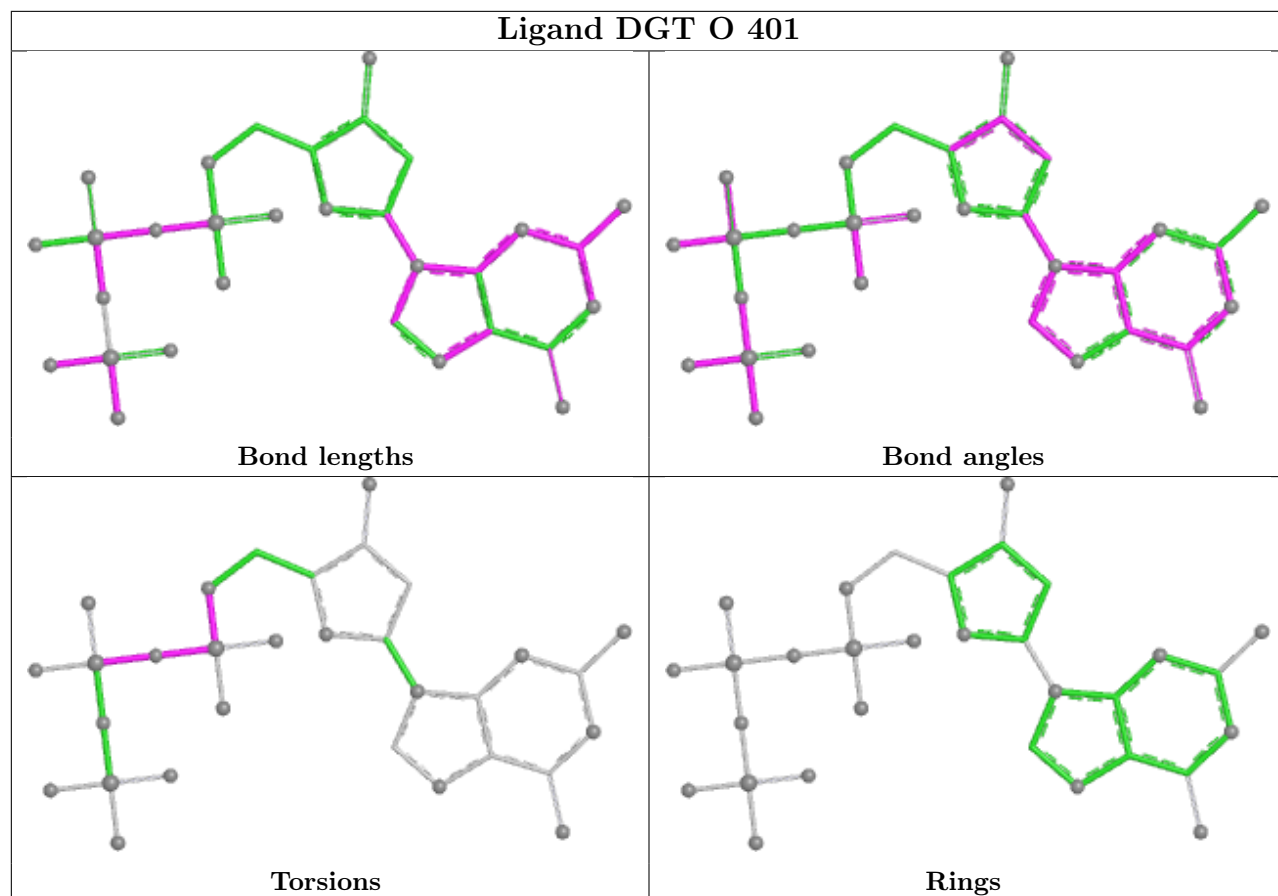


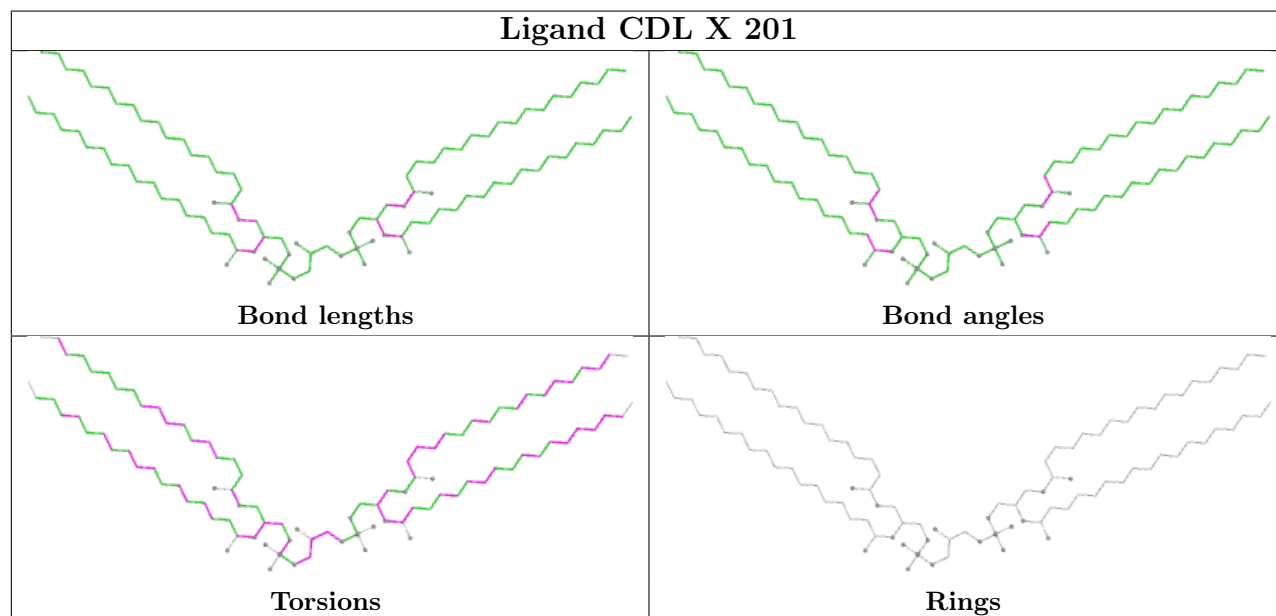
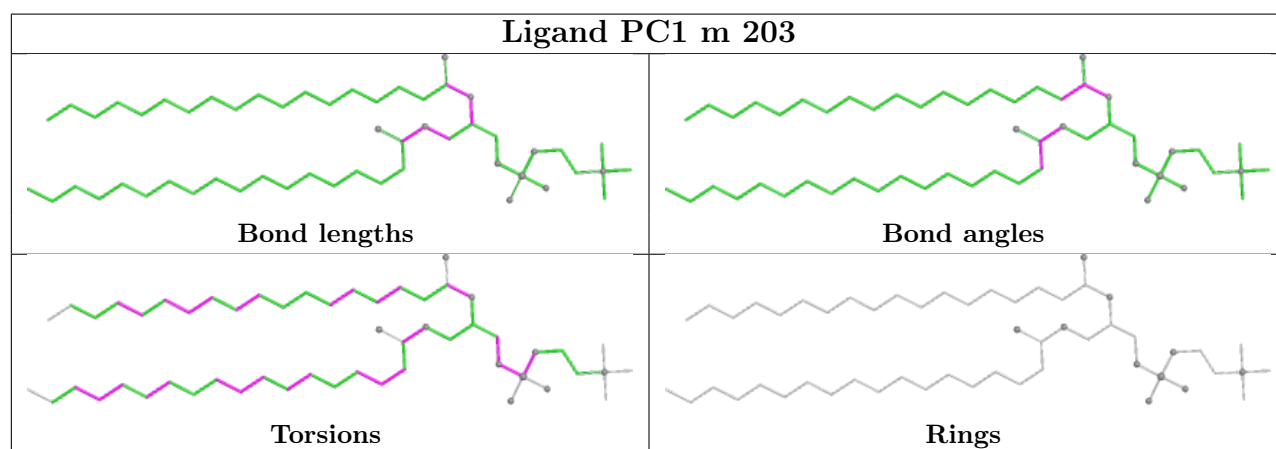
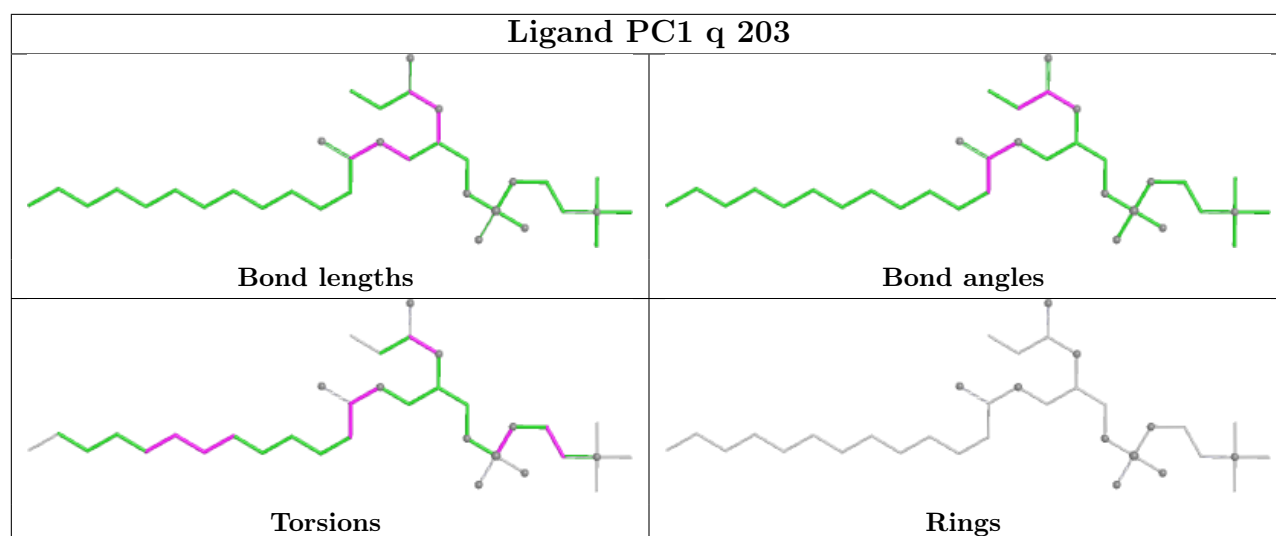


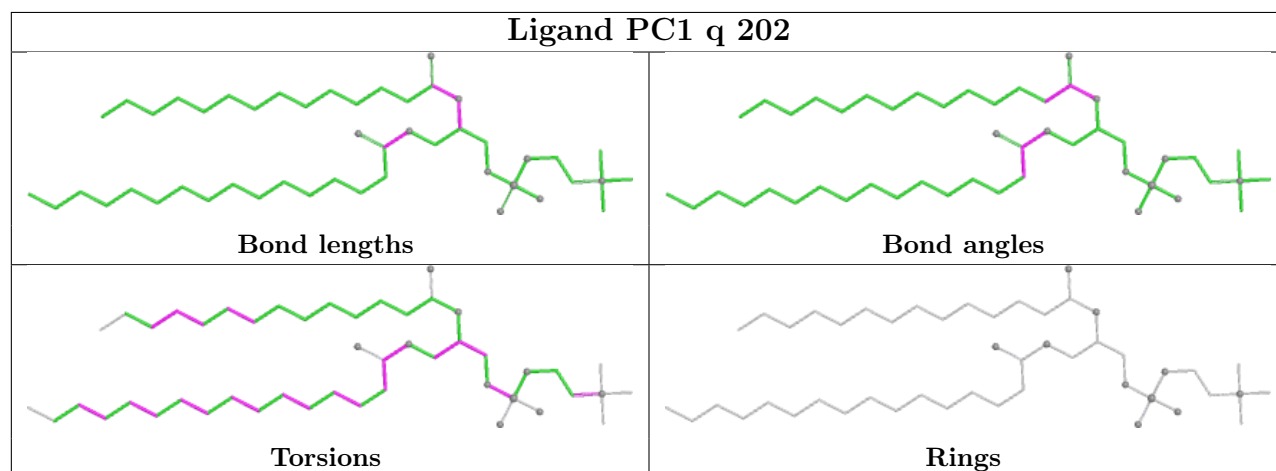
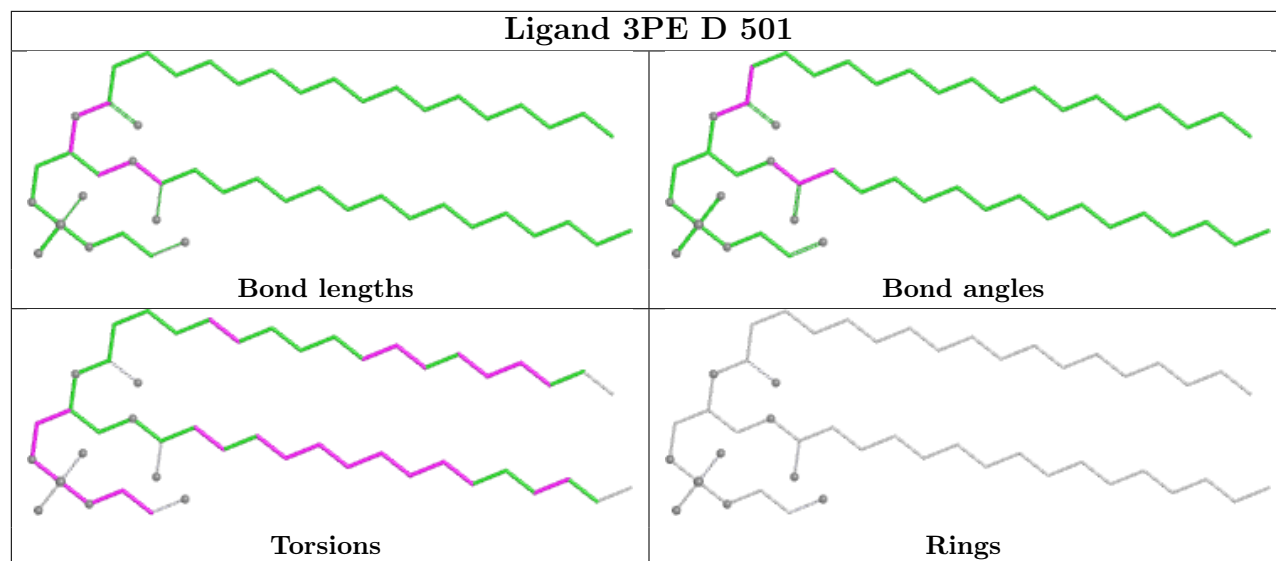


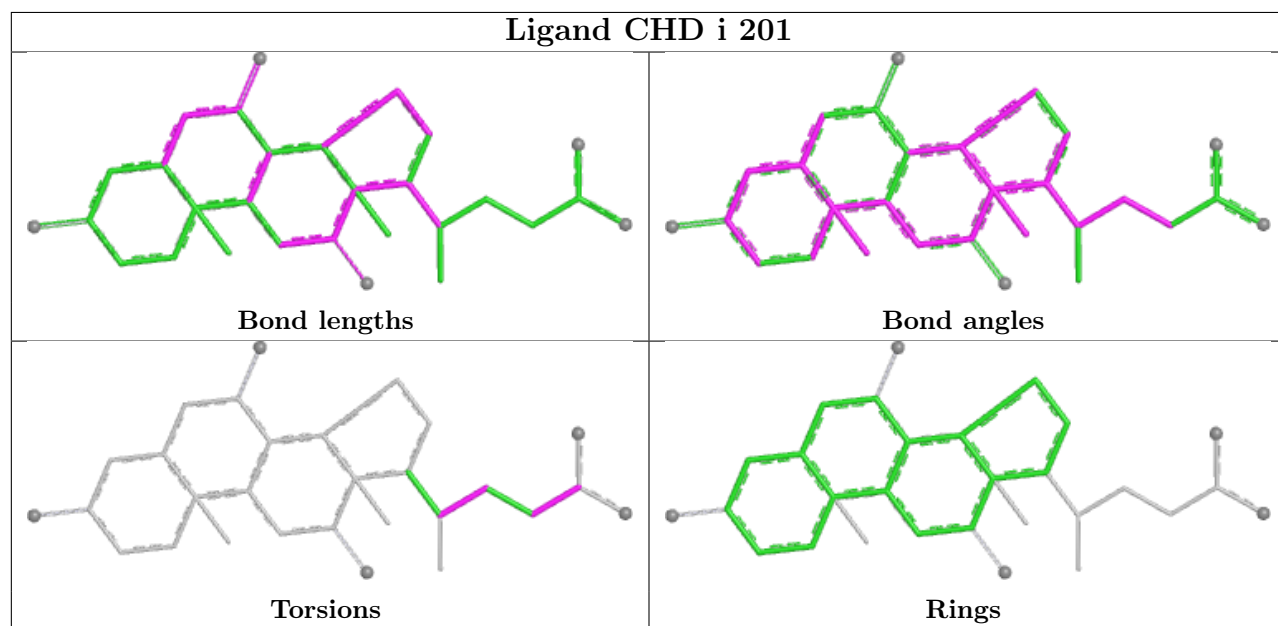
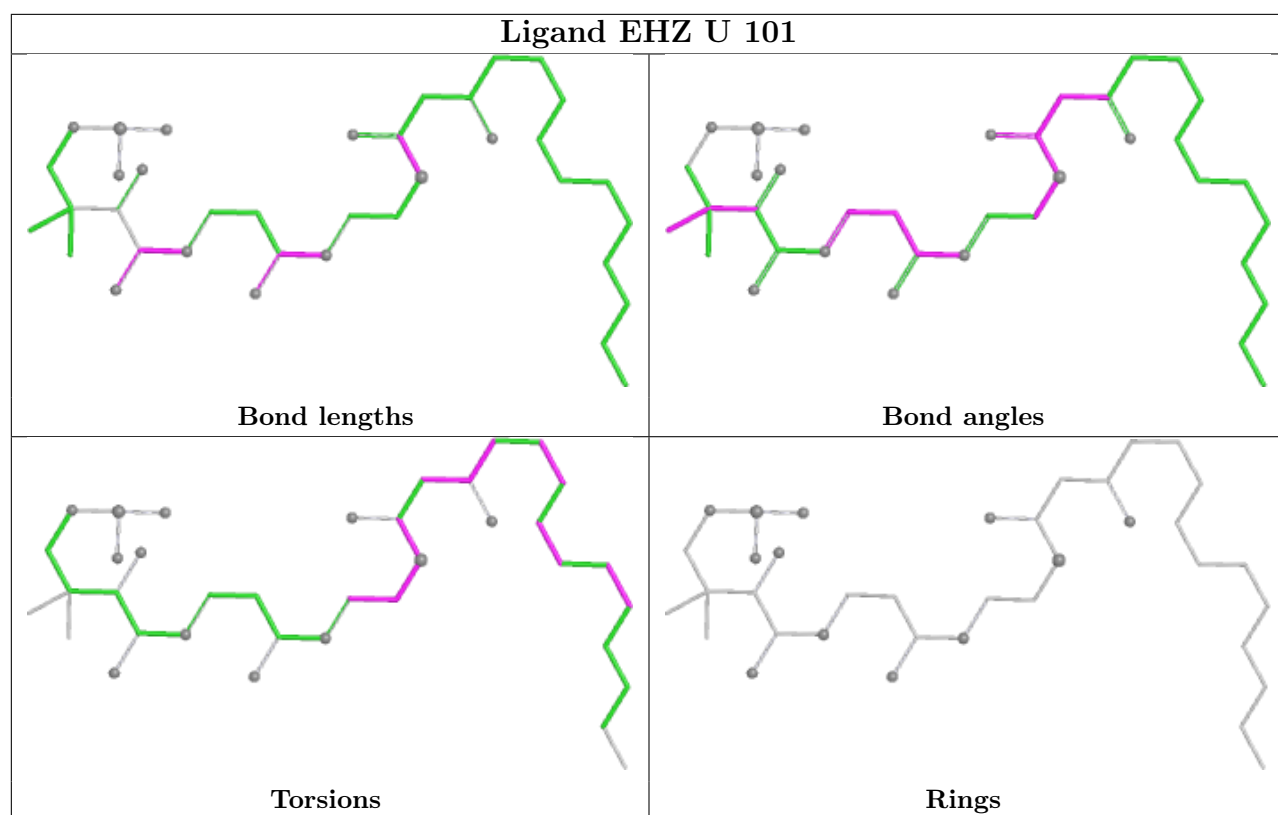


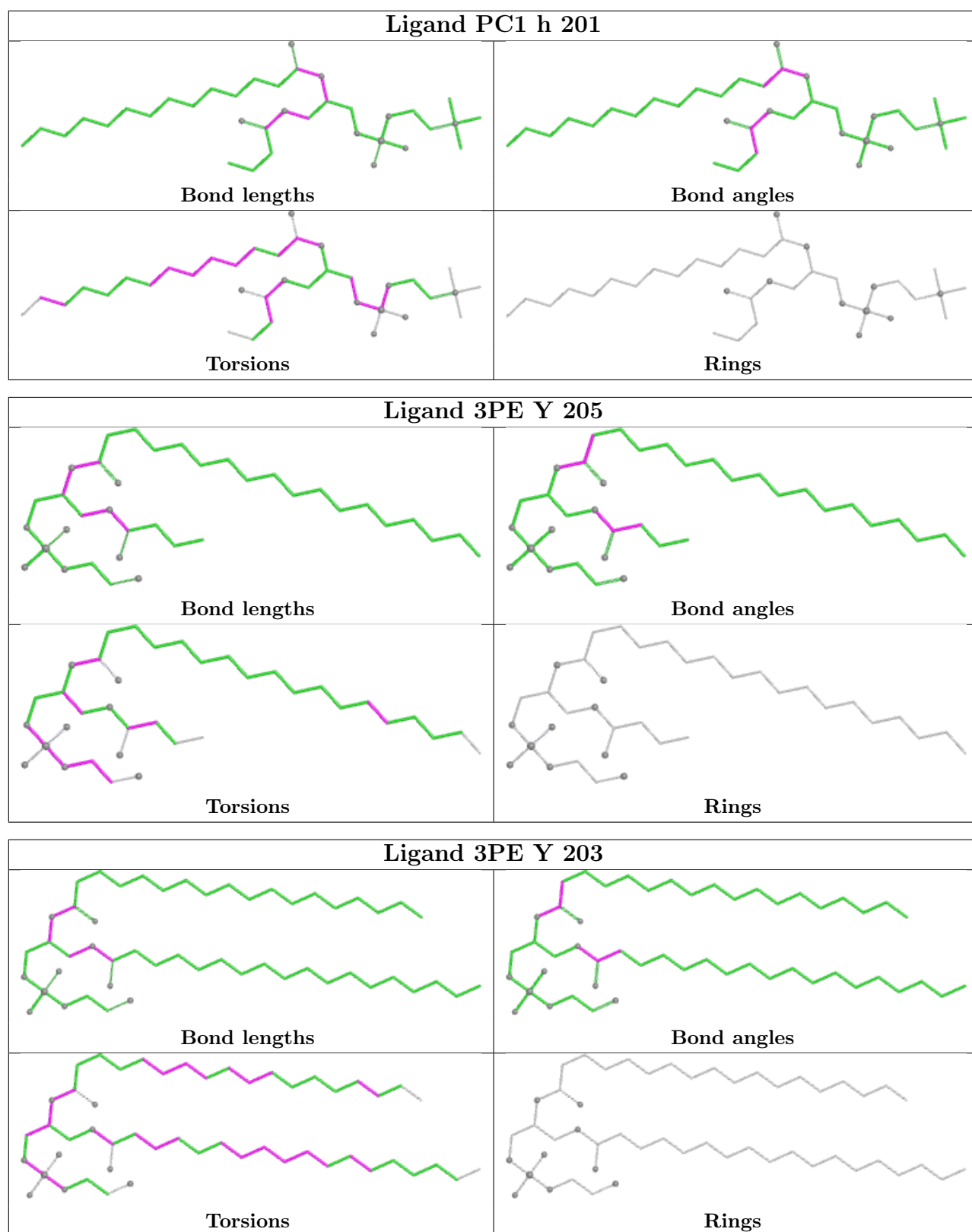


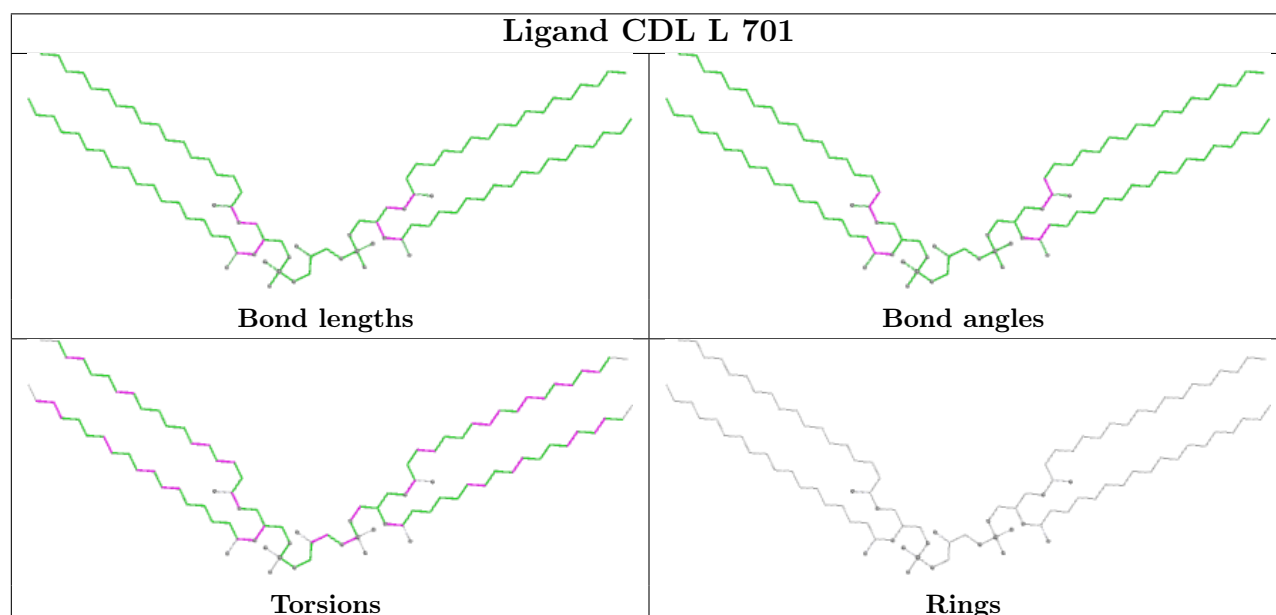
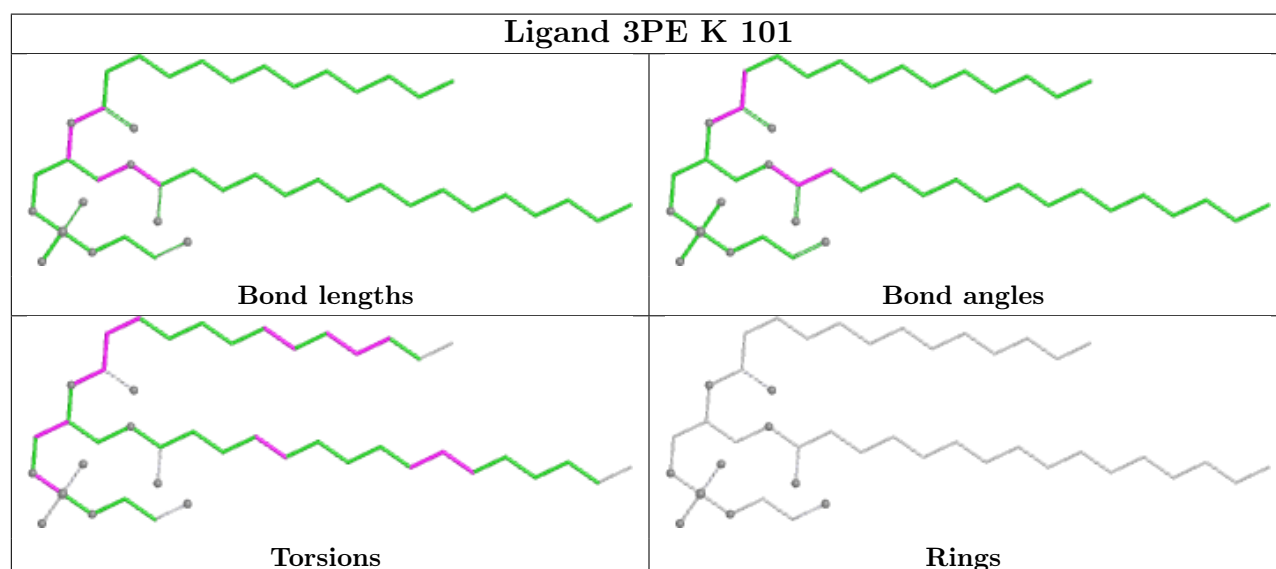
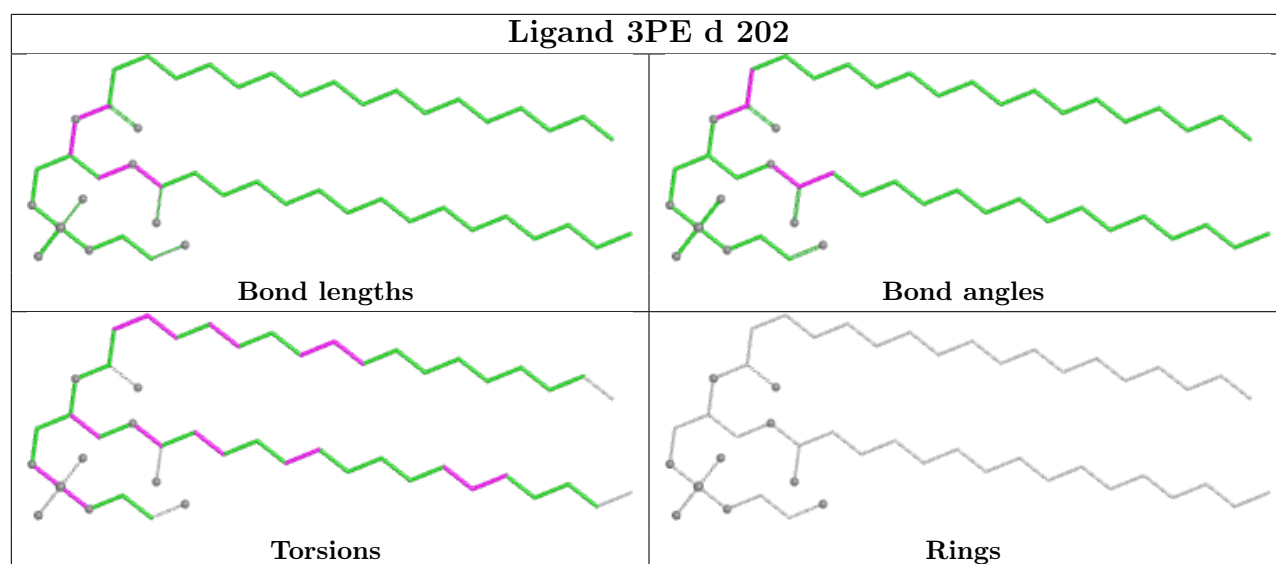


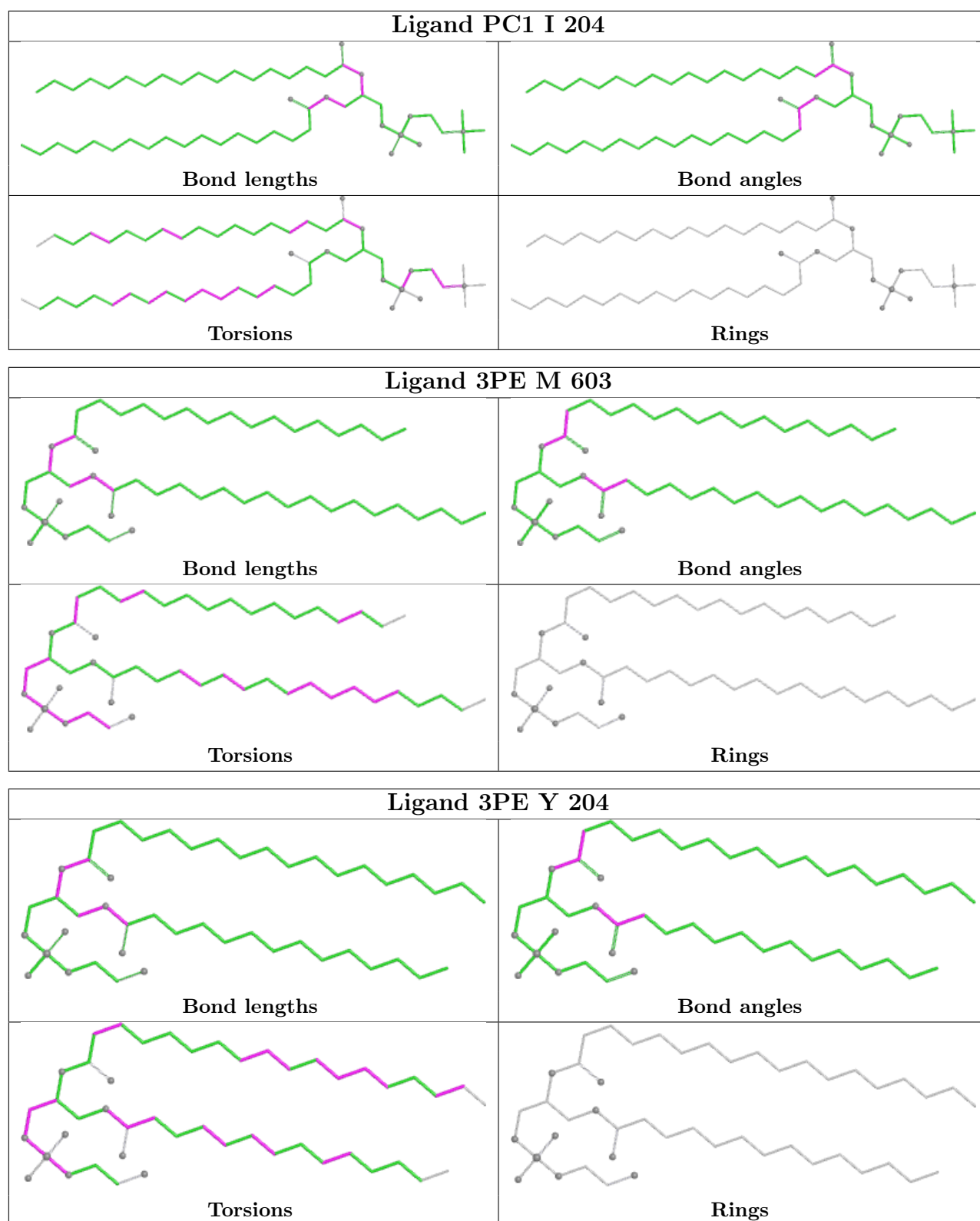


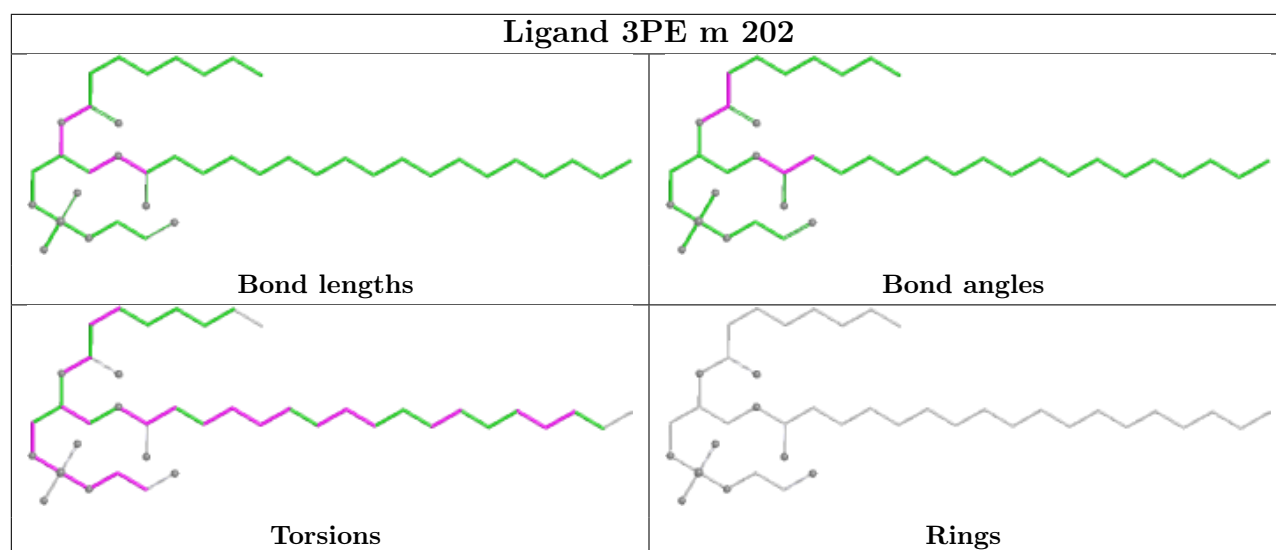
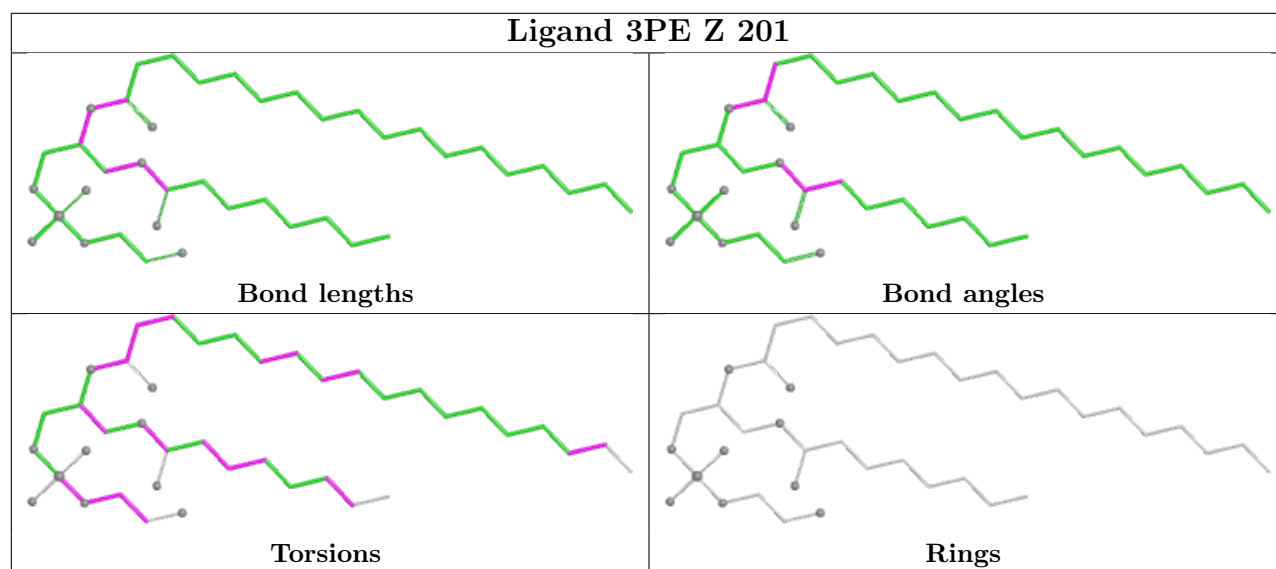
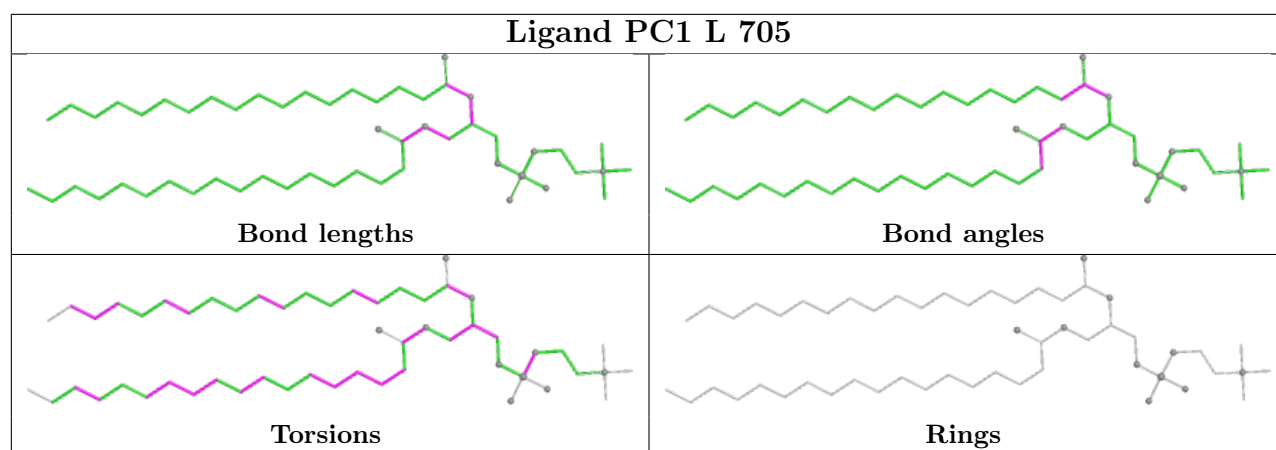


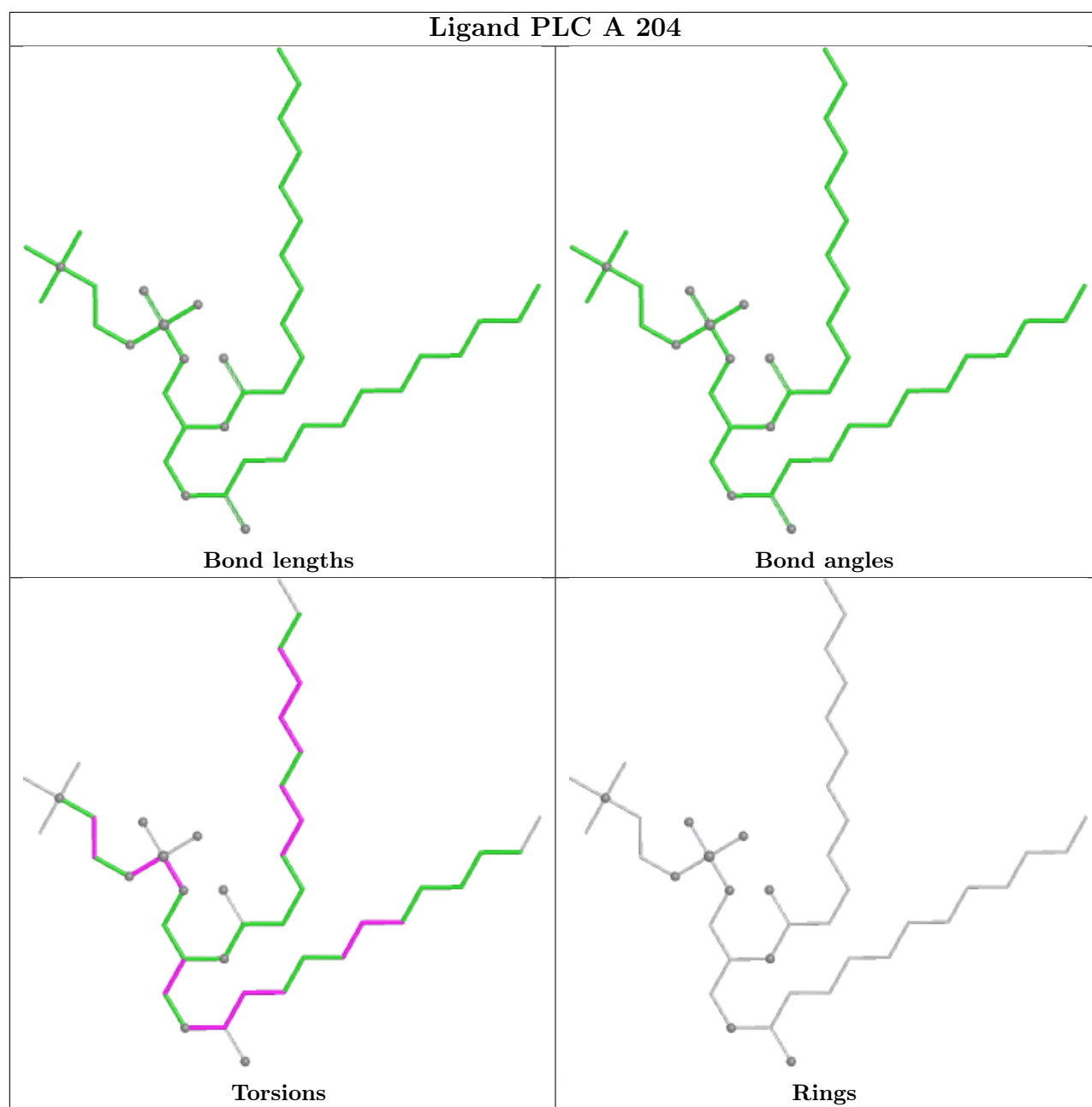


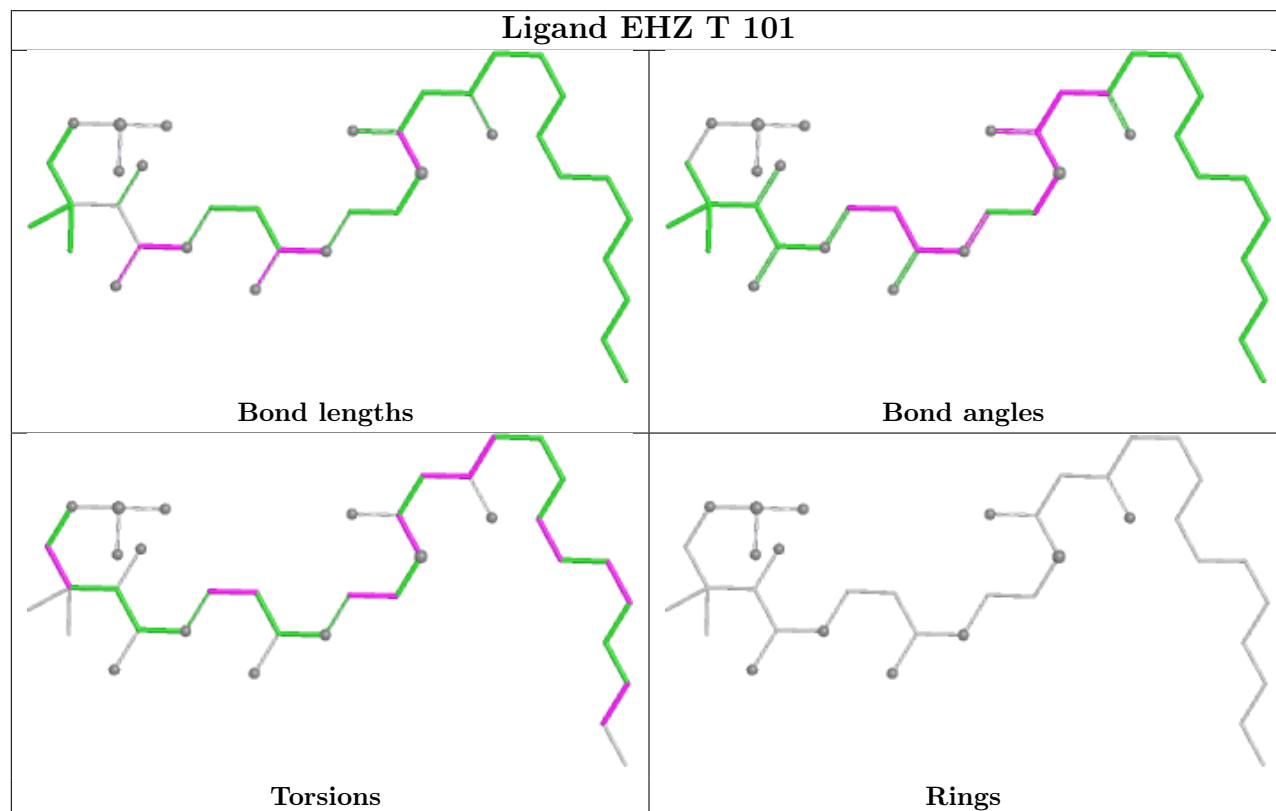
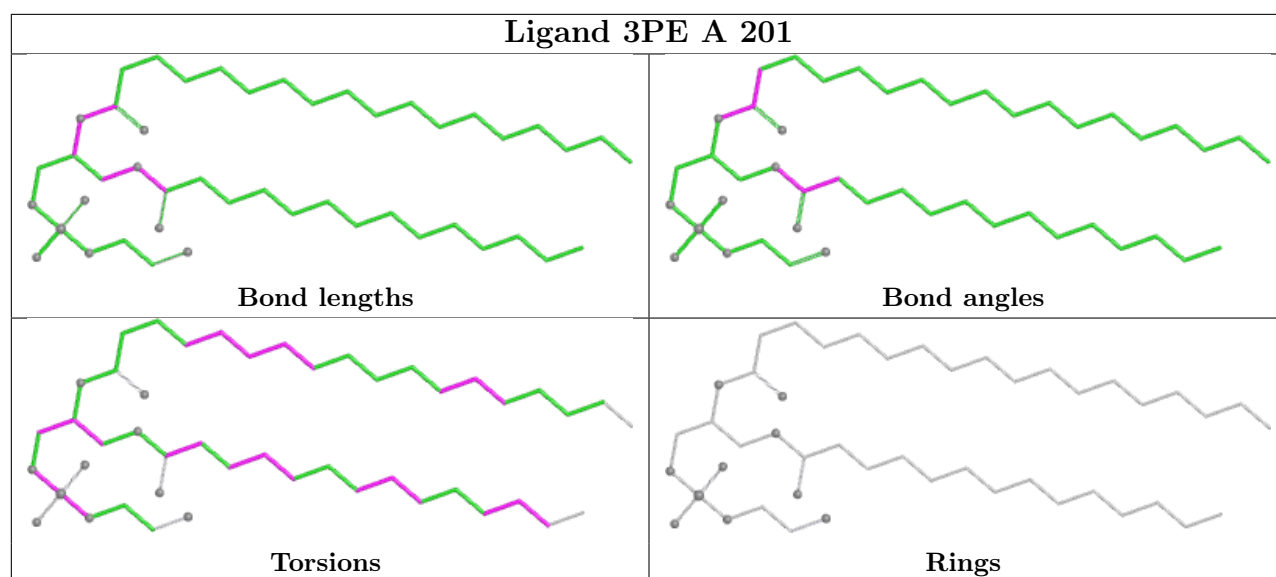


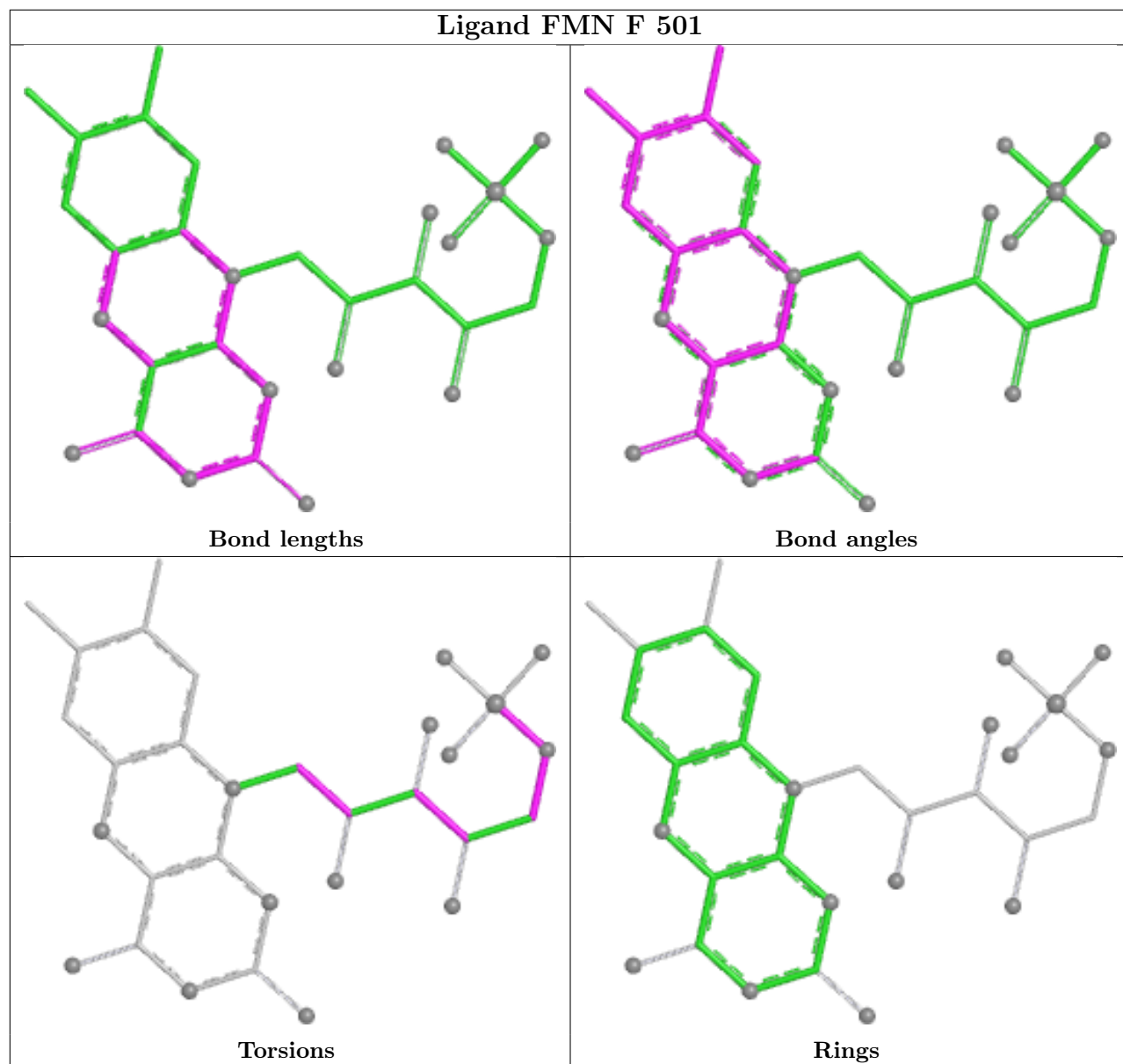


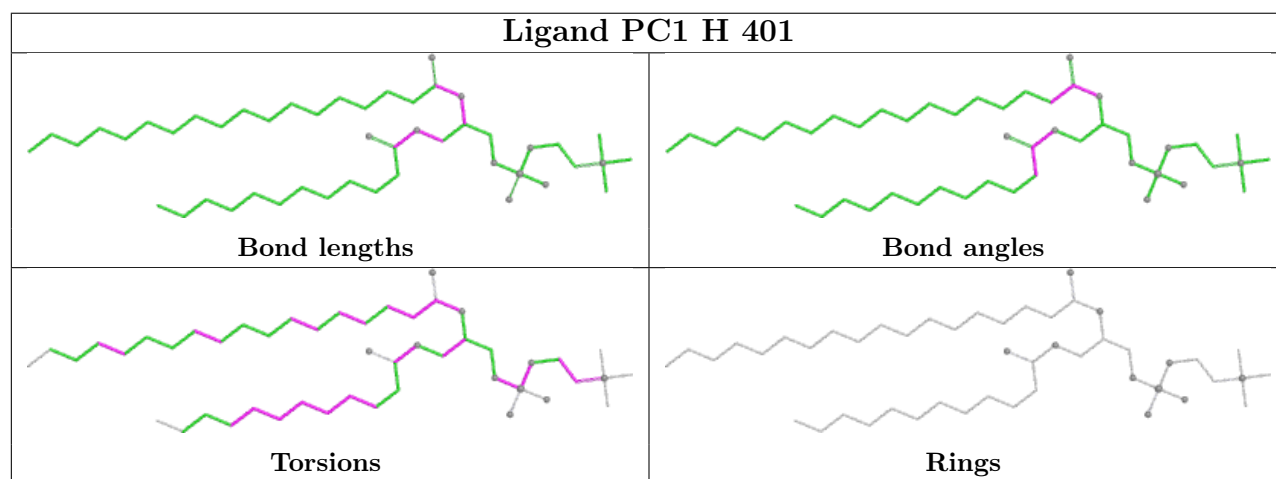
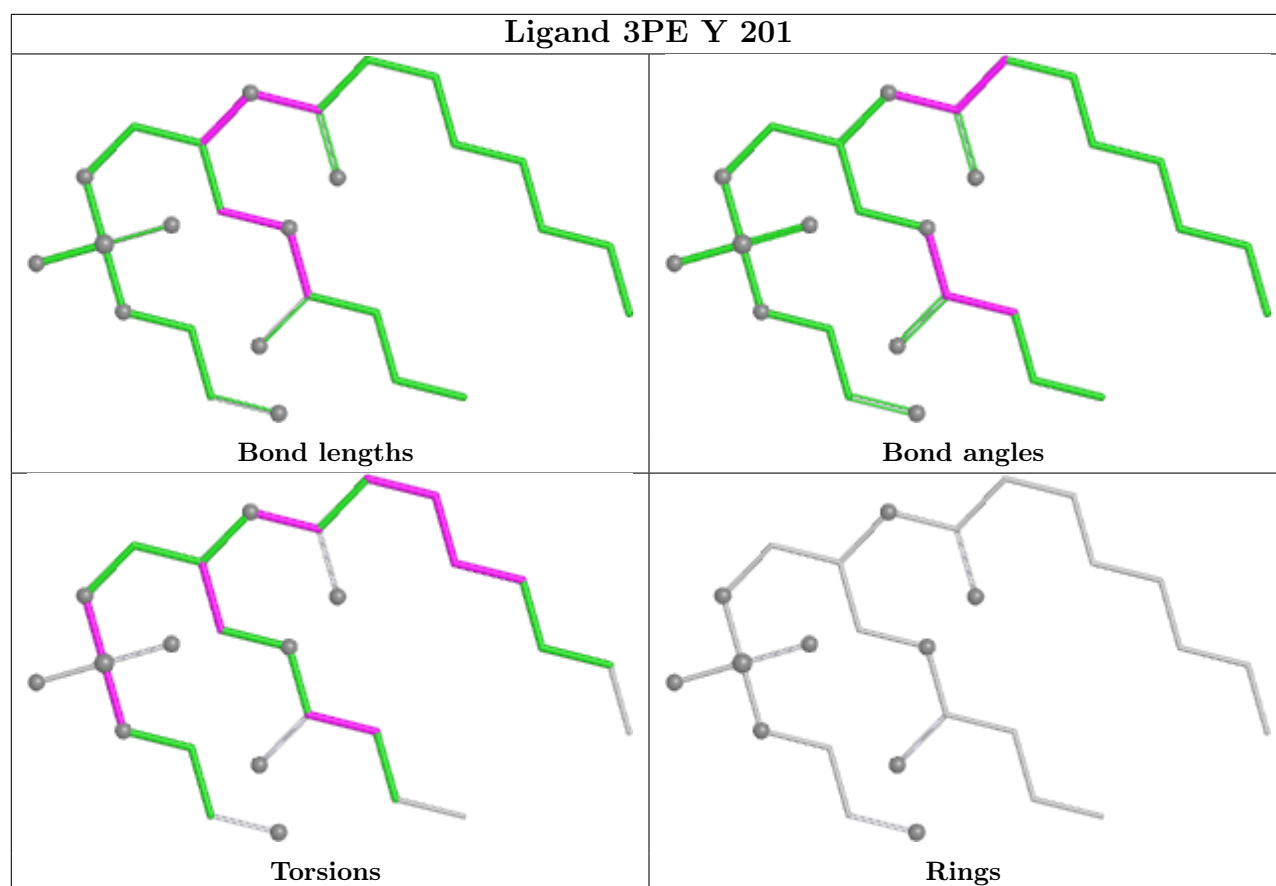


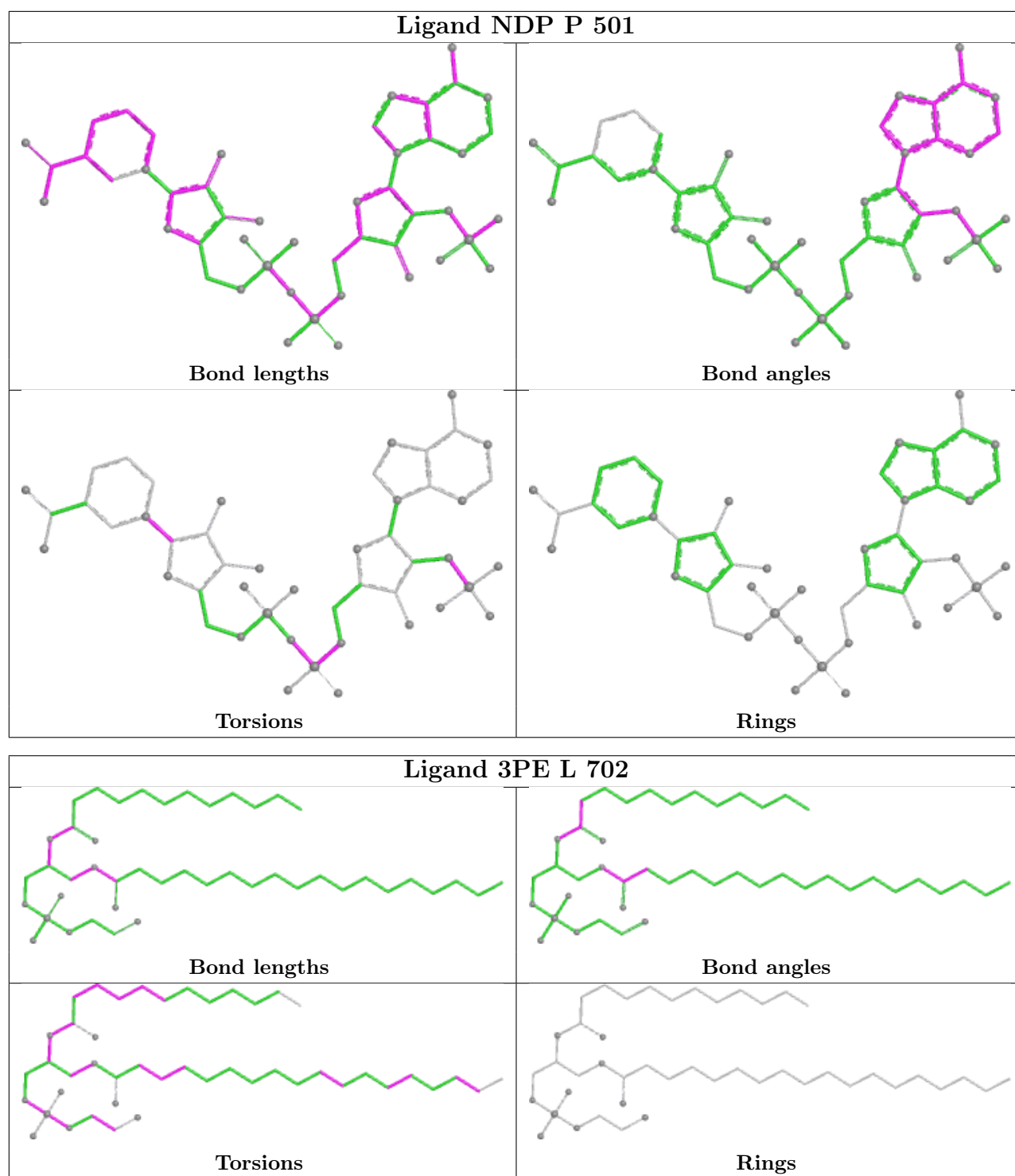












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

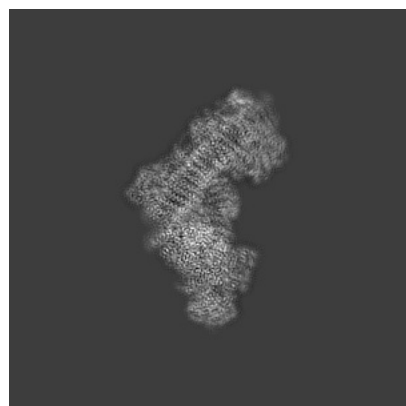
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18052. These allow visual inspection of the internal detail of the map and identification of artifacts.

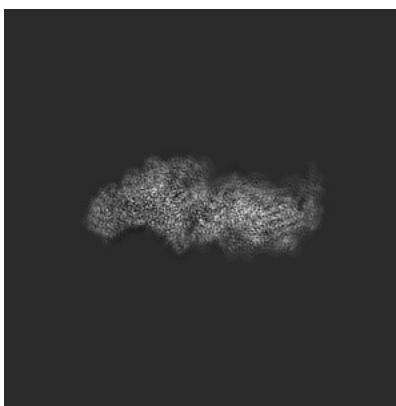
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

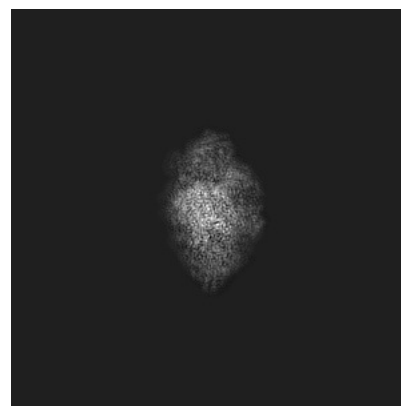
6.1.1 Primary map



X

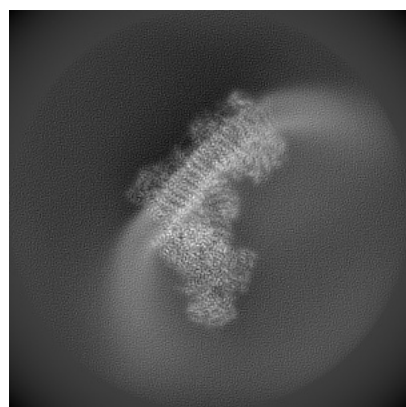


Y

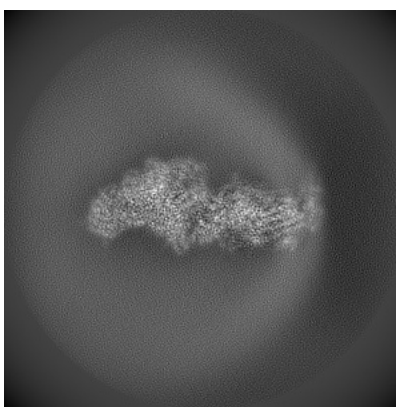


Z

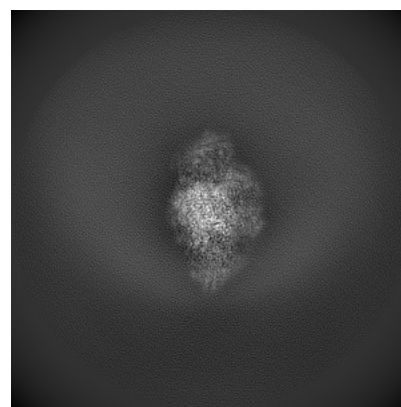
6.1.2 Raw map



X



Y

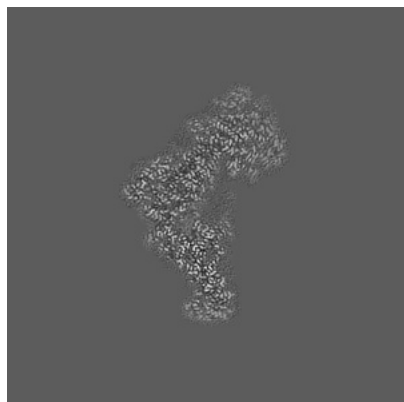


Z

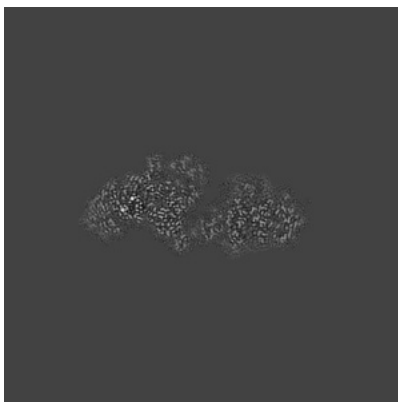
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

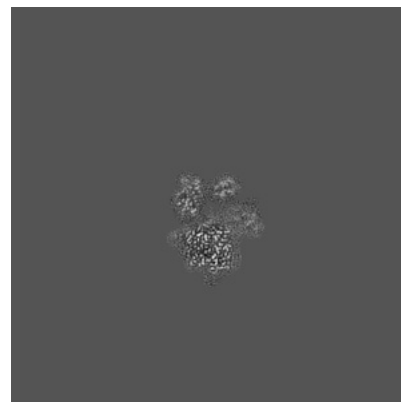
6.2.1 Primary map



X Index: 180

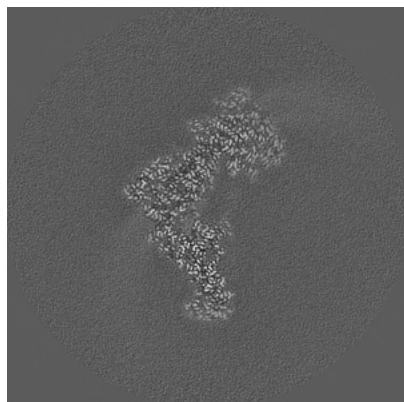


Y Index: 180

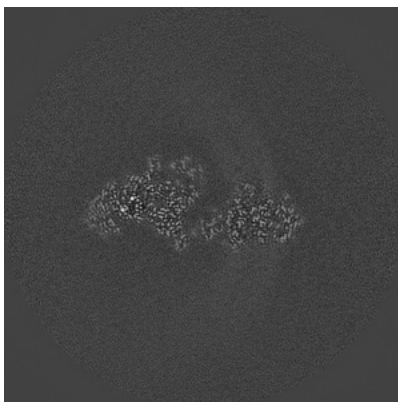


Z Index: 180

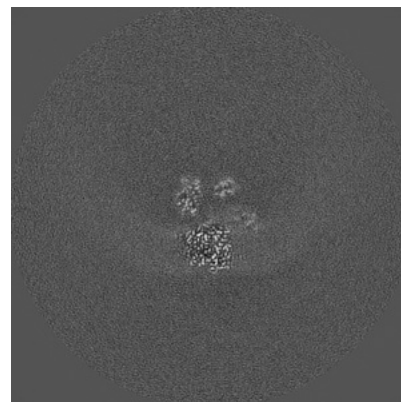
6.2.2 Raw map



X Index: 180



Y Index: 180

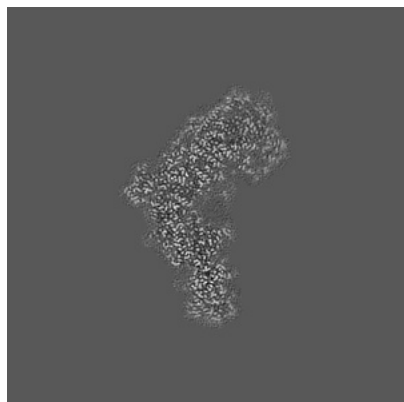


Z Index: 180

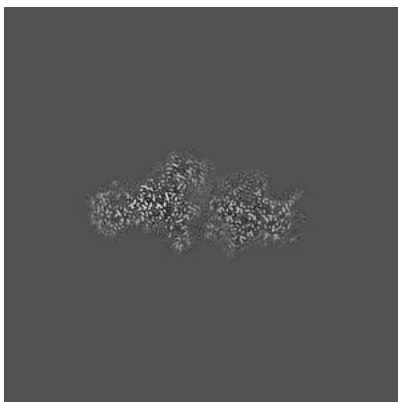
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

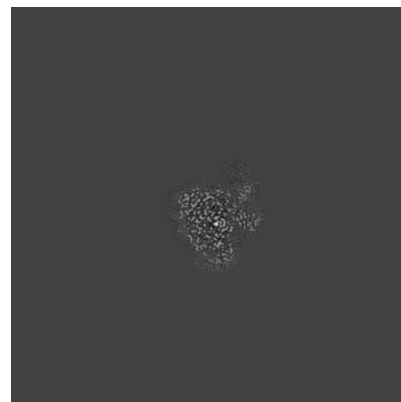
6.3.1 Primary map



X Index: 175

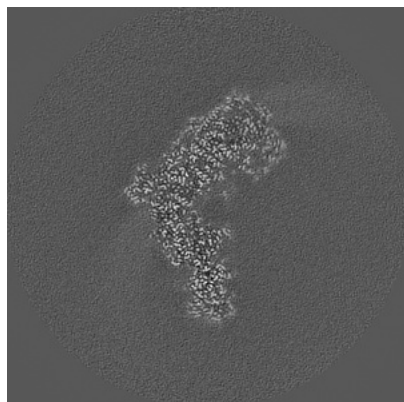


Y Index: 171

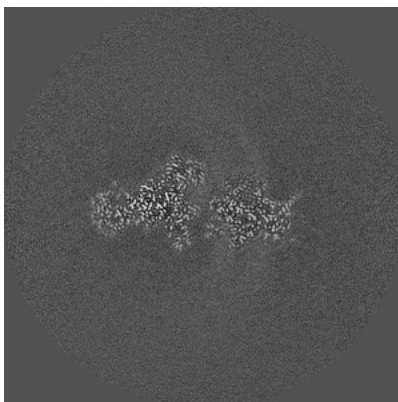


Z Index: 148

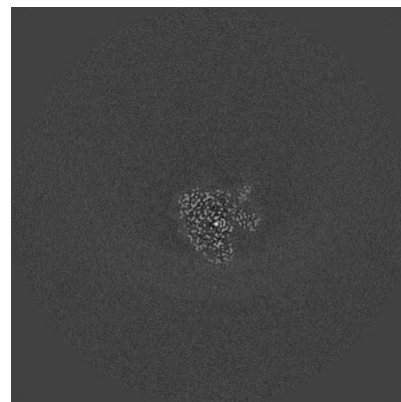
6.3.2 Raw map



X Index: 175



Y Index: 171

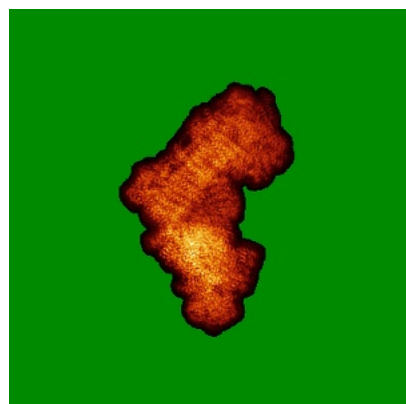


Z Index: 148

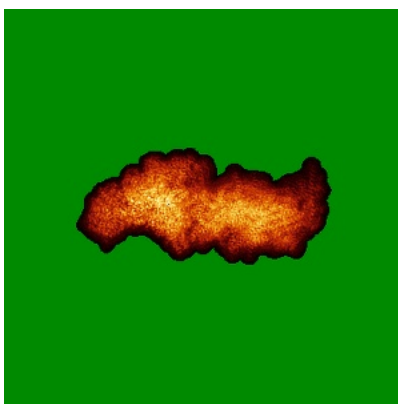
The images above show the largest variance slices of the map in three orthogonal directions.

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

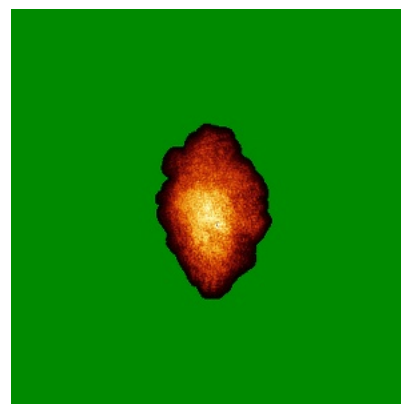
6.4.1 Primary map



X

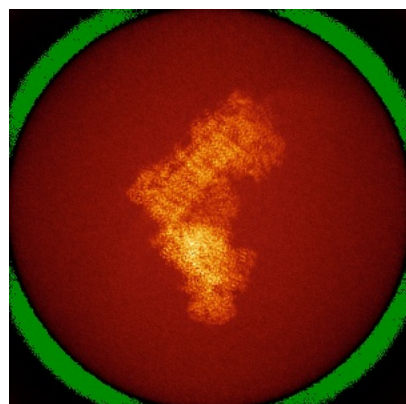


Y

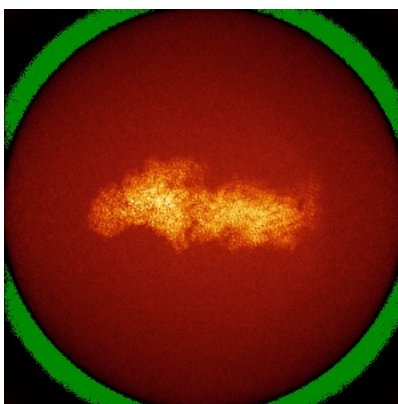


Z

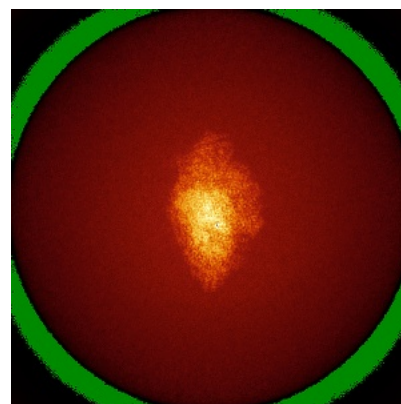
6.4.2 Raw map



X



Y

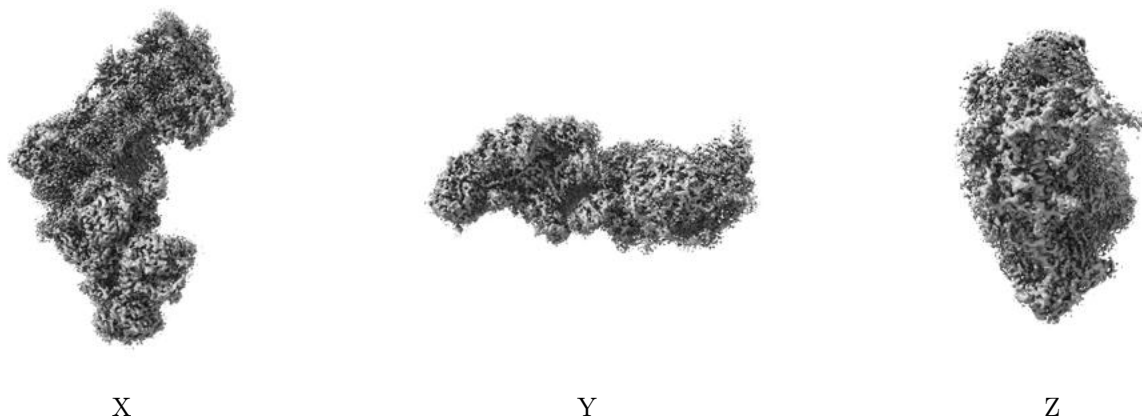


Z

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.

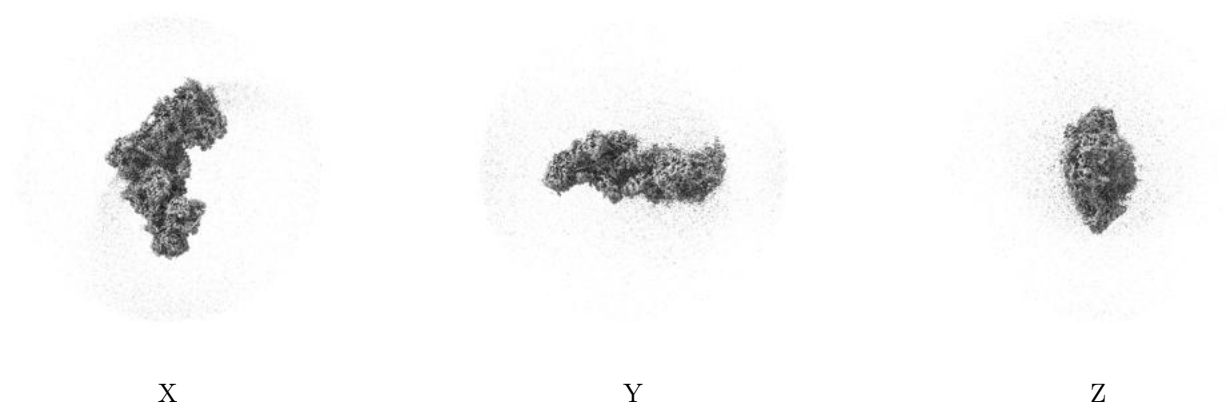
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

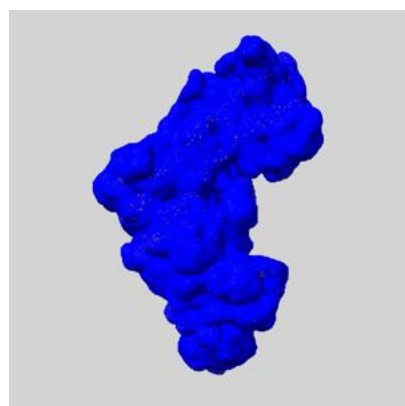
6.6 Mask visualisation [i](#)

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

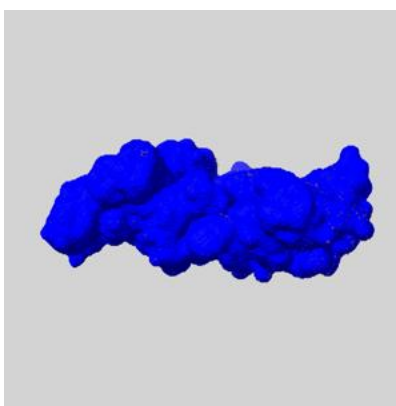
A mask typically either:

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

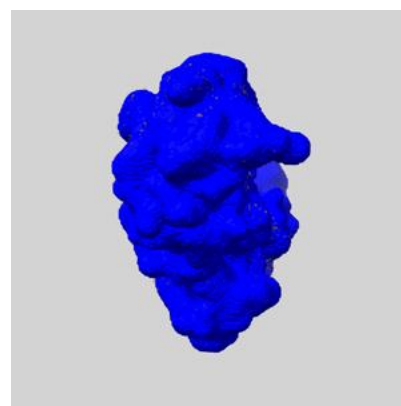
6.6.1 emd_18052_msk_1.map [i](#)



X



Y

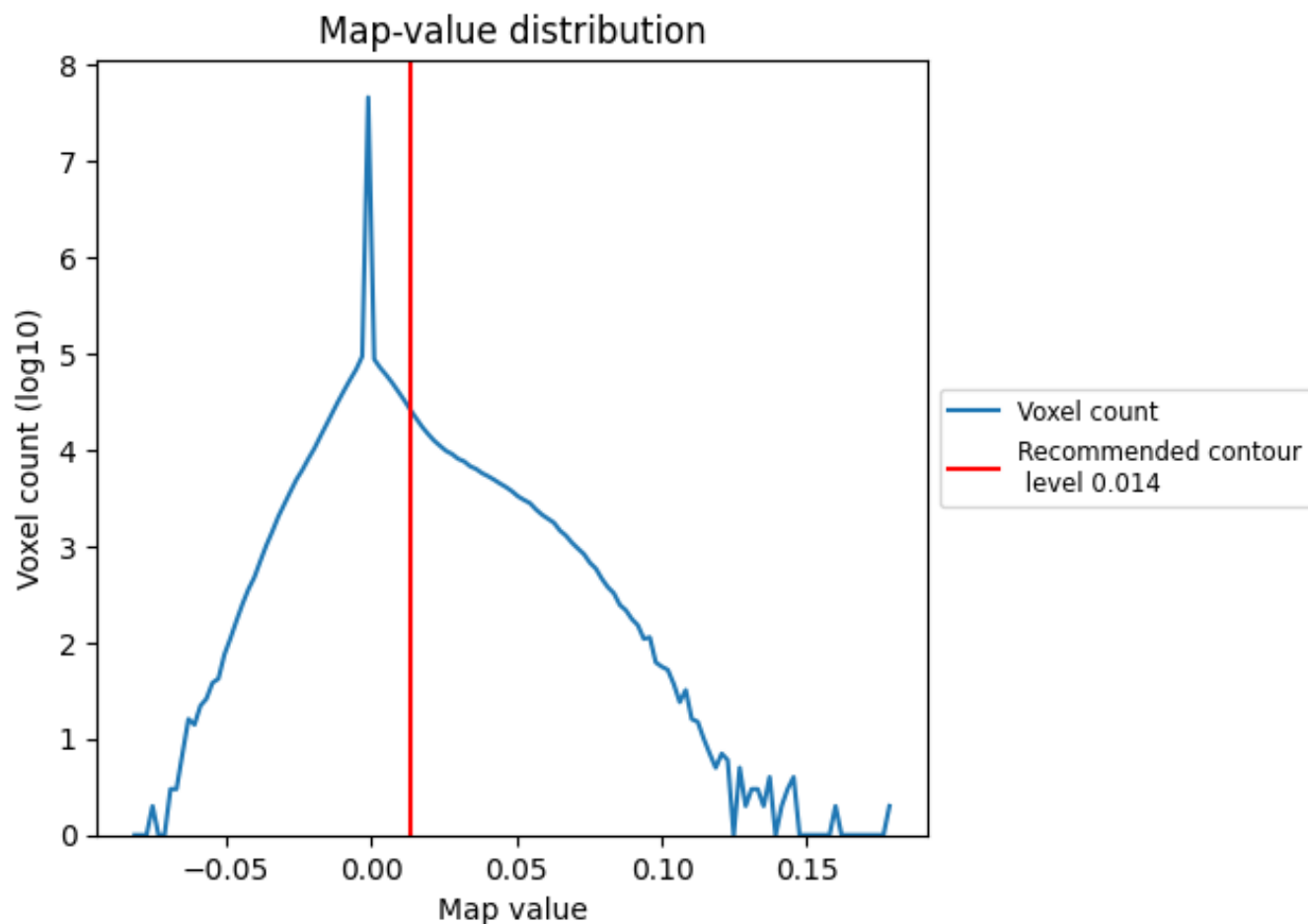


Z

7 Map analysis [i](#)

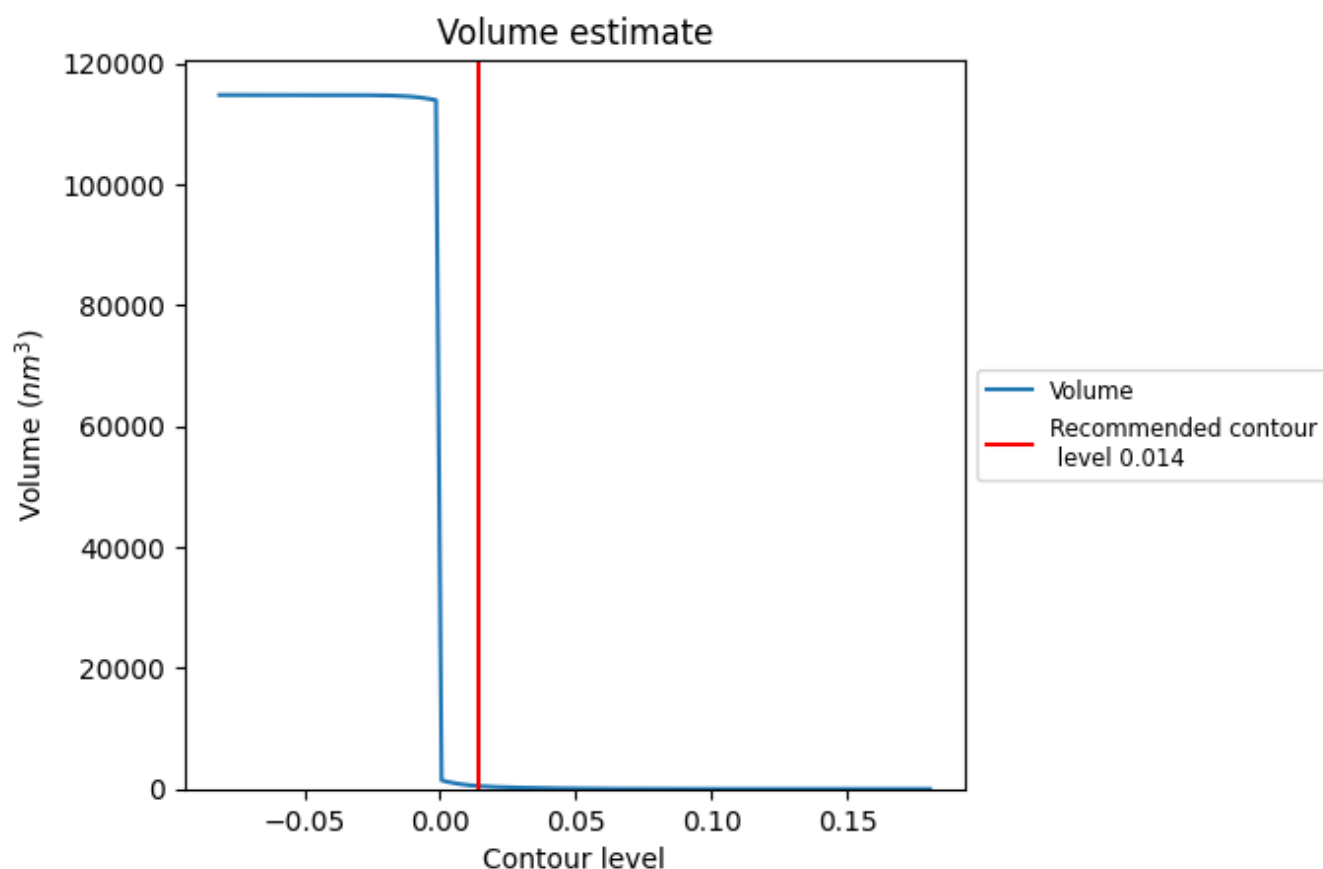
This section contains the results of statistical analysis of the map.

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.

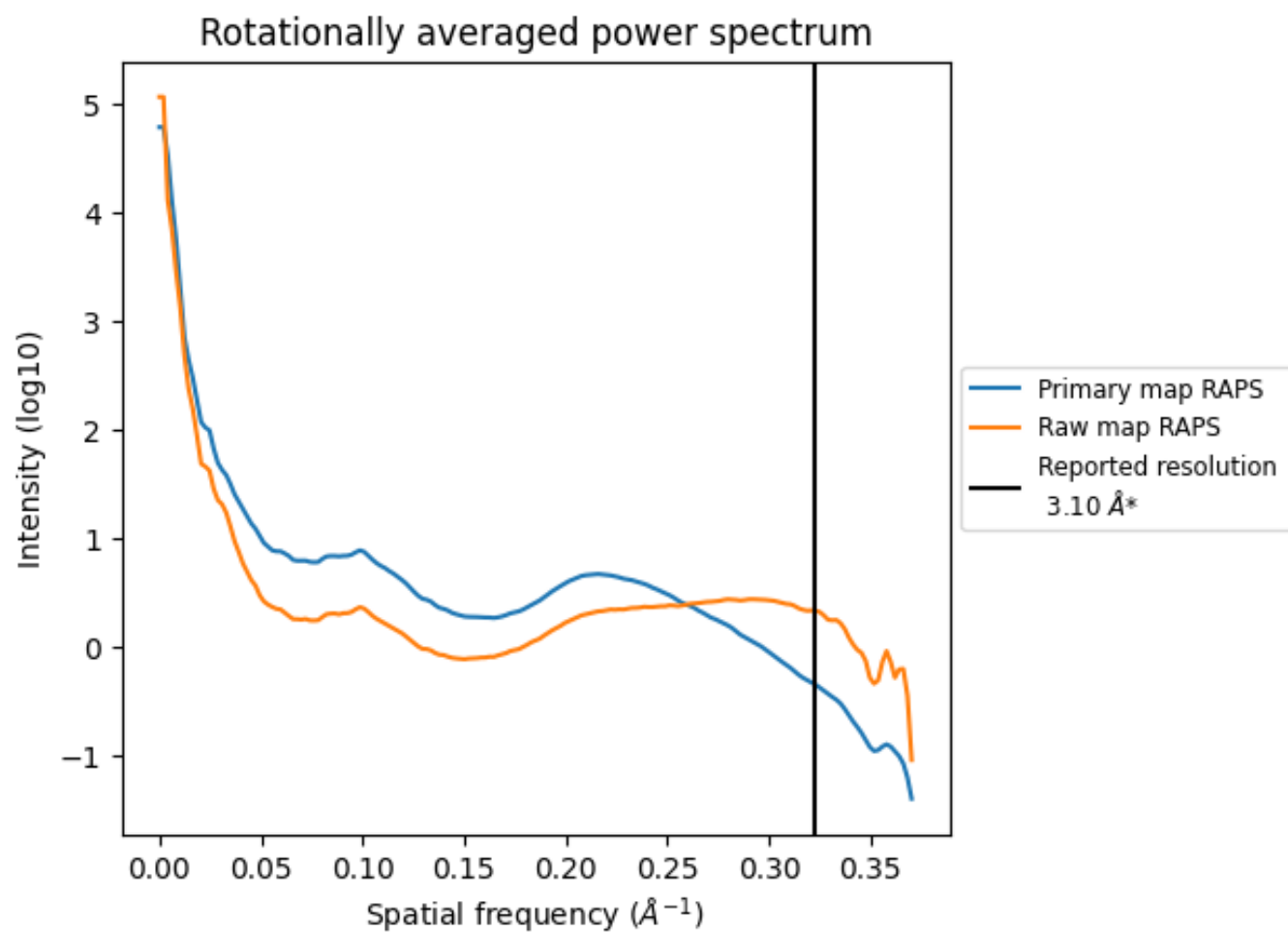
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 492 nm³; this corresponds to an approximate mass of 444 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 ⓘ

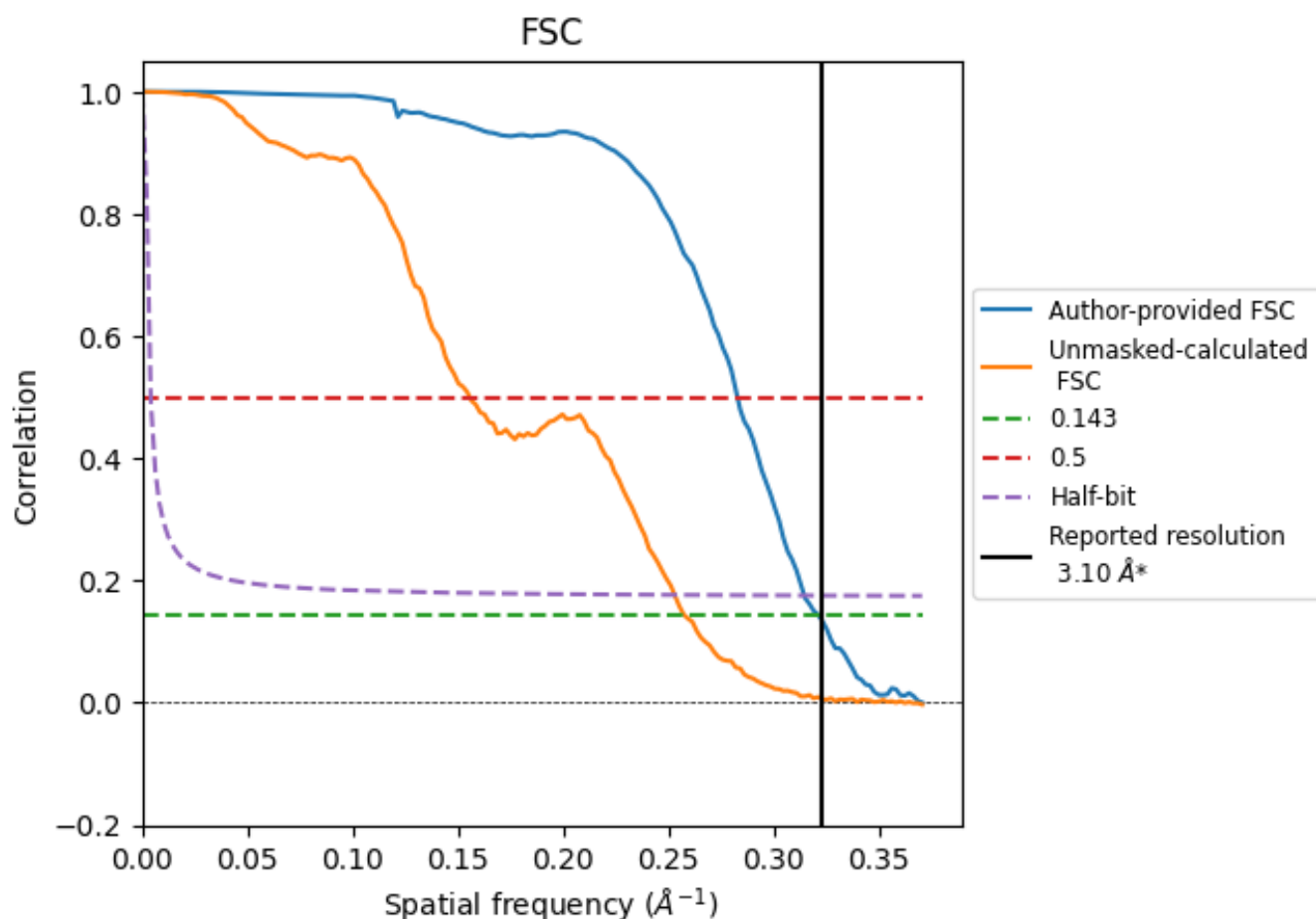


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

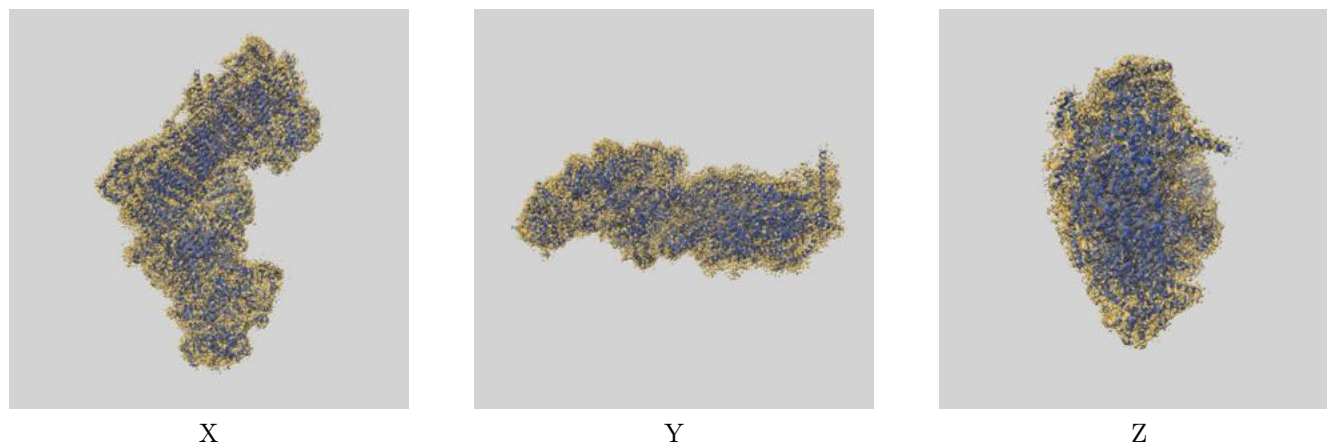
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.54	3.18
Unmasked-calculated*	3.88	6.43	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

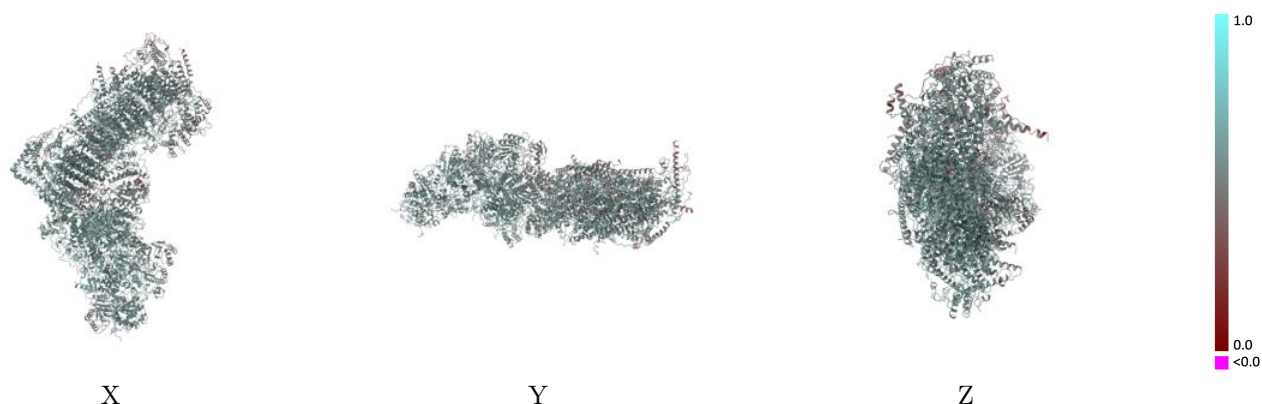
This section contains information regarding the fit between EMDB map EMD-18052 and PDB model 8Q0F. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



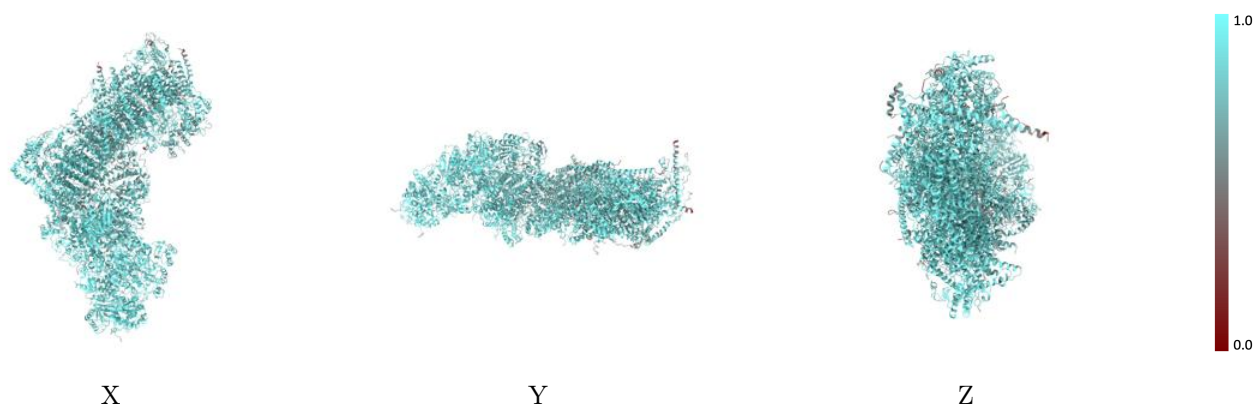
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



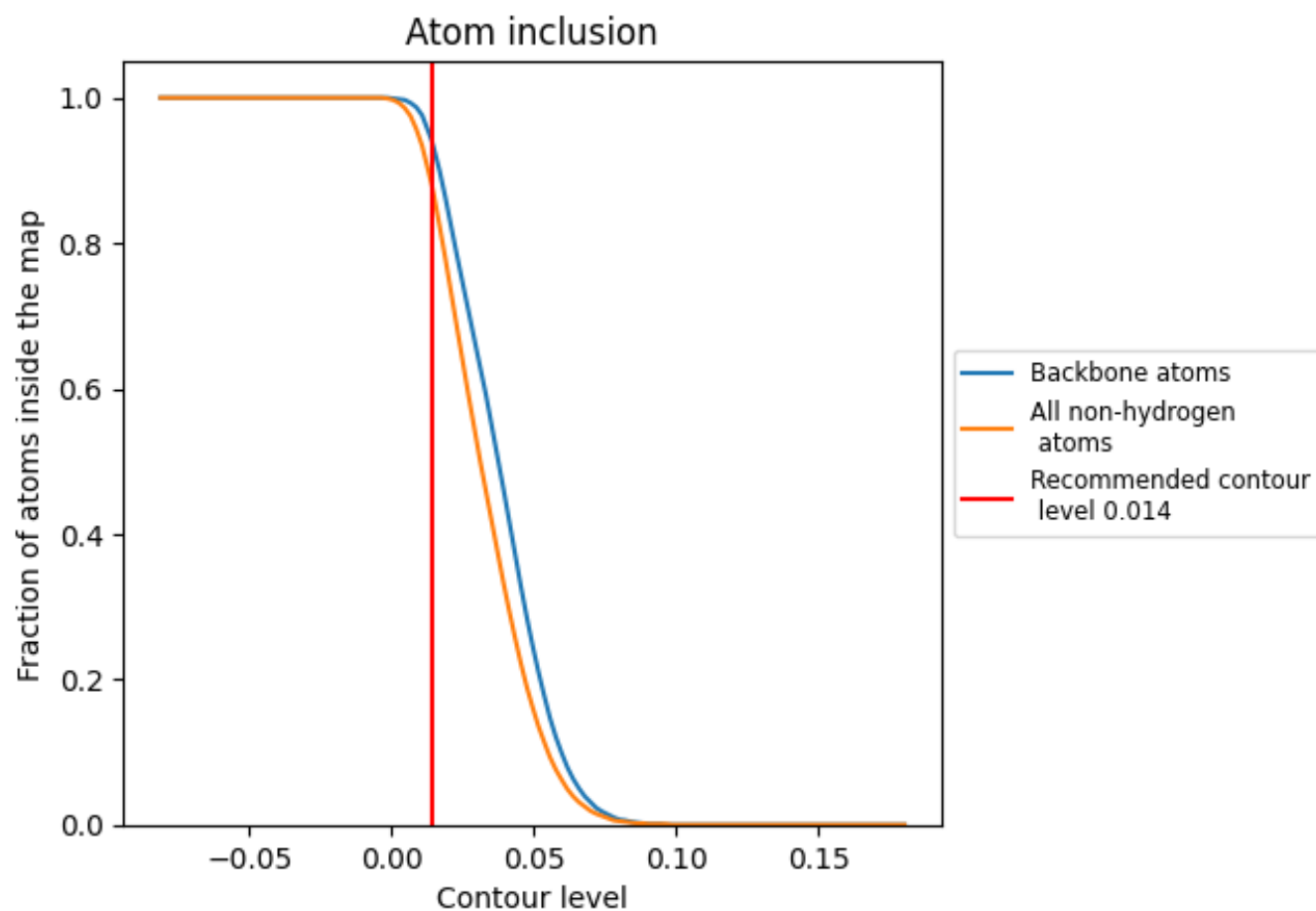
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.5600
A	 0.8620	 0.5630
B	 0.9260	 0.5940
C	 0.9500	 0.6080
D	 0.9330	 0.6050
E	 0.8980	 0.5450
F	 0.9180	 0.5630
G	 0.9100	 0.5710
H	 0.9130	 0.5840
I	 0.9560	 0.6070
J	 0.8670	 0.5530
K	 0.9310	 0.5860
L	 0.8650	 0.5590
M	 0.9200	 0.5950
N	 0.9380	 0.5950
O	 0.8690	 0.5410
P	 0.8390	 0.5310
Q	 0.8940	 0.5810
R	 0.8960	 0.5800
S	 0.8360	 0.5030
T	 0.7670	 0.4400
U	 0.7740	 0.4900
V	 0.8950	 0.5610
W	 0.8750	 0.5540
X	 0.8810	 0.5630
Y	 0.8190	 0.5460
Z	 0.8830	 0.5680
a	 0.9510	 0.5900
b	 0.8710	 0.5580
c	 0.8200	 0.5170
d	 0.8950	 0.5680
e	 0.8850	 0.5520
f	 0.7850	 0.5180
g	 0.8460	 0.5500
h	 0.8960	 0.5700



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7770	 0.4810
j	 0.7750	 0.4990
k	 0.7430	 0.4650
l	 0.8530	 0.5380
m	 0.8220	 0.5400
n	 0.8560	 0.5310
o	 0.7590	 0.4630
p	 0.8460	 0.5340
q	 0.9120	 0.5790
r	 0.9280	 0.5890
s	 0.8260	 0.5100