



Full wwPDB EM Validation Report ⓘ

Apr 18, 2026 – 08:36 am BST

PDB ID : 9SMI / pdb_00009smi
EMDB ID : EMD-55033
Title : Reduced bovine complex I in lipid nanodisc, NADH-deactive
Authors : Chung, I.; Hirst, J.
Deposited on : 2025-09-08
Resolution : 2.01 Å(reported)
Based on initial model : 7QSM

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:

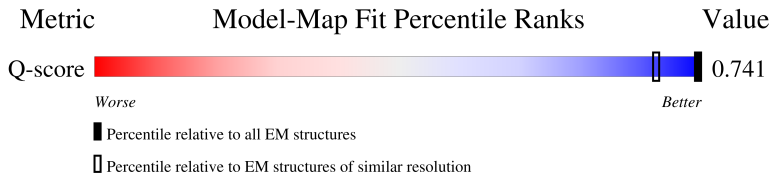
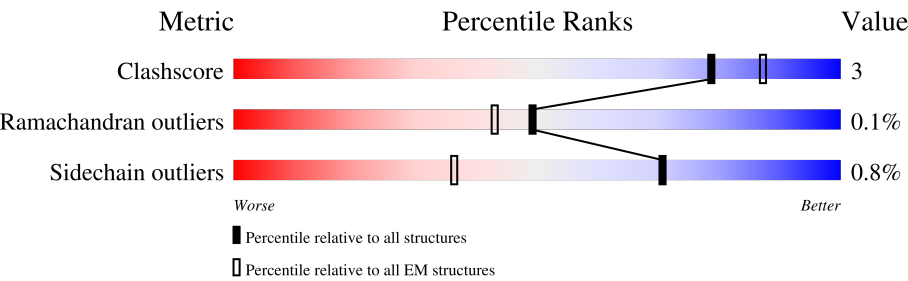
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.01 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	1691 (1.52 - 2.51)

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	 74% 14% 12%
2	B	216	 64% 6% 28%
3	C	266	 76% 22%
4	D	463	 87% 6% 7%

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

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Mol	Chain	Length	Quality of chain
29	d	121	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 72093 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	101	Total	C	N	O	S	0	0
			821	560	119	137	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1242	792	224	212	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	430	Total	C	N	O	S	0	0
			3459	2209	596	629	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	689	Total	C	N	O	S	0	0
			5283	3309	921	1014	39		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	311	Total	C	N	O	S	0	0
			2475	1589	442	439	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	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	83	Total	C	N	O	S	0	0
			674	434	99	136	5		
20	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			977	625	181	167	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	141	Total	C	N	O	S	0	0
			1030	657	176	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	ACE	-	acetylation	UNP Q8HXG6

- 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
			651	425	109	115	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	119	Total	C	N	O	S	0	0
			988	643	171	170	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	1	ACE	-	acetylation	UNP Q02827

- 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	100	Total	C	N	O	S	0	0
			837	539	139	155	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	128	Total	C	N	O	S	0	0
			1097	722	191	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	1	ACE	-	acetylation	UNP Q02367

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			580	381	95	103	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
			1067	684	188	195			

- 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	121	Total	C	N	O	S	0	0
			1040	649	200	182	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1450	909	268	265	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
			1209	778	216	210	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	96	Total	C	N	O	S	0	0
			776	490	144	139	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	1	ACE	-	acetylation	UNP Q05752

- 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).



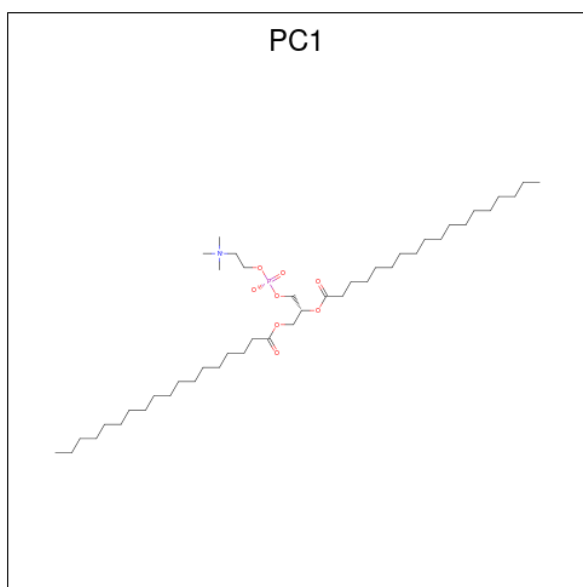
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	K	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	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
			44	34	1	8	1	
45	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			41	31	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	X	1	Total	C	N	O	P	0
			38	28	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
			39	29	1	8	1	
45	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	Y	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	Z	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	h	1	Total	C	N	O	P	0
			51	41	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).



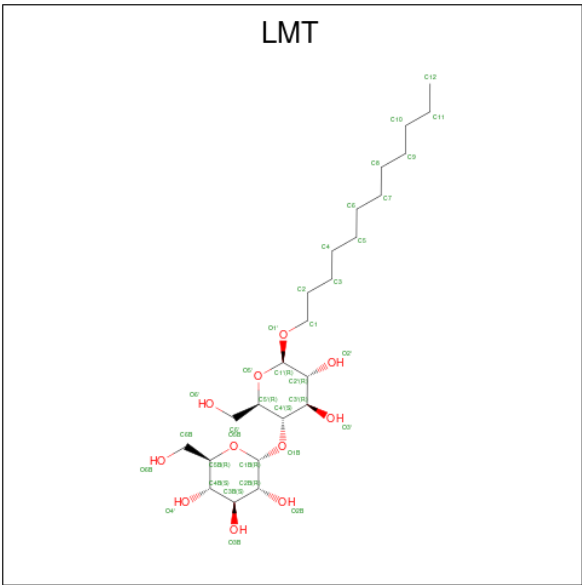
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
46	B	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	J	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	N	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	d	1	Total	C	N	O	P	0
			46	36	1	8	1	

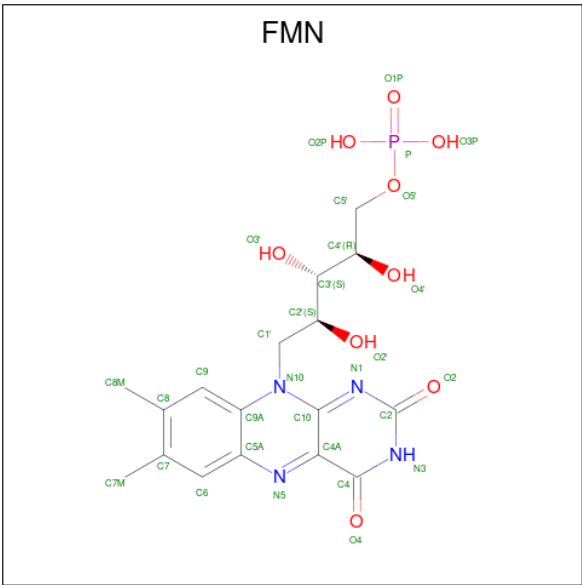
- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

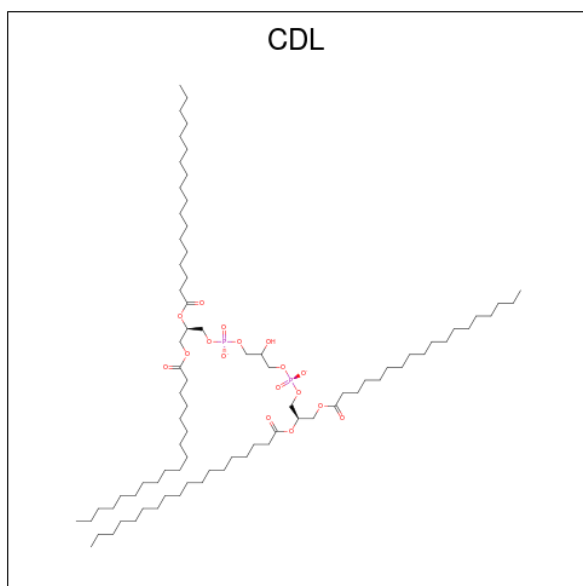
- Molecule 48 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).





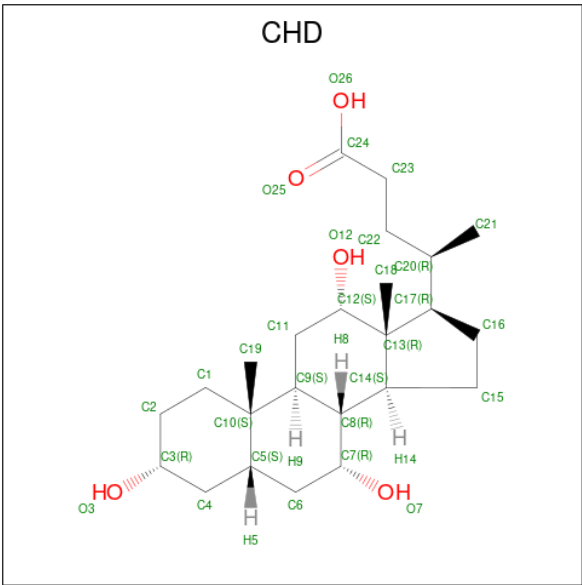
Mol	Chain	Residues	Atoms		AltConf
52	G	1	Total	K	0
			1	1	

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



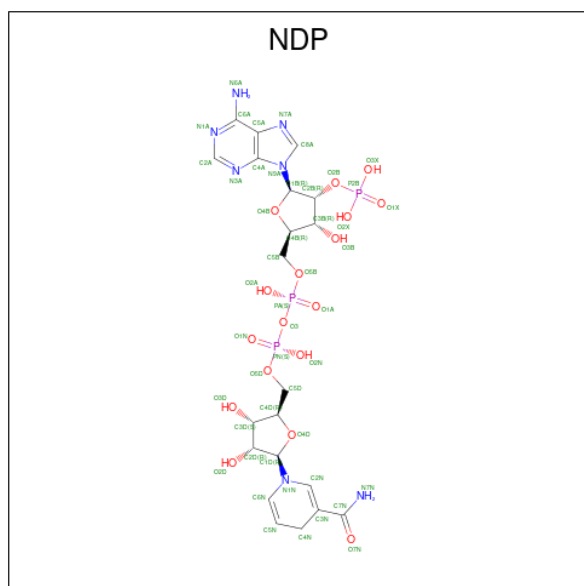
Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			71	52	17	2	
53	N	1	Total	C	O	P	0
			86	67	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			68	49	17	2	
53	q	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 54 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

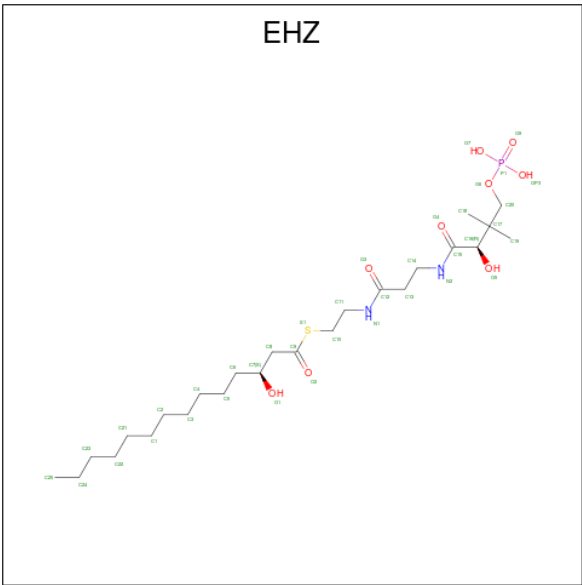


Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

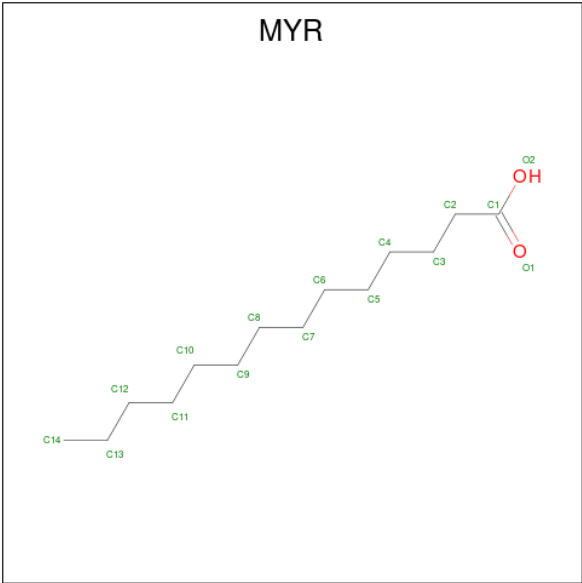
Mol	Chain	Residues	Atoms		AltConf
58	R	1	Total	Zn	0
			1	1	

- Molecule 59 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: $C_{25}H_{49}N_2O_9PS$).



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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	A	26	Total 26	O 26	0
61	B	109	Total 109	O 109	0
61	C	197	Total 197	O 197	0
61	D	344	Total 344	O 344	0
61	E	74	Total 74	O 74	0
61	F	140	Total 140	O 140	0
61	G	389	Total 389	O 389	0
61	H	172	Total 172	O 172	0
61	I	159	Total 159	O 159	0
61	J	49	Total 49	O 49	0
61	K	39	Total 39	O 39	0
61	L	220	Total 220	O 220	0
61	M	248	Total 248	O 248	0
61	N	165	Total 165	O 165	0
61	O	76	Total 76	O 76	0
61	P	116	Total 116	O 116	0
61	Q	153	Total 153	O 153	0
61	R	68	Total 68	O 68	0
61	S	8	Total 8	O 8	0
61	U	23	Total 23	O 23	0
61	V	43	Total 43	O 43	0
61	W	56	Total 56	O 56	0

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Mol	Chain	Residues	Atoms		AltConf
61	X	61	Total 61	O 61	0
61	Y	12	Total 12	O 12	0
61	Z	75	Total 75	O 75	0
61	a	48	Total 48	O 48	0
61	b	28	Total 28	O 28	0
61	c	3	Total 3	O 3	0
61	d	49	Total 49	O 49	0
61	e	63	Total 63	O 63	0
61	f	9	Total 9	O 9	0
61	g	40	Total 40	O 40	0
61	h	68	Total 68	O 68	0
61	i	17	Total 17	O 17	0
61	j	5	Total 5	O 5	0
61	k	6	Total 6	O 6	0
61	l	57	Total 57	O 57	0
61	m	52	Total 52	O 52	0
61	n	80	Total 80	O 80	0
61	o	14	Total 14	O 14	0
61	p	73	Total 73	O 73	0
61	q	86	Total 86	O 86	0
61	r	55	Total 55	O 55	0

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Mol	Chain	Residues	Atoms		AltConf
61	s	22	Total	O	0
			22	22	

3 Residue-property plots [i](#)

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

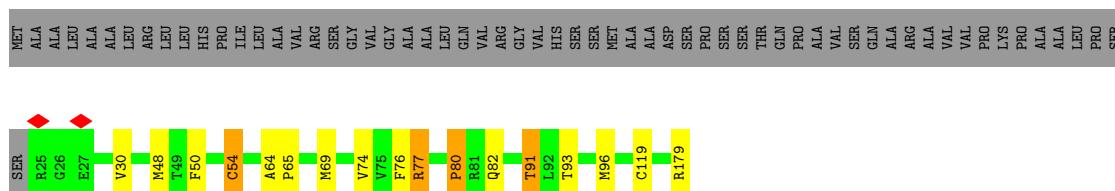
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



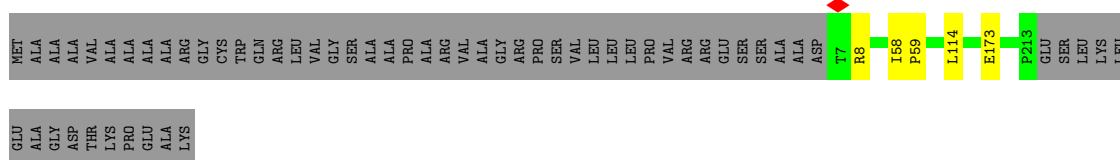
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 




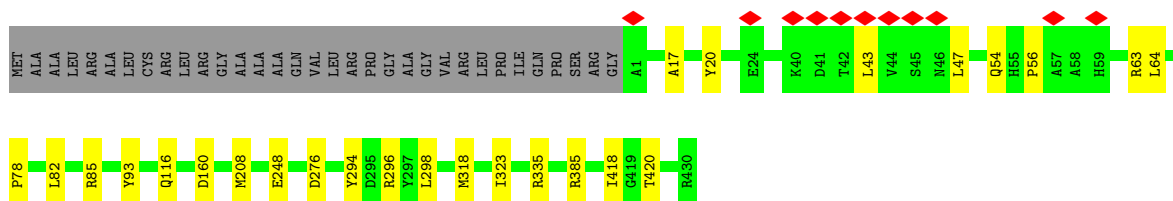
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 

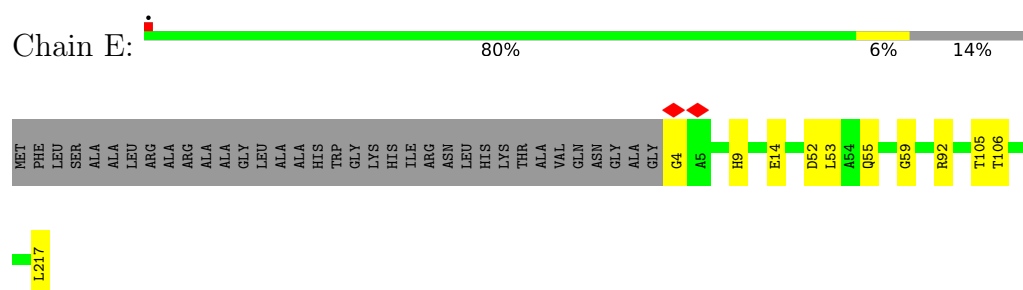


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

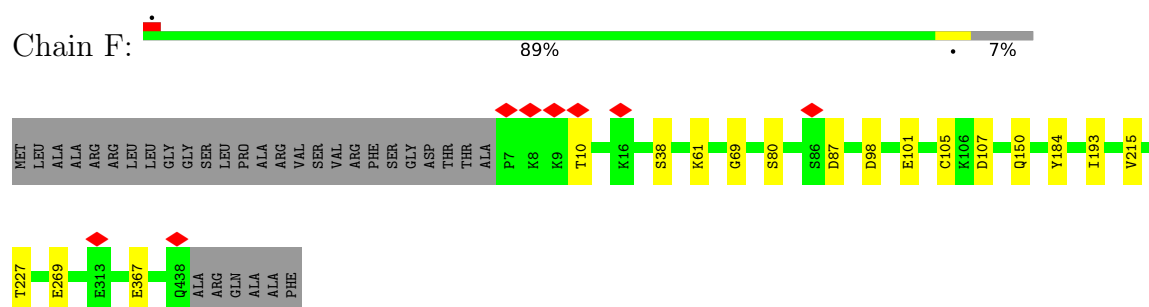
Chain D: 



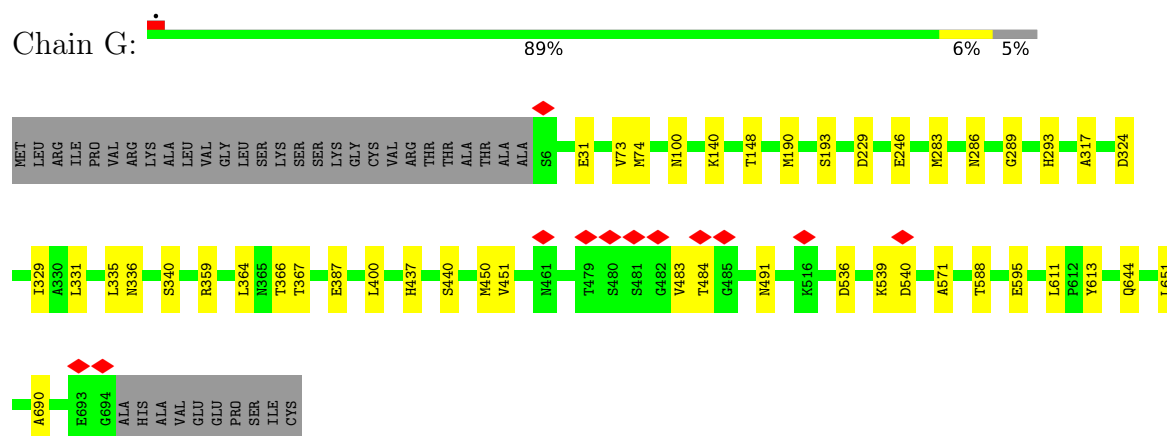
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



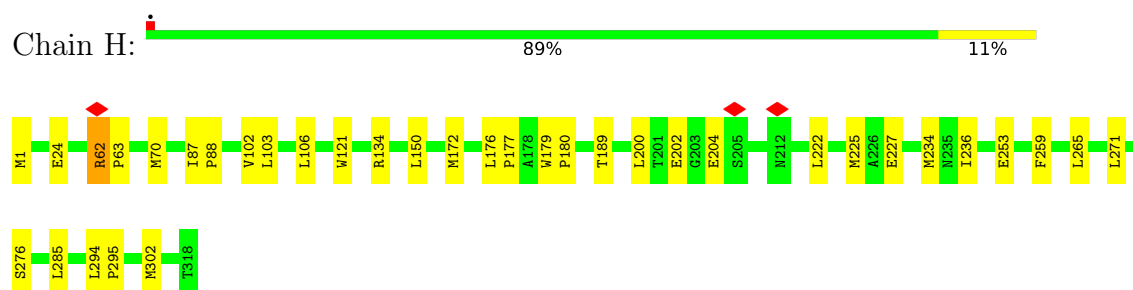
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial




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

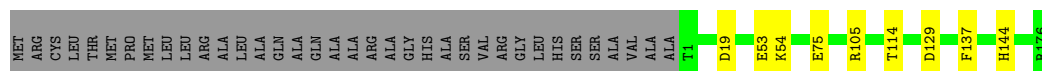


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



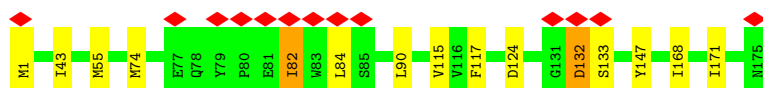
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  79% 17%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  7% 91% 7%



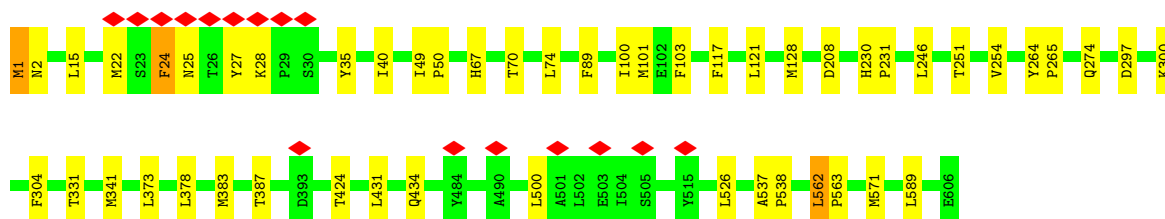
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  93% 7%



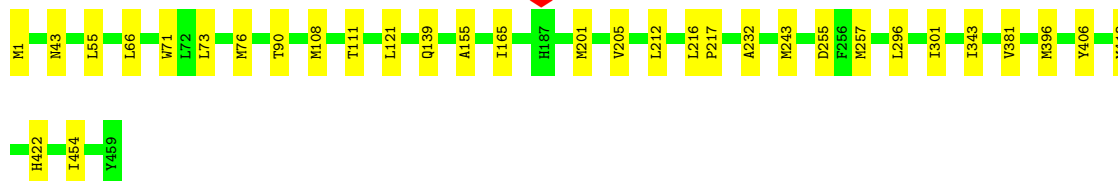
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  92% 8%



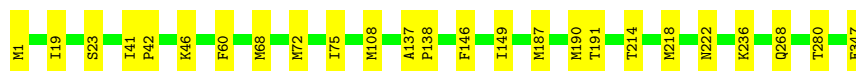
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  93% 7%




- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  93% 7%




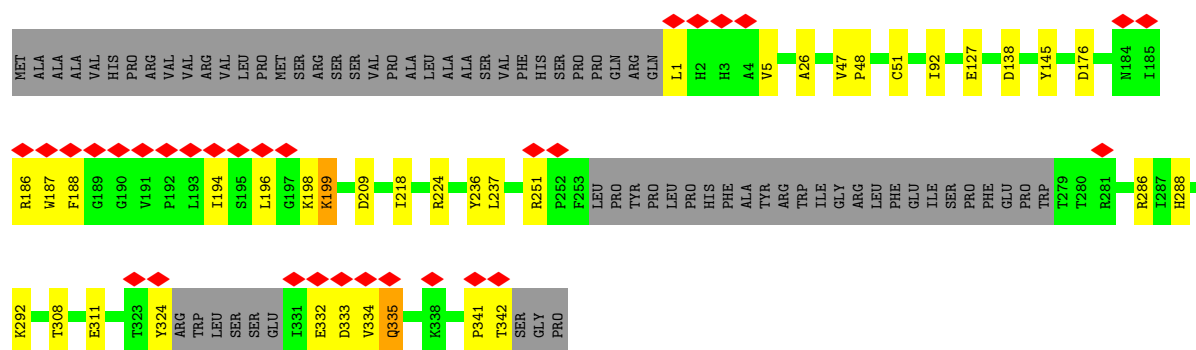
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  87% 6% 7%



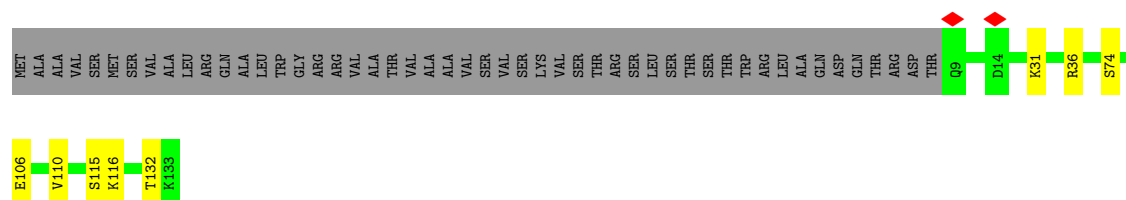
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  8% 72% 9% 18%



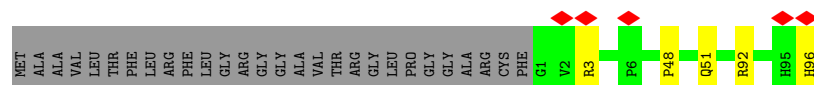
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  67% 5% 29%




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

Chain R:  73% 23%

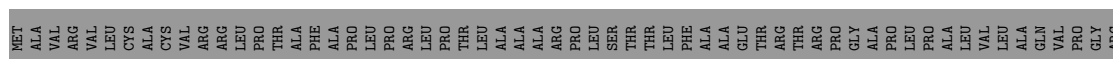


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

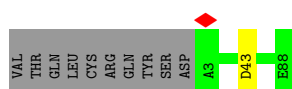
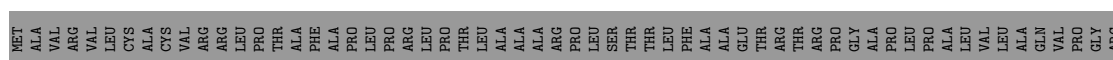
Chain S:  83% 13%



- Molecule 20: Acyl carrier protein, mitochondrial



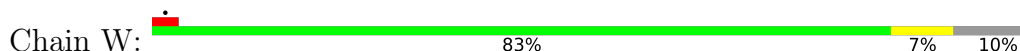
- Molecule 20: Acyl carrier protein, mitochondrial



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



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

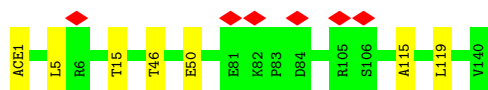


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

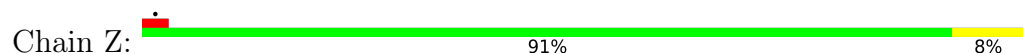


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11





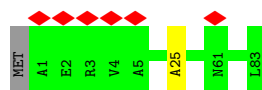
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



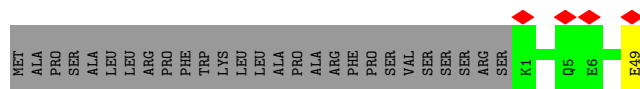
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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



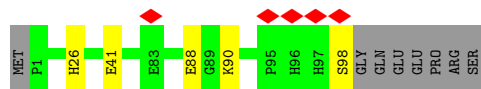
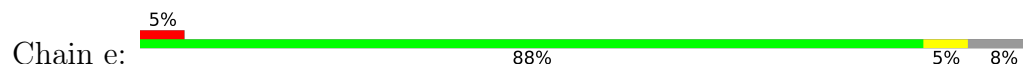
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



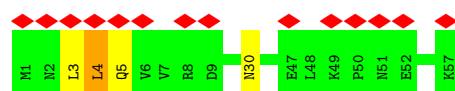
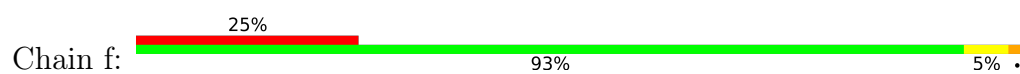
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



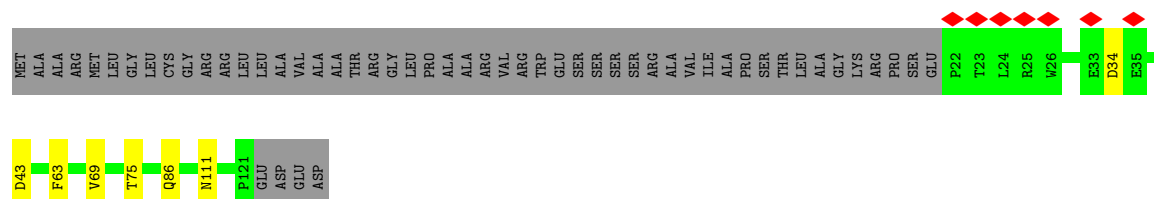
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



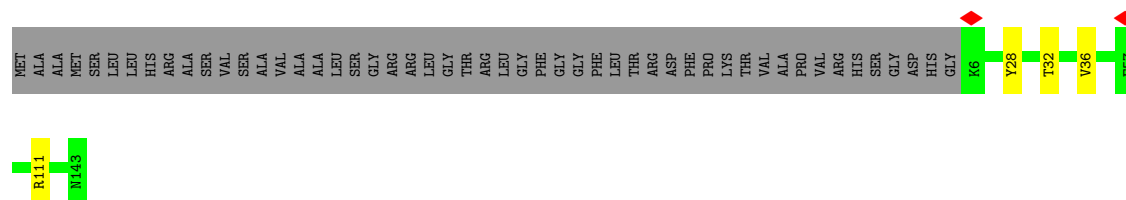
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



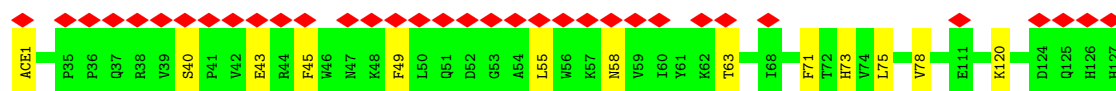
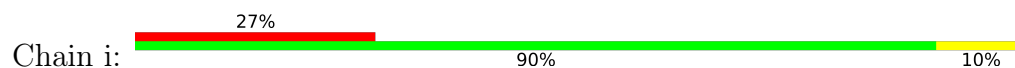
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



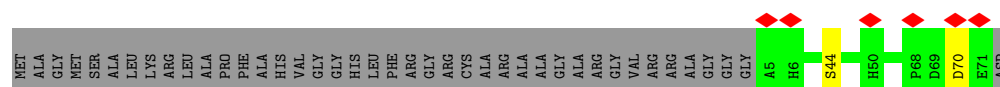
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



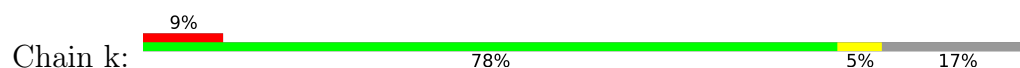
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

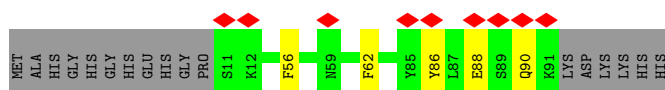


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

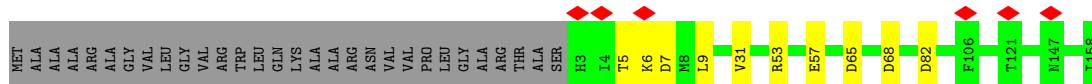
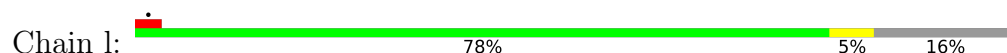


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

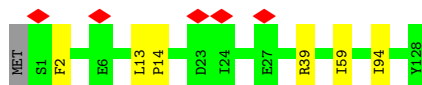




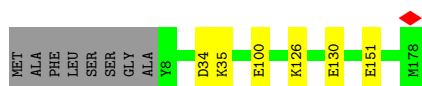
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



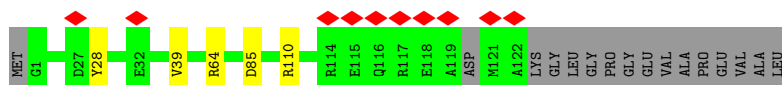
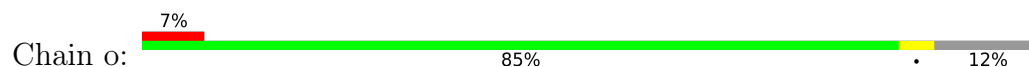
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



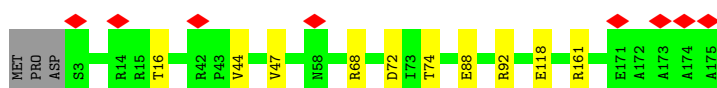
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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



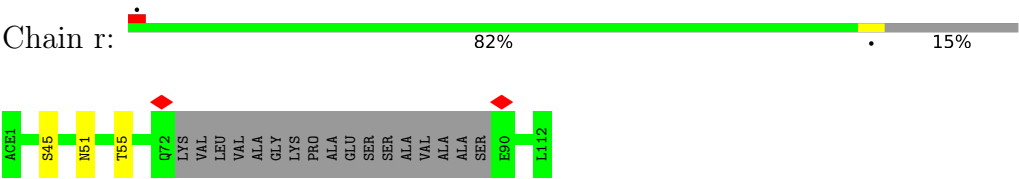
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



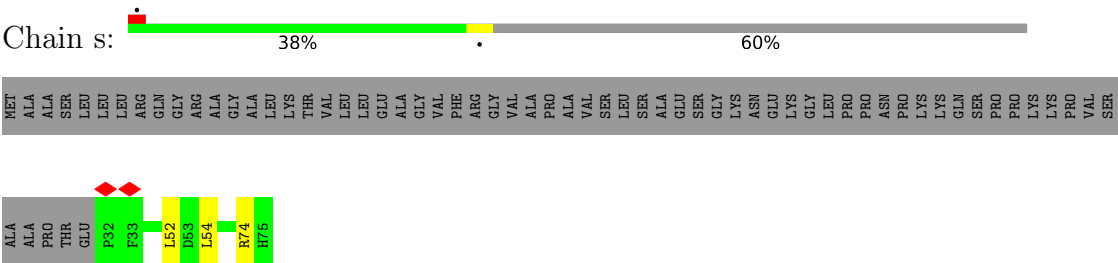
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	521652	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.29	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	57.967	Depositor
Minimum map value	-27.452	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.777	Depositor
Recommended contour level	3	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75375, 0.75375, 0.75375	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, CHD, MG, K, FMN, PC1, FME, MYR, ACE, NDP, FES, ZN, CDL, SF4, ARO, LMT, 3PE, 2MR, EH2, DGT

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	0.10	0/831	0.26	0/1136
2	B	0.14	0/1260	0.32	1/1703 (0.1%)
3	C	0.10	0/1772	0.27	0/2413
4	D	0.10	0/3537	0.25	0/4794
5	E	0.09	0/1699	0.26	0/2312
6	F	0.09	0/3401	0.25	0/4595
7	G	0.09	0/5371	0.27	0/7279
8	H	0.11	0/2571	0.28	0/3513
9	I	0.12	0/1445	0.28	0/1956
10	J	0.09	0/1370	0.24	0/1859
11	K	0.09	0/745	0.23	0/1008
12	L	0.09	0/4920	0.25	0/6694
13	M	0.09	0/3738	0.25	0/5097
14	N	0.10	0/2792	0.25	0/3800
15	O	0.09	0/2651	0.23	0/3587
16	P	0.11	0/2533	0.28	0/3427
17	Q	0.09	0/1039	0.25	0/1404
18	R	0.13	0/753	0.25	0/1014
19	S	0.09	0/702	0.25	0/945
20	T	0.08	0/684	0.23	0/921
20	U	0.08	0/705	0.22	0/952
21	V	0.09	0/948	0.21	0/1284
22	W	0.09	0/1001	0.23	0/1345
23	X	0.09	0/1439	0.24	0/1942
24	Y	0.18	1/1048 (0.1%)	0.20	0/1423
25	Z	0.09	0/1186	0.23	0/1599
26	a	0.12	0/584	0.22	0/786
27	b	0.12	0/672	0.23	0/923
28	c	0.12	0/427	0.20	0/579
29	d	0.08	0/1018	0.24	0/1375
30	e	0.09	0/846	0.24	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.11	0/505	0.27	0/681
32	g	0.09	0/864	0.26	0/1174
33	h	0.09	0/1188	0.23	0/1607
34	i	0.18	1/1134 (0.1%)	0.25	0/1544
35	j	0.08	0/607	0.22	0/833
36	k	0.08	0/672	0.21	0/906
37	l	0.09	0/1369	0.24	0/1873
38	m	0.10	0/1094	0.21	0/1480
39	n	0.08	0/1540	0.22	0/2085
40	o	0.08	0/1064	0.22	0/1423
41	p	0.08	0/1483	0.23	0/2000
42	q	0.10	0/1250	0.25	0/1698
43	r	0.21	0/795	0.28	0/1077
44	s	0.08	0/383	0.25	0/518
All	All	0.10	2/67636 (0.0%)	0.25	1/91695 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	1	ACE	C-N	5.14	1.45	1.34
24	Y	1	ACE	C-N	5.01	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	PRO	CB-CG-CD	-5.09	89.81	106.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	821	0	867	15	0
2	B	1242	0	1250	12	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1721	0	1675	4	0
4	D	3459	0	3404	21	0
5	E	1659	0	1664	13	0
6	F	3326	0	3282	13	0
7	G	5283	0	5304	32	0
8	H	2509	0	2621	30	0
9	I	1414	0	1370	7	0
10	J	1345	0	1352	17	0
11	K	745	0	785	10	0
12	L	4802	0	4960	33	0
13	M	3654	0	3852	26	0
14	N	2733	0	2912	22	0
15	O	2589	0	2566	11	0
16	P	2475	0	2508	22	0
17	Q	1016	0	1014	4	0
18	R	740	0	714	2	0
19	S	691	0	706	5	0
20	T	674	0	669	4	0
20	U	693	0	688	1	0
21	V	928	0	972	3	0
22	W	977	0	994	7	0
23	X	1402	0	1383	7	0
24	Y	1030	0	1039	3	0
25	Z	1157	0	1156	11	0
26	a	569	0	568	6	0
27	b	651	0	662	1	0
28	c	414	0	415	0	0
29	d	988	0	975	4	0
30	e	825	0	826	3	0
31	f	492	0	501	2	0
32	g	837	0	792	8	0
33	h	1154	0	1168	3	0
34	i	1097	0	1108	7	0
35	j	580	0	519	0	0
36	k	653	0	639	2	0
37	l	1314	0	1210	6	0
38	m	1067	0	1067	4	0
39	n	1487	0	1433	4	0
40	o	1040	0	1011	3	0
41	p	1450	0	1426	7	0
42	q	1209	0	1182	4	0
43	r	776	0	782	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	s	371	0	344	4	0
45	A	82	0	115	1	0
45	D	51	0	82	2	0
45	H	89	0	135	3	0
45	I	51	0	82	2	0
45	K	48	0	73	0	0
45	L	131	0	190	0	0
45	M	188	0	284	8	0
45	N	39	0	55	1	0
45	X	38	0	50	2	0
45	Y	227	0	342	6	0
45	Z	76	0	103	4	0
45	d	49	0	75	0	0
45	h	89	0	132	5	0
45	m	41	0	59	1	0
46	B	97	0	148	4	0
46	J	48	0	73	0	0
46	M	92	0	135	2	0
46	N	35	0	44	2	0
46	d	46	0	69	1	0
47	B	8	0	0	1	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	D	35	0	46	2	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	0	0
51	F	44	0	25	3	0
52	G	1	0	0	0	0
53	L	71	0	86	0	0
53	N	86	0	119	1	0
53	d	65	0	77	0	0
53	h	68	0	80	1	0
53	q	64	0	72	6	0
54	L	29	0	38	1	0
55	O	31	0	12	0	0
56	O	1	0	0	0	0
57	P	48	0	26	0	0
58	R	1	0	0	0	0
59	T	37	0	0	0	0
59	U	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	o	15	0	27	0	0
61	A	26	0	0	0	0
61	B	109	0	0	7	0
61	C	197	0	0	1	0
61	D	344	0	0	6	0
61	E	74	0	0	4	0
61	F	140	0	0	5	0
61	G	389	0	0	11	0
61	H	172	0	0	4	0
61	I	159	0	0	2	0
61	J	49	0	0	1	0
61	K	39	0	0	1	0
61	L	220	0	0	3	0
61	M	248	0	0	6	0
61	N	165	0	0	2	0
61	O	76	0	0	3	0
61	P	116	0	0	2	0
61	Q	153	0	0	3	0
61	R	68	0	0	1	0
61	S	8	0	0	0	0
61	U	23	0	0	0	0
61	V	43	0	0	2	0
61	W	56	0	0	1	0
61	X	61	0	0	1	0
61	Y	12	0	0	0	0
61	Z	75	0	0	2	0
61	a	48	0	0	0	0
61	b	28	0	0	0	0
61	c	3	0	0	0	0
61	d	49	0	0	2	0
61	e	63	0	0	1	0
61	f	9	0	0	0	0
61	g	40	0	0	3	0
61	h	68	0	0	1	0
61	i	17	0	0	0	0
61	j	5	0	0	0	0
61	k	6	0	0	0	0
61	l	57	0	0	1	0
61	m	52	0	0	0	0
61	n	80	0	0	1	0
61	o	14	0	0	0	0
61	p	73	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	q	86	0	0	1	0
61	r	55	0	0	0	0
61	s	22	0	0	2	0
All	All	72093	0	69208	381	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 3.

All (381) 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)
13:M:139:GLN:NE2	61:M:703:HOH:O	2.09	0.84
45:M:602:3PE:O14	61:M:701:HOH:O	1.97	0.82
29:d:80:ASP:OD2	61:d:302:HOH:O	1.97	0.82
24:Y:46:THR:OG1	24:Y:50:GLU:OE1	1.97	0.82
10:J:132:ASP:O	61:J:301:HOH:O	2.03	0.76
17:Q:116:LYS:O	61:Q:201:HOH:O	2.03	0.76
37:l:5:THR:OG1	37:l:7:ASP:OD1	2.02	0.76
4:D:385:ARG:NH2	61:D:603:HOH:O	2.18	0.76
13:M:43:ASN:OD1	61:M:702:HOH:O	2.03	0.76
32:g:43:ASP:O	61:g:201:HOH:O	2.02	0.76
1:A:71:LEU:O	10:J:147:TYR:OH	2.03	0.75
16:P:341:PRO:O	16:P:342:THR:OG1	2.04	0.75
21:V:78:GLU:OE1	61:V:201:HOH:O	2.03	0.75
17:Q:110:VAL:O	61:Q:202:HOH:O	2.05	0.75
6:F:269:GLU:OE1	61:F:601:HOH:O	2.05	0.75
41:p:118:GLU:OE2	61:p:201:HOH:O	2.05	0.74
32:g:34:ASP:OD2	61:g:202:HOH:O	2.05	0.73
37:l:65:ASP:OD1	61:l:201:HOH:O	2.06	0.73
2:B:76:PHE:O	61:B:302:HOH:O	2.07	0.73
12:L:22:MET:O	12:L:25:ASN:ND2	2.22	0.73
6:F:87:ASP:OD1	61:F:602:HOH:O	2.06	0.72
16:P:127:GLU:OE1	16:P:224:ARG:NH2	2.23	0.72
13:M:108:MET:HE1	45:X:201:3PE:H3C1	1.71	0.72
46:d:202:PC1:O12	61:d:303:HOH:O	2.06	0.72
16:P:48:PRO:O	61:P:601:HOH:O	2.08	0.71
23:X:125:SER:O	61:X:301:HOH:O	2.08	0.71
2:B:96:MET:N	61:B:301:HOH:O	2.23	0.70
16:P:51:CYS:O	61:P:602:HOH:O	2.09	0.69
33:h:28:TYR:OH	45:h:202:3PE:O12	2.07	0.69
38:m:39:ARG:NH1	39:n:151:GLU:OE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:ARG:NH1	43:r:55:THR:O	2.26	0.68
13:M:255:ASP:OD1	61:M:704:HOH:O	2.11	0.68
48:D:501:LMT:O2'	61:D:601:HOH:O	2.12	0.67
2:B:82:GLN:NE2	61:B:304:HOH:O	2.27	0.67
32:g:63:PHE:HE2	45:h:202:3PE:H2C2	1.60	0.67
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.28	0.67
22:W:123:TYR:O	61:W:201:HOH:O	2.11	0.67
10:J:132:ASP:N	10:J:132:ASP:OD1	2.27	0.67
12:L:208:ASP:OD1	61:L:802:HOH:O	2.12	0.67
15:O:22:SER:OG	15:O:119:GLY:O	2.08	0.66
39:n:100:GLU:OE2	61:n:201:HOH:O	2.13	0.66
44:s:74:ARG:NH2	61:s:101:HOH:O	2.26	0.66
2:B:93:THR:OG1	61:B:301:HOH:O	1.85	0.66
32:g:86:GLN:OE1	61:g:203:HOH:O	2.14	0.66
8:H:225:MET:SD	61:H:634:HOH:O	2.54	0.66
12:L:274:GLN:OE1	61:L:803:HOH:O	2.14	0.66
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.78	0.66
7:G:31:GLU:OE2	61:G:901:HOH:O	2.13	0.65
9:I:137:PHE:O	61:I:301:HOH:O	2.14	0.65
7:G:246:GLU:OE1	61:G:903:HOH:O	2.15	0.64
12:L:1:FME:HE2	12:L:2:ASN:HA	1.80	0.64
7:G:437:HIS:O	7:G:440:SER:OG	2.15	0.64
39:n:126:LYS:NZ	39:n:130:GLU:OE2	2.25	0.64
12:L:251:THR:O	12:L:254:VAL:HG22	1.98	0.63
5:E:150:ASN:OD1	61:E:401:HOH:O	2.15	0.63
17:Q:36:ARG:NE	17:Q:106:GLU:OE2	2.29	0.62
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.35	0.62
11:K:43:MET:HE1	14:N:72:MET:HE1	1.81	0.62
45:H:401:3PE:H2I2	45:Z:201:3PE:C2A	2.31	0.61
2:B:77:ARO:NH1	61:B:307:HOH:O	2.31	0.60
16:P:1:LEU:HD22	16:P:5:VAL:HG23	1.83	0.60
26:a:6:LEU:CD1	53:q:201:CDL:H732	2.32	0.60
23:X:87:CYS:SG	23:X:102:GLN:NE2	2.74	0.60
25:Z:127:LEU:HD12	25:Z:127:LEU:O	2.01	0.60
7:G:229:ASP:OD2	61:G:904:HOH:O	2.17	0.59
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.83	0.59
7:G:283:MET:HE1	42:q:139:PRO:HG3	1.85	0.59
19:S:18:ILE:HD11	19:S:93:VAL:HG11	1.84	0.59
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.33	0.59
10:J:124:ASP:OD1	11:K:2:SER:OG	2.21	0.59
14:N:347:GLU:OE2	61:N:501:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:GLU:O	61:G:905:HOH:O	2.17	0.59
53:h:201:CDL:H581	41:p:47:VAL:HG21	1.84	0.59
14:N:214:THR:HG22	14:N:218:MET:HE2	1.86	0.58
34:i:71:PHE:CD1	34:i:75:LEU:HD23	2.37	0.58
16:P:332:GLU:OE1	16:P:333:ASP:N	2.36	0.58
2:B:48:MET:HE2	4:D:56:PRO:HG3	1.86	0.58
4:D:63:ARG:NH1	61:D:609:HOH:O	2.27	0.57
5:E:52:ASP:OD1	61:E:402:HOH:O	2.17	0.57
39:n:34:ASP:OD1	39:n:35:LYS:N	2.37	0.57
7:G:366:THR:HB	7:G:450:MET:HE3	1.86	0.57
42:q:32:ASP:OD1	61:q:301:HOH:O	2.17	0.57
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.85	0.57
8:H:276:SER:O	61:H:501:HOH:O	2.16	0.57
1:A:18:VAL:HG22	8:H:222:LEU:HD12	1.87	0.57
40:o:28:TYR:OH	40:o:110:ARG:NH1	2.37	0.57
15:O:290:ASP:OD1	61:O:502:HOH:O	2.17	0.57
38:m:13:LEU:HD12	38:m:14:PRO:HD2	1.87	0.57
54:L:704:CHD:H212	54:L:704:CHD:H183	1.87	0.56
4:D:93:TYR:OH	61:D:602:HOH:O	2.14	0.56
6:F:184:TYR:OH	51:F:503:NAI:H5N	2.06	0.56
13:M:201:MET:HG3	45:M:601:3PE:H2G2	1.86	0.56
21:V:110:GLN:OE1	61:V:202:HOH:O	2.17	0.56
13:M:90:THR:HG21	45:M:602:3PE:H12	1.88	0.56
4:D:160:ASP:OD2	61:D:604:HOH:O	2.18	0.56
31:f:4:LEU:O	31:f:4:LEU:HD23	2.05	0.56
45:M:601:3PE:H2A1	14:N:280:THR:HG21	1.88	0.55
8:H:103:LEU:HD21	10:J:55:MET:HE3	1.87	0.55
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.42	0.55
46:M:605:PC1:H3C1	46:M:605:PC1:H372	1.88	0.55
7:G:451:VAL:HG23	61:G:933:HOH:O	2.06	0.55
1:A:94:LEU:HD12	10:J:147:TYR:HE1	1.70	0.55
8:H:227:GLU:OE2	61:H:502:HOH:O	2.18	0.55
11:K:73:LEU:HD12	14:N:60:PHE:CD2	2.41	0.55
26:a:6:LEU:HD13	53:q:201:CDL:H732	1.89	0.54
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.88	0.54
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.36	0.54
10:J:55:MET:HE2	10:J:55:MET:HA	1.87	0.54
5:E:105:THR:HG22	5:E:106:THR:H	1.73	0.54
13:M:108:MET:HE1	45:X:201:3PE:C3C	2.36	0.54
46:B:203:PC1:H3G1	48:D:501:LMT:H121	1.88	0.54
13:M:55:LEU:HD23	61:M:793:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:O	1:A:114:THR:OG1	2.23	0.54
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.91	0.53
22:W:52:LEU:HD22	22:W:104:MET:SD	2.48	0.53
8:H:204:GLU:OE1	8:H:204:GLU:N	2.36	0.53
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.44	0.53
8:H:106:LEU:HD11	8:H:150:LEU:HD23	1.91	0.53
46:M:605:PC1:O13	46:M:605:PC1:H133	2.09	0.53
17:Q:132:THR:O	61:Q:203:HOH:O	2.18	0.53
45:D:502:3PE:O22	12:L:571:MET:HE3	2.09	0.53
37:l:53:ARG:NH1	37:l:57:GLU:OE1	2.38	0.53
11:K:43:MET:CE	14:N:72:MET:HE1	2.38	0.53
6:F:98:ASP:OD2	61:F:603:HOH:O	2.19	0.52
14:N:146:PHE:HA	14:N:149:ILE:HD12	1.91	0.52
16:P:332:GLU:O	16:P:333:ASP:CG	2.51	0.52
4:D:20:TYR:CE1	12:L:571:MET:HE2	2.43	0.52
25:Z:75:LEU:HD12	61:Z:346:HOH:O	2.09	0.52
7:G:190:MET:HE1	7:G:690:ALA:HB1	1.91	0.52
12:L:434:GLN:NE2	36:k:56:PHE:O	2.42	0.52
16:P:198:LYS:O	16:P:199:LYS:CB	2.58	0.52
41:p:92:ARG:NH2	61:p:205:HOH:O	2.42	0.52
7:G:644:GLN:N	7:G:644:GLN:OE1	2.42	0.52
25:Z:51:MET:SD	45:Z:202:3PE:H221	2.50	0.52
41:p:88:GLU:OE2	61:p:202:HOH:O	2.19	0.52
15:O:80:GLU:OE1	15:O:80:GLU:N	2.39	0.52
29:d:9:ALA:HB1	29:d:12:GLN:CD	2.35	0.52
34:i:120:LYS:HG2	40:o:39:VAL:HG13	1.92	0.52
42:q:78:ASP:OD2	42:q:80:SER:OG	2.24	0.52
4:D:64:LEU:HD11	4:D:418:ILE:HD11	1.91	0.51
2:B:179:ARG:NE	46:B:201:PC1:O12	2.39	0.51
9:I:54:LYS:NZ	61:I:308:HOH:O	2.40	0.51
23:X:14:VAL:HG22	23:X:15:GLN:N	2.25	0.51
12:L:373:LEU:HD23	12:L:431:LEU:HD11	1.92	0.51
13:M:343:ILE:HG13	13:M:413:MET:HE2	1.92	0.51
8:H:189:THR:HG22	8:H:234:MET:HE2	1.93	0.51
1:A:18:VAL:HG22	8:H:222:LEU:CD1	2.40	0.51
3:C:173:GLU:OE2	61:C:301:HOH:O	2.19	0.51
6:F:61:LYS:NZ	6:F:80:SER:OG	2.43	0.51
8:H:102:VAL:CG1	8:H:150:LEU:HD21	2.41	0.51
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.40	0.51
11:K:73:LEU:C	11:K:73:LEU:HD13	2.36	0.51
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:216:LEU:HD23	13:M:216:LEU:C	2.36	0.51
30:e:26:HIS:ND1	61:e:201:HOH:O	2.33	0.51
7:G:400:LEU:O	61:G:906:HOH:O	2.19	0.50
18:R:48:PRO:O	61:R:301:HOH:O	2.18	0.50
7:G:283:MET:HE3	7:G:293:HIS:CE1	2.46	0.50
8:H:253:GLU:OE2	26:a:25:ARG:NH2	2.40	0.50
9:I:19:ASP:OD1	25:Z:32:GLY:N	2.39	0.50
14:N:19:ILE:O	14:N:23:SER:OG	2.20	0.50
5:E:55:GLN:O	5:E:59:GLY:N	2.41	0.50
23:X:154:GLU:OE1	23:X:154:GLU:N	2.45	0.50
25:Z:48:TRP:HB2	45:Z:202:3PE:H231	1.92	0.50
13:M:155:ALA:HB1	45:Y:205:3PE:H2I1	1.94	0.50
10:J:84:LEU:HB3	10:J:90:LEU:HD13	1.94	0.49
2:B:54:CYS:HB2	47:B:202:SF4:S1	2.52	0.49
23:X:74:LYS:NZ	26:a:69:ILE:O	2.32	0.49
7:G:450:MET:N	61:G:933:HOH:O	2.44	0.49
25:Z:110:VAL:HG22	61:Z:324:HOH:O	2.12	0.49
30:e:88:GLU:OE1	30:e:90:LYS:NZ	2.37	0.49
12:L:378:LEU:HD22	12:L:383:MET:HE2	1.95	0.49
8:H:227:GLU:HA	8:H:227:GLU:OE1	2.12	0.49
12:L:74:LEU:HD13	61:L:963:HOH:O	2.12	0.48
14:N:68:MET:HE2	14:N:68:MET:HA	1.94	0.48
45:M:602:3PE:H2B2	45:M:606:3PE:H2B2	1.93	0.48
14:N:108:MET:HE1	14:N:191:THR:OG1	2.13	0.48
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.94	0.48
22:W:96:VAL:HG12	22:W:96:VAL:O	2.13	0.48
34:i:45:PHE:O	34:i:49:PHE:N	2.46	0.48
8:H:106:LEU:CD1	8:H:150:LEU:HD23	2.43	0.48
8:H:200:LEU:HD22	8:H:285:LEU:HD21	1.95	0.48
46:N:402:PC1:H351	46:N:402:PC1:H381	1.49	0.48
7:G:611:LEU:HD13	7:G:613:TYR:OH	2.12	0.48
16:P:334:VAL:O	16:P:335:GLN:HB2	2.13	0.48
25:Z:129:ALA:O	25:Z:133:VAL:HG23	2.14	0.48
7:G:283:MET:HE3	7:G:293:HIS:ND1	2.29	0.48
45:H:401:3PE:H2C2	45:I:203:3PE:H2G1	1.95	0.48
2:B:91:THR:HA	2:B:119:CYS:HB3	1.95	0.48
15:O:129:TYR:OH	61:O:501:HOH:O	2.03	0.48
53:q:201:CDL:OB6	53:q:201:CDL:H531	2.07	0.48
1:A:51:PHE:C	1:A:51:PHE:CD1	2.92	0.47
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.96	0.47
26:a:6:LEU:HD11	53:q:201:CDL:H732	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:5:LEU:HD13	45:Y:203:3PE:O32	2.13	0.47
45:A:201:3PE:H2G1	27:b:25:ALA:HB1	1.97	0.47
2:B:80:PRO:O	61:B:303:HOH:O	2.20	0.47
7:G:588:THR:OG1	61:G:902:HOH:O	2.14	0.47
4:D:54:GLN:NE2	8:H:202:GLU:O	2.45	0.47
7:G:73:VAL:O	7:G:74:MET:HE2	2.15	0.47
7:G:359:ARG:NH1	61:G:911:HOH:O	2.46	0.47
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.49	0.47
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.41	0.47
33:h:111:ARG:NH1	61:h:305:HOH:O	2.41	0.47
40:o:64:ARG:NH2	40:o:85:ASP:OD2	2.45	0.47
8:H:134:ARG:NH2	61:H:513:HOH:O	2.36	0.47
15:O:186:LYS:NZ	61:O:504:HOH:O	2.47	0.47
13:M:296:LEU:HD22	13:M:381:VAL:HG11	1.96	0.47
16:P:26:ALA:HB3	16:P:47:VAL:HG13	1.97	0.47
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.97	0.47
13:M:232:ALA:HB3	61:M:840:HOH:O	2.15	0.47
16:P:198:LYS:HE3	16:P:237:LEU:HD11	1.97	0.47
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.97	0.46
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.97	0.46
12:L:27:TYR:CD1	12:L:28:LYS:N	2.83	0.46
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.46
15:O:311:ASP:OD1	15:O:311:ASP:N	2.48	0.46
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.98	0.46
4:D:208:MET:HE1	4:D:318:MET:CB	2.45	0.46
14:N:187:MET:HE2	14:N:190:MET:CE	2.46	0.46
15:O:272:TYR:O	15:O:275:ILE:HG23	2.14	0.46
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.32	0.46
16:P:333:ASP:OD1	16:P:333:ASP:C	2.57	0.46
6:F:69:GLY:O	51:F:503:NAI:H2N	2.15	0.46
46:N:402:PC1:C28	46:N:402:PC1:H352	2.46	0.46
12:L:128:MET:HG2	12:L:251:THR:HG22	1.98	0.46
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.51	0.45
7:G:140:LYS:O	7:G:148:THR:OG1	2.26	0.45
19:S:18:ILE:HD11	19:S:93:VAL:CG1	2.46	0.45
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.40	0.45
41:p:72:ASP:OD1	41:p:74:THR:OG1	2.34	0.45
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.98	0.45
6:F:227:THR:HG23	61:F:607:HOH:O	2.16	0.45
8:H:70:MET:HE1	8:H:121:TRP:CE3	2.51	0.45
8:H:172:MET:SD	8:H:176:LEU:HD23	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:46:LYS:NZ	61:N:509:HOH:O	2.43	0.45
10:J:171:ILE:HD11	14:N:42:PRO:HA	1.99	0.45
13:M:108:MET:HB3	13:M:121:LEU:HD13	1.98	0.45
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.98	0.45
19:S:18:ILE:CD1	19:S:93:VAL:HG11	2.47	0.45
25:Z:51:MET:HE3	25:Z:52:LYS:HD2	1.99	0.45
34:i:43:GLU:OE1	34:i:43:GLU:N	2.43	0.45
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.50	0.45
19:S:13:LEU:N	19:S:13:LEU:HD22	2.31	0.45
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.47	0.45
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.97	0.45
5:E:162:GLU:OE1	61:E:403:HOH:O	2.21	0.45
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.99	0.45
16:P:138:ASP:OD2	16:P:292:LYS:NZ	2.50	0.45
25:Z:51:MET:HE3	25:Z:52:LYS:CD	2.46	0.45
44:s:74:ARG:NH1	61:s:102:HOH:O	2.49	0.45
1:A:94:LEU:HD12	10:J:147:TYR:CE1	2.51	0.44
12:L:562:LEU:CB	12:L:563:PRO:CD	2.95	0.44
53:q:201:CDL:H722	53:q:201:CDL:C35	2.47	0.44
7:G:651:LEU:HD11	19:S:45:LYS:HD3	2.00	0.44
12:L:230:HIS:N	12:L:231:PRO:CD	2.80	0.44
21:V:68:GLU:OE2	21:V:76:ILE:N	2.44	0.44
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.99	0.44
8:H:176:LEU:HB3	8:H:177:PRO:HD3	1.99	0.44
12:L:24:PHE:CD1	12:L:24:PHE:N	2.86	0.44
14:N:222:ASN:OD1	14:N:236:LYS:NZ	2.51	0.44
46:B:201:PC1:H142	46:B:201:PC1:O13	2.17	0.44
7:G:317:ALA:HB1	7:G:331:LEU:HD21	2.00	0.44
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.53	0.44
11:K:40:LEU:HD22	14:N:75:ILE:HD12	1.99	0.44
12:L:589:LEU:HD21	45:Y:204:3PE:C25	2.48	0.44
20:U:43:ASP:OD1	20:U:43:ASP:N	2.50	0.44
12:L:331:THR:HB	12:L:387:THR:HG22	1.99	0.44
4:D:64:LEU:HD23	4:D:78:PRO:HA	1.99	0.44
4:D:208:MET:HE1	4:D:318:MET:HB2	2.00	0.44
7:G:484:THR:O	61:G:907:HOH:O	2.21	0.44
1:A:65:PHE:CD2	1:A:98:LEU:HD11	2.53	0.44
7:G:336:ASN:ND2	7:G:340:SER:O	2.46	0.44
53:q:201:CDL:H711	53:q:201:CDL:H741	1.71	0.44
2:B:69:MET:HE2	2:B:74:VAL:HG12	2.00	0.43
4:D:20:TYR:OH	45:D:502:3PE:O12	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:454:ILE:HD12	13:M:454:ILE:C	2.43	0.43
24:Y:115:ALA:O	24:Y:119:LEU:HD23	2.18	0.43
25:Z:51:MET:CE	45:Z:202:3PE:H221	2.48	0.43
41:p:16:THR:HG23	41:p:16:THR:O	2.18	0.43
5:E:149:VAL:HG22	6:F:105:CYS:SG	2.58	0.43
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.51	0.43
20:T:12:LYS:O	20:T:16:LEU:HD23	2.18	0.43
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.53	0.43
59:U:101:EHZ:O2	59:U:101:EHZ:O1	2.35	0.43
8:H:265:LEU:HD13	45:H:401:3PE:H272	2.00	0.43
12:L:100:ILE:HD13	12:L:246:LEU:HB2	2.01	0.43
13:M:257:MET:HE1	45:M:604:3PE:H372	2.00	0.43
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.54	0.43
10:J:43:ILE:HG22	11:K:46:LEU:HD11	2.01	0.43
37:l:6:LYS:HD3	37:l:9:LEU:HD12	2.00	0.43
38:m:94:ILE:HG13	45:m:201:3PE:H2F2	2.01	0.43
4:D:248:GLU:OE2	61:D:605:HOH:O	2.22	0.43
10:J:132:ASP:O	10:J:133:SER:HB3	2.18	0.43
45:M:601:3PE:H381	45:Y:203:3PE:H2A1	1.99	0.43
12:L:15:LEU:HD22	12:L:40:ILE:HD13	2.01	0.43
13:M:73:LEU:HA	13:M:76:MET:HE3	2.00	0.43
22:W:25:MET:HE2	22:W:74:THR:HA	2.01	0.43
22:W:25:MET:HE1	22:W:79:VAL:HG21	2.01	0.42
3:C:114:LEU:HD23	22:W:81:LEU:HD12	2.01	0.42
16:P:209:ASP:OD2	16:P:308:THR:N	2.48	0.42
45:h:202:3PE:H271	45:h:202:3PE:H2A2	1.73	0.42
1:A:51:PHE:CD1	10:J:74:MET:HE2	2.54	0.42
46:B:203:PC1:H143	46:B:203:PC1:O13	2.19	0.42
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.59	0.42
20:T:49:GLU:OE2	22:W:64:ARG:NH2	2.53	0.42
6:F:101:GLU:HB2	51:F:503:NAI:H42N	2.02	0.42
7:G:286:ASN:OD1	7:G:289:GLY:N	2.52	0.42
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.47	0.42
16:P:176:ASP:OD1	16:P:176:ASP:C	2.63	0.42
16:P:332:GLU:CD	16:P:333:ASP:H	2.27	0.42
33:h:32:THR:O	33:h:36:VAL:HG23	2.18	0.42
14:N:108:MET:SD	14:N:191:THR:HG21	2.60	0.42
15:O:130:SER:O	15:O:133:VAL:HG22	2.19	0.42
16:P:145:TYR:CD1	16:P:286:ARG:HD3	2.55	0.42
23:X:33:ALA:HB2	23:X:119:PRO:HG3	2.00	0.42
37:l:68:ASP:N	37:l:68:ASP:OD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PHE:HB2	10:J:74:MET:HE1	2.02	0.42
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.49	0.42
45:I:203:3PE:N	25:Z:30:LEU:O	2.39	0.42
43:r:45:SER:O	43:r:51:ASN:ND2	2.48	0.42
8:H:62:ARG:HB3	8:H:63:PRO:HA	2.02	0.42
8:H:253:GLU:CD	8:H:253:GLU:H	2.28	0.42
10:J:115:VAL:O	10:J:117:PHE:N	2.49	0.42
18:R:51:GLN:OE1	18:R:92:ARG:NH2	2.51	0.42
5:E:9:HIS:O	61:E:404:HOH:O	2.22	0.42
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.02	0.42
9:I:75:GLU:O	9:I:105:ARG:NH1	2.52	0.41
12:L:89:PHE:HZ	12:L:251:THR:HG23	1.84	0.41
1:A:18:VAL:HA	8:H:222:LEU:HD11	2.02	0.41
4:D:296:ARG:HH21	4:D:420:THR:HG21	1.85	0.41
10:J:82:ILE:HD12	10:J:82:ILE:N	2.35	0.41
7:G:74:MET:HE2	7:G:74:MET:HA	2.01	0.41
61:K:238:HOH:O	14:N:68:MET:HE1	2.20	0.41
12:L:264:TYR:N	12:L:265:PRO:CD	2.84	0.41
16:P:188:PHE:O	16:P:188:PHE:CG	2.72	0.41
5:E:4:GLY:O	5:E:92:ARG:NH2	2.53	0.41
7:G:595:GLU:OE2	61:G:908:HOH:O	2.22	0.41
1:A:115:GLU:N	1:A:115:GLU:OE2	2.53	0.41
45:N:403:3PE:H2E2	45:N:403:3PE:H2I2	2.03	0.41
20:T:19:LEU:HD22	20:T:25:ILE:HD13	2.02	0.41
34:i:71:PHE:CE1	34:i:75:LEU:HD23	2.55	0.41
1:A:14:ALA:O	1:A:18:VAL:HG23	2.21	0.41
5:E:181:ILE:N	5:E:181:ILE:HD12	2.36	0.41
11:K:40:LEU:HD21	14:N:72:MET:HE2	2.02	0.41
13:M:406:TYR:CD1	13:M:406:TYR:C	2.99	0.41
45:Y:201:3PE:C1	45:Y:201:3PE:C31	2.99	0.41
7:G:364:LEU:HD12	7:G:491:ASN:HB3	2.03	0.41
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.55	0.41
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.02	0.41
11:K:73:LEU:HD13	11:K:73:LEU:O	2.21	0.41
2:B:64:ALA:HB1	2:B:65:PRO:CD	2.51	0.41
12:L:297:ASP:OD1	12:L:300:LYS:N	2.46	0.41
45:M:606:3PE:H2A2	45:M:606:3PE:H2D2	1.59	0.41
16:P:334:VAL:O	16:P:335:GLN:CB	2.68	0.41
23:X:146:ARG:NH2	30:e:41:GLU:OE1	2.54	0.41
32:g:75:THR:HG21	45:h:203:3PE:H2C1	2.03	0.41
34:i:75:LEU:O	34:i:78:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:82:ASP:OD1	37:l:82:ASP:N	2.53	0.41
6:F:107:ASP:OD2	61:F:604:HOH:O	2.22	0.41
12:L:589:LEU:HD21	45:Y:204:3PE:H252	2.03	0.41
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.02	0.41
13:M:296:LEU:HD21	13:M:396:MET:SD	2.62	0.41
4:D:323:ILE:HD12	4:D:323:ILE:C	2.46	0.40
13:M:205:VAL:HG22	13:M:212:LEU:HD13	2.02	0.40
14:N:347:GLU:HB2	29:d:82:MET:HE2	2.03	0.40
53:N:401:CDL:H771	53:N:401:CDL:H742	1.82	0.40
31:f:3:LEU:C	31:f:5:GLN:H	2.28	0.40
7:G:539:LYS:O	7:G:540:ASP:OD2	2.39	0.40
32:g:63:PHE:CE2	45:h:202:3PE:H2C2	2.49	0.40
61:B:301:HOH:O	4:D:82:LEU:HA	2.20	0.40
5:E:14:GLU:O	5:E:14:GLU:HG2	2.20	0.40
6:F:150:GLN:HB3	44:s:54:LEU:HD13	2.03	0.40
12:L:40:ILE:HG13	12:L:101:MET:SD	2.62	0.40
12:L:424:THR:HG23	36:k:62:PHE:CE1	2.55	0.40
14:N:41:ILE:N	14:N:42:PRO:HD2	2.36	0.40
16:P:194:ILE:HD12	16:P:288:HIS:CE1	2.57	0.40
4:D:47:LEU:H	4:D:47:LEU:HD23	1.86	0.40
5:E:105:THR:HG22	5:E:106:THR:N	2.36	0.40
7:G:366:THR:O	7:G:367:THR:OG1	2.31	0.40
20:T:58:PHE:CE2	20:T:80:ILE:HD13	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
2	B	152/216 (70%)	148 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	205/266 (77%)	201 (98%)	4 (2%)	0	100	100
4	D	427/463 (92%)	416 (97%)	11 (3%)	0	100	100
5	E	212/249 (85%)	208 (98%)	4 (2%)	0	100	100
6	F	430/464 (93%)	424 (99%)	6 (1%)	0	100	100
7	G	687/727 (94%)	674 (98%)	13 (2%)	0	100	100
8	H	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	173/175 (99%)	166 (96%)	6 (4%)	1 (1%)	21	17
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	584 (97%)	19 (3%)	1 (0%)	43	42
13	M	457/459 (100%)	455 (100%)	2 (0%)	0	100	100
14	N	345/347 (99%)	342 (99%)	3 (1%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	305/380 (80%)	293 (96%)	10 (3%)	2 (1%)	18	14
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	94/124 (76%)	93 (99%)	1 (1%)	0	100	100
19	S	84/99 (85%)	84 (100%)	0	0	100	100
20	T	81/156 (52%)	79 (98%)	2 (2%)	0	100	100
20	U	84/156 (54%)	84 (100%)	0	0	100	100
21	V	113/116 (97%)	113 (100%)	0	0	100	100
22	W	113/128 (88%)	111 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
25	Z	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	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	117/121 (97%)	116 (99%)	1 (1%)	0	100	100
30	e	96/106 (91%)	96 (100%)	0	0	100	100
31	f	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
32	g	98/154 (64%)	92 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
35	j	65/108 (60%)	64 (98%)	1 (2%)	0	100	100
36	k	79/98 (81%)	79 (100%)	0	0	100	100
37	l	154/186 (83%)	148 (96%)	6 (4%)	0	100	100
38	m	126/129 (98%)	125 (99%)	0	1 (1%)	16	11
39	n	169/179 (94%)	164 (97%)	5 (3%)	0	100	100
40	o	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
41	p	171/176 (97%)	171 (100%)	0	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	92/113 (81%)	90 (98%)	2 (2%)	0	100	100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8120/9214 (88%)	7969 (98%)	146 (2%)	5 (0%)	49	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
16	P	199	LYS
16	P	335	GLN
10	J	82	ILE
38	m	2	PHE

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	89/100 (89%)	87 (98%)	2 (2%)	45	50
2	B	130/174 (75%)	126 (97%)	4 (3%)	35	37
3	C	188/228 (82%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	370/392 (94%)	369 (100%)	1 (0%)	86	91
5	E	183/205 (89%)	182 (100%)	1 (0%)	81	87
6	F	346/368 (94%)	344 (99%)	2 (1%)	78	85
7	G	578/608 (95%)	573 (99%)	5 (1%)	70	78
8	H	274/274 (100%)	273 (100%)	1 (0%)	84	89
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	141/141 (100%)	140 (99%)	1 (1%)	76	82
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	531 (100%)	2 (0%)	84	89
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	280 (99%)	3 (1%)	65	73
16	P	267/327 (82%)	262 (98%)	5 (2%)	50	56
17	Q	112/153 (73%)	109 (97%)	3 (3%)	39	42
18	R	79/97 (81%)	77 (98%)	2 (2%)	42	45
19	S	76/82 (93%)	76 (100%)	0	100	100
20	T	77/135 (57%)	75 (97%)	2 (3%)	40	44
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	75
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	154/155 (99%)	153 (99%)	1 (1%)	78	85
24	Y	101/101 (100%)	100 (99%)	1 (1%)	68	75
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	80
26	a	59/59 (100%)	58 (98%)	1 (2%)	53	60
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	44 (98%)	1 (2%)	45	50
29	d	105/106 (99%)	104 (99%)	1 (1%)	68	75
30	e	89/96 (93%)	88 (99%)	1 (1%)	65	73
31	f	54/54 (100%)	52 (96%)	2 (4%)	30	30
32	g	91/131 (70%)	91 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	i	121/121 (100%)	117 (97%)	4 (3%)	33	34
35	j	61/84 (73%)	59 (97%)	2 (3%)	33	34
36	k	63/76 (83%)	60 (95%)	3 (5%)	23	21
37	l	140/159 (88%)	139 (99%)	1 (1%)	76	82
38	m	114/115 (99%)	114 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	109/120 (91%)	109 (100%)	0	100	100
41	p	154/157 (98%)	152 (99%)	2 (1%)	61	68
42	q	131/131 (100%)	129 (98%)	2 (2%)	57	64
43	r	85/96 (88%)	85 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7164/7891 (91%)	7106 (99%)	58 (1%)	70	80

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	TRP
1	A	112	GLU
2	B	30	VAL
2	B	50	PHE
2	B	54	CYS
2	B	91	THR
4	D	43	LEU
5	E	217	LEU
6	F	10	THR
6	F	38	SER
7	G	193	SER
7	G	329	ILE
7	G	335	LEU
7	G	483	VAL
7	G	536	ASP
8	H	62	ARG
10	J	132	ASP
12	L	24	PHE
12	L	500	LEU
15	O	1	LEU
15	O	181	SER
15	O	279	LEU

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Mol	Chain	Res	Type
16	P	186	ARG
16	P	187	TRP
16	P	196	LEU
16	P	251	ARG
16	P	324	TYR
17	Q	31	LYS
17	Q	74	SER
17	Q	115	SER
18	R	3	ARG
18	R	96	HIS
20	T	32	VAL
20	T	34	SER
21	V	6	LYS
23	X	63	ASN
24	Y	15	THR
25	Z	130	SER
26	a	69	ILE
28	c	49	GLU
29	d	3	THR
30	e	98	SER
31	f	4	LEU
31	f	30	ASN
34	i	40	SER
34	i	55	LEU
34	i	58	ASN
34	i	63	THR
35	j	44	SER
35	j	70	ASP
36	k	86	TYR
36	k	88	GLU
36	k	90	GLN
37	l	31	VAL
41	p	44	VAL
41	p	68	ARG
42	q	142	THR
42	q	144	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	39	GLN
5	E	37	ASN

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Mol	Chain	Res	Type
5	E	74	GLN
5	E	91	ASN
5	E	155	GLN
6	F	29	HIS
6	F	398	GLN
6	F	421	HIS
7	G	259	ASN
7	G	336	ASN
8	H	47	GLN
9	I	144	HIS
12	L	56	HIS
12	L	205	ASN
12	L	296	ASN
12	L	541	ASN
12	L	546	GLN
13	M	103	GLN
13	M	138	ASN
13	M	144	ASN
13	M	175	ASN
13	M	331	ASN
13	M	415	GLN
14	N	47	ASN
14	N	48	HIS
15	O	271	ASN
18	R	96	HIS
19	S	85	GLN
20	T	74	GLN
21	V	85	ASN
23	X	102	GLN
28	c	9	HIS
30	e	6	GLN
32	g	27	GLN
32	g	41	ASN
34	i	37	GLN
35	j	24	GLN
36	k	58	ASN
37	l	136	ASN
38	m	74	ASN
39	n	77	GLN
40	o	75	ASN
41	p	58	ASN
41	p	122	GLN

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Mol	Chain	Res	Type
42	q	17	HIS
42	q	69	ASN
42	q	112	ASN
42	q	135	GLN
44	s	55	ASN
44	s	75	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	H	1	8	8,9,10	1.50	1 (12%)	7,9,11	1.64	2 (28%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.84	1 (14%)
14	FME	N	1	14	8,9,10	1.53	1 (12%)	7,9,11	1.51	1 (14%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	7,9,11	1.64	2 (28%)
13	FME	M	1	13	8,9,10	1.52	1 (12%)	7,9,11	1.65	1 (14%)
12	FME	L	1	12	8,9,10	1.51	1 (12%)	7,9,11	1.69	3 (42%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	7,9,11	1.59	2 (28%)
4	2MR	D	85	4	10,12,13	2.45	2 (20%)	5,13,15	1.23	1 (20%)
2	ARO	B	77	2	9,11,12	2.53	2 (22%)	7,13,15	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	H	1	8	-	3/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
2	ARO	B	77	2	-	4/10/11/13	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	ARO	CZ-NE	6.70	1.46	1.33
4	D	85	2MR	CZ-NH2	5.44	1.45	1.33
4	D	85	2MR	CZ-NE	5.20	1.45	1.34
14	N	1	FME	CN-N	3.73	1.45	1.33
11	K	1	FME	CN-N	3.69	1.45	1.33
13	M	1	FME	CN-N	3.69	1.45	1.33
12	L	1	FME	CN-N	3.68	1.45	1.33
10	J	1	FME	CN-N	3.68	1.45	1.33
1	A	1	FME	CN-N	3.66	1.45	1.33
8	H	1	FME	CN-N	3.61	1.45	1.33
2	B	77	ARO	CZ-NH1	-2.24	1.25	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CE-SD-CG	3.47	112.33	100.40
14	N	1	FME	CE-SD-CG	2.98	110.64	100.40
13	M	1	FME	CE-SD-CG	2.69	109.65	100.40
10	J	1	FME	CE-SD-CG	2.60	109.34	100.40
12	L	1	FME	CE-SD-CG	2.59	109.28	100.40
11	K	1	FME	CE-SD-CG	2.58	109.27	100.40
8	H	1	FME	CE-SD-CG	2.44	108.77	100.40
4	D	85	2MR	CD-NE-CZ	-2.28	119.14	123.41
12	L	1	FME	CA-N-CN	-2.09	119.61	122.82
11	K	1	FME	O1-CN-N	-2.05	119.87	125.27
8	H	1	FME	O1-CN-N	-2.04	119.91	125.27
12	L	1	FME	O1-CN-N	-2.04	119.91	125.27
10	J	1	FME	O1-CN-N	-2.03	119.92	125.27

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
2	B	77	ARO	CA-CB-CG-OH
8	H	1	FME	O1-CN-N-CA
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CA-N-CN
12	L	1	FME	CA-CB-CG-SD
1	A	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
8	H	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
12	L	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
14	N	1	FME	C-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD
2	B	77	ARO	CA-CB-CG-CD
2	B	77	ARO	N-CA-CB-CG
13	M	1	FME	CB-CA-N-CN
2	B	77	ARO	C-CA-CB-CG
1	A	1	FME	N-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	FME	1	0
2	B	77	ARO	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 59 ligands modelled in this entry, 3 are monoatomic - leaving 56 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	A	201	-	46,46,50	0.89	3 (6%)	49,51,55	1.02	2 (4%)
53	CDL	N	401	-	85,85,99	0.98	7 (8%)	91,97,111	1.01	4 (4%)
47	SF4	B	202	2	0,12,12	-	-	-	-	-
59	EHZ	T	101	20	29,36,37	1.71	5 (17%)	35,44,47	1.46	4 (11%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
45	3PE	Z	201	-	42,42,50	0.94	4 (9%)	45,47,55	1.15	2 (4%)
60	MYR	o	201	40	14,14,15	0.45	0	13,13,15	0.87	0
45	3PE	D	502	-	50,50,50	0.87	4 (8%)	53,55,55	0.96	1 (1%)
45	3PE	L	703	-	44,44,50	0.92	4 (9%)	47,49,55	1.04	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
46	PC1	B	203	-	46,46,53	1.35	6 (13%)	52,54,61	1.02	2 (3%)
45	3PE	A	202	-	34,34,50	1.02	4 (11%)	37,39,55	1.12	2 (5%)
45	3PE	M	601	-	44,44,50	0.91	3 (6%)	47,49,55	1.08	2 (4%)
55	DGT	O	401	56	29,33,33	3.21	14 (48%)	44,52,52	1.98	12 (27%)
57	NDP	P	501	-	49,52,52	3.97	25 (51%)	66,80,80	2.00	14 (21%)
46	PC1	B	201	-	49,49,53	1.34	6 (12%)	55,57,61	0.98	2 (3%)
45	3PE	Z	202	-	32,32,50	1.04	4 (12%)	35,37,55	1.12	2 (5%)
51	NAI	F	503	-	45,48,48	3.72	19 (42%)	60,73,73	1.78	13 (21%)
45	3PE	d	201	-	48,48,50	0.89	4 (8%)	51,53,55	1.01	2 (3%)
45	3PE	H	401	-	37,37,50	1.00	3 (8%)	40,42,55	1.16	2 (5%)
45	3PE	X	201	-	37,37,50	0.99	4 (10%)	40,42,55	1.14	3 (7%)
45	3PE	Y	202	-	50,50,50	0.88	4 (8%)	53,55,55	0.98	2 (3%)
46	PC1	J	201	-	47,47,53	1.34	6 (12%)	53,55,61	1.01	2 (3%)
45	3PE	N	403	-	38,38,50	0.99	4 (10%)	41,43,55	1.10	2 (4%)
46	PC1	N	402	-	34,34,53	1.53	6 (17%)	40,42,61	1.08	2 (5%)
48	LMT	D	501	-	36,36,36	1.14	2 (5%)	47,47,47	0.99	2 (4%)
45	3PE	L	701	-	41,41,50	0.95	4 (9%)	44,46,55	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	FES	G	803	7	0,4,4	-	-	-		
45	3PE	M	606	-	40,40,50	0.95	3 (7%)	43,45,55	1.07	2 (4%)
45	3PE	L	705	-	43,43,50	0.94	4 (9%)	46,48,55	1.07	2 (4%)
45	3PE	h	203	-	50,50,50	0.87	4 (8%)	53,55,55	0.95	2 (3%)
45	3PE	K	101	-	47,47,50	0.88	4 (8%)	50,52,55	1.10	2 (4%)
46	PC1	M	605	-	45,45,53	1.40	6 (13%)	51,53,61	0.97	2 (3%)
59	EHZ	U	101	20	29,36,37	1.68	5 (17%)	35,44,47	1.60	5 (14%)
53	CDL	L	702	-	70,70,99	1.06	7 (10%)	76,82,111	1.07	4 (5%)
46	PC1	M	603	-	45,45,53	1.37	6 (13%)	51,53,61	0.96	2 (3%)
45	3PE	M	604	-	50,50,50	0.85	4 (8%)	53,55,55	1.06	3 (5%)
47	SF4	F	502	6	0,12,12	-	-	-		
45	3PE	h	202	-	37,37,50	0.99	4 (10%)	40,42,55	1.05	2 (5%)
45	3PE	Y	201	-	50,50,50	0.86	3 (6%)	53,55,55	1.04	2 (3%)
46	PC1	d	202	-	45,45,53	1.39	6 (13%)	51,53,61	1.04	2 (3%)
47	SF4	I	201	9	0,12,12	-	-	-		
45	3PE	Y	204	-	40,40,50	0.95	4 (10%)	43,45,55	1.09	2 (4%)
54	CHD	L	704	-	32,32,32	3.21	10 (31%)	51,51,51	1.78	14 (27%)
45	3PE	Y	205	-	44,44,50	0.91	3 (6%)	47,49,55	1.11	2 (4%)
45	3PE	I	203	-	50,50,50	0.86	3 (6%)	53,55,55	0.99	2 (3%)
45	3PE	m	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.10	2 (4%)
47	SF4	I	202	9	0,12,12	-	-	-		
47	SF4	G	802	7	0,12,12	-	-	-		
53	CDL	q	201	-	63,63,99	1.11	6 (9%)	69,75,111	1.09	4 (5%)
53	CDL	d	203	-	64,64,99	1.09	7 (10%)	70,76,111	1.12	4 (5%)
50	FMN	F	501	-	33,33,33	2.78	10 (30%)	48,50,50	1.76	13 (27%)
45	3PE	Y	203	-	38,38,50	0.98	4 (10%)	41,43,55	1.06	2 (4%)
53	CDL	h	201	-	67,67,99	1.10	7 (10%)	73,79,111	1.17	4 (5%)
45	3PE	H	402	-	50,50,50	0.87	4 (8%)	53,55,55	0.95	2 (3%)
45	3PE	M	602	-	50,50,50	0.86	4 (8%)	53,55,55	1.04	2 (3%)

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	A	201	-	-	19/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	N	401	-	-	34/96/96/110	-
59	EHZ	T	101	20	-	6/42/44/45	-
47	SF4	B	202	2	-	-	0/6/5/5
49	FES	E	301	5	-	-	0/1/1/1
45	3PE	Z	201	-	-	21/46/46/54	-
60	MYR	o	201	40	-	3/11/12/13	-
45	3PE	D	502	-	-	24/54/54/54	-
45	3PE	L	703	-	-	24/48/48/54	-
47	SF4	G	801	7	-	-	0/6/5/5
46	PC1	B	203	-	-	22/50/50/57	-
45	3PE	A	202	-	-	12/38/38/54	-
45	3PE	M	601	-	-	26/48/48/54	-
55	DGT	O	401	56	-	4/22/34/34	0/3/3/3
57	NDP	P	501	-	-	6/34/77/77	0/5/5/5
46	PC1	B	201	-	-	19/53/53/57	-
45	3PE	Z	202	-	-	16/36/36/54	-
51	NAI	F	503	-	-	3/29/72/72	0/5/5/5
45	3PE	d	201	-	-	24/52/52/54	-
45	3PE	H	401	-	-	18/41/41/54	-
45	3PE	X	201	-	-	17/41/41/54	-
45	3PE	Y	202	-	-	23/54/54/54	-
46	PC1	J	201	-	-	15/51/51/57	-
45	3PE	N	403	-	-	21/42/42/54	-
46	PC1	N	402	-	-	14/38/38/57	-
48	LMT	D	501	-	-	2/21/61/61	0/2/2/2
45	3PE	L	701	-	-	19/45/45/54	-
49	FES	G	803	7	-	-	0/1/1/1
45	3PE	M	606	-	-	23/44/44/54	-
45	3PE	L	705	-	-	26/47/47/54	-
45	3PE	h	203	-	-	26/54/54/54	-
45	3PE	K	101	-	-	11/51/51/54	-
46	PC1	M	605	-	-	21/49/49/57	-
59	EHZ	U	101	20	-	14/42/44/45	-
53	CDL	L	702	-	-	39/81/81/110	-
46	PC1	M	603	-	-	14/49/49/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	M	604	-	-	18/54/54/54	-
47	SF4	F	502	6	-	-	0/6/5/5
45	3PE	h	202	-	-	14/41/41/54	-
45	3PE	Y	201	-	-	28/54/54/54	-
46	PC1	d	202	-	-	24/49/49/57	-
47	SF4	I	201	9	-	-	0/6/5/5
45	3PE	Y	204	-	-	18/44/44/54	-
54	CHD	L	704	-	-	8/9/74/74	0/4/4/4
45	3PE	Y	205	-	-	21/48/48/54	-
45	3PE	I	203	-	-	26/54/54/54	-
45	3PE	m	201	-	-	25/44/44/54	-
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
53	CDL	q	201	-	-	39/74/74/110	-
53	CDL	d	203	-	-	39/75/75/110	-
50	FMN	F	501	-	-	1/18/18/18	0/3/3/3
45	3PE	Y	203	-	-	17/42/42/54	-
53	CDL	h	201	-	-	40/78/78/110	-
45	3PE	H	402	-	-	20/54/54/54	-
45	3PE	M	602	-	-	23/54/54/54	-

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	C6N-C5N	12.19	1.55	1.33
51	F	503	NAI	C6N-C5N	11.11	1.53	1.33
54	L	704	CHD	C11-C12	8.81	1.68	1.53
51	F	503	NAI	O4B-C1B	8.52	1.62	1.42
57	P	501	NDP	C2B-C1B	-8.50	1.31	1.53
57	P	501	NDP	O4B-C1B	8.42	1.61	1.42
51	F	503	NAI	O4D-C1D	8.30	1.61	1.42
57	P	501	NDP	C7N-N7N	8.28	1.55	1.33
57	P	501	NDP	O4D-C1D	8.15	1.61	1.42
55	O	401	DGT	C2'-C3'	-7.62	1.32	1.52
50	F	501	FMN	C4A-N5	7.19	1.44	1.30
54	L	704	CHD	C16-C15	7.13	1.73	1.54
57	P	501	NDP	C2D-C1D	-7.11	1.30	1.53
51	F	503	NAI	C2B-C1B	-6.95	1.31	1.53
51	F	503	NAI	C2D-C1D	-6.67	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	F	501	FMN	C10-N1	6.60	1.46	1.33
55	O	401	DGT	C4-N3	6.58	1.49	1.34
51	F	503	NAI	O4D-C4D	-6.51	1.30	1.45
51	F	503	NAI	C2N-C3N	6.38	1.52	1.34
57	P	501	NDP	O4D-C4D	-6.35	1.30	1.45
51	F	503	NAI	O4B-C4B	-6.26	1.31	1.45
54	L	704	CHD	C13-C17	5.96	1.65	1.55
57	P	501	NDP	C6A-N6A	5.58	1.48	1.34
59	T	101	EHZ	C15-N2	5.47	1.45	1.33
57	P	501	NDP	P2B-O2B	5.43	1.69	1.59
59	T	101	EHZ	C12-N1	5.42	1.45	1.33
59	U	101	EHZ	C15-N2	5.40	1.45	1.33
54	L	704	CHD	C8-C9	5.37	1.64	1.53
55	O	401	DGT	O4'-C4'	5.23	1.56	1.45
59	U	101	EHZ	C12-N1	5.19	1.45	1.33
55	O	401	DGT	C2-N2	5.18	1.46	1.34
54	L	704	CHD	O12-C12	-5.17	1.35	1.43
50	F	501	FMN	C9A-N10	5.17	1.50	1.41
55	O	401	DGT	O4'-C1'	-5.15	1.30	1.42
57	P	501	NDP	O4B-C4B	-5.14	1.33	1.45
50	F	501	FMN	C5A-N5	5.12	1.49	1.39
55	O	401	DGT	C2-N3	4.82	1.44	1.33
50	F	501	FMN	C2-N1	4.78	1.48	1.36
57	P	501	NDP	C2N-C3N	4.73	1.48	1.34
54	L	704	CHD	C20-C17	-4.66	1.46	1.54
51	F	503	NAI	C7N-N7N	4.63	1.45	1.33
51	F	503	NAI	C6A-N6A	4.63	1.45	1.34
54	L	704	CHD	C6-C5	4.56	1.61	1.53
54	L	704	CHD	C15-C14	4.28	1.63	1.54
50	F	501	FMN	C2-N3	4.23	1.48	1.39
55	O	401	DGT	C5'-C4'	-4.17	1.38	1.51
55	O	401	DGT	C2'-C1'	4.11	1.63	1.52
54	L	704	CHD	C6-C7	4.06	1.59	1.52
57	P	501	NDP	O2D-C2D	3.98	1.52	1.43
57	P	501	NDP	O7N-C7N	-3.98	1.15	1.24
46	M	605	PC1	O31-C31	3.88	1.44	1.33
57	P	501	NDP	C5A-C4A	-3.83	1.31	1.39
46	N	402	PC1	O31-C31	3.81	1.44	1.33
46	B	201	PC1	O31-C31	3.79	1.44	1.33
50	F	501	FMN	C4-N3	3.78	1.45	1.38
50	F	501	FMN	C10-N10	3.77	1.45	1.37
46	d	202	PC1	O31-C31	3.77	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	M	603	PC1	O31-C31	3.76	1.44	1.33
46	J	201	PC1	O31-C31	3.74	1.44	1.33
46	B	203	PC1	O31-C31	3.68	1.44	1.33
46	d	202	PC1	O21-C21	3.61	1.44	1.34
46	N	402	PC1	O21-C21	3.60	1.44	1.34
46	J	201	PC1	O21-C21	3.57	1.44	1.34
46	B	201	PC1	O21-C21	3.57	1.44	1.34
46	B	203	PC1	O21-C21	3.54	1.44	1.34
57	P	501	NDP	C8A-N9A	-3.51	1.31	1.37
46	M	605	PC1	O21-C21	3.50	1.44	1.34
46	M	603	PC1	O21-C21	3.47	1.44	1.34
57	P	501	NDP	C4N-C3N	3.38	1.56	1.49
48	D	501	LMT	O5B-C1B	3.37	1.50	1.41
51	F	503	NAI	C6N-N1N	3.27	1.45	1.37
55	O	401	DGT	C5-N7	-3.25	1.32	1.39
48	D	501	LMT	O5'-C1'	3.24	1.50	1.41
50	F	501	FMN	O2-C2	-3.08	1.18	1.24
51	F	503	NAI	O2D-C2D	2.97	1.50	1.43
51	F	503	NAI	O3B-C3B	-2.95	1.36	1.43
51	F	503	NAI	O2B-C2B	2.95	1.49	1.43
51	F	503	NAI	O3D-C3D	-2.92	1.36	1.43
55	O	401	DGT	O3'-C3'	2.85	1.49	1.43
55	O	401	DGT	C2-N1	2.84	1.44	1.37
53	N	401	CDL	OB8-CB7	2.79	1.41	1.33
57	P	501	NDP	C4N-C5N	2.77	1.56	1.48
53	q	201	CDL	OA6-CA4	-2.74	1.39	1.46
53	L	702	CDL	OB8-CB7	2.69	1.41	1.33
51	F	503	NAI	C5A-C4A	-2.68	1.34	1.39
50	F	501	FMN	O4-C4	-2.68	1.18	1.23
53	q	201	CDL	OB8-CB7	2.68	1.41	1.33
45	L	703	3PE	O21-C2	-2.65	1.40	1.46
53	L	702	CDL	OA6-CA4	-2.64	1.40	1.46
53	d	203	CDL	OA6-CA4	-2.62	1.40	1.46
46	M	603	PC1	O21-C2	-2.60	1.40	1.46
53	h	201	CDL	OB6-CB5	2.60	1.41	1.34
53	N	401	CDL	OA8-CA7	2.58	1.40	1.33
45	h	202	3PE	O21-C2	-2.57	1.40	1.46
45	Y	202	3PE	O31-C31	2.57	1.40	1.33
53	h	201	CDL	OB8-CB7	2.57	1.40	1.33
46	B	201	PC1	O21-C2	-2.56	1.40	1.46
57	P	501	NDP	C6N-N1N	2.56	1.43	1.37
45	h	203	3PE	O21-C2	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	h	201	CDL	OA6-CA4	-2.55	1.40	1.46
46	M	605	PC1	O21-C2	-2.55	1.40	1.46
45	Y	201	3PE	O31-C31	2.55	1.40	1.33
46	N	402	PC1	O21-C2	-2.54	1.40	1.46
57	P	501	NDP	C5A-N7A	-2.54	1.34	1.39
53	d	203	CDL	OB8-CB7	2.53	1.40	1.33
45	H	402	3PE	O21-C2	-2.53	1.40	1.46
45	I	203	3PE	O21-C2	-2.53	1.40	1.46
45	Y	201	3PE	O21-C2	-2.52	1.40	1.46
53	d	203	CDL	OB6-CB5	2.52	1.41	1.34
53	q	201	CDL	OB6-CB5	2.52	1.41	1.34
45	X	201	3PE	O21-C2	-2.51	1.40	1.46
45	K	101	3PE	O21-C2	-2.51	1.40	1.46
45	D	502	3PE	O31-C31	2.51	1.40	1.33
53	h	201	CDL	OA8-CA7	2.50	1.40	1.33
45	d	201	3PE	O31-C31	2.50	1.40	1.33
46	J	201	PC1	O21-C2	-2.49	1.40	1.46
45	Y	205	3PE	O31-C31	2.48	1.40	1.33
45	N	403	3PE	O31-C31	2.48	1.40	1.33
45	M	601	3PE	O31-C31	2.48	1.40	1.33
53	N	401	CDL	OA6-CA4	-2.48	1.40	1.46
45	I	203	3PE	O31-C31	2.47	1.40	1.33
45	M	602	3PE	O21-C2	-2.47	1.40	1.46
55	O	401	DGT	C6-N1	2.47	1.43	1.38
45	Y	204	3PE	O31-C31	2.46	1.40	1.33
53	L	702	CDL	OB6-CB4	-2.46	1.40	1.46
45	A	202	3PE	O21-C2	-2.46	1.40	1.46
45	m	201	3PE	O31-C31	2.46	1.40	1.33
45	h	203	3PE	O31-C31	2.45	1.40	1.33
51	F	503	NAI	C5A-N7A	-2.45	1.34	1.39
53	L	702	CDL	OA8-CA7	2.45	1.40	1.33
45	M	606	3PE	O31-C31	2.44	1.40	1.33
53	L	702	CDL	OB6-CB5	2.44	1.41	1.34
45	Y	202	3PE	O21-C2	-2.44	1.40	1.46
57	P	501	NDP	O3B-C3B	-2.44	1.37	1.43
45	N	403	3PE	O21-C2	-2.44	1.40	1.46
45	L	705	3PE	O21-C2	-2.43	1.40	1.46
45	L	705	3PE	O31-C31	2.43	1.40	1.33
53	N	401	CDL	OB6-CB5	2.43	1.41	1.34
45	H	401	3PE	O31-C31	2.43	1.40	1.33
57	P	501	NDP	O3D-C3D	-2.43	1.37	1.43
45	D	502	3PE	O21-C2	-2.43	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Z	201	3PE	O31-C31	2.42	1.40	1.33
59	T	101	EHZ	C9-S1	2.42	1.82	1.76
45	A	201	3PE	O21-C2	-2.42	1.40	1.46
45	M	602	3PE	O31-C31	2.42	1.40	1.33
46	B	203	PC1	O21-C2	-2.41	1.40	1.46
45	A	202	3PE	O31-C31	2.41	1.40	1.33
45	d	201	3PE	O21-C2	-2.41	1.40	1.46
45	A	201	3PE	O31-C31	2.40	1.40	1.33
45	M	606	3PE	O21-C2	-2.39	1.40	1.46
45	Z	201	3PE	O21-C2	-2.39	1.40	1.46
53	d	203	CDL	OB6-CB4	-2.39	1.40	1.46
46	M	605	PC1	P-O11	2.39	1.69	1.59
45	Y	203	3PE	O31-C31	2.39	1.40	1.33
46	d	202	PC1	O21-C2	-2.38	1.40	1.46
51	F	503	NAI	O7N-C7N	-2.38	1.18	1.24
53	q	201	CDL	OB6-CB4	-2.38	1.40	1.46
45	H	402	3PE	O31-C31	2.38	1.40	1.33
54	L	704	CHD	C13-C12	-2.38	1.50	1.54
57	P	501	NDP	C7N-C3N	2.38	1.53	1.48
45	K	101	3PE	O31-C31	2.38	1.40	1.33
53	q	201	CDL	OA8-CA7	2.38	1.40	1.33
53	d	203	CDL	OA8-CA7	2.37	1.40	1.33
45	L	703	3PE	O31-C31	2.37	1.40	1.33
45	h	202	3PE	O31-C31	2.35	1.40	1.33
45	Z	202	3PE	O31-C31	2.35	1.40	1.33
59	U	101	EHZ	C9-S1	2.34	1.81	1.76
45	L	701	3PE	O21-C21	2.34	1.40	1.34
45	X	201	3PE	O31-C31	2.33	1.40	1.33
45	H	401	3PE	O21-C2	-2.32	1.40	1.46
53	h	201	CDL	OB6-CB4	-2.32	1.40	1.46
46	B	201	PC1	P-O11	2.32	1.68	1.59
46	N	402	PC1	P-O11	2.32	1.68	1.59
46	d	202	PC1	P-O11	2.31	1.68	1.59
45	M	604	3PE	O31-C31	2.31	1.40	1.33
45	L	701	3PE	O31-C31	2.31	1.40	1.33
55	O	401	DGT	O6-C6	-2.31	1.19	1.23
46	M	603	PC1	P-O11	2.31	1.68	1.59
46	N	402	PC1	C22-C21	2.31	1.57	1.50
45	m	201	3PE	O21-C21	2.30	1.40	1.34
45	Y	203	3PE	O21-C2	-2.30	1.40	1.46
45	L	701	3PE	O21-C2	-2.30	1.40	1.46
55	O	401	DGT	C5-C6	2.30	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	U	101	EHZ	O3-C12	-2.29	1.18	1.23
59	U	101	EHZ	O4-C15	-2.29	1.18	1.23
45	M	606	3PE	O21-C21	2.29	1.40	1.34
46	M	605	PC1	C22-C21	2.29	1.57	1.50
45	Y	204	3PE	O21-C2	-2.29	1.40	1.46
45	N	403	3PE	O21-C21	2.28	1.40	1.34
45	m	201	3PE	O21-C2	-2.28	1.40	1.46
46	B	203	PC1	P-O11	2.27	1.68	1.59
45	Y	205	3PE	O21-C2	-2.27	1.40	1.46
46	d	202	PC1	C22-C21	2.26	1.57	1.50
45	M	601	3PE	O21-C21	2.26	1.40	1.34
45	Y	204	3PE	O21-C21	2.26	1.40	1.34
46	B	201	PC1	C22-C21	2.26	1.57	1.50
53	N	401	CDL	OB6-CB4	-2.25	1.41	1.46
57	P	501	NDP	PA-O5B	2.25	1.68	1.59
46	J	201	PC1	C22-C21	2.25	1.57	1.50
45	D	502	3PE	O21-C21	2.24	1.40	1.34
45	H	401	3PE	O21-C21	2.24	1.40	1.34
45	Z	202	3PE	O21-C2	-2.24	1.41	1.46
45	L	703	3PE	O31-C3	-2.24	1.40	1.45
59	T	101	EHZ	O4-C15	-2.23	1.19	1.23
46	B	203	PC1	C22-C21	2.23	1.57	1.50
45	Y	203	3PE	O21-C21	2.23	1.40	1.34
57	P	501	NDP	P2B-O1X	2.22	1.57	1.50
53	d	203	CDL	OA8-CA6	-2.22	1.40	1.45
45	Z	201	3PE	O31-C3	-2.21	1.40	1.45
45	M	604	3PE	O21-C2	-2.21	1.41	1.46
45	Y	202	3PE	O21-C21	2.21	1.40	1.34
45	M	602	3PE	O21-C21	2.21	1.40	1.34
45	d	201	3PE	O21-C21	2.20	1.40	1.34
45	L	705	3PE	O21-C21	2.20	1.40	1.34
46	M	603	PC1	C22-C21	2.20	1.57	1.50
45	H	402	3PE	O21-C21	2.19	1.40	1.34
45	X	201	3PE	O31-C3	-2.19	1.40	1.45
45	L	701	3PE	O31-C3	-2.19	1.40	1.45
45	L	705	3PE	O31-C3	-2.19	1.40	1.45
45	H	402	3PE	O31-C3	-2.19	1.40	1.45
45	A	201	3PE	O21-C21	2.18	1.40	1.34
45	Y	205	3PE	O21-C21	2.17	1.40	1.34
59	T	101	EHZ	O3-C12	-2.17	1.18	1.23
45	Z	202	3PE	O21-C21	2.17	1.40	1.34
46	M	605	PC1	P-O13	2.17	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	604	3PE	O31-C3	-2.17	1.40	1.45
46	N	402	PC1	P-O13	2.16	1.68	1.59
46	J	201	PC1	P-O11	2.16	1.68	1.59
51	F	503	NAI	C7N-C3N	2.15	1.53	1.48
45	M	601	3PE	O21-C2	-2.15	1.41	1.46
53	N	401	CDL	OA6-CA5	2.15	1.40	1.34
45	Z	201	3PE	O21-C21	2.15	1.40	1.34
45	K	101	3PE	O21-C21	2.14	1.40	1.34
46	M	603	PC1	P-O13	2.13	1.67	1.59
46	d	202	PC1	P-O13	2.13	1.67	1.59
45	h	203	3PE	O21-C21	2.13	1.40	1.34
53	d	203	CDL	OA6-CA5	2.13	1.40	1.34
45	A	202	3PE	O21-C21	2.12	1.40	1.34
45	h	202	3PE	O21-C21	2.11	1.40	1.34
45	M	604	3PE	O21-C21	2.11	1.40	1.34
45	Z	202	3PE	O31-C3	-2.11	1.40	1.45
45	h	202	3PE	O31-C3	-2.10	1.40	1.45
45	d	201	3PE	O31-C3	-2.10	1.40	1.45
45	Y	203	3PE	O31-C3	-2.10	1.40	1.45
45	X	201	3PE	O21-C21	2.09	1.40	1.34
45	m	201	3PE	O31-C3	-2.09	1.40	1.45
53	L	702	CDL	OA8-CA6	-2.09	1.40	1.45
53	N	401	CDL	OA8-CA6	-2.09	1.40	1.45
46	B	203	PC1	P-O13	2.09	1.67	1.59
45	M	602	3PE	O31-C3	-2.08	1.40	1.45
53	h	201	CDL	OA8-CA6	-2.08	1.40	1.45
45	Y	201	3PE	O21-C21	2.08	1.40	1.34
45	K	101	3PE	O31-C3	-2.08	1.40	1.45
53	L	702	CDL	OA6-CA5	2.06	1.40	1.34
45	I	203	3PE	O21-C21	2.06	1.40	1.34
45	A	202	3PE	O31-C3	-2.06	1.40	1.45
53	q	201	CDL	OA8-CA6	-2.06	1.40	1.45
45	L	703	3PE	O21-C21	2.05	1.40	1.34
57	P	501	NDP	C5B-C4B	2.04	1.58	1.51
53	h	201	CDL	OA6-CA5	2.04	1.40	1.34
45	h	203	3PE	O31-C3	-2.04	1.40	1.45
45	D	502	3PE	O31-C3	-2.04	1.40	1.45
45	Y	202	3PE	O31-C3	-2.04	1.40	1.45
46	J	201	PC1	P-O13	2.04	1.67	1.59
46	B	201	PC1	P-O13	2.03	1.67	1.59
45	N	403	3PE	O31-C3	-2.03	1.40	1.45
45	Y	204	3PE	O31-C3	-2.03	1.40	1.45

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	U	101	EHZ	C8-C9-S1	5.71	120.69	113.63
57	P	501	NDP	N6A-C6A-N1A	-5.61	106.06	118.35
57	P	501	NDP	C5A-C4A-N3A	-5.51	119.56	126.75
51	F	503	NAI	N3A-C2A-N1A	-5.42	120.12	128.60
57	P	501	NDP	N3A-C2A-N1A	-5.40	120.16	128.60
59	T	101	EHZ	C8-C9-S1	5.34	120.24	113.63
54	L	704	CHD	C17-C13-C12	5.17	122.38	117.67
51	F	503	NAI	C5A-C4A-N3A	-5.13	120.06	126.75
57	P	501	NDP	C4A-N9A-C1B	-5.11	114.42	126.59
55	O	401	DGT	C1'-N9-C8	4.89	138.82	127.85
55	O	401	DGT	C2-N3-C4	4.88	121.00	112.30
53	h	201	CDL	OB6-CB5-C51	4.79	121.83	111.50
45	Z	201	3PE	O21-C21-C22	4.77	121.79	111.50
50	F	501	FMN	C9-C8-C7	4.76	126.49	119.67
55	O	401	DGT	C1'-N9-C4	-4.59	112.75	125.48
57	P	501	NDP	C5A-C6A-N6A	4.58	133.40	123.43
57	P	501	NDP	C1B-N9A-C8A	4.57	137.46	127.14
45	H	401	3PE	O21-C21-C22	4.47	121.14	111.50
50	F	501	FMN	C7M-C7-C6	4.46	127.73	119.49
45	N	403	3PE	O21-C21-C22	4.41	121.01	111.50
46	d	202	PC1	O21-C21-C22	4.37	120.91	111.50
45	L	701	3PE	O21-C21-C22	4.34	120.85	111.50
45	Z	202	3PE	O21-C21-C22	4.30	120.76	111.50
45	Y	205	3PE	O21-C21-C22	4.25	120.66	111.50
51	F	503	NAI	N9A-C8A-N7A	-4.24	108.11	113.91
45	m	201	3PE	O21-C21-C22	4.24	120.63	111.50
57	P	501	NDP	N9A-C8A-N7A	-4.21	108.15	113.91
45	Y	204	3PE	O21-C21-C22	4.13	120.41	111.50
55	O	401	DGT	C5-C4-N3	-4.11	121.79	128.46
45	d	201	3PE	O21-C21-C22	4.05	120.22	111.50
51	F	503	NAI	N6A-C6A-N1A	-4.04	109.50	118.35
46	N	402	PC1	O21-C21-C22	4.01	120.15	111.50
45	M	604	3PE	O21-C21-C22	3.99	120.10	111.50
45	X	201	3PE	O21-C21-C22	3.98	120.08	111.50
53	d	203	CDL	OA6-CA5-C11	3.98	120.07	111.50
45	A	202	3PE	O21-C21-C22	3.95	120.02	111.50
53	h	201	CDL	OA6-CA5-C11	3.94	120.00	111.50
54	L	704	CHD	C11-C12-C13	3.91	115.26	111.24
53	L	702	CDL	OB6-CB5-C51	3.90	119.90	111.50
45	M	606	3PE	O21-C21-C22	3.88	119.85	111.50
45	L	705	3PE	O21-C21-C22	3.87	119.85	111.50
53	q	201	CDL	OB6-CB5-C51	3.86	119.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	J	201	PC1	O21-C21-C22	3.85	119.80	111.50
46	B	201	PC1	O21-C21-C22	3.84	119.79	111.50
46	B	203	PC1	O21-C21-C22	3.83	119.76	111.50
45	Y	203	3PE	O21-C21-C22	3.82	119.73	111.50
45	M	602	3PE	O21-C21-C22	3.75	119.58	111.50
57	P	501	NDP	C2A-N3A-C4A	3.70	120.49	111.75
45	Y	201	3PE	O21-C21-C22	3.69	119.46	111.50
45	K	101	3PE	O21-C21-C22	3.65	119.37	111.50
45	Y	202	3PE	O21-C21-C22	3.64	119.35	111.50
45	A	201	3PE	O21-C21-C22	3.62	119.30	111.50
46	M	605	PC1	O21-C21-C22	3.55	119.16	111.50
45	h	203	3PE	O21-C21-C22	3.55	119.14	111.50
45	L	703	3PE	O21-C21-C22	3.54	119.12	111.50
53	L	702	CDL	OA6-CA5-C11	3.51	119.07	111.50
53	N	401	CDL	OA6-CA5-C11	3.49	119.03	111.50
51	F	503	NAI	C2A-N3A-C4A	3.48	119.97	111.75
53	d	203	CDL	OB6-CB5-C51	3.47	120.48	110.80
57	P	501	NDP	N3A-C4A-N9A	3.46	132.78	127.08
45	h	202	3PE	O21-C21-C22	3.45	118.95	111.50
50	F	501	FMN	C8M-C8-C7	-3.45	113.66	120.74
55	O	401	DGT	N2-C2-N1	3.44	124.05	116.71
45	D	502	3PE	O21-C21-C22	3.43	118.90	111.50
45	M	601	3PE	O21-C21-C22	3.41	118.86	111.50
46	M	603	PC1	O21-C21-C22	3.41	118.84	111.50
55	O	401	DGT	N1-C2-N3	-3.40	116.98	123.32
53	q	201	CDL	OA6-CA5-C11	3.38	118.79	111.50
54	L	704	CHD	C17-C13-C14	3.37	103.49	100.09
50	F	501	FMN	C4-N3-C2	-3.29	119.56	125.64
54	L	704	CHD	C18-C13-C14	-3.29	106.06	111.21
51	F	503	NAI	C5A-C6A-N6A	3.27	130.55	123.43
53	N	401	CDL	OB6-CB5-C51	3.27	118.55	111.50
45	K	101	3PE	O31-C31-C32	3.16	121.82	111.91
54	L	704	CHD	C21-C20-C22	-3.14	105.44	110.36
45	I	203	3PE	O21-C21-C22	3.13	118.24	111.50
51	F	503	NAI	C5A-N7A-C8A	3.12	107.95	103.51
57	P	501	NDP	C5A-N7A-C8A	3.09	107.91	103.51
55	O	401	DGT	PB-O3B-PG	-3.01	122.49	132.83
51	F	503	NAI	N3A-C4A-N9A	3.01	132.04	127.08
45	H	402	3PE	O21-C21-C22	2.95	117.86	111.50
54	L	704	CHD	C14-C13-C12	2.90	110.10	107.40
50	F	501	FMN	C6-C7-C8	-2.88	115.55	119.67
45	Y	201	3PE	O31-C31-C32	2.87	120.90	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	M	605	PC1	O31-C31-C32	2.85	120.85	111.91
45	L	705	3PE	O31-C31-C32	2.85	120.84	111.91
54	L	704	CHD	C6-C5-C4	-2.83	107.93	111.19
53	h	201	CDL	OA8-CA7-C31	2.81	120.73	111.91
53	L	702	CDL	OB8-CB7-C71	2.80	120.69	111.91
53	q	201	CDL	OA8-CA7-C31	2.77	120.58	111.91
45	I	203	3PE	O31-C31-C32	2.76	120.58	111.91
45	Y	203	3PE	O31-C31-C32	2.76	120.58	111.91
54	L	704	CHD	C18-C13-C17	-2.71	106.97	111.21
55	O	401	DGT	N9-C8-N7	-2.70	108.30	113.39
45	M	601	3PE	O31-C31-C32	2.67	120.28	111.91
45	A	201	3PE	O31-C31-C32	2.66	120.24	111.91
46	B	203	PC1	O31-C31-C32	2.65	120.23	111.91
46	N	402	PC1	O31-C31-C32	2.65	120.22	111.91
45	X	201	3PE	O31-C31-C32	2.63	120.15	111.91
45	Y	205	3PE	O31-C31-C32	2.63	120.15	111.91
55	O	401	DGT	N9-C4-N3	2.63	131.21	125.94
50	F	501	FMN	C4A-C10-N10	2.62	120.32	116.48
45	M	606	3PE	O31-C31-C32	2.62	120.13	111.91
45	h	202	3PE	O31-C31-C32	2.61	120.08	111.91
46	J	201	PC1	O31-C31-C32	2.60	120.06	111.91
45	A	202	3PE	O31-C31-C32	2.59	120.05	111.91
45	Y	202	3PE	O31-C31-C32	2.58	119.99	111.91
45	L	703	3PE	O31-C31-C32	2.57	119.97	111.91
53	h	201	CDL	OB8-CB7-C71	2.56	119.93	111.91
59	U	101	EHZ	C7-C8-C9	-2.55	108.07	113.89
45	H	401	3PE	O31-C31-C32	2.54	119.86	111.91
57	P	501	NDP	PN-O3-PA	-2.52	124.18	132.83
46	B	201	PC1	O31-C31-C32	2.51	119.78	111.91
46	d	202	PC1	O31-C31-C32	2.50	119.76	111.91
54	L	704	CHD	C6-C7-C8	2.50	114.15	111.48
46	M	603	PC1	O31-C31-C32	2.49	119.73	111.91
54	L	704	CHD	C14-C8-C9	2.48	113.12	109.71
45	d	201	3PE	O31-C31-C32	2.47	119.67	111.91
55	O	401	DGT	PA-O3A-PB	-2.47	124.34	132.83
59	T	101	EHZ	C10-S1-C9	2.47	109.57	101.87
53	N	401	CDL	OB8-CB7-C71	2.47	119.65	111.91
50	F	501	FMN	C9A-C5A-N5	-2.46	119.75	122.43
45	m	201	3PE	O31-C31-C32	2.46	119.63	111.91
45	Z	201	3PE	O31-C31-C32	2.46	119.61	111.91
53	q	201	CDL	OB8-CB7-C71	2.45	119.60	111.91
45	N	403	3PE	O31-C31-C32	2.45	119.59	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	F	503	NAI	PN-O3-PA	-2.44	124.44	132.83
45	Y	204	3PE	O31-C31-C32	2.44	119.57	111.91
50	F	501	FMN	C6-C5A-C9A	2.43	122.37	118.94
53	d	203	CDL	OB8-CB7-C71	2.43	119.52	111.91
50	F	501	FMN	C4A-C4-N3	2.42	119.34	113.19
45	M	602	3PE	O31-C31-C32	2.41	119.47	111.91
54	L	704	CHD	C15-C14-C8	2.41	121.70	118.33
50	F	501	FMN	O4-C4-C4A	-2.40	120.23	126.60
53	L	702	CDL	OA8-CA7-C31	2.40	119.44	111.91
45	h	203	3PE	O31-C31-C32	2.40	119.43	111.91
53	d	203	CDL	OA8-CA7-C31	2.39	119.39	111.91
50	F	501	FMN	C4-C4A-C10	2.38	120.78	116.79
55	O	401	DGT	C5-C6-N1	2.36	119.19	113.19
53	N	401	CDL	OA8-CA7-C31	2.34	119.27	111.91
48	D	501	LMT	C1B-O1B-C4'	-2.34	112.17	117.96
59	T	101	EHZ	O2-C9-S1	-2.34	119.57	122.61
59	U	101	EHZ	O2-C9-S1	-2.32	119.60	122.61
50	F	501	FMN	C10-C4A-N5	-2.32	119.94	124.86
45	Z	202	3PE	O31-C31-C32	2.30	119.12	111.91
57	P	501	NDP	C2B-C1B-N9A	-2.29	109.68	113.53
45	M	604	3PE	O31-C31-C32	2.29	119.08	111.91
51	F	503	NAI	C4D-O4D-C1D	-2.27	104.47	109.47
59	U	101	EHZ	C14-C13-C12	-2.26	108.59	112.36
45	H	402	3PE	O31-C31-C32	2.24	118.94	111.91
54	L	704	CHD	C19-C10-C5	-2.24	106.56	110.36
54	L	704	CHD	C18-C13-C12	-2.23	106.80	109.07
45	L	701	3PE	O31-C31-C32	2.22	118.86	111.91
57	P	501	NDP	C4A-N9A-C8A	2.21	108.12	105.73
45	M	604	3PE	C3-C2-C1	-2.18	106.63	111.79
45	X	201	3PE	C2-O21-C21	-2.16	112.47	117.79
50	F	501	FMN	C4A-C10-N1	-2.14	119.77	124.73
59	U	101	EHZ	C13-C12-N1	2.14	120.02	116.42
51	F	503	NAI	C4A-C5A-N7A	-2.13	108.03	110.62
51	F	503	NAI	C4A-N9A-C8A	2.12	108.03	105.73
51	F	503	NAI	C3D-C2D-C1D	2.10	105.42	101.43
59	T	101	EHZ	C13-C12-N1	2.08	119.93	116.42
48	D	501	LMT	C2'-C3'-C4'	2.04	114.34	109.68
54	L	704	CHD	O12-C12-C13	-2.02	107.61	111.03
57	P	501	NDP	C4A-C5A-N7A	-2.02	108.16	110.62
55	O	401	DGT	C3'-C2'-C1'	2.00	107.55	102.54

There are no chirality outliers.

All (927) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	202	3PE	C22-C21-O21-C2
45	D	502	3PE	C1-O11-P-O12
45	D	502	3PE	C1-O11-P-O13
45	D	502	3PE	C1-O11-P-O14
45	H	401	3PE	C1-O11-P-O12
45	H	401	3PE	C1-O11-P-O14
45	H	402	3PE	C1-O11-P-O12
45	H	402	3PE	C1-O11-P-O14
45	I	203	3PE	C1-O11-P-O12
45	I	203	3PE	C11-O13-P-O14
45	I	203	3PE	C22-C21-O21-C2
45	K	101	3PE	O13-C11-C12-N
45	L	705	3PE	C1-O11-P-O12
45	L	705	3PE	C1-O11-P-O13
45	L	705	3PE	C1-O11-P-O14
45	L	705	3PE	C12-C11-O13-P
45	M	601	3PE	C1-O11-P-O12
45	M	601	3PE	C1-O11-P-O14
45	M	601	3PE	C11-O13-P-O11
45	M	601	3PE	C1-C2-O21-C21
45	M	602	3PE	C1-O11-P-O12
45	M	602	3PE	C1-O11-P-O13
45	M	602	3PE	C1-O11-P-O14
45	M	602	3PE	C12-C11-O13-P
45	M	602	3PE	O13-C11-C12-N
45	M	604	3PE	C22-C21-O21-C2
45	M	606	3PE	O13-C11-C12-N
45	M	606	3PE	O22-C21-O21-C2
45	N	403	3PE	C1-O11-P-O12
45	N	403	3PE	C1-O11-P-O13
45	N	403	3PE	C11-O13-P-O12
45	N	403	3PE	C11-O13-P-O14
45	N	403	3PE	C12-C11-O13-P
45	N	403	3PE	O13-C11-C12-N
45	N	403	3PE	O22-C21-O21-C2
45	N	403	3PE	C22-C21-O21-C2
45	X	201	3PE	C1-O11-P-O12
45	X	201	3PE	C1-O11-P-O14
45	X	201	3PE	C22-C21-O21-C2
45	Y	201	3PE	C1-O11-P-O12
45	Y	201	3PE	C1-O11-P-O14
45	Y	201	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	O22-C21-O21-C2
45	Y	201	3PE	C22-C21-O21-C2
45	Y	202	3PE	C1-O11-P-O12
45	Y	202	3PE	C1-O11-P-O14
45	Y	202	3PE	O13-C11-C12-N
45	Y	204	3PE	C2-C1-O11-P
45	Y	204	3PE	O21-C2-C3-O31
45	Y	205	3PE	C1-O11-P-O12
45	Y	205	3PE	C1-O11-P-O13
45	Y	205	3PE	C1-O11-P-O14
45	Y	205	3PE	C22-C21-O21-C2
45	Z	201	3PE	C1-O11-P-O14
45	Z	202	3PE	C1-O11-P-O12
45	Z	202	3PE	C1-O11-P-O13
45	Z	202	3PE	C1-O11-P-O14
45	Z	202	3PE	O22-C21-O21-C2
45	Z	202	3PE	C22-C21-O21-C2
45	d	201	3PE	C11-O13-P-O14
45	d	201	3PE	O13-C11-C12-N
45	h	202	3PE	C1-O11-P-O14
45	h	202	3PE	C12-C11-O13-P
45	h	203	3PE	C11-O13-P-O14
45	m	201	3PE	O22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
46	B	201	PC1	C1-O11-P-O14
46	B	203	PC1	O22-C21-O21-C2
46	B	203	PC1	C22-C21-O21-C2
46	M	605	PC1	O21-C2-C3-O31
46	N	402	PC1	C12-C11-O13-P
46	N	402	PC1	O13-C11-C12-N
46	N	402	PC1	O22-C21-O21-C2
46	N	402	PC1	C22-C21-O21-C2
46	d	202	PC1	C11-O13-P-O12
46	d	202	PC1	C11-O13-P-O14
46	d	202	PC1	C11-O13-P-O11
46	d	202	PC1	C1-O11-P-O14
53	L	702	CDL	CA2-OA2-PA1-OA3
53	L	702	CDL	CA2-OA2-PA1-OA4
53	L	702	CDL	CA2-OA2-PA1-OA5
53	L	702	CDL	CB2-OB2-PB2-OB3
53	N	401	CDL	CA2-OA2-PA1-OA3
53	N	401	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
53	N	401	CDL	C51-CB5-OB6-CB4
53	d	203	CDL	CA2-OA2-PA1-OA4
53	d	203	CDL	CA3-OA5-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA3-OA5-PA1-OA3
53	h	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	C51-CB5-OB6-CB4
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB2-OB2-PB2-OB3
53	q	201	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CB3-OB5-PB2-OB3
54	L	704	CHD	C16-C17-C20-C22
57	P	501	NDP	C2B-O2B-P2B-O1X
59	T	101	EHZ	C11-C10-S1-C9
59	U	101	EHZ	C8-C9-S1-C10
46	N	402	PC1	O32-C31-O31-C3
46	d	202	PC1	O32-C31-O31-C3
45	L	705	3PE	O32-C31-O31-C3
45	M	606	3PE	O32-C31-O31-C3
45	Y	201	3PE	O32-C31-O31-C3
45	d	201	3PE	O32-C31-O31-C3
46	M	603	PC1	O32-C31-O31-C3
53	L	702	CDL	OB9-CB7-OB8-CB6
53	d	203	CDL	OA9-CA7-OA8-CA6
45	A	202	3PE	O22-C21-O21-C2
45	I	203	3PE	O22-C21-O21-C2
45	M	604	3PE	O22-C21-O21-C2
45	Y	205	3PE	O22-C21-O21-C2
45	L	705	3PE	C32-C31-O31-C3
45	M	606	3PE	C32-C31-O31-C3
45	Y	201	3PE	C32-C31-O31-C3
45	d	201	3PE	C32-C31-O31-C3
46	M	603	PC1	C32-C31-O31-C3
46	N	402	PC1	C32-C31-O31-C3
46	d	202	PC1	C32-C31-O31-C3
53	L	702	CDL	C71-CB7-OB8-CB6
45	M	606	3PE	C22-C21-O21-C2
45	Y	203	3PE	O32-C31-O31-C3
45	Z	201	3PE	O32-C31-O31-C3
45	L	703	3PE	C32-C31-O31-C3
53	d	203	CDL	C31-CA7-OA8-CA6
45	X	201	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
53	N	401	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	OA7-CA5-OA6-CA4
53	h	201	CDL	OB9-CB7-OB8-CB6
54	L	704	CHD	C13-C17-C20-C21
53	L	702	CDL	O1-C1-CB2-OB2
53	q	201	CDL	O1-C1-CB2-OB2
45	X	201	3PE	C32-C31-O31-C3
45	h	202	3PE	C32-C31-O31-C3
46	J	201	PC1	C32-C31-O31-C3
53	h	201	CDL	C71-CB7-OB8-CB6
45	h	202	3PE	O32-C31-O31-C3
53	q	201	CDL	C11-CA5-OA6-CA4
45	Y	201	3PE	C2-C3-O31-C31
46	B	201	PC1	C3D-C3E-C3F-C3G
53	N	401	CDL	C51-C52-C53-C54
54	L	704	CHD	C16-C17-C20-C21
45	D	502	3PE	C35-C36-C37-C38
45	Y	203	3PE	C32-C31-O31-C3
45	Z	201	3PE	C32-C31-O31-C3
45	L	703	3PE	O32-C31-O31-C3
53	q	201	CDL	CB5-C51-C52-C53
45	X	201	3PE	O32-C31-O31-C3
45	M	602	3PE	C32-C31-O31-C3
46	N	402	PC1	C35-C36-C37-C38
54	L	704	CHD	C17-C20-C22-C23
46	J	201	PC1	O32-C31-O31-C3
53	h	201	CDL	C51-C52-C53-C54
45	Y	205	3PE	C32-C31-O31-C3
53	h	201	CDL	C31-CA7-OA8-CA6
53	h	201	CDL	CA5-C11-C12-C13
53	L	702	CDL	C12-C13-C14-C15
45	m	201	3PE	O11-C1-C2-O21
46	N	402	PC1	C32-C33-C34-C35
54	L	704	CHD	C21-C20-C22-C23
45	M	602	3PE	C21-C22-C23-C24
45	Y	202	3PE	C31-C32-C33-C34
53	L	702	CDL	CB5-C51-C52-C53
45	D	502	3PE	O21-C2-C3-O31
45	Y	205	3PE	O32-C31-O31-C3
53	h	201	CDL	OA9-CA7-OA8-CA6
53	d	203	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	C31-C32-C33-C34
46	M	605	PC1	C21-C22-C23-C24
45	Y	201	3PE	C22-C23-C24-C25
45	Y	203	3PE	C31-C32-C33-C34
45	Y	204	3PE	C21-C22-C23-C24
53	N	401	CDL	CA7-C31-C32-C33
45	M	601	3PE	C31-C32-C33-C34
45	X	201	3PE	C31-C32-C33-C34
53	N	401	CDL	CB5-C51-C52-C53
53	d	203	CDL	CA5-C11-C12-C13
53	q	201	CDL	CA5-C11-C12-C13
53	q	201	CDL	CB7-C71-C72-C73
48	D	501	LMT	O5'-C5'-C6'-O6'
53	d	203	CDL	OA7-CA5-OA6-CA4
45	M	602	3PE	O32-C31-O31-C3
45	I	203	3PE	C3B-C3C-C3D-C3E
46	d	202	PC1	C35-C36-C37-C38
60	o	201	MYR	C2-C3-C4-C5
45	A	201	3PE	C1-O11-P-O13
45	H	401	3PE	C1-O11-P-O13
45	H	402	3PE	C1-O11-P-O13
45	M	601	3PE	C1-O11-P-O13
45	M	606	3PE	C1-O11-P-O13
45	N	403	3PE	C11-O13-P-O11
45	X	201	3PE	C1-O11-P-O13
45	Y	201	3PE	C1-O11-P-O13
45	Y	202	3PE	C1-O11-P-O13
45	Y	203	3PE	C1-O11-P-O13
45	Y	204	3PE	C1-O11-P-O13
45	Z	201	3PE	C1-O11-P-O13
45	d	201	3PE	C11-O13-P-O11
45	h	202	3PE	C1-O11-P-O13
46	B	201	PC1	C1-O11-P-O13
53	L	702	CDL	CB2-OB2-PB2-OB5
53	N	401	CDL	CA2-OA2-PA1-OA5
53	d	203	CDL	CA2-OA2-PA1-OA5
53	d	203	CDL	CA3-OA5-PA1-OA2
53	d	203	CDL	CB2-OB2-PB2-OB5
53	h	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CB2-OB2-PB2-OB5
53	d	203	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	CA2-C1-CB2-OB2
54	L	704	CHD	C13-C17-C20-C22
45	A	201	3PE	C2D-C2E-C2F-C2G
45	Y	202	3PE	C3C-C3D-C3E-C3F
45	M	601	3PE	C22-C21-O21-C2
45	H	402	3PE	C2B-C2C-C2D-C2E
45	K	101	3PE	C27-C28-C29-C2A
45	Y	205	3PE	C23-C24-C25-C26
45	Y	205	3PE	C2C-C2D-C2E-C2F
45	M	602	3PE	C26-C27-C28-C29
45	h	202	3PE	C32-C33-C34-C35
53	N	401	CDL	C77-C78-C79-C80
53	q	201	CDL	C17-C18-C19-C20
45	Y	205	3PE	C1-C2-O21-C21
45	M	601	3PE	O22-C21-O21-C2
45	L	701	3PE	C31-C32-C33-C34
53	d	203	CDL	CB7-C71-C72-C73
45	I	203	3PE	O11-C1-C2-O21
45	N	403	3PE	O11-C1-C2-O21
45	D	502	3PE	C23-C24-C25-C26
45	M	604	3PE	C33-C34-C35-C36
45	M	604	3PE	C3E-C3F-C3G-C3H
46	N	402	PC1	C34-C35-C36-C37
53	N	401	CDL	C54-C55-C56-C57
46	d	202	PC1	C21-C22-C23-C24
45	Y	203	3PE	C33-C34-C35-C36
46	M	605	PC1	C26-C27-C28-C29
53	L	702	CDL	C51-C52-C53-C54
53	h	201	CDL	C35-C36-C37-C38
53	h	201	CDL	C54-C55-C56-C57
45	Y	203	3PE	C39-C3A-C3B-C3C
45	Z	201	3PE	C3C-C3D-C3E-C3F
45	h	203	3PE	C37-C38-C39-C3A
46	B	203	PC1	C32-C33-C34-C35
46	M	603	PC1	C2B-C2C-C2D-C2E
45	h	203	3PE	C2-C3-O31-C31
45	H	402	3PE	C3A-C3B-C3C-C3D
45	I	203	3PE	C2C-C2D-C2E-C2F
45	N	403	3PE	C2D-C2E-C2F-C2G
53	h	201	CDL	C73-C74-C75-C76
46	B	201	PC1	C3B-C3C-C3D-C3E
46	M	605	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C35-C36-C37-C38
45	H	402	3PE	C38-C39-C3A-C3B
45	A	201	3PE	C38-C39-C3A-C3B
45	H	401	3PE	C26-C27-C28-C29
45	H	402	3PE	C33-C34-C35-C36
45	L	701	3PE	C38-C39-C3A-C3B
45	L	705	3PE	C2B-C2C-C2D-C2E
45	Y	204	3PE	C33-C34-C35-C36
53	h	201	CDL	C74-C75-C76-C77
45	I	203	3PE	C2D-C2E-C2F-C2G
45	h	203	3PE	C2E-C2F-C2G-C2H
53	h	201	CDL	C36-C37-C38-C39
53	q	201	CDL	C71-C72-C73-C74
59	U	101	EHZ	C3-C4-C5-C6
45	L	705	3PE	O13-C11-C12-N
45	A	201	3PE	C3A-C3B-C3C-C3D
45	N	403	3PE	C2A-C2B-C2C-C2D
45	d	201	3PE	C23-C24-C25-C26
46	B	203	PC1	C34-C35-C36-C37
46	M	605	PC1	C37-C38-C39-C3A
59	U	101	EHZ	C1-C21-C22-C23
45	D	502	3PE	C3A-C3B-C3C-C3D
45	L	701	3PE	C34-C35-C36-C37
46	d	202	PC1	C33-C34-C35-C36
53	q	201	CDL	C13-C14-C15-C16
46	B	201	PC1	C32-C31-O31-C3
45	h	202	3PE	C33-C34-C35-C36
45	m	201	3PE	C2E-C2F-C2G-C2H
46	J	201	PC1	C34-C35-C36-C37
45	M	606	3PE	C34-C35-C36-C37
53	N	401	CDL	C76-C77-C78-C79
45	L	703	3PE	C32-C33-C34-C35
45	d	201	3PE	C3C-C3D-C3E-C3F
46	d	202	PC1	C24-C25-C26-C27
45	Y	205	3PE	C1-C2-C3-O31
46	B	203	PC1	C22-C23-C24-C25
45	m	201	3PE	C31-C32-C33-C34
53	L	702	CDL	CA5-C11-C12-C13
46	B	201	PC1	C3E-C3F-C3G-C3H
45	L	703	3PE	C22-C21-O21-C2
45	h	202	3PE	C22-C21-O21-C2
45	h	203	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
46	B	201	PC1	C22-C21-O21-C2
53	h	201	CDL	C11-CA5-OA6-CA4
46	J	201	PC1	C32-C33-C34-C35
60	o	201	MYR	C6-C7-C8-C9
45	M	601	3PE	C34-C35-C36-C37
45	M	601	3PE	C22-C23-C24-C25
46	d	202	PC1	C25-C26-C27-C28
45	L	703	3PE	C3B-C3C-C3D-C3E
53	N	401	CDL	C37-C38-C39-C40
45	D	502	3PE	C37-C38-C39-C3A
45	L	703	3PE	O22-C21-O21-C2
45	h	203	3PE	O22-C21-O21-C2
46	B	201	PC1	O22-C21-O21-C2
53	h	201	CDL	OA7-CA5-OA6-CA4
46	J	201	PC1	C38-C39-C3A-C3B
53	N	401	CDL	C38-C39-C40-C41
45	M	602	3PE	C37-C38-C39-C3A
45	Y	202	3PE	C22-C23-C24-C25
53	h	201	CDL	C71-C72-C73-C74
46	M	603	PC1	C21-C22-C23-C24
53	h	201	CDL	CB5-C51-C52-C53
53	q	201	CDL	C31-CA7-OA8-CA6
45	H	401	3PE	C28-C29-C2A-C2B
45	M	602	3PE	C2E-C2F-C2G-C2H
45	N	403	3PE	C2B-C2C-C2D-C2E
45	Y	201	3PE	C3B-C3C-C3D-C3E
45	Y	204	3PE	C3B-C3C-C3D-C3E
45	Y	204	3PE	C3D-C3E-C3F-C3G
45	Z	201	3PE	C39-C3A-C3B-C3C
46	B	201	PC1	O32-C31-O31-C3
45	A	202	3PE	C36-C37-C38-C39
45	d	201	3PE	O22-C21-O21-C2
45	h	202	3PE	O22-C21-O21-C2
45	M	604	3PE	C21-C22-C23-C24
45	I	203	3PE	C32-C31-O31-C3
45	Z	202	3PE	C32-C31-O31-C3
46	B	203	PC1	C32-C31-O31-C3
45	L	703	3PE	C25-C26-C27-C28
45	L	705	3PE	C22-C23-C24-C25
45	Y	203	3PE	C26-C27-C28-C29
45	Y	205	3PE	C26-C27-C28-C29
53	N	401	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
45	d	201	3PE	C38-C39-C3A-C3B
53	L	702	CDL	C57-C58-C59-C60
45	M	602	3PE	C23-C24-C25-C26
45	h	203	3PE	C2A-C2B-C2C-C2D
53	N	401	CDL	C53-C54-C55-C56
53	h	201	CDL	C56-C57-C58-C59
45	H	402	3PE	C28-C29-C2A-C2B
45	K	101	3PE	C25-C26-C27-C28
45	Y	201	3PE	C34-C35-C36-C37
45	d	201	3PE	C22-C21-O21-C2
46	M	605	PC1	C22-C21-O21-C2
46	d	202	PC1	C22-C21-O21-C2
53	L	702	CDL	C11-CA5-OA6-CA4
53	d	203	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	OB5-CB3-CB4-OB6
45	D	502	3PE	C36-C37-C38-C39
46	M	605	PC1	C39-C3A-C3B-C3C
46	d	202	PC1	O22-C21-O21-C2
53	L	702	CDL	OA7-CA5-OA6-CA4
53	d	203	CDL	OB7-CB5-OB6-CB4
45	L	703	3PE	C39-C3A-C3B-C3C
45	Y	202	3PE	O21-C2-C3-O31
53	q	201	CDL	OB6-CB4-CB6-OB8
45	Y	202	3PE	C2A-C2B-C2C-C2D
53	d	203	CDL	C41-C42-C43-C44
45	L	705	3PE	C24-C25-C26-C27
45	I	203	3PE	C36-C37-C38-C39
45	M	606	3PE	C37-C38-C39-C3A
45	M	606	3PE	C28-C29-C2A-C2B
45	Y	203	3PE	C27-C28-C29-C2A
45	M	601	3PE	C2B-C2C-C2D-C2E
53	q	201	CDL	C51-C52-C53-C54
45	I	203	3PE	O32-C31-O31-C3
46	B	203	PC1	O32-C31-O31-C3
46	M	605	PC1	O22-C21-O21-C2
45	Y	201	3PE	C2A-C2B-C2C-C2D
45	I	203	3PE	C11-O13-P-O11
45	L	701	3PE	C1-O11-P-O13
45	L	703	3PE	C1-O11-P-O13
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CB3-OB5-PB2-OB2
45	H	402	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
45	M	606	3PE	C31-C32-C33-C34
45	M	601	3PE	C38-C39-C3A-C3B
53	q	201	CDL	OA9-CA7-OA8-CA6
45	H	401	3PE	O11-C1-C2-C3
45	I	203	3PE	O11-C1-C2-C3
45	M	606	3PE	O11-C1-C2-C3
45	Z	201	3PE	O11-C1-C2-C3
45	m	201	3PE	O11-C1-C2-C3
46	M	605	PC1	O11-C1-C2-C3
53	L	702	CDL	OB5-CB3-CB4-CB6
53	h	201	CDL	OB5-CB3-CB4-CB6
45	Y	202	3PE	C34-C35-C36-C37
53	N	401	CDL	C71-C72-C73-C74
53	L	702	CDL	C53-C54-C55-C56
53	N	401	CDL	CB2-C1-CA2-OA2
53	q	201	CDL	CA2-C1-CB2-OB2
45	H	402	3PE	C3D-C3E-C3F-C3G
45	Z	202	3PE	C25-C26-C27-C28
53	d	203	CDL	C75-C76-C77-C78
45	H	401	3PE	C21-C22-C23-C24
45	L	703	3PE	C33-C34-C35-C36
45	I	203	3PE	C1-C2-C3-O31
45	L	701	3PE	C39-C3A-C3B-C3C
45	L	705	3PE	C1-C2-C3-O31
45	N	403	3PE	C1-C2-C3-O31
45	X	201	3PE	C1-C2-C3-O31
45	Y	204	3PE	C1-C2-C3-O31
45	m	201	3PE	C1-C2-C3-O31
46	B	201	PC1	C1-C2-C3-O31
45	Z	202	3PE	O32-C31-O31-C3
46	B	203	PC1	C33-C34-C35-C36
45	I	203	3PE	C33-C34-C35-C36
46	B	203	PC1	C39-C3A-C3B-C3C
45	L	705	3PE	O21-C21-C22-C23
53	h	201	CDL	C52-C51-CB5-OB6
53	L	702	CDL	CB7-C71-C72-C73
45	M	604	3PE	C32-C31-O31-C3
45	m	201	3PE	C2C-C2D-C2E-C2F
53	h	201	CDL	C53-C54-C55-C56
53	h	201	CDL	C76-C77-C78-C79
53	q	201	CDL	C52-C53-C54-C55
45	M	602	3PE	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C31-C32-C33-C34
45	M	604	3PE	C31-C32-C33-C34
46	M	605	PC1	C31-C32-C33-C34
45	h	203	3PE	C32-C31-O31-C3
45	M	604	3PE	C1-C2-O21-C21
53	h	201	CDL	CB6-CB4-OB6-CB5
59	U	101	EHZ	C22-C23-C24-C25
46	M	603	PC1	C2-C1-O11-P
45	m	201	3PE	C32-C31-O31-C3
45	M	602	3PE	O11-C1-C2-O21
45	Y	201	3PE	O11-C1-C2-O21
53	d	203	CDL	C76-C77-C78-C79
45	h	203	3PE	C29-C2A-C2B-C2C
53	N	401	CDL	O1-C1-CA2-OA2
53	N	401	CDL	C58-C59-C60-C61
45	Y	202	3PE	C32-C33-C34-C35
45	m	201	3PE	C27-C28-C29-C2A
45	L	703	3PE	O21-C21-C22-C23
45	A	202	3PE	O21-C2-C3-O31
46	J	201	PC1	C25-C26-C27-C28
45	M	604	3PE	O32-C31-O31-C3
45	M	601	3PE	C23-C24-C25-C26
46	M	603	PC1	C29-C2A-C2B-C2C
45	Y	205	3PE	C28-C29-C2A-C2B
53	L	702	CDL	C33-C34-C35-C36
53	L	702	CDL	C14-C15-C16-C17
53	q	201	CDL	C14-C15-C16-C17
45	M	601	3PE	C2E-C2F-C2G-C2H
53	N	401	CDL	C61-C62-C63-C64
45	N	403	3PE	C29-C2A-C2B-C2C
45	Z	201	3PE	C27-C28-C29-C2A
45	m	201	3PE	C2D-C2E-C2F-C2G
46	M	605	PC1	C3B-C3C-C3D-C3E
45	Y	205	3PE	C29-C2A-C2B-C2C
46	M	603	PC1	C2F-C2G-C2H-C2I
45	X	201	3PE	C35-C36-C37-C38
45	N	403	3PE	C27-C28-C29-C2A
45	A	201	3PE	O11-C1-C2-C3
45	L	703	3PE	O11-C1-C2-C3
45	N	403	3PE	O11-C1-C2-C3
45	Y	201	3PE	O11-C1-C2-C3
45	Y	202	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
45	D	502	3PE	O13-C11-C12-N
45	h	202	3PE	O13-C11-C12-N
45	A	201	3PE	C34-C35-C36-C37
45	M	604	3PE	C24-C25-C26-C27
45	A	201	3PE	C28-C29-C2A-C2B
53	N	401	CDL	C56-C57-C58-C59
45	h	203	3PE	O32-C31-O31-C3
45	M	606	3PE	C32-C33-C34-C35
53	d	203	CDL	C33-C34-C35-C36
46	d	202	PC1	C23-C24-C25-C26
45	D	502	3PE	C32-C31-O31-C3
45	H	401	3PE	O21-C21-C22-C23
45	Y	202	3PE	C2-C1-O11-P
45	M	601	3PE	C25-C26-C27-C28
59	U	101	EHZ	C21-C1-C2-C3
45	Y	201	3PE	C2E-C2F-C2G-C2H
45	A	202	3PE	C1-C2-C3-O31
45	D	502	3PE	C1-C2-C3-O31
45	L	701	3PE	C1-C2-C3-O31
45	Y	202	3PE	C1-C2-C3-O31
45	d	201	3PE	C1-C2-C3-O31
45	h	203	3PE	C1-C2-C3-O31
46	B	203	PC1	C1-C2-C3-O31
46	M	605	PC1	C1-C2-C3-O31
53	L	702	CDL	CB3-CB4-CB6-OB8
53	q	201	CDL	CB3-CB4-CB6-OB8
53	d	203	CDL	C31-C32-C33-C34
45	I	203	3PE	C1-O11-P-O13
45	m	201	3PE	C11-O13-P-O11
53	q	201	CDL	CB3-OB5-PB2-OB2
53	N	401	CDL	C39-C40-C41-C42
53	q	201	CDL	C54-C55-C56-C57
46	B	203	PC1	C3B-C3C-C3D-C3E
46	M	605	PC1	C29-C2A-C2B-C2C
45	Z	201	3PE	O11-C1-C2-O21
53	L	702	CDL	OB5-CB3-CB4-OB6
45	M	601	3PE	C32-C31-O31-C3
45	K	101	3PE	C36-C37-C38-C39
45	M	601	3PE	O21-C21-C22-C23
45	I	203	3PE	C2F-C2G-C2H-C2I
45	Z	201	3PE	C3F-C3G-C3H-C3I
45	m	201	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	M	605	PC1	C36-C37-C38-C39
45	Y	201	3PE	O21-C2-C3-O31
45	Y	203	3PE	O21-C2-C3-O31
45	Z	201	3PE	O21-C2-C3-O31
45	h	203	3PE	O21-C2-C3-O31
45	m	201	3PE	O21-C2-C3-O31
53	L	702	CDL	OB6-CB4-CB6-OB8
46	B	203	PC1	C3D-C3E-C3F-C3G
45	H	402	3PE	C31-C32-C33-C34
45	A	201	3PE	C33-C34-C35-C36
46	B	203	PC1	C3A-C3B-C3C-C3D
45	Z	201	3PE	C36-C37-C38-C39
45	Z	202	3PE	C33-C34-C35-C36
59	U	101	EHZ	O2-C9-S1-C10
45	Z	201	3PE	C22-C23-C24-C25
46	M	605	PC1	C23-C24-C25-C26
46	N	402	PC1	C24-C25-C26-C27
45	D	502	3PE	C31-C32-C33-C34
45	Y	204	3PE	C2-C3-O31-C31
53	N	401	CDL	OB5-CB3-CB4-CB6
45	M	601	3PE	C35-C36-C37-C38
53	q	201	CDL	C31-C32-C33-C34
45	M	604	3PE	C34-C35-C36-C37
45	h	202	3PE	C2C-C2D-C2E-C2F
53	d	203	CDL	C34-C35-C36-C37
45	Y	201	3PE	C35-C36-C37-C38
45	h	203	3PE	C25-C26-C27-C28
60	o	201	MYR	C10-C11-C12-C13
45	m	201	3PE	C23-C24-C25-C26
59	T	101	EHZ	C5-C6-C7-C8
45	H	402	3PE	C3C-C3D-C3E-C3F
45	K	101	3PE	C3F-C3G-C3H-C3I
45	Z	201	3PE	C33-C34-C35-C36
45	d	201	3PE	C37-C38-C39-C3A
45	h	203	3PE	C33-C34-C35-C36
53	N	401	CDL	CB6-CB4-OB6-CB5
45	D	502	3PE	C32-C33-C34-C35
45	M	601	3PE	C37-C38-C39-C3A
45	A	202	3PE	C38-C39-C3A-C3B
45	d	201	3PE	C22-C23-C24-C25
45	A	201	3PE	C1-C2-C3-O31
45	L	703	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	C2-C1-O11-P
45	Y	203	3PE	C1-C2-C3-O31
53	h	201	CDL	CA3-CA4-CA6-OA8
53	L	702	CDL	C51-CB5-OB6-CB4
45	H	401	3PE	O11-C1-C2-O21
45	Y	202	3PE	O11-C1-C2-O21
53	N	401	CDL	OB5-CB3-CB4-OB6
53	d	203	CDL	OB5-CB3-CB4-OB6
45	L	701	3PE	O21-C21-C22-C23
53	q	201	CDL	O1-C1-CA2-OA2
53	L	702	CDL	OB7-CB5-OB6-CB4
59	T	101	EHZ	O1-C7-C8-C9
59	U	101	EHZ	C15-C16-C17-C19
45	D	502	3PE	O32-C31-O31-C3
45	H	401	3PE	O21-C2-C3-O31
45	Y	205	3PE	O21-C2-C3-O31
53	d	203	CDL	OA6-CA4-CA6-OA8
53	h	201	CDL	OA6-CA4-CA6-OA8
45	M	601	3PE	O32-C31-O31-C3
45	A	201	3PE	C26-C27-C28-C29
46	M	603	PC1	C24-C25-C26-C27
55	O	401	DGT	C5'-O5'-PA-O3A
57	P	501	NDP	C2B-O2B-P2B-O3X
45	h	203	3PE	C35-C36-C37-C38
53	d	203	CDL	C39-C40-C41-C42
53	d	203	CDL	C77-C78-C79-C80
45	M	602	3PE	C2F-C2G-C2H-C2I
53	N	401	CDL	C55-C56-C57-C58
53	q	201	CDL	C53-C54-C55-C56
53	q	201	CDL	C11-C12-C13-C14
45	M	604	3PE	C37-C38-C39-C3A
45	L	705	3PE	C26-C27-C28-C29
46	B	201	PC1	C36-C37-C38-C39
45	A	202	3PE	C1-O11-P-O13
45	Z	202	3PE	C11-O13-P-O11
45	m	201	3PE	C1-O11-P-O13
57	P	501	NDP	O4D-C1D-N1N-C6N
45	I	203	3PE	C34-C35-C36-C37
45	I	203	3PE	C29-C2A-C2B-C2C
46	M	603	PC1	C36-C37-C38-C39
45	M	604	3PE	C2-C1-O11-P
46	N	402	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
50	F	501	FMN	C4'-C5'-O5'-P
45	H	402	3PE	C34-C35-C36-C37
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O14
45	A	202	3PE	C1-O11-P-O14
45	I	203	3PE	C1-O11-P-O14
45	L	701	3PE	C1-O11-P-O12
45	L	701	3PE	C1-O11-P-O14
45	L	703	3PE	C1-O11-P-O12
45	L	703	3PE	C1-O11-P-O14
45	M	601	3PE	C11-O13-P-O12
45	M	606	3PE	C1-O11-P-O12
45	N	403	3PE	C1-O11-P-O14
45	Y	203	3PE	C1-O11-P-O12
45	Y	203	3PE	C1-O11-P-O14
45	Y	204	3PE	C1-O11-P-O12
45	Y	204	3PE	C1-O11-P-O14
45	Z	201	3PE	C1-O11-P-O12
45	d	201	3PE	C11-O13-P-O12
45	h	202	3PE	C1-O11-P-O12
45	h	203	3PE	C1-O11-P-O14
45	m	201	3PE	C1-O11-P-O14
53	L	702	CDL	CB2-OB2-PB2-OB4
53	N	401	CDL	CA2-OA2-PA1-OA4
53	d	203	CDL	CA2-OA2-PA1-OA3
53	d	203	CDL	CA3-OA5-PA1-OA4
53	d	203	CDL	CB2-OB2-PB2-OB3
53	d	203	CDL	CB2-OB2-PB2-OB4
53	d	203	CDL	CB3-OB5-PB2-OB4
53	h	201	CDL	CA2-OA2-PA1-OA4
59	T	101	EHZ	C6-C7-C8-C9
45	M	601	3PE	O11-C1-C2-C3
45	A	201	3PE	O21-C21-C22-C23
45	M	606	3PE	C29-C2A-C2B-C2C
46	M	603	PC1	C27-C28-C29-C2A
45	D	502	3PE	C12-C11-O13-P
45	H	402	3PE	C12-C11-O13-P
45	L	701	3PE	C12-C11-O13-P
45	M	606	3PE	C12-C11-O13-P
45	Y	201	3PE	C12-C11-O13-P
45	Y	202	3PE	C12-C11-O13-P
45	Z	201	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
45	Z	202	3PE	C12-C11-O13-P
53	N	401	CDL	CA5-C11-C12-C13
45	Z	201	3PE	C21-C22-C23-C24
45	A	201	3PE	O11-C1-C2-O21
45	L	703	3PE	O11-C1-C2-O21
45	M	606	3PE	O11-C1-C2-O21
46	M	605	PC1	O11-C1-C2-O21
53	q	201	CDL	OA5-CA3-CA4-OA6
59	U	101	EHZ	C15-C16-C17-C20
53	N	401	CDL	C19-C20-C21-C22
45	K	101	3PE	C37-C38-C39-C3A
45	L	703	3PE	C29-C2A-C2B-C2C
45	H	401	3PE	C1-C2-C3-O31
53	d	203	CDL	CA3-CA4-CA6-OA8
59	U	101	EHZ	O5-C16-C17-C20
45	L	701	3PE	O21-C2-C3-O31
45	L	705	3PE	O21-C2-C3-O31
45	N	403	3PE	O21-C2-C3-O31
45	X	201	3PE	O21-C2-C3-O31
45	d	201	3PE	O21-C2-C3-O31
46	B	203	PC1	O21-C2-C3-O31
45	H	401	3PE	C27-C28-C29-C2A
45	M	606	3PE	C2-C1-O11-P
46	B	203	PC1	C2-C1-O11-P
46	M	605	PC1	O32-C31-O31-C3
46	M	605	PC1	C32-C31-O31-C3
46	d	202	PC1	C32-C33-C34-C35
46	M	605	PC1	O31-C31-C32-C33
53	L	702	CDL	CB4-CB6-OB8-CB7
53	h	201	CDL	CA7-C31-C32-C33
45	m	201	3PE	C34-C35-C36-C37
45	N	403	3PE	C2E-C2F-C2G-C2H
45	M	606	3PE	C21-C22-C23-C24
53	N	401	CDL	OA9-CA7-OA8-CA6
45	M	602	3PE	C3F-C3G-C3H-C3I
45	D	502	3PE	C26-C27-C28-C29
45	A	201	3PE	C2B-C2C-C2D-C2E
45	X	201	3PE	C3B-C3C-C3D-C3E
46	J	201	PC1	C23-C24-C25-C26
46	d	202	PC1	C26-C27-C28-C29
45	Z	201	3PE	O21-C21-C22-C23
45	H	401	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
53	d	203	CDL	C73-C74-C75-C76
45	M	606	3PE	C36-C37-C38-C39
53	h	201	CDL	C37-C38-C39-C40
45	M	602	3PE	C33-C34-C35-C36
45	Y	203	3PE	C3-C2-O21-C21
45	Z	202	3PE	C1-C2-O21-C21
45	M	602	3PE	O11-C1-C2-C3
46	J	201	PC1	C2C-C2D-C2E-C2F
45	h	203	3PE	C2-C1-O11-P
45	H	402	3PE	C32-C31-O31-C3
53	N	401	CDL	C31-CA7-OA8-CA6
45	L	701	3PE	O11-C1-C2-O21
45	d	201	3PE	O11-C1-C2-O21
59	U	101	EHZ	C2-C3-C4-C5
45	H	402	3PE	O32-C31-O31-C3
45	I	203	3PE	O21-C2-C3-O31
46	B	201	PC1	O21-C2-C3-O31
45	M	601	3PE	C28-C29-C2A-C2B
45	L	701	3PE	C11-O13-P-O11
45	L	705	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O11
45	Y	205	3PE	C11-O13-P-O11
46	B	203	PC1	C11-O13-P-O11
46	N	402	PC1	C1-O11-P-O13
45	I	203	3PE	C2E-C2F-C2G-C2H
46	M	603	PC1	C23-C24-C25-C26
45	h	203	3PE	C3A-C3B-C3C-C3D
59	U	101	EHZ	O5-C16-C17-C18
45	Y	201	3PE	C1-C2-C3-O31
45	Y	204	3PE	C35-C36-C37-C38
46	M	603	PC1	C34-C35-C36-C37
51	F	503	NAI	O4D-C1D-N1N-C2N
55	O	401	DGT	PG-O3B-PB-O2B
55	O	401	DGT	PB-O3A-PA-O1A
45	M	606	3PE	C35-C36-C37-C38
53	h	201	CDL	C57-C58-C59-C60
53	h	201	CDL	C52-C51-CB5-OB7
45	D	502	3PE	C2-C1-O11-P
45	L	705	3PE	C2-C1-O11-P
46	J	201	PC1	C39-C3A-C3B-C3C
45	M	606	3PE	C2A-C2B-C2C-C2D
46	d	202	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
45	Y	202	3PE	C21-C22-C23-C24
53	L	702	CDL	C58-C59-C60-C61
45	L	703	3PE	C34-C35-C36-C37
59	T	101	EHZ	C2-C1-C21-C22
45	L	705	3PE	O22-C21-C22-C23
59	T	101	EHZ	C5-C6-C7-O1
46	B	201	PC1	O11-C1-C2-O21
46	d	202	PC1	O11-C1-C2-O21
53	L	702	CDL	OA5-CA3-CA4-OA6
46	B	201	PC1	C39-C3A-C3B-C3C
53	L	702	CDL	C54-C55-C56-C57
53	N	401	CDL	C35-C36-C37-C38
53	h	201	CDL	C11-C12-C13-C14
45	M	601	3PE	O21-C2-C3-O31
45	Y	202	3PE	C36-C37-C38-C39
45	L	701	3PE	C32-C31-O31-C3
46	d	202	PC1	C3B-C3C-C3D-C3E
46	J	201	PC1	C2E-C2F-C2G-C2H
45	N	403	3PE	C2F-C2G-C2H-C2I
45	K	101	3PE	O22-C21-O21-C2
51	F	503	NAI	C2D-C1D-N1N-C2N
45	L	703	3PE	C3C-C3D-C3E-C3F
45	Y	205	3PE	C2-C3-O31-C31
59	U	101	EHZ	C4-C5-C6-C7
45	L	705	3PE	C32-C33-C34-C35
46	N	402	PC1	C31-C32-C33-C34
45	A	201	3PE	C27-C28-C29-C2A
45	I	203	3PE	C26-C27-C28-C29
45	d	201	3PE	C2E-C2F-C2G-C2H
48	D	501	LMT	C4'-C5'-C6'-O6'
45	M	604	3PE	C35-C36-C37-C38
53	d	203	CDL	C52-C51-CB5-OB6
46	B	203	PC1	C3F-C3G-C3H-C3I
53	q	201	CDL	C19-C20-C21-C22
45	L	705	3PE	C36-C37-C38-C39
45	L	705	3PE	C2D-C2E-C2F-C2G
45	h	203	3PE	C27-C28-C29-C2A
45	L	701	3PE	O11-C1-C2-C3
45	d	201	3PE	O11-C1-C2-C3
45	M	602	3PE	C3C-C3D-C3E-C3F
46	N	402	PC1	C23-C24-C25-C26
45	L	701	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	H	401	3PE	O22-C21-O21-C2
45	h	203	3PE	C23-C24-C25-C26
45	X	201	3PE	C36-C37-C38-C39
45	A	201	3PE	O21-C2-C3-O31
45	H	402	3PE	C35-C36-C37-C38
45	Z	202	3PE	C32-C33-C34-C35
53	N	401	CDL	CA2-C1-CB2-OB2
45	Y	201	3PE	C24-C25-C26-C27
53	L	702	CDL	C52-C53-C54-C55
45	Y	205	3PE	C33-C34-C35-C36
54	L	704	CHD	C22-C23-C24-O26
57	P	501	NDP	PN-O3-PA-O1A
45	D	502	3PE	C2D-C2E-C2F-C2G
46	M	605	PC1	C28-C29-C2A-C2B
45	L	703	3PE	O22-C21-C22-C23
45	m	201	3PE	C2B-C2C-C2D-C2E
57	P	501	NDP	O4D-C4D-C5D-O5D
45	Y	205	3PE	C34-C35-C36-C37
46	J	201	PC1	C33-C34-C35-C36
45	L	705	3PE	O11-C1-C2-O21
45	K	101	3PE	O31-C31-C32-C33
45	Y	202	3PE	O31-C31-C32-C33
45	L	705	3PE	O11-C1-C2-C3
53	N	401	CDL	OA5-CA3-CA4-CA6
45	X	201	3PE	C21-C22-C23-C24
45	L	705	3PE	C2C-C2D-C2E-C2F
46	B	203	PC1	C28-C29-C2A-C2B
45	L	703	3PE	O21-C2-C3-O31
45	Z	202	3PE	O21-C2-C3-O31
45	Y	204	3PE	C3A-C3B-C3C-C3D
45	K	101	3PE	C22-C21-O21-C2
46	J	201	PC1	C37-C38-C39-C3A
45	A	202	3PE	C32-C31-O31-C3
45	D	502	3PE	C34-C35-C36-C37
45	M	602	3PE	O21-C21-C22-C23
45	Y	203	3PE	O31-C31-C32-C33
45	M	606	3PE	C38-C39-C3A-C3B
45	d	201	3PE	C36-C37-C38-C39
53	L	702	CDL	C32-C33-C34-C35
45	M	606	3PE	C11-O13-P-O11
45	h	203	3PE	C11-O13-P-O11
53	d	203	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
45	H	401	3PE	O22-C21-C22-C23
45	Y	201	3PE	O31-C31-C32-C33
45	Y	205	3PE	O21-C21-C22-C23
45	A	201	3PE	C2A-C2B-C2C-C2D
46	B	201	PC1	C37-C38-C39-C3A
53	L	702	CDL	C55-C56-C57-C58
45	Z	201	3PE	C3B-C3C-C3D-C3E
45	A	202	3PE	O32-C31-O31-C3
53	L	702	CDL	CB3-CB4-OB6-CB5
45	M	602	3PE	C28-C29-C2A-C2B
45	M	604	3PE	C2B-C2C-C2D-C2E
54	L	704	CHD	C22-C23-C24-O25
45	D	502	3PE	O21-C21-C22-C23
45	H	402	3PE	C36-C37-C38-C39
45	d	201	3PE	O21-C21-C22-C23
45	h	203	3PE	O21-C21-C22-C23
45	Z	201	3PE	C1-C2-C3-O31
46	B	203	PC1	C26-C27-C28-C29
45	X	201	3PE	O11-C1-C2-O21
45	A	202	3PE	O31-C31-C32-C33
45	K	101	3PE	O21-C21-C22-C23
46	M	603	PC1	O31-C31-C32-C33
53	d	203	CDL	C12-C11-CA5-OA6
45	I	203	3PE	C35-C36-C37-C38
45	m	201	3PE	C33-C34-C35-C36
45	Z	202	3PE	O31-C31-C32-C33
59	U	101	EHZ	C15-C16-C17-C18
45	X	201	3PE	O11-C1-C2-C3
53	d	203	CDL	OA5-CA3-CA4-CA6
53	q	201	CDL	OA5-CA3-CA4-CA6
45	I	203	3PE	O31-C31-C32-C33
45	Y	202	3PE	O21-C21-C22-C23
45	Y	204	3PE	O31-C31-C32-C33
53	q	201	CDL	C32-C31-CA7-OA8
53	q	201	CDL	C52-C51-CB5-OB6
46	J	201	PC1	O21-C2-C3-O31
53	d	203	CDL	OB6-CB4-CB6-OB8
45	Y	203	3PE	O21-C21-C22-C23
45	m	201	3PE	C32-C33-C34-C35
45	m	201	3PE	C26-C27-C28-C29
53	h	201	CDL	C72-C71-CB7-OB8
45	d	201	3PE	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
45	m	201	3PE	C2F-C2G-C2H-C2I
57	P	501	NDP	O4B-C4B-C5B-O5B
55	O	401	DGT	PB-O3A-PA-O2A
46	B	201	PC1	C25-C26-C27-C28
45	H	401	3PE	C22-C21-O21-C2
45	M	604	3PE	C3D-C3E-C3F-C3G
45	Y	201	3PE	C28-C29-C2A-C2B
45	D	502	3PE	C28-C29-C2A-C2B
45	Y	203	3PE	O32-C31-C32-C33
45	M	602	3PE	O22-C21-C22-C23
45	Y	201	3PE	O32-C31-C32-C33
45	Y	205	3PE	O22-C21-C22-C23
45	d	201	3PE	O22-C21-C22-C23
45	L	705	3PE	C33-C34-C35-C36
46	M	603	PC1	O32-C31-C32-C33
45	h	202	3PE	C2A-C2B-C2C-C2D
45	D	502	3PE	O22-C21-C22-C23
53	q	201	CDL	C52-C51-CB5-OB7
45	H	402	3PE	C3B-C3C-C3D-C3E
45	Y	204	3PE	C32-C33-C34-C35
53	d	203	CDL	CB3-CB4-CB6-OB8
45	Y	204	3PE	O21-C21-C22-C23
53	L	702	CDL	C12-C11-CA5-OA6
45	L	701	3PE	C35-C36-C37-C38
45	X	201	3PE	O21-C21-C22-C23
45	Y	201	3PE	C3D-C3E-C3F-C3G
46	d	202	PC1	C3D-C3E-C3F-C3G
59	U	101	EHZ	C1-C2-C3-C4
46	B	203	PC1	C11-O13-P-O14
46	M	605	PC1	C1-O11-P-O14
53	q	201	CDL	CA2-OA2-PA1-OA3
51	F	503	NAI	C3D-C4D-C5D-O5D
45	h	203	3PE	O22-C21-C22-C23
53	d	203	CDL	C12-C11-CA5-OA7
53	h	201	CDL	C72-C71-CB7-OB9
53	L	702	CDL	C52-C51-CB5-OB6
45	H	401	3PE	O32-C31-O31-C3
46	d	202	PC1	O11-C1-C2-C3
53	d	203	CDL	OB5-CB3-CB4-CB6
45	L	701	3PE	O13-C11-C12-N
45	Y	202	3PE	O22-C21-C22-C23
46	B	201	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	d	202	PC1	O21-C21-C22-C23
45	H	402	3PE	O22-C21-O21-C2
45	I	203	3PE	O32-C31-C32-C33
45	K	101	3PE	O22-C21-C22-C23
45	M	601	3PE	O22-C21-C22-C23
45	Z	202	3PE	O32-C31-C32-C33
53	L	702	CDL	C36-C37-C38-C39
45	Y	204	3PE	C3C-C3D-C3E-C3F
46	J	201	PC1	O21-C21-C22-C23
45	Y	203	3PE	O22-C21-C22-C23
45	Z	201	3PE	C23-C24-C25-C26
45	M	602	3PE	C3B-C3C-C3D-C3E
45	Y	202	3PE	C24-C25-C26-C27
45	M	601	3PE	C12-C11-O13-P
45	d	201	3PE	C12-C11-O13-P
45	h	203	3PE	C12-C11-O13-P
45	m	201	3PE	C12-C11-O13-P
45	A	202	3PE	O32-C31-C32-C33
45	L	701	3PE	O22-C21-C22-C23
53	q	201	CDL	C18-C19-C20-C21
45	M	604	3PE	O21-C21-C22-C23
45	m	201	3PE	O31-C31-C32-C33
46	B	201	PC1	O21-C21-C22-C23
46	d	202	PC1	C37-C38-C39-C3A
45	d	201	3PE	C32-C33-C34-C35
45	Y	202	3PE	C2F-C2G-C2H-C2I
53	q	201	CDL	C55-C56-C57-C58
46	B	203	PC1	C38-C39-C3A-C3B
45	L	703	3PE	O31-C31-C32-C33
45	L	705	3PE	O31-C31-C32-C33
46	J	201	PC1	O11-C1-C2-O21
45	L	703	3PE	O32-C31-C32-C33
45	Y	204	3PE	O22-C21-C22-C23
46	B	201	PC1	O22-C21-C22-C23
53	L	702	CDL	C12-C11-CA5-OA7
45	H	401	3PE	O31-C31-C32-C33
45	h	203	3PE	O31-C31-C32-C33
45	h	203	3PE	O32-C31-C32-C33
45	D	502	3PE	C25-C26-C27-C28
46	d	202	PC1	O22-C21-C22-C23
53	q	201	CDL	C32-C31-CA7-OA9
45	h	202	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	B	203	PC1	C37-C38-C39-C3A
45	L	705	3PE	O32-C31-C32-C33
45	M	604	3PE	O22-C21-C22-C23

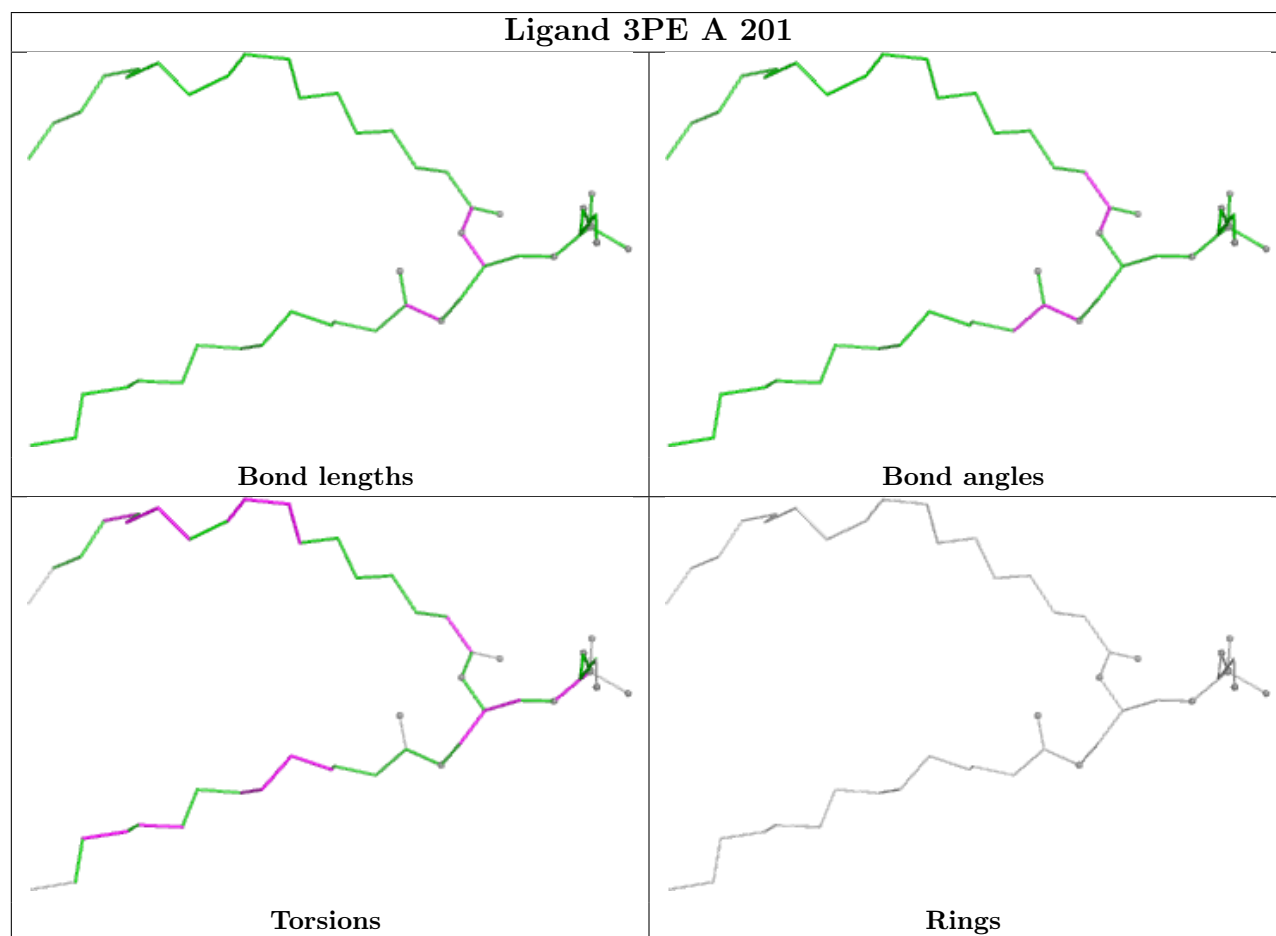
There are no ring outliers.

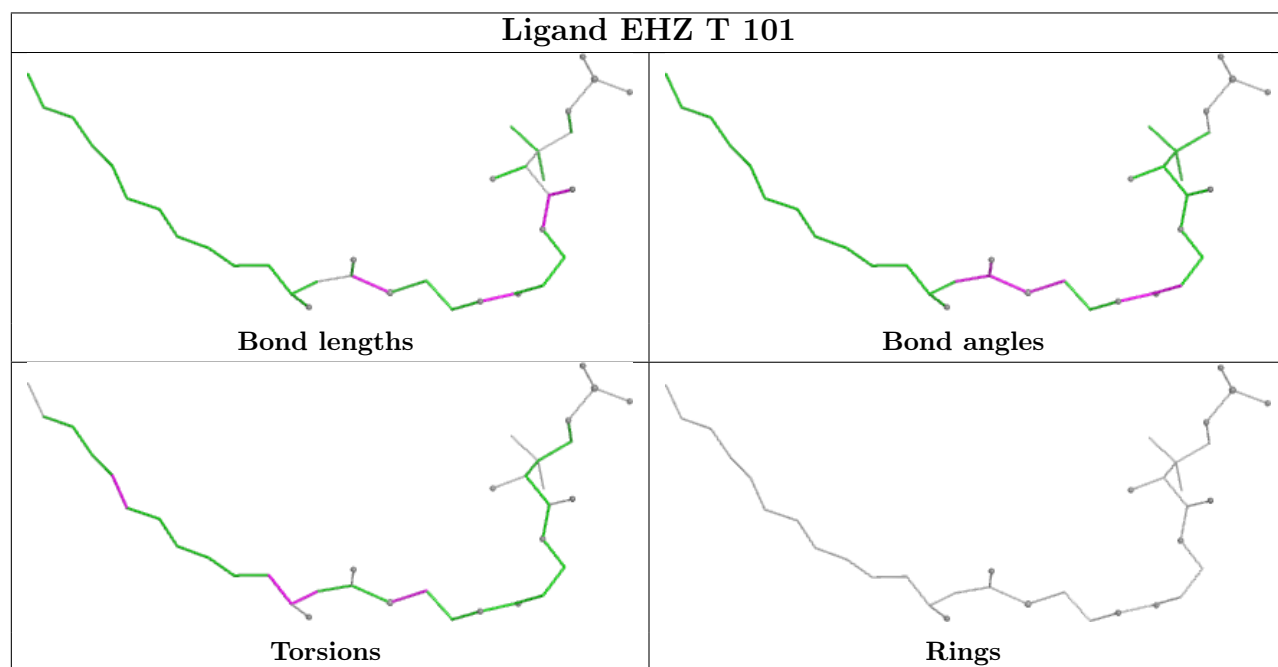
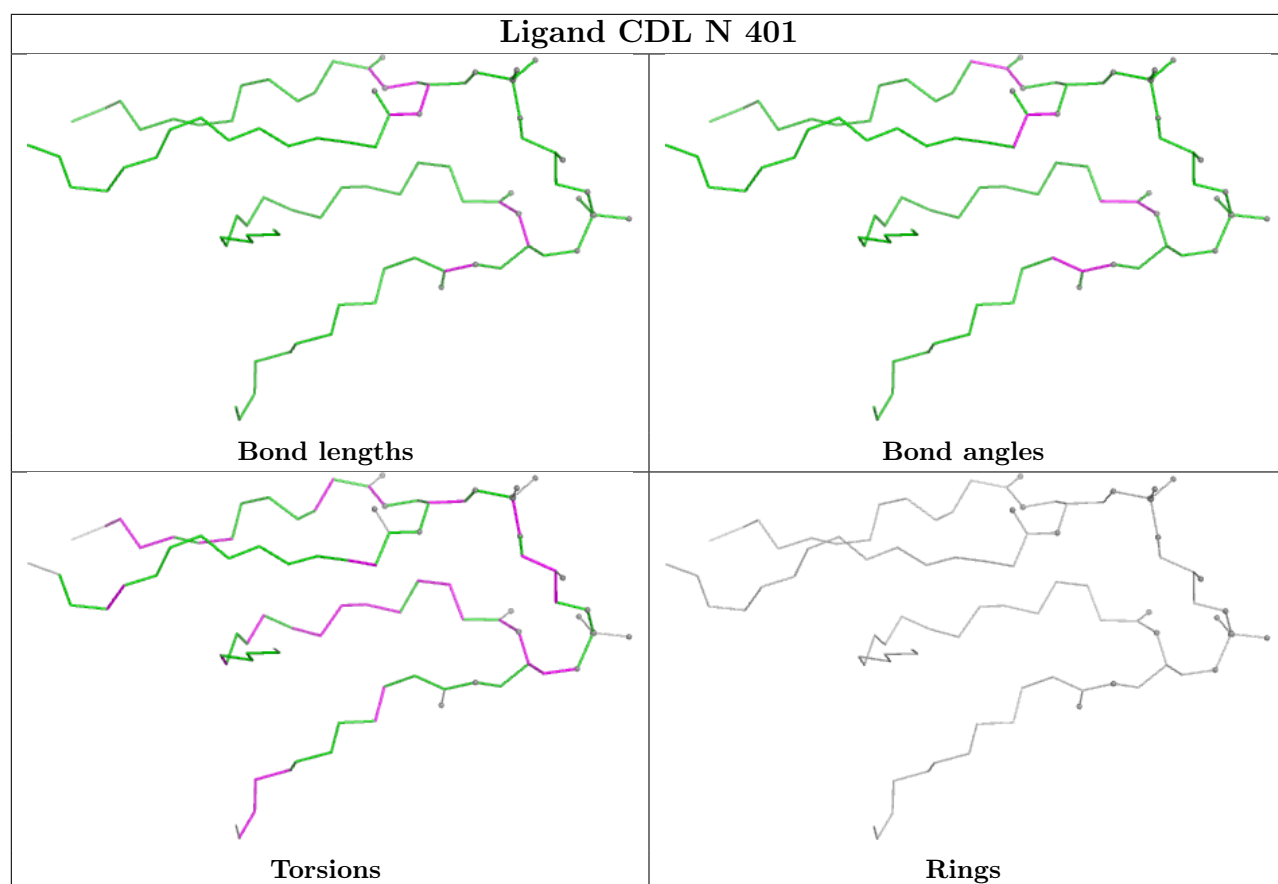
32 monomers are involved in 56 short contacts:

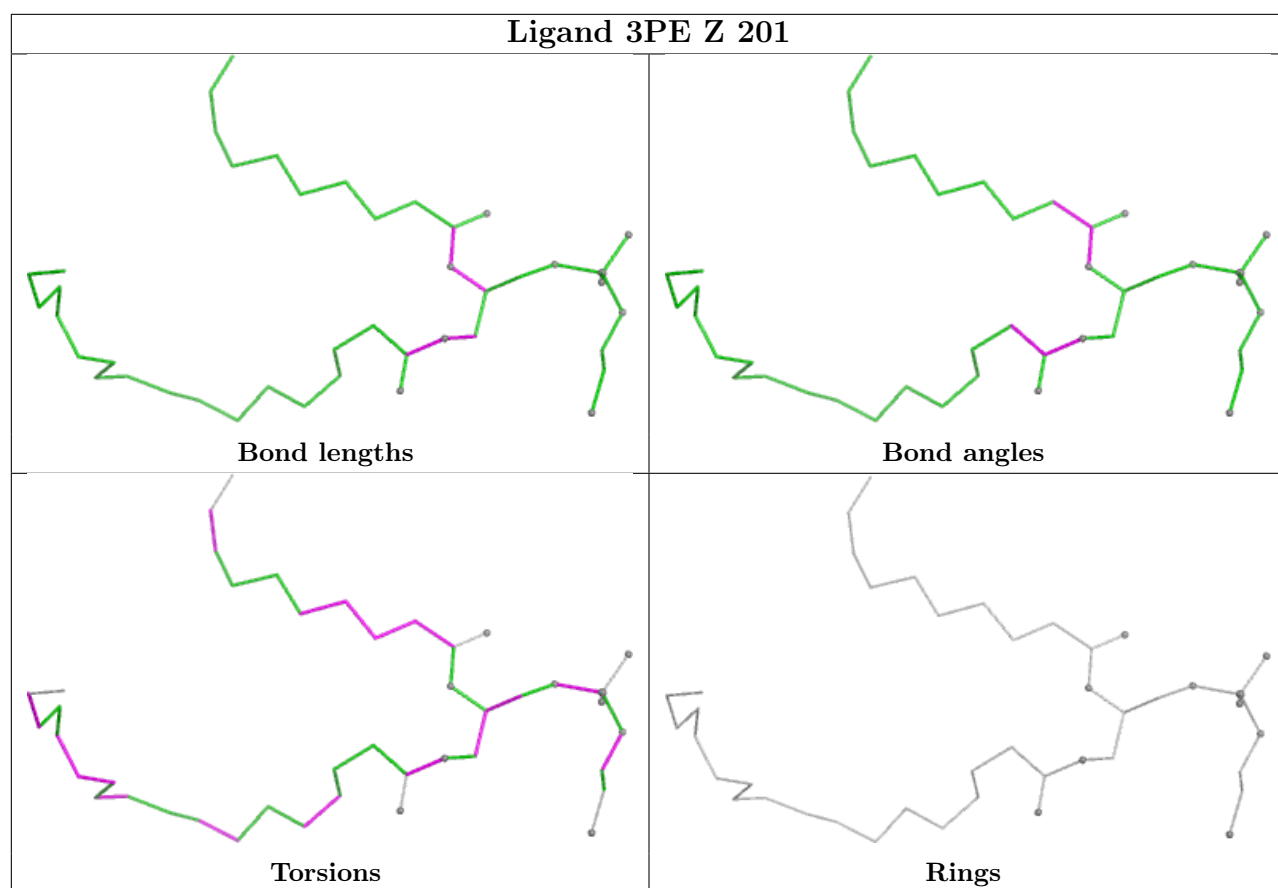
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	201	3PE	1	0
53	N	401	CDL	1	0
47	B	202	SF4	1	0
45	Z	201	3PE	1	0
45	D	502	3PE	2	0
46	B	203	PC1	2	0
45	M	601	3PE	3	0
46	B	201	PC1	2	0
45	Z	202	3PE	3	0
51	F	503	NAI	3	0
45	H	401	3PE	3	0
45	X	201	3PE	2	0
45	N	403	3PE	1	0
46	N	402	PC1	2	0
48	D	501	LMT	2	0
45	M	606	3PE	2	0
45	h	203	3PE	1	0
46	M	605	PC1	2	0
59	U	101	EHZ	1	0
45	M	604	3PE	1	0
45	h	202	3PE	4	0
45	Y	201	3PE	1	0
46	d	202	PC1	1	0
45	Y	204	3PE	2	0
54	L	704	CHD	1	0
45	Y	205	3PE	1	0
45	I	203	3PE	2	0
45	m	201	3PE	1	0
53	q	201	CDL	6	0
45	Y	203	3PE	2	0
53	h	201	CDL	1	0
45	M	602	3PE	3	0

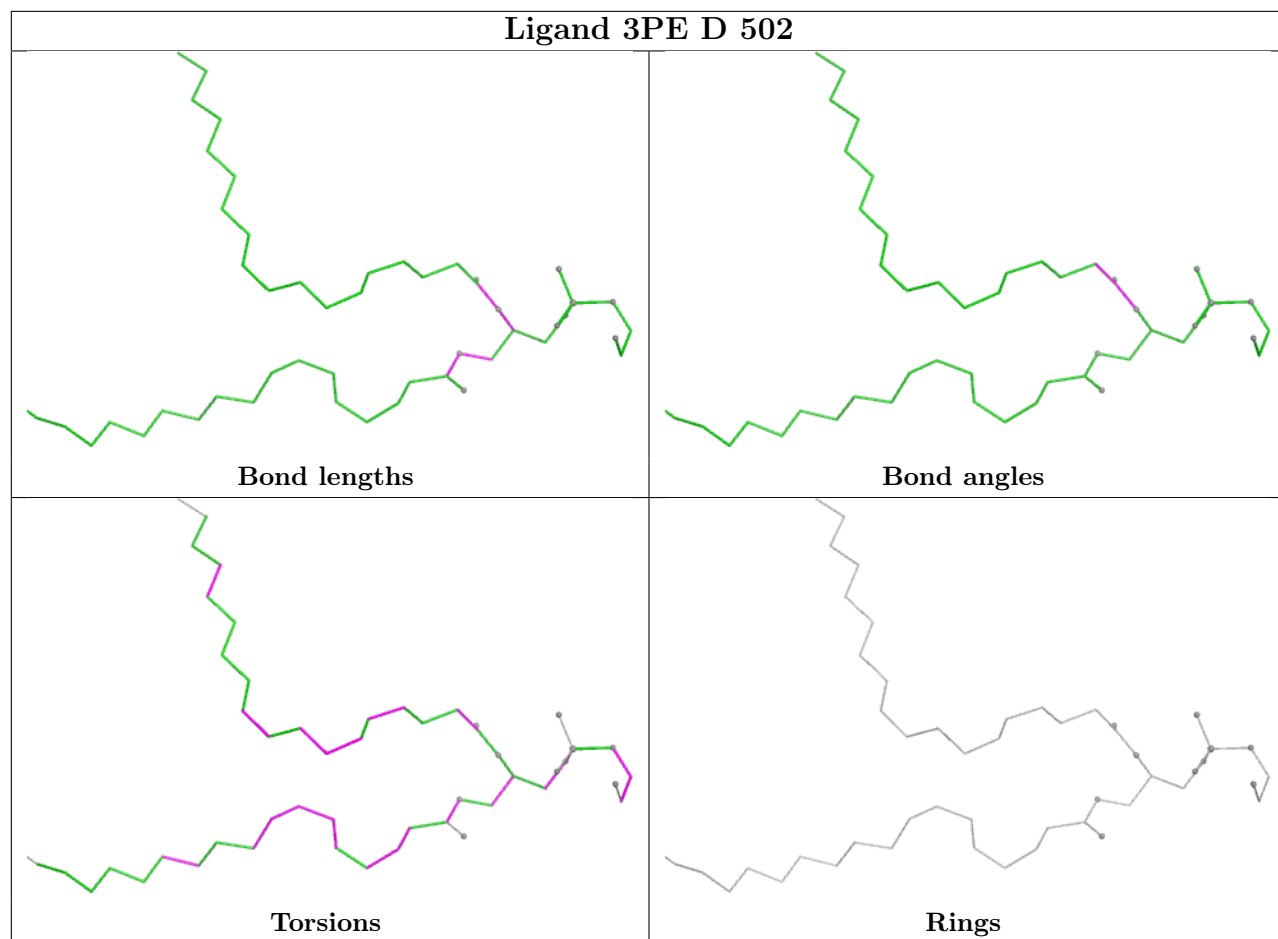
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

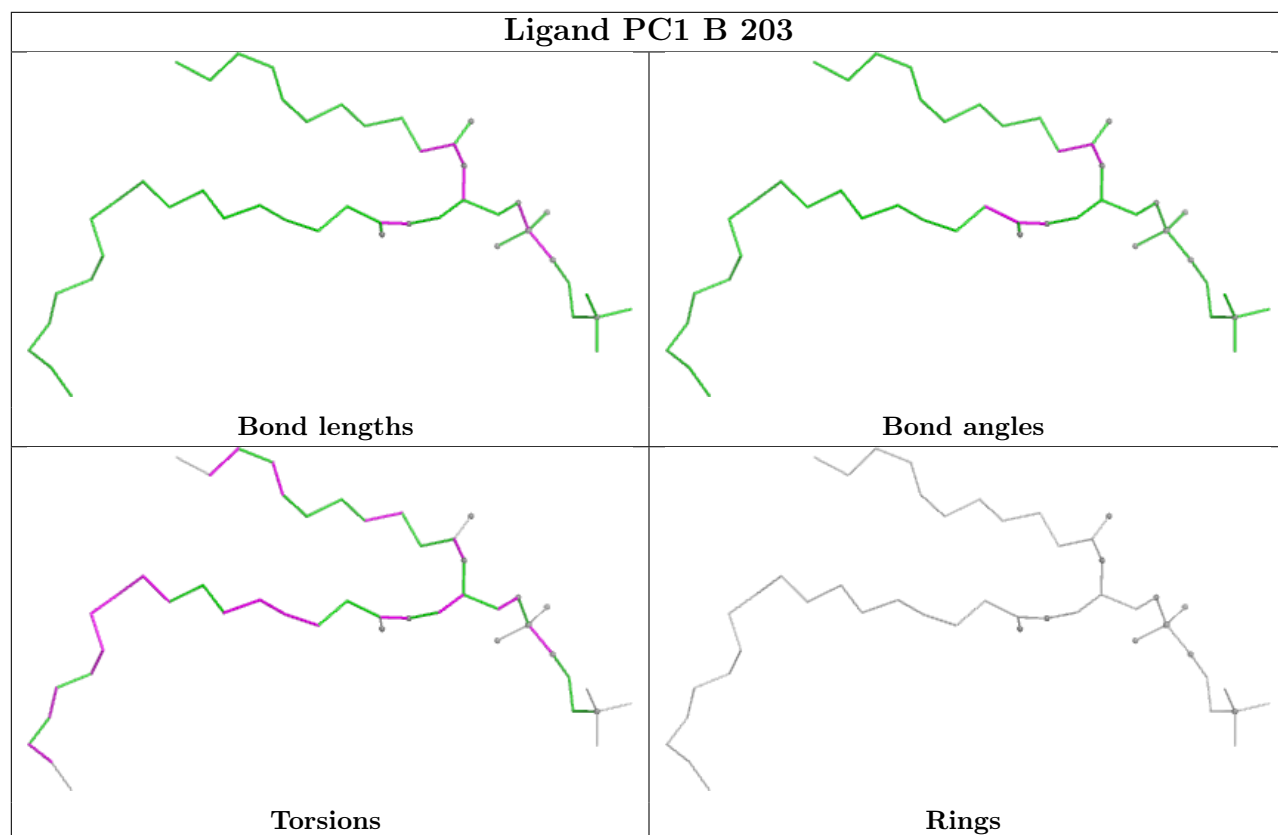
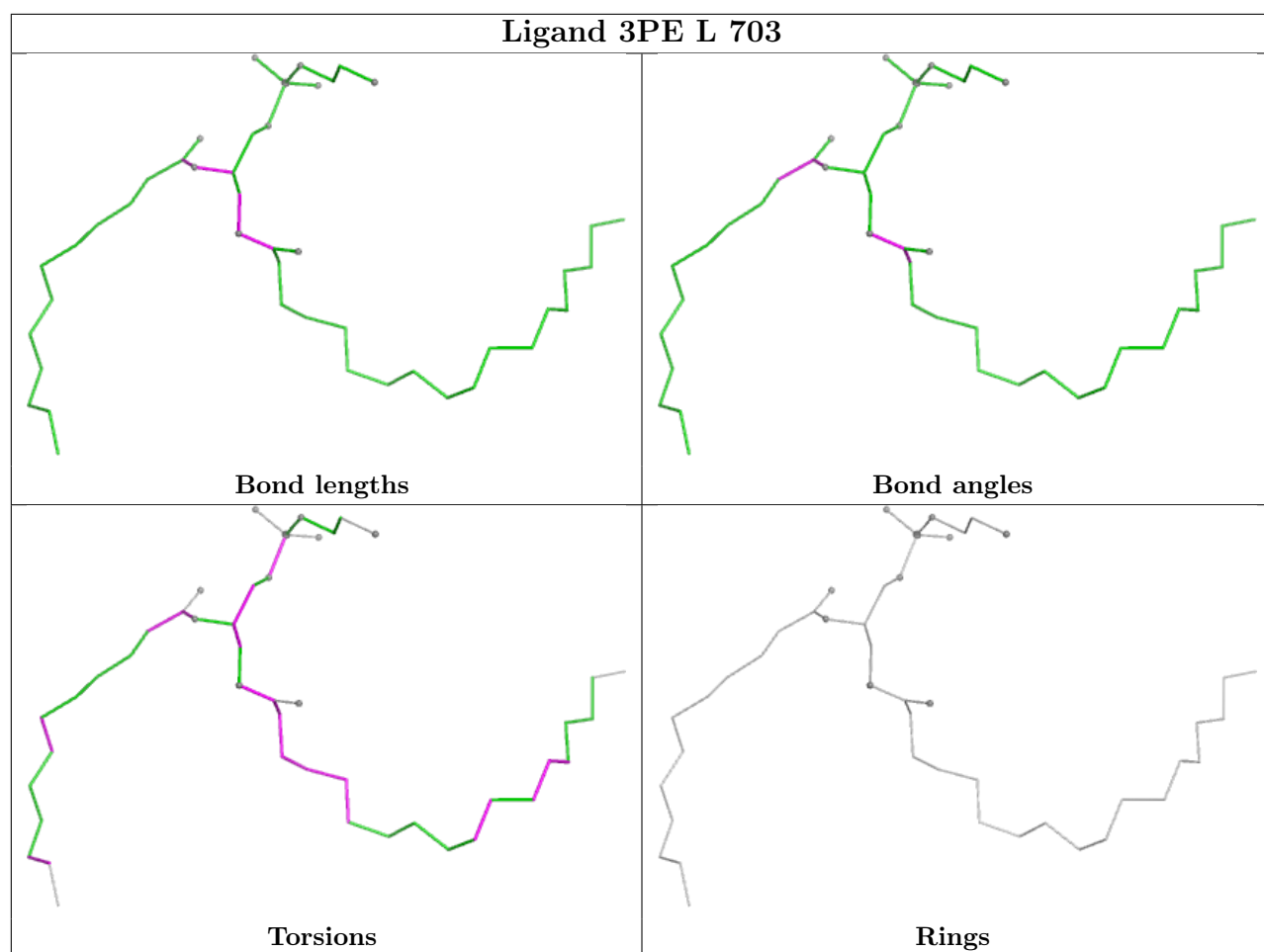
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

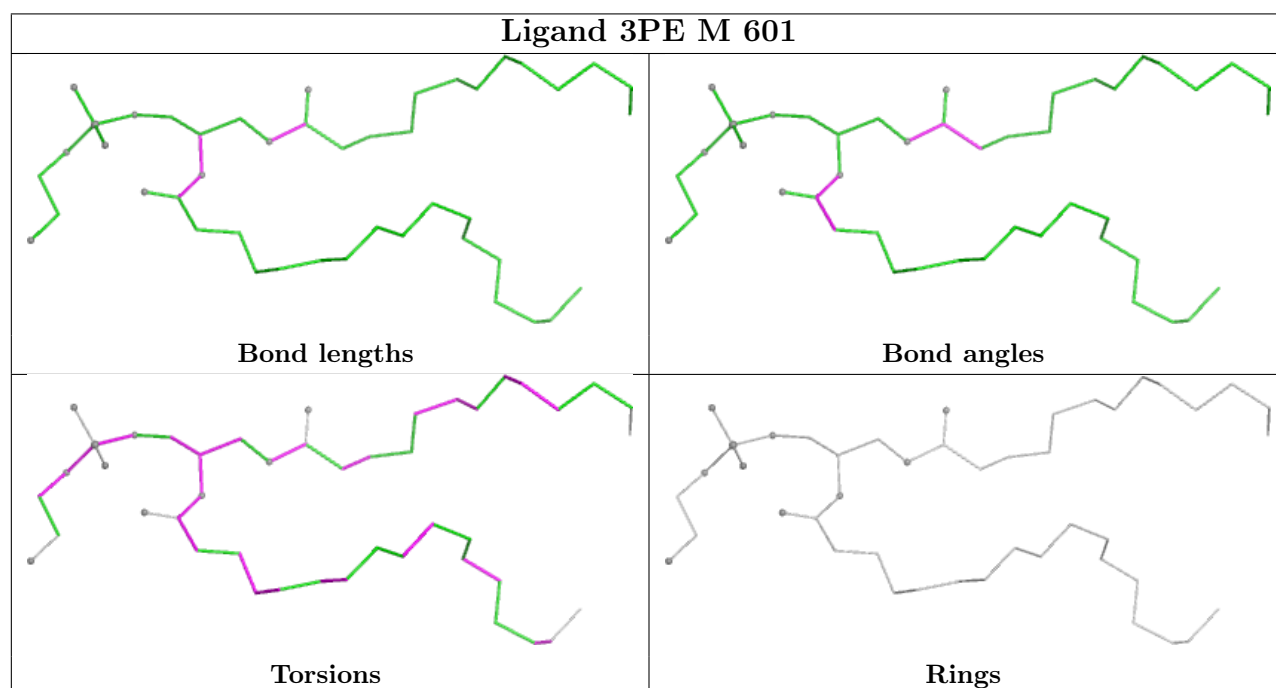
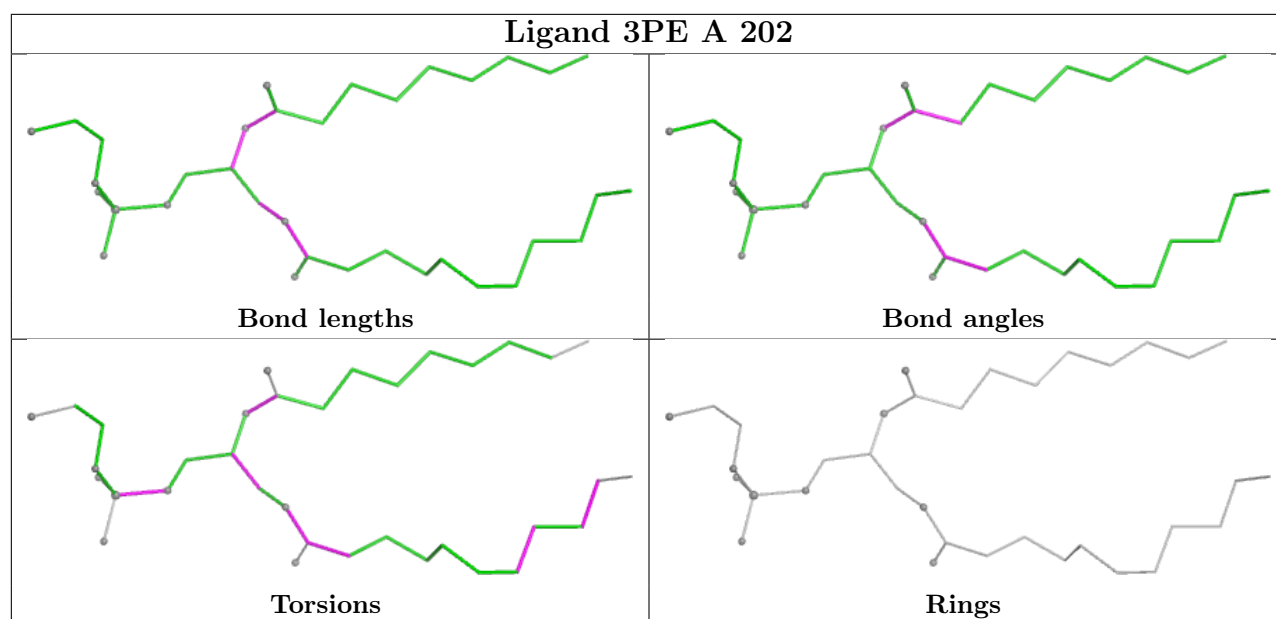


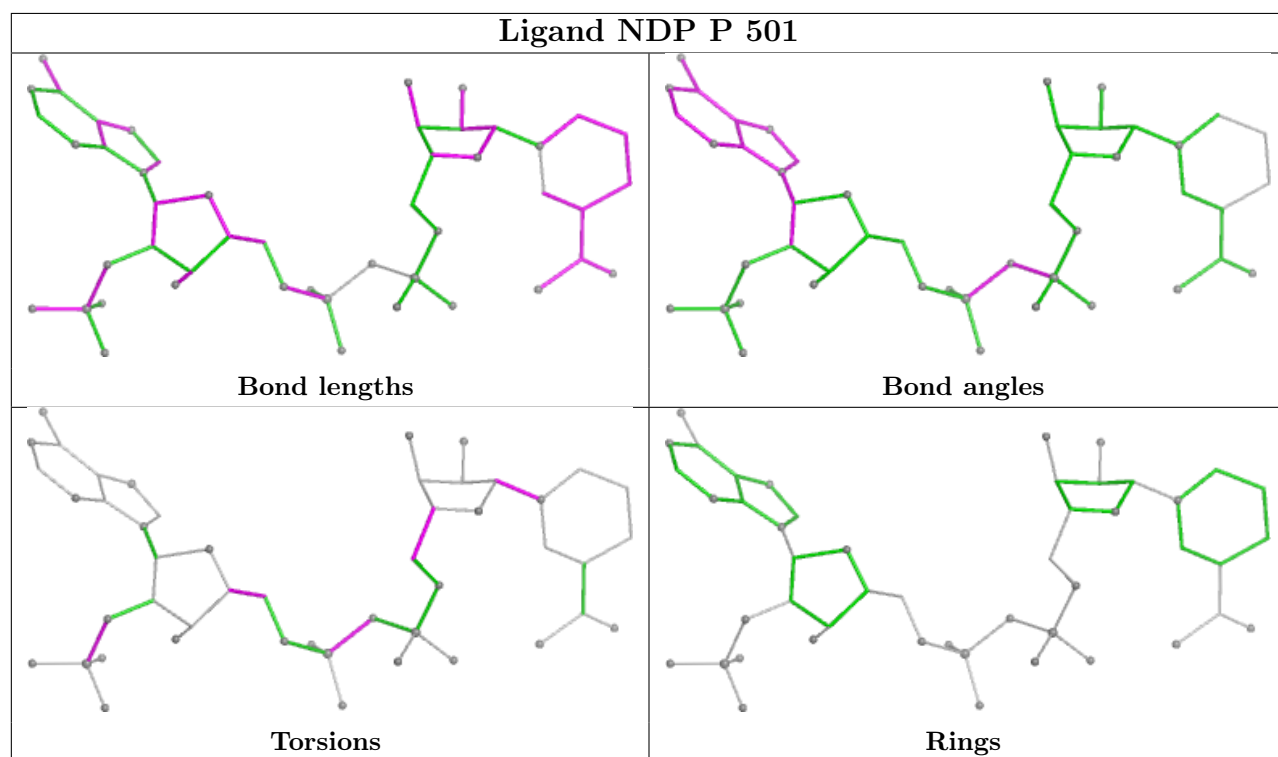
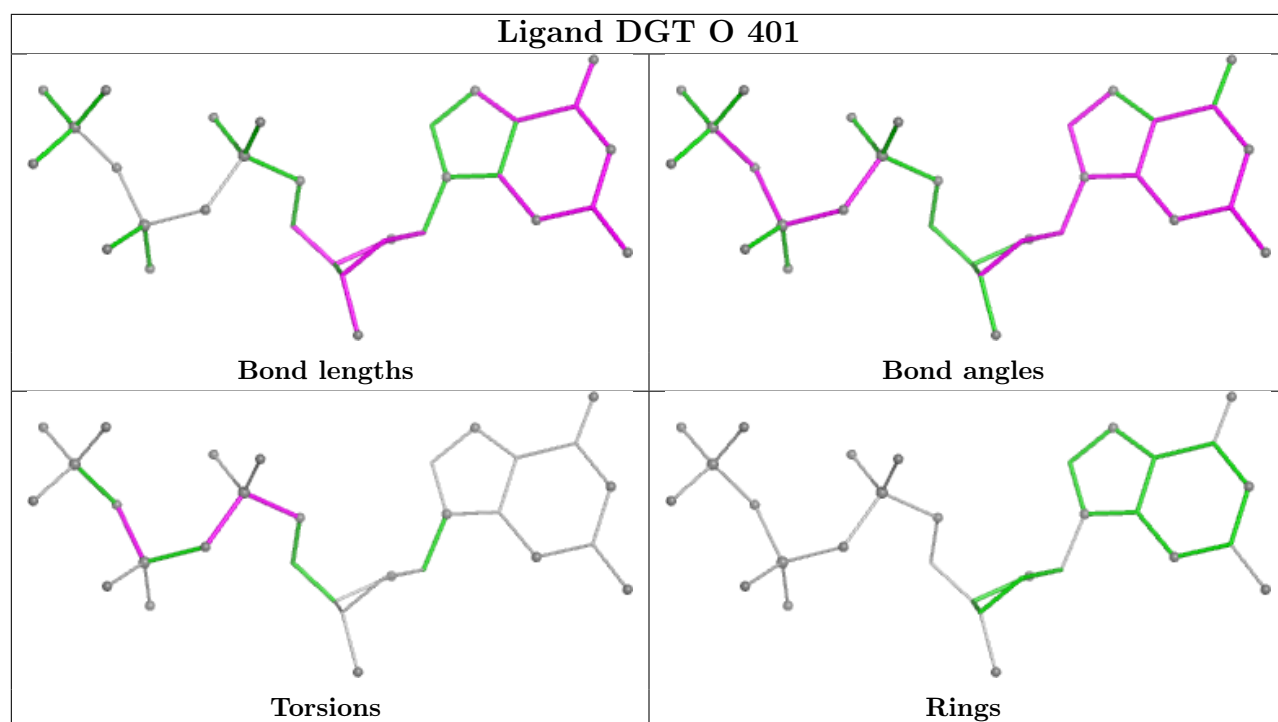


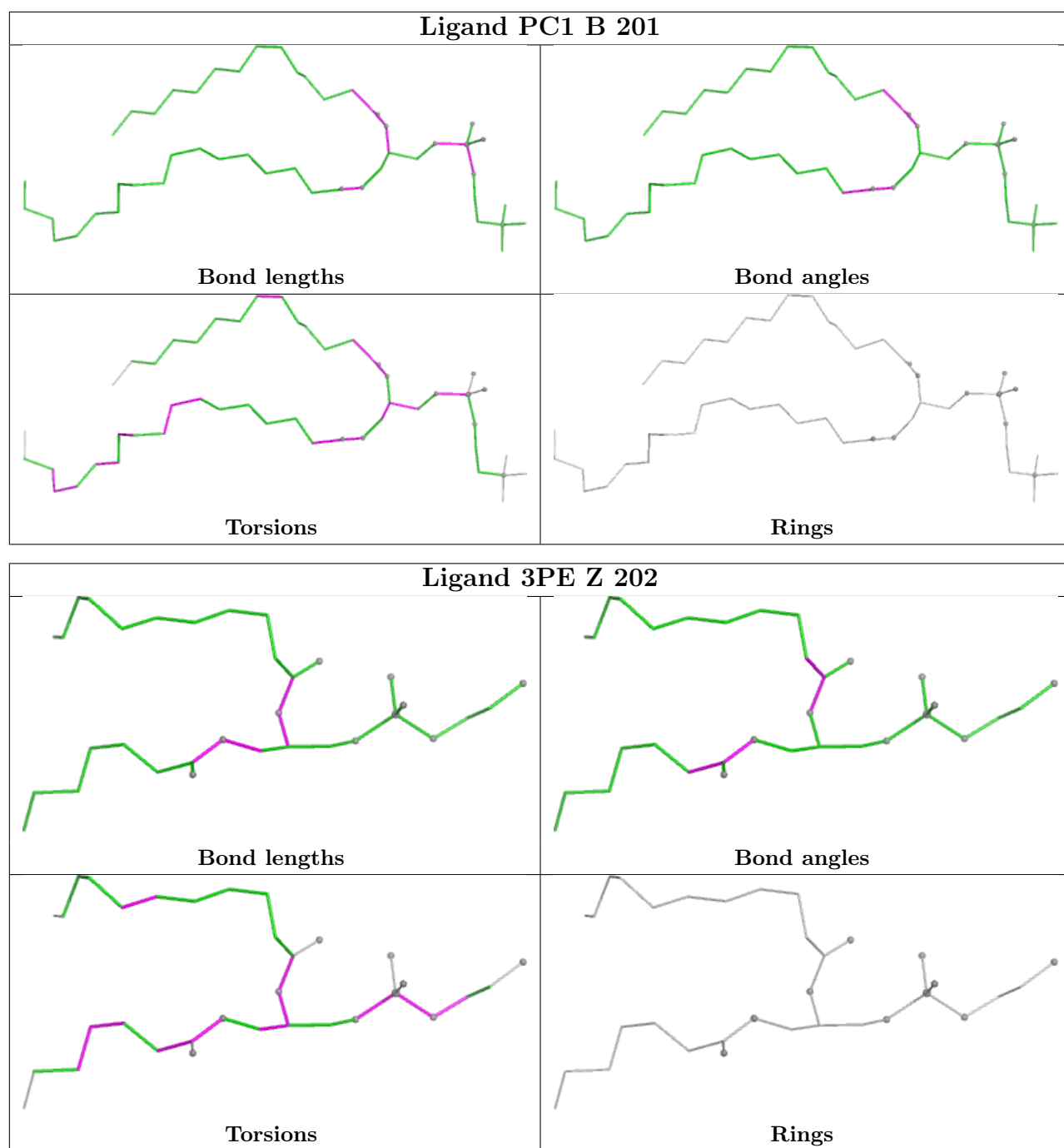


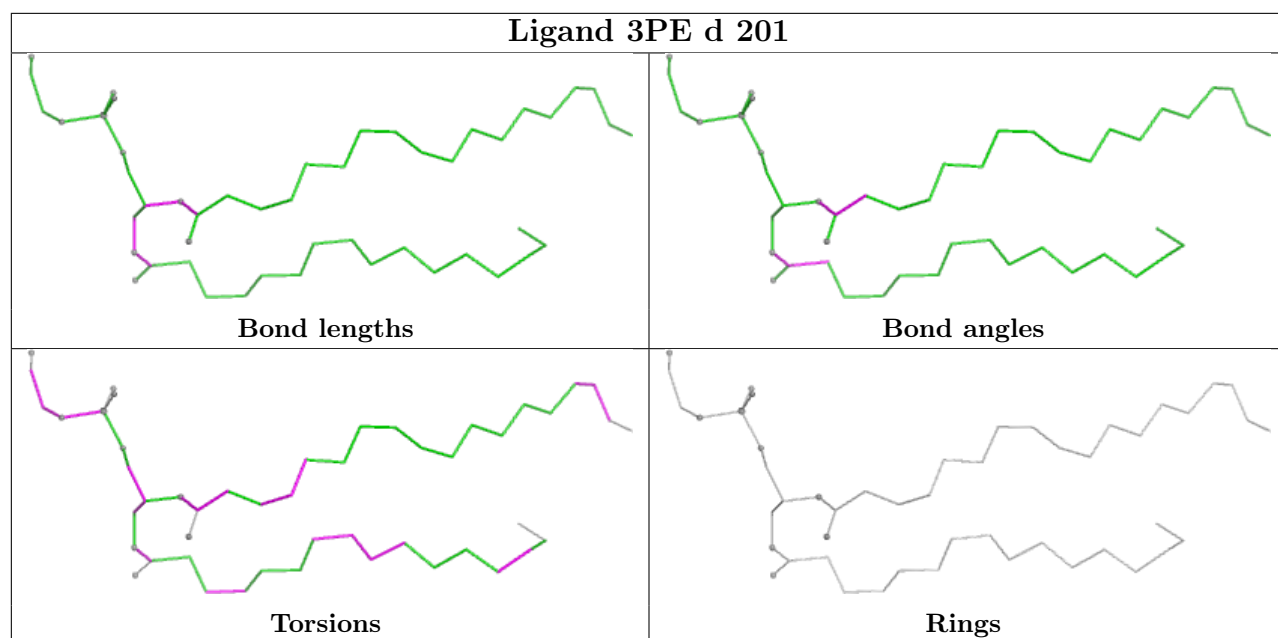
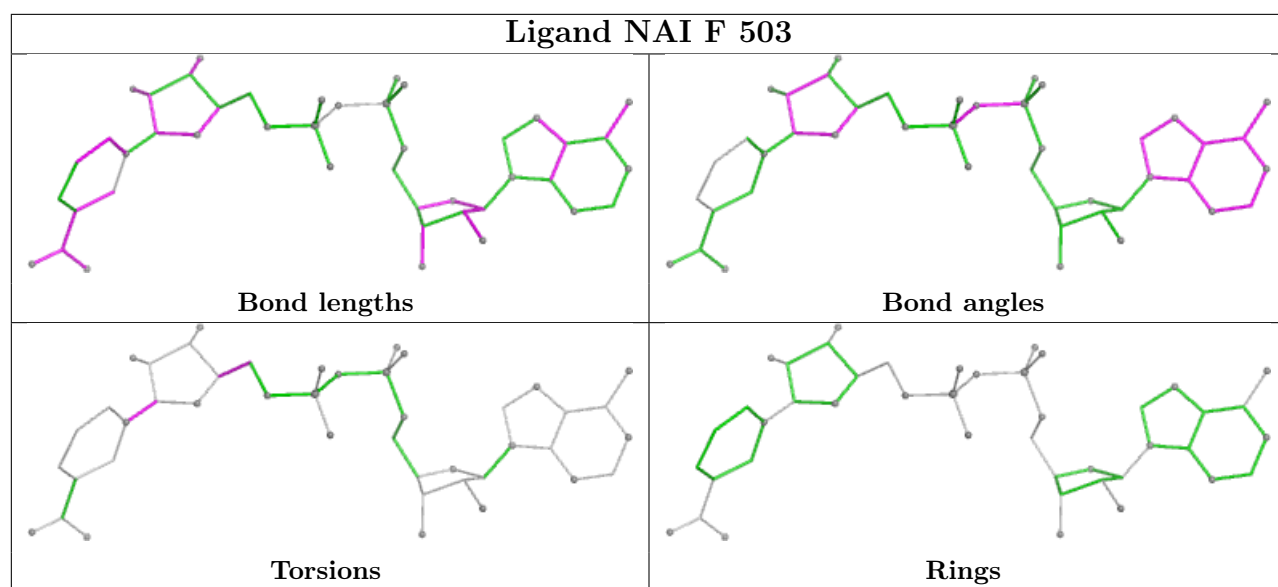


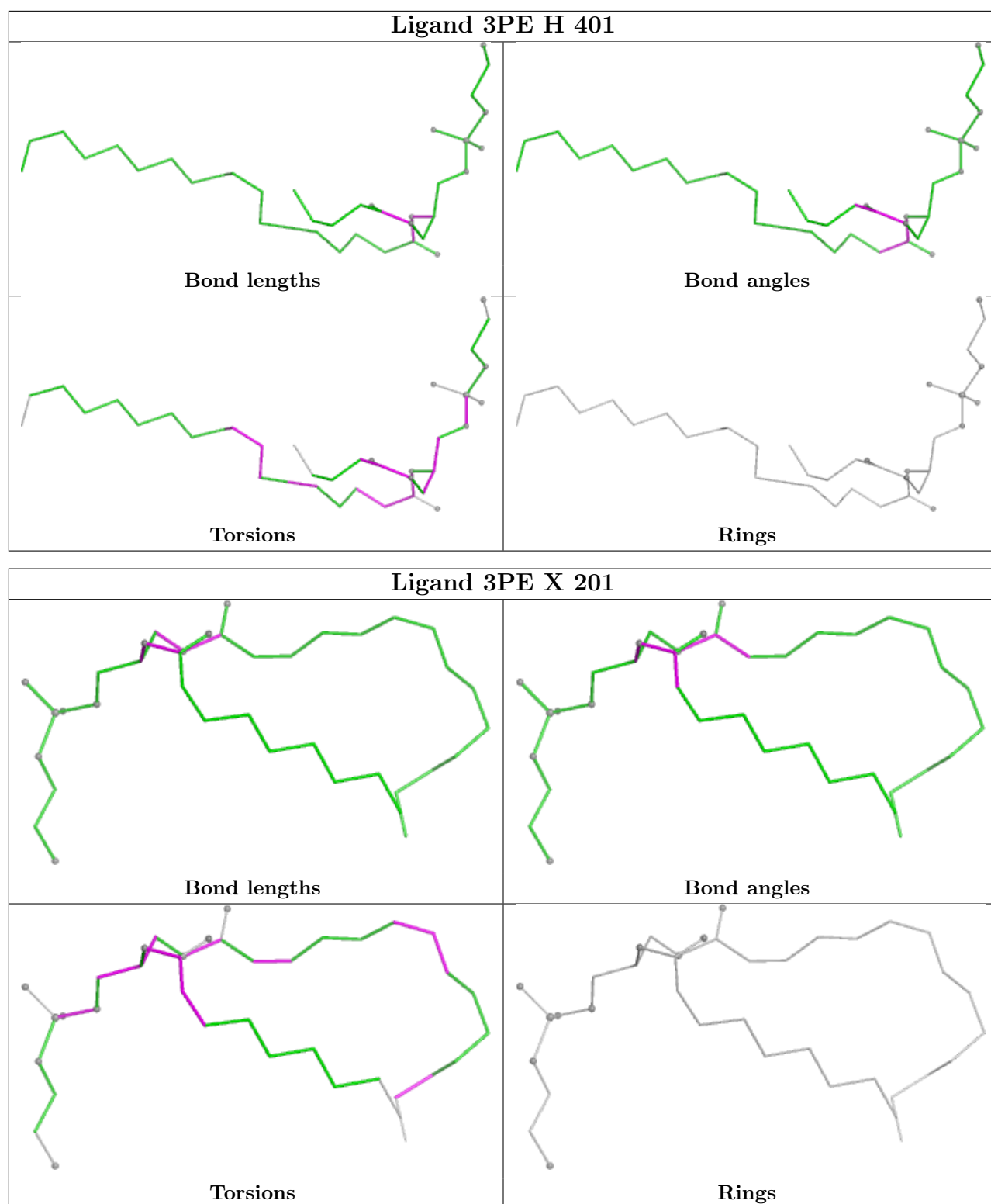


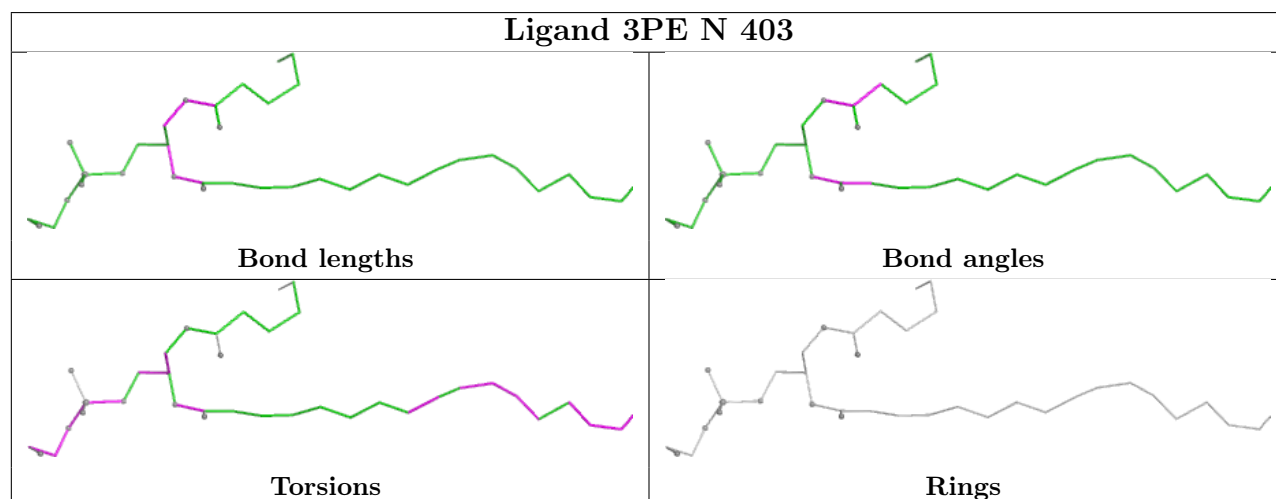
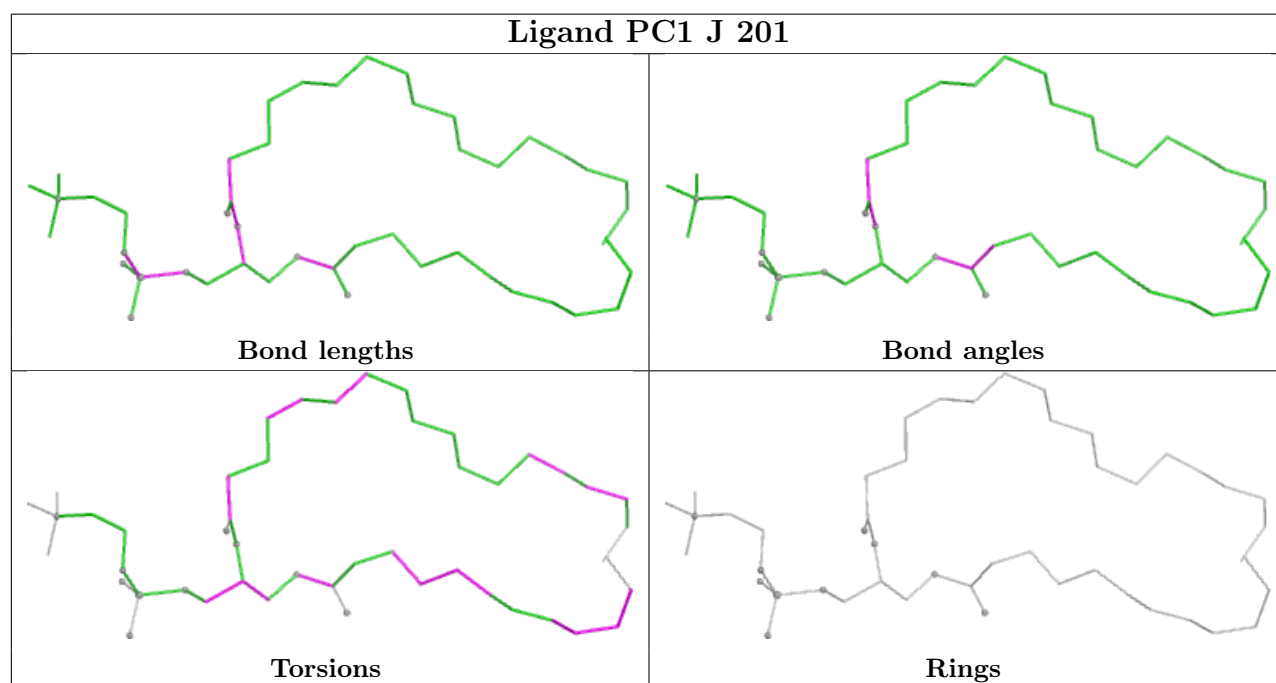
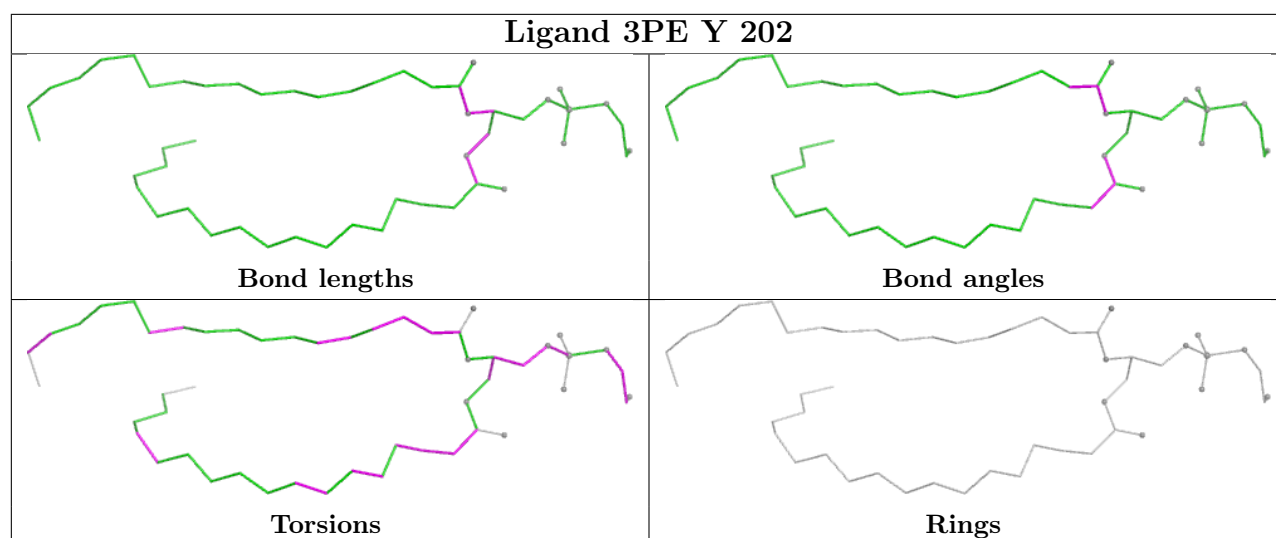


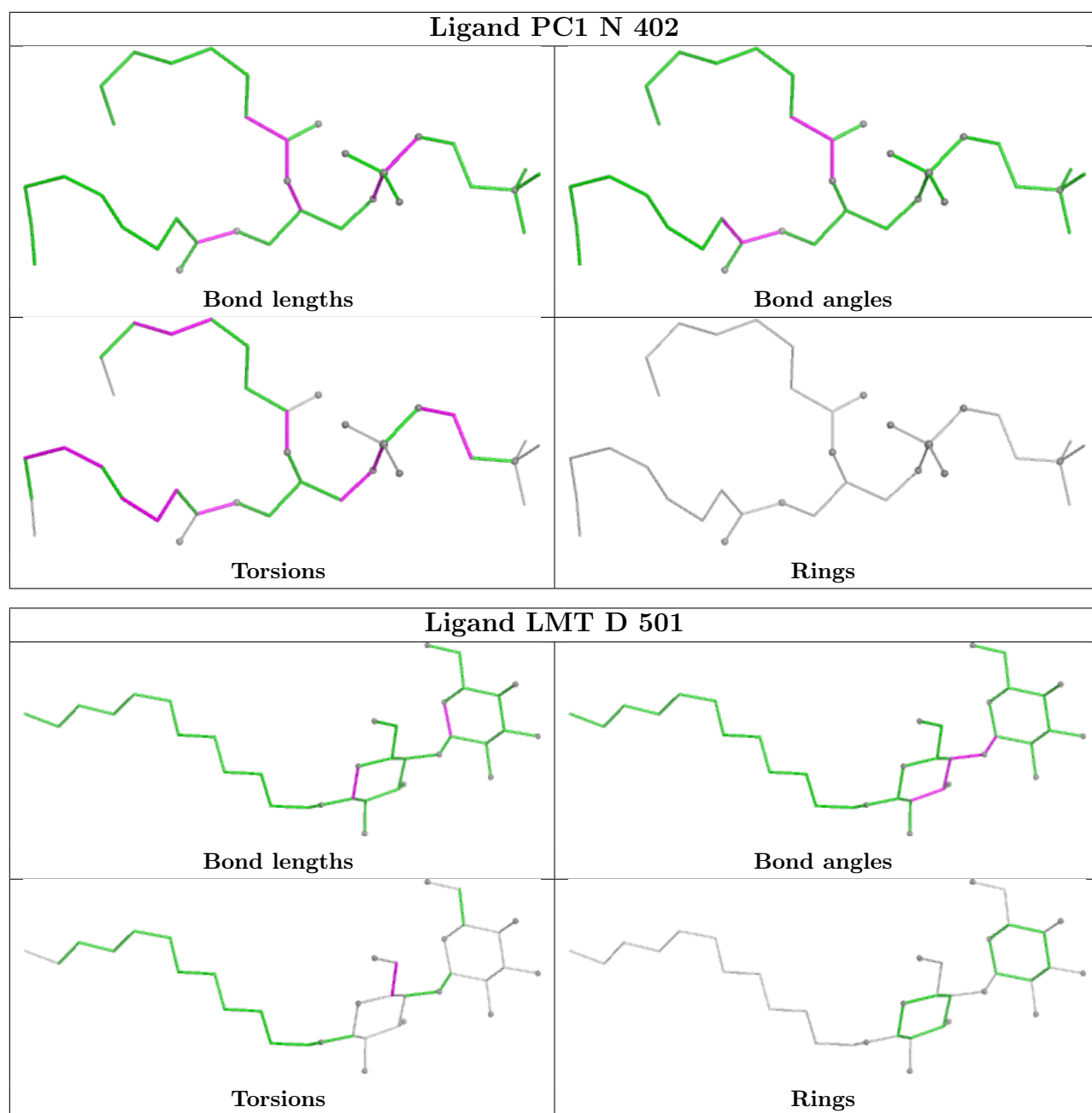


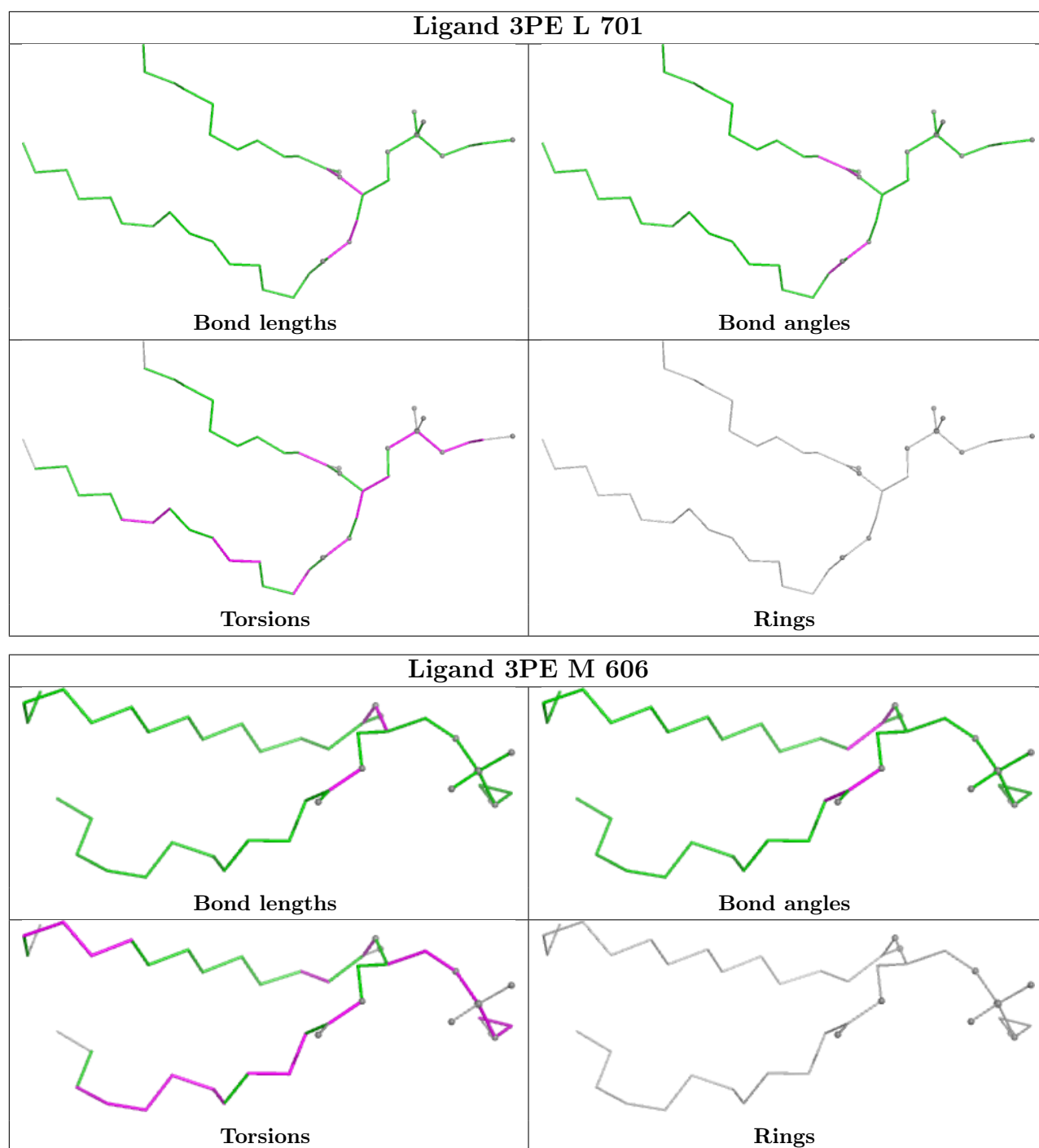


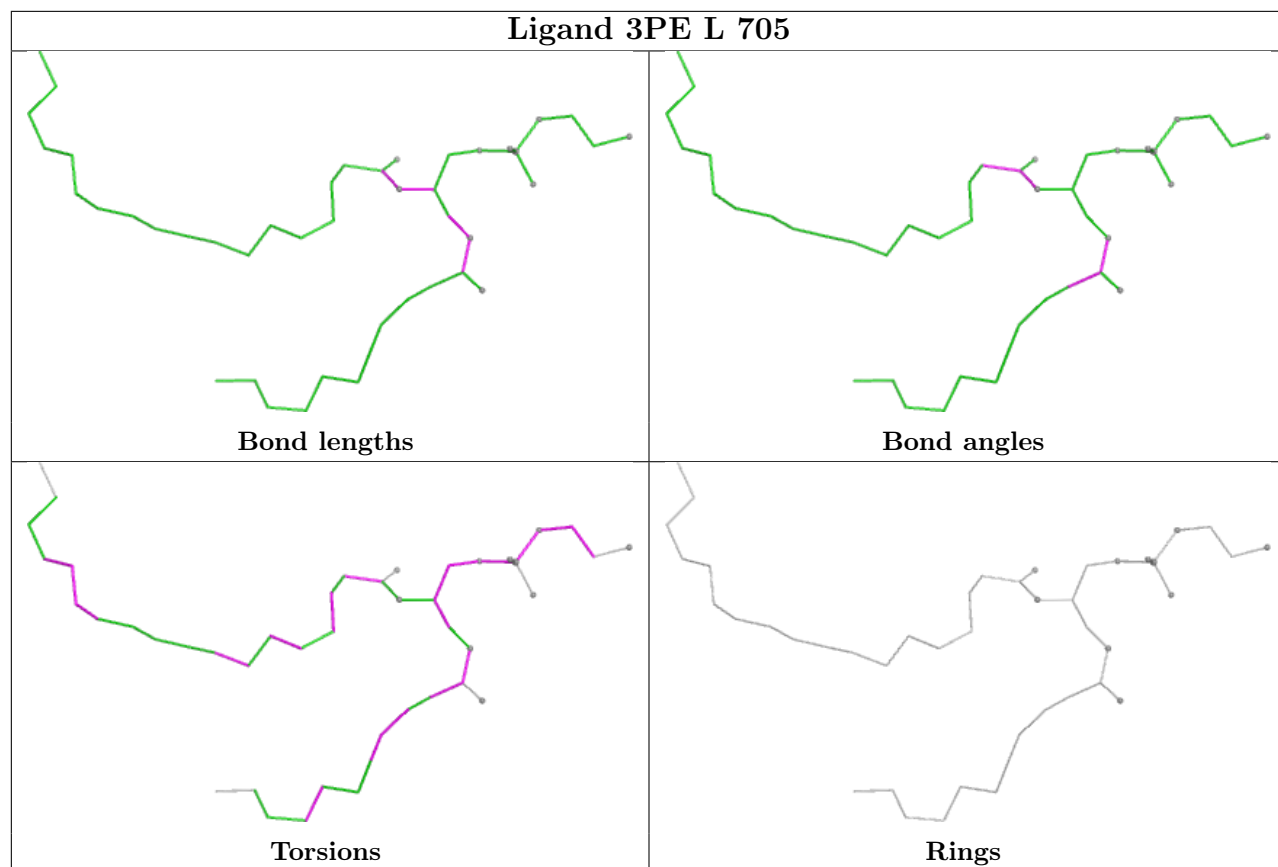


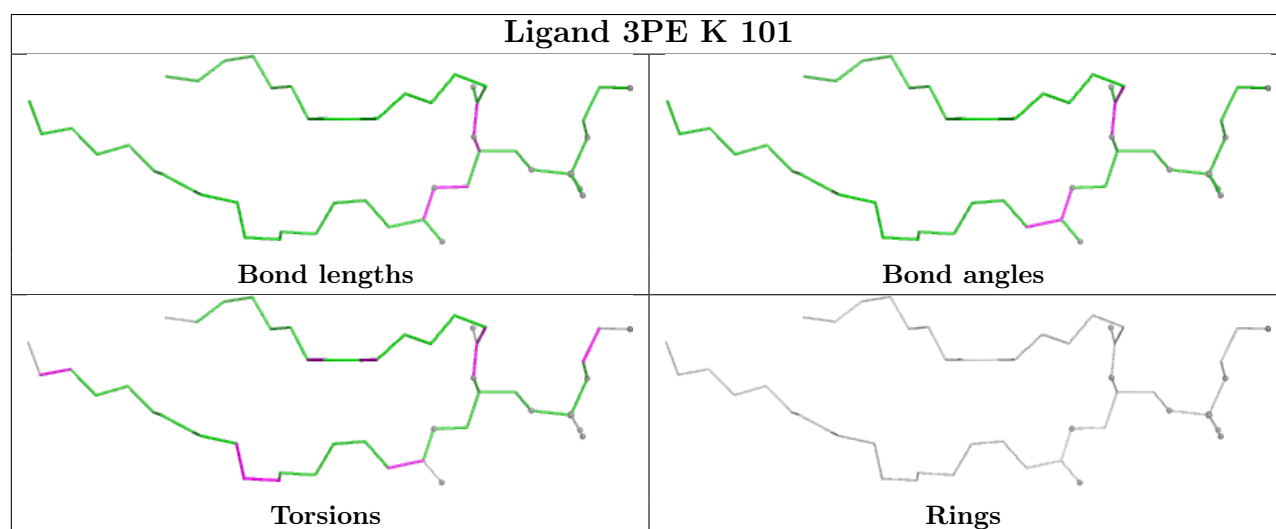
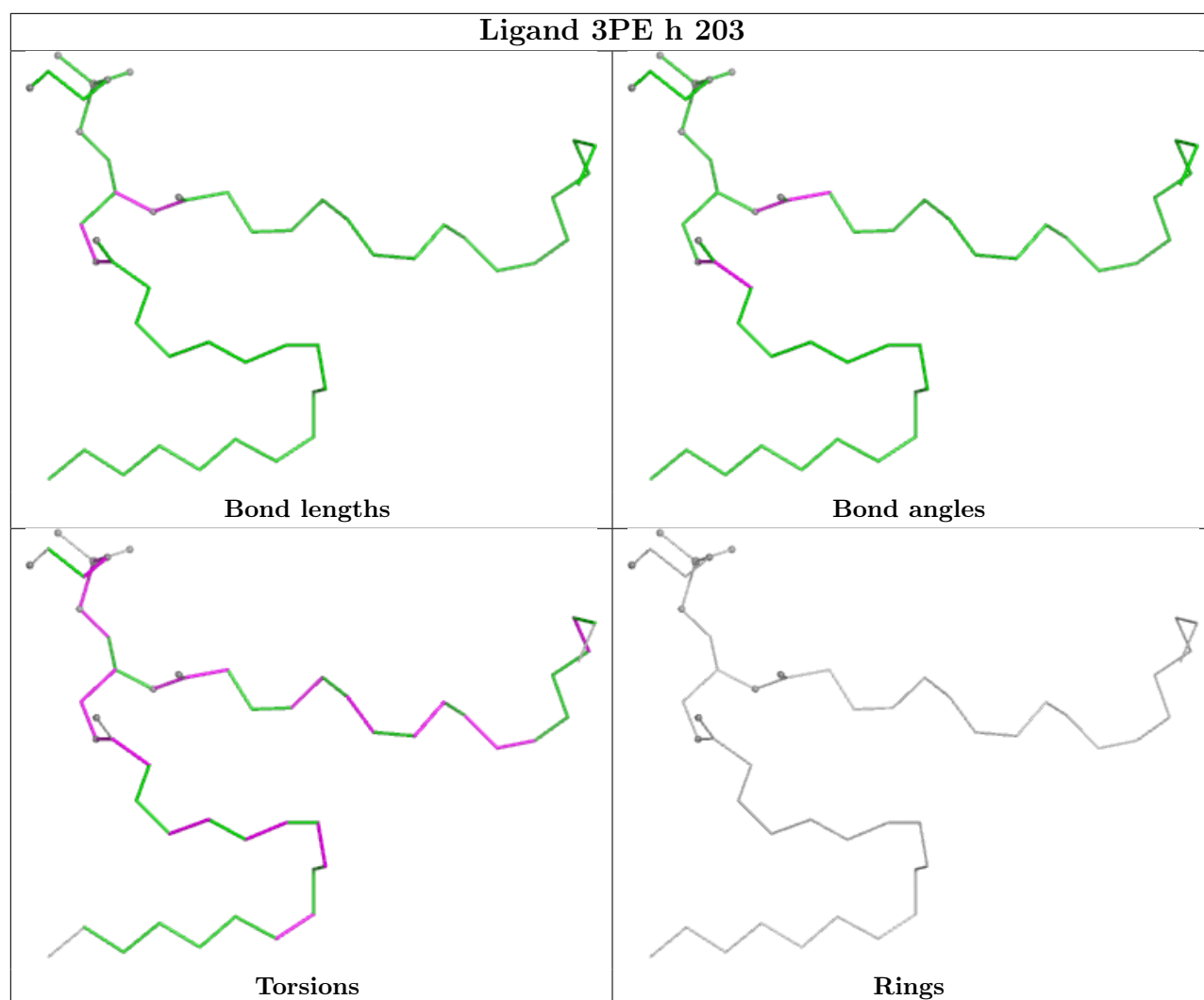


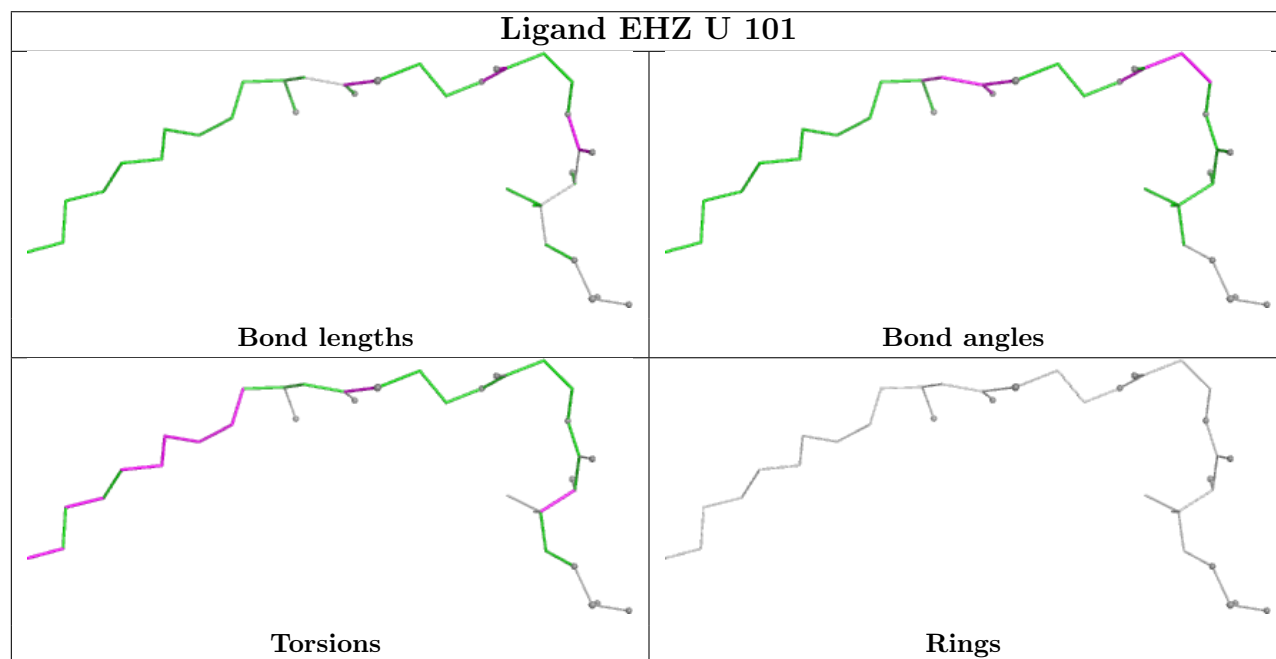
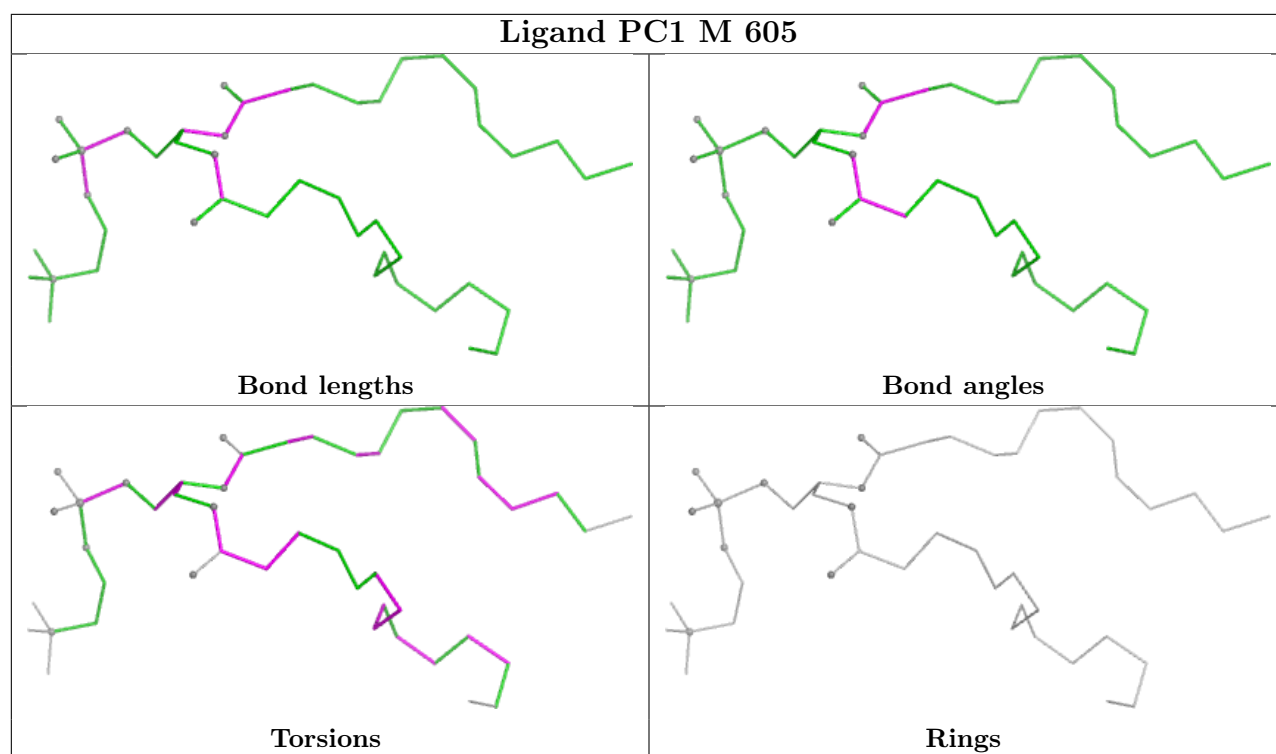


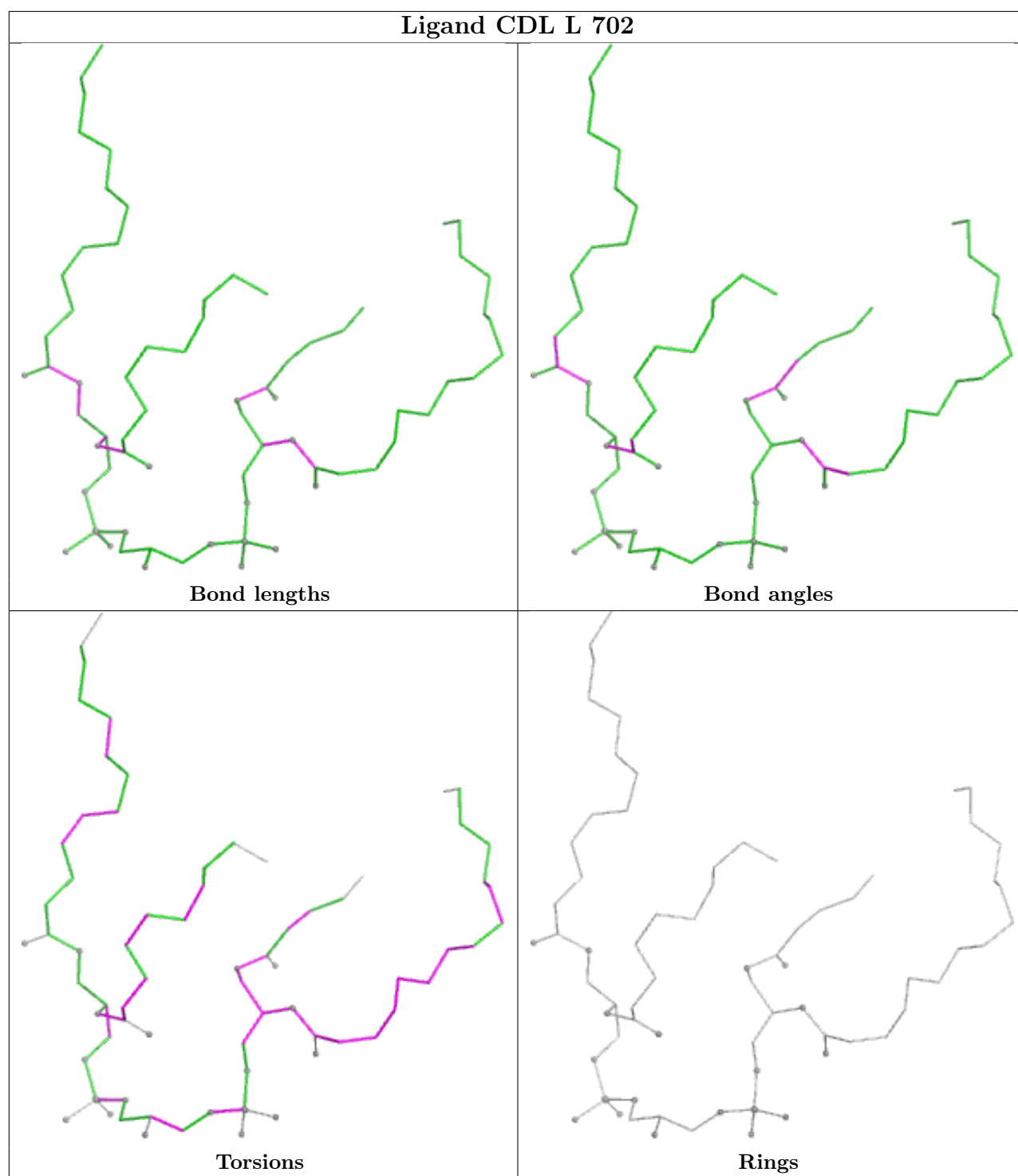


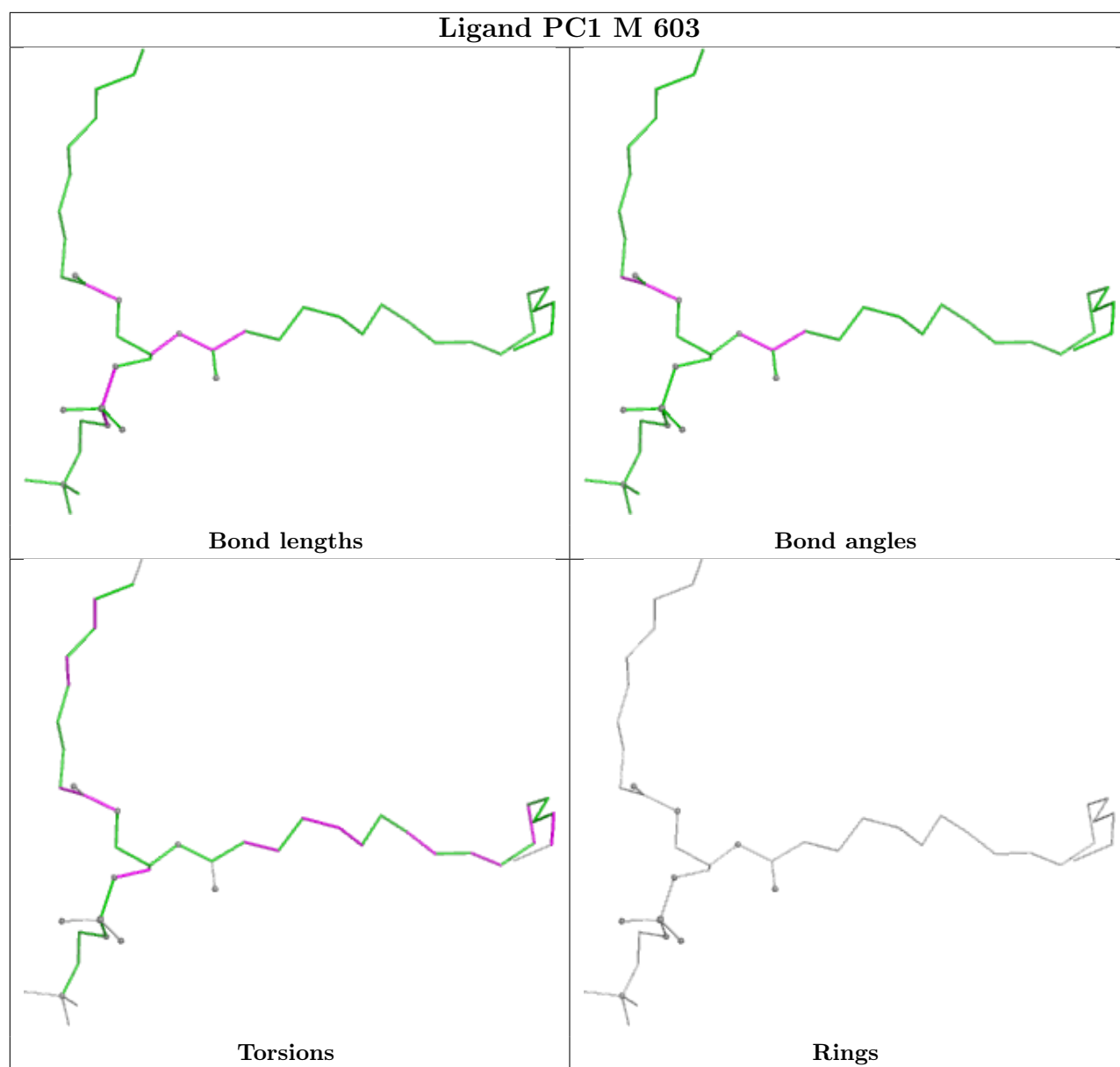


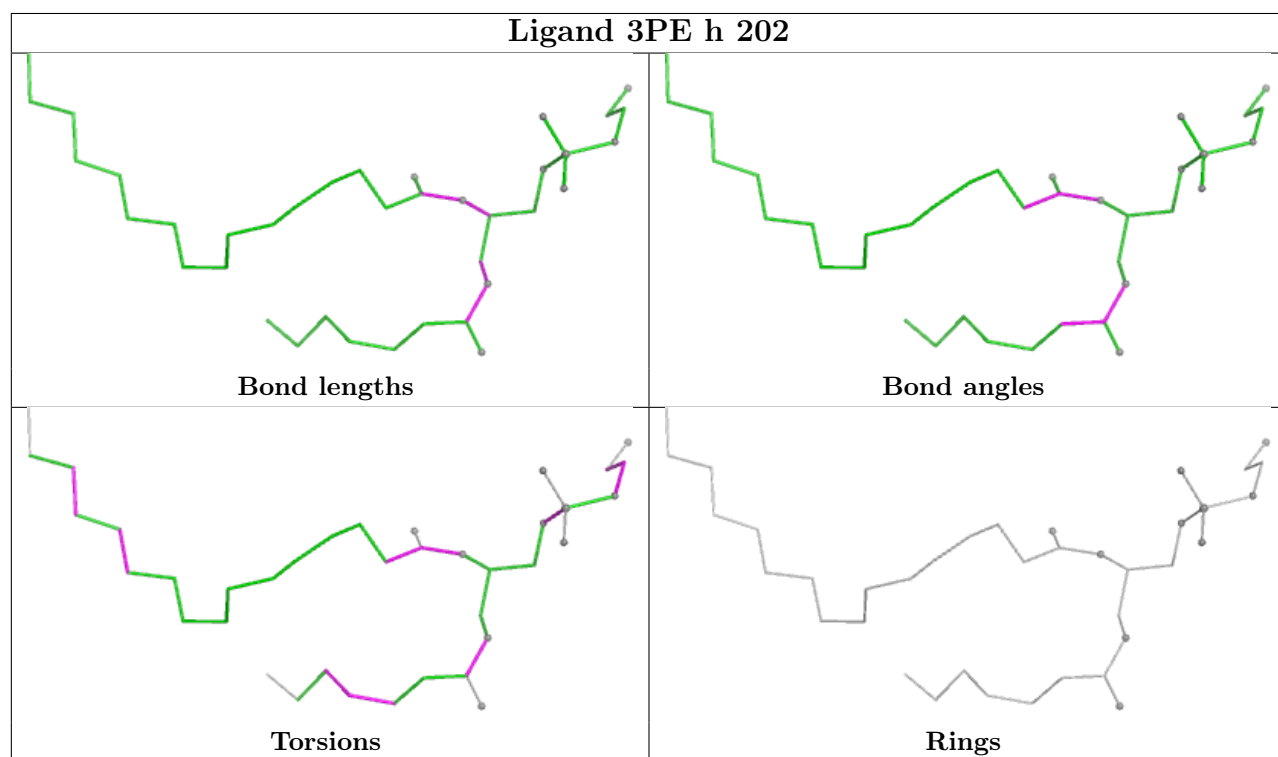
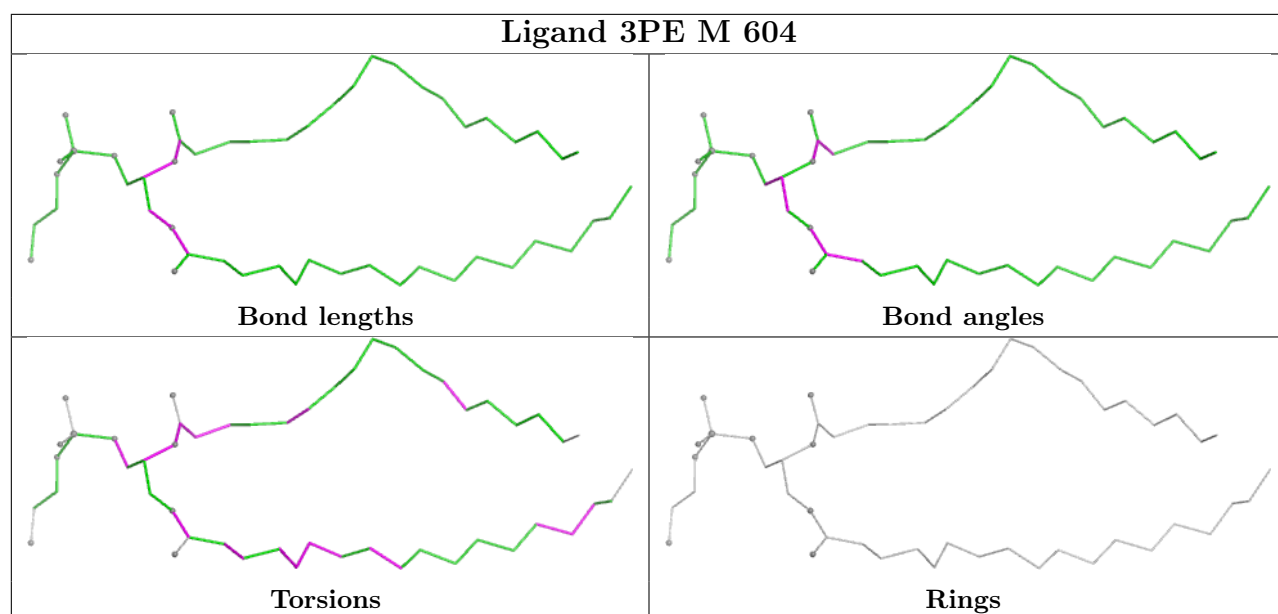


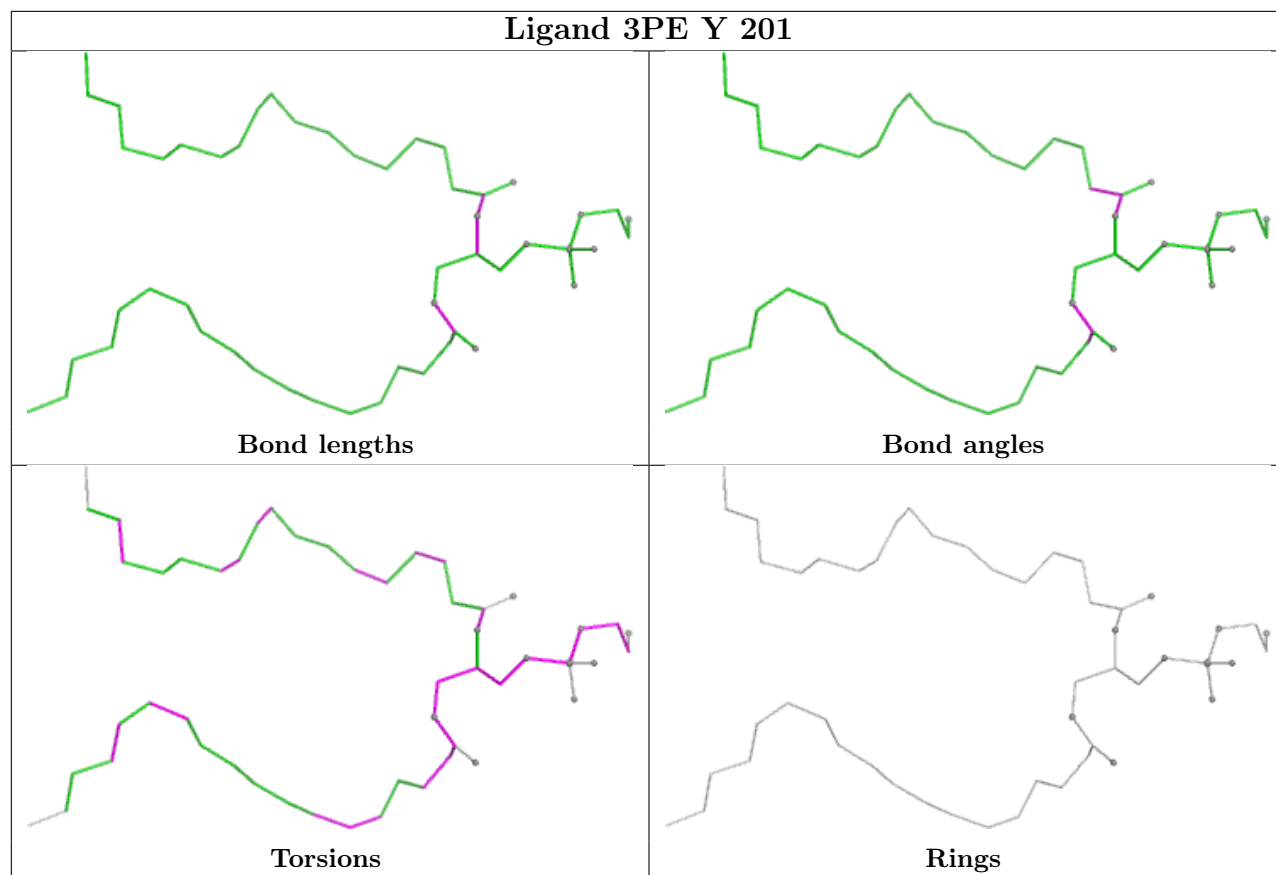


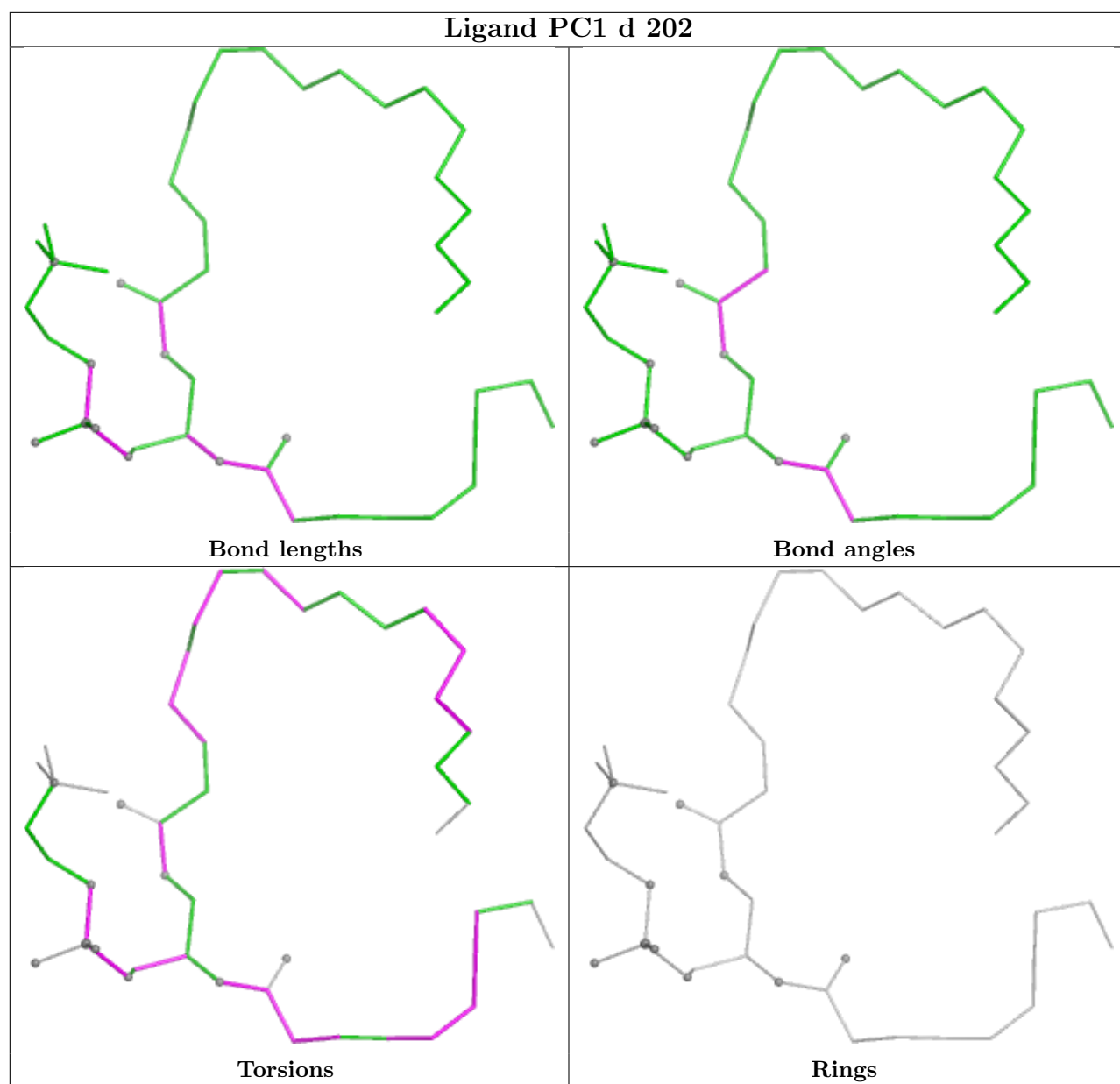


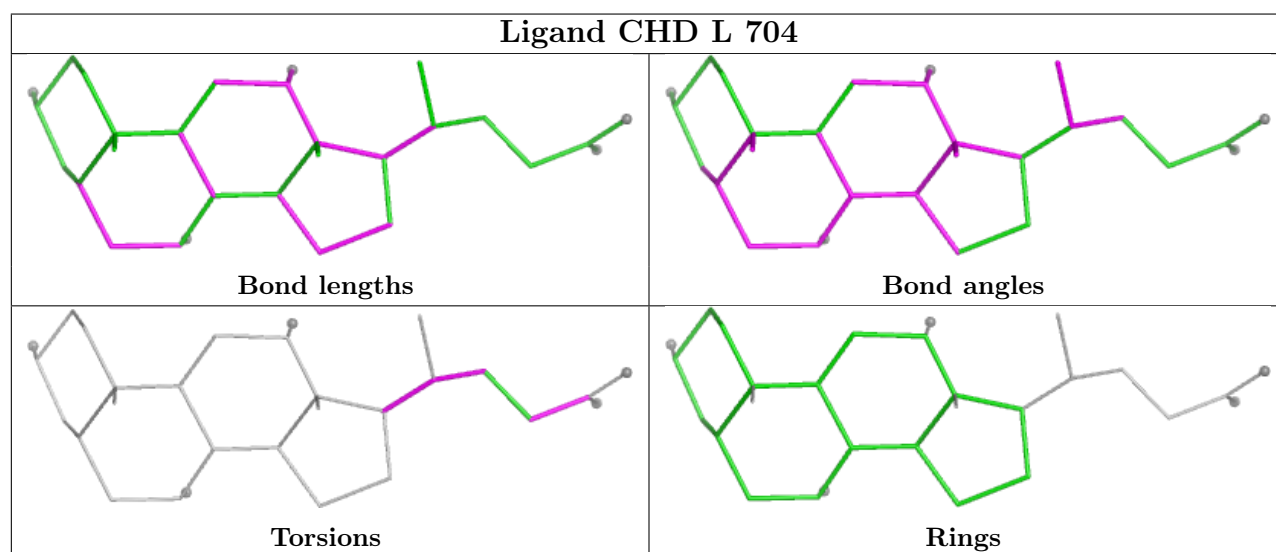
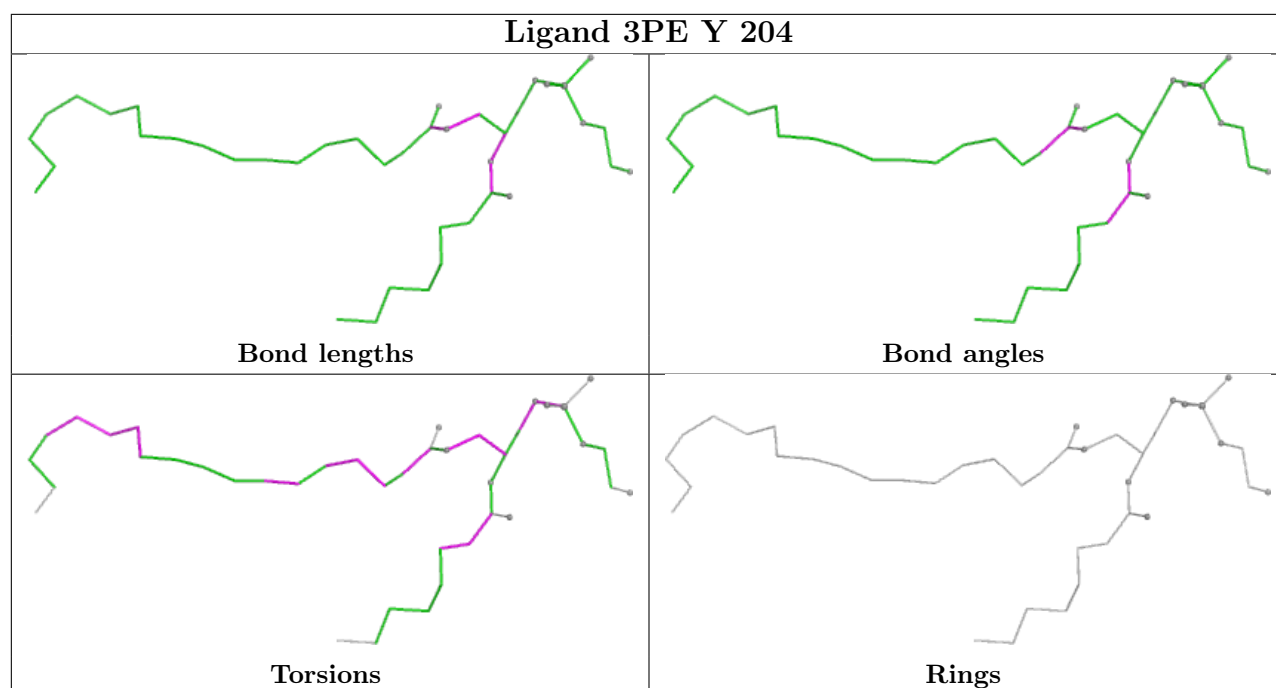


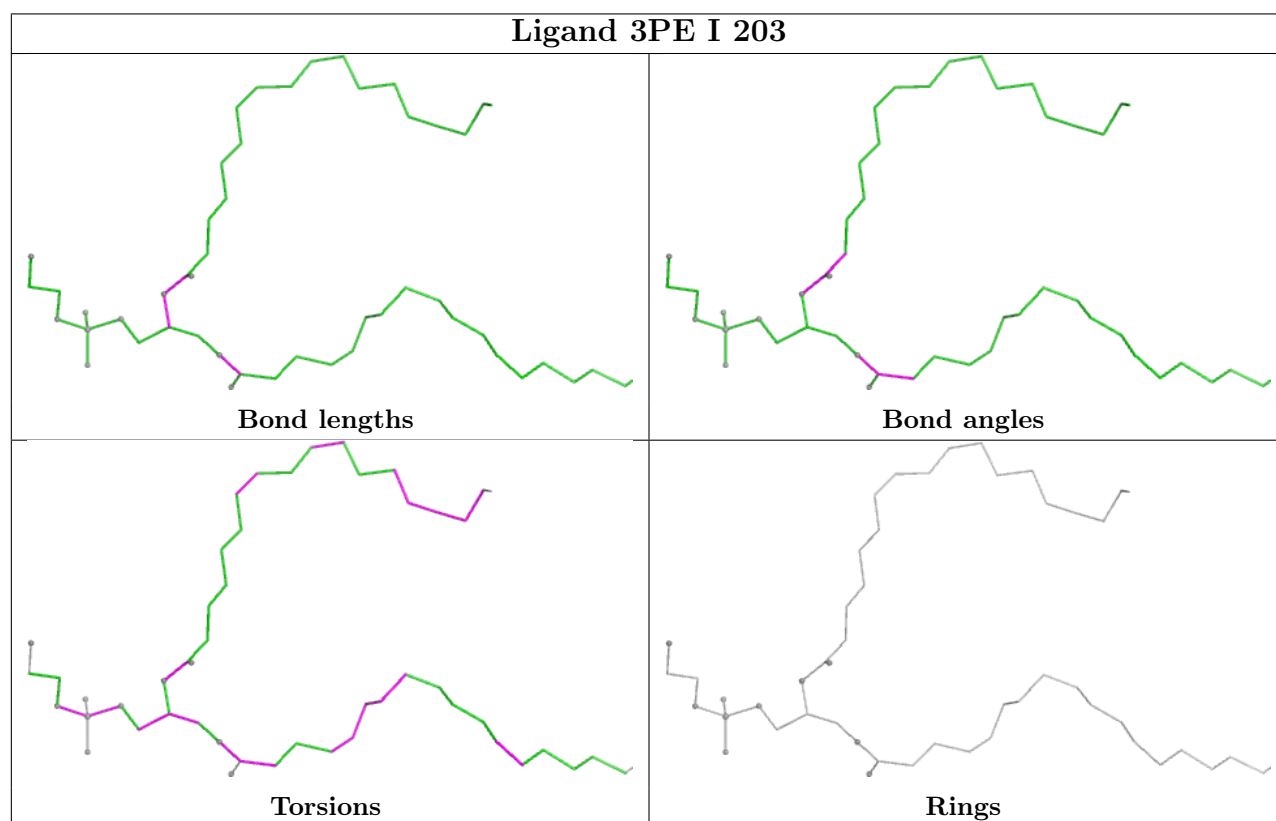
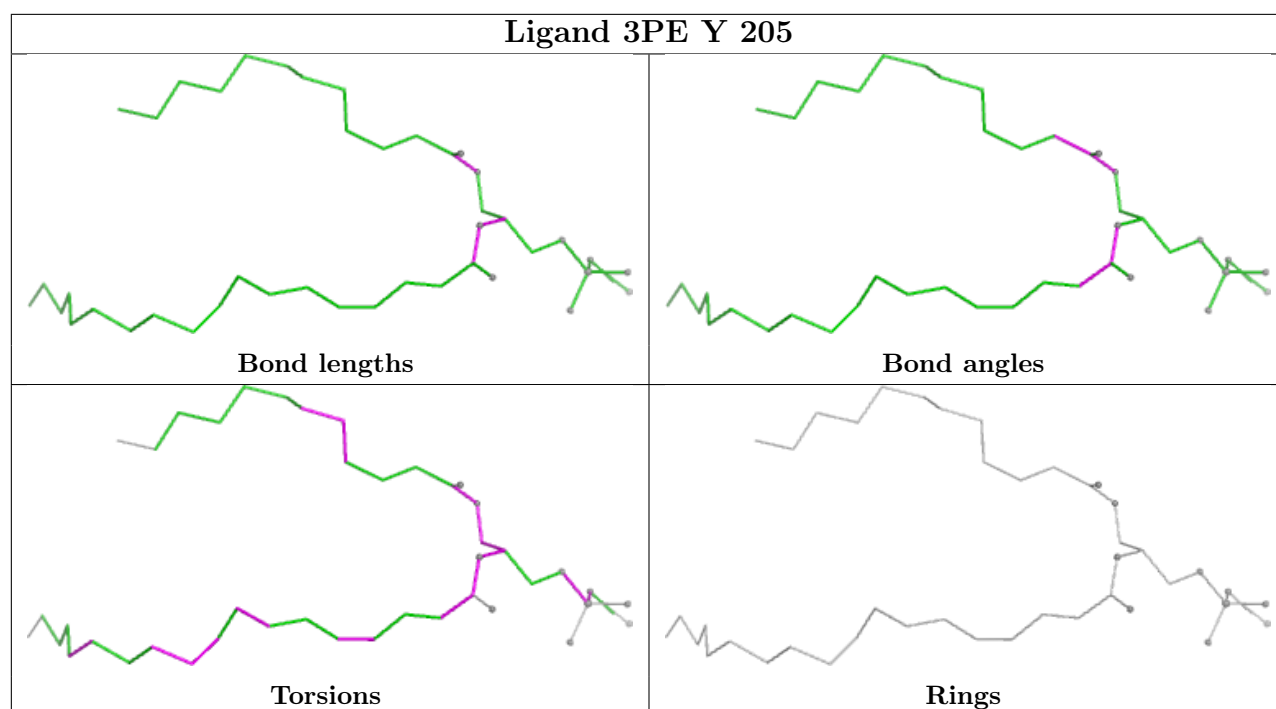


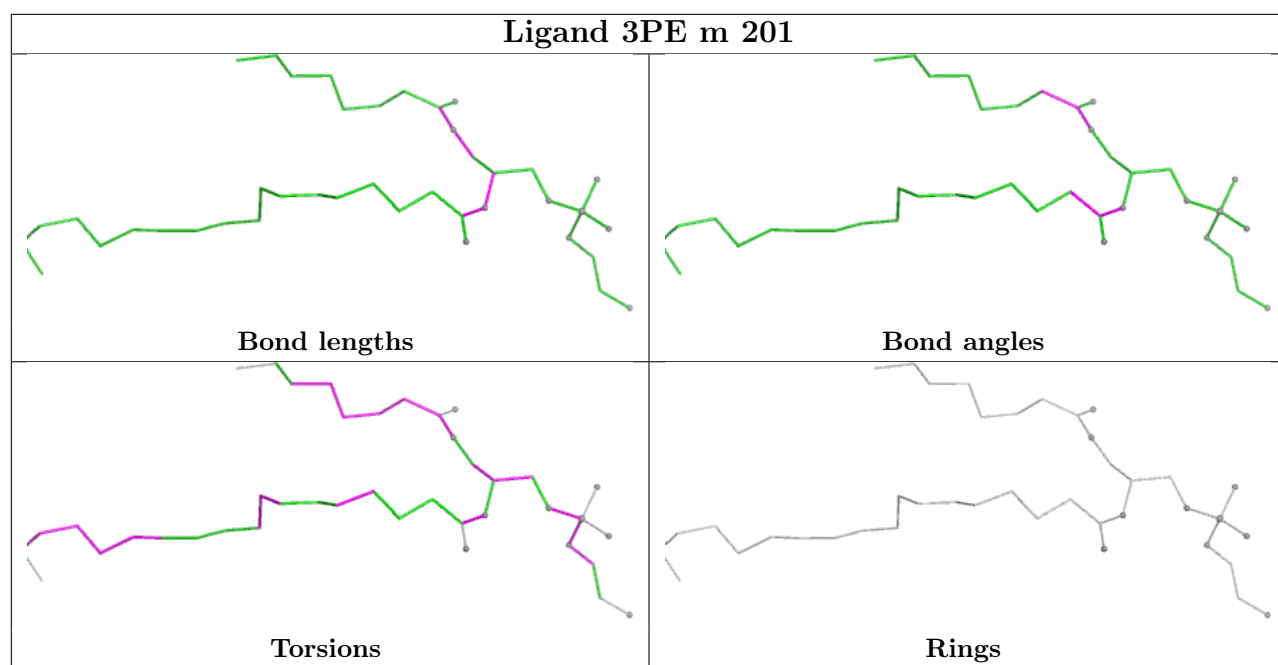


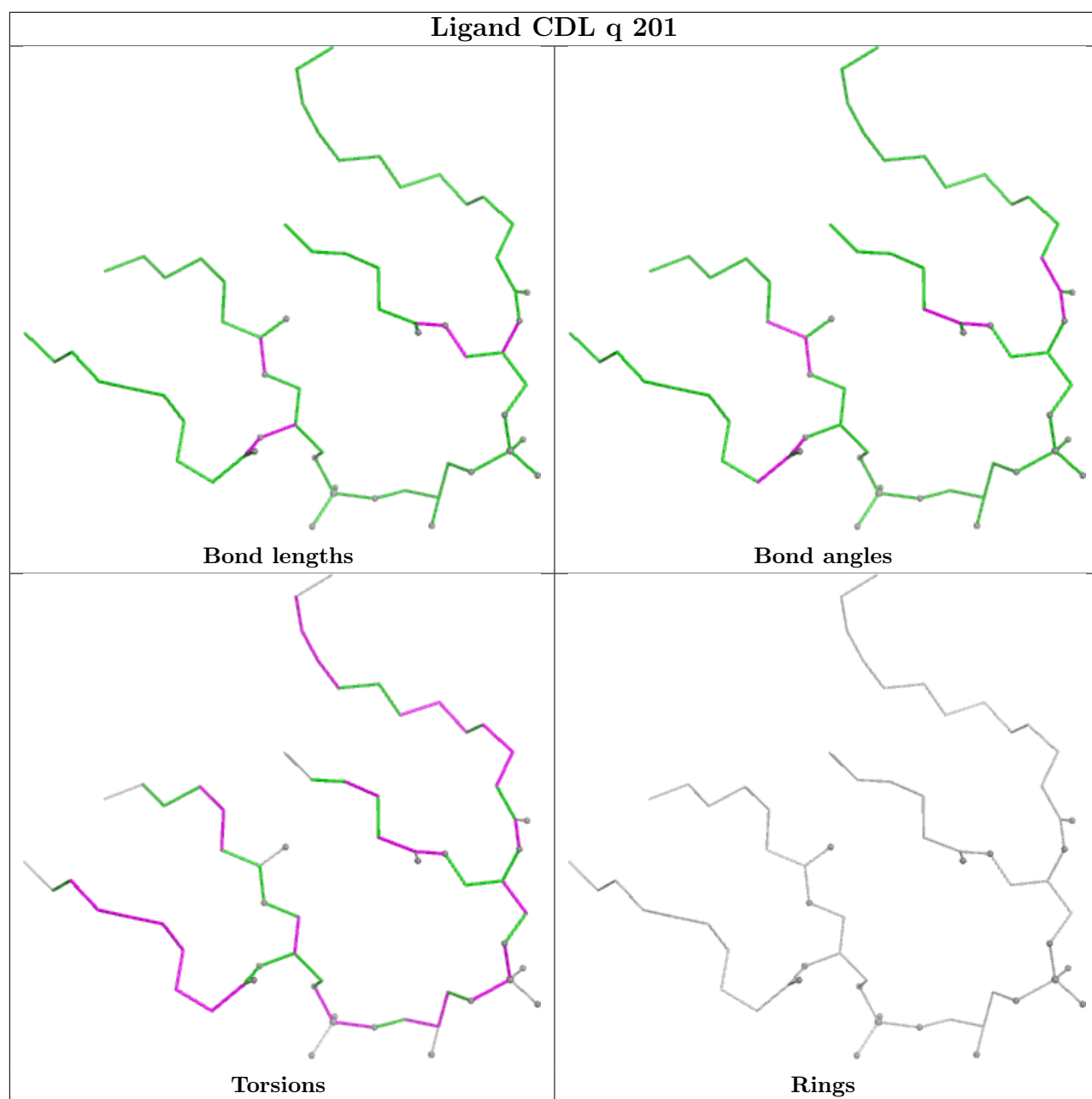


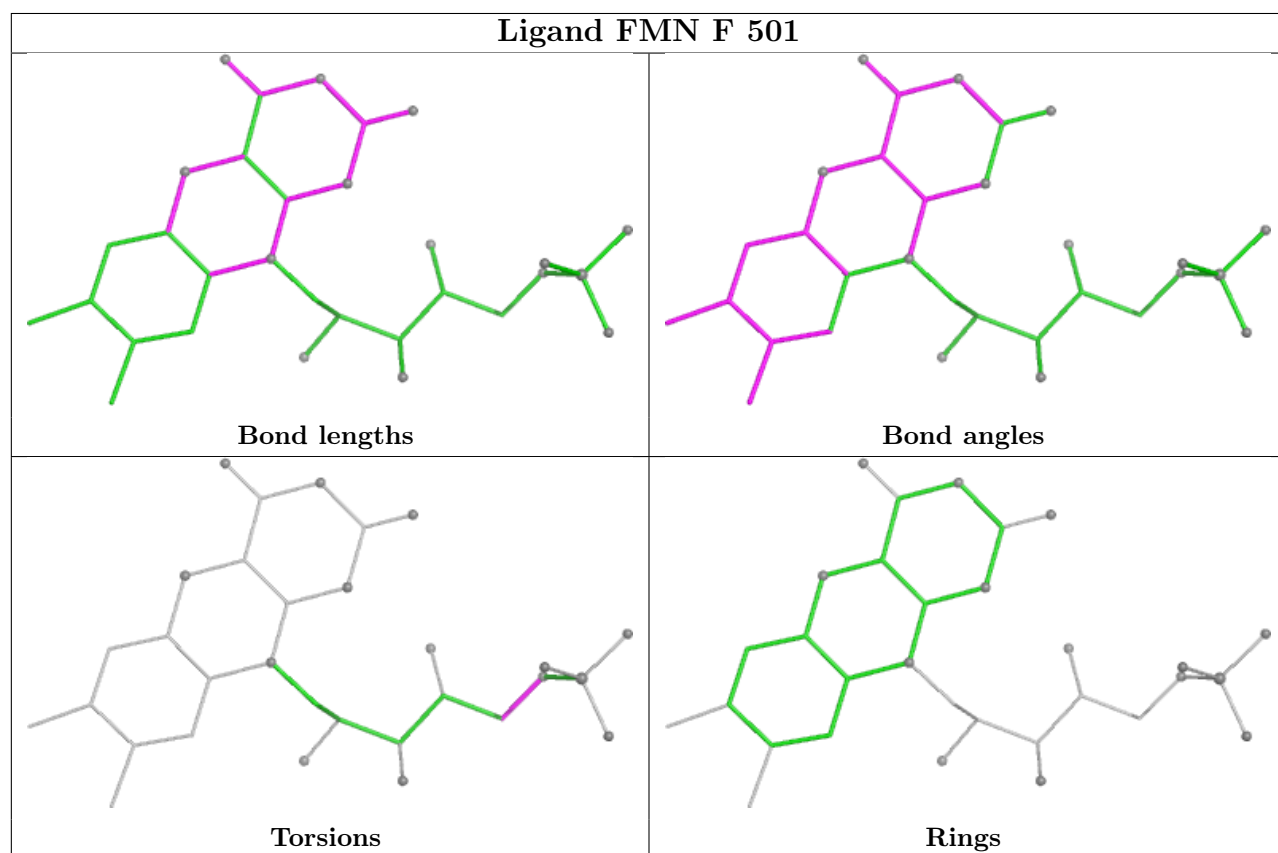
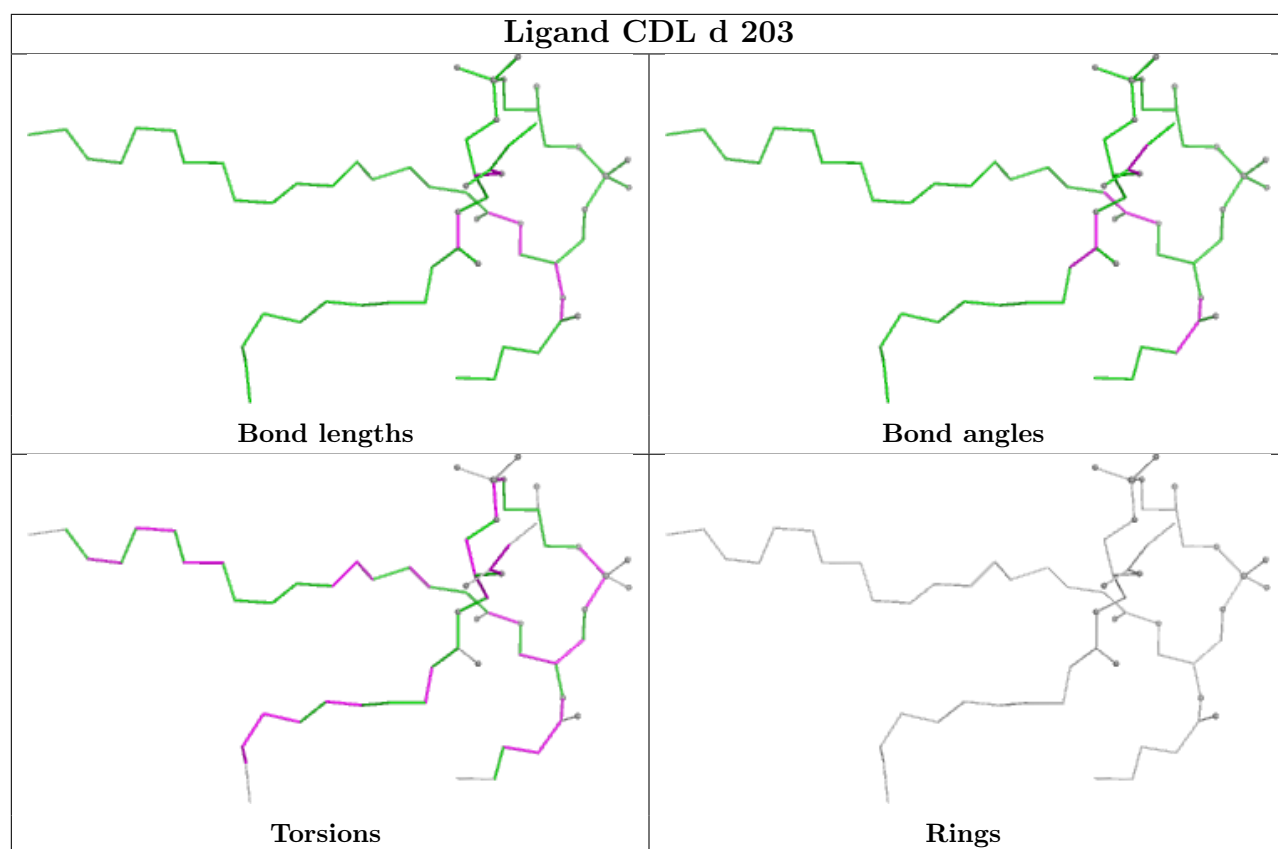


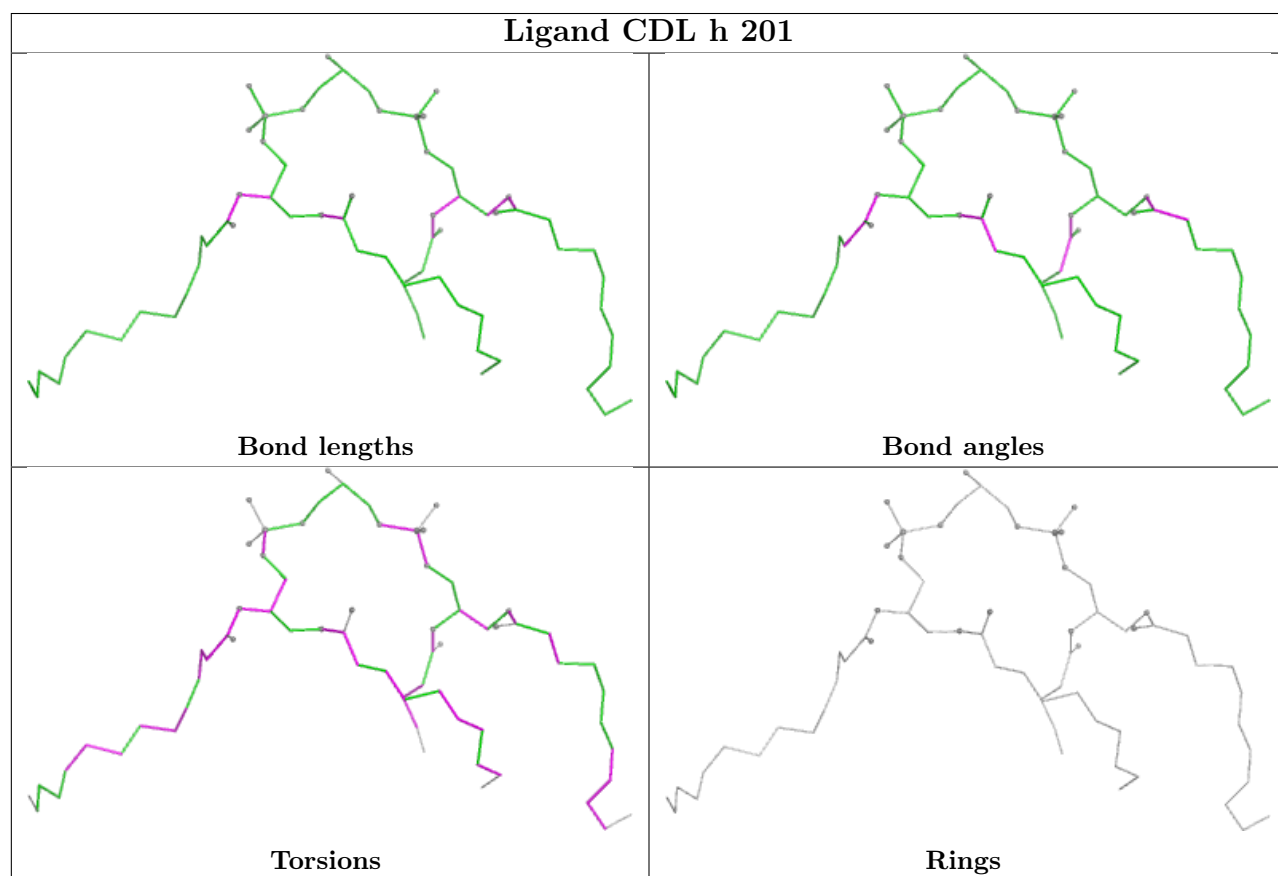
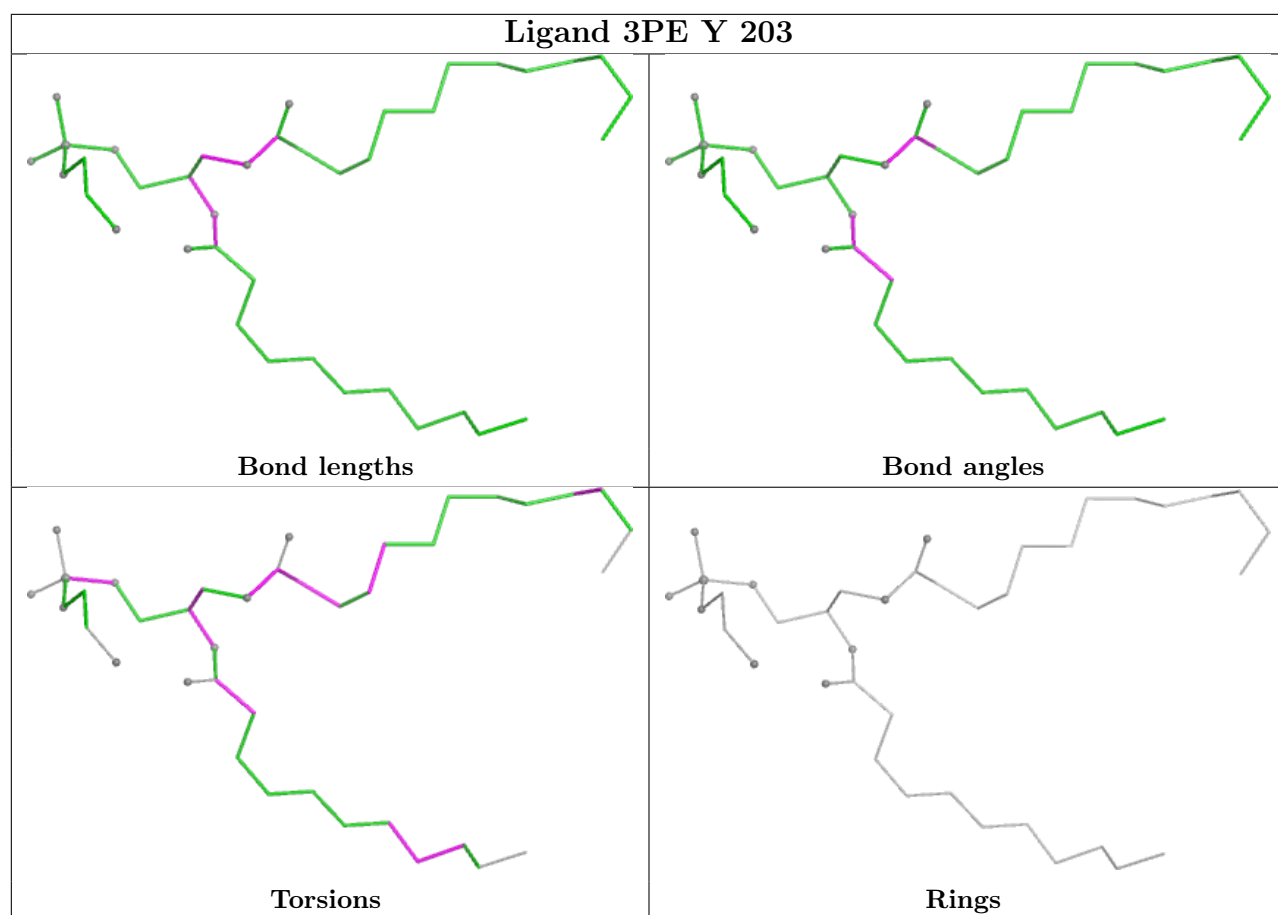


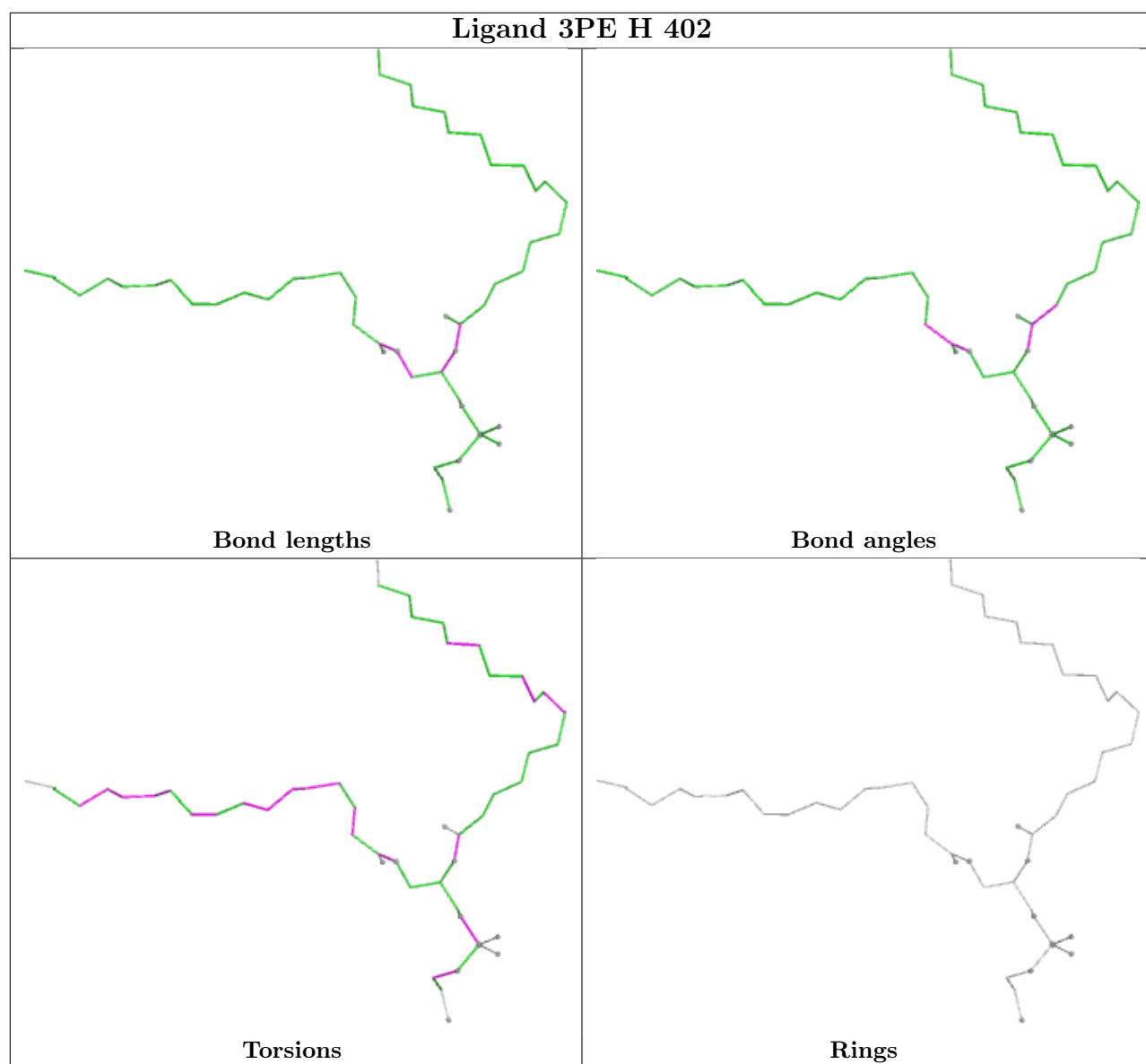


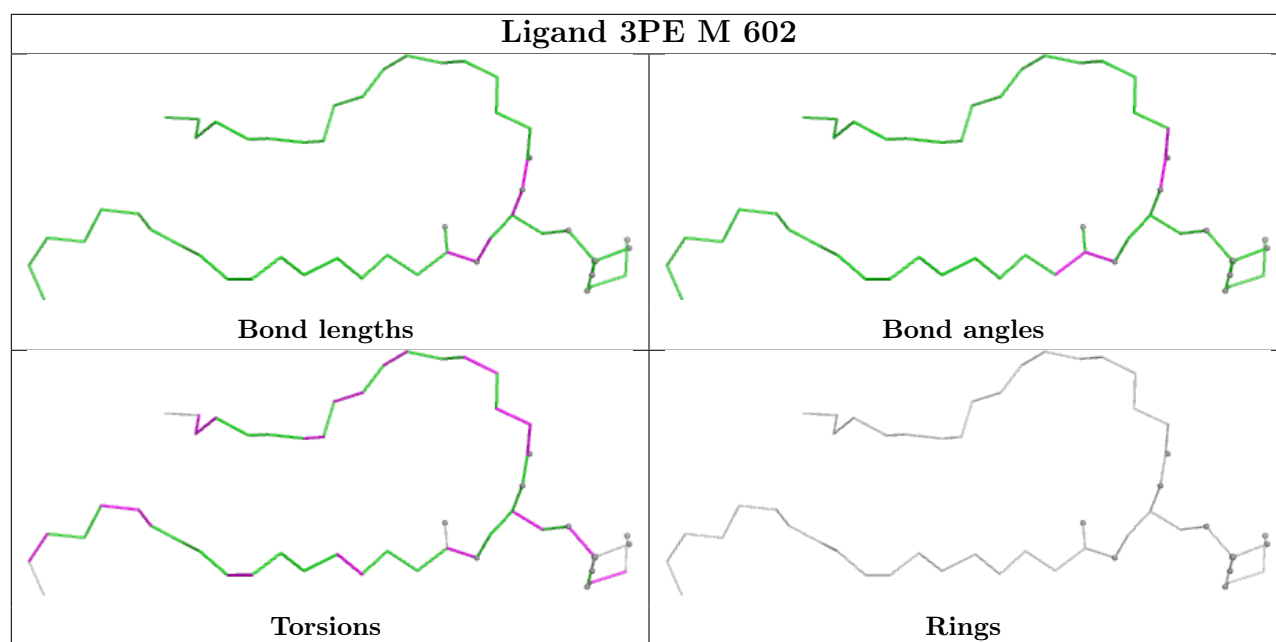












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

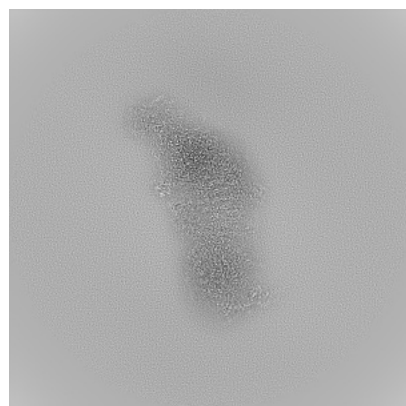
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55033. These allow visual inspection of the internal detail of the map and identification of artifacts.

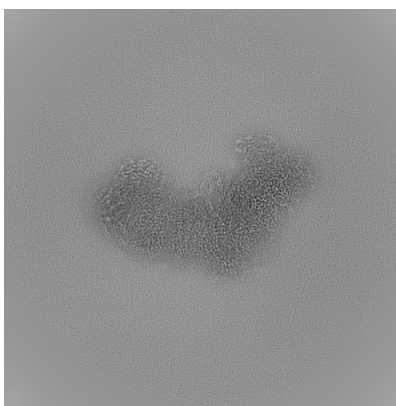
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

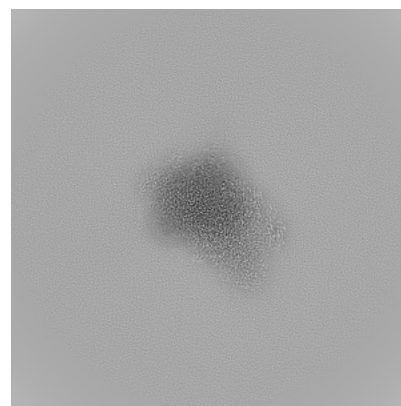
6.1.1 Primary map



X

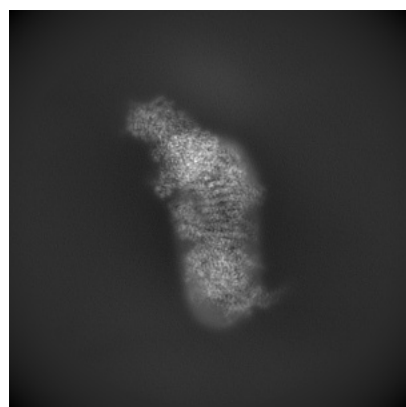


Y

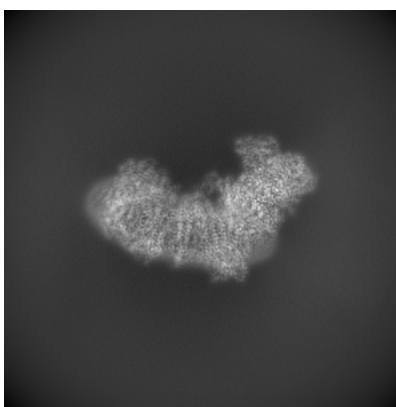


Z

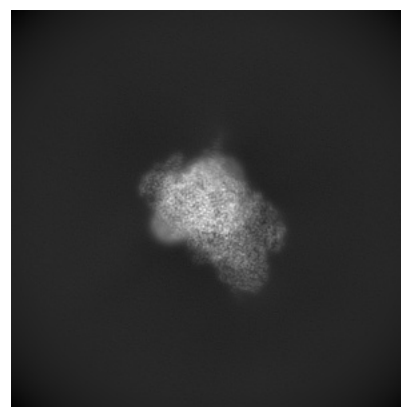
6.1.2 Raw map



X



Y

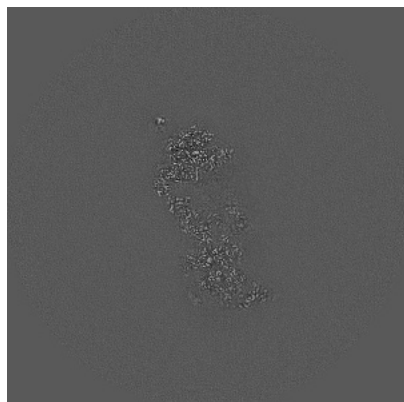


Z

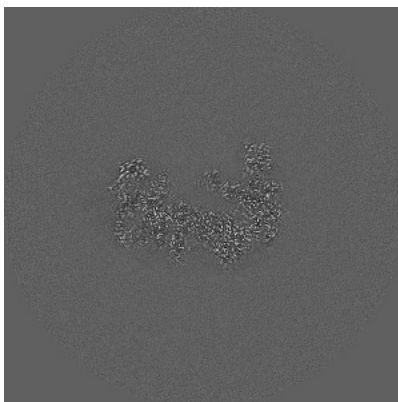
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

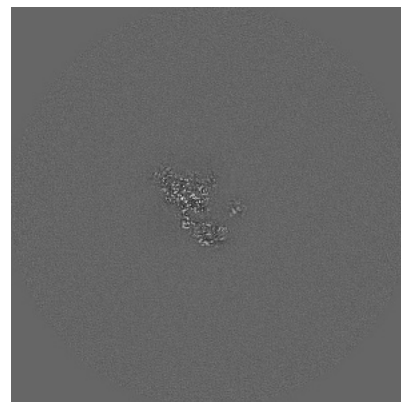
6.2.1 Primary map



X Index: 320

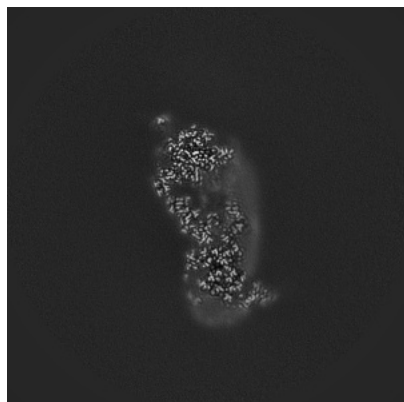


Y Index: 320

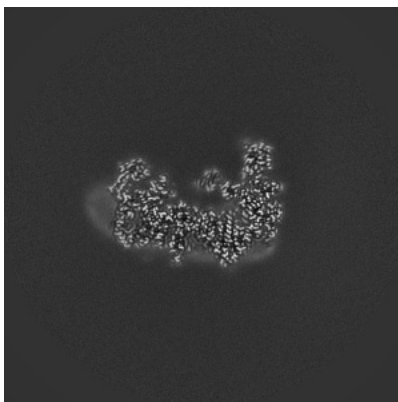


Z Index: 320

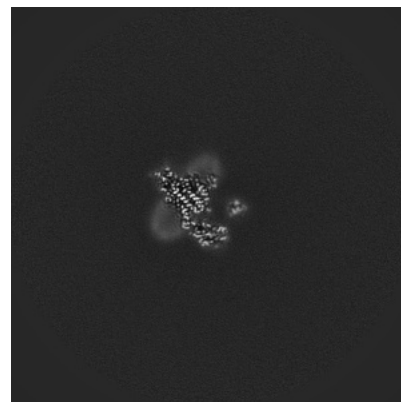
6.2.2 Raw map



X Index: 320



Y Index: 320

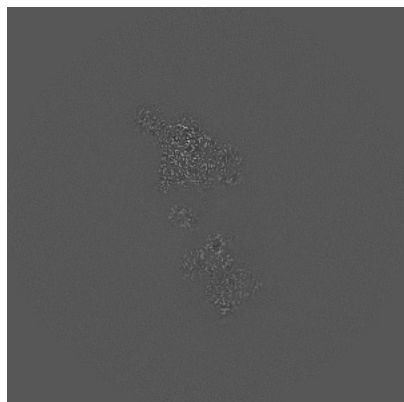


Z Index: 320

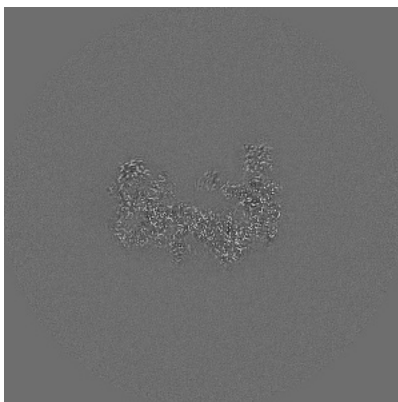
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

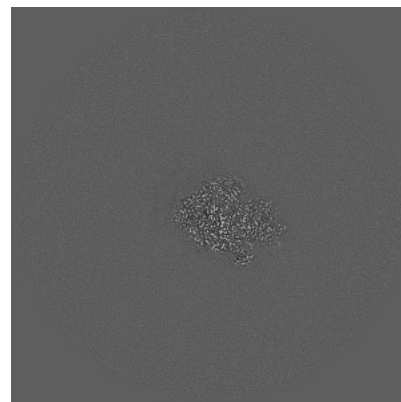
6.3.1 Primary map



X Index: 342

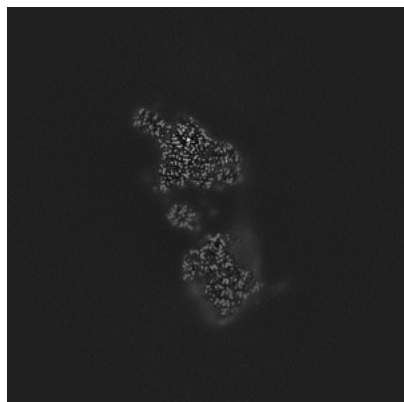


Y Index: 321

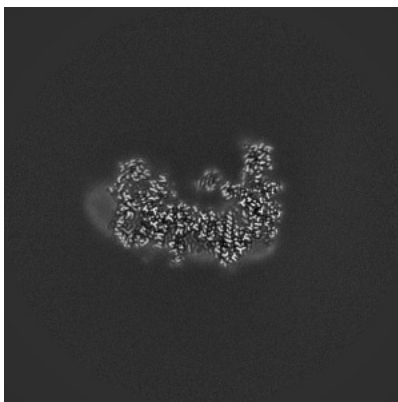


Z Index: 407

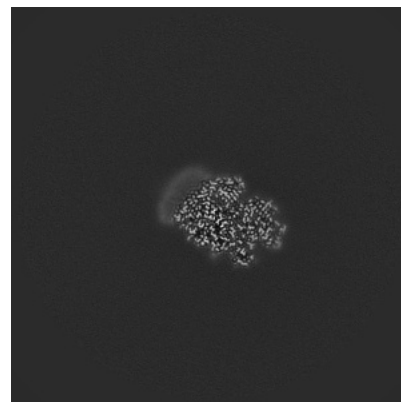
6.3.2 Raw map



X Index: 341



Y Index: 321

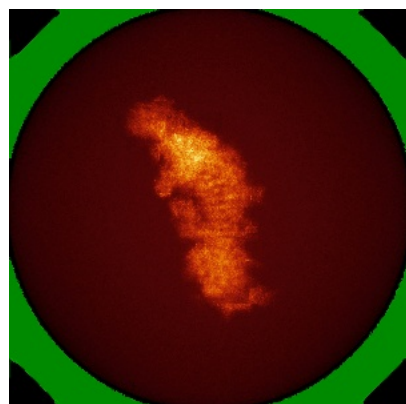


Z Index: 408

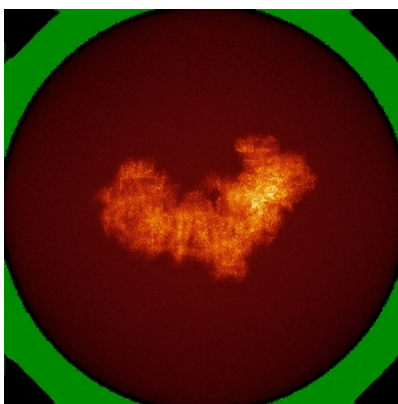
The images above show the largest variance slices of the map in three orthogonal directions.

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

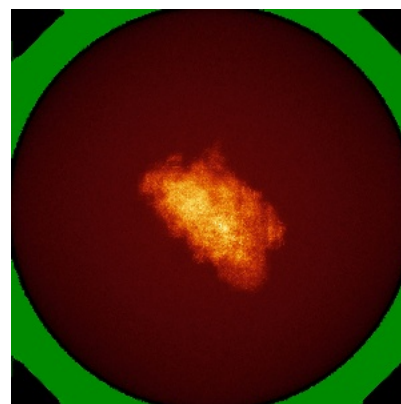
6.4.1 Primary map



X



Y

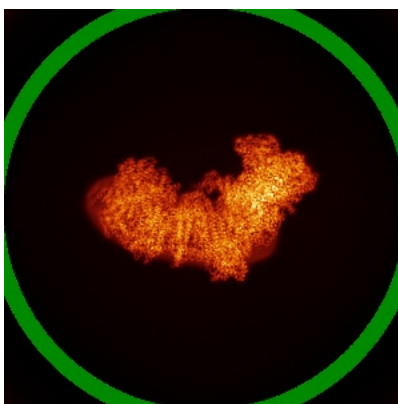


Z

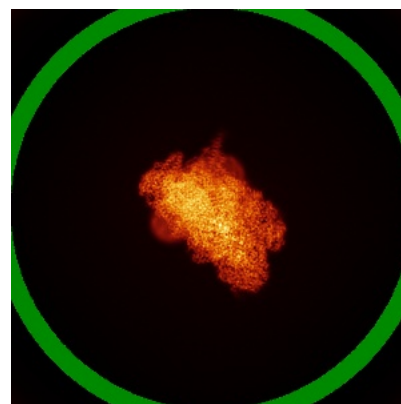
6.4.2 Raw map



X



Y

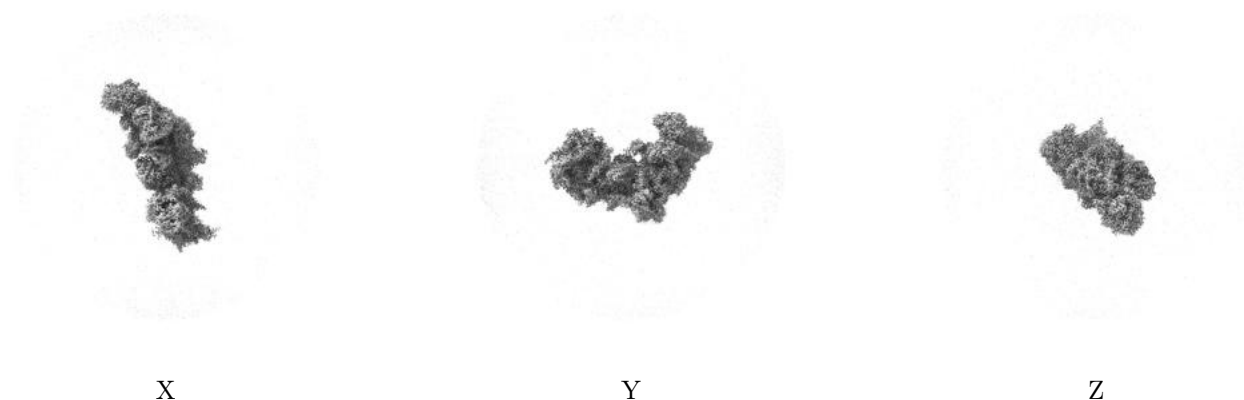


Z

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.

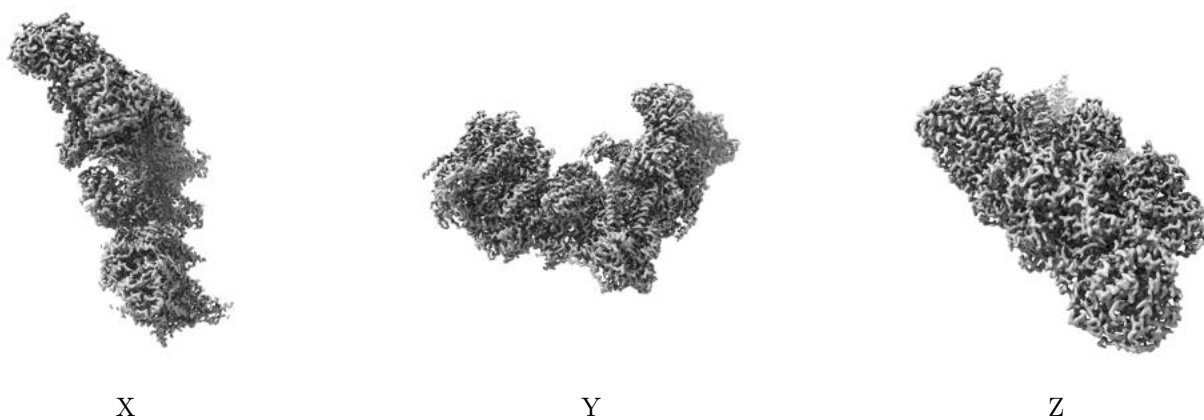
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

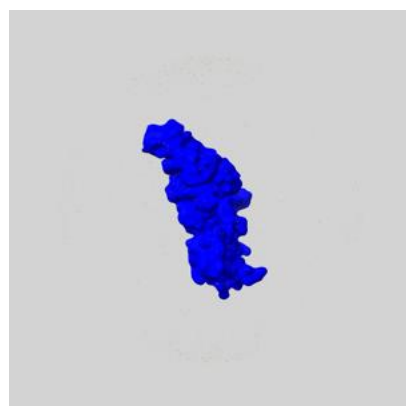
6.6 Mask visualisation [i](#)

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

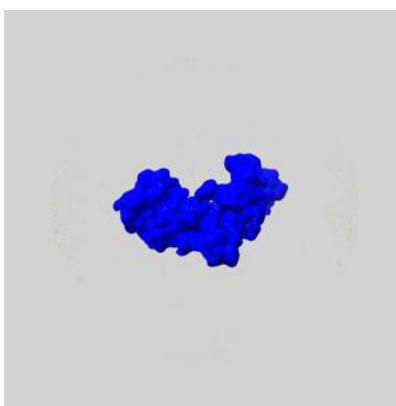
A mask typically either:

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

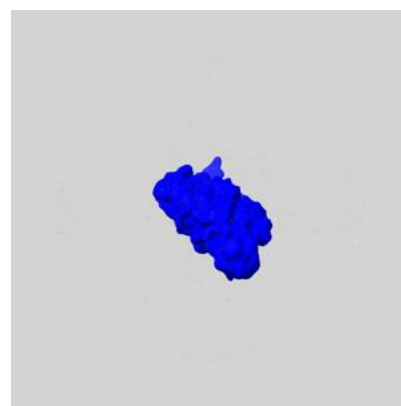
6.6.1 emd_55033_msk_1.map [i](#)



X



Y

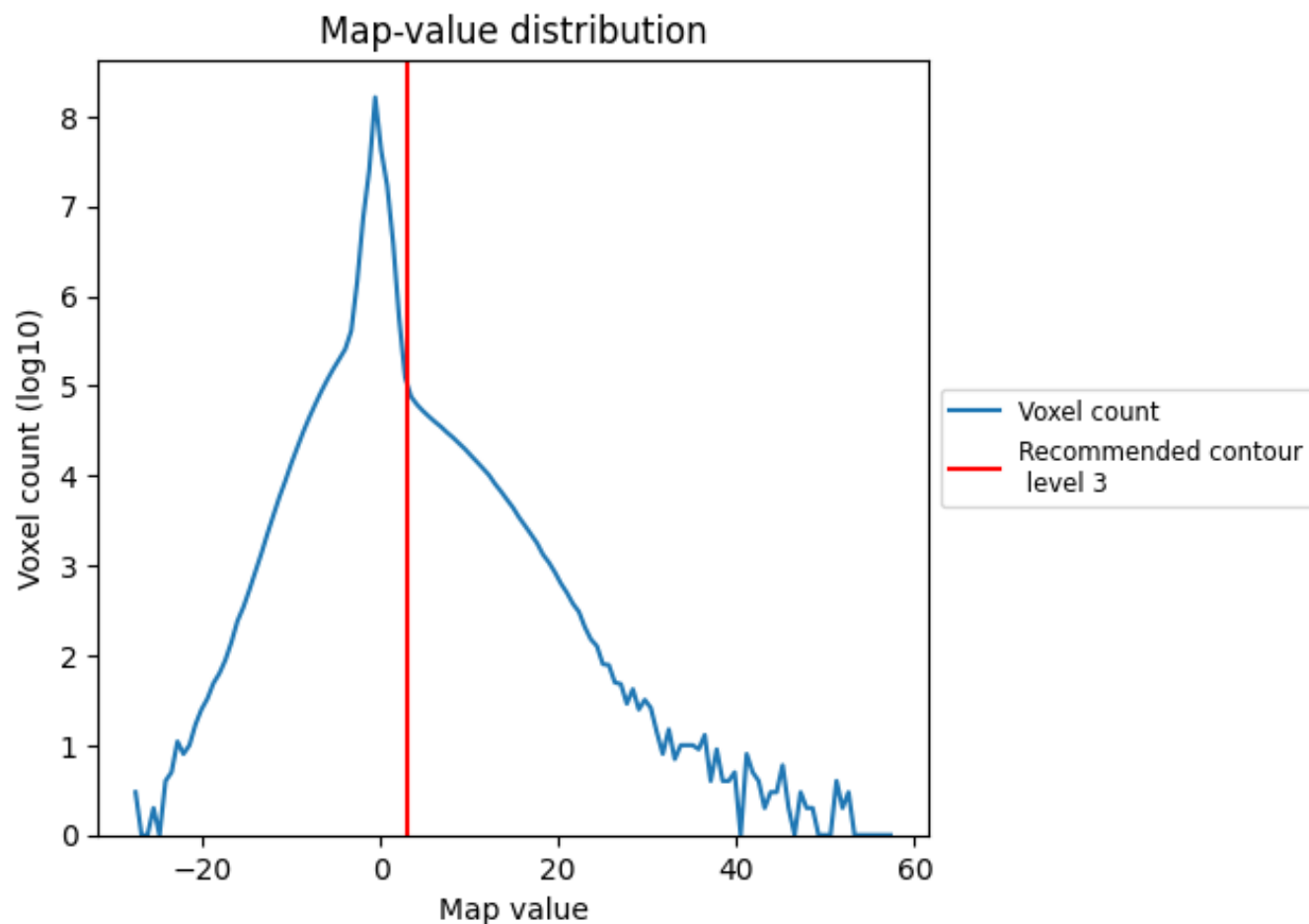


Z

7 Map analysis [i](#)

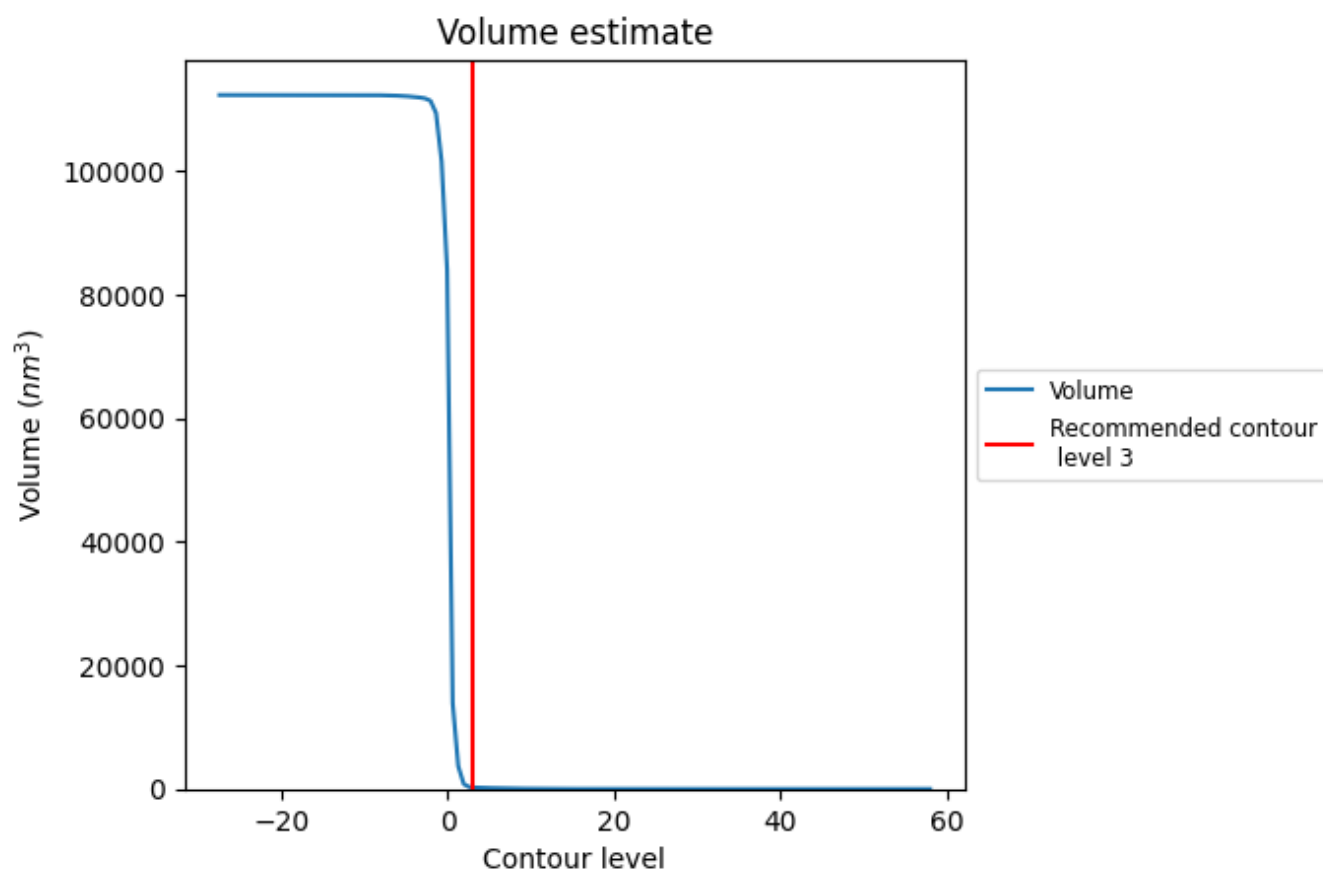
This section contains the results of statistical analysis of the map.

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.

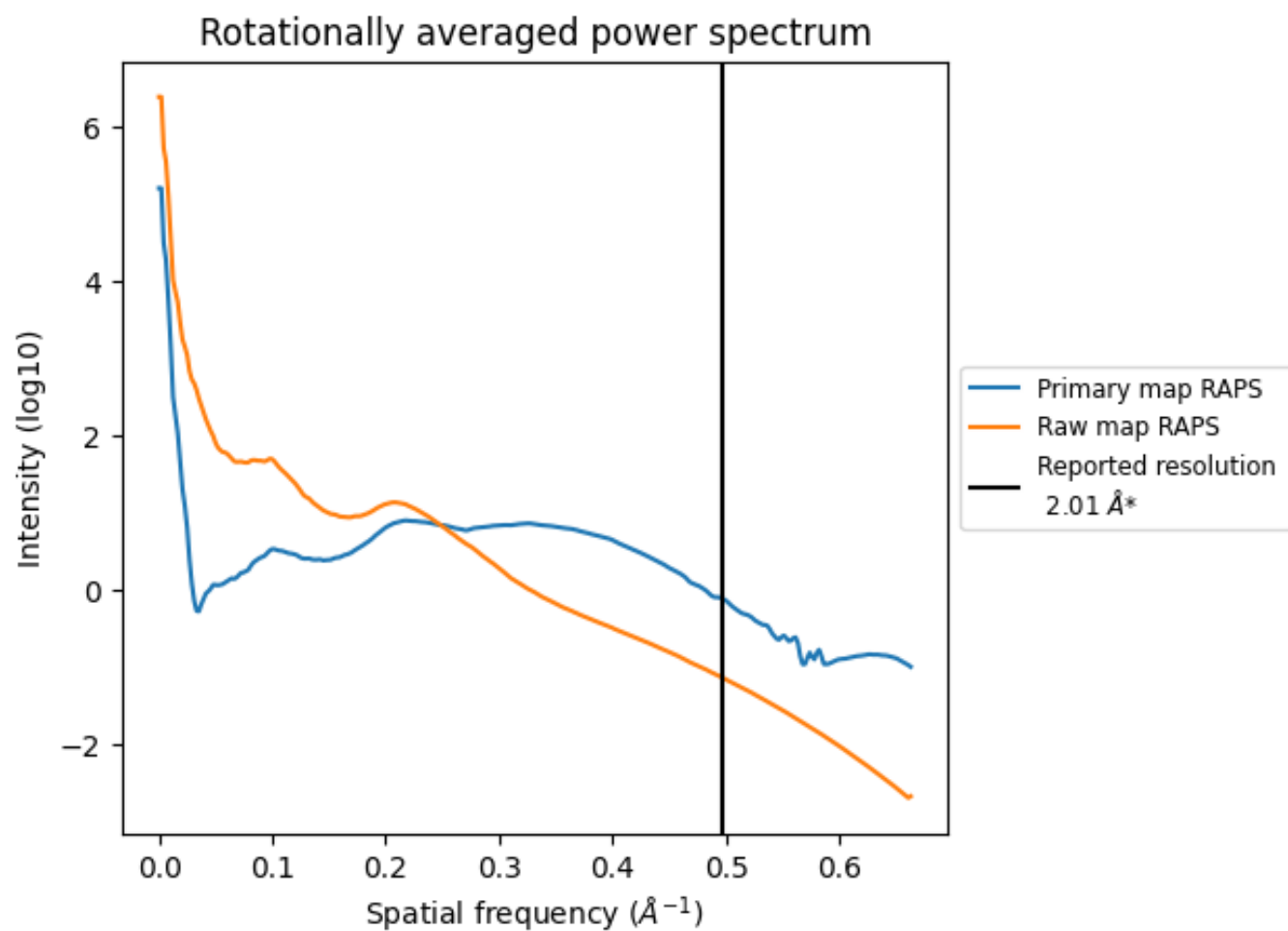
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm^3 ; this corresponds to an approximate mass of 234 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 ⓘ

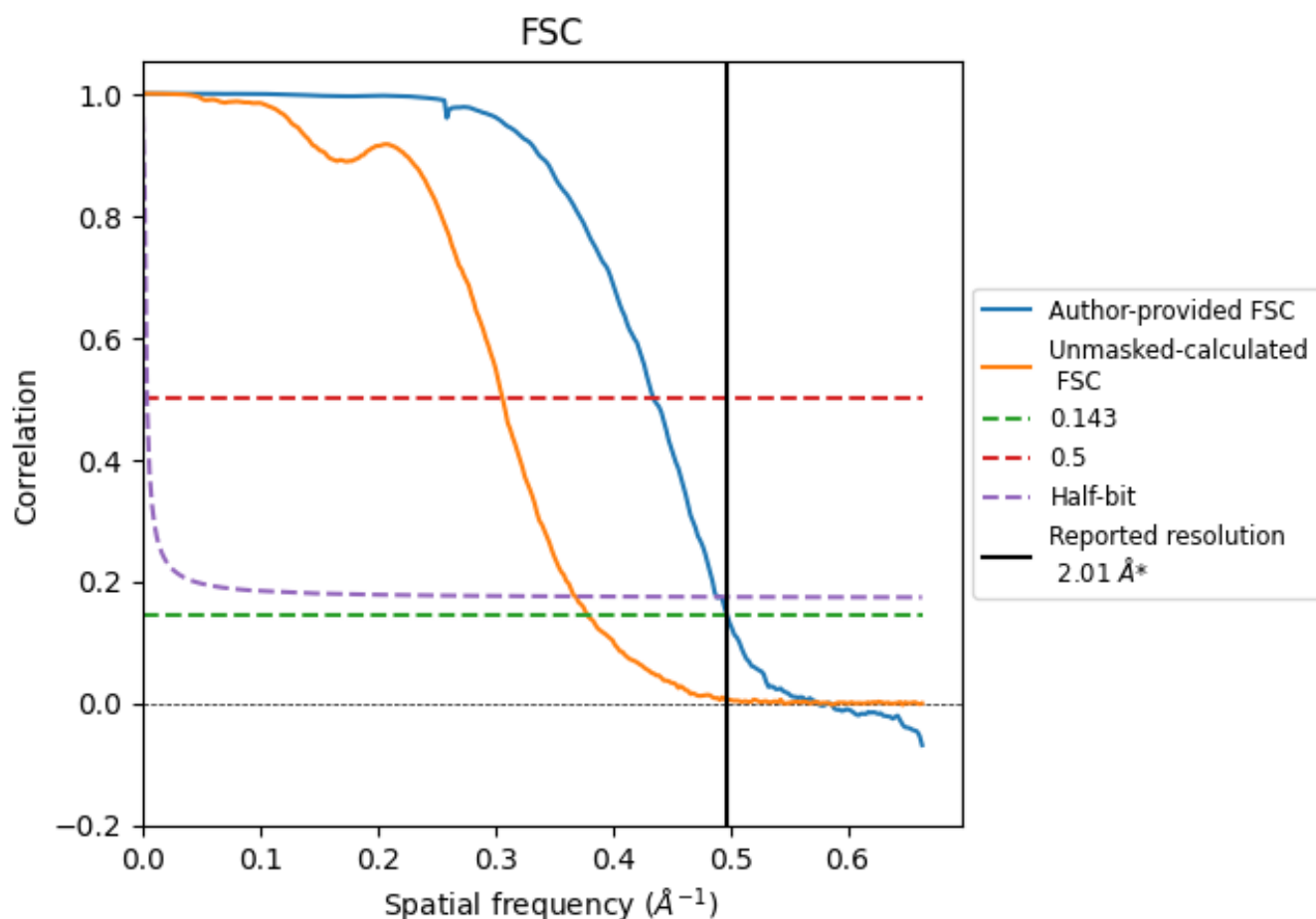


*Reported resolution corresponds to spatial frequency of 0.498 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.498 \AA^{-1}

8.2 Resolution estimates [i](#)

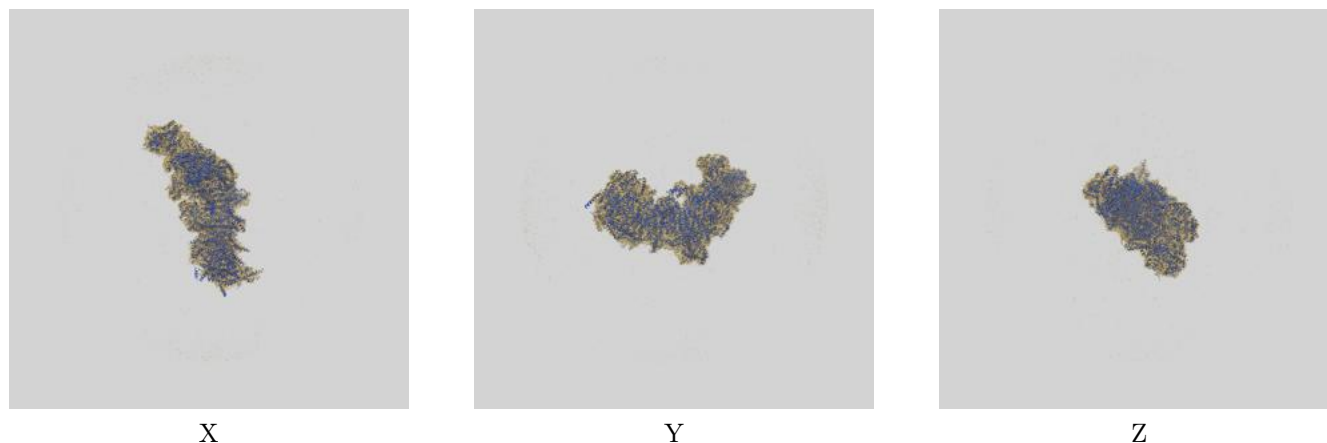
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.30	2.05
Unmasked-calculated*	2.64	3.26	2.71

*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 2.64 differs from the reported value 2.01 by more than 10 %

9 Map-model fit [i](#)

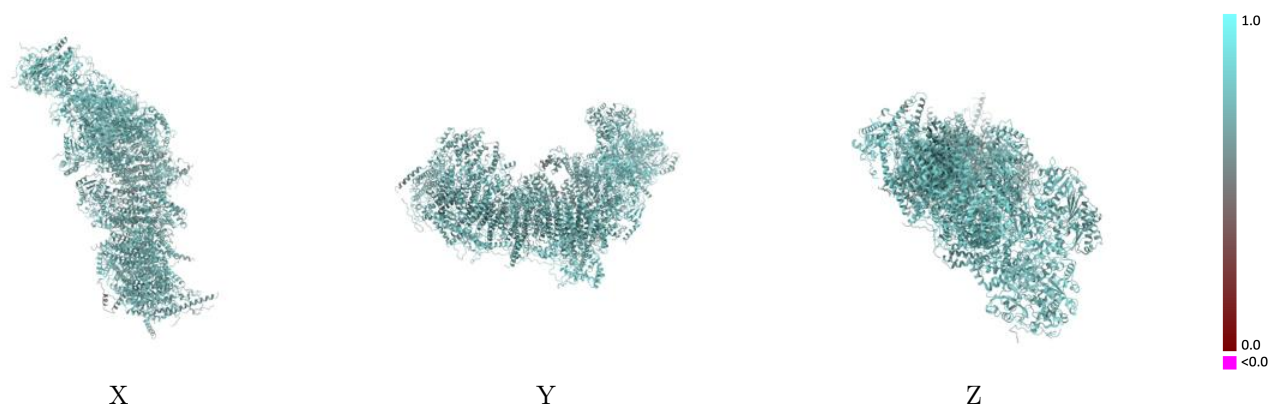
This section contains information regarding the fit between EMDB map EMD-55033 and PDB model 9SMI. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



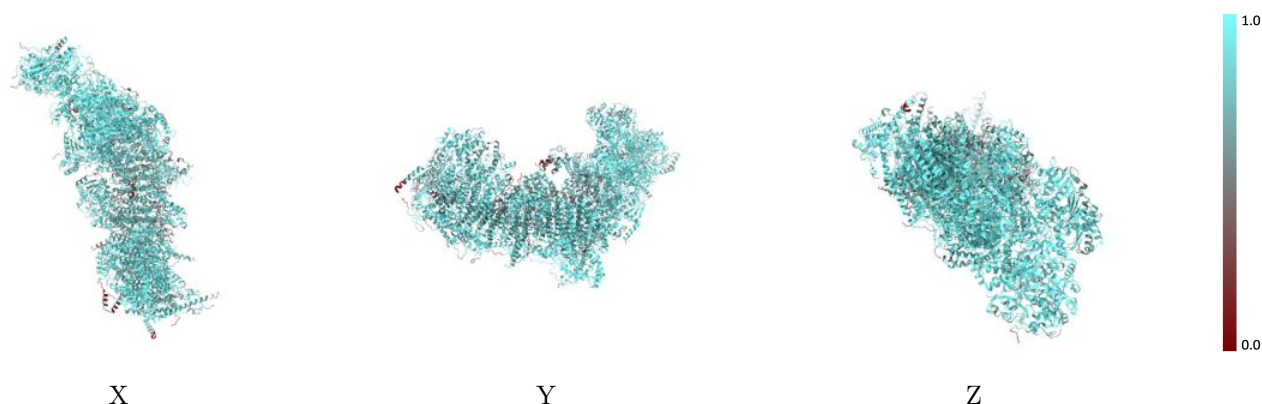
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



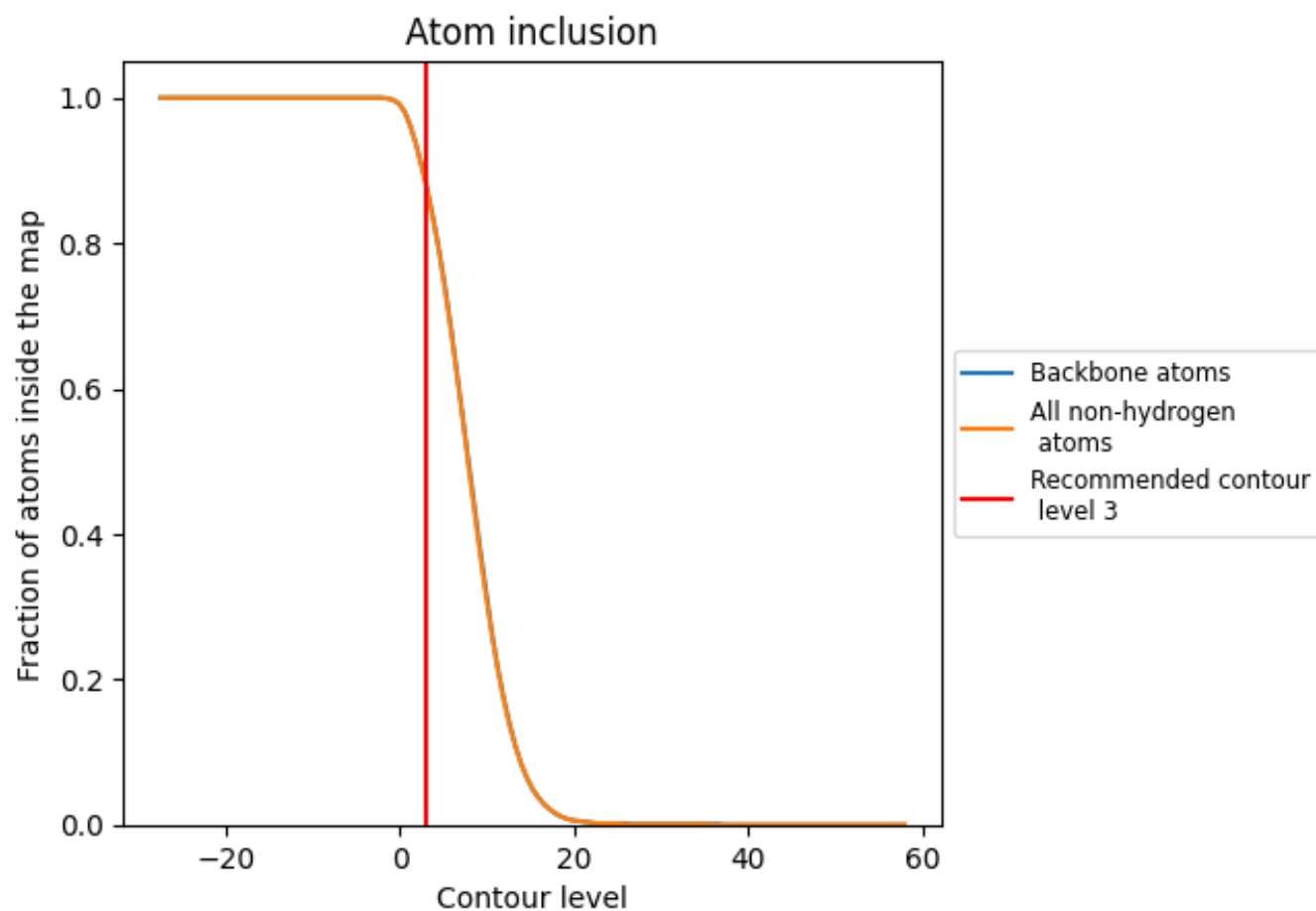
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.7410
A	 0.8400	 0.7310
B	 0.9320	 0.7880
C	 0.9700	 0.7960
D	 0.9440	 0.7920
E	 0.8630	 0.7200
F	 0.9210	 0.7430
G	 0.9240	 0.7540
H	 0.9550	 0.7850
I	 0.9720	 0.8020
J	 0.8460	 0.7360
K	 0.9490	 0.7780
L	 0.8870	 0.7430
M	 0.9430	 0.7780
N	 0.9400	 0.7870
O	 0.8880	 0.7150
P	 0.8000	 0.6970
Q	 0.9240	 0.7800
R	 0.8710	 0.7530
S	 0.8530	 0.6670
T	 0.6170	 0.6040
U	 0.8590	 0.6790
V	 0.8980	 0.7290
W	 0.8680	 0.7260
X	 0.8880	 0.7430
Y	 0.7360	 0.6920
Z	 0.8800	 0.7380
a	 0.9470	 0.7630
b	 0.8650	 0.7380
c	 0.8250	 0.7120
d	 0.8400	 0.7330
e	 0.8590	 0.7390
f	 0.7100	 0.6950
g	 0.8420	 0.7280
h	 0.8530	 0.7440



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Chain	Atom inclusion	Q-score
i	 0.6690	 0.6540
j	 0.7750	 0.6530
k	 0.7550	 0.6460
l	 0.8510	 0.7110
m	 0.8290	 0.7160
n	 0.8790	 0.7000
o	 0.7600	 0.6470
p	 0.8510	 0.7230
q	 0.9060	 0.7570
r	 0.9250	 0.7680
s	 0.8430	 0.7180